



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 3M9S / pdb_00003m9s
Title : Crystal structure of respiratory complex I from *Thermus thermophilus*
Authors : Efremov, R.G.; Baradaran, R.; Sazanov, L.A.
Deposited on : 2010-03-22
Resolution : 4.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

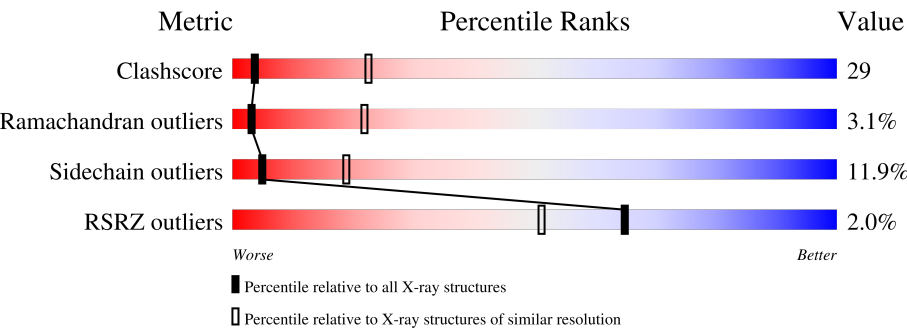
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	438	
1	A	438	
2	2	181	
2	B	181	
3	3	783	
3	C	783	
4	4	409	

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Mol	Chain	Length	Quality of chain
4	D	409	
5	5	207	
5	E	207	
6	6	181	
6	F	181	
7	9	182	
7	G	182	
8	7	129	
8	J	129	
9	L	469	
9	O	469	
10	M	392	
10	P	392	
11	N	379	
11	Q	379	
12	R	274	
12	S	274	
13	H	181	
13	T	181	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	SF4	1	439	-	-	X	-
14	SF4	3	784	-	-	X	-
14	SF4	3	786	-	-	X	-
14	SF4	6	182	-	-	X	-
14	SF4	A	439	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	SF4	C	784	-	-	X	-
14	SF4	C	786	-	-	X	-
14	SF4	F	182	-	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 47664 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			
1	A	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	B	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			
3	C	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			
4	D	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	5	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			
5	E	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			
6	F	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			
7	G	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	J	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 12.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
9	L	469	Total	C	N	0	0	0
			1407	938	469			
9	O	469	Total	C	N	0	0	0
			1407	938	469			

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 13.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
10	M	391	Total	C	N	0	0	0
			1173	782	391			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
10	P	391	Total	C	N	0	0	0
			1173	782	391			

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit 14.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
11	N	378	Total	C	N	0	0	0
			1134	756	378			
11	Q	378	Total	C	N	0	0	0
			1134	756	378			

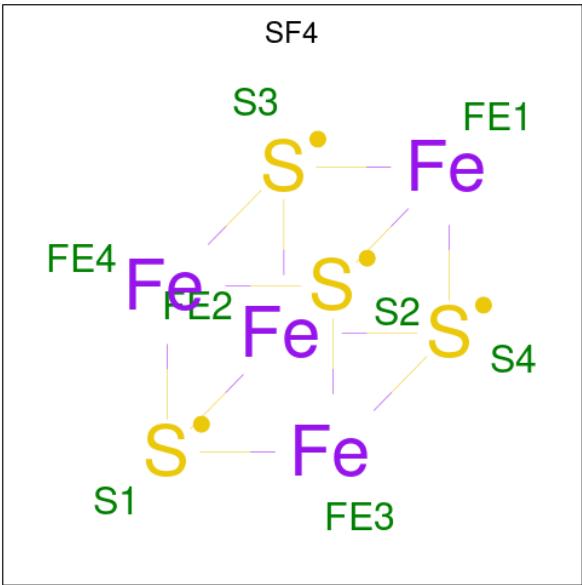
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunits 7, 10 and 11.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
12	R	274	Total	C	N	0	0	0
			822	548	274			
12	S	274	Total	C	N	0	0	0
			822	548	274			

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit 8.

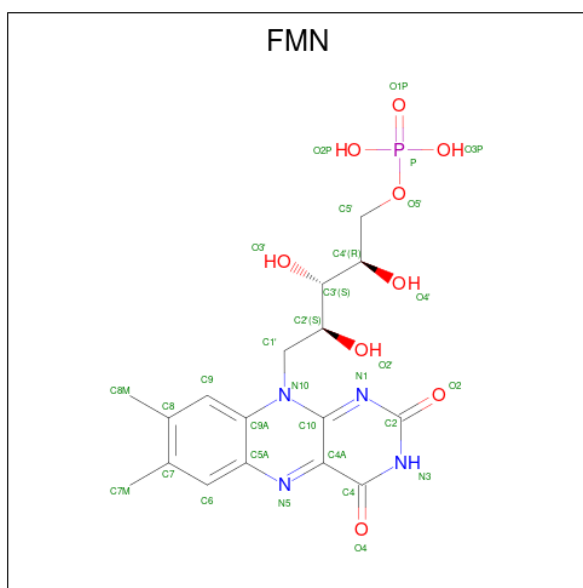
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	H	181	Total	C	N	0	0	0
			543	362	181			
13	T	181	Total	C	N	0	0	0
			543	362	181			

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



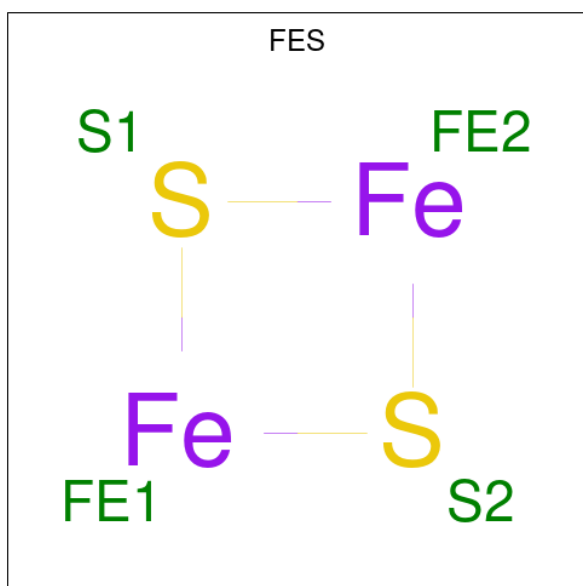
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	1	1	Total	Fe	S	0	0
			8	4	4		
14	3	1	Total	Fe	S	0	0
			8	4	4		
14	3	1	Total	Fe	S	0	0
			8	4	4		
14	3	1	Total	Fe	S	0	0
			8	4	4		
14	6	1	Total	Fe	S	0	0
			8	4	4		
14	9	1	Total	Fe	S	0	0
			8	4	4		
14	9	1	Total	Fe	S	0	0
			8	4	4		
14	A	1	Total	Fe	S	0	0
			8	4	4		
14	C	1	Total	Fe	S	0	0
			8	4	4		
14	C	1	Total	Fe	S	0	0
			8	4	4		
14	C	1	Total	Fe	S	0	0
			8	4	4		
14	F	1	Total	Fe	S	0	0
			8	4	4		
14	G	1	Total	Fe	S	0	0
			8	4	4		
14	G	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 15 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
15	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	2	1	Total	Fe	S	0	0
			4	2	2		

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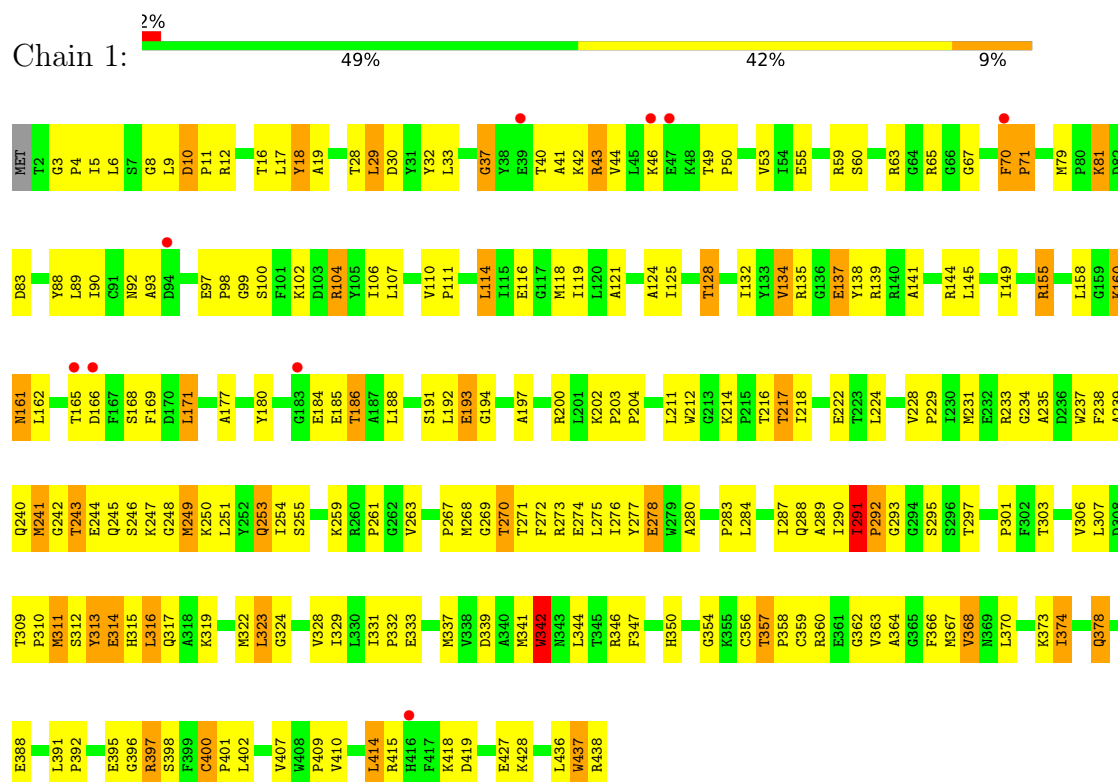
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	3	1	Total 4	Fe 2	S 2	0	0
16	B	1	Total 4	Fe 2	S 2	0	0
16	C	1	Total 4	Fe 2	S 2	0	0

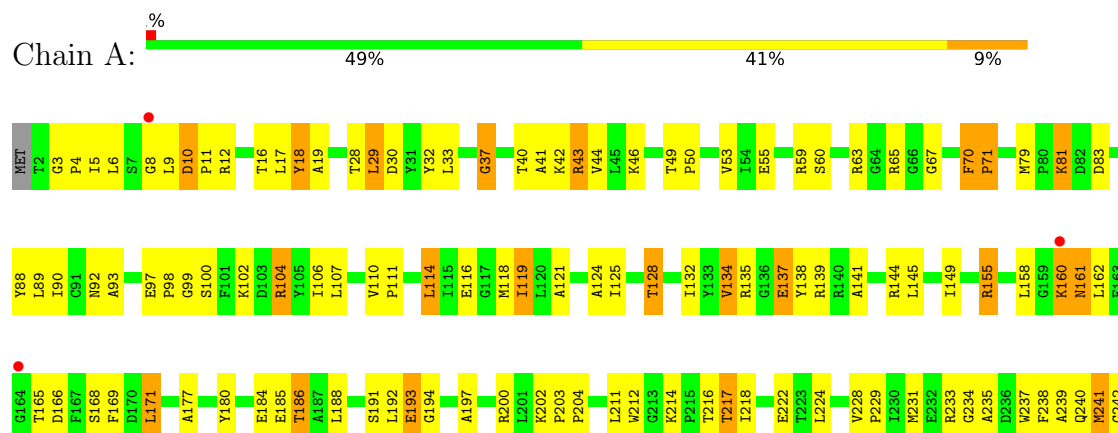
3 Residue-property plots

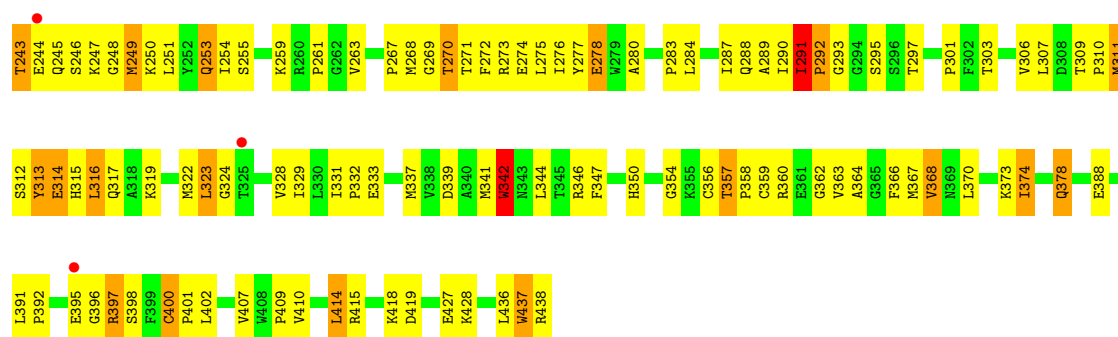
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NADH-quinone oxidoreductase subunit 1

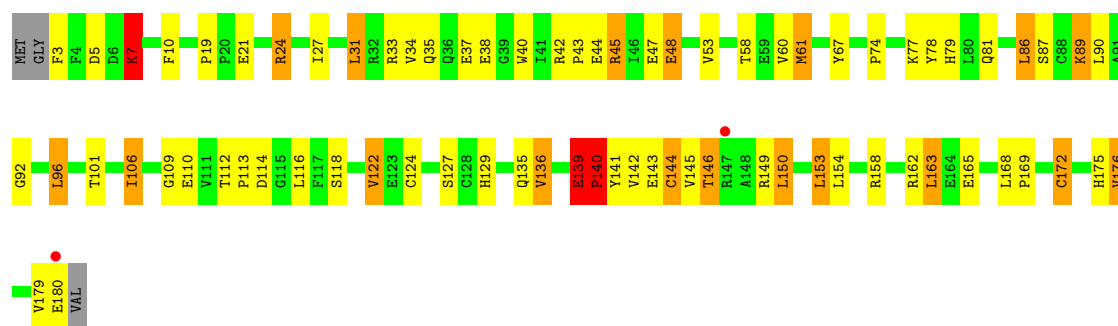


• Molecule 1: NADH-quinone oxidoreductase subunit 1

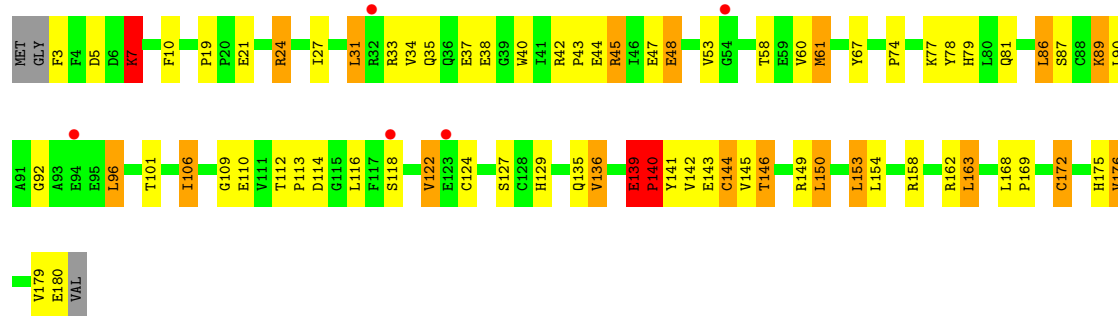




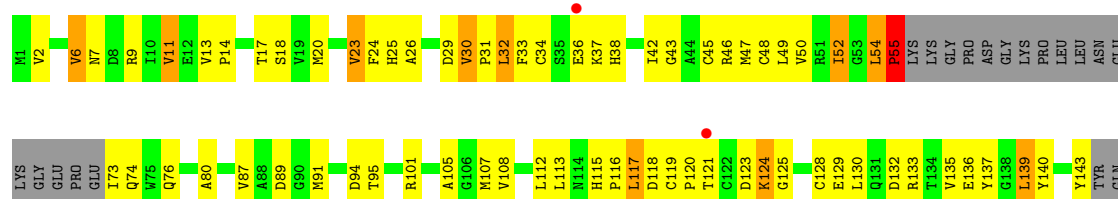
• Molecule 2: NADH-quinone oxidoreductase subunit 2

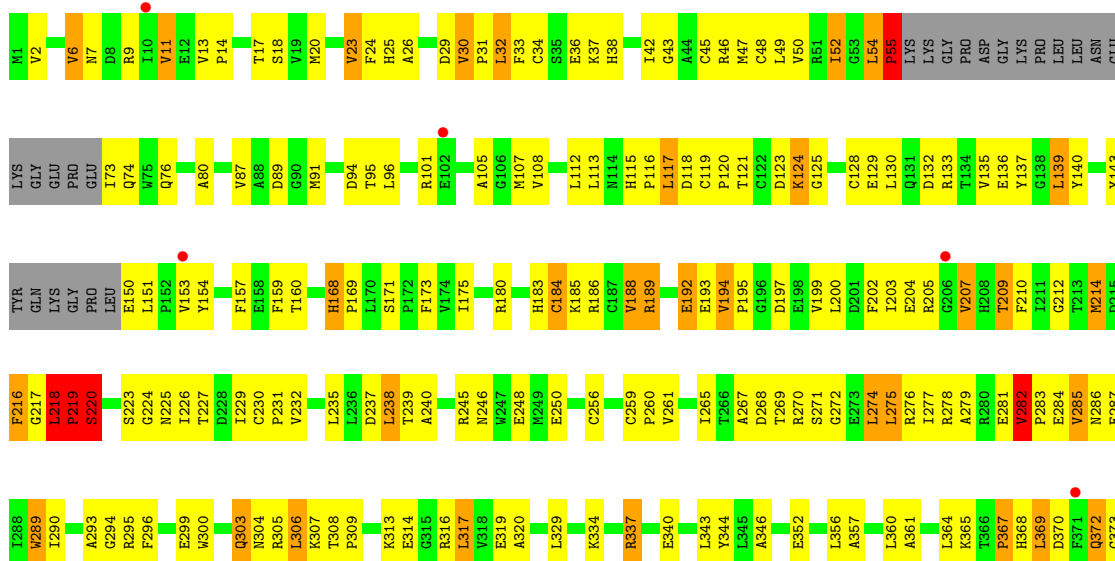
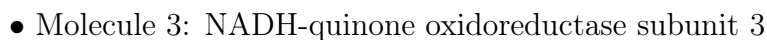


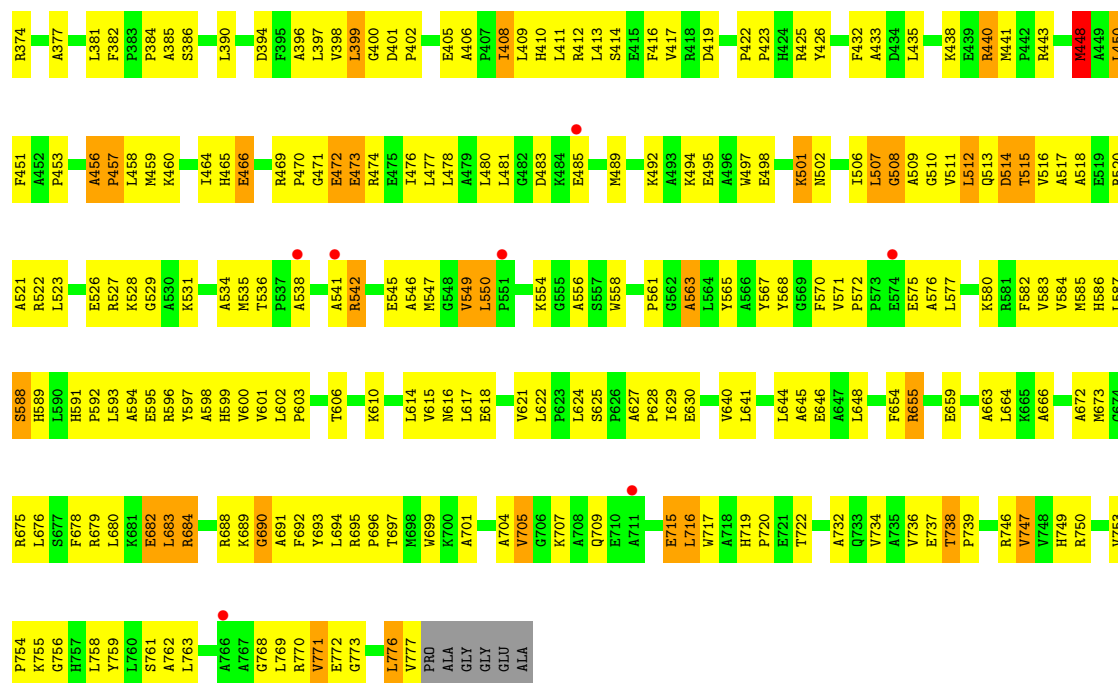
• Molecule 2: NADH-quinone oxidoreductase subunit 2



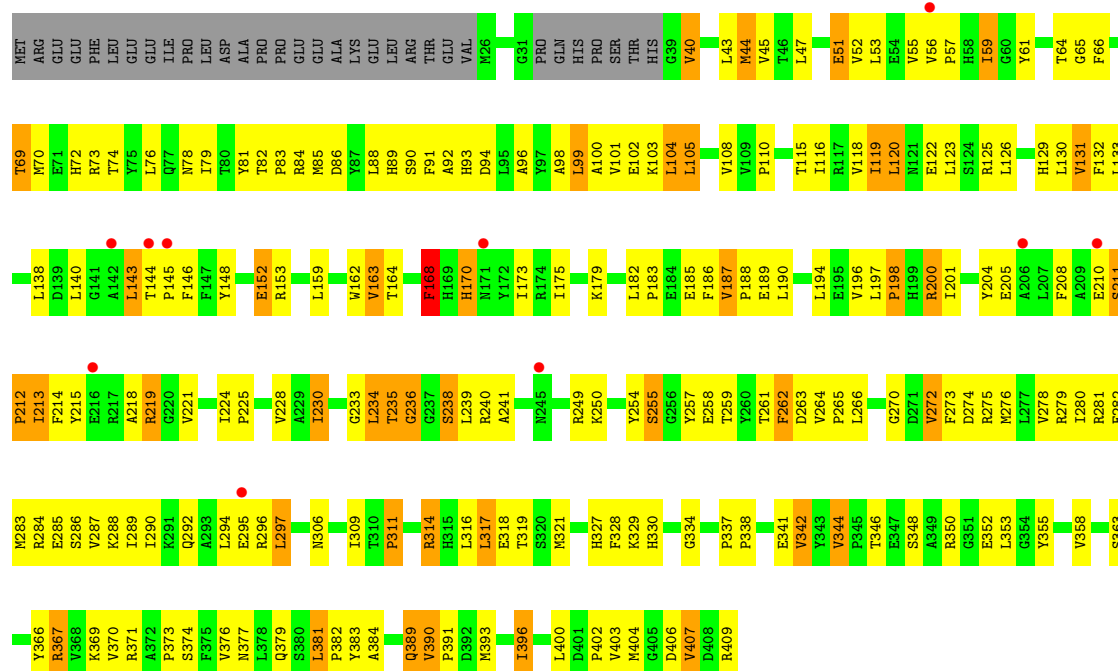
• Molecule 3: NADH-quinone oxidoreductase subunit 3



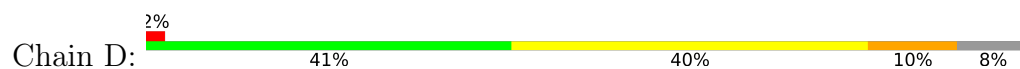


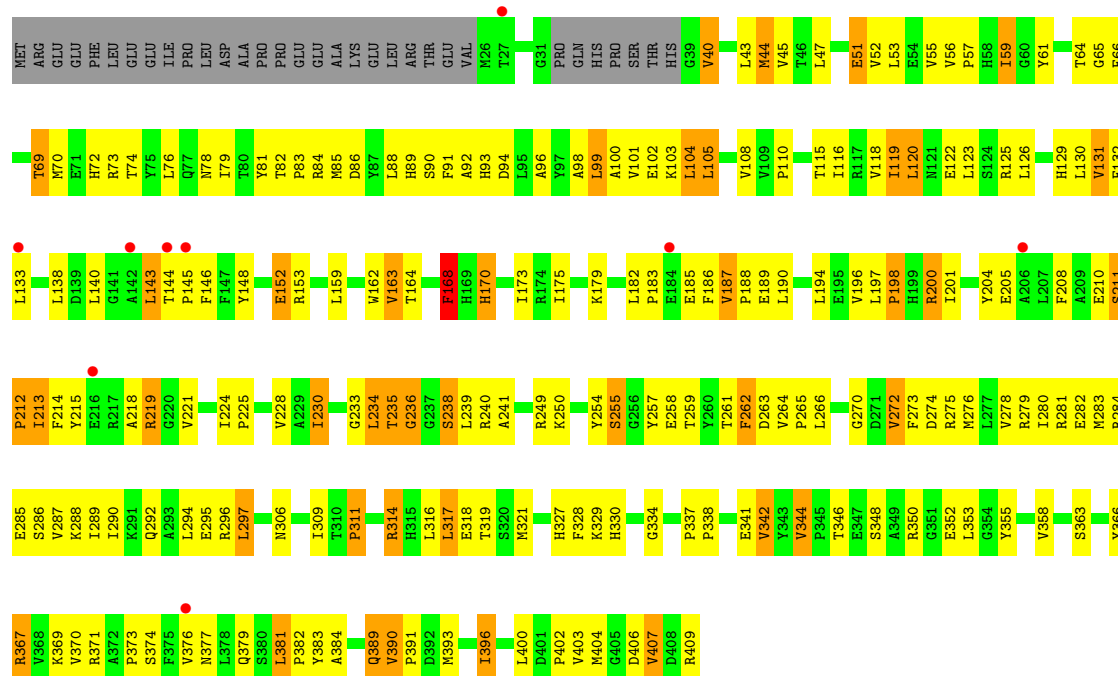


• Molecule 4: NADH-quinone oxidoreductase subunit 4

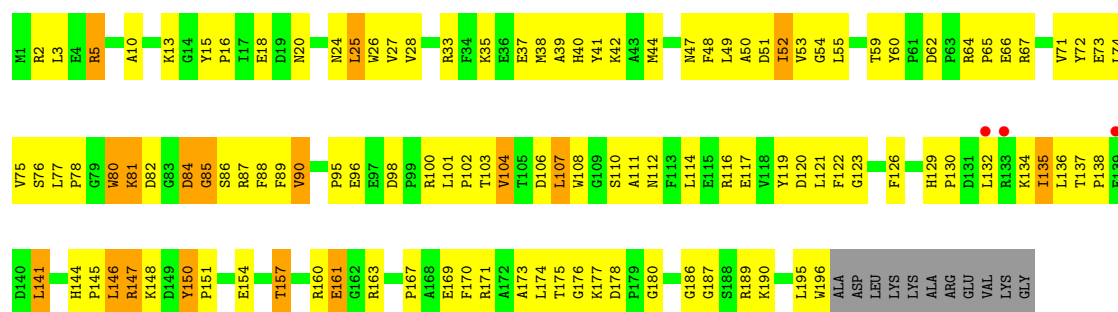


• Molecule 4: NADH-quinone oxidoreductase subunit 4

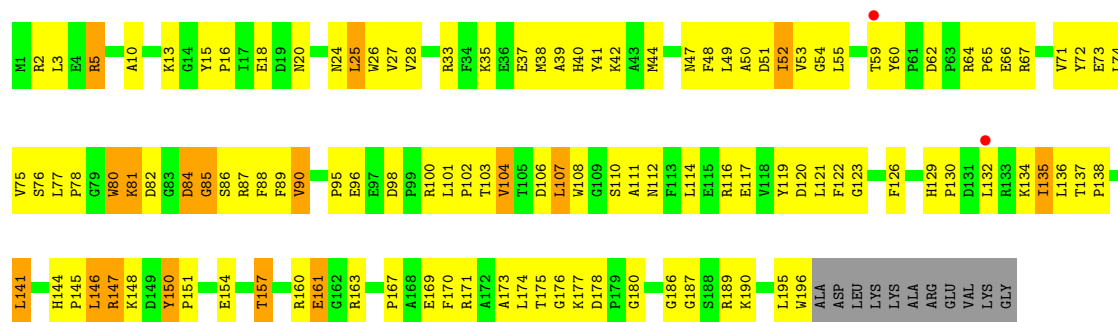




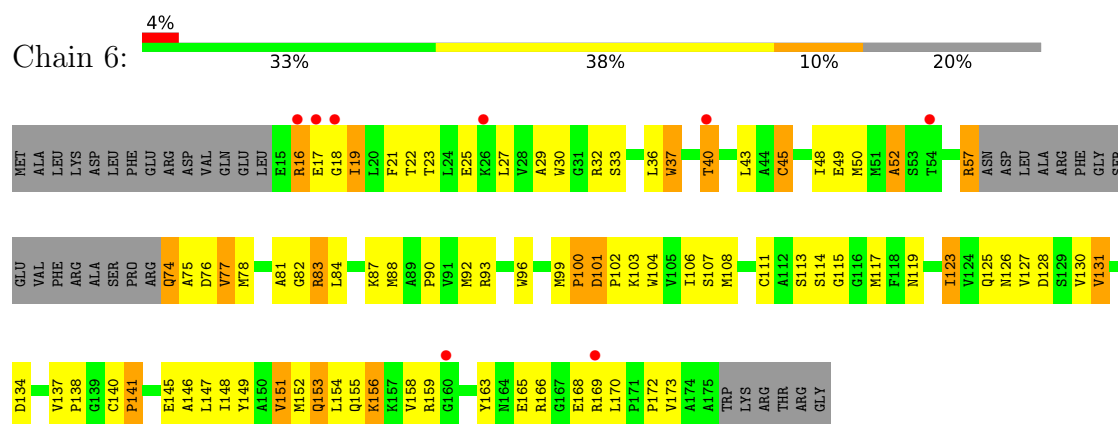
• Molecule 5: NADH-quinone oxidoreductase subunit C



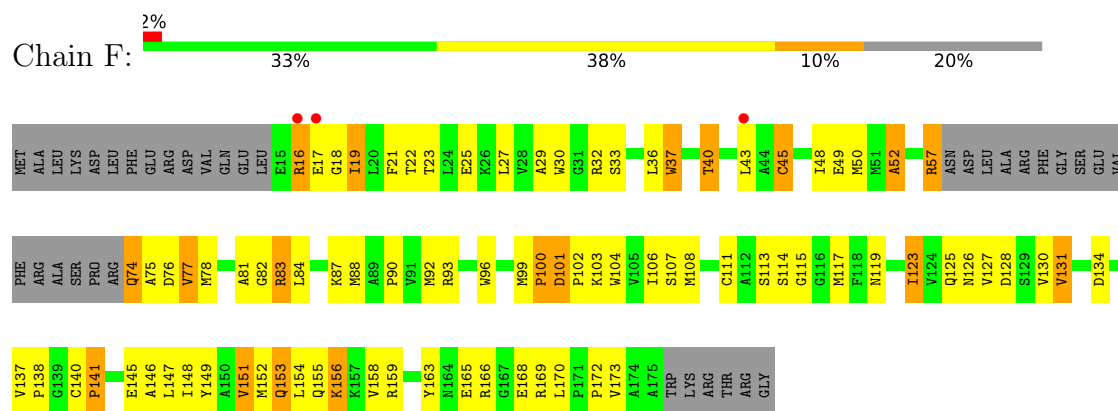
• Molecule 5: NADH-quinone oxidoreductase subunit C



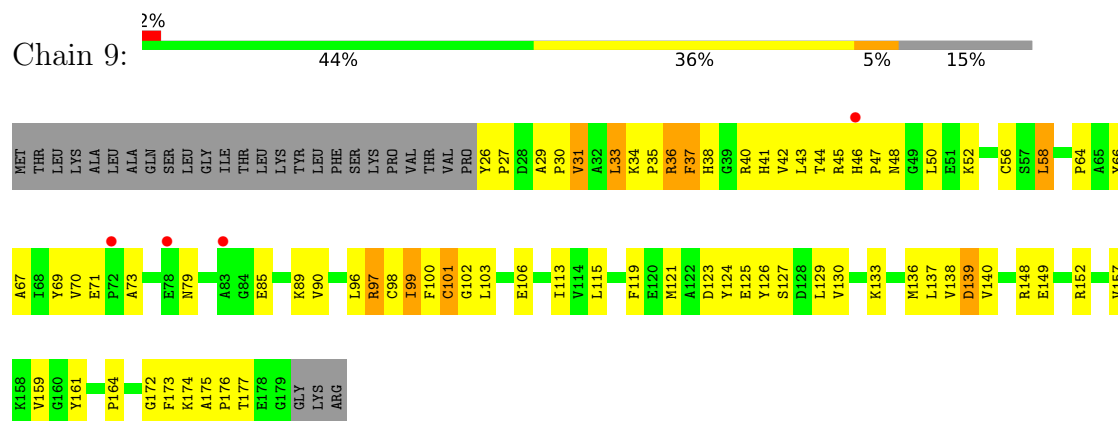
• Molecule 6: NADH-quinone oxidoreductase subunit B



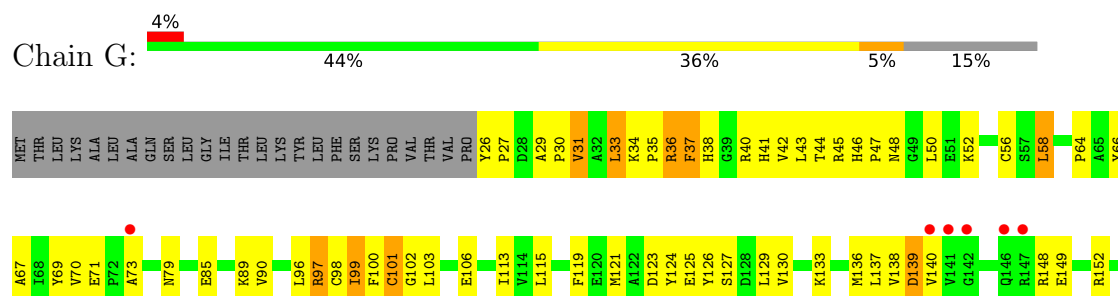
• Molecule 6: NADH-quinone oxidoreductase subunit B

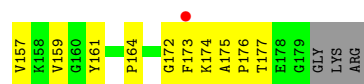


• Molecule 7: NADH-quinone oxidoreductase subunit I



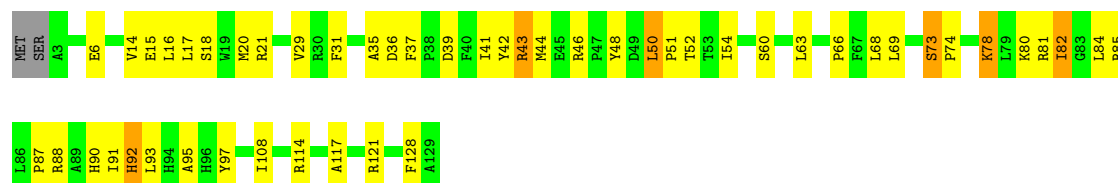
• Molecule 7: NADH-quinone oxidoreductase subunit I





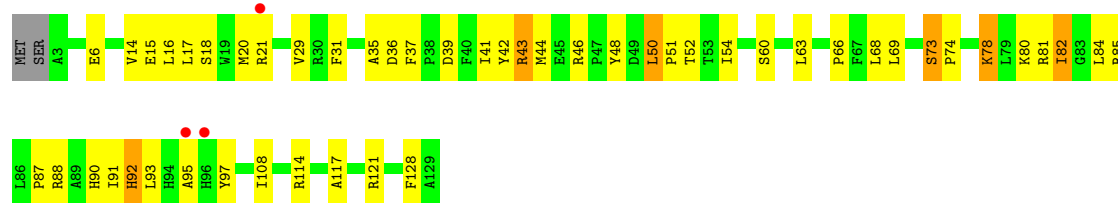
- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7: 60% 34% 5% .



- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain J: 2% 60% 34% 5% .



- Molecule 9: NADH-quinone oxidoreductase subunit 12

Chain L: 94% 6%



- Molecule 9: NADH-quinone oxidoreductase subunit 12

Chain O: 94% 6%



- Molecule 10: NADH-quinone oxidoreductase subunit 13

Chain M: 95%

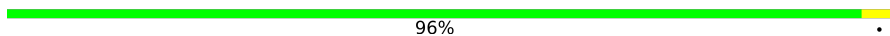


- Molecule 10: NADH-quinone oxidoreductase subunit 13

Chain P: 95%

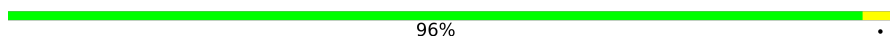


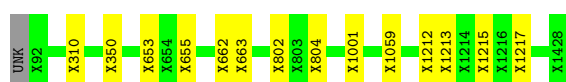
- Molecule 11: NADH-quinone oxidoreductase subunit 14

Chain N:  96%

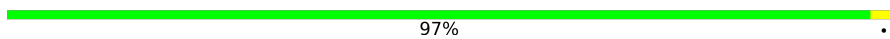


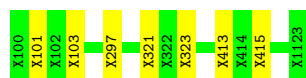
- Molecule 11: NADH-quinone oxidoreductase subunit 14

Chain Q:  96%

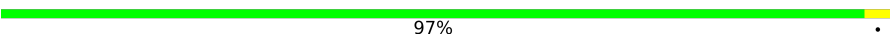


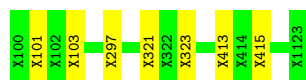
- Molecule 12: NADH-quinone oxidoreductase subunits 7, 10 and 11

Chain R:  97%

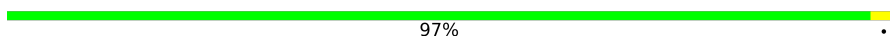


- Molecule 12: NADH-quinone oxidoreductase subunits 7, 10 and 11

Chain S:  97%

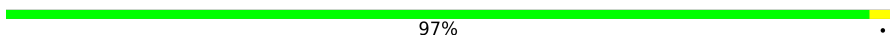


- Molecule 13: NADH-quinone oxidoreductase subunit 8

Chain H:  97%



- Molecule 13: NADH-quinone oxidoreductase subunit 8

Chain T:  97%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.39Å 336.09Å 262.24Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	30.00 – 4.50 30.00 – 4.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-4.50) 75.0 (30.00-4.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 4.42Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) 0.394 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	168.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 308.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.309 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	47664	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FMN, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.62	0/3506	1.05	11/4745 (0.2%)
1	A	0.62	0/3506	1.05	12/4745 (0.3%)
2	2	0.62	0/1439	1.05	6/1953 (0.3%)
2	B	0.62	0/1439	1.05	6/1953 (0.3%)
3	3	0.59	0/6019	1.07	31/8163 (0.4%)
3	C	0.59	0/6019	1.07	32/8163 (0.4%)
4	4	0.57	0/3089	0.99	11/4197 (0.3%)
4	D	0.57	0/3089	0.99	11/4197 (0.3%)
5	5	0.53	0/1656	1.05	14/2246 (0.6%)
5	E	0.53	0/1656	1.05	14/2246 (0.6%)
6	6	0.63	0/1137	1.09	6/1542 (0.4%)
6	F	0.63	0/1137	1.09	6/1542 (0.4%)
7	9	0.64	0/1224	1.04	5/1663 (0.3%)
7	G	0.64	0/1224	1.04	5/1663 (0.3%)
8	7	0.57	0/1059	0.99	7/1429 (0.5%)
8	J	0.57	0/1059	0.99	7/1429 (0.5%)
All	All	0.60	0/38258	1.04	184/51876 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	L	0	2
9	O	0	2
All	All	0	4

There are no bond length outliers.

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	143	TYR	CA-C-O	-18.61	89.16	120.80
3	C	143	TYR	CA-C-O	-18.60	89.18	120.80
4	D	238	SER	N-CA-C	-8.98	101.64	112.59
4	4	238	SER	N-CA-C	-8.96	101.65	112.59
1	A	291	ILE	CA-C-N	8.70	130.72	119.84
1	A	291	ILE	C-N-CA	8.70	130.72	119.84
1	1	291	ILE	CA-C-N	8.70	130.72	119.84
1	1	291	ILE	C-N-CA	8.70	130.72	119.84
3	C	625	SER	CA-C-N	8.60	130.59	119.84
3	C	625	SER	C-N-CA	8.60	130.59	119.84
3	3	625	SER	CA-C-N	8.57	130.56	119.84
3	3	625	SER	C-N-CA	8.57	130.56	119.84
2	B	19	PRO	CA-C-N	7.77	127.32	119.24
2	B	19	PRO	C-N-CA	7.77	127.32	119.24
2	2	19	PRO	CA-C-N	7.76	127.31	119.24
2	2	19	PRO	C-N-CA	7.76	127.31	119.24
5	5	160	ARG	N-CA-C	7.72	119.39	110.97
5	E	160	ARG	N-CA-C	7.69	119.35	110.97
2	B	139	GLU	CA-C-N	7.69	129.45	119.84
2	B	139	GLU	C-N-CA	7.69	129.45	119.84
2	2	139	GLU	CA-C-N	7.67	129.43	119.84
2	2	139	GLU	C-N-CA	7.67	129.43	119.84
6	6	170	LEU	CA-C-N	7.62	128.23	120.38
6	6	170	LEU	C-N-CA	7.62	128.23	120.38
6	F	170	LEU	CA-C-N	7.59	128.20	120.38
6	F	170	LEU	C-N-CA	7.59	128.20	120.38
5	E	135	ILE	CB-CA-C	-7.54	105.30	111.71
5	5	135	ILE	CB-CA-C	-7.53	105.31	111.71
1	1	400	CYS	CA-C-N	7.47	127.50	119.28
1	1	400	CYS	C-N-CA	7.47	127.50	119.28
1	A	400	CYS	CA-C-N	7.43	127.45	119.28
1	A	400	CYS	C-N-CA	7.43	127.45	119.28
5	E	85	GLY	N-CA-C	-7.37	103.92	116.01
5	5	85	GLY	N-CA-C	-7.37	103.92	116.01
7	9	79	ASN	CA-C-N	7.20	127.12	119.85
7	9	79	ASN	C-N-CA	7.20	127.12	119.85
7	G	79	ASN	CA-C-N	7.17	127.09	119.85
7	G	79	ASN	C-N-CA	7.17	127.09	119.85
3	3	14	PRO	CA-C-N	7.05	126.57	119.24
3	3	14	PRO	C-N-CA	7.05	126.57	119.24
3	3	194	VAL	CA-C-N	-7.05	111.03	119.84
3	3	194	VAL	C-N-CA	-7.05	111.03	119.84
3	C	194	VAL	CA-C-N	-7.04	111.04	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	194	VAL	C-N-CA	-7.04	111.04	119.84
3	C	14	PRO	CA-C-N	7.00	126.52	119.24
3	C	14	PRO	C-N-CA	7.00	126.52	119.24
1	A	378	GLN	N-CA-C	-6.72	104.22	112.88
1	1	378	GLN	N-CA-C	-6.70	104.24	112.88
3	C	55	PRO	CB-CA-C	-6.64	97.49	110.10
3	3	55	PRO	CB-CA-C	-6.61	97.53	110.10
3	3	218	LEU	CA-C-N	6.60	128.09	119.84
3	3	218	LEU	C-N-CA	6.60	128.09	119.84
3	C	218	LEU	CA-C-N	6.58	128.06	119.84
3	C	218	LEU	C-N-CA	6.58	128.06	119.84
5	5	60	TYR	CA-C-N	6.51	126.01	119.24
5	5	60	TYR	C-N-CA	6.51	126.01	119.24
5	E	60	TYR	CA-C-N	6.51	126.01	119.24
5	E	60	TYR	C-N-CA	6.51	126.01	119.24
6	6	101	ASP	CA-C-N	-6.35	111.91	119.84
6	6	101	ASP	C-N-CA	-6.35	111.91	119.84
6	F	101	ASP	CA-C-N	-6.35	111.91	119.84
6	F	101	ASP	C-N-CA	-6.35	111.91	119.84
3	3	456	ALA	CA-C-N	6.17	127.56	119.84
3	3	456	ALA	C-N-CA	6.17	127.56	119.84
5	5	160	ARG	CA-C-N	-6.17	114.77	123.03
5	5	160	ARG	C-N-CA	-6.17	114.77	123.03
1	1	137	GLU	N-CA-C	-6.17	106.40	114.04
1	A	137	GLU	N-CA-C	-6.16	106.40	114.04
3	C	456	ALA	CA-C-N	6.15	127.53	119.84
3	C	456	ALA	C-N-CA	6.15	127.53	119.84
3	C	282	VAL	CA-C-N	6.15	126.60	119.47
3	C	282	VAL	C-N-CA	6.15	126.60	119.47
5	E	160	ARG	CA-C-N	-6.14	114.80	123.03
5	E	160	ARG	C-N-CA	-6.14	114.80	123.03
3	3	282	VAL	CA-C-N	6.13	126.59	119.47
3	3	282	VAL	C-N-CA	6.13	126.59	119.47
4	D	306	ASN	CA-C-N	6.09	125.98	119.28
4	D	306	ASN	C-N-CA	6.09	125.98	119.28
4	4	306	ASN	CA-C-N	6.05	125.94	119.28
4	4	306	ASN	C-N-CA	6.05	125.94	119.28
1	A	70	PHE	CA-C-N	6.03	127.37	119.84
1	A	70	PHE	C-N-CA	6.03	127.37	119.84
1	1	70	PHE	CA-C-N	6.00	127.34	119.84
1	1	70	PHE	C-N-CA	6.00	127.34	119.84
3	C	216	PHE	N-CA-C	6.00	121.28	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	216	PHE	N-CA-C	6.00	121.27	111.37
1	A	356	CYS	CB-CA-C	-5.88	99.83	109.53
1	1	356	CYS	CB-CA-C	-5.88	99.84	109.53
3	C	719	HIS	CA-C-N	5.82	127.12	119.84
3	C	719	HIS	C-N-CA	5.82	127.12	119.84
3	3	719	HIS	CA-C-N	5.81	127.10	119.84
3	3	719	HIS	C-N-CA	5.81	127.10	119.84
8	7	35	ALA	N-CA-C	5.69	117.05	108.46
8	J	35	ALA	N-CA-C	5.67	117.03	108.46
1	A	342	TRP	N-CA-C	-5.62	102.09	111.37
1	1	342	TRP	N-CA-C	-5.62	102.10	111.37
2	B	7	LYS	N-CA-C	5.59	116.43	108.54
7	G	102	GLY	N-CA-C	-5.59	107.55	115.43
7	9	102	GLY	N-CA-C	-5.58	107.56	115.43
2	2	7	LYS	N-CA-C	5.57	116.39	108.54
3	C	377	ALA	CA-C-N	5.54	125.82	119.83
3	C	377	ALA	C-N-CA	5.54	125.82	119.83
3	3	377	ALA	CA-C-N	5.51	125.78	119.83
3	3	377	ALA	C-N-CA	5.51	125.78	119.83
5	5	104	VAL	N-CA-C	-5.51	106.94	112.17
3	C	691	ALA	N-CA-C	-5.49	105.70	112.72
5	E	104	VAL	N-CA-C	-5.48	106.97	112.17
3	3	691	ALA	N-CA-C	-5.48	105.71	112.72
4	4	56	VAL	CA-C-N	5.46	125.37	119.85
4	4	56	VAL	C-N-CA	5.46	125.37	119.85
5	E	62	ASP	CA-C-N	5.45	125.21	119.76
5	E	62	ASP	C-N-CA	5.45	125.21	119.76
4	D	344	VAL	CA-C-N	5.44	126.28	120.13
4	D	344	VAL	C-N-CA	5.44	126.28	120.13
5	5	62	ASP	CA-C-N	5.43	125.19	119.76
5	5	62	ASP	C-N-CA	5.43	125.19	119.76
2	2	172	CYS	N-CA-C	5.43	117.27	108.26
4	4	344	VAL	CA-C-N	5.43	126.27	120.13
4	4	344	VAL	C-N-CA	5.43	126.27	120.13
4	D	56	VAL	CA-C-N	5.43	125.33	119.85
4	D	56	VAL	C-N-CA	5.43	125.33	119.85
3	C	448	MET	N-CA-C	5.42	117.42	109.24
2	B	172	CYS	N-CA-C	5.42	117.25	108.26
3	C	52	ILE	N-CA-C	5.40	115.67	108.11
3	3	448	MET	N-CA-C	5.39	117.38	109.24
3	3	52	ILE	N-CA-C	5.39	115.66	108.11
3	3	171	SER	N-CA-C	-5.38	103.29	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	171	SER	N-CA-C	-5.38	103.29	108.07
1	A	67	GLY	N-CA-C	-5.31	108.16	114.48
4	4	119	ILE	CB-CA-C	-5.30	105.18	111.97
1	1	67	GLY	N-CA-C	-5.29	108.18	114.48
7	G	70	VAL	N-CA-C	5.29	115.74	108.12
4	D	119	ILE	CB-CA-C	-5.28	105.21	111.97
7	9	70	VAL	N-CA-C	5.27	115.71	108.12
3	3	406	ALA	CA-C-N	5.26	126.41	119.84
3	3	406	ALA	C-N-CA	5.26	126.41	119.84
8	7	37	PHE	CA-C-N	-5.25	114.26	119.56
8	7	37	PHE	C-N-CA	-5.25	114.26	119.56
3	C	406	ALA	CA-C-N	5.24	126.39	119.84
3	C	406	ALA	C-N-CA	5.24	126.39	119.84
8	J	37	PHE	CA-C-N	-5.22	114.29	119.56
8	J	37	PHE	C-N-CA	-5.22	114.29	119.56
8	J	46	ARG	CA-C-N	5.19	125.09	119.85
8	J	46	ARG	C-N-CA	5.19	125.09	119.85
8	7	46	ARG	CA-C-N	5.18	125.08	119.85
8	7	46	ARG	C-N-CA	5.18	125.08	119.85
3	3	30	VAL	CA-C-N	5.17	125.17	119.89
3	3	30	VAL	C-N-CA	5.17	125.17	119.89
4	4	168	PHE	N-CA-C	5.15	116.13	108.86
3	C	30	VAL	CA-C-N	5.14	125.14	119.89
3	C	30	VAL	C-N-CA	5.14	125.14	119.89
4	4	311	PRO	CA-C-N	5.13	125.67	120.38
4	4	311	PRO	C-N-CA	5.13	125.67	120.38
4	D	311	PRO	CA-C-N	5.13	125.67	120.38
4	D	311	PRO	C-N-CA	5.13	125.67	120.38
4	D	168	PHE	N-CA-C	5.12	116.08	108.86
6	6	52	ALA	N-CA-C	-5.11	106.98	114.39
8	7	73	SER	CA-C-N	5.11	126.23	119.84
8	7	73	SER	C-N-CA	5.11	126.23	119.84
8	J	73	SER	CA-C-N	5.11	126.22	119.84
8	J	73	SER	C-N-CA	5.11	126.22	119.84
6	F	52	ALA	N-CA-C	-5.10	107.00	114.39
6	6	123	ILE	N-CA-C	5.10	115.46	108.12
6	F	123	ILE	N-CA-C	5.09	115.45	108.12
5	E	178	ASP	CA-C-N	5.08	124.69	119.56
5	E	178	ASP	C-N-CA	5.08	124.69	119.56
5	5	178	ASP	CA-C-N	5.07	124.68	119.56
5	5	178	ASP	C-N-CA	5.07	124.68	119.56
3	C	289	TRP	N-CA-C	5.05	117.73	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	289	TRP	N-CA-C	5.05	117.72	109.59
5	E	150	TYR	CA-C-N	5.05	124.96	119.76
5	E	150	TYR	C-N-CA	5.05	124.96	119.76
7	9	64	PRO	N-CA-C	-5.05	107.82	114.03
7	G	64	PRO	N-CA-C	-5.04	107.83	114.03
5	5	150	TYR	CA-C-N	5.04	124.95	119.76
5	5	150	TYR	C-N-CA	5.04	124.95	119.76
3	C	472	GLU	N-CA-C	-5.02	107.11	114.39
3	C	588	SER	N-CA-C	-5.02	107.82	114.04
3	3	472	GLU	N-CA-C	-5.01	107.12	114.39
3	C	466	GLU	N-CA-C	5.01	117.50	108.48
3	3	400	GLY	N-CA-C	-5.01	106.54	111.85
1	A	119	ILE	CB-CA-C	-5.00	105.47	111.88
3	C	400	GLY	N-CA-C	-5.00	106.55	111.85
3	3	466	GLU	N-CA-C	5.00	117.48	108.48

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	L	1212	UNK	Peptide
9	L	1569	UNK	Peptide
9	O	1212	UNK	Peptide
9	O	1569	UNK	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3388	217	0
1	A	3417	0	3388	216	0
2	2	1406	0	1373	77	0
2	B	1406	0	1373	77	0
3	3	5880	0	5911	454	7
3	C	5880	0	5911	433	9
4	4	3011	0	3000	229	0
4	D	3011	0	3000	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	5	1607	0	1574	108	0
5	E	1607	0	1574	108	0
6	6	1113	0	1121	103	2
6	F	1113	0	1121	124	0
7	9	1193	0	1160	71	0
7	G	1193	0	1160	71	0
8	7	1031	0	1029	42	0
8	J	1031	0	1029	42	0
9	L	1407	0	50	15	0
9	O	1407	0	50	15	0
10	M	1173	0	37	15	0
10	P	1173	0	37	15	0
11	N	1134	0	36	12	0
11	Q	1134	0	36	12	0
12	R	822	0	24	4	0
12	S	822	0	24	4	0
13	H	543	0	20	6	0
13	T	543	0	20	6	0
14	1	8	0	0	2	0
14	3	24	0	0	8	0
14	6	8	0	0	4	0
14	9	16	0	0	0	0
14	A	8	0	0	2	0
14	C	24	0	0	7	0
14	F	8	0	0	4	0
14	G	16	0	0	0	0
15	1	31	0	19	8	0
15	A	31	0	19	8	0
16	2	4	0	0	0	0
16	3	4	0	0	1	0
16	B	4	0	0	0	0
16	C	4	0	0	1	0
All	All	47664	0	37484	2470	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (2470) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:1001:UNK:CA	11:N:1059:UNK:C	1.85	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:1001:UNK:CA	11:Q:1059:UNK:C	1.85	1.51
3:3:485:GLU:CD	6:F:16:ARG:HG3	1.39	1.48
9:L:1527:UNK:C	9:L:1530:UNK:N	1.88	1.37
9:O:1527:UNK:C	9:O:1530:UNK:N	1.88	1.37
3:3:485:GLU:O	6:F:16:ARG:CD	1.84	1.25
3:3:679:ARG:CZ	3:C:319:GLU:OE2	1.84	1.23
3:3:485:GLU:OE1	6:F:16:ARG:CG	1.87	1.23
3:3:485:GLU:O	6:F:16:ARG:HD2	1.05	1.21
10:P:920:UNK:CA	10:P:1200:UNK:N	2.03	1.21
10:M:920:UNK:CA	10:M:1200:UNK:N	2.03	1.20
3:3:485:GLU:CG	6:F:16:ARG:HG3	1.73	1.18
3:3:474:ARG:NH2	3:3:516:VAL:HG21	1.60	1.17
3:C:474:ARG:NH2	3:C:516:VAL:HG21	1.60	1.17
3:C:117:LEU:N	4:D:321:MET:HE1	1.62	1.14
3:3:117:LEU:N	4:4:321:MET:HE1	1.62	1.13
6:6:117:MET:HE2	7:9:99:ILE:HG12	1.27	1.12
6:F:117:MET:HE2	7:G:99:ILE:HG12	1.27	1.12
3:3:485:GLU:CD	6:F:16:ARG:CG	2.26	1.08
11:N:310:UNK:CA	11:N:350:UNK:CA	2.31	1.08
11:Q:310:UNK:CA	11:Q:350:UNK:CA	2.32	1.08
7:G:40:ARG:HB2	7:G:121:MET:HE1	1.33	1.07
7:9:40:ARG:HB2	7:9:121:MET:HE1	1.33	1.07
5:E:66:GLU:HG2	5:E:95:PRO:HA	1.16	1.06
3:3:485:GLU:C	6:F:16:ARG:HD2	1.79	1.06
5:5:66:GLU:HG2	5:5:95:PRO:HA	1.16	1.06
3:C:561:PRO:HB3	3:C:576:ALA:HA	1.30	1.06
3:3:440:ARG:HG2	3:3:440:ARG:HH11	1.20	1.05
3:3:561:PRO:HB3	3:3:576:ALA:HA	1.30	1.05
3:C:440:ARG:HG2	3:C:440:ARG:HH11	1.20	1.05
3:3:679:ARG:CZ	3:C:319:GLU:CD	2.29	1.05
3:3:679:ARG:NH2	3:C:319:GLU:CD	2.14	1.05
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.10	1.05
1:A:437:TRP:HB3	2:B:92:GLY:HA3	1.10	1.05
3:3:115:HIS:CD2	3:3:116:PRO:HD2	1.91	1.04
3:C:115:HIS:CD2	3:C:116:PRO:HD2	1.91	1.04
3:3:485:GLU:OE1	6:F:16:ARG:HG3	1.46	1.04
4:4:143:LEU:CD1	13:H:834:UNK:C	2.36	1.02
4:D:143:LEU:CD1	13:T:834:UNK:C	2.36	1.02
3:3:738:THR:HG22	3:3:739:PRO:HD2	1.37	1.02
3:C:738:THR:HG22	3:C:739:PRO:HD2	1.37	1.02
4:4:143:LEU:HD13	13:H:834:UNK:C	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:LEU:HD13	13:T:834:UNK:C	1.90	1.01
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.42	1.01
7:G:41:HIS:HB3	7:G:113:ILE:HD11	1.42	1.01
3:3:655:ARG:HB2	3:3:655:ARG:HH11	1.26	1.00
4:4:367:ARG:HH11	4:4:367:ARG:HG3	1.22	1.00
3:C:655:ARG:HB2	3:C:655:ARG:HH11	1.26	1.00
4:D:367:ARG:HH11	4:D:367:ARG:HG3	1.22	1.00
3:3:485:GLU:OE1	6:F:16:ARG:HG2	1.59	1.00
11:N:1001:UNK:C	11:N:1059:UNK:C	2.40	0.99
11:Q:1001:UNK:C	11:Q:1059:UNK:C	2.40	0.99
1:1:186:THR:HG23	1:1:200:ARG:H	1.27	0.99
1:A:186:THR:HG23	1:A:200:ARG:H	1.27	0.99
3:3:501:LYS:H	3:3:501:LYS:HD2	1.27	0.98
3:C:501:LYS:H	3:C:501:LYS:HD2	1.27	0.98
1:1:16:THR:HG21	1:1:229:PRO:HB3	1.44	0.98
1:A:16:THR:HG21	1:A:229:PRO:HB3	1.44	0.98
6:F:145:GLU:HG2	7:G:31:VAL:HG21	1.43	0.97
6:6:145:GLU:HG2	7:9:31:VAL:HG21	1.43	0.97
10:P:920:UNK:C	10:P:1200:UNK:H2	1.78	0.97
10:M:920:UNK:C	10:M:1200:UNK:H2	1.78	0.97
1:A:90:ILE:HD11	1:A:211:LEU:HD22	1.48	0.96
1:1:90:ILE:HD11	1:1:211:LEU:HD22	1.48	0.95
3:C:474:ARG:HH21	3:C:516:VAL:HG21	1.12	0.95
3:3:474:ARG:HH21	3:3:516:VAL:HG21	1.12	0.95
3:3:440:ARG:HH11	3:3:440:ARG:CG	1.80	0.95
3:C:440:ARG:HH11	3:C:440:ARG:CG	1.80	0.95
3:3:20:MET:HE2	3:3:433:ALA:HB2	1.50	0.94
3:C:20:MET:HE2	3:C:433:ALA:HB2	1.50	0.94
1:A:246:SER:HB3	1:A:268:MET:HG2	1.49	0.94
1:1:246:SER:HB3	1:1:268:MET:HG2	1.50	0.94
1:1:104:ARG:HH21	2:2:127:SER:HB3	1.31	0.94
4:4:254:TYR:HD1	4:4:255:SER:H	1.15	0.94
4:4:238:SER:HB3	4:4:279:ARG:NH2	1.83	0.94
4:D:238:SER:HB3	4:D:279:ARG:NH2	1.83	0.94
1:A:104:ARG:HH21	2:B:127:SER:HB3	1.31	0.94
4:D:254:TYR:HD1	4:D:255:SER:H	1.15	0.94
3:C:509:ALA:HB1	3:C:768:GLY:HA3	1.50	0.93
3:3:509:ALA:HB1	3:3:768:GLY:HA3	1.50	0.93
1:A:358:PRO:O	1:A:362:GLY:HA3	1.66	0.93
1:A:395:GLU:HB2	1:A:407:VAL:HG21	1.50	0.93
1:1:395:GLU:HB2	1:1:407:VAL:HG21	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:343:LEU:HD12	3:3:361:ALA:HB2	1.50	0.93
3:C:343:LEU:HD12	3:C:361:ALA:HB2	1.50	0.93
1:1:358:PRO:O	1:1:362:GLY:HA3	1.66	0.93
1:1:331:ILE:HD12	1:1:337:MET:HE1	1.51	0.93
3:3:486:GLY:HA2	6:F:17:GLU:OE1	1.68	0.93
1:A:331:ILE:HD12	1:A:337:MET:HE1	1.51	0.93
1:1:40:THR:O	1:1:44:VAL:HG23	1.70	0.92
1:A:40:THR:O	1:A:44:VAL:HG23	1.70	0.92
3:3:722:THR:HG21	3:3:756:GLY:H	1.34	0.92
3:C:722:THR:HG21	3:C:756:GLY:H	1.34	0.92
3:3:374:ARG:NH2	3:3:684:ARG:HG3	1.87	0.89
3:C:374:ARG:NH2	3:C:684:ARG:HG3	1.87	0.88
3:3:689:LYS:HE3	3:3:771:VAL:HG13	1.55	0.88
3:C:689:LYS:HE3	3:C:771:VAL:HG13	1.55	0.88
3:3:279:ALA:HB2	3:3:290:ILE:HG12	1.56	0.88
10:M:920:UNK:CA	10:M:1200:UNK:H2	1.77	0.88
3:C:279:ALA:HB2	3:C:290:ILE:HG12	1.56	0.88
10:P:920:UNK:CA	10:P:1200:UNK:H2	1.77	0.88
3:C:115:HIS:CG	3:C:116:PRO:HD2	2.09	0.87
3:3:115:HIS:CG	3:3:116:PRO:HD2	2.09	0.87
9:L:119:UNK:C	9:L:121:UNK:N	2.35	0.87
9:O:119:UNK:C	9:O:121:UNK:N	2.35	0.87
3:3:485:GLU:HG2	6:F:16:ARG:HG3	1.56	0.87
5:5:18:GLU:HB2	5:5:26:TRP:HB2	1.55	0.87
5:E:18:GLU:HB2	5:E:26:TRP:HB2	1.55	0.87
1:A:242:GLY:HA2	1:A:268:MET:O	1.75	0.86
1:1:242:GLY:HA2	1:1:268:MET:O	1.75	0.86
3:3:136:GLU:HG2	5:5:189:ARG:HG2	1.55	0.86
3:C:136:GLU:HG2	5:E:189:ARG:HG2	1.55	0.86
1:A:162:LEU:O	1:A:165:THR:HG22	1.76	0.86
1:1:162:LEU:O	1:1:165:THR:HG22	1.76	0.86
1:1:186:THR:CG2	1:1:200:ARG:H	1.88	0.86
1:A:186:THR:CG2	1:A:200:ARG:H	1.88	0.85
10:P:404:UNK:CA	11:Q:662:UNK:CA	2.53	0.85
1:1:297:THR:HG22	1:1:322:MET:HG3	1.58	0.85
3:3:396:ALA:HB3	3:3:448:MET:HB2	1.57	0.85
10:M:404:UNK:CA	11:N:662:UNK:CA	2.53	0.85
1:A:297:THR:HG22	1:A:322:MET:HG3	1.58	0.85
3:C:396:ALA:HB3	3:C:448:MET:HB2	1.57	0.85
1:1:253:GLN:N	1:1:253:GLN:HE21	1.75	0.85
1:A:253:GLN:N	1:A:253:GLN:HE21	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:87:VAL:HA	3:3:91:MET:HE1	1.58	0.85
8:7:87:PRO:O	8:7:88:ARG:HB2	1.74	0.85
8:J:87:PRO:O	8:J:88:ARG:HB2	1.74	0.85
3:C:87:VAL:HA	3:C:91:MET:HE1	1.58	0.85
3:3:402:PRO:HG3	3:3:535:MET:HE1	1.58	0.84
1:A:245:GLN:HB2	1:A:314:GLU:OE1	1.75	0.84
3:C:402:PRO:HG3	3:C:535:MET:HE1	1.58	0.84
1:1:245:GLN:HB2	1:1:314:GLU:OE1	1.76	0.84
5:5:52:ILE:CG2	5:5:114:LEU:HB3	2.07	0.84
5:E:52:ILE:CG2	5:E:114:LEU:HB3	2.07	0.84
4:4:143:LEU:HD12	13:H:834:UNK:C	2.06	0.84
4:D:143:LEU:HD12	13:T:834:UNK:C	2.06	0.84
4:D:115:THR:HG21	4:D:297:LEU:HD13	1.60	0.84
4:4:115:THR:HG21	4:4:297:LEU:HD13	1.60	0.83
3:C:689:LYS:HG3	3:C:771:VAL:HA	1.59	0.83
3:3:689:LYS:HG3	3:3:771:VAL:HA	1.59	0.83
3:3:226:ILE:HD12	3:3:235:LEU:HD13	1.58	0.83
3:C:226:ILE:HD12	3:C:235:LEU:HD13	1.58	0.83
5:E:121:LEU:HB3	5:E:146:LEU:HB2	1.60	0.83
10:P:704:UNK:C	10:P:706:UNK:N	2.40	0.83
10:M:704:UNK:C	10:M:706:UNK:N	2.40	0.83
5:5:121:LEU:HB3	5:5:146:LEU:HB2	1.60	0.83
3:3:186:ARG:HD2	3:3:231:PRO:HD3	1.61	0.82
3:C:186:ARG:HD2	3:C:231:PRO:HD3	1.61	0.82
4:4:238:SER:HB3	4:4:279:ARG:HH22	1.45	0.82
4:D:238:SER:HB3	4:D:279:ARG:HH22	1.45	0.82
4:4:311:PRO:HD3	4:4:330:HIS:CE1	2.15	0.82
4:D:311:PRO:HD3	4:D:330:HIS:CE1	2.15	0.81
4:D:230:ILE:HD13	5:E:77:LEU:HD12	1.61	0.81
4:4:230:ILE:HD13	5:5:77:LEU:HD12	1.61	0.81
6:F:96:TRP:HA	6:F:99:MET:HE3	1.61	0.81
6:6:96:TRP:HA	6:6:99:MET:HE3	1.61	0.81
3:3:739:PRO:HG2	3:3:771:VAL:CG1	2.11	0.81
3:C:739:PRO:HG2	3:C:771:VAL:CG1	2.11	0.81
3:C:2:VAL:HG13	3:C:89:ASP:HA	1.63	0.81
3:C:117:LEU:H	4:D:321:MET:HE1	1.43	0.81
3:3:2:VAL:HG13	3:3:89:ASP:HA	1.63	0.81
3:3:11:VAL:HG11	3:3:25:HIS:CD2	2.16	0.81
3:3:117:LEU:H	4:4:321:MET:HE1	1.43	0.80
1:A:88:TYR:HB2	1:A:216:THR:HG22	1.60	0.80
3:C:11:VAL:HG11	3:C:25:HIS:CD2	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:161:GLU:HG3	5:E:163:ARG:NH2	1.96	0.80
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.60	0.80
5:5:161:GLU:HG3	5:5:163:ARG:NH2	1.96	0.80
1:1:104:ARG:HH21	2:2:127:SER:CB	1.94	0.80
1:A:104:ARG:HH21	2:B:127:SER:CB	1.94	0.80
3:3:120:PRO:HG2	8:7:42:TYR:OH	1.80	0.80
3:3:250:GLU:HG3	5:5:169:GLU:CD	2.05	0.80
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.64	0.80
3:C:250:GLU:HG3	5:E:169:GLU:CD	2.06	0.80
3:C:584:VAL:HG12	3:C:600:VAL:HB	1.64	0.80
1:1:293:GLY:HA3	1:1:324:GLY:H	1.47	0.80
3:3:679:ARG:NH1	3:C:319:GLU:OE1	2.15	0.80
1:A:293:GLY:HA3	1:A:324:GLY:H	1.47	0.80
3:C:120:PRO:HG2	8:J:42:TYR:OH	1.80	0.80
3:3:722:THR:HG21	3:3:756:GLY:N	1.97	0.80
1:A:104:ARG:NH2	2:B:127:SER:HB3	1.97	0.80
3:C:722:THR:HG21	3:C:756:GLY:N	1.97	0.80
1:1:104:ARG:NH2	2:2:127:SER:HB3	1.97	0.80
15:1:440:FMN:N1	15:1:440:FMN:O3'	2.13	0.79
15:A:440:FMN:N1	15:A:440:FMN:O3'	2.13	0.79
1:A:160:LYS:HG3	1:A:161:ASN:H	1.46	0.79
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.64	0.79
1:1:160:LYS:HG3	1:1:161:ASN:H	1.46	0.79
3:C:694:LEU:HB3	3:C:762:ALA:HB2	1.64	0.79
3:3:237:ASP:OD1	3:3:239:THR:HG22	1.81	0.78
3:C:237:ASP:OD1	3:C:239:THR:HG22	1.81	0.78
4:4:212:PRO:HG2	4:4:213:ILE:HD12	1.64	0.78
1:A:415:ARG:O	1:A:415:ARG:HG2	1.82	0.78
4:D:212:PRO:HG2	4:D:213:ILE:HD12	1.64	0.78
1:1:415:ARG:O	1:1:415:ARG:HG2	1.83	0.78
5:E:37:GLU:O	5:E:41:TYR:HD1	1.67	0.78
5:5:37:GLU:O	5:5:41:TYR:HD1	1.67	0.78
3:3:485:GLU:O	6:F:16:ARG:NH1	2.16	0.77
4:D:249:ARG:HB3	4:D:257:TYR:HD1	1.48	0.77
3:3:561:PRO:CB	3:3:576:ALA:HA	2.12	0.77
4:4:249:ARG:HB3	4:4:257:TYR:HD1	1.48	0.77
3:C:561:PRO:CB	3:C:576:ALA:HA	2.12	0.77
3:3:337:ARG:H	3:3:337:ARG:CD	1.98	0.77
3:C:337:ARG:H	3:C:337:ARG:CD	1.98	0.77
9:O:420:UNK:C	9:O:422:UNK:N	2.44	0.77
3:3:655:ARG:HB2	3:3:655:ARG:NH1	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:420:UNK:C	9:L:422:UNK:N	2.44	0.77
3:C:655:ARG:HB2	3:C:655:ARG:NH1	1.98	0.77
1:1:98:PRO:HA	2:2:124:CYS:SG	2.26	0.77
7:9:33:LEU:HD11	7:9:161:TYR:HB2	1.67	0.77
7:G:33:LEU:HD11	7:G:161:TYR:HB2	1.68	0.77
3:3:368:HIS:CB	3:3:556:ALA:HB3	2.15	0.76
3:C:368:HIS:CB	3:C:556:ALA:HB3	2.15	0.76
1:A:98:PRO:HA	2:B:124:CYS:SG	2.26	0.76
5:5:174:LEU:HD21	5:5:180:GLY:HA2	1.67	0.76
3:C:368:HIS:HB3	3:C:556:ALA:HB3	1.67	0.76
5:E:174:LEU:HD21	5:E:180:GLY:HA2	1.67	0.76
3:3:368:HIS:HB3	3:3:556:ALA:HB3	1.67	0.76
3:3:511:VAL:O	3:3:518:ALA:HB2	1.86	0.76
3:C:511:VAL:O	3:C:518:ALA:HB2	1.86	0.76
4:4:389:GLN:HG3	4:4:390:VAL:H	1.51	0.76
4:D:389:GLN:HG3	4:D:390:VAL:H	1.51	0.76
3:C:337:ARG:H	3:C:337:ARG:HD2	1.51	0.76
3:3:160:THR:OG1	8:7:73:SER:HB3	1.86	0.76
3:C:160:THR:OG1	8:J:73:SER:HB3	1.86	0.76
3:3:337:ARG:H	3:3:337:ARG:HD2	1.51	0.76
4:D:367:ARG:HH11	4:D:367:ARG:CG	1.98	0.76
4:D:390:VAL:HB	4:D:391:PRO:HD3	1.68	0.76
4:4:367:ARG:HH11	4:4:367:ARG:CG	1.99	0.76
4:4:390:VAL:HB	4:4:391:PRO:HD3	1.68	0.76
1:1:243:THR:HG22	1:1:244:GLU:H	1.51	0.75
1:1:437:TRP:CB	2:2:92:GLY:HA3	2.04	0.75
1:A:243:THR:HG22	1:A:244:GLU:H	1.51	0.75
2:2:61:MET:HE2	3:3:214:MET:HG2	1.67	0.75
1:A:437:TRP:CB	2:B:92:GLY:HA3	2.04	0.75
2:B:61:MET:HE2	3:C:214:MET:HG2	1.67	0.75
7:9:44:THR:HA	7:9:138:VAL:CG1	2.16	0.75
7:G:44:THR:HA	7:G:138:VAL:CG1	2.16	0.75
4:4:283:MET:O	4:4:287:VAL:HG23	1.87	0.75
4:D:283:MET:O	4:D:287:VAL:HG23	1.87	0.75
5:5:5:ARG:HH11	5:5:5:ARG:HG3	1.51	0.75
5:E:5:ARG:HH11	5:E:5:ARG:HG3	1.51	0.75
4:4:85:MET:HE3	4:4:409:ARG:HG3	1.69	0.74
6:6:99:MET:HG2	6:6:100:PRO:HD2	1.69	0.74
3:C:186:ARG:HD3	3:C:229:ILE:HG22	1.68	0.74
4:D:85:MET:HE3	4:D:409:ARG:HG3	1.69	0.74
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:MET:HG2	6:F:100:PRO:HD2	1.69	0.74
3:3:690:GLY:HA3	3:3:770:ARG:NH2	2.02	0.74
3:C:690:GLY:HA3	3:C:770:ARG:NH2	2.02	0.74
3:3:440:ARG:CG	3:3:440:ARG:NH1	2.46	0.74
3:C:440:ARG:CG	3:C:440:ARG:NH1	2.46	0.74
9:L:1527:UNK:C	9:L:1529:UNK:N	2.42	0.74
9:O:1527:UNK:C	9:O:1529:UNK:N	2.42	0.74
3:3:101:ARG:HB3	3:3:101:ARG:NH1	2.03	0.73
10:M:651:UNK:C	10:M:653:UNK:N	2.50	0.73
10:P:651:UNK:C	10:P:653:UNK:N	2.50	0.73
3:C:101:ARG:HB3	3:C:101:ARG:NH1	2.04	0.73
3:3:413:LEU:HD13	3:3:448:MET:HE1	1.68	0.73
4:4:371:ARG:NH2	4:4:376:VAL:HG21	2.02	0.73
1:A:360:ARG:O	1:A:364:ALA:HB3	1.88	0.73
4:D:371:ARG:NH2	4:D:376:VAL:HG21	2.02	0.73
1:1:360:ARG:O	1:1:364:ALA:HB3	1.88	0.73
1:1:437:TRP:HB3	2:2:92:GLY:CA	2.05	0.73
3:3:386:SER:HB2	3:3:675:ARG:NH1	2.04	0.73
3:C:386:SER:HB2	3:C:675:ARG:NH1	2.04	0.73
3:C:413:LEU:HD13	3:C:448:MET:HE1	1.68	0.73
4:D:250:LYS:HE2	4:D:262:PHE:HB3	1.69	0.73
4:4:250:LYS:HE2	4:4:262:PHE:HB3	1.70	0.73
1:A:437:TRP:HB3	2:B:92:GLY:CA	2.05	0.73
5:5:103:THR:HG22	5:5:126:PHE:HB3	1.71	0.73
11:N:310:UNK:CA	11:N:350:UNK:N	2.51	0.73
3:C:205:ARG:HA	3:C:209:THR:HG22	1.71	0.73
11:Q:310:UNK:CA	11:Q:350:UNK:N	2.51	0.73
2:2:24:ARG:O	2:2:27:ILE:HG13	1.89	0.73
2:B:24:ARG:O	2:B:27:ILE:HG13	1.89	0.73
5:E:103:THR:HG22	5:E:126:PHE:HB3	1.71	0.73
3:3:116:PRO:O	3:3:117:LEU:HB2	1.88	0.73
3:3:205:ARG:HA	3:3:209:THR:HG22	1.71	0.73
3:3:300:TRP:HB3	3:3:705:VAL:HG21	1.71	0.73
3:C:116:PRO:O	3:C:117:LEU:HB2	1.88	0.73
3:C:300:TRP:HB3	3:C:705:VAL:HG21	1.71	0.73
6:6:165:GLU:HG2	7:9:148:ARG:HH11	1.54	0.73
3:C:738:THR:CG2	3:C:739:PRO:HD2	2.16	0.73
4:D:168:PHE:HE1	6:F:141:PRO:HG3	1.54	0.73
3:3:738:THR:CG2	3:3:739:PRO:HD2	2.17	0.72
4:4:168:PHE:HE1	6:6:141:PRO:HG3	1.54	0.72
5:5:106:ASP:HB2	5:5:107:LEU:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:HA	1:A:284:LEU:HD21	1.72	0.72
5:E:106:ASP:HB2	5:E:107:LEU:HD12	1.71	0.72
1:1:259:LYS:HA	1:1:284:LEU:HD21	1.72	0.72
6:F:165:GLU:HG2	7:G:148:ARG:HH11	1.54	0.72
1:1:270:THR:O	1:1:311:MET:HG3	1.88	0.72
3:3:494:LYS:O	3:3:498:GLU:HG2	1.88	0.72
3:C:494:LYS:O	3:C:498:GLU:HG2	1.88	0.72
3:C:615:VAL:HG22	3:C:621:VAL:HG12	1.70	0.72
1:1:16:THR:HG21	1:1:229:PRO:CB	2.18	0.72
3:3:615:VAL:HG22	3:3:621:VAL:HG12	1.70	0.72
1:A:16:THR:HG21	1:A:229:PRO:CB	2.18	0.72
1:A:270:THR:O	1:A:311:MET:HG3	1.88	0.72
3:C:438:LYS:O	3:C:441:MET:HG3	1.88	0.72
6:F:81:ALA:HA	6:F:108:MET:HB3	1.69	0.72
3:3:438:LYS:O	3:3:441:MET:HG3	1.88	0.72
6:6:81:ALA:HA	6:6:108:MET:HB3	1.69	0.72
7:9:73:ALA:HB2	7:9:89:LYS:HB2	1.71	0.72
3:C:538:ALA:HB3	3:C:541:ALA:HB2	1.72	0.72
7:G:73:ALA:HB2	7:G:89:LYS:HB2	1.71	0.72
3:3:31:PRO:HG3	3:3:137:TYR:CD1	2.24	0.72
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.72	0.72
3:3:679:ARG:NH1	3:C:319:GLU:OE2	2.21	0.72
3:3:300:TRP:HB3	3:3:705:VAL:CG2	2.20	0.72
11:N:653:UNK:C	11:N:655:UNK:N	2.51	0.72
3:C:31:PRO:HG3	3:C:137:TYR:CD1	2.24	0.72
4:4:105:LEU:HD13	4:4:309:ILE:HD13	1.72	0.72
3:C:300:TRP:HB3	3:C:705:VAL:CG2	2.20	0.72
4:D:105:LEU:HD13	4:D:309:ILE:HD13	1.72	0.72
5:E:3:LEU:HB2	5:E:86:SER:HB2	1.70	0.72
11:Q:653:UNK:C	11:Q:655:UNK:N	2.51	0.72
3:3:55:PRO:HD3	3:3:74:GLN:H	1.53	0.72
3:3:679:ARG:NH2	3:C:319:GLU:OE1	2.22	0.72
5:5:3:LEU:HB2	5:5:86:SER:HB2	1.71	0.72
2:2:109:GLY:HA2	8:7:91:ILE:HD13	1.72	0.71
4:4:47:LEU:HD13	4:4:52:VAL:HA	1.72	0.71
6:6:148:ILE:HG21	7:9:27:PRO:HG3	1.70	0.71
9:L:1526:UNK:C	9:L:1528:UNK:N	2.53	0.71
2:B:136:VAL:HG21	2:B:163:LEU:HD13	1.72	0.71
3:C:55:PRO:HD3	3:C:74:GLN:H	1.53	0.71
6:F:148:ILE:HG21	7:G:27:PRO:HG3	1.70	0.71
9:O:1526:UNK:C	9:O:1528:UNK:N	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:LEU:HD13	4:D:52:VAL:HA	1.73	0.71
4:D:314:ARG:HH11	4:D:314:ARG:HG2	1.53	0.71
2:2:136:VAL:HG21	2:2:163:LEU:HD13	1.72	0.71
3:3:501:LYS:HD2	3:3:501:LYS:N	2.02	0.71
4:4:314:ARG:HG2	4:4:314:ARG:HH11	1.53	0.71
2:B:109:GLY:HA2	8:J:91:ILE:HD13	1.72	0.71
3:C:501:LYS:HD2	3:C:501:LYS:N	2.02	0.71
3:3:679:ARG:NH1	3:C:319:GLU:CD	2.48	0.71
1:1:222:GLU:HG3	1:1:251:LEU:HD22	1.72	0.71
3:3:367:PRO:HB2	3:3:554:LYS:HB2	1.73	0.71
1:A:341:MET:HE1	1:A:409:PRO:HB2	1.70	0.71
12:S:413:UNK:C	12:S:415:UNK:N	2.54	0.71
1:1:341:MET:HE1	1:1:409:PRO:HB2	1.70	0.71
1:A:222:GLU:HG3	1:A:251:LEU:HD22	1.72	0.71
3:C:367:PRO:HB2	3:C:554:LYS:HB2	1.73	0.71
3:3:217:GLY:O	3:3:218:LEU:HB2	1.90	0.70
3:3:398:VAL:HB	3:3:450:LEU:HD22	1.71	0.70
12:R:413:UNK:C	12:R:415:UNK:N	2.54	0.70
3:C:217:GLY:O	3:C:218:LEU:HB2	1.90	0.70
3:C:398:VAL:HB	3:C:450:LEU:HD22	1.71	0.70
4:4:371:ARG:HG3	5:5:51:ASP:OD1	1.91	0.70
3:C:185:LYS:HG2	3:C:188:VAL:HG22	1.73	0.70
4:D:371:ARG:HG3	5:E:51:ASP:OD1	1.91	0.70
3:3:185:LYS:HG2	3:3:188:VAL:HG22	1.73	0.70
9:O:1527:UNK:C	9:O:1530:UNK:CA	2.69	0.70
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.25	0.70
7:9:44:THR:HA	7:9:138:VAL:HG13	1.73	0.70
9:L:1527:UNK:C	9:L:1530:UNK:CA	2.69	0.70
4:D:285:GLU:O	4:D:289:ILE:HG12	1.91	0.70
5:E:80:TRP:HA	5:E:80:TRP:CE3	2.25	0.70
7:G:44:THR:HA	7:G:138:VAL:HG13	1.73	0.70
3:3:591:HIS:ND1	3:3:592:PRO:HD2	2.07	0.70
3:C:739:PRO:HG2	3:C:771:VAL:HG12	1.72	0.70
3:3:739:PRO:HG2	3:3:771:VAL:HG12	1.72	0.70
4:4:285:GLU:O	4:4:289:ILE:HG12	1.91	0.70
3:C:101:ARG:NH1	3:C:140:TYR:CD1	2.59	0.70
3:C:591:HIS:ND1	3:C:592:PRO:HD2	2.07	0.70
4:D:371:ARG:HH22	4:D:376:VAL:HG21	1.57	0.70
3:3:101:ARG:NH1	3:3:140:TYR:CD1	2.59	0.70
4:4:371:ARG:HH22	4:4:376:VAL:HG21	1.57	0.70
1:1:267:PRO:O	1:1:270:THR:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:506:ILE:HG21	3:3:535:MET:HE3	1.74	0.70
3:C:506:ILE:HG21	3:C:535:MET:HE3	1.74	0.70
10:P:820:UNK:C	10:P:824:UNK:N	2.55	0.70
10:M:820:UNK:C	10:M:824:UNK:N	2.55	0.70
1:A:267:PRO:O	1:A:270:THR:HG23	1.91	0.70
3:C:309:PRO:HG2	3:C:320:ALA:O	1.92	0.70
3:3:309:PRO:HG2	3:3:320:ALA:O	1.92	0.69
4:D:263:ASP:HB2	4:D:285:GLU:CD	2.17	0.69
4:4:263:ASP:HB2	4:4:285:GLU:CD	2.17	0.69
3:3:459:MET:HG2	3:3:465:HIS:HB2	1.75	0.69
4:D:40:VAL:HG13	4:D:404:MET:HG3	1.73	0.69
1:1:402:LEU:HD13	14:1:439:SF4:S1	2.33	0.69
4:4:40:VAL:HG13	4:4:404:MET:HG3	1.73	0.69
5:5:186:GLY:HA2	5:5:190:LYS:HD3	1.74	0.69
1:A:402:LEU:HD13	14:A:439:SF4:S1	2.33	0.69
5:E:186:GLY:HA2	5:E:190:LYS:HD3	1.74	0.69
6:6:151:VAL:O	6:6:155:GLN:HB2	1.90	0.69
9:L:1522:UNK:C	9:L:1524:UNK:N	2.54	0.69
3:C:459:MET:HG2	3:C:465:HIS:HB2	1.75	0.69
9:O:1522:UNK:C	9:O:1524:UNK:N	2.54	0.69
1:1:203:PRO:HB2	1:1:204:PRO:HD3	1.75	0.69
5:5:33:ARG:O	5:5:37:GLU:HB2	1.92	0.69
1:A:303:THR:OG1	1:A:306:VAL:HG23	1.91	0.69
5:E:33:ARG:O	5:E:37:GLU:HB2	1.92	0.69
6:F:151:VAL:O	6:F:155:GLN:HB2	1.91	0.69
1:1:303:THR:OG1	1:1:306:VAL:HG23	1.91	0.69
3:3:693:TYR:HB3	3:3:759:TYR:HD2	1.57	0.69
4:4:235:THR:HG21	4:4:352:GLU:HB2	1.73	0.69
1:A:203:PRO:HB2	1:A:204:PRO:HD3	1.75	0.69
1:A:312:SER:N	1:A:316:LEU:HD12	2.07	0.69
1:1:312:SER:N	1:1:316:LEU:HD12	2.07	0.69
1:1:370:LEU:O	1:1:374:ILE:HG22	1.92	0.69
3:C:693:TYR:HB3	3:C:759:TYR:HD2	1.57	0.69
4:D:235:THR:HG21	4:D:352:GLU:HB2	1.73	0.69
1:A:370:LEU:O	1:A:374:ILE:HG22	1.92	0.69
4:4:261:THR:H	4:4:292:GLN:HE22	1.39	0.69
1:A:312:SER:H	1:A:316:LEU:HD12	1.58	0.69
1:1:312:SER:H	1:1:316:LEU:HD12	1.59	0.68
4:D:261:THR:H	4:D:292:GLN:HE22	1.39	0.68
6:6:113:SER:HB3	7:9:96:LEU:HD13	1.75	0.68
8:7:121:ARG:HH11	8:7:121:ARG:HG3	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:113:SER:HB3	7:G:96:LEU:HD13	1.75	0.68
8:J:121:ARG:HH11	8:J:121:ARG:HG3	1.58	0.68
1:1:341:MET:CE	1:1:409:PRO:HB2	2.23	0.68
4:4:218:ALA:HB1	4:4:272:VAL:HG22	1.74	0.68
1:A:149:ILE:HD13	1:A:171:LEU:HB3	1.74	0.68
3:C:374:ARG:HH21	3:C:684:ARG:HG3	1.57	0.68
3:C:542:ARG:HB2	3:C:542:ARG:HH11	1.58	0.68
1:1:149:ILE:HD13	1:1:171:LEU:HB3	1.74	0.68
3:3:374:ARG:HH21	3:3:684:ARG:HG3	1.57	0.68
4:4:98:ALA:O	4:4:102:GLU:HG3	1.94	0.68
1:A:29:LEU:HD22	1:A:33:LEU:HG	1.74	0.68
1:A:341:MET:CE	1:A:409:PRO:HB2	2.23	0.68
4:D:98:ALA:O	4:D:102:GLU:HG3	1.94	0.68
1:1:29:LEU:HD22	1:1:33:LEU:HG	1.75	0.68
3:3:175:ILE:HB	3:3:238:LEU:HD22	1.75	0.68
3:3:542:ARG:HB2	3:3:542:ARG:HH11	1.58	0.68
4:4:96:ALA:HB2	4:4:346:THR:HG21	1.76	0.68
4:D:96:ALA:HB2	4:D:346:THR:HG21	1.76	0.68
4:D:218:ALA:HB1	4:D:272:VAL:HG22	1.74	0.68
3:3:567:TYR:HA	3:3:584:VAL:HG23	1.75	0.68
1:A:253:GLN:HE21	1:A:253:GLN:H	1.42	0.68
3:C:175:ILE:HB	3:C:238:LEU:HD22	1.75	0.68
1:1:253:GLN:HE21	1:1:253:GLN:H	1.42	0.68
3:C:567:TYR:HA	3:C:584:VAL:HG23	1.75	0.68
5:5:163:ARG:HD2	7:9:69:TYR:CD1	2.29	0.68
4:D:367:ARG:HG3	4:D:367:ARG:NH1	2.03	0.68
5:E:163:ARG:HD2	7:G:69:TYR:CD1	2.29	0.68
5:5:2:ARG:HG3	5:5:84:ASP:OD2	1.94	0.67
5:E:2:ARG:HG3	5:E:84:ASP:OD2	1.94	0.67
4:4:367:ARG:HG3	4:4:367:ARG:NH1	2.03	0.67
3:C:279:ALA:CB	3:C:290:ILE:HG12	2.24	0.67
3:3:279:ALA:CB	3:3:290:ILE:HG12	2.24	0.67
6:6:163:TYR:HD1	7:9:152:ARG:NH1	1.91	0.67
6:F:163:TYR:HD1	7:G:152:ARG:NH1	1.91	0.67
10:P:401:UNK:CA	11:Q:663:UNK:CA	2.72	0.67
4:4:224:ILE:HD11	4:4:275:ARG:NH1	2.09	0.67
4:D:236:GLY:C	4:D:238:SER:H	2.00	0.67
10:M:401:UNK:CA	11:N:663:UNK:CA	2.72	0.67
4:D:224:ILE:HD11	4:D:275:ARG:NH1	2.09	0.67
4:4:236:GLY:C	4:4:238:SER:H	2.00	0.67
3:3:117:LEU:HD23	4:4:321:MET:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:311:PRO:HD3	4:4:330:HIS:NE2	2.09	0.67
5:5:50:ALA:HB3	5:5:73:GLU:HB3	1.78	0.67
4:D:311:PRO:HD3	4:D:330:HIS:NE2	2.09	0.67
1:1:288:GLN:HB3	1:1:333:GLU:HG2	1.77	0.66
2:2:77:LYS:H	2:2:116:LEU:HA	1.58	0.66
2:B:77:LYS:H	2:B:116:LEU:HA	1.58	0.66
5:E:50:ALA:HB3	5:E:73:GLU:HB3	1.78	0.66
1:A:93:ALA:HB1	1:A:107:LEU:HD11	1.75	0.66
1:A:288:GLN:HB3	1:A:333:GLU:HG2	1.77	0.66
3:C:117:LEU:HD23	4:D:321:MET:HA	1.77	0.66
5:E:5:ARG:HG3	5:E:5:ARG:NH1	2.07	0.66
1:1:93:ALA:HB1	1:1:107:LEU:HD11	1.75	0.66
3:3:586:HIS:NE2	3:3:640:VAL:HG21	2.10	0.66
3:3:679:ARG:CZ	3:C:319:GLU:OE1	2.42	0.66
5:5:5:ARG:HG3	5:5:5:ARG:NH1	2.07	0.66
3:C:586:HIS:NE2	3:C:640:VAL:HG21	2.10	0.66
3:C:132:ASP:O	3:C:136:GLU:HG3	1.95	0.66
3:3:132:ASP:O	3:3:136:GLU:HG3	1.95	0.66
6:6:119:ASN:HA	6:6:125:GLN:HE22	1.61	0.66
6:F:119:ASN:HA	6:F:125:GLN:HE22	1.61	0.66
7:G:40:ARG:HB2	7:G:121:MET:CE	2.18	0.66
4:4:274:ASP:O	4:4:278:VAL:HG23	1.96	0.66
4:D:99:LEU:HB3	4:D:344:VAL:HG21	1.77	0.66
3:3:367:PRO:CB	3:3:554:LYS:HB2	2.26	0.66
4:4:99:LEU:HB3	4:4:344:VAL:HG21	1.77	0.66
4:4:116:ILE:O	4:4:120:LEU:HB2	1.96	0.66
3:3:402:PRO:CG	3:3:535:MET:HE1	2.26	0.66
7:9:40:ARG:HB2	7:9:121:MET:CE	2.18	0.66
3:C:367:PRO:CB	3:C:554:LYS:HB2	2.26	0.66
4:D:116:ILE:O	4:D:120:LEU:HB2	1.96	0.66
4:D:274:ASP:O	4:D:278:VAL:HG23	1.96	0.66
3:3:285:VAL:HG22	3:3:286:ASN:H	1.61	0.66
3:3:485:GLU:CG	6:F:16:ARG:CG	2.65	0.66
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.77	0.66
6:6:117:MET:CE	7:9:99:ILE:HG12	2.17	0.66
3:C:285:VAL:HG22	3:C:286:ASN:H	1.61	0.66
3:C:402:PRO:CG	3:C:535:MET:HE1	2.26	0.66
4:D:341:GLU:HG2	4:D:358:VAL:HG22	1.77	0.65
6:F:117:MET:CE	7:G:99:ILE:HG12	2.17	0.65
1:1:437:TRP:CZ3	2:2:96:LEU:HB2	2.31	0.65
6:F:16:ARG:HA	6:F:21:PHE:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:715:GLU:HB3	3:3:746:ARG:CZ	2.26	0.65
4:4:404:MET:HA	4:4:407:VAL:CG1	2.27	0.65
6:6:16:ARG:HA	6:6:21:PHE:CD2	2.32	0.65
1:A:53:VAL:HG23	1:A:231:MET:HE2	1.77	0.65
1:A:437:TRP:CZ3	2:B:96:LEU:HB2	2.31	0.65
3:C:715:GLU:HB3	3:C:746:ARG:CZ	2.25	0.65
4:D:44:MET:HE2	4:D:44:MET:HA	1.78	0.65
4:D:404:MET:HA	4:D:407:VAL:CG1	2.27	0.65
3:3:117:LEU:CD2	4:4:321:MET:HA	2.26	0.65
4:4:44:MET:HE2	4:4:44:MET:HA	1.78	0.65
3:C:117:LEU:CD2	4:D:321:MET:HA	2.26	0.65
4:D:40:VAL:O	4:D:40:VAL:HG22	1.94	0.65
1:1:53:VAL:HG23	1:1:231:MET:HE2	1.77	0.65
4:4:40:VAL:O	4:4:40:VAL:HG22	1.94	0.65
1:A:272:PHE:HZ	1:A:316:LEU:HD21	1.60	0.65
2:B:86:LEU:O	2:B:90:LEU:HD12	1.96	0.65
3:C:506:ILE:CG2	3:C:535:MET:HE3	2.27	0.65
2:2:86:LEU:O	2:2:90:LEU:HD12	1.96	0.65
3:3:506:ILE:CG2	3:3:535:MET:HE3	2.27	0.65
1:1:272:PHE:HZ	1:1:316:LEU:HD21	1.60	0.65
4:4:254:TYR:CE2	4:4:346:THR:HA	2.31	0.65
4:D:254:TYR:CE2	4:D:346:THR:HA	2.31	0.65
3:C:216:PHE:CZ	8:J:128:PHE:HD2	2.15	0.65
3:3:216:PHE:CZ	8:7:128:PHE:HD2	2.16	0.64
1:A:297:THR:HG22	1:A:322:MET:CG	2.26	0.64
1:1:297:THR:HG22	1:1:322:MET:CG	2.26	0.64
7:9:46:HIS:HB3	7:9:47:PRO:HD2	1.79	0.64
7:G:46:HIS:HB3	7:G:47:PRO:HD2	1.79	0.64
3:3:583:VAL:CG2	3:3:598:ALA:HA	2.27	0.64
3:C:583:VAL:CG2	3:C:598:ALA:HA	2.27	0.64
1:1:274:GLU:HG3	1:1:278:GLU:HG3	1.80	0.64
4:4:65:GLY:O	4:4:69:THR:HG22	1.98	0.64
3:3:489:MET:HE2	3:3:492:LYS:HD2	1.79	0.64
3:3:689:LYS:HE3	3:3:771:VAL:CG1	2.27	0.64
3:C:489:MET:HE2	3:C:492:LYS:HD2	1.79	0.64
3:C:689:LYS:HE3	3:C:771:VAL:CG1	2.27	0.64
4:D:65:GLY:O	4:D:69:THR:HG22	1.98	0.64
1:1:116:GLU:HA	1:1:119:ILE:HD12	1.80	0.64
7:9:101:CYS:HB2	7:9:103:LEU:H	1.63	0.64
1:A:116:GLU:HA	1:A:119:ILE:HD12	1.80	0.64
1:A:274:GLU:HG3	1:A:278:GLU:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:CYS:HB2	7:G:103:LEU:H	1.63	0.64
3:3:205:ARG:C	3:3:209:THR:HG22	2.23	0.64
3:C:205:ARG:C	3:C:209:THR:HG22	2.23	0.64
7:G:56:CYS:SG	7:G:58:LEU:HB2	2.37	0.64
1:1:99:GLY:HA3	1:1:329:ILE:HD11	1.79	0.64
1:1:289:ALA:HB3	1:1:337:MET:HE3	1.79	0.64
7:9:56:CYS:SG	7:9:58:LEU:HB2	2.37	0.64
1:A:99:GLY:HA3	1:A:329:ILE:HD11	1.79	0.64
1:A:289:ALA:HB3	1:A:337:MET:HE3	1.78	0.64
4:4:314:ARG:HG2	4:4:314:ARG:NH1	2.13	0.64
5:5:120:ASP:CG	5:5:134:LYS:HG3	2.22	0.64
3:3:394:ASP:OD2	3:3:501:LYS:HB2	1.98	0.63
3:3:679:ARG:NE	3:C:319:GLU:OE2	2.31	0.63
4:4:93:HIS:CE1	4:4:353:LEU:HD11	2.33	0.63
3:C:205:ARG:CA	3:C:209:THR:HG22	2.27	0.63
3:C:394:ASP:OD2	3:C:501:LYS:HB2	1.98	0.63
4:D:93:HIS:CE1	4:D:353:LEU:HD11	2.33	0.63
4:D:314:ARG:HG2	4:D:314:ARG:NH1	2.13	0.63
3:3:205:ARG:CA	3:3:209:THR:HG22	2.28	0.63
3:3:306:LEU:HD11	3:3:308:THR:O	1.97	0.63
5:E:120:ASP:CG	5:E:134:LYS:HG3	2.22	0.63
3:C:306:LEU:HD11	3:C:308:THR:O	1.98	0.63
5:E:10:ALA:HB1	5:E:15:TYR:HB2	1.81	0.63
3:3:224:GLY:O	3:3:227:THR:HB	1.99	0.63
3:3:304:ASN:O	3:3:589:HIS:CD2	2.52	0.63
5:5:10:ALA:HB1	5:5:15:TYR:HB2	1.81	0.63
5:5:144:HIS:HB2	5:5:147:ARG:HD3	1.79	0.63
3:C:304:ASN:O	3:C:589:HIS:CD2	2.52	0.63
5:E:144:HIS:HB2	5:E:147:ARG:HD3	1.79	0.63
3:3:485:GLU:HG2	6:F:16:ARG:CG	2.28	0.63
3:C:224:GLY:O	3:C:227:THR:HB	1.99	0.63
2:2:40:TRP:CH2	2:2:42:ARG:HG2	2.33	0.63
3:3:11:VAL:HG11	3:3:25:HIS:HD2	1.61	0.63
2:B:40:TRP:CH2	2:B:42:ARG:HG2	2.33	0.63
5:5:107:LEU:HD12	5:5:107:LEU:N	2.14	0.63
3:C:11:VAL:HG11	3:C:25:HIS:HD2	1.60	0.63
3:C:546:ALA:O	3:C:547:MET:HE2	1.98	0.63
4:D:263:ASP:O	4:D:265:PRO:HD3	1.98	0.63
5:E:107:LEU:HD12	5:E:107:LEU:N	2.14	0.63
3:3:546:ALA:O	3:3:547:MET:HE2	1.98	0.62
4:4:70:MET:HG2	4:4:78:ASN:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:83:ARG:HH11	6:6:83:ARG:HG3	1.64	0.62
4:D:70:MET:HG2	4:D:78:ASN:OD1	1.99	0.62
4:4:263:ASP:O	4:4:265:PRO:HD3	1.99	0.62
5:5:72:TYR:HB2	5:5:90:VAL:HG13	1.81	0.62
1:A:401:PRO:HB2	15:A:440:FMN:C8M	2.29	0.62
4:D:225:PRO:HG2	4:D:228:VAL:HB	1.81	0.62
5:E:72:TYR:HB2	5:E:90:VAL:HG13	1.81	0.62
5:E:126:PHE:H	5:E:132:LEU:HD11	1.65	0.62
6:F:83:ARG:HH11	6:F:83:ARG:HG3	1.64	0.62
1:1:401:PRO:HB2	15:1:440:FMN:C8M	2.30	0.62
4:4:225:PRO:HG2	4:4:228:VAL:HB	1.81	0.62
4:4:215:TYR:CE2	4:4:219:ARG:HG3	2.34	0.62
5:5:126:PHE:H	5:5:132:LEU:HD11	1.65	0.62
4:D:215:TYR:CE2	4:D:219:ARG:HG3	2.34	0.62
5:E:37:GLU:O	5:E:41:TYR:CD1	2.52	0.62
6:F:153:GLN:HG3	7:G:124:TYR:OH	1.99	0.62
5:5:37:GLU:O	5:5:41:TYR:CD1	2.52	0.62
6:6:153:GLN:HG3	7:9:124:TYR:OH	1.99	0.62
3:C:716:LEU:HD21	3:C:758:LEU:HB3	1.81	0.62
5:E:39:ALA:HA	5:E:107:LEU:HD23	1.82	0.62
3:3:716:LEU:HD21	3:3:758:LEU:HB3	1.81	0.62
5:5:39:ALA:HA	5:5:107:LEU:HD23	1.82	0.62
5:E:174:LEU:CD2	5:E:180:GLY:HA2	2.30	0.62
3:3:692:PHE:HE1	3:3:773:GLY:O	1.82	0.62
5:5:174:LEU:CD2	5:5:180:GLY:HA2	2.30	0.62
3:C:692:PHE:HE1	3:C:773:GLY:O	1.82	0.62
1:1:50:PRO:O	1:1:53:VAL:HG12	1.99	0.62
1:A:50:PRO:O	1:A:53:VAL:HG12	1.99	0.62
5:E:80:TRP:HA	5:E:80:TRP:HE3	1.65	0.62
3:3:732:ALA:O	3:3:747:VAL:HG12	2.00	0.61
5:5:80:TRP:HA	5:5:80:TRP:HE3	1.65	0.61
3:C:732:ALA:O	3:C:747:VAL:HG12	2.01	0.61
5:5:52:ILE:HG23	5:5:114:LEU:HB3	1.82	0.61
3:C:701:ALA:HB2	3:C:763:LEU:HB2	1.80	0.61
4:D:88:LEU:HD21	6:F:48:ILE:HD13	1.82	0.61
6:F:140:CYS:SG	7:G:99:ILE:HG13	2.39	0.61
4:4:72:HIS:O	4:4:73:ARG:HD2	2.00	0.61
4:4:88:LEU:HD21	6:6:48:ILE:HD13	1.82	0.61
4:D:72:HIS:O	4:D:73:ARG:HD2	2.00	0.61
5:E:52:ILE:HG23	5:E:114:LEU:HB3	1.82	0.61
3:3:750:ARG:HB2	3:3:753:VAL:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:70:MET:HE3	4:4:81:TYR:CB	2.29	0.61
6:6:140:CYS:SG	7:9:99:ILE:HG13	2.39	0.61
1:A:401:PRO:HB2	15:A:440:FMN:HM82	1.81	0.61
3:C:750:ARG:HB2	3:C:753:VAL:HG23	1.82	0.61
4:D:70:MET:HE3	4:D:81:TYR:CB	2.29	0.61
1:1:92:ASN:ND2	15:1:440:FMN:O3'	2.32	0.61
2:2:40:TRP:CD1	2:2:74:PRO:HA	2.36	0.61
3:3:739:PRO:HG2	3:3:771:VAL:HG11	1.79	0.61
1:A:92:ASN:ND2	15:A:440:FMN:O3'	2.32	0.61
3:3:701:ALA:HB2	3:3:763:LEU:HB2	1.80	0.61
5:5:5:ARG:HH11	5:5:5:ARG:CG	2.12	0.61
2:B:40:TRP:CD1	2:B:74:PRO:HA	2.36	0.61
5:5:20:ASN:HD21	5:5:24:ASN:HB2	1.65	0.61
3:C:739:PRO:HG2	3:C:771:VAL:HG11	1.79	0.61
5:E:5:ARG:HH11	5:E:5:ARG:CG	2.12	0.61
1:1:401:PRO:HB2	15:1:440:FMN:HM82	1.81	0.61
5:E:20:ASN:HD21	5:E:24:ASN:HB2	1.65	0.61
6:F:156:LYS:HG2	6:F:156:LYS:O	2.01	0.61
1:1:29:LEU:O	1:1:33:LEU:HG	2.01	0.61
6:6:156:LYS:HG2	6:6:156:LYS:O	2.01	0.61
1:A:29:LEU:O	1:A:33:LEU:HG	2.01	0.61
3:3:368:HIS:CE1	3:3:563:ALA:HB2	2.35	0.60
6:F:163:TYR:HB3	6:F:168:GLU:O	2.01	0.60
6:6:163:TYR:HB3	6:6:168:GLU:O	2.01	0.60
3:C:368:HIS:CE1	3:C:563:ALA:HB2	2.36	0.60
10:P:920:UNK:CA	10:P:1200:UNK:H	2.10	0.60
3:3:360:LEU:O	3:3:364:LEU:HB3	2.00	0.60
8:7:6:GLU:OE1	8:7:80:LYS:HE3	2.01	0.60
3:C:360:LEU:O	3:C:364:LEU:HB3	2.00	0.60
8:J:6:GLU:OE1	8:J:80:LYS:HE3	2.01	0.60
3:3:285:VAL:HG22	3:3:286:ASN:N	2.15	0.60
8:7:6:GLU:CD	8:7:80:LYS:HE3	2.26	0.60
10:M:920:UNK:CA	10:M:1200:UNK:H	2.11	0.60
12:R:101:UNK:C	12:R:103:UNK:N	2.59	0.60
3:C:285:VAL:HG22	3:C:286:ASN:N	2.15	0.60
4:D:263:ASP:HB2	4:D:285:GLU:OE1	2.01	0.60
7:G:45:ARG:NH2	7:G:137:LEU:HD23	2.17	0.60
12:S:101:UNK:C	12:S:103:UNK:N	2.59	0.60
4:4:263:ASP:HB2	4:4:285:GLU:OE1	2.01	0.60
6:6:165:GLU:HG2	7:9:148:ARG:NH1	2.15	0.60
7:9:175:ALA:HB1	7:9:176:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:165:GLU:HG2	7:G:148:ARG:NH1	2.15	0.60
7:G:175:ALA:HB1	7:G:176:PRO:HD2	1.83	0.60
8:J:6:GLU:CD	8:J:80:LYS:HE3	2.26	0.60
4:4:393:MET:HA	4:4:396:ILE:CG2	2.32	0.60
5:5:39:ALA:HA	5:5:107:LEU:CD2	2.32	0.60
7:9:45:ARG:NH2	7:9:137:LEU:HD23	2.17	0.60
4:D:393:MET:HA	4:D:396:ILE:CG2	2.32	0.60
1:1:92:ASN:HD21	15:1:440:FMN:C2	2.14	0.60
6:6:107:SER:O	6:6:137:VAL:HG12	2.01	0.60
1:A:92:ASN:HD21	15:A:440:FMN:C2	2.14	0.60
5:E:39:ALA:HA	5:E:107:LEU:CD2	2.32	0.60
6:F:107:SER:O	6:F:137:VAL:HG12	2.01	0.60
9:O:1324:UNK:C	9:O:1326:UNK:N	2.63	0.60
13:T:119:UNK:C	13:T:121:UNK:N	2.64	0.60
4:4:130:LEU:HD11	4:4:152:GLU:HB3	1.83	0.60
9:L:1324:UNK:C	9:L:1326:UNK:N	2.63	0.60
13:H:119:UNK:C	13:H:121:UNK:N	2.64	0.60
4:D:130:LEU:HD11	4:D:152:GLU:HB3	1.83	0.60
4:4:404:MET:HA	4:4:407:VAL:HG12	1.84	0.60
3:C:512:LEU:HD21	3:C:534:ALA:HB1	1.83	0.60
4:D:404:MET:HA	4:D:407:VAL:HG12	1.84	0.60
3:3:512:LEU:HD21	3:3:534:ALA:HB1	1.83	0.59
3:3:583:VAL:HG21	3:3:598:ALA:HA	1.83	0.59
3:3:282:VAL:HG22	3:3:285:VAL:HG12	1.83	0.59
3:3:693:TYR:HB3	3:3:759:TYR:CD2	2.37	0.59
3:C:282:VAL:HG22	3:C:285:VAL:HG12	1.83	0.59
3:C:583:VAL:HG21	3:C:598:ALA:HA	1.83	0.59
3:3:337:ARG:HD2	3:3:337:ARG:N	2.16	0.59
7:9:43:LEU:O	7:9:138:VAL:HG13	2.03	0.59
10:M:820:UNK:C	10:M:824:UNK:CA	2.80	0.59
11:N:802:UNK:C	11:N:804:UNK:N	2.65	0.59
7:G:43:LEU:O	7:G:138:VAL:HG13	2.03	0.59
10:P:820:UNK:C	10:P:824:UNK:CA	2.80	0.59
11:Q:802:UNK:C	11:Q:804:UNK:N	2.65	0.59
4:D:76:LEU:HD12	4:D:79:ILE:HD12	1.84	0.59
4:4:76:LEU:HD12	4:4:79:ILE:HD12	1.84	0.59
1:A:313:TYR:CE1	1:A:323:LEU:HD13	2.38	0.59
1:1:214:LYS:O	1:1:216:THR:HG23	2.03	0.59
1:1:313:TYR:CE1	1:1:323:LEU:HD13	2.38	0.59
1:1:110:VAL:N	1:1:111:PRO:HD3	2.17	0.59
1:A:110:VAL:N	1:A:111:PRO:HD3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LYS:O	1:A:216:THR:HG23	2.03	0.59
1:A:247:LYS:O	1:A:268:MET:HE2	2.03	0.59
1:1:247:LYS:O	1:1:268:MET:HE2	2.03	0.59
3:3:679:ARG:HH22	3:C:319:GLU:CD	2.08	0.59
1:A:186:THR:HG23	1:A:200:ARG:N	2.09	0.59
1:1:186:THR:HG23	1:1:200:ARG:N	2.09	0.59
3:C:399:LEU:N	3:C:399:LEU:HD12	2.18	0.59
3:3:238:LEU:HD12	3:3:238:LEU:O	2.02	0.59
3:3:399:LEU:N	3:3:399:LEU:HD12	2.18	0.59
5:5:167:PRO:C	5:5:171:ARG:HH12	2.11	0.59
5:5:175:THR:O	5:5:177:LYS:N	2.36	0.59
8:7:60:SER:HA	8:7:66:PRO:HA	1.84	0.59
1:A:6:LEU:HD21	1:A:12:ARG:HG3	1.83	0.59
3:C:337:ARG:HD2	3:C:337:ARG:N	2.16	0.59
5:E:167:PRO:C	5:E:171:ARG:HH12	2.11	0.59
7:G:67:ALA:HB2	7:G:97:ARG:HB3	1.85	0.59
8:J:60:SER:HA	8:J:66:PRO:HA	1.84	0.59
1:1:6:LEU:HD21	1:1:12:ARG:HG3	1.83	0.58
7:9:67:ALA:HB2	7:9:97:ARG:HB3	1.85	0.58
5:E:175:THR:O	5:E:177:LYS:N	2.36	0.58
3:C:238:LEU:HD12	3:C:238:LEU:O	2.02	0.58
1:A:344:LEU:O	1:A:347:PHE:HB3	2.03	0.58
1:1:344:LEU:O	1:1:347:PHE:HB3	2.03	0.58
3:3:546:ALA:HA	3:3:678:PHE:CE2	2.39	0.58
4:4:393:MET:O	4:4:396:ILE:HG22	2.03	0.58
3:C:356:LEU:HD13	3:C:654:PHE:HD1	1.67	0.58
3:C:546:ALA:HA	3:C:678:PHE:CE2	2.39	0.58
4:D:393:MET:O	4:D:396:ILE:HG22	2.03	0.58
2:2:175:HIS:CE1	2:2:176:VAL:HG22	2.38	0.58
3:3:356:LEU:HD13	3:3:654:PHE:HD1	1.67	0.58
4:4:40:VAL:HG23	6:6:88:MET:HE2	1.85	0.58
2:B:175:HIS:CE1	2:B:176:VAL:HG22	2.38	0.58
3:C:738:THR:HG22	3:C:739:PRO:CD	2.22	0.58
1:1:88:TYR:HB2	1:1:216:THR:CG2	2.32	0.58
3:3:290:ILE:HG21	3:3:295:ARG:HB2	1.85	0.58
3:3:738:THR:HG22	3:3:739:PRO:CD	2.22	0.58
10:M:121:UNK:C	10:M:123:UNK:N	2.66	0.58
1:A:88:TYR:HB2	1:A:216:THR:CG2	2.32	0.58
3:C:290:ILE:HG21	3:C:295:ARG:HB2	1.85	0.58
4:D:40:VAL:HG23	6:F:88:MET:HE2	1.85	0.58
10:P:121:UNK:C	10:P:123:UNK:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:300:TRP:CB	3:3:705:VAL:HG21	2.32	0.58
4:4:355:TYR:CE2	4:4:370:VAL:HG22	2.38	0.58
5:5:134:LYS:HD3	5:5:137:THR:OG1	2.03	0.58
3:C:300:TRP:CB	3:C:705:VAL:HG21	2.32	0.58
4:D:115:THR:CG2	4:D:297:LEU:HD13	2.32	0.58
4:D:355:TYR:CE2	4:D:370:VAL:HG22	2.38	0.58
6:F:43:LEU:HB2	6:F:82:GLY:HA3	1.86	0.58
4:4:115:THR:CG2	4:4:297:LEU:HD13	2.32	0.58
6:6:16:ARG:HD3	6:6:17:GLU:OE1	2.04	0.58
6:6:43:LEU:HB2	6:6:82:GLY:HA3	1.86	0.58
1:A:17:LEU:HD12	1:A:251:LEU:HD11	1.86	0.58
5:E:134:LYS:HD3	5:E:137:THR:OG1	2.03	0.58
1:1:17:LEU:HD12	1:1:251:LEU:HD11	1.86	0.58
1:1:185:GLU:HB2	1:1:218:ILE:HD12	1.84	0.58
1:A:185:GLU:HB2	1:A:218:ILE:HD12	1.84	0.58
4:D:241:ALA:CB	4:D:278:VAL:HG21	2.34	0.58
1:1:139:ARG:HG2	2:2:139:GLU:HA	1.85	0.58
3:3:337:ARG:HG2	3:3:340:GLU:HG2	1.86	0.58
4:4:89:HIS:CE1	4:4:92:ALA:HB2	2.39	0.58
6:6:50:MET:HE2	6:6:108:MET:HE2	1.86	0.58
1:A:53:VAL:HG23	1:A:231:MET:CE	2.34	0.58
1:A:139:ARG:HG2	2:B:139:GLU:HA	1.85	0.58
3:C:337:ARG:HG2	3:C:340:GLU:HG2	1.86	0.58
6:F:16:ARG:HD3	6:F:17:GLU:OE1	2.04	0.58
6:F:50:MET:HE2	6:F:108:MET:HE2	1.86	0.58
1:1:53:VAL:HG23	1:1:231:MET:CE	2.34	0.57
4:4:241:ALA:CB	4:4:278:VAL:HG21	2.34	0.57
7:9:33:LEU:H	7:9:33:LEU:HD12	1.69	0.57
4:D:89:HIS:CE1	4:D:92:ALA:HB2	2.39	0.57
3:3:655:ARG:NH1	3:3:659:GLU:HG3	2.18	0.57
3:C:655:ARG:NH1	3:C:659:GLU:HG3	2.18	0.57
7:G:33:LEU:H	7:G:33:LEU:HD12	1.69	0.57
1:1:184:GLU:OE1	1:1:186:THR:HG22	2.04	0.57
2:2:58:THR:HG21	3:3:200:LEU:N	2.19	0.57
2:2:74:PRO:HB2	8:7:121:ARG:HH21	1.70	0.57
1:A:184:GLU:OE1	1:A:186:THR:HG22	2.03	0.57
3:C:495:GLU:O	3:C:498:GLU:HB2	2.04	0.57
1:1:241:MET:HG2	1:1:267:PRO:HB3	1.86	0.57
3:3:495:GLU:O	3:3:498:GLU:HB2	2.04	0.57
4:4:225:PRO:HG3	4:4:383:TYR:OH	2.04	0.57
4:4:278:VAL:O	4:4:282:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:MET:HG2	1:A:267:PRO:HB3	1.86	0.57
2:B:74:PRO:HB2	8:J:121:ARG:HH21	1.70	0.57
3:C:693:TYR:HB3	3:C:759:TYR:CD2	2.37	0.57
4:D:225:PRO:HG3	4:D:383:TYR:OH	2.04	0.57
3:3:655:ARG:HH12	3:3:659:GLU:HG3	1.70	0.57
9:L:1315:UNK:C	9:L:1317:UNK:N	2.67	0.57
2:B:58:THR:HG21	3:C:200:LEU:N	2.20	0.57
3:C:655:ARG:HH12	3:C:659:GLU:HG3	1.70	0.57
9:O:1315:UNK:C	9:O:1317:UNK:N	2.67	0.57
1:1:16:THR:CG2	1:1:229:PRO:HB3	2.28	0.57
3:3:136:GLU:CG	5:5:189:ARG:HG2	2.32	0.57
3:3:197:ASP:O	3:3:199:VAL:HG22	2.05	0.57
1:A:16:THR:CG2	1:A:229:PRO:HB3	2.28	0.57
1:A:104:ARG:NH2	2:B:127:SER:CB	2.64	0.57
3:C:136:GLU:CG	5:E:189:ARG:HG2	2.32	0.57
3:C:197:ASP:O	3:C:199:VAL:HG22	2.05	0.57
4:D:278:VAL:O	4:D:282:GLU:HG3	2.04	0.57
1:1:104:ARG:NH2	2:2:127:SER:CB	2.64	0.57
2:2:146:THR:HG23	2:2:149:ARG:HB2	1.87	0.57
3:3:398:VAL:C	3:3:399:LEU:HD12	2.30	0.57
7:G:46:HIS:HB3	7:G:47:PRO:CD	2.34	0.57
4:4:219:ARG:NH1	4:4:273:PHE:CD2	2.73	0.57
4:4:352:GLU:HB3	4:4:371:ARG:NE	2.20	0.57
7:9:46:HIS:HB3	7:9:47:PRO:CD	2.34	0.57
3:C:398:VAL:C	3:C:399:LEU:HD12	2.30	0.57
4:D:219:ARG:NH1	4:D:273:PHE:CD2	2.73	0.57
4:D:352:GLU:HB3	4:D:371:ARG:NE	2.20	0.57
2:B:146:THR:HG23	2:B:149:ARG:HB2	1.87	0.57
3:3:753:VAL:HG13	3:3:759:TYR:CE1	2.40	0.57
3:C:753:VAL:HG13	3:C:759:TYR:CE1	2.40	0.57
3:3:202:PHE:O	3:3:203:ILE:HD13	2.04	0.56
3:C:202:PHE:O	3:C:203:ILE:HD13	2.04	0.56
7:G:44:THR:OG1	7:G:52:LYS:HD2	2.04	0.56
3:3:309:PRO:HA	3:3:603:PRO:HD2	1.86	0.56
4:4:85:MET:HE3	4:4:409:ARG:HB2	1.86	0.56
6:6:93:ARG:NH1	6:6:96:TRP:CE3	2.73	0.56
7:9:44:THR:OG1	7:9:52:LYS:HD2	2.04	0.56
11:N:310:UNK:CA	11:N:350:UNK:H2	2.19	0.56
1:A:65:ARG:HD2	1:A:250:LYS:HD3	1.86	0.56
1:A:202:LYS:O	1:A:203:PRO:C	2.48	0.56
3:C:309:PRO:HA	3:C:603:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:65:ARG:HD2	1:1:250:LYS:HD3	1.86	0.56
1:1:202:LYS:O	1:1:203:PRO:C	2.48	0.56
1:1:315:HIS:O	1:1:319:LYS:HB2	2.05	0.56
3:3:385:ALA:HB2	3:3:531:LYS:HB2	1.87	0.56
3:3:459:MET:CG	3:3:465:HIS:HB2	2.35	0.56
3:3:583:VAL:HG21	3:3:597:TYR:O	2.04	0.56
4:4:280:ILE:HG23	4:4:283:MET:HE2	1.87	0.56
7:9:26:TYR:N	7:9:27:PRO:HD3	2.19	0.56
1:A:315:HIS:O	1:A:319:LYS:HB2	2.05	0.56
3:C:385:ALA:HB2	3:C:531:LYS:HB2	1.87	0.56
3:C:459:MET:CG	3:C:465:HIS:HB2	2.35	0.56
3:C:583:VAL:HG21	3:C:597:TYR:O	2.04	0.56
4:D:85:MET:HE3	4:D:409:ARG:HB2	1.86	0.56
4:D:280:ILE:HG23	4:D:283:MET:HE2	1.87	0.56
6:F:93:ARG:NH1	6:F:96:TRP:CE3	2.73	0.56
7:G:26:TYR:N	7:G:27:PRO:HD3	2.19	0.56
11:Q:310:UNK:CA	11:Q:350:UNK:H2	2.19	0.56
3:3:509:ALA:HB1	3:3:768:GLY:CA	2.31	0.56
3:3:715:GLU:H	3:3:761:SER:HB2	1.71	0.56
3:C:509:ALA:HB1	3:C:768:GLY:CA	2.31	0.56
3:3:405:GLU:OE1	3:3:508:GLY:HA3	2.06	0.56
2:B:135:GLN:HB2	2:B:141:TYR:HD1	1.70	0.56
3:C:405:GLU:OE1	3:C:508:GLY:HA3	2.06	0.56
3:C:715:GLU:H	3:C:761:SER:HB2	1.71	0.56
4:D:45:VAL:HG13	4:D:55:VAL:HG22	1.87	0.56
1:1:29:LEU:CD1	1:1:155:ARG:HG3	2.36	0.56
2:2:135:GLN:HB2	2:2:141:TYR:HD1	1.70	0.56
4:4:45:VAL:HG13	4:4:55:VAL:HG22	1.87	0.56
4:4:183:PRO:HD3	7:9:36:ARG:NH2	2.20	0.56
4:4:261:THR:N	4:4:292:GLN:HE22	2.03	0.56
1:A:29:LEU:CD1	1:A:155:ARG:HG3	2.36	0.56
1:A:211:LEU:H	1:A:216:THR:HG21	1.71	0.56
4:D:183:PRO:HD3	7:G:36:ARG:NH2	2.20	0.56
4:D:261:THR:N	4:D:292:GLN:HE22	2.03	0.56
1:1:63:ARG:HD3	1:1:313:TYR:HD2	1.71	0.56
1:1:211:LEU:H	1:1:216:THR:HG21	1.71	0.56
3:3:295:ARG:HD2	3:3:296:PHE:CE2	2.41	0.56
3:3:507:LEU:HD22	3:3:511:VAL:HG11	1.88	0.56
3:3:568:TYR:CD1	3:3:572:PRO:HG3	2.40	0.56
3:3:675:ARG:NH1	3:C:316:ARG:HH22	2.03	0.56
3:3:717:TRP:HB2	3:3:759:TYR:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:83:ARG:HD3	14:6:182:SF4:S4	2.44	0.56
1:A:63:ARG:HD3	1:A:313:TYR:HD2	1.71	0.56
3:C:295:ARG:HD2	3:C:296:PHE:CE2	2.41	0.56
3:C:507:LEU:HD22	3:C:511:VAL:HG11	1.88	0.56
3:C:568:TYR:CD1	3:C:572:PRO:HG3	2.40	0.56
3:C:717:TRP:HB2	3:C:759:TYR:HB2	1.88	0.56
3:3:101:ARG:HH12	3:3:140:TYR:HD1	1.47	0.56
3:3:246:ASN:H	3:3:246:ASN:HD22	1.52	0.56
3:3:682:GLU:OE1	3:3:684:ARG:NH2	2.38	0.56
6:6:77:VAL:HA	6:6:104:TRP:O	2.06	0.56
1:A:314:GLU:HA	1:A:317:GLN:HB3	1.87	0.56
3:C:682:GLU:OE1	3:C:684:ARG:NH2	2.38	0.56
6:F:77:VAL:HA	6:F:104:TRP:O	2.06	0.56
6:F:83:ARG:HD3	14:F:182:SF4:S4	2.44	0.56
1:1:314:GLU:HA	1:1:317:GLN:HB3	1.87	0.56
3:3:218:LEU:N	3:3:219:PRO:CD	2.69	0.56
3:3:469:ARG:HB3	3:3:754:PRO:HB3	1.86	0.56
5:5:163:ARG:HD2	7:9:69:TYR:CE1	2.41	0.56
3:C:101:ARG:HH12	3:C:140:TYR:HD1	1.47	0.56
3:C:218:LEU:N	3:C:219:PRO:CD	2.69	0.56
3:C:246:ASN:H	3:C:246:ASN:HD22	1.52	0.56
3:C:469:ARG:HB3	3:C:754:PRO:HB3	1.86	0.56
5:E:163:ARG:HD2	7:G:69:TYR:CE1	2.41	0.56
7:G:175:ALA:O	7:G:177:THR:HG23	2.06	0.56
6:6:163:TYR:HD1	7:9:152:ARG:HH11	1.54	0.56
7:9:45:ARG:HH21	7:9:137:LEU:HD23	1.71	0.56
7:9:175:ALA:O	7:9:177:THR:HG23	2.06	0.56
7:G:45:ARG:HH21	7:G:137:LEU:HD23	1.71	0.56
1:1:310:PRO:HG2	1:1:315:HIS:CD2	2.41	0.55
1:1:312:SER:HG	1:1:315:HIS:HD1	1.53	0.55
1:A:310:PRO:HG2	1:A:315:HIS:CD2	2.41	0.55
1:A:312:SER:O	1:A:316:LEU:HB2	2.06	0.55
6:F:163:TYR:HD1	7:G:152:ARG:HH11	1.54	0.55
1:1:312:SER:O	1:1:316:LEU:HB2	2.06	0.55
3:3:550:LEU:HD12	3:3:550:LEU:N	2.22	0.55
1:A:312:SER:HG	1:A:315:HIS:HD1	1.53	0.55
3:C:183:HIS:C	3:C:184:CYS:O	2.48	0.55
3:C:550:LEU:HD12	3:C:550:LEU:N	2.22	0.55
8:J:82:ILE:HG23	8:J:95:ALA:HB3	1.87	0.55
3:3:183:HIS:C	3:3:184:CYS:O	2.48	0.55
8:7:82:ILE:HG23	8:7:95:ALA:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:138:TYR:HB3	1:1:141:ALA:HB3	1.88	0.55
1:1:177:ALA:HB3	2:2:67:TYR:CG	2.41	0.55
1:A:177:ALA:HB3	2:B:67:TYR:CG	2.41	0.55
1:A:191:SER:HB2	1:A:197:ALA:HB2	1.88	0.55
2:B:10:PHE:CZ	2:B:33:ARG:HG3	2.42	0.55
1:1:366:PHE:CD1	1:1:370:LEU:HD21	2.42	0.55
2:2:10:PHE:CZ	2:2:33:ARG:HG3	2.42	0.55
2:2:86:LEU:O	2:2:89:LYS:HB3	2.07	0.55
2:2:86:LEU:CD1	2:2:90:LEU:HD11	2.35	0.55
3:3:293:ALA:HA	3:3:699:TRP:CZ3	2.42	0.55
3:3:470:PRO:HG3	3:3:759:TYR:HE2	1.71	0.55
4:4:212:PRO:HG2	4:4:213:ILE:H	1.71	0.55
1:A:366:PHE:CD1	1:A:370:LEU:HD21	2.42	0.55
2:B:86:LEU:O	2:B:89:LYS:HB3	2.07	0.55
3:C:293:ALA:HA	3:C:699:TRP:CZ3	2.42	0.55
3:C:470:PRO:HG3	3:C:759:TYR:HE2	1.71	0.55
4:D:70:MET:HE3	4:D:81:TYR:HB3	1.89	0.55
4:D:212:PRO:HG2	4:D:213:ILE:H	1.71	0.55
1:1:191:SER:HB2	1:1:197:ALA:HB2	1.88	0.55
4:4:70:MET:HE3	4:4:81:TYR:HB3	1.89	0.55
4:4:94:ASP:HB3	4:4:173:ILE:HG21	1.88	0.55
1:A:138:TYR:HB3	1:A:141:ALA:HB3	1.89	0.55
2:B:86:LEU:CD1	2:B:90:LEU:HD11	2.36	0.55
7:G:33:LEU:HD22	7:G:37:PHE:CD2	2.41	0.55
2:2:101:THR:HG23	2:2:106:ILE:O	2.07	0.55
3:3:565:TYR:HD1	3:3:582:PHE:CB	2.20	0.55
5:5:167:PRO:C	5:5:171:ARG:NH1	2.65	0.55
7:9:33:LEU:HD22	7:9:37:PHE:CD2	2.41	0.55
7:9:123:ASP:CG	7:9:148:ARG:HH22	2.14	0.55
3:C:565:TYR:HD1	3:C:582:PHE:CB	2.20	0.55
3:C:707:LYS:C	3:C:709:GLN:H	2.14	0.55
4:D:94:ASP:HB3	4:D:173:ILE:HG21	1.88	0.55
5:E:167:PRO:C	5:E:171:ARG:NH1	2.65	0.55
6:F:141:PRO:HB3	14:F:182:SF4:S1	2.46	0.55
7:G:123:ASP:CG	7:G:148:ARG:HH22	2.14	0.55
1:1:29:LEU:HD22	1:1:29:LEU:O	2.07	0.55
3:3:600:VAL:HG12	3:3:602:LEU:HD11	1.88	0.55
3:3:707:LYS:C	3:3:709:GLN:H	2.14	0.55
6:6:76:ASP:O	6:6:77:VAL:HB	2.07	0.55
6:6:141:PRO:HB3	14:6:182:SF4:S1	2.46	0.55
1:A:29:LEU:HD22	1:A:29:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:THR:HG23	2:B:106:ILE:O	2.07	0.55
3:C:600:VAL:HG12	3:C:602:LEU:HD11	1.88	0.55
6:F:76:ASP:O	6:F:77:VAL:HB	2.07	0.55
2:2:27:ILE:HG22	2:2:31:LEU:CD2	2.36	0.55
3:3:474:ARG:NH2	3:3:516:VAL:CG2	2.53	0.55
7:9:41:HIS:CD2	7:9:115:LEU:CD2	2.89	0.55
4:D:250:LYS:CE	4:D:262:PHE:HB3	2.36	0.55
7:G:41:HIS:CD2	7:G:115:LEU:CD2	2.89	0.55
4:4:40:VAL:CG1	4:4:404:MET:HG3	2.36	0.55
4:4:250:LYS:CE	4:4:262:PHE:HB3	2.36	0.55
6:6:40:THR:HB	6:6:50:MET:SD	2.47	0.55
2:B:27:ILE:HG22	2:B:31:LEU:CD2	2.36	0.55
4:D:40:VAL:CG1	4:D:404:MET:HG3	2.36	0.55
6:F:40:THR:HB	6:F:50:MET:SD	2.47	0.55
4:4:86:ASP:O	4:4:90:SER:HA	2.08	0.54
4:4:133:LEU:HD21	4:4:204:TYR:CD2	2.42	0.54
4:4:210:GLU:O	4:4:212:PRO:HD3	2.08	0.54
1:A:107:LEU:O	1:A:111:PRO:HG3	2.06	0.54
3:C:474:ARG:NH2	3:C:516:VAL:CG2	2.53	0.54
3:C:515:THR:HG23	3:C:683:LEU:HD12	1.90	0.54
4:D:86:ASP:O	4:D:90:SER:HA	2.08	0.54
1:1:107:LEU:O	1:1:111:PRO:HG3	2.06	0.54
4:4:197:LEU:HA	4:4:200:ARG:HB3	1.89	0.54
4:4:409:ARG:NH2	5:5:117:GLU:OE2	2.39	0.54
4:D:133:LEU:HD21	4:D:204:TYR:CD2	2.42	0.54
4:D:210:GLU:O	4:D:212:PRO:HD3	2.08	0.54
4:D:409:ARG:NH2	5:E:117:GLU:OE2	2.39	0.54
5:E:25:LEU:HD23	5:E:25:LEU:H	1.72	0.54
3:3:515:THR:HG23	3:3:683:LEU:HD12	1.90	0.54
5:5:25:LEU:HD23	5:5:25:LEU:H	1.72	0.54
3:C:101:ARG:NH1	3:C:140:TYR:HD1	2.05	0.54
3:C:216:PHE:CZ	8:J:128:PHE:CD2	2.94	0.54
4:D:197:LEU:HA	4:D:200:ARG:HB3	1.89	0.54
6:F:117:MET:HE2	7:G:99:ILE:CG1	2.19	0.54
3:3:101:ARG:NH1	3:3:140:TYR:HD1	2.05	0.54
3:3:216:PHE:CZ	8:7:128:PHE:CD2	2.94	0.54
6:6:29:ALA:HB1	6:6:158:VAL:O	2.07	0.54
4:D:381:LEU:HD13	4:D:400:LEU:HD12	1.90	0.54
5:E:25:LEU:HD23	5:E:25:LEU:N	2.22	0.54
1:1:332:PRO:HD2	2:2:90:LEU:CD2	2.38	0.54
3:3:124:LYS:HE3	3:3:128:CYS:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:469:ARG:HB3	3:3:754:PRO:CB	2.38	0.54
4:4:208:PHE:O	4:4:211:SER:HB3	2.06	0.54
4:4:374:SER:HB2	4:4:406:ASP:HB3	1.88	0.54
5:5:25:LEU:HD23	5:5:25:LEU:N	2.22	0.54
6:6:117:MET:HE2	7:9:99:ILE:CG1	2.19	0.54
8:7:50:LEU:HD12	8:7:51:PRO:HD3	1.90	0.54
1:A:332:PRO:HD2	2:B:90:LEU:CD2	2.38	0.54
3:C:124:LYS:HE3	3:C:128:CYS:HA	1.89	0.54
3:C:469:ARG:HB3	3:C:754:PRO:CB	2.38	0.54
4:D:208:PHE:O	4:D:211:SER:HB3	2.06	0.54
4:D:374:SER:HB2	4:D:406:ASP:HB3	1.89	0.54
6:F:29:ALA:HB1	6:F:158:VAL:O	2.07	0.54
8:J:50:LEU:HD12	8:J:51:PRO:HD3	1.90	0.54
1:1:272:PHE:CD2	1:1:311:MET:HE3	2.43	0.54
3:3:294:GLY:HA3	14:3:786:SF4:S4	2.48	0.54
4:4:70:MET:HE3	4:4:81:TYR:HB2	1.89	0.54
4:4:85:MET:HE3	4:4:409:ARG:CG	2.35	0.54
4:4:381:LEU:HD13	4:4:400:LEU:HD12	1.90	0.54
1:A:272:PHE:CD2	1:A:311:MET:HE3	2.43	0.54
3:C:294:GLY:HA3	14:C:786:SF4:S4	2.48	0.54
4:D:70:MET:HE3	4:D:81:TYR:HB2	1.89	0.54
1:1:301:PRO:HB2	1:1:303:THR:HG23	1.89	0.54
2:2:27:ILE:HG22	2:2:31:LEU:HD22	1.90	0.54
3:3:52:ILE:O	3:3:76:GLN:HG2	2.07	0.54
3:3:268:ASP:OD2	3:3:278:ARG:NH1	2.41	0.54
6:6:138:PRO:CG	7:9:121:MET:HG3	2.38	0.54
4:D:85:MET:HE3	4:D:409:ARG:CG	2.35	0.54
3:3:55:PRO:HG3	3:3:74:GLN:HB2	1.90	0.54
3:3:401:ASP:OD2	3:3:457:PRO:HD2	2.08	0.54
6:6:57:ARG:C	6:6:57:ARG:NE	2.66	0.54
6:6:130:VAL:HG23	6:6:131:VAL:HG13	1.89	0.54
7:9:133:LYS:O	7:9:137:LEU:HD13	2.07	0.54
1:A:301:PRO:HB2	1:A:303:THR:HG23	1.89	0.54
1:A:332:PRO:HD2	2:B:90:LEU:HD23	1.89	0.54
3:C:52:ILE:O	3:C:76:GLN:HG2	2.07	0.54
3:C:268:ASP:OD2	3:C:278:ARG:NH1	2.41	0.54
3:C:401:ASP:OD2	3:C:457:PRO:HD2	2.08	0.54
6:F:130:VAL:HG23	6:F:131:VAL:HG13	1.89	0.54
6:F:138:PRO:CG	7:G:121:MET:HG3	2.38	0.54
7:G:133:LYS:O	7:G:137:LEU:HD13	2.07	0.54
1:1:332:PRO:HD2	2:2:90:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:117:LEU:CA	4:4:321:MET:HE1	2.34	0.54
3:3:352:GLU:HG3	3:3:664:LEU:HD11	1.90	0.54
3:3:473:GLU:O	3:3:477:LEU:CD1	2.56	0.54
4:4:179:LYS:HE3	7:9:106:GLU:OE1	2.07	0.54
5:5:123:GLY:HA2	5:5:144:HIS:CE1	2.43	0.54
6:6:83:ARG:HA	6:6:111:CYS:HB3	1.89	0.54
2:B:27:ILE:HG22	2:B:31:LEU:HD22	1.90	0.54
3:C:229:ILE:O	3:C:230:CYS:C	2.51	0.54
3:C:352:GLU:HG3	3:C:664:LEU:HD11	1.90	0.54
3:C:473:GLU:O	3:C:477:LEU:CD1	2.56	0.54
4:D:179:LYS:HE3	7:G:106:GLU:OE1	2.07	0.54
5:E:16:PRO:HB2	5:E:28:VAL:HG12	1.90	0.54
6:F:57:ARG:C	6:F:57:ARG:NE	2.66	0.54
3:3:229:ILE:O	3:3:230:CYS:C	2.51	0.54
5:5:16:PRO:HB2	5:5:28:VAL:HG12	1.90	0.54
6:6:96:TRP:HA	6:6:99:MET:CE	2.34	0.54
6:6:104:TRP:NE1	6:6:158:VAL:HG12	2.23	0.54
3:C:43:GLY:HA2	16:C:787:FES:S1	2.48	0.54
3:C:55:PRO:HG3	3:C:74:GLN:HB2	1.90	0.54
3:C:117:LEU:CA	4:D:321:MET:HE1	2.34	0.54
3:C:410:HIS:HA	3:C:458:LEU:HD21	1.89	0.54
4:D:261:THR:H	4:D:292:GLN:NE2	2.04	0.54
5:E:123:GLY:HA2	5:E:144:HIS:CE1	2.43	0.54
6:F:83:ARG:HA	6:F:111:CYS:HB3	1.89	0.54
1:1:89:LEU:HD12	1:1:217:THR:HG22	1.90	0.53
3:3:43:GLY:HA2	16:3:787:FES:S1	2.48	0.53
3:3:410:HIS:HA	3:3:458:LEU:HD21	1.90	0.53
4:4:261:THR:H	4:4:292:GLN:NE2	2.04	0.53
1:A:89:LEU:HD12	1:A:217:THR:HG22	1.90	0.53
6:F:96:TRP:HA	6:F:99:MET:CE	2.34	0.53
6:F:104:TRP:NE1	6:F:158:VAL:HG12	2.23	0.53
1:A:354:GLY:O	1:A:360:ARG:NH1	2.38	0.53
2:2:106:ILE:CG2	2:2:110:GLU:HB2	2.38	0.53
3:3:305:ARG:HG2	3:3:588:SER:O	2.08	0.53
3:3:356:LEU:HD13	3:3:654:PHE:CD1	2.43	0.53
3:3:684:ARG:HG2	3:3:684:ARG:HH11	1.73	0.53
4:4:105:LEU:HD13	4:4:309:ILE:CD1	2.36	0.53
2:B:106:ILE:CG2	2:B:110:GLU:HB2	2.38	0.53
3:C:305:ARG:HG2	3:C:588:SER:O	2.08	0.53
3:C:356:LEU:HD13	3:C:654:PHE:CD1	2.43	0.53
3:C:684:ARG:HG2	3:C:684:ARG:HH11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:105:LEU:HD13	4:D:309:ILE:CD1	2.36	0.53
1:1:354:GLY:O	1:1:360:ARG:NH1	2.38	0.53
3:3:20:MET:HE3	3:3:432:PHE:HB3	1.91	0.53
3:3:31:PRO:HD3	3:3:137:TYR:CE2	2.44	0.53
3:3:218:LEU:N	3:3:219:PRO:HD3	2.23	0.53
3:C:20:MET:HE3	3:C:432:PHE:HB3	1.91	0.53
3:C:31:PRO:HD3	3:C:137:TYR:CE2	2.44	0.53
3:C:279:ALA:HB2	3:C:290:ILE:CG1	2.35	0.53
3:3:279:ALA:HB2	3:3:290:ILE:CG1	2.35	0.53
3:3:367:PRO:HB2	3:3:554:LYS:CB	2.39	0.53
4:4:262:PHE:CD1	4:4:289:ILE:HD11	2.43	0.53
5:5:53:VAL:HG13	5:5:71:VAL:HB	1.91	0.53
3:C:218:LEU:N	3:C:219:PRO:HD3	2.24	0.53
3:C:367:PRO:HB2	3:C:554:LYS:CB	2.39	0.53
4:D:262:PHE:CD1	4:D:289:ILE:HD11	2.43	0.53
5:E:53:VAL:HG13	5:E:71:VAL:HB	1.91	0.53
1:1:41:ALA:HB2	1:1:116:GLU:HG3	1.90	0.53
3:3:225:ASN:HD21	3:3:289:TRP:HB3	1.74	0.53
3:3:232:VAL:HB	14:3:784:SF4:S2	2.49	0.53
3:3:282:VAL:HG22	3:3:282:VAL:O	2.08	0.53
4:4:105:LEU:CD1	4:4:309:ILE:HD13	2.37	0.53
6:6:128:ASP:HA	6:6:131:VAL:O	2.08	0.53
1:A:9:LEU:O	1:A:9:LEU:HG	2.08	0.53
3:C:101:ARG:NH1	3:C:140:TYR:CE1	2.77	0.53
3:C:225:ASN:HD21	3:C:289:TRP:HB3	1.74	0.53
3:C:232:VAL:HB	14:C:784:SF4:S2	2.49	0.53
3:C:261:VAL:CG2	14:C:786:SF4:S2	2.97	0.53
3:C:701:ALA:HB2	3:C:763:LEU:CB	2.39	0.53
1:1:9:LEU:O	1:1:9:LEU:HG	2.08	0.53
3:3:101:ARG:NH1	3:3:140:TYR:CE1	2.77	0.53
3:3:261:VAL:CG2	14:3:786:SF4:S2	2.97	0.53
3:3:299:GLU:O	3:3:303:GLN:HB2	2.09	0.53
3:3:701:ALA:HB2	3:3:763:LEU:CB	2.39	0.53
1:A:41:ALA:HB2	1:A:116:GLU:HG3	1.90	0.53
1:A:283:PRO:HB3	1:A:287:ILE:HD13	1.90	0.53
3:C:282:VAL:HG22	3:C:282:VAL:O	2.09	0.53
3:C:299:GLU:O	3:C:303:GLN:HB2	2.09	0.53
4:D:105:LEU:CD1	4:D:309:ILE:HD13	2.37	0.53
5:E:42:LYS:HB2	5:E:108:TRP:CZ2	2.43	0.53
6:F:128:ASP:HA	6:F:131:VAL:O	2.08	0.53
1:1:283:PRO:HB3	1:1:287:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:451:PHE:HE1	3:3:466:GLU:HB3	1.74	0.53
3:3:510:GLY:O	3:3:514:ASP:HB3	2.08	0.53
5:5:42:LYS:HB2	5:5:108:TRP:CZ2	2.44	0.53
3:C:451:PHE:HE1	3:C:466:GLU:HB3	1.74	0.53
3:3:248:GLU:HG2	5:5:170:PHE:CE1	2.44	0.52
3:C:248:GLU:HG2	5:E:170:PHE:CE1	2.44	0.52
3:C:510:GLY:O	3:C:514:ASP:HB3	2.08	0.52
5:E:66:GLU:CG	5:E:95:PRO:HA	2.11	0.52
1:1:8:GLY:C	1:1:10:ASP:H	2.17	0.52
1:1:60:SER:HA	1:1:235:ALA:HB1	1.91	0.52
4:4:393:MET:C	4:4:396:ILE:HG22	2.34	0.52
5:5:66:GLU:CG	5:5:95:PRO:HA	2.11	0.52
1:A:60:SER:HA	1:A:235:ALA:HB1	1.91	0.52
1:A:313:TYR:HE1	1:A:323:LEU:HD13	1.74	0.52
3:C:385:ALA:HB2	3:C:531:LYS:CB	2.40	0.52
4:D:393:MET:C	4:D:396:ILE:HG22	2.34	0.52
1:1:42:LYS:HG3	1:1:46:LYS:HE3	1.91	0.52
1:1:313:TYR:HE1	1:1:323:LEU:HD13	1.74	0.52
3:3:385:ALA:HB2	3:3:531:LYS:CB	2.40	0.52
6:6:90:PRO:O	6:6:93:ARG:HB3	2.09	0.52
1:A:8:GLY:C	1:A:10:ASP:H	2.17	0.52
1:A:42:LYS:HG3	1:A:46:LYS:HE3	1.91	0.52
4:D:197:LEU:N	4:D:198:PRO:HD2	2.24	0.52
6:F:90:PRO:O	6:F:93:ARG:HB3	2.09	0.52
3:3:481:LEU:HD22	3:3:527:ARG:NH1	2.25	0.52
4:4:197:LEU:N	4:4:198:PRO:HD2	2.24	0.52
4:4:381:LEU:H	4:4:382:PRO:HD2	1.74	0.52
3:C:481:LEU:HD22	3:C:527:ARG:NH1	2.25	0.52
1:1:139:ARG:CG	2:2:140:PRO:HD3	2.39	0.52
3:3:720:PRO:HG3	3:3:749:HIS:HB3	1.91	0.52
4:4:85:MET:HE3	4:4:409:ARG:CB	2.39	0.52
4:4:294:LEU:O	4:4:294:LEU:HD23	2.09	0.52
5:5:144:HIS:O	5:5:147:ARG:HG2	2.10	0.52
6:6:138:PRO:HG2	7:9:121:MET:HG3	1.92	0.52
8:7:117:ALA:O	8:7:121:ARG:HG2	2.10	0.52
1:A:139:ARG:CG	2:B:140:PRO:HD3	2.39	0.52
1:A:246:SER:HB3	1:A:268:MET:CG	2.32	0.52
1:A:289:ALA:HB3	1:A:337:MET:CE	2.40	0.52
4:D:85:MET:HE3	4:D:409:ARG:CB	2.39	0.52
4:D:381:LEU:H	4:D:382:PRO:HD2	1.74	0.52
5:E:144:HIS:O	5:E:147:ARG:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:138:PRO:HG2	7:G:121:MET:HG3	1.92	0.52
1:1:289:ALA:HB3	1:1:337:MET:CE	2.40	0.52
2:2:139:GLU:CB	2:2:140:PRO:HD2	2.40	0.52
3:3:29:ASP:OD2	5:5:187:GLY:N	2.38	0.52
6:6:50:MET:C	6:6:52:ALA:H	2.16	0.52
2:B:139:GLU:CB	2:B:140:PRO:HD2	2.40	0.52
3:C:46:ARG:O	3:C:107:MET:HG2	2.10	0.52
3:C:720:PRO:HG3	3:C:749:HIS:HB3	1.91	0.52
4:D:153:ARG:HH11	4:D:153:ARG:HG3	1.75	0.52
4:D:294:LEU:O	4:D:294:LEU:HD23	2.10	0.52
6:F:50:MET:C	6:F:52:ALA:H	2.16	0.52
8:J:117:ALA:O	8:J:121:ARG:HG2	2.10	0.52
1:1:246:SER:HB3	1:1:268:MET:CG	2.32	0.52
2:2:135:GLN:HB2	2:2:141:TYR:CD1	2.44	0.52
3:3:46:ARG:O	3:3:107:MET:HG2	2.10	0.52
6:6:78:MET:O	6:6:78:MET:HG3	2.10	0.52
11:N:1001:UNK:CA	11:N:1059:UNK:CA	2.81	0.52
2:B:135:GLN:HB2	2:B:141:TYR:CD1	2.44	0.52
3:C:29:ASP:OD2	5:E:187:GLY:N	2.38	0.52
6:F:78:MET:O	6:F:78:MET:HG3	2.10	0.52
11:Q:1001:UNK:CA	11:Q:1059:UNK:CA	2.81	0.52
4:4:153:ARG:HH11	4:4:153:ARG:HG3	1.75	0.52
6:6:83:ARG:HG3	6:6:83:ARG:NH1	2.25	0.52
8:7:15:GLU:O	8:7:18:SER:HB3	2.09	0.52
8:7:81:ARG:O	8:7:81:ARG:HD3	2.10	0.52
1:A:160:LYS:HG3	1:A:161:ASN:N	2.21	0.52
3:C:157:PHE:CZ	3:C:159:PHE:HB2	2.44	0.52
8:J:15:GLU:O	8:J:18:SER:HB3	2.09	0.52
8:J:81:ARG:O	8:J:81:ARG:HD3	2.10	0.52
1:1:160:LYS:HG3	1:1:161:ASN:N	2.21	0.52
1:1:391:LEU:N	1:1:392:PRO:HD2	2.25	0.52
3:3:36:GLU:HG2	3:3:229:ILE:HG23	1.92	0.52
3:3:55:PRO:HD3	3:3:74:GLN:N	2.23	0.52
3:3:157:PHE:CZ	3:3:159:PHE:HB2	2.45	0.52
3:3:200:LEU:HD12	3:3:212:GLY:O	2.09	0.52
4:4:393:MET:HA	4:4:396:ILE:HG22	1.91	0.52
1:A:391:LEU:N	1:A:392:PRO:HD2	2.25	0.52
2:B:116:LEU:HD23	2:B:116:LEU:N	2.24	0.52
3:C:36:GLU:HG2	3:C:229:ILE:HG23	1.92	0.52
3:C:55:PRO:HD3	3:C:74:GLN:N	2.23	0.52
3:C:575:GLU:OE1	3:C:575:GLU:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:83:ARG:HG3	6:F:83:ARG:NH1	2.25	0.52
1:1:238:PHE:HE1	1:1:249:MET:HE1	1.75	0.52
2:2:116:LEU:HD23	2:2:116:LEU:N	2.24	0.52
3:3:575:GLU:OE1	3:3:575:GLU:HA	2.10	0.52
4:4:85:MET:HE1	4:4:370:VAL:HG21	1.92	0.52
1:A:238:PHE:HE1	1:A:249:MET:HE1	1.75	0.52
3:C:200:LEU:HD12	3:C:212:GLY:O	2.09	0.52
4:D:393:MET:HA	4:D:396:ILE:HG22	1.91	0.52
1:1:118:MET:HG2	1:1:224:LEU:HD13	1.92	0.51
2:2:143:GLU:C	2:2:144:CYS:SG	2.92	0.51
1:A:118:MET:HG2	1:A:224:LEU:HD13	1.92	0.51
2:B:143:GLU:C	2:B:144:CYS:SG	2.92	0.51
4:D:85:MET:HE1	4:D:370:VAL:HG21	1.92	0.51
4:D:140:LEU:HD11	4:D:214:PHE:HB2	1.90	0.51
1:1:261:PRO:HB2	2:2:129:HIS:HB2	1.91	0.51
3:3:54:LEU:H	3:3:55:PRO:HD3	1.73	0.51
6:6:74:GLN:OE1	6:6:74:GLN:HA	2.10	0.51
1:A:243:THR:HG21	1:A:315:HIS:HE1	1.75	0.51
1:A:261:PRO:HB2	2:B:129:HIS:HB2	1.91	0.51
6:F:74:GLN:OE1	6:F:74:GLN:HA	2.10	0.51
1:1:243:THR:HG21	1:1:315:HIS:HE1	1.75	0.51
3:3:87:VAL:CA	3:3:91:MET:HE1	2.35	0.51
4:4:140:LEU:HD11	4:4:214:PHE:HB2	1.90	0.51
6:6:22:THR:HA	6:6:25:GLU:HG2	1.92	0.51
1:1:436:LEU:HD23	2:2:90:LEU:HA	1.91	0.51
3:3:130:LEU:HD23	14:3:784:SF4:S4	2.50	0.51
4:4:59:ILE:HD11	5:5:135:ILE:HG23	1.93	0.51
4:4:254:TYR:HE2	4:4:346:THR:HA	1.72	0.51
1:A:436:LEU:HD23	2:B:90:LEU:HA	1.91	0.51
3:C:54:LEU:H	3:C:55:PRO:HD3	1.73	0.51
3:C:130:LEU:HD23	14:C:784:SF4:S4	2.50	0.51
4:D:254:TYR:HE2	4:D:346:THR:HA	1.72	0.51
6:F:22:THR:HA	6:F:25:GLU:HG2	1.92	0.51
3:3:361:ALA:HB3	3:3:369:LEU:HD13	1.92	0.51
5:5:75:VAL:HG12	5:5:76:SER:N	2.26	0.51
3:C:87:VAL:CA	3:C:91:MET:HE1	2.36	0.51
3:C:168:HIS:C	3:C:168:HIS:CD2	2.89	0.51
3:C:361:ALA:HB3	3:C:369:LEU:HD13	1.92	0.51
4:D:59:ILE:HD11	5:E:135:ILE:HG23	1.93	0.51
5:E:75:VAL:HG12	5:E:76:SER:N	2.26	0.51
3:3:168:HIS:C	3:3:168:HIS:CD2	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:591:HIS:ND1	3:3:592:PRO:CD	2.72	0.51
3:C:440:ARG:HG2	3:C:440:ARG:NH1	2.03	0.51
3:C:591:HIS:ND1	3:C:592:PRO:CD	2.72	0.51
3:3:23:VAL:HG12	3:3:24:PHE:N	2.26	0.51
3:3:440:ARG:HG2	3:3:440:ARG:NH1	2.03	0.51
3:3:594:ALA:O	3:3:598:ALA:HB3	2.10	0.51
4:4:197:LEU:O	4:4:198:PRO:C	2.54	0.51
4:4:236:GLY:C	4:4:238:SER:N	2.65	0.51
4:4:249:ARG:HB2	4:4:262:PHE:HE2	1.76	0.51
3:C:2:VAL:CG1	3:C:89:ASP:HA	2.39	0.51
3:C:23:VAL:HG12	3:C:24:PHE:N	2.26	0.51
3:C:594:ALA:O	3:C:598:ALA:HB3	2.10	0.51
4:D:197:LEU:O	4:D:198:PRO:C	2.54	0.51
4:D:230:ILE:HG22	4:D:230:ILE:O	2.11	0.51
4:D:249:ARG:HB2	4:D:262:PHE:HE2	1.76	0.51
1:1:291:ILE:O	1:1:328:VAL:HA	2.11	0.51
3:3:2:VAL:CG1	3:3:89:ASP:HA	2.39	0.51
4:4:317:LEU:HD21	4:4:327:HIS:CD2	2.46	0.51
3:C:343:LEU:HB2	3:C:369:LEU:HB2	1.93	0.51
4:D:317:LEU:HD21	4:D:327:HIS:CD2	2.46	0.51
3:3:343:LEU:HB2	3:3:369:LEU:HB2	1.93	0.51
6:6:49:GLU:OE1	6:6:49:GLU:HA	2.11	0.51
1:A:291:ILE:O	1:A:328:VAL:HA	2.11	0.51
4:D:263:ASP:O	4:D:285:GLU:HG3	2.11	0.51
6:F:49:GLU:OE1	6:F:49:GLU:HA	2.11	0.51
8:J:121:ARG:HG3	8:J:121:ARG:NH1	2.26	0.51
4:4:84:ARG:CZ	6:6:117:MET:HE1	2.42	0.51
4:4:211:SER:HB2	4:4:214:PHE:HB3	1.92	0.51
4:4:263:ASP:O	4:4:285:GLU:HG3	2.11	0.51
6:6:104:TRP:CE2	6:6:173:VAL:HG22	2.46	0.51
8:7:121:ARG:HG3	8:7:121:ARG:NH1	2.26	0.51
9:L:1119:UNK:C	9:L:1121:UNK:N	2.72	0.51
4:D:211:SER:HB2	4:D:214:PHE:HB3	1.92	0.51
6:F:104:TRP:CE2	6:F:173:VAL:HG22	2.46	0.51
9:O:1119:UNK:C	9:O:1121:UNK:N	2.72	0.51
1:1:359:CYS:HB3	14:1:439:SF4:S3	2.51	0.50
3:3:456:ALA:O	3:3:459:MET:HB2	2.11	0.50
3:C:216:PHE:HZ	8:J:128:PHE:CD2	2.28	0.50
3:C:456:ALA:O	3:C:459:MET:HB2	2.11	0.50
4:D:236:GLY:C	4:D:238:SER:N	2.65	0.50
6:F:77:VAL:O	6:F:77:VAL:HG12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:197:ASP:OD2	3:3:220:SER:HB2	2.12	0.50
3:3:216:PHE:HZ	8:7:128:PHE:CD2	2.28	0.50
3:3:357:ALA:HB2	3:3:641:LEU:HD11	1.92	0.50
4:4:230:ILE:HG22	4:4:230:ILE:O	2.11	0.50
6:6:50:MET:HB2	6:6:108:MET:CE	2.40	0.50
1:A:359:CYS:HB3	14:A:439:SF4:S3	2.51	0.50
3:C:197:ASP:OD2	3:C:220:SER:HB2	2.12	0.50
3:C:357:ALA:HB2	3:C:641:LEU:HD11	1.92	0.50
4:D:84:ARG:CZ	6:F:117:MET:HE1	2.42	0.50
6:F:50:MET:HB2	6:F:108:MET:CE	2.40	0.50
6:F:156:LYS:HA	6:F:159:ARG:HD2	1.92	0.50
1:1:185:GLU:HB2	1:1:218:ILE:CD1	2.41	0.50
3:3:46:ARG:HG2	3:3:46:ARG:HH11	1.76	0.50
3:3:368:HIS:CG	3:3:556:ALA:HB3	2.46	0.50
4:4:234:LEU:C	4:4:236:GLY:H	2.18	0.50
5:5:98:ASP:OD1	5:5:100:ARG:HD3	2.11	0.50
6:6:156:LYS:HA	6:6:159:ARG:HD2	1.92	0.50
8:7:108:ILE:HD12	8:7:108:ILE:N	2.25	0.50
1:A:185:GLU:HB2	1:A:218:ILE:CD1	2.41	0.50
3:C:46:ARG:HG2	3:C:46:ARG:HH11	1.76	0.50
3:C:185:LYS:HB3	3:C:189:ARG:HD3	1.93	0.50
3:C:368:HIS:CG	3:C:556:ALA:HB3	2.46	0.50
3:3:185:LYS:HB3	3:3:189:ARG:HD3	1.93	0.50
3:3:317:LEU:HD22	3:3:317:LEU:N	2.27	0.50
3:3:352:GLU:HG3	3:3:664:LEU:CD1	2.41	0.50
3:C:352:GLU:HG3	3:C:664:LEU:CD1	2.41	0.50
4:D:234:LEU:C	4:D:236:GLY:H	2.18	0.50
5:E:98:ASP:OD1	5:E:100:ARG:HD3	2.11	0.50
3:3:473:GLU:O	3:3:477:LEU:HD13	2.12	0.50
3:3:570:PHE:O	3:3:585:MET:HE2	2.12	0.50
3:3:572:PRO:HD2	3:3:577:LEU:HD21	1.92	0.50
4:4:381:LEU:O	4:4:381:LEU:HG	2.11	0.50
3:C:317:LEU:HD22	3:C:317:LEU:N	2.27	0.50
3:C:473:GLU:O	3:C:477:LEU:HD13	2.12	0.50
5:E:157:THR:HG21	7:G:66:TYR:HB2	1.92	0.50
3:3:101:ARG:HB3	3:3:101:ARG:CZ	2.42	0.50
3:3:344:TYR:CD1	3:3:568:TYR:CE1	2.99	0.50
3:3:614:LEU:HD11	3:3:624:LEU:CD1	2.42	0.50
5:5:157:THR:HG21	7:9:66:TYR:HB2	1.92	0.50
9:L:1528:UNK:C	9:L:1530:UNK:N	2.64	0.50
3:C:101:ARG:HB3	3:C:101:ARG:CZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:570:PHE:O	3:C:585:MET:HE2	2.12	0.50
3:C:572:PRO:HD2	3:C:577:LEU:HD21	1.93	0.50
3:C:614:LEU:HD11	3:C:624:LEU:CD1	2.42	0.50
4:D:381:LEU:O	4:D:381:LEU:HG	2.12	0.50
8:J:108:ILE:N	8:J:108:ILE:HD12	2.25	0.50
9:O:1528:UNK:C	9:O:1530:UNK:N	2.64	0.50
1:1:145:LEU:O	1:1:149:ILE:HG13	2.12	0.50
2:2:112:THR:OG1	2:2:113:PRO:HD2	2.12	0.50
3:3:169:PRO:HA	3:3:175:ILE:HA	1.94	0.50
3:3:192:GLU:HG3	3:3:193:GLU:HG3	1.93	0.50
3:3:272:GLY:O	3:3:629:ILE:HA	2.11	0.50
2:B:7:LYS:O	2:B:7:LYS:HG2	2.12	0.50
2:B:112:THR:OG1	2:B:113:PRO:HD2	2.12	0.50
3:C:169:PRO:HA	3:C:175:ILE:HA	1.94	0.50
3:C:192:GLU:HG3	3:C:193:GLU:HG3	1.93	0.50
3:C:272:GLY:O	3:C:629:ILE:HA	2.11	0.50
3:C:344:TYR:CD1	3:C:568:TYR:CE1	2.99	0.50
3:C:734:VAL:HG12	3:C:736:VAL:HG23	1.94	0.50
2:2:7:LYS:O	2:2:7:LYS:HG2	2.12	0.50
3:3:20:MET:CE	3:3:433:ALA:HB2	2.30	0.50
3:3:409:LEU:HD12	3:3:535:MET:HE2	1.93	0.50
3:3:472:GLU:O	3:3:476:ILE:HD12	2.12	0.50
3:3:734:VAL:HG12	3:3:736:VAL:HG23	1.94	0.50
5:5:167:PRO:CB	5:5:171:ARG:HH12	2.24	0.50
1:A:145:LEU:O	1:A:149:ILE:HG13	2.12	0.50
3:C:472:GLU:O	3:C:476:ILE:HD12	2.12	0.50
4:D:241:ALA:HB2	4:D:278:VAL:HG21	1.92	0.50
5:E:167:PRO:CB	5:E:171:ARG:HH12	2.24	0.50
6:F:153:GLN:HG3	7:G:124:TYR:CZ	2.46	0.50
4:4:241:ALA:HB2	4:4:278:VAL:HG21	1.92	0.50
6:6:153:GLN:HG3	7:9:124:TYR:CZ	2.46	0.50
4:D:64:THR:HB	4:D:66:PHE:CE1	2.46	0.50
3:3:459:MET:HG2	3:3:465:HIS:CB	2.42	0.49
4:4:43:LEU:HD23	4:4:57:PRO:HA	1.93	0.49
4:4:44:MET:HA	4:4:44:MET:CE	2.41	0.49
4:4:64:THR:HB	4:4:66:PHE:CE1	2.46	0.49
6:6:77:VAL:O	6:6:77:VAL:HG12	2.10	0.49
8:7:16:LEU:O	8:7:20:MET:HG3	2.12	0.49
3:C:409:LEU:HD12	3:C:535:MET:HE2	1.93	0.49
4:D:44:MET:HA	4:D:44:MET:CE	2.41	0.49
5:E:119:TYR:O	5:E:122:PHE:O	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:92:HIS:N	8:J:92:HIS:CD2	2.78	0.49
11:Q:1212:UNK:N	11:Q:1213:UNK:CA	2.75	0.49
1:1:272:PHE:CD1	1:1:311:MET:HG2	2.47	0.49
5:5:25:LEU:N	5:5:25:LEU:CD2	2.75	0.49
8:7:92:HIS:N	8:7:92:HIS:CD2	2.78	0.49
11:N:1212:UNK:N	11:N:1213:UNK:CA	2.75	0.49
3:C:20:MET:CE	3:C:433:ALA:HB2	2.30	0.49
3:C:459:MET:HG2	3:C:465:HIS:CB	2.42	0.49
3:C:684:ARG:HG2	3:C:684:ARG:NH1	2.28	0.49
5:E:25:LEU:N	5:E:25:LEU:CD2	2.75	0.49
8:J:16:LEU:O	8:J:20:MET:HG3	2.12	0.49
1:1:323:LEU:C	1:1:323:LEU:CD2	2.84	0.49
1:1:331:ILE:HG21	1:1:337:MET:HE2	1.94	0.49
1:1:350:HIS:O	3:3:205:ARG:NH1	2.45	0.49
3:3:684:ARG:HG2	3:3:684:ARG:NH1	2.28	0.49
5:5:119:TYR:O	5:5:122:PHE:O	2.28	0.49
7:9:40:ARG:NH1	7:9:41:HIS:O	2.45	0.49
1:A:272:PHE:CD1	1:A:311:MET:HG2	2.47	0.49
1:A:323:LEU:C	1:A:323:LEU:CD2	2.84	0.49
1:A:331:ILE:HG21	1:A:337:MET:HE2	1.94	0.49
1:A:350:HIS:O	3:C:205:ARG:NH1	2.45	0.49
4:D:43:LEU:HD23	4:D:57:PRO:HA	1.94	0.49
3:3:300:TRP:HB3	3:3:705:VAL:HG23	1.95	0.49
3:3:697:THR:HG21	3:3:761:SER:OG	2.12	0.49
3:3:722:THR:CG2	3:3:755:LYS:HG3	2.42	0.49
4:4:218:ALA:CB	4:4:272:VAL:HG22	2.42	0.49
4:4:238:SER:HB2	4:4:275:ARG:HG2	1.94	0.49
1:A:339:ASP:OD2	2:B:89:LYS:HE2	2.12	0.49
3:C:550:LEU:HD21	3:C:680:LEU:HD11	1.93	0.49
4:D:238:SER:HB2	4:D:275:ARG:HG2	1.94	0.49
5:E:145:PRO:HA	5:E:150:TYR:CD2	2.47	0.49
7:G:40:ARG:NH1	7:G:41:HIS:O	2.45	0.49
8:J:68:LEU:C	8:J:68:LEU:HD13	2.37	0.49
1:1:97:GLU:O	1:1:100:SER:HB3	2.12	0.49
3:3:360:LEU:HD13	3:3:645:ALA:HB2	1.94	0.49
3:3:550:LEU:HD21	3:3:680:LEU:HD11	1.93	0.49
5:5:145:PRO:HA	5:5:150:TYR:CD2	2.47	0.49
8:7:68:LEU:C	8:7:68:LEU:HD13	2.37	0.49
3:C:300:TRP:HB3	3:C:705:VAL:HG23	1.95	0.49
3:C:697:THR:HG21	3:C:761:SER:OG	2.12	0.49
3:C:722:THR:CG2	3:C:755:LYS:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:ALA:CB	4:D:272:VAL:HG22	2.42	0.49
1:1:339:ASP:OD2	2:2:89:LYS:HE2	2.12	0.49
1:A:97:GLU:O	1:A:100:SER:HB3	2.12	0.49
1:A:367:MET:HE1	1:A:410:VAL:HG21	1.93	0.49
3:C:116:PRO:O	3:C:117:LEU:CB	2.60	0.49
3:C:360:LEU:HD13	3:C:645:ALA:HB2	1.95	0.49
5:E:135:ILE:HG22	5:E:136:LEU:HG	1.94	0.49
1:1:114:LEU:O	1:1:118:MET:HG3	2.13	0.49
1:1:177:ALA:O	2:2:67:TYR:HB3	2.13	0.49
1:1:367:MET:HE1	1:1:410:VAL:HG21	1.93	0.49
2:2:33:ARG:HH21	2:2:37:GLU:CG	2.25	0.49
3:3:116:PRO:O	3:3:117:LEU:CB	2.60	0.49
3:3:337:ARG:HD3	3:3:340:GLU:HG3	1.93	0.49
3:3:592:PRO:HA	3:3:595:GLU:HG2	1.93	0.49
4:4:64:THR:OG1	6:6:83:ARG:NH1	2.46	0.49
1:A:342:TRP:O	1:A:342:TRP:HE3	1.96	0.49
2:B:33:ARG:HH21	2:B:37:GLU:CG	2.25	0.49
4:D:84:ARG:O	6:F:83:ARG:NH2	2.45	0.49
1:1:342:TRP:O	1:1:342:TRP:HE3	1.96	0.49
3:3:202:PHE:HA	3:3:210:PHE:O	2.13	0.49
4:4:84:ARG:O	6:6:83:ARG:NH2	2.45	0.49
4:4:213:ILE:HD12	4:4:213:ILE:H	1.78	0.49
5:5:135:ILE:HG22	5:5:136:LEU:HG	1.94	0.49
1:A:114:LEU:O	1:A:118:MET:HG3	2.13	0.49
1:A:177:ALA:O	2:B:67:TYR:HB3	2.13	0.49
3:C:592:PRO:HA	3:C:595:GLU:HG2	1.93	0.49
4:D:64:THR:OG1	6:F:83:ARG:NH1	2.46	0.49
4:4:99:LEU:O	4:4:103:LYS:HG2	2.13	0.49
3:C:202:PHE:HA	3:C:210:PHE:O	2.13	0.49
3:C:337:ARG:HD3	3:C:340:GLU:HG3	1.93	0.49
4:D:213:ILE:HD12	4:D:213:ILE:H	1.78	0.49
3:3:186:ARG:CD	3:3:231:PRO:HD3	2.37	0.49
3:3:259:CYS:SG	3:3:261:VAL:HG22	2.53	0.49
5:5:101:LEU:O	5:5:126:PHE:HA	2.13	0.49
6:6:104:TRP:HB3	6:6:154:LEU:HD11	1.95	0.49
3:C:186:ARG:CD	3:C:231:PRO:HD3	2.37	0.49
3:C:259:CYS:SG	3:C:261:VAL:HG22	2.53	0.49
3:C:565:TYR:HD1	3:C:582:PHE:HB3	1.76	0.49
5:E:101:LEU:O	5:E:126:PHE:HA	2.13	0.49
3:3:565:TYR:HD1	3:3:582:PHE:HB3	1.76	0.48
4:4:346:THR:HG22	4:4:353:LEU:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:37:TRP:O	6:6:75:ALA:HB1	2.13	0.48
1:A:93:ALA:CB	1:A:107:LEU:HD11	2.43	0.48
1:A:128:THR:O	1:A:169:PHE:HA	2.12	0.48
4:D:99:LEU:O	4:D:103:LYS:HG2	2.13	0.48
4:D:346:THR:HG22	4:D:353:LEU:O	2.12	0.48
5:E:20:ASN:ND2	5:E:26:TRP:HZ3	2.10	0.48
6:F:37:TRP:O	6:F:75:ALA:HB1	2.13	0.48
6:F:104:TRP:HB3	6:F:154:LEU:HD11	1.95	0.48
1:1:93:ALA:CB	1:1:107:LEU:HD11	2.43	0.48
3:3:545:GLU:HA	3:3:550:LEU:HD11	1.95	0.48
4:4:59:ILE:H	4:4:59:ILE:HD13	1.77	0.48
4:4:381:LEU:H	4:4:382:PRO:CD	2.26	0.48
5:5:20:ASN:ND2	5:5:26:TRP:HZ3	2.10	0.48
6:6:156:LYS:NZ	7:9:149:GLU:OE1	2.46	0.48
3:C:545:GLU:HA	3:C:550:LEU:HD11	1.95	0.48
4:D:381:LEU:H	4:D:382:PRO:CD	2.26	0.48
6:F:156:LYS:NZ	7:G:149:GLU:OE1	2.46	0.48
1:1:128:THR:O	1:1:169:PHE:HA	2.12	0.48
2:2:144:CYS:O	2:2:149:ARG:HD3	2.13	0.48
3:3:112:LEU:CD2	3:3:130:LEU:HD21	2.42	0.48
3:3:225:ASN:ND2	3:3:289:TRP:HB3	2.28	0.48
4:4:185:GLU:O	4:4:189:GLU:HG2	2.12	0.48
4:4:233:GLY:HA2	5:5:48:PHE:CE1	2.49	0.48
2:B:144:CYS:O	2:B:149:ARG:HD3	2.13	0.48
3:C:225:ASN:ND2	3:C:289:TRP:HB3	2.29	0.48
3:C:515:THR:HG23	3:C:683:LEU:CD1	2.42	0.48
4:D:59:ILE:H	4:D:59:ILE:HD13	1.77	0.48
4:D:125:ARG:HD2	4:D:286:SER:OG	2.13	0.48
4:D:233:GLY:HA2	5:E:48:PHE:CE1	2.49	0.48
6:F:37:TRP:CD1	6:F:75:ALA:HB2	2.48	0.48
6:F:50:MET:HG3	6:F:108:MET:HE1	1.94	0.48
3:3:11:VAL:CG1	3:3:25:HIS:CD2	2.92	0.48
3:3:229:ILE:HD11	3:3:289:TRP:HZ3	1.77	0.48
4:4:125:ARG:HD2	4:4:286:SER:OG	2.14	0.48
4:4:205:GLU:OE2	4:4:281:ARG:NE	2.27	0.48
5:5:129:HIS:CD2	5:5:130:PRO:HD2	2.48	0.48
6:6:50:MET:HG3	6:6:108:MET:HE1	1.94	0.48
3:C:11:VAL:CG1	3:C:25:HIS:CD2	2.92	0.48
3:C:31:PRO:HG3	3:C:137:TYR:CG	2.48	0.48
3:C:112:LEU:CD2	3:C:130:LEU:HD21	2.42	0.48
3:C:229:ILE:HD11	3:C:289:TRP:HZ3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:185:GLU:O	4:D:189:GLU:HG2	2.12	0.48
4:D:205:GLU:OE2	4:D:281:ARG:NE	2.27	0.48
9:O:1523:UNK:C	9:O:1525:UNK:N	2.72	0.48
3:3:31:PRO:HG3	3:3:137:TYR:CG	2.49	0.48
3:3:515:THR:HG23	3:3:683:LEU:CD1	2.42	0.48
4:4:83:PRO:HD3	4:4:94:ASP:OD1	2.13	0.48
4:4:84:ARG:NE	6:6:117:MET:HE1	2.29	0.48
4:4:379:GLN:OE1	5:5:112:ASN:HB3	2.12	0.48
5:5:59:THR:O	5:5:59:THR:HG22	2.13	0.48
6:6:37:TRP:CD1	6:6:75:ALA:HB2	2.49	0.48
8:7:68:LEU:HD13	8:7:69:LEU:N	2.29	0.48
9:L:901:UNK:CA	9:L:1199:UNK:CA	2.91	0.48
9:L:1523:UNK:C	9:L:1525:UNK:N	2.72	0.48
3:C:205:ARG:HA	3:C:209:THR:CG2	2.43	0.48
4:D:83:PRO:HD3	4:D:94:ASP:OD1	2.13	0.48
4:D:84:ARG:NE	6:F:117:MET:HE1	2.29	0.48
5:E:59:THR:HG22	5:E:59:THR:O	2.13	0.48
8:J:68:LEU:HD13	8:J:69:LEU:N	2.29	0.48
9:O:901:UNK:CA	9:O:1199:UNK:CA	2.91	0.48
1:1:358:PRO:O	1:1:362:GLY:CA	2.52	0.48
1:1:427:GLU:O	1:1:428:LYS:C	2.57	0.48
7:9:172:GLY:O	7:9:174:LYS:N	2.47	0.48
1:A:427:GLU:O	1:A:428:LYS:C	2.57	0.48
4:D:366:TYR:CZ	5:E:148:LYS:HE3	2.49	0.48
4:D:379:GLN:OE1	5:E:112:ASN:HB3	2.12	0.48
5:E:129:HIS:CD2	5:E:130:PRO:HD2	2.48	0.48
7:G:172:GLY:O	7:G:174:LYS:N	2.47	0.48
12:S:321:UNK:C	12:S:323:UNK:N	2.70	0.48
1:1:192:LEU:HD22	1:1:211:LEU:HD11	1.95	0.48
3:3:205:ARG:HA	3:3:209:THR:CG2	2.43	0.48
3:3:478:LEU:HD12	3:3:520:ARG:CZ	2.44	0.48
3:3:646:GLU:C	3:3:648:LEU:H	2.22	0.48
4:4:85:MET:CE	4:4:409:ARG:HG3	2.43	0.48
4:4:366:TYR:CZ	5:5:148:LYS:HE3	2.49	0.48
6:6:82:GLY:HA2	14:6:182:SF4:S4	2.53	0.48
12:R:321:UNK:C	12:R:323:UNK:N	2.70	0.48
1:A:358:PRO:O	1:A:362:GLY:CA	2.52	0.48
2:B:179:VAL:HG12	2:B:180:GLU:N	2.29	0.48
6:F:92:MET:O	6:F:92:MET:HG2	2.14	0.48
3:3:47:MET:HE1	3:3:108:VAL:HA	1.96	0.48
3:3:113:LEU:HD11	3:3:157:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:92:MET:O	6:6:92:MET:HG2	2.14	0.48
1:A:192:LEU:HD22	1:A:211:LEU:HD11	1.95	0.48
3:C:47:MET:HE1	3:C:108:VAL:HA	1.96	0.48
3:C:478:LEU:HD12	3:C:520:ARG:CZ	2.44	0.48
4:D:85:MET:CE	4:D:409:ARG:HG3	2.43	0.48
6:F:82:GLY:HA2	14:F:182:SF4:S4	2.53	0.48
2:2:179:VAL:HG12	2:2:180:GLU:N	2.29	0.48
3:3:344:TYR:HD1	3:3:568:TYR:CE1	2.31	0.48
7:9:101:CYS:SG	7:9:103:LEU:HD12	2.53	0.48
1:A:342:TRP:HZ3	1:A:368:VAL:HG23	1.78	0.48
3:C:113:LEU:HD11	3:C:157:PHE:CD1	2.49	0.48
3:C:344:TYR:HD1	3:C:568:TYR:CE1	2.31	0.48
3:C:646:GLU:C	3:C:648:LEU:H	2.22	0.48
5:E:20:ASN:HD22	5:E:26:TRP:HZ3	1.62	0.48
5:E:123:GLY:H	5:E:147:ARG:HH11	1.60	0.48
6:F:92:MET:HE1	6:F:127:VAL:HG13	1.94	0.48
6:F:92:MET:HE2	6:F:92:MET:HB3	1.77	0.48
1:1:283:PRO:HB3	1:1:287:ILE:CD1	2.43	0.48
1:1:301:PRO:HB2	1:1:303:THR:CG2	2.44	0.48
1:1:342:TRP:HZ3	1:1:368:VAL:HG23	1.78	0.48
3:3:160:THR:OG1	8:7:73:SER:CB	2.60	0.48
3:3:522:ARG:O	3:3:526:GLU:HG3	2.14	0.48
5:5:20:ASN:HD22	5:5:26:TRP:HZ3	1.62	0.48
5:5:123:GLY:H	5:5:147:ARG:HH11	1.60	0.48
1:A:283:PRO:HB3	1:A:287:ILE:CD1	2.43	0.48
1:A:301:PRO:HB2	1:A:303:THR:CG2	2.44	0.48
3:C:160:THR:OG1	8:J:73:SER:CB	2.60	0.48
3:C:522:ARG:O	3:C:526:GLU:HG3	2.14	0.48
7:G:101:CYS:SG	7:G:103:LEU:HD12	2.53	0.48
1:1:6:LEU:HD12	1:1:240:GLN:O	2.14	0.47
1:1:81:LYS:HA	1:1:81:LYS:HE3	1.96	0.47
3:3:55:PRO:CD	3:3:74:GLN:H	2.24	0.47
3:3:105:ALA:CB	3:3:140:TYR:HB2	2.44	0.47
3:3:329:LEU:CD1	3:3:584:VAL:HG11	2.45	0.47
3:3:478:LEU:HD12	3:3:520:ARG:NH2	2.29	0.47
6:6:149:TYR:CE1	6:6:153:GLN:NE2	2.81	0.47
1:A:6:LEU:HD12	1:A:240:GLN:O	2.14	0.47
3:C:55:PRO:CD	3:C:74:GLN:H	2.24	0.47
3:C:105:ALA:CB	3:C:140:TYR:HB2	2.43	0.47
4:D:101:VAL:O	4:D:104:LEU:N	2.47	0.47
1:1:29:LEU:HD12	1:1:155:ARG:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:38:GLU:OE2	2:2:45:ARG:NH1	2.47	0.47
4:4:101:VAL:O	4:4:104:LEU:N	2.47	0.47
4:4:115:THR:O	4:4:118:VAL:HG22	2.14	0.47
6:6:36:LEU:HD22	6:6:77:VAL:HG21	1.97	0.47
6:6:92:MET:HE1	6:6:127:VAL:HG13	1.94	0.47
1:A:29:LEU:HD12	1:A:155:ARG:HG3	1.95	0.47
1:A:400:CYS:HB2	1:A:401:PRO:HD2	1.96	0.47
3:C:329:LEU:CD1	3:C:584:VAL:HG11	2.45	0.47
3:C:478:LEU:HD12	3:C:520:ARG:NH2	2.29	0.47
3:C:616:ASN:ND2	3:C:622:LEU:HD11	2.28	0.47
6:F:36:LEU:HD22	6:F:77:VAL:HG21	1.97	0.47
6:F:149:TYR:CE1	6:F:153:GLN:NE2	2.81	0.47
1:1:400:CYS:HB2	1:1:401:PRO:HD2	1.96	0.47
3:3:616:ASN:ND2	3:3:622:LEU:HD11	2.28	0.47
6:6:92:MET:HE2	6:6:92:MET:HB3	1.77	0.47
6:6:158:VAL:HA	6:6:172:PRO:HB3	1.95	0.47
1:A:81:LYS:HA	1:A:81:LYS:HE3	1.96	0.47
2:B:38:GLU:OE2	2:B:45:ARG:NH1	2.47	0.47
1:1:92:ASN:ND2	15:1:440:FMN:C2	2.77	0.47
2:2:86:LEU:HD11	2:2:90:LEU:HD11	1.96	0.47
3:3:229:ILE:HD11	3:3:289:TRP:CZ3	2.49	0.47
4:4:212:PRO:CG	4:4:213:ILE:HD12	2.41	0.47
5:5:40:HIS:NE2	5:5:44:MET:CE	2.77	0.47
1:A:92:ASN:ND2	15:A:440:FMN:C2	2.77	0.47
3:C:229:ILE:HD11	3:C:289:TRP:CZ3	2.49	0.47
4:D:115:THR:O	4:D:118:VAL:HG22	2.14	0.47
4:D:212:PRO:CG	4:D:213:ILE:HD12	2.41	0.47
5:E:40:HIS:NE2	5:E:44:MET:CE	2.77	0.47
6:F:158:VAL:HA	6:F:172:PRO:HB3	1.95	0.47
15:1:440:FMN:H9	15:1:440:FMN:H1'1	1.64	0.47
3:3:31:PRO:HD3	3:3:137:TYR:CZ	2.49	0.47
7:9:35:PRO:HD3	7:9:164:PRO:CG	2.45	0.47
3:C:31:PRO:HD3	3:C:137:TYR:CZ	2.49	0.47
4:D:205:GLU:OE1	4:D:284:ARG:NH2	2.47	0.47
6:F:23:THR:O	6:F:23:THR:HG22	2.14	0.47
1:1:188:LEU:HD23	1:1:188:LEU:C	2.40	0.47
3:3:697:THR:OG1	3:3:763:LEU:HD23	2.15	0.47
4:4:47:LEU:HD13	4:4:52:VAL:CA	2.42	0.47
4:4:205:GLU:OE1	4:4:284:ARG:NH2	2.47	0.47
6:6:23:THR:O	6:6:23:THR:HG22	2.14	0.47
1:A:32:TYR:OH	1:A:116:GLU:OE1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LEU:HD23	1:A:188:LEU:C	2.40	0.47
15:A:440:FMN:H9	15:A:440:FMN:H1'1	1.64	0.47
2:B:86:LEU:HD11	2:B:90:LEU:HD11	1.96	0.47
3:C:185:LYS:HG3	3:C:202:PHE:HE2	1.79	0.47
3:C:697:THR:OG1	3:C:763:LEU:HD23	2.15	0.47
7:G:35:PRO:HD3	7:G:164:PRO:CG	2.45	0.47
1:1:32:TYR:OH	1:1:116:GLU:OE1	2.29	0.47
1:1:395:GLU:O	1:1:396:GLY:C	2.56	0.47
2:2:77:LYS:HE3	2:2:78:TYR:CZ	2.50	0.47
2:2:116:LEU:HD23	2:2:116:LEU:H	1.78	0.47
3:3:101:ARG:HB3	3:3:101:ARG:HH11	1.77	0.47
3:3:185:LYS:HG3	3:3:202:PHE:HE2	1.80	0.47
3:3:337:ARG:CD	3:3:340:GLU:HG3	2.45	0.47
3:3:360:LEU:HD13	3:3:645:ALA:CB	2.44	0.47
3:3:474:ARG:HA	3:3:517:ALA:HB2	1.97	0.47
4:4:363:SER:HB3	5:5:173:ALA:HB1	1.95	0.47
5:5:49:LEU:HD13	5:5:74:LEU:HD23	1.97	0.47
5:5:54:GLY:C	5:5:55:LEU:HD12	2.40	0.47
5:5:72:TYR:O	5:5:89:PHE:HA	2.15	0.47
1:A:395:GLU:O	1:A:396:GLY:C	2.56	0.47
2:B:77:LYS:HE3	2:B:78:TYR:CZ	2.50	0.47
2:B:116:LEU:HD23	2:B:116:LEU:H	1.78	0.47
3:C:337:ARG:CD	3:C:340:GLU:HG3	2.45	0.47
3:C:474:ARG:HA	3:C:517:ALA:HB2	1.97	0.47
3:C:586:HIS:CE1	3:C:640:VAL:HG21	2.50	0.47
4:D:47:LEU:HD13	4:D:52:VAL:CA	2.42	0.47
4:D:363:SER:HB3	5:E:173:ALA:HB1	1.94	0.47
5:E:49:LEU:HD13	5:E:74:LEU:HD23	1.97	0.47
5:E:54:GLY:C	5:E:55:LEU:HD12	2.40	0.47
5:E:72:TYR:O	5:E:89:PHE:HA	2.15	0.47
10:P:653:UNK:CA	10:P:711:UNK:CA	2.92	0.47
3:3:227:THR:HG21	3:3:237:ASP:HB2	1.97	0.47
3:3:586:HIS:CE1	3:3:640:VAL:HG21	2.50	0.47
10:M:653:UNK:CA	10:M:711:UNK:CA	2.92	0.47
1:A:239:ALA:C	1:A:241:MET:H	2.23	0.47
3:C:360:LEU:HD13	3:C:645:ALA:CB	2.44	0.47
4:D:88:LEU:HD12	4:D:403:VAL:CG2	2.44	0.47
3:3:214:MET:O	3:3:216:PHE:CE1	2.67	0.47
3:3:485:GLU:O	6:F:16:ARG:CZ	2.63	0.47
4:4:88:LEU:HD12	4:4:403:VAL:CG2	2.44	0.47
3:C:227:THR:HG21	3:C:237:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:132:ILE:HG21	1:1:145:LEU:HD11	1.96	0.47
3:3:413:LEU:HD13	3:3:448:MET:CE	2.43	0.47
3:3:478:LEU:CD2	3:3:483:ASP:HB2	2.45	0.47
6:6:115:GLY:HA3	6:6:125:GLN:OE1	2.15	0.47
2:B:21:GLU:O	2:B:21:GLU:HG2	2.14	0.47
2:B:33:ARG:HH21	2:B:37:GLU:HG3	1.80	0.47
3:C:214:MET:O	3:C:216:PHE:CE1	2.67	0.47
3:C:478:LEU:CD2	3:C:483:ASP:HB2	2.45	0.47
6:F:115:GLY:HA3	6:F:125:GLN:OE1	2.15	0.47
1:1:239:ALA:C	1:1:241:MET:H	2.23	0.46
2:2:21:GLU:O	2:2:21:GLU:HG2	2.14	0.46
3:3:309:PRO:HA	3:3:603:PRO:CD	2.45	0.46
3:3:668:LYS:NZ	3:C:592:PRO:HG3	2.30	0.46
2:B:175:HIS:ND1	2:B:175:HIS:N	2.61	0.46
3:C:101:ARG:HB3	3:C:101:ARG:HH11	1.77	0.46
3:C:309:PRO:HA	3:C:603:PRO:CD	2.45	0.46
1:1:259:LYS:HB3	1:1:280:ALA:O	2.15	0.46
2:2:33:ARG:HH21	2:2:37:GLU:HG3	1.80	0.46
2:2:175:HIS:ND1	2:2:175:HIS:N	2.61	0.46
4:4:138:LEU:HD11	4:4:146:PHE:CD1	2.50	0.46
4:4:317:LEU:HD12	4:4:317:LEU:HA	1.78	0.46
1:A:132:ILE:HG21	1:A:145:LEU:HD11	1.96	0.46
1:A:259:LYS:HB3	1:A:280:ALA:O	2.15	0.46
1:A:273:ARG:HB2	1:A:307:LEU:O	2.15	0.46
3:C:413:LEU:HD13	3:C:448:MET:CE	2.43	0.46
4:D:317:LEU:HD12	4:D:317:LEU:HA	1.78	0.46
4:D:350:ARG:O	4:D:373:PRO:HB2	2.14	0.46
1:1:273:ARG:HB2	1:1:307:LEU:O	2.15	0.46
1:1:301:PRO:O	1:1:306:VAL:HG21	2.15	0.46
3:3:602:LEU:HD12	3:3:602:LEU:N	2.31	0.46
4:4:187:VAL:HB	4:4:188:PRO:CD	2.45	0.46
6:6:16:ARG:NH1	6:6:17:GLU:OE2	2.48	0.46
1:A:301:PRO:O	1:A:306:VAL:HG21	2.15	0.46
3:C:34:CYS:HA	3:C:184:CYS:HB2	1.96	0.46
3:C:602:LEU:HD12	3:C:602:LEU:N	2.31	0.46
3:C:672:ALA:O	3:C:673:MET:HB2	2.15	0.46
4:D:138:LEU:HD11	4:D:146:PHE:CD1	2.50	0.46
6:F:16:ARG:NH1	6:F:17:GLU:OE2	2.48	0.46
1:1:254:ILE:HD12	1:1:275:LEU:HD22	1.96	0.46
3:3:34:CYS:HA	3:3:184:CYS:HB2	1.96	0.46
4:4:350:ARG:O	4:4:373:PRO:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:HD12	1:A:275:LEU:HD22	1.96	0.46
4:D:241:ALA:HA	4:D:278:VAL:HG21	1.98	0.46
1:1:132:ILE:HG22	1:1:134:VAL:HG12	1.98	0.46
1:1:233:ARG:O	1:1:237:TRP:HB3	2.16	0.46
3:3:274:LEU:HD12	3:3:275:LEU:N	2.30	0.46
3:3:672:ALA:O	3:3:673:MET:HB2	2.15	0.46
5:5:116:ARG:HB3	5:5:135:ILE:HG13	1.98	0.46
1:A:132:ILE:HG22	1:A:134:VAL:HG12	1.98	0.46
1:A:233:ARG:O	1:A:237:TRP:HB3	2.16	0.46
2:B:145:VAL:HG12	2:B:150:LEU:HB2	1.98	0.46
3:C:274:LEU:HD12	3:C:275:LEU:N	2.30	0.46
4:D:70:MET:C	4:D:72:HIS:H	2.23	0.46
4:D:84:ARG:HG2	14:F:182:SF4:S2	2.56	0.46
4:D:187:VAL:HB	4:D:188:PRO:CD	2.45	0.46
5:E:2:ARG:HG3	5:E:84:ASP:CG	2.39	0.46
5:E:116:ARG:HB3	5:E:135:ILE:HG13	1.98	0.46
8:J:84:LEU:HB2	8:J:93:LEU:HB2	1.98	0.46
2:2:145:VAL:HG12	2:2:150:LEU:HB2	1.98	0.46
3:3:13:VAL:HG22	3:3:17:THR:OG1	2.15	0.46
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.98	0.46
3:3:272:GLY:HA2	3:3:628:PRO:O	2.16	0.46
3:3:402:PRO:CB	3:3:535:MET:HE1	2.46	0.46
4:4:70:MET:C	4:4:72:HIS:H	2.23	0.46
4:4:84:ARG:HG2	14:6:182:SF4:S2	2.56	0.46
4:4:241:ALA:HA	4:4:278:VAL:HG21	1.98	0.46
5:5:2:ARG:HG3	5:5:84:ASP:CG	2.39	0.46
8:7:73:SER:OG	8:7:80:LYS:HA	2.16	0.46
8:7:84:LEU:HB2	8:7:93:LEU:HB2	1.98	0.46
3:C:13:VAL:HG22	3:C:17:THR:OG1	2.15	0.46
3:C:194:VAL:HG12	3:C:411:LEU:HD22	1.98	0.46
3:C:402:PRO:CB	3:C:535:MET:HE1	2.46	0.46
8:J:73:SER:OG	8:J:80:LYS:HA	2.16	0.46
1:1:18:TYR:CZ	1:1:263:VAL:HG11	2.51	0.46
2:2:79:HIS:ND1	2:2:118:SER:HB2	2.31	0.46
2:B:79:HIS:ND1	2:B:118:SER:HB2	2.31	0.46
3:C:33:PHE:HB2	3:C:45:CYS:SG	2.56	0.46
3:C:49:LEU:HA	3:C:80:ALA:O	2.15	0.46
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.56	0.46
3:3:49:LEU:HA	3:3:80:ALA:O	2.15	0.46
3:3:184:CYS:SG	3:3:186:ARG:HB2	2.55	0.46
3:3:469:ARG:HG2	3:3:469:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:690:GLY:HA3	3:3:770:ARG:HH21	1.79	0.46
4:4:108:VAL:O	4:4:110:PRO:HD3	2.16	0.46
1:A:18:TYR:CZ	1:A:263:VAL:HG11	2.51	0.46
3:C:184:CYS:SG	3:C:186:ARG:HB2	2.55	0.46
3:C:272:GLY:HA2	3:C:628:PRO:O	2.16	0.46
3:C:690:GLY:HA3	3:C:770:ARG:HH21	1.79	0.46
4:D:108:VAL:O	4:D:110:PRO:HD3	2.16	0.46
4:4:51:GLU:O	4:4:52:VAL:HG23	2.16	0.46
4:4:190:LEU:O	4:4:194:LEU:HB2	2.16	0.46
4:4:215:TYR:O	4:4:219:ARG:HB2	2.15	0.46
1:A:79:MET:HG3	1:A:125:ILE:HB	1.98	0.46
3:C:469:ARG:HG2	3:C:469:ARG:HH11	1.81	0.46
4:D:190:LEU:O	4:D:194:LEU:HB2	2.16	0.46
1:1:63:ARG:HD3	1:1:313:TYR:CD2	2.50	0.46
1:1:79:MET:HG3	1:1:125:ILE:HB	1.98	0.46
1:1:135:ARG:C	1:1:137:GLU:H	2.24	0.46
1:1:291:ILE:HD11	1:1:331:ILE:HD11	1.97	0.46
15:1:440:FMN:C2	15:1:440:FMN:HO3'	2.17	0.46
3:3:270:ARG:HH11	3:3:270:ARG:HG3	1.81	0.46
4:4:85:MET:HG2	4:4:409:ARG:HB2	1.98	0.46
5:5:52:ILE:HG22	5:5:114:LEU:HB3	1.91	0.46
3:C:346:ALA:HA	3:C:372:GLN:HB2	1.98	0.46
4:D:51:GLU:O	4:D:52:VAL:HG23	2.16	0.46
4:D:85:MET:HG2	4:D:409:ARG:HB2	1.98	0.46
4:D:215:TYR:O	4:D:219:ARG:HB2	2.15	0.46
1:1:193:GLU:HG3	1:1:212:TRP:NE1	2.31	0.45
1:1:398:SER:HA	3:3:46:ARG:CD	2.47	0.45
2:2:109:GLY:CA	8:7:91:ILE:HD13	2.45	0.45
3:3:426:TYR:N	3:3:426:TYR:CD1	2.83	0.45
1:A:63:ARG:HD3	1:A:313:TYR:CD2	2.50	0.45
1:A:135:ARG:C	1:A:137:GLU:H	2.24	0.45
1:A:193:GLU:HG3	1:A:212:TRP:NE1	2.31	0.45
1:A:291:ILE:HD11	1:A:331:ILE:HD11	1.97	0.45
1:A:398:SER:HA	3:C:46:ARG:CD	2.47	0.45
15:A:440:FMN:C2	15:A:440:FMN:HO3'	2.17	0.45
3:C:426:TYR:N	3:C:426:TYR:CD1	2.84	0.45
5:E:52:ILE:HG22	5:E:114:LEU:HB3	1.91	0.45
8:J:29:VAL:HG22	8:J:60:SER:O	2.16	0.45
3:3:694:LEU:CB	3:3:762:ALA:HB2	2.42	0.45
4:4:187:VAL:N	4:4:188:PRO:HD2	2.32	0.45
8:7:29:VAL:HG22	8:7:60:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:GLY:CA	8:J:91:ILE:HD13	2.45	0.45
3:C:270:ARG:HH11	3:C:270:ARG:HG3	1.81	0.45
4:D:367:ARG:CG	4:D:367:ARG:NH1	2.65	0.45
10:P:823:UNK:C	10:P:825:UNK:N	2.77	0.45
1:1:17:LEU:C	1:1:19:ALA:H	2.25	0.45
3:3:346:ALA:HA	3:3:372:GLN:HB2	1.98	0.45
6:6:163:TYR:CE1	7:9:152:ARG:HD2	2.51	0.45
7:9:99:ILE:HD12	7:9:99:ILE:HA	1.85	0.45
8:7:36:ASP:HB2	8:7:41:ILE:HD11	1.98	0.45
10:M:823:UNK:C	10:M:825:UNK:N	2.77	0.45
1:A:17:LEU:C	1:A:19:ALA:H	2.25	0.45
4:D:187:VAL:N	4:D:188:PRO:HD2	2.32	0.45
5:E:13:LYS:HZ3	5:E:33:ARG:HH21	1.63	0.45
7:G:99:ILE:HA	7:G:99:ILE:HD12	1.85	0.45
4:4:126:LEU:O	4:4:130:LEU:HB2	2.17	0.45
4:4:221:VAL:HG23	4:4:272:VAL:CG1	2.46	0.45
5:5:13:LYS:HZ3	5:5:33:ARG:HH21	1.63	0.45
6:6:18:GLY:O	6:6:19:ILE:C	2.60	0.45
6:6:100:PRO:O	6:6:103:LYS:HD3	2.16	0.45
7:9:29:ALA:HA	7:9:30:PRO:HD2	1.83	0.45
3:C:694:LEU:CB	3:C:762:ALA:HB2	2.42	0.45
4:D:221:VAL:HG23	4:D:272:VAL:CG1	2.46	0.45
6:F:18:GLY:O	6:F:19:ILE:C	2.60	0.45
6:F:163:TYR:CE1	7:G:152:ARG:HD2	2.51	0.45
8:J:36:ASP:HB2	8:J:41:ILE:HD11	1.98	0.45
3:3:270:ARG:O	3:3:271:SER:HB2	2.17	0.45
4:4:367:ARG:CG	4:4:367:ARG:NH1	2.65	0.45
5:5:67:ARG:HD3	5:5:96:GLU:HG3	1.99	0.45
5:5:195:LEU:O	5:5:196:TRP:C	2.60	0.45
6:6:166:ARG:HD3	6:6:168:GLU:OE2	2.16	0.45
4:D:126:LEU:O	4:D:130:LEU:HB2	2.17	0.45
5:E:67:ARG:HD3	5:E:96:GLU:HG3	1.99	0.45
5:E:195:LEU:O	5:E:196:TRP:C	2.60	0.45
6:F:100:PRO:O	6:F:103:LYS:HD3	2.16	0.45
6:F:166:ARG:HD3	6:F:168:GLU:OE2	2.17	0.45
1:1:192:LEU:C	1:1:194:GLY:H	2.25	0.45
3:3:20:MET:SD	3:3:32:LEU:CD2	3.05	0.45
3:3:546:ALA:C	3:3:547:MET:HE2	2.42	0.45
3:3:694:LEU:HB3	3:3:762:ALA:CB	2.42	0.45
4:4:40:VAL:HG23	6:6:88:MET:CE	2.46	0.45
4:4:91:PHE:CE1	4:4:120:LEU:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:53:VAL:HG22	5:5:55:LEU:CD1	2.46	0.45
1:A:192:LEU:C	1:A:194:GLY:H	2.25	0.45
1:A:357:THR:N	1:A:358:PRO:HD2	2.32	0.45
3:C:20:MET:SD	3:C:32:LEU:CD2	3.05	0.45
4:D:40:VAL:HG23	6:F:88:MET:CE	2.46	0.45
4:D:257:TYR:C	4:D:259:THR:H	2.25	0.45
8:J:108:ILE:HG22	8:J:114:ARG:NH1	2.32	0.45
1:1:269:GLY:O	1:1:270:THR:C	2.60	0.45
1:1:357:THR:N	1:1:358:PRO:HD2	2.32	0.45
3:3:408:ILE:HD12	3:3:408:ILE:HA	1.83	0.45
3:3:583:VAL:HG23	3:3:598:ALA:HA	1.99	0.45
4:4:257:TYR:C	4:4:259:THR:H	2.25	0.45
6:6:99:MET:CG	6:6:100:PRO:HD2	2.42	0.45
6:6:154:LEU:O	6:6:158:VAL:HG13	2.16	0.45
7:9:126:TYR:HD1	7:9:126:TYR:C	2.25	0.45
8:7:108:ILE:HG22	8:7:114:ARG:NH1	2.32	0.45
3:C:546:ALA:C	3:C:547:MET:HE2	2.42	0.45
3:C:583:VAL:HG23	3:C:598:ALA:HA	1.99	0.45
3:C:694:LEU:HB3	3:C:762:ALA:CB	2.42	0.45
4:D:91:PHE:CE1	4:D:120:LEU:HD12	2.52	0.45
5:E:53:VAL:HG22	5:E:55:LEU:CD1	2.46	0.45
6:F:154:LEU:O	6:F:158:VAL:HG13	2.16	0.45
7:G:29:ALA:HA	7:G:30:PRO:HD2	1.83	0.45
3:3:202:PHE:C	3:3:203:ILE:HD13	2.41	0.45
3:3:550:LEU:N	3:3:550:LEU:CD1	2.79	0.45
3:3:688:ARG:HD3	3:3:688:ARG:HA	1.71	0.45
3:3:707:LYS:C	3:3:709:GLN:N	2.75	0.45
1:A:139:ARG:HG2	2:B:140:PRO:HD3	1.99	0.45
1:A:269:GLY:O	1:A:270:THR:C	2.60	0.45
3:C:202:PHE:C	3:C:203:ILE:HD13	2.41	0.45
3:C:408:ILE:HD12	3:C:408:ILE:HA	1.83	0.45
3:C:707:LYS:C	3:C:709:GLN:N	2.75	0.45
7:G:126:TYR:C	7:G:126:TYR:HD1	2.25	0.45
10:P:920:UNK:C	10:P:1200:UNK:N	2.52	0.45
1:1:139:ARG:HG2	2:2:140:PRO:HD3	1.99	0.45
4:4:162:TRP:CE2	7:9:34:LYS:HD2	2.52	0.45
4:4:197:LEU:N	4:4:198:PRO:CD	2.80	0.45
3:C:550:LEU:N	3:C:550:LEU:CD1	2.79	0.45
3:C:688:ARG:HD3	3:C:688:ARG:HA	1.71	0.45
4:D:162:TRP:CE2	7:G:34:LYS:HD2	2.52	0.45
4:D:197:LEU:N	4:D:198:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:236:GLY:HA3	4:D:377:ASN:HD21	1.82	0.45
2:2:81:GLN:HB3	2:2:122:VAL:HG21	1.98	0.44
3:3:621:VAL:O	3:3:621:VAL:HG23	2.16	0.44
3:3:689:LYS:HG3	3:3:771:VAL:CA	2.38	0.44
4:4:236:GLY:HA3	4:4:377:ASN:HD21	1.82	0.44
10:M:920:UNK:C	10:M:1200:UNK:N	2.52	0.44
2:B:81:GLN:HB3	2:B:122:VAL:HG21	1.98	0.44
6:F:76:ASP:O	6:F:77:VAL:CB	2.66	0.44
6:F:99:MET:CG	6:F:100:PRO:HD2	2.42	0.44
2:2:106:ILE:HG22	2:2:110:GLU:HB2	1.98	0.44
3:3:240:ALA:HB2	3:3:276:ARG:HB2	1.99	0.44
4:4:99:LEU:HA	4:4:99:LEU:HD13	1.55	0.44
6:6:76:ASP:O	6:6:77:VAL:CB	2.66	0.44
3:C:29:ASP:OD1	3:C:29:ASP:N	2.50	0.44
3:C:230:CYS:HA	14:C:785:SF4:S2	2.57	0.44
3:C:240:ALA:HB2	3:C:276:ARG:HB2	1.99	0.44
3:C:621:VAL:O	3:C:621:VAL:HG23	2.16	0.44
3:C:689:LYS:HG3	3:C:771:VAL:CA	2.38	0.44
4:D:99:LEU:HA	4:D:99:LEU:HD13	1.55	0.44
1:1:398:SER:HA	3:3:46:ARG:HD3	1.98	0.44
3:3:29:ASP:OD1	3:3:29:ASP:N	2.50	0.44
3:3:230:CYS:HA	14:3:785:SF4:S2	2.58	0.44
3:3:715:GLU:O	3:3:715:GLU:OE2	2.36	0.44
4:4:196:VAL:O	4:4:196:VAL:HG22	2.17	0.44
4:4:389:GLN:HG3	4:4:390:VAL:N	2.26	0.44
7:9:126:TYR:C	7:9:126:TYR:CD1	2.95	0.44
1:A:398:SER:HA	3:C:46:ARG:HD3	1.98	0.44
3:C:715:GLU:O	3:C:715:GLU:OE2	2.36	0.44
4:D:196:VAL:O	4:D:196:VAL:HG22	2.17	0.44
7:G:126:TYR:C	7:G:126:TYR:CD1	2.95	0.44
1:1:332:PRO:CD	2:2:90:LEU:HD23	2.47	0.44
2:2:154:LEU:O	2:2:158:ARG:HB2	2.17	0.44
4:4:262:PHE:HD1	4:4:289:ILE:HD11	1.81	0.44
1:A:332:PRO:CD	2:B:90:LEU:HD23	2.47	0.44
2:B:106:ILE:HG22	2:B:110:GLU:HB2	1.99	0.44
2:B:154:LEU:O	2:B:158:ARG:HB2	2.17	0.44
4:D:262:PHE:HD1	4:D:289:ILE:HD11	1.81	0.44
5:E:167:PRO:HB2	5:E:171:ARG:HH12	1.83	0.44
6:F:78:MET:HE2	6:F:99:MET:HE1	1.97	0.44
3:3:115:HIS:C	4:4:321:MET:HE3	2.43	0.44
3:3:394:ASP:OD2	3:3:502:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:61:TYR:CZ	6:6:87:LYS:HE2	2.53	0.44
4:4:131:VAL:HG12	4:4:132:PHE:N	2.33	0.44
5:5:167:PRO:HB2	5:5:171:ARG:HH12	1.83	0.44
6:6:78:MET:HE2	6:6:99:MET:HE1	1.97	0.44
3:C:394:ASP:OD2	3:C:502:ASN:N	2.50	0.44
4:D:131:VAL:HG12	4:D:132:PHE:N	2.33	0.44
4:D:389:GLN:HG3	4:D:390:VAL:N	2.26	0.44
6:F:78:MET:CE	6:F:99:MET:HE1	2.47	0.44
3:3:6:VAL:HG12	3:3:7:ASN:N	2.32	0.44
3:3:101:ARG:CZ	3:3:101:ARG:CB	2.94	0.44
3:3:256:CYS:HB2	3:3:265:ILE:HD13	1.98	0.44
3:3:663:ALA:O	3:3:666:ALA:HB3	2.18	0.44
4:4:144:THR:N	4:4:145:PRO:CD	2.81	0.44
5:5:101:LEU:HA	5:5:102:PRO:HD2	1.86	0.44
1:A:10:ASP:OD1	1:A:11:PRO:HD2	2.18	0.44
3:C:6:VAL:HG12	3:C:7:ASN:N	2.32	0.44
3:C:101:ARG:CZ	3:C:101:ARG:CB	2.94	0.44
3:C:115:HIS:C	4:D:321:MET:HE3	2.43	0.44
3:C:116:PRO:HG3	3:C:180:ARG:HG2	1.99	0.44
3:C:256:CYS:HB2	3:C:265:ILE:HD13	1.99	0.44
3:C:663:ALA:O	3:C:666:ALA:HB3	2.18	0.44
4:D:61:TYR:CZ	6:F:87:LYS:HE2	2.53	0.44
4:D:144:THR:N	4:D:145:PRO:CD	2.81	0.44
4:D:250:LYS:HE2	4:D:262:PHE:CD2	2.53	0.44
1:1:10:ASP:OD1	1:1:11:PRO:HD2	2.18	0.44
1:1:93:ALA:O	1:1:134:VAL:HA	2.17	0.44
3:3:116:PRO:HG3	3:3:180:ARG:HG2	1.99	0.44
3:3:240:ALA:CB	3:3:276:ARG:HB2	2.47	0.44
4:4:159:LEU:O	4:4:162:TRP:HB2	2.18	0.44
6:6:78:MET:CE	6:6:99:MET:HE1	2.47	0.44
1:A:93:ALA:O	1:A:134:VAL:HA	2.17	0.44
3:C:240:ALA:CB	3:C:276:ARG:HB2	2.48	0.44
8:J:31:PHE:CD1	8:J:31:PHE:C	2.96	0.44
8:J:78:LYS:HD3	8:J:78:LYS:HA	1.76	0.44
3:3:38:HIS:CE1	3:3:287:GLU:HB3	2.52	0.44
3:3:115:HIS:HB3	4:4:321:MET:HE3	2.00	0.44
4:4:100:ALA:O	4:4:342:VAL:HG11	2.17	0.44
4:4:250:LYS:HE2	4:4:262:PHE:CD2	2.53	0.44
5:5:163:ARG:CD	7:9:69:TYR:CE1	3.00	0.44
8:7:31:PHE:CD1	8:7:31:PHE:C	2.96	0.44
8:7:97:TYR:C	8:7:97:TYR:CD2	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:HIS:CE1	3:C:287:GLU:HB3	2.52	0.44
3:C:115:HIS:HB3	4:D:321:MET:HE3	2.00	0.44
4:D:159:LEU:O	4:D:162:TRP:HB2	2.18	0.44
5:E:163:ARG:CD	7:G:69:TYR:CE1	3.00	0.44
8:J:97:TYR:C	8:J:97:TYR:CD2	2.95	0.44
3:3:173:PHE:HB3	3:3:296:PHE:CE1	2.53	0.44
3:3:334:LYS:NZ	3:3:334:LYS:HB3	2.33	0.44
7:9:41:HIS:CD2	7:9:115:LEU:HD21	2.53	0.44
8:7:78:LYS:HD3	8:7:78:LYS:HA	1.76	0.44
8:7:90:HIS:O	8:7:90:HIS:ND1	2.49	0.44
3:C:173:PHE:HB3	3:C:296:PHE:CE1	2.53	0.44
3:C:334:LYS:NZ	3:C:334:LYS:HB3	2.33	0.44
3:C:606:THR:O	3:C:610:LYS:HG3	2.18	0.44
4:D:100:ALA:O	4:D:342:VAL:HG11	2.17	0.44
5:E:101:LEU:HA	5:E:102:PRO:HD2	1.86	0.44
8:J:87:PRO:O	8:J:88:ARG:CB	2.53	0.44
8:J:90:HIS:O	8:J:90:HIS:ND1	2.49	0.44
1:1:18:TYR:CE2	1:1:263:VAL:HG11	2.53	0.43
1:1:110:VAL:O	1:1:110:VAL:HG23	2.18	0.43
3:3:151:LEU:HD23	3:3:151:LEU:HA	1.86	0.43
3:3:259:CYS:CB	3:3:260:PRO:CD	2.96	0.43
3:3:270:ARG:HB3	3:3:275:LEU:HD21	2.00	0.43
3:3:274:LEU:HD12	3:3:274:LEU:C	2.43	0.43
6:6:37:TRP:CE3	6:6:37:TRP:HA	2.53	0.43
8:7:87:PRO:O	8:7:88:ARG:CB	2.53	0.43
1:A:110:VAL:O	1:A:110:VAL:HG23	2.18	0.43
3:C:270:ARG:HB3	3:C:275:LEU:HD21	2.00	0.43
3:C:561:PRO:HG3	3:C:575:GLU:O	2.18	0.43
5:E:84:ASP:OD1	5:E:84:ASP:N	2.51	0.43
5:E:146:LEU:HD22	5:E:146:LEU:HA	1.86	0.43
6:F:37:TRP:CE3	6:F:37:TRP:HA	2.53	0.43
7:G:41:HIS:CD2	7:G:115:LEU:HD21	2.53	0.43
1:1:134:VAL:HG23	1:1:135:ARG:O	2.17	0.43
1:1:211:LEU:HB2	1:1:216:THR:HG21	2.00	0.43
3:3:561:PRO:HG3	3:3:575:GLU:O	2.18	0.43
3:3:606:THR:O	3:3:610:LYS:HG3	2.18	0.43
4:4:329:LYS:HD2	4:4:329:LYS:HA	1.87	0.43
5:5:84:ASP:OD1	5:5:84:ASP:N	2.51	0.43
1:A:18:TYR:CE2	1:A:263:VAL:HG11	2.53	0.43
1:A:134:VAL:HG23	1:A:135:ARG:O	2.17	0.43
1:A:211:LEU:HB2	1:A:216:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:LEU:HD23	3:C:151:LEU:HA	1.86	0.43
3:C:259:CYS:CB	3:C:260:PRO:CD	2.96	0.43
3:C:274:LEU:HD12	3:C:274:LEU:C	2.43	0.43
3:3:55:PRO:CD	3:3:74:GLN:N	2.80	0.43
3:3:675:ARG:NH1	3:C:316:ARG:NH2	2.67	0.43
3:3:689:LYS:HB2	3:3:772:GLU:HG2	2.00	0.43
3:C:55:PRO:CD	3:C:74:GLN:N	2.80	0.43
3:C:451:PHE:CE1	3:C:466:GLU:HB3	2.53	0.43
6:F:16:ARG:HG2	6:F:21:PHE:HE2	1.83	0.43
8:J:16:LEU:HD13	8:J:16:LEU:C	2.43	0.43
3:3:116:PRO:C	4:4:321:MET:HE1	2.38	0.43
3:3:370:ASP:OD2	3:3:558:TRP:HD1	2.00	0.43
3:3:451:PHE:CE1	3:3:466:GLU:HB3	2.53	0.43
4:4:233:GLY:CA	5:5:48:PHE:HE1	2.31	0.43
5:5:146:LEU:HD22	5:5:146:LEU:HA	1.86	0.43
6:6:16:ARG:HG2	6:6:21:PHE:HE2	1.83	0.43
7:9:127:SER:O	7:9:130:VAL:HG12	2.18	0.43
3:C:370:ASP:OD2	3:C:558:TRP:HD1	2.00	0.43
3:C:689:LYS:HB2	3:C:772:GLU:HG2	2.00	0.43
4:D:153:ARG:HG3	4:D:153:ARG:NH1	2.33	0.43
4:D:329:LYS:HD2	4:D:329:LYS:HA	1.87	0.43
7:G:127:SER:O	7:G:130:VAL:HG12	2.18	0.43
1:1:186:THR:CG2	1:1:200:ARG:N	2.69	0.43
3:3:627:ALA:HA	3:3:628:PRO:HD3	1.80	0.43
4:4:153:ARG:HG3	4:4:153:ARG:NH1	2.33	0.43
6:6:78:MET:HE3	6:6:96:TRP:HB2	2.00	0.43
6:6:104:TRP:NE1	6:6:173:VAL:HG22	2.33	0.43
8:7:16:LEU:HD13	8:7:16:LEU:C	2.43	0.43
1:A:186:THR:CG2	1:A:200:ARG:N	2.69	0.43
3:C:116:PRO:C	4:D:321:MET:HE1	2.38	0.43
3:C:409:LEU:HD23	3:C:409:LEU:HA	1.72	0.43
4:D:233:GLY:CA	5:E:48:PHE:HE1	2.31	0.43
6:F:104:TRP:NE1	6:F:173:VAL:HG22	2.33	0.43
1:1:89:LEU:HD21	1:1:121:ALA:HB3	1.99	0.43
1:1:253:GLN:N	1:1:253:GLN:NE2	2.57	0.43
3:3:571:VAL:HG11	3:3:591:HIS:CD2	2.54	0.43
7:9:41:HIS:CE1	7:9:98:CYS:SG	3.12	0.43
8:7:92:HIS:O	8:7:93:LEU:HD12	2.18	0.43
12:R:297:UNK:CA	13:H:500:UNK:CA	2.96	0.43
3:C:571:VAL:HG11	3:C:591:HIS:CD2	2.54	0.43
6:F:78:MET:HE3	6:F:96:TRP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:41:HIS:CE1	7:G:98:CYS:SG	3.12	0.43
8:J:92:HIS:O	8:J:93:LEU:HD12	2.18	0.43
1:1:291:ILE:HA	1:1:292:PRO:HD2	1.64	0.43
3:3:9:ARG:HE	3:3:9:ARG:HB2	1.65	0.43
3:3:497:TRP:O	3:3:528:LYS:HE3	2.18	0.43
13:H:414:UNK:CA	13:H:515:UNK:CA	2.97	0.43
1:A:89:LEU:HD21	1:A:121:ALA:HB3	1.99	0.43
1:A:253:GLN:N	1:A:253:GLN:NE2	2.57	0.43
3:C:384:PRO:HG3	3:C:542:ARG:HE	1.83	0.43
3:C:497:TRP:O	3:C:528:LYS:HE3	2.18	0.43
3:C:627:ALA:HA	3:C:628:PRO:HD3	1.80	0.43
12:S:297:UNK:CA	13:T:500:UNK:CA	2.96	0.43
13:T:414:UNK:CA	13:T:515:UNK:CA	2.97	0.43
3:3:384:PRO:HG3	3:3:542:ARG:HE	1.83	0.43
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.72	0.43
3:3:567:TYR:HE1	3:3:586:HIS:HB2	1.83	0.43
5:5:167:PRO:HB3	7:9:66:TYR:CE2	2.53	0.43
7:9:99:ILE:HG22	7:9:101:CYS:SG	2.58	0.43
1:A:228:VAL:HB	1:A:229:PRO:CD	2.49	0.43
3:C:567:TYR:HE1	3:C:586:HIS:HB2	1.82	0.43
5:E:167:PRO:HB3	7:G:66:TYR:CE2	2.53	0.43
6:F:106:ILE:CD1	6:F:151:VAL:HG12	2.49	0.43
8:J:121:ARG:NH1	8:J:121:ARG:CG	2.81	0.43
1:1:228:VAL:HB	1:1:229:PRO:CD	2.49	0.43
3:3:237:ASP:CG	3:3:239:THR:HG22	2.43	0.43
3:3:513:GLN:HG2	3:3:769:LEU:HD23	2.01	0.43
3:3:753:VAL:HA	3:3:754:PRO:HD2	1.83	0.43
4:4:163:VAL:HG13	4:4:164:THR:HG23	2.00	0.43
6:6:106:ILE:CD1	6:6:151:VAL:HG12	2.49	0.43
8:7:121:ARG:NH1	8:7:121:ARG:CG	2.81	0.43
1:A:291:ILE:HA	1:A:292:PRO:HD2	1.64	0.43
3:C:237:ASP:CG	3:C:239:THR:HG22	2.43	0.43
3:C:513:GLN:HG2	3:C:769:LEU:HD23	2.01	0.43
3:C:753:VAL:HA	3:C:754:PRO:HD2	1.83	0.43
4:D:240:ARG:HB2	4:D:266:LEU:HD23	2.01	0.43
3:3:120:PRO:HG2	8:7:42:TYR:CZ	2.53	0.43
3:3:715:GLU:OE2	3:3:715:GLU:C	2.62	0.43
4:4:76:LEU:HD12	4:4:76:LEU:O	2.19	0.43
4:4:82:THR:N	4:4:83:PRO:HD2	2.33	0.43
4:4:240:ARG:HB2	4:4:266:LEU:HD23	2.01	0.43
1:A:414:LEU:O	1:A:418:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:PRO:HG2	8:J:42:TYR:CZ	2.53	0.43
3:C:715:GLU:CD	3:C:761:SER:HB2	2.44	0.43
4:D:76:LEU:HD12	4:D:76:LEU:O	2.19	0.43
4:D:163:VAL:HG13	4:D:164:THR:HG23	2.01	0.43
7:G:99:ILE:HG22	7:G:101:CYS:SG	2.58	0.43
1:1:177:ALA:HB3	2:2:67:TYR:CD2	2.54	0.42
1:1:414:LEU:O	1:1:418:LYS:HB2	2.19	0.42
3:3:45:CYS:SG	3:3:47:MET:HB2	2.59	0.42
3:3:471:GLY:HA2	3:3:473:GLU:OE2	2.19	0.42
3:3:715:GLU:CD	3:3:761:SER:HB2	2.44	0.42
4:4:328:PHE:C	4:4:328:PHE:CD2	2.97	0.42
6:6:104:TRP:HA	6:6:134:ASP:OD2	2.19	0.42
1:A:28:THR:C	1:A:30:ASP:N	2.77	0.42
1:A:114:LEU:C	1:A:114:LEU:CD2	2.91	0.42
1:A:177:ALA:HB3	2:B:67:TYR:CD2	2.54	0.42
3:C:270:ARG:O	3:C:271:SER:HB2	2.17	0.42
3:C:471:GLY:HA2	3:C:473:GLU:OE2	2.19	0.42
4:D:82:THR:N	4:D:83:PRO:HD2	2.33	0.42
4:D:122:GLU:CD	4:D:125:ARG:HE	2.27	0.42
4:D:328:PHE:C	4:D:328:PHE:CD2	2.97	0.42
1:1:6:LEU:HB2	1:1:241:MET:HA	2.00	0.42
1:1:28:THR:C	1:1:30:ASP:N	2.77	0.42
1:1:114:LEU:C	1:1:114:LEU:CD2	2.91	0.42
3:3:55:PRO:HG3	3:3:74:GLN:CB	2.49	0.42
3:3:260:PRO:HG3	3:3:536:THR:O	2.19	0.42
4:4:119:ILE:O	4:4:123:LEU:HB2	2.19	0.42
4:4:122:GLU:CD	4:4:125:ARG:HE	2.27	0.42
4:4:257:TYR:C	4:4:259:THR:N	2.77	0.42
1:A:6:LEU:HB2	1:A:241:MET:HA	2.00	0.42
3:C:9:ARG:HE	3:C:9:ARG:HB2	1.65	0.42
3:C:45:CYS:SG	3:C:47:MET:HB2	2.59	0.42
3:C:260:PRO:HG3	3:C:536:THR:O	2.19	0.42
3:C:715:GLU:OE2	3:C:715:GLU:C	2.62	0.42
3:C:776:LEU:N	3:C:776:LEU:HD23	2.34	0.42
4:D:257:TYR:C	4:D:259:THR:N	2.77	0.42
1:1:211:LEU:HA	1:1:211:LEU:HD12	1.65	0.42
2:2:79:HIS:O	2:2:136:VAL:O	2.38	0.42
3:3:716:LEU:CD2	3:3:758:LEU:HB3	2.47	0.42
3:3:776:LEU:N	3:3:776:LEU:HD23	2.34	0.42
4:4:64:THR:N	4:4:409:ARG:OXT	2.52	0.42
6:6:32:ARG:NH1	6:6:102:PRO:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:163:TYR:CD2	6:6:169:ARG:HA	2.54	0.42
1:A:211:LEU:HD12	1:A:211:LEU:HA	1.65	0.42
2:B:79:HIS:O	2:B:136:VAL:O	2.38	0.42
3:C:55:PRO:HG3	3:C:74:GLN:CB	2.49	0.42
3:C:716:LEU:CD2	3:C:758:LEU:HB3	2.47	0.42
4:D:119:ILE:O	4:D:123:LEU:HB2	2.19	0.42
5:E:134:LYS:HB2	5:E:134:LYS:HE3	1.67	0.42
6:F:32:ARG:NH1	6:F:102:PRO:HG2	2.34	0.42
6:F:104:TRP:HA	6:F:134:ASP:OD2	2.19	0.42
6:F:163:TYR:CD2	6:F:169:ARG:HA	2.54	0.42
1:1:5:ILE:HG22	1:1:6:LEU:N	2.34	0.42
1:1:392:PRO:O	1:1:397:ARG:NH1	2.52	0.42
3:3:33:PHE:CE2	3:3:47:MET:HE3	2.54	0.42
3:3:695:ARG:HD2	3:3:717:TRP:CZ3	2.54	0.42
5:5:134:LYS:HB2	5:5:134:LYS:HE3	1.67	0.42
7:9:136:MET:O	7:9:137:LEU:C	2.60	0.42
1:A:5:ILE:HG22	1:A:6:LEU:N	2.34	0.42
1:A:42:LYS:O	1:A:43:ARG:C	2.62	0.42
1:A:392:PRO:O	1:A:397:ARG:NH1	2.52	0.42
2:B:168:LEU:HA	2:B:169:PRO:HD2	1.79	0.42
3:C:33:PHE:CE2	3:C:47:MET:HE3	2.54	0.42
3:C:120:PRO:O	3:C:245:ARG:NH1	2.53	0.42
3:C:516:VAL:O	3:C:520:ARG:HG3	2.19	0.42
4:D:64:THR:N	4:D:409:ARG:OXT	2.52	0.42
7:G:136:MET:O	7:G:137:LEU:C	2.60	0.42
1:1:42:LYS:O	1:1:43:ARG:C	2.62	0.42
1:1:248:GLY:O	1:1:268:MET:HB2	2.19	0.42
2:2:27:ILE:HD13	2:2:60:VAL:HG22	2.01	0.42
2:2:61:MET:HB2	3:3:214:MET:HG3	2.01	0.42
2:2:168:LEU:HA	2:2:169:PRO:HD2	1.79	0.42
3:3:120:PRO:O	3:3:245:ARG:NH1	2.53	0.42
3:3:516:VAL:O	3:3:520:ARG:HG3	2.19	0.42
3:3:753:VAL:HG13	3:3:759:TYR:CD1	2.55	0.42
5:5:16:PRO:HD2	5:5:28:VAL:HG13	2.01	0.42
1:A:248:GLY:O	1:A:268:MET:HB2	2.19	0.42
2:B:27:ILE:HD13	2:B:60:VAL:HG22	2.01	0.42
2:B:61:MET:HB2	3:C:214:MET:HG3	2.01	0.42
3:C:695:ARG:HD2	3:C:717:TRP:CZ3	2.54	0.42
4:D:65:GLY:O	4:D:69:THR:CG2	2.67	0.42
5:E:16:PRO:HD2	5:E:28:VAL:HG13	2.01	0.42
7:G:41:HIS:HE1	7:G:98:CYS:SG	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:364:ALA:HB3	3:3:207:VAL:HG13	2.01	0.42
1:1:367:MET:HE2	1:1:367:MET:HB3	1.74	0.42
2:2:43:PRO:O	2:2:47:GLU:HG3	2.19	0.42
3:3:11:VAL:HG21	3:3:26:ALA:HB2	2.00	0.42
3:3:616:ASN:C	3:3:618:GLU:H	2.28	0.42
4:4:65:GLY:O	4:4:69:THR:CG2	2.67	0.42
4:4:234:LEU:O	4:4:236:GLY:N	2.53	0.42
7:9:41:HIS:HE1	7:9:98:CYS:SG	2.42	0.42
10:M:916:UNK:C	10:M:1203:UNK:CA	2.97	0.42
1:A:364:ALA:HB3	3:C:207:VAL:HG13	2.01	0.42
1:A:367:MET:HE2	1:A:367:MET:HB3	1.74	0.42
2:B:43:PRO:O	2:B:47:GLU:HG3	2.19	0.42
3:C:11:VAL:HG21	3:C:26:ALA:HB2	1.99	0.42
4:D:234:LEU:O	4:D:236:GLY:N	2.53	0.42
1:1:272:PHE:HB3	1:1:276:ILE:HD11	2.02	0.42
2:2:3:PHE:HB3	2:2:48:GLU:OE1	2.20	0.42
2:2:27:ILE:O	2:2:31:LEU:HD22	2.20	0.42
3:3:485:GLU:O	6:F:16:ARG:NE	2.47	0.42
3:3:547:MET:HE2	3:3:547:MET:HA	2.02	0.42
4:4:143:LEU:HD23	4:4:143:LEU:O	2.19	0.42
4:4:297:LEU:HD12	4:4:297:LEU:HA	1.85	0.42
5:5:87:ARG:O	5:5:88:PHE:HB3	2.19	0.42
1:A:17:LEU:HD12	1:A:251:LEU:CD1	2.49	0.42
1:A:272:PHE:HB3	1:A:276:ILE:HD11	2.01	0.42
2:B:27:ILE:O	2:B:31:LEU:HD22	2.20	0.42
3:C:139:LEU:HD11	3:C:154:TYR:CD1	2.54	0.42
3:C:547:MET:HE2	3:C:547:MET:HA	2.02	0.42
3:C:616:ASN:C	3:C:618:GLU:H	2.28	0.42
3:C:753:VAL:HG13	3:C:759:TYR:CD1	2.55	0.42
4:D:297:LEU:HD12	4:D:297:LEU:HA	1.85	0.42
5:E:120:ASP:OD1	5:E:134:LYS:HG3	2.19	0.42
10:P:916:UNK:C	10:P:1203:UNK:CA	2.98	0.42
1:1:17:LEU:HD12	1:1:251:LEU:CD1	2.49	0.42
1:1:249:MET:HA	1:1:267:PRO:HA	2.02	0.42
3:3:139:LEU:HD11	3:3:154:TYR:CD1	2.54	0.42
4:4:182:LEU:HD22	4:4:186:PHE:CD2	2.54	0.42
4:4:196:VAL:O	4:4:200:ARG:HB2	2.20	0.42
4:4:197:LEU:O	4:4:200:ARG:HB3	2.20	0.42
5:5:53:VAL:HG22	5:5:55:LEU:HD12	2.02	0.42
5:5:120:ASP:OD1	5:5:134:LYS:HG3	2.19	0.42
8:7:14:VAL:O	8:7:17:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:CG	1:A:71:PRO:HD2	2.54	0.42
1:A:211:LEU:CB	1:A:216:THR:HG21	2.50	0.42
1:A:249:MET:HA	1:A:267:PRO:HA	2.02	0.42
2:B:3:PHE:HB3	2:B:48:GLU:OE1	2.20	0.42
3:C:414:SER:OG	3:C:443:ARG:NH2	2.53	0.42
4:D:143:LEU:HD23	4:D:143:LEU:O	2.19	0.42
4:D:182:LEU:HD22	4:D:186:PHE:CD2	2.54	0.42
4:D:196:VAL:O	4:D:200:ARG:HB2	2.20	0.42
4:D:197:LEU:O	4:D:200:ARG:HB3	2.20	0.42
5:E:66:GLU:HG2	5:E:95:PRO:CA	2.12	0.42
5:E:87:ARG:O	5:E:88:PHE:HB3	2.19	0.42
8:J:14:VAL:O	8:J:17:LEU:HB2	2.20	0.42
1:1:211:LEU:CB	1:1:216:THR:HG21	2.50	0.42
1:1:228:VAL:O	1:1:229:PRO:C	2.63	0.42
3:3:261:VAL:HG23	14:3:786:SF4:S2	2.60	0.42
3:3:414:SER:OG	3:3:443:ARG:NH2	2.53	0.42
3:3:460:LYS:HB2	3:3:460:LYS:HE2	1.84	0.42
4:4:250:LYS:HG3	4:4:264:VAL:HG21	2.01	0.42
4:4:393:MET:CA	4:4:396:ILE:HG22	2.49	0.42
7:9:96:LEU:HD21	7:9:129:LEU:HD13	2.01	0.42
8:7:108:ILE:N	8:7:108:ILE:CD1	2.83	0.42
1:A:228:VAL:O	1:A:229:PRO:C	2.63	0.42
3:C:194:VAL:HG12	3:C:195:PRO:HD3	2.02	0.42
3:C:261:VAL:HG23	14:C:786:SF4:S2	2.60	0.42
3:C:460:LYS:HB2	3:C:460:LYS:HE2	1.84	0.42
4:D:88:LEU:HD23	4:D:88:LEU:HA	1.92	0.42
4:D:393:MET:CA	4:D:396:ILE:HG22	2.49	0.42
5:E:53:VAL:HG22	5:E:55:LEU:HD12	2.02	0.42
5:E:64:ARG:HB3	5:E:65:PRO:HD2	2.02	0.42
5:E:78:PRO:HG3	5:E:85:GLY:CA	2.49	0.42
7:G:96:LEU:HD21	7:G:129:LEU:HD13	2.01	0.42
1:1:70:PHE:CG	1:1:71:PRO:HD2	2.54	0.42
2:2:142:VAL:HG11	2:2:153:LEU:HG	2.02	0.42
3:3:194:VAL:HG12	3:3:195:PRO:HD3	2.02	0.42
3:3:591:HIS:ND1	3:3:592:PRO:N	2.68	0.42
3:3:692:PHE:HE1	3:3:773:GLY:C	2.28	0.42
5:5:64:ARG:HB3	5:5:65:PRO:HD2	2.02	0.42
5:5:66:GLU:HG2	5:5:95:PRO:CA	2.12	0.42
5:5:78:PRO:HG3	5:5:85:GLY:CA	2.49	0.42
6:6:96:TRP:O	6:6:99:MET:HB2	2.20	0.42
6:6:138:PRO:HG3	7:9:121:MET:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:591:HIS:ND1	3:C:592:PRO:N	2.68	0.42
4:D:250:LYS:HG3	4:D:264:VAL:HG21	2.01	0.42
4:D:348:SER:C	4:D:350:ARG:H	2.27	0.42
4:D:400:LEU:HD23	4:D:400:LEU:HA	1.86	0.42
2:2:33:ARG:O	2:2:34:VAL:C	2.63	0.41
3:3:501:LYS:N	3:3:501:LYS:CD	2.73	0.41
4:4:348:SER:C	4:4:350:ARG:H	2.27	0.41
2:B:142:VAL:HG11	2:B:153:LEU:HG	2.02	0.41
3:C:267:ALA:HA	3:C:277:ILE:HD13	2.01	0.41
3:C:397:LEU:HD21	3:C:480:LEU:HD13	2.01	0.41
6:F:96:TRP:O	6:F:99:MET:HB2	2.20	0.41
6:F:138:PRO:HG3	7:G:121:MET:HG3	2.02	0.41
8:J:108:ILE:N	8:J:108:ILE:CD1	2.83	0.41
1:1:97:GLU:HB2	1:1:180:TYR:HE1	1.85	0.41
3:3:168:HIS:HA	3:3:169:PRO:HD2	1.93	0.41
3:3:308:THR:C	3:3:603:PRO:HG3	2.46	0.41
3:3:397:LEU:HD21	3:3:480:LEU:HD13	2.01	0.41
4:4:88:LEU:HD23	4:4:88:LEU:HA	1.93	0.41
4:4:400:LEU:HD23	4:4:400:LEU:HA	1.86	0.41
9:L:119:UNK:C	9:L:122:UNK:N	2.83	0.41
1:A:97:GLU:HB2	1:A:180:TYR:HE1	1.85	0.41
2:B:33:ARG:O	2:B:34:VAL:C	2.63	0.41
3:C:168:HIS:HA	3:C:169:PRO:HD2	1.93	0.41
3:C:308:THR:C	3:C:603:PRO:HG3	2.46	0.41
3:C:501:LYS:N	3:C:501:LYS:CD	2.73	0.41
3:C:692:PHE:HE1	3:C:773:GLY:C	2.28	0.41
9:O:119:UNK:C	9:O:122:UNK:N	2.83	0.41
1:1:188:LEU:HD23	1:1:188:LEU:O	2.20	0.41
1:1:273:ARG:O	1:1:277:TYR:HB2	2.21	0.41
3:3:267:ALA:HA	3:3:277:ILE:HD13	2.01	0.41
3:3:390:LEU:O	3:3:416:PHE:CD1	2.73	0.41
3:3:694:LEU:HD12	3:3:769:LEU:HB2	2.01	0.41
6:6:146:ALA:HB2	7:9:119:PHE:HD1	1.85	0.41
1:A:391:LEU:N	1:A:392:PRO:CD	2.83	0.41
1:A:438:ARG:HD2	1:A:438:ARG:H	1.85	0.41
3:C:337:ARG:HD3	3:C:340:GLU:CG	2.50	0.41
3:C:694:LEU:HD12	3:C:769:LEU:HB2	2.01	0.41
6:F:146:ALA:HB2	7:G:119:PHE:HD1	1.85	0.41
1:1:391:LEU:N	1:1:392:PRO:CD	2.83	0.41
1:1:438:ARG:H	1:1:438:ARG:HD2	1.85	0.41
1:1:438:ARG:HD2	1:1:438:ARG:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:30:VAL:HG22	3:3:48:CYS:HA	2.03	0.41
3:3:337:ARG:HD3	3:3:340:GLU:CG	2.50	0.41
3:3:487:SER:HB3	6:F:17:GLU:HB2	2.02	0.41
4:4:215:TYR:C	4:4:215:TYR:CD2	2.99	0.41
1:A:246:SER:O	1:A:268:MET:HG2	2.20	0.41
1:A:273:ARG:O	1:A:277:TYR:HB2	2.21	0.41
1:A:438:ARG:HD2	1:A:438:ARG:N	2.35	0.41
3:C:33:PHE:CZ	3:C:130:LEU:HD12	2.56	0.41
3:C:390:LEU:O	3:C:416:PHE:CD1	2.73	0.41
4:D:40:VAL:O	4:D:40:VAL:CG2	2.64	0.41
4:D:215:TYR:C	4:D:215:TYR:CD2	2.99	0.41
1:1:246:SER:O	1:1:268:MET:HG2	2.20	0.41
3:3:33:PHE:CZ	3:3:130:LEU:HD12	2.56	0.41
3:3:91:MET:HE2	3:3:91:MET:HB3	1.90	0.41
3:3:473:GLU:O	3:3:477:LEU:HD12	2.20	0.41
3:3:486:GLY:CA	6:F:17:GLU:OE1	2.54	0.41
3:3:487:SER:HB3	6:F:17:GLU:CB	2.50	0.41
3:3:695:ARG:HA	3:3:696:PRO:HD2	1.91	0.41
4:4:40:VAL:O	4:4:40:VAL:CG2	2.64	0.41
4:4:146:PHE:C	4:4:148:TYR:N	2.77	0.41
5:5:144:HIS:HA	5:5:145:PRO:HD2	1.86	0.41
7:9:37:PHE:CG	7:9:38:HIS:N	2.89	0.41
7:9:121:MET:HG3	7:9:121:MET:O	2.20	0.41
1:A:188:LEU:HD23	1:A:188:LEU:O	2.20	0.41
2:B:44:GLU:CD	2:B:44:GLU:N	2.78	0.41
3:C:91:MET:HE2	3:C:91:MET:HB3	1.90	0.41
3:C:473:GLU:O	3:C:477:LEU:HD12	2.20	0.41
4:D:146:PHE:C	4:D:148:TYR:N	2.77	0.41
7:G:37:PHE:CG	7:G:38:HIS:N	2.89	0.41
7:G:121:MET:HG3	7:G:121:MET:O	2.20	0.41
2:2:44:GLU:CD	2:2:44:GLU:N	2.78	0.41
3:3:281:GLU:HG3	3:3:283:PRO:HD3	2.03	0.41
4:4:337:PRO:HA	4:4:338:PRO:HD3	1.90	0.41
3:C:30:VAL:HG22	3:C:48:CYS:HA	2.03	0.41
3:C:313:LYS:HB3	3:C:314:GLU:H	1.74	0.41
4:D:337:PRO:HA	4:D:338:PRO:HD3	1.90	0.41
1:1:83:ASP:OD1	1:1:83:ASP:N	2.48	0.41
3:3:33:PHE:HZ	3:3:130:LEU:HD12	1.86	0.41
3:3:583:VAL:HG23	3:3:599:HIS:H	1.84	0.41
11:N:1215:UNK:C	11:N:1217:UNK:N	2.83	0.41
1:A:83:ASP:OD1	1:A:83:ASP:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HG23	1:A:110:VAL:HG23	2.00	0.41
3:C:33:PHE:HZ	3:C:130:LEU:HD12	1.86	0.41
3:C:594:ALA:C	3:C:596:ARG:H	2.28	0.41
3:C:695:ARG:HA	3:C:696:PRO:HD2	1.91	0.41
4:D:381:LEU:HA	4:D:384:ALA:HB3	2.03	0.41
5:E:137:THR:HB	5:E:141:LEU:HD22	2.02	0.41
7:G:138:VAL:HG23	7:G:139:ASP:N	2.36	0.41
11:Q:1215:UNK:C	11:Q:1217:UNK:N	2.83	0.41
1:1:158:LEU:HD23	1:1:158:LEU:HA	1.86	0.41
3:3:129:GLU:CD	3:3:186:ARG:HH12	2.28	0.41
3:3:317:LEU:HD22	3:3:317:LEU:H	1.85	0.41
3:3:594:ALA:C	3:3:596:ARG:H	2.28	0.41
4:4:381:LEU:HA	4:4:384:ALA:HB3	2.03	0.41
5:5:137:THR:HB	5:5:141:LEU:HD22	2.02	0.41
6:6:147:LEU:O	6:6:147:LEU:HD13	2.20	0.41
6:6:148:ILE:O	6:6:152:MET:HG3	2.21	0.41
7:9:71:GLU:HB2	7:9:90:VAL:HB	2.02	0.41
7:9:138:VAL:HG23	7:9:139:ASP:N	2.36	0.41
1:A:53:VAL:HG13	1:A:124:ALA:HB2	2.03	0.41
3:C:281:GLU:HG3	3:C:283:PRO:HD3	2.03	0.41
3:C:592:PRO:HA	3:C:595:GLU:OE2	2.20	0.41
5:E:81:LYS:HB2	5:E:82:ASP:H	1.58	0.41
5:E:144:HIS:HA	5:E:145:PRO:HD2	1.86	0.41
5:E:150:TYR:HA	5:E:151:PRO:HD3	1.77	0.41
6:F:148:ILE:O	6:F:152:MET:HG3	2.21	0.41
7:G:71:GLU:HB2	7:G:90:VAL:HB	2.02	0.41
1:1:32:TYR:O	1:1:37:GLY:HA2	2.20	0.41
1:1:53:VAL:HG13	1:1:124:ALA:HB2	2.03	0.41
1:1:106:ILE:HG23	1:1:110:VAL:HG23	2.01	0.41
1:1:169:PHE:CE2	1:1:171:LEU:CD1	3.03	0.41
1:1:273:ARG:HA	1:1:307:LEU:HD22	2.03	0.41
3:3:17:THR:HG22	3:3:18:SER:O	2.21	0.41
3:3:30:VAL:CG2	3:3:48:CYS:HA	2.50	0.41
3:3:36:GLU:O	3:3:37:LYS:C	2.64	0.41
3:3:50:VAL:HG12	3:3:95:THR:HG22	2.02	0.41
3:3:118:ASP:HB2	14:3:784:SF4:S1	2.61	0.41
3:3:361:ALA:CB	3:3:369:LEU:HD13	2.50	0.41
3:3:469:ARG:HB2	3:3:470:PRO:HD2	2.03	0.41
3:3:477:LEU:CD2	3:3:521:ALA:HB2	2.50	0.41
3:3:592:PRO:HA	3:3:595:GLU:OE2	2.20	0.41
3:3:695:ARG:NH1	3:3:697:THR:HG22	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:47:LEU:HA	4:4:53:LEU:HD23	2.03	0.41
4:4:224:ILE:HD11	4:4:275:ARG:CZ	2.50	0.41
5:5:81:LYS:HB2	5:5:82:ASP:H	1.58	0.41
5:5:150:TYR:HA	5:5:151:PRO:HD3	1.77	0.41
6:6:40:THR:OG1	6:6:50:MET:HE1	2.20	0.41
9:L:1506:UNK:C	9:L:1508:UNK:N	2.84	0.41
1:A:32:TYR:O	1:A:37:GLY:HA2	2.20	0.41
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.86	0.41
1:A:169:PHE:CE2	1:A:171:LEU:CD1	3.03	0.41
1:A:272:PHE:HB3	1:A:276:ILE:CD1	2.51	0.41
1:A:273:ARG:HA	1:A:307:LEU:HD22	2.03	0.41
3:C:30:VAL:CG2	3:C:48:CYS:HA	2.50	0.41
3:C:36:GLU:O	3:C:37:LYS:C	2.64	0.41
3:C:50:VAL:HG12	3:C:95:THR:HG22	2.02	0.41
3:C:118:ASP:HB2	14:C:784:SF4:S1	2.61	0.41
3:C:129:GLU:CD	3:C:186:ARG:HH12	2.28	0.41
3:C:317:LEU:HD22	3:C:317:LEU:H	1.85	0.41
3:C:469:ARG:HB2	3:C:470:PRO:HD2	2.03	0.41
3:C:477:LEU:CD2	3:C:521:ALA:HB2	2.50	0.41
3:C:583:VAL:HG23	3:C:599:HIS:H	1.85	0.41
3:C:695:ARG:NH1	3:C:697:THR:HG22	2.36	0.41
5:E:16:PRO:HB2	5:E:28:VAL:CG1	2.51	0.41
5:E:106:ASP:HB2	5:E:107:LEU:CD1	2.47	0.41
5:E:132:LEU:HD23	5:E:132:LEU:HA	1.58	0.41
6:F:147:LEU:O	6:F:147:LEU:HD13	2.20	0.41
1:1:55:GLU:O	1:1:59:ARG:HG3	2.20	0.41
1:1:63:ARG:NH1	1:1:313:TYR:HB3	2.36	0.41
1:1:102:LYS:HG2	1:1:253:GLN:OE1	2.21	0.41
1:1:107:LEU:CD2	1:1:114:LEU:HD12	2.51	0.41
1:1:272:PHE:HB3	1:1:276:ILE:CD1	2.51	0.41
3:3:487:SER:N	6:F:17:GLU:HB2	2.35	0.41
3:3:549:VAL:C	3:3:550:LEU:HD12	2.46	0.41
3:3:737:GLU:O	3:3:773:GLY:HA3	2.20	0.41
4:4:40:VAL:CG2	6:6:88:MET:HE2	2.51	0.41
4:4:102:GLU:HG2	4:4:175:ILE:O	2.21	0.41
4:4:383:TYR:CD1	4:4:383:TYR:C	2.99	0.41
5:5:16:PRO:HB2	5:5:28:VAL:CG1	2.51	0.41
5:5:107:LEU:N	5:5:107:LEU:CD1	2.82	0.41
1:A:63:ARG:NH1	1:A:313:TYR:HB3	2.36	0.41
1:A:102:LYS:HG2	1:A:253:GLN:OE1	2.21	0.41
1:A:107:LEU:CD2	1:A:114:LEU:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLU:CD	2:B:44:GLU:H	2.28	0.41
3:C:17:THR:HG22	3:C:18:SER:O	2.21	0.41
3:C:549:VAL:C	3:C:550:LEU:HD12	2.46	0.41
4:D:47:LEU:HA	4:D:53:LEU:HD23	2.03	0.41
4:D:224:ILE:HD11	4:D:275:ARG:CZ	2.50	0.41
4:D:383:TYR:CD1	4:D:383:TYR:C	2.99	0.41
5:E:107:LEU:N	5:E:107:LEU:CD1	2.82	0.41
9:O:1506:UNK:C	9:O:1508:UNK:N	2.84	0.41
2:2:44:GLU:CD	2:2:44:GLU:H	2.28	0.40
2:2:79:HIS:ND1	2:2:118:SER:CB	2.85	0.40
3:3:307:LYS:HE2	3:3:307:LYS:HB3	1.75	0.40
3:3:601:VAL:C	3:3:602:LEU:HD12	2.46	0.40
4:4:316:LEU:C	4:4:318:GLU:H	2.29	0.40
5:5:106:ASP:HB2	5:5:107:LEU:CD1	2.47	0.40
5:5:132:LEU:HD23	5:5:132:LEU:HA	1.58	0.40
6:6:137:VAL:HG13	6:6:137:VAL:O	2.19	0.40
6:6:154:LEU:O	6:6:154:LEU:HG	2.20	0.40
1:A:55:GLU:O	1:A:59:ARG:HG3	2.20	0.40
2:B:79:HIS:ND1	2:B:118:SER:CB	2.85	0.40
2:B:106:ILE:HG23	2:B:110:GLU:HB2	2.01	0.40
3:C:300:TRP:CD1	3:C:300:TRP:H	2.38	0.40
3:C:361:ALA:CB	3:C:369:LEU:HD13	2.50	0.40
3:C:422:PRO:HA	3:C:423:PRO:HD2	1.91	0.40
3:C:601:VAL:C	3:C:602:LEU:HD12	2.46	0.40
3:C:737:GLU:O	3:C:773:GLY:HA3	2.20	0.40
4:D:40:VAL:CG2	6:F:88:MET:HE2	2.51	0.40
4:D:102:GLU:HG2	4:D:175:ILE:O	2.21	0.40
6:F:40:THR:OG1	6:F:50:MET:HE1	2.20	0.40
2:2:106:ILE:HG23	2:2:110:GLU:HB2	2.02	0.40
3:3:300:TRP:CD1	3:3:300:TRP:H	2.38	0.40
4:4:164:THR:OG1	4:4:170:HIS:HB3	2.21	0.40
5:5:2:ARG:HD2	5:5:84:ASP:OD1	2.21	0.40
3:C:307:LYS:HE2	3:C:307:LYS:HB3	1.75	0.40
3:C:440:ARG:NH1	3:C:440:ARG:HG3	2.34	0.40
3:C:629:ILE:HG22	3:C:630:GLU:N	2.37	0.40
4:D:164:THR:OG1	4:D:170:HIS:HB3	2.21	0.40
4:D:295:GLU:C	4:D:297:LEU:H	2.29	0.40
6:F:137:VAL:HG13	6:F:137:VAL:O	2.19	0.40
6:F:154:LEU:O	6:F:154:LEU:HG	2.20	0.40
1:1:312:SER:C	1:1:314:GLU:H	2.30	0.40
1:1:373:LYS:HE2	1:1:378:GLN:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:382:PHE:CD1	3:3:382:PHE:N	2.90	0.40
3:3:422:PRO:HA	3:3:423:PRO:HD2	1.91	0.40
3:3:440:ARG:NH1	3:3:440:ARG:HG3	2.34	0.40
3:3:571:VAL:HA	3:3:572:PRO:HD3	1.90	0.40
3:3:629:ILE:HG22	3:3:630:GLU:N	2.37	0.40
7:9:125:GLU:O	7:9:126:TYR:C	2.65	0.40
1:A:312:SER:C	1:A:314:GLU:H	2.30	0.40
1:A:373:LYS:HE2	1:A:378:GLN:O	2.22	0.40
3:C:382:PHE:CD1	3:C:382:PHE:N	2.89	0.40
4:D:316:LEU:C	4:D:318:GLU:H	2.29	0.40
7:G:125:GLU:O	7:G:126:TYR:C	2.65	0.40
3:3:197:ASP:O	3:3:199:VAL:N	2.55	0.40
3:3:223:SER:O	3:3:226:ILE:HG12	2.21	0.40
3:3:373:GLY:HA3	3:3:538:ALA:HB2	2.03	0.40
3:3:454:TYR:HB2	3:3:752:ASP:OD2	2.20	0.40
3:3:701:ALA:N	3:3:763:LEU:O	2.51	0.40
4:4:200:ARG:HG3	4:4:204:TYR:HE1	1.86	0.40
4:4:234:LEU:O	4:4:234:LEU:HD13	2.22	0.40
4:4:295:GLU:C	4:4:297:LEU:H	2.29	0.40
4:4:393:MET:HE2	4:4:393:MET:HB3	1.89	0.40
5:5:110:SER:C	5:5:112:ASN:H	2.29	0.40
6:6:30:TRP:CD1	6:6:30:TRP:C	2.99	0.40
8:7:43:ARG:HH11	8:7:48:TYR:CB	2.33	0.40
3:C:197:ASP:O	3:C:199:VAL:N	2.55	0.40
3:C:223:SER:O	3:C:226:ILE:HG12	2.21	0.40
3:C:571:VAL:HA	3:C:572:PRO:HD3	1.90	0.40
3:C:701:ALA:N	3:C:763:LEU:O	2.51	0.40
4:D:234:LEU:O	4:D:234:LEU:HD13	2.22	0.40
4:D:288:LYS:HD3	4:D:288:LYS:HA	1.85	0.40
5:E:2:ARG:HD2	5:E:84:ASP:OD1	2.21	0.40
5:E:110:SER:C	5:E:112:ASN:H	2.29	0.40
6:F:30:TRP:CD1	6:F:30:TRP:C	2.99	0.40
8:J:43:ARG:HH11	8:J:48:TYR:CB	2.33	0.40
1:1:396:GLY:C	1:1:397:ARG:HG3	2.46	0.40
2:2:163:LEU:C	2:2:165:GLU:H	2.29	0.40
3:3:54:LEU:N	3:3:55:PRO:HD3	2.36	0.40
3:3:118:ASP:O	3:3:119:CYS:C	2.64	0.40
3:3:261:VAL:HG22	14:3:786:SF4:S2	2.62	0.40
4:4:131:VAL:HG23	4:4:153:ARG:NH1	2.36	0.40
4:4:200:ARG:HA	4:4:200:ARG:HE	1.86	0.40
4:4:276:MET:O	4:4:280:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:288:LYS:HD3	4:4:288:LYS:HA	1.85	0.40
2:B:136:VAL:HG21	2:B:163:LEU:CD1	2.47	0.40
3:C:7:ASN:OD1	3:C:96:LEU:HD12	2.22	0.40
3:C:118:ASP:O	3:C:119:CYS:C	2.64	0.40
3:C:373:GLY:HA3	3:C:538:ALA:HB2	2.03	0.40
4:D:200:ARG:HA	4:D:200:ARG:HE	1.86	0.40
4:D:276:MET:O	4:D:280:ILE:HG13	2.21	0.40
4:D:393:MET:HE2	4:D:393:MET:HB3	1.89	0.40
6:F:137:VAL:HA	6:F:138:PRO:HD2	1.95	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:319:GLU:OE2	3:C:679:ARG:CZ[1_655]	1.75	0.45
3:3:319:GLU:OE1	3:C:679:ARG:NH1[1_655]	1.84	0.36
6:6:16:ARG:CG	3:C:485:GLU:OE1[1_655]	1.91	0.29
6:6:16:ARG:CD	3:C:485:GLU:O[1_655]	1.99	0.21
3:3:319:GLU:CD	3:C:679:ARG:CZ[1_655]	2.07	0.13
3:3:319:GLU:OE2	3:C:679:ARG:NH1[1_655]	2.07	0.13
3:3:319:GLU:CD	3:C:679:ARG:NH2[1_655]	2.09	0.11
3:3:319:GLU:OE2	3:C:679:ARG:NE[1_655]	2.12	0.08
3:3:319:GLU:OE1	3:C:679:ARG:NH2[1_655]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	435/438 (99%)	362 (83%)	58 (13%)	15 (3%)	3	21
1	A	435/438 (99%)	362 (83%)	58 (13%)	15 (3%)	3	21
2	2	176/181 (97%)	156 (89%)	16 (9%)	4 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	176/181 (97%)	156 (89%)	16 (9%)	4 (2%)	5	28
3	3	748/783 (96%)	634 (85%)	91 (12%)	23 (3%)	3	22
3	C	748/783 (96%)	634 (85%)	91 (12%)	23 (3%)	3	22
4	4	373/409 (91%)	322 (86%)	37 (10%)	14 (4%)	2	19
4	D	373/409 (91%)	321 (86%)	38 (10%)	14 (4%)	2	19
5	5	194/207 (94%)	165 (85%)	23 (12%)	6 (3%)	3	22
5	E	194/207 (94%)	165 (85%)	23 (12%)	6 (3%)	3	22
6	6	141/181 (78%)	114 (81%)	22 (16%)	5 (4%)	3	20
6	F	141/181 (78%)	114 (81%)	22 (16%)	5 (4%)	3	20
7	9	152/182 (84%)	131 (86%)	17 (11%)	4 (3%)	4	26
7	G	152/182 (84%)	131 (86%)	17 (11%)	4 (3%)	4	26
8	7	125/129 (97%)	112 (90%)	12 (10%)	1 (1%)	16	53
8	J	125/129 (97%)	112 (90%)	12 (10%)	1 (1%)	16	53
All	All	4688/5020 (93%)	3991 (85%)	553 (12%)	144 (3%)	3	22

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
1	1	81	LYS
2	2	86	LEU
2	2	136	VAL
2	2	140	PRO
3	3	6	VAL
3	3	117	LEU
3	3	580	LYS
7	9	173	PHE
1	A	4	PRO
1	A	81	LYS
2	B	86	LEU
2	B	136	VAL
2	B	140	PRO
3	C	6	VAL
3	C	117	LEU
3	C	580	LYS
7	G	173	PHE
1	1	37	GLY

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Mol	Chain	Res	Type
1	1	160	LYS
3	3	125	GLY
3	3	184	CYS
3	3	204	GLU
3	3	285	VAL
3	3	563	ALA
4	4	51	GLU
4	4	236	GLY
4	4	258	GLU
4	4	334	GLY
5	5	176	GLY
6	6	45	CYS
6	6	77	VAL
6	6	126	ASN
1	A	37	GLY
1	A	160	LYS
3	C	125	GLY
3	C	184	CYS
3	C	204	GLU
3	C	285	VAL
3	C	563	ALA
4	D	51	GLU
4	D	236	GLY
4	D	258	GLU
4	D	334	GLY
5	E	176	GLY
6	F	45	CYS
6	F	77	VAL
6	F	126	ASN
1	1	18	TYR
1	1	166	ASP
1	1	311	MET
3	3	220	SER
3	3	365	LYS
4	4	235	THR
4	4	389	GLN
5	5	47	ASN
7	9	37	PHE
7	9	48	ASN
1	A	18	TYR
1	A	166	ASP
1	A	311	MET

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Mol	Chain	Res	Type
3	C	220	SER
3	C	365	LYS
4	D	235	THR
4	D	389	GLN
5	E	47	ASN
7	G	37	PHE
7	G	48	ASN
1	1	43	ARG
1	1	314	GLU
3	3	139	LEU
3	3	219	PRO
4	4	255	SER
4	4	390	VAL
5	5	81	LYS
5	5	111	ALA
5	5	138	PRO
1	A	43	ARG
1	A	314	GLU
3	C	139	LEU
3	C	219	PRO
4	D	255	SER
4	D	390	VAL
5	E	81	LYS
5	E	138	PRO
1	1	292	PRO
1	1	313	TYR
2	2	48	GLU
3	3	54	LEU
3	3	372	GLN
3	3	704	ALA
4	4	211	SER
4	4	381	LEU
5	5	35	LYS
7	9	100	PHE
1	A	292	PRO
1	A	313	TYR
2	B	48	GLU
3	C	54	LEU
3	C	372	GLN
3	C	704	ALA
4	D	211	SER
4	D	381	LEU

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Mol	Chain	Res	Type
5	E	35	LYS
5	E	111	ALA
7	G	100	PHE
1	1	193	GLU
3	3	682	GLU
1	A	193	GLU
3	C	682	GLU
1	1	71	PRO
3	3	457	PRO
8	7	74	PRO
1	A	71	PRO
3	C	457	PRO
8	J	74	PRO
1	1	234	GLY
3	3	453	PRO
3	3	529	GLY
4	4	198	PRO
4	4	212	PRO
4	4	270	GLY
1	A	234	GLY
3	C	453	PRO
3	C	529	GLY
4	D	198	PRO
4	D	270	GLY
3	3	367	PRO
3	3	690	GLY
3	C	367	PRO
3	C	690	GLY
4	D	212	PRO
1	1	3	GLY
3	3	549	VAL
4	4	402	PRO
6	6	100	PRO
6	6	101	ASP
1	A	3	GLY
3	C	549	VAL
4	D	402	PRO
6	F	100	PRO
6	F	101	ASP
3	3	508	GLY
3	C	508	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	355/356 (100%)	316 (89%)	39 (11%)	6	21
1	A	355/356 (100%)	316 (89%)	39 (11%)	6	21
2	2	150/152 (99%)	126 (84%)	24 (16%)	2	12
2	B	150/152 (99%)	126 (84%)	24 (16%)	2	12
3	3	607/628 (97%)	535 (88%)	72 (12%)	5	19
3	C	607/628 (97%)	535 (88%)	72 (12%)	5	19
4	4	325/355 (92%)	288 (89%)	37 (11%)	5	20
4	D	325/355 (92%)	288 (89%)	37 (11%)	5	20
5	5	167/175 (95%)	151 (90%)	16 (10%)	8	25
5	E	167/175 (95%)	151 (90%)	16 (10%)	8	25
6	6	118/149 (79%)	100 (85%)	18 (15%)	3	13
6	F	118/149 (79%)	100 (85%)	18 (15%)	3	13
7	9	126/150 (84%)	112 (89%)	14 (11%)	6	21
7	G	126/150 (84%)	112 (89%)	14 (11%)	6	21
8	7	104/106 (98%)	92 (88%)	12 (12%)	5	19
8	J	104/106 (98%)	92 (88%)	12 (12%)	5	19
All	All	3904/4142 (94%)	3440 (88%)	464 (12%)	5	19

All (464) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	10	ASP
1	1	29	LEU
1	1	49	THR
1	1	104	ARG
1	1	114	LEU
1	1	128	THR
1	1	134	VAL
1	1	144	ARG

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Mol	Chain	Res	Type
1	1	155	ARG
1	1	161	ASN
1	1	168	SER
1	1	171	LEU
1	1	186	THR
1	1	217	THR
1	1	241	MET
1	1	243	THR
1	1	249	MET
1	1	253	GLN
1	1	255	SER
1	1	270	THR
1	1	271	THR
1	1	278	GLU
1	1	290	ILE
1	1	291	ILE
1	1	295	SER
1	1	309	THR
1	1	316	LEU
1	1	323	LEU
1	1	342	TRP
1	1	346	ARG
1	1	357	THR
1	1	363	VAL
1	1	368	VAL
1	1	374	ILE
1	1	388	GLU
1	1	397	ARG
1	1	414	LEU
1	1	419	ASP
1	1	437	TRP
2	2	5	ASP
2	2	7	LYS
2	2	24	ARG
2	2	31	LEU
2	2	35	GLN
2	2	45	ARG
2	2	53	VAL
2	2	61	MET
2	2	87	SER
2	2	89	LYS
2	2	96	LEU

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Mol	Chain	Res	Type
2	2	106	ILE
2	2	114	ASP
2	2	122	VAL
2	2	139	GLU
2	2	140	PRO
2	2	144	CYS
2	2	146	THR
2	2	150	LEU
2	2	153	LEU
2	2	162	ARG
2	2	163	LEU
2	2	172	CYS
2	2	176	VAL
3	3	11	VAL
3	3	23	VAL
3	3	32	LEU
3	3	42	ILE
3	3	55	PRO
3	3	73	ILE
3	3	94	ASP
3	3	121	THR
3	3	123	ASP
3	3	124	LYS
3	3	133	ARG
3	3	135	VAL
3	3	150	GLU
3	3	153	VAL
3	3	168	HIS
3	3	188	VAL
3	3	189	ARG
3	3	192	GLU
3	3	207	VAL
3	3	209	THR
3	3	214	MET
3	3	218	LEU
3	3	219	PRO
3	3	220	SER
3	3	238	LEU
3	3	269	THR
3	3	274	LEU
3	3	275	LEU
3	3	282	VAL

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Mol	Chain	Res	Type
3	3	284	GLU
3	3	303	GLN
3	3	306	LEU
3	3	317	LEU
3	3	337	ARG
3	3	369	LEU
3	3	381	LEU
3	3	399	LEU
3	3	408	ILE
3	3	412	ARG
3	3	417	VAL
3	3	419	ASP
3	3	425	ARG
3	3	435	LEU
3	3	440	ARG
3	3	448	MET
3	3	450	LEU
3	3	464	ILE
3	3	473	GLU
3	3	501	LYS
3	3	507	LEU
3	3	512	LEU
3	3	514	ASP
3	3	515	THR
3	3	523	LEU
3	3	542	ARG
3	3	550	LEU
3	3	587	LEU
3	3	593	LEU
3	3	617	LEU
3	3	644	LEU
3	3	655	ARG
3	3	676	LEU
3	3	683	LEU
3	3	684	ARG
3	3	705	VAL
3	3	715	GLU
3	3	716	LEU
3	3	738	THR
3	3	747	VAL
3	3	771	VAL
3	3	776	LEU

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Mol	Chain	Res	Type
3	3	777	VAL
4	4	40	VAL
4	4	44	MET
4	4	59	ILE
4	4	69	THR
4	4	74	THR
4	4	99	LEU
4	4	104	LEU
4	4	105	LEU
4	4	120	LEU
4	4	129	HIS
4	4	131	VAL
4	4	143	LEU
4	4	152	GLU
4	4	163	VAL
4	4	168	PHE
4	4	170	HIS
4	4	187	VAL
4	4	200	ARG
4	4	201	ILE
4	4	213	ILE
4	4	219	ARG
4	4	230	ILE
4	4	234	LEU
4	4	239	LEU
4	4	262	PHE
4	4	272	VAL
4	4	290	ILE
4	4	296	ARG
4	4	297	LEU
4	4	314	ARG
4	4	317	LEU
4	4	319	THR
4	4	342	VAL
4	4	367	ARG
4	4	369	LYS
4	4	396	ILE
4	4	407	VAL
5	5	5	ARG
5	5	25	LEU
5	5	27	VAL
5	5	38	MET

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Mol	Chain	Res	Type
5	5	52	ILE
5	5	80	TRP
5	5	84	ASP
5	5	90	VAL
5	5	104	VAL
5	5	107	LEU
5	5	141	LEU
5	5	146	LEU
5	5	147	ARG
5	5	154	GLU
5	5	157	THR
5	5	161	GLU
6	6	16	ARG
6	6	19	ILE
6	6	27	LEU
6	6	33	SER
6	6	37	TRP
6	6	40	THR
6	6	45	CYS
6	6	57	ARG
6	6	74	GLN
6	6	83	ARG
6	6	84	LEU
6	6	114	SER
6	6	123	ILE
6	6	131	VAL
6	6	141	PRO
6	6	151	VAL
6	6	153	GLN
6	6	156	LYS
7	9	31	VAL
7	9	33	LEU
7	9	36	ARG
7	9	42	VAL
7	9	50	LEU
7	9	58	LEU
7	9	85	GLU
7	9	97	ARG
7	9	99	ILE
7	9	101	CYS
7	9	139	ASP
7	9	140	VAL

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Mol	Chain	Res	Type
7	9	157	VAL
7	9	159	VAL
8	7	21	ARG
8	7	39	ASP
8	7	43	ARG
8	7	44	MET
8	7	50	LEU
8	7	52	THR
8	7	54	ILE
8	7	63	LEU
8	7	78	LYS
8	7	82	ILE
8	7	85	ARG
8	7	92	HIS
1	A	10	ASP
1	A	29	LEU
1	A	49	THR
1	A	104	ARG
1	A	114	LEU
1	A	128	THR
1	A	134	VAL
1	A	144	ARG
1	A	155	ARG
1	A	161	ASN
1	A	168	SER
1	A	171	LEU
1	A	186	THR
1	A	217	THR
1	A	241	MET
1	A	243	THR
1	A	249	MET
1	A	253	GLN
1	A	255	SER
1	A	270	THR
1	A	271	THR
1	A	278	GLU
1	A	290	ILE
1	A	291	ILE
1	A	295	SER
1	A	309	THR
1	A	316	LEU
1	A	323	LEU

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Mol	Chain	Res	Type
1	A	342	TRP
1	A	346	ARG
1	A	357	THR
1	A	363	VAL
1	A	368	VAL
1	A	374	ILE
1	A	388	GLU
1	A	397	ARG
1	A	414	LEU
1	A	419	ASP
1	A	437	TRP
2	B	5	ASP
2	B	7	LYS
2	B	24	ARG
2	B	31	LEU
2	B	35	GLN
2	B	45	ARG
2	B	53	VAL
2	B	61	MET
2	B	87	SER
2	B	89	LYS
2	B	96	LEU
2	B	106	ILE
2	B	114	ASP
2	B	122	VAL
2	B	139	GLU
2	B	140	PRO
2	B	144	CYS
2	B	146	THR
2	B	150	LEU
2	B	153	LEU
2	B	162	ARG
2	B	163	LEU
2	B	172	CYS
2	B	176	VAL
3	C	11	VAL
3	C	23	VAL
3	C	32	LEU
3	C	42	ILE
3	C	55	PRO
3	C	73	ILE
3	C	94	ASP

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Mol	Chain	Res	Type
3	C	121	THR
3	C	123	ASP
3	C	124	LYS
3	C	133	ARG
3	C	135	VAL
3	C	150	GLU
3	C	153	VAL
3	C	168	HIS
3	C	188	VAL
3	C	189	ARG
3	C	192	GLU
3	C	207	VAL
3	C	209	THR
3	C	214	MET
3	C	218	LEU
3	C	219	PRO
3	C	220	SER
3	C	238	LEU
3	C	269	THR
3	C	274	LEU
3	C	275	LEU
3	C	282	VAL
3	C	284	GLU
3	C	303	GLN
3	C	306	LEU
3	C	317	LEU
3	C	337	ARG
3	C	369	LEU
3	C	381	LEU
3	C	399	LEU
3	C	408	ILE
3	C	412	ARG
3	C	417	VAL
3	C	419	ASP
3	C	425	ARG
3	C	435	LEU
3	C	440	ARG
3	C	448	MET
3	C	450	LEU
3	C	464	ILE
3	C	473	GLU
3	C	501	LYS

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Mol	Chain	Res	Type
3	C	507	LEU
3	C	512	LEU
3	C	514	ASP
3	C	515	THR
3	C	523	LEU
3	C	542	ARG
3	C	550	LEU
3	C	587	LEU
3	C	593	LEU
3	C	617	LEU
3	C	644	LEU
3	C	655	ARG
3	C	676	LEU
3	C	683	LEU
3	C	684	ARG
3	C	705	VAL
3	C	715	GLU
3	C	716	LEU
3	C	738	THR
3	C	747	VAL
3	C	771	VAL
3	C	776	LEU
3	C	777	VAL
4	D	40	VAL
4	D	44	MET
4	D	59	ILE
4	D	69	THR
4	D	74	THR
4	D	99	LEU
4	D	104	LEU
4	D	105	LEU
4	D	120	LEU
4	D	129	HIS
4	D	131	VAL
4	D	143	LEU
4	D	152	GLU
4	D	163	VAL
4	D	168	PHE
4	D	170	HIS
4	D	187	VAL
4	D	200	ARG
4	D	201	ILE

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Mol	Chain	Res	Type
4	D	213	ILE
4	D	219	ARG
4	D	230	ILE
4	D	234	LEU
4	D	239	LEU
4	D	262	PHE
4	D	272	VAL
4	D	290	ILE
4	D	296	ARG
4	D	297	LEU
4	D	314	ARG
4	D	317	LEU
4	D	319	THR
4	D	342	VAL
4	D	367	ARG
4	D	369	LYS
4	D	396	ILE
4	D	407	VAL
5	E	5	ARG
5	E	25	LEU
5	E	27	VAL
5	E	38	MET
5	E	52	ILE
5	E	80	TRP
5	E	84	ASP
5	E	90	VAL
5	E	104	VAL
5	E	107	LEU
5	E	141	LEU
5	E	146	LEU
5	E	147	ARG
5	E	154	GLU
5	E	157	THR
5	E	161	GLU
6	F	16	ARG
6	F	19	ILE
6	F	27	LEU
6	F	33	SER
6	F	37	TRP
6	F	40	THR
6	F	45	CYS
6	F	57	ARG

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Mol	Chain	Res	Type
6	F	74	GLN
6	F	83	ARG
6	F	84	LEU
6	F	114	SER
6	F	123	ILE
6	F	131	VAL
6	F	141	PRO
6	F	151	VAL
6	F	153	GLN
6	F	156	LYS
7	G	31	VAL
7	G	33	LEU
7	G	36	ARG
7	G	42	VAL
7	G	50	LEU
7	G	58	LEU
7	G	85	GLU
7	G	97	ARG
7	G	99	ILE
7	G	101	CYS
7	G	139	ASP
7	G	140	VAL
7	G	157	VAL
7	G	159	VAL
8	J	21	ARG
8	J	39	ASP
8	J	43	ARG
8	J	44	MET
8	J	50	LEU
8	J	52	THR
8	J	54	ILE
8	J	63	LEU
8	J	78	LYS
8	J	82	ILE
8	J	85	ARG
8	J	92	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	92	ASN
1	1	220	ASN

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Mol	Chain	Res	Type
2	2	120	GLN
2	2	135	GLN
3	3	38	HIS
3	3	168	HIS
3	3	246	ASN
3	3	368	HIS
3	3	410	HIS
3	3	661	GLN
3	3	702	HIS
3	3	749	HIS
4	4	292	GLN
4	4	327	HIS
4	4	330	HIS
4	4	336	HIS
4	4	377	ASN
5	5	129	HIS
5	5	144	HIS
6	6	153	GLN
7	9	38	HIS
7	9	46	HIS
8	7	92	HIS
1	A	92	ASN
1	A	220	ASN
2	B	120	GLN
2	B	135	GLN
3	C	38	HIS
3	C	168	HIS
3	C	246	ASN
3	C	368	HIS
3	C	410	HIS
3	C	661	GLN
3	C	702	HIS
3	C	749	HIS
4	D	292	GLN
4	D	327	HIS
4	D	330	HIS
4	D	336	HIS
4	D	377	ASN
5	E	129	HIS
5	E	144	HIS
6	F	98	GLN
6	F	153	GLN

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Mol	Chain	Res	Type
7	G	38	HIS
7	G	46	HIS
8	J	92	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	SF4	G	183	7	0,12,12	-	-	-		
14	SF4	C	784	3	0,12,12	-	-	-		
14	SF4	9	183	7	0,12,12	-	-	-		
14	SF4	C	785	3	0,12,12	-	-	-		
14	SF4	C	786	3	0,12,12	-	-	-		
16	FES	3	787	3	0,4,4	-	-	-		
15	FMN	1	440	-	33,33,33	1.33	3 (9%)	48,50,50	1.61	15 (31%)
14	SF4	6	182	6	0,12,12	-	-	-		
14	SF4	F	182	6	0,12,12	-	-	-		
16	FES	B	182	2	0,4,4	-	-	-		
14	SF4	A	439	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	SF4	G	184	7	0,12,12	-	-	-		
14	SF4	3	786	3	0,12,12	-	-	-		
14	SF4	9	184	7	0,12,12	-	-	-		
14	SF4	3	785	3	0,12,12	-	-	-		
16	FES	C	787	3	0,4,4	-	-	-		
14	SF4	3	784	3	0,12,12	-	-	-		
16	FES	2	182	2	0,4,4	-	-	-		
15	FMN	A	440	-	33,33,33	1.33	3 (9%)	48,50,50	1.61	15 (31%)
14	SF4	1	439	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	G	183	7	-	-	0/6/5/5
14	SF4	C	784	3	-	-	0/6/5/5
14	SF4	9	183	7	-	-	0/6/5/5
14	SF4	C	785	3	-	-	0/6/5/5
14	SF4	C	786	3	-	-	0/6/5/5
16	FES	3	787	3	-	-	0/1/1/1
15	FMN	1	440	-	-	10/18/18/18	0/3/3/3
14	SF4	6	182	6	-	-	0/6/5/5
14	SF4	F	182	6	-	-	0/6/5/5
16	FES	B	182	2	-	-	0/1/1/1
14	SF4	A	439	1	-	-	0/6/5/5
14	SF4	G	184	7	-	-	0/6/5/5
14	SF4	3	786	3	-	-	0/6/5/5
14	SF4	9	184	7	-	-	0/6/5/5
14	SF4	3	785	3	-	-	0/6/5/5
16	FES	C	787	3	-	-	0/1/1/1
14	SF4	3	784	3	-	-	0/6/5/5
16	FES	2	182	2	-	-	0/1/1/1
15	FMN	A	440	-	-	10/18/18/18	0/3/3/3
14	SF4	1	439	1	-	-	0/6/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	440	FMN	C4A-N5	3.55	1.38	1.30
15	A	440	FMN	C4A-N5	3.52	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	440	FMN	C9A-N10	-3.22	1.35	1.41
15	1	440	FMN	C9A-N10	-3.18	1.35	1.41
15	1	440	FMN	C4A-C10	-2.15	1.37	1.44
15	A	440	FMN	C4A-C10	-2.14	1.37	1.44

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	440	FMN	C4-N3-C2	-3.00	120.32	125.64
15	1	440	FMN	O4'-C4'-C3'	-3.00	102.23	109.25
15	A	440	FMN	O4'-C4'-C3'	-2.99	102.25	109.25
15	1	440	FMN	C4-N3-C2	-2.97	120.36	125.64
15	A	440	FMN	O4'-C4'-C5'	-2.72	103.99	109.99
15	1	440	FMN	O4'-C4'-C5'	-2.71	104.00	109.99
15	A	440	FMN	O2'-C2'-C3'	2.70	115.57	109.25
15	1	440	FMN	O2'-C2'-C3'	2.69	115.55	109.25
15	1	440	FMN	C9-C9A-N10	-2.67	118.26	121.85
15	A	440	FMN	C9-C9A-N10	-2.66	118.28	121.85
15	A	440	FMN	C9A-C5A-N5	-2.59	119.71	122.45
15	A	440	FMN	C4A-C4-N3	2.58	119.82	113.25
15	1	440	FMN	C4A-C4-N3	2.57	119.79	113.25
15	1	440	FMN	C9A-C5A-N5	-2.57	119.73	122.45
15	A	440	FMN	O4-C4-C4A	-2.53	119.84	126.53
15	1	440	FMN	O4-C4-C4A	-2.52	119.88	126.53
15	1	440	FMN	C4A-C10-N10	2.48	120.03	116.48
15	A	440	FMN	C4A-C10-N10	2.46	120.01	116.48
15	1	440	FMN	C10-C4A-N5	-2.41	119.88	124.81
15	1	440	FMN	C5A-C9A-N10	2.41	120.15	117.97
15	A	440	FMN	C5A-C9A-N10	2.41	120.15	117.97
15	A	440	FMN	C10-C4A-N5	-2.41	119.88	124.81
15	A	440	FMN	C4-C4A-N5	2.41	121.53	118.21
15	1	440	FMN	C4-C4A-N5	2.40	121.52	118.21
15	1	440	FMN	O2-C2-N1	-2.33	117.92	121.80
15	A	440	FMN	O2-C2-N1	-2.32	117.94	121.80
15	1	440	FMN	C5'-C4'-C3'	2.07	116.12	112.22
15	A	440	FMN	C5'-C4'-C3'	2.05	116.08	112.22
15	1	440	FMN	O3'-C3'-C4'	2.04	113.57	108.93
15	A	440	FMN	O3'-C3'-C4'	2.03	113.55	108.93

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	1	440	FMN	N10-C1'-C2'-O2'
15	1	440	FMN	N10-C1'-C2'-C3'
15	1	440	FMN	C3'-C4'-C5'-O5'
15	1	440	FMN	O4'-C4'-C5'-O5'
15	A	440	FMN	N10-C1'-C2'-O2'
15	A	440	FMN	N10-C1'-C2'-C3'
15	A	440	FMN	C3'-C4'-C5'-O5'
15	A	440	FMN	O4'-C4'-C5'-O5'
15	1	440	FMN	O2'-C2'-C3'-C4'
15	A	440	FMN	O2'-C2'-C3'-C4'
15	1	440	FMN	C2'-C3'-C4'-O4'
15	A	440	FMN	C2'-C3'-C4'-O4'
15	1	440	FMN	O2'-C2'-C3'-O3'
15	A	440	FMN	O2'-C2'-C3'-O3'
15	1	440	FMN	C4'-C5'-O5'-P
15	A	440	FMN	C4'-C5'-O5'-P
15	1	440	FMN	C1'-C2'-C3'-O3'
15	A	440	FMN	C1'-C2'-C3'-O3'
15	1	440	FMN	O3'-C3'-C4'-O4'
15	A	440	FMN	O3'-C3'-C4'-O4'

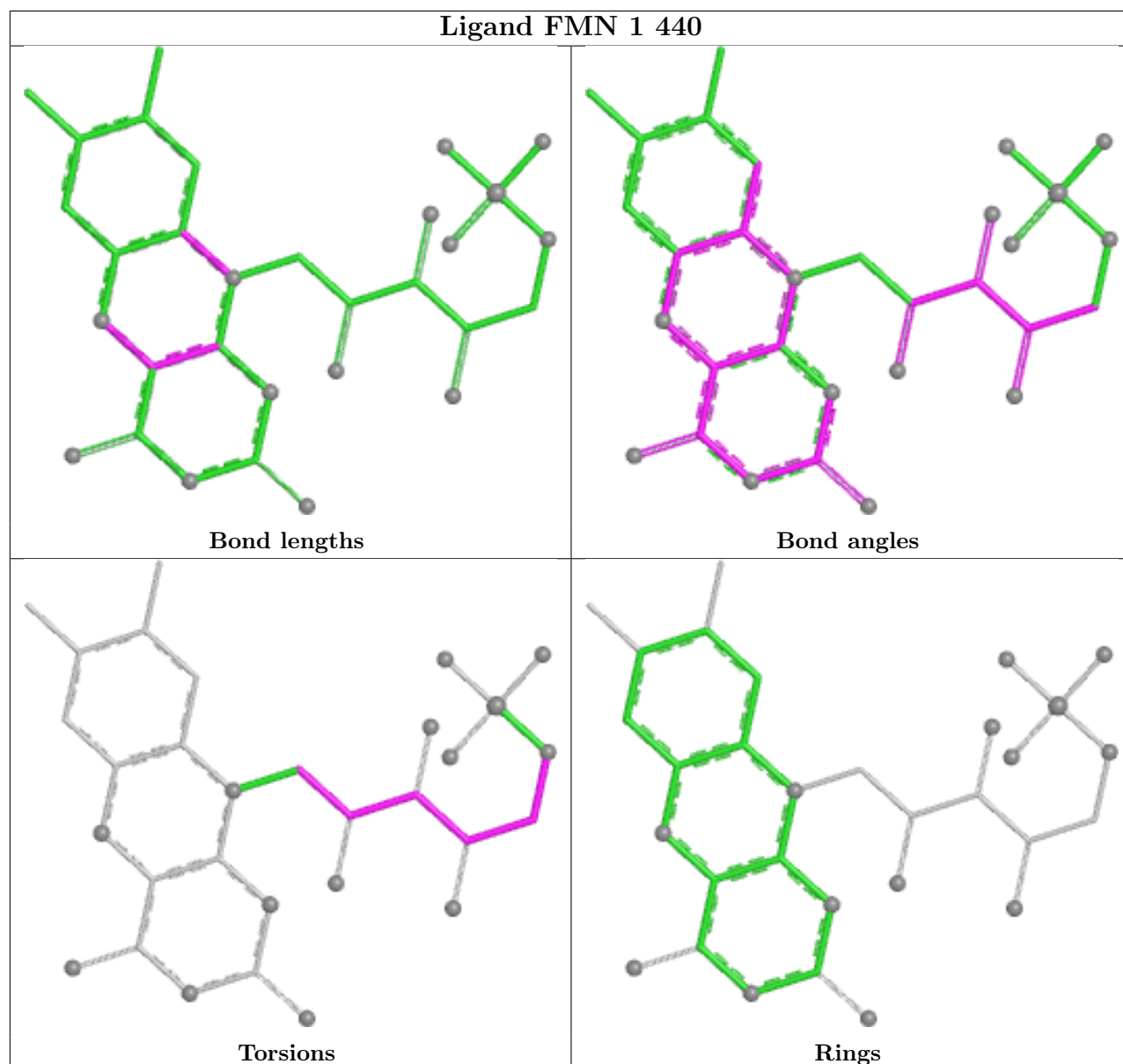
There are no ring outliers.

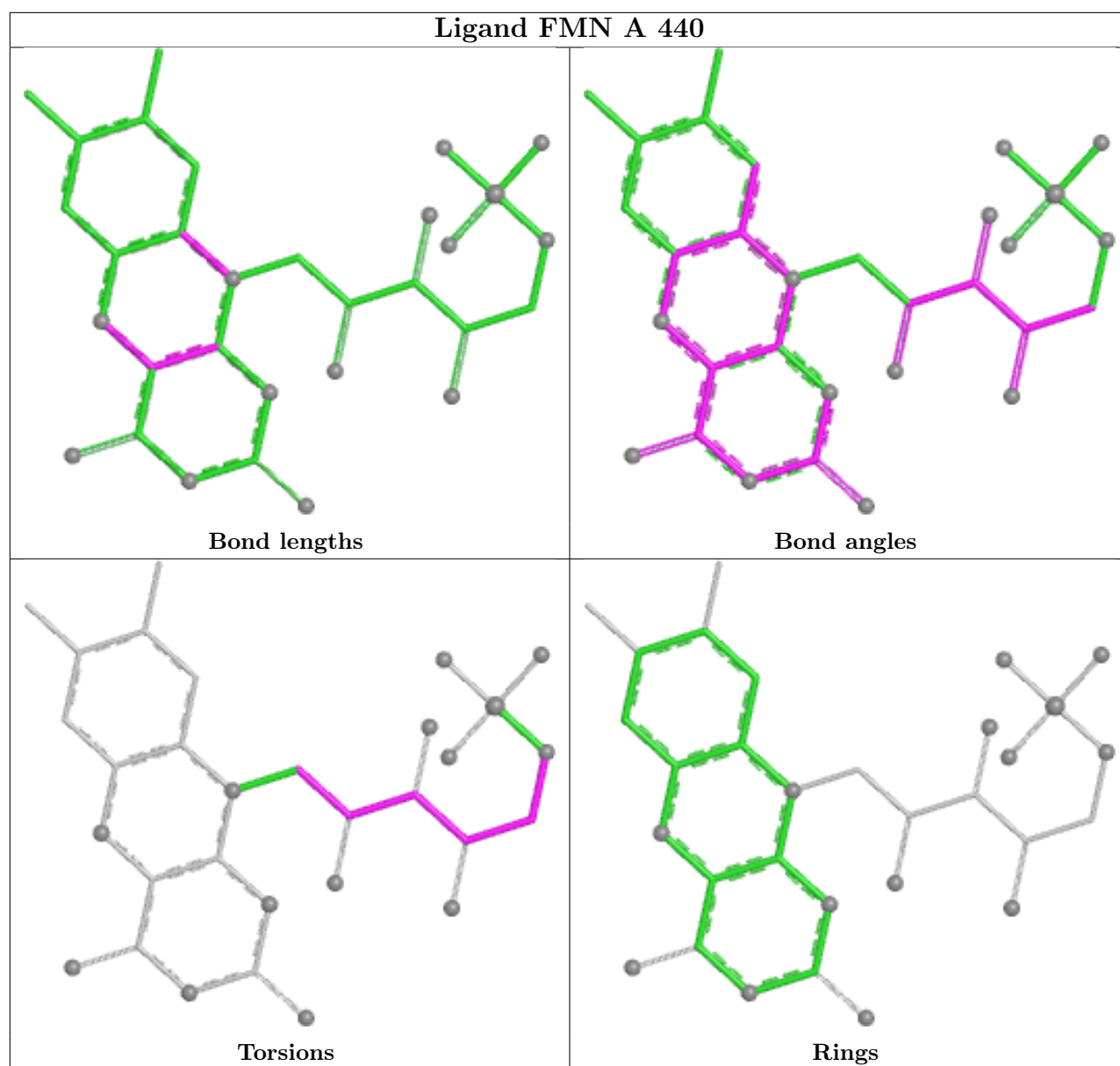
14 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	784	SF4	3	0
14	C	785	SF4	1	0
14	C	786	SF4	3	0
16	3	787	FES	1	0
15	1	440	FMN	8	0
14	6	182	SF4	4	0
14	F	182	SF4	4	0
14	A	439	SF4	2	0
14	3	786	SF4	4	0
14	3	785	SF4	1	0
16	C	787	FES	1	0
14	3	784	SF4	3	0
15	A	440	FMN	8	0
14	1	439	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	L	20
9	O	20
10	M	16

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Mol	Chain	Number of breaks
10	P	16
11	N	16
11	Q	16
12	R	10
12	S	10
13	H	8
13	T	8

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	428:UNK	C	495:UNK	N	56.90
1	O	428:UNK	C	495:UNK	N	56.90
1	M	1024:UNK	C	1050:UNK	N	55.04
1	P	1024:UNK	C	1050:UNK	N	55.04
1	N	366:UNK	C	395:UNK	N	50.88
1	Q	366:UNK	C	395:UNK	N	50.88
1	L	1417:UNK	C	1501:UNK	N	47.71
1	O	1417:UNK	C	1501:UNK	N	47.71
1	N	665:UNK	C	700:UNK	N	47.65
1	Q	665:UNK	C	700:UNK	N	47.65
1	N	524:UNK	C	601:UNK	N	47.16
1	Q	524:UNK	C	601:UNK	N	47.16
1	L	1326:UNK	C	1401:UNK	N	46.61
1	O	1326:UNK	C	1401:UNK	N	46.60
1	N	428:UNK	C	501:UNK	N	46.47
1	Q	428:UNK	C	501:UNK	N	46.47
1	M	1328:UNK	C	1399:UNK	N	43.88
1	P	1328:UNK	C	1399:UNK	N	43.88
1	M	829:UNK	C	899:UNK	N	43.18
1	P	829:UNK	C	899:UNK	N	43.18
1	N	1222:UNK	C	1295:UNK	N	42.97
1	Q	1222:UNK	C	1295:UNK	N	42.97
1	M	520:UNK	C	601:UNK	N	42.94
1	P	520:UNK	C	601:UNK	N	42.94
1	H	625:UNK	C	700:UNK	N	42.29
1	T	625:UNK	C	700:UNK	N	42.29
1	R	725:UNK	C	800:UNK	N	42.19
1	S	725:UNK	C	800:UNK	N	42.19
1	N	923:UNK	C	1001:UNK	N	41.07
1	Q	923:UNK	C	1001:UNK	N	41.07
1	R	524:UNK	C	603:UNK	N	40.88
1	S	524:UNK	C	603:UNK	N	40.88

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	1022:UNK	C	1050:UNK	N	40.59
1	O	1022:UNK	C	1050:UNK	N	40.59
1	L	520:UNK	C	601:UNK	N	40.17
1	O	520:UNK	C	601:UNK	N	40.17
1	M	228:UNK	C	301:UNK	N	39.55
1	P	228:UNK	C	301:UNK	N	39.55
1	L	922:UNK	C	1003:UNK	N	39.30
1	O	922:UNK	C	1003:UNK	N	39.30
1	N	1059:UNK	C	1096:UNK	N	38.87
1	Q	1059:UNK	C	1096:UNK	N	38.87
1	R	624:UNK	C	702:UNK	N	37.28
1	S	624:UNK	C	702:UNK	N	37.28
1	N	226:UNK	C	301:UNK	N	37.24
1	Q	226:UNK	C	301:UNK	N	37.24
1	L	229:UNK	C	301:UNK	N	36.09
1	O	229:UNK	C	301:UNK	N	36.09
1	N	1022:UNK	C	1050:UNK	N	35.98
1	Q	1022:UNK	C	1050:UNK	N	35.98
1	R	820:UNK	C	900:UNK	N	35.39
1	S	820:UNK	C	900:UNK	N	35.39
1	H	322:UNK	C	400:UNK	N	34.95
1	T	322:UNK	C	400:UNK	N	34.95
1	M	923:UNK	C	1002:UNK	N	34.04
1	P	923:UNK	C	1002:UNK	N	34.04
1	L	360:UNK	C	401:UNK	N	33.91
1	O	360:UNK	C	401:UNK	N	33.91
1	N	723:UNK	C	801:UNK	N	33.47
1	Q	723:UNK	C	801:UNK	N	33.47
1	H	718:UNK	C	800:UNK	N	31.72
1	T	718:UNK	C	800:UNK	N	31.72
1	M	1065:UNK	C	1100:UNK	N	30.93
1	P	1065:UNK	C	1100:UNK	N	30.93
1	H	130:UNK	C	201:UNK	N	29.78
1	T	130:UNK	C	201:UNK	N	29.78
1	N	121:UNK	C	202:UNK	N	29.63
1	Q	121:UNK	C	202:UNK	N	29.63
1	M	123:UNK	C	201:UNK	N	28.64
1	P	123:UNK	C	201:UNK	N	28.64
1	L	1061:UNK	C	1101:UNK	N	28.15
1	O	1061:UNK	C	1101:UNK	N	28.15
1	H	414:UNK	C	500:UNK	N	25.75
1	T	414:UNK	C	500:UNK	N	25.75

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	424:UNK	C	495:UNK	N	16.18
1	P	424:UNK	C	495:UNK	N	16.18
1	L	824:UNK	C	901:UNK	N	15.99
1	O	824:UNK	C	901:UNK	N	15.99
1	M	367:UNK	C	398:UNK	N	15.97
1	P	367:UNK	C	398:UNK	N	15.97
1	L	666:UNK	C	704:UNK	N	15.22
1	O	666:UNK	C	704:UNK	N	15.22
1	P	1121:UNK	C	1200:UNK	N	14.33
1	M	1121:UNK	C	1200:UNK	N	14.32
1	L	732:UNK	C	802:UNK	N	14.14
1	O	732:UNK	C	802:UNK	N	14.14
1	H	219:UNK	C	300:UNK	N	13.65
1	T	219:UNK	C	300:UNK	N	13.65
1	N	823:UNK	C	903:UNK	N	13.62
1	Q	823:UNK	C	903:UNK	N	13.62
1	M	734:UNK	C	800:UNK	N	12.90
1	P	734:UNK	C	800:UNK	N	12.90
1	R	919:UNK	C	997:UNK	N	12.22
1	S	919:UNK	C	997:UNK	N	12.22
1	R	125:UNK	C	202:UNK	N	11.40
1	S	125:UNK	C	202:UNK	N	11.40
1	M	1222:UNK	C	1300:UNK	N	11.26
1	P	1222:UNK	C	1300:UNK	N	11.26
1	L	613:UNK	C	650:UNK	N	11.20
1	O	613:UNK	C	650:UNK	N	11.20
1	N	1122:UNK	C	1200:UNK	N	11.16
1	Q	1122:UNK	C	1200:UNK	N	11.16
1	N	1320:UNK	C	1401:UNK	N	11.09
1	Q	1320:UNK	C	1401:UNK	N	11.09
1	R	423:UNK	C	494:UNK	N	10.86
1	S	423:UNK	C	494:UNK	N	10.86
1	M	663:UNK	C	704:UNK	N	10.34
1	P	663:UNK	C	704:UNK	N	10.34
1	N	615:UNK	C	650:UNK	N	10.27
1	Q	615:UNK	C	650:UNK	N	10.27
1	L	1123:UNK	C	1195:UNK	N	9.83
1	O	1123:UNK	C	1195:UNK	N	9.82
1	L	127:UNK	C	201:UNK	N	9.74
1	O	127:UNK	C	201:UNK	N	9.74
1	R	324:UNK	C	397:UNK	N	9.72
1	S	324:UNK	C	397:UNK	N	9.72

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	615:UNK	C	650:UNK	N	9.60
1	P	615:UNK	C	650:UNK	N	9.60
1	H	520:UNK	C	600:UNK	N	9.55
1	T	520:UNK	C	600:UNK	N	9.55
1	L	1218:UNK	C	1298:UNK	N	9.44
1	O	1218:UNK	C	1298:UNK	N	9.44
1	L	1563:UNK	C	1569:UNK	N	9.11
1	O	1563:UNK	C	1569:UNK	N	9.11
1	R	223:UNK	C	295:UNK	N	8.96
1	S	223:UNK	C	295:UNK	N	8.96
1	L	311:UNK	C	350:UNK	N	6.99
1	O	311:UNK	C	350:UNK	N	6.99
1	N	313:UNK	C	350:UNK	N	6.87
1	Q	313:UNK	C	350:UNK	N	6.87
1	R	1021:UNK	C	1098:UNK	N	6.64
1	S	1021:UNK	C	1098:UNK	N	6.64
1	L	1543:UNK	C	1545:UNK	N	5.82
1	O	1543:UNK	C	1545:UNK	N	5.82
1	M	313:UNK	C	350:UNK	N	5.71
1	P	313:UNK	C	350:UNK	N	5.71
1	H	812:UNK	C	820:UNK	N	4.89
1	T	812:UNK	C	820:UNK	N	4.88
1	L	1595:UNK	C	1601:UNK	N	4.61
1	O	1595:UNK	C	1601:UNK	N	4.61

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	437/438 (99%)	-0.28	9 (2%) 63 50	80, 80, 80, 80	0
1	A	437/438 (99%)	-0.39	6 (1%) 73 58	80, 80, 80, 80	0
2	2	178/181 (98%)	-0.40	2 (1%) 78 63	80, 80, 80, 80	0
2	B	178/181 (98%)	-0.46	5 (2%) 55 43	80, 80, 80, 80	0
3	3	754/783 (96%)	-0.40	10 (1%) 75 60	80, 80, 80, 80	0
3	C	754/783 (96%)	-0.34	12 (1%) 70 55	80, 80, 80, 80	0
4	4	377/409 (92%)	-0.26	10 (2%) 56 44	80, 80, 80, 80	0
4	D	377/409 (92%)	-0.33	9 (2%) 59 47	80, 80, 80, 80	0
5	5	196/207 (94%)	-0.35	3 (1%) 72 57	80, 80, 80, 80	0
5	E	196/207 (94%)	-0.32	2 (1%) 79 64	80, 80, 80, 80	0
6	6	145/181 (80%)	0.01	8 (5%) 30 29	80, 80, 80, 80	0
6	F	145/181 (80%)	-0.24	3 (2%) 63 50	80, 80, 80, 80	0
7	9	154/182 (84%)	-0.13	4 (2%) 57 44	80, 80, 80, 80	0
7	G	154/182 (84%)	-0.16	7 (4%) 38 34	80, 80, 80, 80	0
8	7	127/129 (98%)	-0.41	0 100 100	80, 80, 80, 80	0
8	J	127/129 (98%)	-0.50	3 (2%) 59 47	80, 80, 80, 80	0
9	L	0/469	-	-	-	-
9	O	0/469	-	-	-	-
10	M	0/392	-	-	-	-
10	P	0/392	-	-	-	-
11	N	0/379	-	-	-	-
11	Q	0/379	-	-	-	-
12	R	0/274	-	-	-	-
12	S	0/274	-	-	-	-
13	H	0/181	-	-	-	-
13	T	0/181	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	4736/8410 (56%)	-0.33	93 (1%)	65 51	80, 80, 80, 80	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	4	144	THR	11.6
1	1	165	THR	9.0
6	6	18	GLY	7.6
4	4	245	ASN	7.0
7	9	72	PRO	6.7
4	4	216	GLU	6.5
4	D	142	ALA	6.2
4	D	184	GLU	5.4
6	F	16	ARG	5.3
6	6	16	ARG	5.2
2	B	123	GLU	5.2
2	B	54	GLY	5.0
3	3	219	PRO	5.0
7	G	141	VAL	4.9
5	E	132	LEU	4.9
7	9	78	GLU	4.6
6	6	17	GLU	4.5
1	A	160	LYS	4.5
5	5	139	GLU	4.4
4	4	56	VAL	4.4
3	C	541	ALA	4.4
7	G	142	GLY	4.3
6	6	160	GLY	4.2
7	G	147	ARG	4.2
3	C	10	ILE	4.0
2	2	180	GLU	3.9
1	A	244	GLU	3.9
4	D	145	PRO	3.7
1	A	164	GLY	3.6
4	4	145	PRO	3.4
3	C	153	VAL	3.4
1	1	183	GLY	3.3
3	3	36	GLU	3.3
3	C	574	GLU	3.3
6	6	26	LYS	3.2
1	1	70	PHE	3.2
7	G	140	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
3	3	336	ALA	3.2
2	B	94	GLU	3.2
6	6	54	THR	3.2
1	1	39	GLU	3.1
3	C	538	ALA	3.1
7	9	83	ALA	3.1
1	1	46	LYS	3.0
8	J	21	ARG	3.0
4	D	144	THR	3.0
3	3	307	LYS	2.7
4	D	206	ALA	2.7
3	C	485	GLU	2.7
1	1	94	ASP	2.7
1	A	8	GLY	2.7
2	B	32	ARG	2.7
1	1	166	ASP	2.6
3	3	319	GLU	2.6
1	1	416	HIS	2.6
4	D	27	THR	2.6
4	D	376	VAL	2.6
8	J	95	ALA	2.6
7	G	146	GLN	2.6
6	6	40	THR	2.6
3	C	551	PRO	2.5
5	5	132	LEU	2.5
3	C	206	GLY	2.5
5	E	59	THR	2.5
4	4	210	GLU	2.5
3	3	217	GLY	2.5
8	J	96	HIS	2.4
4	4	171	ASN	2.4
6	6	169	ARG	2.4
4	D	216	GLU	2.4
3	3	349	ALA	2.4
7	G	73	ALA	2.3
6	F	43	LEU	2.3
1	1	47	GLU	2.3
1	A	395	GLU	2.3
1	A	325	THR	2.3
2	B	118	SER	2.3
3	3	121	THR	2.3
3	C	102	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
5	5	133	ARG	2.2
4	4	295	GLU	2.2
2	2	147	ARG	2.2
6	F	17	GLU	2.2
3	3	745	ALA	2.2
3	3	221	GLY	2.1
3	C	766	ALA	2.1
7	9	46	HIS	2.1
4	4	142	ALA	2.1
3	C	371	PHE	2.0
7	G	173	PHE	2.0
4	4	206	ALA	2.0
4	D	133	LEU	2.0
3	C	711	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

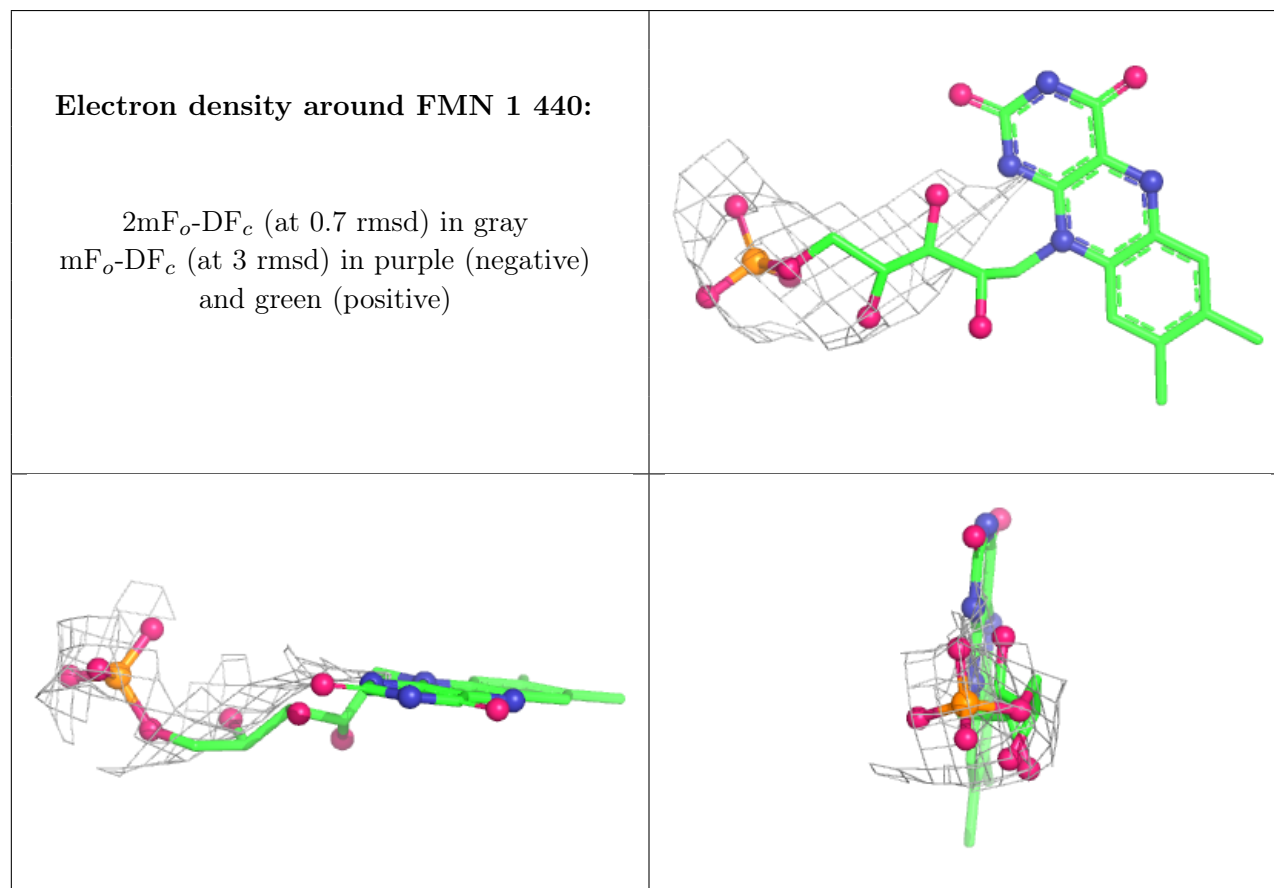
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	FMN	1	440	31/31	0.98	0.11	80,80,80,80	0
14	SF4	9	184	8/8	0.99	0.04	80,80,80,80	0
14	SF4	3	786	8/8	0.99	0.05	80,80,80,80	0
15	FMN	A	440	31/31	0.99	0.06	80,80,80,80	0
14	SF4	6	182	8/8	1.00	0.06	80,80,80,80	0
14	SF4	9	183	8/8	1.00	0.02	80,80,80,80	0
14	SF4	3	784	8/8	1.00	0.06	80,80,80,80	0
14	SF4	A	439	8/8	1.00	0.03	80,80,80,80	0
14	SF4	C	784	8/8	1.00	0.04	80,80,80,80	0

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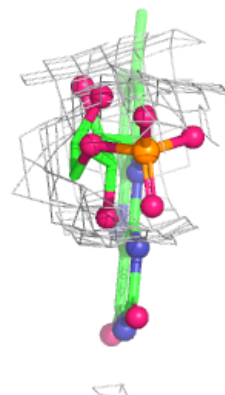
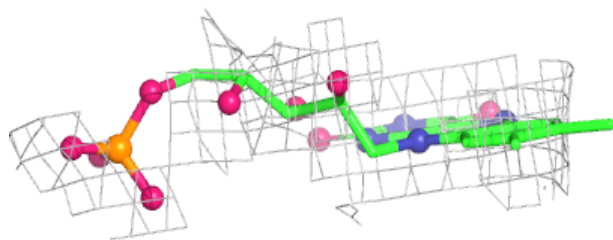
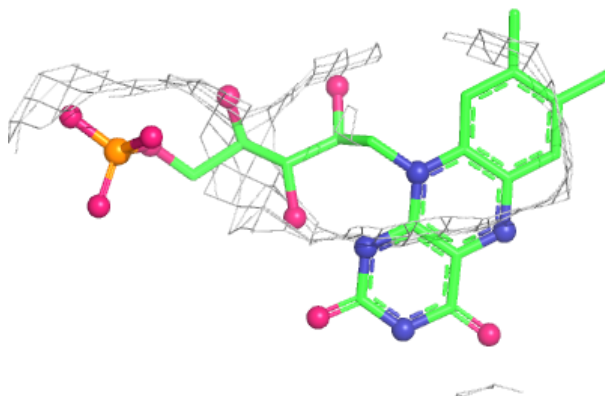
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	SF4	C	785	8/8	1.00	0.04	80,80,80,80	0
14	SF4	C	786	8/8	1.00	0.04	80,80,80,80	0
14	SF4	F	182	8/8	1.00	0.02	80,80,80,80	0
14	SF4	G	183	8/8	1.00	0.03	80,80,80,80	0
14	SF4	G	184	8/8	1.00	0.03	80,80,80,80	0
14	SF4	3	785	8/8	1.00	0.03	80,80,80,80	0
14	SF4	1	439	8/8	1.00	0.04	80,80,80,80	0
16	FES	2	182	4/4	1.00	0.03	80,80,80,80	0
16	FES	3	787	4/4	1.00	0.06	80,80,80,80	0
16	FES	B	182	4/4	1.00	0.02	80,80,80,80	0
16	FES	C	787	4/4	1.00	0.02	80,80,80,80	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around FMN A 440:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.