



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 11:11 AM UTC

PDB ID : 1KN0 / pdb_00001kn0
Title : Crystal Structure of the human Rad52 protein
Authors : Kagawa, W.; Kurumizaka, H.; Ishitani, R.; Fukai, S.; Nureki, O.; Shibata, T.;
Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2001-12-18
Resolution : 2.85 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

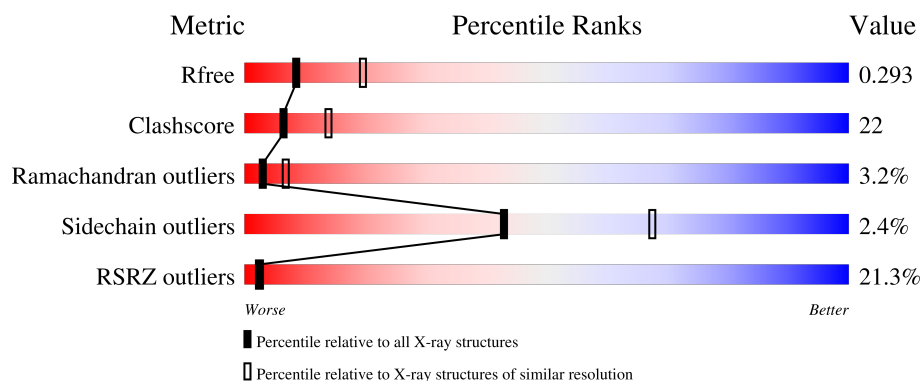
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	212	9% 48% 35% 13%
1	B	212	13% 50% 34% 13%
1	C	212	12% 50% 33% 13%
1	D	212	19% 49% 34% 13%
1	E	212	26% 46% 36% 13%

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Mol	Chain	Length	Quality of chain
1	F	212	
1	G	212	
1	H	212	
1	I	212	
1	J	212	
1	K	212	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16032 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 Rad52.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	B	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	C	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	D	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	E	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	F	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	G	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	H	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	I	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	J	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	K	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	12	Total	O	0	0
			12	12		
2	C	9	Total	O	0	0
			9	9		

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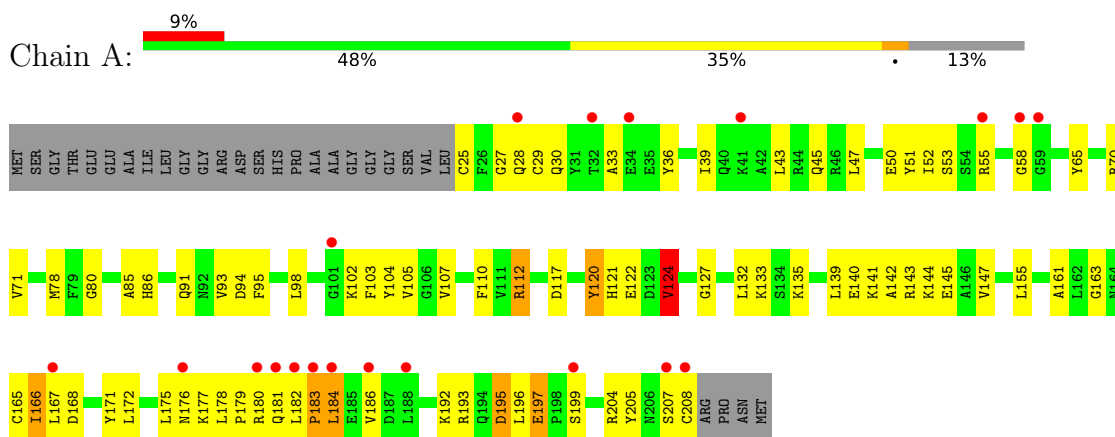
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	6	Total 6	O 6	0	0
2	E	3	Total 3	O 3	0	0
2	F	2	Total 2	O 2	0	0
2	G	8	Total 8	O 8	0	0
2	H	10	Total 10	O 10	0	0
2	I	7	Total 7	O 7	0	0
2	J	9	Total 9	O 9	0	0
2	K	7	Total 7	O 7	0	0

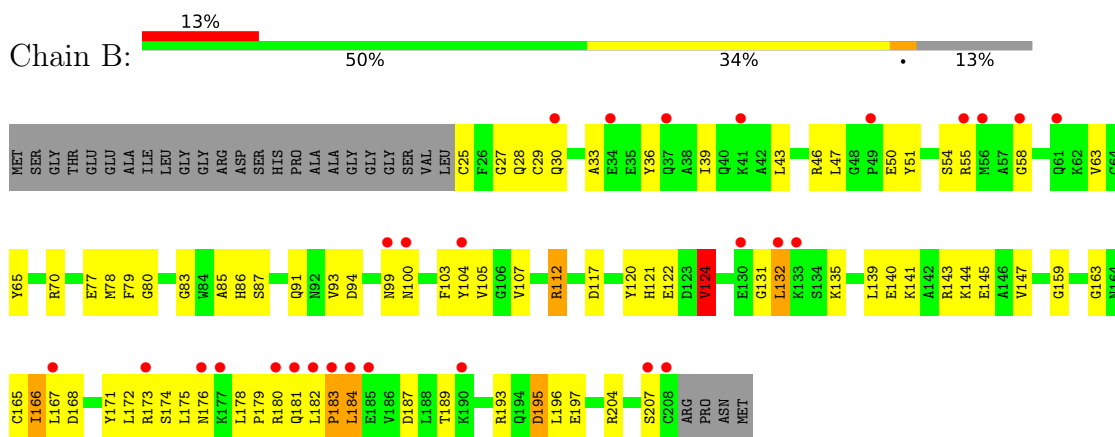
3 Residue-property plots [i](#)

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.

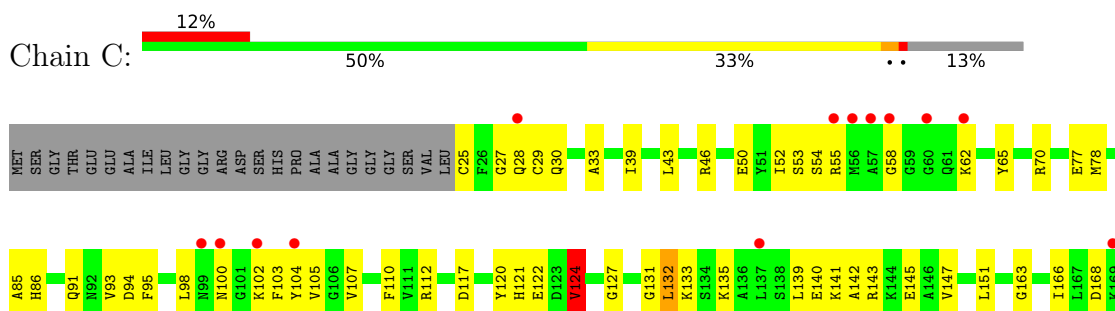
• Molecule 1: Rad52

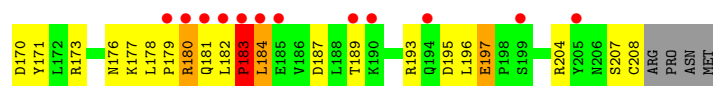


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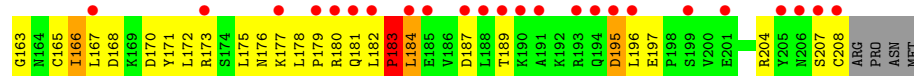
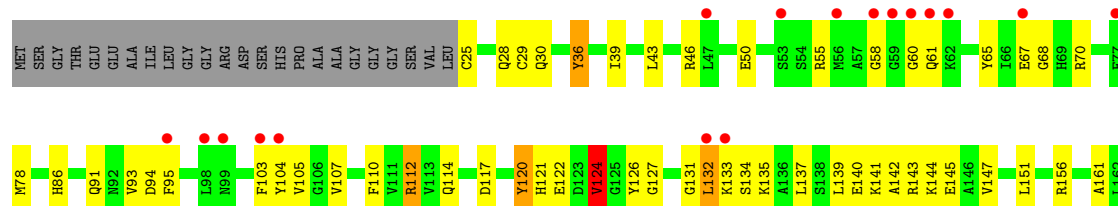


• Molecule 1: Rad52

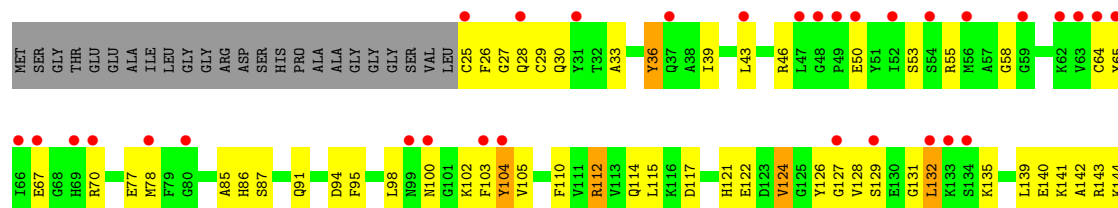




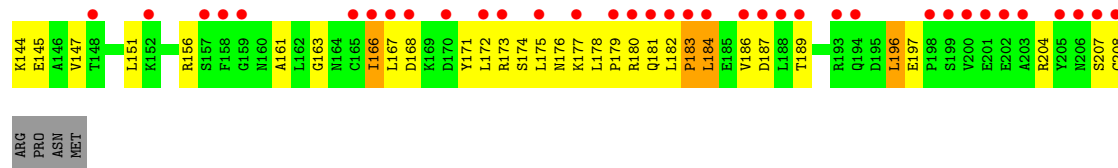
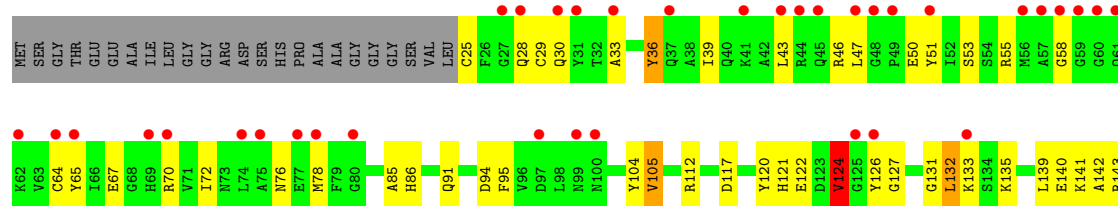
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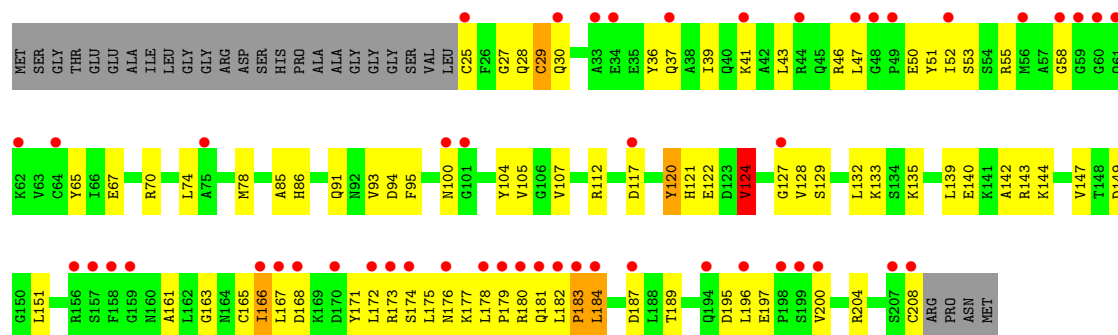
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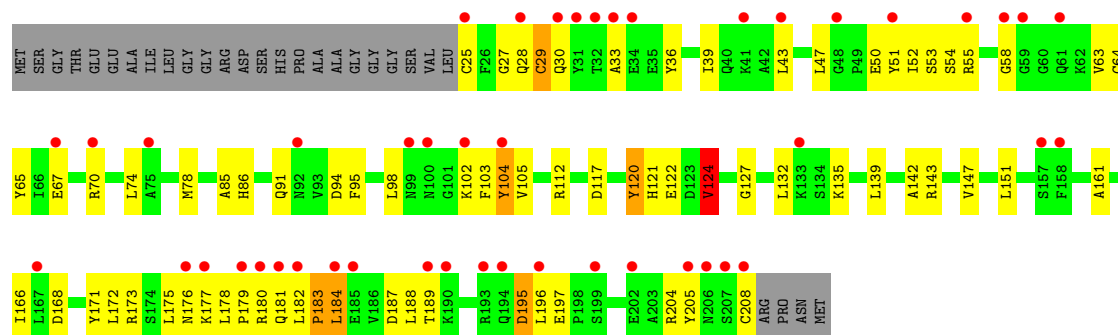
• Molecule 1: Rad52



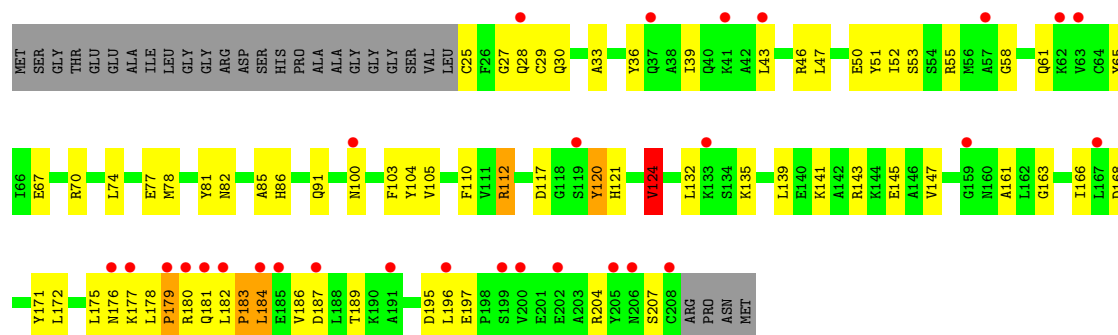
• Molecule 1: Rad52



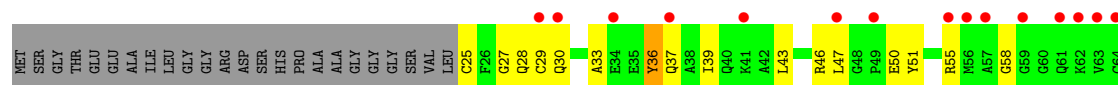
• Molecule 1: Rad52

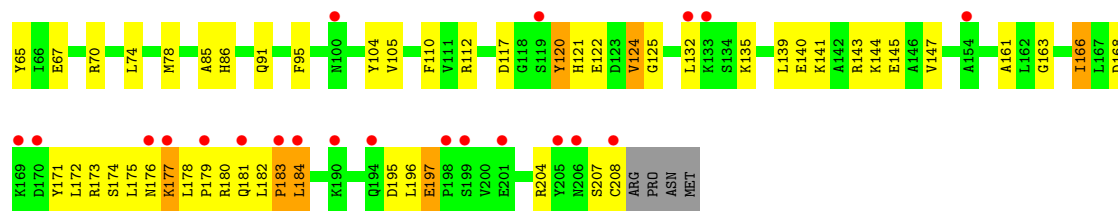


• Molecule 1: Rad52

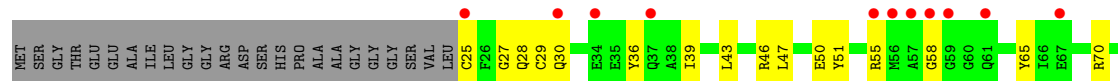


• Molecule 1: Rad52





● Molecule 1: Rad52



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	145.61Å 145.61Å 247.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.85) 99.2 (50.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.06 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.297 0.270 , 0.293	Depositor DCC
R_{free} test set	6303 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 80.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	16032	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.31% 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	0.54	0/1474	0.93	8/1981 (0.4%)
1	B	0.55	0/1474	0.92	5/1981 (0.3%)
1	C	0.53	0/1474	0.90	6/1981 (0.3%)
1	D	0.48	0/1474	0.91	5/1981 (0.3%)
1	E	0.45	0/1474	0.89	2/1981 (0.1%)
1	F	0.46	0/1474	0.86	3/1981 (0.2%)
1	G	0.50	0/1474	0.92	6/1981 (0.3%)
1	H	0.51	0/1474	0.88	5/1981 (0.3%)
1	I	0.51	0/1474	0.91	5/1981 (0.3%)
1	J	0.48	0/1474	0.91	7/1981 (0.4%)
1	K	0.51	0/1474	0.89	5/1981 (0.3%)
All	All	0.50	0/16214	0.90	57/21791 (0.3%)

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	D	0	1
1	E	0	1
1	F	0	1
1	J	0	1
All	All	0	4

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLY	N-CA-C	-7.33	105.97	114.69
1	B	124	VAL	CB-CA-C	-7.05	101.03	110.98
1	K	195	ASP	N-CA-C	6.75	118.33	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	27	GLY	N-CA-C	-6.69	107.12	115.08
1	K	125	GLY	N-CA-C	-6.68	100.89	111.18
1	G	195	ASP	N-CA-C	6.62	118.19	110.97
1	E	27	GLY	N-CA-C	-6.36	107.51	115.08
1	J	195	ASP	N-CA-C	6.34	117.88	110.97
1	G	105	VAL	N-CA-C	6.33	117.04	108.17
1	J	27	GLY	N-CA-C	-6.26	107.25	114.69
1	I	27	GLY	N-CA-C	-6.23	107.66	115.08
1	H	195	ASP	N-CA-C	6.09	117.60	110.97
1	I	195	ASP	N-CA-C	6.07	117.59	110.97
1	G	27	GLY	N-CA-C	-6.03	107.91	115.08
1	E	195	ASP	N-CA-C	5.99	117.50	110.97
1	I	124	VAL	CB-CA-C	-5.90	102.66	110.98
1	D	124	VAL	CB-CA-C	-5.89	101.85	110.81
1	F	124	VAL	CB-CA-C	-5.81	102.79	110.98
1	F	105	VAL	N-CA-C	5.78	116.25	108.17
1	B	195	ASP	N-CA-C	5.77	117.26	110.97
1	K	105	VAL	N-CA-C	5.77	116.19	108.11
1	A	197	GLU	CA-C-N	5.76	125.23	119.24
1	A	197	GLU	C-N-CA	5.76	125.23	119.24
1	B	27	GLY	N-CA-C	-5.72	108.28	115.08
1	J	105	VAL	N-CA-C	5.67	116.65	108.48
1	G	124	VAL	CB-CA-C	-5.64	103.48	111.21
1	J	120	TYR	N-CA-C	5.58	117.57	108.76
1	D	68	GLY	N-CA-C	5.57	119.37	112.64
1	C	133	LYS	N-CA-C	-5.55	106.67	113.50
1	A	195	ASP	N-CA-C	5.55	117.02	110.97
1	K	120	TYR	N-CA-C	5.46	117.39	108.76
1	C	195	ASP	N-CA-C	5.42	116.88	110.97
1	H	120	TYR	N-CA-C	5.39	117.28	108.76
1	D	133	LYS	N-CA-C	-5.38	106.89	113.50
1	D	120	TYR	N-CA-C	5.34	117.19	108.76
1	G	133	LYS	N-CA-C	-5.31	106.65	113.23
1	H	124	VAL	CB-CA-C	-5.29	103.96	111.21
1	K	27	GLY	N-CA-C	-5.29	108.33	115.21
1	F	133	LYS	N-CA-C	-5.28	107.00	113.50
1	H	52	ILE	N-CA-C	5.27	116.81	109.80
1	A	120	TYR	N-CA-C	5.25	117.05	109.07
1	B	80	GLY	N-CA-C	-5.23	106.16	112.48
1	B	159	GLY	N-CA-C	5.20	117.63	110.56
1	H	27	GLY	N-CA-C	-5.19	108.51	114.69
1	D	195	ASP	N-CA-C	5.19	116.62	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	120	TYR	N-CA-C	5.18	116.94	109.07
1	I	105	VAL	N-CA-C	5.16	115.39	108.17
1	A	124	VAL	CB-CA-C	-5.12	103.03	110.81
1	A	80	GLY	N-CA-C	-5.12	105.32	112.18
1	J	197	GLU	CA-C-N	5.09	124.53	119.24
1	J	197	GLU	C-N-CA	5.09	124.53	119.24
1	I	120	TYR	N-CA-C	5.09	116.98	108.99
1	A	133	LYS	N-CA-C	-5.09	106.92	113.23
1	C	197	GLU	CA-C-N	5.04	124.48	119.24
1	C	197	GLU	C-N-CA	5.04	124.48	119.24
1	C	124	VAL	CB-CA-C	-5.04	103.88	110.98
1	J	125	GLY	N-CA-C	-5.03	102.81	111.57

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	36	TYR	Sidechain
1	E	36	TYR	Sidechain
1	F	36	TYR	Sidechain
1	J	36	TYR	Sidechain

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	1450	0	1433	74	0
1	B	1450	0	1433	76	0
1	C	1450	0	1433	78	0
1	D	1450	0	1433	83	1
1	E	1450	0	1433	88	1
1	F	1450	0	1433	82	0
1	G	1450	0	1433	90	1
1	H	1450	0	1433	72	0
1	I	1450	0	1433	72	0
1	J	1450	0	1433	78	0
1	K	1450	0	1433	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	9	0	0	2	0
2	B	12	0	0	0	0
2	C	9	0	0	0	0
2	D	6	0	0	0	0
2	E	3	0	0	0	0
2	F	2	0	0	0	0
2	G	8	0	0	0	0
2	H	10	0	0	0	0
2	I	7	0	0	0	0
2	J	9	0	0	0	0
2	K	7	0	0	0	0
All	All	16032	0	15763	694	2

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 22.

All (694) 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:G:182:LEU:HD12	1:G:183:PRO:HD2	1.43	0.99
1:A:86:HIS:HD2	1:B:121:HIS:HD2	1.09	0.98
1:G:182:LEU:CD1	1:G:183:PRO:HD2	1.96	0.95
1:A:121:HIS:HD2	1:K:86:HIS:HD2	1.14	0.93
1:B:86:HIS:HD2	1:C:121:HIS:HD2	1.14	0.93
1:J:86:HIS:HD2	1:K:121:HIS:HD2	1.15	0.89
1:B:147:VAL:HG21	1:C:124:VAL:CG2	2.04	0.88
1:G:182:LEU:HD12	1:G:183:PRO:CD	2.04	0.87
1:H:86:HIS:HD2	1:I:121:HIS:HD2	1.23	0.85
1:K:91:GLN:NE2	1:K:143:ARG:HE	1.75	0.85
1:I:86:HIS:HD2	1:J:121:HIS:HD2	1.23	0.85
1:J:147:VAL:HG21	1:K:124:VAL:CG2	2.09	0.82
1:F:86:HIS:CD2	1:G:121:HIS:HD2	1.97	0.82
1:A:39:ILE:HG23	1:A:78:MET:CE	2.10	0.82
1:A:86:HIS:CD2	1:B:121:HIS:HD2	1.96	0.82
1:E:39:ILE:HG23	1:E:78:MET:CE	2.09	0.81
1:G:43:LEU:HG	1:G:78:MET:HE2	1.62	0.81
1:F:86:HIS:HD2	1:G:121:HIS:HD2	1.24	0.81
1:A:86:HIS:HD2	1:B:121:HIS:CD2	1.97	0.80
1:B:86:HIS:HD2	1:C:121:HIS:CD2	2.00	0.79
1:G:86:HIS:CD2	1:H:121:HIS:HD2	2.00	0.79
1:C:39:ILE:HG23	1:C:78:MET:CE	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:LYS:HE2	1:E:145:GLU:OE2	1.83	0.78
1:D:147:VAL:HG21	1:E:124:VAL:CG2	2.13	0.78
1:D:91:GLN:NE2	1:D:143:ARG:HE	1.80	0.78
1:H:39:ILE:HG23	1:H:78:MET:CE	2.14	0.78
1:J:86:HIS:HD2	1:K:121:HIS:CD2	2.03	0.77
1:H:43:LEU:HG	1:H:78:MET:HE2	1.65	0.77
1:I:39:ILE:HG23	1:I:78:MET:CE	2.15	0.77
1:G:50:GLU:HG3	1:G:181:GLN:HE22	1.49	0.77
1:H:91:GLN:NE2	1:H:143:ARG:HE	1.83	0.76
1:K:39:ILE:HG23	1:K:78:MET:CE	2.15	0.76
1:F:39:ILE:HG23	1:F:78:MET:CE	2.16	0.75
1:C:86:HIS:HD2	1:D:121:HIS:HD2	1.33	0.75
1:A:121:HIS:CD2	1:K:86:HIS:HD2	2.02	0.75
1:I:147:VAL:HG21	1:J:124:VAL:CG2	2.17	0.75
1:F:50:GLU:HG3	1:F:181:GLN:HE22	1.52	0.74
1:D:86:HIS:CD2	1:E:121:HIS:HD2	2.05	0.74
1:F:86:HIS:HD2	1:G:121:HIS:CD2	2.05	0.74
1:C:86:HIS:CD2	1:D:121:HIS:HD2	2.05	0.74
1:I:182:LEU:HG	1:I:183:PRO:HD2	1.69	0.73
1:J:50:GLU:HG3	1:J:181:GLN:HE22	1.51	0.73
1:H:147:VAL:HG21	1:I:124:VAL:CG2	2.18	0.73
1:I:50:GLU:HG3	1:I:181:GLN:HE22	1.54	0.73
1:J:86:HIS:CD2	1:K:121:HIS:HD2	2.04	0.73
1:C:91:GLN:NE2	1:C:143:ARG:HE	1.87	0.73
1:D:39:ILE:HG23	1:D:78:MET:CE	2.19	0.73
1:G:147:VAL:HG21	1:H:124:VAL:CG2	2.17	0.73
1:H:86:HIS:CD2	1:I:121:HIS:HD2	2.07	0.72
1:H:28:GLN:HE21	1:H:28:GLN:HA	1.54	0.72
1:K:50:GLU:HG3	1:K:181:GLN:HE22	1.54	0.72
1:G:39:ILE:HG23	1:G:78:MET:CE	2.19	0.72
1:H:50:GLU:HG3	1:H:181:GLN:HE22	1.54	0.72
1:J:39:ILE:HG23	1:J:78:MET:CE	2.20	0.72
1:J:50:GLU:HG3	1:J:181:GLN:NE2	2.05	0.72
1:K:43:LEU:HG	1:K:78:MET:HE2	1.72	0.72
1:B:50:GLU:HG3	1:B:181:GLN:HE22	1.54	0.71
1:E:43:LEU:HG	1:E:78:MET:HE2	1.71	0.71
1:I:85:ALA:HB1	1:J:120:TYR:O	1.91	0.71
1:B:182:LEU:HG	1:B:183:PRO:HD2	1.72	0.70
1:I:91:GLN:NE2	1:I:143:ARG:HE	1.88	0.70
1:I:43:LEU:HG	1:I:78:MET:HE2	1.73	0.70
1:A:124:VAL:CG2	1:K:147:VAL:HG21	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:28:GLN:HA	1:K:28:GLN:HE21	1.54	0.70
1:E:50:GLU:HG3	1:E:181:GLN:HE22	1.55	0.70
1:F:204:ARG:HD2	1:H:36:TYR:OH	1.91	0.70
1:G:50:GLU:HG3	1:G:181:GLN:NE2	2.07	0.70
1:I:86:HIS:HD2	1:J:121:HIS:CD2	2.08	0.70
1:F:50:GLU:HG3	1:F:181:GLN:NE2	2.06	0.70
1:B:86:HIS:CD2	1:C:121:HIS:HD2	2.04	0.70
1:G:184:LEU:HD22	1:G:184:LEU:H	1.57	0.70
1:H:184:LEU:H	1:H:184:LEU:HD22	1.56	0.70
1:H:50:GLU:HG3	1:H:181:GLN:NE2	2.06	0.70
1:J:43:LEU:HG	1:J:78:MET:HE2	1.74	0.70
1:H:112:ARG:HG3	1:H:122:GLU:HB2	1.74	0.69
1:A:50:GLU:HG3	1:A:181:GLN:HE22	1.58	0.69
1:J:28:GLN:HA	1:J:28:GLN:HE21	1.58	0.69
1:B:39:ILE:HG23	1:B:78:MET:CE	2.22	0.69
1:F:147:VAL:HG21	1:G:124:VAL:CG2	2.23	0.69
1:G:86:HIS:HD2	1:H:121:HIS:HD2	1.39	0.69
1:I:50:GLU:HG3	1:I:181:GLN:NE2	2.08	0.69
1:J:91:GLN:NE2	1:J:143:ARG:HE	1.91	0.69
1:E:28:GLN:HE21	1:E:28:GLN:HA	1.58	0.69
1:A:147:VAL:HG21	1:B:124:VAL:CG2	2.23	0.68
1:G:28:GLN:HE21	1:G:28:GLN:HA	1.58	0.68
1:I:184:LEU:HD22	1:I:184:LEU:H	1.58	0.68
1:J:184:LEU:HD22	1:J:184:LEU:H	1.58	0.68
1:C:86:HIS:HD2	1:D:121:HIS:CD2	2.11	0.68
1:D:70:ARG:HG3	1:D:70:ARG:HH11	1.57	0.68
1:E:50:GLU:HG3	1:E:181:GLN:NE2	2.08	0.68
1:F:43:LEU:HG	1:F:78:MET:HE2	1.74	0.68
1:F:184:LEU:H	1:F:184:LEU:HD22	1.57	0.68
1:F:25:CYS:HA	1:G:30:GLN:HG2	1.76	0.68
1:K:50:GLU:HG3	1:K:181:GLN:NE2	2.08	0.68
1:A:28:GLN:HA	1:A:28:GLN:HE21	1.59	0.67
1:B:50:GLU:HG3	1:B:181:GLN:NE2	2.09	0.67
1:D:25:CYS:HA	1:E:30:GLN:HG2	1.76	0.67
1:H:182:LEU:HG	1:H:183:PRO:HD2	1.76	0.67
1:A:121:HIS:HD2	1:K:86:HIS:CD2	2.05	0.67
1:K:184:LEU:H	1:K:184:LEU:HD22	1.60	0.67
1:A:184:LEU:H	1:A:184:LEU:HD22	1.59	0.67
1:G:86:HIS:CD2	1:H:121:HIS:CD2	2.83	0.67
1:C:147:VAL:HG21	1:D:124:VAL:CG2	2.24	0.66
1:E:204:ARG:HD2	1:G:36:TYR:OH	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:HG3	1:A:181:GLN:NE2	2.10	0.66
1:E:25:CYS:HA	1:F:30:GLN:HG2	1.75	0.66
1:E:147:VAL:HG21	1:F:124:VAL:CG2	2.25	0.66
1:F:28:GLN:HA	1:F:28:GLN:HE21	1.58	0.66
1:G:70:ARG:HG3	1:G:70:ARG:HH11	1.60	0.66
1:G:86:HIS:HD2	1:H:121:HIS:CD2	2.14	0.66
1:A:78:MET:O	1:K:204:ARG:NH2	2.29	0.66
1:E:112:ARG:HG3	1:E:122:GLU:HB2	1.78	0.66
1:H:208:CYS:HB2	1:J:33:ALA:HB2	1.78	0.66
1:C:184:LEU:HD22	1:C:184:LEU:H	1.60	0.66
1:B:28:GLN:HA	1:B:28:GLN:HE21	1.60	0.66
1:I:70:ARG:HG3	1:I:70:ARG:HH11	1.61	0.66
1:A:39:ILE:HG23	1:A:78:MET:HE1	1.77	0.66
1:A:91:GLN:NE2	1:A:143:ARG:HE	1.93	0.66
2:A:213:HOH:O	1:B:121:HIS:HE1	1.79	0.65
1:D:184:LEU:H	1:D:184:LEU:HD22	1.61	0.65
1:F:182:LEU:HG	1:F:183:PRO:HD2	1.78	0.65
1:A:204:ARG:NH2	1:B:78:MET:O	2.29	0.65
1:D:50:GLU:HG3	1:D:181:GLN:HE22	1.59	0.65
1:F:91:GLN:NE2	1:F:143:ARG:HE	1.94	0.65
1:D:86:HIS:CD2	1:E:121:HIS:CD2	2.85	0.65
1:A:93:VAL:HA	1:A:107:VAL:HG22	1.79	0.65
1:B:91:GLN:NE2	1:B:143:ARG:HE	1.94	0.65
1:C:50:GLU:HG3	1:C:181:GLN:HE22	1.61	0.65
1:K:196:LEU:HD12	1:K:197:GLU:H	1.61	0.65
1:E:39:ILE:HG23	1:E:78:MET:HE1	1.78	0.64
1:E:196:LEU:HD12	1:E:197:GLU:H	1.62	0.64
1:D:141:LYS:HE2	1:D:145:GLU:OE2	1.98	0.64
1:E:86:HIS:CD2	1:F:121:HIS:HD2	2.15	0.64
1:I:28:GLN:HE21	1:I:28:GLN:HA	1.63	0.64
1:I:39:ILE:HG23	1:I:78:MET:HE1	1.78	0.64
1:B:70:ARG:HG3	1:B:70:ARG:HH11	1.63	0.64
1:B:43:LEU:HG	1:B:78:MET:HE2	1.79	0.64
1:E:91:GLN:NE2	1:E:143:ARG:HE	1.96	0.64
1:D:182:LEU:HG	1:D:183:PRO:HD2	1.80	0.64
1:B:184:LEU:HD22	1:B:184:LEU:H	1.63	0.63
1:K:182:LEU:HG	1:K:183:PRO:HD2	1.80	0.63
1:D:28:GLN:HE21	1:D:28:GLN:HA	1.64	0.63
1:E:184:LEU:HD22	1:E:184:LEU:H	1.63	0.63
1:J:182:LEU:HG	1:J:183:PRO:HD2	1.81	0.63
1:B:141:LYS:HE2	1:B:145:GLU:OE2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:GLU:HG3	1:D:181:GLN:NE2	2.14	0.63
1:C:50:GLU:HG3	1:C:181:GLN:NE2	2.14	0.63
1:E:182:LEU:HG	1:E:183:PRO:HD2	1.81	0.63
1:G:85:ALA:HB1	1:H:120:TYR:O	1.97	0.62
1:H:85:ALA:HB1	1:I:120:TYR:O	1.99	0.62
1:D:147:VAL:HG21	1:E:124:VAL:HG22	1.81	0.62
1:H:70:ARG:HG3	1:H:70:ARG:HH11	1.63	0.62
1:J:70:ARG:HH11	1:J:70:ARG:HG3	1.64	0.62
1:B:204:ARG:HD2	1:D:36:TYR:OH	1.98	0.62
1:B:135:LYS:HG2	1:C:95:PHE:CE2	2.35	0.62
1:C:29:CYS:O	1:C:117:ASP:HA	2.00	0.62
1:I:29:CYS:O	1:I:117:ASP:HA	1.99	0.62
1:D:135:LYS:HG2	1:E:95:PHE:CE2	2.34	0.61
1:F:208:CYS:HB2	1:H:33:ALA:HB2	1.80	0.61
1:H:86:HIS:HD2	1:I:121:HIS:CD2	2.10	0.61
1:J:29:CYS:O	1:J:117:ASP:HA	2.00	0.61
1:I:86:HIS:CD2	1:J:121:HIS:HD2	2.11	0.61
1:A:124:VAL:HG22	1:K:147:VAL:HG21	1.80	0.61
1:F:86:HIS:CD2	1:G:121:HIS:CD2	2.83	0.61
1:G:25:CYS:HA	1:H:30:GLN:HG2	1.82	0.61
1:J:86:HIS:CD2	1:K:121:HIS:CD2	2.86	0.61
1:E:29:CYS:O	1:E:117:ASP:HA	2.00	0.61
1:G:29:CYS:O	1:G:117:ASP:HA	2.00	0.61
1:J:112:ARG:HG3	1:J:122:GLU:HB2	1.82	0.61
1:A:192:LYS:NZ	1:A:197:GLU:OE2	2.30	0.60
1:F:196:LEU:HD12	1:F:197:GLU:H	1.65	0.60
1:G:55:ARG:HD3	1:G:65:TYR:CE2	2.37	0.60
1:C:105:VAL:HG11	1:C:139:LEU:HD23	1.83	0.60
1:C:182:LEU:HG	1:C:183:PRO:HD2	1.82	0.60
1:J:25:CYS:HA	1:K:30:GLN:HG2	1.84	0.60
1:A:86:HIS:CD2	1:B:121:HIS:CD2	2.81	0.60
1:B:29:CYS:O	1:B:117:ASP:HA	2.01	0.60
1:G:112:ARG:HG3	1:G:122:GLU:HB2	1.82	0.60
1:A:30:GLN:HG2	1:K:25:CYS:HA	1.84	0.60
1:A:196:LEU:HD12	1:A:197:GLU:H	1.66	0.60
1:B:36:TYR:OH	1:K:204:ARG:HD2	2.02	0.60
1:G:43:LEU:HG	1:G:78:MET:CE	2.31	0.59
1:F:147:VAL:HG21	1:G:124:VAL:HG22	1.84	0.59
1:E:55:ARG:HD3	1:E:65:TYR:CE2	2.37	0.59
1:E:110:PHE:CE2	1:E:124:VAL:HG13	2.37	0.59
1:C:39:ILE:HG23	1:C:78:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:CYS:O	1:A:117:ASP:HA	2.03	0.59
1:G:208:CYS:HB2	1:I:33:ALA:HB2	1.85	0.59
1:F:112:ARG:HG3	1:F:122:GLU:HB2	1.83	0.59
1:F:204:ARG:NH2	1:G:78:MET:O	2.36	0.59
1:G:204:ARG:HD2	1:I:36:TYR:OH	2.02	0.59
1:A:182:LEU:HG	1:A:183:PRO:HD2	1.83	0.59
1:F:135:LYS:HG2	1:G:95:PHE:CE2	2.38	0.59
1:B:147:VAL:HG21	1:C:124:VAL:HG22	1.86	0.58
1:G:43:LEU:CG	1:G:78:MET:HE2	2.33	0.58
1:J:147:VAL:HG21	1:K:124:VAL:HG22	1.83	0.58
1:A:47:LEU:HD12	1:A:51:TYR:CD1	2.38	0.58
1:G:182:LEU:CG	1:G:183:PRO:HD2	2.33	0.58
1:I:196:LEU:HD12	1:I:197:GLU:H	1.67	0.58
1:J:196:LEU:HD12	1:J:197:GLU:H	1.68	0.58
1:H:39:ILE:HG23	1:H:78:MET:HE1	1.83	0.58
1:B:168:ASP:HB3	1:B:171:TYR:HB3	1.86	0.58
1:H:184:LEU:HD22	1:H:184:LEU:N	2.18	0.58
1:I:25:CYS:HA	1:J:30:GLN:HG2	1.84	0.58
1:D:55:ARG:HD3	1:D:65:TYR:CE2	2.39	0.58
1:K:70:ARG:HG3	1:K:70:ARG:HH11	1.67	0.58
1:E:70:ARG:HH11	1:E:70:ARG:HG3	1.67	0.57
1:G:91:GLN:NE2	1:G:143:ARG:HE	2.01	0.57
1:H:29:CYS:O	1:H:117:ASP:HA	2.04	0.57
1:A:70:ARG:HG3	1:A:70:ARG:HH11	1.68	0.57
1:F:55:ARG:HD3	1:F:65:TYR:CE2	2.39	0.57
1:C:86:HIS:CD2	1:D:121:HIS:CD2	2.89	0.57
1:D:50:GLU:OE1	1:D:50:GLU:N	2.36	0.57
1:F:39:ILE:HG23	1:F:78:MET:HE1	1.86	0.57
1:F:70:ARG:HG3	1:F:70:ARG:HH11	1.68	0.57
1:J:55:ARG:HD3	1:J:65:TYR:CE2	2.39	0.57
1:D:112:ARG:HG3	1:D:122:GLU:HB2	1.87	0.57
1:C:208:CYS:HB2	1:E:33:ALA:HB2	1.87	0.57
1:F:29:CYS:O	1:F:117:ASP:HA	2.05	0.57
1:C:28:GLN:HA	1:C:28:GLN:HE21	1.70	0.56
1:H:103:PHE:CE1	1:H:135:LYS:HB2	2.40	0.56
1:A:121:HIS:CD2	1:K:86:HIS:CD2	2.87	0.56
1:D:204:ARG:HD2	1:F:36:TYR:OH	2.04	0.56
1:H:168:ASP:HB3	1:H:171:TYR:HB3	1.87	0.56
1:H:196:LEU:HD12	1:H:197:GLU:H	1.69	0.56
1:B:86:HIS:CD2	1:C:121:HIS:CD2	2.85	0.56
1:C:184:LEU:HD22	1:C:184:LEU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:LEU:HD12	1:D:197:GLU:H	1.71	0.56
1:C:93:VAL:HA	1:C:107:VAL:HG22	1.88	0.56
1:D:176:ASN:C	1:D:178:LEU:H	2.14	0.56
1:G:37:GLN:HG2	1:G:41:LYS:HE2	1.87	0.56
1:G:196:LEU:HD12	1:G:197:GLU:H	1.71	0.56
1:I:182:LEU:CG	1:I:183:PRO:HD2	2.36	0.56
1:A:147:VAL:HG21	1:B:124:VAL:HG22	1.86	0.56
1:C:147:VAL:HG21	1:D:124:VAL:HG22	1.88	0.56
1:E:85:ALA:HB1	1:F:120:TYR:O	2.06	0.56
1:I:184:LEU:HD22	1:I:184:LEU:N	2.21	0.56
1:A:55:ARG:HD3	1:A:65:TYR:CE2	2.41	0.55
1:B:196:LEU:HD12	1:B:197:GLU:H	1.69	0.55
1:F:184:LEU:HD22	1:F:184:LEU:N	2.20	0.55
1:C:43:LEU:HG	1:C:78:MET:HE2	1.87	0.55
1:A:85:ALA:HB1	1:B:120:TYR:O	2.05	0.55
1:H:205:TYR:CE1	1:J:37:GLN:NE2	2.75	0.55
1:I:55:ARG:HD3	1:I:65:TYR:CE2	2.42	0.55
1:A:143:ARG:NH1	1:B:94:ASP:OD1	2.40	0.55
1:B:182:LEU:CG	1:B:183:PRO:HD2	2.37	0.55
1:G:135:LYS:HG2	1:H:95:PHE:CE2	2.42	0.55
1:J:184:LEU:HD22	1:J:184:LEU:N	2.21	0.55
1:A:112:ARG:HG3	1:A:122:GLU:HB2	1.88	0.55
1:H:25:CYS:HA	1:I:30:GLN:HG2	1.88	0.55
1:I:176:ASN:C	1:I:178:LEU:H	2.15	0.55
1:H:86:HIS:CD2	1:I:121:HIS:CD2	2.91	0.54
1:K:140:GLU:HG3	1:K:144:LYS:HE3	1.88	0.54
1:B:33:ALA:HB2	1:K:208:CYS:HB2	1.87	0.54
1:F:141:LYS:HE2	1:F:145:GLU:OE2	2.07	0.54
1:B:87:SER:HA	1:C:122:GLU:HB3	1.89	0.54
1:A:184:LEU:HD22	1:A:184:LEU:N	2.21	0.54
1:J:176:ASN:C	1:J:178:LEU:H	2.15	0.54
1:J:143:ARG:NH1	1:K:94:ASP:OD1	2.41	0.54
1:K:112:ARG:HG3	1:K:122:GLU:HB2	1.90	0.54
1:E:86:HIS:HD2	1:F:121:HIS:HD2	1.56	0.54
1:G:176:ASN:C	1:G:178:LEU:H	2.15	0.54
1:H:43:LEU:HG	1:H:78:MET:CE	2.36	0.54
1:E:140:GLU:HB2	1:F:126:TYR:CD2	2.42	0.54
1:F:85:ALA:HB1	1:G:120:TYR:O	2.08	0.54
1:F:187:ASP:OD1	1:F:189:THR:HG23	2.08	0.54
1:E:86:HIS:CD2	1:F:121:HIS:CD2	2.97	0.53
1:E:135:LYS:HG2	1:F:95:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:ASP:HB3	1:F:171:TYR:HB3	1.90	0.53
1:A:176:ASN:C	1:A:178:LEU:H	2.16	0.53
1:J:139:LEU:O	1:J:143:ARG:HG3	2.08	0.53
1:C:182:LEU:CG	1:C:183:PRO:HD2	2.39	0.53
1:D:184:LEU:HD22	1:D:184:LEU:N	2.23	0.53
1:E:86:HIS:HD2	1:F:121:HIS:CD2	2.27	0.53
1:G:184:LEU:HD22	1:G:184:LEU:N	2.21	0.53
1:C:85:ALA:HB1	1:D:120:TYR:O	2.08	0.53
1:C:182:LEU:CD1	1:C:183:PRO:HD2	2.38	0.53
1:H:28:GLN:HA	1:H:28:GLN:NE2	2.24	0.53
1:F:176:ASN:C	1:F:178:LEU:H	2.17	0.53
1:C:187:ASP:OD1	1:C:189:THR:HG23	2.08	0.53
1:A:91:GLN:HE22	1:A:143:ARG:HB3	1.75	0.52
1:A:91:GLN:HE21	1:A:143:ARG:HE	1.58	0.52
1:D:29:CYS:O	1:D:117:ASP:HA	2.09	0.52
1:D:86:HIS:HD2	1:E:121:HIS:CD2	2.25	0.52
1:F:67:GLU:O	1:F:70:ARG:HB2	2.10	0.52
1:B:184:LEU:HD22	1:B:184:LEU:N	2.23	0.52
1:C:176:ASN:C	1:C:178:LEU:H	2.17	0.52
1:G:143:ARG:NH1	1:H:94:ASP:OD1	2.42	0.52
1:K:141:LYS:HE2	1:K:145:GLU:OE2	2.10	0.52
1:D:103:PHE:CE1	1:D:135:LYS:HB2	2.44	0.52
1:D:86:HIS:CE1	1:D:151:LEU:HD22	2.44	0.52
1:I:86:HIS:CD2	1:J:121:HIS:CD2	2.92	0.52
1:C:112:ARG:HG3	1:C:122:GLU:HB2	1.90	0.52
1:G:168:ASP:HB3	1:G:171:TYR:HB3	1.92	0.52
1:A:94:ASP:OD1	1:K:143:ARG:NH1	2.43	0.52
1:D:179:PRO:O	1:D:181:GLN:N	2.43	0.52
1:I:43:LEU:HG	1:I:78:MET:CE	2.39	0.52
1:C:70:ARG:HG3	1:C:70:ARG:HH11	1.75	0.52
1:E:67:GLU:O	1:E:70:ARG:HB2	2.10	0.52
1:A:172:LEU:O	1:A:175:LEU:HB2	2.10	0.51
1:A:208:CYS:HB2	1:C:33:ALA:HB2	1.92	0.51
1:B:93:VAL:HA	1:B:107:VAL:HG22	1.92	0.51
1:D:105:VAL:HG11	1:D:139:LEU:HD23	1.92	0.51
1:F:135:LYS:HE3	1:G:95:PHE:CG	2.45	0.51
1:H:176:ASN:C	1:H:178:LEU:H	2.18	0.51
1:K:55:ARG:HD3	1:K:65:TYR:CE2	2.46	0.51
1:B:187:ASP:OD1	1:B:189:THR:HG23	2.10	0.51
1:G:50:GLU:CG	1:G:181:GLN:HE22	2.22	0.51
1:J:135:LYS:HG2	1:K:95:PHE:CE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:140:GLU:HG3	1:J:144:LYS:HE3	1.91	0.51
1:B:85:ALA:HB1	1:C:120:TYR:O	2.10	0.51
1:C:204:ARG:O	1:C:207:SER:HB3	2.10	0.51
1:E:103:PHE:CE1	1:E:135:LYS:HB2	2.45	0.51
1:H:54:SER:HA	1:H:63:VAL:O	2.10	0.51
1:E:204:ARG:CD	1:G:36:TYR:OH	2.58	0.51
1:G:187:ASP:OD1	1:G:189:THR:HG23	2.10	0.51
1:I:172:LEU:O	1:I:175:LEU:HB2	2.11	0.51
1:B:105:VAL:HG11	1:B:139:LEU:HD23	1.92	0.51
1:E:176:ASN:C	1:E:178:LEU:H	2.18	0.51
1:E:182:LEU:CG	1:E:183:PRO:HD2	2.41	0.51
1:E:184:LEU:HD22	1:E:184:LEU:N	2.25	0.51
1:E:204:ARG:NH2	1:F:78:MET:O	2.43	0.51
1:B:143:ARG:NH1	1:C:94:ASP:OD1	2.43	0.51
1:C:55:ARG:HD3	1:C:65:TYR:CE2	2.46	0.50
1:D:140:GLU:HG3	1:D:144:LYS:HE3	1.93	0.50
1:F:46:ARG:HD3	1:F:171:TYR:CD1	2.47	0.50
1:G:52:ILE:HG22	1:G:53:SER:N	2.27	0.50
1:K:93:VAL:HA	1:K:107:VAL:HG22	1.93	0.50
1:H:182:LEU:CG	1:H:183:PRO:HD2	2.39	0.50
1:K:29:CYS:O	1:K:117:ASP:HA	2.11	0.50
1:K:39:ILE:HG23	1:K:78:MET:HE1	1.91	0.50
1:A:36:TYR:OH	1:J:204:ARG:HD2	2.12	0.50
1:C:141:LYS:HE2	1:C:145:GLU:OE2	2.10	0.50
1:D:43:LEU:HA	1:D:161:ALA:HB3	1.94	0.50
1:D:182:LEU:CG	1:D:183:PRO:HD2	2.41	0.50
1:H:55:ARG:HD3	1:H:65:TYR:CE2	2.47	0.50
1:E:135:LYS:HE3	1:F:95:PHE:CG	2.46	0.50
1:H:47:LEU:HD12	1:H:51:TYR:CD1	2.47	0.50
1:K:28:GLN:HA	1:K:28:GLN:NE2	2.24	0.50
1:A:163:GLY:O	1:A:166:ILE:HG22	2.12	0.50
1:D:163:GLY:O	1:D:166:ILE:HG22	2.12	0.50
1:E:179:PRO:O	1:E:181:GLN:N	2.45	0.50
1:I:135:LYS:HG2	1:J:95:PHE:CE2	2.46	0.50
1:J:204:ARG:NH2	1:K:78:MET:O	2.45	0.50
1:K:163:GLY:O	1:K:166:ILE:HG22	2.12	0.50
1:G:47:LEU:HD12	1:G:51:TYR:CD1	2.46	0.49
1:K:104:TYR:CD1	1:K:104:TYR:N	2.80	0.49
1:B:140:GLU:O	1:B:144:LYS:HG3	2.12	0.49
1:D:135:LYS:HE3	1:E:95:PHE:CD2	2.47	0.49
1:D:187:ASP:OD1	1:D:189:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:ARG:HH11	1:G:173:ARG:HB3	1.77	0.49
1:H:53:SER:O	1:H:64:CYS:HA	2.12	0.49
1:K:182:LEU:CG	1:K:183:PRO:HD2	2.42	0.49
1:D:156:ARG:NH1	1:D:167:LEU:HD21	2.27	0.49
1:I:47:LEU:HD12	1:I:51:TYR:CD1	2.47	0.49
1:J:141:LYS:HE2	1:J:145:GLU:OE2	2.13	0.49
1:B:195:ASP:HB3	1:C:77:GLU:HG3	1.94	0.49
1:D:110:PHE:CE2	1:D:124:VAL:HG13	2.47	0.49
1:G:86:HIS:HA	1:G:112:ARG:O	2.12	0.49
1:E:143:ARG:NH1	1:F:94:ASP:OD1	2.45	0.49
1:G:28:GLN:HA	1:G:28:GLN:NE2	2.27	0.49
1:H:172:LEU:O	1:H:175:LEU:HB2	2.13	0.49
1:I:179:PRO:O	1:I:181:GLN:N	2.46	0.49
1:C:140:GLU:HB2	1:D:126:TYR:CD2	2.48	0.49
1:E:168:ASP:HB3	1:E:171:TYR:HB3	1.94	0.49
1:A:25:CYS:HA	1:B:30:GLN:HG2	1.94	0.49
1:A:139:LEU:O	1:A:143:ARG:HG3	2.12	0.49
1:E:163:GLY:O	1:E:166:ILE:HG22	2.13	0.49
1:F:143:ARG:NH1	1:G:94:ASP:OD1	2.46	0.49
1:G:179:PRO:O	1:G:181:GLN:N	2.46	0.49
1:H:139:LEU:O	1:H:143:ARG:HG3	2.12	0.49
1:J:173:ARG:HH11	1:J:173:ARG:HB3	1.78	0.49
1:C:131:GLY:O	1:C:132:LEU:O	2.31	0.48
1:I:91:GLN:HE21	1:I:143:ARG:HE	1.61	0.48
1:A:168:ASP:HB3	1:A:171:TYR:HB3	1.94	0.48
1:E:187:ASP:OD1	1:E:189:THR:HG23	2.12	0.48
1:H:204:ARG:HD2	1:J:36:TYR:OH	2.13	0.48
1:J:39:ILE:HG23	1:J:78:MET:HE1	1.94	0.48
1:J:85:ALA:HB1	1:K:120:TYR:O	2.13	0.48
1:K:184:LEU:HD22	1:K:184:LEU:N	2.25	0.48
1:E:112:ARG:NH2	1:E:114:GLN:HE21	2.12	0.48
1:J:163:GLY:O	1:J:166:ILE:HG22	2.14	0.48
1:K:43:LEU:HA	1:K:161:ALA:HB3	1.95	0.48
1:B:112:ARG:HG3	1:B:122:GLU:HB2	1.96	0.48
1:C:168:ASP:HB3	1:C:171:TYR:HB3	1.96	0.48
1:G:104:TYR:N	1:G:104:TYR:CD1	2.81	0.48
1:H:187:ASP:OD1	1:H:189:THR:HG23	2.14	0.48
1:K:46:ARG:HD3	1:K:171:TYR:CD1	2.49	0.48
1:C:104:TYR:CD1	1:C:104:TYR:N	2.82	0.48
1:C:193:ARG:HD3	1:D:50:GLU:OE2	2.13	0.48
1:F:182:LEU:CG	1:F:183:PRO:HD2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:VAL:HG21	1:I:124:VAL:HG22	1.95	0.48
1:F:173:ARG:HB3	1:F:173:ARG:HH11	1.78	0.48
1:C:179:PRO:O	1:C:181:GLN:N	2.47	0.48
1:F:163:GLY:O	1:F:166:ILE:HG22	2.13	0.48
1:B:46:ARG:HD3	1:B:171:TYR:CD1	2.48	0.48
1:J:182:LEU:CG	1:J:183:PRO:HD2	2.43	0.48
1:K:176:ASN:C	1:K:178:LEU:H	2.21	0.48
1:B:25:CYS:HA	1:C:30:GLN:HG2	1.96	0.47
1:B:204:ARG:NH2	1:C:78:MET:O	2.47	0.47
1:D:70:ARG:HG3	1:D:70:ARG:NH1	2.28	0.47
1:G:67:GLU:O	1:G:70:ARG:HB2	2.13	0.47
1:F:179:PRO:O	1:F:181:GLN:N	2.47	0.47
1:A:50:GLU:CG	1:A:181:GLN:HE22	2.27	0.47
1:A:110:PHE:CE2	1:A:124:VAL:HG13	2.49	0.47
1:C:163:GLY:O	1:C:166:ILE:HG22	2.14	0.47
1:G:127:GLY:HA3	1:G:142:ALA:O	2.13	0.47
1:H:179:PRO:O	1:H:181:GLN:N	2.47	0.47
1:C:25:CYS:HA	1:D:30:GLN:HG2	1.96	0.47
1:H:104:TYR:N	1:H:104:TYR:CD1	2.80	0.47
1:D:135:LYS:HE3	1:E:95:PHE:CG	2.48	0.47
1:D:140:GLU:HB2	1:E:126:TYR:CD2	2.50	0.47
1:D:168:ASP:HB3	1:D:171:TYR:HB3	1.95	0.47
1:D:183:PRO:HB3	1:E:170:ASP:OD1	2.15	0.47
1:D:208:CYS:HB2	1:F:33:ALA:HB2	1.95	0.47
1:F:28:GLN:HA	1:F:28:GLN:NE2	2.27	0.47
1:H:43:LEU:CG	1:H:78:MET:HE2	2.38	0.47
1:E:104:TYR:CD1	1:E:104:TYR:N	2.83	0.47
1:G:151:LEU:HD12	1:G:151:LEU:O	2.14	0.47
1:I:74:LEU:HD13	1:I:161:ALA:O	2.14	0.47
1:E:131:GLY:O	1:E:132:LEU:O	2.33	0.47
1:F:104:TYR:CD1	1:F:104:TYR:N	2.83	0.47
1:I:186:VAL:HB	1:J:174:SER:OG	2.15	0.47
1:K:47:LEU:HD12	1:K:51:TYR:CD1	2.49	0.47
1:K:91:GLN:HE21	1:K:143:ARG:HE	1.58	0.47
1:A:71:VAL:HG12	1:A:155:LEU:HD13	1.97	0.47
1:D:50:GLU:CG	1:D:181:GLN:HE22	2.28	0.47
1:E:28:GLN:HA	1:E:28:GLN:NE2	2.26	0.47
1:K:192:LYS:NZ	1:K:197:GLU:OE2	2.35	0.47
1:C:182:LEU:HD12	1:C:183:PRO:HD2	1.96	0.47
1:C:204:ARG:HD2	1:E:36:TYR:OH	2.15	0.47
1:K:172:LEU:O	1:K:175:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:SER:HB3	1:D:137:LEU:HB2	1.96	0.47
1:D:204:ARG:NH2	1:E:78:MET:O	2.48	0.47
1:D:204:ARG:O	1:D:207:SER:HB3	2.14	0.47
1:A:186:VAL:HB	1:B:174:SER:OG	2.15	0.46
1:B:39:ILE:HG23	1:B:78:MET:HE1	1.93	0.46
1:E:127:GLY:HA3	1:E:142:ALA:O	2.15	0.46
1:G:140:GLU:HG3	1:G:144:LYS:HE3	1.97	0.46
1:H:127:GLY:HA3	1:H:142:ALA:O	2.15	0.46
1:H:195:ASP:HB3	1:I:77:GLU:HG3	1.96	0.46
1:A:204:ARG:O	1:A:207:SER:HB3	2.16	0.46
1:B:172:LEU:O	1:B:175:LEU:HB2	2.15	0.46
1:G:139:LEU:O	1:G:143:ARG:HG3	2.15	0.46
1:B:204:ARG:O	1:B:207:SER:HB3	2.16	0.46
1:E:105:VAL:HG11	1:E:139:LEU:HD23	1.96	0.46
1:A:50:GLU:OE1	1:A:50:GLU:N	2.40	0.46
1:C:182:LEU:HD12	1:C:183:PRO:CD	2.46	0.46
1:G:171:TYR:CE2	1:G:175:LEU:HD11	2.50	0.46
1:H:50:GLU:CG	1:H:181:GLN:HE22	2.25	0.46
1:H:86:HIS:HA	1:H:112:ARG:O	2.15	0.46
1:J:204:ARG:O	1:J:207:SER:HB3	2.16	0.46
1:A:120:TYR:O	1:K:85:ALA:HB1	2.15	0.46
1:I:46:ARG:HD3	1:I:171:TYR:CD1	2.51	0.46
1:D:39:ILE:HG23	1:D:78:MET:HE1	1.96	0.46
1:E:115:LEU:HD11	1:E:158:PHE:CE2	2.51	0.46
1:B:176:ASN:C	1:B:178:LEU:H	2.24	0.46
1:C:143:ARG:NH1	1:D:94:ASP:OD1	2.49	0.46
1:E:151:LEU:HD12	1:E:151:LEU:O	2.15	0.46
1:G:147:VAL:HG21	1:H:124:VAL:HG22	1.97	0.46
1:K:179:PRO:O	1:K:181:GLN:N	2.48	0.46
1:K:187:ASP:OD1	1:K:189:THR:HG23	2.16	0.46
1:A:165:CYS:O	1:A:167:LEU:N	2.49	0.46
1:B:50:GLU:CG	1:B:181:GLN:HE22	2.27	0.46
1:D:165:CYS:O	1:D:167:LEU:N	2.49	0.46
1:F:156:ARG:NH1	1:F:167:LEU:HD21	2.30	0.46
1:I:135:LYS:HE3	1:J:95:PHE:CG	2.51	0.46
1:C:46:ARG:HD3	1:C:171:TYR:CD1	2.51	0.46
1:D:131:GLY:O	1:D:132:LEU:O	2.34	0.46
1:J:173:ARG:NH1	1:J:173:ARG:CB	2.79	0.46
1:B:163:GLY:O	1:B:166:ILE:HG22	2.16	0.45
1:D:91:GLN:NE2	1:E:110:PHE:HZ	2.13	0.45
1:I:147:VAL:HG21	1:J:124:VAL:HG22	1.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:104:TYR:N	1:J:104:TYR:CD1	2.84	0.45
1:J:172:LEU:O	1:J:175:LEU:HB2	2.17	0.45
1:A:33:ALA:HB2	1:J:208:CYS:HB2	1.98	0.45
1:B:183:PRO:HB3	1:C:170:ASP:OD1	2.16	0.45
1:C:183:PRO:HB3	1:D:170:ASP:OD1	2.16	0.45
1:E:43:LEU:HA	1:E:161:ALA:HB3	1.98	0.45
1:E:140:GLU:HG3	1:E:144:LYS:HE3	1.98	0.45
1:I:104:TYR:N	1:I:104:TYR:CD1	2.84	0.45
1:J:173:ARG:O	1:J:177:LYS:HG3	2.16	0.45
1:A:140:GLU:HG3	1:A:144:LYS:HE3	1.99	0.45
1:C:173:ARG:HH11	1:C:173:ARG:HB3	1.82	0.45
1:G:39:ILE:HG23	1:G:78:MET:HE1	1.94	0.45
1:K:50:GLU:CG	1:K:181:GLN:HE22	2.26	0.45
1:D:46:ARG:HD3	1:D:171:TYR:CD1	2.51	0.45
1:D:112:ARG:NH2	1:D:114:GLN:HE21	2.14	0.45
1:G:93:VAL:HA	1:G:107:VAL:HG22	1.97	0.45
1:I:70:ARG:HG3	1:I:70:ARG:NH1	2.30	0.45
1:J:43:LEU:HG	1:J:78:MET:CE	2.46	0.45
1:A:141:LYS:HE2	1:A:145:GLU:OE2	2.17	0.45
1:B:179:PRO:O	1:B:181:GLN:N	2.49	0.45
1:F:173:ARG:NH1	1:F:173:ARG:CB	2.80	0.45
1:G:172:LEU:O	1:G:175:LEU:HB2	2.17	0.45
1:G:173:ARG:NH1	1:G:173:ARG:CB	2.80	0.45
1:E:43:LEU:CG	1:E:78:MET:HE2	2.42	0.45
1:F:43:LEU:HA	1:F:161:ALA:HB3	1.97	0.45
1:H:70:ARG:HG3	1:H:70:ARG:NH1	2.31	0.45
1:C:196:LEU:HD12	1:C:197:GLU:H	1.81	0.45
1:J:173:ARG:HH11	1:J:173:ARG:CB	2.29	0.45
1:J:179:PRO:O	1:J:181:GLN:N	2.49	0.45
1:K:168:ASP:HB3	1:K:171:TYR:HB3	1.99	0.45
1:A:104:TYR:N	1:A:104:TYR:CD1	2.85	0.45
1:B:135:LYS:HE3	1:C:95:PHE:CG	2.52	0.45
1:E:28:GLN:HE21	1:E:28:GLN:CA	2.23	0.45
1:E:43:LEU:HG	1:E:78:MET:CE	2.42	0.45
1:F:184:LEU:H	1:F:184:LEU:CD2	2.28	0.45
1:A:98:LEU:HD12	1:A:102:LYS:O	2.17	0.45
1:B:173:ARG:HH11	1:B:173:ARG:HB3	1.82	0.45
1:D:182:LEU:CD1	1:D:183:PRO:HD2	2.46	0.45
1:A:179:PRO:O	1:A:181:GLN:N	2.50	0.45
1:E:147:VAL:HG21	1:F:124:VAL:HG22	1.97	0.45
1:E:182:LEU:CD1	1:E:183:PRO:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168:ASP:HB3	1:I:171:TYR:HB3	1.99	0.45
1:D:112:ARG:HH21	1:D:114:GLN:NE2	2.14	0.44
1:G:39:ILE:HG23	1:G:78:MET:HE3	1.97	0.44
1:G:43:LEU:CD2	1:G:78:MET:HE2	2.47	0.44
1:B:55:ARG:HD3	1:B:65:TYR:CE2	2.52	0.44
1:C:25:CYS:O	1:C:29:CYS:SG	2.67	0.44
1:D:172:LEU:O	1:D:175:LEU:HB2	2.17	0.44
1:I:43:LEU:CG	1:I:78:MET:HE2	2.43	0.44
1:K:43:LEU:HG	1:K:78:MET:CE	2.45	0.44
1:A:199:SER:HB3	2:A:218:HOH:O	2.16	0.44
1:C:204:ARG:NH2	1:D:78:MET:O	2.51	0.44
1:D:104:TYR:CD1	1:D:104:TYR:N	2.86	0.44
1:F:43:LEU:HG	1:F:78:MET:CE	2.47	0.44
1:G:70:ARG:HG3	1:G:70:ARG:NH1	2.31	0.44
1:G:182:LEU:HD12	1:G:183:PRO:HD3	1.93	0.44
1:H:105:VAL:HG11	1:H:139:LEU:HD23	1.99	0.44
1:J:86:HIS:HA	1:J:112:ARG:O	2.17	0.44
1:D:173:ARG:HB3	1:D:173:ARG:HH11	1.82	0.44
1:E:135:LYS:HE3	1:F:95:PHE:CD2	2.53	0.44
1:I:139:LEU:O	1:I:143:ARG:HG3	2.16	0.44
1:H:67:GLU:O	1:H:70:ARG:HB2	2.18	0.44
1:B:104:TYR:N	1:B:104:TYR:CD1	2.85	0.44
1:E:172:LEU:O	1:E:175:LEU:HB2	2.17	0.44
1:I:28:GLN:HA	1:I:28:GLN:NE2	2.30	0.44
1:J:46:ARG:HD3	1:J:171:TYR:CD1	2.53	0.44
1:J:47:LEU:HD12	1:J:51:TYR:CD1	2.52	0.44
1:G:184:LEU:H	1:G:184:LEU:CD2	2.28	0.44
1:A:43:LEU:HA	1:A:161:ALA:HB3	2.00	0.44
1:A:182:LEU:CG	1:A:183:PRO:HD2	2.45	0.44
1:G:163:GLY:O	1:G:166:ILE:HG22	2.17	0.44
1:I:141:LYS:HE2	1:I:145:GLU:OE2	2.18	0.44
1:J:74:LEU:HD13	1:J:161:ALA:O	2.18	0.44
1:H:182:LEU:CD1	1:H:183:PRO:HD2	2.48	0.43
1:I:81:TYR:CE1	1:I:82:ASN:HB3	2.53	0.43
1:D:112:ARG:NH2	1:D:114:GLN:NE2	2.66	0.43
1:F:186:VAL:HB	1:G:174:SER:OG	2.18	0.43
1:C:50:GLU:CG	1:C:181:GLN:HE22	2.31	0.43
1:G:182:LEU:HG	1:G:183:PRO:HD2	1.98	0.43
1:I:135:LYS:HE3	1:J:95:PHE:CD2	2.53	0.43
1:I:187:ASP:OD1	1:I:189:THR:HG23	2.18	0.43
1:C:184:LEU:H	1:C:184:LEU:CD2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:ARG:HH11	1:E:173:ARG:HB3	1.84	0.43
1:F:53:SER:O	1:F:64:CYS:HA	2.19	0.43
1:H:184:LEU:H	1:H:184:LEU:CD2	2.27	0.43
1:I:50:GLU:CG	1:I:181:GLN:HE22	2.26	0.43
1:J:168:ASP:HB3	1:J:171:TYR:HB3	2.00	0.43
1:A:205:TYR:CE1	1:C:33:ALA:HB1	2.53	0.43
1:E:46:ARG:HD3	1:E:171:TYR:CD1	2.54	0.43
1:F:140:GLU:O	1:F:144:LYS:HG3	2.18	0.43
1:J:43:LEU:HA	1:J:161:ALA:HB3	2.01	0.43
1:J:184:LEU:H	1:J:184:LEU:CD2	2.30	0.43
1:B:131:GLY:O	1:B:132:LEU:O	2.36	0.43
1:E:193:ARG:HB3	1:F:50:GLU:OE2	2.18	0.43
1:I:171:TYR:CE2	1:I:175:LEU:HD11	2.53	0.43
1:J:50:GLU:CG	1:J:181:GLN:HE22	2.23	0.43
1:K:158:PHE:HB2	1:K:162:LEU:HD12	2.00	0.43
1:J:67:GLU:O	1:J:70:ARG:HB2	2.19	0.43
1:A:193:ARG:HD3	1:B:50:GLU:OE2	2.19	0.43
1:E:86:HIS:CE1	1:E:151:LEU:HD22	2.53	0.43
1:E:98:LEU:HD12	1:E:102:LYS:O	2.19	0.43
1:H:43:LEU:HA	1:H:161:ALA:HB3	2.00	0.43
1:H:151:LEU:HD12	1:H:151:LEU:O	2.18	0.43
1:I:204:ARG:NH2	1:J:78:MET:O	2.51	0.43
1:D:55:ARG:HD3	1:D:65:TYR:CD2	2.54	0.43
1:G:46:ARG:HD3	1:G:171:TYR:CD1	2.53	0.43
1:I:61:GLN:OE1	1:I:61:GLN:N	2.52	0.43
1:I:103:PHE:CE1	1:I:135:LYS:HB2	2.54	0.43
1:I:184:LEU:H	1:I:184:LEU:CD2	2.29	0.43
1:K:173:ARG:HB3	1:K:173:ARG:HH11	1.83	0.43
1:C:173:ARG:CB	1:C:173:ARG:NH1	2.82	0.43
1:D:93:VAL:HA	1:D:107:VAL:HG22	2.01	0.43
1:F:127:GLY:HA3	1:F:142:ALA:O	2.19	0.43
1:G:168:ASP:HB3	1:G:171:TYR:CB	2.48	0.43
1:B:165:CYS:O	1:B:167:LEU:N	2.52	0.42
1:E:112:ARG:HH21	1:E:114:GLN:NE2	2.17	0.42
1:F:55:ARG:HD3	1:F:65:TYR:CD2	2.54	0.42
1:I:50:GLU:OE1	1:I:50:GLU:N	2.42	0.42
1:J:28:GLN:HA	1:J:28:GLN:NE2	2.30	0.42
1:J:147:VAL:CG2	1:K:124:VAL:CG2	2.90	0.42
1:F:72:ILE:HG22	1:F:76:ASN:ND2	2.35	0.42
1:G:86:HIS:CE1	1:G:151:LEU:HD22	2.55	0.42
1:B:47:LEU:HD12	1:B:51:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ASP:HB3	1:E:77:GLU:HG3	2.01	0.42
1:C:52:ILE:HG22	1:C:53:SER:N	2.34	0.42
1:F:172:LEU:O	1:F:175:LEU:HB2	2.19	0.42
1:D:173:ARG:NH1	1:D:173:ARG:CB	2.82	0.42
1:E:171:TYR:CE2	1:E:175:LEU:HD11	2.55	0.42
1:F:50:GLU:CG	1:F:181:GLN:HE22	2.26	0.42
1:F:131:GLY:O	1:F:132:LEU:O	2.37	0.42
1:J:182:LEU:CD1	1:J:183:PRO:HD2	2.50	0.42
1:E:87:SER:HA	1:F:122:GLU:HB3	2.02	0.42
1:G:173:ARG:HH11	1:G:173:ARG:CB	2.32	0.42
1:A:105:VAL:HG11	1:A:139:LEU:HD23	2.01	0.42
1:B:193:ARG:HH11	1:B:193:ARG:HG3	1.84	0.42
1:G:128:VAL:HG12	1:G:129:SER:N	2.35	0.42
1:J:47:LEU:N	1:J:47:LEU:HD22	2.35	0.42
1:J:110:PHE:CE2	1:J:124:VAL:HG13	2.55	0.42
1:J:147:VAL:HG21	1:K:124:VAL:HG23	1.96	0.42
1:J:173:ARG:NH1	1:J:173:ARG:HB2	2.34	0.42
1:B:103:PHE:CE1	1:B:135:LYS:HB2	2.54	0.42
1:E:128:VAL:HG12	1:E:129:SER:N	2.35	0.42
1:A:95:PHE:CE2	1:K:135:LYS:HG2	2.55	0.41
1:F:86:HIS:CE1	1:F:151:LEU:HD22	2.55	0.41
1:J:70:ARG:HG3	1:J:70:ARG:NH1	2.32	0.41
1:K:182:LEU:CD1	1:K:183:PRO:HD2	2.49	0.41
1:A:127:GLY:HA3	1:A:142:ALA:O	2.20	0.41
1:A:184:LEU:H	1:A:184:LEU:CD2	2.31	0.41
1:G:175:LEU:O	1:G:178:LEU:HB2	2.20	0.41
1:H:39:ILE:HG23	1:H:78:MET:HE3	1.98	0.41
1:I:47:LEU:N	1:I:47:LEU:HD22	2.35	0.41
1:C:98:LEU:HD12	1:C:102:LYS:O	2.20	0.41
1:G:165:CYS:O	1:G:168:ASP:N	2.52	0.41
1:H:98:LEU:HD12	1:H:102:LYS:O	2.20	0.41
1:F:39:ILE:HG23	1:F:78:MET:HE3	1.98	0.41
1:G:74:LEU:HD13	1:G:161:ALA:O	2.20	0.41
1:G:140:GLU:O	1:G:144:LYS:HG3	2.20	0.41
1:A:52:ILE:HG22	1:A:53:SER:N	2.35	0.41
1:B:99:ASN:C	1:B:100:ASN:OD1	2.64	0.41
1:D:67:GLU:O	1:D:70:ARG:HB2	2.21	0.41
1:H:168:ASP:HB3	1:H:171:TYR:CB	2.50	0.41
1:A:103:PHE:CE1	1:A:135:LYS:HB2	2.56	0.41
1:E:186:VAL:HB	1:F:174:SER:OG	2.21	0.41
1:F:105:VAL:HG11	1:F:139:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:LEU:HD13	1:H:161:ALA:O	2.21	0.41
1:A:195:ASP:HB3	1:B:77:GLU:HG3	2.02	0.41
1:D:165:CYS:O	1:D:168:ASP:N	2.52	0.41
1:E:204:ARG:O	1:E:207:SER:HB3	2.21	0.41
1:I:86:HIS:HA	1:I:112:ARG:O	2.20	0.41
1:C:54:SER:CB	1:C:62:LYS:HE3	2.51	0.41
1:C:110:PHE:CE2	1:C:124:VAL:HG13	2.55	0.41
1:D:127:GLY:HA3	1:D:142:ALA:O	2.21	0.41
1:D:140:GLU:O	1:D:144:LYS:HG3	2.21	0.41
1:E:53:SER:O	1:E:64:CYS:HA	2.21	0.41
1:F:140:GLU:HG3	1:F:144:LYS:HE3	2.02	0.41
1:G:55:ARG:HD3	1:G:65:TYR:CD2	2.56	0.41
1:G:85:ALA:CB	1:H:120:TYR:O	2.68	0.41
1:I:67:GLU:O	1:I:70:ARG:HB2	2.20	0.41
1:J:171:TYR:CE2	1:J:175:LEU:HD11	2.56	0.41
1:A:193:ARG:HG3	1:A:193:ARG:HH11	1.86	0.41
1:B:79:PHE:O	1:B:83:GLY:HA3	2.20	0.41
1:D:61:GLN:OE1	1:D:61:GLN:N	2.52	0.41
1:H:173:ARG:HB3	1:H:173:ARG:HH11	1.85	0.41
1:I:163:GLY:O	1:I:166:ILE:HG22	2.21	0.41
1:I:204:ARG:HD2	1:K:36:TYR:OH	2.21	0.41
1:K:43:LEU:HA	1:K:161:ALA:CB	2.51	0.41
1:C:103:PHE:CE1	1:C:135:LYS:HB2	2.56	0.41
1:E:26:PHE:C	1:E:28:GLN:H	2.29	0.41
1:F:204:ARG:O	1:F:207:SER:HB3	2.21	0.41
1:I:70:ARG:HH11	1:I:70:ARG:CG	2.31	0.41
1:B:28:GLN:HA	1:B:28:GLN:NE2	2.30	0.40
1:B:43:LEU:HG	1:B:78:MET:CE	2.48	0.40
1:D:143:ARG:NH1	1:E:94:ASP:OD1	2.53	0.40
1:G:200:VAL:HG13	1:H:39:ILE:HG13	2.03	0.40
1:I:204:ARG:O	1:I:207:SER:HB3	2.20	0.40
1:J:25:CYS:SG	1:J:28:GLN:HG3	2.62	0.40
1:K:184:LEU:H	1:K:184:LEU:CD2	2.31	0.40
1:B:33:ALA:HB2	1:K:208:CYS:CB	2.51	0.40
1:C:86:HIS:CE1	1:C:151:LEU:HD22	2.56	0.40
1:F:47:LEU:HD12	1:F:51:TYR:CD1	2.56	0.40
1:I:52:ILE:HG22	1:I:53:SER:N	2.36	0.40
1:B:54:SER:HA	1:B:63:VAL:O	2.20	0.40
1:B:182:LEU:CD1	1:B:183:PRO:HD2	2.51	0.40
1:E:55:ARG:HD3	1:E:65:TYR:CD2	2.56	0.40
1:G:165:CYS:O	1:G:167:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:43:LEU:CG	1:K:78:MET:HE2	2.46	0.40
1:K:139:LEU:O	1:K:143:ARG:HG3	2.20	0.40
1:A:186:VAL:HG21	1:B:171:TYR:HA	2.02	0.40
1:C:176:ASN:C	1:C:178:LEU:N	2.80	0.40
1:F:144:LYS:NZ	1:G:149:ASP:OD2	2.38	0.40
1:F:182:LEU:CD1	1:F:183:PRO:HD2	2.51	0.40
1:G:165:CYS:C	1:G:167:LEU:N	2.80	0.40
1:H:188:LEU:HD12	1:I:178:LEU:HD11	2.02	0.40
1:A:182:LEU:CD1	1:A:183:PRO:HD2	2.52	0.40
1:C:127:GLY:HA3	1:C:142:ALA:O	2.22	0.40
1:C:135:LYS:HG2	1:D:95:PHE:CE2	2.56	0.40
1:C:180:ARG:CZ	1:C:181:GLN:O	2.69	0.40
1:E:70:ARG:HG3	1:E:70:ARG:NH1	2.35	0.40
1:I:110:PHE:CE2	1:I:124:VAL:HG13	2.57	0.40
1:K:173:ARG:CB	1:K:173:ARG:NH1	2.84	0.40
1:K:204:ARG:O	1:K:207:SER:HB3	2.21	0.40

All (2) 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:D:60:GLY:O	1:G:37:GLN:OE1[6_456]	2.14	0.06
1:E:185:GLU:OE2	1:E:185:GLU:OE2[8_666]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	182/212 (86%)	165 (91%)	11 (6%)	6 (3%)	3 7
1	B	182/212 (86%)	166 (91%)	12 (7%)	4 (2%)	5 12
1	C	182/212 (86%)	165 (91%)	11 (6%)	6 (3%)	3 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	182/212 (86%)	166 (91%)	10 (6%)	6 (3%)	3	7
1	E	182/212 (86%)	163 (90%)	12 (7%)	7 (4%)	2	5
1	F	182/212 (86%)	158 (87%)	18 (10%)	6 (3%)	3	7
1	G	182/212 (86%)	162 (89%)	13 (7%)	7 (4%)	2	5
1	H	182/212 (86%)	162 (89%)	14 (8%)	6 (3%)	3	7
1	I	182/212 (86%)	165 (91%)	11 (6%)	6 (3%)	3	7
1	J	182/212 (86%)	167 (92%)	10 (6%)	5 (3%)	4	9
1	K	182/212 (86%)	164 (90%)	13 (7%)	5 (3%)	4	9
All	All	2002/2332 (86%)	1803 (90%)	135 (7%)	64 (3%)	3	7

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	B	132	LEU
1	C	132	LEU
1	D	132	LEU
1	E	132	LEU
1	F	132	LEU
1	G	132	LEU
1	H	132	LEU
1	I	132	LEU
1	J	132	LEU
1	K	132	LEU
1	A	180	ARG
1	D	166	ILE
1	D	180	ARG
1	E	180	ARG
1	I	180	ARG
1	A	166	ILE
1	A	177	LYS
1	C	180	ARG
1	D	177	LYS
1	F	180	ARG
1	G	180	ARG
1	H	58	GLY
1	H	180	ARG
1	I	177	LYS
1	J	177	LYS

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Mol	Chain	Res	Type
1	J	180	ARG
1	K	58	GLY
1	K	180	ARG
1	B	180	ARG
1	C	58	GLY
1	C	177	LYS
1	E	177	LYS
1	F	177	LYS
1	F	196	LEU
1	G	29	CYS
1	G	58	GLY
1	G	100	ASN
1	H	177	LYS
1	J	58	GLY
1	A	45	GLN
1	A	58	GLY
1	B	58	GLY
1	B	166	ILE
1	C	100	ASN
1	E	100	ASN
1	E	196	LEU
1	F	58	GLY
1	G	177	LYS
1	H	29	CYS
1	I	58	GLY
1	I	100	ASN
1	K	177	LYS
1	D	58	GLY
1	E	58	GLY
1	E	166	ILE
1	F	166	ILE
1	G	166	ILE
1	K	100	ASN
1	D	183	PRO
1	H	166	ILE
1	I	179	PRO
1	J	166	ILE
1	C	183	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	153/172 (89%)	149 (97%)	4 (3%)	40	65
1	B	153/172 (89%)	149 (97%)	4 (3%)	40	65
1	C	153/172 (89%)	150 (98%)	3 (2%)	48	71
1	D	153/172 (89%)	149 (97%)	4 (3%)	40	65
1	E	153/172 (89%)	148 (97%)	5 (3%)	33	58
1	F	153/172 (89%)	150 (98%)	3 (2%)	48	71
1	G	153/172 (89%)	150 (98%)	3 (2%)	48	71
1	H	153/172 (89%)	149 (97%)	4 (3%)	40	65
1	I	153/172 (89%)	149 (97%)	4 (3%)	40	65
1	J	153/172 (89%)	150 (98%)	3 (2%)	48	71
1	K	153/172 (89%)	149 (97%)	4 (3%)	40	65
All	All	1683/1892 (89%)	1642 (98%)	41 (2%)	43	67

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
1	A	124	VAL
1	A	183	PRO
1	A	184	LEU
1	B	112	ARG
1	B	124	VAL
1	B	183	PRO
1	B	184	LEU
1	C	124	VAL
1	C	183	PRO
1	C	184	LEU
1	D	112	ARG
1	D	124	VAL
1	D	183	PRO
1	D	184	LEU

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Mol	Chain	Res	Type
1	E	104	TYR
1	E	112	ARG
1	E	124	VAL
1	E	183	PRO
1	E	184	LEU
1	F	124	VAL
1	F	183	PRO
1	F	184	LEU
1	G	124	VAL
1	G	183	PRO
1	G	184	LEU
1	H	104	TYR
1	H	124	VAL
1	H	183	PRO
1	H	184	LEU
1	I	112	ARG
1	I	124	VAL
1	I	183	PRO
1	I	184	LEU
1	J	124	VAL
1	J	183	PRO
1	J	184	LEU
1	K	112	ARG
1	K	124	VAL
1	K	183	PRO
1	K	184	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	37	GLN
1	A	45	GLN
1	A	86	HIS
1	A	91	GLN
1	A	114	GLN
1	A	121	HIS
1	A	181	GLN
1	B	28	GLN
1	B	37	GLN
1	B	45	GLN
1	B	73	ASN

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Mol	Chain	Res	Type
1	B	86	HIS
1	B	91	GLN
1	B	121	HIS
1	B	181	GLN
1	C	28	GLN
1	C	37	GLN
1	C	45	GLN
1	C	73	ASN
1	C	86	HIS
1	C	91	GLN
1	C	121	HIS
1	C	160	ASN
1	C	181	GLN
1	D	28	GLN
1	D	37	GLN
1	D	45	GLN
1	D	73	ASN
1	D	86	HIS
1	D	91	GLN
1	D	92	ASN
1	D	114	GLN
1	D	121	HIS
1	D	160	ASN
1	D	181	GLN
1	E	28	GLN
1	E	30	GLN
1	E	37	GLN
1	E	45	GLN
1	E	73	ASN
1	E	86	HIS
1	E	91	GLN
1	E	114	GLN
1	E	121	HIS
1	E	160	ASN
1	E	181	GLN
1	F	28	GLN
1	F	37	GLN
1	F	45	GLN
1	F	73	ASN
1	F	86	HIS
1	F	91	GLN
1	F	114	GLN

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Mol	Chain	Res	Type
1	F	160	ASN
1	F	181	GLN
1	G	28	GLN
1	G	30	GLN
1	G	37	GLN
1	G	45	GLN
1	G	73	ASN
1	G	86	HIS
1	G	91	GLN
1	G	114	GLN
1	G	121	HIS
1	G	160	ASN
1	G	181	GLN
1	H	28	GLN
1	H	30	GLN
1	H	37	GLN
1	H	45	GLN
1	H	73	ASN
1	H	86	HIS
1	H	91	GLN
1	H	121	HIS
1	H	160	ASN
1	H	181	GLN
1	I	28	GLN
1	I	37	GLN
1	I	45	GLN
1	I	73	ASN
1	I	86	HIS
1	I	91	GLN
1	I	121	HIS
1	I	160	ASN
1	I	176	ASN
1	I	181	GLN
1	J	28	GLN
1	J	37	GLN
1	J	45	GLN
1	J	73	ASN
1	J	86	HIS
1	J	91	GLN
1	J	121	HIS
1	J	160	ASN
1	J	181	GLN

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Mol	Chain	Res	Type
1	K	28	GLN
1	K	37	GLN
1	K	45	GLN
1	K	86	HIS
1	K	91	GLN
1	K	121	HIS
1	K	160	ASN
1	K	181	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	184/212 (86%)	0.63	20 (10%) 10 8	25, 60, 136, 198	0
1	B	184/212 (86%)	0.71	28 (15%) 5 4	25, 56, 150, 200	0
1	C	184/212 (86%)	0.77	25 (13%) 7 5	25, 61, 166, 200	0
1	D	184/212 (86%)	1.21	41 (22%) 2 2	28, 78, 156, 200	0
1	E	184/212 (86%)	1.51	55 (29%) 1 1	33, 85, 170, 200	0
1	F	184/212 (86%)	1.67	72 (39%) 1 0	38, 87, 163, 199	0
1	G	184/212 (86%)	1.49	50 (27%) 1 1	37, 82, 170, 200	0
1	H	184/212 (86%)	1.19	46 (25%) 2 1	30, 72, 149, 198	0
1	I	184/212 (86%)	0.94	29 (15%) 5 4	31, 69, 139, 185	0
1	J	184/212 (86%)	1.00	36 (19%) 3 3	31, 70, 158, 200	0
1	K	184/212 (86%)	0.85	30 (16%) 4 4	30, 65, 154, 182	0
All	All	2024/2332 (86%)	1.09	432 (21%) 2 2	25, 72, 160, 200	0

All (432) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	159	GLY	6.4
1	E	167	LEU	5.5
1	F	167	LEU	5.4
1	B	176	ASN	5.4
1	B	182	LEU	5.1
1	G	49	PRO	5.1
1	A	101	GLY	5.1
1	E	184	LEU	4.9
1	G	182	LEU	4.9
1	G	184	LEU	4.8
1	B	184	LEU	4.7
1	E	49	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	168	ASP	4.6
1	E	48	GLY	4.6
1	H	58	GLY	4.6
1	H	208	CYS	4.5
1	A	58	GLY	4.5
1	H	181	GLN	4.5
1	D	99	ASN	4.4
1	G	166	ILE	4.3
1	D	199	SER	4.3
1	D	61	GLN	4.3
1	E	183	PRO	4.3
1	F	30	GLN	4.2
1	H	167	LEU	4.2
1	J	184	LEU	4.2
1	E	80	GLY	4.2
1	K	167	LEU	4.2
1	E	207	SER	4.2
1	E	181	GLN	4.1
1	H	100	ASN	4.1
1	F	31	TYR	4.1
1	K	208	CYS	4.1
1	A	167	LEU	4.1
1	G	101	GLY	4.1
1	G	208	CYS	4.1
1	F	168	ASP	4.0
1	I	182	LEU	4.0
1	E	208	CYS	4.0
1	G	167	LEU	4.0
1	G	194	GLN	4.0
1	D	56	MET	4.0
1	C	194	GLN	4.0
1	J	37	GLN	4.0
1	G	62	LYS	4.0
1	F	188	LEU	3.9
1	G	207	SER	3.9
1	F	133	LYS	3.9
1	J	177	LYS	3.9
1	D	207	SER	3.9
1	C	205	TYR	3.9
1	E	67	GLU	3.8
1	F	159	GLY	3.8
1	G	30	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	184	LEU	3.8
1	J	61	GLN	3.8
1	E	203	ALA	3.8
1	A	182	LEU	3.8
1	K	184	LEU	3.8
1	I	185	GLU	3.8
1	I	184	LEU	3.7
1	G	59	GLY	3.7
1	J	181	GLN	3.7
1	H	206	ASN	3.7
1	D	181	GLN	3.7
1	G	48	GLY	3.6
1	A	184	LEU	3.6
1	F	194	GLN	3.6
1	J	199	SER	3.6
1	I	167	LEU	3.6
1	E	62	LYS	3.5
1	G	41	LYS	3.5
1	F	207	SER	3.5
1	H	182	LEU	3.5
1	B	37	GLN	3.5
1	G	37	GLN	3.5
1	D	208	CYS	3.5
1	B	181	GLN	3.5
1	J	208	CYS	3.5
1	F	206	ASN	3.5
1	D	59	GLY	3.4
1	D	62	LYS	3.4
1	D	184	LEU	3.4
1	D	182	LEU	3.4
1	A	207	SER	3.4
1	B	173	ARG	3.4
1	E	37	GLN	3.4
1	E	196	LEU	3.4
1	H	70	ARG	3.4
1	E	56	MET	3.4
1	I	37	GLN	3.4
1	E	63	VAL	3.3
1	G	34	GLU	3.3
1	I	208	CYS	3.3
1	F	181	GLN	3.3
1	E	65	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	205	TYR	3.3
1	G	196	LEU	3.3
1	C	100	ASN	3.3
1	K	190	LYS	3.3
1	E	59	GLY	3.3
1	F	48	GLY	3.3
1	K	34	GLU	3.3
1	F	177	LYS	3.3
1	C	190	LYS	3.2
1	C	181	GLN	3.2
1	F	186	VAL	3.2
1	F	27	GLY	3.2
1	B	49	PRO	3.2
1	E	206	ASN	3.2
1	H	33	ALA	3.2
1	E	176	ASN	3.2
1	B	180	ARG	3.2
1	A	181	GLN	3.2
1	J	34	GLU	3.2
1	H	207	SER	3.2
1	F	158	PHE	3.2
1	D	133	LYS	3.2
1	B	41	LYS	3.1
1	C	199	SER	3.1
1	G	75	ALA	3.1
1	I	199	SER	3.1
1	F	99	ASN	3.1
1	H	190	LYS	3.1
1	B	207	SER	3.1
1	G	157	SER	3.1
1	G	174	SER	3.1
1	K	59	GLY	3.1
1	G	44	ARG	3.1
1	H	199	SER	3.1
1	G	127	GLY	3.1
1	I	43	LEU	3.1
1	H	104	TYR	3.0
1	D	173	ARG	3.0
1	I	177	LYS	3.0
1	C	104	TYR	3.0
1	F	100	ASN	3.0
1	K	30	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	58	GLY	3.0
1	F	170	ASP	3.0
1	H	48	GLY	3.0
1	I	100	ASN	3.0
1	I	159	GLY	3.0
1	F	184	LEU	3.0
1	J	132	LEU	3.0
1	K	207	SER	3.0
1	C	182	LEU	3.0
1	B	100	ASN	3.0
1	K	201	GLU	3.0
1	E	70	ARG	2.9
1	F	74	LEU	2.9
1	F	198	PRO	2.9
1	G	176	ASN	2.9
1	C	62	LYS	2.9
1	E	201	GLU	2.9
1	I	57	ALA	2.9
1	H	59	GLY	2.9
1	J	198	PRO	2.9
1	J	201	GLU	2.9
1	E	69	HIS	2.9
1	C	56	MET	2.9
1	G	56	MET	2.9
1	J	63	VAL	2.9
1	D	58	GLY	2.8
1	D	194	GLN	2.8
1	K	61	GLN	2.8
1	F	97	ASP	2.8
1	H	32	THR	2.8
1	G	64	CYS	2.8
1	J	55	ARG	2.8
1	H	30	GLN	2.8
1	H	194	GLN	2.8
1	H	184	LEU	2.8
1	G	170	ASP	2.8
1	C	189	THR	2.8
1	G	61	GLN	2.8
1	G	181	GLN	2.8
1	H	61	GLN	2.8
1	F	203	ALA	2.8
1	H	41	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	157	SER	2.8
1	B	58	GLY	2.8
1	G	58	GLY	2.8
1	E	52	ILE	2.7
1	E	133	LYS	2.7
1	F	56	MET	2.7
1	C	179	PRO	2.7
1	B	55	ARG	2.7
1	F	175	LEU	2.7
1	K	205	TYR	2.7
1	F	41	LYS	2.7
1	K	100	ASN	2.7
1	F	80	GLY	2.7
1	E	182	LEU	2.7
1	H	43	LEU	2.7
1	H	196	LEU	2.7
1	F	62	LYS	2.7
1	C	183	PRO	2.7
1	F	180	ARG	2.7
1	K	183	PRO	2.7
1	E	134	SER	2.7
1	B	167	LEU	2.7
1	E	178	LEU	2.7
1	G	158	PHE	2.7
1	I	41	LYS	2.7
1	E	64	CYS	2.7
1	A	180	ARG	2.7
1	C	180	ARG	2.7
1	D	179	PRO	2.7
1	F	61	GLN	2.7
1	I	200	VAL	2.7
1	H	177	LYS	2.6
1	H	205	TYR	2.6
1	J	29	CYS	2.6
1	G	179	PRO	2.6
1	J	49	PRO	2.6
1	B	34	GLU	2.6
1	B	177	LYS	2.6
1	D	188	LEU	2.6
1	F	77	GLU	2.6
1	F	59	GLY	2.6
1	I	62	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	43	LEU	2.6
1	F	182	LEU	2.6
1	G	172	LEU	2.6
1	D	195	ASP	2.6
1	G	187	ASP	2.6
1	K	180	ARG	2.6
1	B	208	CYS	2.6
1	D	167	LEU	2.6
1	I	196	LEU	2.6
1	D	196	LEU	2.6
1	E	186	VAL	2.6
1	G	25	CYS	2.6
1	J	64	CYS	2.6
1	B	185	GLU	2.6
1	F	187	ASP	2.6
1	D	177	LYS	2.5
1	G	60	GLY	2.5
1	E	31	TYR	2.5
1	F	200	VAL	2.5
1	D	77	GLU	2.5
1	D	189	THR	2.5
1	H	34	GLU	2.5
1	H	202	GLU	2.5
1	A	208	CYS	2.5
1	I	181	GLN	2.5
1	G	33	ALA	2.5
1	J	100	ASN	2.5
1	I	187	ASP	2.5
1	B	190	LYS	2.5
1	E	172	LEU	2.5
1	F	49	PRO	2.5
1	F	183	PRO	2.5
1	K	182	LEU	2.5
1	K	56	MET	2.5
1	D	201	GLU	2.5
1	B	61	GLN	2.5
1	F	165	CYS	2.5
1	K	25	CYS	2.5
1	J	169	LYS	2.5
1	J	183	PRO	2.5
1	A	186	VAL	2.5
1	H	31	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	67	GLU	2.5
1	H	28	GLN	2.5
1	E	177	LYS	2.5
1	K	175	LEU	2.5
1	E	54	SER	2.5
1	E	179	PRO	2.5
1	F	199	SER	2.5
1	J	205	TYR	2.5
1	E	173	ARG	2.5
1	E	180	ARG	2.5
1	F	75	ALA	2.5
1	H	180	ARG	2.5
1	E	127	GLY	2.4
1	I	202	GLU	2.4
1	D	191	ALA	2.4
1	E	104	TYR	2.4
1	J	41	LYS	2.4
1	K	194	GLN	2.4
1	F	69	HIS	2.4
1	G	100	ASN	2.4
1	D	60	GLY	2.4
1	D	67	GLU	2.4
1	J	133	LYS	2.4
1	K	185	GLU	2.4
1	E	28	GLN	2.4
1	F	28	GLN	2.4
1	F	45	GLN	2.4
1	J	30	GLN	2.4
1	D	206	ASN	2.4
1	H	92	ASN	2.4
1	K	176	ASN	2.4
1	K	206	ASN	2.4
1	E	25	CYS	2.4
1	F	179	PRO	2.4
1	J	170	ASP	2.4
1	A	41	LYS	2.4
1	C	55	ARG	2.4
1	F	173	ARG	2.4
1	G	156	ARG	2.4
1	E	129	SER	2.4
1	K	57	ALA	2.4
1	G	47	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	179	PRO	2.4
1	E	169	LYS	2.4
1	F	60	GLY	2.4
1	F	44	ARG	2.4
1	B	104	TYR	2.4
1	E	205	TYR	2.4
1	D	98	LEU	2.4
1	K	196	LEU	2.4
1	A	176	ASN	2.3
1	B	99	ASN	2.3
1	H	99	ASN	2.3
1	H	193	ARG	2.3
1	B	130	GLU	2.3
1	C	57	ALA	2.3
1	B	30	GLN	2.3
1	K	181	GLN	2.3
1	B	132	LEU	2.3
1	D	205	TYR	2.3
1	G	52	ILE	2.3
1	G	183	PRO	2.3
1	I	176	ASN	2.3
1	E	103	PHE	2.3
1	E	50	GLU	2.3
1	F	202	GLU	2.3
1	H	25	CYS	2.3
1	D	53	SER	2.3
1	E	43	LEU	2.3
1	I	119	SER	2.3
1	C	169	LYS	2.3
1	H	133	LYS	2.3
1	J	190	LYS	2.3
1	A	55	ARG	2.3
1	D	180	ARG	2.3
1	G	180	ARG	2.3
1	C	60	GLY	2.3
1	J	176	ASN	2.3
1	A	34	GLU	2.3
1	B	56	MET	2.3
1	A	32	THR	2.3
1	H	189	THR	2.3
1	F	51	TYR	2.3
1	E	100	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	57	ALA	2.3
1	J	62	LYS	2.3
1	F	70	ARG	2.3
1	H	157	SER	2.3
1	F	126	TYR	2.3
1	F	201	GLU	2.2
1	J	57	ALA	2.2
1	C	28	GLN	2.2
1	E	187	ASP	2.2
1	K	55	ARG	2.2
1	B	183	PRO	2.2
1	J	154	ALA	2.2
1	D	190	LYS	2.2
1	F	47	LEU	2.2
1	A	183	PRO	2.2
1	H	179	PRO	2.2
1	F	65	TYR	2.2
1	H	51	TYR	2.2
1	F	125	GLY	2.2
1	D	132	LEU	2.2
1	D	185	GLU	2.2
1	E	47	LEU	2.2
1	F	172	LEU	2.2
1	H	176	ASN	2.2
1	G	198	PRO	2.2
1	G	200	VAL	2.2
1	I	63	VAL	2.2
1	F	189	THR	2.2
1	F	78	MET	2.2
1	G	199	SER	2.2
1	J	59	GLY	2.2
1	C	102	LYS	2.2
1	D	95	PHE	2.2
1	I	191	ALA	2.2
1	F	193	ARG	2.2
1	K	37	GLN	2.2
1	D	187	ASP	2.2
1	F	208	CYS	2.2
1	A	199	SER	2.2
1	G	178	LEU	2.2
1	E	66	ILE	2.1
1	G	173	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	37	GLN	2.1
1	J	206	ASN	2.1
1	J	179	PRO	2.1
1	A	59	GLY	2.1
1	D	104	TYR	2.1
1	H	55	ARG	2.1
1	F	152	LYS	2.1
1	G	117	ASP	2.1
1	C	58	GLY	2.1
1	I	205	TYR	2.1
1	E	166	ILE	2.1
1	I	28	GLN	2.1
1	J	56	MET	2.1
1	J	47	LEU	2.1
1	K	104	TYR	2.1
1	B	133	LYS	2.1
1	E	78	MET	2.1
1	E	99	ASN	2.1
1	I	206	ASN	2.1
1	E	132	LEU	2.1
1	D	103	PHE	2.1
1	F	58	GLY	2.1
1	D	193	ARG	2.1
1	F	166	ILE	2.1
1	C	185	GLU	2.1
1	I	133	LYS	2.0
1	J	194	GLN	2.0
1	C	99	ASN	2.0
1	C	137	LEU	2.0
1	D	47	LEU	2.0
1	H	158	PHE	2.0
1	F	33	ALA	2.0
1	H	185	GLU	2.0
1	K	67	GLU	2.0
1	H	102	LYS	2.0
1	A	28	GLN	2.0
1	J	119	SER	2.0
1	F	64	CYS	2.0
1	A	188	LEU	2.0
1	I	180	ARG	2.0
1	F	148	THR	2.0
1	H	75	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.