



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:51 AM UTC

PDB ID : 1BR2 / pdb_00001br2
Title : SMOOTH MUSCLE MYOSIN MOTOR DOMAIN COMPLEXED WITH
MGADP.ALF4
Authors : Dominguez, R.; Trybus, K.M.; Cohen, C.
Deposited on : 1998-08-26
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

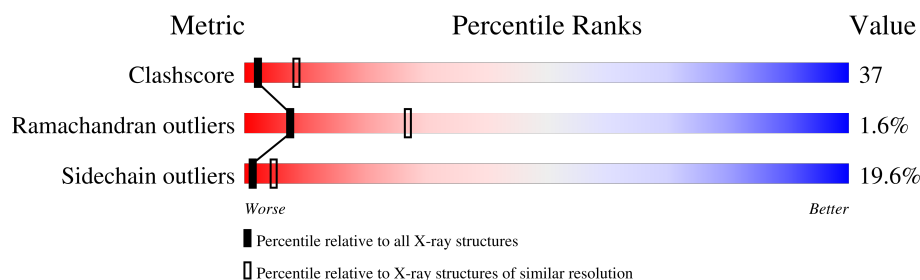
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	791	
1	B	791	
1	C	791	
1	D	791	
1	E	791	
1	F	791	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ALF	D	999	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31830 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.

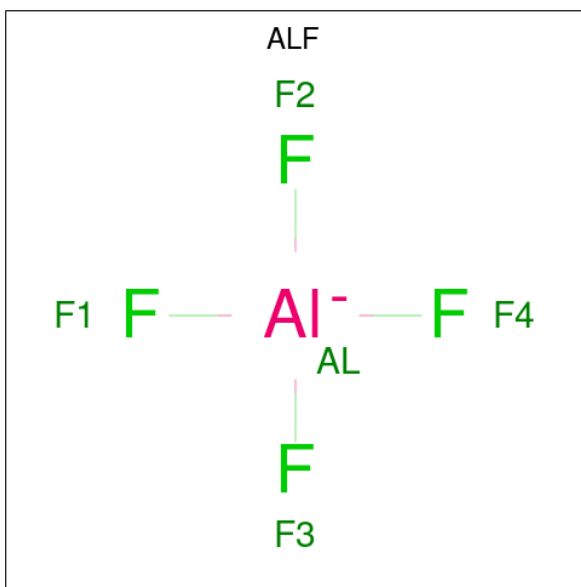
- Molecule 1 is a protein called MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			
1	B	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			
1	C	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			
1	D	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			
1	E	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			
1	F	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

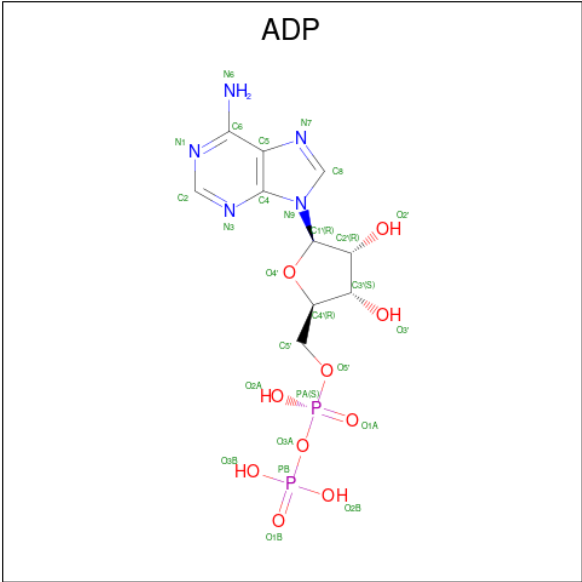
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		
3	B	1	Total	Al	F	0	0
			5	1	4		
3	C	1	Total	Al	F	0	0
			5	1	4		
3	D	1	Total	Al	F	0	0
			5	1	4		
3	E	1	Total	Al	F	0	0
			5	1	4		
3	F	1	Total	Al	F	0	0
			5	1	4		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

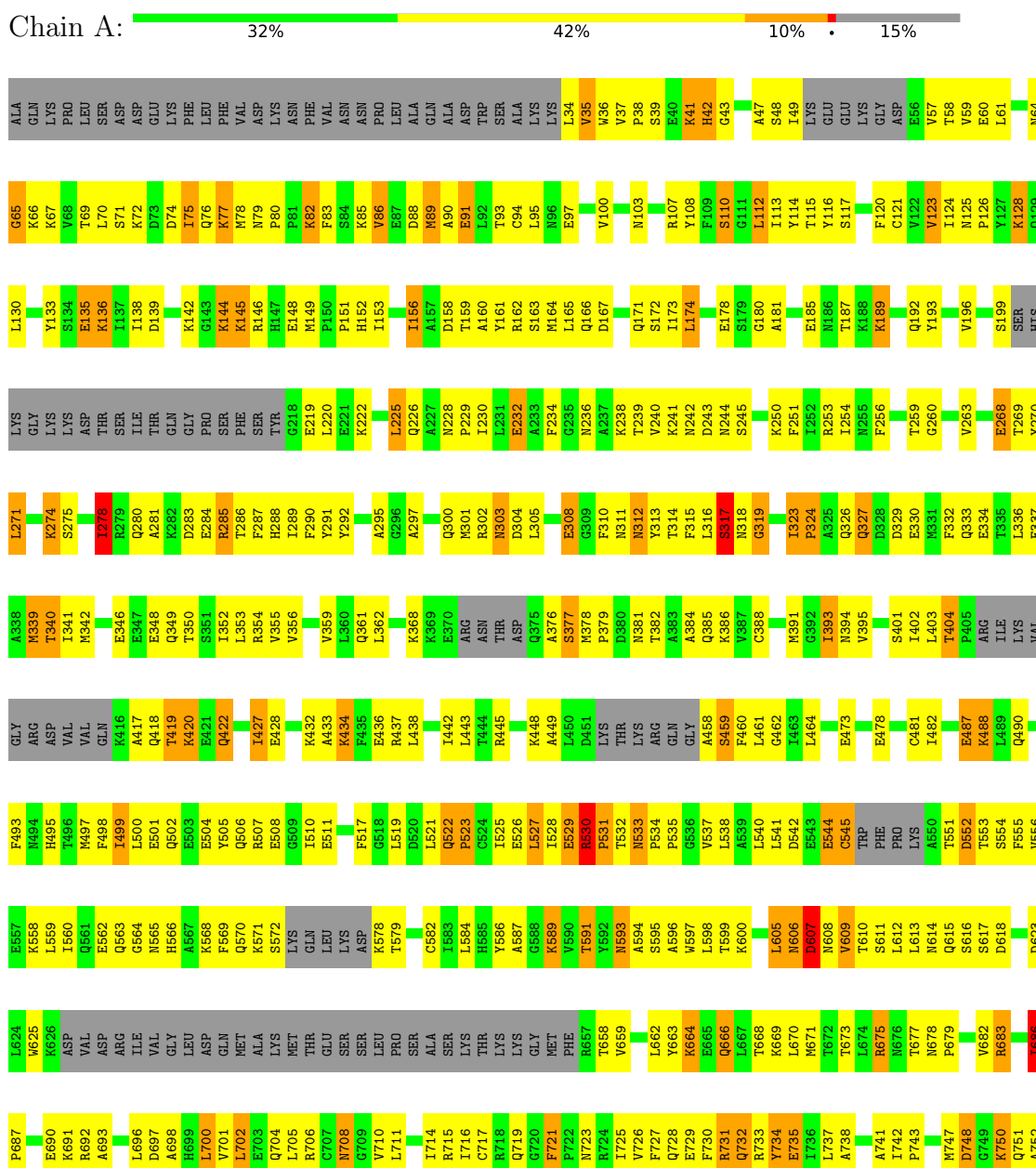
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	2	Total	O	0	0
			2	2		
5	C	2	Total	O	0	0
			2	2		
5	D	2	Total	O	0	0
			2	2		
5	E	2	Total	O	0	0
			2	2		
5	F	2	Total	O	0	0
			2	2		

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. 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. 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.

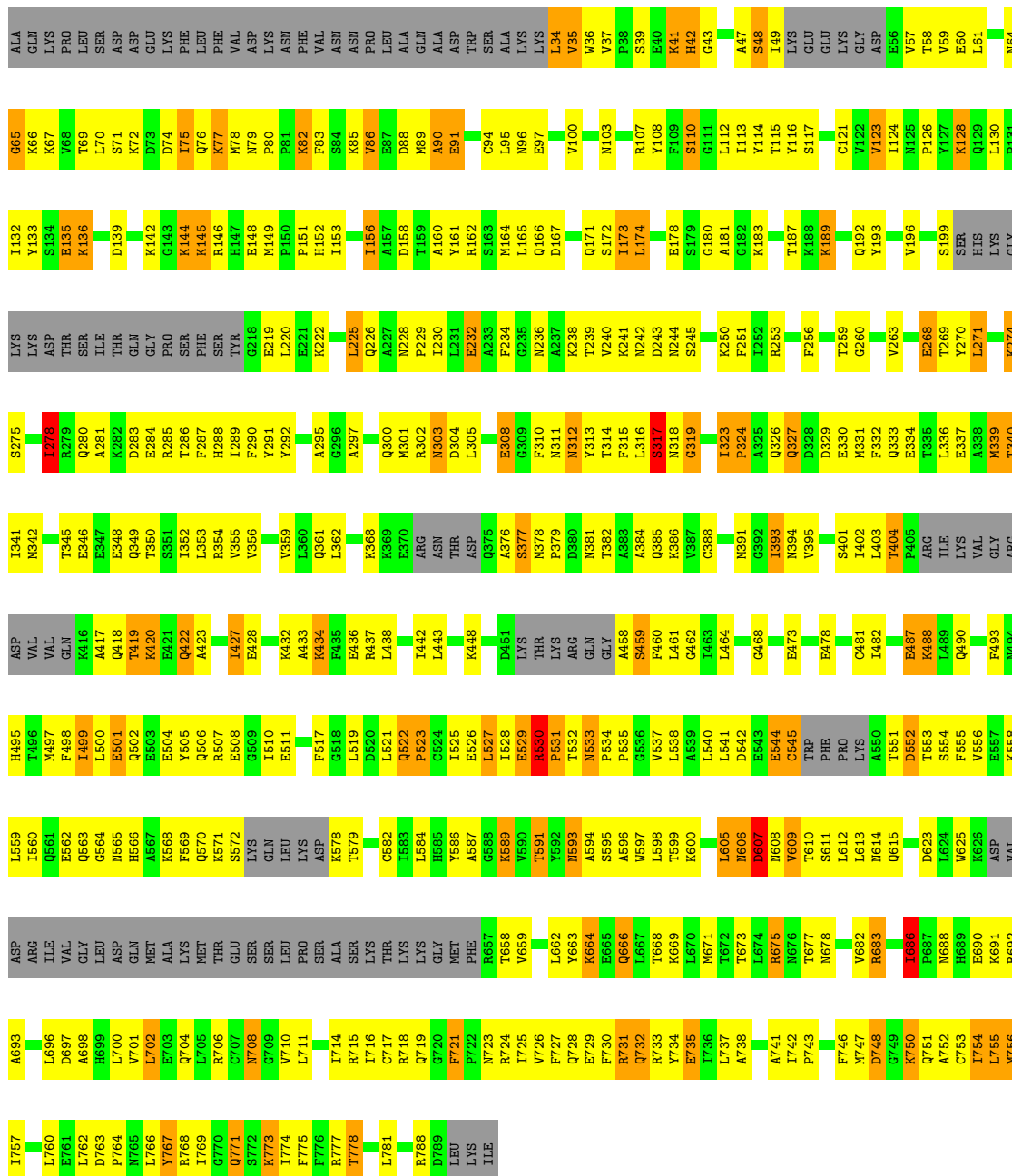
Note EDS was not executed.

• Molecule 1: MYOSIN

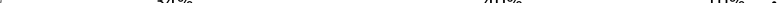


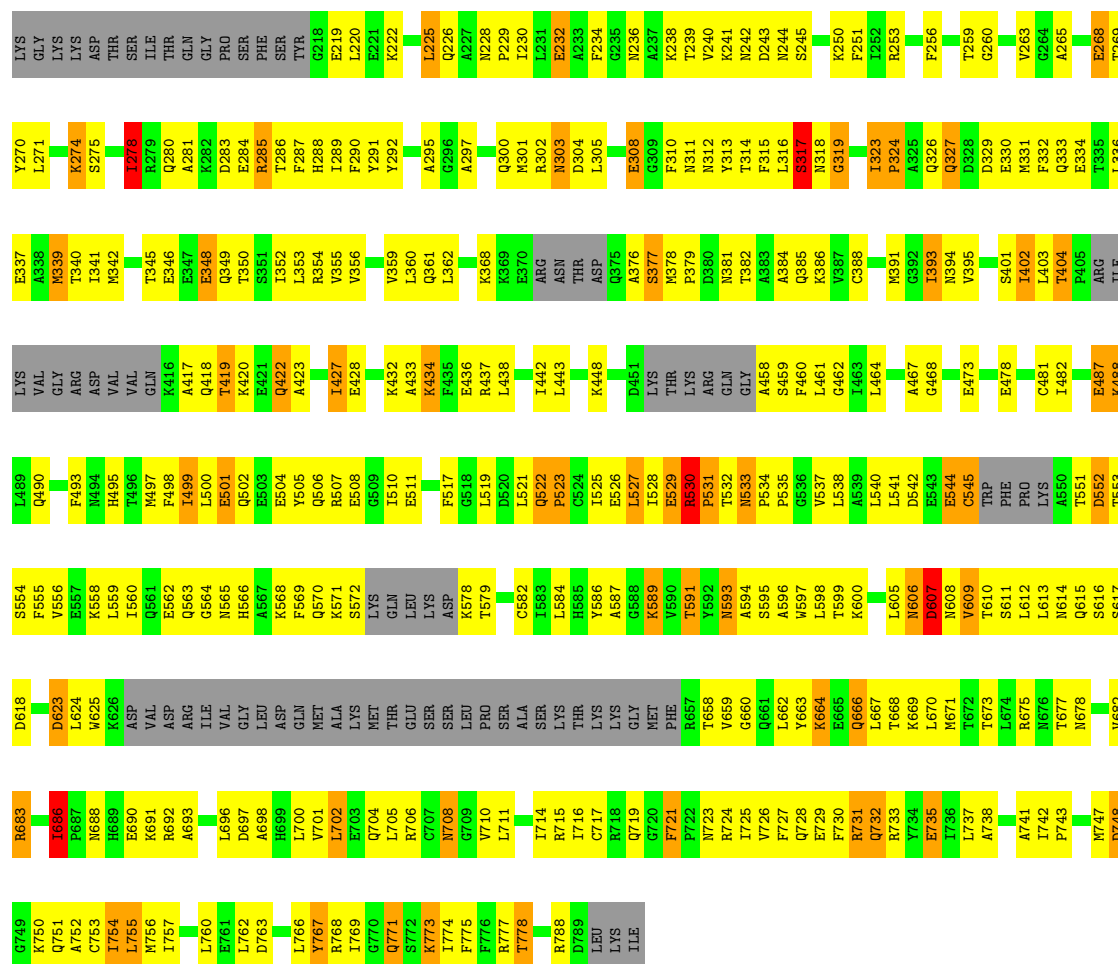
- Molecule 1: MYOSIN

Chain B:  33% 41% 11% • 15%



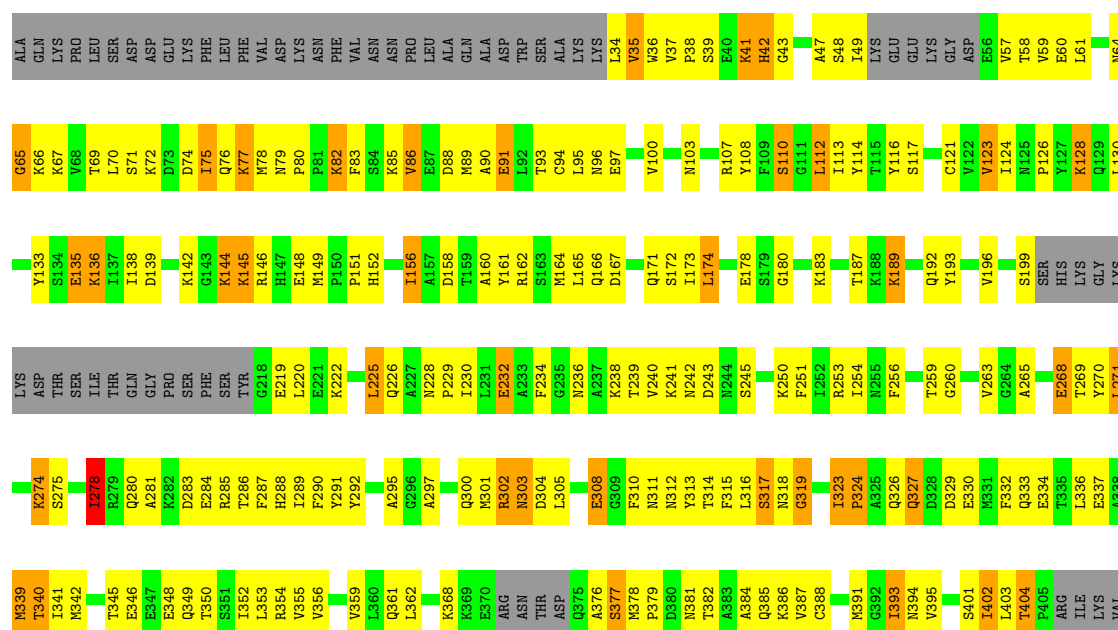
- Molecule 1: MYOSIN

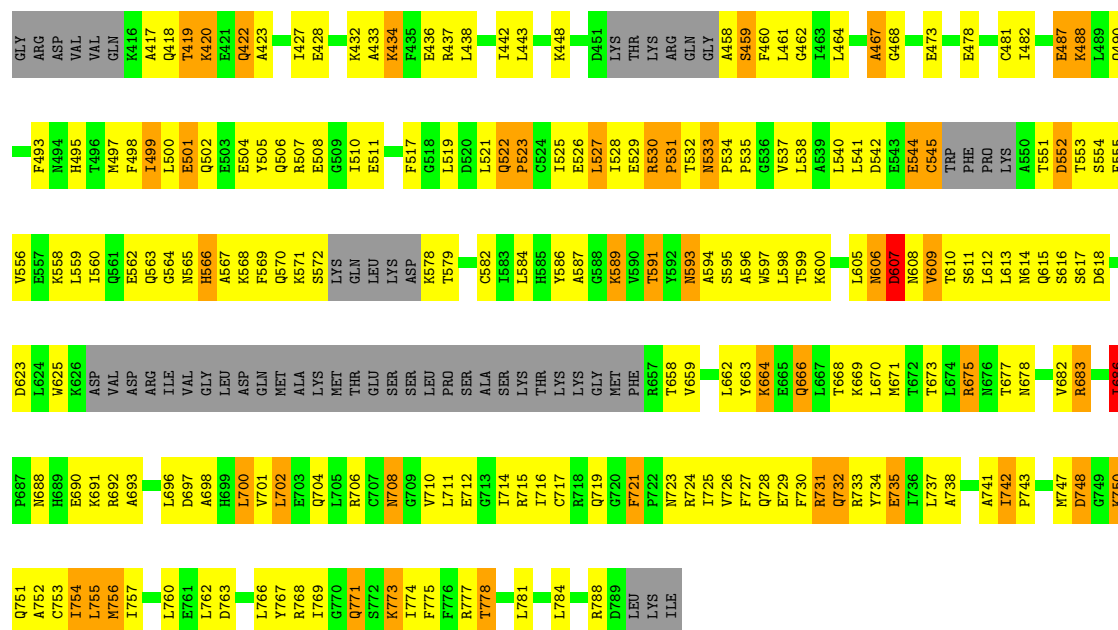
Chain C:  34% 40% 10% 1% 15%



• Molecule 1: MYOSIN

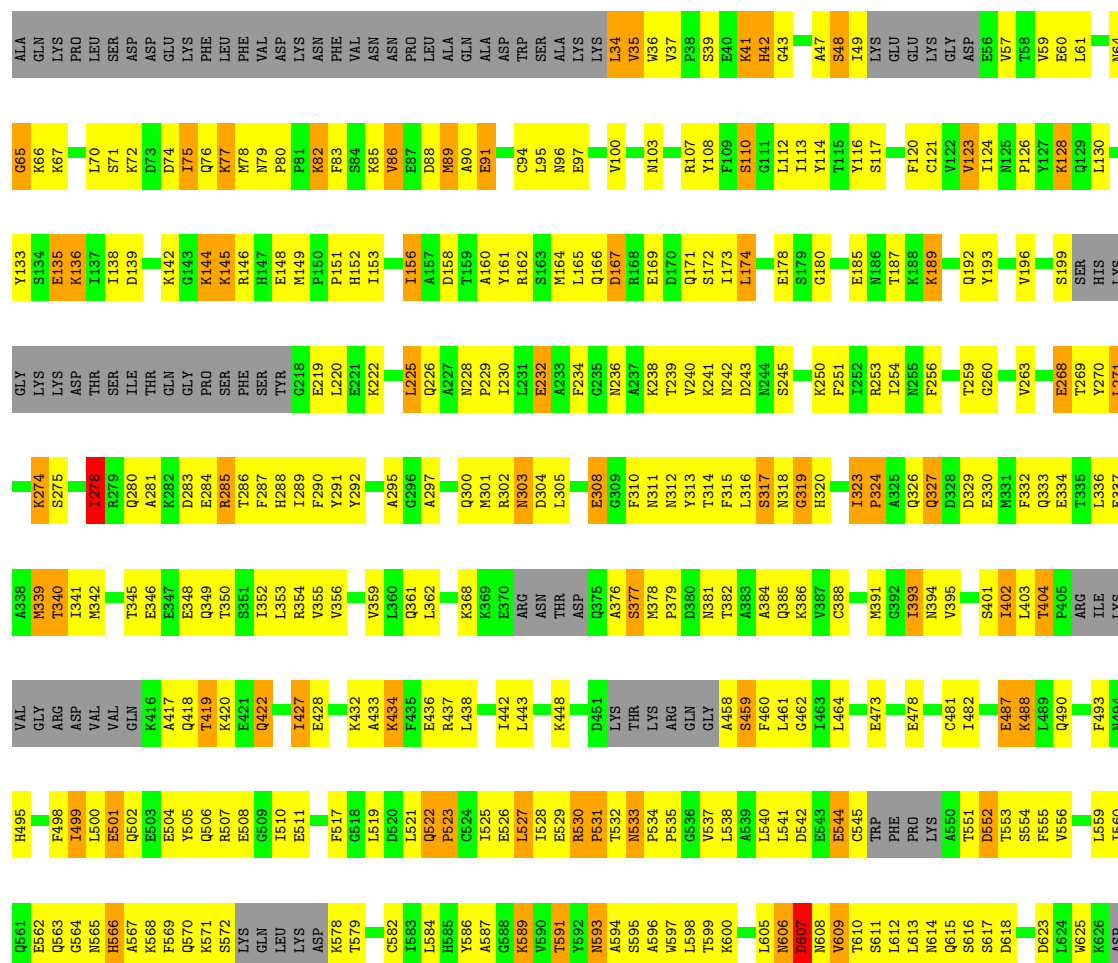
Chain E: 33% 41% 11% 15%

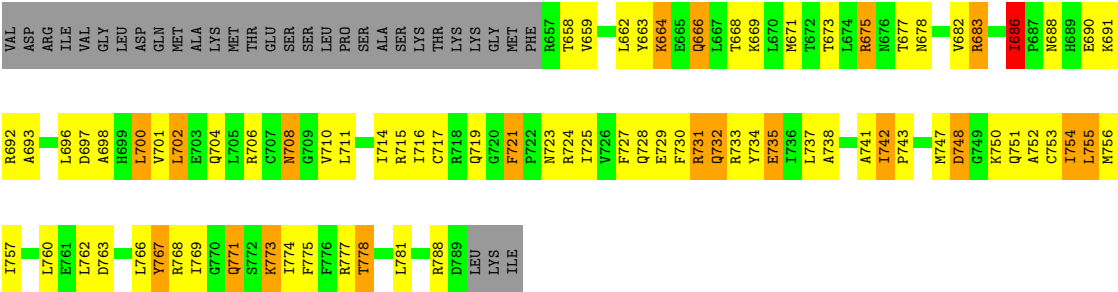




• Molecule 1: MYOSIN

Chain F: 34% 40% 11% 15%





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.01Å 107.67Å 188.31Å 90.00° 90.66° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	83.1 (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.232 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31830	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, ADP, MG

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	A	0.58	0/5364	0.95	22/7253 (0.3%)
1	B	0.56	0/5364	0.94	18/7253 (0.2%)
1	C	0.60	0/5364	0.95	21/7253 (0.3%)
1	D	0.62	0/5364	0.95	21/7253 (0.3%)
1	E	0.56	0/5364	0.92	19/7253 (0.3%)
1	F	0.56	0/5364	0.91	18/7253 (0.2%)
All	All	0.58	0/32184	0.94	119/43518 (0.3%)

There are no bond length outliers.

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	278	ILE	N-CA-C	7.18	119.79	112.90
1	E	65	GLY	N-CA-C	-7.07	104.70	114.67
1	F	65	GLY	N-CA-C	-6.97	104.84	114.67
1	D	65	GLY	N-CA-C	-6.89	104.95	114.67
1	A	65	GLY	N-CA-C	-6.85	105.01	114.67
1	B	65	GLY	N-CA-C	-6.85	105.02	114.67
1	C	65	GLY	N-CA-C	-6.79	105.09	114.67
1	F	90	ALA	N-CA-C	-6.73	104.33	112.54
1	E	90	ALA	N-CA-C	-6.67	104.40	112.54
1	D	90	ALA	N-CA-C	-6.67	104.40	112.54
1	C	278	ILE	N-CA-C	6.58	119.21	112.90
1	D	686	ILE	N-CA-C	-6.57	100.30	108.05
1	C	90	ALA	N-CA-C	-6.51	104.27	111.82
1	B	90	ALA	N-CA-C	-6.49	104.29	111.82
1	D	682	VAL	N-CA-C	-6.45	98.34	107.75
1	D	721	PHE	CA-C-N	6.40	125.63	118.97
1	D	721	PHE	C-N-CA	6.40	125.63	118.97
1	A	90	ALA	N-CA-C	-6.36	104.45	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	278	ILE	N-CA-C	6.33	118.97	112.90
1	E	160	ALA	N-CA-C	-6.28	104.52	111.36
1	A	278	ILE	N-CA-C	6.25	119.16	113.10
1	D	552	ASP	N-CA-C	-6.24	104.47	111.28
1	B	552	ASP	N-CA-C	-6.23	104.49	111.28
1	F	160	ALA	N-CA-C	-6.21	104.59	111.36
1	D	571	LYS	N-CA-C	-6.21	101.74	110.50
1	F	721	PHE	CA-C-N	6.21	125.42	118.97
1	F	721	PHE	C-N-CA	6.21	125.42	118.97
1	A	686	ILE	N-CA-C	-6.18	100.76	108.05
1	B	160	ALA	N-CA-C	-6.15	104.66	111.36
1	E	187	THR	N-CA-C	-6.11	104.62	111.28
1	C	160	ALA	N-CA-C	-6.10	104.71	111.36
1	D	339	MET	N-CA-C	-6.04	104.70	111.28
1	C	686	ILE	N-CA-C	-6.04	100.93	108.05
1	A	552	ASP	N-CA-C	-6.01	104.72	111.28
1	A	160	ALA	N-CA-C	-6.01	104.81	111.36
1	B	571	LYS	N-CA-C	-5.98	102.22	110.35
1	F	339	MET	N-CA-C	-5.93	104.82	111.28
1	B	278	ILE	N-CA-C	5.92	118.59	112.90
1	B	686	ILE	N-CA-C	-5.91	101.08	108.05
1	F	552	ASP	N-CA-C	-5.90	104.84	111.28
1	A	187	THR	N-CA-C	-5.90	104.85	111.28
1	C	571	LYS	N-CA-C	-5.89	102.19	110.50
1	C	339	MET	N-CA-C	-5.89	104.86	111.28
1	F	571	LYS	N-CA-C	-5.89	102.19	110.50
1	E	571	LYS	N-CA-C	-5.88	102.22	110.50
1	C	187	THR	N-CA-C	-5.87	104.88	111.28
1	A	721	PHE	CA-C-N	5.86	125.06	118.97
1	A	721	PHE	C-N-CA	5.86	125.06	118.97
1	E	721	PHE	CA-C-N	5.86	125.06	118.97
1	E	721	PHE	C-N-CA	5.86	125.06	118.97
1	F	187	THR	N-CA-C	-5.83	104.92	111.28
1	A	682	VAL	N-CA-C	-5.83	98.02	107.28
1	B	135	GLU	N-CA-C	-5.82	105.28	112.90
1	D	135	GLU	N-CA-C	-5.81	105.29	112.90
1	C	138	ILE	N-CA-C	-5.80	104.70	110.62
1	A	135	GLU	N-CA-C	-5.78	105.32	112.90
1	A	571	LYS	N-CA-C	-5.78	102.35	110.50
1	E	686	ILE	N-CA-C	-5.77	101.24	108.05
1	B	187	THR	N-CA-C	-5.77	104.99	111.28
1	B	682	VAL	N-CA-C	-5.74	98.15	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	552	ASP	N-CA-C	-5.74	105.02	111.28
1	D	278	ILE	N-CA-C	5.74	118.67	113.10
1	A	339	MET	N-CA-C	-5.72	105.05	111.28
1	B	721	PHE	CA-C-N	5.67	124.86	118.97
1	B	721	PHE	C-N-CA	5.67	124.86	118.97
1	C	682	VAL	N-CA-C	-5.65	98.30	107.28
1	C	552	ASP	N-CA-C	-5.62	105.15	111.28
1	D	187	THR	N-CA-C	-5.61	105.16	111.28
1	B	339	MET	N-CA-C	-5.61	105.17	111.28
1	F	686	ILE	N-CA-C	-5.60	101.44	108.05
1	A	138	ILE	N-CA-C	-5.58	104.93	110.62
1	F	135	GLU	N-CA-C	-5.55	105.63	112.90
1	E	135	GLU	N-CA-C	-5.52	105.67	112.90
1	C	617	SER	N-CA-C	-5.51	105.66	112.38
1	F	700	LEU	N-CA-C	-5.48	105.31	111.28
1	C	464	LEU	N-CA-C	5.45	117.55	108.02
1	F	682	VAL	N-CA-C	-5.45	98.62	107.28
1	C	721	PHE	CA-C-N	5.44	124.63	118.97
1	C	721	PHE	C-N-CA	5.44	124.63	118.97
1	F	464	LEU	N-CA-C	5.40	117.54	107.99
1	C	423	ALA	N-CA-C	-5.39	105.06	111.69
1	F	767	TYR	N-CA-C	5.39	115.65	108.38
1	E	138	ILE	N-CA-C	-5.38	105.14	110.62
1	E	423	ALA	N-CA-C	-5.36	105.10	111.69
1	A	767	TYR	N-CA-C	5.35	115.61	108.38
1	C	312	ASN	N-CA-C	-5.35	106.76	113.72
1	E	700	LEU	N-CA-C	-5.35	105.45	111.28
1	D	467	ALA	N-CA-C	-5.35	101.26	109.76
1	B	530	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	D	617	SER	N-CA-C	-5.32	105.89	112.38
1	D	423	ALA	N-CA-C	-5.30	105.17	111.69
1	D	160	ALA	N-CA-C	-5.30	105.17	111.69
1	F	617	SER	N-CA-C	-5.29	105.93	112.38
1	C	135	GLU	N-CA-C	-5.28	105.98	112.90
1	C	530	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	E	339	MET	N-CA-C	-5.27	105.53	111.28
1	A	464	LEU	N-CA-C	5.26	117.22	108.02
1	A	530	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	B	423	ALA	N-CA-C	-5.25	105.23	111.69
1	D	464	LEU	N-CA-C	5.25	117.20	108.02
1	E	464	LEU	N-CA-C	5.25	117.27	107.99
1	E	617	SER	N-CA-C	-5.22	106.01	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	530	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	767	TYR	N-CA-C	5.16	115.35	108.38
1	E	682	VAL	N-CA-C	-5.16	99.07	107.28
1	A	312	ASN	N-CA-C	-5.16	107.02	113.72
1	D	348	GLU	N-CA-C	-5.15	105.75	111.36
1	A	348	GLU	N-CA-C	-5.14	105.75	111.36
1	D	138	ILE	N-CA-C	-5.14	105.38	110.62
1	C	467	ALA	N-CA-C	-5.14	101.59	109.76
1	A	734	TYR	N-CA-C	5.13	119.08	112.41
1	A	617	SER	N-CA-C	-5.11	106.14	112.38
1	D	767	TYR	N-CA-C	5.11	115.28	108.38
1	B	464	LEU	N-CA-C	5.07	116.89	108.02
1	A	700	LEU	N-CA-C	-5.06	105.84	111.36
1	E	467	ALA	N-CA-C	-5.02	101.78	109.76
1	F	138	ILE	N-CA-C	-5.02	104.78	111.05
1	C	700	LEU	N-CA-C	-5.02	105.89	111.36
1	B	312	ASN	N-CA-C	-5.01	107.21	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	A	5270	0	5145	396	0
1	B	5270	0	5145	390	0
1	C	5270	0	5145	389	0
1	D	5270	0	5145	382	0
1	E	5270	0	5145	386	0
1	F	5270	0	5145	371	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
3	D	5	0	0	2	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
All	All	31830	0	30942	2306	0

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 37.

All (2306) 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)
1:D:529:GLU:O	1:D:531:PRO:HD3	1.30	1.27
1:A:529:GLU:O	1:A:531:PRO:HD3	1.30	1.24
1:C:529:GLU:O	1:C:531:PRO:HD3	1.30	1.24
1:B:529:GLU:O	1:B:531:PRO:HD3	1.30	1.23
1:D:323:ILE:CG2	1:D:324:PRO:HD2	1.68	1.23
1:B:323:ILE:CG2	1:B:324:PRO:HD2	1.68	1.23
1:C:323:ILE:CG2	1:C:324:PRO:HD2	1.68	1.22
1:A:323:ILE:CG2	1:A:324:PRO:HD2	1.68	1.21
1:D:323:ILE:HG23	1:D:324:PRO:HD2	1.15	1.15
1:D:533:ASN:HB2	1:D:534:PRO:HD2	1.24	1.14
1:B:533:ASN:HB2	1:B:534:PRO:HD2	1.24	1.14
1:F:323:ILE:HG23	1:F:324:PRO:HD2	1.18	1.13
1:A:533:ASN:CB	1:A:534:PRO:CD	2.27	1.12
1:A:533:ASN:HB2	1:A:534:PRO:HD2	1.24	1.12
1:B:533:ASN:CB	1:B:534:PRO:CD	2.27	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:ASN:CB	1:D:534:PRO:CD	2.27	1.12
1:F:529:GLU:O	1:F:531:PRO:HD3	1.47	1.12
1:B:323:ILE:HG23	1:B:324:PRO:HD2	1.15	1.12
1:C:323:ILE:HG23	1:C:324:PRO:HD2	1.15	1.11
1:C:533:ASN:CB	1:C:534:PRO:CD	2.27	1.11
1:E:323:ILE:HG23	1:E:324:PRO:HD2	1.19	1.10
1:E:529:GLU:O	1:E:531:PRO:HD3	1.50	1.09
1:C:533:ASN:HB2	1:C:534:PRO:HD2	1.24	1.09
1:A:323:ILE:HG23	1:A:324:PRO:HD2	1.15	1.08
1:E:323:ILE:CG2	1:E:324:PRO:HD2	1.86	1.05
1:E:533:ASN:HB2	1:E:534:PRO:HD2	1.40	1.03
1:F:323:ILE:CG2	1:F:324:PRO:HD2	1.87	1.03
1:F:533:ASN:HB2	1:F:534:PRO:HD2	1.41	1.01
1:D:533:ASN:HB3	1:D:534:PRO:HD3	1.43	1.01
1:C:533:ASN:HB3	1:C:534:PRO:HD3	1.43	1.01
1:B:533:ASN:HB3	1:B:534:PRO:HD3	1.43	1.01
1:B:533:ASN:CB	1:B:534:PRO:HD2	1.89	1.00
1:A:533:ASN:HB3	1:A:534:PRO:HD3	1.43	1.00
1:D:533:ASN:CB	1:D:534:PRO:HD2	1.89	0.98
1:E:533:ASN:CB	1:E:534:PRO:CD	2.41	0.98
1:A:533:ASN:CB	1:A:534:PRO:HD2	1.89	0.97
1:C:533:ASN:CB	1:C:534:PRO:HD2	1.89	0.97
1:A:533:ASN:HB2	1:A:534:PRO:CD	1.94	0.96
1:F:533:ASN:CB	1:F:534:PRO:CD	2.42	0.96
1:C:533:ASN:HB3	1:C:534:PRO:CD	1.94	0.95
1:C:533:ASN:HB2	1:C:534:PRO:CD	1.94	0.95
1:C:544:GLU:HB3	1:C:598:LEU:HD21	1.49	0.94
1:F:544:GLU:HB3	1:F:598:LEU:HD21	1.49	0.94
1:B:568:LYS:HA	1:B:584:LEU:HD12	1.49	0.93
1:A:533:ASN:HB3	1:A:534:PRO:CD	1.94	0.92
1:E:568:LYS:HA	1:E:584:LEU:HD12	1.51	0.92
1:F:533:ASN:CB	1:F:534:PRO:HD2	1.99	0.92
1:A:568:LYS:HA	1:A:584:LEU:HD12	1.51	0.92
1:A:696:LEU:HD21	1:A:701:VAL:HG21	1.50	0.91
1:D:544:GLU:HB3	1:D:598:LEU:HD21	1.50	0.91
1:A:584:LEU:HD23	1:A:589:LYS:HG3	1.51	0.91
1:E:544:GLU:HB3	1:E:598:LEU:HD21	1.49	0.91
1:A:544:GLU:HB3	1:A:598:LEU:HD21	1.53	0.91
1:B:529:GLU:O	1:B:531:PRO:CD	2.19	0.91
1:C:568:LYS:HA	1:C:584:LEU:HD12	1.53	0.91
1:B:696:LEU:HD21	1:B:701:VAL:HG21	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:696:LEU:HD21	1:F:701:VAL:HG21	1.52	0.90
1:E:584:LEU:HD23	1:E:589:LYS:HG3	1.51	0.90
1:D:748:ASP:OD1	1:D:751:GLN:N	2.05	0.90
1:B:544:GLU:HB3	1:B:598:LEU:HD21	1.53	0.90
1:C:606:ASN:ND2	1:C:608:ASN:HB2	1.87	0.90
1:C:584:LEU:HD23	1:C:589:LYS:HG3	1.52	0.90
1:A:748:ASP:OD1	1:A:751:GLN:N	2.05	0.89
1:C:529:GLU:O	1:C:531:PRO:CD	2.19	0.89
1:B:748:ASP:OD1	1:B:751:GLN:N	2.05	0.89
1:B:323:ILE:CG2	1:B:324:PRO:CD	2.51	0.89
1:B:533:ASN:HB3	1:B:534:PRO:CD	1.94	0.89
1:A:323:ILE:CG2	1:A:324:PRO:CD	2.51	0.89
1:C:748:ASP:OD1	1:C:751:GLN:N	2.05	0.89
1:D:584:LEU:HD23	1:D:589:LYS:HG3	1.55	0.89
1:A:529:GLU:O	1:A:531:PRO:CD	2.19	0.89
1:D:568:LYS:HA	1:D:584:LEU:HD12	1.55	0.89
1:A:751:GLN:CD	1:C:692:ARG:HH22	1.81	0.89
1:E:533:ASN:CB	1:E:534:PRO:HD2	1.99	0.89
1:E:696:LEU:HD21	1:E:701:VAL:HG21	1.53	0.89
1:B:584:LEU:HD23	1:B:589:LYS:HG3	1.55	0.88
1:D:323:ILE:CG2	1:D:324:PRO:CD	2.51	0.88
1:F:568:LYS:HA	1:F:584:LEU:HD12	1.52	0.88
1:D:533:ASN:HB3	1:D:534:PRO:CD	1.94	0.88
1:A:606:ASN:ND2	1:A:608:ASN:HB2	1.88	0.88
1:D:696:LEU:HD21	1:D:701:VAL:HG21	1.54	0.87
1:E:378:MET:HE2	1:E:381:ASN:HA	1.55	0.87
1:E:533:ASN:HB3	1:E:534:PRO:CD	2.03	0.87
1:F:584:LEU:HD23	1:F:589:LYS:HG3	1.54	0.87
1:F:533:ASN:HB3	1:F:534:PRO:CD	2.04	0.87
1:C:606:ASN:HD21	1:C:608:ASN:HB2	1.40	0.87
1:B:323:ILE:HG23	1:B:324:PRO:CD	2.04	0.86
1:D:323:ILE:HG23	1:D:324:PRO:CD	2.04	0.86
1:A:751:GLN:NE2	1:C:692:ARG:HH22	1.73	0.86
1:C:323:ILE:CG2	1:C:324:PRO:CD	2.51	0.86
1:D:378:MET:HE2	1:D:381:ASN:HA	1.55	0.86
1:A:742:ILE:HD11	1:A:752:ALA:O	1.75	0.86
1:B:742:ILE:HD11	1:B:752:ALA:O	1.75	0.86
1:B:606:ASN:ND2	1:B:608:ASN:HB2	1.91	0.85
1:F:606:ASN:ND2	1:F:608:ASN:HB2	1.90	0.85
1:D:529:GLU:O	1:D:531:PRO:CD	2.19	0.85
1:F:742:ILE:HD11	1:F:752:ALA:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:MET:HE2	1:A:381:ASN:HA	1.59	0.85
1:A:323:ILE:HG23	1:A:324:PRO:CD	2.04	0.84
1:C:378:MET:HE2	1:C:381:ASN:HA	1.60	0.84
1:D:606:ASN:ND2	1:D:608:ASN:HB2	1.92	0.84
1:B:145:LYS:HB2	1:B:148:GLU:HG3	1.59	0.84
1:C:544:GLU:HG3	1:C:555:PHE:HB2	1.59	0.84
1:A:606:ASN:HD21	1:A:608:ASN:HB2	1.42	0.84
1:C:145:LYS:HB2	1:C:148:GLU:HG3	1.58	0.84
1:D:145:LYS:HB2	1:D:148:GLU:HG3	1.60	0.83
1:C:696:LEU:HD21	1:C:701:VAL:HG21	1.57	0.83
1:E:742:ILE:HD11	1:E:752:ALA:O	1.79	0.83
1:F:145:LYS:HB2	1:F:148:GLU:HG3	1.61	0.83
1:A:323:ILE:HG22	1:A:324:PRO:HD2	1.61	0.82
1:F:606:ASN:HD21	1:F:608:ASN:HB2	1.43	0.82
1:A:544:GLU:HG3	1:A:555:PHE:HB2	1.62	0.82
1:A:145:LYS:HB2	1:A:148:GLU:HG3	1.59	0.82
1:E:533:ASN:HB3	1:E:534:PRO:HD3	1.61	0.82
1:B:378:MET:HE2	1:B:381:ASN:HA	1.61	0.82
1:B:606:ASN:HD21	1:B:608:ASN:HB2	1.45	0.82
1:E:606:ASN:ND2	1:E:608:ASN:HB2	1.95	0.82
1:C:323:ILE:HG23	1:C:324:PRO:CD	2.04	0.81
1:D:419:THR:H	1:D:422:GLN:HG3	1.45	0.81
1:E:43:GLY:H	1:E:698:ALA:HB1	1.44	0.81
1:F:544:GLU:HG3	1:F:555:PHE:HB2	1.62	0.81
1:C:742:ILE:HD11	1:C:752:ALA:O	1.79	0.81
1:E:49:ILE:HA	1:E:59:VAL:HG12	1.63	0.81
1:F:49:ILE:HA	1:F:59:VAL:HG12	1.63	0.81
1:D:544:GLU:HG3	1:D:555:PHE:HB2	1.61	0.81
1:D:742:ILE:HD11	1:D:752:ALA:O	1.80	0.81
1:E:419:THR:H	1:E:422:GLN:HG3	1.46	0.81
1:B:156:ILE:HG22	1:B:173:ILE:HD13	1.63	0.81
1:C:323:ILE:HG22	1:C:324:PRO:HD2	1.61	0.81
1:C:593:ASN:HD22	1:C:595:SER:H	1.28	0.81
1:E:715:ARG:HH11	1:E:715:ARG:HG3	1.45	0.81
1:F:378:MET:HE2	1:F:381:ASN:HA	1.60	0.81
1:B:419:THR:H	1:B:422:GLN:HG3	1.44	0.80
1:E:145:LYS:HB2	1:E:148:GLU:HG3	1.62	0.80
1:E:544:GLU:HG3	1:E:555:PHE:HB2	1.63	0.80
1:B:593:ASN:HD22	1:B:595:SER:H	1.29	0.80
1:A:49:ILE:HA	1:A:59:VAL:HG12	1.64	0.80
1:D:606:ASN:HD21	1:D:608:ASN:HB2	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:GLY:H	1:F:698:ALA:HB1	1.47	0.80
1:B:715:ARG:HH11	1:B:715:ARG:HG3	1.47	0.80
1:B:43:GLY:H	1:B:698:ALA:HB1	1.47	0.80
1:A:128:LYS:HD3	1:A:693:ALA:HB1	1.63	0.80
1:D:323:ILE:HG22	1:D:324:PRO:HD2	1.62	0.80
1:B:323:ILE:HG22	1:B:324:PRO:HD2	1.61	0.79
1:C:49:ILE:HA	1:C:59:VAL:HG12	1.63	0.79
1:A:85:LYS:HB3	1:A:107:ARG:HG2	1.64	0.79
1:B:49:ILE:HA	1:B:59:VAL:HG12	1.63	0.79
1:F:533:ASN:HB3	1:F:534:PRO:HD3	1.64	0.79
1:D:715:ARG:HG3	1:D:715:ARG:HH11	1.47	0.79
1:A:593:ASN:HD22	1:A:595:SER:H	1.29	0.79
1:D:49:ILE:HA	1:D:59:VAL:HG12	1.65	0.79
1:E:593:ASN:HD22	1:E:595:SER:H	1.30	0.79
1:A:751:GLN:HE22	1:C:692:ARG:NH2	1.80	0.79
1:C:715:ARG:HH11	1:C:715:ARG:HG3	1.48	0.79
1:D:43:GLY:H	1:D:698:ALA:HB1	1.46	0.79
1:D:85:LYS:HB3	1:D:107:ARG:HG2	1.64	0.79
1:F:715:ARG:HH11	1:F:715:ARG:HG3	1.47	0.78
1:E:737:LEU:HD21	1:E:788:ARG:HA	1.65	0.78
1:F:85:LYS:HB3	1:F:107:ARG:HG2	1.63	0.78
1:A:743:PRO:HG2	1:A:747:MET:SD	2.24	0.78
1:C:85:LYS:HB3	1:C:107:ARG:HG2	1.64	0.78
1:A:419:THR:H	1:A:422:GLN:HG3	1.48	0.78
1:D:593:ASN:HD22	1:D:595:SER:H	1.27	0.78
1:F:128:LYS:HD3	1:F:693:ALA:HB1	1.66	0.78
1:B:544:GLU:HG3	1:B:555:PHE:HB2	1.64	0.78
1:F:743:PRO:HG2	1:F:747:MET:SD	2.23	0.78
1:B:743:PRO:HG2	1:B:747:MET:SD	2.24	0.78
1:C:498:PHE:O	1:C:502:GLN:HG3	1.84	0.78
1:E:128:LYS:HD3	1:E:693:ALA:HB1	1.66	0.78
1:E:748:ASP:OD1	1:E:751:GLN:N	2.16	0.78
1:F:156:ILE:HG22	1:F:173:ILE:HD13	1.65	0.78
1:B:128:LYS:HD3	1:B:693:ALA:HB1	1.65	0.78
1:A:751:GLN:OE1	1:C:692:ARG:NH2	2.16	0.78
1:C:743:PRO:HG2	1:C:747:MET:SD	2.24	0.78
1:A:419:THR:HG23	1:A:422:GLN:NE2	1.99	0.77
1:E:606:ASN:HD21	1:E:608:ASN:HB2	1.49	0.77
1:F:593:ASN:HD22	1:F:595:SER:H	1.32	0.77
1:C:128:LYS:HD3	1:C:693:ALA:HB1	1.66	0.77
1:D:743:PRO:HG2	1:D:747:MET:SD	2.24	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:ARG:HH11	1:A:715:ARG:HG3	1.48	0.77
1:A:43:GLY:H	1:A:698:ALA:HB1	1.49	0.77
1:B:498:PHE:O	1:B:502:GLN:HG3	1.85	0.77
1:F:419:THR:H	1:F:422:GLN:HG3	1.49	0.77
1:E:85:LYS:HB3	1:E:107:ARG:HG2	1.67	0.77
1:D:419:THR:HG23	1:D:422:GLN:NE2	2.00	0.76
1:D:742:ILE:HG13	1:D:747:MET:HG2	1.67	0.76
1:B:742:ILE:HG13	1:B:747:MET:HG2	1.67	0.76
1:D:128:LYS:HD3	1:D:693:ALA:HB1	1.67	0.76
1:E:156:ILE:HG22	1:E:173:ILE:HD13	1.67	0.76
1:C:156:ILE:HG22	1:C:173:ILE:HD13	1.65	0.76
1:F:498:PHE:O	1:F:502:GLN:HG3	1.86	0.76
1:C:742:ILE:HG13	1:C:747:MET:HG2	1.67	0.76
1:C:419:THR:HG23	1:C:422:GLN:NE2	2.00	0.76
1:C:43:GLY:H	1:C:698:ALA:HB1	1.48	0.75
1:C:419:THR:H	1:C:422:GLN:HG3	1.48	0.75
1:D:156:ILE:HG22	1:D:173:ILE:HD13	1.68	0.75
1:A:419:THR:H	1:A:422:GLN:HE21	1.34	0.75
1:B:85:LYS:HB3	1:B:107:ARG:HG2	1.67	0.75
1:F:529:GLU:O	1:F:531:PRO:CD	2.32	0.75
1:D:582:CYS:SG	1:D:591:THR:HB	2.27	0.75
1:F:737:LEU:HD21	1:F:788:ARG:HA	1.68	0.75
1:E:743:PRO:HG2	1:E:747:MET:SD	2.27	0.75
1:A:742:ILE:HG13	1:A:747:MET:HG2	1.67	0.74
1:E:527:LEU:O	1:E:527:LEU:HD12	1.87	0.74
1:B:737:LEU:HD21	1:B:788:ARG:HA	1.69	0.74
1:F:323:ILE:CG2	1:F:324:PRO:CD	2.66	0.74
1:D:378:MET:HE1	1:D:384:ALA:HB2	1.68	0.74
1:E:742:ILE:HG13	1:E:747:MET:HG2	1.70	0.74
1:F:748:ASP:OD1	1:F:751:GLN:N	2.20	0.74
1:A:747:MET:HE3	1:A:751:GLN:HB2	1.68	0.74
1:E:323:ILE:CG2	1:E:324:PRO:CD	2.65	0.74
1:A:156:ILE:HG22	1:A:173:ILE:HD13	1.67	0.74
1:D:737:LEU:HD21	1:D:788:ARG:HA	1.70	0.74
1:E:738:ALA:HB1	1:E:741:ALA:HB2	1.69	0.74
1:B:391:MET:HG2	1:B:434:LYS:HZ1	1.53	0.74
1:A:737:LEU:HD21	1:A:788:ARG:HA	1.68	0.74
1:D:419:THR:H	1:D:422:GLN:HE21	1.36	0.74
1:C:540:LEU:HD13	1:C:559:LEU:HA	1.70	0.73
1:F:743:PRO:CG	1:F:747:MET:SD	2.76	0.73
1:A:747:MET:HE3	1:A:751:GLN:CB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:498:PHE:O	1:E:502:GLN:HG3	1.89	0.73
1:B:419:THR:HG23	1:B:422:GLN:NE2	2.03	0.73
1:E:529:GLU:O	1:E:531:PRO:CD	2.35	0.73
1:D:391:MET:HE2	1:D:434:LYS:CE	2.19	0.73
1:E:419:THR:HG23	1:E:422:GLN:NE2	2.03	0.73
1:B:540:LEU:HD13	1:B:559:LEU:HA	1.69	0.73
1:B:747:MET:HE3	1:B:751:GLN:CB	2.19	0.73
1:C:747:MET:HE3	1:C:751:GLN:HB2	1.70	0.73
1:A:527:LEU:HD12	1:A:527:LEU:O	1.87	0.73
1:A:540:LEU:HD13	1:A:559:LEU:HA	1.70	0.73
1:C:391:MET:HG2	1:C:434:LYS:HZ1	1.54	0.73
1:A:498:PHE:O	1:A:502:GLN:HG3	1.88	0.73
1:C:737:LEU:HD21	1:C:788:ARG:HA	1.69	0.73
1:F:280:GLN:OE1	1:F:317:SER:HB2	1.88	0.73
1:C:419:THR:H	1:C:422:GLN:HE21	1.35	0.73
1:E:508:GLU:HG2	1:E:775:PHE:HE1	1.54	0.73
1:C:401:SER:HB3	1:C:608:ASN:HB3	1.71	0.72
1:B:747:MET:HE3	1:B:751:GLN:HB2	1.70	0.72
1:C:747:MET:HE3	1:C:751:GLN:CB	2.19	0.72
1:A:535:PRO:O	1:A:563:GLN:NE2	2.22	0.72
1:B:378:MET:HE1	1:B:384:ALA:HB2	1.70	0.72
1:C:743:PRO:CG	1:C:747:MET:SD	2.77	0.72
1:D:747:MET:HE3	1:D:751:GLN:HB2	1.69	0.72
1:C:535:PRO:O	1:C:563:GLN:NE2	2.22	0.72
1:D:743:PRO:CG	1:D:747:MET:SD	2.77	0.72
1:F:419:THR:HG23	1:F:422:GLN:NE2	2.04	0.72
1:D:535:PRO:O	1:D:563:GLN:NE2	2.22	0.72
1:A:743:PRO:CG	1:A:747:MET:SD	2.77	0.72
1:A:738:ALA:HB1	1:A:741:ALA:HB2	1.71	0.72
1:B:508:GLU:HG2	1:B:775:PHE:HE1	1.55	0.72
1:B:535:PRO:O	1:B:563:GLN:NE2	2.22	0.72
1:D:498:PHE:O	1:D:502:GLN:HG3	1.90	0.72
1:D:738:ALA:HB1	1:D:741:ALA:HB2	1.71	0.72
1:E:747:MET:HE3	1:E:751:GLN:HB2	1.72	0.72
1:B:419:THR:H	1:B:422:GLN:HE21	1.35	0.71
1:B:743:PRO:CG	1:B:747:MET:SD	2.77	0.71
1:E:747:MET:HE3	1:E:751:GLN:CB	2.19	0.71
1:F:540:LEU:HD13	1:F:559:LEU:HA	1.71	0.71
1:F:747:MET:HE3	1:F:751:GLN:HB2	1.72	0.71
1:D:508:GLU:HG2	1:D:775:PHE:HE1	1.54	0.71
1:E:419:THR:H	1:E:422:GLN:HE21	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:419:THR:H	1:F:422:GLN:HE21	1.36	0.71
1:B:419:THR:N	1:B:422:GLN:HE21	1.89	0.71
1:B:738:ALA:HB1	1:B:741:ALA:HB2	1.71	0.71
1:C:738:ALA:HB1	1:C:741:ALA:HB2	1.71	0.71
1:D:527:LEU:HD12	1:D:527:LEU:O	1.91	0.71
1:D:747:MET:HE3	1:D:751:GLN:CB	2.19	0.71
1:A:242:ASN:HB3	1:A:245:SER:HB2	1.72	0.71
1:C:242:ASN:HB3	1:C:245:SER:HB2	1.72	0.71
1:A:401:SER:HB3	1:A:608:ASN:HB3	1.73	0.71
1:B:527:LEU:O	1:B:527:LEU:HD12	1.91	0.71
1:D:731:ARG:HH21	1:D:742:ILE:HG21	1.55	0.71
1:F:569:PHE:CD1	1:F:570:GLN:N	2.59	0.71
1:E:391:MET:HG2	1:E:434:LYS:HZ1	1.56	0.70
1:E:540:LEU:HD13	1:E:559:LEU:HA	1.71	0.70
1:D:391:MET:HE2	1:D:434:LYS:HE3	1.73	0.70
1:D:731:ARG:HH11	1:D:731:ARG:HG3	1.57	0.70
1:F:742:ILE:HG13	1:F:747:MET:HG2	1.72	0.70
1:B:526:GLU:O	1:B:530:ARG:HB2	1.92	0.70
1:C:280:GLN:OE1	1:C:317:SER:HB2	1.90	0.70
1:C:378:MET:HE1	1:C:384:ALA:HB2	1.74	0.70
1:E:569:PHE:CD1	1:E:570:GLN:N	2.60	0.70
1:A:731:ARG:HH11	1:A:731:ARG:HG3	1.57	0.70
1:F:527:LEU:HD12	1:F:527:LEU:O	1.90	0.70
1:A:731:ARG:NH2	1:A:742:ILE:HG21	2.07	0.70
1:C:527:LEU:HD12	1:C:527:LEU:O	1.91	0.70
1:A:378:MET:HE1	1:A:384:ALA:HB2	1.74	0.70
1:B:533:ASN:HB2	1:B:534:PRO:CD	1.94	0.70
1:C:731:ARG:HH21	1:C:742:ILE:HG21	1.57	0.70
1:D:731:ARG:NH2	1:D:742:ILE:HG21	2.07	0.70
1:B:401:SER:HB3	1:B:608:ASN:HB3	1.74	0.69
1:E:419:THR:N	1:E:422:GLN:HE21	1.90	0.69
1:F:533:ASN:HB2	1:F:534:PRO:CD	2.13	0.69
1:E:378:MET:HE1	1:E:384:ALA:HB2	1.74	0.69
1:F:731:ARG:HH21	1:F:742:ILE:HG21	1.55	0.69
1:D:391:MET:HG2	1:D:434:LYS:HZ1	1.56	0.69
1:E:346:GLU:O	1:E:350:THR:HG23	1.93	0.69
1:F:508:GLU:HG2	1:F:775:PHE:HE1	1.56	0.69
1:F:346:GLU:O	1:F:350:THR:HG23	1.92	0.69
1:D:540:LEU:HD13	1:D:559:LEU:HA	1.75	0.69
1:A:419:THR:N	1:A:422:GLN:HE21	1.89	0.69
1:E:743:PRO:CG	1:E:747:MET:SD	2.81	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:ARG:NH2	1:C:742:ILE:HG21	2.08	0.69
1:D:72:LYS:HA	1:D:75:ILE:HD12	1.73	0.69
1:F:378:MET:HE1	1:F:384:ALA:HB2	1.72	0.69
1:A:72:LYS:HA	1:A:75:ILE:HD12	1.74	0.69
1:A:569:PHE:CD1	1:A:570:GLN:N	2.61	0.69
1:A:731:ARG:HH21	1:A:742:ILE:HG21	1.57	0.69
1:A:751:GLN:OE1	1:C:692:ARG:NH1	2.26	0.69
1:D:526:GLU:O	1:D:530:ARG:HB2	1.93	0.69
1:F:747:MET:HE3	1:F:751:GLN:CB	2.23	0.69
1:A:537:VAL:HG22	1:A:559:LEU:HD11	1.74	0.69
1:C:391:MET:HE2	1:C:434:LYS:CE	2.23	0.69
1:C:419:THR:N	1:C:422:GLN:HE21	1.91	0.69
1:C:569:PHE:CD1	1:C:570:GLN:N	2.61	0.69
1:A:274:LYS:HG2	1:A:436:GLU:HB2	1.75	0.69
1:B:280:GLN:OE1	1:B:317:SER:HB2	1.92	0.69
1:E:582:CYS:SG	1:E:591:THR:HB	2.33	0.69
1:F:731:ARG:NH2	1:F:742:ILE:HG21	2.07	0.69
1:C:607:ASP:HA	1:C:610:THR:HB	1.75	0.68
1:D:419:THR:N	1:D:422:GLN:HE21	1.89	0.68
1:E:72:LYS:HA	1:E:75:ILE:HD12	1.74	0.68
1:E:526:GLU:O	1:E:530:ARG:HB2	1.93	0.68
1:F:323:ILE:HG23	1:F:324:PRO:CD	2.11	0.68
1:E:537:VAL:HG22	1:E:559:LEU:HD11	1.75	0.68
1:E:391:MET:HE2	1:E:434:LYS:CE	2.24	0.68
1:E:418:GLN:HA	1:E:422:GLN:NE2	2.08	0.68
1:B:708:ASN:HD22	1:B:708:ASN:N	1.91	0.68
1:C:274:LYS:HG2	1:C:436:GLU:HB2	1.75	0.68
1:C:537:VAL:HG22	1:C:559:LEU:HD11	1.74	0.68
1:A:728:GLN:O	1:A:732:GLN:HG2	1.94	0.68
1:D:401:SER:HB3	1:D:608:ASN:HB3	1.76	0.68
1:E:280:GLN:OE1	1:E:317:SER:HB2	1.93	0.68
1:A:582:CYS:SG	1:A:591:THR:HB	2.34	0.68
1:B:537:VAL:HG22	1:B:559:LEU:HD11	1.74	0.68
1:B:731:ARG:HH21	1:B:742:ILE:HG21	1.59	0.68
1:C:72:LYS:HA	1:C:75:ILE:HD12	1.75	0.68
1:D:242:ASN:HB3	1:D:245:SER:HB2	1.74	0.68
1:C:731:ARG:HG3	1:C:731:ARG:HH11	1.59	0.68
1:D:569:PHE:CD1	1:D:570:GLN:N	2.62	0.68
1:B:72:LYS:HA	1:B:75:ILE:HD12	1.74	0.68
1:D:196:VAL:HG12	1:D:196:VAL:O	1.94	0.68
1:F:72:LYS:HA	1:F:75:ILE:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LYS:HG2	1:D:436:GLU:HB2	1.75	0.67
1:E:116:TYR:CZ	1:E:151:PRO:HA	2.29	0.67
1:F:401:SER:HB3	1:F:608:ASN:HB3	1.75	0.67
1:A:508:GLU:HG2	1:A:775:PHE:HE1	1.57	0.67
1:B:527:LEU:CD1	1:B:563:GLN:HG3	2.25	0.67
1:F:281:ALA:O	1:F:284:GLU:HB2	1.95	0.67
1:A:596:ALA:O	1:A:600:LYS:HG3	1.94	0.67
1:F:332:PHE:CE2	1:F:336:LEU:HD11	2.29	0.67
1:F:535:PRO:O	1:F:563:GLN:NE2	2.27	0.67
1:F:686:ILE:HG22	1:F:704:GLN:NE2	2.10	0.67
1:A:116:TYR:CZ	1:A:151:PRO:HA	2.29	0.67
1:A:280:GLN:OE1	1:A:317:SER:HB2	1.95	0.67
1:B:232:GLU:O	1:B:236:ASN:HB2	1.95	0.67
1:C:508:GLU:HG2	1:C:775:PHE:HE1	1.57	0.67
1:F:79:ASN:ND2	1:F:94:CYS:HB2	2.10	0.67
1:E:401:SER:HB3	1:E:608:ASN:HB3	1.74	0.67
1:F:274:LYS:HB3	1:F:432:LYS:HB3	1.76	0.67
1:B:391:MET:HE2	1:B:434:LYS:CE	2.24	0.67
1:D:332:PHE:CE2	1:D:336:LEU:HD11	2.30	0.67
1:D:418:GLN:HA	1:D:422:GLN:NE2	2.10	0.67
1:E:535:PRO:O	1:E:563:GLN:NE2	2.28	0.67
1:B:274:LYS:HB3	1:B:432:LYS:HB3	1.76	0.67
1:C:526:GLU:O	1:C:530:ARG:HB2	1.94	0.67
1:D:116:TYR:CZ	1:D:151:PRO:HA	2.30	0.67
1:F:419:THR:N	1:F:422:GLN:HE21	1.92	0.67
1:A:332:PHE:CE2	1:A:336:LEU:HD11	2.30	0.67
1:B:274:LYS:HG2	1:B:436:GLU:HB2	1.77	0.67
1:B:731:ARG:NH2	1:B:742:ILE:HG21	2.09	0.67
1:D:725:ILE:HD11	1:D:730:PHE:HD1	1.60	0.67
1:F:391:MET:HE2	1:F:434:LYS:CE	2.24	0.67
1:B:116:TYR:CZ	1:B:151:PRO:HA	2.30	0.67
1:B:418:GLN:HA	1:B:422:GLN:NE2	2.09	0.67
1:C:232:GLU:O	1:C:236:ASN:HB2	1.94	0.67
1:D:280:GLN:OE1	1:D:317:SER:HB2	1.94	0.67
1:B:569:PHE:CD1	1:B:570:GLN:N	2.63	0.67
1:C:419:THR:HG23	1:C:422:GLN:CD	2.20	0.67
1:C:79:ASN:ND2	1:C:94:CYS:HB2	2.10	0.66
1:F:537:VAL:HG22	1:F:559:LEU:HD11	1.76	0.66
1:B:725:ILE:HD11	1:B:730:PHE:HD1	1.60	0.66
1:D:537:VAL:HG22	1:D:559:LEU:HD11	1.77	0.66
1:E:332:PHE:CE2	1:E:336:LEU:HD11	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:731:ARG:HH21	1:E:742:ILE:HG21	1.60	0.66
1:B:242:ASN:HB3	1:B:245:SER:HB2	1.76	0.66
1:B:540:LEU:CD1	1:B:559:LEU:HA	2.26	0.66
1:D:281:ALA:O	1:D:284:GLU:HB2	1.95	0.66
1:D:433:ALA:O	1:D:437:ARG:HG3	1.96	0.66
1:A:526:GLU:O	1:A:530:ARG:HB2	1.94	0.66
1:B:103:ASN:O	1:B:107:ARG:HG3	1.95	0.66
1:B:107:ARG:HB3	1:B:112:LEU:HB2	1.78	0.66
1:B:728:GLN:O	1:B:732:GLN:HG2	1.96	0.66
1:C:582:CYS:SG	1:C:591:THR:HB	2.35	0.66
1:C:686:ILE:HG22	1:C:704:GLN:NE2	2.09	0.66
1:E:731:ARG:NH2	1:E:742:ILE:HG21	2.11	0.66
1:E:731:ARG:HH11	1:E:731:ARG:HG3	1.60	0.66
1:F:728:GLN:O	1:F:732:GLN:HG2	1.95	0.66
1:C:274:LYS:HB3	1:C:432:LYS:HB3	1.76	0.66
1:C:596:ALA:O	1:C:600:LYS:HG3	1.96	0.66
1:E:274:LYS:HB3	1:E:432:LYS:HB3	1.77	0.66
1:A:308:GLU:HB3	1:A:312:ASN:HB2	1.77	0.66
1:D:308:GLU:HB3	1:D:312:ASN:HB2	1.77	0.66
1:D:527:LEU:CD1	1:D:563:GLN:HG3	2.26	0.66
1:A:708:ASN:N	1:A:708:ASN:HD22	1.93	0.66
1:B:346:GLU:O	1:B:350:THR:HG23	1.95	0.66
1:C:346:GLU:O	1:C:350:THR:HG23	1.95	0.66
1:C:708:ASN:HD22	1:C:708:ASN:N	1.94	0.66
1:E:433:ALA:O	1:E:437:ARG:HG3	1.95	0.66
1:E:232:GLU:O	1:E:236:ASN:HB2	1.96	0.66
1:F:607:ASP:HA	1:F:610:THR:HB	1.77	0.66
1:A:79:ASN:ND2	1:A:94:CYS:HB2	2.12	0.65
1:A:391:MET:HG2	1:A:434:LYS:HZ1	1.61	0.65
1:A:607:ASP:HA	1:A:610:THR:HB	1.78	0.65
1:C:418:GLN:HA	1:C:422:GLN:NE2	2.11	0.65
1:C:769:ILE:HD13	1:C:774:ILE:HG23	1.78	0.65
1:E:596:ALA:O	1:E:600:LYS:HG3	1.96	0.65
1:A:419:THR:HG23	1:A:422:GLN:CD	2.20	0.65
1:A:725:ILE:HD11	1:A:730:PHE:HD1	1.61	0.65
1:C:728:GLN:O	1:C:732:GLN:HG2	1.96	0.65
1:B:79:ASN:ND2	1:B:94:CYS:HB2	2.11	0.65
1:B:433:ALA:O	1:B:437:ARG:HG3	1.96	0.65
1:B:731:ARG:HH11	1:B:731:ARG:HG3	1.61	0.65
1:D:346:GLU:O	1:D:350:THR:HG23	1.95	0.65
1:C:116:TYR:CZ	1:C:151:PRO:HA	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ALA:O	1:C:284:GLU:HB2	1.97	0.65
1:E:725:ILE:HD11	1:E:730:PHE:HD1	1.60	0.65
1:F:242:ASN:HB3	1:F:245:SER:HB2	1.76	0.65
1:A:391:MET:HE2	1:A:434:LYS:CE	2.26	0.65
1:B:281:ALA:O	1:B:284:GLU:HB2	1.96	0.65
1:C:433:ALA:O	1:C:437:ARG:HG3	1.96	0.65
1:D:686:ILE:HG22	1:D:704:GLN:NE2	2.11	0.65
1:A:77:LYS:H	1:A:77:LYS:CE	2.09	0.65
1:A:433:ALA:O	1:A:437:ARG:HG3	1.96	0.65
1:C:540:LEU:CD1	1:C:559:LEU:HA	2.27	0.65
1:F:391:MET:HG2	1:F:434:LYS:HZ1	1.60	0.65
1:B:332:PHE:CE2	1:B:336:LEU:HD11	2.31	0.65
1:D:596:ALA:O	1:D:600:LYS:HG3	1.97	0.65
1:D:731:ARG:HG3	1:D:731:ARG:NH1	2.11	0.65
1:F:433:ALA:O	1:F:437:ARG:HG3	1.97	0.65
1:A:696:LEU:CD2	1:A:701:VAL:HG21	2.27	0.65
1:B:305:LEU:HD22	1:B:354:ARG:HA	1.79	0.65
1:D:103:ASN:O	1:D:107:ARG:HG3	1.96	0.65
1:E:715:ARG:HG3	1:E:715:ARG:NH1	2.12	0.65
1:F:582:CYS:SG	1:F:591:THR:HB	2.36	0.65
1:F:731:ARG:HH11	1:F:731:ARG:HG3	1.60	0.65
1:F:769:ILE:HD13	1:F:774:ILE:HG23	1.79	0.65
1:E:607:ASP:HA	1:E:610:THR:HB	1.78	0.65
1:F:596:ALA:O	1:F:600:LYS:HG3	1.97	0.65
1:B:419:THR:HG23	1:B:422:GLN:CD	2.22	0.65
1:C:488:LYS:HE2	1:C:529:GLU:OE1	1.97	0.65
1:D:232:GLU:O	1:D:236:ASN:HB2	1.96	0.65
1:D:488:LYS:HE2	1:D:529:GLU:OE1	1.96	0.65
1:E:708:ASN:HD22	1:E:708:ASN:N	1.94	0.65
1:F:526:GLU:O	1:F:530:ARG:HB2	1.96	0.65
1:A:145:LYS:HB2	1:A:148:GLU:CG	2.27	0.64
1:A:540:LEU:CD1	1:A:559:LEU:HA	2.26	0.64
1:D:769:ILE:HD13	1:D:774:ILE:HG23	1.79	0.64
1:E:242:ASN:HB3	1:E:245:SER:HB2	1.80	0.64
1:F:738:ALA:HB1	1:F:741:ALA:HB2	1.78	0.64
1:D:419:THR:HG23	1:D:422:GLN:CD	2.22	0.64
1:D:593:ASN:HD22	1:D:593:ASN:C	2.04	0.64
1:D:728:GLN:O	1:D:732:GLN:HG2	1.96	0.64
1:E:274:LYS:HG2	1:E:436:GLU:HB2	1.78	0.64
1:F:540:LEU:CD1	1:F:559:LEU:HA	2.27	0.64
1:A:232:GLU:O	1:A:236:ASN:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:CYS:SG	1:B:591:THR:HB	2.37	0.64
1:C:391:MET:HE2	1:C:434:LYS:HE3	1.77	0.64
1:A:89:MET:HE1	1:A:100:VAL:HG13	1.79	0.64
1:B:57:VAL:HB	1:B:75:ILE:HD11	1.80	0.64
1:C:332:PHE:CE2	1:C:336:LEU:HD11	2.32	0.64
1:D:607:ASP:HA	1:D:610:THR:HB	1.79	0.64
1:E:728:GLN:O	1:E:732:GLN:HG2	1.97	0.64
1:A:305:LEU:HD22	1:A:354:ARG:HA	1.80	0.64
1:F:376:ALA:HB2	1:F:420:LYS:N	2.13	0.64
1:A:103:ASN:O	1:A:107:ARG:HG3	1.97	0.64
1:A:281:ALA:O	1:A:284:GLU:HB2	1.96	0.64
1:A:418:GLN:HA	1:A:422:GLN:NE2	2.12	0.64
1:A:527:LEU:CD1	1:A:563:GLN:HG3	2.27	0.64
1:B:596:ALA:O	1:B:600:LYS:HG3	1.98	0.64
1:C:145:LYS:HB2	1:C:148:GLU:CG	2.25	0.64
1:E:79:ASN:ND2	1:E:94:CYS:HB2	2.11	0.64
1:E:281:ALA:O	1:E:284:GLU:HB2	1.97	0.64
1:F:274:LYS:HG2	1:F:436:GLU:HB2	1.78	0.64
1:B:715:ARG:HG3	1:B:715:ARG:NH1	2.13	0.64
1:D:79:ASN:ND2	1:D:94:CYS:HB2	2.12	0.64
1:D:274:LYS:HB3	1:D:432:LYS:HB3	1.79	0.64
1:B:607:ASP:HA	1:B:610:THR:HB	1.77	0.64
1:D:593:ASN:ND2	1:D:595:SER:H	1.95	0.64
1:C:527:LEU:CD1	1:C:563:GLN:HG3	2.28	0.64
1:A:196:VAL:O	1:A:196:VAL:HG12	1.98	0.64
1:A:593:ASN:HD22	1:A:593:ASN:C	2.06	0.64
1:C:725:ILE:HD11	1:C:730:PHE:HD1	1.63	0.64
1:E:391:MET:HE2	1:E:434:LYS:HE3	1.79	0.64
1:F:107:ARG:HB3	1:F:112:LEU:HB2	1.80	0.64
1:F:725:ILE:HD11	1:F:730:PHE:HD1	1.63	0.64
1:A:346:GLU:O	1:A:350:THR:HG23	1.97	0.63
1:A:673:THR:O	1:A:677:THR:HG23	1.98	0.63
1:C:593:ASN:HD22	1:C:593:ASN:C	2.05	0.63
1:F:308:GLU:HB3	1:F:312:ASN:HB2	1.81	0.63
1:A:715:ARG:HG3	1:A:715:ARG:NH1	2.13	0.63
1:B:89:MET:HE1	1:B:100:VAL:HG13	1.78	0.63
1:F:708:ASN:HD22	1:F:708:ASN:N	1.94	0.63
1:A:488:LYS:HE2	1:A:529:GLU:OE1	1.98	0.63
1:B:391:MET:HE2	1:B:434:LYS:HE3	1.79	0.63
1:C:103:ASN:O	1:C:107:ARG:HG3	1.99	0.63
1:D:742:ILE:HG23	1:D:743:PRO:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:PHE:CE2	1:B:716:ILE:HD13	2.34	0.63
1:C:196:VAL:O	1:C:196:VAL:HG12	1.97	0.63
1:D:107:ARG:HB3	1:D:112:LEU:HB2	1.79	0.63
1:E:103:ASN:O	1:E:107:ARG:HG3	1.99	0.63
1:C:305:LEU:HD22	1:C:354:ARG:HA	1.79	0.63
1:E:145:LYS:HB2	1:E:148:GLU:CG	2.27	0.63
1:A:742:ILE:HG23	1:A:743:PRO:HD2	1.81	0.63
1:B:145:LYS:HB2	1:B:148:GLU:CG	2.27	0.63
1:C:57:VAL:HB	1:C:75:ILE:HD11	1.80	0.63
1:C:308:GLU:HB3	1:C:312:ASN:HB2	1.79	0.63
1:D:305:LEU:HD22	1:D:354:ARG:HA	1.81	0.63
1:D:708:ASN:HD22	1:D:708:ASN:N	1.95	0.63
1:E:308:GLU:HB3	1:E:312:ASN:HB2	1.80	0.63
1:F:116:TYR:CZ	1:F:151:PRO:HA	2.34	0.63
1:F:271:LEU:HD23	1:F:482:ILE:HG13	1.81	0.63
1:C:107:ARG:HB3	1:C:112:LEU:HB2	1.79	0.63
1:D:174:LEU:N	1:D:174:LEU:HD23	2.13	0.63
1:F:174:LEU:N	1:F:174:LEU:HD23	2.14	0.63
1:F:305:LEU:HD22	1:F:354:ARG:HA	1.81	0.63
1:C:742:ILE:HG23	1:C:743:PRO:HD2	1.81	0.63
1:D:517:PHE:CE2	1:D:716:ILE:HD13	2.33	0.63
1:F:593:ASN:HD22	1:F:593:ASN:C	2.06	0.63
1:F:715:ARG:HG3	1:F:715:ARG:NH1	2.12	0.63
1:B:308:GLU:HB3	1:B:312:ASN:HB2	1.80	0.62
1:A:748:ASP:OD1	1:A:748:ASP:O	2.18	0.62
1:E:107:ARG:HB3	1:E:112:LEU:HB2	1.80	0.62
1:E:517:PHE:CE2	1:E:716:ILE:HD13	2.34	0.62
1:F:391:MET:HE2	1:F:434:LYS:HE3	1.79	0.62
1:E:593:ASN:HD22	1:E:593:ASN:C	2.07	0.62
1:A:107:ARG:HB3	1:A:112:LEU:HB2	1.80	0.62
1:A:274:LYS:HB3	1:A:432:LYS:HB3	1.82	0.62
1:A:686:ILE:HG22	1:A:704:GLN:NE2	2.15	0.62
1:B:488:LYS:HE2	1:B:529:GLU:OE1	1.99	0.62
1:B:673:THR:O	1:B:677:THR:HG23	1.99	0.62
1:B:748:ASP:OD1	1:B:748:ASP:O	2.17	0.62
1:C:715:ARG:HG3	1:C:715:ARG:NH1	2.13	0.62
1:D:748:ASP:OD1	1:D:748:ASP:O	2.18	0.62
1:F:145:LYS:HB2	1:F:148:GLU:CG	2.28	0.62
1:F:418:GLN:HA	1:F:422:GLN:NE2	2.13	0.62
1:A:174:LEU:N	1:A:174:LEU:HD23	2.14	0.62
1:B:174:LEU:N	1:B:174:LEU:HD23	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:ARG:HG3	1:B:731:ARG:NH1	2.15	0.62
1:C:731:ARG:HG3	1:C:731:ARG:NH1	2.13	0.62
1:F:673:THR:O	1:F:677:THR:HG23	1.98	0.62
1:A:377:SER:O	1:A:379:PRO:HD3	2.00	0.62
1:D:715:ARG:HG3	1:D:715:ARG:NH1	2.13	0.62
1:F:527:LEU:CD1	1:F:563:GLN:HG3	2.30	0.62
1:B:377:SER:O	1:B:379:PRO:HD3	2.00	0.62
1:C:748:ASP:OD1	1:C:748:ASP:O	2.18	0.62
1:E:731:ARG:HG3	1:E:731:ARG:NH1	2.14	0.62
1:C:376:ALA:HB2	1:C:420:LYS:N	2.14	0.61
1:E:540:LEU:CD1	1:E:559:LEU:HA	2.30	0.61
1:A:271:LEU:HD23	1:A:482:ILE:HG13	1.81	0.61
1:B:196:VAL:O	1:B:196:VAL:HG12	1.99	0.61
1:B:271:LEU:HD23	1:B:482:ILE:HG13	1.83	0.61
1:B:552:ASP:O	1:B:555:PHE:HB3	2.00	0.61
1:C:517:PHE:CE2	1:C:716:ILE:HD13	2.35	0.61
1:F:232:GLU:O	1:F:236:ASN:HB2	2.00	0.61
1:A:288:HIS:HB3	1:A:292:TYR:CZ	2.35	0.61
1:C:508:GLU:HG3	1:C:771:GLN:H	1.65	0.61
1:E:419:THR:HG23	1:E:422:GLN:CD	2.25	0.61
1:E:488:LYS:HE2	1:E:529:GLU:OE1	2.00	0.61
1:F:225:LEU:N	1:F:225:LEU:HD23	2.15	0.61
1:A:57:VAL:HB	1:A:75:ILE:HD11	1.82	0.61
1:B:742:ILE:HG23	1:B:743:PRO:HD2	1.81	0.61
1:C:271:LEU:HD23	1:C:482:ILE:HG13	1.81	0.61
1:C:673:THR:O	1:C:677:THR:HG23	2.00	0.61
1:F:757:ILE:HA	1:F:760:LEU:HD12	1.82	0.61
1:F:89:MET:HE1	1:F:100:VAL:HG13	1.82	0.61
1:D:145:LYS:HB2	1:D:148:GLU:CG	2.28	0.61
1:E:552:ASP:O	1:E:555:PHE:HB3	2.01	0.61
1:F:103:ASN:O	1:F:107:ARG:HG3	2.00	0.61
1:A:234:PHE:CE2	1:A:289:ILE:HG12	2.36	0.61
1:F:295:ALA:HB2	1:F:310:PHE:HZ	1.65	0.61
1:E:686:ILE:HG22	1:E:704:GLN:NE2	2.16	0.61
1:F:196:VAL:O	1:F:196:VAL:HG12	2.00	0.61
1:F:731:ARG:HG3	1:F:731:ARG:NH1	2.14	0.61
1:A:133:TYR:CD1	1:A:189:LYS:HD2	2.36	0.61
1:A:769:ILE:HD13	1:A:774:ILE:HG23	1.83	0.61
1:D:673:THR:O	1:D:677:THR:HG23	2.01	0.61
1:B:593:ASN:ND2	1:B:595:SER:H	1.98	0.61
1:D:77:LYS:H	1:D:77:LYS:CE	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:VAL:HB	1:F:75:ILE:HD11	1.83	0.61
1:A:731:ARG:HG3	1:A:731:ARG:NH1	2.10	0.60
1:C:593:ASN:ND2	1:C:595:SER:H	1.97	0.60
1:D:271:LEU:HD23	1:D:482:ILE:HG13	1.82	0.60
1:B:323:ILE:HG22	1:B:324:PRO:CD	2.26	0.60
1:B:522:GLN:N	1:B:523:PRO:HD2	2.15	0.60
1:C:174:LEU:HD23	1:C:174:LEU:N	2.16	0.60
1:D:388:CYS:SG	1:D:393:ILE:HG22	2.41	0.60
1:D:757:ILE:HA	1:D:760:LEU:HD12	1.84	0.60
1:E:742:ILE:HG23	1:E:743:PRO:HD2	1.83	0.60
1:B:89:MET:CE	1:B:100:VAL:HG13	2.32	0.60
1:C:522:GLN:N	1:C:523:PRO:HD2	2.16	0.60
1:E:174:LEU:N	1:E:174:LEU:HD23	2.16	0.60
1:E:664:LYS:O	1:E:668:THR:HG23	2.00	0.60
1:E:769:ILE:HD13	1:E:774:ILE:HG23	1.82	0.60
1:A:323:ILE:HG22	1:A:324:PRO:CD	2.26	0.60
1:A:593:ASN:ND2	1:A:595:SER:H	1.98	0.60
1:B:288:HIS:HB3	1:B:292:TYR:CZ	2.37	0.60
1:D:391:MET:HG2	1:D:434:LYS:NZ	2.16	0.60
1:E:225:LEU:N	1:E:225:LEU:HD23	2.16	0.60
1:E:673:THR:O	1:E:677:THR:HG23	2.01	0.60
1:A:522:GLN:N	1:A:523:PRO:HD2	2.15	0.60
1:C:664:LYS:O	1:C:668:THR:HG23	2.02	0.60
1:F:419:THR:HG23	1:F:422:GLN:CD	2.26	0.60
1:A:376:ALA:HB2	1:A:420:LYS:N	2.16	0.60
1:D:225:LEU:N	1:D:225:LEU:HD23	2.15	0.60
1:A:382:THR:O	1:A:385:GLN:HB2	2.02	0.60
1:B:418:GLN:HA	1:B:422:GLN:HE21	1.66	0.60
1:B:686:ILE:HG22	1:B:704:GLN:NE2	2.16	0.60
1:E:57:VAL:HB	1:E:75:ILE:HD11	1.83	0.60
1:E:288:HIS:HB3	1:E:292:TYR:CZ	2.36	0.60
1:E:305:LEU:HD22	1:E:354:ARG:HA	1.82	0.60
1:E:377:SER:O	1:E:379:PRO:HD3	2.01	0.60
1:E:757:ILE:HA	1:E:760:LEU:HD12	1.84	0.60
1:F:133:TYR:CD1	1:F:189:LYS:HD2	2.36	0.60
1:A:285:ARG:HB2	1:A:291:TYR:CZ	2.37	0.60
1:B:376:ALA:HB2	1:B:420:LYS:N	2.17	0.60
1:D:664:LYS:O	1:D:668:THR:HG23	2.02	0.60
1:F:696:LEU:CD2	1:F:701:VAL:HG21	2.28	0.60
1:B:77:LYS:CE	1:B:77:LYS:H	2.15	0.60
1:C:77:LYS:CE	1:C:77:LYS:H	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:MET:HE1	1:C:100:VAL:HG13	1.83	0.60
1:E:593:ASN:ND2	1:E:595:SER:H	1.98	0.60
1:F:664:LYS:O	1:F:668:THR:HG23	2.02	0.60
1:C:288:HIS:HB3	1:C:292:TYR:CZ	2.36	0.60
1:C:391:MET:HG2	1:C:434:LYS:NZ	2.16	0.60
1:D:234:PHE:CE2	1:D:289:ILE:HG12	2.37	0.60
1:E:80:PRO:HD2	1:E:83:PHE:CE2	2.37	0.60
1:E:527:LEU:CD1	1:E:563:GLN:HG3	2.31	0.60
1:F:171:GLN:OE1	1:F:678:ASN:HB3	2.02	0.60
1:A:751:GLN:OE1	1:C:692:ARG:CZ	2.50	0.59
1:B:225:LEU:N	1:B:225:LEU:HD23	2.16	0.59
1:E:391:MET:HG2	1:E:434:LYS:NZ	2.17	0.59
1:A:508:GLU:HG3	1:A:771:GLN:H	1.66	0.59
1:B:664:LYS:O	1:B:668:THR:HG23	2.02	0.59
1:F:144:LYS:HG3	1:F:149:MET:HG3	1.83	0.59
1:F:517:PHE:CE1	1:F:716:ILE:HD13	2.37	0.59
1:A:88:ASP:O	1:A:91:GLU:HB2	2.02	0.59
1:F:77:LYS:CE	1:F:77:LYS:H	2.14	0.59
1:F:403:LEU:O	1:F:404:THR:HG23	2.02	0.59
1:A:391:MET:HG2	1:A:434:LYS:NZ	2.17	0.59
1:B:382:THR:O	1:B:385:GLN:HB2	2.02	0.59
1:F:508:GLU:HG3	1:F:771:GLN:H	1.68	0.59
1:D:288:HIS:HB3	1:D:292:TYR:CZ	2.38	0.59
1:A:552:ASP:O	1:A:555:PHE:HB3	2.02	0.59
1:B:234:PHE:CE2	1:B:289:ILE:HG12	2.38	0.59
1:B:593:ASN:HD22	1:B:593:ASN:C	2.10	0.59
1:B:696:LEU:CD2	1:B:701:VAL:HG21	2.30	0.59
1:B:767:TYR:O	1:B:768:ARG:NH1	2.35	0.59
1:C:285:ARG:HB2	1:C:291:TYR:CZ	2.37	0.59
1:C:323:ILE:HG22	1:C:324:PRO:CD	2.26	0.59
1:D:696:LEU:CD2	1:D:701:VAL:HG21	2.30	0.59
1:F:488:LYS:HE2	1:F:529:GLU:OE1	2.03	0.59
1:F:767:TYR:O	1:F:768:ARG:NH1	2.36	0.59
1:A:136:LYS:O	1:A:139:ASP:HB2	2.03	0.59
1:A:757:ILE:HG12	1:A:762:LEU:HD12	1.85	0.59
1:D:171:GLN:OE1	1:D:678:ASN:HB3	2.02	0.59
1:D:377:SER:O	1:D:379:PRO:HD3	2.02	0.59
1:E:271:LEU:HD23	1:E:482:ILE:HG13	1.83	0.59
1:F:552:ASP:O	1:F:555:PHE:HB3	2.02	0.59
1:D:522:GLN:N	1:D:523:PRO:HD2	2.17	0.59
1:E:80:PRO:HD2	1:E:83:PHE:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:535:PRO:HB2	1:E:540:LEU:HD21	1.84	0.59
1:C:710:VAL:O	1:C:714:ILE:HG13	2.03	0.59
1:E:376:ALA:HB2	1:E:420:LYS:N	2.18	0.59
1:F:753:CYS:HA	1:F:756:MET:HE3	1.85	0.59
1:C:133:TYR:CD1	1:C:189:LYS:HD2	2.37	0.59
1:C:377:SER:O	1:C:379:PRO:HD3	2.02	0.59
1:E:61:LEU:O	1:E:65:GLY:HA2	2.03	0.59
1:E:77:LYS:CE	1:E:77:LYS:H	2.15	0.59
1:F:593:ASN:ND2	1:F:595:SER:H	2.00	0.59
1:A:77:LYS:H	1:A:77:LYS:HZ2	1.51	0.58
1:B:80:PRO:HD2	1:B:83:PHE:CD2	2.38	0.58
1:B:419:THR:N	1:B:422:GLN:HG3	2.18	0.58
1:B:606:ASN:HB3	1:B:609:VAL:CG1	2.33	0.58
1:D:535:PRO:HB2	1:D:540:LEU:HD21	1.84	0.58
1:D:540:LEU:CD1	1:D:559:LEU:HA	2.33	0.58
1:E:136:LYS:O	1:E:139:ASP:HB2	2.04	0.58
1:B:748:ASP:OD1	1:B:748:ASP:C	2.46	0.58
1:C:225:LEU:N	1:C:225:LEU:HD23	2.17	0.58
1:D:152:HIS:O	1:D:156:ILE:HD12	2.03	0.58
1:F:368:LYS:O	1:F:376:ALA:HA	2.03	0.58
1:B:742:ILE:HD11	1:B:752:ALA:C	2.28	0.58
1:B:757:ILE:HA	1:B:760:LEU:HD12	1.86	0.58
1:C:89:MET:CE	1:C:100:VAL:HG13	2.33	0.58
1:C:544:GLU:HG3	1:C:555:PHE:CB	2.31	0.58
1:E:522:GLN:N	1:E:523:PRO:HD2	2.18	0.58
1:E:731:ARG:HG2	1:E:756:MET:HE1	1.85	0.58
1:B:757:ILE:HG12	1:B:762:LEU:HD12	1.85	0.58
1:D:748:ASP:OD1	1:D:748:ASP:C	2.46	0.58
1:E:144:LYS:HG3	1:E:149:MET:HG3	1.85	0.58
1:E:180:GLY:C	1:E:686:ILE:HD12	2.27	0.58
1:A:225:LEU:N	1:A:225:LEU:HD23	2.17	0.58
1:A:606:ASN:HB3	1:A:609:VAL:CG1	2.32	0.58
1:D:349:GLN:O	1:D:353:LEU:HG	2.03	0.58
1:E:696:LEU:CD2	1:E:701:VAL:HG21	2.29	0.58
1:A:403:LEU:O	1:A:404:THR:HG23	2.03	0.58
1:D:382:THR:O	1:D:385:GLN:HB2	2.03	0.58
1:B:508:GLU:HG3	1:B:771:GLN:H	1.69	0.58
1:B:769:ILE:HD13	1:B:774:ILE:HG23	1.85	0.58
1:C:748:ASP:OD1	1:C:748:ASP:C	2.46	0.58
1:C:757:ILE:HA	1:C:760:LEU:HD12	1.85	0.58
1:F:288:HIS:HB3	1:F:292:TYR:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:748:ASP:OD1	1:F:748:ASP:C	2.47	0.58
1:E:133:TYR:CD1	1:E:189:LYS:HD2	2.38	0.58
1:E:285:ARG:HB2	1:E:291:TYR:CZ	2.39	0.58
1:F:61:LEU:O	1:F:65:GLY:HA2	2.04	0.58
1:F:173:ILE:C	1:F:174:LEU:HD23	2.28	0.58
1:A:368:LYS:O	1:A:376:ALA:HA	2.04	0.58
1:B:538:LEU:HD12	1:B:664:LYS:HD2	1.85	0.58
1:C:368:LYS:O	1:C:376:ALA:HA	2.04	0.58
1:D:295:ALA:HB2	1:D:310:PHE:HZ	1.69	0.58
1:E:196:VAL:O	1:E:196:VAL:HG12	2.02	0.58
1:F:88:ASP:O	1:F:91:GLU:HB2	2.04	0.58
1:F:544:GLU:HG3	1:F:555:PHE:CB	2.33	0.58
1:A:517:PHE:CE2	1:A:716:ILE:HD13	2.39	0.58
1:B:133:TYR:CD1	1:B:189:LYS:HD2	2.39	0.58
1:C:753:CYS:HA	1:C:756:MET:HE3	1.85	0.58
1:D:173:ILE:C	1:D:174:LEU:HD23	2.28	0.58
1:D:376:ALA:HB2	1:D:420:LYS:N	2.17	0.58
1:D:418:GLN:HA	1:D:422:GLN:HE21	1.68	0.58
1:E:234:PHE:CE2	1:E:289:ILE:HG12	2.39	0.58
1:E:418:GLN:HA	1:E:422:GLN:HE21	1.68	0.58
1:A:80:PRO:HD2	1:A:83:PHE:CD2	2.39	0.57
1:C:144:LYS:HG3	1:C:149:MET:HG3	1.86	0.57
1:D:88:ASP:O	1:D:91:GLU:HB2	2.04	0.57
1:E:606:ASN:HB3	1:E:609:VAL:CG1	2.33	0.57
1:F:391:MET:HG2	1:F:434:LYS:NZ	2.19	0.57
1:A:180:GLY:C	1:A:686:ILE:HD12	2.28	0.57
1:A:295:ALA:HB2	1:A:310:PHE:HZ	1.68	0.57
1:A:538:LEU:HD12	1:A:664:LYS:HD2	1.86	0.57
1:A:544:GLU:HG3	1:A:555:PHE:CB	2.32	0.57
1:B:80:PRO:HD2	1:B:83:PHE:CE2	2.39	0.57
1:C:80:PRO:HD2	1:C:83:PHE:CD2	2.39	0.57
1:C:382:THR:O	1:C:385:GLN:HB2	2.04	0.57
1:E:594:ALA:HA	1:E:597:TRP:CD1	2.39	0.57
1:F:606:ASN:HB3	1:F:609:VAL:CG1	2.34	0.57
1:B:171:GLN:OE1	1:B:678:ASN:HB3	2.04	0.57
1:B:288:HIS:HB3	1:B:292:TYR:CE1	2.39	0.57
1:C:77:LYS:H	1:C:77:LYS:HZ2	1.52	0.57
1:C:418:GLN:HA	1:C:422:GLN:HE21	1.68	0.57
1:D:57:VAL:HB	1:D:75:ILE:HD11	1.83	0.57
1:D:144:LYS:HG3	1:D:149:MET:HG3	1.86	0.57
1:A:144:LYS:HG3	1:A:149:MET:HG3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:MET:HE2	1:A:434:LYS:HE3	1.84	0.57
1:A:748:ASP:OD1	1:A:748:ASP:C	2.46	0.57
1:B:88:ASP:O	1:B:91:GLU:HB2	2.04	0.57
1:B:725:ILE:HD11	1:B:730:PHE:CD1	2.39	0.57
1:C:180:GLY:C	1:C:686:ILE:HD12	2.30	0.57
1:D:606:ASN:HB3	1:D:609:VAL:CG1	2.35	0.57
1:E:702:LEU:O	1:E:706:ARG:HG3	2.05	0.57
1:A:80:PRO:HD2	1:A:83:PHE:CE2	2.38	0.57
1:A:742:ILE:HD11	1:A:752:ALA:C	2.29	0.57
1:B:77:LYS:H	1:B:77:LYS:HZ2	1.51	0.57
1:C:295:ALA:HB2	1:C:310:PHE:HZ	1.68	0.57
1:C:552:ASP:O	1:C:555:PHE:HB3	2.04	0.57
1:D:41:LYS:HB2	1:D:42:HIS:CE1	2.39	0.57
1:D:565:ASN:O	1:D:566:HIS:C	2.48	0.57
1:F:377:SER:O	1:F:379:PRO:HD3	2.04	0.57
1:E:178:GLU:OE2	1:E:686:ILE:HG21	2.05	0.57
1:E:295:ALA:HB2	1:E:310:PHE:HZ	1.70	0.57
1:F:742:ILE:HD11	1:F:752:ALA:C	2.29	0.57
1:A:288:HIS:HB3	1:A:292:TYR:CE1	2.40	0.57
1:D:725:ILE:HD11	1:D:730:PHE:CD1	2.40	0.57
1:D:767:TYR:O	1:D:768:ARG:NH1	2.37	0.57
1:F:80:PRO:HD2	1:F:83:PHE:CD2	2.40	0.57
1:B:180:GLY:C	1:B:686:ILE:HD12	2.29	0.57
1:B:540:LEU:HD12	1:B:559:LEU:HD12	1.87	0.57
1:B:710:VAL:O	1:B:714:ILE:HG13	2.04	0.57
1:C:61:LEU:O	1:C:65:GLY:HA2	2.05	0.57
1:C:79:ASN:HD21	1:C:94:CYS:HB2	1.70	0.57
1:D:753:CYS:HA	1:D:756:MET:HE3	1.87	0.57
1:E:368:LYS:O	1:E:376:ALA:HA	2.05	0.57
1:E:544:GLU:HG3	1:E:555:PHE:CB	2.34	0.57
1:B:61:LEU:O	1:B:65:GLY:HA2	2.04	0.57
1:B:368:LYS:O	1:B:376:ALA:HA	2.05	0.57
1:B:565:ASN:O	1:B:566:HIS:C	2.48	0.57
1:D:552:ASP:O	1:D:555:PHE:HB3	2.04	0.57
1:D:738:ALA:O	1:D:741:ALA:CB	2.53	0.57
1:F:418:GLN:HA	1:F:422:GLN:HE21	1.70	0.57
1:F:522:GLN:N	1:F:523:PRO:HD2	2.19	0.57
1:A:361:GLN:HG2	1:A:386:LYS:HB2	1.87	0.57
1:C:565:ASN:O	1:C:566:HIS:C	2.48	0.57
1:D:86:VAL:HG23	1:D:103:ASN:ND2	2.20	0.57
1:E:79:ASN:HD21	1:E:94:CYS:HB2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:538:LEU:HD12	1:E:664:LYS:HD2	1.87	0.57
1:F:89:MET:CE	1:F:100:VAL:HG13	2.35	0.57
1:F:382:THR:O	1:F:385:GLN:HB2	2.04	0.57
1:A:171:GLN:OE1	1:A:678:ASN:HB3	2.05	0.56
1:B:391:MET:HG2	1:B:434:LYS:NZ	2.18	0.56
1:C:403:LEU:O	1:C:404:THR:HG23	2.05	0.56
1:E:278:ILE:HD13	1:E:432:LYS:HD3	1.87	0.56
1:E:376:ALA:O	1:E:403:LEU:HD22	2.05	0.56
1:E:743:PRO:HD2	1:E:747:MET:HG2	1.87	0.56
1:E:767:TYR:O	1:E:768:ARG:NH1	2.36	0.56
1:F:742:ILE:HG23	1:F:743:PRO:HD2	1.86	0.56
1:A:767:TYR:O	1:A:768:ARG:NH1	2.36	0.56
1:C:738:ALA:O	1:C:741:ALA:CB	2.53	0.56
1:D:80:PRO:HD2	1:D:83:PHE:CD2	2.40	0.56
1:D:288:HIS:HB3	1:D:292:TYR:CE1	2.40	0.56
1:E:403:LEU:O	1:E:404:THR:HG23	2.05	0.56
1:E:508:GLU:HG3	1:E:771:GLN:H	1.70	0.56
1:E:725:ILE:HD11	1:E:730:PHE:CD1	2.39	0.56
1:E:753:CYS:HA	1:E:756:MET:HE3	1.87	0.56
1:F:757:ILE:HG23	1:F:762:LEU:HB2	1.87	0.56
1:A:256:PHE:O	1:A:458:ALA:HB3	2.05	0.56
1:B:318:ASN:O	1:B:319:GLY:C	2.49	0.56
1:B:731:ARG:HG2	1:B:756:MET:HE1	1.86	0.56
1:B:753:CYS:HA	1:B:756:MET:HE3	1.86	0.56
1:C:136:LYS:O	1:C:139:ASP:HB2	2.05	0.56
1:C:686:ILE:HG22	1:C:704:GLN:HE22	1.71	0.56
1:D:133:TYR:CD1	1:D:189:LYS:HD2	2.40	0.56
1:D:323:ILE:HG22	1:D:324:PRO:CD	2.26	0.56
1:E:70:LEU:HD12	1:E:71:SER:O	2.06	0.56
1:E:323:ILE:HG23	1:E:324:PRO:CD	2.12	0.56
1:A:738:ALA:O	1:A:741:ALA:CB	2.53	0.56
1:B:41:LYS:HB2	1:B:42:HIS:CE1	2.41	0.56
1:B:144:LYS:HG3	1:B:149:MET:HG3	1.88	0.56
1:B:295:ALA:HB2	1:B:310:PHE:HZ	1.69	0.56
1:C:540:LEU:HD12	1:C:559:LEU:HD12	1.87	0.56
1:C:540:LEU:HD21	1:C:562:GLU:HG3	1.87	0.56
1:C:742:ILE:HD11	1:C:752:ALA:C	2.30	0.56
1:A:731:ARG:HG2	1:A:756:MET:HE1	1.88	0.56
1:B:738:ALA:O	1:B:741:ALA:CB	2.53	0.56
1:D:742:ILE:HD11	1:D:752:ALA:C	2.30	0.56
1:A:173:ILE:C	1:A:174:LEU:HD23	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LEU:HD21	1:A:562:GLU:HG3	1.87	0.56
1:B:361:GLN:HG2	1:B:386:LYS:HB2	1.87	0.56
1:C:88:ASP:O	1:C:91:GLU:HB2	2.05	0.56
1:D:710:VAL:O	1:D:714:ILE:HG13	2.06	0.56
1:E:288:HIS:HB3	1:E:292:TYR:CE1	2.41	0.56
1:F:308:GLU:HB2	1:F:313:TYR:CZ	2.41	0.56
1:A:89:MET:CE	1:A:100:VAL:HG13	2.36	0.56
1:A:108:TYR:CD2	1:A:696:LEU:HD12	2.40	0.56
1:B:278:ILE:HD13	1:B:432:LYS:HD3	1.87	0.56
1:D:256:PHE:O	1:D:458:ALA:HB3	2.04	0.56
1:D:544:GLU:HG3	1:D:555:PHE:CB	2.33	0.56
1:E:88:ASP:O	1:E:91:GLU:HB2	2.06	0.56
1:E:382:THR:O	1:E:385:GLN:HB2	2.04	0.56
1:F:80:PRO:HD2	1:F:83:PHE:CE2	2.40	0.56
1:F:748:ASP:OD1	1:F:748:ASP:O	2.24	0.56
1:A:41:LYS:HB2	1:A:42:HIS:CE1	2.40	0.56
1:B:403:LEU:O	1:B:404:THR:HG23	2.05	0.56
1:D:361:GLN:HG2	1:D:386:LYS:HB2	1.88	0.56
1:F:285:ARG:HB2	1:F:291:TYR:CZ	2.41	0.56
1:A:70:LEU:HD12	1:A:71:SER:O	2.06	0.56
1:A:565:ASN:O	1:A:566:HIS:C	2.48	0.56
1:A:664:LYS:O	1:A:668:THR:HG23	2.05	0.56
1:C:80:PRO:HD2	1:C:83:PHE:CE2	2.40	0.56
1:D:318:ASN:O	1:D:319:GLY:C	2.49	0.56
1:E:41:LYS:HB2	1:E:42:HIS:CE1	2.41	0.56
1:B:578:LYS:C	1:B:579:THR:HG23	2.31	0.56
1:C:278:ILE:HD13	1:C:432:LYS:HD3	1.88	0.56
1:E:171:GLN:OE1	1:E:678:ASN:HB3	2.05	0.56
1:E:308:GLU:HB2	1:E:313:TYR:CZ	2.41	0.56
1:E:563:GLN:O	1:E:565:ASN:N	2.39	0.56
1:F:41:LYS:HB2	1:F:42:HIS:CE1	2.41	0.56
1:A:308:GLU:HB2	1:A:313:TYR:CZ	2.41	0.55
1:A:710:VAL:O	1:A:714:ILE:HG13	2.05	0.55
1:A:757:ILE:HA	1:A:760:LEU:HD12	1.88	0.55
1:C:725:ILE:HD11	1:C:730:PHE:CD1	2.42	0.55
1:D:80:PRO:HD2	1:D:83:PHE:CE2	2.42	0.55
1:F:594:ALA:HA	1:F:597:TRP:CD1	2.42	0.55
1:F:743:PRO:CD	1:F:747:MET:SD	2.95	0.55
1:B:301:MET:HA	1:B:304:ASP:HB3	1.88	0.55
1:B:517:PHE:CZ	1:B:716:ILE:HD13	2.41	0.55
1:D:89:MET:HE1	1:D:100:VAL:HG13	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:GLY:C	1:D:686:ILE:HD12	2.31	0.55
1:E:361:GLN:HG2	1:E:386:LYS:HB2	1.88	0.55
1:E:757:ILE:HG12	1:E:762:LEU:HD12	1.87	0.55
1:A:61:LEU:O	1:A:65:GLY:HA2	2.06	0.55
1:C:41:LYS:HB2	1:C:42:HIS:CE1	2.42	0.55
1:D:61:LEU:O	1:D:65:GLY:HA2	2.07	0.55
1:D:301:MET:HA	1:D:304:ASP:HB3	1.89	0.55
1:E:89:MET:CE	1:E:100:VAL:HG13	2.37	0.55
1:E:578:LYS:C	1:E:579:THR:HG23	2.31	0.55
1:F:540:LEU:HD21	1:F:562:GLU:HG3	1.88	0.55
1:F:690:GLU:HG2	1:F:692:ARG:NH2	2.22	0.55
1:A:349:GLN:O	1:A:353:LEU:HG	2.06	0.55
1:A:753:CYS:HA	1:A:756:MET:HE3	1.88	0.55
1:B:79:ASN:HD21	1:B:94:CYS:HB2	1.71	0.55
1:C:318:ASN:O	1:C:319:GLY:C	2.49	0.55
1:D:97:GLU:HA	1:D:711:LEU:HD11	1.88	0.55
1:D:578:LYS:C	1:D:579:THR:HG23	2.31	0.55
1:E:89:MET:HE1	1:E:100:VAL:HG13	1.86	0.55
1:E:349:GLN:O	1:E:353:LEU:HG	2.06	0.55
1:B:327:GLN:O	1:B:330:GLU:HB2	2.07	0.55
1:C:152:HIS:O	1:C:156:ILE:HD12	2.07	0.55
1:C:173:ILE:C	1:C:174:LEU:HD23	2.32	0.55
1:C:308:GLU:HB2	1:C:313:TYR:CZ	2.42	0.55
1:C:696:LEU:CD2	1:C:701:VAL:HG21	2.33	0.55
1:A:70:LEU:HD13	1:A:74:ASP:HB2	1.88	0.55
1:A:460:PHE:CD1	1:A:460:PHE:C	2.85	0.55
1:B:544:GLU:HG3	1:B:555:PHE:CB	2.34	0.55
1:C:757:ILE:HG12	1:C:762:LEU:HD12	1.87	0.55
1:D:419:THR:N	1:D:422:GLN:HG3	2.19	0.55
1:A:86:VAL:HG23	1:A:103:ASN:ND2	2.22	0.55
1:B:95:LEU:HD11	1:B:714:ILE:HG21	1.89	0.55
1:B:285:ARG:HB2	1:B:291:TYR:CZ	2.42	0.55
1:C:234:PHE:CE2	1:C:289:ILE:HG12	2.42	0.55
1:C:594:ALA:HA	1:C:597:TRP:CD1	2.41	0.55
1:D:285:ARG:HB2	1:D:291:TYR:CZ	2.41	0.55
1:E:747:MET:HE3	1:E:751:GLN:HB3	1.89	0.55
1:F:70:LEU:HD12	1:F:71:SER:O	2.06	0.55
1:F:79:ASN:HD21	1:F:94:CYS:HB2	1.70	0.55
1:A:318:ASN:O	1:A:319:GLY:C	2.49	0.55
1:B:108:TYR:CD2	1:B:696:LEU:HD12	2.42	0.55
1:D:178:GLU:OE2	1:D:686:ILE:HG21	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:LEU:O	1:D:404:THR:HG23	2.07	0.55
1:E:742:ILE:HD11	1:E:752:ALA:C	2.31	0.55
1:A:278:ILE:HD13	1:A:432:LYS:HD3	1.89	0.55
1:B:594:ALA:HA	1:B:597:TRP:CD1	2.42	0.55
1:C:702:LEU:O	1:C:706:ARG:HG3	2.07	0.55
1:E:748:ASP:OD1	1:E:748:ASP:C	2.50	0.55
1:F:535:PRO:HB2	1:F:540:LEU:HD21	1.88	0.55
1:F:540:LEU:HD12	1:F:559:LEU:HD12	1.89	0.55
1:A:702:LEU:O	1:A:706:ARG:HG3	2.06	0.55
1:B:376:ALA:O	1:B:403:LEU:HD22	2.07	0.55
1:C:171:GLN:OE1	1:C:678:ASN:HB3	2.06	0.55
1:E:757:ILE:HG23	1:E:762:LEU:HB2	1.88	0.55
1:F:349:GLN:O	1:F:353:LEU:HG	2.08	0.55
1:A:418:GLN:HA	1:A:422:GLN:HE21	1.70	0.54
1:A:725:ILE:HD11	1:A:730:PHE:CD1	2.40	0.54
1:B:308:GLU:HB2	1:B:313:TYR:CZ	2.42	0.54
1:B:540:LEU:HD21	1:B:562:GLU:HG3	1.88	0.54
1:B:173:ILE:C	1:B:174:LEU:HD23	2.32	0.54
1:C:538:LEU:HD12	1:C:664:LYS:HD2	1.89	0.54
1:D:243:ASP:OD2	1:D:324:PRO:HG3	2.07	0.54
1:F:77:LYS:H	1:F:77:LYS:HZ2	1.55	0.54
1:F:136:LYS:O	1:F:139:ASP:HB2	2.07	0.54
1:F:757:ILE:HG12	1:F:762:LEU:HD12	1.88	0.54
1:B:136:LYS:O	1:B:139:ASP:HB2	2.07	0.54
1:C:301:MET:HA	1:C:304:ASP:HB3	1.89	0.54
1:E:725:ILE:O	1:E:773:LYS:HB2	2.07	0.54
1:D:368:LYS:O	1:D:376:ALA:HA	2.08	0.54
1:D:757:ILE:HG12	1:D:762:LEU:HD12	1.89	0.54
1:F:578:LYS:C	1:F:579:THR:HG23	2.33	0.54
1:F:710:VAL:O	1:F:714:ILE:HG13	2.06	0.54
1:A:97:GLU:HA	1:A:711:LEU:HD11	1.89	0.54
1:B:349:GLN:O	1:B:353:LEU:HG	2.06	0.54
1:C:97:GLU:HA	1:C:711:LEU:HD11	1.89	0.54
1:C:535:PRO:HB2	1:C:540:LEU:HD21	1.89	0.54
1:D:136:LYS:O	1:D:139:ASP:HB2	2.07	0.54
1:D:508:GLU:HG3	1:D:771:GLN:H	1.71	0.54
1:E:70:LEU:HD13	1:E:74:ASP:HB2	1.90	0.54
1:E:86:VAL:HG23	1:E:103:ASN:ND2	2.22	0.54
1:F:180:GLY:C	1:F:686:ILE:HD12	2.32	0.54
1:A:37:VAL:HG11	1:A:59:VAL:HG21	1.90	0.54
1:B:286:THR:OG1	1:B:287:PHE:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:GLU:HB2	1:D:313:TYR:CZ	2.42	0.54
1:E:243:ASP:OD2	1:E:324:PRO:HG3	2.08	0.54
1:F:117:SER:HB2	1:F:714:ILE:HD11	1.89	0.54
1:F:565:ASN:O	1:F:566:HIS:C	2.50	0.54
1:B:535:PRO:HB2	1:B:540:LEU:HD21	1.89	0.54
1:B:757:ILE:HG23	1:B:762:LEU:HB2	1.88	0.54
1:C:286:THR:OG1	1:C:287:PHE:N	2.40	0.54
1:C:578:LYS:C	1:C:579:THR:HG23	2.32	0.54
1:C:606:ASN:HB3	1:C:609:VAL:CG1	2.38	0.54
1:F:702:LEU:O	1:F:706:ARG:HG3	2.07	0.54
1:A:152:HIS:O	1:A:156:ILE:HD12	2.07	0.54
1:B:70:LEU:HD13	1:B:74:ASP:HB2	1.89	0.54
1:B:256:PHE:O	1:B:458:ALA:HB3	2.08	0.54
1:D:89:MET:CE	1:D:100:VAL:HG13	2.37	0.54
1:E:173:ILE:C	1:E:174:LEU:HD23	2.33	0.54
1:E:517:PHE:CZ	1:E:716:ILE:HD13	2.43	0.54
1:E:743:PRO:HD2	1:E:747:MET:CG	2.38	0.54
1:F:278:ILE:HD13	1:F:432:LYS:HD3	1.88	0.54
1:F:686:ILE:HG22	1:F:704:GLN:HE22	1.72	0.54
1:C:731:ARG:HG2	1:C:756:MET:HE1	1.90	0.54
1:D:79:ASN:HD21	1:D:94:CYS:HB2	1.72	0.54
1:E:499:ILE:HG22	1:E:500:LEU:N	2.22	0.54
1:F:301:MET:HA	1:F:304:ASP:HB3	1.90	0.54
1:A:747:MET:HE3	1:A:751:GLN:HB3	1.90	0.54
1:A:757:ILE:HG23	1:A:762:LEU:HB2	1.90	0.54
1:C:269:THR:HG23	1:C:443:LEU:HD22	1.90	0.54
1:C:767:TYR:O	1:C:768:ARG:NH1	2.38	0.54
1:A:578:LYS:C	1:A:579:THR:HG23	2.32	0.53
1:A:594:ALA:HA	1:A:597:TRP:CD1	2.43	0.53
1:A:751:GLN:NE2	1:C:692:ARG:NH2	2.40	0.53
1:E:540:LEU:HD12	1:E:559:LEU:HD12	1.88	0.53
1:F:85:LYS:HE2	1:F:110:SER:OG	2.07	0.53
1:A:540:LEU:HD12	1:A:559:LEU:HD12	1.90	0.53
1:D:278:ILE:HD13	1:D:432:LYS:HD3	1.89	0.53
1:E:535:PRO:HB2	1:E:540:LEU:CD2	2.39	0.53
1:F:86:VAL:HG23	1:F:103:ASN:ND2	2.23	0.53
1:F:725:ILE:HD11	1:F:730:PHE:CD1	2.42	0.53
1:A:79:ASN:HD21	1:A:94:CYS:HB2	1.71	0.53
1:B:97:GLU:HA	1:B:711:LEU:HD11	1.90	0.53
1:B:743:PRO:HD2	1:B:747:MET:HG2	1.90	0.53
1:C:108:TYR:CD2	1:C:696:LEU:HD12	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:GLN:O	1:C:565:ASN:N	2.41	0.53
1:D:72:LYS:HA	1:D:75:ILE:CD1	2.38	0.53
1:E:419:THR:N	1:E:422:GLN:HG3	2.20	0.53
1:F:361:GLN:HG2	1:F:386:LYS:HB2	1.90	0.53
1:F:538:LEU:HD12	1:F:664:LYS:HD2	1.90	0.53
1:F:563:GLN:O	1:F:565:ASN:N	2.41	0.53
1:A:563:GLN:O	1:A:565:ASN:N	2.41	0.53
1:B:70:LEU:HD12	1:B:71:SER:O	2.07	0.53
1:B:219:GLU:O	1:B:220:LEU:C	2.52	0.53
1:C:35:VAL:HG22	1:C:36:TRP:H	1.74	0.53
1:C:70:LEU:HD12	1:C:71:SER:O	2.08	0.53
1:D:563:GLN:O	1:D:565:ASN:N	2.41	0.53
1:E:565:ASN:O	1:E:566:HIS:C	2.50	0.53
1:F:97:GLU:HA	1:F:711:LEU:HD11	1.90	0.53
1:F:256:PHE:O	1:F:458:ALA:HB3	2.07	0.53
1:F:460:PHE:CD1	1:F:460:PHE:C	2.86	0.53
1:A:77:LYS:H	1:A:77:LYS:NZ	2.06	0.53
1:A:743:PRO:HD2	1:A:747:MET:HG2	1.90	0.53
1:B:37:VAL:HG11	1:B:59:VAL:HG21	1.90	0.53
1:C:86:VAL:HG23	1:C:103:ASN:ND2	2.24	0.53
1:C:349:GLN:O	1:C:353:LEU:HG	2.08	0.53
1:C:419:THR:HG23	1:C:422:GLN:CG	2.39	0.53
1:D:510:ILE:HD12	1:D:768:ARG:HB3	1.89	0.53
1:D:517:PHE:CZ	1:D:716:ILE:HD13	2.43	0.53
1:D:725:ILE:O	1:D:773:LYS:HB2	2.08	0.53
1:E:97:GLU:HA	1:E:711:LEU:HD11	1.90	0.53
1:E:318:ASN:O	1:E:319:GLY:C	2.51	0.53
1:E:738:ALA:O	1:E:741:ALA:CB	2.57	0.53
1:F:35:VAL:HG22	1:F:36:TRP:H	1.73	0.53
1:A:72:LYS:HA	1:A:75:ILE:CD1	2.39	0.53
1:B:747:MET:HE3	1:B:751:GLN:HB3	1.89	0.53
1:E:748:ASP:OD1	1:E:748:ASP:O	2.26	0.53
1:F:152:HIS:O	1:F:156:ILE:HD12	2.09	0.53
1:A:419:THR:N	1:A:422:GLN:HG3	2.21	0.53
1:B:303:ASN:HD22	1:B:304:ASP:N	2.07	0.53
1:C:36:TRP:CE2	1:C:78:MET:HG2	2.44	0.53
1:C:743:PRO:CD	1:C:747:MET:SD	2.97	0.53
1:D:281:ALA:O	1:D:318:ASN:ND2	2.41	0.53
1:D:743:PRO:CD	1:D:747:MET:SD	2.97	0.53
1:E:556:VAL:HG21	1:E:579:THR:CA	2.39	0.53
1:F:376:ALA:O	1:F:403:LEU:HD22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:419:THR:N	1:F:422:GLN:HG3	2.23	0.53
1:A:743:PRO:CD	1:A:747:MET:SD	2.97	0.53
1:B:86:VAL:HG23	1:B:103:ASN:ND2	2.24	0.53
1:B:743:PRO:CD	1:B:747:MET:SD	2.97	0.53
1:C:361:GLN:HG2	1:C:386:LYS:HB2	1.91	0.53
1:D:196:VAL:O	1:D:196:VAL:CG1	2.57	0.53
1:D:219:GLU:O	1:D:220:LEU:C	2.52	0.53
1:F:295:ALA:HB2	1:F:310:PHE:CZ	2.44	0.53
1:F:499:ILE:HG22	1:F:500:LEU:N	2.23	0.53
1:A:243:ASP:OD2	1:A:324:PRO:HG3	2.08	0.53
1:B:178:GLU:OE2	1:B:686:ILE:HG21	2.09	0.53
1:C:85:LYS:HE2	1:C:110:SER:OG	2.08	0.53
1:C:288:HIS:HB3	1:C:292:TYR:CE1	2.44	0.53
1:C:303:ASN:HD22	1:C:304:ASP:N	2.07	0.53
1:C:376:ALA:O	1:C:403:LEU:HD22	2.08	0.53
1:C:743:PRO:HD2	1:C:747:MET:HG2	1.90	0.53
1:D:743:PRO:HD2	1:D:747:MET:HG2	1.90	0.53
1:E:152:HIS:O	1:E:156:ILE:HD12	2.09	0.53
1:E:502:GLN:O	1:E:505:TYR:HB2	2.09	0.53
1:E:556:VAL:HG21	1:E:579:THR:HA	1.91	0.53
1:F:725:ILE:O	1:F:773:LYS:HB2	2.09	0.53
1:A:751:GLN:CD	1:C:692:ARG:NH2	2.59	0.52
1:B:419:THR:H	1:B:422:GLN:NE2	2.06	0.52
1:B:563:GLN:O	1:B:565:ASN:N	2.41	0.52
1:B:702:LEU:O	1:B:706:ARG:HG3	2.10	0.52
1:B:738:ALA:CB	1:B:741:ALA:HB2	2.39	0.52
1:A:303:ASN:HD22	1:A:304:ASP:N	2.07	0.52
1:C:460:PHE:CD1	1:C:460:PHE:C	2.86	0.52
1:D:738:ALA:CB	1:D:741:ALA:HB2	2.39	0.52
1:F:108:TYR:CD2	1:F:696:LEU:HD12	2.44	0.52
1:F:238:LYS:NZ	1:F:283:ASP:O	2.42	0.52
1:F:743:PRO:HD2	1:F:747:MET:CG	2.40	0.52
1:A:161:TYR:O	1:A:164:MET:HB3	2.09	0.52
1:A:499:ILE:HG22	1:A:500:LEU:N	2.25	0.52
1:B:85:LYS:HE2	1:B:110:SER:OG	2.10	0.52
1:C:243:ASP:OD2	1:C:324:PRO:HG3	2.09	0.52
1:F:288:HIS:HB3	1:F:292:TYR:CE1	2.44	0.52
1:A:419:THR:HG23	1:A:422:GLN:CG	2.39	0.52
1:D:540:LEU:HD21	1:D:562:GLU:HG3	1.92	0.52
1:F:161:TYR:O	1:F:164:MET:HB3	2.09	0.52
1:A:219:GLU:O	1:A:220:LEU:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ALA:O	1:A:403:LEU:HD22	2.10	0.52
1:B:746:PHE:HD1	1:C:389:HIS:CD2	2.28	0.52
1:D:70:LEU:HD12	1:D:71:SER:O	2.09	0.52
1:F:517:PHE:CZ	1:F:716:ILE:HD13	2.44	0.52
1:A:327:GLN:O	1:A:330:GLU:HB2	2.10	0.52
1:A:725:ILE:O	1:A:773:LYS:HB2	2.10	0.52
1:C:158:ASP:O	1:C:162:ARG:HG2	2.10	0.52
1:C:256:PHE:O	1:C:458:ALA:HB3	2.09	0.52
1:D:85:LYS:HE2	1:D:110:SER:OG	2.10	0.52
1:B:230:ILE:HD11	1:B:342:MET:HB2	1.92	0.52
1:C:690:GLU:HG2	1:C:692:ARG:NH2	2.25	0.52
1:D:540:LEU:HD12	1:D:559:LEU:HD12	1.92	0.52
1:D:594:ALA:HA	1:D:597:TRP:CD1	2.45	0.52
1:F:70:LEU:HD13	1:F:74:ASP:HB2	1.90	0.52
1:F:219:GLU:O	1:F:220:LEU:C	2.53	0.52
1:F:731:ARG:HA	1:F:756:MET:HE1	1.91	0.52
1:A:158:ASP:O	1:A:162:ARG:HG2	2.10	0.52
1:A:508:GLU:HG3	1:A:508:GLU:O	2.10	0.52
1:A:535:PRO:HB2	1:A:540:LEU:HD21	1.90	0.52
1:B:510:ILE:HD12	1:B:768:ARG:HB3	1.90	0.52
1:B:556:VAL:HG21	1:B:579:THR:CA	2.40	0.52
1:C:219:GLU:O	1:C:220:LEU:C	2.51	0.52
1:C:743:PRO:HD2	1:C:747:MET:CG	2.40	0.52
1:C:747:MET:HE3	1:C:751:GLN:HB3	1.91	0.52
1:D:77:LYS:H	1:D:77:LYS:HZ2	1.56	0.52
1:E:540:LEU:HD21	1:E:562:GLU:HG3	1.92	0.52
1:C:487:GLU:HG3	1:C:521:LEU:HD13	1.92	0.52
1:C:499:ILE:HG22	1:C:500:LEU:N	2.24	0.52
1:D:43:GLY:H	1:D:698:ALA:CB	2.21	0.52
1:D:460:PHE:CD1	1:D:460:PHE:C	2.88	0.52
1:D:535:PRO:HB2	1:D:540:LEU:CD2	2.39	0.52
1:D:686:ILE:HG22	1:D:704:GLN:HE22	1.73	0.52
1:D:702:LEU:O	1:D:706:ARG:HG3	2.10	0.52
1:E:161:TYR:O	1:E:164:MET:HB3	2.09	0.52
1:F:743:PRO:HD2	1:F:747:MET:HG2	1.92	0.52
1:A:510:ILE:HD12	1:A:768:ARG:HB3	1.92	0.51
1:B:243:ASP:OD2	1:B:324:PRO:HG3	2.11	0.51
1:B:327:GLN:HB2	1:B:330:GLU:CD	2.35	0.51
1:D:747:MET:HE3	1:D:751:GLN:HB3	1.90	0.51
1:A:117:SER:HB2	1:A:714:ILE:HD11	1.92	0.51
1:B:77:LYS:H	1:B:77:LYS:NZ	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:GLU:HG2	1:B:692:ARG:NH2	2.26	0.51
1:D:743:PRO:HD2	1:D:747:MET:CG	2.40	0.51
1:F:535:PRO:HB2	1:F:540:LEU:CD2	2.40	0.51
1:A:690:GLU:HG2	1:A:692:ARG:NH2	2.25	0.51
1:B:419:THR:HG23	1:B:422:GLN:CG	2.40	0.51
1:B:460:PHE:C	1:B:460:PHE:CD1	2.88	0.51
1:D:303:ASN:HD22	1:D:304:ASP:N	2.07	0.51
1:B:161:TYR:O	1:B:164:MET:HB3	2.10	0.51
1:C:556:VAL:HG21	1:C:579:THR:CA	2.41	0.51
1:D:586:TYR:CG	1:D:587:ALA:N	2.78	0.51
1:E:219:GLU:O	1:E:220:LEU:C	2.52	0.51
1:E:301:MET:HA	1:E:304:ASP:HB3	1.93	0.51
1:B:43:GLY:H	1:B:698:ALA:CB	2.22	0.51
1:B:327:GLN:O	1:B:330:GLU:N	2.44	0.51
1:B:499:ILE:HG22	1:B:500:LEU:N	2.24	0.51
1:C:77:LYS:H	1:C:77:LYS:NZ	2.09	0.51
1:D:70:LEU:HD13	1:D:74:ASP:HB2	1.92	0.51
1:D:286:THR:OG1	1:D:287:PHE:N	2.44	0.51
1:E:419:THR:H	1:E:422:GLN:NE2	2.07	0.51
1:E:586:TYR:CG	1:E:587:ALA:N	2.78	0.51
1:A:301:MET:HA	1:A:304:ASP:HB3	1.91	0.51
1:C:327:GLN:O	1:C:330:GLU:N	2.44	0.51
1:D:37:VAL:HG11	1:D:59:VAL:HG21	1.92	0.51
1:D:161:TYR:O	1:D:164:MET:HB3	2.10	0.51
1:D:238:LYS:NZ	1:D:283:ASP:O	2.44	0.51
1:E:690:GLU:HG2	1:E:692:ARG:NH2	2.26	0.51
1:F:234:PHE:CE2	1:F:289:ILE:HG12	2.45	0.51
1:B:152:HIS:O	1:B:156:ILE:HD12	2.10	0.51
1:B:743:PRO:HD2	1:B:747:MET:CG	2.40	0.51
1:C:527:LEU:HD22	1:C:566:HIS:CD2	2.46	0.51
1:D:36:TRP:CE2	1:D:78:MET:HG2	2.45	0.51
1:D:108:TYR:CD2	1:D:696:LEU:HD12	2.45	0.51
1:D:499:ILE:HG22	1:D:500:LEU:N	2.25	0.51
1:F:36:TRP:CE2	1:F:78:MET:HG2	2.46	0.51
1:F:158:ASP:O	1:F:162:ARG:HG2	2.11	0.51
1:F:766:LEU:HA	1:F:777:ARG:HG3	1.93	0.51
1:A:743:PRO:HD2	1:A:747:MET:CG	2.40	0.51
1:C:388:CYS:SG	1:C:393:ILE:HG22	2.51	0.51
1:C:757:ILE:HG23	1:C:762:LEU:HB2	1.92	0.51
1:D:757:ILE:HG23	1:D:762:LEU:HB2	1.92	0.51
1:B:35:VAL:HG22	1:B:36:TRP:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:CD1	1:B:714:ILE:HG21	2.40	0.51
1:C:37:VAL:HG11	1:C:59:VAL:HG21	1.93	0.51
1:C:70:LEU:HD13	1:C:74:ASP:HB2	1.92	0.51
1:D:327:GLN:O	1:D:330:GLU:N	2.43	0.51
1:E:35:VAL:HG12	1:E:47:ALA:O	2.11	0.51
1:E:37:VAL:HG11	1:E:59:VAL:HG21	1.92	0.51
1:E:72:LYS:HA	1:E:75:ILE:CD1	2.40	0.51
1:E:269:THR:HG23	1:E:443:LEU:HD22	1.92	0.51
1:E:286:THR:OG1	1:E:287:PHE:N	2.43	0.51
1:A:36:TRP:CE2	1:A:78:MET:HG2	2.45	0.51
1:D:376:ALA:O	1:D:403:LEU:HD22	2.11	0.51
1:E:743:PRO:CD	1:E:747:MET:SD	2.99	0.51
1:F:158:ASP:O	1:F:161:TYR:HB3	2.11	0.51
1:F:731:ARG:HG2	1:F:756:MET:HE1	1.91	0.51
1:A:556:VAL:HG21	1:A:579:THR:HA	1.93	0.50
1:A:766:LEU:HA	1:A:777:ARG:HG3	1.92	0.50
1:B:226:GLN:C	1:B:229:PRO:HD2	2.35	0.50
1:B:527:LEU:HD22	1:B:566:HIS:CD2	2.46	0.50
1:C:327:GLN:O	1:C:330:GLU:HB2	2.10	0.50
1:E:85:LYS:HE2	1:E:110:SER:OG	2.10	0.50
1:F:419:THR:H	1:F:422:GLN:NE2	2.08	0.50
1:F:490:GLN:O	1:F:493:PHE:HB3	2.11	0.50
1:A:556:VAL:HG21	1:A:579:THR:CA	2.41	0.50
1:C:117:SER:HB2	1:C:714:ILE:HD11	1.93	0.50
1:E:281:ALA:O	1:E:318:ASN:ND2	2.45	0.50
1:E:303:ASN:HD22	1:E:304:ASP:N	2.09	0.50
1:E:460:PHE:C	1:E:460:PHE:CD1	2.89	0.50
1:E:710:VAL:O	1:E:714:ILE:HG13	2.11	0.50
1:F:381:ASN:O	1:F:382:THR:C	2.54	0.50
1:C:378:MET:HG3	1:C:378:MET:O	2.12	0.50
1:C:517:PHE:CZ	1:C:716:ILE:HD13	2.46	0.50
1:D:77:LYS:H	1:D:77:LYS:NZ	2.10	0.50
1:D:327:GLN:O	1:D:330:GLU:HB2	2.11	0.50
1:F:243:ASP:OD2	1:F:324:PRO:HG3	2.12	0.50
1:F:378:MET:HG3	1:F:378:MET:O	2.10	0.50
1:A:527:LEU:HD22	1:A:566:HIS:CD2	2.46	0.50
1:B:72:LYS:HA	1:B:75:ILE:CD1	2.41	0.50
1:B:434:LYS:HG2	1:B:625:TRP:HZ2	1.76	0.50
1:B:725:ILE:O	1:B:773:LYS:HB2	2.11	0.50
1:D:60:GLU:HA	1:D:67:LYS:HA	1.93	0.50
1:F:487:GLU:HG3	1:F:521:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HD11	1:A:342:MET:HB2	1.93	0.50
1:B:269:THR:HG23	1:B:443:LEU:HD22	1.94	0.50
1:B:586:TYR:CG	1:B:587:ALA:N	2.80	0.50
1:D:35:VAL:HG12	1:D:47:ALA:O	2.11	0.50
1:E:117:SER:HB2	1:E:714:ILE:HD11	1.92	0.50
1:E:510:ILE:HD12	1:E:768:ARG:HB3	1.92	0.50
1:F:72:LYS:HA	1:F:75:ILE:CD1	2.42	0.50
1:B:766:LEU:HA	1:B:777:ARG:HG3	1.93	0.50
1:D:165:LEU:HD21	1:D:260:GLY:HA2	1.94	0.50
1:F:37:VAL:HG11	1:F:59:VAL:HG21	1.92	0.50
1:A:165:LEU:HD21	1:A:260:GLY:HA2	1.94	0.50
1:A:178:GLU:OE2	1:A:686:ILE:HG21	2.11	0.50
1:B:556:VAL:HG21	1:B:579:THR:HA	1.92	0.50
1:B:611:SER:O	1:B:614:ASN:HB3	2.10	0.50
1:C:43:GLY:H	1:C:698:ALA:CB	2.22	0.50
1:C:438:LEU:O	1:C:442:ILE:HG13	2.12	0.50
1:C:738:ALA:CB	1:C:741:ALA:HB2	2.39	0.50
1:E:388:CYS:SG	1:E:393:ILE:HG22	2.52	0.50
1:F:318:ASN:O	1:F:319:GLY:C	2.54	0.50
1:F:556:VAL:HG21	1:F:579:THR:CA	2.41	0.50
1:A:60:GLU:HA	1:A:67:LYS:HA	1.94	0.50
1:A:355:VAL:O	1:A:359:VAL:HG23	2.12	0.50
1:B:158:ASP:O	1:B:161:TYR:HB3	2.12	0.50
1:B:238:LYS:NZ	1:B:283:ASP:O	2.44	0.50
1:B:754:ILE:HD13	1:F:692:ARG:NH2	2.27	0.50
1:C:434:LYS:HG2	1:C:625:TRP:HZ2	1.77	0.50
1:D:690:GLU:HG2	1:D:692:ARG:NH2	2.27	0.50
1:E:230:ILE:HD11	1:E:342:MET:HB2	1.94	0.50
1:F:688:ASN:ND2	1:F:692:ARG:O	2.33	0.50
1:A:316:LEU:O	1:A:317:SER:C	2.55	0.50
1:A:526:GLU:HA	1:A:526:GLU:OE1	2.12	0.50
1:D:36:TRP:NE1	1:D:78:MET:HG2	2.27	0.50
1:E:256:PHE:O	1:E:458:ALA:HB3	2.12	0.50
1:E:337:GLU:O	1:E:341:ILE:HG13	2.12	0.50
1:F:43:GLY:H	1:F:698:ALA:CB	2.21	0.50
1:F:77:LYS:H	1:F:77:LYS:NZ	2.09	0.50
1:A:278:ILE:HD12	1:A:428:GLU:HG2	1.93	0.49
1:A:731:ARG:HA	1:A:756:MET:HE1	1.94	0.49
1:B:117:SER:HB2	1:B:714:ILE:HD11	1.92	0.49
1:B:339:MET:HE2	1:B:352:ILE:HD13	1.95	0.49
1:B:381:ASN:O	1:B:382:THR:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TRP:NE1	1:C:78:MET:HG2	2.27	0.49
1:C:281:ALA:O	1:C:318:ASN:ND2	2.45	0.49
1:C:510:ILE:HD12	1:C:768:ARG:HB3	1.94	0.49
1:C:611:SER:O	1:C:614:ASN:HB3	2.12	0.49
1:D:659:VAL:HA	1:D:662:LEU:HD12	1.95	0.49
1:E:108:TYR:CD2	1:E:696:LEU:HD12	2.47	0.49
1:E:738:ALA:CB	1:E:741:ALA:HB2	2.39	0.49
1:E:754:ILE:HG22	1:E:755:LEU:HD23	1.94	0.49
1:F:60:GLU:HA	1:F:67:LYS:HA	1.94	0.49
1:F:556:VAL:HG21	1:F:579:THR:HA	1.94	0.49
1:A:490:GLN:O	1:A:493:PHE:HB3	2.12	0.49
1:B:498:PHE:CE2	1:B:519:LEU:HD13	2.48	0.49
1:C:381:ASN:O	1:C:382:THR:C	2.55	0.49
1:E:165:LEU:HD21	1:E:260:GLY:HA2	1.93	0.49
1:F:303:ASN:HD22	1:F:304:ASP:N	2.09	0.49
1:F:566:HIS:CD2	1:F:568:LYS:H	2.30	0.49
1:A:226:GLN:C	1:A:229:PRO:HD2	2.37	0.49
1:A:586:TYR:CG	1:A:587:ALA:N	2.80	0.49
1:B:36:TRP:CE2	1:B:78:MET:HG2	2.47	0.49
1:B:158:ASP:O	1:B:162:ARG:HG2	2.11	0.49
1:B:538:LEU:CD1	1:B:664:LYS:HD2	2.42	0.49
1:C:238:LYS:NZ	1:C:283:ASP:O	2.44	0.49
1:D:230:ILE:HD11	1:D:342:MET:HB2	1.94	0.49
1:F:327:GLN:HB2	1:F:330:GLU:CD	2.38	0.49
1:F:339:MET:HE2	1:F:352:ILE:HD13	1.95	0.49
1:A:327:GLN:O	1:A:330:GLU:N	2.45	0.49
1:A:738:ALA:CB	1:A:741:ALA:HB2	2.39	0.49
1:B:35:VAL:HG12	1:B:47:ALA:O	2.12	0.49
1:B:535:PRO:HB2	1:B:540:LEU:CD2	2.43	0.49
1:C:538:LEU:CD1	1:C:664:LYS:HD2	2.43	0.49
1:D:487:GLU:HG3	1:D:521:LEU:HD13	1.93	0.49
1:E:36:TRP:CE2	1:E:78:MET:HG2	2.47	0.49
1:E:419:THR:HG23	1:E:422:GLN:CG	2.43	0.49
1:C:161:TYR:O	1:C:164:MET:HB3	2.11	0.49
1:D:117:SER:HB2	1:D:714:ILE:HD11	1.94	0.49
1:D:556:VAL:HG21	1:D:579:THR:CA	2.41	0.49
1:D:606:ASN:HB3	1:D:609:VAL:HG13	1.94	0.49
1:F:290:PHE:CE1	1:F:356:VAL:HG13	2.47	0.49
1:F:586:TYR:CG	1:F:587:ALA:N	2.80	0.49
1:A:35:VAL:HG22	1:A:36:TRP:H	1.76	0.49
1:B:526:GLU:OE1	1:B:526:GLU:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:TYR:O	1:B:768:ARG:HG2	2.13	0.49
1:C:297:ALA:HB1	1:C:301:MET:HG2	1.94	0.49
1:C:725:ILE:O	1:C:773:LYS:HB2	2.12	0.49
1:D:337:GLU:O	1:D:341:ILE:HG13	2.13	0.49
1:D:566:HIS:CD2	1:D:568:LYS:H	2.31	0.49
1:E:60:GLU:HA	1:E:67:LYS:HA	1.93	0.49
1:E:77:LYS:H	1:E:77:LYS:HZ2	1.59	0.49
1:F:240:VAL:HG23	1:F:241:LYS:HG2	1.95	0.49
1:A:434:LYS:HG2	1:A:625:TRP:HZ2	1.78	0.49
1:A:697:ASP:HB3	1:A:700:LEU:HB3	1.94	0.49
1:C:165:LEU:HD21	1:C:260:GLY:HA2	1.94	0.49
1:D:271:LEU:HG	1:D:271:LEU:O	2.12	0.49
1:D:295:ALA:HB2	1:D:310:PHE:CZ	2.48	0.49
1:D:434:LYS:HG2	1:D:625:TRP:HZ2	1.78	0.49
1:D:611:SER:O	1:D:614:ASN:HB3	2.13	0.49
1:D:731:ARG:HG2	1:D:756:MET:HE1	1.93	0.49
1:E:763:ASP:HB3	1:E:766:LEU:HG	1.95	0.49
1:F:508:GLU:HG3	1:F:508:GLU:O	2.12	0.49
1:A:297:ALA:HB1	1:A:301:MET:HG2	1.95	0.49
1:B:337:GLU:O	1:B:341:ILE:HG13	2.12	0.49
1:B:393:ILE:HG13	1:B:612:LEU:HB3	1.94	0.49
1:C:316:LEU:O	1:C:317:SER:C	2.55	0.49
1:C:508:GLU:HG3	1:C:508:GLU:O	2.13	0.49
1:C:767:TYR:CD1	1:C:767:TYR:C	2.90	0.49
1:D:419:THR:H	1:D:422:GLN:NE2	2.06	0.49
1:E:688:ASN:ND2	1:E:692:ARG:O	2.34	0.49
1:E:727:PHE:HA	1:E:753:CYS:SG	2.53	0.49
1:F:278:ILE:HD12	1:F:428:GLU:HG2	1.93	0.49
1:A:566:HIS:CD2	1:A:568:LYS:H	2.31	0.49
1:B:281:ALA:O	1:B:318:ASN:ND2	2.46	0.49
1:B:478:GLU:OE2	1:B:600:LYS:HE2	2.13	0.49
1:D:42:HIS:O	1:D:43:GLY:C	2.55	0.49
1:D:113:ILE:O	1:D:123:VAL:HA	2.12	0.49
1:D:327:GLN:HB2	1:D:330:GLU:CD	2.38	0.49
1:D:419:THR:HG23	1:D:422:GLN:CG	2.43	0.49
1:F:95:LEU:HD11	1:F:714:ILE:HG21	1.93	0.49
1:F:327:GLN:O	1:F:330:GLU:HB2	2.13	0.49
1:C:158:ASP:O	1:C:161:TYR:HB3	2.12	0.49
1:C:178:GLU:OE2	1:C:686:ILE:HG21	2.12	0.49
1:C:271:LEU:HG	1:C:271:LEU:O	2.12	0.49
1:E:36:TRP:NE1	1:E:78:MET:HG2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:434:LYS:HG2	1:E:625:TRP:HZ2	1.78	0.49
1:E:606:ASN:HB3	1:E:609:VAL:HG13	1.94	0.49
1:F:393:ILE:HD11	1:F:613:LEU:HA	1.95	0.49
1:A:35:VAL:HG12	1:A:47:ALA:O	2.13	0.48
1:A:337:GLU:O	1:A:341:ILE:HG13	2.13	0.48
1:A:419:THR:H	1:A:422:GLN:NE2	2.05	0.48
1:E:290:PHE:CE1	1:E:356:VAL:HG13	2.48	0.48
1:E:327:GLN:O	1:E:330:GLU:HB2	2.13	0.48
1:F:35:VAL:HG22	1:F:76:GLN:O	2.13	0.48
1:F:165:LEU:HD21	1:F:260:GLY:HA2	1.94	0.48
1:F:286:THR:OG1	1:F:287:PHE:N	2.45	0.48
1:F:747:MET:HE3	1:F:751:GLN:HB3	1.94	0.48
1:A:77:LYS:HZ2	1:A:77:LYS:N	2.10	0.48
1:A:80:PRO:HB2	1:A:82:LYS:HG2	1.96	0.48
1:A:196:VAL:O	1:A:196:VAL:CG1	2.60	0.48
1:A:295:ALA:HB2	1:A:310:PHE:CZ	2.47	0.48
1:A:606:ASN:HB3	1:A:609:VAL:HG13	1.94	0.48
1:B:42:HIS:O	1:B:43:GLY:C	2.56	0.48
1:B:196:VAL:O	1:B:196:VAL:CG1	2.61	0.48
1:B:508:GLU:HG3	1:B:508:GLU:O	2.14	0.48
1:B:606:ASN:HB3	1:B:609:VAL:HG13	1.94	0.48
1:C:60:GLU:HA	1:C:67:LYS:HA	1.94	0.48
1:C:196:VAL:O	1:C:196:VAL:CG1	2.60	0.48
1:C:278:ILE:HB	1:C:315:PHE:CE1	2.48	0.48
1:C:295:ALA:HB2	1:C:310:PHE:CZ	2.47	0.48
1:C:327:GLN:HB2	1:C:330:GLU:CD	2.38	0.48
1:D:556:VAL:HG21	1:D:579:THR:HA	1.94	0.48
1:B:77:LYS:HZ2	1:B:77:LYS:N	2.12	0.48
1:C:556:VAL:HG21	1:C:579:THR:HA	1.93	0.48
1:F:606:ASN:HB3	1:F:609:VAL:HG13	1.94	0.48
1:A:686:ILE:HG22	1:A:704:GLN:HE22	1.77	0.48
1:B:60:GLU:HA	1:B:67:LYS:HA	1.94	0.48
1:C:219:GLU:O	1:C:222:LYS:N	2.46	0.48
1:C:419:THR:H	1:C:422:GLN:NE2	2.07	0.48
1:C:478:GLU:OE2	1:C:600:LYS:HE2	2.14	0.48
1:D:158:ASP:O	1:D:162:ARG:HG2	2.14	0.48
1:E:43:GLY:H	1:E:698:ALA:CB	2.20	0.48
1:E:158:ASP:O	1:E:161:TYR:HB3	2.13	0.48
1:E:540:LEU:HD11	1:E:562:GLU:HB2	1.95	0.48
1:F:337:GLU:O	1:F:341:ILE:HG13	2.13	0.48
1:F:611:SER:O	1:F:614:ASN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:NZ	1:A:283:ASP:O	2.46	0.48
1:B:355:VAL:O	1:B:359:VAL:HG23	2.14	0.48
1:C:95:LEU:HD11	1:C:714:ILE:HG21	1.96	0.48
1:C:766:LEU:HA	1:C:777:ARG:HG3	1.95	0.48
1:D:490:GLN:O	1:D:493:PHE:HB3	2.14	0.48
1:F:95:LEU:CD1	1:F:714:ILE:HG21	2.44	0.48
1:F:510:ILE:HD12	1:F:768:ARG:HB3	1.94	0.48
1:F:754:ILE:HG22	1:F:755:LEU:HD23	1.94	0.48
1:A:271:LEU:HG	1:A:271:LEU:O	2.13	0.48
1:A:290:PHE:CE1	1:A:356:VAL:HG13	2.49	0.48
1:B:295:ALA:HB2	1:B:310:PHE:CZ	2.48	0.48
1:B:316:LEU:O	1:B:317:SER:C	2.55	0.48
1:B:754:ILE:HG22	1:B:755:LEU:HD23	1.96	0.48
1:C:526:GLU:OE1	1:C:526:GLU:HA	2.14	0.48
1:C:586:TYR:CG	1:C:587:ALA:N	2.82	0.48
1:D:316:LEU:O	1:D:317:SER:C	2.55	0.48
1:D:381:ASN:O	1:D:382:THR:C	2.57	0.48
1:E:42:HIS:O	1:E:43:GLY:C	2.56	0.48
1:E:478:GLU:OE2	1:E:600:LYS:HE2	2.14	0.48
1:E:766:LEU:HA	1:E:777:ARG:HG3	1.95	0.48
1:F:178:GLU:OE2	1:F:686:ILE:HG21	2.13	0.48
1:A:487:GLU:HG3	1:A:521:LEU:HD13	1.95	0.48
1:A:535:PRO:HB2	1:A:540:LEU:CD2	2.43	0.48
1:C:107:ARG:NH1	1:C:114:TYR:O	2.46	0.48
1:E:731:ARG:HG2	1:E:756:MET:CE	2.44	0.48
1:A:85:LYS:HE2	1:A:110:SER:OG	2.13	0.48
1:C:498:PHE:CE2	1:C:519:LEU:HD13	2.49	0.48
1:F:36:TRP:NE1	1:F:78:MET:HG2	2.28	0.48
1:F:540:LEU:HD11	1:F:562:GLU:HB2	1.96	0.48
1:F:697:ASP:HB3	1:F:700:LEU:HB3	1.96	0.48
1:F:763:ASP:HB3	1:F:766:LEU:HG	1.96	0.48
1:C:566:HIS:CD2	1:C:568:LYS:H	2.31	0.48
1:D:508:GLU:HG3	1:D:508:GLU:O	2.13	0.48
1:D:697:ASP:HB3	1:D:700:LEU:HB3	1.96	0.48
1:D:766:LEU:HA	1:D:777:ARG:HG3	1.95	0.48
1:E:228:ASN:O	1:E:229:PRO:C	2.56	0.48
1:E:487:GLU:HG3	1:E:521:LEU:HD13	1.96	0.48
1:F:742:ILE:HG12	1:F:752:ALA:HB1	1.96	0.48
1:A:381:ASN:O	1:A:382:THR:C	2.55	0.48
1:A:517:PHE:CZ	1:A:716:ILE:HD13	2.47	0.48
1:A:538:LEU:CD1	1:A:664:LYS:HD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:VAL:HG21	1:B:75:ILE:HG22	1.96	0.48
1:B:566:HIS:CD2	1:B:568:LYS:H	2.31	0.48
1:D:767:TYR:C	1:D:767:TYR:CD1	2.92	0.48
1:E:77:LYS:H	1:E:77:LYS:NZ	2.11	0.48
1:F:158:ASP:HB2	1:F:193:TYR:CZ	2.49	0.48
1:F:196:VAL:O	1:F:196:VAL:CG1	2.62	0.48
1:A:36:TRP:NE1	1:A:78:MET:HG2	2.29	0.47
1:A:611:SER:O	1:A:614:ASN:HB3	2.14	0.47
1:B:165:LEU:HD21	1:B:260:GLY:HA2	1.95	0.47
1:C:228:ASN:HB2	1:C:229:PRO:HD3	1.96	0.47
1:C:535:PRO:HB2	1:C:540:LEU:CD2	2.43	0.47
1:D:228:ASN:HB2	1:D:229:PRO:HD3	1.96	0.47
1:D:378:MET:CE	1:D:381:ASN:HA	2.38	0.47
1:D:502:GLN:O	1:D:505:TYR:HB2	2.14	0.47
1:E:327:GLN:O	1:E:330:GLU:N	2.47	0.47
1:E:611:SER:O	1:E:614:ASN:HB3	2.13	0.47
1:A:393:ILE:HG13	1:A:612:LEU:HB3	1.96	0.47
1:A:545:CYS:SG	1:A:598:LEU:HD23	2.53	0.47
1:C:490:GLN:O	1:C:493:PHE:HB3	2.14	0.47
1:F:434:LYS:HG2	1:F:625:TRP:HZ2	1.78	0.47
1:D:763:ASP:HB3	1:D:766:LEU:HG	1.96	0.47
1:F:42:HIS:O	1:F:43:GLY:C	2.56	0.47
1:A:327:GLN:HB2	1:A:330:GLU:CD	2.39	0.47
1:A:767:TYR:C	1:A:767:TYR:CD1	2.91	0.47
1:B:686:ILE:HG22	1:B:704:GLN:HE22	1.78	0.47
1:C:393:ILE:HG13	1:C:612:LEU:HB3	1.95	0.47
1:C:754:ILE:HG22	1:C:755:LEU:HD23	1.97	0.47
1:E:268:GLU:HG2	1:E:270:TYR:OH	2.14	0.47
1:E:526:GLU:OE1	1:E:526:GLU:HA	2.13	0.47
1:E:538:LEU:CD1	1:E:664:LYS:HD2	2.44	0.47
1:A:158:ASP:HB2	1:A:193:TYR:CZ	2.49	0.47
1:A:540:LEU:HD11	1:A:562:GLU:HB2	1.96	0.47
1:B:35:VAL:HG22	1:B:76:GLN:O	2.14	0.47
1:B:659:VAL:HA	1:B:662:LEU:HD12	1.97	0.47
1:D:727:PHE:HA	1:D:753:CYS:SG	2.55	0.47
1:F:269:THR:HG23	1:F:443:LEU:HD22	1.95	0.47
1:A:158:ASP:O	1:A:161:TYR:HB3	2.14	0.47
1:B:271:LEU:O	1:B:271:LEU:HG	2.14	0.47
1:B:278:ILE:HB	1:B:315:PHE:CE1	2.50	0.47
1:B:666:GLN:HA	1:B:669:LYS:HD3	1.96	0.47
1:B:697:ASP:HB3	1:B:700:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:THR:N	1:C:422:GLN:HG3	2.21	0.47
1:D:278:ILE:HB	1:D:315:PHE:CE1	2.50	0.47
1:F:35:VAL:HG21	1:F:75:ILE:HG22	1.97	0.47
1:F:226:GLN:C	1:F:229:PRO:HD2	2.40	0.47
1:F:339:MET:CE	1:F:352:ILE:HD13	2.45	0.47
1:A:731:ARG:HG2	1:A:756:MET:CE	2.44	0.47
1:A:754:ILE:HG22	1:A:755:LEU:HD23	1.96	0.47
1:A:767:TYR:O	1:A:768:ARG:HG2	2.15	0.47
1:B:419:THR:H	1:B:422:GLN:CG	2.22	0.47
1:B:487:GLU:HG3	1:B:521:LEU:HD13	1.95	0.47
1:B:742:ILE:HG22	1:B:743:PRO:O	2.15	0.47
1:C:77:LYS:HZ2	1:C:77:LYS:N	2.13	0.47
1:C:337:GLU:O	1:C:341:ILE:HG13	2.15	0.47
1:C:551:THR:CB	1:C:553:THR:HG22	2.45	0.47
1:C:763:ASP:HB3	1:C:766:LEU:HG	1.96	0.47
1:D:35:VAL:HG22	1:D:36:TRP:H	1.80	0.47
1:E:113:ILE:O	1:E:123:VAL:HA	2.15	0.47
1:E:238:LYS:NZ	1:E:283:ASP:O	2.47	0.47
1:E:278:ILE:HB	1:E:315:PHE:CE1	2.49	0.47
1:E:490:GLN:O	1:E:493:PHE:HB3	2.15	0.47
1:F:116:TYR:CZ	1:F:146:ARG:HG2	2.50	0.47
1:F:164:MET:SD	1:F:459:SER:HB2	2.55	0.47
1:F:230:ILE:HD11	1:F:342:MET:HB2	1.97	0.47
1:F:402:ILE:HG22	1:F:403:LEU:N	2.30	0.47
1:A:734:TYR:OH	1:A:781:LEU:HD22	2.15	0.47
1:B:240:VAL:HG23	1:B:241:LYS:HG2	1.97	0.47
1:B:690:GLU:C	1:B:692:ARG:N	2.70	0.47
1:B:731:ARG:HG2	1:B:756:MET:CE	2.43	0.47
1:D:297:ALA:HB1	1:D:301:MET:HG2	1.96	0.47
1:D:393:ILE:HG13	1:D:612:LEU:HB3	1.97	0.47
1:E:381:ASN:O	1:E:382:THR:C	2.56	0.47
1:F:251:PHE:CZ	1:F:462:GLY:HA3	2.50	0.47
1:F:271:LEU:HG	1:F:271:LEU:O	2.15	0.47
1:F:419:THR:HG23	1:F:422:GLN:CG	2.44	0.47
1:F:767:TYR:CD1	1:F:767:TYR:C	2.92	0.47
1:A:607:ASP:CA	1:A:610:THR:HB	2.45	0.47
1:A:666:GLN:HA	1:A:669:LYS:HD3	1.96	0.47
1:B:734:TYR:OH	1:B:781:LEU:HD22	2.14	0.47
1:E:43:GLY:HA3	1:E:702:LEU:CD1	2.45	0.47
1:E:158:ASP:O	1:E:162:ARG:HG2	2.14	0.47
1:E:228:ASN:HB2	1:E:229:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:LEU:HG	1:E:271:LEU:O	2.14	0.47
1:E:327:GLN:HB2	1:E:330:GLU:CD	2.40	0.47
1:E:566:HIS:CD2	1:E:568:LYS:H	2.32	0.47
1:F:43:GLY:HA3	1:F:702:LEU:CD1	2.45	0.47
1:A:107:ARG:NH1	1:A:114:TYR:O	2.48	0.47
1:A:278:ILE:HB	1:A:315:PHE:CE1	2.49	0.47
1:A:742:ILE:HG22	1:A:743:PRO:O	2.15	0.47
1:C:61:LEU:HG	1:C:66:LYS:O	2.15	0.47
1:C:391:MET:HE2	1:C:434:LYS:NZ	2.30	0.47
1:C:711:LEU:O	1:C:715:ARG:HG2	2.15	0.47
1:D:339:MET:CE	1:D:352:ILE:HD13	2.45	0.47
1:E:297:ALA:HB1	1:E:301:MET:HG2	1.97	0.47
1:E:419:THR:H	1:E:422:GLN:CG	2.24	0.47
1:E:502:GLN:HA	1:E:505:TYR:CD2	2.50	0.47
1:E:658:THR:O	1:E:662:LEU:HD12	2.15	0.47
1:F:253:ARG:HG3	1:F:460:PHE:CD1	2.50	0.47
1:F:281:ALA:O	1:F:318:ASN:ND2	2.48	0.47
1:A:42:HIS:O	1:A:43:GLY:C	2.58	0.46
1:C:540:LEU:HD11	1:C:562:GLU:HB2	1.97	0.46
1:D:538:LEU:HD12	1:D:664:LYS:HD2	1.96	0.46
1:D:742:ILE:HG22	1:D:743:PRO:O	2.15	0.46
1:E:417:ALA:C	1:E:418:GLN:HE21	2.22	0.46
1:E:666:GLN:HA	1:E:669:LYS:HD3	1.96	0.46
1:E:686:ILE:HG22	1:E:704:GLN:HE22	1.80	0.46
1:F:228:ASN:O	1:F:229:PRO:C	2.56	0.46
1:F:527:LEU:HD22	1:F:566:HIS:CD2	2.49	0.46
1:F:731:ARG:O	1:F:735:GLU:HB2	2.15	0.46
1:A:57:VAL:HG12	1:A:59:VAL:HG13	1.98	0.46
1:A:236:ASN:ND2	1:A:244:ASN:O	2.49	0.46
1:B:228:ASN:HB2	1:B:229:PRO:HD3	1.97	0.46
1:C:158:ASP:HB2	1:C:193:TYR:CZ	2.50	0.46
1:D:339:MET:HE2	1:D:352:ILE:HD13	1.96	0.46
1:D:393:ILE:HD11	1:D:613:LEU:HA	1.97	0.46
1:D:495:HIS:CD2	1:D:500:LEU:HG	2.50	0.46
1:A:269:THR:HG23	1:A:443:LEU:HD22	1.96	0.46
1:A:551:THR:CB	1:A:553:THR:HG22	2.45	0.46
1:B:57:VAL:HG12	1:B:59:VAL:HG13	1.97	0.46
1:D:278:ILE:HD12	1:D:428:GLU:HG2	1.98	0.46
1:F:731:ARG:HG2	1:F:756:MET:CE	2.45	0.46
1:A:717:CYS:O	1:A:778:THR:HG22	2.15	0.46
1:C:57:VAL:HG12	1:C:59:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ARG:HG3	1:C:460:PHE:CD1	2.50	0.46
1:C:593:ASN:C	1:C:593:ASN:ND2	2.73	0.46
1:D:240:VAL:HG23	1:D:241:LYS:HG2	1.96	0.46
1:D:566:HIS:HD2	1:D:568:LYS:H	1.64	0.46
1:D:754:ILE:HG22	1:D:755:LEU:HD23	1.96	0.46
1:E:607:ASP:CA	1:E:610:THR:HB	2.46	0.46
1:E:697:ASP:HB3	1:E:700:LEU:HB3	1.97	0.46
1:F:532:THR:OG1	1:F:533:ASN:ND2	2.48	0.46
1:C:607:ASP:CA	1:C:610:THR:HB	2.43	0.46
1:E:323:ILE:HG22	1:E:324:PRO:CD	2.45	0.46
1:E:498:PHE:CE2	1:E:519:LEU:HD13	2.50	0.46
1:F:297:ALA:HB1	1:F:301:MET:HG2	1.97	0.46
1:F:303:ASN:HD22	1:F:303:ASN:C	2.24	0.46
1:A:286:THR:OG1	1:A:287:PHE:N	2.46	0.46
1:B:36:TRP:NE1	1:B:78:MET:HG2	2.31	0.46
1:B:427:ILE:HD13	1:B:427:ILE:HA	1.78	0.46
1:C:72:LYS:HA	1:C:75:ILE:CD1	2.43	0.46
1:C:172:SER:HA	1:C:462:GLY:O	2.15	0.46
1:C:290:PHE:CE1	1:C:356:VAL:HG13	2.49	0.46
1:C:731:ARG:O	1:C:735:GLU:HB2	2.16	0.46
1:C:742:ILE:HG22	1:C:743:PRO:O	2.15	0.46
1:D:540:LEU:HD11	1:D:562:GLU:HB2	1.98	0.46
1:D:690:GLU:C	1:D:692:ARG:N	2.72	0.46
1:E:251:PHE:CZ	1:E:462:GLY:HA3	2.51	0.46
1:E:508:GLU:HG3	1:E:508:GLU:O	2.16	0.46
1:F:659:VAL:HA	1:F:662:LEU:HD12	1.98	0.46
1:A:690:GLU:C	1:A:692:ARG:N	2.72	0.46
1:A:738:ALA:O	1:A:741:ALA:HB2	2.16	0.46
1:B:43:GLY:HA3	1:B:702:LEU:CD1	2.46	0.46
1:B:121:CYS:O	1:B:683:ARG:HG2	2.16	0.46
1:B:727:PHE:HA	1:B:753:CYS:SG	2.55	0.46
1:B:756:MET:HE3	1:B:756:MET:HB2	1.76	0.46
1:C:659:VAL:HA	1:C:662:LEU:HD12	1.97	0.46
1:D:36:TRP:HB2	1:D:76:GLN:O	2.16	0.46
1:D:593:ASN:C	1:D:593:ASN:ND2	2.72	0.46
1:E:527:LEU:HD22	1:E:566:HIS:CD2	2.50	0.46
1:E:532:THR:OG1	1:E:533:ASN:ND2	2.49	0.46
1:E:584:LEU:HD23	1:E:589:LYS:CG	2.36	0.46
1:E:712:GLU:OE1	1:E:712:GLU:N	2.43	0.46
1:F:607:ASP:CA	1:F:610:THR:HB	2.45	0.46
1:A:532:THR:OG1	1:A:533:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ILE:HD12	1:B:428:GLU:HG2	1.97	0.46
1:C:606:ASN:HB3	1:C:609:VAL:HG13	1.98	0.46
1:D:391:MET:HE2	1:D:434:LYS:NZ	2.31	0.46
1:D:666:GLN:HA	1:D:669:LYS:HD3	1.98	0.46
1:E:295:ALA:HB2	1:E:310:PHE:CZ	2.49	0.46
1:E:495:HIS:CD2	1:E:500:LEU:HG	2.50	0.46
1:F:727:PHE:HA	1:F:753:CYS:SG	2.56	0.46
1:F:738:ALA:O	1:F:741:ALA:CB	2.64	0.46
1:B:339:MET:CE	1:B:352:ILE:HD13	2.45	0.46
1:B:607:ASP:CA	1:B:610:THR:HB	2.46	0.46
1:C:697:ASP:HB3	1:C:700:LEU:HB3	1.98	0.46
1:C:731:ARG:HA	1:C:756:MET:HE1	1.98	0.46
1:D:34:LEU:HD12	1:D:34:LEU:HA	1.74	0.46
1:D:226:GLN:C	1:D:229:PRO:HD2	2.40	0.46
1:E:57:VAL:HG12	1:E:59:VAL:HG13	1.97	0.46
1:F:478:GLU:OE2	1:F:600:LYS:HE2	2.15	0.46
1:A:35:VAL:HG22	1:A:76:GLN:O	2.16	0.46
1:B:251:PHE:CZ	1:B:462:GLY:HA3	2.51	0.46
1:B:738:ALA:O	1:B:741:ALA:HB2	2.16	0.46
1:C:35:VAL:HG22	1:C:76:GLN:O	2.15	0.46
1:C:35:VAL:HG21	1:C:75:ILE:HG22	1.98	0.46
1:C:508:GLU:HG3	1:C:771:GLN:N	2.29	0.46
1:D:419:THR:H	1:D:422:GLN:CG	2.23	0.46
1:D:502:GLN:HA	1:D:505:TYR:CD2	2.51	0.46
1:D:532:THR:OG1	1:D:533:ASN:ND2	2.49	0.46
1:E:563:GLN:OE1	1:E:563:GLN:HA	2.16	0.46
1:F:239:THR:HG23	1:F:245:SER:HB3	1.98	0.46
1:A:173:ILE:HG13	1:A:461:LEU:HD21	1.99	0.45
1:A:300:GLN:O	1:A:304:ASP:HB2	2.17	0.45
1:A:419:THR:O	1:A:420:LYS:C	2.59	0.45
1:B:290:PHE:CE1	1:B:356:VAL:HG13	2.51	0.45
1:B:508:GLU:HG3	1:B:771:GLN:N	2.31	0.45
1:B:532:THR:OG1	1:B:533:ASN:ND2	2.49	0.45
1:B:540:LEU:HD11	1:B:562:GLU:HB2	1.97	0.45
1:B:566:HIS:HD2	1:B:568:LYS:H	1.64	0.45
1:C:226:GLN:HB2	1:C:342:MET:HE2	1.98	0.45
1:D:268:GLU:HG2	1:D:270:TYR:OH	2.16	0.45
1:D:419:THR:O	1:D:420:LYS:C	2.58	0.45
1:D:526:GLU:OE1	1:D:526:GLU:HA	2.16	0.45
1:E:659:VAL:HA	1:E:662:LEU:HD12	1.97	0.45
1:F:327:GLN:O	1:F:330:GLU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:ILE:HG13	1:F:612:LEU:HB3	1.99	0.45
1:F:502:GLN:HA	1:F:505:TYR:CD2	2.51	0.45
1:F:743:PRO:HD2	1:F:747:MET:SD	2.56	0.45
1:A:393:ILE:HD11	1:A:613:LEU:HA	1.98	0.45
1:A:478:GLU:OE2	1:A:600:LYS:HE2	2.17	0.45
1:A:498:PHE:CE2	1:A:519:LEU:HD13	2.51	0.45
1:A:563:GLN:OE1	1:A:563:GLN:HA	2.17	0.45
1:B:508:GLU:HG2	1:B:775:PHE:CE1	2.44	0.45
3:B:999:ALF:F4	4:B:998:ADP:PB	2.65	0.45
1:C:271:LEU:HD22	1:C:481:CYS:HB2	1.98	0.45
1:D:41:LYS:H	1:D:41:LYS:HG2	1.44	0.45
1:D:607:ASP:CA	1:D:610:THR:HB	2.45	0.45
1:E:35:VAL:HG22	1:E:76:GLN:O	2.16	0.45
1:E:35:VAL:HG22	1:E:36:TRP:H	1.82	0.45
1:E:196:VAL:O	1:E:196:VAL:CG1	2.64	0.45
1:E:756:MET:HE3	1:E:756:MET:HB2	1.78	0.45
1:F:756:MET:HE3	1:F:756:MET:HB2	1.78	0.45
1:C:126:PRO:HB3	1:C:130:LEU:HD11	1.98	0.45
1:C:756:MET:HE3	1:C:756:MET:HB2	1.75	0.45
1:D:417:ALA:C	1:D:418:GLN:HE21	2.24	0.45
1:F:35:VAL:HG13	1:F:36:TRP:N	2.30	0.45
1:F:228:ASN:HB2	1:F:229:PRO:HD3	1.98	0.45
1:F:498:PHE:CE2	1:F:519:LEU:HD13	2.51	0.45
1:F:711:LEU:O	1:F:715:ARG:HG2	2.16	0.45
1:A:43:GLY:HA3	1:A:702:LEU:CD1	2.46	0.45
1:A:97:GLU:HG2	1:A:711:LEU:CD1	2.47	0.45
1:A:251:PHE:CZ	1:A:462:GLY:HA3	2.51	0.45
1:A:659:VAL:HA	1:A:662:LEU:HD12	1.96	0.45
1:C:95:LEU:CD1	1:C:714:ILE:HG21	2.45	0.45
1:C:173:ILE:HG13	1:C:461:LEU:HD21	1.99	0.45
1:C:226:GLN:C	1:C:229:PRO:HD2	2.41	0.45
1:D:551:THR:CB	1:D:553:THR:HG22	2.47	0.45
1:E:253:ARG:HG3	1:E:460:PHE:CD1	2.52	0.45
1:A:228:ASN:HB2	1:A:229:PRO:HD3	1.99	0.45
1:A:281:ALA:O	1:A:318:ASN:ND2	2.47	0.45
1:C:532:THR:OG1	1:C:533:ASN:ND2	2.49	0.45
1:E:738:ALA:O	1:E:741:ALA:HB3	2.16	0.45
1:F:538:LEU:CD1	1:F:664:LYS:HD2	2.46	0.45
1:A:43:GLY:H	1:A:698:ALA:CB	2.24	0.45
1:B:35:VAL:HG11	1:B:75:ILE:CG2	2.47	0.45
1:C:35:VAL:HG11	1:C:75:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASN:O	1:C:229:PRO:C	2.59	0.45
1:C:240:VAL:HG23	1:C:241:LYS:HG2	1.97	0.45
1:C:545:CYS:SG	1:C:598:LEU:HD23	2.56	0.45
1:C:731:ARG:HG2	1:C:756:MET:CE	2.45	0.45
1:D:738:ALA:O	1:D:741:ALA:HB2	2.16	0.45
1:E:80:PRO:HB2	1:E:82:LYS:HG2	1.99	0.45
1:E:393:ILE:HG13	1:E:612:LEU:HB3	1.97	0.45
1:E:731:ARG:O	1:E:735:GLU:HB2	2.17	0.45
1:F:438:LEU:O	1:F:442:ILE:HG13	2.15	0.45
1:A:228:ASN:O	1:A:229:PRO:C	2.60	0.45
1:A:271:LEU:HD22	1:A:481:CYS:HB2	1.97	0.45
1:A:711:LEU:O	1:A:715:ARG:HG2	2.17	0.45
3:A:999:ALF:F4	4:A:998:ADP:PB	2.65	0.45
1:B:552:ASP:HA	1:B:598:LEU:HD12	1.99	0.45
1:C:502:GLN:HA	1:C:505:TYR:CD2	2.51	0.45
1:D:478:GLU:OE2	1:D:600:LYS:HE2	2.17	0.45
1:D:717:CYS:O	1:D:778:THR:HG22	2.17	0.45
1:F:323:ILE:HG22	1:F:324:PRO:CD	2.47	0.45
1:F:566:HIS:HD2	1:F:568:LYS:H	1.64	0.45
1:F:666:GLN:HA	1:F:669:LYS:HD3	1.98	0.45
1:A:268:GLU:HG2	1:A:270:TYR:OH	2.17	0.45
1:A:525:ILE:O	1:A:529:GLU:HG2	2.17	0.45
1:A:658:THR:O	1:A:662:LEU:HD12	2.17	0.45
1:B:80:PRO:HB2	1:B:82:LYS:HG2	1.98	0.45
1:B:238:LYS:HB3	1:B:285:ARG:HG2	1.98	0.45
1:B:525:ILE:O	1:B:529:GLU:HG2	2.17	0.45
1:C:34:LEU:HD12	1:C:34:LEU:HA	1.74	0.45
1:C:35:VAL:HG12	1:C:47:ALA:O	2.17	0.45
1:C:566:HIS:HD2	1:C:568:LYS:H	1.63	0.45
1:D:239:THR:HG23	1:D:245:SER:HB3	1.99	0.45
1:D:242:ASN:OD1	1:D:243:ASP:N	2.49	0.45
1:D:711:LEU:O	1:D:715:ARG:HG2	2.17	0.45
1:E:419:THR:O	1:E:420:LYS:C	2.59	0.45
1:F:316:LEU:O	1:F:317:SER:C	2.60	0.45
1:F:690:GLU:C	1:F:692:ARG:N	2.72	0.45
1:A:95:LEU:HD11	1:A:714:ILE:HG21	1.98	0.45
1:A:219:GLU:O	1:A:222:LYS:N	2.50	0.45
1:A:566:HIS:HD2	1:A:568:LYS:H	1.64	0.45
1:B:490:GLN:O	1:B:493:PHE:HB3	2.16	0.45
1:B:731:ARG:HH11	1:B:731:ARG:CG	2.30	0.45
1:C:268:GLU:HG2	1:C:270:TYR:OH	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:ASP:O	1:D:161:TYR:HB3	2.15	0.45
1:D:538:LEU:CD1	1:D:664:LYS:HD2	2.47	0.45
1:E:242:ASN:OD1	1:E:243:ASP:N	2.50	0.45
1:E:551:THR:CB	1:E:553:THR:HG22	2.47	0.45
1:F:35:VAL:HG11	1:F:75:ILE:CG2	2.46	0.45
1:F:502:GLN:O	1:F:505:TYR:HB2	2.16	0.45
1:A:114:TYR:CE1	1:A:153:ILE:HB	2.52	0.45
1:A:508:GLU:HG3	1:A:771:GLN:N	2.31	0.45
1:B:438:LEU:O	1:B:442:ILE:HG13	2.16	0.45
1:D:95:LEU:CD1	1:D:714:ILE:HG21	2.47	0.45
1:D:427:ILE:HA	1:D:427:ILE:HD13	1.76	0.45
1:D:527:LEU:HD22	1:D:566:HIS:CD2	2.52	0.45
1:D:670:LEU:O	1:D:671:MET:C	2.59	0.45
1:E:303:ASN:HD22	1:E:303:ASN:C	2.24	0.45
1:E:731:ARG:HA	1:E:756:MET:HE1	1.99	0.45
1:A:95:LEU:CD1	1:A:714:ILE:HG21	2.47	0.44
1:A:508:GLU:HG2	1:A:775:PHE:CE1	2.46	0.44
1:A:690:GLU:O	1:A:691:LYS:C	2.60	0.44
1:A:721:PHE:HB2	1:A:775:PHE:HB3	1.98	0.44
1:B:116:TYR:CZ	1:B:146:ARG:HG2	2.52	0.44
1:B:419:THR:O	1:B:420:LYS:C	2.60	0.44
1:C:230:ILE:HD11	1:C:342:MET:HB2	1.99	0.44
1:D:355:VAL:O	1:D:359:VAL:HG23	2.17	0.44
3:D:999:ALF:F4	4:D:998:ADP:PB	2.65	0.44
1:E:271:LEU:HD22	1:E:481:CYS:HB2	1.99	0.44
1:E:734:TYR:OH	1:E:781:LEU:HD22	2.17	0.44
1:F:219:GLU:O	1:F:222:LYS:N	2.50	0.44
1:F:271:LEU:HD22	1:F:481:CYS:HB2	1.99	0.44
1:A:41:LYS:H	1:A:41:LYS:HG2	1.46	0.44
1:A:738:ALA:O	1:A:741:ALA:HB3	2.17	0.44
1:B:297:ALA:HB1	1:B:301:MET:HG2	1.98	0.44
1:B:378:MET:O	1:B:378:MET:HG3	2.16	0.44
1:C:339:MET:HE2	1:C:352:ILE:HD13	1.98	0.44
1:C:738:ALA:O	1:C:741:ALA:HB3	2.17	0.44
1:E:742:ILE:HG12	1:E:752:ALA:HB1	1.99	0.44
1:F:593:ASN:C	1:F:593:ASN:ND2	2.75	0.44
1:A:226:GLN:HB2	1:A:342:MET:HE2	2.00	0.44
1:A:388:CYS:SG	1:A:393:ILE:HG22	2.57	0.44
1:A:502:GLN:HA	1:A:505:TYR:CD2	2.52	0.44
1:B:417:ALA:C	1:B:418:GLN:HE21	2.26	0.44
1:B:746:PHE:CG	1:C:306:LEU:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:THR:HG23	1:C:245:SER:HB3	1.99	0.44
1:C:402:ILE:HG22	1:C:403:LEU:N	2.33	0.44
1:C:563:GLN:OE1	1:C:563:GLN:HA	2.16	0.44
1:D:114:TYR:CE1	1:D:153:ILE:HB	2.53	0.44
1:D:269:THR:HG23	1:D:443:LEU:HD22	2.00	0.44
1:E:355:VAL:O	1:E:359:VAL:HG23	2.17	0.44
1:E:711:LEU:O	1:E:715:ARG:HG2	2.18	0.44
1:F:61:LEU:HG	1:F:66:LYS:O	2.18	0.44
1:F:80:PRO:HB2	1:F:82:LYS:HG2	1.99	0.44
1:F:551:THR:CB	1:F:553:THR:HG22	2.48	0.44
1:F:606:ASN:HD22	1:F:606:ASN:C	2.25	0.44
1:A:164:MET:SD	1:A:459:SER:HB2	2.57	0.44
1:B:219:GLU:O	1:B:222:LYS:N	2.51	0.44
1:C:666:GLN:HA	1:C:669:LYS:HD3	1.98	0.44
1:D:393:ILE:HD11	1:D:612:LEU:O	2.17	0.44
1:D:526:GLU:OE1	1:D:530:ARG:HD3	2.17	0.44
1:D:552:ASP:HA	1:D:598:LEU:HD12	1.99	0.44
1:D:731:ARG:HG2	1:D:756:MET:CE	2.48	0.44
1:E:658:THR:C	1:E:662:LEU:HD12	2.42	0.44
1:F:35:VAL:HG12	1:F:47:ALA:O	2.17	0.44
1:F:584:LEU:HD23	1:F:589:LYS:CG	2.37	0.44
1:B:97:GLU:HG2	1:B:711:LEU:CD1	2.48	0.44
1:B:158:ASP:HB2	1:B:193:TYR:CZ	2.53	0.44
1:B:731:ARG:HA	1:B:756:MET:HE1	1.99	0.44
1:C:42:HIS:O	1:C:43:GLY:C	2.59	0.44
1:D:97:GLU:HG2	1:D:711:LEU:CD1	2.48	0.44
1:D:107:ARG:NH1	1:D:114:TYR:O	2.50	0.44
1:D:300:GLN:O	1:D:304:ASP:HB2	2.17	0.44
1:D:438:LEU:O	1:D:442:ILE:HG13	2.18	0.44
1:E:238:LYS:HB3	1:E:285:ARG:HG2	2.00	0.44
1:E:566:HIS:HD2	1:E:568:LYS:H	1.65	0.44
1:F:385:GLN:HA	1:F:395:VAL:HG22	2.00	0.44
1:F:388:CYS:SG	1:F:393:ILE:HG22	2.57	0.44
1:F:508:GLU:HG3	1:F:771:GLN:N	2.30	0.44
1:F:690:GLU:O	1:F:691:LYS:C	2.60	0.44
1:B:268:GLU:HG2	1:B:270:TYR:OH	2.18	0.44
1:B:747:MET:CE	1:B:751:GLN:HB3	2.47	0.44
1:C:393:ILE:HD11	1:C:613:LEU:HA	1.98	0.44
1:C:434:LYS:HG2	1:C:625:TRP:CZ2	2.53	0.44
1:D:116:TYR:CZ	1:D:146:ARG:HG2	2.53	0.44
1:E:501:GLU:CD	1:E:724:ARG:HH22	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:541:LEU:O	1:E:542:ASP:C	2.61	0.44
1:A:393:ILE:HD11	1:A:612:LEU:C	2.43	0.44
1:A:584:LEU:HD23	1:A:589:LYS:CG	2.35	0.44
1:B:228:ASN:O	1:B:229:PRO:C	2.60	0.44
1:B:242:ASN:OD1	1:B:243:ASP:N	2.51	0.44
1:B:551:THR:CB	1:B:553:THR:HG22	2.47	0.44
1:C:278:ILE:HD12	1:C:428:GLU:HG2	1.99	0.44
3:C:999:ALF:F4	4:C:998:ADP:PB	2.65	0.44
1:D:493:PHE:CZ	1:D:497:MET:HG3	2.52	0.44
1:D:563:GLN:OE1	1:D:563:GLN:HA	2.17	0.44
1:D:688:ASN:ND2	1:D:692:ARG:O	2.35	0.44
1:D:731:ARG:HA	1:D:756:MET:HE1	2.00	0.44
1:E:64:ASN:C	1:E:66:LYS:H	2.26	0.44
1:E:158:ASP:HB2	1:E:193:TYR:CZ	2.52	0.44
1:E:240:VAL:HG23	1:E:241:LYS:HG2	1.99	0.44
1:E:316:LEU:O	1:E:317:SER:C	2.60	0.44
1:E:742:ILE:HG23	1:E:743:PRO:CD	2.47	0.44
1:F:64:ASN:C	1:F:66:LYS:H	2.25	0.44
1:F:173:ILE:HG13	1:F:461:LEU:HD21	1.99	0.44
1:F:340:THR:HG22	1:F:341:ILE:N	2.33	0.44
1:A:222:LYS:O	1:A:226:GLN:HG2	2.18	0.44
1:A:240:VAL:HG23	1:A:241:LYS:HG2	1.99	0.44
1:B:393:ILE:HD11	1:B:613:LEU:HA	1.99	0.44
1:B:690:GLU:O	1:B:691:LYS:C	2.61	0.44
1:B:767:TYR:CD1	1:B:767:TYR:C	2.96	0.44
1:D:251:PHE:CZ	1:D:462:GLY:HA3	2.53	0.44
1:D:545:CYS:SG	1:D:598:LEU:HD23	2.56	0.44
1:E:95:LEU:HD11	1:E:714:ILE:HG21	2.00	0.44
1:E:508:GLU:HG3	1:E:771:GLN:N	2.32	0.44
1:E:751:GLN:O	1:E:755:LEU:HG	2.18	0.44
1:F:36:TRP:HB2	1:F:76:GLN:O	2.18	0.44
1:F:427:ILE:HD13	1:F:427:ILE:HA	1.80	0.44
1:C:97:GLU:HG2	1:C:711:LEU:CD1	2.48	0.44
1:C:164:MET:SD	1:C:459:SER:HB2	2.58	0.44
1:C:251:PHE:CZ	1:C:462:GLY:HA3	2.53	0.44
1:C:738:ALA:O	1:C:741:ALA:HB2	2.16	0.44
1:D:77:LYS:HZ2	1:D:77:LYS:N	2.15	0.44
1:D:225:LEU:N	1:D:225:LEU:CD2	2.81	0.44
1:D:738:ALA:O	1:D:741:ALA:HB3	2.17	0.44
1:D:751:GLN:O	1:D:755:LEU:HG	2.18	0.44
1:E:558:LYS:O	1:E:562:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:767:TYR:CD1	1:E:767:TYR:C	2.96	0.44
1:F:113:ILE:O	1:F:123:VAL:HA	2.18	0.44
1:F:126:PRO:HB3	1:F:130:LEU:HD11	1.99	0.44
1:A:303:ASN:HD22	1:A:303:ASN:C	2.26	0.43
1:A:378:MET:HG3	1:A:378:MET:O	2.18	0.43
1:A:541:LEU:O	1:A:542:ASP:C	2.61	0.43
1:B:495:HIS:CD2	1:B:500:LEU:HG	2.53	0.43
1:C:751:GLN:O	1:C:755:LEU:HG	2.18	0.43
1:E:41:LYS:H	1:E:41:LYS:HG2	1.47	0.43
1:E:508:GLU:HG2	1:E:775:PHE:CE1	2.43	0.43
1:F:116:TYR:CE2	1:F:146:ARG:HG2	2.53	0.43
1:F:355:VAL:O	1:F:359:VAL:HG23	2.17	0.43
1:A:116:TYR:CZ	1:A:146:ARG:HG2	2.53	0.43
1:A:495:HIS:CD2	1:A:500:LEU:HG	2.54	0.43
1:A:742:ILE:HG23	1:A:743:PRO:CD	2.47	0.43
1:B:289:ILE:HD12	1:B:289:ILE:HA	1.85	0.43
1:B:378:MET:CE	1:B:381:ASN:HA	2.42	0.43
1:B:558:LYS:O	1:B:562:GLU:HG2	2.18	0.43
1:C:35:VAL:HG13	1:C:36:TRP:N	2.32	0.43
1:C:734:TYR:OH	1:C:781:LEU:HD22	2.18	0.43
1:D:508:GLU:HG3	1:D:771:GLN:N	2.33	0.43
1:D:558:LYS:O	1:D:562:GLU:HG2	2.18	0.43
1:D:742:ILE:HG23	1:D:743:PRO:CD	2.47	0.43
1:D:747:MET:CE	1:D:751:GLN:HB3	2.48	0.43
1:E:95:LEU:CD1	1:E:714:ILE:HG21	2.48	0.43
1:F:121:CYS:O	1:F:683:ARG:HG2	2.18	0.43
1:F:226:GLN:HB2	1:F:342:MET:HE2	2.01	0.43
1:F:717:CYS:O	1:F:778:THR:HG22	2.17	0.43
1:A:35:VAL:HG11	1:A:75:ILE:CG2	2.49	0.43
1:A:323:ILE:HG22	1:A:324:PRO:N	2.34	0.43
1:A:727:PHE:HA	1:A:753:CYS:SG	2.57	0.43
1:B:96:ASN:O	1:B:97:GLU:C	2.62	0.43
1:B:253:ARG:HG3	1:B:460:PHE:CD1	2.54	0.43
1:B:391:MET:HE2	1:B:434:LYS:NZ	2.33	0.43
1:B:563:GLN:OE1	1:B:563:GLN:HA	2.16	0.43
1:B:717:CYS:O	1:B:778:THR:HG22	2.18	0.43
1:B:731:ARG:O	1:B:735:GLU:HB2	2.18	0.43
1:C:43:GLY:HA3	1:C:702:LEU:CD1	2.47	0.43
1:C:690:GLU:C	1:C:692:ARG:N	2.73	0.43
1:D:158:ASP:HB2	1:D:193:TYR:CZ	2.53	0.43
1:D:498:PHE:CE2	1:D:519:LEU:HD13	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:ILE:HG22	1:E:324:PRO:HD2	1.90	0.43
1:F:501:GLU:CD	1:F:724:ARG:HH22	2.26	0.43
1:F:721:PHE:HB2	1:F:775:PHE:HB3	2.00	0.43
1:B:721:PHE:HB2	1:B:775:PHE:HB3	1.99	0.43
1:C:323:ILE:HG22	1:C:324:PRO:N	2.33	0.43
1:D:35:VAL:N	1:D:47:ALA:O	2.51	0.43
1:E:393:ILE:HD11	1:E:613:LEU:HA	1.98	0.43
1:F:566:HIS:O	1:F:567:ALA:C	2.61	0.43
1:F:751:GLN:O	1:F:755:LEU:HG	2.19	0.43
1:A:239:THR:HG23	1:A:245:SER:HB3	1.99	0.43
1:A:242:ASN:OD1	1:A:243:ASP:N	2.51	0.43
1:A:391:MET:HE2	1:A:434:LYS:NZ	2.32	0.43
1:B:181:ALA:N	1:B:686:ILE:HD12	2.32	0.43
1:C:48:SER:O	1:C:59:VAL:HB	2.19	0.43
1:C:225:LEU:N	1:C:225:LEU:CD2	2.82	0.43
1:D:95:LEU:HD11	1:D:714:ILE:HG21	2.00	0.43
1:D:690:GLU:O	1:D:691:LYS:C	2.61	0.43
1:E:107:ARG:NH1	1:E:114:TYR:O	2.51	0.43
1:E:126:PRO:HB3	1:E:130:LEU:HD11	2.00	0.43
1:E:178:GLU:CD	1:E:686:ILE:HG21	2.44	0.43
1:E:345:THR:HG23	1:E:348:GLU:OE1	2.19	0.43
1:E:767:TYR:O	1:E:768:ARG:HG2	2.18	0.43
1:F:35:VAL:HG21	1:F:75:ILE:CG2	2.48	0.43
1:F:391:MET:HE2	1:F:434:LYS:NZ	2.32	0.43
1:F:417:ALA:C	1:F:418:GLN:HE21	2.26	0.43
1:A:64:ASN:C	1:A:66:LYS:H	2.27	0.43
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.88	0.43
1:B:183:LYS:HZ1	1:B:468:GLY:HA3	1.84	0.43
1:B:303:ASN:HD22	1:B:303:ASN:C	2.26	0.43
1:B:767:TYR:C	1:B:768:ARG:HG2	2.44	0.43
1:C:116:TYR:CZ	1:C:146:ARG:HG2	2.54	0.43
1:C:181:ALA:N	1:C:686:ILE:HD12	2.33	0.43
1:C:242:ASN:OD1	1:C:243:ASP:N	2.51	0.43
1:C:250:LYS:HD2	1:C:252:ILE:HD11	2.01	0.43
1:D:35:VAL:HG21	1:D:75:ILE:HG22	2.01	0.43
1:E:526:GLU:OE1	1:E:530:ARG:HD3	2.18	0.43
1:E:717:CYS:O	1:E:778:THR:HG22	2.19	0.43
1:F:242:ASN:OD1	1:F:243:ASP:N	2.51	0.43
1:F:268:GLU:HG2	1:F:270:TYR:OH	2.19	0.43
1:F:278:ILE:HB	1:F:315:PHE:CE1	2.54	0.43
1:A:35:VAL:HG21	1:A:75:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ILE:HG23	1:A:538:LEU:HG	2.00	0.43
1:A:658:THR:C	1:A:662:LEU:HD12	2.44	0.43
1:B:658:THR:O	1:B:662:LEU:HD12	2.19	0.43
1:C:238:LYS:HB3	1:C:285:ARG:HG2	2.01	0.43
1:D:57:VAL:HG12	1:D:59:VAL:HG13	1.99	0.43
1:D:117:SER:OG	1:D:120:PHE:CE2	2.72	0.43
1:D:468:GLY:N	3:D:999:ALF:F1	2.40	0.43
1:D:663:TYR:O	1:D:664:LYS:C	2.60	0.43
1:E:391:MET:HE2	1:E:434:LYS:NZ	2.33	0.43
1:E:525:ILE:O	1:E:529:GLU:HG2	2.19	0.43
1:F:225:LEU:N	1:F:225:LEU:CD2	2.80	0.43
1:F:526:GLU:OE1	1:F:530:ARG:HD3	2.19	0.43
1:F:663:TYR:O	1:F:664:LYS:C	2.62	0.43
1:A:126:PRO:HB3	1:A:130:LEU:HD11	2.01	0.43
1:A:333:GLN:O	1:A:337:GLU:HB2	2.19	0.43
1:A:493:PHE:CZ	1:A:497:MET:HG3	2.54	0.43
1:A:747:MET:CE	1:A:751:GLN:HB3	2.48	0.43
1:B:64:ASN:C	1:B:66:LYS:H	2.27	0.43
1:B:271:LEU:HD22	1:B:481:CYS:HB2	2.00	0.43
1:B:300:GLN:O	1:B:304:ASP:HB2	2.18	0.43
1:C:300:GLN:O	1:C:304:ASP:HB2	2.18	0.43
1:C:393:ILE:HD11	1:C:612:LEU:C	2.44	0.43
1:C:526:GLU:OE1	1:C:530:ARG:HD3	2.19	0.43
1:D:378:MET:HG3	1:D:378:MET:O	2.19	0.43
1:D:616:SER:C	1:D:618:ASP:N	2.75	0.43
1:D:721:PHE:HB2	1:D:775:PHE:HB3	2.00	0.43
1:E:192:GLN:O	1:E:196:VAL:HG23	2.19	0.43
1:E:219:GLU:O	1:E:222:LYS:N	2.52	0.43
1:E:333:GLN:O	1:E:337:GLU:HB2	2.18	0.43
1:E:339:MET:HE2	1:E:352:ILE:HD13	2.01	0.43
1:E:593:ASN:C	1:E:593:ASN:ND2	2.75	0.43
1:F:747:MET:CE	1:F:751:GLN:HB3	2.49	0.43
1:A:327:GLN:HE21	1:A:327:GLN:HB3	1.73	0.43
1:B:35:VAL:HG13	1:B:36:TRP:N	2.34	0.43
1:B:61:LEU:HG	1:B:66:LYS:O	2.18	0.43
1:B:493:PHE:CZ	1:B:497:MET:HG3	2.54	0.43
1:B:763:ASP:HB3	1:B:766:LEU:HG	2.01	0.43
1:D:501:GLU:CD	1:D:724:ARG:HH22	2.27	0.43
1:E:79:ASN:OD1	1:E:93:THR:HB	2.19	0.43
1:E:528:ILE:HG23	1:E:538:LEU:HG	2.01	0.43
1:E:708:ASN:N	1:E:708:ASN:ND2	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:750:LYS:HE3	1:E:769:ILE:HG22	2.01	0.43
1:F:48:SER:O	1:F:59:VAL:HB	2.19	0.43
1:F:57:VAL:HG12	1:F:59:VAL:HG13	2.00	0.43
1:F:300:GLN:O	1:F:304:ASP:HB2	2.19	0.43
1:F:528:ILE:HG23	1:F:538:LEU:HG	2.01	0.43
1:A:726:VAL:O	1:A:727:PHE:C	2.62	0.43
1:B:172:SER:HA	1:B:462:GLY:O	2.18	0.43
1:B:688:ASN:ND2	1:B:692:ARG:O	2.36	0.43
1:C:493:PHE:CZ	1:C:497:MET:HG3	2.54	0.43
1:C:605:LEU:HD12	1:C:605:LEU:HA	1.85	0.43
1:C:616:SER:C	1:C:618:ASP:N	2.74	0.43
1:D:226:GLN:HB2	1:D:342:MET:HE2	2.00	0.43
1:D:323:ILE:HG22	1:D:324:PRO:N	2.34	0.43
1:E:226:GLN:C	1:E:229:PRO:HD2	2.44	0.43
1:E:616:SER:C	1:E:618:ASP:N	2.76	0.43
1:F:767:TYR:O	1:F:768:ARG:HG2	2.18	0.43
1:A:113:ILE:O	1:A:123:VAL:HA	2.19	0.42
1:A:274:LYS:CG	1:A:436:GLU:HB2	2.46	0.42
1:A:419:THR:H	1:A:422:GLN:CG	2.26	0.42
1:B:501:GLU:CD	1:B:724:ARG:HH22	2.27	0.42
1:C:528:ILE:HG23	1:C:538:LEU:HG	2.01	0.42
1:F:172:SER:HA	1:F:462:GLY:O	2.19	0.42
1:F:495:HIS:CD2	1:F:500:LEU:HG	2.54	0.42
1:F:731:ARG:HH11	1:F:731:ARG:CG	2.30	0.42
1:A:172:SER:HA	1:A:462:GLY:O	2.19	0.42
1:B:48:SER:O	1:B:59:VAL:HB	2.19	0.42
1:B:323:ILE:HG22	1:B:324:PRO:N	2.33	0.42
1:C:355:VAL:O	1:C:359:VAL:HG23	2.19	0.42
1:E:544:GLU:OE1	1:E:544:GLU:HA	2.20	0.42
1:E:721:PHE:HB2	1:E:775:PHE:HB3	2.01	0.42
1:F:526:GLU:OE1	1:F:526:GLU:HA	2.18	0.42
1:A:731:ARG:O	1:A:735:GLU:HB2	2.20	0.42
1:B:126:PRO:HB3	1:B:130:LEU:HD11	2.01	0.42
1:B:164:MET:SD	1:B:459:SER:HB2	2.59	0.42
1:B:225:LEU:N	1:B:225:LEU:CD2	2.82	0.42
1:B:393:ILE:HD11	1:B:612:LEU:C	2.43	0.42
1:B:746:PHE:CD1	1:C:306:LEU:HD11	2.54	0.42
1:C:58:THR:HA	1:C:69:THR:HA	2.01	0.42
1:C:64:ASN:C	1:C:66:LYS:H	2.27	0.42
1:C:291:TYR:HA	1:C:310:PHE:HE1	1.84	0.42
1:C:303:ASN:HD22	1:C:303:ASN:C	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:ASN:HD22	1:C:606:ASN:C	2.26	0.42
1:C:690:GLU:O	1:C:691:LYS:C	2.62	0.42
1:D:80:PRO:HB2	1:D:82:LYS:HG2	2.01	0.42
1:D:271:LEU:HD22	1:D:481:CYS:HB2	2.02	0.42
1:D:345:THR:HG23	1:D:348:GLU:OE1	2.19	0.42
1:D:731:ARG:O	1:D:735:GLU:HB2	2.19	0.42
1:E:36:TRP:HB2	1:E:76:GLN:O	2.19	0.42
1:E:116:TYR:CZ	1:E:146:ARG:HG2	2.55	0.42
1:E:690:GLU:O	1:E:691:LYS:C	2.62	0.42
1:E:756:MET:O	1:E:760:LEU:HG	2.19	0.42
1:F:192:GLN:O	1:F:196:VAL:HG23	2.18	0.42
1:F:508:GLU:HG2	1:F:775:PHE:CE1	2.45	0.42
1:F:527:LEU:HB2	1:F:566:HIS:CE1	2.55	0.42
1:F:563:GLN:OE1	1:F:563:GLN:HA	2.19	0.42
1:A:417:ALA:C	1:A:418:GLN:HE21	2.26	0.42
1:A:537:VAL:HG22	1:A:559:LEU:CD1	2.47	0.42
1:A:750:LYS:HE3	1:A:769:ILE:HG22	2.01	0.42
1:B:173:ILE:HG13	1:B:461:LEU:HD21	2.00	0.42
1:B:239:THR:HG23	1:B:245:SER:HB3	2.00	0.42
1:B:525:ILE:O	1:B:529:GLU:CG	2.67	0.42
1:B:593:ASN:ND2	1:B:593:ASN:C	2.77	0.42
1:C:525:ILE:O	1:C:529:GLU:HG2	2.19	0.42
1:D:61:LEU:HG	1:D:66:LYS:O	2.19	0.42
1:D:162:ARG:HG2	1:D:162:ARG:H	1.68	0.42
1:D:290:PHE:CE1	1:D:356:VAL:HG13	2.54	0.42
1:D:401:SER:HB3	1:D:608:ASN:CB	2.48	0.42
1:D:686:ILE:HG22	1:D:704:GLN:CD	2.44	0.42
1:F:77:LYS:HZ2	1:F:77:LYS:N	2.16	0.42
1:A:117:SER:OG	1:A:120:PHE:CE2	2.73	0.42
1:A:339:MET:CE	1:A:352:ILE:HD13	2.49	0.42
1:A:339:MET:HE2	1:A:352:ILE:HD13	2.00	0.42
1:A:605:LEU:HD12	1:A:605:LEU:HA	1.88	0.42
1:B:35:VAL:HG21	1:B:75:ILE:CG2	2.49	0.42
1:B:663:TYR:O	1:B:664:LYS:C	2.62	0.42
1:C:271:LEU:HD22	1:C:481:CYS:CB	2.49	0.42
1:C:417:ALA:C	1:C:418:GLN:HE21	2.27	0.42
1:C:495:HIS:CD2	1:C:500:LEU:HG	2.55	0.42
1:C:686:ILE:HG22	1:C:704:GLN:CD	2.45	0.42
1:D:521:LEU:O	1:D:522:GLN:C	2.62	0.42
1:E:724:ARG:HG3	1:E:724:ARG:O	2.20	0.42
1:E:747:MET:CE	1:E:751:GLN:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:ILE:O	1:F:529:GLU:HG2	2.20	0.42
1:F:738:ALA:CB	1:F:741:ALA:HB2	2.47	0.42
1:A:253:ARG:HG3	1:A:460:PHE:CD1	2.54	0.42
1:B:292:TYR:CE2	1:B:331:MET:HB3	2.54	0.42
1:B:528:ILE:HG23	1:B:538:LEU:HG	2.01	0.42
1:B:541:LEU:O	1:B:542:ASP:C	2.62	0.42
1:B:711:LEU:O	1:B:715:ARG:HG2	2.20	0.42
1:C:36:TRP:HB2	1:C:76:GLN:O	2.20	0.42
1:C:333:GLN:O	1:C:337:GLU:HB2	2.19	0.42
1:C:385:GLN:HA	1:C:395:VAL:HG22	2.00	0.42
1:C:558:LYS:O	1:C:562:GLU:HG2	2.19	0.42
1:C:750:LYS:HE3	1:C:769:ILE:HG22	2.01	0.42
1:D:64:ASN:C	1:D:66:LYS:H	2.28	0.42
1:D:172:SER:HA	1:D:462:GLY:O	2.20	0.42
1:D:219:GLU:O	1:D:222:LYS:N	2.52	0.42
1:D:228:ASN:O	1:D:229:PRO:C	2.60	0.42
1:D:236:ASN:ND2	1:D:244:ASN:O	2.52	0.42
1:E:173:ILE:HG13	1:E:461:LEU:HD21	2.00	0.42
1:E:225:LEU:N	1:E:225:LEU:CD2	2.82	0.42
1:E:339:MET:CE	1:E:352:ILE:HD13	2.50	0.42
1:E:545:CYS:SG	1:E:598:LEU:HD23	2.60	0.42
1:F:97:GLU:HG2	1:F:711:LEU:CD1	2.49	0.42
1:F:254:ILE:O	1:F:460:PHE:HA	2.20	0.42
1:F:724:ARG:O	1:F:724:ARG:HG3	2.20	0.42
1:A:61:LEU:HG	1:A:66:LYS:O	2.20	0.42
1:A:192:GLN:O	1:A:196:VAL:HG23	2.19	0.42
1:A:606:ASN:HD22	1:A:606:ASN:C	2.27	0.42
1:A:756:MET:HE3	1:A:756:MET:HB2	1.77	0.42
1:A:763:ASP:HB3	1:A:766:LEU:HG	2.01	0.42
1:B:41:LYS:H	1:B:41:LYS:HG2	1.44	0.42
1:B:333:GLN:O	1:B:337:GLU:HB2	2.19	0.42
1:B:393:ILE:HD11	1:B:612:LEU:O	2.19	0.42
1:B:502:GLN:HA	1:B:505:TYR:CD2	2.54	0.42
1:B:750:LYS:HE3	1:B:769:ILE:HG22	2.02	0.42
1:C:427:ILE:HA	1:C:427:ILE:HD13	1.75	0.42
1:C:742:ILE:HG12	1:C:752:ALA:HB1	2.00	0.42
1:D:253:ARG:HG3	1:D:460:PHE:CD1	2.54	0.42
1:D:291:TYR:HA	1:D:310:PHE:HE1	1.84	0.42
1:D:541:LEU:O	1:D:542:ASP:C	2.62	0.42
1:D:743:PRO:HD2	1:D:747:MET:SD	2.60	0.42
1:E:278:ILE:HD12	1:E:428:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:LEU:HD12	1:F:34:LEU:HA	1.75	0.42
1:F:78:MET:HE2	1:F:78:MET:HB3	1.92	0.42
1:F:434:LYS:HG2	1:F:625:TRP:CZ2	2.55	0.42
1:A:308:GLU:HB3	1:A:312:ASN:CB	2.48	0.42
1:A:393:ILE:HD11	1:A:612:LEU:O	2.20	0.42
1:A:401:SER:HB3	1:A:608:ASN:CB	2.47	0.42
1:A:521:LEU:O	1:A:522:GLN:C	2.61	0.42
1:A:671:MET:O	1:A:675:ARG:HD2	2.20	0.42
1:A:743:PRO:HD2	1:A:747:MET:SD	2.60	0.42
1:B:340:THR:HG22	1:B:341:ILE:N	2.35	0.42
1:B:388:CYS:SG	1:B:393:ILE:HG22	2.60	0.42
1:B:526:GLU:OE1	1:B:530:ARG:HD3	2.19	0.42
1:B:545:CYS:SG	1:B:598:LEU:HD23	2.59	0.42
1:B:742:ILE:HG12	1:B:752:ALA:HB1	2.02	0.42
1:C:80:PRO:HB2	1:C:82:LYS:HG2	2.01	0.42
1:C:540:LEU:HD12	1:C:559:LEU:CD1	2.50	0.42
1:C:717:CYS:O	1:C:778:THR:HG22	2.19	0.42
1:D:96:ASN:O	1:D:97:GLU:C	2.61	0.42
1:E:671:MET:O	1:E:675:ARG:HD2	2.20	0.42
1:A:107:ARG:HD3	1:A:115:THR:OG1	2.20	0.42
1:A:271:LEU:HD22	1:A:481:CYS:CB	2.50	0.42
1:A:663:TYR:O	1:A:664:LYS:C	2.62	0.42
1:B:58:THR:OG1	1:B:69:THR:HG23	2.20	0.42
1:B:385:GLN:HA	1:B:395:VAL:HG22	2.02	0.42
1:C:222:LYS:O	1:C:226:GLN:HG2	2.19	0.42
1:C:274:LYS:CG	1:C:436:GLU:HB2	2.47	0.42
1:C:541:LEU:O	1:C:542:ASP:C	2.62	0.42
1:D:385:GLN:HA	1:D:395:VAL:HG22	2.02	0.42
1:D:402:ILE:HG22	1:D:403:LEU:N	2.33	0.42
1:D:659:VAL:O	1:D:660:GLY:C	2.62	0.42
1:D:726:VAL:O	1:D:727:PHE:C	2.62	0.42
1:E:97:GLU:HG2	1:E:711:LEU:CD1	2.49	0.42
1:E:162:ARG:HG2	1:E:162:ARG:H	1.64	0.42
1:E:183:LYS:HZ1	1:E:468:GLY:HA3	1.85	0.42
1:E:401:SER:HB3	1:E:608:ASN:CB	2.45	0.42
1:B:274:LYS:CG	1:B:436:GLU:HB2	2.48	0.42
1:B:606:ASN:C	1:B:606:ASN:HD22	2.28	0.42
1:B:671:MET:O	1:B:675:ARG:HD2	2.19	0.42
1:B:726:VAL:O	1:B:727:PHE:C	2.62	0.42
1:C:663:TYR:O	1:C:664:LYS:C	2.63	0.42
1:D:121:CYS:O	1:D:683:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:PHE:HD1	1:D:360:LEU:HD11	1.85	0.42
1:D:393:ILE:HD11	1:D:612:LEU:C	2.45	0.42
1:E:61:LEU:O	1:E:65:GLY:CA	2.68	0.42
1:E:385:GLN:HA	1:E:395:VAL:HG22	2.01	0.42
1:E:402:ILE:HD13	1:E:402:ILE:HA	1.93	0.42
1:E:606:ASN:C	1:E:606:ASN:HD22	2.28	0.42
1:A:527:LEU:HB2	1:A:566:HIS:CE1	2.54	0.41
1:B:58:THR:HA	1:B:69:THR:HA	2.02	0.41
1:B:113:ILE:O	1:B:123:VAL:HA	2.20	0.41
1:B:658:THR:C	1:B:662:LEU:HD12	2.45	0.41
1:B:742:ILE:HG23	1:B:743:PRO:CD	2.47	0.41
1:C:743:PRO:HD2	1:C:747:MET:SD	2.60	0.41
1:D:43:GLY:HA3	1:D:702:LEU:CD1	2.49	0.41
1:D:72:LYS:O	1:D:75:ILE:HD12	2.20	0.41
1:D:173:ILE:HG13	1:D:461:LEU:HD21	2.02	0.41
1:E:38:PRO:HD3	1:E:74:ASP:O	2.20	0.41
1:E:271:LEU:HD22	1:E:481:CYS:CB	2.50	0.41
1:E:566:HIS:O	1:E:567:ALA:C	2.62	0.41
1:F:616:SER:C	1:F:618:ASP:N	2.74	0.41
1:A:185:GLU:O	1:A:189:LYS:HG2	2.20	0.41
1:A:438:LEU:O	1:A:442:ILE:HG13	2.20	0.41
1:A:616:SER:C	1:A:618:ASP:N	2.76	0.41
1:A:721:PHE:CB	1:A:775:PHE:HB3	2.50	0.41
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.89	0.41
1:B:107:ARG:NH1	1:B:114:TYR:O	2.54	0.41
1:B:291:TYR:HA	1:B:310:PHE:HE1	1.85	0.41
1:C:747:MET:CE	1:C:751:GLN:HB3	2.49	0.41
1:D:58:THR:OG1	1:D:69:THR:HG23	2.20	0.41
1:D:525:ILE:O	1:D:529:GLU:HG2	2.20	0.41
1:E:323:ILE:HG22	1:E:324:PRO:N	2.34	0.41
1:E:362:LEU:HD23	1:E:387:VAL:HG21	2.01	0.41
1:E:606:ASN:O	1:E:609:VAL:HG13	2.21	0.41
1:F:362:LEU:HD23	1:F:362:LEU:HA	1.90	0.41
1:F:609:VAL:O	1:F:612:LEU:HB2	2.19	0.41
1:F:742:ILE:HG23	1:F:743:PRO:CD	2.51	0.41
1:A:38:PRO:HD3	1:A:74:ASP:O	2.21	0.41
1:A:77:LYS:H	1:A:77:LYS:CD	2.32	0.41
1:A:181:ALA:N	1:A:686:ILE:HD12	2.34	0.41
1:A:385:GLN:HA	1:A:395:VAL:HG22	2.02	0.41
1:A:525:ILE:O	1:A:529:GLU:CG	2.68	0.41
1:A:558:LYS:O	1:A:562:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:VAL:CG2	1:B:75:ILE:HG22	2.51	0.41
1:B:192:GLN:O	1:B:196:VAL:HG23	2.20	0.41
1:B:605:LEU:HD12	1:B:605:LEU:HA	1.85	0.41
1:C:96:ASN:O	1:C:97:GLU:C	2.62	0.41
1:C:340:THR:HG22	1:C:341:ILE:N	2.36	0.41
1:C:727:PHE:HA	1:C:753:CYS:SG	2.59	0.41
1:D:333:GLN:O	1:D:337:GLU:HB2	2.20	0.41
1:D:362:LEU:HD23	1:D:362:LEU:HA	1.87	0.41
1:E:172:SER:HA	1:E:462:GLY:O	2.20	0.41
1:E:434:LYS:HG2	1:E:625:TRP:CZ2	2.54	0.41
1:E:467:ALA:HB3	1:E:482:ILE:HG12	2.02	0.41
1:F:715:ARG:NH1	1:F:715:ARG:CG	2.81	0.41
1:A:767:TYR:C	1:A:768:ARG:HG2	2.45	0.41
1:B:738:ALA:O	1:B:741:ALA:HB3	2.17	0.41
1:C:419:THR:O	1:C:420:LYS:C	2.62	0.41
1:D:183:LYS:HZ1	1:D:468:GLY:HA3	1.86	0.41
1:D:300:GLN:O	1:D:303:ASN:ND2	2.53	0.41
1:D:303:ASN:HD22	1:D:303:ASN:C	2.26	0.41
1:D:508:GLU:HG2	1:D:775:PHE:CE1	2.43	0.41
1:E:88:ASP:HA	1:E:116:TYR:O	2.20	0.41
1:F:671:MET:O	1:F:675:ARG:HD2	2.20	0.41
1:F:686:ILE:HG22	1:F:704:GLN:CD	2.45	0.41
1:F:721:PHE:CB	1:F:775:PHE:HB3	2.51	0.41
1:B:345:THR:HG23	1:B:348:GLU:OE1	2.21	0.41
1:B:721:PHE:CB	1:B:775:PHE:HB3	2.51	0.41
1:C:393:ILE:HD11	1:C:612:LEU:O	2.20	0.41
1:C:521:LEU:O	1:C:522:GLN:C	2.63	0.41
1:C:527:LEU:HB2	1:C:566:HIS:CE1	2.55	0.41
1:E:527:LEU:HB2	1:E:566:HIS:CE1	2.55	0.41
1:A:58:THR:HA	1:A:69:THR:HA	2.02	0.41
1:B:114:TYR:CE1	1:B:153:ILE:HB	2.55	0.41
1:B:238:LYS:HB3	1:B:285:ARG:HD3	2.03	0.41
1:B:271:LEU:HD22	1:B:481:CYS:CB	2.50	0.41
1:C:192:GLN:O	1:C:196:VAL:HG23	2.20	0.41
1:D:35:VAL:HG22	1:D:76:GLN:O	2.19	0.41
1:D:116:TYR:CE2	1:D:146:ARG:HG2	2.55	0.41
1:D:192:GLN:O	1:D:196:VAL:HG23	2.20	0.41
1:D:327:GLN:HE21	1:D:327:GLN:HB3	1.73	0.41
1:D:606:ASN:C	1:D:606:ASN:HD22	2.29	0.41
1:E:300:GLN:O	1:E:304:ASP:HB2	2.20	0.41
1:E:340:THR:HG22	1:E:341:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:438:LEU:O	1:E:442:ILE:HG13	2.20	0.41
1:E:743:PRO:HD2	1:E:747:MET:SD	2.61	0.41
1:E:781:LEU:HD23	1:E:784:LEU:HD12	2.01	0.41
1:F:289:ILE:HD12	1:F:289:ILE:HA	1.81	0.41
1:F:658:THR:O	1:F:662:LEU:HD12	2.21	0.41
1:A:254:ILE:O	1:A:460:PHE:HA	2.21	0.41
1:C:82:LYS:HE2	1:C:82:LYS:HB3	1.90	0.41
1:D:178:GLU:CD	1:D:686:ILE:HG21	2.46	0.41
1:D:292:TYR:CE2	1:D:331:MET:HB3	2.56	0.41
1:D:528:ILE:HG23	1:D:538:LEU:HG	2.02	0.41
1:D:701:VAL:O	1:D:705:LEU:HG	2.19	0.41
1:E:61:LEU:HG	1:E:66:LYS:O	2.20	0.41
1:E:121:CYS:O	1:E:683:ARG:HG2	2.21	0.41
1:E:254:ILE:O	1:E:460:PHE:HA	2.20	0.41
1:B:362:LEU:HA	1:B:362:LEU:HD23	1.86	0.41
1:B:566:HIS:O	1:B:569:PHE:N	2.53	0.41
1:D:434:LYS:HG2	1:D:625:TRP:CZ2	2.56	0.41
1:E:222:LYS:O	1:E:226:GLN:HG2	2.21	0.41
1:E:540:LEU:HD12	1:E:559:LEU:CD1	2.51	0.41
1:E:690:GLU:C	1:E:692:ARG:N	2.73	0.41
1:E:767:TYR:C	1:E:768:ARG:HG2	2.46	0.41
1:A:35:VAL:HG21	1:A:75:ILE:CG2	2.51	0.41
1:A:159:THR:O	1:A:163:SER:HB2	2.21	0.41
1:A:427:ILE:HD13	1:A:427:ILE:HA	1.75	0.41
1:A:670:LEU:O	1:A:671:MET:C	2.61	0.41
1:A:677:THR:O	1:A:679:PRO:HD3	2.21	0.41
1:A:742:ILE:HG12	1:A:752:ALA:HB1	2.03	0.41
1:A:781:LEU:O	1:A:782:ALA:C	2.64	0.41
1:B:34:LEU:HD12	1:B:34:LEU:HA	1.74	0.41
1:B:107:ARG:HD3	1:B:115:THR:OG1	2.21	0.41
1:B:527:LEU:HB2	1:B:566:HIS:CE1	2.56	0.41
1:C:41:LYS:H	1:C:41:LYS:HG2	1.46	0.41
1:C:113:ILE:O	1:C:123:VAL:HA	2.21	0.41
1:C:671:MET:O	1:C:675:ARG:HD2	2.21	0.41
1:D:78:MET:HE2	1:D:78:MET:HB3	1.90	0.41
1:D:663:TYR:CE2	1:D:667:LEU:HD22	2.56	0.41
1:E:291:TYR:HA	1:E:310:PHE:HE1	1.86	0.41
1:E:297:ALA:HB3	1:E:302:ARG:HD2	2.03	0.41
1:E:670:LEU:O	1:E:671:MET:C	2.64	0.41
1:E:726:VAL:O	1:E:727:PHE:C	2.64	0.41
1:E:731:ARG:HH11	1:E:731:ARG:CG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:ARG:NH1	1:F:114:TYR:O	2.54	0.41
1:F:114:TYR:CE1	1:F:153:ILE:HB	2.56	0.41
1:F:310:PHE:CE1	1:F:320:HIS:HD2	2.39	0.41
1:F:541:LEU:O	1:F:542:ASP:C	2.64	0.41
1:A:121:CYS:O	1:A:683:ARG:HG2	2.21	0.41
1:A:178:GLU:CD	1:A:686:ILE:HG21	2.46	0.41
1:A:225:LEU:N	1:A:225:LEU:CD2	2.82	0.41
1:A:552:ASP:HA	1:A:598:LEU:HD12	2.03	0.41
1:B:36:TRP:HB2	1:B:76:GLN:O	2.21	0.41
1:B:90:ALA:O	1:B:718:ARG:NH1	2.53	0.41
1:B:434:LYS:HG2	1:B:625:TRP:CZ2	2.53	0.41
1:B:743:PRO:HD2	1:B:747:MET:SD	2.60	0.41
1:C:38:PRO:HD3	1:C:74:ASP:O	2.21	0.41
1:C:184:THR:HG22	1:C:188:LYS:HE3	2.02	0.41
1:C:403:LEU:HD23	1:C:403:LEU:HA	1.94	0.41
1:C:781:LEU:HD23	1:C:784:LEU:HD12	2.02	0.41
1:D:658:THR:C	1:D:662:LEU:HD12	2.46	0.41
1:E:35:VAL:HG21	1:E:75:ILE:HG22	2.02	0.41
1:E:96:ASN:O	1:E:97:GLU:C	2.63	0.41
1:E:164:MET:SD	1:E:459:SER:HB2	2.61	0.41
1:E:239:THR:HG23	1:E:245:SER:HB3	2.03	0.41
1:E:663:TYR:O	1:E:664:LYS:C	2.63	0.41
1:F:393:ILE:HD11	1:F:612:LEU:O	2.21	0.41
1:F:419:THR:O	1:F:420:LYS:C	2.63	0.41
1:A:79:ASN:OD1	1:A:93:THR:HB	2.21	0.40
1:A:721:PHE:CD1	1:A:721:PHE:N	2.89	0.40
1:B:763:ASP:OD1	1:B:764:PRO:HD2	2.21	0.40
1:C:178:GLU:CD	1:C:686:ILE:HG21	2.46	0.40
1:C:419:THR:H	1:C:422:GLN:CG	2.26	0.40
1:D:58:THR:HA	1:D:69:THR:HA	2.02	0.40
1:D:145:LYS:CB	1:D:148:GLU:HG3	2.43	0.40
1:D:189:LYS:HZ2	1:D:189:LYS:HG2	1.77	0.40
1:F:291:TYR:HA	1:F:310:PHE:HE1	1.85	0.40
1:A:125:ASN:O	1:A:687:PRO:HG3	2.21	0.40
1:A:340:THR:HG22	1:A:341:ILE:N	2.36	0.40
1:A:606:ASN:O	1:A:609:VAL:HG13	2.21	0.40
1:B:521:LEU:O	1:B:522:GLN:C	2.63	0.40
1:C:35:VAL:HG21	1:C:75:ILE:CG2	2.51	0.40
1:C:721:PHE:HB2	1:C:775:PHE:HB3	2.02	0.40
1:C:747:MET:HG3	1:C:752:ALA:HB2	2.03	0.40
1:D:184:THR:HG22	1:D:188:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:623:ASP:O	1:D:624:LEU:C	2.64	0.40
1:E:35:VAL:N	1:E:47:ALA:O	2.51	0.40
1:E:402:ILE:HG22	1:E:403:LEU:N	2.36	0.40
1:F:167:ASP:HB2	1:F:169:GLU:HG2	2.03	0.40
1:F:323:ILE:HG22	1:F:324:PRO:N	2.35	0.40
1:F:345:THR:HG23	1:F:348:GLU:OE1	2.21	0.40
1:F:734:TYR:OH	1:F:781:LEU:HD22	2.21	0.40
1:A:445:ARG:HH12	1:A:449:ALA:HB2	1.86	0.40
1:A:541:LEU:O	1:A:544:GLU:N	2.54	0.40
1:C:35:VAL:N	1:C:47:ALA:O	2.55	0.40
1:C:61:LEU:O	1:C:65:GLY:CA	2.70	0.40
1:C:107:ARG:HD3	1:C:115:THR:OG1	2.21	0.40
1:C:501:GLU:CD	1:C:724:ARG:HH22	2.27	0.40
1:C:742:ILE:HG23	1:C:743:PRO:CD	2.47	0.40
1:D:38:PRO:HD3	1:D:74:ASP:O	2.22	0.40
1:D:126:PRO:HB3	1:D:130:LEU:HD11	2.03	0.40
1:D:185:GLU:O	1:D:189:LYS:HG2	2.22	0.40
1:E:493:PHE:CZ	1:E:497:MET:HG3	2.56	0.40
1:E:721:PHE:CB	1:E:775:PHE:HB3	2.50	0.40
1:F:96:ASN:O	1:F:97:GLU:C	2.64	0.40
1:F:117:SER:OG	1:F:120:PHE:CE2	2.72	0.40
1:F:185:GLU:O	1:F:189:LYS:HG2	2.21	0.40
1:F:333:GLN:O	1:F:337:GLU:HB2	2.20	0.40
1:B:226:GLN:HB2	1:B:342:MET:HE2	2.04	0.40
1:C:285:ARG:HB2	1:C:291:TYR:CE2	2.56	0.40
1:C:525:ILE:O	1:C:529:GLU:CG	2.70	0.40
1:E:35:VAL:HG11	1:E:75:ILE:CG2	2.51	0.40
1:E:378:MET:HG3	1:E:378:MET:O	2.22	0.40
1:E:521:LEU:O	1:E:522:GLN:C	2.64	0.40
1:A:526:GLU:OE1	1:A:530:ARG:HD3	2.22	0.40
1:A:701:VAL:O	1:A:705:LEU:HG	2.21	0.40
1:B:236:ASN:ND2	1:B:244:ASN:O	2.55	0.40
1:C:339:MET:CE	1:C:352:ILE:HD13	2.52	0.40
1:E:58:THR:HA	1:E:69:THR:HA	2.04	0.40
1:E:278:ILE:CD1	1:E:432:LYS:HD3	2.52	0.40
1:F:544:GLU:OE1	1:F:544:GLU:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	655/791 (83%)	582 (89%)	63 (10%)	10 (2%)	8	28
1	B	655/791 (83%)	586 (90%)	59 (9%)	10 (2%)	8	28
1	C	655/791 (83%)	583 (89%)	63 (10%)	9 (1%)	9	30
1	D	655/791 (83%)	583 (89%)	62 (10%)	10 (2%)	8	28
1	E	655/791 (83%)	581 (89%)	62 (10%)	12 (2%)	6	25
1	F	655/791 (83%)	585 (89%)	59 (9%)	11 (2%)	7	26
All	All	3930/4746 (83%)	3500 (89%)	368 (9%)	62 (2%)	7	27

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	SER
1	A	324	PRO
1	A	533	ASN
1	A	564	GLY
1	B	317	SER
1	B	324	PRO
1	B	533	ASN
1	B	564	GLY
1	C	317	SER
1	C	324	PRO
1	C	533	ASN
1	C	564	GLY
1	D	317	SER
1	D	324	PRO
1	D	533	ASN
1	D	564	GLY
1	E	317	SER
1	E	533	ASN
1	E	564	GLY
1	F	317	SER

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Mol	Chain	Res	Type
1	F	324	PRO
1	F	533	ASN
1	F	564	GLY
1	A	319	GLY
1	A	530	ARG
1	A	607	ASP
1	B	319	GLY
1	B	530	ARG
1	B	607	ASP
1	C	319	GLY
1	C	530	ARG
1	C	607	ASP
1	D	319	GLY
1	D	530	ARG
1	E	319	GLY
1	E	324	PRO
1	E	607	ASP
1	F	319	GLY
1	F	607	ASP
1	D	607	ASP
1	E	531	PRO
1	F	531	PRO
1	A	531	PRO
1	B	531	PRO
1	C	531	PRO
1	D	531	PRO
1	E	530	ARG
1	F	530	ARG
1	A	523	PRO
1	B	523	PRO
1	C	523	PRO
1	D	265	ALA
1	D	523	PRO
1	E	265	ALA
1	E	523	PRO
1	F	271	LEU
1	F	523	PRO
1	A	271	LEU
1	B	271	LEU
1	E	271	LEU
1	E	566	HIS
1	F	566	HIS

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	A	555/696 (80%)	445 (80%)	110 (20%)	1	5
1	B	555/696 (80%)	445 (80%)	110 (20%)	1	5
1	C	555/696 (80%)	447 (80%)	108 (20%)	1	5
1	D	555/696 (80%)	446 (80%)	109 (20%)	1	5
1	E	555/696 (80%)	447 (80%)	108 (20%)	1	5
1	F	555/696 (80%)	448 (81%)	107 (19%)	1	5
All	All	3330/4176 (80%)	2678 (80%)	652 (20%)	1	5

All (652) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	35	VAL
1	A	39	SER
1	A	41	LYS
1	A	42	HIS
1	A	48	SER
1	A	75	ILE
1	A	77	LYS
1	A	82	LYS
1	A	86	VAL
1	A	89	MET
1	A	91	GLU
1	A	110	SER
1	A	112	LEU
1	A	123	VAL
1	A	124	ILE
1	A	128	LYS
1	A	135	GLU
1	A	136	LYS
1	A	142	LYS
1	A	144	LYS
1	A	145	LYS

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Mol	Chain	Res	Type
1	A	156	ILE
1	A	166	GLN
1	A	167	ASP
1	A	174	LEU
1	A	189	LYS
1	A	199	SER
1	A	225	LEU
1	A	232	GLU
1	A	250	LYS
1	A	259	THR
1	A	263	VAL
1	A	268	GLU
1	A	274	LYS
1	A	275	SER
1	A	278	ILE
1	A	285	ARG
1	A	302	ARG
1	A	303	ASN
1	A	308	GLU
1	A	311	ASN
1	A	314	THR
1	A	317	SER
1	A	323	ILE
1	A	326	GLN
1	A	327	GLN
1	A	329	ASP
1	A	334	GLU
1	A	340	THR
1	A	377	SER
1	A	393	ILE
1	A	394	ASN
1	A	402	ILE
1	A	404	THR
1	A	419	THR
1	A	420	LYS
1	A	422	GLN
1	A	427	ILE
1	A	434	LYS
1	A	448	LYS
1	A	459	SER
1	A	473	GLU
1	A	487	GLU

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Mol	Chain	Res	Type
1	A	488	LYS
1	A	499	ILE
1	A	501	GLU
1	A	504	GLU
1	A	506	GLN
1	A	507	ARG
1	A	511	GLU
1	A	522	GLN
1	A	527	LEU
1	A	529	GLU
1	A	544	GLU
1	A	545	CYS
1	A	554	SER
1	A	560	ILE
1	A	572	SER
1	A	589	LYS
1	A	591	THR
1	A	593	ASN
1	A	599	THR
1	A	605	LEU
1	A	606	ASN
1	A	607	ASP
1	A	609	VAL
1	A	615	GLN
1	A	623	ASP
1	A	664	LYS
1	A	666	GLN
1	A	675	ARG
1	A	683	ARG
1	A	686	ILE
1	A	702	LEU
1	A	708	ASN
1	A	719	GLN
1	A	723	ASN
1	A	729	GLU
1	A	731	ARG
1	A	732	GLN
1	A	733	ARG
1	A	735	GLU
1	A	748	ASP
1	A	750	LYS
1	A	754	ILE

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Mol	Chain	Res	Type
1	A	755	LEU
1	A	771	GLN
1	A	773	LYS
1	A	778	THR
1	B	34	LEU
1	B	35	VAL
1	B	39	SER
1	B	41	LYS
1	B	42	HIS
1	B	48	SER
1	B	75	ILE
1	B	77	LYS
1	B	82	LYS
1	B	86	VAL
1	B	91	GLU
1	B	110	SER
1	B	123	VAL
1	B	124	ILE
1	B	128	LYS
1	B	132	ILE
1	B	135	GLU
1	B	136	LYS
1	B	142	LYS
1	B	144	LYS
1	B	145	LYS
1	B	156	ILE
1	B	166	GLN
1	B	167	ASP
1	B	173	ILE
1	B	174	LEU
1	B	189	LYS
1	B	199	SER
1	B	225	LEU
1	B	232	GLU
1	B	250	LYS
1	B	259	THR
1	B	263	VAL
1	B	268	GLU
1	B	274	LYS
1	B	275	SER
1	B	278	ILE
1	B	302	ARG

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Mol	Chain	Res	Type
1	B	303	ASN
1	B	308	GLU
1	B	311	ASN
1	B	314	THR
1	B	317	SER
1	B	323	ILE
1	B	326	GLN
1	B	327	GLN
1	B	329	ASP
1	B	334	GLU
1	B	340	THR
1	B	377	SER
1	B	393	ILE
1	B	394	ASN
1	B	402	ILE
1	B	404	THR
1	B	419	THR
1	B	420	LYS
1	B	422	GLN
1	B	427	ILE
1	B	434	LYS
1	B	448	LYS
1	B	459	SER
1	B	473	GLU
1	B	487	GLU
1	B	488	LYS
1	B	499	ILE
1	B	501	GLU
1	B	504	GLU
1	B	506	GLN
1	B	507	ARG
1	B	511	GLU
1	B	522	GLN
1	B	527	LEU
1	B	529	GLU
1	B	544	GLU
1	B	545	CYS
1	B	554	SER
1	B	560	ILE
1	B	572	SER
1	B	589	LYS
1	B	591	THR

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Mol	Chain	Res	Type
1	B	593	ASN
1	B	599	THR
1	B	605	LEU
1	B	606	ASN
1	B	607	ASP
1	B	609	VAL
1	B	615	GLN
1	B	623	ASP
1	B	664	LYS
1	B	666	GLN
1	B	675	ARG
1	B	683	ARG
1	B	686	ILE
1	B	702	LEU
1	B	708	ASN
1	B	719	GLN
1	B	723	ASN
1	B	729	GLU
1	B	731	ARG
1	B	732	GLN
1	B	733	ARG
1	B	735	GLU
1	B	748	ASP
1	B	750	LYS
1	B	754	ILE
1	B	755	LEU
1	B	756	MET
1	B	771	GLN
1	B	773	LYS
1	B	778	THR
1	C	34	LEU
1	C	35	VAL
1	C	39	SER
1	C	41	LYS
1	C	42	HIS
1	C	48	SER
1	C	75	ILE
1	C	77	LYS
1	C	82	LYS
1	C	86	VAL
1	C	91	GLU
1	C	110	SER

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Mol	Chain	Res	Type
1	C	112	LEU
1	C	123	VAL
1	C	124	ILE
1	C	128	LYS
1	C	135	GLU
1	C	136	LYS
1	C	142	LYS
1	C	144	LYS
1	C	145	LYS
1	C	156	ILE
1	C	166	GLN
1	C	167	ASP
1	C	173	ILE
1	C	174	LEU
1	C	189	LYS
1	C	199	SER
1	C	225	LEU
1	C	232	GLU
1	C	250	LYS
1	C	259	THR
1	C	263	VAL
1	C	268	GLU
1	C	274	LYS
1	C	275	SER
1	C	278	ILE
1	C	302	ARG
1	C	303	ASN
1	C	308	GLU
1	C	311	ASN
1	C	314	THR
1	C	317	SER
1	C	323	ILE
1	C	326	GLN
1	C	327	GLN
1	C	329	ASP
1	C	334	GLU
1	C	340	THR
1	C	377	SER
1	C	393	ILE
1	C	394	ASN
1	C	402	ILE
1	C	404	THR

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Mol	Chain	Res	Type
1	C	419	THR
1	C	422	GLN
1	C	427	ILE
1	C	434	LYS
1	C	448	LYS
1	C	459	SER
1	C	473	GLU
1	C	487	GLU
1	C	488	LYS
1	C	499	ILE
1	C	501	GLU
1	C	504	GLU
1	C	506	GLN
1	C	507	ARG
1	C	511	GLU
1	C	522	GLN
1	C	527	LEU
1	C	529	GLU
1	C	544	GLU
1	C	545	CYS
1	C	554	SER
1	C	560	ILE
1	C	572	SER
1	C	589	LYS
1	C	591	THR
1	C	593	ASN
1	C	599	THR
1	C	605	LEU
1	C	606	ASN
1	C	607	ASP
1	C	609	VAL
1	C	615	GLN
1	C	623	ASP
1	C	664	LYS
1	C	666	GLN
1	C	675	ARG
1	C	683	ARG
1	C	686	ILE
1	C	702	LEU
1	C	708	ASN
1	C	719	GLN
1	C	723	ASN

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Mol	Chain	Res	Type
1	C	729	GLU
1	C	731	ARG
1	C	732	GLN
1	C	733	ARG
1	C	735	GLU
1	C	748	ASP
1	C	750	LYS
1	C	754	ILE
1	C	755	LEU
1	C	771	GLN
1	C	773	LYS
1	C	778	THR
1	D	34	LEU
1	D	35	VAL
1	D	39	SER
1	D	41	LYS
1	D	42	HIS
1	D	48	SER
1	D	75	ILE
1	D	77	LYS
1	D	82	LYS
1	D	86	VAL
1	D	89	MET
1	D	91	GLU
1	D	110	SER
1	D	112	LEU
1	D	123	VAL
1	D	124	ILE
1	D	128	LYS
1	D	135	GLU
1	D	136	LYS
1	D	142	LYS
1	D	144	LYS
1	D	145	LYS
1	D	156	ILE
1	D	166	GLN
1	D	167	ASP
1	D	174	LEU
1	D	189	LYS
1	D	199	SER
1	D	225	LEU
1	D	232	GLU

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Mol	Chain	Res	Type
1	D	250	LYS
1	D	259	THR
1	D	263	VAL
1	D	268	GLU
1	D	274	LYS
1	D	275	SER
1	D	278	ILE
1	D	285	ARG
1	D	302	ARG
1	D	303	ASN
1	D	308	GLU
1	D	311	ASN
1	D	314	THR
1	D	317	SER
1	D	323	ILE
1	D	326	GLN
1	D	327	GLN
1	D	329	ASP
1	D	334	GLU
1	D	340	THR
1	D	377	SER
1	D	393	ILE
1	D	394	ASN
1	D	402	ILE
1	D	404	THR
1	D	419	THR
1	D	422	GLN
1	D	427	ILE
1	D	434	LYS
1	D	448	LYS
1	D	459	SER
1	D	473	GLU
1	D	487	GLU
1	D	488	LYS
1	D	499	ILE
1	D	501	GLU
1	D	504	GLU
1	D	506	GLN
1	D	507	ARG
1	D	511	GLU
1	D	522	GLN
1	D	527	LEU

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Mol	Chain	Res	Type
1	D	529	GLU
1	D	544	GLU
1	D	545	CYS
1	D	554	SER
1	D	560	ILE
1	D	572	SER
1	D	589	LYS
1	D	591	THR
1	D	593	ASN
1	D	599	THR
1	D	605	LEU
1	D	606	ASN
1	D	607	ASP
1	D	609	VAL
1	D	615	GLN
1	D	623	ASP
1	D	664	LYS
1	D	666	GLN
1	D	675	ARG
1	D	683	ARG
1	D	686	ILE
1	D	702	LEU
1	D	708	ASN
1	D	719	GLN
1	D	723	ASN
1	D	729	GLU
1	D	731	ARG
1	D	732	GLN
1	D	733	ARG
1	D	735	GLU
1	D	748	ASP
1	D	750	LYS
1	D	754	ILE
1	D	755	LEU
1	D	771	GLN
1	D	773	LYS
1	D	778	THR
1	E	34	LEU
1	E	35	VAL
1	E	39	SER
1	E	41	LYS
1	E	42	HIS

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Mol	Chain	Res	Type
1	E	48	SER
1	E	75	ILE
1	E	77	LYS
1	E	82	LYS
1	E	86	VAL
1	E	91	GLU
1	E	110	SER
1	E	112	LEU
1	E	123	VAL
1	E	124	ILE
1	E	128	LYS
1	E	135	GLU
1	E	136	LYS
1	E	142	LYS
1	E	144	LYS
1	E	145	LYS
1	E	156	ILE
1	E	166	GLN
1	E	167	ASP
1	E	174	LEU
1	E	189	LYS
1	E	199	SER
1	E	225	LEU
1	E	232	GLU
1	E	250	LYS
1	E	259	THR
1	E	263	VAL
1	E	268	GLU
1	E	274	LYS
1	E	275	SER
1	E	278	ILE
1	E	302	ARG
1	E	303	ASN
1	E	308	GLU
1	E	311	ASN
1	E	314	THR
1	E	323	ILE
1	E	326	GLN
1	E	327	GLN
1	E	329	ASP
1	E	334	GLU
1	E	340	THR

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Mol	Chain	Res	Type
1	E	377	SER
1	E	393	ILE
1	E	394	ASN
1	E	402	ILE
1	E	404	THR
1	E	419	THR
1	E	420	LYS
1	E	422	GLN
1	E	427	ILE
1	E	434	LYS
1	E	448	LYS
1	E	459	SER
1	E	473	GLU
1	E	487	GLU
1	E	488	LYS
1	E	499	ILE
1	E	501	GLU
1	E	504	GLU
1	E	506	GLN
1	E	507	ARG
1	E	511	GLU
1	E	522	GLN
1	E	527	LEU
1	E	544	GLU
1	E	545	CYS
1	E	554	SER
1	E	560	ILE
1	E	572	SER
1	E	589	LYS
1	E	591	THR
1	E	593	ASN
1	E	599	THR
1	E	605	LEU
1	E	606	ASN
1	E	607	ASP
1	E	609	VAL
1	E	615	GLN
1	E	623	ASP
1	E	664	LYS
1	E	666	GLN
1	E	675	ARG
1	E	683	ARG

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Mol	Chain	Res	Type
1	E	686	ILE
1	E	702	LEU
1	E	708	ASN
1	E	719	GLN
1	E	723	ASN
1	E	729	GLU
1	E	731	ARG
1	E	732	GLN
1	E	733	ARG
1	E	735	GLU
1	E	742	ILE
1	E	748	ASP
1	E	750	LYS
1	E	754	ILE
1	E	755	LEU
1	E	756	MET
1	E	771	GLN
1	E	773	LYS
1	E	778	THR
1	F	34	LEU
1	F	35	VAL
1	F	39	SER
1	F	41	LYS
1	F	42	HIS
1	F	48	SER
1	F	75	ILE
1	F	77	LYS
1	F	82	LYS
1	F	86	VAL
1	F	89	MET
1	F	91	GLU
1	F	110	SER
1	F	123	VAL
1	F	124	ILE
1	F	128	LYS
1	F	135	GLU
1	F	136	LYS
1	F	142	LYS
1	F	144	LYS
1	F	145	LYS
1	F	156	ILE
1	F	166	GLN

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Mol	Chain	Res	Type
1	F	167	ASP
1	F	174	LEU
1	F	189	LYS
1	F	199	SER
1	F	225	LEU
1	F	232	GLU
1	F	250	LYS
1	F	259	THR
1	F	263	VAL
1	F	268	GLU
1	F	274	LYS
1	F	275	SER
1	F	278	ILE
1	F	285	ARG
1	F	302	ARG
1	F	303	ASN
1	F	308	GLU
1	F	311	ASN
1	F	314	THR
1	F	323	ILE
1	F	326	GLN
1	F	327	GLN
1	F	329	ASP
1	F	334	GLU
1	F	340	THR
1	F	377	SER
1	F	393	ILE
1	F	394	ASN
1	F	402	ILE
1	F	404	THR
1	F	419	THR
1	F	422	GLN
1	F	427	ILE
1	F	434	LYS
1	F	448	LYS
1	F	459	SER
1	F	473	GLU
1	F	487	GLU
1	F	488	LYS
1	F	499	ILE
1	F	501	GLU
1	F	504	GLU

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Mol	Chain	Res	Type
1	F	506	GLN
1	F	507	ARG
1	F	511	GLU
1	F	522	GLN
1	F	527	LEU
1	F	544	GLU
1	F	545	CYS
1	F	554	SER
1	F	560	ILE
1	F	572	SER
1	F	589	LYS
1	F	591	THR
1	F	593	ASN
1	F	599	THR
1	F	605	LEU
1	F	606	ASN
1	F	607	ASP
1	F	609	VAL
1	F	615	GLN
1	F	623	ASP
1	F	664	LYS
1	F	666	GLN
1	F	675	ARG
1	F	683	ARG
1	F	686	ILE
1	F	702	LEU
1	F	708	ASN
1	F	719	GLN
1	F	723	ASN
1	F	729	GLU
1	F	731	ARG
1	F	732	GLN
1	F	733	ARG
1	F	735	GLU
1	F	742	ILE
1	F	748	ASP
1	F	750	LYS
1	F	754	ILE
1	F	755	LEU
1	F	771	GLN
1	F	773	LYS
1	F	778	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	255	ASN
1	A	303	ASN
1	A	327	GLN
1	A	333	GLN
1	A	361	GLN
1	A	418	GLN
1	A	422	GLN
1	A	533	ASN
1	A	566	HIS
1	A	593	ASN
1	A	606	ASN
1	A	614	ASN
1	A	689	HIS
1	A	708	ASN
1	B	228	ASN
1	B	255	ASN
1	B	303	ASN
1	B	327	GLN
1	B	333	GLN
1	B	361	GLN
1	B	418	GLN
1	B	422	GLN
1	B	533	ASN
1	B	566	HIS
1	B	593	ASN
1	B	606	ASN
1	B	614	ASN
1	B	680	ASN
1	B	689	HIS
1	B	708	ASN
1	B	732	GLN
1	C	228	ASN
1	C	255	ASN
1	C	303	ASN
1	C	327	GLN
1	C	333	GLN
1	C	361	GLN
1	C	389	HIS
1	C	418	GLN
1	C	422	GLN

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Mol	Chain	Res	Type
1	C	533	ASN
1	C	566	HIS
1	C	593	ASN
1	C	606	ASN
1	C	614	ASN
1	C	689	HIS
1	C	699	HIS
1	C	708	ASN
1	C	732	GLN
1	C	751	GLN
1	D	228	ASN
1	D	236	ASN
1	D	255	ASN
1	D	303	ASN
1	D	327	GLN
1	D	333	GLN
1	D	361	GLN
1	D	418	GLN
1	D	422	GLN
1	D	533	ASN
1	D	566	HIS
1	D	593	ASN
1	D	606	ASN
1	D	608	ASN
1	D	614	ASN
1	D	689	HIS
1	D	708	ASN
1	D	732	GLN
1	D	751	GLN
1	E	228	ASN
1	E	255	ASN
1	E	303	ASN
1	E	327	GLN
1	E	333	GLN
1	E	361	GLN
1	E	418	GLN
1	E	422	GLN
1	E	533	ASN
1	E	566	HIS
1	E	593	ASN
1	E	606	ASN
1	E	614	ASN

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Mol	Chain	Res	Type
1	E	689	HIS
1	E	708	ASN
1	E	732	GLN
1	E	751	GLN
1	F	228	ASN
1	F	255	ASN
1	F	303	ASN
1	F	327	GLN
1	F	333	GLN
1	F	361	GLN
1	F	418	GLN
1	F	422	GLN
1	F	533	ASN
1	F	566	HIS
1	F	593	ASN
1	F	606	ASN
1	F	614	ASN
1	F	689	HIS
1	F	699	HIS
1	F	708	ASN
1	F	732	GLN
1	F	751	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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
3	ALF	A	999	2,5,4	4,4,4	1.46	0	-		
3	ALF	B	999	1,2,5,4	4,4,4	1.46	0	-		
3	ALF	C	999	2,5,4	4,4,4	1.46	0	-		
4	ADP	A	998	3,2	28,29,29	0.90	0	43,45,45	0.87	2 (4%)
4	ADP	D	998	3,2	28,29,29	0.90	0	43,45,45	0.87	2 (4%)
4	ADP	E	998	3,2	28,29,29	0.99	0	43,45,45	0.79	0
3	ALF	E	999	2,4	4,4,4	1.22	0	-		
4	ADP	B	998	3,2	28,29,29	0.90	0	43,45,45	0.87	2 (4%)
4	ADP	F	998	3,2	28,29,29	1.13	2 (7%)	43,45,45	0.79	1 (2%)
4	ADP	C	998	3,2	28,29,29	0.89	0	43,45,45	0.87	2 (4%)
3	ALF	D	999	1,2,5,4	4,4,4	1.46	0	-		
3	ALF	F	999	1,2,4	4,4,4	1.17	0	-		

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
4	ADP	A	998	3,2	-	5/16/32/32	0/3/3/3
4	ADP	D	998	3,2	-	5/16/32/32	0/3/3/3
4	ADP	E	998	3,2	-	5/16/32/32	0/3/3/3
4	ADP	B	998	3,2	-	5/16/32/32	0/3/3/3
4	ADP	F	998	3,2	-	5/16/32/32	0/3/3/3
4	ADP	C	998	3,2	-	5/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	998	ADP	PB-O3B	-2.30	1.46	1.54
4	F	998	ADP	PA-O3A	-2.27	1.57	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	998	ADP	O3'-C3'-C2'	2.47	119.72	111.82
4	D	998	ADP	O3'-C3'-C2'	2.46	119.69	111.82
4	B	998	ADP	O3'-C3'-C2'	2.45	119.66	111.82
4	C	998	ADP	O3'-C3'-C2'	2.44	119.63	111.82
4	F	998	ADP	O3'-C3'-C2'	2.33	119.27	111.82
4	C	998	ADP	O2B-PB-O3A	2.26	112.23	104.64
4	B	998	ADP	O2B-PB-O3A	2.26	112.20	104.64
4	D	998	ADP	O2B-PB-O3A	2.26	112.20	104.64
4	A	998	ADP	O2B-PB-O3A	2.25	112.17	104.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	998	ADP	C5'-O5'-PA-O1A
4	A	998	ADP	C5'-O5'-PA-O2A
4	A	998	ADP	C5'-O5'-PA-O3A
4	B	998	ADP	C5'-O5'-PA-O1A
4	B	998	ADP	C5'-O5'-PA-O2A
4	B	998	ADP	C5'-O5'-PA-O3A
4	C	998	ADP	C5'-O5'-PA-O1A
4	C	998	ADP	C5'-O5'-PA-O2A
4	C	998	ADP	C5'-O5'-PA-O3A
4	D	998	ADP	C5'-O5'-PA-O1A
4	D	998	ADP	C5'-O5'-PA-O2A
4	D	998	ADP	C5'-O5'-PA-O3A
4	E	998	ADP	C5'-O5'-PA-O1A
4	E	998	ADP	C5'-O5'-PA-O2A
4	E	998	ADP	C5'-O5'-PA-O3A
4	F	998	ADP	C5'-O5'-PA-O1A
4	F	998	ADP	C5'-O5'-PA-O2A
4	F	998	ADP	C5'-O5'-PA-O3A
4	A	998	ADP	O4'-C4'-C5'-O5'
4	B	998	ADP	O4'-C4'-C5'-O5'
4	C	998	ADP	O4'-C4'-C5'-O5'
4	D	998	ADP	O4'-C4'-C5'-O5'
4	A	998	ADP	C3'-C4'-C5'-O5'
4	B	998	ADP	C3'-C4'-C5'-O5'
4	C	998	ADP	C3'-C4'-C5'-O5'
4	D	998	ADP	C3'-C4'-C5'-O5'
4	E	998	ADP	O4'-C4'-C5'-O5'
4	F	998	ADP	O4'-C4'-C5'-O5'
4	E	998	ADP	C3'-C4'-C5'-O5'

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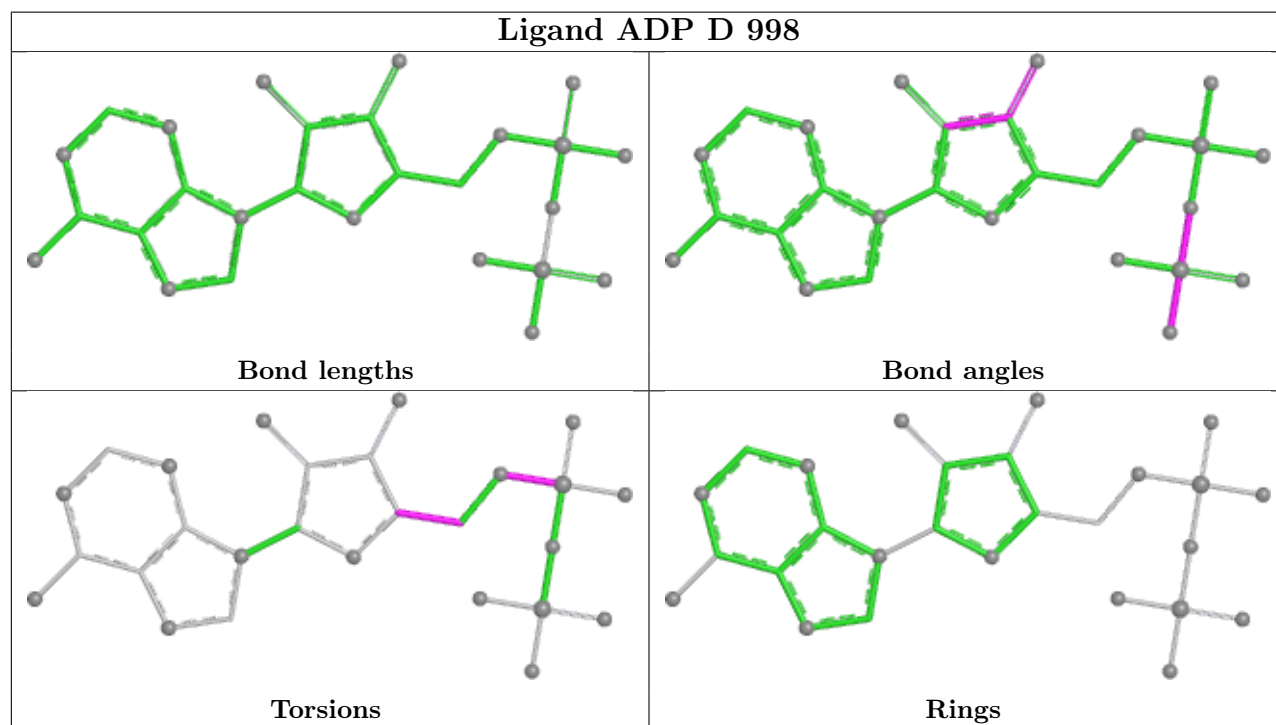
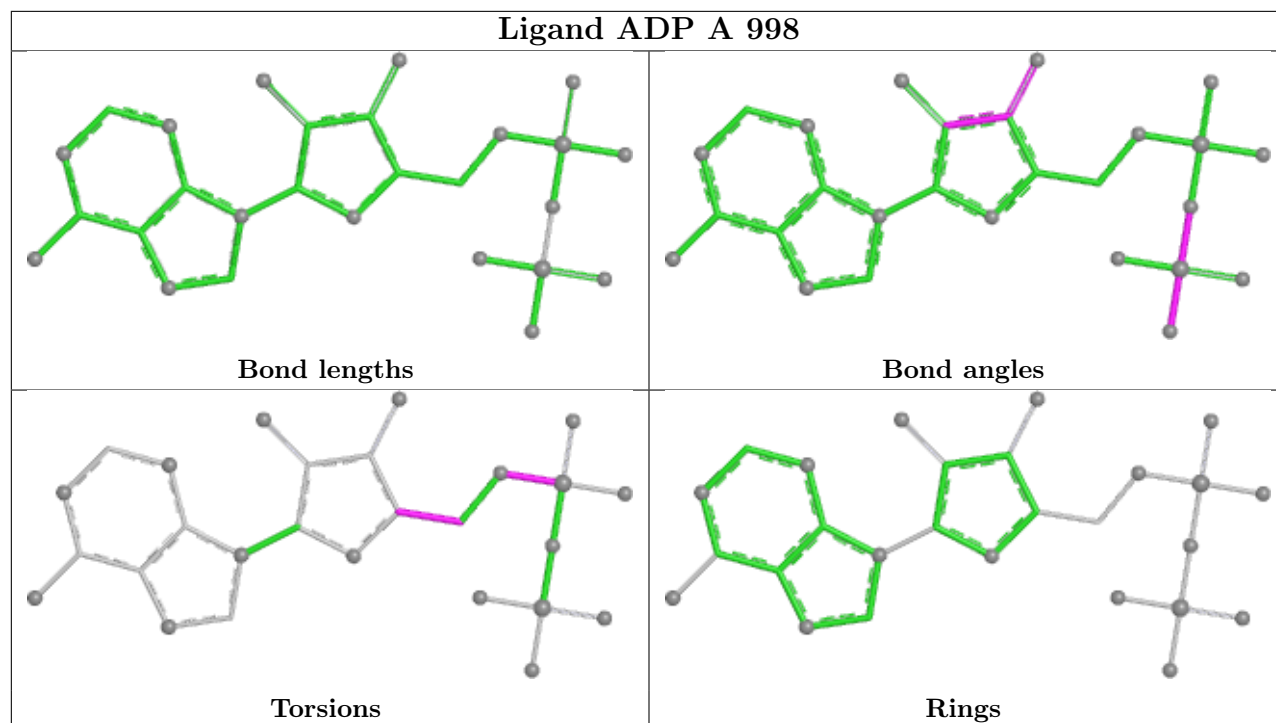
Mol	Chain	Res	Type	Atoms
4	F	998	ADP	C3'-C4'-C5'-O5'

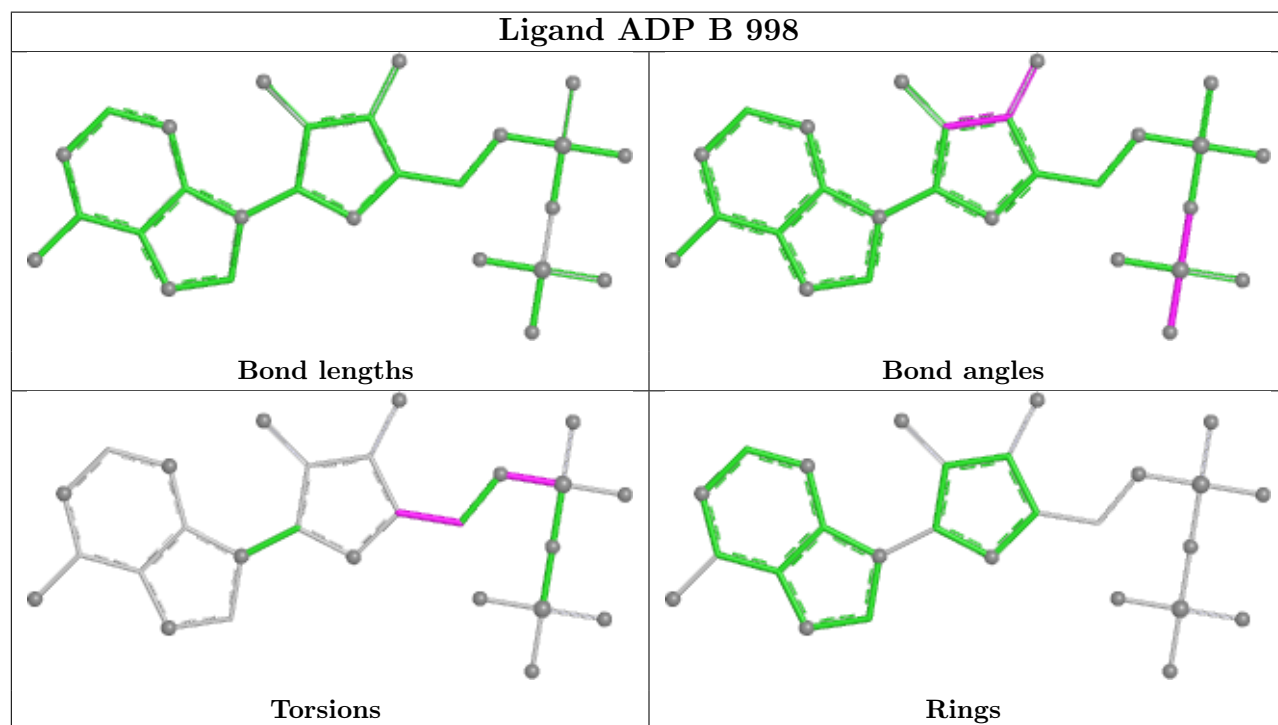
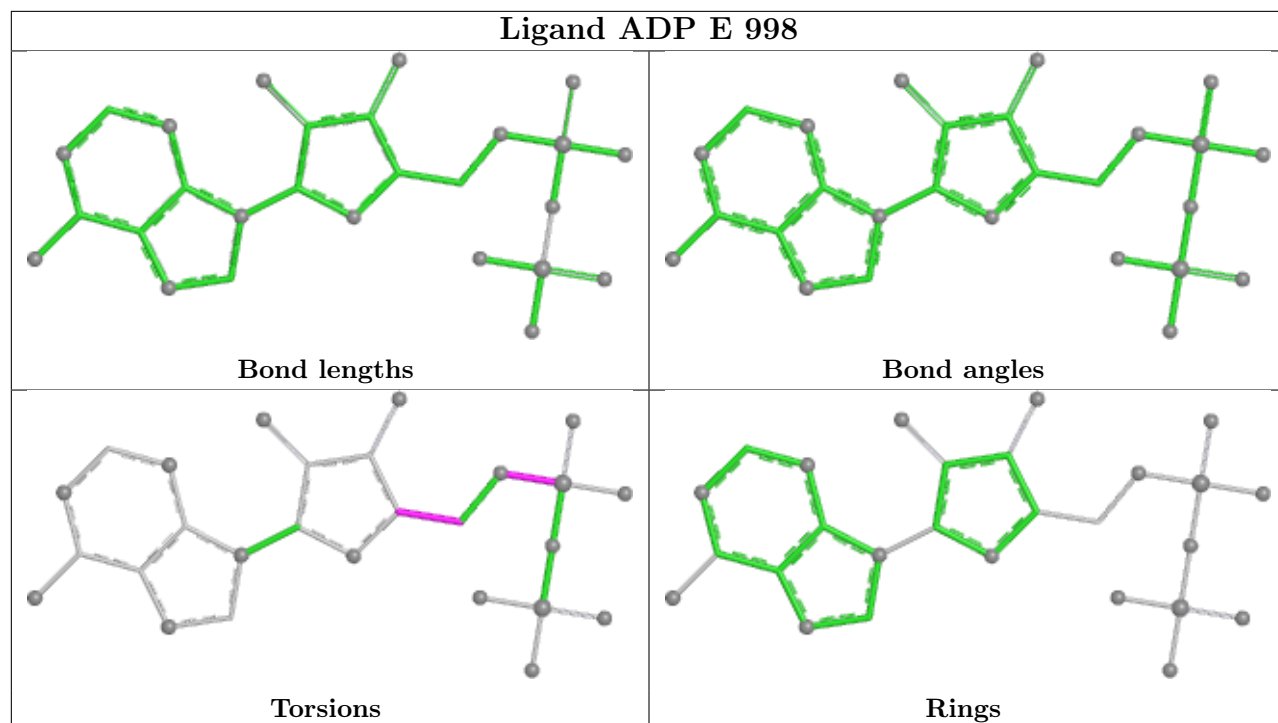
There are no ring outliers.

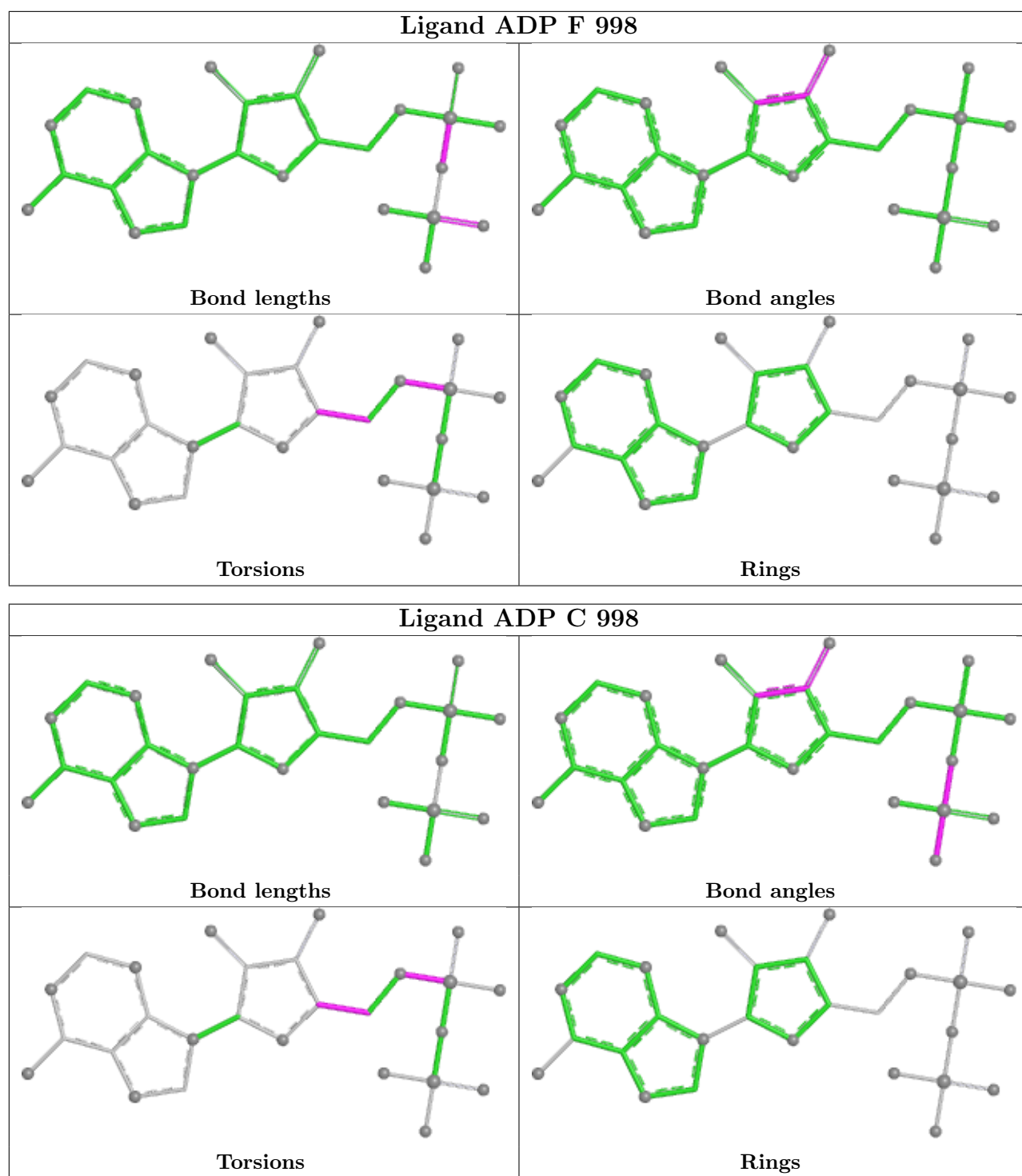
8 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	ALF	1	0
3	B	999	ALF	1	0
3	C	999	ALF	1	0
4	A	998	ADP	1	0
4	D	998	ADP	1	0
4	B	998	ADP	1	0
4	C	998	ADP	1	0
3	D	999	ALF	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.