



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:46 PM UTC

PDB ID : 4HRE / pdb_00004hre
Title : Crystal Structure of p11/Annexin A2 Heterotetramer in Complex with SMARCA3 Peptide
Authors : Gao, P.; Patel, D.J.
Deposited on : 2012-10-27
Resolution : 2.79 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

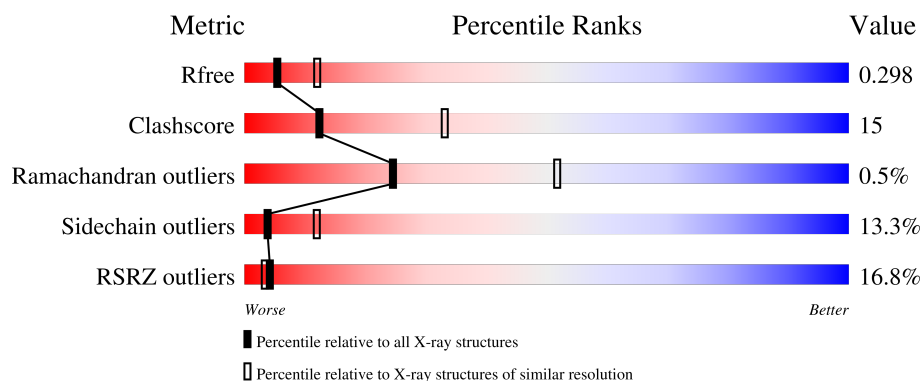
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	339	12% 68% 27% 5%
1	B	339	10% 68% 25% 6%
1	C	339	11% 65% 28% 6%
1	D	339	9% 62% 32% 5%
2	E	97	40% 38% 49% 6% 6%

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Mol	Chain	Length	Quality of chain
2	F	97	25%49%31%13%6%
2	I	97	34%45%38%10%6%
2	J	97	33%45%38%9%6%
3	G	14	57%21%21%21%36%
3	H	14	36%21%29%14%36%
3	K	14	43%50%14%36%
3	L	14	43%29%29%7%36%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14088 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 Annexin A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2705	1700	463	529	13			
1	C	338	Total	C	N	O	S	0	0	0
			2705	1700	463	529	13			
1	B	338	Total	C	N	O	S	0	0	0
			2705	1700	463	529	13			
1	D	338	Total	C	N	O	S	0	0	0
			2701	1699	463	526	13			

- Molecule 2 is a protein called Protein S100-A10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	91	Total	C	N	O	S	0	0	0
			733	472	118	134	9			
2	F	91	Total	C	N	O	S	0	0	0
			733	472	118	134	9			
2	I	91	Total	C	N	O	S	0	0	0
			733	472	118	134	9			
2	J	91	Total	C	N	O	S	0	0	0
			733	472	118	134	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	expression tag	UNP P60903
F	0	SER	-	expression tag	UNP P60903
I	0	SER	-	expression tag	UNP P60903
J	0	SER	-	expression tag	UNP P60903

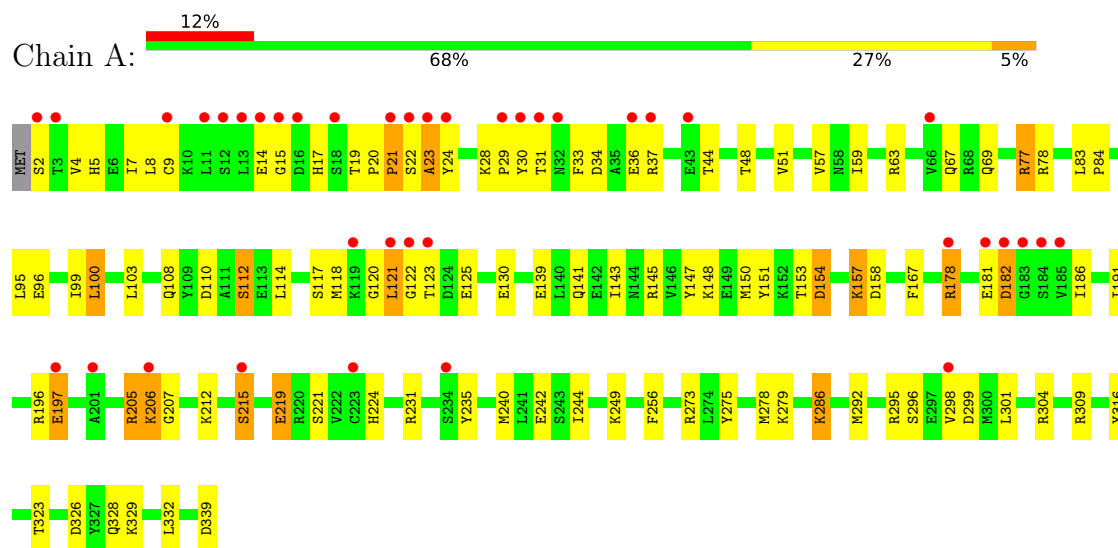
- Molecule 3 is a protein called Helicase-like transcription factor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	9	Total 85	C 61	N 12	O 12	0	0	0
3	H	9	Total 85	C 61	N 12	O 12	0	0	0
3	K	9	Total 85	C 61	N 12	O 12	0	0	0
3	L	9	Total 85	C 61	N 12	O 12	0	0	0

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: Annexin A2

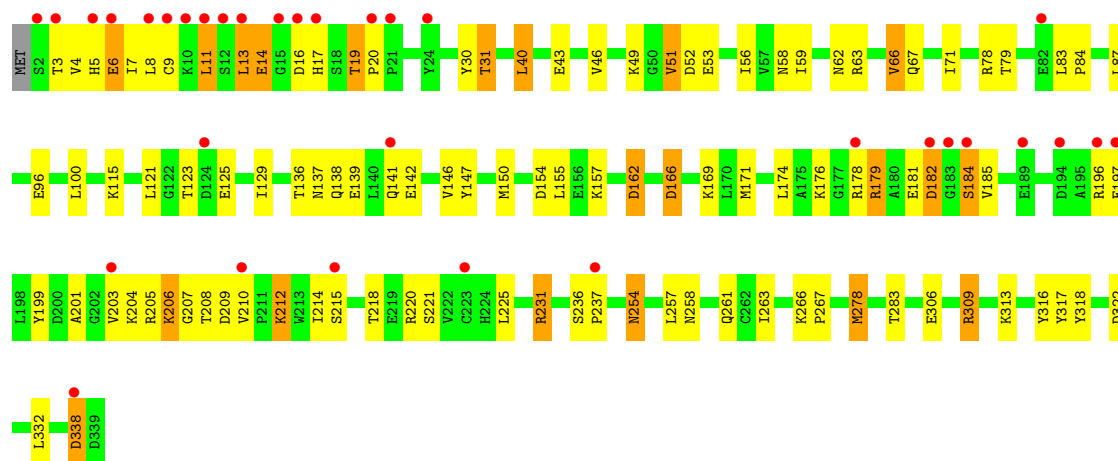


• Molecule 1: Annexin A2

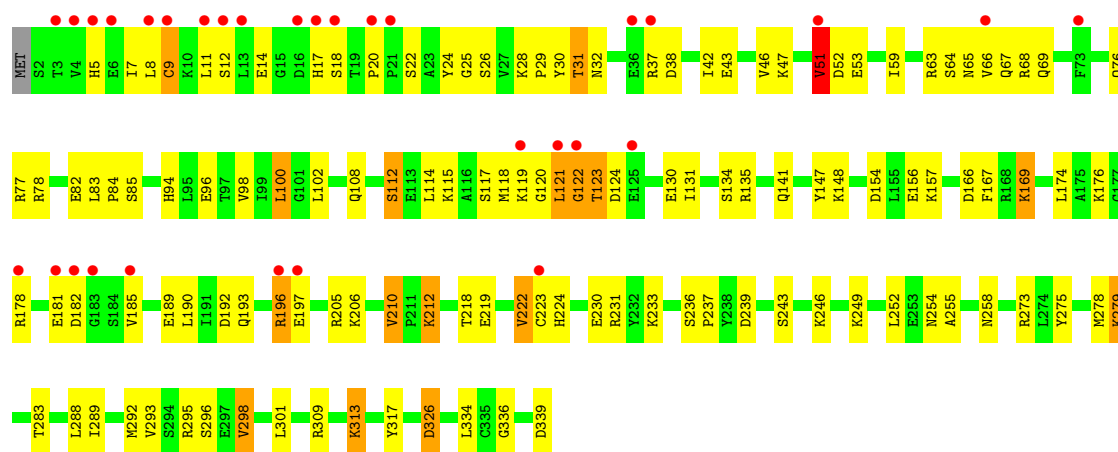


• Molecule 1: Annexin A2

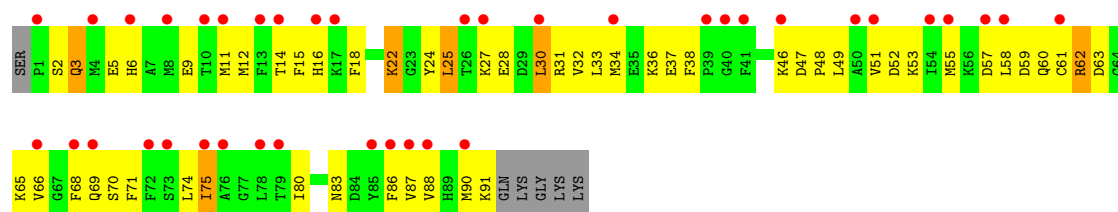




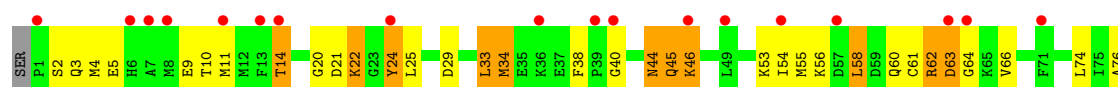
• Molecule 1: Annexin A2

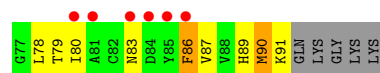


• Molecule 2: Protein S100-A10

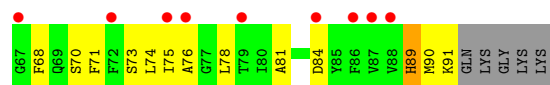
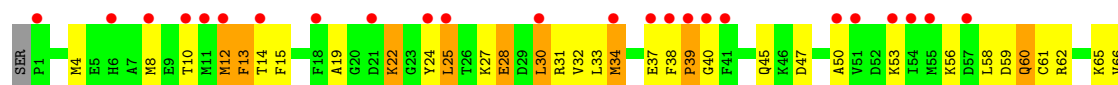
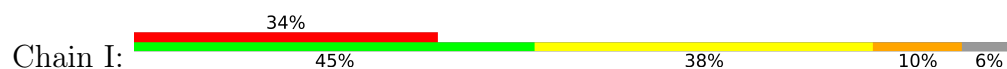


• Molecule 2: Protein S100-A10

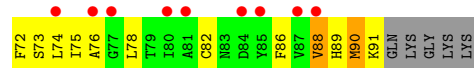
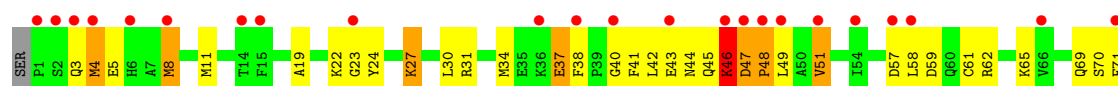




• Molecule 2: Protein S100-A10



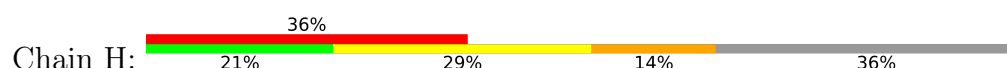
• Molecule 2: Protein S100-A10



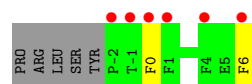
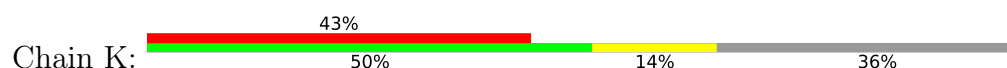
• Molecule 3: Helicase-like transcription factor



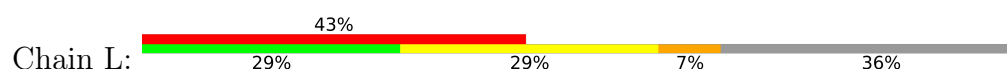
• Molecule 3: Helicase-like transcription factor



• Molecule 3: Helicase-like transcription factor



• Molecule 3: Helicase-like transcription factor



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.79Å 74.35Å 154.47Å 90.14° 96.56° 108.37°	Depositor
Resolution (Å)	47.34 – 2.79 47.34 – 2.79	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.34-2.79) 95.3 (47.34-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.249 , 0.296 0.260 , 0.298	Depositor DCC
R_{free} test set	2586 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,h+k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14088	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4504e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.50	0/2744	0.91	3/3687 (0.1%)
1	B	0.51	0/2744	0.96	7/3687 (0.2%)
1	C	0.50	0/2744	0.98	10/3687 (0.3%)
1	D	0.51	0/2740	0.94	8/3682 (0.2%)
2	E	0.41	0/749	0.96	3/1000 (0.3%)
2	F	0.38	0/749	0.94	1/1000 (0.1%)
2	I	0.39	0/749	0.89	0/1000
2	J	0.48	1/749 (0.1%)	1.03	4/1000 (0.4%)
3	G	0.46	0/90	0.78	0/120
3	H	0.43	0/90	0.86	0/120
3	K	0.47	0/90	0.75	0/120
3	L	0.39	0/90	0.74	0/120
All	All	0.48	1/14328 (0.0%)	0.94	36/19223 (0.2%)

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	1
1	C	0	1
1	D	0	3
2	J	0	1
3	H	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	48	PRO	N-CD	6.96	1.57	1.47

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	LEU	N-CA-C	-8.66	102.25	113.17
2	E	37	GLU	N-CA-C	8.15	119.95	111.14
1	D	20	PRO	N-CA-C	7.71	120.11	110.70
1	D	12	SER	CB-CA-C	7.22	127.39	112.44
1	C	53	GLU	N-CA-C	-7.19	104.13	113.12
1	B	51	VAL	N-CA-C	6.57	122.99	109.34
1	C	51	VAL	N-CA-C	6.28	122.39	109.34
1	B	53	GLU	N-CA-C	-6.18	105.39	113.12
1	D	122	GLY	N-CA-C	-6.15	102.95	112.85
1	C	236	SER	CA-C-N	6.12	125.74	119.56
1	C	236	SER	C-N-CA	6.12	125.74	119.56
2	J	47	ASP	CB-CA-C	6.12	122.23	110.17
1	C	183	GLY	N-CA-C	6.08	120.00	112.64
1	D	51	VAL	N-CA-C	6.00	121.83	109.34
1	B	19	THR	CA-C-N	-5.99	114.21	120.38
1	B	19	THR	C-N-CA	-5.99	114.21	120.38
1	D	53	GLU	N-CA-C	-5.98	105.64	113.12
1	C	20	PRO	N-CA-C	5.92	117.92	110.70
1	C	11	LEU	N-CA-C	5.90	118.19	109.69
1	A	21	PRO	CB-CA-C	-5.81	101.98	111.56
1	B	184	SER	N-CA-C	5.78	118.45	111.40
2	J	89	HIS	N-CA-C	5.74	118.65	111.24
1	C	181	GLU	N-CA-C	5.73	120.55	113.50
1	C	299	ASP	N-CA-C	5.62	120.13	112.88
1	A	31	THR	N-CA-C	5.60	117.07	110.97
2	E	38	PHE	CA-C-N	5.55	124.90	118.85
2	E	38	PHE	C-N-CA	5.55	124.90	118.85
1	D	123	THR	N-CA-C	-5.29	99.66	108.07
1	A	23	ALA	N-CA-C	5.26	122.01	110.80
1	B	338	ASP	N-CA-C	5.23	117.36	109.41
1	B	31	THR	N-CA-C	5.15	116.75	111.03
1	D	279	LYS	N-CA-C	5.13	119.25	112.89
2	J	47	ASP	C-N-CD	-5.09	104.13	125.00
1	C	338	ASP	N-CA-C	5.08	117.27	109.95
2	F	22	LYS	N-CA-C	-5.08	105.74	111.28
2	J	48	PRO	N-CA-C	-5.08	102.01	112.47

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	GLU	Peptide
1	C	15	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	D	120	GLY	Peptide
1	D	121	LEU	Peptide
1	D	181	GLU	Peptide
3	H	-1	THR	Peptide
2	J	46	LYS	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	2705	0	2737	86	0
1	B	2705	0	2737	73	0
1	C	2705	0	2737	74	0
1	D	2701	0	2732	71	0
2	E	733	0	723	41	0
2	F	733	0	723	35	0
2	I	733	0	723	40	0
2	J	733	0	723	41	0
3	G	85	0	78	9	0
3	H	85	0	78	5	0
3	K	85	0	78	0	0
3	L	85	0	78	2	0
All	All	14088	0	14147	434	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (434) 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:B:197:GLU:OE1	1:B:212:LYS:CE	1.82	1.27
1:A:118:MET:O	1:A:123:THR:HG21	1.42	1.17
1:A:120:GLY:CA	1:A:123:THR:HG22	1.76	1.16
1:A:120:GLY:HA3	1:A:123:THR:HG22	1.28	1.11
2:I:4:MET:HB2	2:J:37:GLU:HG3	1.14	1.11
1:B:197:GLU:OE1	1:B:212:LYS:HE2	1.47	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLU:OE1	1:B:212:LYS:HE3	1.50	1.07
1:B:6:GLU:HA	1:B:9:CYS:SG	1.94	1.06
2:I:4:MET:CB	2:J:37:GLU:HG3	1.87	1.04
1:A:215:SER:O	1:A:219:GLU:HG3	1.63	0.99
2:F:86:PHE:O	2:F:90:MET:HB3	1.62	0.99
1:C:23:ALA:O	1:C:301:LEU:HD12	1.68	0.94
2:I:4:MET:HG3	2:J:37:GLU:HG2	1.53	0.91
1:A:120:GLY:HA3	1:A:122:GLY:O	1.70	0.91
1:D:5:HIS:O	1:D:9:CYS:SG	2.33	0.86
1:D:30:TYR:N	1:D:67:GLN:HE22	1.75	0.85
1:A:5:HIS:O	1:A:9:CYS:SG	2.35	0.85
1:A:121:LEU:HB3	1:A:122:GLY:HA3	1.56	0.85
1:D:30:TYR:H	1:D:67:GLN:HE22	1.24	0.83
1:A:120:GLY:CA	1:A:122:GLY:O	2.25	0.83
1:A:197:GLU:HG2	1:A:212:LYS:HZ2	1.42	0.83
2:F:25:LEU:HB2	2:F:66:VAL:HB	1.62	0.82
1:D:5:HIS:CD2	1:D:9:CYS:SG	2.72	0.82
2:I:4:MET:CG	2:J:37:GLU:HG2	2.10	0.81
2:I:38:PHE:HD1	2:J:5:GLU:OE2	1.62	0.80
1:C:19:THR:C	1:C:21:PRO:HD3	2.06	0.79
2:I:58:LEU:HD11	2:I:74:LEU:HD12	1.65	0.79
2:E:66:VAL:HG13	2:E:70:SER:HB2	1.63	0.79
2:E:31:ARG:HA	2:E:51:VAL:HG11	1.65	0.78
1:A:215:SER:O	1:A:219:GLU:CG	2.32	0.78
1:D:222:VAL:HG12	1:D:223:CYS:N	1.97	0.78
2:I:4:MET:CG	2:J:37:GLU:CG	2.62	0.78
1:A:120:GLY:CA	1:A:123:THR:CG2	2.62	0.77
2:F:86:PHE:O	2:F:90:MET:CB	2.33	0.76
2:I:4:MET:HB2	2:J:37:GLU:CG	2.06	0.76
1:A:120:GLY:N	1:A:123:THR:HG22	2.01	0.76
1:B:83:LEU:N	1:B:84:PRO:HD2	2.01	0.75
1:C:192:ASP:O	1:C:196:ARG:HG3	1.87	0.74
1:A:197:GLU:HG2	1:A:212:LYS:NZ	2.02	0.74
2:F:89:HIS:O	2:F:90:MET:HE3	1.88	0.74
1:C:23:ALA:O	1:C:301:LEU:CD1	2.35	0.73
1:D:83:LEU:N	1:D:84:PRO:HD2	2.04	0.73
1:D:192:ASP:O	1:D:196:ARG:HG3	1.87	0.73
1:C:316:TYR:HB3	1:C:338:ASP:HB3	1.70	0.73
2:I:4:MET:CB	2:J:37:GLU:CG	2.67	0.72
1:C:13:LEU:HD13	1:C:14:GLU:H	1.53	0.71
1:D:30:TYR:H	1:D:67:GLN:NE2	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:8:MET:HE1	2:J:75:ILE:HD12	1.73	0.70
1:C:8:LEU:HD21	2:F:78:LEU:HD23	1.74	0.69
1:C:42:ILE:O	1:C:46:VAL:HG23	1.93	0.69
1:D:156:GLU:OE2	1:D:176:LYS:HE3	1.93	0.68
1:C:14:GLU:HB3	1:C:17:HIS:HB2	1.75	0.68
1:D:222:VAL:CG1	1:D:223:CYS:N	2.57	0.68
1:B:5:HIS:O	1:B:9:CYS:SG	2.50	0.68
1:B:197:GLU:CD	1:B:212:LYS:HE2	2.19	0.68
1:B:6:GLU:CA	1:B:9:CYS:SG	2.79	0.67
2:I:4:MET:HG3	2:J:37:GLU:CG	2.24	0.67
1:C:13:LEU:HD22	1:C:14:GLU:HG2	1.75	0.67
2:F:86:PHE:HD2	2:F:90:MET:HG2	1.60	0.67
1:D:82:GLU:HB2	1:D:85:SER:OG	1.95	0.67
1:A:117:SER:O	1:A:123:THR:HB	1.94	0.66
1:A:96:GLU:HG2	1:A:100:LEU:HD23	1.78	0.66
1:B:306:GLU:OE2	1:B:309:ARG:NH2	2.28	0.66
1:B:51:VAL:O	1:B:52:ASP:C	2.37	0.66
1:A:17:HIS:ND1	1:A:19:THR:OG1	2.24	0.65
1:A:118:MET:O	1:A:123:THR:CG2	2.35	0.65
2:F:89:HIS:O	2:F:90:MET:HB2	1.96	0.65
1:A:120:GLY:C	1:A:122:GLY:O	2.40	0.65
1:C:164:SER:HA	1:C:168:ARG:HH21	1.62	0.65
1:A:121:LEU:CB	1:A:122:GLY:HA3	2.21	0.64
2:I:76:ALA:HA	2:J:72:PHE:CE1	2.33	0.64
1:A:24:TYR:O	1:A:301:LEU:HG	1.96	0.64
1:A:83:LEU:N	1:A:84:PRO:HD2	2.13	0.64
1:D:130:GLU:OE1	1:D:273:ARG:NH2	2.31	0.64
1:C:182:ASP:HB2	1:C:221:SER:OG	1.97	0.64
1:D:154:ASP:HB2	1:D:157:LYS:HD3	1.80	0.62
1:A:120:GLY:HA3	1:A:123:THR:CG2	2.19	0.62
2:F:62:ARG:NH1	2:F:63:ASP:OD1	2.32	0.62
1:C:13:LEU:HB2	3:H:4:PHE:HD1	1.65	0.62
1:A:206:LYS:HD3	1:A:207:GLY:H	1.64	0.62
1:C:132:ILE:HG13	1:C:171:MET:HE3	1.82	0.62
1:C:59:ILE:O	1:C:63:ARG:HG2	2.00	0.62
2:I:38:PHE:CD1	2:J:5:GLU:OE2	2.51	0.61
2:J:46:LYS:HD3	2:J:46:LYS:H	1.66	0.61
1:D:17:HIS:N	1:D:18:SER:HA	2.16	0.60
1:D:42:ILE:O	1:D:46:VAL:HG23	2.01	0.60
1:A:286:LYS:HE3	1:A:286:LYS:H	1.66	0.60
1:C:83:LEU:HB3	1:C:84:PRO:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:18:PHE:CZ	2:E:36:LYS:HG3	2.36	0.60
1:B:316:TYR:CB	1:B:338:ASP:HB3	2.31	0.60
1:B:56:ILE:HG21	1:B:87:LEU:HD21	1.84	0.60
2:J:19:ALA:HB1	2:J:23:GLY:HA2	1.84	0.59
1:A:14:GLU:H	1:A:15:GLY:HA2	1.67	0.59
2:E:18:PHE:HB2	2:E:33:LEU:HD12	1.84	0.59
1:A:30:TYR:N	1:A:67:GLN:HE22	1.98	0.59
1:D:5:HIS:HA	1:D:8:LEU:HD12	1.82	0.59
1:A:14:GLU:HB3	1:A:15:GLY:C	2.28	0.59
1:B:166:ASP:N	1:B:166:ASP:OD1	2.35	0.59
1:C:316:TYR:CB	1:C:338:ASP:HB3	2.31	0.59
1:A:33:PHE:CE1	1:A:67:GLN:HB3	2.38	0.59
1:A:121:LEU:N	1:A:122:GLY:O	2.36	0.58
1:D:313:LYS:HE2	1:D:313:LYS:HA	1.85	0.58
2:E:59:ASP:HA	3:G:0:PHE:HD1	1.67	0.58
1:C:124:ASP:OD1	1:C:286:LYS:NZ	2.32	0.58
2:F:46:LYS:H	2:F:46:LYS:HD3	1.69	0.58
1:D:230:GLU:OE2	1:D:233:LYS:NZ	2.26	0.58
3:G:1:PHE:HD1	3:G:1:PHE:H	1.51	0.58
1:B:63:ARG:HG3	1:B:71:ILE:HD11	1.86	0.58
1:A:28:LYS:HB3	1:A:29:PRO:HD2	1.86	0.58
1:C:12:SER:HB3	2:F:45:GLN:HG3	1.86	0.58
1:C:58:ASN:O	1:C:62:ASN:HB2	2.04	0.58
2:E:71:PHE:CZ	2:E:75:ILE:HD11	2.39	0.58
1:C:179:ARG:NH1	1:C:220:ARG:O	2.33	0.58
1:B:225:LEU:HD13	1:B:263:ILE:HD13	1.86	0.58
1:C:30:TYR:N	1:C:67:GLN:HE22	2.02	0.58
1:B:283:THR:CG2	1:B:322:ASP:HB3	2.34	0.57
2:E:32:VAL:O	2:E:36:LYS:HG2	2.05	0.57
3:G:-2:PRO:HA	3:H:0:PHE:HA	1.86	0.57
3:G:-1:THR:H	3:H:-1:THR:HG22	1.70	0.57
1:D:176:LYS:HD2	1:D:178:ARG:NH2	2.19	0.57
2:I:4:MET:O	2:I:8:MET:HG2	2.04	0.57
1:A:191:ILE:HG13	1:A:224:HIS:CE1	2.39	0.56
1:D:96:GLU:HG2	1:D:100:LEU:HD23	1.87	0.56
2:E:16:HIS:HE1	2:F:83:ASN:HD21	1.51	0.56
1:B:40:LEU:HG	1:B:78:ARG:NH1	2.21	0.56
2:I:59:ASP:HB2	2:I:70:SER:HA	1.88	0.56
1:A:44:THR:O	1:A:48:THR:OG1	2.23	0.56
2:I:70:SER:O	2:I:73:SER:OG	2.22	0.56
2:J:59:ASP:OD2	2:J:69:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:VAL:O	1:C:52:ASP:C	2.48	0.56
1:C:224:HIS:O	1:C:228:VAL:HG23	2.05	0.56
2:J:31:ARG:HB2	2:J:51:VAL:HG21	1.88	0.56
2:F:2:SER:HB3	2:F:5:GLU:HG3	1.87	0.56
2:J:3:GLN:C	2:J:5:GLU:H	2.13	0.55
1:A:182:ASP:HB2	1:A:221:SER:OG	2.07	0.55
1:C:96:GLU:HG2	1:C:100:LEU:HD23	1.89	0.55
1:D:102:LEU:HD23	1:D:293:VAL:HG13	1.88	0.55
2:I:28:GLU:CD	2:I:28:GLU:H	2.14	0.55
3:G:1:PHE:O	3:G:3:ARG:NH1	2.40	0.55
2:I:71:PHE:HZ	2:J:4:MET:HE1	1.72	0.55
2:J:41:PHE:O	2:J:45:GLN:HG2	2.07	0.55
1:A:154:ASP:OD1	1:A:154:ASP:N	2.37	0.55
1:D:222:VAL:HG12	1:D:223:CYS:H	1.70	0.55
2:J:74:LEU:O	2:J:78:LEU:HB2	2.06	0.55
1:A:110:ASP:HB2	1:A:143:ILE:HD12	1.89	0.55
1:B:30:TYR:N	1:B:67:GLN:HE22	2.05	0.54
2:F:86:PHE:HA	2:F:90:MET:HB2	1.88	0.54
1:C:83:LEU:N	1:C:84:PRO:CD	2.70	0.54
1:B:154:ASP:HB2	1:B:157:LYS:HD3	1.89	0.54
1:D:59:ILE:O	1:D:63:ARG:HG2	2.07	0.54
1:C:3:THR:O	1:C:7:ILE:HG12	2.08	0.54
1:A:34:ASP:OD2	1:A:36:GLU:HG3	2.08	0.54
1:C:7:ILE:HD11	2:F:90:MET:SD	2.48	0.54
2:F:76:ALA:O	2:F:80:ILE:HG13	2.08	0.54
1:C:29:PRO:HA	1:C:64:SER:HB3	1.89	0.53
1:A:120:GLY:N	1:A:123:THR:CG2	2.71	0.53
2:E:49:LEU:HB3	2:E:53:LYS:HE3	1.90	0.53
1:A:22:SER:O	1:A:23:ALA:HB3	2.07	0.53
1:A:83:LEU:N	1:A:84:PRO:CD	2.71	0.53
1:A:197:GLU:HG2	1:A:212:LYS:CE	2.38	0.53
1:C:130:GLU:O	1:C:134:SER:OG	2.26	0.53
1:D:326:ASP:N	1:D:326:ASP:OD1	2.39	0.53
1:C:128:LEU:O	1:C:132:ILE:HG12	2.08	0.53
2:E:57:ASP:N	2:E:61:CYS:SG	2.82	0.53
2:E:80:ILE:HD12	3:G:1:PHE:HE2	1.72	0.53
2:J:40:GLY:O	2:J:44:ASN:HB2	2.09	0.53
2:I:22:LYS:HB2	2:I:24:TYR:CZ	2.43	0.53
1:D:197:GLU:HG2	1:D:212:LYS:HG2	1.90	0.53
1:C:244:ILE:HD11	1:C:260:VAL:HG21	1.91	0.52
2:F:60:GLN:HB3	2:F:62:ARG:CZ	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LYS:HB2	1:B:318:TYR:HE1	1.74	0.52
1:C:83:LEU:N	1:C:84:PRO:HD2	2.25	0.52
1:D:295:ARG:HA	1:D:298:VAL:HG23	1.90	0.52
1:A:33:PHE:CZ	1:A:67:GLN:HB3	2.45	0.52
2:I:27:LYS:HZ2	2:I:31:ARG:HE	1.56	0.52
1:A:120:GLY:C	1:A:123:THR:CG2	2.83	0.52
1:C:24:TYR:HB2	1:C:298:VAL:O	2.10	0.52
1:D:7:ILE:O	1:D:11:LEU:HG	2.10	0.52
2:E:2:SER:N	2:E:5:GLU:OE1	2.42	0.51
1:B:206:LYS:HD3	1:B:207:GLY:H	1.75	0.51
1:D:108:GLN:O	1:D:112:SER:OG	2.28	0.51
1:D:131:ILE:O	1:D:135:ARG:HG2	2.09	0.51
2:E:16:HIS:HE1	2:F:83:ASN:ND2	2.08	0.51
1:D:134:SER:OG	1:D:135:ARG:NH1	2.43	0.51
2:I:60:GLN:HE22	2:I:62:ARG:HG3	1.75	0.51
1:C:283:THR:HG21	1:C:322:ASP:HB3	1.92	0.51
2:J:73:SER:OG	3:L:0:PHE:O	2.25	0.51
1:C:130:GLU:OE1	1:C:290:ARG:NH2	2.28	0.51
1:A:316:TYR:CD2	1:A:332:LEU:HD22	2.45	0.51
1:B:59:ILE:O	1:B:63:ARG:HG2	2.11	0.51
1:B:146:VAL:HG12	1:B:150:MET:SD	2.51	0.51
1:C:30:TYR:OH	1:D:219:GLU:OE1	2.21	0.51
2:J:30:LEU:O	2:J:34:MET:HG3	2.10	0.51
1:A:196:ARG:HD2	1:A:235:TYR:CZ	2.46	0.50
2:F:24:TYR:HD1	2:F:24:TYR:H	1.58	0.50
1:B:182:ASP:HB2	1:B:221:SER:OG	2.11	0.50
2:J:22:LYS:HG2	2:J:24:TYR:HD1	1.76	0.50
1:B:16:ASP:HB3	1:B:17:HIS:HA	1.93	0.50
2:I:30:LEU:HA	2:I:33:LEU:HD23	1.93	0.50
1:A:21:PRO:HG3	1:A:29:PRO:HD3	1.92	0.50
1:C:51:VAL:O	1:C:51:VAL:HG12	2.12	0.50
1:C:56:ILE:HG21	1:C:87:LEU:HD21	1.93	0.50
1:B:174:LEU:HD23	1:B:218:THR:HG22	1.93	0.50
1:B:206:LYS:HD3	1:B:207:GLY:N	2.26	0.50
1:B:40:LEU:HG	1:B:78:ARG:HH12	1.77	0.50
1:D:83:LEU:N	1:D:84:PRO:CD	2.74	0.50
1:A:292:MET:O	1:A:296:SER:HB3	2.12	0.50
2:J:58:LEU:HB3	2:J:70:SER:HB3	1.93	0.50
1:B:83:LEU:N	1:B:84:PRO:CD	2.73	0.50
1:B:58:ASN:O	1:B:62:ASN:ND2	2.45	0.49
1:B:137:ASN:ND2	1:B:179:ARG:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:THR:O	2:F:14:THR:OG1	2.30	0.49
1:B:316:TYR:CD1	1:B:332:LEU:HD22	2.46	0.49
1:A:295:ARG:HH21	1:A:299:ASP:CG	2.19	0.49
1:A:121:LEU:C	1:A:121:LEU:CD2	2.86	0.49
1:C:166:ASP:HA	1:C:169:LYS:HB2	1.94	0.49
1:A:121:LEU:N	1:A:122:GLY:CA	2.74	0.49
1:A:139:GLU:O	1:A:143:ILE:HG12	2.12	0.49
2:E:16:HIS:CE1	2:F:83:ASN:HD21	2.29	0.49
2:J:71:PHE:O	2:J:74:LEU:HB3	2.11	0.49
1:D:166:ASP:HB2	1:D:252:LEU:HD22	1.95	0.49
1:A:182:ASP:H	1:A:221:SER:HB3	1.77	0.49
1:C:17:HIS:HA	1:C:18:SER:HA	1.50	0.49
1:D:94:HIS:O	1:D:98:VAL:HG23	2.12	0.49
2:J:3:GLN:C	2:J:5:GLU:N	2.69	0.49
2:E:3:GLN:HB2	2:F:10:THR:HG21	1.94	0.48
1:A:328:GLN:OE1	1:A:329:LYS:HE3	2.13	0.48
1:A:121:LEU:HB3	1:A:122:GLY:CA	2.35	0.48
1:D:26:SER:HB2	1:D:336:GLY:HA3	1.96	0.48
1:A:95:LEU:HD22	1:A:326:ASP:HB3	1.95	0.48
2:E:24:TYR:CG	2:E:65:LYS:HD2	2.49	0.48
2:I:10:THR:HA	2:I:13:PHE:CE1	2.49	0.48
1:C:87:LEU:HD12	1:C:103:LEU:HD11	1.96	0.48
1:B:5:HIS:CE1	2:I:40:GLY:H	2.31	0.48
1:B:8:LEU:HD11	2:J:8:MET:HE1	1.95	0.48
2:E:25:LEU:HD11	2:E:33:LEU:HD13	1.95	0.48
1:B:197:GLU:CG	1:B:212:LYS:HE2	2.44	0.48
2:J:8:MET:HA	2:J:11:MET:HG3	1.96	0.48
1:C:292:MET:O	1:C:296:SER:HB3	2.14	0.48
1:D:122:GLY:O	1:D:123:THR:OG1	2.29	0.48
1:C:4:VAL:HB	2:E:9:GLU:HB2	1.95	0.48
2:I:13:PHE:HD1	2:I:14:THR:N	2.12	0.48
1:B:136:THR:OG1	1:B:139:GLU:HG3	2.14	0.47
2:I:12:MET:HE3	2:I:12:MET:HB3	1.76	0.47
2:E:22:LYS:HB2	2:E:24:TYR:CE2	2.49	0.47
2:J:42:LEU:HD12	2:J:42:LEU:H	1.79	0.47
1:B:257:LEU:O	1:B:261:GLN:HG3	2.14	0.47
1:D:190:LEU:HD23	1:D:224:HIS:CE1	2.49	0.47
1:C:2:SER:HB2	1:C:4:VAL:HG12	1.95	0.47
1:C:13:LEU:HB2	3:H:4:PHE:CD1	2.49	0.47
2:E:47:ASP:OD2	2:E:53:LYS:NZ	2.40	0.47
1:B:179:ARG:HD3	1:B:220:ARG:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:LYS:HD3	2:J:24:TYR:HB2	1.96	0.47
1:C:22:SER:O	1:C:24:TYR:N	2.47	0.47
1:D:22:SER:O	1:D:28:LYS:NZ	2.47	0.47
1:D:25:GLY:O	1:D:28:LYS:HE2	2.14	0.47
1:D:174:LEU:HD23	1:D:218:THR:HG22	1.97	0.47
2:I:15:PHE:CG	2:I:68:PHE:HD1	2.32	0.47
2:I:30:LEU:HD12	2:I:34:MET:HE1	1.96	0.47
1:A:57:VAL:HG22	1:A:99:ILE:HD11	1.97	0.47
1:A:59:ILE:O	1:A:63:ARG:HG2	2.14	0.47
1:A:178:ARG:HE	1:A:178:ARG:HB2	1.41	0.47
2:E:6:HIS:HA	2:E:9:GLU:HB3	1.96	0.47
2:E:15:PHE:CD2	2:E:68:PHE:HD2	2.33	0.47
2:E:27:LYS:HB3	2:E:55:MET:SD	2.55	0.47
1:B:13:LEU:HD12	2:I:53:LYS:HB3	1.96	0.47
1:B:316:TYR:HB3	1:B:338:ASP:HB3	1.95	0.47
1:D:64:SER:O	1:D:68:ARG:HG3	2.14	0.47
1:A:275:TYR:O	1:A:279:LYS:HB3	2.14	0.47
1:B:49:LYS:HB3	1:B:49:LYS:HE2	1.63	0.47
1:C:62:ASN:HD21	1:D:178:ARG:HD2	1.80	0.46
2:E:22:LYS:H	2:E:22:LYS:HG2	1.49	0.46
1:B:30:TYR:HB2	1:B:63:ARG:HD3	1.98	0.46
2:J:88:VAL:O	2:J:91:LYS:NZ	2.43	0.46
2:F:90:MET:O	2:F:91:LYS:C	2.58	0.46
1:A:83:LEU:HB3	1:A:84:PRO:HD3	1.97	0.46
1:C:22:SER:C	1:C:24:TYR:N	2.72	0.46
2:F:20:GLY:HA3	2:F:22:LYS:HE3	1.98	0.46
1:D:28:LYS:HB3	1:D:29:PRO:HD2	1.97	0.46
1:C:13:LEU:HD23	3:H:5:GLU:HG3	1.96	0.46
2:I:66:VAL:HG13	2:I:70:SER:OG	2.15	0.46
2:E:80:ILE:HD12	3:G:1:PHE:CE2	2.49	0.46
1:D:51:VAL:O	1:D:52:ASP:C	2.58	0.46
2:I:12:MET:HE1	2:J:86:PHE:CD2	2.51	0.46
2:J:90:MET:HB2	2:J:90:MET:HE3	1.70	0.46
2:E:24:TYR:HB2	2:E:65:LYS:HB3	1.98	0.46
2:E:25:LEU:HB2	2:E:66:VAL:O	2.16	0.46
2:E:63:ASP:C	2:E:65:LYS:H	2.24	0.46
1:A:304:ARG:HB3	1:A:339:ASP:OD2	2.16	0.46
1:A:96:GLU:O	1:A:100:LEU:HB2	2.15	0.45
1:D:24:TYR:HA	1:D:301:LEU:HD12	1.98	0.45
1:D:292:MET:O	1:D:296:SER:HB3	2.16	0.45
2:I:22:LYS:H	2:I:22:LYS:HG2	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:THR:CG2	1:C:322:ASP:HB3	2.45	0.45
2:E:87:VAL:HA	2:E:91:LYS:HB2	1.97	0.45
1:B:129:ILE:HA	1:B:171:MET:HE1	1.98	0.45
1:B:13:LEU:HD22	1:B:14:GLU:H	1.81	0.45
1:B:19:THR:HB	1:B:20:PRO:HD2	1.99	0.45
1:B:43:GLU:OE1	1:B:79:THR:HG22	2.17	0.45
1:A:21:PRO:O	1:A:22:SER:CB	2.65	0.45
1:B:197:GLU:HG2	1:B:212:LYS:HE2	1.98	0.45
1:D:115:LYS:HD2	1:D:147:TYR:OH	2.17	0.45
1:A:323:THR:O	1:A:328:GLN:NE2	2.50	0.45
2:J:47:ASP:HB2	2:J:49:LEU:HB2	1.98	0.45
1:A:215:SER:C	1:A:219:GLU:HG3	2.37	0.44
1:B:11:LEU:HD21	2:I:81:ALA:HB1	2.00	0.44
1:A:154:ASP:HB2	1:A:157:LYS:HD3	1.99	0.44
1:B:174:LEU:CD2	1:B:218:THR:HG22	2.47	0.44
1:A:2:SER:HA	2:F:9:GLU:OE1	2.17	0.44
1:C:34:ASP:HB3	1:C:37:ARG:HD3	1.98	0.44
2:F:53:LYS:O	2:F:56:LYS:HG2	2.17	0.44
1:B:17:HIS:HB2	1:B:66:VAL:HG11	2.00	0.44
2:F:55:MET:O	2:F:61:CYS:HB2	2.17	0.44
1:B:5:HIS:NE2	2:I:39:PRO:HG2	2.32	0.44
2:E:28:GLU:O	2:E:31:ARG:HB2	2.18	0.44
1:B:142:GLU:O	1:B:146:VAL:HG23	2.18	0.44
1:B:210:VAL:O	1:B:214:ILE:HG13	2.18	0.44
1:D:166:ASP:HA	1:D:169:LYS:HG3	2.00	0.44
1:A:77:ARG:HE	1:A:77:ARG:HB3	1.53	0.44
1:A:197:GLU:HG2	1:A:212:LYS:HE3	1.98	0.44
2:F:11:MET:HA	2:F:14:THR:OG1	2.18	0.44
1:D:114:LEU:O	1:D:118:MET:HG2	2.18	0.44
1:A:125:GLU:HG2	1:A:167:PHE:CE2	2.53	0.43
1:C:54:VAL:HG21	1:D:182:ASP:HA	1.99	0.43
1:C:313:LYS:NZ	1:C:314:SER:H	2.16	0.43
1:A:125:GLU:HG2	1:A:167:PHE:CZ	2.53	0.43
1:A:316:TYR:CE2	1:A:332:LEU:HD22	2.53	0.43
1:C:46:VAL:HG13	1:C:90:ALA:HB2	1.99	0.43
1:A:130:GLU:OE1	1:A:273:ARG:NH2	2.25	0.43
1:A:244:ILE:HD13	1:A:256:PHE:HB3	1.99	0.43
2:E:34:MET:SD	2:E:51:VAL:HG13	2.57	0.43
1:B:231:ARG:HA	1:B:231:ARG:HD3	1.86	0.43
1:A:240:MET:HA	1:A:240:MET:HE3	2.01	0.43
1:C:236:SER:HA	1:C:237:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:GLY:O	2:F:44:ASN:HB2	2.18	0.43
1:B:283:THR:HG22	1:B:322:ASP:HB3	2.00	0.43
1:B:123:THR:OG1	1:B:162:ASP:OD2	2.29	0.43
1:D:17:HIS:HE2	1:D:29:PRO:HD3	1.82	0.43
1:D:51:VAL:O	1:D:51:VAL:HG12	2.18	0.43
1:C:75:TYR:CZ	1:C:79:THR:HG21	2.53	0.43
1:B:201:ALA:HB1	1:B:209:ASP:HB3	2.00	0.43
1:D:38:ASP:O	1:D:42:ILE:HG13	2.19	0.43
1:A:206:LYS:HD3	1:A:207:GLY:N	2.31	0.43
2:F:11:MET:O	2:F:14:THR:OG1	2.33	0.43
1:A:147:TYR:OH	1:A:158:ASP:OD2	2.29	0.43
1:C:63:ARG:HG3	1:C:71:ILE:HD11	2.01	0.43
1:B:166:ASP:HA	1:B:169:LYS:HB2	1.99	0.43
1:D:42:ILE:CG1	1:D:59:ILE:HD11	2.49	0.43
1:D:117:SER:HB2	1:D:124:ASP:HB3	2.01	0.43
1:D:254:ASN:O	1:D:258:ASN:ND2	2.49	0.43
1:A:108:GLN:O	1:A:112:SER:HB3	2.19	0.42
2:J:27:LYS:HE2	2:J:27:LYS:HB2	1.76	0.42
1:A:21:PRO:O	1:A:22:SER:OG	2.28	0.42
1:B:266:LYS:HB3	1:B:267:PRO:HD3	1.99	0.42
2:E:69:GLN:HE21	3:G:-1:THR:HG22	1.84	0.42
1:B:147:TYR:CE1	1:B:155:LEU:HA	2.53	0.42
1:A:20:PRO:C	1:A:22:SER:H	2.27	0.42
2:F:58:LEU:HD12	2:F:61:CYS:SG	2.59	0.42
1:B:212:LYS:HD3	1:B:212:LYS:HA	1.88	0.42
1:D:167:PHE:HE1	1:D:255:ALA:HB2	1.85	0.42
1:C:199:TYR:CE2	1:C:204:LYS:HB2	2.54	0.42
2:E:71:PHE:O	2:E:74:LEU:HB3	2.20	0.42
2:E:60:GLN:HA	2:E:62:ARG:NH1	2.34	0.42
1:C:225:LEU:HD13	1:C:263:ILE:HD13	2.00	0.42
1:C:249:LYS:HA	1:C:253:GLU:OE1	2.20	0.42
1:C:300:MET:HE1	1:C:315:LEU:HD23	2.02	0.42
1:B:316:TYR:CG	1:B:338:ASP:HB3	2.54	0.42
1:C:100:LEU:HD13	1:C:100:LEU:HA	1.85	0.42
1:B:51:VAL:O	1:B:51:VAL:HG12	2.19	0.42
1:C:205:ARG:HH21	1:C:209:ASP:HB2	1.85	0.42
2:E:11:MET:HE3	2:E:11:MET:HB2	1.84	0.42
1:B:278:MET:HB3	1:B:322:ASP:CG	2.45	0.42
2:J:24:TYR:HB3	2:J:65:LYS:HB3	2.01	0.42
1:A:148:LYS:HE2	1:A:148:LYS:HB3	1.91	0.42
1:C:199:TYR:CZ	1:C:204:LYS:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:LYS:O	2:E:30:LEU:HB3	2.20	0.41
2:E:47:ASP:HA	2:E:48:PRO:HD3	1.86	0.41
1:B:123:THR:HB	1:B:125:GLU:CD	2.45	0.41
1:B:313:LYS:HD3	1:B:317:TYR:CD2	2.55	0.41
1:D:43:GLU:O	1:D:47:LYS:HG3	2.20	0.41
2:I:71:PHE:HZ	2:J:4:MET:CE	2.31	0.41
1:C:191:ILE:HG13	1:C:224:HIS:CE1	2.55	0.41
2:E:46:LYS:HB2	2:E:46:LYS:HE3	1.72	0.41
2:F:29:ASP:O	2:F:33:LEU:HB2	2.20	0.41
1:B:199:TYR:CE2	1:B:204:LYS:HG3	2.55	0.41
1:D:98:VAL:HG22	1:D:289:ILE:HG12	2.02	0.41
2:I:47:ASP:O	2:I:50:ALA:HB2	2.21	0.41
2:J:8:MET:HE2	2:J:8:MET:HB2	1.91	0.41
1:A:150:MET:HE2	1:A:151:TYR:CZ	2.55	0.41
1:C:129:ILE:HA	1:C:171:MET:HE1	2.03	0.41
1:D:189:GLU:O	1:D:193:GLN:HB2	2.21	0.41
2:I:27:LYS:O	2:I:30:LEU:N	2.53	0.41
2:I:89:HIS:O	2:I:91:LYS:NZ	2.36	0.41
1:B:137:ASN:HD21	1:B:179:ARG:N	2.19	0.41
1:D:65:ASN:O	1:D:69:GLN:HG2	2.21	0.41
1:D:210:VAL:HG11	1:D:252:LEU:HD21	2.02	0.41
2:I:19:ALA:HA	2:I:25:LEU:HD23	2.02	0.41
3:L:2:PRO:HA	3:L:3:ARG:NH1	2.36	0.41
1:D:102:LEU:HD11	1:D:334:LEU:HD11	2.01	0.41
1:A:121:LEU:N	1:A:122:GLY:C	2.79	0.41
1:C:19:THR:O	1:C:21:PRO:HD3	2.19	0.41
1:B:283:THR:HG21	1:B:322:ASP:HB3	2.02	0.41
2:J:72:PHE:O	2:J:76:ALA:N	2.52	0.41
1:C:201:ALA:HB1	1:C:209:ASP:HB3	2.02	0.41
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.92	0.41
1:A:121:LEU:N	1:A:122:GLY:HA3	2.36	0.41
1:C:123:THR:OG1	1:C:162:ASP:OD2	2.27	0.41
1:C:246:LYS:HE2	1:C:246:LYS:HB3	1.90	0.41
2:E:11:MET:HE1	2:F:11:MET:SD	2.60	0.41
2:F:34:MET:HE3	2:F:74:LEU:HD21	2.02	0.41
2:F:61:CYS:O	2:F:64:GLY:N	2.31	0.41
1:B:254:ASN:O	1:B:258:ASN:ND2	2.43	0.41
2:I:27:LYS:NZ	2:I:31:ARG:HE	2.19	0.41
2:J:65:LYS:HE3	2:J:65:LYS:HB2	1.73	0.41
1:C:94:HIS:HB3	1:C:327:TYR:CE1	2.56	0.41
3:G:1:PHE:CD1	3:G:1:PHE:N	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:HD2	1:A:207:GLY:O	2.21	0.40
2:E:12:MET:HA	2:E:68:PHE:CE2	2.56	0.40
1:B:67:GLN:O	1:B:71:ILE:HG13	2.20	0.40
1:B:115:LYS:HA	1:B:115:LYS:HD2	1.89	0.40
1:D:275:TYR:O	1:D:279:LYS:HB3	2.21	0.40
1:D:288:LEU:O	1:D:292:MET:HG2	2.21	0.40
2:E:83:ASN:O	2:E:86:PHE:HB3	2.21	0.40
2:F:62:ARG:H	2:F:62:ARG:HG3	1.66	0.40
1:D:96:GLU:HG2	1:D:100:LEU:CD2	2.50	0.40
1:D:236:SER:HA	1:D:237:PRO:HD3	1.91	0.40
1:D:313:LYS:HD3	1:D:317:TYR:CG	2.56	0.40
1:C:38:ASP:O	1:C:42:ILE:HG13	2.21	0.40
1:C:166:ASP:HB3	1:C:210:VAL:HG11	2.03	0.40
1:D:5:HIS:NE2	1:D:9:CYS:SG	2.93	0.40
1:D:239:ASP:O	1:D:243:SER:OG	2.37	0.40
1:D:334:LEU:HD23	1:D:334:LEU:HA	1.83	0.40
1:A:114:LEU:O	1:A:118:MET:HB2	2.21	0.40
1:B:236:SER:HA	1:B:237:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/339 (99%)	319 (95%)	16 (5%)	1 (0%)	36	63
1	B	336/339 (99%)	328 (98%)	8 (2%)	0	100	100
1	C	336/339 (99%)	316 (94%)	16 (5%)	4 (1%)	10	30
1	D	336/339 (99%)	318 (95%)	16 (5%)	2 (1%)	21	47
2	E	89/97 (92%)	81 (91%)	8 (9%)	0	100	100
2	F	89/97 (92%)	82 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	89/97 (92%)	78 (88%)	10 (11%)	1 (1%)	11	32
2	J	89/97 (92%)	74 (83%)	15 (17%)	0	100	100
3	G	7/14 (50%)	7 (100%)	0	0	100	100
3	H	7/14 (50%)	7 (100%)	0	0	100	100
3	K	7/14 (50%)	7 (100%)	0	0	100	100
3	L	7/14 (50%)	7 (100%)	0	0	100	100
All	All	1728/1800 (96%)	1624 (94%)	96 (6%)	8 (0%)	24	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	23	ALA
1	C	21	PRO
1	C	130	GLU
1	D	31	THR
1	D	51	VAL
1	A	51	VAL
1	C	51	VAL
2	I	39	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	300/301 (100%)	270 (90%)	30 (10%)	7	21
1	B	300/301 (100%)	264 (88%)	36 (12%)	5	15
1	C	300/301 (100%)	268 (89%)	32 (11%)	6	19
1	D	298/301 (99%)	266 (89%)	32 (11%)	6	19
2	E	80/85 (94%)	69 (86%)	11 (14%)	3	11
2	F	80/85 (94%)	61 (76%)	19 (24%)	1	2
2	I	80/85 (94%)	61 (76%)	19 (24%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	80/85 (94%)	65 (81%)	15 (19%)	1	5
3	G	9/14 (64%)	5 (56%)	4 (44%)	0	0
3	H	9/14 (64%)	6 (67%)	3 (33%)	0	0
3	K	9/14 (64%)	7 (78%)	2 (22%)	1	3
3	L	9/14 (64%)	6 (67%)	3 (33%)	0	0
All	All	1554/1600 (97%)	1348 (87%)	206 (13%)	4	12

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	7	ILE
1	A	8	LEU
1	A	37	ARG
1	A	69	GLN
1	A	77	ARG
1	A	78	ARG
1	A	100	LEU
1	A	112	SER
1	A	121	LEU
1	A	141	GLN
1	A	145	ARG
1	A	153	THR
1	A	154	ASP
1	A	157	LYS
1	A	178	ARG
1	A	182	ASP
1	A	186	ILE
1	A	197	GLU
1	A	205	ARG
1	A	206	LYS
1	A	215	SER
1	A	219	GLU
1	A	231	ARG
1	A	242	GLU
1	A	249	LYS
1	A	278	MET
1	A	286	LYS
1	A	298	VAL
1	A	309	ARG

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Mol	Chain	Res	Type
1	C	3	THR
1	C	6	GLU
1	C	11	LEU
1	C	12	SER
1	C	13	LEU
1	C	14	GLU
1	C	37	ARG
1	C	40	LEU
1	C	62	ASN
1	C	76	GLN
1	C	77	ARG
1	C	78	ARG
1	C	100	LEU
1	C	121	LEU
1	C	134	SER
1	C	157	LYS
1	C	162	ASP
1	C	166	ASP
1	C	176	LYS
1	C	181	GLU
1	C	193	GLN
1	C	196	ARG
1	C	204	LYS
1	C	205	ARG
1	C	212	LYS
1	C	215	SER
1	C	254	ASN
1	C	278	MET
1	C	283	THR
1	C	313	LYS
1	C	324	LYS
1	C	339	ASP
2	E	3	GLN
2	E	14	THR
2	E	22	LYS
2	E	25	LEU
2	E	30	LEU
2	E	52	ASP
2	E	58	LEU
2	E	62	ARG
2	E	75	ILE
2	E	88	VAL

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Mol	Chain	Res	Type
2	E	90	MET
2	F	3	GLN
2	F	4	MET
2	F	14	THR
2	F	21	ASP
2	F	24	TYR
2	F	33	LEU
2	F	34	MET
2	F	38	PHE
2	F	44	ASN
2	F	45	GLN
2	F	46	LYS
2	F	54	ILE
2	F	58	LEU
2	F	62	ARG
2	F	63	ASP
2	F	79	THR
2	F	86	PHE
2	F	87	VAL
2	F	90	MET
3	G	-1	THR
3	G	0	PHE
3	G	1	PHE
3	G	5	GLU
3	H	3	ARG
3	H	5	GLU
3	H	6	PHE
1	B	3	THR
1	B	4	VAL
1	B	6	GLU
1	B	7	ILE
1	B	11	LEU
1	B	13	LEU
1	B	14	GLU
1	B	31	THR
1	B	40	LEU
1	B	46	VAL
1	B	66	VAL
1	B	96	GLU
1	B	100	LEU
1	B	121	LEU
1	B	138	GLN

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Mol	Chain	Res	Type
1	B	141	GLN
1	B	162	ASP
1	B	166	ASP
1	B	176	LYS
1	B	178	ARG
1	B	179	ARG
1	B	181	GLU
1	B	182	ASP
1	B	184	SER
1	B	185	VAL
1	B	196	ARG
1	B	203	VAL
1	B	205	ARG
1	B	206	LYS
1	B	208	THR
1	B	212	LYS
1	B	215	SER
1	B	231	ARG
1	B	254	ASN
1	B	278	MET
1	B	309	ARG
1	D	9	CYS
1	D	14	GLU
1	D	31	THR
1	D	32	ASN
1	D	37	ARG
1	D	66	VAL
1	D	76	GLN
1	D	77	ARG
1	D	78	ARG
1	D	100	LEU
1	D	112	SER
1	D	119	LYS
1	D	141	GLN
1	D	148	LYS
1	D	169	LYS
1	D	185	VAL
1	D	196	ARG
1	D	205	ARG
1	D	206	LYS
1	D	210	VAL
1	D	212	LYS

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Mol	Chain	Res	Type
1	D	222	VAL
1	D	231	ARG
1	D	246	LYS
1	D	249	LYS
1	D	278	MET
1	D	283	THR
1	D	298	VAL
1	D	309	ARG
1	D	313	LYS
1	D	326	ASP
1	D	339	ASP
2	I	12	MET
2	I	13	PHE
2	I	22	LYS
2	I	25	LEU
2	I	28	GLU
2	I	30	LEU
2	I	32	VAL
2	I	34	MET
2	I	37	GLU
2	I	45	GLN
2	I	56	LYS
2	I	60	GLN
2	I	61	CYS
2	I	65	LYS
2	I	75	ILE
2	I	78	LEU
2	I	84	ASP
2	I	89	HIS
2	I	90	MET
2	J	4	MET
2	J	8	MET
2	J	27	LYS
2	J	37	GLU
2	J	38	PHE
2	J	43	GLU
2	J	46	LYS
2	J	48	PRO
2	J	51	VAL
2	J	57	ASP
2	J	61	CYS
2	J	62	ARG

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Mol	Chain	Res	Type
2	J	82	CYS
2	J	88	VAL
2	J	90	MET
3	K	0	PHE
3	K	6	PHE
3	L	-1	THR
3	L	3	ARG
3	L	5	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	76	GLN
1	A	254	ASN
1	C	41	ASN
1	C	76	GLN
1	C	141	GLN
1	C	254	ASN
1	C	321	GLN
2	E	3	GLN
2	E	16	HIS
2	E	45	GLN
2	E	69	GLN
2	F	44	ASN
2	F	69	GLN
1	B	32	ASN
1	B	76	GLN
1	B	137	ASN
1	B	141	GLN
1	B	328	GLN
1	D	5	HIS
1	D	94	HIS
1	D	108	GLN
2	J	3	GLN
2	J	45	GLN
2	J	69	GLN

5.3.3 RNA ⓘ

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	338/339 (99%)	0.60	39 (11%) 9 7	27, 54, 112, 197	0
1	B	338/339 (99%)	0.64	33 (9%) 13 10	26, 55, 124, 168	0
1	C	338/339 (99%)	0.71	38 (11%) 10 8	25, 51, 128, 188	0
1	D	338/339 (99%)	0.56	31 (9%) 14 11	23, 50, 111, 210	0
2	E	91/97 (93%)	1.86	39 (42%) 0 0	88, 146, 209, 277	0
2	F	91/97 (93%)	1.63	24 (26%) 1 1	77, 139, 204, 267	0
2	I	91/97 (93%)	1.78	33 (36%) 1 0	69, 142, 204, 291	0
2	J	91/97 (93%)	1.84	32 (35%) 1 0	85, 139, 182, 217	0
3	G	9/14 (64%)	2.80	8 (88%) 0 0	105, 118, 159, 193	0
3	H	9/14 (64%)	3.17	5 (55%) 0 0	136, 156, 169, 211	0
3	K	9/14 (64%)	2.62	6 (66%) 0 0	90, 122, 150, 166	0
3	L	9/14 (64%)	3.10	6 (66%) 0 0	106, 126, 152, 158	0
All	All	1752/1800 (97%)	0.91	294 (16%) 4 3	23, 60, 168, 291	0

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	GLY	7.6
1	B	9	CYS	7.5
1	C	9	CYS	7.4
1	D	183	GLY	6.8
1	A	22	SER	6.6
2	E	40	GLY	6.6
1	A	9	CYS	6.4
1	D	9	CYS	6.3
1	C	183	GLY	6.2
2	F	40	GLY	6.1
3	H	-2	PRO	6.1

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Mol	Chain	Res	Type	RSRZ
3	H	4	PHE	6.0
2	J	74	LEU	6.0
3	L	-2	PRO	5.8
1	B	183	GLY	5.7
1	D	17	HIS	5.6
2	I	54	ILE	5.3
1	D	121	LEU	5.3
3	G	6	PHE	5.1
1	C	23	ALA	4.9
2	E	54	ILE	4.8
3	H	6	PHE	4.8
1	A	178	ARG	4.7
3	L	4	PHE	4.7
1	D	182	ASP	4.6
1	D	223	CYS	4.6
2	J	1	PRO	4.6
1	A	21	PRO	4.5
1	C	13	LEU	4.5
1	A	183	GLY	4.5
1	C	12	SER	4.4
1	D	16	ASP	4.4
1	C	223	CYS	4.4
3	K	0	PHE	4.3
1	B	10	LYS	4.1
2	I	40	GLY	4.1
1	D	12	SER	4.1
1	D	66	VAL	4.1
1	B	8	LEU	4.1
2	E	76	ALA	4.0
1	B	11	LEU	4.0
2	E	72	PHE	3.9
2	I	72	PHE	3.9
2	I	39	PRO	3.8
1	A	197	GLU	3.8
3	L	6	PHE	3.8
1	C	11	LEU	3.8
1	A	223	CYS	3.8
1	C	14	GLU	3.8
1	A	18	SER	3.7
1	B	197	GLU	3.7
2	J	54	ILE	3.7
1	B	223	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	4	VAL	3.6
3	G	-1	THR	3.6
1	B	16	ASP	3.6
2	E	39	PRO	3.6
1	C	4	VAL	3.6
2	F	11	MET	3.5
3	L	2	PRO	3.5
2	J	58	LEU	3.5
1	C	182	ASP	3.5
2	J	80	ILE	3.4
2	J	57	ASP	3.4
2	I	6	HIS	3.4
3	K	4	PHE	3.4
1	D	185	VAL	3.4
2	E	8	MET	3.4
1	D	178	ARG	3.4
2	I	75	ILE	3.4
2	J	46	LYS	3.4
1	C	19	THR	3.4
1	B	17	HIS	3.4
2	E	79	THR	3.4
3	K	-1	THR	3.4
3	H	2	PRO	3.4
1	C	15	GLY	3.3
2	I	18	PHE	3.3
1	C	141	GLN	3.3
2	I	34	MET	3.3
2	I	55	MET	3.3
1	B	182	ASP	3.3
1	B	178	ARG	3.2
2	I	14	THR	3.2
2	I	38	PHE	3.2
1	C	178	ARG	3.2
2	F	54	ILE	3.2
1	A	13	LEU	3.2
2	E	10	THR	3.2
2	I	67	GLY	3.2
2	J	71	PHE	3.2
1	C	121	LEU	3.1
1	A	15	GLY	3.1
2	E	68	PHE	3.1
2	F	13	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	J	43	GLU	3.1
1	B	141	GLN	3.1
2	F	64	GLY	3.1
2	E	88	VAL	3.1
2	F	8	MET	3.1
1	C	17	HIS	3.1
1	C	203	VAL	3.1
3	L	0	PHE	3.1
2	J	85	TYR	3.1
2	E	58	LEU	3.1
1	A	36	GLU	3.1
1	C	196	ARG	3.1
2	F	86	PHE	3.1
2	F	81	ALA	3.0
1	B	184	SER	3.0
2	F	39	PRO	3.0
1	B	12	SER	3.0
1	D	122	GLY	3.0
2	I	41	PHE	3.0
2	I	86	PHE	3.0
1	A	121	LEU	3.0
2	E	57	ASP	3.0
1	D	13	LEU	2.9
1	C	5	HIS	2.9
2	I	79	THR	2.9
1	A	182	ASP	2.9
2	F	85	TYR	2.9
3	K	-2	PRO	2.9
1	A	185	VAL	2.9
3	G	4	PHE	2.9
1	C	197	GLU	2.9
1	B	20	PRO	2.9
1	A	234	SER	2.9
2	J	14	THR	2.9
2	E	78	LEU	2.9
2	E	13	PHE	2.9
3	G	0	PHE	2.9
1	D	197	GLU	2.8
2	J	84	ASP	2.8
1	A	24	TYR	2.8
1	A	123	THR	2.8
1	C	66	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	5	HIS	2.8
2	F	36	LYS	2.8
1	B	13	LEU	2.8
1	D	18	SER	2.8
2	F	6	HIS	2.8
2	J	38	PHE	2.8
2	J	51	VAL	2.8
2	I	53	LYS	2.7
1	C	18	SER	2.7
1	B	82	GLU	2.7
2	E	14	THR	2.7
2	E	34	MET	2.7
2	I	11	MET	2.7
2	E	66	VAL	2.7
2	J	88	VAL	2.7
3	K	1	PHE	2.7
2	I	1	PRO	2.7
2	E	50	ALA	2.7
2	E	55	MET	2.7
1	A	31	THR	2.7
3	K	6	PHE	2.7
2	F	80	ILE	2.6
1	A	215	SER	2.6
2	E	41	PHE	2.6
2	F	1	PRO	2.6
2	J	48	PRO	2.6
1	D	119	LYS	2.6
1	C	181	GLU	2.6
2	J	87	VAL	2.6
2	I	10	THR	2.6
1	A	14	GLU	2.6
1	A	181	GLU	2.6
1	C	125	GLU	2.5
1	B	203	VAL	2.5
1	D	21	PRO	2.5
3	G	1	PHE	2.5
2	F	14	THR	2.5
1	A	37	ARG	2.5
1	B	5	HIS	2.5
2	E	85	TYR	2.5
3	G	-2	PRO	2.5
2	E	51	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	81	ALA	2.5
1	C	97	THR	2.5
1	C	22	SER	2.5
1	B	2	SER	2.5
2	E	6	HIS	2.5
1	B	21	PRO	2.5
2	J	8	MET	2.5
2	J	15	PHE	2.5
2	E	26	THR	2.5
2	F	83	ASN	2.5
2	J	36	LYS	2.5
2	E	73	SER	2.5
2	I	84	ASP	2.5
1	D	6	GLU	2.5
2	I	24	TYR	2.5
2	J	2	SER	2.4
2	I	88	VAL	2.4
1	C	37	ARG	2.4
2	J	47	ASP	2.4
1	C	242	GLU	2.4
1	A	66	VAL	2.4
2	I	50	ALA	2.4
2	I	21	ASP	2.4
2	E	4	MET	2.4
2	I	8	MET	2.4
2	F	46	LYS	2.4
1	A	30	TYR	2.4
2	F	7	ALA	2.4
1	A	12	SER	2.4
1	D	181	GLU	2.4
2	F	63	ASP	2.4
1	D	11	LEU	2.3
2	I	30	LEU	2.3
1	A	32	ASN	2.3
1	D	36	GLU	2.3
1	A	2	SER	2.3
1	B	338	ASP	2.3
1	B	237	PRO	2.3
2	J	40	GLY	2.3
2	J	77	GLY	2.3
1	B	196	ARG	2.3
1	C	45	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	3	THR	2.3
1	D	3	THR	2.3
1	C	206	LYS	2.3
1	D	51	VAL	2.3
1	A	201	ALA	2.3
1	D	8	LEU	2.3
2	E	11	MET	2.3
2	E	17	LYS	2.3
2	J	4	MET	2.3
1	D	20	PRO	2.3
1	C	24	TYR	2.3
1	A	16	ASP	2.3
1	C	20	PRO	2.3
2	E	30	LEU	2.3
2	E	61	CYS	2.2
1	B	3	THR	2.2
1	D	125	GLU	2.2
1	C	2	SER	2.2
2	F	57	ASP	2.2
2	I	57	ASP	2.2
2	J	6	HIS	2.2
1	D	196	ARG	2.2
2	J	66	VAL	2.2
1	B	6	GLU	2.2
3	G	5	GLU	2.2
3	L	5	GLU	2.2
1	B	15	GLY	2.2
2	E	90	MET	2.2
2	J	3	GLN	2.2
1	B	124	ASP	2.2
2	I	12	MET	2.2
1	B	210	VAL	2.2
3	H	0	PHE	2.2
2	I	76	ALA	2.1
1	C	82	GLU	2.1
1	D	37	ARG	2.1
1	A	29	PRO	2.1
2	E	16	HIS	2.1
2	I	87	VAL	2.1
1	A	23	ALA	2.1
2	E	27	LYS	2.1
1	B	24	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	49	LEU	2.1
1	B	194	ASP	2.1
1	A	184	SER	2.1
2	J	76	ALA	2.1
1	B	189	GLU	2.1
2	E	69	GLN	2.1
1	C	8	LEU	2.1
1	C	330	ALA	2.1
2	I	37	GLU	2.1
1	A	119	LYS	2.1
2	E	1	PRO	2.1
1	A	11	LEU	2.1
2	F	49	LEU	2.1
1	C	7	ILE	2.1
2	F	24	TYR	2.1
1	A	298	VAL	2.1
1	D	73	PHE	2.1
2	E	86	PHE	2.1
2	F	71	PHE	2.1
2	E	46	LYS	2.0
3	G	2	PRO	2.0
2	I	25	LEU	2.0
2	I	51	VAL	2.0
1	A	43	GLU	2.0
1	C	154	ASP	2.0
2	F	84	ASP	2.0
1	A	206	LYS	2.0
1	B	215	SER	2.0
2	E	75	ILE	2.0
2	J	23	GLY	2.0
2	E	87	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.