



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:10 AM UTC

PDB ID : 5B04 / pdb_00005b04
Title : Crystal structure of the eukaryotic translation initiation factor 2B from *Schizosaccharomyces pombe*
Authors : Kashiwagi, K.; Ito, T.; Yokoyama, S.
Deposited on : 2015-10-27
Resolution : 2.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

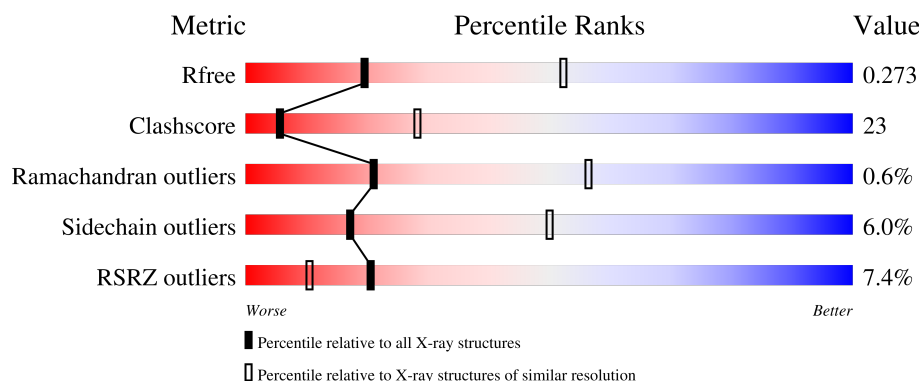
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	341	6% 56% 29% 7% 7%
1	B	341	4% 73% 18% 6%
2	C	399	4% 64% 19% 13%
2	D	399	3% 67% 19% 13%
3	E	458	14% 41% 30% 10% 16%

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Mol	Chain	Length	Quality of chain
3	F	458	15% 35% 33% 13% • 16%
4	G	467	4% 55% 16% • 25%
4	H	467	3% 61% 13% • 25%
5	I	678	2% 46% 13% • • 37%
5	J	678	4% 42% 17% • • 37%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28584 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2472	1571	430	458	13			
1	B	319	Total	C	N	O	S	0	0	0
			2489	1582	434	460	13			

- Molecule 2 is a protein called Probable translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	349	Total	C	N	O	S	0	0	0
			2702	1714	459	515	14			
2	D	346	Total	C	N	O	S	0	0	0
			2674	1697	453	511	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q9UT76
C	-4	PRO	-	expression tag	UNP Q9UT76
C	-3	ILE	-	expression tag	UNP Q9UT76
C	-2	SER	-	expression tag	UNP Q9UT76
C	-1	GLU	-	expression tag	UNP Q9UT76
C	0	PHE	-	expression tag	UNP Q9UT76
D	-5	GLY	-	expression tag	UNP Q9UT76
D	-4	PRO	-	expression tag	UNP Q9UT76
D	-3	ILE	-	expression tag	UNP Q9UT76
D	-2	SER	-	expression tag	UNP Q9UT76
D	-1	GLU	-	expression tag	UNP Q9UT76
D	0	PHE	-	expression tag	UNP Q9UT76

- Molecule 3 is a protein called Probable translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	384	Total	C	N	O	S	0	0	0
			2976	1895	511	553	17			
3	F	383	Total	C	N	O	S	0	0	0
			2967	1890	509	551	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	157	TYR	ILE	engineered mutation	UNP P56288
E	158	THR	TYR	engineered mutation	UNP P56288
E	159	VAL	GLY	engineered mutation	UNP P56288
F	157	TYR	ILE	engineered mutation	UNP P56288
F	158	THR	TYR	engineered mutation	UNP P56288
F	159	VAL	GLY	engineered mutation	UNP P56288

- Molecule 4 is a protein called Probable translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	349	Total	C	N	O	S	0	0	0
			2755	1763	466	513	13			
4	H	349	Total	C	N	O	S	0	0	0
			2755	1763	466	513	13			

- Molecule 5 is a protein called Probable translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	428	Total	C	N	O	S	0	0	0
			3377	2123	592	647	15			
5	J	428	Total	C	N	O	S	0	0	0
			3372	2119	591	647	15			

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

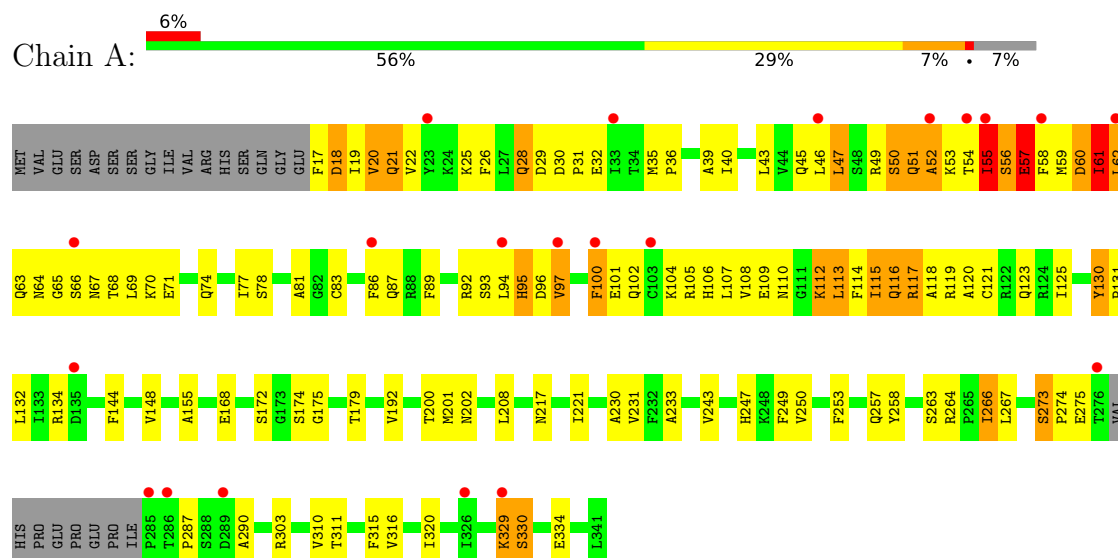


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		
6	I	1	Total	O	P	0	0
			5	4	1		

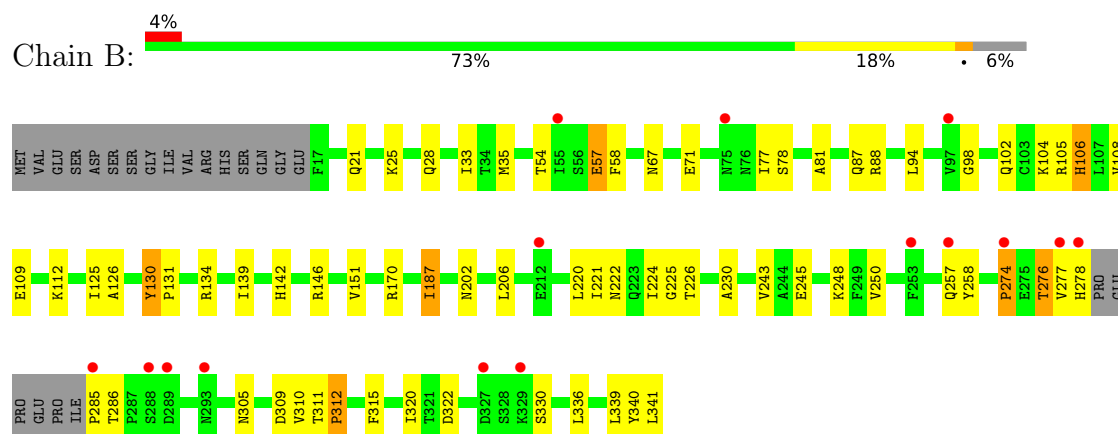
3 Residue-property plots [i](#)

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

- Molecule 1: Translation initiation factor eIF-2B subunit alpha

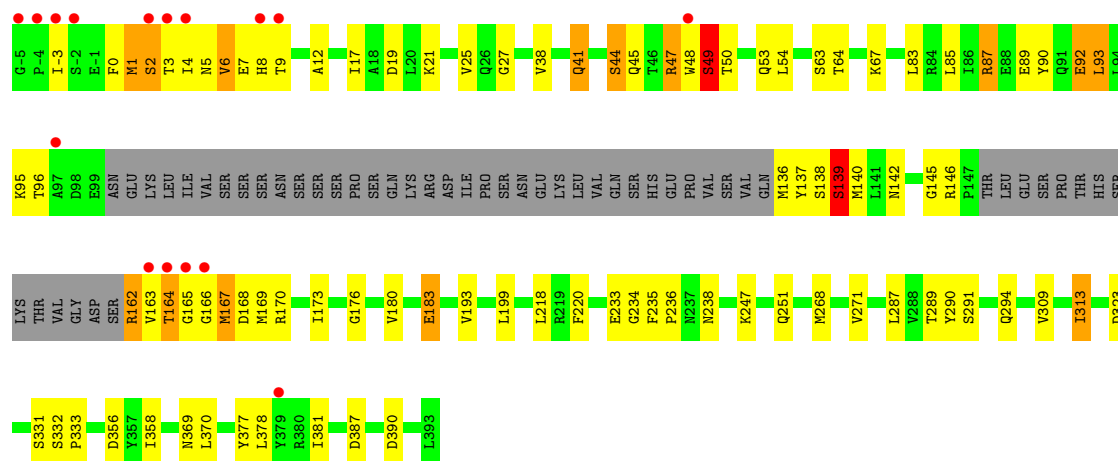


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

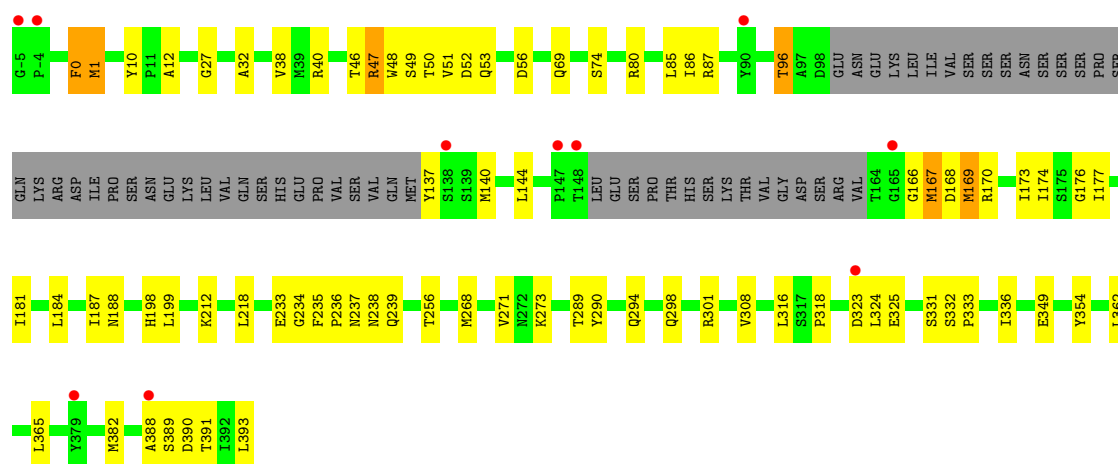


- Molecule 2: Probable translation initiation factor eIF-2B subunit beta

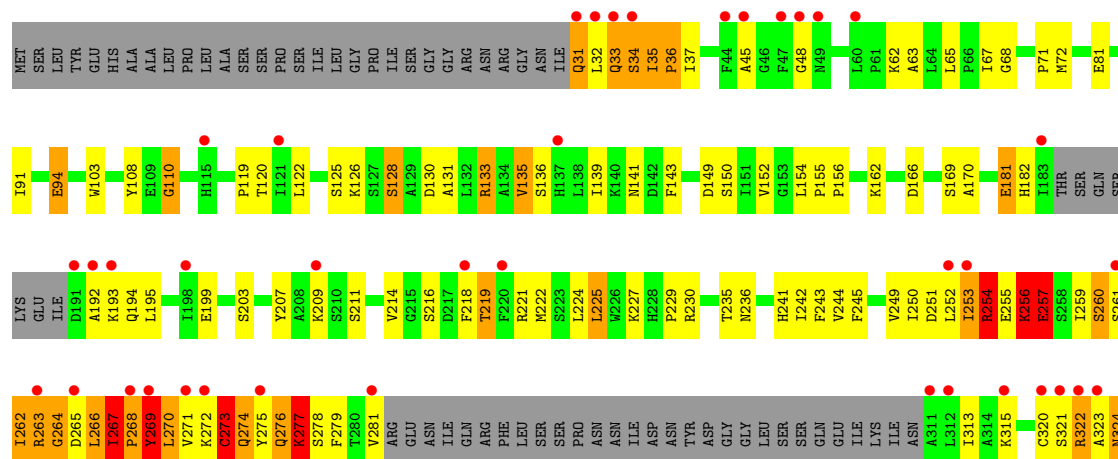




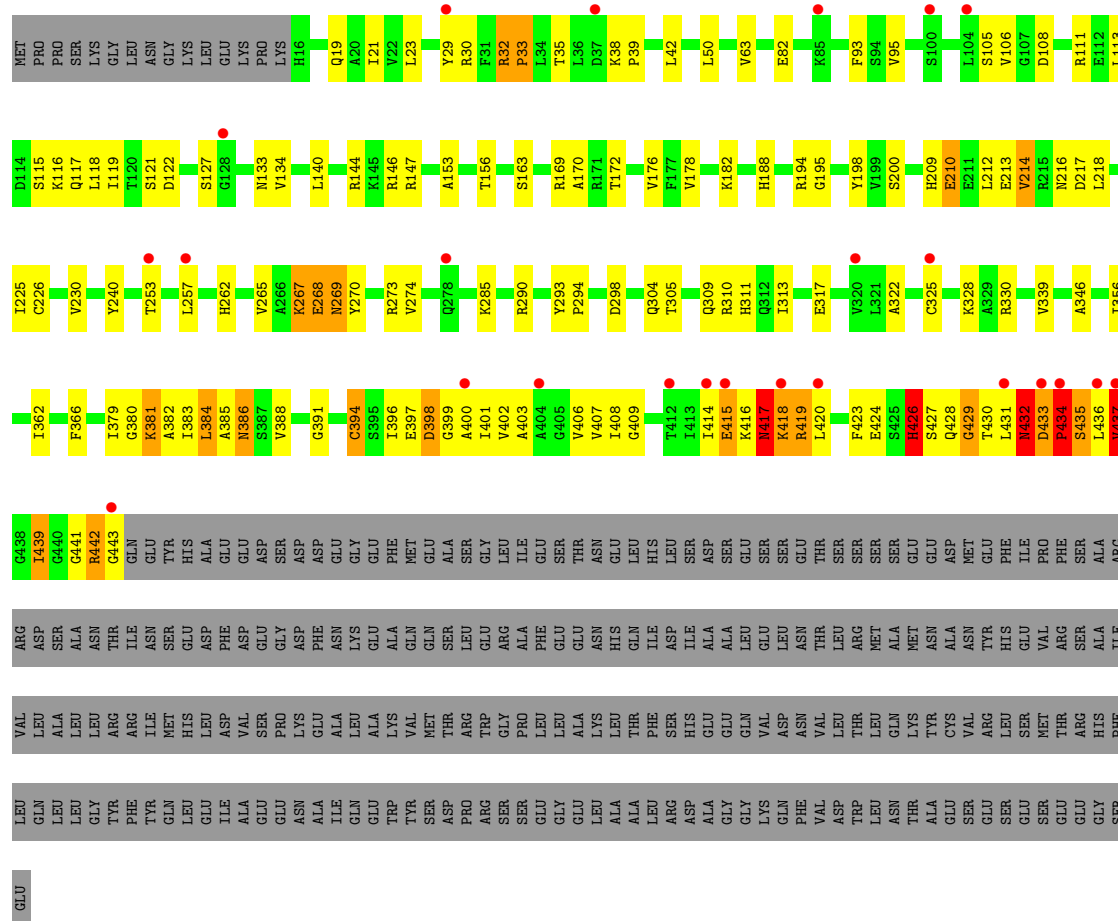
• Molecule 2: Probable translation initiation factor eIF-2B subunit beta



• Molecule 3: Probable translation initiation factor eIF-2B subunit gamma







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	144.50Å 209.23Å 223.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.99 49.29 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.29-2.99) 99.6 (49.29-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.222 , 0.271 0.229 , 0.273	Depositor DCC
R_{free} test set	6815 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	80.9	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28584	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.46	0/2519	1.03	20/3409 (0.6%)
1	B	0.39	0/2537	0.86	8/3434 (0.2%)
2	C	0.45	1/2747 (0.0%)	0.85	9/3726 (0.2%)
2	D	0.35	0/2719	0.84	9/3690 (0.2%)
3	E	0.75	5/3029 (0.2%)	1.33	53/4100 (1.3%)
3	F	0.74	7/3020 (0.2%)	1.67	73/4088 (1.8%)
4	G	0.51	1/2802 (0.0%)	0.96	15/3797 (0.4%)
4	H	0.38	0/2802	0.78	1/3797 (0.0%)
5	I	0.60	2/3437 (0.1%)	1.14	31/4658 (0.7%)
5	J	0.59	3/3432 (0.1%)	1.00	21/4652 (0.5%)
All	All	0.55	19/29044 (0.1%)	1.09	240/39351 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	E	0	5
3	F	0	6
4	H	0	1
5	I	0	1
5	J	0	1
All	All	0	16

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	268	PRO	N-CD	-13.69	1.28	1.47
3	F	382	ASN	CA-C	9.46	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	434	PRO	N-CD	-9.32	1.34	1.47
5	J	33	PRO	N-CD	8.94	1.60	1.47
3	F	211	SER	CA-C	8.22	1.67	1.52
3	E	371	ASN	CA-C	7.63	1.62	1.52
3	F	422	LYS	CA-C	7.48	1.62	1.53
5	I	434	PRO	N-CD	7.20	1.57	1.47
3	E	419	ILE	CA-CB	7.20	1.61	1.55
2	C	47	ARG	CA-C	6.11	1.59	1.52
5	J	433	ASP	CA-C	5.89	1.60	1.52
3	E	253	ILE	CA-C	5.66	1.59	1.52
3	E	35	ILE	C-N	5.53	1.40	1.33
4	G	413	PRO	N-CD	5.49	1.55	1.47
3	F	268	PRO	N-CD	5.33	1.55	1.47
3	F	384	VAL	N-CA	5.25	1.52	1.46
3	F	368	ILE	CA-C	5.16	1.59	1.52
3	F	119	PRO	N-CD	5.03	1.54	1.47
5	I	203	PRO	N-CD	5.03	1.54	1.47

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	370	ASP	N-CA-C	30.64	155.28	110.24
3	F	384	VAL	N-CA-C	21.52	141.57	108.87
3	F	370	ASP	CB-CA-C	-20.77	78.69	109.84
3	F	371	ASN	N-CA-C	20.44	139.45	111.24
5	I	433	ASP	N-CA-C	19.79	138.70	110.20
5	I	431	LEU	N-CA-C	19.55	141.31	108.67
3	F	213	ASP	N-CA-C	18.92	142.99	113.28
5	I	429	GLY	N-CA-C	17.54	154.74	113.18
3	F	382	ASN	N-CA-C	17.34	134.02	112.86
3	F	213	ASP	CB-CA-C	-16.93	85.68	110.06
5	I	432	ASN	CB-CA-C	-15.07	80.44	110.42
1	A	116	GLN	N-CA-C	15.00	129.12	111.11
4	G	405	GLY	N-CA-C	14.74	129.59	112.50
3	E	370	ASP	N-CA-C	13.74	128.43	110.43
5	J	434	PRO	N-CA-CB	-13.18	89.41	103.25
3	E	419	ILE	CB-CA-C	-13.00	99.52	111.74
5	I	433	ASP	N-CA-CB	-12.92	91.44	110.05
3	F	353	ARG	N-CA-C	-12.45	94.10	110.53
3	F	210	SER	N-CA-C	-12.12	94.19	110.55
5	I	432	ASN	N-CA-C	11.92	136.19	110.80
3	E	353	ARG	CB-CA-C	-11.70	87.84	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	30	ARG	N-CA-C	-11.59	99.24	113.50
3	E	444	GLY	N-CA-C	11.27	129.26	110.56
5	J	415	GLU	N-CA-C	11.19	125.64	108.96
3	F	352	GLU	N-CA-C	11.09	125.16	110.53
3	F	382	ASN	CA-C-O	10.77	133.03	120.32
3	E	110	GLY	N-CA-C	10.57	125.28	112.49
3	E	435	ARG	N-CA-C	10.53	124.82	109.14
3	F	366	THR	N-CA-C	10.32	126.21	109.59
3	F	383	CYS	N-CA-CB	10.30	126.95	110.77
3	F	212	ALA	CB-CA-C	9.91	130.15	110.42
3	F	385	ILE	N-CA-CB	9.86	127.62	111.45
3	F	422	LYS	N-CA-C	9.54	124.62	111.74
3	E	435	ARG	N-CA-CB	-9.54	96.16	111.62
3	F	280	THR	N-CA-C	-9.53	101.21	113.12
3	F	449	ASP	N-CA-C	9.49	123.26	110.35
5	J	269	ASN	N-CA-C	9.49	122.74	108.31
1	A	95	HIS	CB-CA-C	9.44	129.21	110.42
3	F	211	SER	CB-CA-C	-9.09	93.53	110.36
1	A	116	GLN	N-CA-CB	-9.09	96.39	109.94
3	F	382	ASN	CB-CA-C	-8.79	97.03	111.36
5	J	434	PRO	N-CD-CG	-8.70	90.16	103.20
3	E	354	ALA	N-CA-C	-8.54	102.88	113.38
3	E	340	THR	CA-C-N	8.38	130.32	119.84
3	E	340	THR	C-N-CA	8.38	130.32	119.84
1	A	330	SER	N-CA-C	-8.36	102.64	113.17
5	I	425	SER	N-CA-C	8.27	119.48	108.07
2	C	6	VAL	N-CA-C	-8.26	103.30	112.80
5	I	430	THR	N-CA-C	8.26	122.86	110.64
3	E	419	ILE	N-CA-C	8.22	117.73	107.70
4	G	242	ILE	N-CA-C	-8.21	102.81	110.53
1	A	117	ARG	N-CA-C	-8.16	101.11	112.45
4	H	408	ASP	N-CA-C	8.12	119.91	111.14
5	J	417	ASN	N-CA-C	8.00	122.48	112.24
2	D	169	MET	N-CA-C	-7.96	103.14	113.17
3	F	212	ALA	N-CA-CB	7.95	123.92	110.49
3	E	435	ARG	CG-CD-NE	7.92	129.41	112.00
5	I	211	GLU	N-CA-C	-7.91	96.49	108.52
3	F	33	GLN	N-CA-C	-7.80	101.81	112.03
3	E	257	GLU	N-CA-C	7.79	127.39	110.80
5	J	172	THR	N-CA-C	7.73	119.70	111.28
3	F	384	VAL	CB-CA-C	-7.71	100.65	111.21
3	F	364	GLU	N-CA-CB	-7.66	98.21	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	431	LEU	CB-CA-C	-7.60	106.89	117.23
3	F	364	GLU	N-CA-C	7.55	121.69	110.52
5	I	433	ASP	CB-CA-C	-7.46	95.71	109.51
3	F	397	MET	N-CA-C	7.44	124.99	110.56
2	C	139	SER	N-CA-C	-7.43	104.73	113.88
3	F	434	HIS	N-CA-C	7.43	121.14	107.99
5	I	269	ASN	N-CA-C	7.41	118.97	108.00
3	E	278	SER	N-CA-C	7.35	121.65	112.24
3	F	211	SER	CA-C-O	7.32	130.50	119.23
3	E	269	TYR	N-CA-C	-7.28	104.55	113.50
4	G	228	ASP	CB-CA-C	-7.22	101.26	111.65
4	G	240	GLU	N-CA-C	7.21	123.26	111.37
5	J	32	ARG	CA-C-N	-7.20	111.00	118.85
5	J	32	ARG	C-N-CA	-7.20	111.00	118.85
3	E	254	ARG	CA-C-N	7.17	130.11	120.65
3	E	254	ARG	C-N-CA	7.17	130.11	120.65
4	G	241	LYS	N-CA-C	-7.16	104.81	113.97
3	F	418	GLN	CA-C-N	-7.09	113.14	122.99
3	F	418	GLN	C-N-CA	-7.09	113.14	122.99
3	E	324	ASN	N-CA-C	7.04	119.89	108.41
3	F	275	TYR	N-CA-C	7.02	121.23	112.24
3	F	397	MET	CB-CA-C	-7.01	99.44	112.00
3	F	384	VAL	N-CA-CB	-7.01	100.88	110.56
3	F	449	ASP	N-CA-CB	-6.99	99.76	110.04
5	I	211	GLU	CB-CA-C	6.98	121.22	109.99
3	F	339	LEU	N-CA-C	-6.97	104.66	113.02
3	F	194	GLN	N-CA-CB	-6.91	99.17	110.43
3	E	35	ILE	CA-C-N	-6.89	113.69	120.52
3	E	35	ILE	C-N-CA	-6.89	113.69	120.52
3	F	369	LYS	N-CA-C	6.89	120.82	110.14
1	B	330	SER	N-CA-C	-6.87	104.58	114.12
3	F	118	ALA	CA-C-N	-6.83	112.95	119.85
3	F	118	ALA	C-N-CA	-6.83	112.95	119.85
3	E	125	SER	N-CA-C	-6.78	104.88	113.02
3	F	211	SER	N-CA-C	6.78	121.22	113.15
3	F	386	GLY	N-CA-C	6.77	120.45	110.63
1	A	95	HIS	N-CA-C	-6.74	96.44	110.80
3	E	404	ASP	CB-CA-C	-6.74	98.73	111.06
3	F	420	GLY	N-CA-C	6.71	120.94	111.42
5	I	433	ASP	C-N-CD	6.68	135.29	120.60
3	F	194	GLN	N-CA-C	6.64	120.06	109.24
3	E	323	ALA	N-CA-C	6.63	123.79	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	256	LYS	CA-C-N	-6.62	108.89	121.54
3	E	256	LYS	C-N-CA	-6.62	108.89	121.54
3	F	214	VAL	N-CA-CB	6.62	122.15	111.23
3	F	214	VAL	N-CA-C	-6.61	95.60	109.34
3	E	371	ASN	CA-C-O	6.58	129.91	120.51
5	I	32	ARG	CA-C-N	-6.49	111.73	119.84
5	I	32	ARG	C-N-CA	-6.49	111.73	119.84
3	F	444	GLY	N-CA-C	6.49	119.39	111.93
3	E	267	ILE	O-C-N	6.46	124.55	120.42
2	D	27	GLY	CA-C-N	6.45	125.95	119.24
2	D	27	GLY	C-N-CA	6.45	125.95	119.24
3	F	267	ILE	O-C-N	6.41	124.62	120.07
2	D	0	PHE	CB-CA-C	-6.40	97.68	110.42
4	G	239	LEU	CA-C-N	6.35	130.34	120.82
4	G	239	LEU	C-N-CA	6.35	130.34	120.82
5	J	417	ASN	N-CA-CB	-6.33	102.68	112.30
5	I	430	THR	CB-CA-C	6.32	117.57	109.80
5	I	435	SER	N-CA-C	6.28	118.64	110.53
2	C	49	SER	N-CA-C	6.26	124.14	110.80
3	F	422	LYS	CB-CA-C	-6.25	102.85	111.73
3	F	128	SER	N-CA-C	6.25	118.61	111.11
3	E	403	GLU	N-CA-C	6.23	120.18	108.65
4	G	275	LEU	N-CA-C	6.22	118.60	108.08
5	I	121	SER	N-CA-C	6.22	124.05	110.80
3	E	419	ILE	N-CA-CB	6.20	118.02	109.84
3	F	399	ASN	N-CA-CB	-6.10	102.64	111.91
5	J	429	GLY	N-CA-C	6.10	120.36	112.68
2	D	96	THR	N-CA-C	-6.09	105.81	113.18
3	F	424	LYS	CA-CB-CG	6.05	126.19	114.10
3	F	369	LYS	CA-C-N	6.04	129.69	121.05
3	F	369	LYS	C-N-CA	6.04	129.69	121.05
1	A	57	GLU	N-CA-C	-6.04	104.26	111.69
1	B	58	PHE	N-CA-C	-6.04	104.82	111.82
2	C	167	MET	CB-CA-C	-6.03	99.54	111.60
1	B	102	GLN	N-CA-C	-6.01	104.73	111.28
2	C	166	GLY	N-CA-C	6.00	121.16	111.38
3	E	279	PHE	N-CA-C	5.97	118.01	110.24
5	I	440	GLY	N-CA-C	-5.97	99.02	113.18
3	E	267	ILE	CB-CA-C	-5.95	106.20	114.00
5	J	433	ASP	N-CA-C	5.93	122.92	109.81
5	I	36	LEU	N-CA-C	-5.92	105.71	113.17
5	J	117	GLN	N-CA-C	-5.88	105.40	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	29	TYR	CB-CA-C	-5.88	99.95	111.06
3	F	346	VAL	N-CA-C	5.87	117.91	109.51
3	E	352	GLU	N-CA-C	5.85	119.68	112.54
4	G	230	THR	N-CA-C	-5.83	102.42	110.35
3	F	267	ILE	CB-CA-C	-5.80	108.20	114.35
3	F	369	LYS	CG-CD-CE	5.80	124.63	111.30
3	E	227	LYS	N-CA-C	-5.78	102.90	110.53
5	J	117	GLN	CA-CB-CG	-5.78	102.55	114.10
1	A	130	TYR	CA-C-N	-5.77	113.86	119.87
1	A	130	TYR	C-N-CA	-5.77	113.86	119.87
5	I	434	PRO	N-CD-CG	-5.75	96.90	103.80
1	A	273	SER	CA-C-N	-5.75	112.66	119.84
1	A	273	SER	C-N-CA	-5.75	112.66	119.84
3	F	252	LEU	N-CA-C	-5.73	105.78	112.89
3	F	363	ASN	N-CA-C	-5.73	100.05	109.80
5	J	433	ASP	CA-C-N	-5.73	112.68	119.84
5	J	433	ASP	C-N-CA	-5.73	112.68	119.84
1	A	55	ILE	N-CA-C	-5.73	104.78	110.62
3	E	332	LEU	N-CA-C	-5.67	105.10	111.28
3	F	200	GLU	N-CA-C	-5.65	103.03	110.43
5	I	205	ILE	CB-CA-C	-5.64	104.52	112.14
5	J	426	HIS	N-CA-C	5.64	117.43	111.28
1	B	274	PRO	CA-N-CD	-5.63	104.11	112.00
3	F	347	ASP	N-CA-C	5.62	118.17	111.71
3	F	398	ASP	N-CA-C	5.62	117.06	108.52
1	A	56	SER	N-CA-C	-5.58	105.20	111.28
1	A	52	ALA	N-CA-C	5.58	116.78	108.31
4	G	186	LEU	N-CA-C	5.56	118.06	111.33
2	C	165	GLY	N-CA-C	-5.53	104.89	111.36
3	E	264	GLY	N-CA-C	-5.51	105.72	112.77
3	F	267	ILE	CA-C-N	-5.50	113.20	120.96
3	F	267	ILE	C-N-CA	-5.50	113.20	120.96
3	E	216	SER	N-CA-C	-5.47	105.32	111.28
2	D	389	SER	N-CA-C	-5.46	107.26	114.31
3	F	58	ASP	N-CA-C	-5.46	106.62	113.72
3	E	371	ASN	N-CA-CB	-5.45	101.28	110.49
2	D	1	MET	N-CA-CB	5.43	119.67	110.49
5	J	380	GLY	CA-C-O	-5.42	116.18	121.06
3	E	364	GLU	N-CA-C	5.40	117.65	110.53
3	F	386	GLY	CA-C-N	5.39	129.79	122.19
3	F	386	GLY	C-N-CA	5.39	129.79	122.19
1	A	115	ILE	N-CA-C	-5.39	106.25	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	268	PRO	N-CD-CG	5.37	111.26	103.20
3	F	351	SER	N-CA-C	5.36	117.83	108.76
3	F	344	ARG	N-CA-C	5.36	117.85	110.35
1	B	312	PRO	CA-C-N	5.36	125.02	119.56
1	B	312	PRO	C-N-CA	5.36	125.02	119.56
1	B	130	TYR	CA-C-N	-5.34	114.32	119.87
1	B	130	TYR	C-N-CA	-5.34	114.32	119.87
1	A	116	GLN	CB-CA-C	-5.32	102.30	110.81
5	I	211	GLU	N-CA-CB	5.31	119.69	111.24
3	E	353	ARG	N-CA-CB	-5.31	105.85	113.65
5	J	163	SER	CA-C-N	-5.30	113.17	119.05
5	J	163	SER	C-N-CA	-5.30	113.17	119.05
4	G	229	LEU	N-CA-CB	-5.29	102.26	110.46
3	E	257	GLU	CB-CG-CD	-5.26	103.66	112.60
4	G	404	MET	N-CA-C	-5.26	103.08	110.50
3	E	133	ARG	N-CA-C	5.25	116.69	111.07
3	E	251	ASP	N-CA-C	-5.25	106.84	113.20
4	G	241	LYS	CB-CG-CD	5.24	123.36	111.30
5	J	170	ALA	N-CA-C	5.23	118.16	109.94
5	J	268	GLU	CB-CA-C	5.22	122.07	111.11
3	E	128	SER	N-CA-C	5.21	117.70	111.71
3	E	277	LYS	N-CA-C	5.20	121.87	110.80
3	F	435	ARG	N-CA-C	-5.20	102.79	110.48
1	A	311	THR	CA-C-N	5.19	123.45	119.66
1	A	311	THR	C-N-CA	5.19	123.45	119.66
3	F	193	LYS	N-CA-C	5.18	117.39	110.35
3	E	219	THR	N-CA-C	5.17	117.33	108.90
2	C	27	GLY	CA-C-N	5.16	124.61	119.24
2	C	27	GLY	C-N-CA	5.16	124.61	119.24
3	E	266	LEU	N-CA-C	5.15	117.29	111.11
5	I	120	THR	N-CA-C	-5.15	102.16	110.14
3	E	326	LEU	CA-C-N	-5.14	113.41	119.84
3	E	326	LEU	C-N-CA	-5.14	113.41	119.84
3	E	36	PRO	CA-N-CD	-5.14	104.81	112.00
3	F	337	ALA	O-C-N	5.14	127.57	122.12
5	I	432	ASN	N-CA-CB	-5.14	101.81	110.49
2	D	69	GLN	CA-C-N	5.11	124.72	119.56
2	D	69	GLN	C-N-CA	5.11	124.72	119.56
3	F	155	PRO	CA-C-N	5.10	124.72	119.05
3	F	155	PRO	C-N-CA	5.10	124.72	119.05
3	E	404	ASP	N-CA-C	5.10	120.90	113.40
1	A	20	VAL	CB-CA-C	-5.10	105.26	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	78	ARG	N-CA-C	-5.08	105.74	111.28
1	A	45	GLN	N-CA-C	-5.06	107.06	113.18
2	C	95	LYS	N-CA-C	-5.05	105.77	111.28
5	I	28	ASN	N-CA-C	-5.05	100.04	110.80
3	E	256	LYS	N-CA-C	5.05	116.87	107.99
3	E	322	ARG	N-CA-C	5.03	117.06	109.41
5	I	209	HIS	N-CA-C	5.01	119.00	112.13
4	G	436	PRO	CA-C-N	5.01	124.61	119.05
4	G	436	PRO	C-N-CA	5.01	124.61	119.05

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	LYS	Peptide
1	A	60	ASP	Peptide
3	E	257	GLU	Peptide
3	E	260	SER	Peptide
3	E	269	TYR	Peptide
3	E	340	THR	Peptide
3	E	442	ALA	Peptide
3	F	269	TYR	Peptide
3	F	369	LYS	Peptide
3	F	370	ASP	Peptide
3	F	383	CYS	Peptide
3	F	403	GLU	Peptide
3	F	447	LEU	Peptide
4	H	355	ARG	Peptide
5	I	31	PHE	Peptide
5	J	432	ASN	Peptide

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	2472	0	2492	156	0
1	B	2489	0	2512	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2702	0	2744	103	0
2	D	2674	0	2714	56	1
3	E	2976	0	3032	278	0
3	F	2967	0	3022	341	7
4	G	2755	0	2841	93	0
4	H	2755	0	2841	45	0
5	I	3377	0	3361	145	1
5	J	3372	0	3351	135	7
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	1	0
6	G	10	0	0	1	0
6	H	10	0	0	0	0
6	I	5	0	0	1	0
All	All	28584	0	28910	1343	8

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 23.

All (1343) 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)
3:F:218:PHE:CE2	5:I:203:PRO:HB3	1.37	1.58
3:F:368:ILE:HA	3:F:385:ILE:O	1.17	1.24
3:F:212:ALA:O	3:F:213:ASP:CG	1.81	1.23
3:E:355:LEU:HD21	3:E:369:LYS:O	1.05	1.23
3:F:218:PHE:HE2	5:I:203:PRO:CB	1.54	1.21
3:E:37:ILE:HD11	3:E:141:ASN:CG	1.66	1.21
3:F:265:ASP:O	3:F:268:PRO:HD2	1.35	1.21
1:A:62:LEU:O	1:A:65:GLY:N	1.72	1.20
3:E:355:LEU:CD2	3:E:369:LYS:O	1.89	1.20
3:E:371:ASN:O	3:E:388:GLY:HA2	1.42	1.19
1:A:18:ASP:HB3	1:A:21:GLN:HG3	1.25	1.18
3:E:276:GLN:O	3:E:277:LYS:CG	1.92	1.18
3:E:276:GLN:O	3:E:277:LYS:HG2	1.02	1.17
3:E:276:GLN:C	3:E:277:LYS:HG2	1.66	1.14
3:F:368:ILE:CA	3:F:385:ILE:O	1.94	1.14
3:F:348:VAL:CG1	3:F:364:GLU:HG2	1.78	1.13
1:A:52:ALA:O	1:A:57:GLU:OE1	1.67	1.13
3:E:355:LEU:HD23	3:E:370:ASP:HA	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:238:LEU:O	4:G:240:GLU:OE1	1.66	1.12
5:J:399:GLY:O	5:J:417:ASN:HA	1.49	1.12
1:B:106:HIS:CE1	2:C:146:ARG:HG2	1.86	1.10
5:I:18:LEU:CD2	5:I:63:VAL:HA	1.82	1.10
3:F:201:LYS:HE3	4:G:409:PHE:HE1	1.01	1.10
2:D:48:TRP:NE1	2:D:166:GLY:O	1.83	1.10
5:J:439:ILE:HG22	5:J:441:GLY:H	1.14	1.09
1:A:53:LYS:CE	1:A:104:LYS:NZ	2.15	1.09
3:F:201:LYS:CE	4:G:409:PHE:HE1	1.63	1.08
3:E:269:TYR:CE1	3:E:270:LEU:HD23	1.88	1.08
3:F:351:SER:OG	3:F:355:LEU:HD11	1.51	1.08
5:I:439:ILE:HD12	5:I:440:GLY:N	1.66	1.08
1:A:53:LYS:NZ	1:A:104:LYS:CE	2.15	1.08
5:I:431:LEU:HD23	5:I:432:ASN:H	1.17	1.08
3:E:149:ASP:HB2	3:E:327:PRO:HD2	1.38	1.06
3:F:397:MET:O	3:F:398:ASP:OD1	1.72	1.06
5:I:33:PRO:HG2	5:I:419:ARG:HG2	1.37	1.06
3:F:218:PHE:CE2	5:I:203:PRO:CB	2.31	1.06
4:G:403:ASN:ND2	4:G:404:MET:O	1.88	1.06
3:F:218:PHE:CD2	5:I:203:PRO:HB3	1.90	1.06
5:J:439:ILE:HD12	5:J:439:ILE:H	1.19	1.06
3:F:385:ILE:HG12	3:F:402:VAL:HB	1.35	1.03
1:A:62:LEU:C	1:A:65:GLY:H	1.66	1.03
3:F:265:ASP:C	3:F:268:PRO:HD2	1.82	1.03
3:E:355:LEU:CD2	3:E:370:ASP:HA	1.88	1.03
3:F:348:VAL:HG11	3:F:364:GLU:HG2	1.08	1.02
3:E:355:LEU:HD21	3:E:369:LYS:C	1.83	1.02
3:E:211:SER:HA	3:E:214:VAL:CG1	1.90	1.02
3:F:201:LYS:HE3	4:G:409:PHE:CE1	1.93	1.02
5:I:187:VAL:HG11	5:I:205:ILE:CG2	1.90	1.02
3:E:418:GLN:OE1	3:E:435:ARG:NH1	1.92	1.01
3:F:343:GLN:HG3	3:F:344:ARG:H	1.21	1.01
1:A:115:ILE:HG22	1:A:115:ILE:O	1.59	1.00
3:F:385:ILE:HG12	3:F:402:VAL:CB	1.91	1.00
2:C:47:ARG:HG2	2:C:167:MET:HE1	1.42	1.00
5:I:32:ARG:O	5:I:33:PRO:C	2.01	0.99
5:I:439:ILE:HD12	5:I:440:GLY:C	1.87	0.99
3:F:343:GLN:HG3	3:F:344:ARG:HG3	1.43	0.99
3:F:421:ALA:O	3:F:438:ALA:HA	1.61	0.99
3:F:446:ARG:HG2	3:F:447:LEU:HB2	1.44	0.99
3:E:355:LEU:HD23	3:E:370:ASP:C	1.88	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:239:GLN:NE2	4:H:404:MET:HB2	1.76	0.98
3:F:123:ASP:OD1	3:F:124:ASP:N	1.95	0.98
3:F:447:LEU:O	3:F:448:VAL:HG23	1.64	0.98
5:I:430:THR:O	5:I:439:ILE:HD13	1.63	0.97
3:E:37:ILE:HD11	3:E:141:ASN:OD1	1.61	0.97
5:I:18:LEU:HD21	5:I:63:VAL:HA	1.43	0.97
3:E:355:LEU:HD23	3:E:370:ASP:CA	1.96	0.96
3:F:363:ASN:OD1	3:F:364:GLU:N	1.99	0.95
5:I:407:VAL:O	5:I:431:LEU:O	1.83	0.95
3:E:274:GLN:HB3	3:E:276:GLN:HE22	1.27	0.95
3:F:193:LYS:O	3:F:211:SER:HB3	1.65	0.94
3:F:352:GLU:O	3:F:355:LEU:HG	1.65	0.94
3:F:201:LYS:NZ	4:G:409:PHE:CE1	2.34	0.94
3:F:363:ASN:OD1	3:F:381:LYS:HG3	1.67	0.94
3:E:91:ILE:HG21	3:E:131:ALA:HB1	1.49	0.94
3:F:191:ASP:N	3:F:329:TYR:CZ	2.36	0.94
3:F:424:LYS:C	3:F:425:LEU:HD12	1.92	0.94
5:I:431:LEU:HD23	5:I:432:ASN:N	1.83	0.94
3:E:269:TYR:CD1	3:E:270:LEU:HA	2.02	0.93
5:J:418:LYS:HZ1	5:J:420:LEU:HA	1.31	0.93
1:A:52:ALA:C	1:A:57:GLU:OE1	2.10	0.93
3:E:37:ILE:CD1	3:E:141:ASN:CG	2.41	0.93
3:F:336:ILE:HD12	3:F:395:ILE:HD13	1.50	0.93
5:J:418:LYS:NZ	5:J:420:LEU:HD23	1.83	0.92
3:E:355:LEU:HB3	3:E:372:SER:O	1.70	0.92
3:F:348:VAL:HG11	3:F:364:GLU:CG	2.00	0.92
4:G:238:LEU:C	4:G:240:GLU:OE1	2.11	0.92
1:A:46:LEU:O	1:A:50:SER:OG	1.87	0.92
3:F:367:THR:O	3:F:385:ILE:N	2.02	0.92
1:A:60:ASP:C	1:A:61:ILE:HD12	1.95	0.92
3:E:37:ILE:HD11	3:E:141:ASN:ND2	1.85	0.92
3:F:446:ARG:CG	3:F:447:LEU:HB2	1.99	0.91
3:F:201:LYS:CE	4:G:409:PHE:CE1	2.50	0.91
3:F:351:SER:OG	3:F:355:LEU:CD1	2.19	0.91
1:A:53:LYS:CE	1:A:104:LYS:HZ1	1.81	0.90
3:F:191:ASP:N	3:F:329:TYR:CE2	2.38	0.90
2:C:167:MET:HG2	2:C:168:ASP:H	1.33	0.90
5:J:409:GLY:HA3	5:J:433:ASP:O	1.70	0.90
3:F:349:THR:OG1	3:F:366:THR:O	1.90	0.90
4:H:402:VAL:O	4:H:404:MET:HE2	1.72	0.89
5:I:430:THR:OG1	5:I:441:GLY:HA2	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:397:GLU:HG3	5:J:398:ASP:H	1.34	0.89
1:A:62:LEU:O	1:A:65:GLY:CA	2.20	0.88
3:F:193:LYS:O	3:F:211:SER:CB	2.22	0.88
3:F:199:GLU:OE1	3:F:202:THR:OG1	1.91	0.88
5:I:431:LEU:CD2	5:I:432:ASN:H	1.86	0.88
5:I:18:LEU:HD21	5:I:63:VAL:CA	2.04	0.88
3:F:426:ARG:HE	3:F:442:ALA:HB1	1.37	0.88
3:F:385:ILE:CG1	3:F:402:VAL:HB	2.04	0.87
2:C:87:ARG:HG3	2:C:87:ARG:HH11	1.36	0.87
5:J:439:ILE:CG2	5:J:442:ARG:H	1.86	0.87
5:J:418:LYS:HE2	5:J:420:LEU:HG	1.56	0.87
3:E:320:CYS:SG	3:E:321:SER:N	2.47	0.87
1:A:62:LEU:O	1:A:66:SER:N	2.08	0.86
3:F:366:THR:HG22	3:F:383:CYS:H	1.38	0.86
1:A:62:LEU:HD12	1:A:63:GLN:N	1.90	0.86
3:F:434:HIS:CD2	3:F:448:VAL:HG23	2.10	0.86
3:F:212:ALA:O	3:F:213:ASP:OD1	1.93	0.86
3:F:366:THR:HB	3:F:383:CYS:O	1.76	0.85
5:I:28:ASN:O	5:I:29:TYR:HD1	1.58	0.85
5:I:33:PRO:CG	5:I:419:ARG:HG2	2.06	0.85
1:B:105:ARG:HG3	1:B:105:ARG:HH11	1.40	0.85
5:J:33:PRO:CG	5:J:419:ARG:HB3	2.06	0.85
1:A:55:ILE:HA	1:A:58:PHE:HB3	1.59	0.85
1:A:18:ASP:CB	1:A:21:GLN:HG3	2.05	0.85
3:F:366:THR:HG21	3:F:380:GLY:O	1.77	0.85
3:F:396:LEU:HD23	3:F:413:VAL:HG22	1.58	0.85
3:F:354:ALA:HB3	3:F:370:ASP:OD1	1.77	0.84
2:C:93:LEU:O	2:C:96:THR:OG1	1.93	0.84
5:J:418:LYS:HZ1	5:J:420:LEU:HD23	1.41	0.84
2:C:47:ARG:CG	2:C:167:MET:HE1	2.05	0.84
3:E:368:ILE:HG22	3:E:385:ILE:HB	1.59	0.84
1:A:47:LEU:HA	1:A:50:SER:OG	1.78	0.84
3:F:396:LEU:HD22	3:F:413:VAL:HG21	1.60	0.83
2:C:136:MET:HG3	2:C:138:SER:O	1.78	0.83
3:F:265:ASP:O	3:F:268:PRO:CD	2.25	0.83
3:F:434:HIS:CD2	3:F:448:VAL:CG2	2.62	0.83
1:A:61:ILE:HD13	1:A:62:LEU:HD12	1.60	0.82
1:B:105:ARG:O	1:B:109:GLU:HG3	1.79	0.82
5:I:187:VAL:HG11	5:I:205:ILE:HG22	1.60	0.82
3:F:367:THR:HB	3:F:384:VAL:HG12	1.58	0.82
3:E:348:VAL:HG21	3:E:364:GLU:HG2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:187:VAL:CG1	5:I:205:ILE:CG2	2.58	0.81
2:C:47:ARG:HG3	2:C:167:MET:SD	2.20	0.81
4:H:402:VAL:O	4:H:404:MET:CE	2.27	0.81
1:A:55:ILE:HG13	1:A:56:SER:H	1.46	0.81
5:I:187:VAL:HG11	5:I:205:ILE:HG21	1.63	0.81
3:E:274:GLN:HB3	3:E:276:GLN:NE2	1.96	0.81
3:F:446:ARG:CB	3:F:447:LEU:HB2	2.10	0.81
3:F:396:LEU:CD2	3:F:413:VAL:CG2	2.58	0.81
3:E:211:SER:HA	3:E:214:VAL:HG11	1.60	0.81
3:E:329:TYR:HB2	3:E:331:GLU:OE1	1.79	0.81
1:A:113:LEU:HA	1:A:116:GLN:HG3	1.62	0.80
3:F:341:PRO:C	3:F:342:GLU:HG2	2.05	0.80
3:E:130:ASP:HA	3:E:133:ARG:CZ	2.13	0.79
4:G:228:ASP:CB	4:G:229:LEU:HD12	2.13	0.79
3:E:385:ILE:HG23	3:E:389:VAL:HG21	1.64	0.79
5:I:18:LEU:HD23	5:I:63:VAL:HA	1.62	0.79
3:E:352:GLU:O	3:E:353:ARG:CG	2.29	0.79
5:I:202:ASP:OD1	5:I:205:ILE:HD11	1.82	0.79
3:E:396:LEU:HD22	3:E:400:ILE:HD11	1.64	0.79
5:I:187:VAL:CG1	5:I:205:ILE:HG21	2.13	0.79
5:I:429:GLY:HA3	5:I:436:LEU:HD23	1.64	0.79
3:E:211:SER:C	3:E:214:VAL:HG13	2.06	0.79
1:A:25:LYS:HA	1:A:28:GLN:OE1	1.83	0.78
3:F:434:HIS:CG	3:F:448:VAL:HG23	2.19	0.78
3:F:363:ASN:CG	3:F:381:LYS:HG3	2.07	0.78
5:J:397:GLU:HG3	5:J:398:ASP:N	1.94	0.78
5:J:409:GLY:CA	5:J:433:ASP:O	2.32	0.78
3:F:367:THR:O	3:F:384:VAL:CA	2.32	0.78
2:D:50:THR:HB	2:D:53:GLN:HG3	1.65	0.78
3:F:421:ALA:O	3:F:438:ALA:CA	2.30	0.78
5:J:33:PRO:HG3	5:J:419:ARG:HB3	1.64	0.78
1:A:94:LEU:C	1:A:95:HIS:O	2.22	0.78
5:J:381:LYS:HB3	5:J:398:ASP:HA	1.66	0.78
3:F:265:ASP:C	3:F:268:PRO:CD	2.57	0.78
3:E:267:ILE:HD13	3:E:267:ILE:N	1.98	0.78
5:J:399:GLY:C	5:J:417:ASN:HA	2.09	0.78
3:E:352:GLU:O	3:E:353:ARG:CB	2.32	0.77
5:I:439:ILE:CD1	5:I:441:GLY:N	2.47	0.77
3:F:366:THR:CB	3:F:383:CYS:O	2.32	0.77
5:I:439:ILE:CD1	5:I:440:GLY:C	2.56	0.77
1:B:106:HIS:NE2	2:C:146:ARG:CG	2.46	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:MET:HG2	2:C:168:ASP:N	1.98	0.77
3:E:211:SER:CA	3:E:214:VAL:CG1	2.63	0.77
3:E:397:MET:HE3	3:E:414:ALA:HA	1.64	0.77
4:G:228:ASP:HB2	4:G:229:LEU:CD1	2.13	0.77
2:C:48:TRP:CD1	2:C:54:LEU:HB2	2.18	0.77
2:D:48:TRP:HE1	2:D:166:GLY:C	1.92	0.77
3:F:358:ALA:N	3:F:360:CYS:SG	2.58	0.77
2:D:316:LEU:HG	2:D:382:MET:HE3	1.67	0.76
4:G:278:SER:OG	6:G:501:PO4:O4	2.02	0.76
2:D:0:PHE:O	2:D:1:MET:HG3	1.86	0.76
1:B:106:HIS:CE1	2:C:146:ARG:CG	2.68	0.76
2:C:162:ARG:HA	2:C:162:ARG:NE	1.97	0.76
2:C:93:LEU:HA	2:C:96:THR:CG2	2.16	0.76
5:I:205:ILE:HD13	5:I:205:ILE:H	1.50	0.76
3:E:182:HIS:CD2	3:E:334:LYS:HE3	2.21	0.76
3:F:343:GLN:HE21	3:F:343:GLN:HA	1.50	0.76
1:A:63:GLN:O	1:A:67:ASN:OD1	2.02	0.75
3:F:343:GLN:CG	3:F:344:ARG:H	1.99	0.75
4:G:240:GLU:CD	4:G:241:LYS:H	1.93	0.75
1:A:59:MET:C	1:A:61:ILE:HG13	2.11	0.75
1:A:61:ILE:HD13	1:A:62:LEU:N	2.00	0.75
3:E:369:LYS:HB2	3:E:386:GLY:CA	2.17	0.75
3:F:385:ILE:HG12	3:F:402:VAL:CG2	2.16	0.75
3:F:181:GLU:H	3:F:334:LYS:HE3	1.52	0.75
3:E:369:LYS:HB2	3:E:386:GLY:HA3	1.68	0.75
5:J:386:ASN:H	5:J:386:ASN:ND2	1.84	0.75
3:E:269:TYR:CD1	3:E:270:LEU:CA	2.70	0.75
5:J:431:LEU:O	5:J:432:ASN:HB2	1.86	0.75
1:A:63:GLN:O	1:A:67:ASN:CG	2.29	0.74
3:F:343:GLN:HA	3:F:343:GLN:NE2	2.03	0.74
5:I:32:ARG:O	5:I:34:LEU:N	2.19	0.74
5:I:205:ILE:HD13	5:I:205:ILE:N	2.03	0.74
1:A:62:LEU:HD12	1:A:63:GLN:H	1.51	0.74
3:F:269:TYR:CD1	3:F:270:LEU:HA	2.21	0.74
3:F:396:LEU:HD22	3:F:413:VAL:CG2	2.16	0.74
3:F:426:ARG:HE	3:F:442:ALA:CB	2.00	0.74
3:F:361:MET:HB2	3:F:378:ILE:HD13	1.70	0.74
1:A:22:VAL:O	1:A:25:LYS:HB2	1.88	0.74
4:G:241:LYS:HA	4:G:244:SER:HB2	1.68	0.74
5:I:188:HIS:HD2	5:I:201:MET:HB3	1.52	0.74
3:E:352:GLU:C	3:E:353:ARG:HG2	2.13	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:447:LEU:O	3:F:448:VAL:CG2	2.36	0.74
3:E:252:LEU:HD12	3:E:256:LYS:HE3	1.70	0.73
1:A:18:ASP:HB3	1:A:21:GLN:CG	2.14	0.73
3:E:269:TYR:HD1	3:E:270:LEU:CA	2.01	0.73
3:F:266:LEU:O	3:F:269:TYR:HD2	1.71	0.73
3:F:371:ASN:O	3:F:388:GLY:HA2	1.88	0.73
4:G:410:GLU:C	4:G:411:GLU:HG3	2.14	0.73
2:C:50:THR:OG1	2:C:53:GLN:OE1	2.06	0.73
5:I:430:THR:OG1	5:I:439:ILE:HD11	1.88	0.73
3:F:119:PRO:HG2	3:F:122:LEU:HG	1.70	0.73
3:F:430:ILE:HA	3:F:446:ARG:O	1.89	0.73
5:I:28:ASN:O	5:I:29:TYR:CD1	2.40	0.73
1:A:26:PHE:HA	1:A:29:ASP:CG	2.13	0.73
3:F:397:MET:O	3:F:398:ASP:CG	2.31	0.73
5:I:430:THR:O	5:I:439:ILE:CD1	2.35	0.73
5:I:437:VAL:HG22	5:I:438:GLY:H	1.54	0.73
2:C:87:ARG:HG3	2:C:87:ARG:NH1	1.98	0.72
3:F:366:THR:CA	3:F:383:CYS:O	2.36	0.72
1:A:25:LYS:O	1:A:28:GLN:OE1	2.06	0.72
1:A:26:PHE:O	1:A:29:ASP:N	2.22	0.72
1:A:115:ILE:O	1:A:115:ILE:CG2	2.31	0.72
3:E:182:HIS:CD2	3:E:334:LYS:CE	2.72	0.72
3:F:418:GLN:O	3:F:435:ARG:HA	1.89	0.72
5:I:439:ILE:HD12	5:I:441:GLY:N	2.05	0.72
3:E:81:GLU:OE2	3:E:110:GLY:O	2.07	0.72
1:A:53:LYS:HZ1	1:A:104:LYS:CE	1.93	0.72
3:E:269:TYR:CE1	3:E:270:LEU:HA	2.24	0.72
1:A:61:ILE:HD13	1:A:62:LEU:CD1	2.19	0.72
3:F:267:ILE:HD13	3:F:267:ILE:N	2.05	0.72
3:F:320:CYS:SG	3:F:321:SER:N	2.60	0.72
5:J:416:LYS:C	5:J:417:ASN:ND2	2.48	0.72
5:J:418:LYS:NZ	5:J:420:LEU:HA	2.03	0.72
3:F:124:ASP:OD1	3:F:125:SER:N	2.23	0.72
2:C:377:TYR:OH	4:H:460:ASN:ND2	2.23	0.72
5:I:433:ASP:HA	5:I:434:PRO:C	2.15	0.72
5:J:385:ALA:O	5:J:388:VAL:HG23	1.90	0.72
3:E:276:GLN:C	3:E:277:LYS:CG	2.53	0.71
3:E:274:GLN:CB	3:E:276:GLN:HE22	2.02	0.71
5:J:414:ILE:C	5:J:415:GLU:HG2	2.15	0.71
1:A:57:GLU:O	1:A:61:ILE:HG23	1.91	0.71
1:B:104:LYS:O	1:B:108:VAL:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:446:ARG:HG2	3:F:447:LEU:CB	2.19	0.71
1:B:106:HIS:NE2	2:C:146:ARG:HG2	2.06	0.71
3:E:349:THR:OG1	3:E:366:THR:O	2.04	0.71
5:I:436:LEU:C	5:I:436:LEU:HD12	2.16	0.71
5:J:418:LYS:HE2	5:J:420:LEU:CG	2.21	0.71
2:C:235:PHE:HE1	4:G:405:GLY:HA3	1.55	0.71
2:D:51:VAL:HG13	2:D:52:ASP:OD1	1.91	0.71
4:G:228:ASP:HB3	4:G:229:LEU:HD12	1.71	0.71
3:E:352:GLU:C	3:E:353:ARG:CG	2.63	0.71
3:E:355:LEU:HD23	3:E:371:ASN:N	2.05	0.71
2:C:47:ARG:CG	2:C:167:MET:CE	2.68	0.71
3:F:426:ARG:NE	3:F:442:ALA:HB1	2.04	0.71
5:J:383:ILE:C	5:J:384:LEU:HD23	2.15	0.71
5:J:439:ILE:HG22	5:J:441:GLY:N	1.99	0.71
3:E:170:ALA:HB3	3:E:315:LYS:HG2	1.74	0.70
3:F:387:LYS:HB2	3:F:404:ASP:HB3	1.73	0.70
5:I:130:VAL:HG12	5:I:273:ARG:HG2	1.73	0.70
5:I:437:VAL:HG22	5:I:438:GLY:N	2.04	0.70
5:J:391:GLY:C	5:J:394:CYS:SG	2.73	0.70
3:E:269:TYR:CD1	3:E:270:LEU:N	2.58	0.70
2:C:167:MET:CG	2:C:168:ASP:H	2.04	0.70
3:E:387:LYS:HD3	3:E:404:ASP:HA	1.73	0.70
3:F:122:LEU:HD11	3:F:131:ALA:HA	1.74	0.70
1:A:53:LYS:HZ3	1:A:104:LYS:CE	1.94	0.70
3:E:371:ASN:O	3:E:388:GLY:CA	2.33	0.70
3:E:403:GLU:O	3:E:406:VAL:HG13	1.90	0.70
3:F:212:ALA:O	3:F:213:ASP:CB	2.39	0.70
5:J:418:LYS:HE3	5:J:420:LEU:N	2.05	0.70
3:F:373:ASN:N	3:F:389:VAL:O	2.23	0.69
1:A:59:MET:CA	1:A:61:ILE:HG13	2.22	0.69
5:J:439:ILE:HG21	5:J:442:ARG:H	1.55	0.69
3:F:127:SER:HB3	3:F:261:SER:HB2	1.74	0.69
3:F:396:LEU:CD2	3:F:413:VAL:HG21	2.20	0.69
5:I:188:HIS:CD2	5:I:201:MET:HB3	2.27	0.69
5:J:418:LYS:CE	5:J:420:LEU:HG	2.22	0.69
1:A:64:ASN:O	1:A:68:THR:OG1	2.01	0.69
5:I:439:ILE:HD11	5:I:441:GLY:CA	2.22	0.69
5:J:409:GLY:N	5:J:433:ASP:O	2.25	0.69
5:J:418:LYS:HE2	5:J:420:LEU:CD2	2.23	0.69
3:E:211:SER:C	3:E:214:VAL:CG1	2.65	0.69
3:F:368:ILE:HG22	3:F:385:ILE:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:433:ASP:HB2	5:J:434:PRO:HD3	1.73	0.69
2:C:47:ARG:HG3	2:C:167:MET:CE	2.22	0.69
2:C:48:TRP:HH2	2:C:170:ARG:HG2	1.56	0.69
3:E:339:LEU:C	3:E:341:PRO:HD2	2.18	0.69
3:F:180:TYR:OH	3:F:331:GLU:OE2	2.09	0.69
3:E:276:GLN:H	3:E:276:GLN:CD	2.01	0.69
5:I:433:ASP:O	5:I:433:ASP:OD2	2.11	0.69
2:C:333:PRO:HD3	5:I:290:ARG:HB2	1.75	0.69
4:G:229:LEU:HD23	4:G:233:GLU:CB	2.23	0.69
3:F:407:ARG:HD2	3:F:424:LYS:HE3	1.75	0.69
5:J:400:ALA:O	5:J:401:ILE:HG13	1.92	0.68
3:E:37:ILE:CD1	3:E:141:ASN:OD1	2.40	0.68
5:I:18:LEU:HD21	5:I:63:VAL:N	2.07	0.68
3:E:387:LYS:CD	3:E:404:ASP:HA	2.24	0.68
3:F:368:ILE:C	3:F:385:ILE:O	2.37	0.68
3:F:403:GLU:CB	3:F:420:GLY:HA2	2.23	0.68
1:B:105:ARG:HG3	1:B:105:ARG:NH1	2.09	0.68
3:E:355:LEU:HD11	3:E:368:ILE:HG13	1.75	0.68
5:I:257:LEU:O	5:I:259:LYS:HG2	1.93	0.68
5:I:439:ILE:HD12	5:I:439:ILE:C	2.18	0.68
5:J:111:ARG:NH2	5:J:240:TYR:O	2.27	0.68
2:C:291:SER:HA	2:C:356:ASP:HB2	1.75	0.68
3:F:343:GLN:HG3	3:F:344:ARG:N	2.03	0.68
4:H:411:GLU:N	4:H:411:GLU:OE1	2.27	0.68
5:J:290:ARG:NH1	5:J:298:ASP:OD1	2.27	0.67
5:J:439:ILE:H	5:J:439:ILE:CD1	1.94	0.67
1:A:28:GLN:H	1:A:28:GLN:CD	2.02	0.67
3:E:255:GLU:HG2	3:E:256:LYS:HD3	1.75	0.67
4:G:228:ASP:CB	4:G:229:LEU:CD1	2.72	0.67
3:E:133:ARG:NE	3:E:257:GLU:OE1	2.27	0.67
3:E:355:LEU:HD22	3:E:372:SER:HB2	1.77	0.67
5:J:406:VAL:HG11	5:J:420:LEU:HD13	1.76	0.67
5:J:418:LYS:HZ1	5:J:420:LEU:CA	2.07	0.67
3:E:68:GLY:HA3	3:E:339:LEU:HD22	1.75	0.67
3:F:407:ARG:HB2	3:F:424:LYS:HD3	1.76	0.67
2:D:50:THR:HG22	2:D:52:ASP:H	1.60	0.67
3:E:249:VAL:O	3:E:253:ILE:HG13	1.94	0.67
5:J:169:ARG:NH1	5:J:218:LEU:O	2.27	0.67
3:E:274:GLN:OE1	3:E:274:GLN:N	2.27	0.67
3:E:385:ILE:HA	3:E:402:VAL:O	1.94	0.67
5:I:209:HIS:O	5:I:210:GLU:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:NZ	1:A:104:LYS:NZ	0.69	0.66
5:I:290:ARG:NH1	5:I:298:ASP:OD1	2.24	0.66
2:C:93:LEU:HA	2:C:96:THR:HG21	1.76	0.66
1:A:55:ILE:O	1:A:59:MET:N	2.27	0.66
3:F:161:ASP:OD1	4:G:134:THR:CG2	2.44	0.66
3:F:403:GLU:HB3	3:F:420:GLY:HA2	1.76	0.66
3:F:397:MET:SD	3:F:414:ALA:HA	2.36	0.66
4:H:117:GLU:O	4:H:119:GLN:NE2	2.29	0.66
5:J:33:PRO:HG2	5:J:419:ARG:HB3	1.77	0.66
3:E:413:VAL:HG22	3:E:430:ILE:HD12	1.78	0.66
3:F:91:ILE:HG21	3:F:131:ALA:HB1	1.78	0.66
5:I:439:ILE:HG13	5:I:441:GLY:HA3	1.78	0.66
1:B:339:LEU:HD23	1:B:340:TYR:CE2	2.29	0.65
3:E:211:SER:HA	3:E:214:VAL:HG12	1.75	0.65
3:F:144:VAL:HG22	3:F:244:VAL:HG12	1.77	0.65
1:A:55:ILE:HG13	1:A:56:SER:N	2.07	0.65
3:F:363:ASN:CG	3:F:364:GLU:H	2.02	0.65
1:A:59:MET:HA	1:A:61:ILE:HG13	1.79	0.65
3:F:391:VAL:HG12	3:F:408:LEU:HB2	1.78	0.65
5:I:18:LEU:CD2	5:I:62:GLY:O	2.45	0.65
3:E:352:GLU:O	3:E:353:ARG:HB2	1.97	0.65
4:H:405:GLY:O	4:H:406:VAL:HG12	1.96	0.65
3:E:385:ILE:HG12	3:E:402:VAL:HB	1.79	0.65
4:H:408:ASP:OD1	4:H:408:ASP:N	2.27	0.65
5:I:18:LEU:CD2	5:I:63:VAL:CA	2.64	0.65
3:E:348:VAL:HG21	3:E:364:GLU:CG	2.27	0.64
3:F:262:ILE:HG23	3:F:266:LEU:HD13	1.79	0.64
3:F:420:GLY:N	3:F:436:VAL:O	2.26	0.64
4:G:407:ASP:OD1	4:G:408:ASP:N	2.30	0.64
3:E:221:ARG:NH1	5:J:198:TYR:OH	2.30	0.64
3:E:355:LEU:CD2	3:E:370:ASP:CA	2.64	0.64
4:G:237:LEU:HD12	4:G:238:LEU:N	2.12	0.64
3:E:418:GLN:OE1	3:E:435:ARG:HD3	1.96	0.64
1:A:47:LEU:CA	1:A:50:SER:OG	2.44	0.64
3:F:396:LEU:CD2	3:F:413:VAL:HG22	2.18	0.64
1:A:58:PHE:O	1:A:61:ILE:HG21	1.97	0.64
3:F:446:ARG:CA	3:F:447:LEU:HB2	2.28	0.64
3:F:202:THR:O	3:F:203:SER:HB2	1.97	0.64
5:I:348:THR:HG21	5:I:362:ILE:HG22	1.79	0.64
2:C:87:ARG:NH1	2:C:387:ASP:OD2	2.31	0.64
3:F:212:ALA:C	3:F:213:ASP:CG	2.66	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:241:LYS:O	4:G:245:TYR:HB2	1.96	0.64
5:J:226:CYS:HB3	5:J:230:VAL:HG21	1.78	0.64
5:I:50:LEU:HD11	5:I:274:VAL:HG21	1.80	0.64
3:E:37:ILE:CD1	3:E:141:ASN:ND2	2.56	0.63
3:F:202:THR:HB	3:F:204:ARG:HG2	1.79	0.63
5:I:29:TYR:CD2	5:I:29:TYR:O	2.51	0.63
3:E:352:GLU:HG3	3:E:370:ASP:N	2.13	0.63
3:F:339:LEU:HD13	3:F:339:LEU:O	1.99	0.63
2:C:-3:ILE:HG22	2:C:64:THR:HG21	1.80	0.63
1:A:53:LYS:HZ1	1:A:104:LYS:NZ	0.69	0.63
1:A:53:LYS:HD3	1:A:53:LYS:N	2.13	0.63
2:C:92:GLU:O	2:C:96:THR:HG23	1.99	0.63
4:G:444:VAL:HG22	4:G:449:LEU:HG	1.80	0.63
2:C:93:LEU:HA	2:C:96:THR:HG23	1.80	0.63
5:I:436:LEU:HA	5:I:437:VAL:C	2.23	0.63
2:D:47:ARG:HG3	2:D:167:MET:HE1	1.78	0.63
3:F:367:THR:CB	3:F:384:VAL:HG12	2.29	0.63
3:E:385:ILE:CG2	3:E:389:VAL:HG21	2.29	0.62
5:I:154:ILE:HD11	5:I:259:LYS:HE3	1.80	0.62
1:B:106:HIS:NE2	2:C:146:ARG:HG3	2.13	0.62
5:J:386:ASN:H	5:J:386:ASN:HD22	1.46	0.62
1:A:117:ARG:O	1:A:120:ALA:N	2.32	0.62
3:F:423:SER:OG	3:F:438:ALA:O	2.18	0.62
5:I:420:LEU:HA	5:I:428:GLN:O	1.98	0.62
3:E:274:GLN:CD	3:E:274:GLN:H	2.07	0.62
4:G:228:ASP:HB2	4:G:229:LEU:HD13	1.81	0.62
2:C:163:VAL:HG12	2:C:164:THR:OG1	1.99	0.62
2:D:50:THR:HB	2:D:53:GLN:CG	2.30	0.62
3:F:194:GLN:HB2	3:F:237:LEU:O	2.00	0.62
5:J:418:LYS:HE3	5:J:419:ARG:C	2.24	0.62
5:J:430:THR:HG22	5:J:431:LEU:H	1.64	0.62
1:A:25:LYS:CA	1:A:28:GLN:OE1	2.47	0.62
2:C:136:MET:O	2:C:137:TYR:HB2	2.00	0.62
3:E:48:GLY:HA2	3:E:62:LYS:HD2	1.80	0.62
3:E:352:GLU:HG3	3:E:369:LYS:HA	1.81	0.62
2:C:0:PHE:C	2:C:1:MET:HG3	2.23	0.61
3:F:363:ASN:OD1	3:F:381:LYS:CG	2.43	0.61
2:C:294:GLN:HG2	4:G:330:SER:HB2	1.81	0.61
2:D:198:HIS:O	2:D:273:LYS:NZ	2.32	0.61
5:J:391:GLY:O	5:J:394:CYS:SG	2.58	0.61
5:I:439:ILE:CD1	5:I:441:GLY:CA	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:261:SER:O	3:E:262:ILE:HB	1.99	0.61
3:E:355:LEU:HD22	3:E:372:SER:N	2.15	0.61
1:B:336:LEU:O	1:B:340:TYR:HD2	1.82	0.61
1:A:117:ARG:O	1:A:121:CYS:N	2.26	0.61
1:A:168:GLU:OE2	1:B:170:ARG:NH1	2.32	0.61
1:B:25:LYS:HA	1:B:28:GLN:NE2	2.15	0.61
3:E:354:ALA:HB3	3:E:370:ASP:HB3	1.83	0.61
3:E:396:LEU:HD22	3:E:400:ILE:CD1	2.30	0.61
3:F:273:CYS:O	3:F:275:TYR:HD2	1.83	0.61
5:I:439:ILE:HD12	5:I:440:GLY:CA	2.31	0.61
5:J:439:ILE:HD12	5:J:439:ILE:N	2.04	0.61
3:E:119:PRO:HG2	3:E:122:LEU:HG	1.82	0.61
5:J:156:THR:HG22	5:J:262:HIS:HB2	1.82	0.61
3:E:182:HIS:CD2	3:E:334:LYS:HE2	2.35	0.61
3:E:389:VAL:HG12	3:E:406:VAL:N	2.16	0.61
3:F:426:ARG:HG3	3:F:426:ARG:O	2.01	0.61
4:G:114:ILE:HG22	4:G:116:GLU:H	1.65	0.61
2:C:136:MET:HE3	2:C:142:ASN:ND2	2.16	0.61
2:D:239:GLN:CD	4:H:404:MET:HB2	2.25	0.61
3:E:418:GLN:OE1	3:E:435:ARG:CD	2.49	0.61
3:E:437:GLU:H	3:E:437:GLU:CD	2.08	0.61
1:A:101:GLU:O	1:A:105:ARG:HG2	2.01	0.60
4:G:356:ALA:HA	4:G:433:ASP:HB2	1.83	0.60
1:A:51:GLN:O	1:A:53:LYS:HG2	2.01	0.60
1:A:113:LEU:HD12	1:A:113:LEU:O	2.01	0.60
3:F:218:PHE:CD2	5:I:203:PRO:CB	2.76	0.60
1:A:172:SER:HB2	1:B:286:THR:HG21	1.83	0.60
3:F:269:TYR:CE1	3:F:270:LEU:HA	2.35	0.60
4:G:272:LEU:HD12	4:G:336:VAL:HG21	1.82	0.60
3:F:366:THR:HG22	3:F:383:CYS:N	2.12	0.60
5:J:407:VAL:HB	5:J:431:LEU:HG	1.83	0.60
1:A:113:LEU:HA	1:A:116:GLN:CG	2.30	0.60
3:E:32:LEU:HD23	3:E:32:LEU:O	2.02	0.60
1:A:95:HIS:CD2	1:A:96:ASP:H	2.20	0.60
3:F:161:ASP:OD1	4:G:134:THR:HG23	2.01	0.60
3:F:213:ASP:OD1	3:F:214:VAL:N	2.35	0.60
2:C:93:LEU:CA	2:C:96:THR:HG23	2.32	0.60
3:E:404:ASP:OD2	3:E:421:ALA:N	2.28	0.60
3:F:403:GLU:HG2	3:F:421:ALA:H	1.67	0.60
3:F:270:LEU:N	3:F:270:LEU:HD23	2.17	0.60
3:F:367:THR:O	3:F:384:VAL:C	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:154:LEU:HD12	3:E:155:PRO:HD2	1.84	0.59
3:E:162:LYS:NZ	3:E:166:ASP:OD2	2.35	0.59
3:E:380:GLY:N	3:E:396:LEU:O	2.35	0.59
3:F:183:ILE:HG22	3:F:183:ILE:O	2.01	0.59
1:A:25:LYS:C	1:A:28:GLN:OE1	2.45	0.59
3:E:182:HIS:HD2	3:E:334:LYS:HE2	1.67	0.59
3:E:269:TYR:HD1	3:E:270:LEU:HA	1.53	0.59
3:F:336:ILE:CD1	3:F:395:ILE:HD13	2.30	0.59
2:C:48:TRP:N	2:C:167:MET:HE2	2.18	0.59
3:F:346:VAL:HG12	3:F:348:VAL:H	1.67	0.59
3:F:419:ILE:HB	3:F:436:VAL:HB	1.83	0.59
3:F:449:ASP:OD1	3:F:450:MET:N	2.35	0.59
3:F:251:ASP:HA	3:F:254:ARG:HB2	1.82	0.59
5:J:416:LYS:C	5:J:417:ASN:HD22	2.09	0.59
3:F:154:LEU:HD12	3:F:155:PRO:HD2	1.83	0.59
3:F:214:VAL:HG23	3:F:218:PHE:CD1	2.38	0.59
2:C:136:MET:HG2	2:C:137:TYR:H	1.68	0.59
3:E:65:LEU:HB2	3:E:72:MET:HE3	1.85	0.59
3:E:387:LYS:HB2	3:E:404:ASP:H	1.68	0.59
5:J:398:ASP:N	5:J:398:ASP:OD1	2.32	0.59
3:E:441:ILE:HG13	3:E:443:ARG:HH21	1.66	0.58
3:E:224:LEU:HD23	3:E:225:LEU:HD12	1.84	0.58
2:D:10:TYR:OH	2:D:46:THR:OG1	1.79	0.58
3:E:256:LYS:O	3:E:259:ILE:CG1	2.51	0.58
3:F:367:THR:O	3:F:384:VAL:HA	2.01	0.58
4:G:240:GLU:OE1	4:G:241:LYS:N	2.28	0.58
3:F:194:GLN:HG3	3:F:238:SER:HA	1.86	0.58
4:G:237:LEU:HD12	4:G:238:LEU:H	1.69	0.58
2:C:19:ASP:HB3	2:C:25:VAL:HG12	1.85	0.58
2:C:93:LEU:C	2:C:96:THR:HG23	2.28	0.58
5:I:18:LEU:CD2	5:I:62:GLY:C	2.77	0.58
5:I:409:GLY:HA3	5:I:434:PRO:HA	1.86	0.58
1:A:61:ILE:CD1	1:A:62:LEU:HD12	2.32	0.58
3:E:434:HIS:CG	3:E:447:LEU:HA	2.39	0.58
3:F:424:LYS:O	3:F:425:LEU:HD12	2.03	0.58
3:F:446:ARG:HG2	3:F:447:LEU:HD22	1.85	0.58
5:J:33:PRO:HG2	5:J:419:ARG:HG2	1.85	0.58
5:J:285:LYS:HE2	5:J:330:ARG:HH21	1.69	0.58
3:F:368:ILE:HA	3:F:385:ILE:C	2.17	0.58
5:I:202:ASP:CG	5:I:205:ILE:HD11	2.28	0.58
5:J:418:LYS:CE	5:J:420:LEU:HD23	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:240:GLU:CD	4:G:241:LYS:N	2.61	0.58
1:A:113:LEU:CD1	1:A:116:GLN:HG3	2.34	0.58
2:D:46:THR:O	2:D:170:ARG:NH2	2.36	0.58
3:E:260:SER:OG	3:E:264:GLY:HA3	2.03	0.58
3:E:328:ASN:OD1	3:E:328:ASN:N	2.30	0.58
3:E:133:ARG:NE	3:E:257:GLU:CD	2.62	0.57
4:H:258:VAL:HA	4:H:283:VAL:HG22	1.86	0.57
2:C:41:GLN:HA	2:C:44:SER:HB3	1.85	0.57
2:C:5:ASN:O	2:C:9:THR:OG1	2.16	0.57
3:E:195:LEU:HD23	3:E:218:PHE:CE2	2.39	0.57
3:E:211:SER:CA	3:E:214:VAL:HG11	2.29	0.57
5:J:267:LYS:C	5:J:268:GLU:HG3	2.30	0.57
3:F:122:LEU:HD11	3:F:131:ALA:CB	2.34	0.57
3:F:161:ASP:CG	4:G:134:THR:HG23	2.28	0.57
1:A:74:GLN:HB3	1:A:263:SER:HB2	1.86	0.57
3:F:122:LEU:CD1	3:F:131:ALA:CB	2.82	0.57
4:G:160:SER:HB3	4:G:344:HIS:HD2	1.70	0.57
5:I:226:CYS:HB3	5:I:230:VAL:HG21	1.85	0.57
5:J:429:GLY:HA2	5:J:436:LEU:HD21	1.85	0.57
1:A:61:ILE:HD13	1:A:62:LEU:H	1.68	0.57
1:A:67:ASN:O	1:A:71:GLU:HG3	2.03	0.57
4:H:411:GLU:O	4:H:412:LYS:HG2	2.04	0.57
2:D:12:ALA:HB1	2:D:38:VAL:HG22	1.85	0.57
2:D:236:PRO:HG3	2:D:336:ILE:HG22	1.87	0.57
3:E:136:SER:HB2	3:E:254:ARG:HH11	1.70	0.57
3:E:256:LYS:O	3:E:259:ILE:HG13	2.05	0.57
3:E:357:GLY:HA3	3:E:374:ILE:HG13	1.87	0.57
3:E:369:LYS:HB2	3:E:386:GLY:HA2	1.86	0.57
3:F:122:LEU:HD13	3:F:131:ALA:HB2	1.85	0.57
3:F:123:ASP:CG	3:F:124:ASP:N	2.63	0.57
3:F:430:ILE:HD12	3:F:430:ILE:O	2.04	0.57
5:I:431:LEU:CD2	5:I:432:ASN:N	2.57	0.57
4:H:117:GLU:C	4:H:119:GLN:HE21	2.12	0.57
1:A:201:MET:HE2	1:A:233:ALA:HA	1.87	0.57
3:F:401:VAL:HG23	3:F:401:VAL:O	2.05	0.57
4:G:231:ASP:O	4:G:234:GLY:N	2.37	0.57
2:C:136:MET:HE2	2:C:139:SER:HA	1.86	0.56
2:D:325:GLU:OE2	5:J:310:ARG:NE	2.37	0.56
3:F:413:VAL:HA	3:F:430:ILE:HG13	1.87	0.56
4:H:213:ASN:OD1	4:H:216:ARG:NH1	2.37	0.56
5:I:24:SER:O	5:I:25:ASP:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:LYS:HE3	5:I:301:LEU:HA	1.86	0.56
3:E:355:LEU:CD2	3:E:370:ASP:C	2.71	0.56
3:E:182:HIS:H	3:E:334:LYS:HE3	1.70	0.56
3:F:212:ALA:C	3:F:213:ASP:OD1	2.49	0.56
3:F:380:GLY:HA3	3:F:397:MET:O	2.06	0.56
3:F:447:LEU:HG	3:F:448:VAL:N	2.19	0.56
4:G:234:GLY:O	4:G:237:LEU:HD12	2.05	0.56
5:I:186:CYS:HB3	5:I:261:ILE:HG23	1.88	0.56
3:F:229:PRO:HB3	5:I:164:PRO:HG3	1.88	0.56
3:F:343:GLN:HE21	3:F:343:GLN:CA	2.16	0.56
3:E:255:GLU:OE1	3:E:255:GLU:N	2.31	0.56
3:F:385:ILE:HG12	3:F:402:VAL:HG21	1.86	0.56
3:F:398:ASP:O	3:F:399:ASN:HB2	2.04	0.56
1:A:117:ARG:HA	1:A:120:ALA:HB3	1.86	0.56
4:G:232:ASP:OD1	4:G:232:ASP:N	2.39	0.56
5:I:409:GLY:HA3	5:I:433:ASP:HB2	1.88	0.56
5:J:415:GLU:HB3	5:J:416:LYS:HG2	1.88	0.56
3:F:369:LYS:N	3:F:385:ILE:O	2.38	0.56
2:D:166:GLY:HA2	2:D:169:MET:HE2	1.88	0.56
5:I:348:THR:HG22	5:I:365:ALA:H	1.70	0.56
5:J:127:SER:O	5:J:273:ARG:NH1	2.37	0.56
1:A:266:ILE:HG12	1:A:267:LEU:HG	1.87	0.55
4:G:229:LEU:HD23	4:G:233:GLU:HB2	1.86	0.55
3:F:69:ASN:HB3	3:F:363:ASN:HD22	1.71	0.55
3:F:363:ASN:HB3	3:F:380:GLY:C	2.30	0.55
3:E:152:VAL:HG11	3:E:242:ILE:HD11	1.89	0.55
3:F:367:THR:CA	3:F:384:VAL:HG12	2.37	0.55
3:F:447:LEU:HD12	3:F:448:VAL:H	1.72	0.55
3:F:342:GLU:OE1	3:F:361:MET:CE	2.55	0.55
3:F:387:LYS:CG	3:F:404:ASP:HB3	2.36	0.55
5:J:433:ASP:CB	5:J:434:PRO:HD3	2.36	0.55
2:C:2:SER:HB3	2:C:4:ILE:HG22	1.89	0.55
3:E:260:SER:C	3:E:261:SER:HG	2.14	0.55
5:I:403:ALA:HB3	5:I:421:THR:HA	1.88	0.55
1:A:62:LEU:O	1:A:65:GLY:C	2.50	0.55
3:E:236:ASN:N	5:J:210:GLU:OE1	2.40	0.55
5:I:35:THR:HA	5:I:38:LYS:O	2.07	0.55
5:I:416:LYS:HB3	5:I:417:ASN:ND2	2.22	0.55
1:A:26:PHE:CA	1:A:29:ASP:CG	2.74	0.55
1:A:287:PRO:HG2	1:A:290:ALA:HB2	1.89	0.55
3:E:386:GLY:O	3:E:389:VAL:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLN:O	1:A:53:LYS:HE2	2.07	0.55
2:C:234:GLY:HA3	2:C:238:ASN:HB2	1.88	0.55
3:E:108:TYR:CZ	3:E:110:GLY:HA3	2.41	0.55
3:F:269:TYR:CD1	3:F:269:TYR:C	2.85	0.55
5:J:434:PRO:HD2	5:J:434:PRO:O	2.06	0.55
2:D:48:TRP:NE1	2:D:166:GLY:C	2.59	0.55
5:I:17:ALA:HA	5:I:64:GLN:HG3	1.88	0.55
3:E:352:GLU:O	3:E:353:ARG:HG3	2.08	0.54
1:A:58:PHE:CE2	1:A:94:LEU:HD21	2.43	0.54
3:F:385:ILE:CG1	3:F:402:VAL:CG2	2.83	0.54
3:F:401:VAL:O	3:F:403:GLU:N	2.40	0.54
1:A:35:MET:HE2	1:A:78:SER:HB2	1.88	0.54
3:F:366:THR:CG2	3:F:380:GLY:O	2.52	0.54
4:G:229:LEU:HD23	4:G:233:GLU:HB3	1.89	0.54
5:J:39:PRO:HG2	5:J:42:LEU:HB2	1.89	0.54
5:J:178:VAL:HB	5:J:188:HIS:HB3	1.89	0.54
5:J:418:LYS:CE	5:J:420:LEU:CD2	2.86	0.54
1:A:83:CYS:HB3	1:A:87:GLN:HE22	1.72	0.54
1:B:222:ASN:HB3	1:B:226:THR:HG21	1.90	0.54
2:C:48:TRP:H	2:C:167:MET:HE2	1.72	0.54
3:F:149:ASP:O	3:F:327:PRO:HD2	2.07	0.54
3:F:432:VAL:O	3:F:434:HIS:CD2	2.60	0.54
3:E:255:GLU:H	3:E:255:GLU:CD	2.16	0.54
3:E:269:TYR:CD1	3:E:269:TYR:C	2.85	0.54
3:F:161:ASP:OD1	4:G:134:THR:HG21	2.07	0.54
5:I:433:ASP:O	5:I:433:ASP:CG	2.48	0.54
2:D:237:ASN:ND2	2:D:354:TYR:HA	2.21	0.54
3:F:92:CYS:SG	3:F:93:MET:N	2.80	0.54
2:C:48:TRP:CD2	2:C:54:LEU:HD13	2.43	0.54
3:E:91:ILE:HG12	3:E:135:VAL:HG21	1.89	0.54
3:E:275:TYR:HD1	3:E:275:TYR:O	1.91	0.54
3:E:352:GLU:HG2	3:E:368:ILE:O	2.07	0.54
3:F:32:LEU:HD12	3:F:33:GLN:N	2.23	0.54
3:F:161:ASP:OD2	4:G:134:THR:HG23	2.07	0.54
1:B:224:ILE:HA	1:B:309:ASP:HB2	1.90	0.54
2:D:86:ILE:HG12	2:D:173:ILE:HD12	1.89	0.54
3:E:218:PHE:CD1	3:E:218:PHE:C	2.85	0.54
3:E:253:ILE:HG22	3:E:253:ILE:O	2.08	0.54
5:J:397:GLU:CG	5:J:398:ASP:H	2.14	0.54
1:A:61:ILE:HD13	1:A:63:GLN:H	1.73	0.54
1:B:54:THR:HG22	1:B:57:GLU:CD	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:ASN:O	2:C:145:GLY:N	2.30	0.54
3:F:279:PHE:CD1	3:F:279:PHE:C	2.85	0.54
5:I:187:VAL:HG12	5:I:205:ILE:HG21	1.90	0.54
3:F:53:PRO:HG2	3:F:429:GLU:HG3	1.90	0.54
3:F:169:SER:HB2	3:F:315:LYS:HZ3	1.72	0.54
3:F:193:LYS:O	3:F:211:SER:HB2	2.05	0.54
3:F:366:THR:HA	3:F:383:CYS:O	2.08	0.54
5:I:431:LEU:CG	5:I:432:ASN:N	2.67	0.54
1:A:113:LEU:HD13	1:A:116:GLN:HG3	1.90	0.53
5:I:439:ILE:CG1	5:I:441:GLY:HA3	2.37	0.53
3:F:446:ARG:HA	3:F:447:LEU:HB2	1.90	0.53
1:A:273:SER:O	1:A:275:GLU:N	2.41	0.53
1:B:312:PRO:HG2	1:B:315:PHE:CD2	2.44	0.53
3:E:355:LEU:HD22	3:E:372:SER:H	1.72	0.53
3:E:396:LEU:HB3	3:E:400:ILE:HD11	1.91	0.53
3:F:67:ILE:HA	3:F:336:ILE:HG12	1.90	0.53
3:F:353:ARG:O	3:F:354:ALA:HB3	2.07	0.53
3:F:429:GLU:HG3	3:F:445:GLU:CB	2.38	0.53
3:F:429:GLU:O	3:F:445:GLU:HA	2.09	0.53
5:I:202:ASP:O	5:I:205:ILE:HG12	2.08	0.53
3:E:414:ALA:HB3	3:E:431:GLY:C	2.33	0.53
4:G:191:THR:HB	4:G:222:ILE:HG21	1.90	0.53
5:I:205:ILE:H	5:I:205:ILE:CD1	2.15	0.53
3:E:389:VAL:HG12	3:E:406:VAL:H	1.73	0.53
3:F:204:ARG:HH11	3:F:204:ARG:HB3	1.73	0.53
3:F:425:LEU:HD12	3:F:425:LEU:N	2.22	0.53
5:I:29:TYR:O	5:I:29:TYR:CG	2.57	0.53
2:C:49:SER:CA	2:C:167:MET:HE3	2.38	0.53
3:E:149:ASP:O	3:E:327:PRO:HD2	2.08	0.53
3:E:355:LEU:HD22	3:E:372:SER:CB	2.39	0.53
1:A:60:ASP:O	1:A:61:ILE:HD12	2.08	0.53
3:F:181:GLU:H	3:F:334:LYS:CE	2.22	0.53
5:I:436:LEU:HD12	5:I:437:VAL:N	2.24	0.53
5:J:439:ILE:HG22	5:J:442:ARG:H	1.69	0.53
2:D:301:ARG:HH21	2:D:362:LEU:HA	1.74	0.53
1:A:40:ILE:HG23	1:A:86:PHE:HD2	1.73	0.52
1:A:61:ILE:CD1	1:A:62:LEU:CD1	2.85	0.52
3:E:81:GLU:CD	3:E:110:GLY:O	2.52	0.52
3:E:434:HIS:HB2	3:E:448:VAL:HG23	1.91	0.52
3:F:379:ILE:HA	3:F:396:LEU:HB2	1.91	0.52
3:F:403:GLU:HG3	3:F:404:ASP:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:419:ILE:HG22	3:F:436:VAL:CG2	2.39	0.52
3:E:182:HIS:HD2	3:E:334:LYS:CE	2.16	0.52
3:E:45:ALA:HB1	3:E:63:ALA:HB2	1.92	0.52
3:F:119:PRO:CG	3:F:122:LEU:HG	2.38	0.52
4:G:195:ASN:OD1	4:G:219:LYS:NZ	2.43	0.52
1:A:192:VAL:HG11	1:A:200:THR:HG21	1.92	0.52
3:E:261:SER:HG	3:E:264:GLY:H	1.58	0.52
3:F:413:VAL:HB	3:F:430:ILE:HD11	1.91	0.52
5:I:18:LEU:HD21	5:I:62:GLY:C	2.34	0.52
5:I:431:LEU:CG	5:I:432:ASN:H	2.19	0.52
5:J:384:LEU:HD23	5:J:384:LEU:N	2.24	0.52
1:B:257:GLN:HA	1:B:310:VAL:HB	1.90	0.52
2:C:87:ARG:NH2	2:C:390:ASP:OD1	2.43	0.52
5:I:437:VAL:CG2	5:I:438:GLY:H	2.22	0.52
5:I:437:VAL:CG2	5:I:438:GLY:N	2.73	0.52
1:A:53:LYS:NZ	1:A:104:LYS:HZ1	0.72	0.52
2:D:268:MET:HE3	2:D:271:VAL:HB	1.92	0.52
2:D:333:PRO:HD3	5:J:290:ARG:HB2	1.92	0.52
5:I:155:MET:HE2	5:I:261:ILE:HD11	1.91	0.52
1:A:55:ILE:CG1	1:A:56:SER:N	2.73	0.52
2:C:235:PHE:CE2	4:G:325:MET:HE2	2.45	0.52
3:E:269:TYR:HE1	3:E:270:LEU:HD23	1.62	0.52
3:F:429:GLU:CG	3:F:445:GLU:HB3	2.40	0.52
4:G:237:LEU:CD1	4:G:238:LEU:N	2.73	0.52
2:D:234:GLY:HA3	2:D:238:ASN:HB2	1.91	0.52
3:F:447:LEU:CG	3:F:448:VAL:N	2.72	0.52
4:G:228:ASP:OD1	4:G:228:ASP:N	2.43	0.52
5:I:435:SER:O	5:I:436:LEU:C	2.53	0.52
5:J:418:LYS:CE	5:J:420:LEU:CG	2.85	0.52
3:E:384:VAL:O	3:E:402:VAL:N	2.43	0.52
3:F:122:LEU:HD11	3:F:131:ALA:CA	2.39	0.52
3:F:162:LYS:HE3	3:F:318:ILE:HD13	1.92	0.52
1:B:245:GLU:H	1:B:248:LYS:HE3	1.75	0.51
1:B:312:PRO:HG2	1:B:315:PHE:HD2	1.75	0.51
3:E:340:THR:N	3:E:341:PRO:HD2	2.25	0.51
5:J:396:ILE:HG22	5:J:397:GLU:N	2.26	0.51
3:E:126:LYS:HD2	3:E:130:ASP:HB3	1.92	0.51
3:E:348:VAL:CG2	3:E:364:GLU:HG2	2.36	0.51
3:F:446:ARG:CB	3:F:447:LEU:CB	2.85	0.51
5:I:16:HIS:O	5:I:16:HIS:ND1	2.43	0.51
1:A:81:ALA:HB2	1:A:250:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:257:GLU:HA	3:E:259:ILE:H	1.75	0.51
4:H:168:LEU:HD21	4:H:214:ALA:HB1	1.92	0.51
2:C:136:MET:CG	2:C:137:TYR:N	2.73	0.51
3:F:32:LEU:HD12	3:F:33:GLN:H	1.75	0.51
3:F:108:TYR:OH	3:F:112:MET:HB3	2.10	0.51
5:J:418:LYS:CE	5:J:420:LEU:N	2.73	0.51
1:A:202:ASN:HB3	1:B:258:TYR:CE2	2.45	0.51
2:D:308:VAL:HG22	2:D:365:LEU:HB3	1.92	0.51
3:E:385:ILE:CG2	3:E:389:VAL:CG2	2.89	0.51
4:G:137:ILE:HG23	4:G:137:ILE:O	2.10	0.51
2:D:48:TRP:CE2	2:D:166:GLY:O	2.63	0.51
2:D:323:ASP:OD1	2:D:324:LEU:N	2.44	0.51
3:E:199:GLU:O	3:E:203:SER:N	2.43	0.51
3:F:379:ILE:HG12	3:F:396:LEU:HD12	1.92	0.51
3:E:255:GLU:HG2	3:E:256:LYS:N	2.25	0.51
3:E:434:HIS:HB2	3:E:448:VAL:N	2.25	0.51
3:F:263:ARG:O	3:F:267:ILE:HD11	2.10	0.51
3:F:378:ILE:O	3:F:396:LEU:N	2.37	0.51
5:I:107:GLY:HA2	5:I:110:LEU:HB2	1.93	0.51
3:E:428:CYS:SG	3:E:442:ALA:O	2.69	0.51
1:A:17:PHE:CD2	1:A:46:LEU:HD12	2.46	0.51
1:A:95:HIS:O	1:A:96:ASP:OD1	2.29	0.51
3:E:194:GLN:O	3:E:235:THR:HA	2.11	0.51
3:E:423:SER:OG	3:E:439:GLY:O	2.22	0.51
3:F:224:LEU:O	3:F:224:LEU:HG	2.11	0.51
4:G:410:GLU:O	4:G:411:GLU:HG3	2.10	0.51
5:J:115:SER:C	5:J:116:LYS:HD2	2.35	0.51
5:J:381:LYS:HB3	5:J:398:ASP:CA	2.39	0.51
4:H:411:GLU:H	4:H:411:GLU:CD	2.18	0.51
4:H:444:VAL:HG22	4:H:449:LEU:HG	1.93	0.51
2:C:85:LEU:HD11	2:C:176:GLY:HA3	1.92	0.50
3:E:34:SER:C	3:E:35:ILE:HG13	2.36	0.50
3:E:126:LYS:HB3	3:E:130:ASP:HB2	1.93	0.50
3:F:215:GLY:HA2	3:F:218:PHE:CZ	2.46	0.50
3:F:385:ILE:HG23	3:F:389:VAL:HG21	1.93	0.50
5:J:305:THR:HB	5:J:317:GLU:HG3	1.92	0.50
2:C:49:SER:HA	2:C:167:MET:HE3	1.93	0.50
3:F:35:ILE:HG22	4:G:142:HIS:HA	1.92	0.50
3:F:195:LEU:O	3:F:196:ILE:HD13	2.11	0.50
3:F:387:LYS:CB	3:F:404:ASP:HB3	2.40	0.50
5:I:435:SER:OG	5:I:436:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:169:SER:HB2	3:F:315:LYS:NZ	2.27	0.50
3:F:202:THR:CB	3:F:204:ARG:HG2	2.41	0.50
1:B:125:ILE:HG21	1:B:243:VAL:HG13	1.93	0.50
2:C:87:ARG:HH22	2:C:390:ASP:CG	2.19	0.50
2:D:199:LEU:HD11	2:D:218:LEU:HD23	1.94	0.50
3:F:446:ARG:HG2	3:F:447:LEU:CD2	2.42	0.50
5:J:439:ILE:HG21	5:J:442:ARG:N	2.26	0.50
1:A:29:ASP:OD1	1:A:30:ASP:N	2.45	0.50
2:C:313:ILE:HG21	2:C:370:LEU:HD22	1.92	0.50
3:E:37:ILE:O	3:E:37:ILE:HG13	2.11	0.50
3:F:386:GLY:O	3:F:404:ASP:HA	2.11	0.50
5:J:328:LYS:HD3	5:J:346:ALA:HB2	1.94	0.50
1:B:67:ASN:O	1:B:71:GLU:HG3	2.12	0.50
3:E:130:ASP:HA	3:E:133:ARG:NH2	2.26	0.50
4:G:228:ASP:HB2	4:G:229:LEU:HD12	1.77	0.50
5:J:116:LYS:HD2	5:J:116:LYS:N	2.27	0.50
1:B:134:ARG:NH1	2:C:323:ASP:OD2	2.45	0.50
3:F:419:ILE:HG22	3:F:436:VAL:HG23	1.94	0.50
1:A:63:GLN:O	1:A:67:ASN:CB	2.59	0.50
3:E:218:PHE:C	3:E:218:PHE:HD1	2.20	0.50
3:F:218:PHE:HE2	5:I:203:PRO:HB3	0.78	0.50
3:F:251:ASP:O	3:F:255:GLU:HG3	2.11	0.50
1:A:18:ASP:CG	1:A:21:GLN:CG	2.85	0.49
2:C:287:LEU:HD11	2:C:309:VAL:HG21	1.94	0.49
4:H:271:ILE:HG21	4:H:284:LEU:HD21	1.93	0.49
5:J:133:ASN:OD1	5:J:269:ASN:HB3	2.11	0.49
3:E:276:GLN:NE2	3:E:276:GLN:N	2.60	0.49
5:I:27:TYR:C	5:I:28:ASN:O	2.51	0.49
2:C:136:MET:HG2	2:C:137:TYR:N	2.27	0.49
3:E:271:VAL:O	3:E:272:LYS:HD3	2.12	0.49
3:E:437:GLU:N	3:E:437:GLU:OE1	2.45	0.49
4:H:406:VAL:HG13	4:H:406:VAL:O	2.10	0.49
5:I:140:LEU:O	5:I:144:ARG:HG3	2.12	0.49
5:J:147:ARG:NH1	5:J:153:ALA:O	2.44	0.49
2:C:49:SER:N	2:C:167:MET:HE3	2.27	0.49
2:D:167:MET:HG3	2:D:168:ASP:N	2.28	0.49
3:F:280:THR:OG1	3:F:281:VAL:N	2.45	0.49
5:J:414:ILE:O	5:J:415:GLU:HG2	2.12	0.49
1:A:28:GLN:CD	1:A:28:GLN:N	2.71	0.49
1:A:96:ASP:O	1:A:97:VAL:HG22	2.12	0.49
1:A:115:ILE:O	1:A:119:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:262:ILE:HA	3:E:265:ASP:HB3	1.94	0.49
3:F:318:ILE:C	3:F:319:ILE:HG13	2.38	0.49
1:A:257:GLN:HA	1:A:310:VAL:HB	1.95	0.49
2:D:51:VAL:HG13	2:D:52:ASP:N	2.28	0.49
3:E:255:GLU:N	3:E:255:GLU:CD	2.71	0.49
3:F:61:PRO:HD2	3:F:64:LEU:HD12	1.95	0.49
5:J:418:LYS:HZ2	5:J:419:ARG:C	2.21	0.49
3:E:352:GLU:CG	3:E:369:LYS:HA	2.43	0.49
3:E:421:ALA:HB1	3:E:438:ALA:HB2	1.93	0.49
3:F:367:THR:HB	3:F:384:VAL:CG1	2.36	0.49
3:E:384:VAL:HB	3:E:401:VAL:HG13	1.94	0.49
3:F:169:SER:CB	3:F:315:LYS:HZ3	2.25	0.49
3:F:400:ILE:HD13	3:F:413:VAL:HG23	1.95	0.49
5:I:202:ASP:OD1	5:I:202:ASP:N	2.40	0.49
5:J:293:TYR:CG	5:J:294:PRO:HA	2.48	0.49
5:J:418:LYS:C	5:J:418:LYS:CD	2.85	0.49
2:C:12:ALA:HB1	2:C:38:VAL:HG22	1.94	0.49
2:D:85:LEU:HD21	2:D:176:GLY:HA3	1.95	0.49
2:D:169:MET:O	2:D:173:ILE:HG12	2.12	0.49
3:E:400:ILE:HG22	3:E:417:ALA:H	1.77	0.49
3:F:275:TYR:HD1	3:F:275:TYR:O	1.96	0.49
1:A:59:MET:C	1:A:61:ILE:CD1	2.86	0.48
1:A:66:SER:OG	1:A:83:CYS:SG	2.67	0.48
1:A:104:LYS:O	1:A:108:VAL:HG23	2.13	0.48
2:C:48:TRP:CH2	2:C:170:ARG:HG2	2.44	0.48
3:E:260:SER:O	3:E:264:GLY:CA	2.61	0.48
3:E:269:TYR:HD1	3:E:270:LEU:N	2.03	0.48
3:F:58:ASP:O	3:F:99:HIS:NE2	2.46	0.48
3:F:385:ILE:CD1	3:F:402:VAL:HG21	2.43	0.48
4:H:406:VAL:O	4:H:406:VAL:HG22	2.13	0.48
5:I:431:LEU:HD23	5:I:432:ASN:CA	2.43	0.48
1:A:39:ALA:O	1:A:43:LEU:HG	2.13	0.48
3:F:182:HIS:ND1	3:F:183:ILE:N	2.60	0.48
5:I:33:PRO:HG2	5:I:419:ARG:CG	2.26	0.48
5:J:194:ARG:HD3	5:J:195:GLY:N	2.28	0.48
5:J:418:LYS:C	5:J:418:LYS:HD2	2.39	0.48
3:E:218:PHE:HD1	3:E:219:THR:N	2.11	0.48
5:J:418:LYS:CE	5:J:419:ARG:C	2.85	0.48
1:A:112:LYS:O	1:A:116:GLN:HG2	2.14	0.48
1:B:106:HIS:CD2	2:C:146:ARG:HD3	2.48	0.48
3:E:252:LEU:HD12	3:E:256:LYS:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:269:TYR:HD1	3:F:271:VAL:HG13	1.79	0.48
1:B:77:ILE:HG21	1:B:221:ILE:HD12	1.95	0.48
3:E:352:GLU:C	3:E:354:ALA:H	2.20	0.48
3:F:71:PRO:HG2	3:F:103:TRP:CE2	2.49	0.48
3:F:321:SER:O	3:F:321:SER:OG	2.28	0.48
3:F:368:ILE:HA	3:F:385:ILE:H	1.78	0.48
4:G:121:SER:HB3	4:G:124:SER:HB3	1.94	0.48
4:G:210:SER:HB3	4:G:380:LYS:HG2	1.96	0.48
1:A:59:MET:C	1:A:61:ILE:CG1	2.85	0.48
1:A:230:ALA:HB1	1:A:315:PHE:HB3	1.96	0.48
1:B:94:LEU:HA	1:B:98:GLY:HA2	1.95	0.48
3:E:149:ASP:O	3:E:327:PRO:CD	2.61	0.48
3:E:149:ASP:CB	3:E:327:PRO:HD2	2.25	0.48
3:F:199:GLU:CD	3:F:202:THR:HG1	2.07	0.48
4:G:286:HIS:O	4:G:290:VAL:HG23	2.13	0.48
1:A:61:ILE:CD1	1:A:62:LEU:N	2.73	0.48
2:C:87:ARG:HH11	2:C:87:ARG:CG	2.12	0.48
4:G:416:LEU:HD13	4:G:427:LEU:HD11	1.96	0.48
4:H:312:LYS:NZ	4:H:316:GLU:OE2	2.44	0.48
5:I:327:ILE:HG22	5:I:345:VAL:HB	1.96	0.48
1:A:17:PHE:HE2	1:A:46:LEU:HB2	1.79	0.48
3:E:130:ASP:HA	3:E:133:ARG:NH1	2.28	0.48
3:E:349:THR:OG1	3:E:350:VAL:N	2.47	0.48
1:A:106:HIS:ND1	1:A:110:ASN:OD1	2.45	0.48
3:E:441:ILE:HG13	3:E:443:ARG:NH2	2.28	0.48
3:E:149:ASP:HB2	3:E:327:PRO:CD	2.26	0.48
3:F:383:CYS:CB	3:F:400:ILE:O	2.62	0.48
4:G:240:GLU:OE1	4:G:240:GLU:N	2.47	0.48
5:J:21:ILE:HG12	5:J:113:LEU:HD11	1.94	0.48
5:J:426:HIS:ND1	5:J:426:HIS:C	2.72	0.48
2:D:388:ALA:HA	2:D:391:THR:HG23	1.96	0.47
3:E:269:TYR:CE1	3:E:270:LEU:CD2	2.80	0.47
3:F:340:THR:N	3:F:341:PRO:HD3	2.29	0.47
1:A:46:LEU:C	1:A:50:SER:HG	2.04	0.47
1:A:59:MET:HA	1:A:61:ILE:CG1	2.43	0.47
3:E:276:GLN:O	3:E:277:LYS:CD	2.58	0.47
3:E:379:ILE:HA	3:E:396:LEU:HB2	1.96	0.47
3:F:269:TYR:CD1	3:F:271:VAL:HG13	2.49	0.47
5:J:169:ARG:NH2	5:J:216:ASN:OD1	2.47	0.47
1:A:89:PHE:HE2	1:A:107:LEU:HD21	1.79	0.47
1:B:28:GLN:CD	1:B:28:GLN:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:LEU:O	2:C:87:ARG:HG3	2.14	0.47
3:F:241:HIS:HB2	3:F:326:LEU:HD21	1.95	0.47
3:F:419:ILE:CB	3:F:436:VAL:HB	2.43	0.47
4:G:308:ARG:NH2	4:G:406:VAL:O	2.47	0.47
5:J:29:TYR:CE2	5:J:30:ARG:CD	2.97	0.47
1:A:54:THR:H	1:A:57:GLU:HB3	1.80	0.47
2:C:199:LEU:HD11	2:C:218:LEU:HD23	1.95	0.47
3:E:260:SER:O	3:E:261:SER:OG	2.27	0.47
3:E:370:ASP:N	3:E:370:ASP:OD1	2.36	0.47
1:A:130:TYR:HB2	1:A:155:ALA:HB2	1.95	0.47
2:C:3:THR:O	2:C:6:VAL:HG12	2.14	0.47
2:C:4:ILE:O	2:C:7:GLU:HB2	2.15	0.47
2:C:7:GLU:OE2	5:I:90:SER:OG	2.24	0.47
2:C:169:MET:O	2:C:173:ILE:HG12	2.14	0.47
5:I:416:LYS:C	5:I:417:ASN:ND2	2.73	0.47
1:A:316:VAL:HB	1:A:329:LYS:HE3	1.96	0.47
2:D:233:GLU:OE1	4:H:302:ARG:HD3	2.15	0.47
3:E:230:ARG:NH2	5:J:213:GLU:OE2	2.41	0.47
3:F:182:HIS:ND1	3:F:183:ILE:C	2.73	0.47
3:F:440:ARG:O	3:F:441:ILE:HG13	2.14	0.47
5:I:421:THR:OG1	5:I:422:THR:N	2.47	0.47
3:E:218:PHE:O	5:J:200:SER:HA	2.14	0.47
3:E:245:PHE:HB3	3:E:249:VAL:HG21	1.97	0.47
3:E:256:LYS:O	3:E:259:ILE:HG12	2.15	0.47
3:E:346:VAL:HG13	3:E:348:VAL:HG22	1.97	0.47
3:F:243:PHE:CE2	3:F:262:ILE:HG21	2.49	0.47
3:F:336:ILE:HD12	3:F:395:ILE:CD1	2.35	0.47
3:F:447:LEU:C	3:F:448:VAL:HG23	2.36	0.47
4:H:117:GLU:C	4:H:119:GLN:NE2	2.73	0.47
4:H:220:LEU:O	4:H:224:VAL:HG23	2.15	0.47
5:I:27:TYR:O	5:I:28:ASN:C	2.58	0.47
5:I:178:VAL:HB	5:I:188:HIS:HB3	1.96	0.47
1:A:53:LYS:N	1:A:53:LYS:CD	2.73	0.47
3:F:329:TYR:HB2	3:F:331:GLU:HG3	1.95	0.47
1:A:249:PHE:HB2	2:D:140:MET:HE1	1.97	0.47
3:F:399:ASN:HB2	3:F:416:GLY:H	1.80	0.47
1:A:100:PHE:N	1:A:100:PHE:CD1	2.78	0.47
1:B:125:ILE:HG23	1:B:320:ILE:HG22	1.96	0.47
3:E:218:PHE:CD1	3:E:219:THR:N	2.83	0.47
3:E:241:HIS:HA	3:E:243:PHE:CE2	2.50	0.47
3:E:352:GLU:HG3	3:E:369:LYS:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:413:VAL:HG12	3:F:430:ILE:HG12	1.97	0.47
4:G:274:TYR:CD1	4:G:275:LEU:HG	2.49	0.47
5:J:418:LYS:NZ	5:J:419:ARG:C	2.72	0.47
2:D:349:GLU:OE2	5:J:311:HIS:HA	2.15	0.46
3:E:274:GLN:N	3:E:274:GLN:CD	2.72	0.46
3:E:355:LEU:CD2	3:E:372:SER:H	2.27	0.46
3:F:124:ASP:C	3:F:126:LYS:H	2.21	0.46
3:F:155:PRO:HA	3:F:156:PRO:HD3	1.80	0.46
3:F:206:LEU:HB3	3:F:224:LEU:HD11	1.98	0.46
3:F:235:THR:HG21	5:I:206:PHE:HB3	1.97	0.46
5:I:30:ARG:NH2	6:I:701:PO4:O3	2.48	0.46
5:I:332:LEU:HD22	5:I:349:ILE:HG23	1.97	0.46
3:E:260:SER:O	3:E:264:GLY:HA3	2.16	0.46
3:F:267:ILE:O	3:F:270:LEU:HD21	2.14	0.46
2:C:167:MET:CG	2:C:168:ASP:N	2.67	0.46
3:E:274:GLN:C	3:E:276:GLN:NE2	2.73	0.46
3:F:344:ARG:H	3:F:344:ARG:HG3	1.43	0.46
4:G:175:ILE:HG12	4:G:190:LEU:HD11	1.98	0.46
1:A:47:LEU:C	1:A:50:SER:OG	2.58	0.46
1:A:114:PHE:CE1	2:D:144:LEU:HA	2.50	0.46
3:E:128:SER:N	3:E:261:SER:HA	2.30	0.46
3:F:224:LEU:HD12	3:F:272:LYS:HD2	1.97	0.46
5:I:439:ILE:CD1	5:I:440:GLY:N	2.57	0.46
1:A:19:ILE:HD12	1:A:46:LEU:HD13	1.97	0.46
2:C:313:ILE:HG12	2:C:370:LEU:HD13	1.96	0.46
3:E:397:MET:HG3	3:E:413:VAL:O	2.16	0.46
3:F:388:GLY:C	3:F:405:GLY:HA2	2.40	0.46
1:A:61:ILE:HD13	1:A:62:LEU:CG	2.46	0.46
3:E:320:CYS:SG	3:E:322:ARG:N	2.89	0.46
3:F:127:SER:CB	3:F:261:SER:HB2	2.43	0.46
4:G:218:LEU:O	4:G:222:ILE:HG12	2.16	0.46
4:H:416:LEU:HD22	4:H:425:LEU:HD21	1.98	0.46
5:I:16:HIS:ND1	5:I:16:HIS:C	2.74	0.46
3:E:369:LYS:N	3:E:385:ILE:O	2.34	0.46
4:G:240:GLU:O	4:G:244:SER:OG	2.20	0.46
4:G:403:ASN:ND2	4:G:403:ASN:C	2.73	0.46
5:J:19:GLN:OE1	5:J:119:ILE:HA	2.15	0.46
1:A:92:ARG:CZ	2:D:137:TYR:HD2	2.29	0.46
2:C:162:ARG:HA	2:C:162:ARG:HE	1.74	0.46
2:C:268:MET:HE3	2:C:271:VAL:HB	1.98	0.46
3:E:257:GLU:HG3	3:E:259:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:362:VAL:O	3:E:362:VAL:HG13	2.15	0.46
3:F:193:LYS:C	3:F:211:SER:CB	2.89	0.46
3:F:341:PRO:C	3:F:342:GLU:CG	2.86	0.46
2:C:63:SER:OG	2:C:67:LYS:NZ	2.48	0.46
3:F:241:HIS:HA	3:F:243:PHE:CZ	2.51	0.46
3:F:274:GLN:O	3:F:275:TYR:CG	2.69	0.46
3:F:382:ASN:ND2	3:F:399:ASN:OD1	2.45	0.46
4:H:411:GLU:N	4:H:411:GLU:CD	2.73	0.46
5:I:436:LEU:C	5:I:436:LEU:CD1	2.85	0.46
1:B:187:ILE:HD12	1:B:187:ILE:HA	1.88	0.45
3:E:34:SER:O	3:E:35:ILE:HG13	2.16	0.45
3:F:205:LEU:C	3:F:206:LEU:HD12	2.41	0.45
3:F:381:LYS:O	3:F:382:ASN:HB2	2.16	0.45
4:G:240:GLU:CD	4:G:241:LYS:HG2	2.41	0.45
1:A:125:ILE:HG21	1:A:243:VAL:HG13	1.98	0.45
2:C:48:TRP:CD1	2:C:48:TRP:O	2.69	0.45
3:E:364:GLU:C	3:E:366:THR:H	2.23	0.45
4:H:386:GLN:CD	4:H:392:TYR:HB2	2.41	0.45
5:J:33:PRO:HG2	5:J:419:ARG:CB	2.46	0.45
3:E:346:VAL:CG1	3:E:348:VAL:HG22	2.46	0.45
3:F:164:ARG:NH1	4:G:134:THR:HG21	2.31	0.45
5:I:416:LYS:CB	5:I:417:ASN:ND2	2.79	0.45
1:A:18:ASP:CG	1:A:21:GLN:HG3	2.41	0.45
1:A:66:SER:O	1:A:70:LYS:N	2.39	0.45
1:A:202:ASN:HB3	1:B:258:TYR:CZ	2.51	0.45
3:E:266:LEU:C	3:E:266:LEU:HD23	2.41	0.45
3:E:274:GLN:HB3	3:E:276:GLN:CD	2.41	0.45
5:I:418:LYS:HD2	5:I:418:LYS:HA	1.90	0.45
1:A:22:VAL:O	1:A:25:LYS:N	2.50	0.45
1:A:192:VAL:HA	1:B:305:ASN:HD21	1.82	0.45
2:C:180:VAL:HA	2:C:183:GLU:HG3	1.99	0.45
3:E:181:GLU:OE1	3:E:182:HIS:CG	2.69	0.45
3:E:448:VAL:HG12	3:E:449:ASP:N	2.31	0.45
3:F:122:LEU:HD13	3:F:131:ALA:CB	2.46	0.45
3:F:125:SER:O	3:F:126:LYS:HG2	2.17	0.45
5:I:401:ILE:HB	5:I:419:ARG:HG3	1.97	0.45
5:J:402:VAL:HG22	5:J:420:LEU:HD12	1.97	0.45
2:C:162:ARG:NE	2:C:162:ARG:CA	2.75	0.45
2:C:247:LYS:NZ	2:C:251:GLN:OE1	2.45	0.45
4:H:409:PHE:O	4:H:409:PHE:CD1	2.70	0.45
5:I:419:ARG:C	5:I:420:LEU:HD23	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:146:ARG:HD2	5:J:262:HIS:CE1	2.51	0.45
5:J:309:GLN:HB2	5:J:313:ILE:HG13	1.99	0.45
5:J:339:VAL:HA	5:J:356:ILE:HB	1.98	0.45
1:B:220:LEU:HB2	1:B:311:THR:HB	1.97	0.45
2:D:80:ARG:NH1	2:D:391:THR:O	2.50	0.45
3:E:35:ILE:HD11	4:H:140:ASP:HA	1.97	0.45
3:E:133:ARG:CZ	3:E:257:GLU:CD	2.90	0.45
3:E:192:ALA:HB3	3:E:329:TYR:OH	2.17	0.45
3:F:71:PRO:HG2	3:F:103:TRP:NE1	2.32	0.45
3:F:178:LEU:HD23	3:F:178:LEU:HA	1.79	0.45
4:G:240:GLU:HG2	4:G:241:LYS:HG2	1.99	0.45
4:G:436:PRO:HA	4:G:437:PRO:HD3	1.86	0.45
1:A:117:ARG:O	1:A:118:ALA:C	2.60	0.45
3:E:71:PRO:HG2	3:E:103:TRP:NE1	2.32	0.45
3:E:275:TYR:C	3:E:275:TYR:CD1	2.95	0.45
3:E:366:THR:HG23	3:E:383:CYS:HB2	1.99	0.45
3:F:275:TYR:O	3:F:275:TYR:CD1	2.70	0.45
4:G:408:ASP:O	4:G:409:PHE:CG	2.70	0.45
5:I:439:ILE:HG13	5:I:441:GLY:CA	2.44	0.45
1:A:19:ILE:HG23	1:A:20:VAL:N	2.32	0.44
1:A:36:PRO:HG2	1:A:247:HIS:HD2	1.82	0.44
3:E:434:HIS:HA	3:E:448:VAL:HG23	1.99	0.44
3:F:181:GLU:CG	3:F:182:HIS:N	2.79	0.44
3:F:259:ILE:HD12	3:F:259:ILE:O	2.17	0.44
3:F:332:LEU:O	3:F:336:ILE:HG13	2.17	0.44
4:G:274:TYR:CE1	4:G:275:LEU:HG	2.53	0.44
4:G:408:ASP:O	4:G:409:PHE:CD2	2.70	0.44
5:J:23:LEU:HD21	5:J:106:VAL:HA	1.99	0.44
3:E:155:PRO:HA	3:E:156:PRO:HD3	1.76	0.44
3:E:262:ILE:O	3:E:262:ILE:HG22	2.16	0.44
3:E:273:CYS:O	3:E:275:TYR:CD2	2.70	0.44
3:E:275:TYR:O	3:E:275:TYR:CD1	2.70	0.44
3:F:181:GLU:HG3	3:F:182:HIS:N	2.32	0.44
4:G:257:ILE:HG23	4:G:444:VAL:HG12	2.00	0.44
4:G:348:SER:OG	4:G:382:THR:O	2.31	0.44
4:G:409:PHE:O	4:G:409:PHE:CD1	2.70	0.44
4:H:221:GLU:OE1	4:H:241:LYS:NZ	2.40	0.44
4:H:277:SER:OG	4:H:342:GLY:HA3	2.17	0.44
5:I:24:SER:O	5:I:25:ASP:CB	2.63	0.44
5:J:418:LYS:NZ	5:J:420:LEU:CA	2.73	0.44
2:C:17:ILE:HG22	2:C:21:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:181:GLU:OE1	3:E:182:HIS:CE1	2.70	0.44
3:E:229:PRO:HB2	5:J:217:ASP:HB3	1.99	0.44
3:E:402:VAL:HA	3:E:419:ILE:HG13	1.99	0.44
3:F:381:LYS:N	3:F:398:ASP:OD1	2.51	0.44
4:H:115:PHE:CE1	4:H:117:GLU:O	2.71	0.44
5:J:430:THR:O	5:J:435:SER:OG	2.32	0.44
1:B:35:MET:HE2	1:B:78:SER:HB2	1.99	0.44
2:C:8:HIS:CD2	5:I:89:PRO:HG3	2.53	0.44
2:D:87:ARG:NH1	2:D:390:ASP:OD2	2.38	0.44
3:E:139:ILE:HB	3:E:250:ILE:HD13	1.98	0.44
3:F:92:CYS:SG	3:F:100:ILE:HD12	2.57	0.44
1:B:88:ARG:HH22	1:B:341:LEU:HD12	1.82	0.44
2:C:47:ARG:HB2	2:C:170:ARG:NH2	2.33	0.44
3:E:35:ILE:HG23	4:H:143:PRO:HD3	1.98	0.44
3:E:360:CYS:HB2	3:E:377:SER:O	2.18	0.44
3:F:182:HIS:CE1	3:F:183:ILE:O	2.71	0.44
3:F:214:VAL:CG2	3:F:218:PHE:CD1	3.01	0.44
3:F:267:ILE:N	3:F:268:PRO:CD	2.81	0.44
3:F:333:ASN:HB2	3:F:412:ILE:HD11	1.99	0.44
3:F:339:LEU:HD22	3:F:339:LEU:HA	1.76	0.44
4:G:354:SER:OG	4:G:355:ARG:N	2.50	0.44
2:C:93:LEU:O	2:C:96:THR:HG23	2.17	0.44
3:E:274:GLN:O	3:E:275:TYR:CD1	2.70	0.44
3:F:183:ILE:N	3:F:183:ILE:CD1	2.81	0.44
3:F:397:MET:HB3	3:F:415:SER:OG	2.17	0.44
4:G:408:ASP:OD1	4:G:409:PHE:CD2	2.71	0.44
1:A:58:PHE:O	1:A:58:PHE:CD1	2.70	0.44
1:B:33:ILE:O	1:B:146:ARG:NH1	2.46	0.44
2:D:256:THR:N	4:H:424:ASN:O	2.49	0.44
3:E:434:HIS:CG	3:E:435:ARG:N	2.86	0.44
3:E:434:HIS:CD2	3:E:447:LEU:HA	2.52	0.44
3:F:122:LEU:CD1	3:F:131:ALA:HB2	2.48	0.44
3:F:274:GLN:O	3:F:275:TYR:CD2	2.70	0.44
4:G:408:ASP:OD1	4:G:409:PHE:CE2	2.70	0.44
1:A:17:PHE:O	1:A:17:PHE:CD1	2.70	0.44
1:A:130:TYR:CD2	1:A:131:PRO:HD3	2.52	0.44
1:B:25:LYS:HA	1:B:28:GLN:HE22	1.81	0.44
1:B:106:HIS:ND1	1:B:106:HIS:C	2.73	0.44
3:E:181:GLU:OE1	3:E:182:HIS:CD2	2.70	0.44
3:E:261:SER:C	3:E:263:ARG:H	2.26	0.44
3:E:396:LEU:HD23	3:E:413:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:385:ALA:HB3	5:J:403:ALA:HA	2.00	0.44
1:A:52:ALA:C	1:A:53:LYS:CG	2.90	0.44
1:A:59:MET:O	1:A:61:ILE:HD11	2.17	0.44
2:D:184:LEU:O	2:D:187:ILE:HG12	2.18	0.44
2:D:331:SER:OG	2:D:332:SER:N	2.51	0.44
3:E:181:GLU:OE2	3:E:182:HIS:CE1	2.70	0.44
3:E:245:PHE:CD1	3:E:249:VAL:HG11	2.52	0.44
3:E:276:GLN:NE2	3:E:276:GLN:H	2.15	0.44
3:F:383:CYS:HB2	3:F:400:ILE:O	2.18	0.44
4:G:208:SER:HB2	4:G:344:HIS:NE2	2.33	0.44
3:F:47:PHE:CE2	3:F:93:MET:HE2	2.52	0.43
3:F:354:ALA:CB	3:F:370:ASP:OD1	2.56	0.43
4:H:329:LEU:HD21	4:H:361:ILE:HA	2.00	0.43
5:I:18:LEU:HD23	5:I:62:GLY:O	2.15	0.43
5:J:322:ALA:O	5:J:325:CYS:HB3	2.18	0.43
1:A:52:ALA:CA	1:A:57:GLU:OE1	2.65	0.43
2:C:313:ILE:H	2:C:313:ILE:HG13	1.60	0.43
3:F:204:ARG:HB3	3:F:204:ARG:NH1	2.33	0.43
4:G:258:VAL:HA	4:G:283:VAL:HG22	2.00	0.43
3:F:214:VAL:HG23	3:F:218:PHE:HD1	1.81	0.43
3:F:315:LYS:HD2	3:F:315:LYS:N	2.33	0.43
3:F:355:LEU:C	3:F:355:LEU:HD12	2.43	0.43
3:F:434:HIS:CG	3:F:447:LEU:O	2.71	0.43
4:G:186:LEU:HD11	4:G:190:LEU:HD22	2.01	0.43
5:J:366:PHE:N	5:J:382:ALA:O	2.45	0.43
2:D:289:THR:OG1	2:D:290:TYR:N	2.52	0.43
3:F:51:LEU:HD22	3:F:54:LEU:HD12	2.00	0.43
3:F:314:ALA:N	3:F:315:LYS:HZ2	2.17	0.43
3:F:446:ARG:CA	3:F:447:LEU:CB	2.93	0.43
4:H:411:GLU:O	4:H:412:LYS:CG	2.66	0.43
5:I:178:VAL:HG22	5:I:214:VAL:HG22	2.00	0.43
2:C:48:TRP:CE2	2:C:54:LEU:HD22	2.53	0.43
2:C:89:GLU:C	2:C:89:GLU:CD	2.85	0.43
2:C:136:MET:CG	2:C:137:TYR:H	2.28	0.43
3:E:260:SER:O	3:E:264:GLY:N	2.51	0.43
3:E:276:GLN:CD	3:E:276:GLN:N	2.73	0.43
4:G:238:LEU:C	4:G:240:GLU:CD	2.85	0.43
1:B:54:THR:O	1:B:57:GLU:HG2	2.18	0.43
3:E:327:PRO:O	3:E:327:PRO:HG2	2.19	0.43
3:F:269:TYR:CD1	3:F:270:LEU:CA	2.96	0.43
5:I:203:PRO:O	5:I:205:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:267:LYS:C	5:I:268:GLU:HG3	2.42	0.43
5:J:362:ILE:HA	5:J:379:ILE:O	2.18	0.43
1:B:134:ARG:HD3	1:B:134:ARG:HA	1.69	0.43
3:E:355:LEU:CD1	3:E:368:ILE:HG13	2.44	0.43
3:F:88:ALA:HB2	3:F:112:MET:HE2	2.00	0.43
5:I:242:ASP:O	5:I:246:ASP:HB2	2.19	0.43
5:J:29:TYR:CE2	5:J:30:ARG:HD3	2.54	0.43
1:A:113:LEU:HD12	1:A:116:GLN:HG3	2.01	0.43
3:E:274:GLN:CB	3:E:276:GLN:NE2	2.73	0.43
3:F:93:MET:HB3	3:F:93:MET:HE3	1.67	0.43
3:F:199:GLU:C	3:F:200:GLU:O	2.57	0.43
1:A:105:ARG:O	1:A:109:GLU:HG3	2.18	0.43
1:B:139:ILE:HD12	1:B:206:LEU:HD22	2.00	0.43
2:D:318:PRO:N	2:D:382:MET:HE1	2.33	0.43
3:E:355:LEU:CB	3:E:372:SER:O	2.56	0.43
3:E:375:LYS:O	3:E:392:SER:HA	2.18	0.43
3:F:213:ASP:OD1	3:F:214:VAL:HG22	2.19	0.43
3:F:247:HIS:O	3:F:250:ILE:HG22	2.19	0.43
4:H:348:SER:OG	4:H:383:GLU:HA	2.18	0.43
5:J:178:VAL:HG22	5:J:214:VAL:HG13	1.99	0.43
1:A:54:THR:O	1:A:57:GLU:N	2.51	0.43
1:A:60:ASP:N	1:A:61:ILE:HG13	2.34	0.43
1:A:77:ILE:HG21	1:A:221:ILE:HD12	2.01	0.43
2:C:140:MET:HB3	2:C:140:MET:HE2	1.65	0.43
3:E:67:ILE:HA	3:E:336:ILE:HG12	2.01	0.43
3:F:101:ASN:O	3:F:105:ARG:HG2	2.18	0.43
3:F:155:PRO:O	3:F:158:THR:OG1	2.36	0.43
2:C:233:GLU:OE2	4:G:302:ARG:HD3	2.19	0.42
3:F:262:ILE:HA	3:F:265:ASP:HB3	2.01	0.42
3:F:339:LEU:C	3:F:341:PRO:HD3	2.43	0.42
5:J:209:HIS:HB3	5:J:212:LEU:HD21	2.01	0.42
5:J:423:PHE:HB3	5:J:424:GLU:H	1.58	0.42
1:B:130:TYR:CD2	1:B:131:PRO:HD3	2.54	0.42
2:D:187:ILE:HG13	2:D:188:ASN:H	1.84	0.42
3:E:143:PHE:CE1	3:E:250:ILE:HG23	2.54	0.42
3:F:401:VAL:HG22	3:F:418:GLN:HA	2.01	0.42
5:J:50:LEU:HD22	5:J:274:VAL:HG21	2.00	0.42
5:J:121:SER:OG	5:J:122:ASP:N	2.50	0.42
5:J:400:ALA:O	5:J:401:ILE:CG1	2.62	0.42
5:J:414:ILE:HG22	5:J:415:GLU:N	2.34	0.42
2:D:177:ILE:O	2:D:181:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:ASN:HD21	2:D:354:TYR:HA	1.84	0.42
3:E:31:GLN:HB3	3:E:33:GLN:OE1	2.19	0.42
3:E:334:LYS:HA	3:E:334:LYS:HD2	1.88	0.42
3:F:368:ILE:HG22	3:F:385:ILE:CB	2.46	0.42
3:F:429:GLU:HG3	3:F:445:GLU:HB3	1.98	0.42
5:J:116:LYS:HB2	5:J:118:LEU:HG	2.02	0.42
1:A:258:TYR:CE2	1:B:202:ASN:HB3	2.54	0.42
3:E:257:GLU:HA	3:E:259:ILE:HG12	2.01	0.42
3:E:381:LYS:O	3:E:399:ASN:N	2.41	0.42
3:E:389:VAL:HG12	3:E:405:GLY:CA	2.49	0.42
3:F:55:THR:HG21	3:F:62:LYS:HB2	2.00	0.42
3:F:351:SER:OG	3:F:355:LEU:HD13	2.14	0.42
3:F:385:ILE:HD11	3:F:402:VAL:HG21	2.00	0.42
3:F:425:LEU:N	3:F:425:LEU:CD1	2.83	0.42
4:G:419:TRP:CZ2	4:G:420:LYS:HD3	2.54	0.42
5:J:35:THR:HA	5:J:38:LYS:O	2.19	0.42
1:B:21:GLN:O	1:B:25:LYS:HB2	2.20	0.42
2:D:393:LEU:HD12	2:D:393:LEU:HA	1.88	0.42
3:F:205:LEU:HD21	3:F:208:ALA:HB2	2.01	0.42
5:I:53:TYR:CG	5:I:131:VAL:HG12	2.55	0.42
3:F:382:ASN:HB2	3:F:399:ASN:H	1.84	0.42
3:F:387:LYS:HB2	3:F:404:ASP:CB	2.45	0.42
4:G:135:GLU:O	4:G:136:ASN:HB2	2.20	0.42
4:G:241:LYS:HA	4:G:244:SER:CB	2.42	0.42
5:I:197:HIS:C	5:I:198:TYR:HD1	2.28	0.42
5:J:116:LYS:HE3	5:J:116:LYS:HA	2.02	0.42
5:J:304:GLN:OE1	5:J:304:GLN:N	2.50	0.42
5:J:386:ASN:ND2	5:J:386:ASN:N	2.60	0.42
1:B:257:GLN:H	1:B:257:GLN:HG3	1.58	0.42
2:C:53:GLN:OE1	2:C:53:GLN:N	2.53	0.42
3:E:271:VAL:C	3:E:272:LYS:HG2	2.45	0.42
3:E:272:LYS:O	3:E:273:CYS:HB2	2.20	0.42
3:E:384:VAL:HB	3:E:401:VAL:HG22	2.01	0.42
5:J:134:VAL:HG23	5:J:270:TYR:O	2.19	0.42
1:A:22:VAL:HA	1:A:25:LYS:HG3	2.02	0.42
1:A:53:LYS:NZ	1:A:104:LYS:HZ2	0.94	0.42
2:D:212:LYS:N	6:D:401:PO4:O4	2.53	0.42
3:E:36:PRO:HD2	4:H:143:PRO:HG2	2.02	0.42
3:E:365:GLY:C	3:E:382:ASN:HA	2.44	0.42
3:E:442:ALA:O	3:E:444:GLY:N	2.53	0.42
3:F:147:SER:HB2	3:F:241:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:193:LYS:C	3:F:211:SER:HB3	2.40	0.42
3:F:385:ILE:CG1	3:F:402:VAL:HG21	2.46	0.42
5:J:33:PRO:HG2	5:J:419:ARG:CG	2.49	0.42
5:J:105:SER:OG	5:J:108:ASP:OD2	2.32	0.42
5:J:431:LEU:HD23	5:J:432:ASN:N	2.35	0.42
2:C:93:LEU:HD12	2:C:96:THR:OG1	2.19	0.42
3:E:267:ILE:HB	3:E:268:PRO:HD3	2.02	0.42
3:E:342:GLU:OE2	3:E:361:MET:HE3	2.19	0.42
3:F:401:VAL:O	3:F:402:VAL:C	2.61	0.42
4:H:122:ILE:HD11	4:H:123:PHE:CZ	2.55	0.42
4:H:208:SER:HB2	4:H:344:HIS:NE2	2.35	0.42
5:I:63:VAL:O	5:I:93:PHE:HB3	2.19	0.42
5:I:211:GLU:O	5:I:212:LEU:HG	2.19	0.42
5:I:290:ARG:HH12	5:I:298:ASP:CG	2.24	0.42
1:B:106:HIS:HE2	2:C:146:ARG:HG3	1.84	0.42
3:E:207:TYR:CE1	3:E:209:LYS:HB2	2.55	0.42
3:E:169:SER:OG	3:E:313:ILE:HG13	2.20	0.41
3:E:274:GLN:C	3:E:276:GLN:HE22	2.27	0.41
3:F:199:GLU:O	3:F:200:GLU:C	2.62	0.41
5:I:19:GLN:OE1	5:I:120:THR:N	2.45	0.41
1:A:175:GLY:O	1:A:179:THR:OG1	2.30	0.41
3:E:81:GLU:OE1	3:E:110:GLY:O	2.38	0.41
3:E:222:MET:HE1	5:J:176:VAL:HG21	2.01	0.41
3:E:355:LEU:HD21	3:E:370:ASP:HA	1.83	0.41
3:F:274:GLN:H	3:F:274:GLN:HG3	1.57	0.41
3:F:367:THR:O	3:F:384:VAL:CB	2.68	0.41
3:F:385:ILE:CG2	3:F:386:GLY:N	2.82	0.41
2:C:287:LEU:HB2	2:C:358:ILE:HB	2.02	0.41
3:F:169:SER:CB	3:F:315:LYS:NZ	2.83	0.41
3:F:172:ALA:O	3:F:317:GLY:HA2	2.20	0.41
3:F:280:THR:O	3:F:281:VAL:HB	2.20	0.41
3:F:423:SER:HA	3:F:438:ALA:O	2.21	0.41
4:H:347:LEU:HD23	4:H:386:GLN:H	1.85	0.41
5:I:409:GLY:CA	5:I:433:ASP:HB2	2.50	0.41
1:B:276:THR:HG23	1:B:278:HIS:HB3	1.28	0.41
1:B:322:ASP:OD1	1:B:322:ASP:N	2.41	0.41
3:E:266:LEU:HB3	3:E:267:ILE:HD13	2.03	0.41
3:F:274:GLN:C	3:F:275:TYR:CD2	2.98	0.41
4:G:175:ILE:O	4:G:178:TYR:HB3	2.20	0.41
5:I:416:LYS:C	5:I:417:ASN:HD22	2.27	0.41
1:A:264:ARG:CZ	1:A:303:ARG:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:SER:O	1:A:334:GLU:HG3	2.20	0.41
2:C:193:VAL:HA	2:C:220:PHE:CE1	2.55	0.41
2:C:378:LEU:HD23	2:C:381:ILE:HD12	2.02	0.41
3:E:181:GLU:OE1	3:E:182:HIS:N	2.53	0.41
3:F:335:CYS:O	3:F:338:LYS:HB3	2.21	0.41
5:I:34:LEU:O	5:I:35:THR:OG1	2.26	0.41
5:J:140:LEU:O	5:J:144:ARG:HG3	2.21	0.41
5:J:383:ILE:O	5:J:384:LEU:HD23	2.20	0.41
1:A:66:SER:HA	1:A:69:LEU:HB3	2.02	0.41
1:B:81:ALA:HB2	1:B:250:VAL:HB	2.03	0.41
3:E:434:HIS:ND1	3:E:448:VAL:HA	2.35	0.41
3:F:129:ALA:HB2	3:F:262:ILE:HD12	2.02	0.41
3:F:278:SER:O	3:F:278:SER:OG	2.26	0.41
5:I:230:VAL:HB	5:I:231:PRO:HD3	2.02	0.41
5:I:439:ILE:CD1	5:I:439:ILE:C	2.85	0.41
5:J:436:LEU:HA	5:J:437:VAL:HA	1.97	0.41
3:E:332:LEU:O	3:E:336:ILE:HG13	2.19	0.41
5:I:160:ARG:HB3	5:I:219:ILE:HB	2.03	0.41
5:I:293:TYR:CG	5:I:294:PRO:HA	2.56	0.41
1:A:95:HIS:O	1:A:96:ASP:CG	2.64	0.41
1:A:148:VAL:HG13	1:A:208:LEU:HD23	2.03	0.41
2:C:377:TYR:HH	4:H:460:ASN:ND2	2.17	0.41
3:F:214:VAL:CG2	3:F:218:PHE:HD1	2.33	0.41
4:G:139:LYS:H	4:G:139:LYS:CD	2.32	0.41
4:G:241:LYS:O	4:G:245:TYR:CB	2.67	0.41
4:G:403:ASN:ND2	4:G:407:ASP:O	2.54	0.41
5:I:293:TYR:CD1	5:I:294:PRO:HA	2.56	0.41
5:J:267:LYS:C	5:J:268:GLU:CG	2.93	0.41
5:J:293:TYR:CD1	5:J:294:PRO:HA	2.56	0.41
1:A:19:ILE:CG2	1:A:20:VAL:N	2.84	0.41
1:A:21:GLN:O	1:A:25:LYS:HG3	2.21	0.41
1:A:52:ALA:C	1:A:53:LYS:HG2	2.46	0.41
1:A:217:ASN:HB3	1:A:253:PHE:CZ	2.56	0.41
1:B:126:ALA:HA	1:B:151:VAL:HG22	2.03	0.41
2:C:90:TYR:HB2	2:C:169:MET:HE1	2.03	0.41
2:C:289:THR:OG1	2:C:290:TYR:N	2.54	0.41
2:C:313:ILE:HG13	2:C:369:ASN:OD1	2.21	0.41
2:D:187:ILE:HG13	2:D:188:ASN:N	2.36	0.41
2:D:294:GLN:HG2	2:D:298:GLN:HG2	2.02	0.41
3:F:125:SER:C	3:F:126:LYS:HG2	2.46	0.41
3:F:353:ARG:O	3:F:354:ALA:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:368:ILE:CG2	3:F:385:ILE:HB	2.47	0.41
3:F:429:GLU:HG3	3:F:445:GLU:HB2	2.03	0.41
3:F:434:HIS:CD2	3:F:448:VAL:HG21	2.52	0.41
4:G:238:LEU:HD23	4:G:238:LEU:HA	1.76	0.41
4:G:274:TYR:CZ	4:G:275:LEU:HD11	2.55	0.41
4:H:332:ILE:HD12	4:H:332:ILE:HA	1.96	0.41
5:I:322:ALA:O	5:I:325:CYS:HB3	2.20	0.41
1:A:62:LEU:H	1:A:62:LEU:HG	1.61	0.41
2:C:235:PHE:CD1	2:C:236:PRO:HA	2.56	0.41
3:E:267:ILE:HD13	3:E:267:ILE:H	1.78	0.41
3:F:49:ASN:OD1	3:F:49:ASN:N	2.53	0.41
3:F:352:GLU:C	3:F:353:ARG:O	2.57	0.41
3:F:355:LEU:CD2	3:F:368:ILE:O	2.69	0.41
1:A:144:PHE:HB3	1:A:174:SER:HB3	2.03	0.40
3:E:94:GLU:OE2	3:E:120:THR:HA	2.22	0.40
3:E:414:ALA:HB3	3:E:431:GLY:O	2.20	0.40
3:F:169:SER:H	3:F:315:LYS:HZ1	1.68	0.40
3:F:259:ILE:H	3:F:259:ILE:HG13	1.60	0.40
3:F:275:TYR:O	3:F:277:LYS:N	2.51	0.40
3:F:340:THR:HG23	3:F:342:GLU:HG3	2.03	0.40
4:H:300:ASP:OD1	4:H:301:SER:N	2.50	0.40
5:J:63:VAL:O	5:J:93:PHE:HB3	2.21	0.40
5:J:431:LEU:O	5:J:432:ASN:CB	2.62	0.40
1:A:132:LEU:HD12	1:A:320:ILE:HD11	2.02	0.40
1:B:142:HIS:CE1	1:B:225:GLY:HA3	2.56	0.40
1:B:341:LEU:HD12	1:B:341:LEU:HA	1.91	0.40
2:D:235:PHE:CD1	2:D:236:PRO:HA	2.56	0.40
3:E:67:ILE:HG22	3:E:68:GLY:N	2.36	0.40
3:E:333:ASN:HB2	3:E:412:ILE:HD11	2.04	0.40
1:A:31:PRO:HB3	1:B:285:PRO:HD3	2.03	0.40
3:E:211:SER:O	3:E:214:VAL:HG13	2.19	0.40
3:E:249:VAL:C	3:E:252:LEU:H	2.28	0.40
3:E:272:LYS:O	3:E:273:CYS:CB	2.68	0.40
3:E:354:ALA:HB3	3:E:370:ASP:CB	2.50	0.40
3:F:275:TYR:CD1	3:F:275:TYR:C	2.98	0.40
4:G:288:LYS:HE3	4:G:288:LYS:HB2	1.90	0.40
4:G:402:VAL:O	4:G:404:MET:HE2	2.21	0.40
4:H:418:ASN:O	4:H:422:VAL:HG23	2.21	0.40
5:I:337:THR:HG23	5:I:354:CYS:HB2	2.04	0.40
5:I:381:LYS:HD3	5:I:381:LYS:HA	1.93	0.40
1:A:62:LEU:C	1:A:65:GLY:N	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:331:SER:OG	2:C:332:SER:N	2.52	0.40
2:D:32:ALA:HB2	2:D:74:SER:OG	2.22	0.40
2:D:40:ARG:HG3	2:D:174:ILE:HD12	2.04	0.40
4:G:134:THR:O	4:G:137:ILE:HB	2.22	0.40
4:G:264:LYS:HA	4:G:264:LYS:HD3	1.85	0.40
5:I:57:PHE:CD1	5:I:132:SER:HB3	2.57	0.40
5:I:257:LEU:O	5:I:259:LYS:HD3	2.22	0.40
5:J:140:LEU:HD23	5:J:225:ILE:HD13	2.02	0.40
1:B:230:ALA:HB1	1:B:315:PHE:HB3	2.03	0.40
3:F:367:THR:N	3:F:383:CYS:O	2.55	0.40
4:G:273:THR:O	4:G:273:THR:HG23	2.21	0.40
4:H:202:VAL:HG22	4:H:207:LEU:HG	2.03	0.40
5:I:439:ILE:HD11	5:I:441:GLY:HA2	2.00	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:113:ARG:NH2	5:J:443:GLY:C[2_555]	0.64	1.56
3:F:113:ARG:CZ	5:J:443:GLY:O[2_555]	0.66	1.54
3:F:113:ARG:NH2	5:J:443:GLY:O[2_555]	0.96	1.24
3:F:113:ARG:NH1	5:J:443:GLY:O[2_555]	1.51	0.69
3:F:113:ARG:CZ	5:J:443:GLY:C[2_555]	1.76	0.44
3:F:113:ARG:NE	5:J:443:GLY:O[2_555]	1.83	0.37
2:D:56:ASP:OD2	5:I:432:ASN:OD1[3_645]	1.95	0.25
3:F:113:ARG:NH2	5:J:443:GLY:CA[2_555]	2.04	0.16

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	313/341 (92%)	293 (94%)	17 (5%)	3 (1%)	12 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	315/341 (92%)	302 (96%)	12 (4%)	1 (0%)	36	70
2	C	343/399 (86%)	330 (96%)	13 (4%)	0	100	100
2	D	340/399 (85%)	327 (96%)	13 (4%)	0	100	100
3	E	378/458 (82%)	334 (88%)	36 (10%)	8 (2%)	5	27
3	F	377/458 (82%)	334 (89%)	40 (11%)	3 (1%)	16	50
4	G	347/467 (74%)	331 (95%)	15 (4%)	1 (0%)	36	70
4	H	347/467 (74%)	339 (98%)	8 (2%)	0	100	100
5	I	426/678 (63%)	400 (94%)	24 (6%)	2 (0%)	24	60
5	J	426/678 (63%)	385 (90%)	37 (9%)	4 (1%)	14	48
All	All	3612/4686 (77%)	3375 (93%)	215 (6%)	22 (1%)	21	56

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	262	ILE
3	E	442	ALA
3	E	270	LEU
3	E	277	LYS
5	J	432	ASN
5	I	432	ASN
1	A	61	ILE
3	E	273	CYS
3	E	340	THR
1	B	274	PRO
3	E	327	PRO
3	F	331	GLU
3	F	341	PRO
3	E	150	SER
5	J	32	ARG
5	J	434	PRO
1	A	97	VAL
1	A	274	PRO
3	F	402	VAL
5	J	437	VAL
5	I	33	PRO
4	G	303	PRO

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	276/298 (93%)	255 (92%)	21 (8%)	12	41
1	B	278/298 (93%)	271 (98%)	7 (2%)	42	72
2	C	301/350 (86%)	287 (95%)	14 (5%)	23	58
2	D	298/350 (85%)	294 (99%)	4 (1%)	61	81
3	E	330/395 (84%)	295 (89%)	35 (11%)	6	27
3	F	329/395 (83%)	293 (89%)	36 (11%)	6	26
4	G	314/408 (77%)	297 (95%)	17 (5%)	20	53
4	H	314/408 (77%)	300 (96%)	14 (4%)	24	59
5	I	379/596 (64%)	360 (95%)	19 (5%)	22	56
5	J	378/596 (63%)	352 (93%)	26 (7%)	14	45
All	All	3197/4094 (78%)	3004 (94%)	193 (6%)	17	50

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	21	GLN
1	A	28	GLN
1	A	32	GLU
1	A	47	LEU
1	A	49	ARG
1	A	50	SER
1	A	51	GLN
1	A	55	ILE
1	A	57	GLU
1	A	61	ILE
1	A	62	LEU
1	A	93	SER
1	A	100	PHE
1	A	102	GLN
1	A	112	LYS

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Mol	Chain	Res	Type
1	A	113	LEU
1	A	123	GLN
1	A	134	ARG
1	A	231	VAL
1	A	266	ILE
1	B	57	GLU
1	B	87	GLN
1	B	106	HIS
1	B	112	LYS
1	B	187	ILE
1	B	276	THR
1	B	277	VAL
2	C	1	MET
2	C	2	SER
2	C	41	GLN
2	C	44	SER
2	C	45	GLN
2	C	49	SER
2	C	87	ARG
2	C	92	GLU
2	C	93	LEU
2	C	139	SER
2	C	162	ARG
2	C	164	THR
2	C	183	GLU
2	C	313	ILE
2	D	47	ARG
2	D	49	SER
2	D	96	THR
2	D	167	MET
3	E	31	GLN
3	E	33	GLN
3	E	34	SER
3	E	94	GLU
3	E	135	VAL
3	E	181	GLU
3	E	193	LYS
3	E	225	LEU
3	E	244	VAL
3	E	254	ARG
3	E	256	LYS
3	E	263	ARG

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Mol	Chain	Res	Type
3	E	267	ILE
3	E	273	CYS
3	E	274	GLN
3	E	276	GLN
3	E	277	LYS
3	E	281	VAL
3	E	324	ASN
3	E	326	LEU
3	E	327	PRO
3	E	328	ASN
3	E	331	GLU
3	E	332	LEU
3	E	346	VAL
3	E	353	ARG
3	E	355	LEU
3	E	367	THR
3	E	368	ILE
3	E	370	ASP
3	E	381	LYS
3	E	397	MET
3	E	424	LYS
3	E	443	ARG
3	E	448	VAL
3	F	42	VAL
3	F	100	ILE
3	F	109	GLU
3	F	113	ARG
3	F	120	THR
3	F	183	ILE
3	F	200	GLU
3	F	204	ARG
3	F	221	ARG
3	F	254	ARG
3	F	259	ILE
3	F	262	ILE
3	F	267	ILE
3	F	268	PRO
3	F	270	LEU
3	F	272	LYS
3	F	277	LYS
3	F	279	PHE
3	F	281	VAL

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Mol	Chain	Res	Type
3	F	315	LYS
3	F	319	ILE
3	F	322	ARG
3	F	339	LEU
3	F	342	GLU
3	F	344	ARG
3	F	345	LEU
3	F	360	CYS
3	F	407	ARG
3	F	419	ILE
3	F	428	CYS
3	F	429	GLU
3	F	435	ARG
3	F	440	ARG
3	F	443	ARG
3	F	446	ARG
3	F	450	MET
4	G	116	GLU
4	G	117	GLU
4	G	127	ASP
4	G	151	LYS
4	G	157	ILE
4	G	179	GLN
4	G	225	LEU
4	G	228	ASP
4	G	232	ASP
4	G	237	LEU
4	G	240	GLU
4	G	278	SER
4	G	288	LYS
4	G	293	LYS
4	G	401	LEU
4	G	403	ASN
4	G	412	LYS
4	H	116	GLU
4	H	120	VAL
4	H	156	LYS
4	H	157	ILE
4	H	179	GLN
4	H	227	ILE
4	H	293	LYS
4	H	355	ARG

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Mol	Chain	Res	Type
4	H	383	GLU
4	H	404	MET
4	H	407	ASP
4	H	408	ASP
4	H	410	GLU
4	H	411	GLU
5	I	16	HIS
5	I	18	LEU
5	I	29	TYR
5	I	83	LYS
5	I	106	VAL
5	I	187	VAL
5	I	205	ILE
5	I	210	GLU
5	I	245	LYS
5	I	268	GLU
5	I	292	VAL
5	I	418	LYS
5	I	419	ARG
5	I	424	GLU
5	I	430	THR
5	I	431	LEU
5	I	432	ASN
5	I	436	LEU
5	I	439	ILE
5	J	82	GLU
5	J	95	VAL
5	J	182	LYS
5	J	210	GLU
5	J	214	VAL
5	J	253	THR
5	J	257	LEU
5	J	265	VAL
5	J	267	LYS
5	J	381	LYS
5	J	384	LEU
5	J	386	ASN
5	J	394	CYS
5	J	398	ASP
5	J	408	ILE
5	J	417	ASN
5	J	418	LYS

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Mol	Chain	Res	Type
5	J	419	ARG
5	J	426	HIS
5	J	427	SER
5	J	428	GLN
5	J	432	ASN
5	J	435	SER
5	J	437	VAL
5	J	439	ILE
5	J	442	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	95	HIS
1	B	223	GLN
1	B	228	GLN
1	B	247	HIS
1	B	305	ASN
2	C	26	GLN
2	C	194	GLN
2	C	202	ASN
2	D	26	GLN
2	D	69	GLN
2	D	194	GLN
2	D	352	ASN
3	E	111	HIS
3	E	182	HIS
3	E	276	GLN
3	F	247	HIS
3	F	325	ASN
3	F	343	GLN
4	G	154	ASN
4	G	281	ASN
4	G	400	GLN
4	G	403	ASN
4	G	460	ASN
4	H	119	GLN
4	H	460	ASN
5	I	188	HIS
5	I	312	GLN
5	I	347	ASN

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Mol	Chain	Res	Type
5	I	376	ASN
5	I	393	ASN
5	I	417	ASN
5	J	76	GLN
5	J	152	ASN
5	J	237	ASN
5	J	359	ASN
5	J	386	ASN
5	J	393	ASN
5	J	411	ASN
5	J	417	ASN
5	J	432	ASN

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](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PO4	G	501	-	4,4,4	0.96	0	6,6,6	0.46	0
6	PO4	I	701	-	4,4,4	0.94	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PO4	H	502	-	4,4,4	0.97	0	6,6,6	0.49	0
6	PO4	C	401	-	4,4,4	0.95	0	6,6,6	0.45	0
6	PO4	D	401	-	4,4,4	0.97	0	6,6,6	0.47	0
6	PO4	H	501	-	4,4,4	0.95	0	6,6,6	0.48	0
6	PO4	B	401	-	4,4,4	0.99	0	6,6,6	0.48	0
6	PO4	A	401	-	4,4,4	0.98	0	6,6,6	0.46	0
6	PO4	G	502	-	4,4,4	0.96	0	6,6,6	0.45	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	501	PO4	1	0
6	I	701	PO4	1	0
6	D	401	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	317/341 (92%)	0.51	21 (6%)	24	12	55, 86, 150, 173	0
1	B	319/341 (93%)	0.36	15 (4%)	36	19	49, 80, 123, 180	0
2	C	349/399 (87%)	0.17	16 (4%)	37	20	42, 68, 138, 165	0
2	D	346/399 (86%)	0.02	10 (2%)	53	31	41, 66, 111, 161	0
3	E	384/458 (83%)	1.02	65 (16%)	4	3	61, 99, 142, 163	0
3	F	383/458 (83%)	1.14	69 (18%)	3	2	66, 108, 153, 168	0
4	G	349/467 (74%)	0.32	19 (5%)	31	16	44, 75, 136, 167	0
4	H	349/467 (74%)	0.07	14 (4%)	42	23	44, 65, 116, 153	0
5	I	428/678 (63%)	0.20	16 (3%)	45	25	42, 73, 115, 148	0
5	J	428/678 (63%)	0.43	24 (5%)	30	15	50, 87, 122, 153	0
All	All	3652/4686 (77%)	0.43	269 (7%)	20	10	41, 80, 137, 180	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	405	GLY	7.2
3	F	423	SER	6.8
5	I	432	ASN	6.0
1	A	285	PRO	5.6
3	E	183	ILE	5.3
3	E	311	ALA	5.1
5	I	429	GLY	4.9
3	E	419	ILE	4.8
4	H	408	ASP	4.7
5	J	433	ASP	4.4
5	J	257	LEU	4.4
4	G	157	ILE	4.3
3	E	281	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
3	E	315	LYS	4.3
3	E	263	ARG	4.2
3	F	263	ARG	4.2
3	E	32	LEU	4.2
3	E	252	LEU	4.2
1	A	58	PHE	4.2
1	B	329	LYS	4.1
4	G	406	VAL	4.1
3	E	265	ASP	4.1
3	F	32	LEU	4.0
3	F	401	VAL	4.0
2	C	-4	PRO	4.0
3	F	183	ILE	4.0
3	F	60	LEU	4.0
3	F	384	VAL	3.9
5	J	437	VAL	3.9
3	F	441	ILE	3.9
5	J	436	LEU	3.8
5	J	404	ALA	3.8
3	F	281	VAL	3.8
3	E	356	VAL	3.7
1	A	55	ILE	3.7
2	D	165	GLY	3.7
2	C	163	VAL	3.7
3	F	211	SER	3.7
3	F	47	PHE	3.7
3	E	330	PHE	3.6
3	F	434	HIS	3.5
3	F	345	LEU	3.5
5	I	430	THR	3.5
3	E	350	VAL	3.5
5	J	434	PRO	3.5
3	F	44	PHE	3.4
4	G	115	PHE	3.4
3	E	407	ARG	3.3
3	E	320	CYS	3.3
3	F	330	PHE	3.3
3	F	346	VAL	3.3
3	F	350	VAL	3.3
2	D	-5	GLY	3.3
3	F	358	ALA	3.3
3	E	192	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
3	E	268	PRO	3.2
4	G	185	THR	3.2
3	F	218	PHE	3.2
3	E	415	SER	3.1
3	F	252	LEU	3.1
1	B	278	HIS	3.1
1	B	277	VAL	3.1
4	H	114	ILE	3.1
3	E	271	VAL	3.1
3	F	406	VAL	3.1
1	A	289	ASP	3.1
3	F	421	ALA	3.0
4	H	405	GLY	3.0
3	F	355	LEU	3.0
5	I	16	HIS	3.0
2	C	-5	GLY	3.0
3	F	145	CYS	3.0
3	E	346	VAL	3.0
2	C	48	TRP	3.0
2	C	379	TYR	3.0
3	F	440	ARG	3.0
5	J	100	SER	3.0
4	G	186	LEU	2.9
1	B	274	PRO	2.9
3	F	48	GLY	2.9
3	F	275	TYR	2.9
3	E	218	PHE	2.9
3	F	407	ARG	2.9
5	J	37	ASP	2.9
1	A	66	SER	2.9
3	F	264	GLY	2.8
2	D	-4	PRO	2.8
1	A	329	LYS	2.8
3	E	272	LYS	2.8
3	E	446	ARG	2.8
2	C	4	ILE	2.8
3	E	367	THR	2.8
4	H	119	GLN	2.8
3	F	279	PHE	2.8
4	H	158	PHE	2.8
5	I	17	ALA	2.8
2	C	8	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
3	F	265	ASP	2.8
3	E	404	ASP	2.8
5	J	85	LYS	2.8
3	E	333	ASN	2.7
3	E	340	THR	2.7
4	G	184	THR	2.7
5	J	104	LEU	2.7
3	E	269	TYR	2.7
5	I	29	TYR	2.7
3	E	49	ASN	2.7
3	F	404	ASP	2.7
5	I	433	ASP	2.7
4	H	115	PHE	2.7
5	J	29	TYR	2.7
5	J	443	GLY	2.7
3	E	321	SER	2.7
3	E	348	VAL	2.7
3	E	405	GLY	2.7
4	H	413	PRO	2.7
5	J	128	GLY	2.7
5	J	415	GLU	2.7
2	C	2	SER	2.7
3	E	332	LEU	2.7
3	F	438	ALA	2.6
2	D	90	TYR	2.6
3	F	269	TYR	2.6
2	C	166	GLY	2.6
2	C	3	THR	2.6
3	E	275	TYR	2.6
1	A	54	THR	2.6
3	F	356	VAL	2.6
4	G	225	LEU	2.6
5	J	253	THR	2.6
1	A	33	ILE	2.6
3	E	31	GLN	2.6
4	H	409	PHE	2.6
4	G	155	TYR	2.6
1	B	75	ASN	2.6
1	B	327	ASP	2.6
4	G	226	ASP	2.6
1	A	23	TYR	2.5
3	E	220	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
5	I	442	ARG	2.5
2	D	147	PRO	2.5
4	G	413	PRO	2.5
3	F	402	VAL	2.5
4	H	116	GLU	2.5
2	C	164	THR	2.5
3	E	355	LEU	2.5
3	F	332	LEU	2.5
3	F	212	ALA	2.5
3	E	312	LEU	2.4
1	B	285	PRO	2.4
3	F	368	ILE	2.4
3	F	419	ILE	2.4
1	A	97	VAL	2.4
3	E	44	PHE	2.4
4	H	304	GLU	2.4
3	E	327	PRO	2.4
4	H	406	VAL	2.4
3	F	351	SER	2.4
3	E	253	ILE	2.4
3	F	91	ILE	2.4
5	J	320	VAL	2.4
1	A	100	PHE	2.4
3	F	220	PHE	2.4
3	E	329	TYR	2.4
3	F	393	ASN	2.4
1	B	253	PHE	2.4
3	E	47	PHE	2.4
2	D	388	ALA	2.4
3	E	323	ALA	2.4
2	D	138	SER	2.4
3	F	326	LEU	2.4
4	G	189	HIS	2.4
3	F	348	VAL	2.3
3	E	357	GLY	2.3
3	E	352	GLU	2.3
3	F	34	SER	2.3
3	F	321	SER	2.3
4	G	404	MET	2.3
3	F	447	LEU	2.3
1	B	257	GLN	2.3
4	H	184	THR	2.3

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Mol	Chain	Res	Type	RSRZ
5	J	414	ILE	2.3
3	E	193	LYS	2.3
5	I	15	LYS	2.3
3	E	48	GLY	2.3
3	E	417	ALA	2.3
1	A	276	THR	2.3
3	E	436	VAL	2.3
3	F	333	ASN	2.3
4	G	241	LYS	2.3
2	C	-3	ILE	2.3
2	C	97	ALA	2.2
1	A	286	THR	2.2
1	B	97	VAL	2.2
1	B	288	SER	2.2
3	F	127	SER	2.2
1	A	86	PHE	2.2
3	E	60	LEU	2.2
1	A	135	ASP	2.2
3	E	440	ARG	2.2
1	A	326	ILE	2.2
3	E	198	ILE	2.2
4	G	227	ILE	2.2
3	F	182	HIS	2.2
5	J	412	THR	2.2
5	I	435	SER	2.2
1	A	94	LEU	2.2
3	F	270	LEU	2.2
1	A	52	ALA	2.2
5	J	400	ALA	2.2
3	F	385	ILE	2.2
3	E	115	HIS	2.2
5	I	426	HIS	2.2
4	H	303	PRO	2.2
5	I	255	ASP	2.2
2	C	165	GLY	2.2
3	F	431	GLY	2.2
1	A	46	LEU	2.2
3	F	312	LEU	2.2
5	I	425	SER	2.2
3	E	421	ALA	2.2
3	E	322	ARG	2.1
3	F	315	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	387	LYS	2.1
3	F	444	GLY	2.1
5	J	431	LEU	2.1
3	E	261	SER	2.1
3	F	261	SER	2.1
3	F	352	GLU	2.1
4	G	132	ARG	2.1
3	F	412	ILE	2.1
2	D	323	ASP	2.1
2	C	9	THR	2.1
4	G	182	TYR	2.1
3	E	34	SER	2.1
5	J	325	CYS	2.1
3	E	209	LYS	2.1
5	J	418	LYS	2.1
3	F	370	ASP	2.1
3	F	439	GLY	2.1
5	I	257	LEU	2.1
5	J	420	LEU	2.1
2	D	379	TYR	2.1
3	E	121	ILE	2.1
2	C	-2	SER	2.1
4	H	429	SER	2.1
3	E	33	GLN	2.1
5	J	278	GLN	2.1
3	E	137	HIS	2.1
3	E	448	VAL	2.1
3	F	271	VAL	2.1
3	F	369	LYS	2.1
1	B	293	ASN	2.1
1	A	62	LEU	2.1
1	B	55	ILE	2.1
3	E	351	SER	2.0
1	A	103	CYS	2.0
3	F	424	LYS	2.0
4	G	412	LYS	2.0
5	I	245	LYS	2.0
1	B	289	ASP	2.0
3	E	191	ASP	2.0
3	F	259	ILE	2.0
5	I	322	ALA	2.0
3	F	181	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
4	G	178	TYR	2.0
2	D	148	THR	2.0
3	E	45	ALA	2.0
1	B	212	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PO4	I	701	5/5	0.75	0.12	101,102,127,141	0
6	PO4	G	501	5/5	0.83	0.16	91,94,118,136	0
6	PO4	H	501	5/5	0.86	0.15	81,85,101,134	0
6	PO4	G	502	5/5	0.86	0.11	62,67,102,104	0
6	PO4	A	401	5/5	0.94	0.08	70,71,84,89	0
6	PO4	H	502	5/5	0.95	0.07	71,82,90,98	0
6	PO4	B	401	5/5	0.95	0.10	63,67,86,93	0
6	PO4	D	401	5/5	0.98	0.05	50,53,72,73	0
6	PO4	C	401	5/5	0.98	0.05	51,53,68,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.