Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2021 – 01:10 PM EDT

PDB ID	:	2ZCT
Title	:	Oxidation of archaeal peroxiredoxin involves a hypervalent sulfur intermediate
Authors	:	Nakamura, T.; Hagihara, Y.; Abe, M.; Inoue, T.; Yamamoto, T.; Matsumura, H.
Deposited on	:	2007-11-12
Resolution	:	1.70 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 (i) symbol.

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

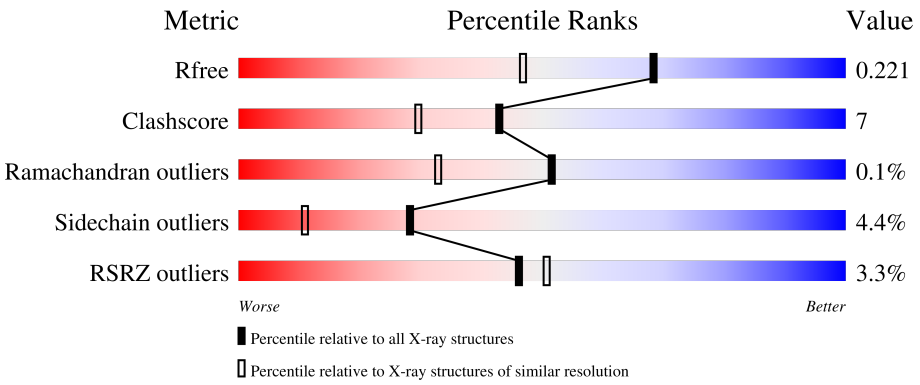
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	249	4%, 82%, 12%, • 5%
1	B	249	2%, 81%, 13%, 6%
1	C	249	4%, 81%, 11%, • 5%
1	D	249	6%, 82%, 12%, • •
1	E	249	3%, 79%, 15%, • 5%

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Mol	Chain	Length	Quality of chain
1	F	249	4% 84% 10% 5%
1	G	249	2% 79% 12% 5%
1	H	249	3% 80% 13% 6%
1	I	249	2% 84% 10% 6%
1	J	249	2% 85% 10% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSO	E	50	-	-	X	-
1	CSO	H	50	-	-	X	-
1	CSO	J	50	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20821 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 Probable peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	236	1919	1235	337	341	6	0	0	0
1	B	234	1905	1227	335	337	6	0	0	0
1	C	237	1927	1241	338	342	6	0	0	0
1	D	238	1934	1244	339	345	6	0	0	0
1	E	236	1922	1238	337	341	6	0	0	0
1	F	237	1927	1241	338	342	6	0	0	0
1	G	237	1928	1241	338	343	6	0	0	0
1	H	235	1913	1233	336	338	6	0	0	0
1	I	235	1913	1233	336	338	6	0	0	0
1	J	236	1922	1238	337	341	6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	SER	CYS	engineered mutation	UNP Q9Y9L0
B	207	SER	CYS	engineered mutation	UNP Q9Y9L0
C	207	SER	CYS	engineered mutation	UNP Q9Y9L0
D	207	SER	CYS	engineered mutation	UNP Q9Y9L0
E	207	SER	CYS	engineered mutation	UNP Q9Y9L0
F	207	SER	CYS	engineered mutation	UNP Q9Y9L0
G	207	SER	CYS	engineered mutation	UNP Q9Y9L0
H	207	SER	CYS	engineered mutation	UNP Q9Y9L0
I	207	SER	CYS	engineered mutation	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	207	SER	CYS	engineered mutation	UNP Q9Y9L0

- Molecule 2 is water.

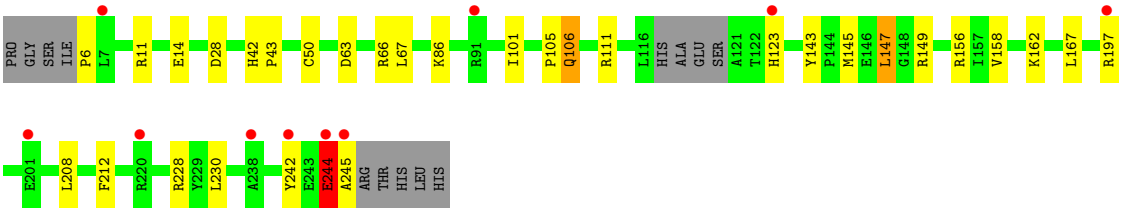
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	184	184	184	0	0
2	B	158	158	158	0	0
2	C	131	131	131	0	0
2	D	163	163	163	0	0
2	E	154	154	154	0	0
2	F	172	172	172	0	0
2	G	160	160	160	0	0
2	H	150	150	150	0	0
2	I	164	164	164	0	0
2	J	175	175	175	0	0

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.

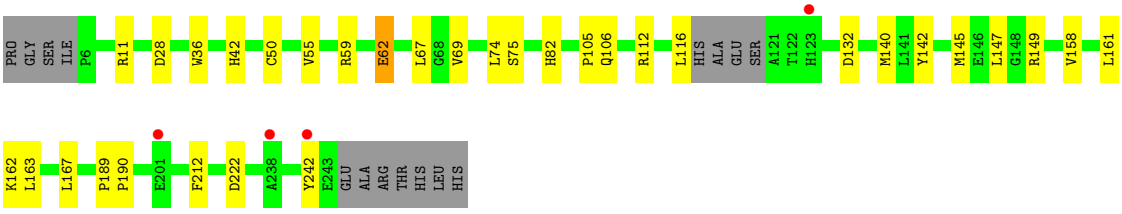
• Molecule 1: Probable peroxiredoxin

Chain A:



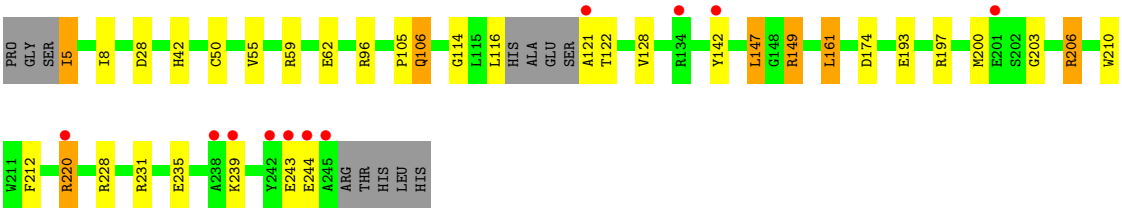
• Molecule 1: Probable peroxiredoxin

Chain B:



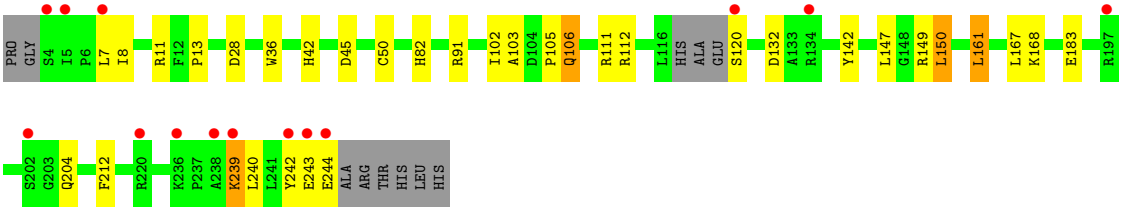
• Molecule 1: Probable peroxiredoxin

Chain C:



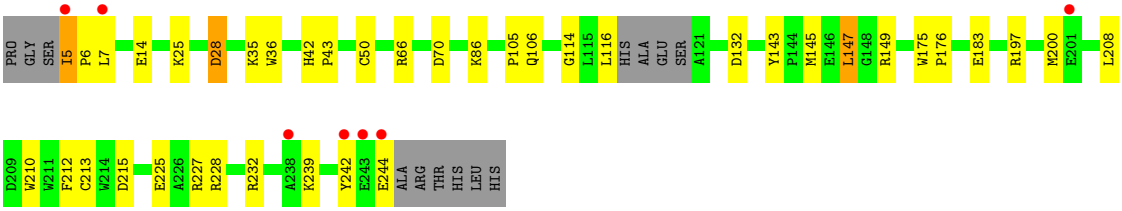
• Molecule 1: Probable peroxiredoxin

Chain D:



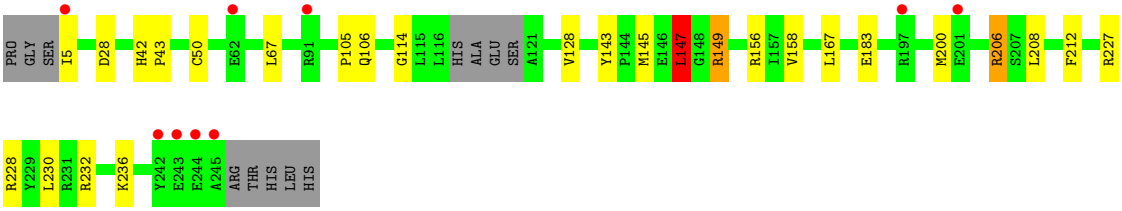
• Molecule 1: Probable peroxiredoxin

Chain E:



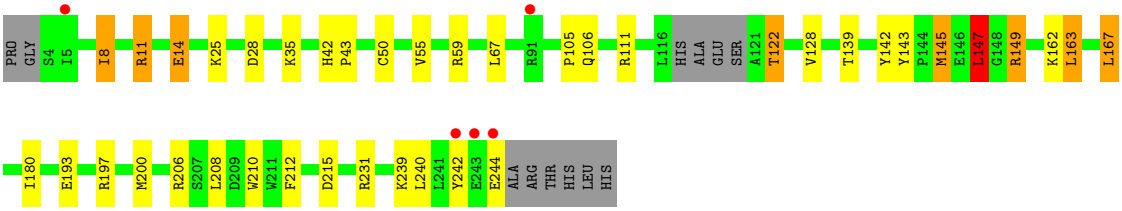
• Molecule 1: Probable peroxiredoxin

Chain F:



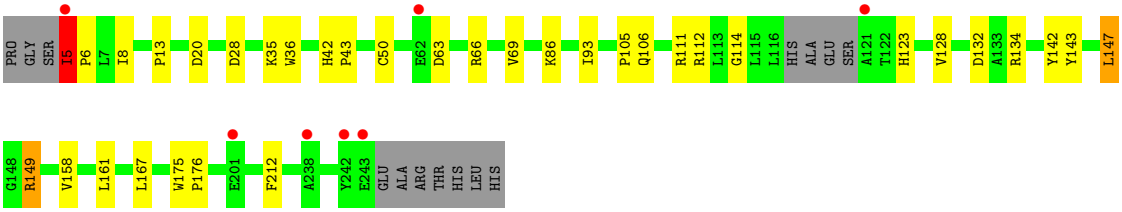
• Molecule 1: Probable peroxiredoxin

Chain G:



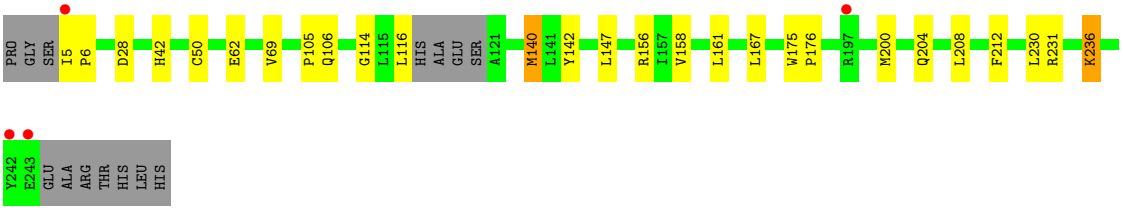
• Molecule 1: Probable peroxiredoxin

Chain H:



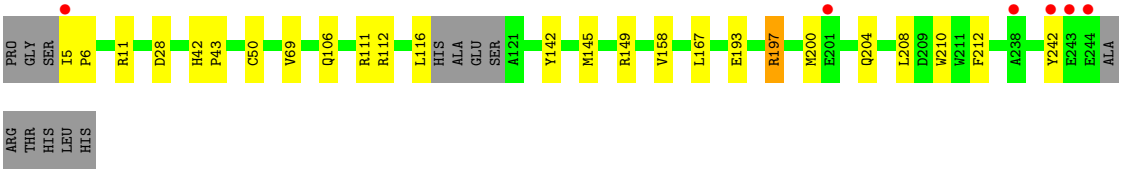
• Molecule 1: Probable peroxiredoxin

Chain I:



• Molecule 1: Probable peroxiredoxin

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.12Å 103.05Å 104.44Å 105.80° 105.30° 92.68°	Depositor
Resolution (Å)	19.96 – 1.70 19.95 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.96-1.70) 91.3 (19.95-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.190 , 0.221 0.190 , 0.221	Depositor DCC
R_{free} test set	14786 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20821	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.69	0/1963	0.72	0/2665
1	B	0.66	0/1949	0.71	0/2646
1	C	0.63	0/1971	0.74	3/2677 (0.1%)
1	D	0.66	0/1978	0.72	0/2686
1	E	0.72	0/1966	0.74	1/2670 (0.0%)
1	F	0.71	0/1971	0.83	6/2677 (0.2%)
1	G	0.71	0/1972	0.83	5/2678 (0.2%)
1	H	0.69	0/1957	0.80	4/2658 (0.2%)
1	I	0.72	0/1957	0.75	0/2658
1	J	0.73	0/1966	0.72	0/2670
All	All	0.69	0/19650	0.76	19/26685 (0.1%)

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	H	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	149	ARG	NE-CZ-NH1	14.64	127.62	120.30
1	H	149	ARG	NE-CZ-NH1	13.74	127.17	120.30
1	G	149	ARG	NE-CZ-NH1	13.72	127.16	120.30
1	F	149	ARG	NE-CZ-NH2	-12.87	113.87	120.30
1	G	149	ARG	NE-CZ-NH2	-12.17	114.21	120.30
1	H	149	ARG	NE-CZ-NH2	-11.14	114.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	149	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	C	149	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	G	147	LEU	CB-CG-CD2	5.71	120.70	111.00
1	F	147	LEU	CB-CG-CD2	5.51	120.37	111.00
1	F	227	ARG	CG-CD-NE	-5.40	100.46	111.80
1	C	161	LEU	CA-CB-CG	5.37	127.66	115.30
1	H	149	ARG	CB-CG-CD	5.36	125.53	111.60
1	G	215	ASP	CB-CG-OD1	5.32	123.09	118.30
1	G	149	ARG	CD-NE-CZ	5.29	131.00	123.60
1	F	149	ARG	CD-NE-CZ	5.27	130.98	123.60
1	H	149	ARG	CD-NE-CZ	5.21	130.90	123.60
1	E	215	ASP	CB-CG-OD1	5.10	122.89	118.30
1	F	149	ARG	CB-CG-CD	5.03	124.67	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	5	ILE	Peptide

5.2 Too-close contacts (i)

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	1919	0	1909	32	0
1	B	1905	0	1898	17	1
1	C	1927	0	1919	36	0
1	D	1934	0	1924	24	0
1	E	1922	0	1914	36	0
1	F	1927	0	1919	20	0
1	G	1928	0	1919	34	1
1	H	1913	0	1908	28	0
1	I	1913	0	1908	32	0
1	J	1922	0	1914	26	0
2	A	184	0	0	6	0
2	B	158	0	0	3	0
2	C	131	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	163	0	0	7	0
2	E	154	0	0	11	0
2	F	172	0	0	5	0
2	G	160	0	0	5	0
2	H	150	0	0	8	0
2	I	164	0	0	5	0
2	J	175	0	0	6	0
All	All	20821	0	19132	260	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (260) 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:I:42:HIS:ND1	1:I:50:CSO:SG	2.04	1.28
1:G:42:HIS:ND1	1:G:50:CSO:SG	2.08	1.26
1:J:42:HIS:ND1	1:J:50:CSO:SG	2.05	1.25
1:A:42:HIS:ND1	1:A:50:CSO:SG	2.15	1.18
1:E:42:HIS:ND1	1:E:50:CSO:SG	2.17	1.16
1:H:42:HIS:ND1	1:H:50:CSO:SG	2.22	1.12
1:C:42:HIS:ND1	1:C:50:CSO:SG	2.23	1.11
1:B:50:CSO:OD	2:B:406:HOH:O	1.71	1.08
1:A:50:CSO:OD	2:A:427:HOH:O	1.72	1.02
1:D:42:HIS:ND1	1:D:50:CSO:SG	2.34	1.00
1:B:42:HIS:ND1	1:B:50:CSO:SG	2.34	0.99
1:G:50:CSO:OD	2:G:453:HOH:O	1.74	0.98
1:E:183:GLU:OE1	2:E:394:HOH:O	1.82	0.97
1:F:42:HIS:ND1	1:F:50:CSO:SG	2.39	0.94
1:F:200:MET:HE2	1:F:200:MET:HA	1.53	0.91
1:E:105:PRO:O	1:E:106:GLN:HB2	1.71	0.90
1:C:206:ARG:HG2	1:C:206:ARG:HH11	1.38	0.88
1:E:66:ARG:HD3	2:E:374:HOH:O	1.73	0.88
1:E:14:GLU:HG2	2:E:381:HOH:O	1.74	0.87
1:E:43:PRO:HG2	1:E:145:MET:HE3	1.57	0.85
1:D:105:PRO:O	1:D:106:GLN:HB2	1.76	0.84
1:A:111:ARG:HH21	1:J:106:GLN:HE21	1.23	0.83
1:I:50:CSO:OD	2:I:571:HOH:O	1.75	0.83
1:J:50:CSO:OD	2:J:569:HOH:O	1.99	0.80
1:C:121:ALA:HA	2:C:372:HOH:O	1.81	0.79
1:A:106:GLN:HE21	1:J:111:ARG:HH21	1.26	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:208:LEU:HD11	1:J:242:TYR:CD1	2.18	0.79
1:A:228:ARG:HD3	2:A:336:HOH:O	1.84	0.78
1:I:208:LEU:HD11	1:J:242:TYR:HD1	1.49	0.77
1:I:105:PRO:O	1:I:106:GLN:HB2	1.84	0.77
1:I:5:ILE:CG2	2:J:544:HOH:O	2.34	0.76
1:H:5:ILE:HG23	1:H:6:PRO:HD2	1.69	0.74
1:D:45:ASP:OD2	1:D:82:HIS:HD2	1.69	0.74
1:G:111:ARG:NH1	2:G:441:HOH:O	2.14	0.72
1:C:206:ARG:HG2	1:C:206:ARG:NH1	2.00	0.72
1:A:106:GLN:O	1:A:111:ARG:NH2	2.23	0.71
1:B:105:PRO:O	1:B:106:GLN:HB2	1.90	0.71
1:A:105:PRO:O	1:A:106:GLN:HB2	1.89	0.71
1:A:197:ARG:HH22	1:C:96:ARG:NH2	1.89	0.70
1:I:69:VAL:HG21	1:I:158:VAL:HG11	1.74	0.70
1:D:111:ARG:HH21	1:E:106:GLN:HE21	1.39	0.70
1:E:228:ARG:NH2	2:E:365:HOH:O	2.23	0.70
1:I:5:ILE:HG22	2:J:544:HOH:O	1.92	0.69
1:J:43:PRO:HG2	1:J:145:MET:HE3	1.74	0.69
1:G:163:LEU:HD22	1:G:167:LEU:HD22	1.73	0.68
1:D:106:GLN:O	1:D:111:ARG:NH2	2.27	0.68
1:G:206:ARG:HD3	2:H:398:HOH:O	1.94	0.67
1:J:69:VAL:HG21	1:J:158:VAL:HG11	1.75	0.67
1:G:14:GLU:OE1	1:G:25:LYS:HE3	1.94	0.67
1:F:42:HIS:CE1	1:F:149:ARG:HH22	2.13	0.67
1:F:228:ARG:HD3	2:F:424:HOH:O	1.93	0.67
1:C:105:PRO:O	1:C:106:GLN:HB3	1.94	0.66
1:E:5:ILE:HG23	1:E:114:GLY:HA3	1.75	0.66
1:F:43:PRO:HG2	1:F:145:MET:HE3	1.77	0.66
1:H:105:PRO:O	1:H:106:GLN:HB2	1.94	0.66
1:C:5:ILE:HB	1:C:114:GLY:HA3	1.77	0.66
1:F:105:PRO:O	1:F:106:GLN:HB2	1.94	0.66
1:H:5:ILE:HG13	1:H:114:GLY:HA3	1.79	0.65
1:H:111:ARG:HH21	1:I:106:GLN:HE21	1.43	0.65
1:J:42:HIS:CG	1:J:50:CSO:SG	2.88	0.65
1:B:69:VAL:HG21	1:B:158:VAL:HG11	1.79	0.65
1:G:105:PRO:O	1:G:106:GLN:HB2	1.96	0.64
1:D:91:ARG:HD3	2:D:378:HOH:O	1.98	0.64
1:A:6:PRO:N	2:A:412:HOH:O	2.31	0.64
1:A:106:GLN:NE2	1:J:111:ARG:HH21	1.95	0.64
1:E:239:LYS:HD3	1:E:244:GLU:HG2	1.78	0.64
1:G:14:GLU:OE1	1:G:25:LYS:CE	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:ARG:NH1	2:H:389:HOH:O	2.28	0.63
1:G:8:ILE:HD11	1:G:139:THR:HA	1.80	0.63
1:D:105:PRO:O	1:D:106:GLN:CB	2.46	0.63
1:E:225:GLU:OE2	2:E:386:HOH:O	2.16	0.62
1:F:42:HIS:CE1	1:F:149:ARG:NH2	2.68	0.62
1:H:149:ARG:HD3	2:H:252:HOH:O	1.99	0.61
1:E:50:CSO:OD	2:E:404:HOH:O	1.72	0.61
1:A:106:GLN:HE21	1:J:111:ARG:NH2	1.96	0.60
1:D:239:LYS:HE2	1:D:244:GLU:HB3	1.83	0.60
1:A:197:ARG:NH2	1:C:96:ARG:NH2	2.50	0.60
1:B:142:TYR:HD2	2:B:368:HOH:O	1.82	0.60
1:I:5:ILE:N	1:I:6:PRO:HD2	2.17	0.60
1:A:67:LEU:O	1:A:162:LYS:NZ	2.24	0.60
1:F:67:LEU:HD13	1:F:158:VAL:HG23	1.82	0.60
1:H:123:HIS:HB2	2:H:374:HOH:O	2.00	0.60
1:A:106:GLN:CA	1:J:106:GLN:HA	2.32	0.60
1:C:105:PRO:O	1:C:106:GLN:CB	2.49	0.59
1:I:231:ARG:NH2	2:I:486:HOH:O	2.36	0.59
1:E:105:PRO:O	1:E:106:GLN:CB	2.49	0.59
1:F:200:MET:HE2	1:F:200:MET:CA	2.30	0.59
1:G:11:ARG:HD3	2:G:338:HOH:O	2.02	0.58
1:E:66:ARG:HD2	2:E:365:HOH:O	2.03	0.58
1:A:244:GLU:CB	1:A:245:ALA:HA	2.33	0.58
1:E:42:HIS:CG	1:E:50:CSO:SG	2.97	0.57
1:G:193:GLU:O	1:G:197:ARG:HG2	2.04	0.57
1:C:200:MET:HE3	1:C:210:TRP:HA	1.87	0.57
1:G:43:PRO:HG2	1:G:145:MET:CE	2.35	0.57
1:G:231:ARG:NH2	2:G:320:HOH:O	2.35	0.57
1:H:50:CSO:OD	2:H:400:HOH:O	1.93	0.57
1:E:14:GLU:OE1	1:E:25:LYS:HE2	2.05	0.57
1:H:42:HIS:CE1	1:H:149:ARG:HH22	2.23	0.57
1:I:200:MET:HA	1:I:200:MET:HE2	1.86	0.57
1:I:208:LEU:CD1	1:J:242:TYR:CD1	2.87	0.57
2:C:300:HOH:O	1:D:150:LEU:HD22	2.04	0.56
1:H:106:GLN:O	1:H:111:ARG:NH2	2.37	0.56
1:I:5:ILE:HG21	2:J:544:HOH:O	2.03	0.56
1:E:35:LYS:HD3	1:E:70:ASP:OD2	2.06	0.56
1:A:14:GLU:HG2	2:A:358:HOH:O	2.06	0.55
1:F:200:MET:HA	1:F:200:MET:CE	2.31	0.55
1:D:82:HIS:HE1	1:D:102:ILE:O	1.89	0.55
1:E:228:ARG:CZ	2:E:390:HOH:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:HIS:CE1	1:H:149:ARG:NH2	2.74	0.55
1:J:11:ARG:NH1	2:J:560:HOH:O	2.38	0.55
1:G:239:LYS:HE2	1:G:244:GLU:HG2	1.89	0.55
1:A:244:GLU:HB3	1:A:245:ALA:HA	1.89	0.54
1:C:8:ILE:HD11	1:D:142:TYR:O	2.06	0.54
1:B:105:PRO:O	1:B:106:GLN:CB	2.55	0.54
1:H:69:VAL:HG21	1:H:158:VAL:HG11	1.89	0.54
1:E:228:ARG:NE	2:E:390:HOH:O	2.40	0.54
1:C:193:GLU:OE2	1:E:86:LYS:HD3	2.06	0.54
1:G:67:LEU:O	1:G:162:LYS:HE3	2.08	0.54
1:A:43:PRO:HG2	1:A:145:MET:HE3	1.90	0.54
1:D:120:SER:O	1:E:106:GLN:OE1	2.26	0.53
1:F:206:ARG:HD3	2:F:409:HOH:O	2.07	0.53
1:C:206:ARG:HD2	2:C:378:HOH:O	2.07	0.53
1:G:142:TYR:O	1:H:8:ILE:HD11	2.08	0.53
1:H:128:VAL:HG21	1:H:149:ARG:HD2	1.89	0.53
1:A:197:ARG:HH22	1:C:96:ARG:HH22	1.56	0.53
1:F:5:ILE:HG12	1:F:114:GLY:HA3	1.91	0.53
1:H:142:TYR:HD2	2:H:397:HOH:O	1.92	0.52
1:C:42:HIS:CE1	1:C:149:ARG:HH22	2.28	0.52
1:E:232:ARG:O	2:E:330:HOH:O	2.18	0.52
1:I:200:MET:HE2	1:I:200:MET:CA	2.40	0.52
1:C:206:ARG:HH11	1:C:206:ARG:CG	2.16	0.52
1:G:240:LEU:O	1:G:244:GLU:HG3	2.09	0.52
1:C:121:ALA:CA	2:C:372:HOH:O	2.49	0.51
1:I:42:HIS:CG	1:I:50:CSO:SG	2.97	0.51
1:A:106:GLN:C	1:J:106:GLN:HA	2.30	0.51
1:A:63:ASP:OD1	1:A:66:ARG:NH1	2.42	0.51
1:F:105:PRO:O	1:F:106:GLN:CB	2.59	0.51
1:C:231:ARG:O	1:C:235:GLU:HG3	2.11	0.50
1:C:220:ARG:HA	2:C:361:HOH:O	2.11	0.50
1:D:168:LYS:HD2	2:D:394:HOH:O	2.11	0.50
1:E:143:TYR:HD2	1:E:147:LEU:HD13	1.77	0.50
1:C:142:TYR:HD2	2:C:368:HOH:O	1.94	0.49
1:G:43:PRO:HG2	1:G:145:MET:HE3	1.94	0.49
1:H:105:PRO:HA	2:H:338:HOH:O	2.12	0.49
1:I:236:LYS:HE2	2:J:516:HOH:O	2.12	0.49
1:E:5:ILE:N	1:E:6:PRO:HD2	2.28	0.49
1:C:149:ARG:HD3	2:C:251:HOH:O	2.11	0.48
1:D:11:ARG:HD3	2:D:349:HOH:O	2.12	0.48
1:A:123:HIS:HB2	2:A:371:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:SER:HB3	1:B:82:HIS:CE1	2.49	0.48
1:I:62:GLU:HG2	2:I:521:HOH:O	2.12	0.48
1:D:82:HIS:CE1	1:D:103:ALA:HA	2.49	0.48
1:G:43:PRO:HB3	1:G:122:THR:HG23	1.95	0.48
1:H:42:HIS:CG	1:H:50:CSO:SG	3.03	0.48
1:J:5:ILE:HG13	1:J:6:PRO:HD3	1.96	0.48
1:J:42:HIS:HB3	1:J:50:CSO:SG	2.54	0.48
1:G:239:LYS:CE	1:G:244:GLU:HG2	2.44	0.47
1:I:5:ILE:N	1:I:6:PRO:CD	2.77	0.47
1:C:239:LYS:HD3	1:C:243:GLU:OE1	2.14	0.47
1:G:105:PRO:O	1:G:106:GLN:CB	2.62	0.47
1:G:239:LYS:CD	1:G:244:GLU:HG2	2.44	0.47
1:E:14:GLU:CG	2:E:381:HOH:O	2.48	0.47
1:I:156:ARG:HD3	1:I:230:LEU:HD21	1.97	0.47
1:A:42:HIS:CG	1:A:50:CSO:SG	2.99	0.47
1:G:128:VAL:HG21	1:G:149:ARG:HD2	1.94	0.47
1:A:143:TYR:HD2	1:A:147:LEU:HD13	1.78	0.47
1:A:67:LEU:HD13	1:A:158:VAL:HG23	1.97	0.47
1:H:175:TRP:CG	1:H:176:PRO:HA	2.50	0.47
1:C:59:ARG:HD3	2:D:405:HOH:O	2.15	0.46
1:H:63:ASP:OD1	1:H:66:ARG:NH1	2.46	0.46
1:H:143:TYR:HD2	1:H:147:LEU:HD13	1.81	0.46
1:G:200:MET:HE3	1:G:210:TRP:HA	1.98	0.46
1:C:174:ASP:HB3	2:D:367:HOH:O	2.14	0.46
2:A:432:HOH:O	1:J:145:MET:HE1	2.16	0.46
1:J:69:VAL:CG2	1:J:158:VAL:HG11	2.43	0.46
1:C:142:TYR:O	1:D:8:ILE:HD11	2.16	0.46
1:C:55:VAL:O	1:C:59:ARG:HG3	2.16	0.45
1:I:5:ILE:HG23	1:I:114:GLY:HA3	1.98	0.45
1:E:36:TRP:CD2	1:E:132:ASP:HA	2.51	0.45
1:B:163:LEU:HD11	1:B:222:ASP:HB3	1.99	0.45
1:E:143:TYR:CD2	1:E:147:LEU:HD13	2.52	0.45
1:G:14:GLU:OE1	1:G:25:LYS:HE2	2.17	0.45
1:A:105:PRO:O	1:A:106:GLN:CB	2.57	0.45
1:C:42:HIS:CE1	1:C:149:ARG:NH2	2.84	0.45
1:I:200:MET:HE2	1:I:200:MET:N	2.31	0.45
1:G:43:PRO:O	1:G:122:THR:HG21	2.17	0.45
1:I:208:LEU:CD1	1:J:242:TYR:CE1	2.98	0.45
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.51	0.45
1:F:149:ARG:HD3	2:F:288:HOH:O	2.16	0.45
1:B:42:HIS:CE1	1:B:149:ARG:HH22	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:HIS:CG	1:C:50:CSO:SG	3.05	0.44
1:G:143:TYR:HD2	1:G:147:LEU:HD13	1.82	0.44
1:J:200:MET:HE3	1:J:210:TRP:HA	1.99	0.44
1:F:143:TYR:HD2	1:F:147:LEU:HD13	1.82	0.44
1:G:55:VAL:O	1:G:59:ARG:HG3	2.17	0.44
1:I:175:TRP:CG	1:I:176:PRO:HA	2.52	0.44
1:F:156:ARG:HD3	1:F:230:LEU:HD21	2.00	0.44
1:B:69:VAL:CG2	1:B:158:VAL:HG11	2.48	0.44
1:H:42:HIS:HB3	1:H:50:CSO:SG	2.58	0.43
1:J:106:GLN:O	1:J:111:ARG:NH2	2.51	0.43
1:D:240:LEU:O	1:D:243:GLU:HG2	2.17	0.43
1:I:105:PRO:O	1:I:106:GLN:CB	2.57	0.43
1:F:128:VAL:HG21	1:F:149:ARG:HD2	1.99	0.43
1:G:42:HIS:CE1	1:G:149:ARG:NH2	2.86	0.43
1:I:69:VAL:CG2	1:I:158:VAL:HG11	2.44	0.43
1:I:200:MET:HA	1:I:200:MET:CE	2.48	0.43
1:B:67:LEU:O	1:B:162:LYS:HE3	2.19	0.43
1:E:42:HIS:HB3	1:E:50:CSO:SG	2.58	0.43
1:C:203:GLY:HA2	2:C:364:HOH:O	2.19	0.43
1:C:128:VAL:HG21	1:C:149:ARG:HD2	2.00	0.43
1:C:147:LEU:HG	1:D:161:LEU:HD13	2.00	0.43
2:C:363:HOH:O	1:D:7:LEU:HD22	2.18	0.43
1:E:227:ARG:NH2	1:F:236:LYS:HD2	2.34	0.43
1:E:239:LYS:HD3	1:E:244:GLU:CG	2.45	0.43
1:J:193:GLU:HG2	1:J:197:ARG:NH2	2.34	0.43
1:A:106:GLN:HA	1:J:106:GLN:HA	2.00	0.43
1:B:145:MET:HB2	1:B:145:MET:HE2	1.81	0.43
1:F:232:ARG:O	2:F:311:HOH:O	2.22	0.43
1:G:149:ARG:HD3	2:G:296:HOH:O	2.18	0.43
1:A:86:LYS:HE3	1:A:101:ILE:CD1	2.49	0.43
1:F:183:GLU:HG2	2:F:337:HOH:O	2.18	0.43
2:H:338:HOH:O	1:I:105:PRO:HA	2.18	0.43
1:I:204:GLN:NE2	2:I:508:HOH:O	2.51	0.43
1:G:42:HIS:CE1	1:G:149:ARG:HH22	2.37	0.42
1:G:42:HIS:HA	1:G:43:PRO:HD3	1.90	0.42
1:H:36:TRP:CD2	1:H:132:ASP:HA	2.54	0.42
1:A:42:HIS:CE1	1:A:149:ARG:HH22	2.38	0.42
1:A:156:ARG:HD3	1:A:230:LEU:HD21	2.00	0.42
1:I:140:MET:HG3	1:J:142:TYR:CD1	2.55	0.42
1:I:105:PRO:O	2:I:562:HOH:O	2.21	0.42
1:C:5:ILE:HD13	2:D:361:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:MET:CE	1:C:210:TRP:HA	2.49	0.42
1:C:228:ARG:HD3	2:C:299:HOH:O	2.19	0.42
1:E:28:ASP:OD1	1:E:28:ASP:N	2.53	0.42
1:H:42:HIS:HA	1:H:43:PRO:HD3	1.96	0.42
1:B:55:VAL:O	1:B:59:ARG:HG3	2.19	0.42
1:D:183:GLU:HG2	2:D:275:HOH:O	2.19	0.42
1:E:7:LEU:N	1:E:7:LEU:HD12	2.35	0.42
1:H:13:PRO:HB3	1:H:112:ARG:NH2	2.34	0.42
1:D:42:HIS:CE1	1:D:149:ARG:HH22	2.38	0.42
1:E:42:HIS:CE1	1:E:149:ARG:HH22	2.38	0.42
1:G:42:HIS:CG	1:G:50:CSO:SG	3.02	0.42
1:B:163:LEU:HD21	1:B:222:ASP:OD2	2.21	0.41
1:D:36:TRP:CD2	1:D:132:ASP:HA	2.55	0.41
1:H:20:ASP:OD2	1:H:86:LYS:NZ	2.48	0.41
1:C:239:LYS:HD2	1:C:244:GLU:HG2	2.03	0.41
1:A:42:HIS:HA	1:A:43:PRO:HD3	1.92	0.41
1:G:180:ILE:HD13	1:H:93:ILE:HD13	2.02	0.41
1:J:42:HIS:CE1	1:J:149:ARG:HH22	2.38	0.40
1:B:140:MET:HE1	2:B:396:HOH:O	2.20	0.40
1:E:200:MET:HE3	1:E:213:CYS:SG	2.61	0.40
1:E:200:MET:HE3	1:E:210:TRP:HA	2.03	0.40
1:B:189:PRO:HA	1:B:190:PRO:HD3	1.98	0.40
1:C:96:ARG:NH1	2:C:333:HOH:O	2.36	0.40
2:C:375:HOH:O	1:D:242:TYR:HD1	2.03	0.40
1:D:13:PRO:HB3	1:D:112:ARG:CZ	2.52	0.40
1:E:175:TRP:CG	1:E:176:PRO:HA	2.56	0.40
1:H:175:TRP:CD1	1:H:176:PRO:HA	2.57	0.40
1:I:175:TRP:CD1	1:I:176:PRO:HA	2.56	0.40
1:A:143:TYR:CD2	1:A:147:LEU:HD13	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLU:OE1	1:G:59:ARG:NH2[1_445]	1.95	0.25

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	231/249 (93%)	223 (96%)	7 (3%)	1 (0%)	34	18
1	B	229/249 (92%)	224 (98%)	5 (2%)	0	100	100
1	C	232/249 (93%)	225 (97%)	7 (3%)	0	100	100
1	D	233/249 (94%)	226 (97%)	5 (2%)	2 (1%)	17	5
1	E	231/249 (93%)	225 (97%)	6 (3%)	0	100	100
1	F	232/249 (93%)	225 (97%)	7 (3%)	0	100	100
1	G	232/249 (93%)	225 (97%)	7 (3%)	0	100	100
1	H	230/249 (92%)	222 (96%)	8 (4%)	0	100	100
1	I	230/249 (92%)	224 (97%)	6 (3%)	0	100	100
1	J	231/249 (93%)	223 (96%)	8 (4%)	0	100	100
All	All	2311/2490 (93%)	2242 (97%)	66 (3%)	3 (0%)	51	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
1	D	239	LYS
1	D	106	GLN

5.3.2 Protein sidechains (i)

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	203/214 (95%)	194 (96%)	9 (4%)	28	11
1	B	202/214 (94%)	191 (95%)	11 (5%)	22	7
1	C	204/214 (95%)	192 (94%)	12 (6%)	19	6
1	D	206/214 (96%)	199 (97%)	7 (3%)	37	18
1	E	204/214 (95%)	196 (96%)	8 (4%)	32	13
1	F	204/214 (95%)	198 (97%)	6 (3%)	42	23
1	G	205/214 (96%)	192 (94%)	13 (6%)	18	5
1	H	203/214 (95%)	196 (97%)	7 (3%)	37	18
1	I	203/214 (95%)	194 (96%)	9 (4%)	28	11
1	J	204/214 (95%)	196 (96%)	8 (4%)	32	13
All	All	2038/2140 (95%)	1948 (96%)	90 (4%)	28	11

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	28	ASP
1	A	106	GLN
1	A	147	LEU
1	A	167	LEU
1	A	208	LEU
1	A	212	PHE
1	A	242	TYR
1	A	244	GLU
1	B	11	ARG
1	B	28	ASP
1	B	62	GLU
1	B	74	LEU
1	B	112	ARG
1	B	116	LEU
1	B	147	LEU
1	B	161	LEU
1	B	167	LEU
1	B	212	PHE
1	B	242	TYR
1	C	5	ILE
1	C	28	ASP
1	C	62	GLU
1	C	106	GLN

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Mol	Chain	Res	Type
1	C	116	LEU
1	C	122	THR
1	C	147	LEU
1	C	161	LEU
1	C	197	ARG
1	C	206	ARG
1	C	212	PHE
1	C	220	ARG
1	D	28	ASP
1	D	147	LEU
1	D	150	LEU
1	D	161	LEU
1	D	167	LEU
1	D	204	GLN
1	D	212	PHE
1	E	5	ILE
1	E	28	ASP
1	E	116	LEU
1	E	147	LEU
1	E	197	ARG
1	E	208	LEU
1	E	212	PHE
1	E	242	TYR
1	F	28	ASP
1	F	147	LEU
1	F	167	LEU
1	F	206	ARG
1	F	208	LEU
1	F	212	PHE
1	G	8	ILE
1	G	11	ARG
1	G	14	GLU
1	G	28	ASP
1	G	35	LYS
1	G	122	THR
1	G	145	MET
1	G	147	LEU
1	G	163	LEU
1	G	167	LEU
1	G	208	LEU
1	G	212	PHE
1	G	242	TYR

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Mol	Chain	Res	Type
1	H	5	ILE
1	H	28	ASP
1	H	35	LYS
1	H	147	LEU
1	H	161	LEU
1	H	167	LEU
1	H	212	PHE
1	I	28	ASP
1	I	116	LEU
1	I	140	MET
1	I	142	TYR
1	I	147	LEU
1	I	161	LEU
1	I	167	LEU
1	I	212	PHE
1	I	236	LYS
1	J	28	ASP
1	J	112	ARG
1	J	116	LEU
1	J	167	LEU
1	J	197	ARG
1	J	204	GLN
1	J	208	LEU
1	J	212	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	204	GLN
1	B	204	GLN
1	C	204	GLN
1	D	82	HIS
1	E	106	GLN
1	E	204	GLN
1	F	106	GLN
1	F	204	GLN
1	G	106	GLN
1	G	204	GLN
1	I	106	GLN
1	I	204	GLN
1	J	106	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)

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSO	E	50	1	3,6,7	0.45	0	0,6,8	-	-
1	CSO	A	50	1	3,6,7	0.62	0	0,6,8	-	-
1	CSO	C	50	1	3,6,7	0.71	0	0,6,8	-	-
1	CSO	G	50	1	3,6,7	0.54	0	0,6,8	-	-
1	CSO	F	50	1	3,6,7	0.33	0	0,6,8	-	-
1	CSO	H	50	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	I	50	1	3,6,7	0.57	0	0,6,8	-	-
1	CSO	D	50	1	3,6,7	0.42	0	0,6,8	-	-
1	CSO	J	50	1	3,6,7	0.72	0	0,6,8	-	-
1	CSO	B	50	1	3,6,7	0.66	0	0,6,8	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	E	50	1	-	0/1/5/7	-
1	CSO	A	50	1	-	0/1/5/7	-
1	CSO	C	50	1	-	0/1/5/7	-
1	CSO	G	50	1	-	0/1/5/7	-
1	CSO	F	50	1	-	0/1/5/7	-
1	CSO	H	50	1	-	0/1/5/7	-
1	CSO	I	50	1	-	0/1/5/7	-
1	CSO	D	50	1	-	0/1/5/7	-
1	CSO	J	50	1	-	0/1/5/7	-
1	CSO	B	50	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	50	CSO	4	0
1	A	50	CSO	3	0
1	C	50	CSO	2	0
1	G	50	CSO	3	0
1	F	50	CSO	1	0
1	H	50	CSO	4	0
1	I	50	CSO	3	0
1	D	50	CSO	1	0
1	J	50	CSO	4	0
1	B	50	CSO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	235/249 (94%)	-0.10	10 (4%)	35	39	16, 22, 34, 56	0
1	B	233/249 (93%)	-0.12	4 (1%)	70	74	16, 23, 35, 42	0
1	C	236/249 (94%)	0.11	11 (4%)	31	35	18, 26, 41, 59	0
1	D	237/249 (95%)	0.05	14 (5%)	22	24	16, 24, 41, 60	0
1	E	235/249 (94%)	-0.08	7 (2%)	50	54	16, 22, 35, 52	0
1	F	236/249 (94%)	-0.09	9 (3%)	40	45	15, 22, 35, 57	0
1	G	236/249 (94%)	-0.10	5 (2%)	63	67	16, 22, 36, 50	0
1	H	234/249 (93%)	-0.09	7 (2%)	50	54	16, 23, 36, 47	0
1	I	234/249 (93%)	-0.20	4 (1%)	70	74	15, 21, 34, 43	0
1	J	235/249 (94%)	-0.14	6 (2%)	56	60	14, 21, 34, 50	0
All	All	2351/2490 (94%)	-0.08	77 (3%)	46	51	14, 23, 37, 60	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	8.4
1	F	245	ALA	6.8
1	D	242	TYR	5.9
1	H	5	ILE	5.6
1	D	238	ALA	5.6
1	C	245	ALA	5.5
1	D	120	SER	5.5
1	H	242	TYR	5.3
1	B	242	TYR	4.7
1	J	242	TYR	4.5
1	C	244	GLU	4.0
1	C	238	ALA	4.0
1	G	242	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	244	GLU	3.9
1	E	242	TYR	3.9
1	E	244	GLU	3.7
1	F	5	ILE	3.6
1	D	5	ILE	3.5
1	A	244	GLU	3.3
1	J	238	ALA	3.2
1	A	242	TYR	3.2
1	J	243	GLU	3.2
1	D	243	GLU	3.2
1	C	239	LYS	3.1
1	D	239	LYS	3.1
1	E	5	ILE	3.0
1	F	242	TYR	3.0
1	B	201	GLU	3.0
1	C	242	TYR	3.0
1	E	238	ALA	2.9
1	A	7	LEU	2.9
1	A	220	ARG	2.9
1	D	4	SER	2.9
1	I	242	TYR	2.8
1	E	7	LEU	2.8
1	G	244	GLU	2.8
1	C	243	GLU	2.7
1	C	121	ALA	2.7
1	H	201	GLU	2.6
1	D	134	ARG	2.6
1	G	5	ILE	2.5
1	I	5	ILE	2.5
1	D	220	ARG	2.5
1	C	201	GLU	2.5
1	A	123	HIS	2.5
1	H	62	GLU	2.5
1	C	220	ARG	2.4
1	A	201	GLU	2.4
1	A	91	ARG	2.4
1	A	238	ALA	2.4
1	F	62	GLU	2.4
1	J	201	GLU	2.3
1	J	244	GLU	2.3
1	G	91	ARG	2.3
1	A	197	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	197	ARG	2.3
1	B	123	HIS	2.3
1	B	238	ALA	2.3
1	H	243	GLU	2.3
1	C	142	TYR	2.3
1	J	5	ILE	2.3
1	F	197	ARG	2.3
1	F	91	ARG	2.2
1	H	121	ALA	2.2
1	F	244	GLU	2.2
1	I	243	GLU	2.2
1	D	197	ARG	2.2
1	H	238	ALA	2.2
1	D	236	LYS	2.2
1	F	201	GLU	2.1
1	G	243	GLU	2.1
1	F	243	GLU	2.1
1	E	243	GLU	2.1
1	C	134	ARG	2.0
1	E	201	GLU	2.0
1	D	202	SER	2.0
1	D	7	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSO	D	50	7/8	0.93	0.09	18,18,25,32	0
1	CSO	G	50	7/8	0.93	0.09	17,18,23,23	0
1	CSO	A	50	7/8	0.94	0.09	17,17,26,28	0
1	CSO	I	50	7/8	0.94	0.08	14,15,22,24	0
1	CSO	H	50	7/8	0.95	0.08	16,17,23,27	0
1	CSO	B	50	7/8	0.95	0.07	17,18,25,25	0
1	CSO	F	50	7/8	0.96	0.09	18,19,27,30	0
1	CSO	C	50	7/8	0.96	0.06	18,20,28,33	0
1	CSO	J	50	7/8	0.96	0.07	16,16,23,25	0
1	CSO	E	50	7/8	0.97	0.06	17,18,24,27	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.