



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:37 AM UTC

PDB ID : 1IJG / pdb_00001ijg
Title : Structure of the Bacteriophage phi29 Head-Tail Connector Protein
Authors : Simpson, A.A.; Leiman, P.G.; Tao, Y.; He, Y.; Badasso, M.; Jardine, P.J.;
Anderson, D.L.; Rossmann, M.G.
Deposited on : 2001-04-26
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

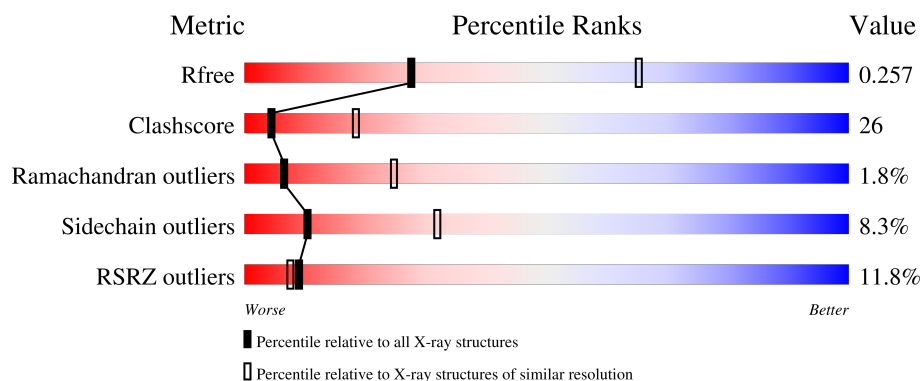
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	309	7% 49% 28% 6% 17%
1	B	309	11% 49% 30% 5% 17%
1	C	309	7% 47% 29% 7% 17%
1	D	309	12% 44% 33% 6% 17%
1	E	309	15% 47% 31% 5% 17%

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Mol	Chain	Length	Quality of chain
1	F	309	13%38%39%6%17%
1	G	309	8%42%36%6%17%
1	H	309	9%45%34%17%
1	I	309	7%49%28%6%17%
1	J	309	6%49%29%5%17%
1	K	309	13%42%35%6%17%
1	L	309	8%41%37%5%17%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 25977 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 UPPER COLLAR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	B	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	C	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	D	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	E	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	F	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	G	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	H	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	I	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	J	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	K	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	L	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	68	Total	O	0	0
			68	68		
2	B	55	Total	O	0	0
			55	55		

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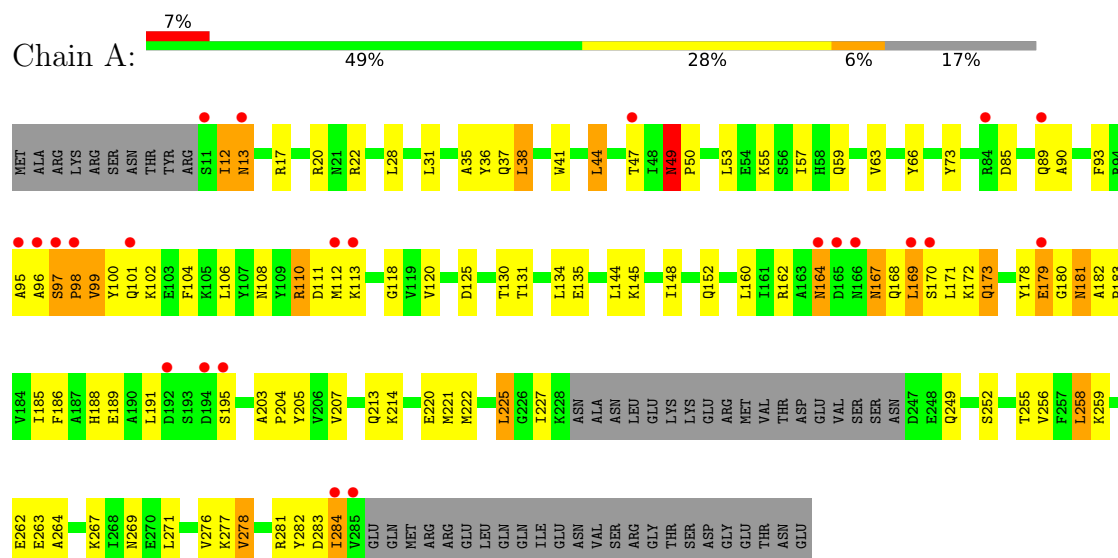
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	56	Total 56	O 56	0	0
2	D	67	Total 67	O 67	0	0
2	E	35	Total 35	O 35	0	0
2	F	69	Total 69	O 69	0	0
2	G	59	Total 59	O 59	0	0
2	H	65	Total 65	O 65	0	0
2	I	73	Total 73	O 73	0	0
2	J	67	Total 67	O 67	0	0
2	K	68	Total 68	O 68	0	0
2	L	71	Total 71	O 71	0	0

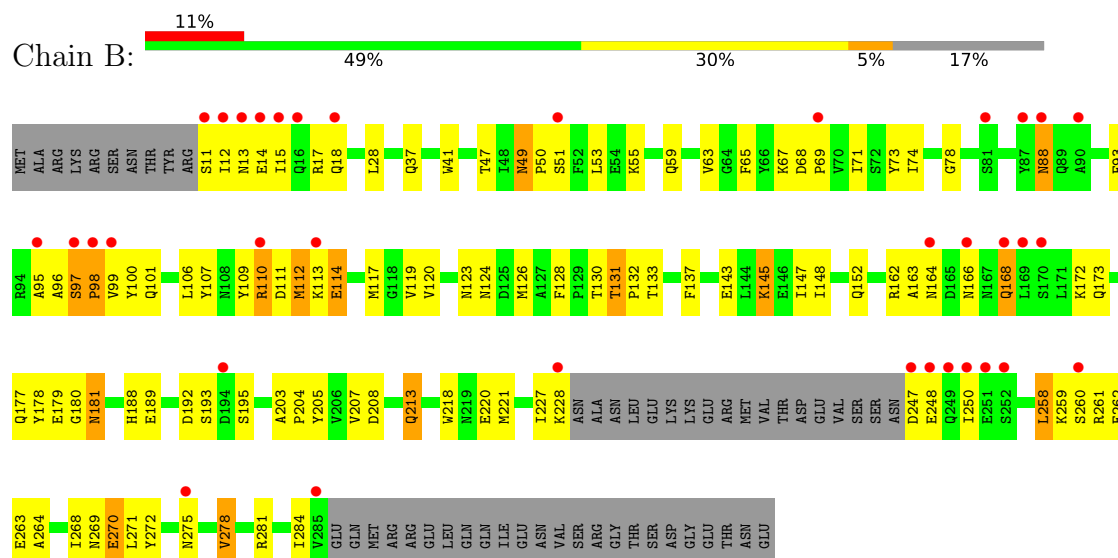
3 Residue-property plots

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

• Molecule 1: UPPER COLLAR PROTEIN

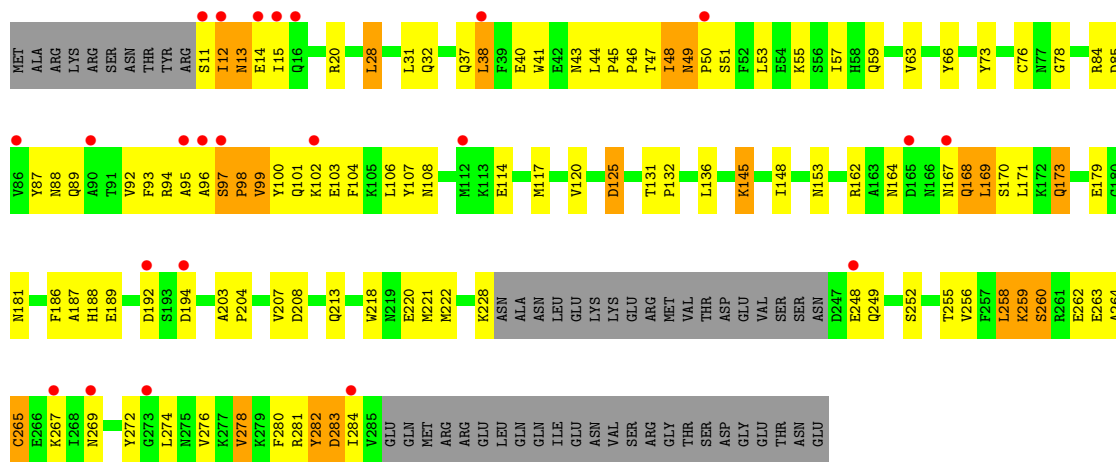


• Molecule 1: UPPER COLLAR PROTEIN

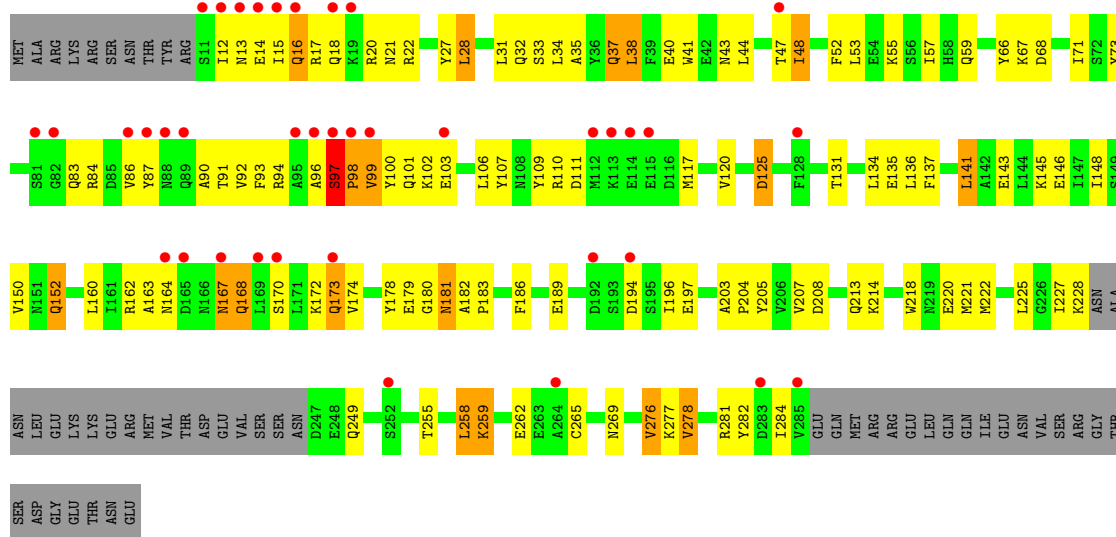


• Molecule 1: UPPER COLLAR PROTEIN

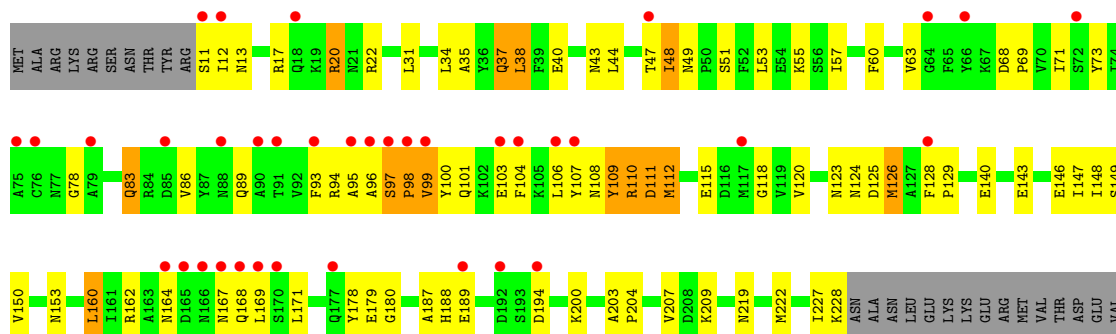


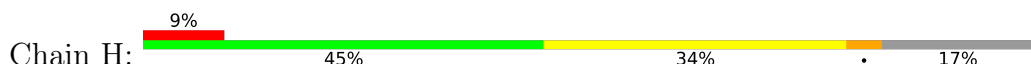


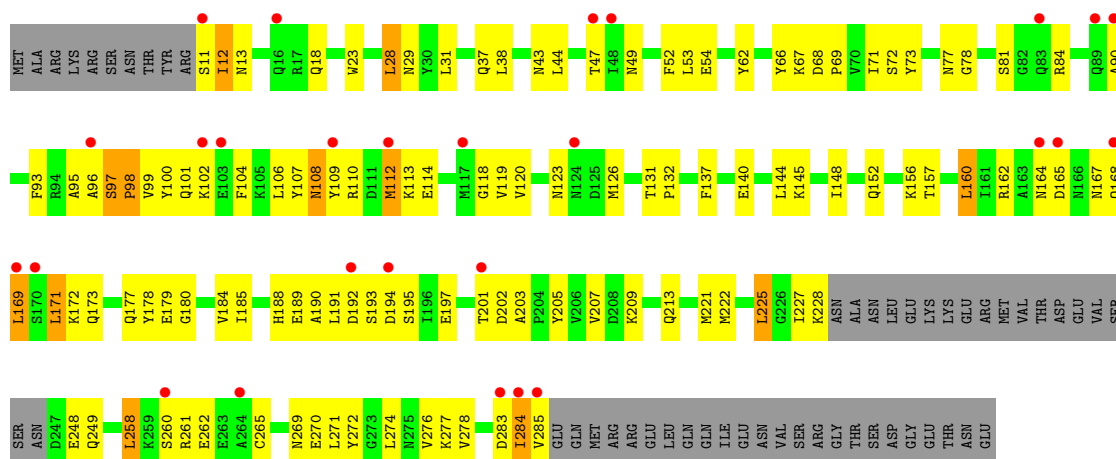
• Molecule 1: UPPER COLLAR PROTEIN



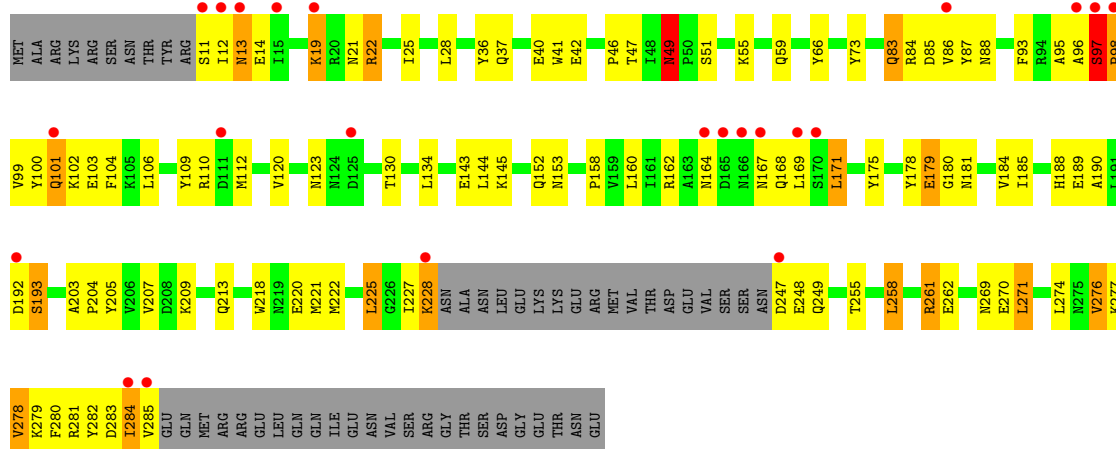
• Molecule 1: UPPER COLLAR PROTEIN



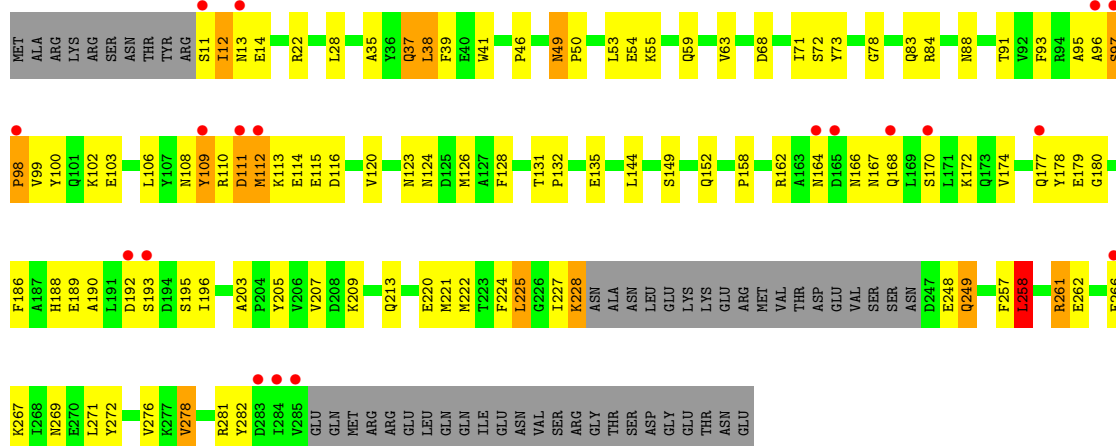




• Molecule 1: UPPER COLLAR PROTEIN



• Molecule 1: UPPER COLLAR PROTEIN



• Molecule 1: UPPER COLLAR PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	176.75Å 171.57Å 184.71Å 90.00° 112.21° 90.00°	Depositor
Resolution (Å)	500.00 – 2.90 171.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (500.00-2.90) 97.8 (171.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.09 (at 2.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.264 0.221 , 0.257	Depositor DCC
R_{free} test set	2500 reflections (2.27%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25977	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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 ⓘ

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	0.49	0/2147	0.87	5/2909 (0.2%)
1	B	0.46	0/2147	0.87	4/2909 (0.1%)
1	C	0.47	0/2147	0.90	5/2909 (0.2%)
1	D	0.46	0/2147	0.90	5/2909 (0.2%)
1	E	0.42	0/2147	0.85	3/2909 (0.1%)
1	F	0.46	0/2147	0.89	6/2909 (0.2%)
1	G	0.46	0/2147	0.89	4/2909 (0.1%)
1	H	0.44	0/2147	0.88	2/2909 (0.1%)
1	I	0.49	0/2147	0.90	5/2909 (0.2%)
1	J	0.49	0/2147	0.91	5/2909 (0.2%)
1	K	0.45	0/2147	0.86	2/2909 (0.1%)
1	L	0.50	0/2147	0.90	3/2909 (0.1%)
All	All	0.47	0/25764	0.89	49/34908 (0.1%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	99	VAL	N-CA-C	-9.67	103.20	112.29
1	I	99	VAL	N-CA-C	-9.28	103.57	112.29
1	C	99	VAL	N-CA-C	-9.27	103.57	112.29
1	D	99	VAL	N-CA-C	-9.24	103.60	112.29
1	H	99	VAL	N-CA-C	-9.01	103.82	112.29
1	E	99	VAL	N-CA-C	-8.99	103.84	112.29
1	A	99	VAL	N-CA-C	-8.95	103.87	112.29
1	J	99	VAL	N-CA-C	-8.95	103.88	112.29
1	K	99	VAL	N-CA-C	-8.94	103.88	112.29
1	L	99	VAL	N-CA-C	-8.90	103.92	112.29
1	F	99	VAL	N-CA-C	-8.87	103.95	112.29
1	B	99	VAL	N-CA-C	-8.63	104.18	112.29
1	F	116	ASP	N-CA-C	-7.18	104.10	112.86
1	E	112	MET	N-CA-C	-6.90	104.16	112.58
1	C	283	ASP	N-CA-C	-6.78	96.37	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	38	LEU	N-CA-C	5.97	118.31	111.02
1	E	283	ASP	N-CA-C	5.94	119.89	109.80
1	J	112	MET	N-CA-C	5.90	119.13	109.76
1	C	220	GLU	N-CA-C	-5.85	104.81	111.07
1	A	220	GLU	N-CA-C	-5.80	104.87	111.07
1	L	220	GLU	N-CA-C	-5.59	105.10	111.14
1	K	220	GLU	N-CA-C	-5.54	105.24	111.28
1	I	220	GLU	N-CA-C	-5.54	105.32	111.36
1	J	220	GLU	N-CA-C	-5.50	105.29	111.28
1	C	38	LEU	N-CA-C	5.48	122.48	110.80
1	G	284	ILE	N-CA-C	5.41	116.56	109.58
1	J	109	TYR	N-CA-C	5.37	117.81	107.44
1	D	220	GLU	N-CA-C	-5.32	105.56	111.36
1	B	220	GLU	N-CA-C	-5.32	105.56	111.36
1	A	49	ASN	CA-C-N	5.32	124.77	119.24
1	A	49	ASN	C-N-CA	5.32	124.77	119.24
1	F	220	GLU	N-CA-C	-5.28	105.42	111.07
1	F	39	PHE	N-CA-C	5.19	118.58	110.32
1	F	38	LEU	N-CA-C	5.18	121.84	110.80
1	A	110	ARG	N-CA-C	-5.16	100.37	108.63
1	D	284	ILE	N-CA-C	5.16	115.90	108.93
1	F	258	LEU	N-CA-C	5.14	116.57	111.07
1	J	258	LEU	N-CA-C	5.10	116.53	111.07
1	L	258	LEU	N-CA-C	5.09	116.52	111.07
1	G	220	GLU	N-CA-C	-5.09	105.73	111.28
1	B	258	LEU	N-CA-C	5.08	116.51	111.07
1	I	49	ASN	CA-C-N	5.08	124.52	119.24
1	I	49	ASN	C-N-CA	5.08	124.52	119.24
1	C	282	TYR	N-CA-C	5.07	117.40	107.57
1	I	193	SER	N-CA-C	-5.05	107.17	113.38
1	G	258	LEU	N-CA-C	5.05	116.47	111.07
1	D	152	GLN	CB-CA-C	-5.02	102.99	110.88
1	B	193	SER	N-CA-C	-5.01	107.17	113.28
1	D	258	LEU	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2102	0	2050	114	0
1	B	2102	0	2050	109	0
1	C	2102	0	2050	130	0
1	D	2102	0	2050	122	0
1	E	2102	0	2050	113	0
1	F	2102	0	2050	158	0
1	G	2102	0	2050	128	0
1	H	2102	0	2050	138	0
1	I	2102	0	2050	108	0
1	J	2102	0	2050	101	0
1	K	2102	0	2050	137	1
1	L	2102	0	2050	126	0
2	A	68	0	0	3	0
2	B	55	0	0	3	0
2	C	56	0	0	4	0
2	D	67	0	0	7	0
2	E	35	0	0	1	0
2	F	69	0	0	3	0
2	G	59	0	0	4	0
2	H	65	0	0	4	0
2	I	73	0	0	11	0
2	J	67	0	0	4	0
2	K	68	0	0	3	0
2	L	71	0	0	1	0
All	All	25977	0	24600	1317	1

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 26.

All (1317) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:HD21	1:A:276:VAL:HG12	1.18	1.01
1:F:249:GLN:HG2	1:G:222:MET:HE2	1.41	0.98
1:H:283:ASP:HB3	1:H:285:VAL:HG12	1.44	0.97
1:F:55:LYS:HG2	1:F:59:GLN:HE21	1.26	0.96
1:K:89:GLN:HB3	1:K:108:ASN:HD21	1.29	0.96
1:F:93:PHE:HB2	1:F:106:LEU:HD21	1.50	0.94
1:J:213:GLN:HA	1:J:213:GLN:HE21	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:THR:HG21	1:G:281:ARG:HD3	1.51	0.91
1:B:168:GLN:HG2	1:B:188:HIS:NE2	1.85	0.91
1:J:168:GLN:HG2	1:J:188:HIS:CE1	2.07	0.90
1:F:110:ARG:NH1	1:F:113:LYS:HG2	1.85	0.90
1:F:168:GLN:HG2	1:F:188:HIS:CE1	2.07	0.89
1:C:12:ILE:H	1:C:12:ILE:HD12	1.35	0.89
1:A:55:LYS:O	1:A:59:GLN:HG3	1.73	0.89
1:E:11:SER:HB2	1:E:12:ILE:HD12	1.53	0.89
1:A:49:ASN:HD22	1:A:49:ASN:C	1.79	0.88
1:K:119:VAL:HG21	1:K:268:ILE:HG12	1.55	0.88
1:E:93:PHE:HB2	1:E:106:LEU:HD21	1.56	0.87
1:B:137:PHE:HB2	1:B:221:MET:HE2	1.54	0.87
1:G:105:LYS:N	1:G:105:LYS:HD2	1.89	0.87
1:J:168:GLN:HG2	1:J:188:HIS:NE2	1.89	0.87
1:I:19:LYS:HE3	1:I:19:LYS:HA	1.56	0.86
1:E:123:ASN:HA	1:E:261:ARG:HH12	1.39	0.85
1:B:37:GLN:HG2	1:B:281:ARG:HD2	1.58	0.85
1:C:255:THR:HG21	1:D:281:ARG:HD3	1.58	0.85
1:E:269:ASN:HD21	1:E:276:VAL:HG22	1.40	0.85
1:L:55:LYS:O	1:L:59:GLN:HG3	1.75	0.85
1:F:55:LYS:HG2	1:F:59:GLN:NE2	1.92	0.84
1:A:269:ASN:HD21	1:A:276:VAL:CG1	1.91	0.83
1:A:269:ASN:ND2	1:A:276:VAL:HG12	1.93	0.83
1:H:188:HIS:CD2	1:H:190:ALA:H	1.96	0.83
1:K:91:THR:HG23	1:K:92:VAL:HG23	1.60	0.83
1:H:93:PHE:HB2	1:H:106:LEU:HD21	1.60	0.83
1:J:249:GLN:HB3	1:K:222:MET:HE2	1.60	0.83
1:D:37:GLN:HG2	1:D:281:ARG:HD2	1.60	0.83
1:I:168:GLN:HG2	1:I:188:HIS:CD2	2.12	0.83
1:I:188:HIS:CD2	1:I:190:ALA:H	1.97	0.81
1:F:168:GLN:HG2	1:F:188:HIS:NE2	1.95	0.81
1:G:257:PHE:O	1:G:261:ARG:HD2	1.81	0.81
1:F:40:GLU:HG3	1:F:281:ARG:NH2	1.96	0.81
1:C:162:ARG:HG3	1:C:162:ARG:HH11	1.46	0.80
1:K:119:VAL:HG21	1:K:268:ILE:CG1	2.11	0.80
1:L:269:ASN:HD21	1:L:276:VAL:H	1.30	0.80
1:B:114:GLU:CD	1:B:114:GLU:H	1.90	0.79
1:E:162:ARG:HH11	1:E:162:ARG:HG3	1.47	0.79
1:L:266:GLU:O	1:L:270:GLU:HG3	1.82	0.79
1:J:113:LYS:O	1:J:114:GLU:HG3	1.83	0.79
1:F:248:GLU:HB3	1:G:227:ILE:HG23	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:TYR:OH	1:H:110:ARG:HA	1.83	0.79
1:L:91:THR:HG22	1:L:92:VAL:HG23	1.65	0.79
1:L:258:LEU:HD22	1:L:262:GLU:HG3	1.62	0.79
1:C:93:PHE:HB2	1:C:106:LEU:HD21	1.65	0.79
1:D:167:ASN:ND2	1:D:168:GLN:HE21	1.80	0.79
1:A:282:TYR:CE2	1:L:248:GLU:HA	2.18	0.79
1:I:168:GLN:HG2	1:I:188:HIS:CG	2.18	0.79
1:A:93:PHE:HB2	1:A:106:LEU:HD21	1.64	0.78
1:J:249:GLN:NE2	1:K:218:TRP:HE1	1.81	0.78
1:A:188:HIS:HB3	1:A:191:LEU:HD13	1.66	0.78
1:G:115:GLU:H	1:G:115:GLU:CD	1.91	0.78
1:J:258:LEU:HD22	1:J:262:GLU:HG3	1.66	0.78
1:L:107:TYR:HA	1:L:117:MET:HE3	1.66	0.78
1:J:49:ASN:C	1:J:49:ASN:HD22	1.91	0.77
1:J:55:LYS:O	1:J:59:GLN:HG3	1.83	0.77
1:H:12:ILE:HD12	1:H:12:ILE:H	1.49	0.77
1:J:213:GLN:HA	1:J:213:GLN:NE2	1.97	0.77
1:G:13:ASN:O	1:G:17:ARG:HG3	1.85	0.77
1:G:113:LYS:HA	1:G:117:MET:HE1	1.66	0.77
1:H:258:LEU:HD22	1:H:262:GLU:HG3	1.66	0.77
1:F:137:PHE:CG	1:F:221:MET:HG2	2.20	0.76
1:D:28:LEU:O	1:D:32:GLN:HG3	1.84	0.76
1:E:269:ASN:ND2	1:E:276:VAL:HG22	1.99	0.76
1:E:222:MET:HE3	1:E:227:ILE:HG21	1.68	0.76
1:B:168:GLN:HG2	1:B:188:HIS:CE1	2.20	0.76
1:E:89:GLN:NE2	1:E:108:ASN:HD21	1.83	0.76
1:G:205:TYR:CE2	1:G:207:VAL:HB	2.21	0.76
1:G:126:MET:HG2	1:G:128:PHE:CZ	2.20	0.75
1:K:14:GLU:CD	1:K:14:GLU:H	1.94	0.75
1:A:167:ASN:ND2	1:A:168:GLN:HG2	2.01	0.75
1:E:261:ARG:HH11	1:E:261:ARG:HG2	1.51	0.75
1:B:49:ASN:C	1:B:49:ASN:HD22	1.92	0.75
1:H:201:THR:HG21	2:I:310:HOH:O	1.86	0.75
1:A:222:MET:HE3	1:A:227:ILE:HG21	1.68	0.75
1:G:85:ASP:OD1	1:G:89:GLN:HB2	1.85	0.74
1:K:55:LYS:HG2	1:K:59:GLN:NE2	2.02	0.74
1:K:55:LYS:HG2	1:K:59:GLN:HE21	1.51	0.74
1:B:213:GLN:HG3	1:C:207:VAL:HG11	1.69	0.74
1:A:249:GLN:NE2	1:B:218:TRP:HE1	1.85	0.74
1:B:55:LYS:O	1:B:59:GLN:HG3	1.88	0.74
1:C:269:ASN:HD21	1:C:276:VAL:HG22	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:ASN:ND2	1:J:179:GLU:HG2	2.03	0.74
1:D:167:ASN:HD22	1:D:168:GLN:NE2	1.85	0.74
1:C:248:GLU:HB3	1:D:227:ILE:HG23	1.70	0.74
1:L:102:LYS:HD3	1:L:103:GLU:H	1.52	0.74
1:B:137:PHE:CB	1:B:221:MET:HE2	2.18	0.73
1:E:51:SER:O	1:E:55:LYS:HG3	1.88	0.73
1:G:145:LYS:O	1:G:145:LYS:HD3	1.88	0.73
1:C:249:GLN:HG2	1:D:222:MET:HE2	1.69	0.73
1:D:222:MET:HE3	1:D:227:ILE:HB	1.69	0.73
1:I:168:GLN:HG3	1:I:169:LEU:N	2.04	0.73
1:F:96:ALA:HB1	1:F:101:GLN:HG2	1.71	0.73
1:C:168:GLN:H	1:C:168:GLN:HE21	1.37	0.73
1:F:42:GLU:HG3	1:F:277:LYS:HB2	1.71	0.73
1:L:172:LYS:NZ	1:L:176:ASN:HD21	1.87	0.73
1:D:213:GLN:HE21	1:D:213:GLN:HA	1.54	0.72
1:A:106:LEU:HD22	1:A:120:VAL:HG23	1.69	0.72
1:A:167:ASN:HD22	1:A:168:GLN:H	1.36	0.72
1:C:264:ALA:HA	1:C:267:LYS:HE3	1.70	0.72
1:J:269:ASN:HD21	1:J:276:VAL:H	1.38	0.72
1:B:106:LEU:HD22	1:B:120:VAL:HG23	1.71	0.72
1:G:145:LYS:HD3	1:G:145:LYS:C	2.15	0.72
1:A:131:THR:O	1:A:135:GLU:HG3	1.90	0.71
1:D:93:PHE:HB2	1:D:106:LEU:HD21	1.70	0.71
1:J:222:MET:HE3	1:J:227:ILE:HG21	1.70	0.71
1:K:249:GLN:HG2	1:L:222:MET:HE2	1.71	0.71
1:J:188:HIS:CD2	1:J:190:ALA:H	2.08	0.71
1:B:114:GLU:HA	1:B:117:MET:SD	2.29	0.71
1:G:93:PHE:HB2	1:G:106:LEU:HD21	1.71	0.71
1:K:162:ARG:HG2	1:K:162:ARG:HH11	1.55	0.71
1:L:14:GLU:H	1:L:14:GLU:CD	1.99	0.71
1:A:264:ALA:HA	1:A:267:LYS:NZ	2.04	0.71
1:H:171:LEU:HD13	1:I:185:ILE:HD13	1.73	0.71
1:B:162:ARG:HG3	1:B:162:ARG:HH11	1.55	0.70
1:A:179:GLU:CD	1:A:179:GLU:H	2.00	0.70
1:L:102:LYS:HD3	1:L:103:GLU:N	2.05	0.70
1:B:269:ASN:ND2	1:B:275:ASN:HA	2.06	0.70
1:D:17:ARG:HG2	1:D:20:ARG:NH2	2.05	0.70
1:D:107:TYR:OH	1:D:110:ARG:HA	1.92	0.70
1:F:106:LEU:HD22	1:F:120:VAL:HG22	1.73	0.70
1:B:148:ILE:HG23	1:B:207:VAL:HG13	1.72	0.70
1:F:28:LEU:O	1:F:32:GLN:HG3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:LEU:HD22	1:G:48:ILE:HG21	1.73	0.70
1:B:96:ALA:O	1:B:97:SER:HB2	1.91	0.70
1:F:56:SER:HB2	1:F:63:VAL:HG11	1.72	0.70
1:H:168:GLN:CD	1:H:168:GLN:H	1.99	0.70
1:I:258:LEU:HD22	1:I:262:GLU:HG3	1.72	0.70
1:F:265:CYS:SG	1:F:276:VAL:HG23	2.31	0.70
1:H:157:THR:O	1:H:201:THR:HG23	1.92	0.70
1:C:192:ASP:HB2	1:C:194:ASP:OD1	1.91	0.70
1:H:107:TYR:CD2	1:H:271:LEU:HB2	2.27	0.70
1:H:269:ASN:HD21	1:H:276:VAL:HG22	1.55	0.70
1:H:269:ASN:HD21	1:H:276:VAL:H	1.39	0.70
1:B:111:ASP:O	1:B:112:MET:HG2	1.91	0.69
1:E:271:LEU:HD23	1:E:271:LEU:O	1.92	0.69
1:A:167:ASN:HD22	1:A:167:ASN:N	1.91	0.69
1:B:124:ASN:HD21	1:B:128:PHE:H	1.39	0.69
1:K:68:ASP:OD2	1:K:71:ILE:HG12	1.91	0.69
1:C:283:ASP:O	1:C:284:ILE:HG12	1.93	0.69
1:B:53:LEU:HD12	1:B:63:VAL:HG11	1.73	0.69
1:H:165:ASP:OD1	1:H:191:LEU:HD23	1.92	0.69
1:E:13:ASN:O	1:E:17:ARG:HG3	1.91	0.69
1:E:86:VAL:HG11	1:F:74:ILE:HD11	1.74	0.69
1:I:87:TYR:HD1	1:I:109:TYR:HH	1.41	0.68
1:B:93:PHE:HB2	1:B:106:LEU:HD21	1.75	0.68
1:F:137:PHE:CD1	1:F:221:MET:HE3	2.28	0.68
1:H:123:ASN:OD1	1:H:261:ARG:NH2	2.27	0.68
1:C:49:ASN:C	1:C:49:ASN:HD22	2.00	0.68
1:F:107:TYR:HB2	1:F:117:MET:HE3	1.76	0.68
1:J:144:LEU:HD21	1:K:152:GLN:NE2	2.08	0.68
1:D:227:ILE:O	1:D:228:LYS:HB3	1.94	0.68
1:E:269:ASN:HD21	1:E:276:VAL:H	1.41	0.68
1:D:40:GLU:HG3	1:D:281:ARG:HH21	1.59	0.68
1:E:148:ILE:HG23	1:E:207:VAL:HG13	1.76	0.68
1:I:98:PRO:HG2	1:I:100:TYR:H	1.59	0.68
1:B:166:ASN:ND2	1:C:187:ALA:HB1	2.08	0.68
1:I:167:ASN:HB2	1:J:189:GLU:OE2	1.94	0.68
1:G:105:LYS:HD2	1:G:105:LYS:H	1.58	0.67
1:B:65:PHE:CD2	1:B:268:ILE:HD12	2.30	0.67
1:K:107:TYR:HD2	1:K:271:LEU:HD13	1.58	0.67
1:G:167:ASN:HB3	1:G:168:GLN:NE2	2.09	0.67
1:A:44:LEU:HD12	1:A:44:LEU:H	1.60	0.67
1:H:84:ARG:NH1	1:H:84:ARG:HB3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:ASN:OD1	1:I:261:ARG:NH2	2.28	0.67
1:D:164:ASN:O	1:E:189:GLU:HA	1.95	0.67
1:K:45:PRO:HG3	1:K:274:LEU:HD11	1.77	0.67
1:D:106:LEU:HD22	1:D:120:VAL:HG23	1.76	0.66
1:F:96:ALA:HB2	1:F:101:GLN:HE21	1.61	0.66
1:G:113:LYS:HE2	1:G:270:GLU:HG3	1.76	0.66
1:I:283:ASP:O	1:I:284:ILE:HB	1.96	0.66
1:G:205:TYR:CZ	1:G:207:VAL:HB	2.30	0.66
1:L:123:ASN:OD1	1:L:261:ARG:NH2	2.28	0.66
1:C:267:LYS:HG2	2:C:313:HOH:O	1.95	0.66
1:A:222:MET:HE3	1:A:227:ILE:CG2	2.25	0.66
1:B:88:ASN:CG	1:B:88:ASN:O	2.38	0.66
1:D:213:GLN:HA	1:D:213:GLN:NE2	2.10	0.66
1:I:93:PHE:HB2	1:I:106:LEU:HD21	1.77	0.66
1:H:248:GLU:HG3	1:I:282:TYR:CD2	2.30	0.66
1:D:137:PHE:O	1:D:141:LEU:HD22	1.95	0.66
1:D:167:ASN:HD22	1:D:168:GLN:HE21	1.39	0.66
1:G:221:MET:HE3	1:G:225:LEU:HG	1.75	0.66
1:A:181:ASN:ND2	1:A:181:ASN:H	1.90	0.66
1:G:51:SER:O	1:G:55:LYS:HG3	1.95	0.66
1:I:167:ASN:HB2	1:J:189:GLU:CD	2.21	0.66
1:A:264:ALA:HA	1:A:267:LYS:HZ3	1.60	0.66
1:K:274:LEU:CD2	1:K:275:ASN:H	2.07	0.66
1:H:73:TYR:HE2	1:H:272:TYR:CD1	2.14	0.65
1:I:106:LEU:HD22	1:I:120:VAL:HG23	1.77	0.65
1:J:96:ALA:O	1:J:97:SER:HB2	1.94	0.65
1:K:98:PRO:HG2	1:K:100:TYR:H	1.59	0.65
1:B:137:PHE:CG	1:B:221:MET:HE2	2.31	0.65
1:E:12:ILE:HD12	1:E:12:ILE:H	1.61	0.65
1:I:144:LEU:HD21	1:J:152:GLN:NE2	2.12	0.65
1:D:16:GLN:O	1:D:20:ARG:HD3	1.95	0.65
1:L:49:ASN:C	1:L:49:ASN:HD22	2.02	0.65
1:D:21:ASN:HB2	2:D:322:HOH:O	1.96	0.65
1:F:82:GLY:HA3	1:F:92:VAL:HG23	1.79	0.65
1:F:213:GLN:HE21	1:F:213:GLN:HA	1.62	0.65
1:F:56:SER:HB2	1:F:63:VAL:CG1	2.26	0.65
1:K:107:TYR:CD2	1:K:271:LEU:HD13	2.32	0.65
1:F:213:GLN:HA	1:F:213:GLN:NE2	2.12	0.65
1:H:173:GLN:HG3	1:H:177:GLN:NE2	2.11	0.65
1:H:12:ILE:HD12	1:H:12:ILE:N	2.11	0.64
1:K:227:ILE:O	1:K:228:LYS:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:THR:HG23	1:G:92:VAL:HG23	1.79	0.64
1:H:269:ASN:ND2	1:H:276:VAL:HG22	2.13	0.64
1:I:269:ASN:HD21	1:I:276:VAL:HG13	1.63	0.64
1:K:47:THR:HG23	1:K:73:TYR:HB2	1.79	0.64
1:F:222:MET:HE3	1:F:227:ILE:HG21	1.80	0.64
1:H:167:ASN:HB2	1:H:168:GLN:NE2	2.13	0.64
1:C:12:ILE:HD12	1:C:12:ILE:N	2.12	0.64
1:D:148:ILE:O	1:D:152:GLN:HG3	1.98	0.64
1:G:265:CYS:SG	1:G:276:VAL:HG23	2.38	0.64
1:K:221:MET:HE2	1:K:225:LEU:HD13	1.78	0.64
1:E:160:LEU:HD23	1:F:184:VAL:HG12	1.79	0.64
1:F:86:VAL:HG12	1:G:100:TYR:HB2	1.80	0.64
1:J:35:ALA:O	1:J:38:LEU:HB2	1.98	0.64
1:C:168:GLN:H	1:C:168:GLN:NE2	1.95	0.64
1:C:167:ASN:HB2	1:D:189:GLU:CD	2.23	0.64
1:I:98:PRO:HA	2:I:325:HOH:O	1.98	0.64
1:C:41:TRP:CE3	1:C:278:VAL:HG13	2.32	0.63
1:C:106:LEU:HD22	1:C:120:VAL:HG23	1.80	0.63
1:F:268:ILE:HG22	1:F:274:LEU:HD12	1.80	0.63
1:I:19:LYS:HA	1:I:19:LYS:CE	2.29	0.63
1:B:107:TYR:OH	1:B:270:GLU:HG2	1.98	0.63
1:J:68:ASP:OD2	1:J:71:ILE:HG12	1.99	0.63
1:L:68:ASP:OD2	1:L:71:ILE:HG12	1.99	0.63
1:H:160:LEU:HD23	1:I:184:VAL:HG12	1.80	0.63
1:D:17:ARG:HG2	1:D:20:ARG:HH22	1.64	0.63
1:H:98:PRO:HG2	1:H:100:TYR:H	1.62	0.63
1:I:21:ASN:O	1:I:25:ILE:HG12	1.97	0.63
1:J:106:LEU:HD22	1:J:120:VAL:HG23	1.80	0.63
1:D:221:MET:O	1:D:221:MET:HE3	1.98	0.63
1:F:144:LEU:HD21	1:G:152:GLN:NE2	2.13	0.63
1:C:12:ILE:H	1:C:12:ILE:CD1	2.10	0.63
1:D:84:ARG:NH1	1:D:90:ALA:HB2	2.14	0.63
1:F:164:ASN:O	1:G:189:GLU:HA	1.99	0.63
1:J:123:ASN:OD1	1:J:261:ARG:NH2	2.32	0.63
1:B:110:ARG:HG3	1:B:111:ASP:N	2.14	0.63
1:G:128:PHE:CZ	1:H:29:ASN:ND2	2.67	0.63
1:K:213:GLN:HE21	1:K:213:GLN:HA	1.64	0.63
1:D:205:TYR:CE2	1:D:207:VAL:HB	2.34	0.62
1:E:249:GLN:HG3	1:F:222:MET:HE2	1.81	0.62
1:C:269:ASN:ND2	1:C:276:VAL:HG22	2.14	0.62
1:D:173:GLN:HG2	2:D:365:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:104:PHE:CE2	1:K:118:GLY:HA3	2.35	0.62
1:C:265:CYS:SG	1:C:276:VAL:HG23	2.39	0.62
1:E:272:TYR:HB2	1:E:274:LEU:HD13	1.81	0.62
1:G:37:GLN:HG2	1:G:281:ARG:HD2	1.80	0.62
1:F:20:ARG:HD2	1:F:146:GLU:OE2	1.99	0.62
1:K:73:TYR:HE2	1:K:272:TYR:CD1	2.17	0.62
1:J:13:ASN:HD21	1:L:179:GLU:HG2	1.61	0.62
1:J:49:ASN:C	1:J:49:ASN:ND2	2.57	0.62
1:C:145:LYS:HD3	1:C:145:LYS:C	2.24	0.62
1:F:34:LEU:O	1:F:37:GLN:HG3	2.00	0.62
1:F:93:PHE:CE2	1:F:95:ALA:HB2	2.35	0.62
1:G:106:LEU:HD22	1:G:120:VAL:HG23	1.80	0.62
1:H:272:TYR:HB2	1:H:274:LEU:HD23	1.82	0.62
1:J:110:ARG:O	1:J:111:ASP:C	2.41	0.62
1:A:167:ASN:ND2	1:A:168:GLN:H	1.98	0.62
1:G:172:LYS:HG3	2:G:327:HOH:O	1.98	0.62
1:A:35:ALA:O	1:A:38:LEU:HB2	2.01	0.61
1:H:113:LYS:HZ2	1:H:270:GLU:HG3	1.64	0.61
1:D:131:THR:O	1:D:135:GLU:HG3	2.00	0.61
1:H:222:MET:HE3	1:H:227:ILE:HG21	1.83	0.61
1:C:256:VAL:CG1	1:D:33:SER:HB2	2.31	0.61
1:E:94:ARG:HG2	1:E:103:GLU:OE2	2.00	0.61
1:J:222:MET:HE3	1:J:227:ILE:CG2	2.30	0.61
1:A:181:ASN:H	1:A:181:ASN:HD22	1.48	0.61
1:E:107:TYR:CB	1:E:271:LEU:HD12	2.30	0.61
1:A:96:ALA:CB	1:A:101:GLN:HG3	2.30	0.61
1:A:162:ARG:HG3	1:A:162:ARG:HH11	1.66	0.61
1:C:259:LYS:O	1:C:263:GLU:HG3	2.00	0.61
1:G:131:THR:HA	1:G:134:LEU:HD12	1.81	0.61
1:F:20:ARG:NH2	1:F:143:GLU:HG3	2.16	0.61
1:J:110:ARG:O	1:J:112:MET:N	2.34	0.61
1:F:118:GLY:HA2	1:F:272:TYR:OH	2.01	0.61
1:G:188:HIS:CD2	1:G:190:ALA:H	2.19	0.61
1:H:272:TYR:CB	1:H:274:LEU:HD23	2.31	0.61
1:H:283:ASP:CB	1:H:285:VAL:HG12	2.27	0.61
1:I:213:GLN:HA	1:I:213:GLN:HE21	1.66	0.61
1:C:94:ARG:HG2	1:C:103:GLU:HG2	1.81	0.60
1:H:227:ILE:O	1:H:228:LYS:HB3	2.00	0.60
1:K:167:ASN:OD1	1:L:189:GLU:HB3	2.01	0.60
1:E:12:ILE:HD12	1:E:12:ILE:N	2.16	0.60
1:K:222:MET:HE3	1:K:227:ILE:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:213:GLN:HE21	1:L:213:GLN:HA	1.66	0.60
1:B:113:LYS:O	1:B:113:LYS:HG3	2.02	0.60
1:D:13:ASN:O	1:D:17:ARG:HG3	2.00	0.60
1:I:221:MET:O	1:I:221:MET:HE3	2.02	0.60
1:A:258:LEU:HD13	1:A:262:GLU:OE1	2.01	0.60
1:F:41:TRP:CZ2	1:F:261:ARG:HG2	2.36	0.60
1:D:145:LYS:C	1:D:145:LYS:HD3	2.26	0.60
1:I:42:GLU:OE2	1:I:279:LYS:HD3	2.02	0.60
1:A:36:TYR:HD2	1:L:126:MET:HE1	1.67	0.60
1:A:97:SER:OG	1:A:98:PRO:HD3	2.02	0.60
1:F:13:ASN:ND2	1:H:179:GLU:HG2	2.16	0.60
1:F:98:PRO:HG2	1:F:100:TYR:H	1.66	0.60
1:K:258:LEU:HD22	1:K:262:GLU:HG3	1.83	0.60
1:F:94:ARG:HG2	1:F:103:GLU:OE1	2.01	0.60
1:A:164:ASN:OD1	1:A:195:SER:HA	2.00	0.60
1:B:11:SER:C	1:B:13:ASN:H	2.09	0.60
1:F:284:ILE:HD12	2:F:350:HOH:O	2.01	0.60
1:H:84:ARG:HB3	1:H:84:ARG:CZ	2.32	0.60
1:B:213:GLN:HG3	1:C:207:VAL:CG1	2.32	0.60
1:F:107:TYR:CD1	1:F:271:LEU:HD13	2.37	0.59
1:H:188:HIS:HD2	1:H:190:ALA:H	1.44	0.59
1:E:40:GLU:HB2	1:E:281:ARG:HE	1.67	0.59
1:E:128:PHE:HD2	1:E:129:PRO:CD	2.16	0.59
1:I:285:VAL:HB	2:I:362:HOH:O	2.02	0.59
1:K:114:GLU:HB2	1:K:117:MET:SD	2.42	0.59
1:K:131:THR:HB	1:K:132:PRO:HD3	1.84	0.59
1:F:264:ALA:O	1:F:268:ILE:HG12	2.02	0.59
1:G:258:LEU:HD13	1:G:262:GLU:HG3	1.84	0.59
1:A:41:TRP:C	1:A:44:LEU:HD11	2.27	0.59
1:B:164:ASN:O	1:C:189:GLU:HA	2.02	0.59
1:K:213:GLN:HA	1:K:213:GLN:NE2	2.18	0.59
1:L:93:PHE:HB2	1:L:106:LEU:HD21	1.83	0.59
1:G:202:ASP:HA	2:G:314:HOH:O	2.01	0.59
1:G:261:ARG:HG2	1:G:261:ARG:HH11	1.67	0.59
1:H:43:ASN:O	1:H:276:VAL:HG12	2.03	0.59
1:K:43:ASN:O	1:K:276:VAL:HG12	2.02	0.59
1:K:258:LEU:CD2	1:K:262:GLU:HG3	2.33	0.59
1:B:137:PHE:CD1	1:B:221:MET:HE2	2.38	0.59
1:B:284:ILE:HG23	1:B:284:ILE:O	2.03	0.59
1:F:42:GLU:CG	1:F:277:LYS:HB2	2.32	0.59
1:L:84:ARG:HG2	2:L:343:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:MET:CE	1:A:227:ILE:HG21	2.33	0.59
1:B:247:ASP:HB3	2:B:316:HOH:O	2.02	0.58
1:C:96:ALA:HB1	1:C:101:GLN:HG2	1.84	0.58
1:C:98:PRO:HG2	1:C:100:TYR:H	1.66	0.58
1:D:162:ARG:NH1	1:D:197:GLU:OE2	2.36	0.58
1:E:126:MET:HA	1:E:126:MET:HE3	1.83	0.58
1:C:87:TYR:HA	1:D:52:PHE:CE1	2.38	0.58
1:H:265:CYS:SG	1:H:276:VAL:HG23	2.44	0.58
1:E:96:ALA:O	1:E:97:SER:HB2	2.04	0.58
1:F:55:LYS:O	1:F:59:GLN:HG3	2.02	0.58
1:I:55:LYS:O	1:I:59:GLN:HG3	2.03	0.58
1:L:97:SER:OG	1:L:98:PRO:HD3	2.03	0.58
1:L:162:ARG:NH1	1:L:197:GLU:OE1	2.36	0.58
1:L:113:LYS:HA	1:L:117:MET:HE1	1.84	0.58
1:J:84:ARG:HD2	1:J:88:ASN:O	2.04	0.58
1:C:47:THR:CG2	1:C:73:TYR:HB2	2.33	0.58
1:F:248:GLU:HB3	1:G:227:ILE:CG2	2.32	0.58
1:G:223:THR:HG23	1:G:250:ILE:HD13	1.84	0.58
1:K:221:MET:HA	1:K:221:MET:HE3	1.86	0.58
1:I:168:GLN:HG2	1:I:188:HIS:CE1	2.38	0.58
1:L:105:LYS:N	1:L:105:LYS:HD2	2.18	0.58
1:L:168:GLN:HA	1:L:168:GLN:NE2	2.18	0.58
1:E:167:ASN:OD1	1:E:168:GLN:HG2	2.03	0.58
1:F:222:MET:HE3	1:F:227:ILE:CG2	2.33	0.58
1:G:213:GLN:HA	1:G:213:GLN:OE1	2.03	0.58
1:H:144:LEU:HD21	1:I:152:GLN:NE2	2.18	0.58
1:L:181:ASN:H	1:L:181:ASN:ND2	2.01	0.58
1:E:272:TYR:CB	1:E:274:LEU:HD13	2.33	0.58
1:H:113:LYS:NZ	1:H:270:GLU:HG3	2.19	0.58
1:I:49:ASN:C	1:I:49:ASN:HD22	2.11	0.58
1:B:71:ILE:HD11	1:B:74:ILE:HD12	1.85	0.58
1:D:143:GLU:OE2	1:E:153:ASN:ND2	2.26	0.58
1:F:96:ALA:CB	1:F:101:GLN:HG2	2.33	0.58
1:E:107:TYR:CD1	1:E:271:LEU:HB2	2.38	0.57
1:H:97:SER:OG	1:H:98:PRO:HD3	2.04	0.57
1:L:53:LEU:O	1:L:57:ILE:HG13	2.04	0.57
1:C:93:PHE:CE2	1:C:95:ALA:HB2	2.40	0.57
1:C:269:ASN:HD21	1:C:276:VAL:H	1.52	0.57
1:H:249:GLN:OE1	1:I:218:TRP:NE1	2.28	0.57
1:K:106:LEU:HD22	1:K:120:VAL:HG13	1.85	0.57
1:B:130:THR:C	1:B:132:PRO:HD2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ASN:O	1:D:189:GLU:HA	2.04	0.57
1:B:208:ASP:OD2	1:B:208:ASP:N	2.37	0.57
1:D:182:ALA:HB1	1:D:183:PRO:HD2	1.86	0.57
1:K:222:MET:HE3	1:K:227:ILE:CG2	2.33	0.57
1:A:99:VAL:CG2	1:L:86:VAL:HG12	2.33	0.57
1:C:47:THR:HG23	1:C:73:TYR:HB2	1.87	0.57
1:C:148:ILE:HG23	1:C:207:VAL:HG13	1.86	0.57
1:K:123:ASN:OD1	1:K:261:ARG:NH2	2.34	0.57
1:C:258:LEU:HD22	1:C:262:GLU:CG	2.34	0.57
1:H:164:ASN:O	1:I:189:GLU:HA	2.04	0.57
1:D:27:TYR:O	1:D:31:LEU:HG	2.03	0.57
1:H:107:TYR:CZ	1:H:110:ARG:HA	2.39	0.57
1:B:49:ASN:C	1:B:49:ASN:ND2	2.63	0.57
1:B:259:LYS:HE2	2:B:361:HOH:O	2.04	0.57
1:C:44:LEU:HD13	1:C:48:ILE:HG21	1.86	0.57
1:I:37:GLN:O	1:I:281:ARG:HD2	2.04	0.57
1:K:164:ASN:O	1:L:189:GLU:HA	2.04	0.57
1:B:168:GLN:CG	1:B:188:HIS:NE2	2.64	0.57
1:D:162:ARG:NH2	1:D:194:ASP:O	2.37	0.57
1:E:222:MET:HE3	1:E:227:ILE:CG2	2.35	0.57
1:E:261:ARG:HH11	1:E:261:ARG:CG	2.18	0.57
1:I:205:TYR:CZ	1:I:207:VAL:HB	2.40	0.57
1:C:258:LEU:HD22	1:C:262:GLU:HG3	1.87	0.57
1:G:172:LYS:O	1:G:176:ASN:ND2	2.38	0.57
1:J:123:ASN:HD22	1:J:124:ASN:ND2	2.03	0.56
1:G:71:ILE:O	1:G:72:SER:HB3	2.05	0.56
1:G:227:ILE:O	1:G:228:LYS:HB3	2.04	0.56
1:J:168:GLN:HG2	1:J:188:HIS:CD2	2.40	0.56
1:B:114:GLU:CD	1:B:114:GLU:N	2.62	0.56
1:C:259:LYS:HD2	1:D:281:ARG:NH1	2.20	0.56
1:C:283:ASP:O	1:C:284:ILE:CG1	2.53	0.56
1:F:66:TYR:HB2	1:F:104:PHE:CE2	2.40	0.56
1:H:12:ILE:H	1:H:12:ILE:CD1	2.17	0.56
1:I:47:THR:HG23	1:I:73:TYR:HB2	1.88	0.56
1:K:47:THR:CG2	1:K:73:TYR:HB2	2.35	0.56
1:L:68:ASP:OD1	1:L:69:PRO:HD2	2.04	0.56
1:A:249:GLN:HE21	1:B:218:TRP:HE1	1.52	0.56
1:E:107:TYR:HB2	1:E:271:LEU:HD12	1.87	0.56
1:E:128:PHE:HD2	1:E:129:PRO:HD2	1.71	0.56
1:E:250:ILE:N	1:E:250:ILE:HD12	2.20	0.56
1:F:13:ASN:O	1:F:17:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:GLN:NE2	1:F:178:TYR:HA	2.21	0.56
1:G:35:ALA:O	1:G:38:LEU:HB2	2.05	0.56
1:H:47:THR:HG23	1:H:73:TYR:HB2	1.87	0.56
1:K:89:GLN:HB3	1:K:108:ASN:ND2	2.09	0.56
1:L:98:PRO:HG2	1:L:100:TYR:H	1.69	0.56
1:B:112:MET:H	1:B:114:GLU:CD	2.12	0.56
1:F:188:HIS:CD2	1:F:190:ALA:H	2.24	0.56
1:G:113:LYS:CE	1:G:270:GLU:HG3	2.35	0.56
1:L:177:GLN:O	1:L:177:GLN:HG2	2.05	0.56
1:B:119:VAL:HB	1:B:268:ILE:CD1	2.36	0.56
1:F:53:LEU:HD22	1:F:63:VAL:HG21	1.88	0.56
1:H:213:GLN:HA	1:H:213:GLN:NE2	2.21	0.56
1:D:181:ASN:ND2	1:D:181:ASN:H	2.04	0.56
1:G:49:ASN:C	1:G:49:ASN:HD22	2.12	0.56
1:B:123:ASN:ND2	1:B:261:ARG:NH2	2.54	0.56
1:H:284:ILE:HD13	1:H:284:ILE:H	1.70	0.56
1:I:11:SER:O	1:I:12:ILE:HD13	2.05	0.56
1:A:17:ARG:HG3	1:A:20:ARG:HH12	1.71	0.56
1:C:258:LEU:O	1:C:262:GLU:HG3	2.06	0.56
1:E:259:LYS:HG3	1:E:260:SER:N	2.20	0.56
1:F:96:ALA:HB2	1:F:101:GLN:NE2	2.21	0.56
1:F:162:ARG:NH1	1:F:197:GLU:OE2	2.39	0.56
1:I:179:GLU:HB2	1:I:181:ASN:ND2	2.21	0.56
1:K:274:LEU:HD22	1:K:275:ASN:H	1.70	0.56
1:H:71:ILE:HG13	1:H:71:ILE:O	2.06	0.55
1:H:168:GLN:CD	1:H:168:GLN:N	2.63	0.55
1:H:284:ILE:HD13	1:H:284:ILE:N	2.21	0.55
1:C:11:SER:C	1:C:13:ASN:H	2.13	0.55
1:H:104:PHE:CE2	1:H:118:GLY:HA3	2.41	0.55
1:J:49:ASN:HD22	1:J:50:PRO:N	2.03	0.55
1:B:248:GLU:HA	1:C:282:TYR:CE2	2.41	0.55
1:J:41:TRP:CD2	1:J:278:VAL:HG13	2.41	0.55
1:A:41:TRP:CE3	1:A:278:VAL:HG13	2.41	0.55
1:C:41:TRP:CD2	1:C:278:VAL:HG13	2.41	0.55
1:G:259:LYS:HG3	1:G:260:SER:N	2.21	0.55
1:H:145:LYS:HD3	1:H:145:LYS:C	2.31	0.55
1:H:69:PRO:HD2	1:H:102:LYS:NZ	2.21	0.55
1:A:90:ALA:O	1:A:108:ASN:ND2	2.32	0.55
1:D:17:ARG:HG2	1:D:20:ARG:CZ	2.37	0.55
1:L:215:ASN:O	1:L:219:ASN:ND2	2.40	0.55
1:G:54:GLU:CD	1:G:261:ARG:HH12	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:LEU:HD22	1:H:120:VAL:CG2	2.36	0.55
1:A:41:TRP:CD2	1:A:278:VAL:HG13	2.42	0.55
1:H:69:PRO:HD2	1:H:102:LYS:HZ1	1.72	0.55
1:K:107:TYR:HB2	1:K:271:LEU:HD22	1.88	0.55
1:L:85:ASP:C	1:L:85:ASP:OD1	2.49	0.55
1:B:41:TRP:CD2	1:B:278:VAL:HG13	2.42	0.54
1:D:35:ALA:O	1:D:38:LEU:HB2	2.07	0.54
1:H:221:MET:HE2	1:H:225:LEU:HD13	1.88	0.54
1:L:213:GLN:HA	1:L:213:GLN:NE2	2.21	0.54
1:B:181:ASN:C	1:B:181:ASN:HD22	2.15	0.54
1:D:55:LYS:O	1:D:59:GLN:HG3	2.07	0.54
1:F:84:ARG:O	1:G:99:VAL:HG21	2.08	0.54
1:G:41:TRP:CD2	1:G:278:VAL:HG13	2.42	0.54
1:G:53:LEU:HD12	1:G:63:VAL:HG11	1.87	0.54
1:C:162:ARG:HH11	1:C:162:ARG:CG	2.17	0.54
1:D:17:ARG:HA	1:D:20:ARG:CZ	2.36	0.54
1:D:102:LYS:HG3	1:D:103:GLU:N	2.23	0.54
1:F:43:ASN:N	1:F:43:ASN:HD22	2.04	0.54
1:F:107:TYR:CB	1:F:271:LEU:HD22	2.38	0.54
1:J:249:GLN:HE22	1:K:218:TRP:HE1	1.52	0.54
1:A:36:TYR:CD2	1:L:126:MET:HE1	2.43	0.54
1:A:213:GLN:NE2	1:A:213:GLN:HA	2.22	0.54
1:B:113:LYS:O	1:B:113:LYS:CG	2.55	0.54
1:J:162:ARG:HG2	1:J:162:ARG:HH11	1.71	0.54
1:A:167:ASN:CG	1:A:168:GLN:HE21	2.16	0.54
1:C:49:ASN:C	1:C:49:ASN:ND2	2.65	0.54
1:D:205:TYR:CZ	1:D:207:VAL:HB	2.42	0.54
1:F:119:VAL:HB	1:F:268:ILE:CD1	2.38	0.54
1:G:257:PHE:O	1:G:261:ARG:CD	2.53	0.54
1:L:222:MET:HE3	1:L:227:ILE:CG2	2.37	0.54
1:A:181:ASN:HD22	1:A:181:ASN:N	2.04	0.54
1:B:205:TYR:CZ	1:B:207:VAL:HB	2.43	0.54
1:D:167:ASN:ND2	1:D:168:GLN:NE2	2.47	0.54
1:A:44:LEU:HD12	1:A:44:LEU:N	2.21	0.54
1:A:167:ASN:HD22	1:A:168:GLN:N	2.04	0.54
1:C:248:GLU:HB3	1:D:227:ILE:CG2	2.37	0.54
1:D:97:SER:OG	1:D:98:PRO:HD3	2.08	0.54
1:K:130:THR:HG22	1:K:134:LEU:HG	1.89	0.54
1:K:144:LEU:O	1:K:148:ILE:HG13	2.07	0.54
1:A:47:THR:HG23	1:A:73:TYR:HB2	1.88	0.54
1:A:164:ASN:O	1:B:189:GLU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:MET:HA	1:B:112:MET:HE2	1.90	0.54
1:B:259:LYS:HG3	1:B:260:SER:N	2.23	0.54
1:A:222:MET:HE2	1:L:249:GLN:HG2	1.90	0.53
1:C:170:SER:HB3	1:C:173:GLN:HB2	1.90	0.53
1:E:126:MET:HE1	1:F:55:LYS:HD3	1.90	0.53
1:A:37:GLN:O	1:A:281:ARG:HD2	2.09	0.53
1:A:96:ALA:HB1	1:A:101:GLN:HG3	1.90	0.53
1:C:84:ARG:O	1:D:99:VAL:HG21	2.08	0.53
1:C:114:GLU:HG2	1:C:117:MET:HE3	1.90	0.53
1:G:53:LEU:O	1:G:57:ILE:HG13	2.08	0.53
1:B:271:LEU:HD23	1:B:272:TYR:CE1	2.43	0.53
1:K:53:LEU:HD12	1:K:63:VAL:HG11	1.90	0.53
1:B:264:ALA:O	1:B:268:ILE:HG12	2.08	0.53
1:I:109:TYR:HB2	1:I:112:MET:HG2	1.90	0.53
1:K:67:LYS:HB2	1:K:272:TYR:CE1	2.43	0.53
1:F:112:MET:HG2	1:F:113:LYS:N	2.22	0.53
1:E:98:PRO:HG2	1:E:100:TYR:H	1.73	0.53
1:F:35:ALA:O	1:F:38:LEU:HB2	2.09	0.53
1:K:162:ARG:HG2	1:K:162:ARG:NH1	2.22	0.53
1:I:110:ARG:HD3	1:I:270:GLU:OE2	2.09	0.53
1:I:203:ALA:HB1	1:J:158:PRO:HG3	1.91	0.53
1:K:53:LEU:O	1:K:57:ILE:HG13	2.08	0.53
1:L:168:GLN:HA	1:L:168:GLN:HE21	1.73	0.53
1:B:145:LYS:HD3	1:B:145:LYS:C	2.34	0.53
1:E:35:ALA:O	1:E:38:LEU:HB2	2.09	0.53
1:F:269:ASN:OD1	1:F:276:VAL:HG22	2.08	0.53
1:L:222:MET:HE3	1:L:227:ILE:HG21	1.90	0.53
1:E:89:GLN:NE2	1:E:108:ASN:ND2	2.56	0.53
1:F:96:ALA:O	1:F:97:SER:HB2	2.08	0.53
1:F:178:TYR:CZ	1:F:180:GLY:HA2	2.43	0.53
1:C:256:VAL:HG11	1:D:33:SER:HB2	1.89	0.53
1:D:41:TRP:CZ3	1:D:278:VAL:HG22	2.43	0.53
1:E:43:ASN:O	1:E:276:VAL:HG12	2.09	0.53
1:E:162:ARG:HG3	1:E:162:ARG:NH1	2.21	0.53
1:F:113:LYS:HG3	1:F:114:GLU:H	1.73	0.53
1:A:170:SER:HB3	1:A:173:GLN:HB2	1.90	0.52
1:C:213:GLN:HA	1:C:213:GLN:NE2	2.25	0.52
1:C:255:THR:O	1:C:259:LYS:HG2	2.09	0.52
1:K:214:LYS:HE3	2:K:315:HOH:O	2.09	0.52
1:A:41:TRP:HB2	1:A:44:LEU:HD21	1.91	0.52
1:B:227:ILE:O	1:B:228:LYS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ILE:HG23	1:D:207:VAL:HG13	1.91	0.52
1:D:259:LYS:NZ	1:D:259:LYS:HB3	2.24	0.52
1:I:271:LEU:O	1:I:271:LEU:HD22	2.08	0.52
1:J:131:THR:OG1	1:J:132:PRO:HD3	2.09	0.52
1:K:97:SER:OG	1:K:98:PRO:HD3	2.09	0.52
1:L:88:ASN:CG	1:L:88:ASN:O	2.52	0.52
1:B:68:ASP:OD1	1:B:69:PRO:HD2	2.09	0.52
1:H:93:PHE:CE2	1:H:95:ALA:HB2	2.44	0.52
1:L:126:MET:HG2	1:L:128:PHE:CZ	2.44	0.52
1:D:107:TYR:HB2	1:D:117:MET:HG2	1.92	0.52
1:F:137:PHE:CD2	1:F:221:MET:HG2	2.44	0.52
1:G:265:CYS:O	1:G:269:ASN:ND2	2.43	0.52
1:I:221:MET:HE2	1:I:225:LEU:HD13	1.91	0.52
2:I:356:HOH:O	1:J:22:ARG:HD3	2.09	0.52
1:B:124:ASN:HD22	1:B:126:MET:H	1.56	0.52
1:B:166:ASN:HD21	1:C:187:ALA:HB1	1.73	0.52
1:D:84:ARG:HH12	1:D:90:ALA:HB2	1.74	0.52
1:D:98:PRO:HA	2:D:326:HOH:O	2.10	0.52
1:D:174:VAL:HG21	1:D:186:PHE:HD1	1.75	0.52
1:I:213:GLN:HA	1:I:213:GLN:NE2	2.25	0.52
1:J:126:MET:HG2	1:J:128:PHE:CE1	2.45	0.52
1:L:41:TRP:CD2	1:L:278:VAL:HG13	2.44	0.52
1:L:51:SER:O	1:L:55:LYS:HG3	2.10	0.52
1:A:145:LYS:NZ	1:L:140:GLU:OE1	2.42	0.52
1:C:14:GLU:HG2	1:C:15:ILE:N	2.24	0.52
1:A:98:PRO:HG2	1:A:100:TYR:H	1.74	0.52
1:A:222:MET:CE	1:L:249:GLN:HG2	2.39	0.52
1:D:14:GLU:O	1:D:18:GLN:HG2	2.09	0.52
1:I:221:MET:CE	1:I:225:LEU:HD13	2.40	0.52
1:B:166:ASN:CG	1:C:187:ALA:HB1	2.35	0.52
1:B:178:TYR:CZ	1:B:180:GLY:HA2	2.44	0.52
1:C:43:ASN:HB2	1:C:276:VAL:HA	1.90	0.52
1:C:73:TYR:CE2	1:C:274:LEU:HD11	2.45	0.52
1:D:87:TYR:OH	1:E:48:ILE:HA	2.10	0.52
1:D:163:ALA:HB3	1:E:187:ALA:HB2	1.92	0.52
1:E:53:LEU:HD12	1:E:63:VAL:HG11	1.91	0.52
1:F:47:THR:CG2	1:F:73:TYR:HB2	2.39	0.52
1:I:143:GLU:HB2	2:I:331:HOH:O	2.10	0.52
1:L:195:SER:O	1:L:196:ILE:HD13	2.10	0.52
1:A:167:ASN:ND2	1:A:167:ASN:N	2.53	0.52
1:B:137:PHE:HB2	1:B:221:MET:CE	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLU:HA	1:C:282:TYR:CZ	2.45	0.52
1:F:131:THR:HB	1:F:132:PRO:HD3	1.92	0.52
1:H:277:LYS:HE3	1:H:278:VAL:H	1.74	0.52
1:I:97:SER:OG	1:I:98:PRO:HD3	2.09	0.52
1:I:227:ILE:O	1:I:228:LYS:HB3	2.10	0.52
1:L:20:ARG:NH1	1:L:143:GLU:HG3	2.25	0.52
1:F:93:PHE:HE2	1:F:95:ALA:HB2	1.74	0.51
1:F:258:LEU:HD22	1:F:262:GLU:HG3	1.91	0.51
1:G:22:ARG:HD2	2:G:317:HOH:O	2.10	0.51
1:H:110:ARG:HG2	1:H:270:GLU:HG2	1.92	0.51
1:I:85:ASP:OD1	1:I:87:TYR:N	2.39	0.51
1:J:222:MET:CE	1:J:227:ILE:HG21	2.39	0.51
1:A:47:THR:CG2	1:A:73:TYR:HB2	2.40	0.51
1:D:125:ASP:OD2	1:D:259:LYS:HE2	2.11	0.51
1:F:160:LEU:HD23	1:G:184:VAL:HG12	1.90	0.51
1:F:221:MET:HE2	1:F:221:MET:HA	1.91	0.51
1:E:107:TYR:OH	1:E:110:ARG:HA	2.08	0.51
1:H:209:LYS:HD3	1:I:205:TYR:CD2	2.45	0.51
1:L:205:TYR:CZ	1:L:207:VAL:HB	2.45	0.51
1:E:110:ARG:HG2	1:E:111:ASP:OD1	2.10	0.51
1:I:258:LEU:HD22	1:I:262:GLU:CG	2.38	0.51
1:J:13:ASN:ND2	1:L:179:GLU:HG2	2.25	0.51
1:C:114:GLU:HG2	1:C:117:MET:CE	2.39	0.51
1:D:146:GLU:O	1:D:150:VAL:HG23	2.10	0.51
1:H:107:TYR:CD2	1:H:271:LEU:HD13	2.46	0.51
1:C:93:PHE:HE2	1:C:95:ALA:HB2	1.75	0.51
1:E:68:ASP:OD1	1:E:69:PRO:HD2	2.09	0.51
1:F:41:TRP:HB3	1:F:44:LEU:CD1	2.41	0.51
1:G:249:GLN:HG2	1:H:222:MET:HE2	1.93	0.51
1:J:12:ILE:HD13	1:J:12:ILE:N	2.24	0.51
1:K:119:VAL:HG21	1:K:268:ILE:HG13	1.93	0.51
1:K:169:LEU:HD23	1:K:170:SER:H	1.76	0.51
1:K:249:GLN:HG2	1:L:222:MET:CE	2.38	0.51
1:A:188:HIS:HB3	1:A:191:LEU:CD1	2.37	0.51
1:A:221:MET:HE2	1:A:225:LEU:HD22	1.92	0.51
1:C:100:TYR:CE1	1:C:102:LYS:HB2	2.45	0.51
1:E:249:GLN:NE2	1:F:218:TRP:HE1	2.07	0.51
1:I:249:GLN:HG2	1:J:222:MET:HE2	1.91	0.51
1:B:133:THR:HG22	1:B:221:MET:HE1	1.92	0.51
1:D:145:LYS:HG2	2:D:338:HOH:O	2.11	0.51
1:H:173:GLN:HG3	1:H:177:GLN:HE22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:209:LYS:HB3	1:I:205:TYR:CE2	2.46	0.51
1:A:259:LYS:O	1:A:263:GLU:HG3	2.11	0.51
1:B:14:GLU:HG3	1:B:15:ILE:N	2.25	0.51
1:D:87:TYR:CD1	1:E:49:ASN:HB2	2.46	0.51
1:E:264:ALA:HA	1:E:267:LYS:HD3	1.92	0.51
1:F:202:ASP:HA	2:F:328:HOH:O	2.10	0.51
1:B:164:ASN:OD1	1:B:195:SER:HA	2.10	0.51
1:H:131:THR:HB	1:H:132:PRO:HD3	1.93	0.51
1:I:178:TYR:CZ	1:I:180:GLY:HA2	2.46	0.51
1:J:54:GLU:OE1	1:J:261:ARG:NH1	2.43	0.51
1:K:94:ARG:HH21	1:K:94:ARG:HG3	1.75	0.51
1:K:106:LEU:CD2	1:K:120:VAL:HG13	2.41	0.51
1:K:222:MET:CE	1:K:227:ILE:HG21	2.40	0.51
1:L:49:ASN:C	1:L:49:ASN:ND2	2.69	0.51
1:L:67:LYS:HB2	1:L:73:TYR:CE2	2.46	0.51
1:L:165:ASP:HB2	1:L:195:SER:OG	2.10	0.51
1:B:96:ALA:HB1	1:B:101:GLN:HE21	1.76	0.50
1:F:41:TRP:CD2	1:F:278:VAL:HG13	2.46	0.50
1:F:255:THR:CG2	1:G:281:ARG:HD3	2.32	0.50
1:K:53:LEU:CD1	1:K:63:VAL:HG11	2.41	0.50
1:C:53:LEU:HD12	1:C:63:VAL:HG11	1.93	0.50
1:E:162:ARG:HH11	1:E:162:ARG:CG	2.22	0.50
1:G:107:TYR:HB2	1:G:117:MET:HE3	1.93	0.50
1:H:106:LEU:HD22	1:H:120:VAL:HG23	1.92	0.50
1:I:168:GLN:HG2	1:I:188:HIS:NE2	2.26	0.50
1:K:93:PHE:HB2	1:K:106:LEU:HD21	1.93	0.50
1:C:107:TYR:O	1:C:108:ASN:C	2.55	0.50
1:K:104:PHE:CD2	1:K:118:GLY:HA3	2.46	0.50
1:K:260:SER:HA	1:K:263:GLU:OE2	2.11	0.50
1:F:258:LEU:HD12	1:F:280:PHE:CE1	2.47	0.50
1:I:168:GLN:CG	1:I:169:LEU:N	2.65	0.50
1:J:106:LEU:CD2	1:J:120:VAL:HG23	2.41	0.50
1:J:221:MET:HE2	1:J:225:LEU:HD13	1.93	0.50
1:A:49:ASN:C	1:A:49:ASN:ND2	2.53	0.50
1:A:282:TYR:CE1	1:L:248:GLU:HB2	2.47	0.50
1:D:178:TYR:CZ	1:D:180:GLY:HA2	2.46	0.50
1:D:218:TRP:O	1:D:222:MET:HG2	2.11	0.50
1:F:179:GLU:OE2	1:F:180:GLY:N	2.45	0.50
1:G:128:PHE:CE1	1:H:29:ASN:ND2	2.80	0.50
1:H:23:TRP:CD1	1:H:145:LYS:HD2	2.45	0.50
1:K:66:TYR:HB2	1:K:104:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:LYS:NZ	1:G:149:SER:OG	2.42	0.50
1:I:102:LYS:HD3	1:I:103:GLU:H	1.76	0.50
1:F:119:VAL:HB	1:F:268:ILE:HD13	1.93	0.50
1:I:168:GLN:HG3	1:I:169:LEU:H	1.75	0.50
1:F:115:GLU:CD	1:F:115:GLU:H	2.19	0.50
1:F:148:ILE:HG23	1:F:207:VAL:HG13	1.94	0.50
1:H:47:THR:CG2	1:H:73:TYR:HB2	2.41	0.50
1:K:219:ASN:O	1:K:223:THR:HG23	2.12	0.50
1:J:209:LYS:HB3	1:K:205:TYR:CE2	2.47	0.50
1:C:168:GLN:NE2	1:C:168:GLN:N	2.59	0.49
1:D:68:ASP:OD2	1:D:71:ILE:HG12	2.11	0.49
1:F:56:SER:CB	1:F:63:VAL:HG12	2.42	0.49
1:B:258:LEU:HD13	1:B:258:LEU:C	2.36	0.49
1:K:209:LYS:HB3	1:L:205:TYR:CE2	2.47	0.49
1:L:54:GLU:OE1	1:L:261:ARG:NH1	2.44	0.49
1:B:163:ALA:O	1:B:166:ASN:ND2	2.41	0.49
1:C:169:LEU:HB3	1:C:186:PHE:HE1	1.77	0.49
1:I:49:ASN:C	1:I:49:ASN:ND2	2.71	0.49
1:A:99:VAL:HG22	1:L:86:VAL:HA	1.94	0.49
1:F:41:TRP:HB3	1:F:44:LEU:HD13	1.94	0.49
1:F:120:VAL:HB	1:F:122:TYR:CE1	2.48	0.49
1:G:12:ILE:HG22	1:G:12:ILE:O	2.11	0.49
1:I:19:LYS:O	1:I:22:ARG:HB2	2.12	0.49
1:I:162:ARG:NH1	1:J:193:SER:HA	2.27	0.49
1:F:43:ASN:O	1:F:276:VAL:HG12	2.12	0.49
1:F:106:LEU:HD22	1:F:120:VAL:CG2	2.42	0.49
1:G:255:THR:O	1:G:259:LYS:HG2	2.12	0.49
1:H:165:ASP:OD1	1:H:195:SER:HB3	2.12	0.49
1:K:178:TYR:CE2	1:K:184:VAL:HG22	2.48	0.49
1:A:145:LYS:HZ3	1:L:140:GLU:CD	2.19	0.49
1:A:167:ASN:ND2	1:A:168:GLN:N	2.60	0.49
1:C:162:ARG:HG3	1:C:162:ARG:NH1	2.23	0.49
1:E:249:GLN:CD	1:F:218:TRP:HE1	2.21	0.49
1:G:228:LYS:HB3	1:G:228:LYS:NZ	2.27	0.49
1:H:249:GLN:HG2	1:I:222:MET:HE2	1.95	0.49
1:I:66:TYR:HB2	1:I:104:PHE:CZ	2.47	0.49
1:J:131:THR:O	1:J:135:GLU:HG3	2.13	0.49
1:K:197:GLU:HG2	1:K:199:PHE:CE1	2.47	0.49
1:C:51:SER:OG	1:C:55:LYS:HD2	2.13	0.49
1:F:115:GLU:N	1:F:115:GLU:OE1	2.45	0.49
1:J:97:SER:HB3	1:J:98:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLN:HG2	1:B:281:ARG:CD	2.37	0.49
1:C:11:SER:C	1:C:13:ASN:N	2.70	0.49
1:C:28:LEU:O	1:C:32:GLN:HG3	2.11	0.49
1:D:12:ILE:HG23	1:D:15:ILE:HD12	1.94	0.49
1:E:34:LEU:O	1:E:37:GLN:NE2	2.46	0.49
1:E:227:ILE:O	1:E:228:LYS:HB3	2.12	0.49
1:E:271:LEU:HD23	1:E:271:LEU:C	2.37	0.49
1:F:169:LEU:HD23	1:F:170:SER:H	1.78	0.49
1:G:98:PRO:HG2	1:G:100:TYR:H	1.78	0.49
1:J:203:ALA:HB1	1:K:158:PRO:HG3	1.94	0.49
1:L:172:LYS:HZ2	1:L:176:ASN:HD21	1.61	0.49
1:C:55:LYS:HB3	1:C:59:GLN:NE2	2.27	0.49
1:C:258:LEU:HD12	1:C:280:PHE:CE1	2.48	0.49
1:D:16:GLN:HE21	1:D:16:GLN:HA	1.77	0.49
1:E:106:LEU:CD1	1:E:120:VAL:HG13	2.42	0.49
1:E:178:TYR:CZ	1:E:180:GLY:HA2	2.47	0.49
1:F:148:ILE:O	1:F:152:GLN:HG2	2.13	0.49
1:F:227:ILE:HG22	1:F:228:LYS:N	2.28	0.49
1:H:172:LYS:HD3	2:I:368:HOH:O	2.11	0.49
1:J:93:PHE:HB2	1:J:106:LEU:HD21	1.95	0.49
1:J:108:ASN:O	1:J:109:TYR:CD1	2.66	0.49
1:A:49:ASN:HD22	1:A:50:PRO:N	2.09	0.49
1:A:221:MET:HE3	1:A:221:MET:HA	1.94	0.49
1:B:51:SER:O	1:B:55:LYS:HG3	2.13	0.49
1:B:53:LEU:CD1	1:B:63:VAL:HG11	2.42	0.49
1:B:123:ASN:ND2	1:B:261:ARG:HH21	2.11	0.49
1:C:136:LEU:HD13	1:D:22:ARG:HD2	1.95	0.49
1:F:66:TYR:HB2	1:F:104:PHE:CZ	2.47	0.49
1:K:87:TYR:OH	1:L:48:ILE:HD13	2.13	0.49
1:L:168:GLN:HE21	1:L:168:GLN:CA	2.26	0.49
1:C:73:TYR:HE2	1:C:272:TYR:CD1	2.31	0.48
1:F:13:ASN:HD21	1:H:179:GLU:HG2	1.77	0.48
1:F:124:ASN:HA	1:F:260:SER:OG	2.13	0.48
1:F:248:GLU:HG2	1:G:282:TYR:CE2	2.47	0.48
1:G:25:ILE:HG22	1:G:29:ASN:ND2	2.28	0.48
1:G:114:GLU:H	1:G:117:MET:HE2	1.78	0.48
1:H:67:LYS:HD3	1:H:73:TYR:CZ	2.48	0.48
1:J:209:LYS:HD3	1:K:205:TYR:CD2	2.48	0.48
1:K:163:ALA:HB3	1:L:187:ALA:HB2	1.95	0.48
1:K:249:GLN:CG	1:L:222:MET:HE2	2.40	0.48
1:L:221:MET:HE2	1:L:225:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TYR:CZ	1:L:248:GLU:HA	2.47	0.48
1:C:256:VAL:HG13	1:D:33:SER:HB2	1.95	0.48
1:F:96:ALA:CB	1:F:101:GLN:HE21	2.24	0.48
1:K:137:PHE:CD2	1:K:221:MET:HB2	2.49	0.48
1:A:169:LEU:HD23	1:A:170:SER:H	1.78	0.48
1:D:31:LEU:HB3	1:D:134:LEU:HD22	1.96	0.48
1:E:258:LEU:O	1:E:258:LEU:HD22	2.13	0.48
1:G:192:ASP:HB2	1:G:194:ASP:OD1	2.13	0.48
1:J:167:ASN:HD21	1:K:189:GLU:HB3	1.77	0.48
1:G:160:LEU:HD23	1:H:184:VAL:HG12	1.94	0.48
1:H:221:MET:HE3	1:H:221:MET:HA	1.94	0.48
1:K:31:LEU:HB3	1:K:134:LEU:HD22	1.96	0.48
1:K:113:LYS:HE2	1:K:271:LEU:HA	1.94	0.48
1:L:71:ILE:O	1:L:72:SER:OG	2.25	0.48
1:C:11:SER:HB3	1:C:12:ILE:HD12	1.95	0.48
1:F:115:GLU:C	1:F:117:MET:N	2.70	0.48
1:F:168:GLN:HG2	1:F:188:HIS:CD2	2.48	0.48
1:A:255:THR:HG21	1:B:281:ARG:HD3	1.95	0.48
1:C:44:LEU:HD13	1:C:48:ILE:CG2	2.43	0.48
1:H:249:GLN:CG	1:I:222:MET:HE2	2.43	0.48
1:I:96:ALA:O	1:I:97:SER:CB	2.61	0.48
1:K:284:ILE:HG23	1:K:284:ILE:O	2.13	0.48
1:L:122:TYR:O	1:L:260:SER:OG	2.30	0.48
1:B:131:THR:N	1:B:132:PRO:HD2	2.28	0.48
1:G:164:ASN:O	1:H:189:GLU:HA	2.14	0.48
1:L:227:ILE:O	1:L:228:LYS:HB3	2.14	0.48
1:C:167:ASN:ND2	1:C:167:ASN:O	2.46	0.48
2:J:350:HOH:O	1:K:200:LYS:HE3	2.14	0.48
1:K:96:ALA:O	1:K:97:SER:CB	2.62	0.48
1:F:205:TYR:CZ	1:F:207:VAL:HB	2.48	0.48
1:G:162:ARG:NH1	1:G:197:GLU:OE1	2.46	0.48
1:H:107:TYR:CE2	1:H:271:LEU:HB2	2.48	0.48
1:K:259:LYS:O	1:K:263:GLU:HG2	2.13	0.48
1:C:255:THR:CG2	1:D:281:ARG:HD3	2.35	0.48
1:K:93:PHE:CE2	1:K:95:ALA:HB2	2.49	0.48
1:L:283:ASP:O	1:L:285:VAL:N	2.47	0.48
1:C:131:THR:HB	1:C:132:PRO:HD3	1.95	0.47
1:C:145:LYS:HD3	1:C:145:LYS:O	2.14	0.47
1:C:252:SER:O	1:C:256:VAL:HG23	2.14	0.47
1:D:179:GLU:HB2	2:D:336:HOH:O	2.14	0.47
1:E:219:ASN:OD1	1:E:228:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:CYS:SG	1:E:276:VAL:HG23	2.54	0.47
1:L:178:TYR:CZ	1:L:180:GLY:HA2	2.49	0.47
1:A:93:PHE:CE2	1:A:95:ALA:HB2	2.48	0.47
1:C:167:ASN:ND2	1:C:167:ASN:C	2.72	0.47
1:G:68:ASP:CG	1:G:71:ILE:HG12	2.39	0.47
1:H:107:TYR:CG	1:H:271:LEU:HD13	2.49	0.47
1:K:125:ASP:OD1	1:K:259:LYS:NZ	2.40	0.47
1:D:249:GLN:HG2	1:E:222:MET:HE2	1.95	0.47
1:E:104:PHE:CE2	1:E:118:GLY:HA3	2.49	0.47
1:G:144:LEU:HD21	1:H:152:GLN:NE2	2.30	0.47
1:L:19:LYS:HA	1:L:22:ARG:NH1	2.30	0.47
1:A:189:GLU:HA	1:L:164:ASN:O	2.14	0.47
1:B:12:ILE:HG22	1:B:12:ILE:O	2.13	0.47
1:B:269:ASN:HD21	1:B:275:ASN:HA	1.76	0.47
1:C:125:ASP:OD2	1:C:259:LYS:HE3	2.14	0.47
1:C:213:GLN:HA	1:C:213:GLN:HE21	1.80	0.47
1:D:87:TYR:CE1	1:E:47:THR:O	2.68	0.47
1:G:87:TYR:CD1	1:H:49:ASN:HB2	2.49	0.47
1:H:140:GLU:OE1	1:I:145:LYS:HE3	2.14	0.47
1:K:71:ILE:O	1:K:72:SER:HB3	2.14	0.47
1:L:12:ILE:HG22	1:L:12:ILE:O	2.13	0.47
1:D:91:THR:HG23	1:D:92:VAL:HG23	1.97	0.47
1:F:37:GLN:O	1:F:281:ARG:HD2	2.14	0.47
1:I:204:PRO:HD2	2:I:319:HOH:O	2.14	0.47
1:J:164:ASN:O	1:K:189:GLU:HA	2.14	0.47
1:J:221:MET:CE	1:J:225:LEU:HD13	2.44	0.47
1:L:153:ASN:CG	1:L:156:LYS:HZ3	2.22	0.47
1:F:53:LEU:HD13	1:F:53:LEU:C	2.40	0.47
1:F:56:SER:CB	1:F:63:VAL:CG1	2.93	0.47
1:G:249:GLN:HG2	1:H:222:MET:CE	2.45	0.47
1:H:162:ARG:NH1	1:H:197:GLU:OE1	2.48	0.47
1:I:85:ASP:OD1	1:I:85:ASP:C	2.57	0.47
1:K:168:GLN:HG3	1:K:188:HIS:NE2	2.30	0.47
1:A:213:GLN:HA	1:A:213:GLN:HE21	1.78	0.47
1:B:67:LYS:HB2	1:B:272:TYR:CE2	2.50	0.47
1:B:119:VAL:HB	1:B:268:ILE:HD13	1.96	0.47
1:C:14:GLU:HG2	1:C:15:ILE:H	1.80	0.47
1:D:145:LYS:HD3	1:D:145:LYS:O	2.13	0.47
1:E:200:LYS:HG2	2:E:335:HOH:O	2.13	0.47
1:I:87:TYR:HD1	1:I:109:TYR:OH	1.97	0.47
1:K:42:GLU:HB2	1:K:277:LYS:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:PHE:HB3	1:K:119:VAL:HG23	1.97	0.47
1:K:84:ARG:NH1	1:K:90:ALA:HB2	2.30	0.47
1:L:172:LYS:NZ	1:L:176:ASN:ND2	2.59	0.47
1:B:112:MET:N	1:B:114:GLU:OE1	2.44	0.47
1:B:203:ALA:O	1:B:204:PRO:C	2.57	0.47
1:D:17:ARG:HG2	1:D:20:ARG:NH1	2.29	0.47
1:D:265:CYS:SG	1:D:276:VAL:HG22	2.55	0.47
1:F:113:LYS:HG3	1:F:114:GLU:N	2.30	0.47
1:H:178:TYR:CZ	1:H:180:GLY:HA2	2.50	0.47
1:I:218:TRP:O	1:I:222:MET:HG2	2.15	0.47
1:J:37:GLN:O	1:J:281:ARG:HD2	2.14	0.47
2:J:332:HOH:O	1:K:228:LYS:HD2	2.13	0.47
1:A:252:SER:O	1:A:256:VAL:HG23	2.15	0.47
1:B:97:SER:HB3	1:B:98:PRO:HD3	1.95	0.47
1:F:97:SER:HB3	1:F:98:PRO:HD3	1.97	0.47
1:F:163:ALA:HB3	1:G:187:ALA:HB2	1.97	0.47
1:H:96:ALA:O	1:H:97:SER:CB	2.62	0.47
1:H:284:ILE:H	1:H:284:ILE:CD1	2.27	0.47
1:J:126:MET:HE1	1:K:36:TYR:CE2	2.50	0.47
1:K:12:ILE:O	1:K:12:ILE:HG22	2.15	0.47
1:K:107:TYR:C	1:K:107:TYR:HD1	2.22	0.47
1:A:178:TYR:CZ	1:A:180:GLY:HA2	2.50	0.47
1:B:179:GLU:HG2	1:L:13:ASN:CG	2.40	0.47
1:C:87:TYR:HB3	1:D:52:PHE:CD1	2.51	0.47
1:D:83:GLN:OE1	1:D:83:GLN:HA	2.15	0.47
1:E:20:ARG:HG3	1:E:146:GLU:OE1	2.15	0.47
1:G:105:LYS:N	1:G:105:LYS:CD	2.71	0.47
1:G:147:ILE:HG12	1:H:156:LYS:HD2	1.97	0.47
1:D:98:PRO:HG2	1:D:100:TYR:H	1.78	0.46
1:D:170:SER:HB3	1:D:173:GLN:HB2	1.97	0.46
1:E:203:ALA:HB1	1:F:158:PRO:HG3	1.97	0.46
1:F:72:SER:OG	1:F:73:TYR:N	2.49	0.46
1:J:195:SER:O	1:J:196:ILE:HD13	2.15	0.46
1:L:221:MET:HE3	1:L:221:MET:HA	1.96	0.46
1:D:47:THR:CG2	1:D:73:TYR:HB2	2.44	0.46
1:D:53:LEU:O	1:D:57:ILE:HG13	2.14	0.46
1:D:94:ARG:NH1	2:D:361:HOH:O	2.48	0.46
1:F:67:LYS:HB2	1:F:272:TYR:CE2	2.50	0.46
1:I:222:MET:HE3	1:I:227:ILE:CG2	2.46	0.46
1:L:283:ASP:O	1:L:285:VAL:HG12	2.15	0.46
1:A:12:ILE:N	1:A:12:ILE:HD13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ASN:HD21	1:B:51:SER:HB3	1.81	0.46
1:C:49:ASN:HD22	1:C:50:PRO:N	2.12	0.46
1:C:55:LYS:HB3	1:C:59:GLN:HE21	1.80	0.46
1:D:87:TYR:HE1	1:E:47:THR:O	1.99	0.46
1:D:96:ALA:O	1:D:97:SER:CB	2.62	0.46
1:G:167:ASN:HB3	1:G:168:GLN:HE21	1.79	0.46
1:H:283:ASP:C	1:H:285:VAL:N	2.73	0.46
1:J:227:ILE:HG22	1:J:228:LYS:N	2.29	0.46
1:K:73:TYR:CE2	1:K:272:TYR:CD1	3.01	0.46
1:C:265:CYS:SG	1:C:278:VAL:HG22	2.55	0.46
1:H:165:ASP:O	1:H:165:ASP:OD2	2.33	0.46
1:H:165:ASP:CG	1:H:195:SER:HB3	2.41	0.46
1:J:248:GLU:HG3	1:K:282:TYR:CD2	2.49	0.46
1:K:274:LEU:HA	2:K:332:HOH:O	2.15	0.46
1:A:17:ARG:HG3	1:A:20:ARG:NH1	2.31	0.46
1:C:99:VAL:HG12	1:C:99:VAL:O	2.15	0.46
1:D:47:THR:HG23	1:D:73:TYR:HB2	1.98	0.46
1:D:67:LYS:HB2	1:D:73:TYR:CE2	2.51	0.46
1:E:47:THR:CG2	1:E:73:TYR:HB2	2.46	0.46
1:F:222:MET:CE	1:F:227:ILE:HG21	2.43	0.46
1:H:62:TYR:C	1:H:62:TYR:CD2	2.93	0.46
1:H:162:ARG:NH1	1:I:193:SER:HA	2.30	0.46
1:H:283:ASP:C	1:H:285:VAL:H	2.23	0.46
1:I:222:MET:HE3	1:I:227:ILE:HG21	1.97	0.46
1:K:107:TYR:C	1:K:107:TYR:CD1	2.93	0.46
1:L:183:PRO:O	1:L:185:ILE:HG13	2.15	0.46
1:A:214:LYS:HE3	2:A:329:HOH:O	2.16	0.46
1:D:137:PHE:O	1:D:141:LEU:CD2	2.63	0.46
1:E:143:GLU:O	1:E:147:ILE:HG13	2.16	0.46
1:F:107:TYR:CB	1:F:117:MET:HE3	2.45	0.46
1:F:136:LEU:HD13	1:G:22:ARG:HD3	1.97	0.46
1:J:221:MET:HE3	1:J:221:MET:O	2.16	0.46
1:A:130:THR:HG22	1:A:134:LEU:HG	1.97	0.46
1:A:167:ASN:HD21	1:A:168:GLN:HG2	1.78	0.46
1:B:143:GLU:OE2	1:C:153:ASN:ND2	2.44	0.46
1:C:204:PRO:HG2	2:D:328:HOH:O	2.14	0.46
1:C:281:ARG:HG2	2:C:314:HOH:O	2.15	0.46
1:E:255:THR:O	1:E:259:LYS:HG2	2.15	0.46
1:G:28:LEU:O	1:G:32:GLN:HG3	2.15	0.46
1:I:83:GLN:OE1	1:I:83:GLN:HA	2.15	0.46
1:J:178:TYR:CZ	1:J:180:GLY:HA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:82:GLY:HA3	1:K:92:VAL:HG23	1.96	0.46
1:L:277:LYS:HA	1:L:277:LYS:HD3	1.58	0.46
1:A:96:ALA:HB2	1:A:101:GLN:HG3	1.96	0.46
1:A:179:GLU:CD	1:A:179:GLU:N	2.71	0.46
1:C:76:CYS:HA	2:C:326:HOH:O	2.16	0.46
1:C:168:GLN:HG2	1:C:188:HIS:NE2	2.31	0.46
1:D:125:ASP:OD2	1:D:259:LYS:CE	2.64	0.46
1:G:258:LEU:HD13	1:G:258:LEU:C	2.40	0.46
1:H:119:VAL:HA	2:H:318:HOH:O	2.16	0.46
1:A:104:PHE:CE2	1:A:118:GLY:HA3	2.51	0.46
1:J:249:GLN:H	1:J:249:GLN:HG2	1.61	0.46
1:K:104:PHE:HE2	1:K:118:GLY:HA3	1.81	0.46
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.81	0.46
1:C:55:LYS:O	1:C:59:GLN:HG3	2.16	0.46
1:D:222:MET:HE3	1:D:227:ILE:CB	2.44	0.46
1:E:104:PHE:CD2	1:E:118:GLY:HA3	2.51	0.46
1:F:67:LYS:HB3	1:F:272:TYR:HE2	1.80	0.46
1:H:165:ASP:OD1	1:H:191:LEU:CD2	2.63	0.46
1:H:213:GLN:HA	1:H:213:GLN:HE21	1.81	0.46
1:J:102:LYS:HG3	1:J:103:GLU:N	2.30	0.46
1:J:258:LEU:HD22	1:J:258:LEU:O	2.15	0.46
1:A:13:ASN:ND2	1:C:179:GLU:HG2	2.30	0.45
1:B:67:LYS:HB2	1:B:73:TYR:CE2	2.50	0.45
1:E:258:LEU:HD22	1:E:262:GLU:HG3	1.98	0.45
1:F:69:PRO:HA	2:F:335:HOH:O	2.15	0.45
1:I:88:ASN:HA	2:I:373:HOH:O	2.16	0.45
1:J:98:PRO:HG2	1:J:100:TYR:H	1.81	0.45
1:A:22:ARG:NH1	2:A:336:HOH:O	2.48	0.45
1:G:181:ASN:C	1:G:181:ASN:HD22	2.25	0.45
1:K:274:LEU:HD23	1:K:275:ASN:H	1.80	0.45
1:A:66:TYR:HB2	1:A:104:PHE:CZ	2.51	0.45
1:F:110:ARG:HH11	1:F:113:LYS:HG2	1.72	0.45
1:G:172:LYS:HG2	1:H:185:ILE:HD12	1.98	0.45
1:F:54:GLU:OE2	1:F:261:ARG:HD3	2.17	0.45
1:G:37:GLN:HG2	1:G:281:ARG:CD	2.47	0.45
1:I:88:ASN:HB2	2:I:333:HOH:O	2.16	0.45
1:I:188:HIS:CD2	1:I:190:ALA:HB3	2.52	0.45
1:L:48:ILE:O	1:L:50:PRO:HD3	2.16	0.45
1:H:11:SER:C	1:H:13:ASN:N	2.74	0.45
1:I:188:HIS:NE2	1:I:190:ALA:HB3	2.31	0.45
1:A:144:LEU:HD21	1:B:152:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:TRP:CZ2	1:C:222:MET:HE3	2.51	0.45
1:E:47:THR:HG23	1:E:73:TYR:HB2	1.99	0.45
1:E:271:LEU:HD22	1:E:272:TYR:CE1	2.52	0.45
1:G:68:ASP:OD2	1:G:71:ILE:HG12	2.16	0.45
2:H:341:HOH:O	1:I:36:TYR:HB3	2.16	0.45
1:I:19:LYS:HE3	1:I:19:LYS:CA	2.35	0.45
1:J:93:PHE:CE2	1:J:95:ALA:HB2	2.51	0.45
1:C:84:ARG:HD2	1:C:84:ARG:N	2.32	0.45
1:D:222:MET:HE1	1:D:227:ILE:HD12	1.99	0.45
1:E:44:LEU:HD13	1:E:48:ILE:CG2	2.46	0.45
1:F:67:LYS:CB	1:F:272:TYR:HE2	2.30	0.45
1:F:162:ARG:NH2	1:F:194:ASP:O	2.50	0.45
1:H:222:MET:HE3	1:H:227:ILE:CG2	2.46	0.45
1:J:167:ASN:N	1:J:167:ASN:HD22	2.14	0.45
1:K:73:TYR:CE2	1:K:272:TYR:HD1	2.35	0.45
1:D:164:ASN:HA	1:E:188:HIS:O	2.17	0.45
1:I:283:ASP:CG	1:I:284:ILE:N	2.72	0.45
1:L:113:LYS:HA	1:L:117:MET:CE	2.46	0.45
1:B:93:PHE:CE2	1:B:95:ALA:HB2	2.51	0.45
1:B:162:ARG:HG3	1:B:162:ARG:NH1	2.28	0.45
1:D:181:ASN:H	1:D:181:ASN:HD22	1.64	0.45
1:E:164:ASN:O	1:F:189:GLU:HA	2.16	0.45
1:F:199:PHE:HB3	1:G:198:VAL:HG21	1.98	0.45
1:I:40:GLU:OE1	1:I:279:LYS:HE3	2.17	0.45
1:J:39:PHE:HZ	1:J:257:PHE:HB2	1.82	0.45
1:K:255:THR:HG21	1:L:281:ARG:HD3	1.99	0.45
1:I:164:ASN:O	1:J:189:GLU:HA	2.17	0.45
1:J:97:SER:HB3	1:J:98:PRO:CD	2.47	0.45
1:L:93:PHE:HB2	1:L:106:LEU:HD11	1.99	0.45
1:L:181:ASN:ND2	1:L:181:ASN:N	2.62	0.45
1:L:258:LEU:HD22	1:L:262:GLU:CG	2.40	0.45
1:A:96:ALA:O	1:A:97:SER:CB	2.65	0.44
1:C:53:LEU:O	1:C:57:ILE:HG13	2.18	0.44
1:C:162:ARG:CG	1:C:162:ARG:NH1	2.78	0.44
1:E:93:PHE:CB	1:E:106:LEU:HD21	2.36	0.44
1:E:257:PHE:O	1:E:261:ARG:HG3	2.17	0.44
1:B:258:LEU:HD11	1:B:262:GLU:CD	2.42	0.44
1:C:259:LYS:HG3	1:C:260:SER:N	2.32	0.44
1:J:174:VAL:HG21	1:J:186:PHE:HD1	1.83	0.44
1:L:66:TYR:HB2	1:L:104:PHE:CE2	2.52	0.44
1:C:13:ASN:OD1	1:E:179:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:VAL:CG1	1:G:33:SER:HB2	2.46	0.44
1:I:247:ASP:OD2	1:I:247:ASP:C	2.60	0.44
1:J:213:GLN:NE2	1:J:213:GLN:CA	2.69	0.44
1:L:43:ASN:HB2	1:L:276:VAL:HA	1.98	0.44
1:A:282:TYR:O	1:A:283:ASP:HB2	2.16	0.44
1:B:248:GLU:HB2	1:C:282:TYR:CE1	2.52	0.44
1:C:203:ALA:O	1:C:204:PRO:C	2.60	0.44
1:E:83:GLN:HE21	1:E:83:GLN:HB2	1.58	0.44
1:F:49:ASN:C	1:F:49:ASN:ND2	2.74	0.44
1:G:96:ALA:O	1:G:97:SER:CB	2.66	0.44
1:H:43:ASN:HB2	1:H:276:VAL:HA	1.99	0.44
1:G:34:LEU:O	1:G:37:GLN:NE2	2.51	0.44
1:H:205:TYR:CZ	1:H:207:VAL:HB	2.52	0.44
1:K:85:ASP:OD1	1:K:89:GLN:N	2.50	0.44
1:L:96:ALA:O	1:L:97:SER:CB	2.65	0.44
1:D:203:ALA:O	1:D:204:PRO:C	2.60	0.44
1:F:41:TRP:CH2	1:F:261:ARG:HG2	2.52	0.44
1:F:107:TYR:HD1	1:F:271:LEU:HB2	1.83	0.44
1:A:205:TYR:CD2	1:L:209:LYS:HD3	2.53	0.44
1:B:250:ILE:N	1:B:250:ILE:HD12	2.33	0.44
1:C:167:ASN:CB	1:D:189:GLU:OE2	2.65	0.44
1:D:41:TRP:HB2	1:D:44:LEU:HD11	1.98	0.44
1:E:12:ILE:HG22	1:E:12:ILE:O	2.17	0.44
1:I:258:LEU:HD12	1:I:280:PHE:CE1	2.53	0.44
1:K:271:LEU:C	1:K:272:TYR:HD2	2.25	0.44
1:L:45:PRO:HA	1:L:46:PRO:HD3	1.90	0.44
1:L:85:ASP:OD1	1:L:86:VAL:N	2.51	0.44
1:F:96:ALA:O	1:F:97:SER:CB	2.66	0.44
1:J:164:ASN:OD1	1:J:195:SER:HA	2.18	0.44
1:L:113:LYS:HB2	1:L:113:LYS:NZ	2.32	0.44
1:L:203:ALA:O	1:L:204:PRO:C	2.59	0.44
1:A:284:ILE:O	1:A:284:ILE:HG22	2.17	0.44
1:C:85:ASP:OD1	1:C:89:GLN:N	2.47	0.44
1:H:28:LEU:HD23	1:H:28:LEU:O	2.18	0.44
1:I:93:PHE:CE2	1:I:95:ALA:HB2	2.52	0.44
1:J:248:GLU:HG3	1:K:282:TYR:CG	2.52	0.44
1:L:222:MET:CE	1:L:227:ILE:HG21	2.46	0.44
1:C:66:TYR:HB2	1:C:104:PHE:CZ	2.53	0.43
1:E:60:PHE:C	1:E:129:PRO:HG3	2.42	0.43
1:G:16:GLN:C	1:G:16:GLN:CD	2.86	0.43
1:G:178:TYR:CZ	1:G:180:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:ASP:HA	2:H:340:HOH:O	2.18	0.43
1:J:166:ASN:ND2	1:J:170:SER:HA	2.33	0.43
1:A:249:GLN:NE2	1:B:218:TRP:NE1	2.61	0.43
1:F:218:TRP:O	1:F:222:MET:HG2	2.18	0.43
1:G:160:LEU:HD23	1:H:184:VAL:CG1	2.48	0.43
1:H:249:GLN:HG2	1:I:222:MET:CE	2.48	0.43
1:J:11:SER:O	1:J:14:GLU:OE2	2.36	0.43
1:J:271:LEU:HD12	1:J:272:TYR:CZ	2.53	0.43
1:B:97:SER:HB3	1:B:98:PRO:CD	2.48	0.43
1:C:208:ASP:OD2	1:C:208:ASP:N	2.51	0.43
1:G:13:ASN:OD1	1:I:179:GLU:HB3	2.17	0.43
1:G:284:ILE:HD12	1:G:285:VAL:H	1.83	0.43
1:L:11:SER:O	1:L:12:ILE:HD13	2.18	0.43
1:D:66:TYR:CE2	1:D:68:ASP:HA	2.53	0.43
1:E:128:PHE:HD2	1:E:129:PRO:N	2.15	0.43
1:F:56:SER:HB3	1:F:63:VAL:HG12	2.00	0.43
1:H:113:LYS:HZ1	1:H:270:GLU:C	2.26	0.43
1:J:71:ILE:O	1:J:72:SER:HB3	2.19	0.43
2:J:342:HOH:O	1:L:182:ALA:HA	2.19	0.43
1:K:55:LYS:CG	1:K:59:GLN:NE2	2.76	0.43
1:F:73:TYR:OH	1:F:274:LEU:HD21	2.19	0.43
1:G:222:MET:HE3	1:G:227:ILE:CG2	2.49	0.43
1:H:66:TYR:CE2	1:H:68:ASP:HA	2.54	0.43
1:I:209:LYS:HB3	1:J:205:TYR:CE2	2.53	0.43
1:K:140:GLU:CD	1:L:145:LYS:NZ	2.77	0.43
1:K:144:LEU:HD21	1:L:152:GLN:NE2	2.33	0.43
1:K:169:LEU:HD23	1:K:170:SER:N	2.33	0.43
1:L:93:PHE:CE2	1:L:95:ALA:HB2	2.53	0.43
1:L:181:ASN:H	1:L:181:ASN:HD22	1.66	0.43
1:A:205:TYR:CZ	1:A:207:VAL:HB	2.54	0.43
1:B:172:LYS:NZ	1:C:181:ASN:OD1	2.49	0.43
1:C:248:GLU:HG2	1:D:282:TYR:CD2	2.53	0.43
1:D:41:TRP:CB	1:D:44:LEU:HD11	2.48	0.43
1:E:203:ALA:O	1:E:204:PRO:C	2.61	0.43
1:H:109:TYR:CG	1:H:112:MET:SD	3.11	0.43
1:I:168:GLN:HG2	1:I:188:HIS:ND1	2.32	0.43
1:J:227:ILE:O	1:J:228:LYS:HB3	2.16	0.43
1:K:39:PHE:HE2	1:K:280:PHE:CE2	2.36	0.43
1:K:73:TYR:HE2	1:K:272:TYR:HD1	1.66	0.43
1:K:91:THR:HG21	2:K:346:HOH:O	2.18	0.43
1:A:169:LEU:HB3	1:A:186:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:O	1:A:258:LEU:HD22	2.18	0.43
1:C:96:ALA:O	1:C:97:SER:CB	2.67	0.43
1:D:96:ALA:HB2	1:D:101:GLN:HG3	2.00	0.43
1:D:258:LEU:HD13	1:D:258:LEU:C	2.43	0.43
1:E:128:PHE:CD2	1:E:129:PRO:HD2	2.53	0.43
1:E:252:SER:O	1:E:256:VAL:HG23	2.19	0.43
1:G:60:PHE:CD1	1:G:77:ASN:OD1	2.71	0.43
1:H:54:GLU:OE1	1:H:261:ARG:NH1	2.52	0.43
1:H:165:ASP:OD1	1:H:195:SER:CB	2.66	0.43
1:I:248:GLU:HB2	1:J:282:TYR:CE2	2.53	0.43
1:I:258:LEU:O	1:I:262:GLU:HG3	2.18	0.43
1:K:161:ILE:HG12	1:K:198:VAL:HG22	2.01	0.43
1:K:178:TYR:CD2	1:K:184:VAL:HG22	2.54	0.43
1:K:258:LEU:CD2	1:K:258:LEU:C	2.92	0.43
1:B:49:ASN:HD22	1:B:50:PRO:N	2.15	0.43
1:E:160:LEU:HD23	1:F:184:VAL:CG1	2.47	0.43
1:E:271:LEU:HD22	1:E:272:TYR:CD1	2.53	0.43
1:G:208:ASP:OD2	1:G:208:ASP:N	2.52	0.43
1:I:203:ALA:O	1:I:204:PRO:C	2.61	0.43
1:J:78:GLY:HA3	1:J:95:ALA:HA	2.01	0.43
1:A:148:ILE:HG23	1:A:207:VAL:HG13	2.01	0.43
1:A:152:GLN:NE2	1:L:144:LEU:HD21	2.33	0.43
1:C:92:VAL:HG11	1:C:94:ARG:NH1	2.34	0.43
1:D:227:ILE:O	1:D:228:LYS:CB	2.64	0.43
1:G:49:ASN:C	1:G:49:ASN:ND2	2.75	0.43
1:J:167:ASN:OD1	1:K:189:GLU:OE2	2.37	0.43
1:J:168:GLN:CG	1:J:188:HIS:CE1	2.91	0.43
1:K:39:PHE:HZ	1:K:257:PHE:HB2	1.84	0.43
1:K:248:GLU:HG2	1:L:227:ILE:HG23	2.00	0.43
1:K:270:GLU:OE1	1:K:271:LEU:N	2.52	0.43
1:B:213:GLN:CG	1:C:207:VAL:CG1	2.97	0.43
1:C:40:GLU:HA	2:C:315:HOH:O	2.18	0.43
1:C:221:MET:HE3	1:C:221:MET:HA	2.00	0.43
1:D:48:ILE:CD1	1:D:73:TYR:HB3	2.49	0.43
1:F:271:LEU:HD23	1:F:272:TYR:CE1	2.54	0.43
1:G:222:MET:HE3	1:G:227:ILE:HB	2.01	0.43
1:H:164:ASN:OD1	1:H:165:ASP:N	2.52	0.43
1:L:221:MET:HE3	1:L:221:MET:O	2.18	0.43
1:B:13:ASN:ND2	1:B:17:ARG:HH21	2.16	0.42
1:B:67:LYS:CB	1:B:272:TYR:CE2	3.02	0.42
1:B:78:GLY:HA3	1:B:95:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:LEU:CD1	1:E:63:VAL:HG11	2.49	0.42
1:H:137:PHE:CD2	1:H:221:MET:HB2	2.54	0.42
1:K:81:SER:HB2	1:K:94:ARG:NH2	2.32	0.42
1:L:181:ASN:N	1:L:181:ASN:HD22	2.17	0.42
1:C:45:PRO:HA	1:C:46:PRO:HD3	1.96	0.42
1:F:128:PHE:HA	1:F:129:PRO:HD3	1.87	0.42
1:G:66:TYR:CE2	1:G:68:ASP:HA	2.54	0.42
1:G:98:PRO:HB2	1:G:99:VAL:H	1.61	0.42
1:G:107:TYR:OH	1:G:110:ARG:HA	2.20	0.42
1:H:67:LYS:HD3	1:H:73:TYR:CE2	2.54	0.42
1:K:11:SER:O	1:K:12:ILE:HD13	2.19	0.42
1:B:143:GLU:O	1:B:147:ILE:HG13	2.19	0.42
1:C:43:ASN:N	1:C:43:ASN:ND2	2.66	0.42
1:C:167:ASN:HB3	1:D:189:GLU:OE2	2.19	0.42
1:C:218:TRP:CE2	1:C:222:MET:HE3	2.55	0.42
1:F:272:TYR:CD1	1:F:272:TYR:N	2.87	0.42
1:L:130:THR:HG22	1:L:134:LEU:HG	2.02	0.42
1:D:258:LEU:HD13	1:D:262:GLU:HG3	2.00	0.42
1:E:78:GLY:HA3	1:E:95:ALA:HA	2.01	0.42
1:E:203:ALA:CB	1:F:158:PRO:HG3	2.48	0.42
1:G:60:PHE:HD1	1:G:77:ASN:OD1	2.02	0.42
1:H:126:MET:HG3	2:I:346:HOH:O	2.20	0.42
1:H:148:ILE:O	1:H:152:GLN:HG2	2.20	0.42
1:K:271:LEU:HG	1:K:272:TYR:CE2	2.55	0.42
1:A:85:ASP:OD2	1:A:89:GLN:N	2.49	0.42
1:A:97:SER:OG	1:A:98:PRO:CD	2.68	0.42
1:D:43:ASN:HB2	1:D:276:VAL:HA	2.00	0.42
1:D:258:LEU:HD11	1:D:262:GLU:CD	2.44	0.42
1:E:68:ASP:OD2	1:E:71:ILE:HG12	2.20	0.42
1:F:78:GLY:HA3	1:F:95:ALA:HA	2.01	0.42
1:J:205:TYR:CZ	1:J:207:VAL:HB	2.55	0.42
1:K:87:TYR:CD1	1:L:49:ASN:HB2	2.55	0.42
1:L:259:LYS:HG3	1:L:260:SER:N	2.34	0.42
1:A:179:GLU:N	1:A:179:GLU:OE1	2.50	0.42
1:A:205:TYR:CE2	1:L:209:LYS:HB3	2.54	0.42
1:C:11:SER:CB	1:C:12:ILE:HD12	2.50	0.42
1:D:109:TYR:C	1:D:111:ASP:N	2.78	0.42
1:F:71:ILE:O	1:F:72:SER:HB3	2.19	0.42
1:G:28:LEU:C	1:G:28:LEU:HD23	2.45	0.42
1:J:72:SER:OG	1:J:73:TYR:N	2.52	0.42
1:L:144:LEU:O	1:L:148:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:PHE:N	1:E:106:LEU:HD21	2.33	0.42
1:F:203:ALA:O	1:F:204:PRO:C	2.61	0.42
1:G:114:GLU:H	1:G:117:MET:CE	2.33	0.42
1:J:213:GLN:NE2	2:J:340:HOH:O	2.53	0.42
1:K:34:LEU:O	1:K:37:GLN:NE2	2.53	0.42
1:G:16:GLN:NE2	1:G:17:ARG:HA	2.34	0.42
1:G:183:PRO:O	1:G:185:ILE:HG13	2.19	0.42
1:G:228:LYS:HB3	1:G:228:LYS:HZ2	1.84	0.42
1:I:249:GLN:HG2	1:J:222:MET:CE	2.50	0.42
1:I:269:ASN:ND2	1:I:276:VAL:HG13	2.33	0.42
1:L:284:ILE:HG23	1:L:284:ILE:O	2.20	0.42
1:A:93:PHE:HE2	1:A:95:ALA:HB2	1.85	0.42
1:A:144:LEU:O	1:A:148:ILE:HG13	2.19	0.42
1:D:136:LEU:HD13	1:E:22:ARG:HG2	2.01	0.42
1:D:186:PHE:CE2	1:D:196:ILE:HD11	2.55	0.42
1:G:78:GLY:HA3	1:G:95:ALA:HA	2.01	0.42
1:H:73:TYR:OH	1:H:274:LEU:HD21	2.20	0.42
1:L:73:TYR:OH	1:L:272:TYR:HB3	2.19	0.42
1:A:277:LYS:NZ	1:A:278:VAL:H	2.18	0.42
1:J:162:ARG:HG2	1:J:162:ARG:NH1	2.33	0.42
1:L:107:TYR:HD2	1:L:117:MET:CE	2.32	0.42
1:L:170:SER:O	1:L:174:VAL:HG23	2.19	0.42
1:L:188:HIS:CD2	1:L:190:ALA:H	2.37	0.42
1:D:12:ILE:O	1:D:12:ILE:HG22	2.20	0.41
1:D:265:CYS:SG	1:D:276:VAL:O	2.78	0.41
1:F:65:PHE:CD1	1:F:268:ILE:HD12	2.55	0.41
1:G:222:MET:HE3	1:G:227:ILE:HG21	2.02	0.41
1:I:84:ARG:HA	1:I:84:ARG:HD3	1.82	0.41
1:I:249:GLN:NE2	2:I:338:HOH:O	2.50	0.41
1:K:110:ARG:O	1:K:112:MET:N	2.46	0.41
1:L:58:HIS:HD2	1:L:130:THR:OG1	2.03	0.41
1:B:173:GLN:HE21	1:B:177:GLN:CG	2.33	0.41
1:E:93:PHE:CE1	1:E:95:ALA:HB2	2.55	0.41
1:E:124:ASN:HA	1:E:260:SER:HB2	2.01	0.41
1:G:43:ASN:O	1:G:276:VAL:HG12	2.20	0.41
1:H:104:PHE:CD2	1:H:118:GLY:HA3	2.55	0.41
1:J:41:TRP:CE2	1:J:278:VAL:HG13	2.54	0.41
1:J:113:LYS:O	1:J:114:GLU:CG	2.63	0.41
1:L:181:ASN:HD22	1:L:181:ASN:C	2.27	0.41
1:E:250:ILE:N	1:E:250:ILE:CD1	2.84	0.41
1:F:47:THR:HG23	1:F:73:TYR:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:LEU:HD21	1:G:32:GLN:OE1	2.20	0.41
1:G:160:LEU:HB2	2:H:327:HOH:O	2.21	0.41
1:H:67:LYS:HB2	1:H:272:TYR:CE1	2.55	0.41
1:H:109:TYR:HB3	1:H:110:ARG:H	1.71	0.41
1:H:192:ASP:HB2	1:H:194:ASP:OD2	2.20	0.41
1:H:227:ILE:HG22	1:H:228:LYS:N	2.35	0.41
1:H:248:GLU:HB3	1:I:227:ILE:CG2	2.51	0.41
1:I:130:THR:HG22	1:I:134:LEU:HG	2.02	0.41
1:K:113:LYS:HB3	1:K:114:GLU:H	1.53	0.41
1:A:162:ARG:HG3	1:A:162:ARG:NH1	2.34	0.41
1:D:109:TYR:N	1:D:109:TYR:CD2	2.86	0.41
1:F:43:ASN:N	1:F:43:ASN:ND2	2.68	0.41
1:F:105:LYS:O	1:F:117:MET:HG3	2.20	0.41
1:G:72:SER:OG	1:G:73:TYR:N	2.53	0.41
1:I:13:ASN:HD22	1:I:13:ASN:HA	1.56	0.41
1:J:224:PHE:HD2	1:J:225:LEU:CD1	2.33	0.41
1:K:227:ILE:HG22	1:K:228:LYS:N	2.35	0.41
1:A:189:GLU:HG2	2:A:342:HOH:O	2.21	0.41
1:E:44:LEU:HD13	1:E:48:ILE:HG21	2.01	0.41
1:E:261:ARG:CG	1:E:261:ARG:NH1	2.77	0.41
1:F:67:LYS:CB	1:F:272:TYR:CE2	3.04	0.41
1:H:84:ARG:NH1	1:H:84:ARG:CB	2.83	0.41
1:H:90:ALA:O	1:H:108:ASN:OD1	2.38	0.41
1:A:112:MET:O	1:A:112:MET:SD	2.78	0.41
1:C:78:GLY:HA3	1:C:95:ALA:HA	2.02	0.41
1:E:86:VAL:HG22	1:F:99:VAL:CG2	2.51	0.41
1:E:209:LYS:HB3	1:F:205:TYR:CZ	2.55	0.41
1:F:57:ILE:HG12	1:F:63:VAL:HG13	2.02	0.41
1:F:94:ARG:CZ	1:F:94:ARG:HB3	2.51	0.41
1:G:27:TYR:OH	1:G:214:LYS:NZ	2.44	0.41
1:G:261:ARG:HG2	1:G:261:ARG:NH1	2.32	0.41
1:I:51:SER:O	1:I:55:LYS:HG3	2.19	0.41
1:I:106:LEU:CD2	1:I:120:VAL:HG23	2.49	0.41
1:K:43:ASN:HB2	1:K:276:VAL:HA	2.03	0.41
1:K:178:TYR:CZ	1:K:180:GLY:HA2	2.56	0.41
1:K:248:GLU:CD	1:L:227:ILE:HG23	2.45	0.41
1:B:119:VAL:HB	1:B:268:ILE:HD11	2.03	0.41
1:B:145:LYS:HD3	1:B:145:LYS:O	2.21	0.41
1:E:57:ILE:HG21	1:E:261:ARG:NH1	2.35	0.41
1:E:146:GLU:O	1:E:150:VAL:HG23	2.19	0.41
1:F:265:CYS:O	1:F:269:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:ASN:O	1:G:25:ILE:HG12	2.21	0.41
1:G:285:VAL:HG12	1:G:285:VAL:O	2.21	0.41
1:K:172:LYS:HA	1:K:172:LYS:HD2	1.81	0.41
1:K:205:TYR:CZ	1:K:207:VAL:HB	2.55	0.41
1:L:41:TRP:CE2	1:L:278:VAL:HG13	2.56	0.41
1:B:11:SER:C	1:B:13:ASN:N	2.71	0.41
1:E:31:LEU:HD23	1:E:31:LEU:HA	1.95	0.41
1:E:53:LEU:O	1:E:57:ILE:HG13	2.20	0.41
1:G:109:TYR:HB2	1:G:112:MET:HB2	2.02	0.41
1:B:123:ASN:HD21	1:B:261:ARG:HH21	1.69	0.41
1:D:208:ASP:OD2	1:D:208:ASP:N	2.51	0.41
1:E:97:SER:HB3	1:E:98:PRO:HD3	2.02	0.41
1:E:98:PRO:HB2	1:E:99:VAL:H	1.66	0.41
1:E:111:ASP:O	1:E:112:MET:HB3	2.21	0.41
1:E:249:GLN:NE2	1:F:218:TRP:NE1	2.69	0.41
1:F:85:ASP:OD2	1:F:89:GLN:HB3	2.21	0.41
1:G:39:PHE:HZ	1:G:257:PHE:HB2	1.86	0.41
1:G:52:PHE:CD2	1:G:52:PHE:C	2.98	0.41
1:H:168:GLN:HB2	1:H:169:LEU:H	1.66	0.41
1:H:178:TYR:CD1	1:H:184:VAL:HG22	2.56	0.41
1:J:11:SER:C	1:J:12:ILE:HD13	2.46	0.41
1:K:55:LYS:HE2	1:K:59:GLN:NE2	2.36	0.41
1:K:200:LYS:HD3	1:K:200:LYS:HA	1.80	0.41
1:L:113:LYS:HG3	1:L:271:LEU:HD12	2.03	0.41
1:A:98:PRO:HB2	1:A:99:VAL:H	1.70	0.41
1:C:38:LEU:O	1:C:281:ARG:HB3	2.21	0.41
1:C:43:ASN:N	1:C:43:ASN:HD22	2.19	0.41
1:D:269:ASN:OD1	1:D:276:VAL:HG13	2.21	0.41
1:F:62:TYR:CZ	1:F:80:LEU:HG	2.56	0.41
1:G:54:GLU:OE2	1:G:261:ARG:NH1	2.52	0.41
1:H:31:LEU:HD23	1:H:31:LEU:HA	1.82	0.41
1:H:110:ARG:HB3	1:I:46:PRO:HB2	2.02	0.41
1:I:98:PRO:HG2	1:I:100:TYR:N	2.32	0.41
1:I:171:LEU:HD22	1:I:175:TYR:CE1	2.56	0.41
1:J:188:HIS:CD2	1:J:190:ALA:HB3	2.56	0.41
1:L:106:LEU:HD22	1:L:120:VAL:HG23	2.03	0.41
1:L:129:PRO:O	1:L:132:PRO:HD2	2.21	0.41
1:A:181:ASN:HD22	1:A:182:ALA:N	2.20	0.40
1:A:183:PRO:O	1:A:185:ILE:HG13	2.22	0.40
1:A:203:ALA:O	1:A:204:PRO:C	2.60	0.40
1:B:98:PRO:HG2	1:B:100:TYR:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TYR:CE2	1:B:180:GLY:HA2	2.55	0.40
1:C:283:ASP:C	1:C:284:ILE:CG1	2.94	0.40
1:E:140:GLU:OE1	1:F:145:LYS:NZ	2.48	0.40
1:H:71:ILE:O	1:H:72:SER:HB3	2.20	0.40
1:H:78:GLY:HA3	1:H:95:ALA:HA	2.04	0.40
1:H:203:ALA:HB1	1:I:158:PRO:HG3	2.03	0.40
1:I:41:TRP:CZ3	1:I:278:VAL:HG22	2.56	0.40
1:L:227:ILE:HG22	1:L:228:LYS:N	2.35	0.40
1:G:186:PHE:CE2	1:G:196:ILE:HD11	2.56	0.40
1:H:69:PRO:CD	1:H:102:LYS:HZ1	2.34	0.40
1:I:14:GLU:HA	1:I:14:GLU:OE1	2.21	0.40
1:J:53:LEU:HD12	1:J:63:VAL:HG11	2.02	0.40
1:J:109:TYR:HE1	1:J:267:LYS:HG2	1.86	0.40
1:J:115:GLU:O	1:J:116:ASP:CB	2.69	0.40
1:K:65:PHE:HB3	1:K:119:VAL:CG2	2.50	0.40
1:D:277:LYS:HE2	1:D:277:LYS:HB3	1.83	0.40
1:F:170:SER:HB3	1:F:173:GLN:HB2	2.04	0.40
1:G:162:ARG:NH1	1:H:193:SER:HA	2.36	0.40
1:G:167:ASN:HB2	1:H:189:GLU:OE2	2.21	0.40
1:F:172:LYS:HA	1:F:172:LYS:HD2	1.94	0.40
1:G:98:PRO:HA	2:G:312:HOH:O	2.22	0.40
1:G:258:LEU:CD1	1:G:262:GLU:CD	2.94	0.40
1:I:101:GLN:HE21	1:I:101:GLN:HB3	1.58	0.40
1:J:109:TYR:HD2	1:K:46:PRO:O	2.03	0.40
1:K:72:SER:OG	1:K:73:TYR:N	2.53	0.40
1:K:78:GLY:HA3	1:K:95:ALA:HA	2.03	0.40
1:A:53:LEU:O	1:A:57:ILE:HG13	2.21	0.40
1:A:53:LEU:HD12	1:A:63:VAL:HG11	2.02	0.40
1:A:168:GLN:HB2	1:A:169:LEU:H	1.69	0.40
1:B:119:VAL:HA	2:B:357:HOH:O	2.20	0.40
1:C:31:LEU:HD21	1:C:221:MET:HG2	2.03	0.40
1:F:20:ARG:HH22	1:F:143:GLU:HG3	1.82	0.40
1:F:49:ASN:C	1:F:49:ASN:HD22	2.28	0.40
1:F:248:GLU:HG2	1:G:282:TYR:CD2	2.56	0.40
1:F:258:LEU:HD12	1:F:280:PHE:CZ	2.56	0.40
1:H:52:PHE:CZ	1:H:77:ASN:ND2	2.89	0.40
1:H:52:PHE:HZ	1:H:77:ASN:ND2	2.20	0.40
1:K:221:MET:HE3	1:K:221:MET:CA	2.52	0.40
1:L:14:GLU:CD	1:L:14:GLU:N	2.74	0.40

All (1) 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)
1:K:189:GLU:OE1	1:K:189:GLU:OE1[2_556]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/309 (82%)	234 (92%)	13 (5%)	6 (2%)	4	18
1	B	253/309 (82%)	235 (93%)	13 (5%)	5 (2%)	6	22
1	C	253/309 (82%)	237 (94%)	13 (5%)	3 (1%)	10	34
1	D	253/309 (82%)	242 (96%)	8 (3%)	3 (1%)	10	34
1	E	253/309 (82%)	236 (93%)	10 (4%)	7 (3%)	4	15
1	F	253/309 (82%)	235 (93%)	14 (6%)	4 (2%)	7	27
1	G	253/309 (82%)	241 (95%)	9 (4%)	3 (1%)	10	34
1	H	253/309 (82%)	233 (92%)	16 (6%)	4 (2%)	7	27
1	I	253/309 (82%)	236 (93%)	13 (5%)	4 (2%)	7	27
1	J	253/309 (82%)	236 (93%)	13 (5%)	4 (2%)	7	27
1	K	253/309 (82%)	235 (93%)	10 (4%)	8 (3%)	3	13
1	L	253/309 (82%)	238 (94%)	11 (4%)	4 (2%)	7	27
All	All	3036/3708 (82%)	2838 (94%)	143 (5%)	55 (2%)	6	25

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	SER
1	B	97	SER
1	C	97	SER
1	D	97	SER
1	E	97	SER
1	E	284	ILE
1	F	97	SER

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Mol	Chain	Res	Type
1	G	97	SER
1	H	97	SER
1	I	97	SER
1	I	98	PRO
1	I	284	ILE
1	J	97	SER
1	J	111	ASP
1	K	97	SER
1	K	111	ASP
1	K	113	LYS
1	L	97	SER
1	A	98	PRO
1	B	98	PRO
1	B	110	ARG
1	C	98	PRO
1	D	98	PRO
1	E	98	PRO
1	E	109	TYR
1	E	111	ASP
1	F	98	PRO
1	F	108	ASN
1	G	98	PRO
1	H	98	PRO
1	J	98	PRO
1	K	98	PRO
1	K	108	ASN
1	L	98	PRO
1	L	284	ILE
1	A	111	ASP
1	A	113	LYS
1	A	284	ILE
1	H	114	GLU
1	B	112	MET
1	B	192	ASP
1	E	110	ARG
1	K	114	GLU
1	L	192	ASP
1	A	125	ASP
1	C	125	ASP
1	D	125	ASP
1	F	192	ASP
1	G	110	ARG

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Mol	Chain	Res	Type
1	H	108	ASN
1	I	192	ASP
1	J	192	ASP
1	K	12	ILE
1	E	125	ASP
1	K	125	ASP

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	228/277 (82%)	207 (91%)	21 (9%)	8	27
1	B	228/277 (82%)	213 (93%)	15 (7%)	15	43
1	C	228/277 (82%)	209 (92%)	19 (8%)	10	32
1	D	228/277 (82%)	207 (91%)	21 (9%)	8	27
1	E	228/277 (82%)	212 (93%)	16 (7%)	14	40
1	F	228/277 (82%)	205 (90%)	23 (10%)	7	24
1	G	228/277 (82%)	213 (93%)	15 (7%)	15	43
1	H	228/277 (82%)	212 (93%)	16 (7%)	14	40
1	I	228/277 (82%)	205 (90%)	23 (10%)	7	24
1	J	228/277 (82%)	210 (92%)	18 (8%)	11	34
1	K	228/277 (82%)	209 (92%)	19 (8%)	10	32
1	L	228/277 (82%)	207 (91%)	21 (9%)	8	27
All	All	2736/3324 (82%)	2509 (92%)	227 (8%)	10	32

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	13	ASN
1	A	28	LEU
1	A	38	LEU

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Mol	Chain	Res	Type
1	A	44	LEU
1	A	49	ASN
1	A	102	LYS
1	A	110	ARG
1	A	160	LEU
1	A	164	ASN
1	A	167	ASN
1	A	169	LEU
1	A	171	LEU
1	A	172	LYS
1	A	173	GLN
1	A	179	GLU
1	A	181	ASN
1	A	225	LEU
1	A	258	LEU
1	A	271	LEU
1	A	278	VAL
1	B	18	GLN
1	B	28	LEU
1	B	47	THR
1	B	49	ASN
1	B	88	ASN
1	B	109	TYR
1	B	114	GLU
1	B	131	THR
1	B	145	LYS
1	B	168	GLN
1	B	181	ASN
1	B	213	GLN
1	B	263	GLU
1	B	270	GLU
1	B	278	VAL
1	C	12	ILE
1	C	13	ASN
1	C	20	ARG
1	C	28	LEU
1	C	37	GLN
1	C	48	ILE
1	C	49	ASN
1	C	88	ASN
1	C	145	LYS
1	C	168	GLN

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Mol	Chain	Res	Type
1	C	169	LEU
1	C	171	LEU
1	C	173	GLN
1	C	228	LYS
1	C	258	LEU
1	C	259	LYS
1	C	260	SER
1	C	265	CYS
1	C	278	VAL
1	D	16	GLN
1	D	28	LEU
1	D	34	LEU
1	D	37	GLN
1	D	38	LEU
1	D	48	ILE
1	D	86	VAL
1	D	97	SER
1	D	141	LEU
1	D	160	LEU
1	D	167	ASN
1	D	168	GLN
1	D	172	LYS
1	D	173	GLN
1	D	181	ASN
1	D	214	LYS
1	D	225	LEU
1	D	255	THR
1	D	259	LYS
1	D	276	VAL
1	D	278	VAL
1	E	20	ARG
1	E	37	GLN
1	E	38	LEU
1	E	48	ILE
1	E	83	GLN
1	E	101	GLN
1	E	109	TYR
1	E	115	GLU
1	E	126	MET
1	E	149	SER
1	E	160	LEU
1	E	169	LEU

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Mol	Chain	Res	Type
1	E	171	LEU
1	E	194	ASP
1	E	258	LEU
1	E	266	GLU
1	F	21	ASN
1	F	22	ARG
1	F	37	GLN
1	F	38	LEU
1	F	40	GLU
1	F	115	GLU
1	F	120	VAL
1	F	160	LEU
1	F	164	ASN
1	F	166	ASN
1	F	169	LEU
1	F	177	GLN
1	F	179	GLU
1	F	204	PRO
1	F	221	MET
1	F	248	GLU
1	F	258	LEU
1	F	259	LYS
1	F	261	ARG
1	F	275	ASN
1	F	278	VAL
1	F	281	ARG
1	F	284	ILE
1	G	22	ARG
1	G	37	GLN
1	G	42	GLU
1	G	48	ILE
1	G	49	ASN
1	G	115	GLU
1	G	145	LYS
1	G	160	LEU
1	G	169	LEU
1	G	171	LEU
1	G	181	ASN
1	G	228	LYS
1	G	255	THR
1	G	271	LEU
1	G	278	VAL

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Mol	Chain	Res	Type
1	H	12	ILE
1	H	18	GLN
1	H	28	LEU
1	H	37	GLN
1	H	44	LEU
1	H	53	LEU
1	H	81	SER
1	H	101	GLN
1	H	112	MET
1	H	160	LEU
1	H	169	LEU
1	H	171	LEU
1	H	225	LEU
1	H	258	LEU
1	H	260	SER
1	H	284	ILE
1	I	13	ASN
1	I	19	LYS
1	I	22	ARG
1	I	28	LEU
1	I	49	ASN
1	I	83	GLN
1	I	86	VAL
1	I	97	SER
1	I	101	GLN
1	I	153	ASN
1	I	160	LEU
1	I	171	LEU
1	I	179	GLU
1	I	225	LEU
1	I	228	LYS
1	I	255	THR
1	I	258	LEU
1	I	261	ARG
1	I	271	LEU
1	I	274	LEU
1	I	276	VAL
1	I	277	LYS
1	I	278	VAL
1	J	12	ILE
1	J	28	LEU
1	J	37	GLN

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Mol	Chain	Res	Type
1	J	38	LEU
1	J	46	PRO
1	J	49	ASN
1	J	83	GLN
1	J	91	THR
1	J	149	SER
1	J	172	LYS
1	J	177	GLN
1	J	225	LEU
1	J	228	LYS
1	J	249	GLN
1	J	258	LEU
1	J	261	ARG
1	J	266	GLU
1	J	278	VAL
1	K	14	GLU
1	K	28	LEU
1	K	37	GLN
1	K	47	THR
1	K	86	VAL
1	K	89	GLN
1	K	112	MET
1	K	114	GLU
1	K	149	SER
1	K	160	LEU
1	K	166	ASN
1	K	167	ASN
1	K	169	LEU
1	K	225	LEU
1	K	258	LEU
1	K	261	ARG
1	K	270	GLU
1	K	274	LEU
1	K	278	VAL
1	L	14	GLU
1	L	28	LEU
1	L	37	GLN
1	L	47	THR
1	L	49	ASN
1	L	85	ASP
1	L	91	THR
1	L	101	GLN

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Mol	Chain	Res	Type
1	L	102	LYS
1	L	112	MET
1	L	113	LYS
1	L	126	MET
1	L	160	LEU
1	L	171	LEU
1	L	177	GLN
1	L	181	ASN
1	L	193	SER
1	L	258	LEU
1	L	261	ARG
1	L	276	VAL
1	L	278	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (161) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	18	GLN
1	A	32	GLN
1	A	43	ASN
1	A	49	ASN
1	A	88	ASN
1	A	101	GLN
1	A	152	GLN
1	A	167	ASN
1	A	168	GLN
1	A	177	GLN
1	A	181	ASN
1	A	213	GLN
1	A	215	ASN
1	A	249	GLN
1	A	269	ASN
1	B	13	ASN
1	B	32	GLN
1	B	43	ASN
1	B	49	ASN
1	B	59	GLN
1	B	101	GLN
1	B	108	ASN
1	B	123	ASN
1	B	124	ASN

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Mol	Chain	Res	Type
1	B	152	GLN
1	B	155	GLN
1	B	166	ASN
1	B	168	GLN
1	B	173	GLN
1	B	181	ASN
1	B	215	ASN
1	B	249	GLN
1	C	37	GLN
1	C	43	ASN
1	C	49	ASN
1	C	59	GLN
1	C	83	GLN
1	C	152	GLN
1	C	167	ASN
1	C	168	GLN
1	C	213	GLN
1	C	219	ASN
1	C	269	ASN
1	D	16	GLN
1	D	37	GLN
1	D	59	GLN
1	D	88	ASN
1	D	89	GLN
1	D	101	GLN
1	D	108	ASN
1	D	153	ASN
1	D	155	GLN
1	D	168	GLN
1	D	177	GLN
1	D	181	ASN
1	D	213	GLN
1	D	275	ASN
1	E	29	ASN
1	E	37	GLN
1	E	43	ASN
1	E	59	GLN
1	E	83	GLN
1	E	89	GLN
1	E	152	GLN
1	E	177	GLN
1	E	269	ASN

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Mol	Chain	Res	Type
1	E	275	ASN
1	F	13	ASN
1	F	43	ASN
1	F	49	ASN
1	F	59	GLN
1	F	88	ASN
1	F	101	GLN
1	F	108	ASN
1	F	176	ASN
1	F	188	HIS
1	F	213	GLN
1	F	275	ASN
1	G	16	GLN
1	G	29	ASN
1	G	37	GLN
1	G	49	ASN
1	G	59	GLN
1	G	88	ASN
1	G	152	GLN
1	G	168	GLN
1	G	177	GLN
1	G	181	ASN
1	G	188	HIS
1	H	13	ASN
1	H	29	ASN
1	H	32	GLN
1	H	43	ASN
1	H	101	GLN
1	H	108	ASN
1	H	152	GLN
1	H	168	GLN
1	H	176	ASN
1	H	177	GLN
1	H	188	HIS
1	H	213	GLN
1	H	269	ASN
1	I	13	ASN
1	I	18	GLN
1	I	49	ASN
1	I	101	GLN
1	I	108	ASN
1	I	152	GLN

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Mol	Chain	Res	Type
1	I	167	ASN
1	I	168	GLN
1	I	173	GLN
1	I	188	HIS
1	I	213	GLN
1	I	215	ASN
1	I	269	ASN
1	I	275	ASN
1	J	13	ASN
1	J	16	GLN
1	J	32	GLN
1	J	37	GLN
1	J	49	ASN
1	J	101	GLN
1	J	108	ASN
1	J	152	GLN
1	J	153	ASN
1	J	166	ASN
1	J	167	ASN
1	J	176	ASN
1	J	188	HIS
1	J	213	GLN
1	J	249	GLN
1	J	269	ASN
1	J	275	ASN
1	K	13	ASN
1	K	18	GLN
1	K	21	ASN
1	K	32	GLN
1	K	37	GLN
1	K	59	GLN
1	K	88	ASN
1	K	101	GLN
1	K	108	ASN
1	K	152	GLN
1	K	168	GLN
1	K	177	GLN
1	K	213	GLN
1	K	215	ASN
1	K	275	ASN
1	L	37	GLN
1	L	49	ASN

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Mol	Chain	Res	Type
1	L	58	HIS
1	L	59	GLN
1	L	89	GLN
1	L	152	GLN
1	L	168	GLN
1	L	176	ASN
1	L	181	ASN
1	L	213	GLN
1	L	269	ASN
1	L	275	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](#)

There are no ligands in this entry.

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	257/309 (83%)	0.30	23 (8%) 15 13	21, 42, 78, 92	0
1	B	257/309 (83%)	0.66	35 (13%) 7 5	22, 56, 97, 122	0
1	C	257/309 (83%)	0.57	23 (8%) 15 13	24, 51, 84, 103	0
1	D	257/309 (83%)	0.64	38 (14%) 5 4	22, 51, 99, 129	0
1	E	257/309 (83%)	0.86	45 (17%) 4 3	22, 68, 106, 115	0
1	F	257/309 (83%)	0.83	40 (15%) 5 4	24, 59, 99, 108	0
1	G	257/309 (83%)	0.51	26 (10%) 12 10	23, 50, 86, 120	0
1	H	257/309 (83%)	0.56	27 (10%) 11 10	24, 51, 90, 103	0
1	I	257/309 (83%)	0.44	23 (8%) 15 13	21, 45, 85, 125	0
1	J	257/309 (83%)	0.32	19 (7%) 20 17	21, 42, 82, 92	0
1	K	257/309 (83%)	0.76	40 (15%) 5 4	22, 52, 96, 112	0
1	L	257/309 (83%)	0.39	24 (9%) 14 12	17, 44, 81, 125	0
All	All	3084/3708 (83%)	0.57	363 (11%) 9 7	17, 50, 95, 129	0

All (363) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	SER	7.5
1	F	284	ILE	7.2
1	L	99	VAL	6.5
1	D	15	ILE	5.7
1	C	11	SER	5.4
1	E	285	VAL	4.9
1	I	164	ASN	4.8
1	B	18	GLN	4.7
1	H	11	SER	4.6
1	L	15	ILE	4.5
1	D	19	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	14	GLU	4.5
1	J	97	SER	4.5
1	J	112	MET	4.3
1	I	97	SER	4.3
1	G	285	VAL	4.3
1	B	13	ASN	4.2
1	G	284	ILE	4.2
1	D	81	SER	4.1
1	D	16	GLN	4.1
1	E	284	ILE	4.1
1	A	192	ASP	4.0
1	D	82	GLY	4.0
1	C	90	ALA	4.0
1	L	88	ASN	4.0
1	F	95	ALA	4.0
1	B	251	GLU	4.0
1	B	99	VAL	4.0
1	H	285	VAL	3.9
1	K	11	SER	3.9
1	B	15	ILE	3.9
1	B	12	ILE	3.9
1	L	12	ILE	3.9
1	B	95	ALA	3.8
1	D	165	ASP	3.8
1	C	96	ALA	3.8
1	D	192	ASP	3.8
1	F	285	VAL	3.8
1	L	247	ASP	3.8
1	D	12	ILE	3.7
1	C	165	ASP	3.7
1	B	88	ASN	3.7
1	B	97	SER	3.7
1	D	11	SER	3.7
1	B	247	ASP	3.7
1	I	86	VAL	3.7
1	K	15	ILE	3.7
1	I	101	GLN	3.6
1	H	165	ASP	3.6
1	B	98	PRO	3.6
1	C	167	ASN	3.6
1	B	11	SER	3.5
1	C	14	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	285	VAL	3.5
1	E	192	ASP	3.5
1	I	11	SER	3.5
1	F	192	ASP	3.5
1	B	16	GLN	3.5
1	G	15	ILE	3.5
1	G	99	VAL	3.5
1	I	285	VAL	3.4
1	K	70	VAL	3.4
1	G	228	LYS	3.4
1	E	168	GLN	3.4
1	B	248	GLU	3.4
1	I	13	ASN	3.3
1	K	86	VAL	3.3
1	D	128	PHE	3.3
1	G	91	THR	3.3
1	G	16	GLN	3.3
1	L	89	GLN	3.3
1	D	285	VAL	3.3
1	J	13	ASN	3.3
1	J	266	GLU	3.3
1	K	14	GLU	3.3
1	E	169	LEU	3.3
1	E	177	GLN	3.3
1	F	47	THR	3.3
1	C	248	GLU	3.2
1	I	12	ILE	3.2
1	E	167	ASN	3.2
1	F	228	LYS	3.2
1	H	96	ALA	3.2
1	C	112	MET	3.2
1	F	50	PRO	3.2
1	E	170	SER	3.2
1	H	192	ASP	3.2
1	C	15	ILE	3.2
1	D	87	TYR	3.1
1	F	103	GLU	3.1
1	J	11	SER	3.1
1	D	13	ASN	3.1
1	H	284	ILE	3.1
1	G	98	PRO	3.1
1	K	91	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	106	LEU	3.1
1	A	194	ASP	3.1
1	E	117	MET	3.1
1	E	194	ASP	3.1
1	F	194	ASP	3.1
1	G	247	ASP	3.1
1	H	112	MET	3.1
1	A	285	VAL	3.0
1	K	107	TYR	3.0
1	H	194	ASP	3.0
1	C	86	VAL	3.0
1	E	99	VAL	3.0
1	A	101	GLN	3.0
1	B	166	ASN	3.0
1	F	12	ILE	3.0
1	H	90	ALA	3.0
1	C	284	ILE	3.0
1	F	97	SER	3.0
1	D	86	VAL	3.0
1	K	272	TYR	2.9
1	A	164	ASN	2.9
1	A	170	SER	2.9
1	B	249	GLN	2.9
1	I	228	LYS	2.9
1	J	284	ILE	2.9
1	K	165	ASP	2.9
1	D	99	VAL	2.9
1	K	96	ALA	2.9
1	H	89	GLN	2.9
1	H	109	TYR	2.9
1	E	165	ASP	2.9
1	L	285	VAL	2.9
1	D	170	SER	2.9
1	E	11	SER	2.9
1	K	97	SER	2.9
1	I	15	ILE	2.9
1	D	18	GLN	2.8
1	F	177	GLN	2.8
1	E	93	PHE	2.8
1	K	104	PHE	2.8
1	A	97	SER	2.8
1	E	72	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	284	ILE	2.8
1	J	177	GLN	2.8
1	K	167	ASN	2.8
1	B	169	LEU	2.8
1	K	12	ILE	2.8
1	J	109	TYR	2.8
1	I	96	ALA	2.8
1	J	283	ASP	2.8
1	F	102	LYS	2.8
1	K	55	LYS	2.8
1	H	16	GLN	2.8
1	F	276	VAL	2.8
1	G	81	SER	2.8
1	D	89	GLN	2.7
1	F	70	VAL	2.7
1	J	192	ASP	2.7
1	J	285	VAL	2.7
1	D	164	ASN	2.7
1	L	124	ASN	2.7
1	B	110	ARG	2.7
1	C	95	ALA	2.7
1	E	47	THR	2.7
1	B	260	SER	2.7
1	A	169	LEU	2.7
1	F	15	ILE	2.7
1	E	76	CYS	2.7
1	I	165	ASP	2.7
1	L	194	ASP	2.7
1	G	11	SER	2.7
1	D	264	ALA	2.6
1	G	257	PHE	2.6
1	F	275	ASN	2.6
1	B	14	GLU	2.6
1	F	125	ASP	2.6
1	E	79	ALA	2.6
1	D	169	LEU	2.6
1	F	166	ASN	2.6
1	K	271	LEU	2.6
1	K	284	ILE	2.6
1	F	98	PRO	2.6
1	D	115	GLU	2.6
1	G	12	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	124	ASN	2.6
1	D	96	ALA	2.6
1	F	165	ASP	2.6
1	H	264	ALA	2.6
1	K	283	ASP	2.6
1	C	97	SER	2.6
1	E	97	SER	2.6
1	G	260	SER	2.6
1	I	170	SER	2.6
1	E	107	TYR	2.6
1	K	118	GLY	2.6
1	B	285	VAL	2.6
1	H	47	THR	2.6
1	E	248	GLU	2.6
1	E	164	ASN	2.6
1	K	116	ASP	2.6
1	D	97	SER	2.5
1	G	51	SER	2.5
1	L	11	SER	2.5
1	C	50	PRO	2.5
1	C	12	ILE	2.5
1	J	111	ASP	2.5
1	I	19	LYS	2.5
1	F	63	VAL	2.5
1	E	91	THR	2.5
1	A	95	ALA	2.5
1	K	164	ASN	2.5
1	A	165	ASP	2.5
1	F	278	VAL	2.5
1	K	92	VAL	2.5
1	A	47	THR	2.5
1	A	89	GLN	2.5
1	E	128	PHE	2.5
1	K	108	ASN	2.5
1	G	165	ASP	2.5
1	F	179	GLU	2.5
1	C	269	ASN	2.5
1	H	164	ASN	2.5
1	E	247	ASP	2.4
1	H	169	LEU	2.4
1	J	165	ASP	2.4
1	B	69	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	98	PRO	2.4
1	I	98	PRO	2.4
1	F	170	SER	2.4
1	J	193	SER	2.4
1	G	164	ASN	2.4
1	F	114	GLU	2.4
1	E	90	ALA	2.4
1	E	96	ALA	2.4
1	G	167	ASN	2.4
1	J	164	ASN	2.4
1	B	250	ILE	2.4
1	E	98	PRO	2.4
1	E	85	ASP	2.4
1	I	247	ASP	2.4
1	L	192	ASP	2.4
1	A	113	LYS	2.4
1	B	228	LYS	2.4
1	A	112	MET	2.4
1	F	274	LEU	2.4
1	K	21	ASN	2.4
1	A	195	SER	2.4
1	C	16	GLN	2.4
1	L	170	SER	2.4
1	A	98	PRO	2.4
1	F	46	PRO	2.4
1	F	86	VAL	2.3
1	F	93	PHE	2.3
1	E	103	GLU	2.3
1	B	170	SER	2.3
1	G	275	ASN	2.3
1	K	166	ASN	2.3
1	A	179	GLU	2.3
1	F	101	GLN	2.3
1	H	83	GLN	2.3
1	H	117	MET	2.3
1	L	168	GLN	2.3
1	F	271	LEU	2.3
1	J	170	SER	2.3
1	D	113	LYS	2.3
1	A	84	ARG	2.3
1	K	278	VAL	2.3
1	G	166	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	42	GLU	2.3
1	L	177	GLN	2.3
1	L	249	GLN	2.3
1	B	87	TYR	2.3
1	A	166	ASN	2.3
1	E	280	PHE	2.3
1	K	13	ASN	2.3
1	D	114	GLU	2.3
1	G	14	GLU	2.3
1	C	194	ASP	2.3
1	D	194	ASP	2.3
1	G	192	ASP	2.3
1	H	283	ASP	2.3
1	K	267	LYS	2.3
1	F	91	THR	2.3
1	K	51	SER	2.3
1	F	272	TYR	2.3
1	D	95	ALA	2.2
1	K	189	GLU	2.2
1	I	125	ASP	2.2
1	K	117	MET	2.2
1	L	96	ALA	2.2
1	G	13	ASN	2.2
1	I	169	LEU	2.2
1	K	88	ASN	2.2
1	D	173	GLN	2.2
1	B	81	SER	2.2
1	D	252	SER	2.2
1	E	66	TYR	2.2
1	F	81	SER	2.2
1	H	170	SER	2.2
1	E	64	GLY	2.2
1	B	113	LYS	2.2
1	J	96	ALA	2.2
1	K	42	GLU	2.2
1	D	88	ASN	2.2
1	E	88	ASN	2.2
1	K	168	GLN	2.2
1	L	94	ARG	2.2
1	B	194	ASP	2.2
1	C	192	ASP	2.2
1	I	192	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	98	PRO	2.2
1	B	252	SER	2.2
1	E	254	GLY	2.2
1	L	97	SER	2.2
1	G	105	LYS	2.2
1	D	103	GLU	2.2
1	L	248	GLU	2.2
1	B	275	ASN	2.2
1	E	166	ASN	2.2
1	I	166	ASN	2.2
1	I	167	ASN	2.2
1	K	99	VAL	2.2
1	F	51	SER	2.2
1	G	97	SER	2.2
1	A	96	ALA	2.2
1	A	13	ASN	2.1
1	F	164	ASN	2.1
1	L	13	ASN	2.1
1	C	267	LYS	2.1
1	E	104	PHE	2.1
1	L	81	SER	2.1
1	I	284	ILE	2.1
1	J	168	GLN	2.1
1	H	102	LYS	2.1
1	D	283	ASP	2.1
1	K	194	ASP	2.1
1	D	47	THR	2.1
1	L	189	GLU	2.1
1	B	168	GLN	2.1
1	E	18	GLN	2.1
1	L	112	MET	2.1
1	K	98	PRO	2.1
1	F	226	GLY	2.1
1	I	111	ASP	2.1
1	L	91	THR	2.1
1	B	90	ALA	2.1
1	K	264	ALA	2.1
1	E	266	GLU	2.1
1	G	103	GLU	2.1
1	H	260	SER	2.1
1	D	112	MET	2.1
1	B	164	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	167	ASN	2.1
1	C	38	LEU	2.1
1	H	103	GLU	2.1
1	C	102	LYS	2.0
1	H	168	GLN	2.0
1	C	273	GLY	2.0
1	E	12	ILE	2.0
1	H	201	THR	2.0
1	E	95	ALA	2.0
1	E	189	GLU	2.0
1	B	51	SER	2.0
1	K	274	LEU	2.0
1	F	52	PHE	2.0
1	H	48	ILE	2.0
1	E	75	ALA	2.0
1	E	276	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.