Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:16 AM GMT

PDB ID	:	3A2V
Title	:	Peroxiredoxin (C207S) from Aeropyrum pernix K1 complexed with hydrogen peroxide
Authors	:	Nakamura, T.; Kado, Y.; Yamaguchi, F.; Ishikawa, K.; Matsumura, H.; Inoue, T.
Deposited on	:	2009-06-04
Resolution	:	1.65 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

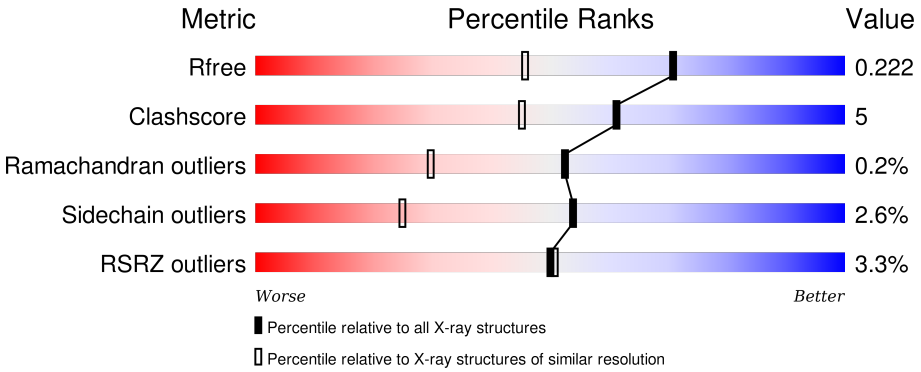
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.65 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}	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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. 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	80% 17%
1	B	249	4% 88% 9%
1	C	249	5% 80% 16%
1	D	249	3% 85% 10%
1	E	249	2% 87% 10%

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Mol	Chain	Length	Quality of chain
1	F	249	3% 86% 12%
1	G	249	4% 86% 10%
1	H	249	4% 87% 9%
1	I	249	3% 88% 9%
1	J	249	3% 80% 16%

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
2	PER	J	251	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20999 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
1	A	243	Total	C	N	O	S	0	15	0
			2050	1334	350	359	7			
1	B	242	Total	C	N	O	S	0	6	0
			1993	1287	348	352	6			
1	C	243	Total	C	N	O	S	0	11	0
			2038	1318	358	354	8			
1	D	240	Total	C	N	O	S	0	7	0
			1978	1276	349	346	7			
1	E	242	Total	C	N	O	S	0	5	0
			1990	1281	352	351	6			
1	F	244	Total	C	N	O	S	0	7	0
			2014	1302	348	357	7			
1	G	243	Total	C	N	O	S	0	5	0
			1998	1288	350	353	7			
1	H	242	Total	C	N	O	S	0	5	0
			1996	1292	349	349	6			
1	I	242	Total	C	N	O	S	0	5	0
			1993	1286	352	349	6			
1	J	243	Total	C	N	O	S	0	6	0
			2019	1300	353	358	8			

There are 10 discrepancies between the modelled and reference sequences:

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

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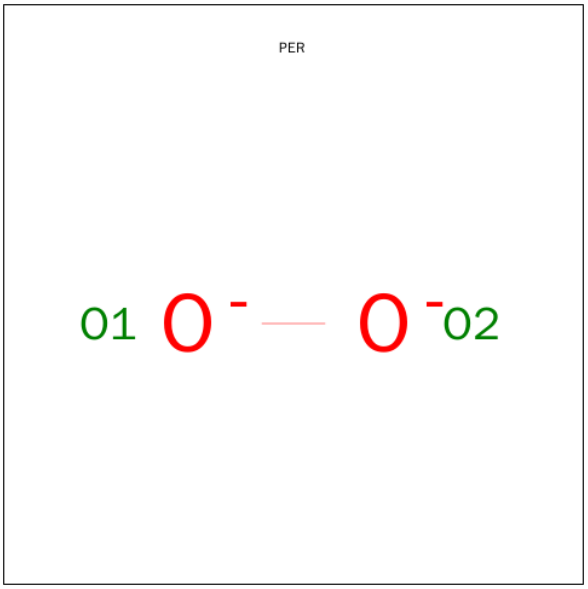
Chain	Residue	Modelled	Actual	Comment	Reference
J	207	SER	CYS	ENGINEERED	UNP Q9Y9L0

- Molecule 2 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



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

- Molecule 3 is water.

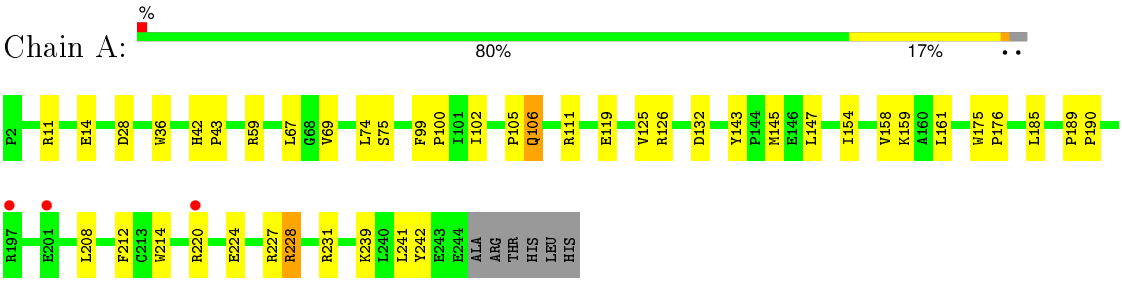
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	106	Total O 106 106	0	0
3	B	79	Total O 79 79	0	0
3	C	77	Total O 77 77	0	0
3	D	88	Total O 88 88	0	0
3	E	79	Total O 79 79	0	0
3	F	76	Total O 76 76	0	0
3	G	93	Total O 93 93	0	0
3	H	85	Total O 85 85	0	0
3	I	124	Total O 124 124	0	0
3	J	103	Total O 103 103	0	0

3 Residue-property plots (i)

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.

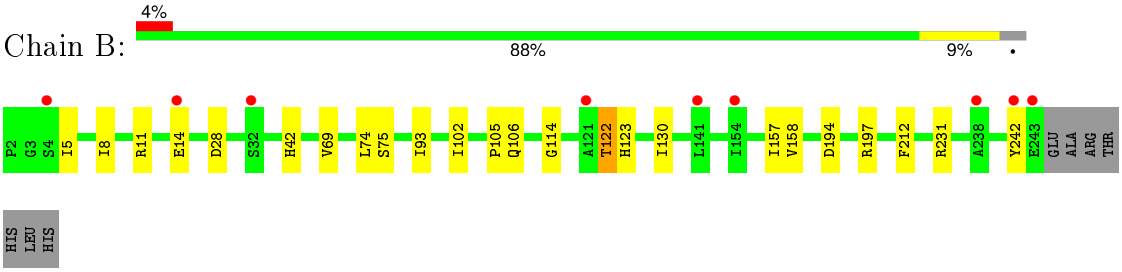
- Molecule 1: Probable peroxiredoxin

Chain A:



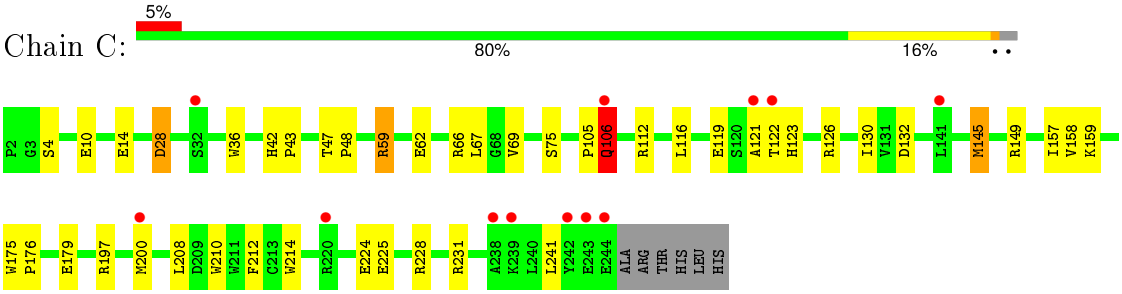
- Molecule 1: Probable peroxiredoxin

Chain B:



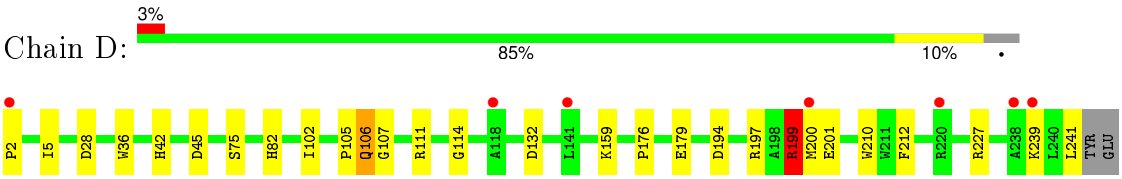
- Molecule 1: Probable peroxiredoxin

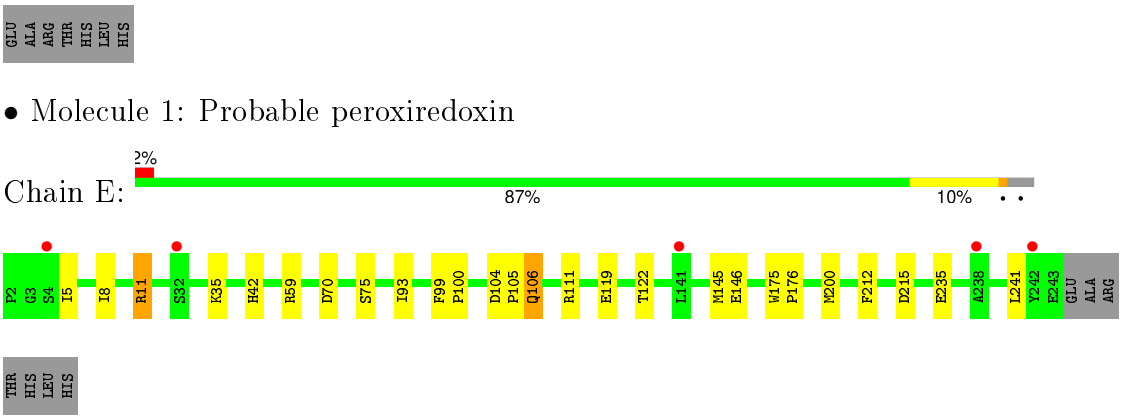
Chain C:

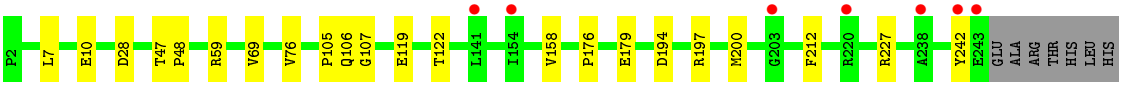


- Molecule 1: Probable peroxiredoxin

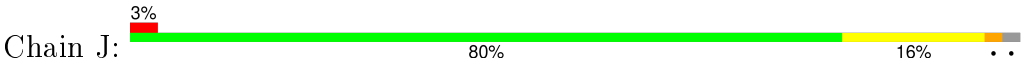
Chain D:

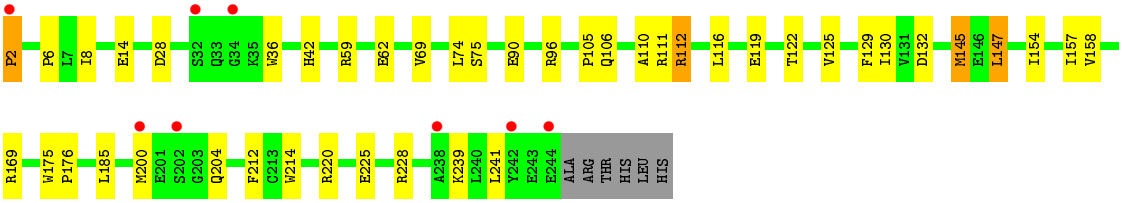



GLU ALA ARG THR HIS LEU HIS
• Molecule 1: Probable peroxiredoxin
Chain E:
2%
87%
10%
P2 G3 S4 I5 I8 R11 S32 K35 H42 R59 D70 S75 I93 F99 P100 D104 P105 Q106 R111 E119 T122 L141 M145 E146 W175 P176 M200 F212 D215 E235 A238 L241 Y242 E243 GLU ALA ARG
THR HIS LEU HIS
• Molecule 1: Probable peroxiredoxin
Chain F:
3%
86%
12%
P2 I5 I8 D28 W36 H42 T47 P48 S75 V79 P105 Q106 E119 S120 A121 T122 F129 D132 M140 L141 Y142 M145 E179 L185 P188 R197 A198 R199 M200 E201 S202 R206 S207 L208 F212 C213 W214 R220
R228 R231 Y242 E243 E244 A245 ARG THR HIS LEU HIS
• Molecule 1: Probable peroxiredoxin
Chain G:
4%
86%
10%
P2 G3 D28 S32 S41 H42 R59 L67 S75 P105 Q106 R111 R112 H117 A118 E119 T122 H123 T124 V125 L141 K162 L163 L167 E179 E183 I186 E193 R197 E201 L208 F212 R220 A238 Y242 E243
E244 ALA ARG THR HIS LEU HIS
• Molecule 1: Probable peroxiredoxin
Chain H:
4%
87%
9%
P2 L7 I8 G9 E10 E14 K25 D28 K35 P48 R59 V69 D70 L74 P105 Q106 R111 R112 T122 H123 I130 R134 L141 M145 I154 I157 V158 E179 T191 M200 E201 F212 R220 K239 Y242
E243 GLU ALA ARG THR HIS LEU HIS
• Molecule 1: Probable peroxiredoxin
Chain I:
3%
88%
9%



• Molecule 1: Probable peroxiredoxin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.21Å 103.11Å 104.40Å 106.02° 104.91° 92.97°	Depositor
Resolution (Å)	39.25 – 1.65 39.24 – 1.65	Depositor EDS
% Data completeness (in resolution range)	94.0 (39.25-1.65) 84.2 (39.24-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.223 0.193 , 0.222	Depositor DCC
R_{free} test set	16633 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 329512 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20999	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 4.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.66	0/2153	0.71	0/2927
1	B	0.63	0/2066	0.69	1/2808 (0.0%)
1	C	0.58	0/2128	0.67	0/2889
1	D	0.63	0/2053	0.72	1/2788 (0.0%)
1	E	0.64	0/2060	0.70	1/2797 (0.0%)
1	F	0.63	0/2093	0.68	0/2846
1	G	0.66	0/2070	0.69	0/2813
1	H	0.63	0/2069	0.71	0/2814
1	I	0.71	0/2065	0.73	0/2807
1	J	0.73	0/2076	0.76	2/2822 (0.1%)
All	All	0.65	0/20833	0.71	5/28311 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	231	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	D	199	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	J	147	LEU	CB-CG-CD2	5.25	119.93	111.00
1	E	215	ASP	CB-CG-OD1	5.05	122.85	118.30
1	J	169	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2050	0	2084	38	0
1	B	1993	0	2004	24	0
1	C	2038	0	2064	34	0
1	D	1978	0	2001	20	0
1	E	1990	0	1998	24	0
1	F	2014	0	2012	31	0
1	G	1998	0	1996	23	0
1	H	1996	0	2000	28	0
1	I	1993	0	1998	24	0
1	J	2019	0	2001	34	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
3	A	106	0	0	1	0
3	B	79	0	0	0	0
3	C	77	0	0	1	0
3	D	88	0	0	1	0
3	E	79	0	0	1	0
3	F	76	0	0	1	0
3	G	93	0	0	0	0
3	H	85	0	0	1	0
3	I	124	0	0	1	0
3	J	103	0	0	1	0
All	All	20999	0	20158	221	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (221) 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:242:TYR:CD1	1:J:214[B]:TRP:HH2	1.55	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:ARG:HD3	1:F:179[B]:GLU:OE1	1.41	1.20
1:E:59:ARG:CD	1:F:179[B]:GLU:OE1	1.91	1.16
1:E:59:ARG:HD2	1:F:179[B]:GLU:OE2	1.49	1.12
1:E:59:ARG:HD2	1:F:179[B]:GLU:CD	1.71	1.10
1:I:242:TYR:CD1	1:J:214[B]:TRP:CH2	2.40	1.09
1:A:214[A]:TRP:HH2	1:B:242:TYR:CD1	1.73	1.05
1:I:242:TYR:CE1	1:J:214[B]:TRP:HH2	1.78	0.99
1:G:105:PRO:O	1:G:106:GLN:HB2	1.66	0.94
1:I:242:TYR:CE1	1:J:214[B]:TRP:CH2	2.54	0.94
1:A:214[A]:TRP:CH2	1:B:242:TYR:CD1	2.56	0.93
1:F:105:PRO:O	1:F:106:GLN:HB2	1.69	0.92
1:C:59:ARG:HD2	1:D:179:GLU:OE2	1.74	0.88
1:B:11[A]:ARG:NH1	1:B:14[A]:GLU:OE2	2.06	0.87
1:B:69:VAL:HG21	1:B:158[A]:VAL:HG11	1.56	0.87
1:C:208[A]:LEU:CD1	1:C:214[A]:TRP:HZ3	1.88	0.85
1:B:194:ASP:OD2	1:B:197:ARG:NH2	2.10	0.85
1:E:105:PRO:O	1:E:106:GLN:HB2	1.73	0.85
1:E:241:LEU:HD11	1:F:179[B]:GLU:OE2	1.78	0.83
1:I:69:VAL:HG21	1:I:158[A]:VAL:HG11	1.61	0.83
1:C:69:VAL:HG21	1:C:158:VAL:HG11	1.59	0.81
1:J:69:VAL:HG21	1:J:158[A]:VAL:HG21	1.64	0.80
1:J:105:PRO:O	1:J:106:GLN:HB2	1.82	0.79
1:D:45:ASP:OD2	1:D:82:HIS:HD2	1.68	0.77
1:A:125[A]:VAL:HG22	1:A:143:TYR:O	1.84	0.76
1:E:8:ILE:HG22	1:F:119:GLU:HG3	1.67	0.76
1:I:179:GLU:OE1	1:J:241:LEU:HD11	1.86	0.75
1:C:208[A]:LEU:CD1	1:C:214[A]:TRP:CZ3	2.70	0.74
1:G:106:GLN:O	1:G:111:ARG:NH2	2.20	0.74
1:F:129:PHE:HE2	1:F:140:MET:HE3	1.53	0.74
1:H:106:GLN:O	1:H:111:ARG:NH2	2.20	0.73
1:H:134:ARG:NH1	3:H:1139:HOH:O	2.22	0.72
1:B:105:PRO:O	1:B:106:GLN:HB2	1.88	0.72
1:D:105:PRO:O	1:D:106:GLN:HB2	1.88	0.71
1:C:179:GLU:OE1	1:D:241:LEU:HD11	1.90	0.71
1:I:200:MET:HE2	1:I:200:MET:HA	1.72	0.70
1:C:119:GLU:HB3	3:C:445:HOH:O	1.92	0.69
1:G:163:LEU:HD22	1:G:167:LEU:HD22	1.74	0.68
1:A:105:PRO:O	1:A:106:GLN:HB2	1.93	0.68
1:C:43:PRO:HG3	1:C:145[A]:MET:HG3	1.74	0.68
1:H:69:VAL:HG21	1:H:158[B]:VAL:HG11	1.76	0.68
1:F:200:MET:HA	1:F:200:MET:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214[A]:TRP:HH2	1:B:242:TYR:CE1	2.12	0.67
1:J:105:PRO:O	1:J:106:GLN:CB	2.43	0.67
1:H:122:THR:HG23	1:H:123:HIS:CD2	2.29	0.66
1:C:208[A]:LEU:HD12	1:C:214[A]:TRP:HZ3	1.59	0.66
1:H:35:LYS:HD3	1:H:70:ASP:OD2	1.96	0.66
1:E:11:ARG:HD3	3:E:392:HOH:O	1.95	0.66
1:C:224:GLU:OE2	1:C:231:ARG:NH1	2.29	0.65
1:H:122:THR:HG21	3:I:627:HOH:O	1.97	0.65
1:A:214[A]:TRP:CH2	1:B:242:TYR:CE1	2.85	0.64
1:A:224[B]:GLU:OE2	1:A:231:ARG:NH2	2.30	0.64
1:F:122:THR:HB	1:G:105:PRO:HG2	1.78	0.63
1:H:122:THR:CG2	1:H:123:HIS:CD2	2.81	0.63
1:J:110:ALA:HB1	1:J:116:LEU:CD2	2.28	0.63
1:C:105:PRO:O	1:C:106[A]:GLN:HB2	1.99	0.63
1:F:129:PHE:CE2	1:F:140:MET:HE3	2.34	0.62
1:F:140:MET:CE	1:F:142:TYR:OH	2.47	0.61
1:F:140:MET:HE1	1:F:142:TYR:OH	2.01	0.61
1:E:59:ARG:CD	1:F:179[B]:GLU:CD	2.45	0.61
1:D:105:PRO:O	1:D:106:GLN:CB	2.48	0.61
1:F:129:PHE:CE2	1:F:140:MET:CE	2.84	0.61
1:J:225:GLU:CD	1:J:228:ARG:HH21	2.05	0.60
1:A:105:PRO:HG2	1:J:122:THR:HB	1.84	0.60
1:I:105:PRO:O	1:I:106:GLN:HB2	2.02	0.59
1:I:176:PRO:HG2	1:I:227:ARG:HG2	1.85	0.59
1:H:105:PRO:O	1:H:106:GLN:HB2	2.03	0.59
1:A:106:GLN:O	1:A:111:ARG:NH2	2.36	0.58
1:A:69:VAL:HG21	1:A:158[A]:VAL:HG11	1.84	0.58
1:B:106:GLN:NE2	1:C:116:LEU:HD22	2.18	0.57
1:B:42:HIS:CE1	1:B:75:SER:HB3	2.38	0.57
1:E:35[B]:LYS:HD2	1:E:70:ASP:OD2	2.03	0.57
1:D:106:GLN:O	1:D:111:ARG:NH2	2.37	0.57
1:D:176:PRO:HG2	1:D:227:ARG:HG2	1.85	0.57
1:A:185:LEU:O	1:A:214[A]:TRP:HB2	2.05	0.57
1:A:106:GLN:HG2	1:J:122:THR:HA	1.87	0.56
1:C:10:GLU:OE2	1:D:2:PRO:HB2	2.05	0.56
1:B:74:LEU:HD23	1:B:102:ILE:HB	1.87	0.56
1:E:119:GLU:OE2	1:E:145:MET:HG2	2.05	0.56
1:G:124:THR:HG23	1:G:125:VAL:O	2.07	0.55
1:I:105:PRO:O	1:I:106:GLN:CB	2.54	0.55
1:C:200[A]:MET:CE	1:C:200[A]:MET:HA	2.37	0.54
1:I:200:MET:HE2	1:I:200:MET:CA	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:PRO:HG2	1:I:122:THR:HB	1.90	0.54
1:A:105:PRO:O	1:A:106:GLN:CB	2.55	0.54
1:B:122:THR:HG23	1:B:123:HIS:CD2	2.42	0.54
1:B:130:ILE:HD13	1:B:157:ILE:HG21	1.89	0.54
1:A:125[A]:VAL:HG21	1:B:8:ILE:HD12	1.89	0.53
1:A:119:GLU:HG3	1:B:8:ILE:HG22	1.91	0.53
1:I:200:MET:CE	1:I:200:MET:HA	2.39	0.53
1:H:106:GLN:HE22	1:I:107:GLY:HA3	1.73	0.52
1:C:105:PRO:O	1:C:106[B]:GLN:CB	2.57	0.52
1:H:130:ILE:HD13	1:H:157:ILE:HG21	1.91	0.52
1:G:59:ARG:HG3	1:H:179:GLU:OE1	2.08	0.52
1:D:105:PRO:HG2	1:E:122:THR:HB	1.92	0.52
1:J:90:GLU:OE2	1:J:96:ARG:HD3	2.09	0.52
1:J:14:GLU:O	1:J:112:ARG:NH2	2.40	0.52
1:A:11:ARG:NH1	1:A:14[A]:GLU:OE2	2.32	0.52
1:I:179:GLU:OE1	1:J:241:LEU:CD1	2.56	0.51
1:A:74[A]:LEU:HD23	1:A:102:ILE:HB	1.92	0.51
1:I:194:ASP:OD1	1:I:197:ARG:NH1	2.43	0.51
1:F:106:GLN:HE22	1:G:111:ARG:HE	1.59	0.51
1:F:105:PRO:HG2	1:G:122:THR:HB	1.93	0.51
1:F:200:MET:CA	1:F:200:MET:HE2	2.40	0.51
1:J:42:HIS:CE1	1:J:75:SER:HB3	2.46	0.51
1:C:208[A]:LEU:HD13	1:C:214[A]:TRP:CZ3	2.46	0.50
1:C:200[A]:MET:HG2	1:C:210:TRP:HB3	1.92	0.50
1:J:185:LEU:O	1:J:214[B]:TRP:HB2	2.11	0.50
1:A:36:TRP:HB2	1:A:69:VAL:HG22	1.94	0.50
1:B:74:LEU:HD23	1:B:102:ILE:CG2	2.42	0.50
1:J:74:LEU:HD13	1:J:74:LEU:C	2.32	0.50
1:C:241:LEU:HD11	1:D:179:GLU:OE1	2.12	0.50
1:A:119:GLU:OE2	1:A:145[B]:MET:HG2	2.11	0.49
1:A:220:ARG:O	1:A:224[A]:GLU:HG3	2.12	0.49
1:E:119:GLU:HG3	1:F:8:ILE:HG22	1.94	0.49
1:C:59:ARG:CD	1:D:179:GLU:OE2	2.55	0.49
1:B:5:ILE:HG22	1:B:114:GLY:HA3	1.93	0.49
1:D:42:HIS:CE1	1:D:75:SER:HB3	2.48	0.49
1:I:242:TYR:CD1	1:J:214[B]:TRP:CZ2	2.98	0.49
1:E:175:TRP:CG	1:E:176:PRO:HA	2.48	0.49
1:B:69:VAL:CG2	1:B:158[A]:VAL:HG11	2.36	0.48
1:C:130:ILE:HD13	1:C:157:ILE:HG21	1.95	0.48
1:B:105:PRO:O	1:B:106:GLN:CB	2.57	0.48
1:E:93:ILE:HD11	1:F:208:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:PRO:O	1:H:106:GLN:CB	2.62	0.48
1:D:82:HIS:HE1	1:D:102:ILE:O	1.97	0.48
1:D:199:ARG:HD3	3:D:472:HOH:O	2.14	0.47
1:J:119:GLU:OE2	1:J:145[B]:MET:HG2	2.14	0.47
1:F:185:LEU:O	1:F:214[A]:TRP:HB2	2.14	0.47
1:J:175:TRP:CG	1:J:176:PRO:HA	2.50	0.47
1:I:179:GLU:OE2	1:J:59:ARG:HG3	2.14	0.47
1:B:106:GLN:HE22	1:C:116:LEU:HD22	1.78	0.47
1:A:125[A]:VAL:HG22	1:A:126:ARG:H	1.79	0.47
1:J:106:GLN:O	1:J:111:ARG:NH2	2.48	0.47
1:C:42:HIS:CE1	1:C:75:SER:HB3	2.50	0.47
1:C:122:THR:HG23	1:C:123:HIS:CD2	2.51	0.47
1:I:119:GLU:HG3	1:J:8:ILE:HG22	1.96	0.46
1:G:208:LEU:CD1	1:H:242[B]:TYR:CD1	2.99	0.46
1:F:140:MET:HE2	1:F:142:TYR:OH	2.15	0.46
1:J:6:PRO:HG2	1:J:129:PHE:HE2	1.81	0.46
1:F:42:HIS:CE1	1:F:75:SER:HB3	2.51	0.46
1:G:119:GLU:HG3	1:H:8:ILE:HG22	1.97	0.46
1:G:179:GLU:OE2	1:H:59:ARG:HG3	2.16	0.46
1:E:5:ILE:HG12	1:F:5:ILE:HG12	1.97	0.46
1:G:193:GLU:O	1:G:197:ARG:HG2	2.15	0.46
1:H:14:GLU:O	1:H:112[B]:ARG:NH2	2.49	0.46
1:G:3:GLY:HA3	1:H:7:LEU:HD21	1.97	0.46
1:E:146:GLU:HG3	3:F:558:HOH:O	2.16	0.46
1:A:67:LEU:HD21	1:A:159:LYS:HD3	1.98	0.46
1:J:204:GLN:NE2	3:J:283:HOH:O	2.48	0.46
1:A:125[A]:VAL:CG2	1:A:143:TYR:O	2.60	0.45
1:G:208:LEU:CD1	1:H:242[B]:TYR:HD1	2.29	0.45
1:H:74:LEU:C	1:H:74:LEU:HD13	2.36	0.45
1:E:42:HIS:CE1	1:E:75:SER:HB3	2.52	0.45
1:G:186:ILE:HG21	1:H:48:PRO:HG2	1.99	0.45
1:C:200[B]:MET:HG3	1:C:210:TRP:HB3	1.98	0.45
1:F:129:PHE:CE2	1:F:140:MET:HE2	2.51	0.44
1:A:99:PHE:HB2	1:A:100:PRO:HD2	1.97	0.44
1:E:99:PHE:HB2	1:E:100:PRO:HD2	1.99	0.44
1:F:47:THR:HB	1:F:48:PRO:HD2	1.97	0.44
1:D:200:MET:CE	1:D:210:TRP:HA	2.48	0.44
1:A:176:PRO:HG2	1:A:227:ARG:HG2	2.00	0.44
1:C:175:TRP:CG	1:C:176:PRO:HA	2.53	0.44
1:J:200[A]:MET:HA	1:J:200[A]:MET:CE	2.48	0.44
1:D:36:TRP:CD2	1:D:132:ASP:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:154:ILE:O	1:J:158[B]:VAL:HG23	2.17	0.44
1:D:200:MET:HE3	1:D:210:TRP:HA	1.99	0.44
1:D:194:ASP:OD1	1:D:197:ARG:NH2	2.49	0.44
1:C:67:LEU:HD21	1:C:159:LYS:HD3	1.99	0.44
1:F:188:PRO:O	1:F:199:ARG:NH2	2.47	0.43
1:C:36:TRP:CD2	1:C:132:ASP:HA	2.53	0.43
1:C:14:GLU:O	1:C:112:ARG:NH2	2.52	0.43
1:A:214[A]:TRP:CZ2	1:B:242:TYR:CD1	3.06	0.43
1:G:122:THR:OG1	1:G:123:HIS:HD2	2.01	0.43
1:A:175:TRP:CG	1:A:176:PRO:HA	2.54	0.43
1:F:79[B]:VAL:HG11	1:H:191:THR:O	2.19	0.43
1:G:41:SER:HB2	1:G:124:THR:HG21	2.00	0.43
1:C:47:THR:HB	1:C:48:PRO:HD2	2.01	0.43
1:E:104:ASP:N	1:E:105:PRO:HD3	2.34	0.43
1:H:106:GLN:HG2	1:I:122:THR:HA	2.01	0.43
1:D:5:ILE:HG22	1:D:114:GLY:HA3	2.01	0.43
1:A:125[A]:VAL:HG22	1:A:126:ARG:N	2.34	0.43
1:E:200:MET:HA	1:E:200:MET:CE	2.49	0.43
1:J:36:TRP:CD2	1:J:132:ASP:HA	2.54	0.42
1:G:208:LEU:HD11	1:H:242[B]:TYR:CD1	2.54	0.42
1:A:59[A]:ARG:HH21	1:A:241:LEU:HD21	1.85	0.42
1:C:28:ASP:N	1:C:28:ASP:OD1	2.51	0.42
1:A:154:ILE:O	1:A:158[A]:VAL:HG23	2.20	0.42
1:A:74[A]:LEU:HD23	1:A:102:ILE:CG2	2.50	0.42
1:F:228:ARG:HG3	1:F:231:ARG:NH1	2.35	0.42
1:B:106:GLN:NE2	1:C:116:LEU:CD2	2.83	0.42
1:F:119:GLU:OE2	1:F:145[B]:MET:HG2	2.20	0.41
1:A:189:PRO:HA	1:A:190:PRO:HD3	1.97	0.41
1:A:42:HIS:CE1	1:A:75:SER:HB3	2.54	0.41
1:G:2:PRO:HB2	1:H:10:GLU:OE2	2.20	0.41
1:A:228:ARG:HD3	3:A:387:HOH:O	2.20	0.41
1:C:126:ARG:HB3	1:C:149:ARG:CZ	2.50	0.41
1:B:106:GLN:NE2	1:C:121:ALA:O	2.53	0.41
1:C:62:GLU:HG2	1:C:66:ARG:NH1	2.35	0.41
1:D:107:GLY:HA3	1:E:106:GLN:NE2	2.36	0.41
1:A:228:ARG:HB3	1:A:228:ARG:CZ	2.51	0.41
1:I:59:ARG:HH11	1:I:59:ARG:HD3	1.74	0.41
1:G:67:LEU:O	1:G:162:LYS:HE3	2.20	0.41
1:J:69:VAL:CG2	1:J:158[A]:VAL:HG21	2.42	0.41
1:E:175:TRP:CD1	1:E:176:PRO:HA	2.56	0.41
1:I:10:GLU:OE2	1:J:2:PRO:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:HIS:CE1	1:G:75:SER:HB3	2.56	0.41
1:G:183:GLU:OE2	1:G:220[B]:ARG:NH2	2.42	0.41
1:J:130:ILE:HD13	1:J:157:ILE:HG21	2.02	0.41
1:H:106:GLN:OE1	1:I:76:VAL:HG11	2.22	0.40
1:A:208:LEU:HD13	1:B:93[A]:ILE:CD1	2.51	0.40
1:J:110:ALA:CB	1:J:116:LEU:CD2	2.97	0.40
1:G:117:HIS:HA	1:H:7:LEU:HD13	2.02	0.40
1:F:36:TRP:CD2	1:F:132:ASP:HA	2.57	0.40
1:A:43:PRO:HB3	1:A:145[B]:MET:CE	2.51	0.40
1:C:225:GLU:O	1:C:228[B]:ARG:HB3	2.22	0.40
1:H:25:LYS:NZ	1:H:28:ASP:OD2	2.54	0.40
1:A:36:TRP:CD2	1:A:132:ASP:HA	2.56	0.40
1:J:6:PRO:HG2	1:J:129:PHE:CE2	2.57	0.40
1:I:47:THR:HB	1:I:48:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

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	256/249 (103%)	251 (98%)	4 (2%)	1 (0%)	39 18
1	B	246/249 (99%)	243 (99%)	3 (1%)	0	100 100
1	C	252/249 (101%)	244 (97%)	6 (2%)	2 (1%)	24 5
1	D	245/249 (98%)	239 (98%)	4 (2%)	2 (1%)	24 5
1	E	245/249 (98%)	238 (97%)	7 (3%)	0	100 100
1	F	249/249 (100%)	245 (98%)	4 (2%)	0	100 100
1	G	246/249 (99%)	241 (98%)	5 (2%)	0	100 100
1	H	245/249 (98%)	240 (98%)	5 (2%)	0	100 100
1	I	245/249 (98%)	241 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	247/249 (99%)	238 (96%)	7 (3%)	2 (1%)	24 5
All	All	2476/2490 (99%)	2420 (98%)	49 (2%)	7 (0%)	52 24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	106[A]	GLN
1	C	106[B]	GLN
1	D	106	GLN
1	A	106	GLN
1	D	239	LYS
1	J	239	LYS
1	J	125	VAL

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	225/215 (105%)	215 (96%)	10 (4%)	35 9
1	B	215/215 (100%)	212 (99%)	3 (1%)	74 53
1	C	221/215 (103%)	212 (96%)	9 (4%)	37 10
1	D	214/215 (100%)	209 (98%)	5 (2%)	58 30
1	E	214/215 (100%)	210 (98%)	4 (2%)	65 40
1	F	217/215 (101%)	212 (98%)	5 (2%)	58 30
1	G	215/215 (100%)	208 (97%)	7 (3%)	45 15
1	H	214/215 (100%)	208 (97%)	6 (3%)	51 21
1	I	214/215 (100%)	211 (99%)	3 (1%)	74 53
1	J	216/215 (100%)	207 (96%)	9 (4%)	36 10
All	All	2165/2150 (101%)	2104 (97%)	61 (3%)	54 21

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	147[A]	LEU
1	A	147[B]	LEU
1	A	161[A]	LEU
1	A	161[B]	LEU
1	A	212	PHE
1	A	228	ARG
1	A	239	LYS
1	A	242[A]	TYR
1	A	242[B]	TYR
1	B	28	ASP
1	B	122	THR
1	B	212	PHE
1	C	4	SER
1	C	28	ASP
1	C	59	ARG
1	C	106[A]	GLN
1	C	106[B]	GLN
1	C	145[A]	MET
1	C	145[B]	MET
1	C	197	ARG
1	C	212	PHE
1	D	28	ASP
1	D	159	LYS
1	D	199	ARG
1	D	201	GLU
1	D	212	PHE
1	E	11	ARG
1	E	106	GLN
1	E	111	ARG
1	E	212	PHE
1	F	28	ASP
1	F	199	ARG
1	F	206	ARG
1	F	212	PHE
1	F	220	ARG
1	G	28	ASP
1	G	112	ARG
1	G	124	THR
1	G	163	LEU
1	G	167	LEU
1	G	208	LEU
1	G	212	PHE

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Mol	Chain	Res	Type
1	H	14	GLU
1	H	28	ASP
1	H	112[A]	ARG
1	H	112[B]	ARG
1	H	122	THR
1	H	212	PHE
1	I	7	LEU
1	I	28	ASP
1	I	212	PHE
1	J	2	PRO
1	J	28	ASP
1	J	62	GLU
1	J	112	ARG
1	J	145[A]	MET
1	J	145[B]	MET
1	J	147	LEU
1	J	212	PHE
1	J	220	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	106	GLN
1	A	123	HIS
1	A	204	GLN
1	B	106	GLN
1	B	123	HIS
1	B	204	GLN
1	C	123	HIS
1	C	204	GLN
1	D	82	HIS
1	E	123	HIS
1	F	106	GLN
1	F	123	HIS
1	F	204	GLN
1	G	123	HIS
1	G	204	GLN
1	H	106	GLN
1	H	123	HIS
1	H	204	GLN
1	I	204	GLN

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Mol	Chain	Res	Type
1	J	204	GLN

5.3.3 RNA

There are no RNA molecules 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	PER	A	1	-	0,1,1	0.00	-	0,0,0	0.00	-
2	PER	B	251	-	0,1,1	0.00	-	0,0,0	0.00	-
2	PER	C	251	-	0,1,1	0.00	-	0,0,0	0.00	-
2	PER	D	251	-	0,1,1	0.00	-	0,0,0	0.00	-
2	PER	E	251	-	0,1,1	0.00	-	0,0,0	0.00	-
2	PER	F	251	-	0,1,1	0.00	-	0,0,0	0.00	-
2	PER	G	251	-	0,1,1	0.00	-	0,0,0	0.00	-
2	PER	H	251	-	0,1,1	0.00	-	0,0,0	0.00	-
2	PER	I	251	-	0,1,1	0.00	-	0,0,0	0.00	-
2	PER	J	251	-	0,1,1	0.00	-	0,0,0	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	PER	A	1	-	-	0/0/0/0	0/0/0/0
2	PER	B	251	-	-	0/0/0/0	0/0/0/0
2	PER	C	251	-	-	0/0/0/0	0/0/0/0
2	PER	D	251	-	-	0/0/0/0	0/0/0/0
2	PER	E	251	-	-	0/0/0/0	0/0/0/0
2	PER	F	251	-	-	0/0/0/0	0/0/0/0
2	PER	G	251	-	-	0/0/0/0	0/0/0/0
2	PER	H	251	-	-	0/0/0/0	0/0/0/0
2	PER	I	251	-	-	0/0/0/0	0/0/0/0
2	PER	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.

No monomer is involved in short contacts.

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, 95^{th} 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%)	-0.19	3 (1%)	81 83	16, 22, 36, 48	0
1	B	242/249 (97%)	0.06	9 (3%)	45 46	16, 25, 40, 48	0
1	C	243/249 (97%)	0.27	12 (4%)	33 31	18, 27, 44, 62	0
1	D	240/249 (96%)	-0.03	7 (2%)	55 56	16, 24, 42, 50	0
1	E	242/249 (97%)	-0.10	5 (2%)	67 70	15, 24, 39, 44	0
1	F	244/249 (97%)	-0.09	8 (3%)	50 51	16, 25, 41, 54	0
1	G	243/249 (97%)	0.06	10 (4%)	41 40	17, 24, 40, 59	0
1	H	242/249 (97%)	0.11	10 (4%)	41 40	16, 24, 36, 47	0
1	I	242/249 (97%)	-0.12	7 (2%)	55 56	13, 20, 35, 45	0
1	J	243/249 (97%)	-0.13	8 (3%)	50 51	14, 21, 37, 56	0
All	All	2424/2490 (97%)	-0.02	79 (3%)	50 51	13, 24, 40, 62	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	245	ALA	7.7
1	D	238	ALA	6.4
1	J	238	ALA	6.2
1	H	242[A]	TYR	4.9
1	G	242	TYR	4.7
1	D	239	LYS	4.4
1	C	238	ALA	4.3
1	C	244	GLU	4.0
1	F	201	GLU	4.0
1	H	200	MET	3.8
1	F	244	GLU	3.6
1	J	242	TYR	3.4
1	C	220	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	239	LYS	3.3
1	I	242	TYR	3.2
1	B	242	TYR	3.2
1	D	200	MET	3.1
1	E	242	TYR	3.0
1	G	244	GLU	3.0
1	F	200	MET	3.0
1	A	201	GLU	2.9
1	C	243	GLU	2.9
1	J	200[A]	MET	2.9
1	H	243	GLU	2.9
1	B	238	ALA	2.9
1	F	242[A]	TYR	2.9
1	H	141	LEU	2.7
1	C	242	TYR	2.7
1	C	141	LEU	2.7
1	J	244	GLU	2.7
1	C	32	SER	2.7
1	G	32	SER	2.7
1	B	4	SER	2.6
1	G	238	ALA	2.6
1	G	118	ALA	2.6
1	I	238	ALA	2.5
1	G	243	GLU	2.5
1	E	32	SER	2.5
1	G	119	GLU	2.5
1	G	141	LEU	2.5
1	H	154	ILE	2.5
1	B	121	ALA	2.5
1	C	106[A]	GLN	2.5
1	D	2	PRO	2.4
1	I	220	ARG	2.4
1	I	243	GLU	2.4
1	A	220	ARG	2.4
1	C	122	THR	2.4
1	D	141	LEU	2.4
1	A	197	ARG	2.4
1	H	201	GLU	2.3
1	H	220	ARG	2.3
1	G	2	PRO	2.3
1	B	141	LEU	2.2
1	F	197	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	121	ALA	2.2
1	C	200[A]	MET	2.2
1	B	14[A]	GLU	2.2
1	J	34	GLY	2.2
1	J	202	SER	2.2
1	B	243	GLU	2.2
1	J	32	SER	2.2
1	I	203	GLY	2.2
1	D	118	ALA	2.2
1	I	141	LEU	2.1
1	E	4	SER	2.1
1	E	238	ALA	2.1
1	D	220	ARG	2.1
1	H	2	PRO	2.1
1	B	32	SER	2.1
1	C	121	ALA	2.1
1	H	239	LYS	2.1
1	F	202	SER	2.1
1	E	141	LEU	2.1
1	I	154	ILE	2.1
1	J	2	PRO	2.0
1	G	201	GLU	2.0
1	B	154	ILE	2.0
1	H	145	MET	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 carbohydrates in this entry.

6.4 Ligands (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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	PER	J	251	2/2	0.91	0.15	2.99	22,22,22,29	0
2	PER	F	251	2/2	0.90	0.15	1.82	28,28,28,37	0
2	PER	B	251	2/2	0.90	0.12	1.70	28,28,28,35	0
2	PER	G	251	2/2	0.94	0.10	1.23	29,29,29,33	0
2	PER	E	251	2/2	0.95	0.09	-0.07	32,32,32,34	0
2	PER	A	1	2/2	0.91	0.08	-0.20	25,25,25,31	0
2	PER	I	251	2/2	0.96	0.08	-0.23	22,22,22,27	0
2	PER	C	251	2/2	0.93	0.09	-0.59	27,27,27,33	0
2	PER	D	251	2/2	0.93	0.07	-0.69	30,30,30,35	0
2	PER	H	251	2/2	0.95	0.06	-1.18	29,29,29,32	0

6.5 Other polymers (i)

There are no such residues in this entry.