



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:06 PM GMT

PDB ID : 3A2X
Title : Peroxiredoxin (C50S) from Aeropyrum pernix K1 (acetate-bound form)
Authors : Nakamura, T.; Kado, Y.; Yamaguchi, F.; Matsumura, H.; Ishikawa, K.; Inoue, T.
Deposited on : 2009-06-04
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

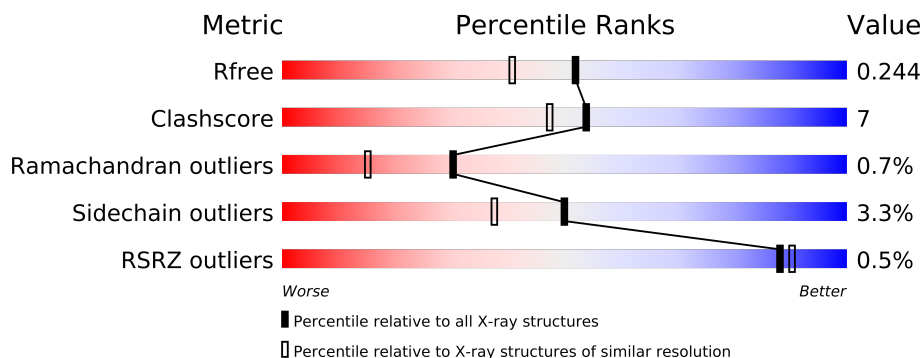
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	249	
1	B	249	
1	C	249	
1	D	249	
1	E	249	
1	F	249	
1	G	249	
1	H	249	
1	I	249	
1	J	249	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACT	H	251	-	X
2	ACT	I	251	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21180 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	243	Total 1968	C 1265	N 346	O 351	S 6	0	0	0
1	B	242	Total 1959	C 1260	N 345	O 348	S 6	0	0	0
1	C	244	Total 1973	C 1268	N 347	O 352	S 6	0	0	0
1	D	243	Total 1968	C 1265	N 346	O 351	S 6	0	0	0
1	E	243	Total 1968	C 1265	N 346	O 351	S 6	0	0	0
1	F	244	Total 1973	C 1268	N 347	O 352	S 6	0	0	0
1	G	243	Total 1968	C 1265	N 346	O 351	S 6	0	0	0
1	H	243	Total 1968	C 1265	N 346	O 351	S 6	0	0	0
1	I	243	Total 1968	C 1265	N 346	O 351	S 6	0	0	0
1	J	243	Total 1968	C 1265	N 346	O 351	S 6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

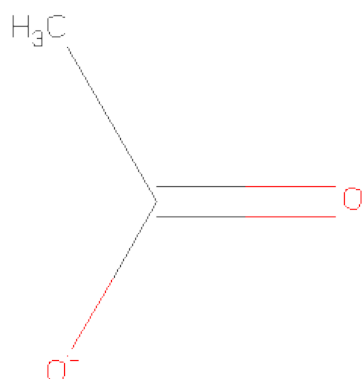
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	SER	CYS	ENGINEERED	UNP Q9Y9L0
B	50	SER	CYS	ENGINEERED	UNP Q9Y9L0
C	50	SER	CYS	ENGINEERED	UNP Q9Y9L0
D	50	SER	CYS	ENGINEERED	UNP Q9Y9L0
E	50	SER	CYS	ENGINEERED	UNP Q9Y9L0
F	50	SER	CYS	ENGINEERED	UNP Q9Y9L0
G	50	SER	CYS	ENGINEERED	UNP Q9Y9L0
H	50	SER	CYS	ENGINEERED	UNP Q9Y9L0
I	50	SER	CYS	ENGINEERED	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	50	SER	CYS	ENGINEERED	UNP Q9Y9L0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

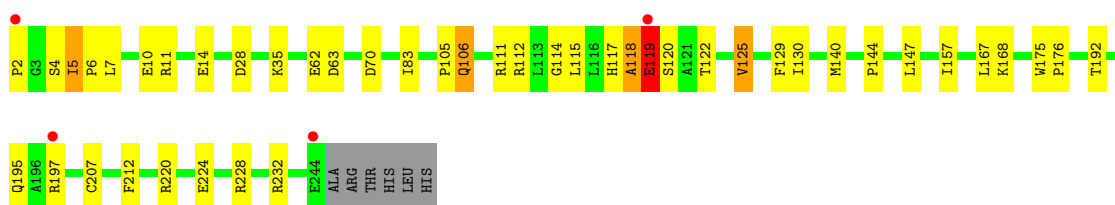
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total 145	O 145	0	0
3	B	148	Total 148	O 148	0	0
3	C	129	Total 129	O 129	0	0
3	D	147	Total 147	O 147	0	0
3	E	142	Total 142	O 142	0	0
3	F	153	Total 153	O 153	0	0
3	G	141	Total 141	O 141	0	0
3	H	147	Total 147	O 147	0	0
3	I	150	Total 150	O 150	0	0
3	J	157	Total 157	O 157	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

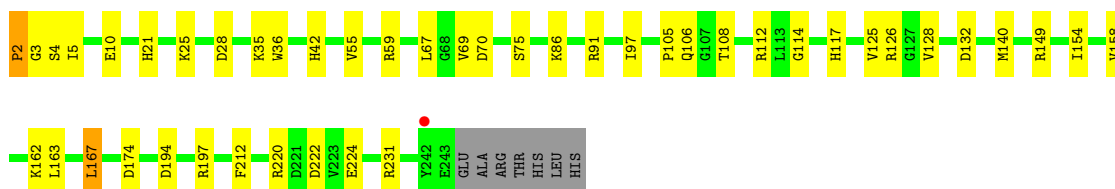
- Molecule 1: Probable peroxiredoxin

Chain A: 



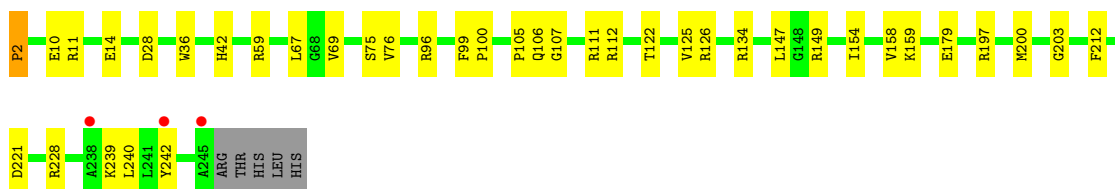
- Molecule 1: Probable peroxiredoxin

Chain B: 



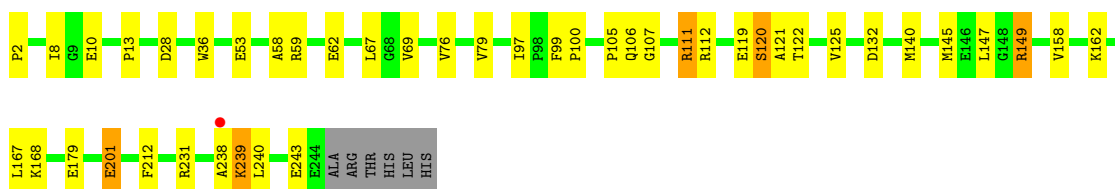
- Molecule 1: Probable peroxiredoxin

Chain C: 



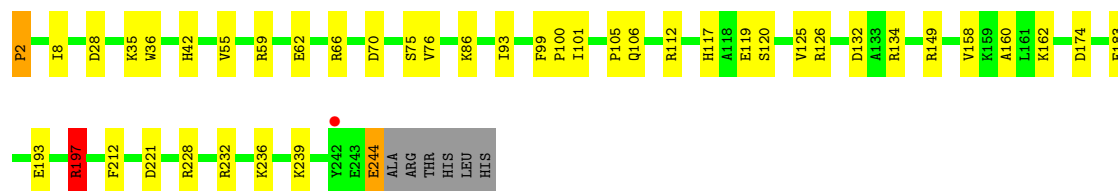
- Molecule 1: Probable peroxiredoxin

Chain D: 



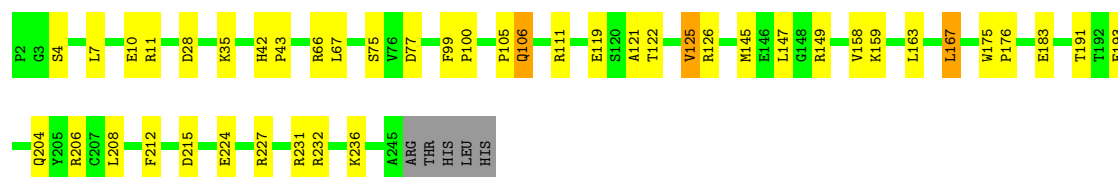
- Molecule 1: Probable peroxiredoxin

Chain E:



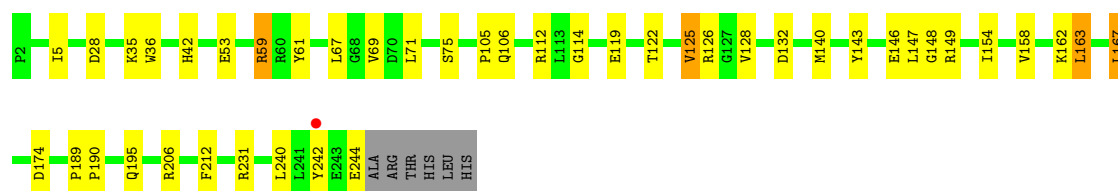
- Molecule 1: Probable peroxiredoxin

Chain F:



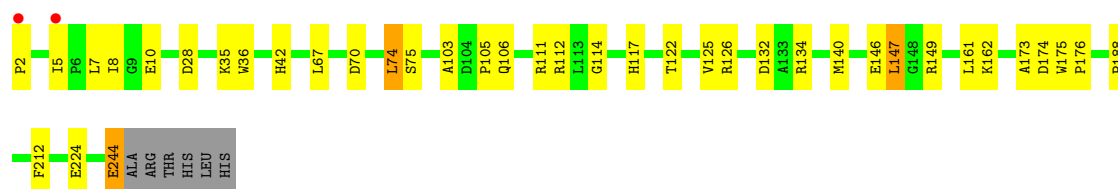
- Molecule 1: Probable peroxiredoxin

Chain G:



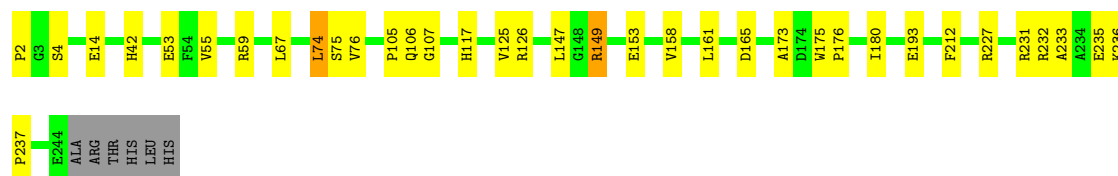
- Molecule 1: Probable peroxiredoxin

Chain H:



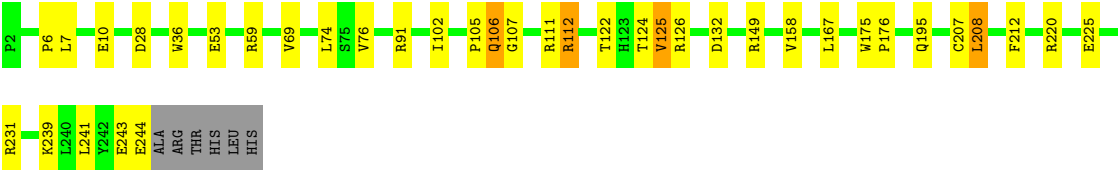
- Molecule 1: Probable peroxiredoxin

Chain I:



- Molecule 1: Probable peroxiredoxin

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.83Å 102.92Å 104.14Å 105.99° 105.12° 92.80°	Depositor
Resolution (Å)	95.78 – 1.90 72.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (95.78-1.90) 93.8 (72.58-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.243 0.196 , 0.244	Depositor DCC
R_{free} test set	10674 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 214068 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21180	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.94	1/2023 (0.0%)	0.87	0/2750
1	B	0.91	0/2014	0.84	1/2738 (0.0%)
1	C	0.86	2/2028 (0.1%)	0.83	1/2757 (0.0%)
1	D	0.88	1/2023 (0.0%)	0.94	2/2750 (0.1%)
1	E	0.91	1/2023 (0.0%)	0.93	5/2750 (0.2%)
1	F	0.91	1/2028 (0.0%)	0.89	2/2757 (0.1%)
1	G	0.89	1/2023 (0.0%)	0.85	0/2750
1	H	0.87	1/2023 (0.0%)	0.81	1/2750 (0.0%)
1	I	0.93	2/2023 (0.1%)	0.93	4/2750 (0.1%)
1	J	1.01	2/2023 (0.1%)	0.89	1/2750 (0.0%)
All	All	0.91	12/20231 (0.1%)	0.88	17/27502 (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	A	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	J	0	1
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	VAL	CB-CG1	7.78	1.69	1.52
1	C	179	GLU	CB-CG	6.51	1.64	1.52
1	C	179	GLU	CG-CD	6.44	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	224	GLU	CG-CD	5.48	1.60	1.51
1	J	225	GLU	CG-CD	5.39	1.60	1.51
1	I	233	ALA	CA-CB	5.36	1.63	1.52
1	I	153	GLU	CB-CG	5.36	1.62	1.52
1	E	160	ALA	CA-CB	5.33	1.63	1.52
1	F	125	VAL	CB-CG1	5.29	1.64	1.52
1	J	207	CYS	CB-SG	-5.14	1.73	1.81
1	G	231	ARG	CG-CD	5.08	1.64	1.51
1	D	179	GLU	CG-CD	5.03	1.59	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	149	ARG	NE-CZ-NH1	-14.01	113.29	120.30
1	D	149	ARG	NE-CZ-NH1	-13.42	113.59	120.30
1	D	149	ARG	NE-CZ-NH2	12.54	126.57	120.30
1	I	149	ARG	NE-CZ-NH2	10.93	125.77	120.30
1	E	228	ARG	NE-CZ-NH2	8.30	124.45	120.30
1	E	120	SER	N-CA-CB	-6.28	101.08	110.50
1	F	215	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	231	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	H	147	LEU	CA-CB-CG	5.59	128.15	115.30
1	I	165	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	E	221	ASP	CB-CG-OD1	5.50	123.25	118.30
1	E	197	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	J	125	VAL	N-CA-C	5.44	125.69	111.00
1	C	221	ASP	CB-CG-OD1	5.42	123.18	118.30
1	F	167	LEU	CA-CB-CG	5.32	127.53	115.30
1	E	120	SER	N-CA-C	5.25	125.17	111.00
1	I	74	LEU	CB-CG-CD1	-5.16	102.23	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	HIS	Peptide
1	A	118	ALA	Peptide
1	D	120	SER	Peptide
1	E	119	GLU	Peptide
1	F	121	ALA	Peptide
1	J	124	THR	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1968	0	1954	39	0
1	B	1959	0	1948	33	0
1	C	1973	0	1959	26	0
1	D	1968	0	1954	28	0
1	E	1968	0	1954	33	0
1	F	1973	0	1959	34	0
1	G	1968	0	1954	35	0
1	H	1968	0	1954	28	0
1	I	1968	0	1954	24	0
1	J	1968	0	1954	35	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
2	G	4	0	3	0	0
2	H	4	0	3	0	0
2	I	4	0	3	0	0
2	J	4	0	3	0	0
3	A	145	0	0	7	1
3	B	148	0	0	3	0
3	C	129	0	0	9	0
3	D	147	0	0	7	0
3	E	142	0	0	5	0
3	F	153	0	0	8	0
3	G	141	0	0	6	0
3	H	147	0	0	6	0
3	I	150	0	0	4	0
3	J	157	0	0	6	1
All	All	21180	0	19574	270	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (270) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:206:ARG:HD3	3:G:1217:HOH:O	1.39	1.21
1:E:76:VAL:HG12	3:E:1314:HOH:O	1.50	1.10
1:F:35:LYS:NZ	3:F:1142:HOH:O	1.84	1.09
1:D:53:GLU:OE2	1:D:149:ARG:HD2	1.54	1.08
1:G:125:VAL:HG12	3:G:1123:HOH:O	1.54	1.07
1:G:59:ARG:HG2	1:G:59:ARG:HH11	1.03	1.06
1:G:69:VAL:HG21	1:G:158:VAL:HG21	1.47	0.96
1:J:112:ARG:HG3	1:J:112:ARG:HH21	1.28	0.95
1:I:53:GLU:OE2	1:I:149:ARG:HD2	1.67	0.95
1:G:59:ARG:NH1	1:G:59:ARG:HG2	1.75	0.95
1:G:105:PRO:O	1:G:106:GLN:HB2	1.65	0.94
1:D:111:ARG:HD2	3:D:1153:HOH:O	1.65	0.94
1:B:222:ASP:OD2	3:B:1134:HOH:O	1.85	0.93
1:F:11:ARG:HH11	1:F:11:ARG:HG2	1.35	0.90
1:E:8:ILE:HG22	1:F:119:GLU:HG3	1.56	0.87
1:G:119:GLU:OE1	3:G:1123:HOH:O	1.92	0.87
1:G:163:LEU:HD22	1:G:167:LEU:HD22	1.57	0.87
1:J:112:ARG:CG	1:J:112:ARG:HH21	1.87	0.86
1:E:134:ARG:NH1	3:E:482:HOH:O	2.08	0.85
1:J:112:ARG:CD	3:J:1023:HOH:O	2.23	0.85
1:C:59:ARG:HD3	3:C:1172:HOH:O	1.76	0.85
1:G:59:ARG:CG	1:G:59:ARG:HH11	1.88	0.84
1:J:105:PRO:O	1:J:106:GLN:HB2	1.77	0.84
1:D:105:PRO:O	1:D:106:GLN:HB2	1.80	0.80
1:F:224:GLU:OE2	1:F:231:ARG:NH2	2.15	0.80
1:F:206:ARG:HD2	3:F:939:HOH:O	1.79	0.80
1:D:53:GLU:OE2	1:D:149:ARG:CD	2.30	0.80
1:J:69:VAL:HG21	1:J:158:VAL:HG11	1.63	0.79
1:D:240:LEU:O	1:D:243:GLU:HG3	1.86	0.76
1:A:118:ALA:H	1:A:119:GLU:HB3	1.50	0.76
1:B:106:GLN:HE22	1:C:107:GLY:HA3	1.49	0.76
1:J:105:PRO:O	1:J:106:GLN:CB	2.34	0.76
1:G:105:PRO:O	1:G:106:GLN:CB	2.28	0.75
1:I:55:VAL:O	1:I:59:ARG:HG2	1.87	0.75
1:I:53:GLU:OE2	1:I:149:ARG:CD	2.33	0.74
1:F:204:GLN:NE2	3:F:737:HOH:O	2.20	0.73
1:C:10:GLU:OE2	1:D:2:PRO:HB2	1.90	0.71
1:E:2:PRO:HB2	1:F:10:GLU:OE2	1.89	0.71
1:H:122:THR:HB	1:I:105:PRO:HG2	1.72	0.71
1:D:168:LYS:NZ	3:D:268:HOH:O	2.23	0.71
1:E:35:LYS:HD3	1:E:70:ASP:OD2	1.91	0.70
1:F:67:LEU:HD13	1:F:158:VAL:HG23	1.73	0.70
1:H:112:ARG:NE	3:H:830:HOH:O	2.24	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:111:ARG:HD3	3:F:1165:HOH:O	1.92	0.69
1:C:112:ARG:NE	3:C:1214:HOH:O	2.18	0.69
1:C:2:PRO:HB2	1:D:10:GLU:OE1	1.92	0.69
1:D:105:PRO:O	1:D:106:GLN:CB	2.42	0.68
1:B:5:ILE:HG22	1:B:114:GLY:HA3	1.76	0.68
1:H:244:GLU:OE1	3:H:1413:HOH:O	2.11	0.68
1:F:11:ARG:NH1	1:F:11:ARG:HG2	2.04	0.68
1:H:188:PRO:O	3:H:659:HOH:O	2.12	0.68
1:H:35:LYS:HD3	1:H:70:ASP:OD2	1.93	0.68
1:A:105:PRO:O	1:A:106:GLN:HB2	1.94	0.67
1:C:96:ARG:HD3	3:C:794:HOH:O	1.92	0.67
1:J:126:ARG:HB3	1:J:149:ARG:CZ	2.25	0.67
1:B:69:VAL:HG21	1:B:158:VAL:HG11	1.76	0.66
1:I:105:PRO:O	3:I:1144:HOH:O	2.14	0.66
1:G:143:TYR:HD2	1:G:147:LEU:HD12	1.61	0.66
1:C:105:PRO:O	1:C:106:GLN:HB2	1.96	0.65
1:F:204:GLN:O	3:F:826:HOH:O	2.14	0.65
1:A:118:ALA:N	1:A:119:GLU:HB3	2.10	0.65
1:E:105:PRO:O	1:E:106:GLN:HB2	1.95	0.65
1:A:10:GLU:OE2	1:B:2:PRO:HB2	1.95	0.65
1:C:126:ARG:HB3	1:C:149:ARG:CZ	2.26	0.65
1:E:239:LYS:HE3	1:E:244:GLU:HG2	1.79	0.65
1:D:62:GLU:OE2	3:D:578:HOH:O	2.14	0.64
1:A:232:ARG:O	3:A:263:HOH:O	2.15	0.64
1:E:183:GLU:OE1	1:F:236:LYS:NZ	2.29	0.63
1:H:126:ARG:HB3	1:H:149:ARG:CZ	2.27	0.63
1:E:126:ARG:HB3	1:E:149:ARG:CZ	2.28	0.63
1:A:111:ARG:HD2	3:A:1051:HOH:O	2.00	0.62
1:H:105:PRO:O	1:H:106:GLN:HB2	1.98	0.62
1:I:235:GLU:OE2	3:I:881:HOH:O	2.16	0.62
1:J:112:ARG:NE	3:J:1023:HOH:O	2.31	0.61
1:A:105:PRO:O	1:A:106:GLN:CB	2.48	0.61
1:A:224:GLU:HG2	3:A:977:HOH:O	2.00	0.60
1:E:193:GLU:O	1:E:197:ARG:CD	2.49	0.60
1:B:105:PRO:O	1:B:106:GLN:HB2	2.01	0.60
1:F:105:PRO:O	1:F:106:GLN:HB2	2.02	0.59
1:B:42:HIS:CE1	1:B:75:SER:HB3	2.37	0.59
1:D:238:ALA:O	1:D:239:LYS:HG2	2.02	0.59
1:G:126:ARG:HB3	1:G:149:ARG:CZ	2.33	0.59
1:E:55:VAL:O	1:E:59:ARG:HG2	2.03	0.59
1:F:43:PRO:HB3	1:F:145:MET:CE	2.33	0.58
1:F:105:PRO:O	1:F:106:GLN:CB	2.49	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:8:ILE:HG13	1:D:140:MET:HE2	1.85	0.58
1:E:62:GLU:OE1	1:E:66:ARG:NH1	2.37	0.58
1:E:99:PHE:HB2	1:E:100:PRO:HD2	1.85	0.58
1:C:67:LEU:HD21	1:C:159:LYS:HD3	1.86	0.57
1:D:13:PRO:HB3	1:D:112:ARG:CZ	2.33	0.57
1:E:193:GLU:O	1:E:197:ARG:HD2	2.04	0.57
1:B:194:ASP:OD2	1:B:197:ARG:NH2	2.37	0.57
1:B:91:ARG:HD2	3:B:682:HOH:O	2.04	0.56
1:C:154:ILE:O	1:C:158:VAL:HG22	2.04	0.56
1:J:112:ARG:CG	1:J:112:ARG:NH2	2.56	0.56
1:A:118:ALA:H	1:A:119:GLU:CB	2.15	0.56
1:G:36:TRP:HB2	1:G:69:VAL:HG22	1.88	0.56
1:B:106:GLN:OE1	1:C:76:VAL:HG11	2.05	0.56
1:D:79:VAL:HG11	1:F:191:THR:O	2.06	0.55
1:A:2:PRO:HB3	1:B:10:GLU:OE2	2.07	0.55
1:G:143:TYR:CD2	1:G:147:LEU:HD12	2.40	0.55
1:D:107:GLY:HA3	1:E:106:GLN:OE1	2.06	0.55
1:C:105:PRO:O	1:C:106:GLN:CB	2.54	0.55
1:C:134:ARG:NH1	3:C:548:HOH:O	2.39	0.55
1:D:120:SER:O	3:D:1085:HOH:O	2.17	0.54
1:F:119:GLU:OE1	1:F:145:MET:HG2	2.07	0.54
1:D:231:ARG:NH2	3:D:1119:HOH:O	2.40	0.54
1:A:4:SER:HA	1:B:4:SER:HA	1.90	0.54
1:J:74:LEU:HD13	1:J:102:ILE:CG2	2.37	0.53
1:E:197:ARG:HD2	1:E:197:ARG:N	2.23	0.53
1:G:67:LEU:O	1:G:162:LYS:HE3	2.08	0.53
1:B:55:VAL:O	1:B:59:ARG:HG3	2.08	0.53
1:B:106:GLN:HE21	1:C:111:ARG:HH22	1.57	0.53
1:I:236:LYS:HD3	1:I:237:PRO:HD2	1.90	0.53
1:G:154:ILE:O	1:G:158:VAL:HG12	2.09	0.52
1:A:11:ARG:NE	3:A:751:HOH:O	2.13	0.52
1:J:69:VAL:CG2	1:J:158:VAL:HG11	2.36	0.52
1:C:42:HIS:CE1	1:C:75:SER:HB3	2.45	0.52
1:F:67:LEU:HD13	1:F:158:VAL:CG2	2.40	0.52
1:E:174:ASP:HB3	3:F:721:HOH:O	2.08	0.52
1:E:66:ARG:CD	3:E:965:HOH:O	2.58	0.51
1:G:140:MET:CE	1:H:117:HIS:HE1	2.23	0.51
1:J:112:ARG:NH2	1:J:112:ARG:HG3	2.10	0.51
1:A:111:ARG:NE	3:A:1208:HOH:O	2.36	0.51
1:H:106:GLN:OE1	1:I:107:GLY:HA3	2.09	0.51
1:D:99:PHE:HB2	1:D:100:PRO:HD2	1.92	0.51
1:A:192:THR:OG1	1:A:195:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:193:GLU:O	1:E:197:ARG:HD3	2.11	0.51
1:J:112:ARG:HD2	3:J:1023:HOH:O	2.02	0.51
1:D:36:TRP:CD2	1:D:132:ASP:HA	2.46	0.51
1:I:126:ARG:HB3	1:I:149:ARG:CZ	2.41	0.51
1:D:122:THR:HB	1:E:105:PRO:HG2	1.92	0.50
1:F:122:THR:HB	1:G:105:PRO:HG2	1.94	0.50
1:E:93:ILE:HD11	1:F:208:LEU:HD23	1.94	0.50
1:A:118:ALA:N	1:A:119:GLU:CB	2.74	0.49
1:A:106:GLN:NE2	1:J:76:VAL:HG11	2.27	0.49
1:A:140:MET:HE1	1:B:117:HIS:HE1	1.76	0.49
1:H:106:GLN:NE2	1:I:76:VAL:HG11	2.27	0.49
1:I:232:ARG:O	3:I:281:HOH:O	2.19	0.49
1:A:130:ILE:HD13	1:A:157:ILE:HG21	1.94	0.49
1:B:35:LYS:HD3	1:B:70:ASP:OD2	2.13	0.49
1:F:176:PRO:HG2	1:F:227:ARG:HG2	1.94	0.49
1:A:83:ILE:HG12	1:I:193:GLU:HG2	1.95	0.49
1:A:5:ILE:HG12	1:B:5:ILE:HG12	1.95	0.49
1:J:74:LEU:HD13	1:J:102:ILE:HG21	1.95	0.48
1:A:140:MET:HE1	1:B:117:HIS:CE1	2.48	0.48
1:I:175:TRP:CG	1:I:176:PRO:HA	2.48	0.48
1:D:112:ARG:NE	3:D:920:HOH:O	2.28	0.48
1:E:232:ARG:O	3:E:525:HOH:O	2.20	0.48
1:A:106:GLN:HE21	1:J:76:VAL:HG11	1.77	0.48
1:B:105:PRO:O	1:B:106:GLN:CB	2.61	0.48
1:C:228:ARG:HG3	3:C:628:HOH:O	2.14	0.48
1:A:119:GLU:HA	1:A:119:GLU:OE2	2.12	0.48
1:A:14:GLU:HG2	3:A:751:HOH:O	2.13	0.48
1:J:36:TRP:CD2	1:J:132:ASP:HA	2.49	0.48
1:H:42:HIS:CE1	1:H:75:SER:HB3	2.48	0.48
1:I:173:ALA:HB2	1:J:53:GLU:HG2	1.96	0.48
1:C:59:ARG:CD	3:C:1172:HOH:O	2.50	0.47
1:F:105:PRO:HG2	1:G:122:THR:HB	1.95	0.47
1:H:105:PRO:O	1:H:106:GLN:CB	2.62	0.47
1:H:2:PRO:N	3:H:1373:HOH:O	2.47	0.47
1:A:5:ILE:HG22	1:A:114:GLY:HA3	1.96	0.47
1:E:36:TRP:CD2	1:E:132:ASP:HA	2.50	0.47
1:I:117:HIS:HA	1:J:7:LEU:HD13	1.97	0.47
1:B:67:LEU:O	1:B:162:LYS:HE3	2.14	0.47
1:B:21:HIS:HB3	3:B:601:HOH:O	2.15	0.47
1:D:36:TRP:HB2	1:D:69:VAL:HG22	1.97	0.47
1:G:174:ASP:HB3	3:G:783:HOH:O	2.14	0.47
1:H:175:TRP:CG	1:H:176:PRO:HA	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:99:PHE:HB2	1:C:100:PRO:HD2	1.96	0.46
1:J:195:GLN:OE1	3:J:1427:HOH:O	2.21	0.46
1:B:220:ARG:O	1:B:224:GLU:HG3	2.15	0.46
1:I:2:PRO:N	1:J:10:GLU:OE2	2.49	0.46
1:J:107:GLY:O	1:J:111:ARG:HG3	2.15	0.46
1:C:59:ARG:NH1	3:C:1172:HOH:O	2.46	0.46
1:D:76:VAL:HG11	1:E:106:GLN:NE2	2.31	0.46
1:E:105:PRO:O	1:E:106:GLN:CB	2.62	0.46
1:G:42:HIS:CE1	1:G:75:SER:HB3	2.51	0.46
1:H:7:LEU:O	1:H:10:GLU:HB2	2.15	0.46
1:F:42:HIS:CE1	1:F:75:SER:HB3	2.51	0.46
1:A:63:ASP:OD2	1:A:228:ARG:NH2	2.49	0.46
1:J:91:ARG:NH2	3:J:280:HOH:O	2.48	0.46
1:F:126:ARG:HB3	1:F:149:ARG:CZ	2.46	0.46
1:H:74:LEU:C	1:H:74:LEU:HD13	2.36	0.46
1:G:240:LEU:HD12	1:G:242:TYR:HE2	1.81	0.46
1:I:105:PRO:O	1:I:106:GLN:HB2	2.16	0.46
1:E:66:ARG:HD3	3:E:965:HOH:O	2.17	0.45
1:C:203:GLY:HA2	3:C:1076:HOH:O	2.16	0.45
1:G:5:ILE:HG22	1:G:114:GLY:HA3	1.98	0.45
1:A:175:TRP:CG	1:A:176:PRO:HA	2.51	0.45
1:F:232:ARG:O	3:F:272:HOH:O	2.21	0.45
1:I:42:HIS:CE1	1:I:75:SER:HB3	2.52	0.45
1:J:239:LYS:HE2	1:J:243:GLU:HB2	1.98	0.45
1:G:163:LEU:HD22	1:G:167:LEU:CD2	2.39	0.45
1:J:243:GLU:O	1:J:244:GLU:HB2	2.17	0.45
1:G:146:GLU:HG3	3:H:1008:HOH:O	2.16	0.45
1:H:134:ARG:NH1	3:H:1181:HOH:O	2.49	0.45
1:F:43:PRO:HB3	1:F:145:MET:HE1	1.99	0.44
1:H:106:GLN:O	1:H:111:ARG:NH2	2.50	0.44
1:H:67:LEU:O	1:H:162:LYS:HE3	2.17	0.44
1:H:5:ILE:HG22	1:H:114:GLY:HA3	1.98	0.44
1:I:227:ARG:HD2	3:I:378:HOH:O	2.18	0.44
1:G:143:TYR:HD2	1:G:147:LEU:CD1	2.30	0.44
1:D:201:GLU:HG2	3:D:1368:HOH:O	2.17	0.44
1:H:36:TRP:CD2	1:H:132:ASP:HA	2.53	0.44
1:C:36:TRP:HB2	1:C:69:VAL:HG22	2.00	0.44
1:J:175:TRP:CG	1:J:176:PRO:HA	2.53	0.44
1:A:220:ARG:NH1	1:A:224:GLU:OE2	2.51	0.44
1:A:144:PRO:HD2	1:A:147:LEU:HB3	2.00	0.44
1:A:105:PRO:HG2	1:J:122:THR:HB	2.00	0.43
1:G:140:MET:HE1	1:H:117:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:128:VAL:O	1:B:140:MET:HA	2.18	0.43
1:E:2:PRO:CB	1:F:10:GLU:OE2	2.64	0.43
1:A:7:LEU:HD21	1:B:3:GLY:HA3	2.00	0.43
3:A:707:HOH:O	1:B:174:ASP:HB3	2.17	0.43
1:J:231:ARG:HD2	1:J:231:ARG:HH11	1.67	0.43
3:G:821:HOH:O	1:H:174:ASP:HB3	2.18	0.43
1:D:162:LYS:HE3	1:D:162:LYS:HB3	1.80	0.43
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.53	0.43
1:F:67:LEU:HD21	1:F:159:LYS:HD3	2.00	0.43
1:B:154:ILE:O	1:B:158:VAL:HG23	2.18	0.43
1:E:86:LYS:HE3	1:E:101:ILE:CD1	2.48	0.43
1:A:5:ILE:HD12	1:A:6:PRO:O	2.18	0.43
1:J:59:ARG:NH2	1:J:59:ARG:HG2	2.33	0.43
1:B:163:LEU:HD22	1:B:167:LEU:HD22	2.00	0.43
1:E:42:HIS:CE1	1:E:75:SER:HB3	2.53	0.43
1:G:128:VAL:O	1:G:140:MET:HA	2.19	0.43
1:J:7:LEU:O	1:J:10:GLU:HB2	2.19	0.43
1:E:117:HIS:HA	1:F:7:LEU:HD13	2.00	0.42
1:A:122:THR:HA	1:J:106:GLN:HG3	1.99	0.42
1:A:4:SER:HB2	1:B:3:GLY:O	2.20	0.42
1:F:175:TRP:CG	1:F:176:PRO:HA	2.55	0.42
1:B:105:PRO:HG2	1:C:122:THR:HB	2.01	0.42
1:D:119:GLU:OE1	1:D:145:MET:HG2	2.20	0.42
1:H:103:ALA:C	1:H:105:PRO:HD3	2.40	0.42
1:B:126:ARG:HB3	1:B:149:ARG:CZ	2.50	0.42
1:C:240:LEU:HD12	1:C:242:TYR:HE2	1.84	0.42
1:J:220:ARG:NE	3:J:1132:HOH:O	2.36	0.41
1:G:61:TYR:HD1	1:G:71:LEU:HD12	1.85	0.41
1:A:115:LEU:HD21	1:A:129:PHE:HE1	1.85	0.41
1:D:58:ALA:HB2	1:D:97:ILE:HD12	2.02	0.41
1:A:197:ARG:HH12	1:C:96:ARG:HH21	1.67	0.41
1:I:175:TRP:CD1	1:I:176:PRO:HA	2.56	0.41
1:A:35:LYS:HG3	1:A:70:ASP:OD2	2.21	0.41
1:G:53:GLU:HG2	1:H:173:ALA:HB2	2.03	0.41
1:J:59:ARG:HH21	1:J:59:ARG:HG2	1.86	0.41
1:I:180:ILE:HA	1:J:241:LEU:HB2	2.03	0.41
1:F:183:GLU:HG2	1:F:183:GLU:H	1.67	0.41
1:I:105:PRO:O	1:I:106:GLN:CB	2.68	0.41
1:G:147:LEU:HD13	1:G:148:GLY:O	2.20	0.41
1:E:197:ARG:HD2	1:E:197:ARG:H	1.85	0.41
1:G:140:MET:HE1	1:H:117:HIS:HE1	1.85	0.41
1:B:86:LYS:HG2	1:B:97:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:8:ILE:HG13	1:H:140:MET:HE2	2.02	0.41
1:F:77:ASP:OD2	3:F:1328:HOH:O	2.22	0.41
1:I:74:LEU:C	1:I:74:LEU:HD23	2.42	0.41
1:D:67:LEU:HD13	1:D:158:VAL:HG23	2.02	0.41
1:F:99:PHE:HB2	1:F:100:PRO:HD2	2.03	0.40
1:G:189:PRO:HA	1:G:190:PRO:HD3	1.89	0.40
1:I:67:LEU:HD13	1:I:158:VAL:HG23	2.03	0.40
3:G:447:HOH:O	1:H:146:GLU:HG3	2.21	0.40
1:E:93:ILE:HD11	1:F:208:LEU:CD2	2.51	0.40
1:C:203:GLY:N	3:C:1076:HOH:O	2.50	0.40
1:C:11:ARG:NH1	1:C:14:GLU:OE1	2.55	0.40
1:E:158:VAL:O	1:E:162:LYS:HG3	2.20	0.40
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.56	0.40
1:J:208:LEU:CD2	1:J:208:LEU:N	2.85	0.40
1:G:190:PRO:HB3	1:G:195:GLN:HG2	2.03	0.40
1:A:112:ARG:HD2	1:A:112:ARG:HA	1.89	0.40
1:A:140:MET:CE	1:B:117:HIS:HE1	2.34	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	Distance(Å)	Clash(Å)
3:A:1031:HOH:O	3:J:1020:HOH:O[1_455]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	241/249 (97%)	232 (96%)	5 (2%)	4 (2%)	14 3
1	B	240/249 (96%)	236 (98%)	3 (1%)	1 (0%)	43 29
1	C	242/249 (97%)	235 (97%)	6 (2%)	1 (0%)	43 29
1	D	241/249 (97%)	229 (95%)	9 (4%)	3 (1%)	19 6
1	E	241/249 (97%)	235 (98%)	5 (2%)	1 (0%)	43 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	242/249 (97%)	234 (97%)	6 (2%)	2 (1%)	27	12
1	G	241/249 (97%)	235 (98%)	5 (2%)	1 (0%)	43	29
1	H	241/249 (97%)	233 (97%)	7 (3%)	1 (0%)	43	29
1	I	241/249 (97%)	234 (97%)	6 (2%)	1 (0%)	43	29
1	J	241/249 (97%)	233 (97%)	6 (2%)	2 (1%)	27	12
All	All	2411/2490 (97%)	2336 (97%)	58 (2%)	17 (1%)	30	15

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	D	121	ALA
1	J	125	VAL
1	D	239	LYS
1	A	120	SER
1	D	125	VAL
1	F	106	GLN
1	F	125	VAL
1	J	106	GLN
1	A	106	GLN
1	A	125	VAL
1	E	125	VAL
1	G	125	VAL
1	I	125	VAL
1	C	125	VAL
1	H	125	VAL
1	B	125	VAL

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	210/215 (98%)	202 (96%)	8 (4%)	44	31
1	B	209/215 (97%)	202 (97%)	7 (3%)	50	37
1	C	210/215 (98%)	203 (97%)	7 (3%)	50	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	210/215 (98%)	203 (97%)	7 (3%)	50	37
1	E	210/215 (98%)	203 (97%)	7 (3%)	50	37
1	F	210/215 (98%)	202 (96%)	8 (4%)	44	31
1	G	210/215 (98%)	202 (96%)	8 (4%)	44	31
1	H	210/215 (98%)	204 (97%)	6 (3%)	55	44
1	I	210/215 (98%)	204 (97%)	6 (3%)	55	44
1	J	210/215 (98%)	204 (97%)	6 (3%)	55	44
All	All	2099/2150 (98%)	2029 (97%)	70 (3%)	50	37

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	28	ASP
1	A	62	GLU
1	A	119	GLU
1	A	167	LEU
1	A	168	LYS
1	A	207	CYS
1	A	212	PHE
1	B	2	PRO
1	B	25	LYS
1	B	28	ASP
1	B	108	THR
1	B	112	ARG
1	B	167	LEU
1	B	212	PHE
1	C	2	PRO
1	C	28	ASP
1	C	147	LEU
1	C	197	ARG
1	C	200	MET
1	C	212	PHE
1	C	239	LYS
1	D	28	ASP
1	D	59	ARG
1	D	111	ARG
1	D	147	LEU
1	D	167	LEU
1	D	201	GLU

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Mol	Chain	Res	Type
1	D	212	PHE
1	E	2	PRO
1	E	28	ASP
1	E	112	ARG
1	E	197	ARG
1	E	212	PHE
1	E	236	LYS
1	E	244	GLU
1	F	4	SER
1	F	28	ASP
1	F	66	ARG
1	F	147	LEU
1	F	163	LEU
1	F	167	LEU
1	F	193	GLU
1	F	212	PHE
1	G	28	ASP
1	G	35	LYS
1	G	59	ARG
1	G	112	ARG
1	G	163	LEU
1	G	167	LEU
1	G	212	PHE
1	G	244	GLU
1	H	28	ASP
1	H	74	LEU
1	H	147	LEU
1	H	161	LEU
1	H	212	PHE
1	H	244	GLU
1	I	4	SER
1	I	14	GLU
1	I	147	LEU
1	I	161	LEU
1	I	212	PHE
1	I	231	ARG
1	J	6	PRO
1	J	28	ASP
1	J	112	ARG
1	J	167	LEU
1	J	208	LEU
1	J	212	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	B	106	GLN
1	B	123	HIS
1	B	204	GLN
1	D	204	GLN
1	E	92	HIS
1	F	92	HIS
1	F	123	HIS
1	F	204	GLN
1	G	204	GLN
1	H	204	GLN
1	I	204	GLN
1	J	204	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	1	-	1,3,3	1.04	0	0,3,3	0.00	-
2	ACT	B	251	-	1,3,3	1.58	0	0,3,3	0.00	-
2	ACT	C	251	-	1,3,3	0.34	0	0,3,3	0.00	-
2	ACT	D	251	-	1,3,3	1.78	0	0,3,3	0.00	-
2	ACT	E	251	-	1,3,3	0.38	0	0,3,3	0.00	-
2	ACT	F	251	-	1,3,3	1.66	0	0,3,3	0.00	-
2	ACT	G	251	-	1,3,3	0.70	0	0,3,3	0.00	-
2	ACT	H	251	-	1,3,3	0.55	0	0,3,3	0.00	-
2	ACT	I	251	-	1,3,3	1.90	0	0,3,3	0.00	-
2	ACT	J	251	-	1,3,3	1.72	0	0,3,3	0.00	-

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
2	ACT	A	1	-	-	0/0/0/0	0/0/0/0
2	ACT	B	251	-	-	0/0/0/0	0/0/0/0
2	ACT	C	251	-	-	0/0/0/0	0/0/0/0
2	ACT	D	251	-	-	0/0/0/0	0/0/0/0
2	ACT	E	251	-	-	0/0/0/0	0/0/0/0
2	ACT	F	251	-	-	0/0/0/0	0/0/0/0
2	ACT	G	251	-	-	0/0/0/0	0/0/0/0
2	ACT	H	251	-	-	0/0/0/0	0/0/0/0
2	ACT	I	251	-	-	0/0/0/0	0/0/0/0
2	ACT	J	251	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	243/249 (97%)	-0.05	4 (1%) 68 70	16, 23, 38, 57	0
1	B	242/249 (97%)	-0.06	1 (0%) 90 91	16, 25, 37, 50	0
1	C	244/249 (97%)	-0.01	3 (1%) 75 78	18, 27, 43, 61	0
1	D	243/249 (97%)	-0.11	1 (0%) 90 91	17, 26, 42, 58	0
1	E	243/249 (97%)	-0.01	1 (0%) 90 91	15, 24, 38, 53	0
1	F	244/249 (97%)	-0.02	0 100 100	16, 24, 37, 53	0
1	G	243/249 (97%)	-0.12	1 (0%) 90 91	17, 24, 40, 51	0
1	H	243/249 (97%)	-0.13	2 (0%) 83 85	17, 25, 39, 51	0
1	I	243/249 (97%)	-0.16	0 100 100	14, 23, 38, 54	0
1	J	243/249 (97%)	-0.00	0 100 100	14, 23, 37, 49	0
All	All	2431/2490 (97%)	-0.07	13 (0%) 88 90	14, 24, 40, 61	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	238	ALA	4.2
1	C	242	TYR	2.9
1	B	242	TYR	2.8
1	A	119	GLU	2.7
1	C	245	ALA	2.6
1	A	2	PRO	2.5
1	C	238	ALA	2.5
1	G	242	TYR	2.5
1	H	5	ILE	2.4
1	H	2	PRO	2.3
1	A	244	GLU	2.3
1	E	242	TYR	2.1
1	A	197	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ACT	I	251	4/4	0.13	6.85	22,23,24,24	0
2	ACT	H	251	4/4	0.12	2.06	20,22,22,23	0
2	ACT	A	1	4/4	0.12	1.41	25,27,27,27	0
2	ACT	B	251	4/4	0.10	0.54	21,22,23,24	0
2	ACT	F	251	4/4	0.10	0.27	22,24,24,25	0
2	ACT	G	251	4/4	0.08	0.00	20,21,21,22	0
2	ACT	C	251	4/4	0.08	-0.11	22,23,24,24	0
2	ACT	J	251	4/4	0.09	-0.23	20,21,22,22	0
2	ACT	E	251	4/4	0.10	-0.45	23,23,24,25	0
2	ACT	D	251	4/4	0.08	-0.61	23,23,24,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.