Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:55 pm BST

PDB ID	:	5XBS
Title	:	Peroxiredoxin from Aeropyrum pernix (6m mutant)
Authors	:	Nakamura, T.; Uegaki, K.
Deposited on	:	2017-03-21
Resolution	:	2.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

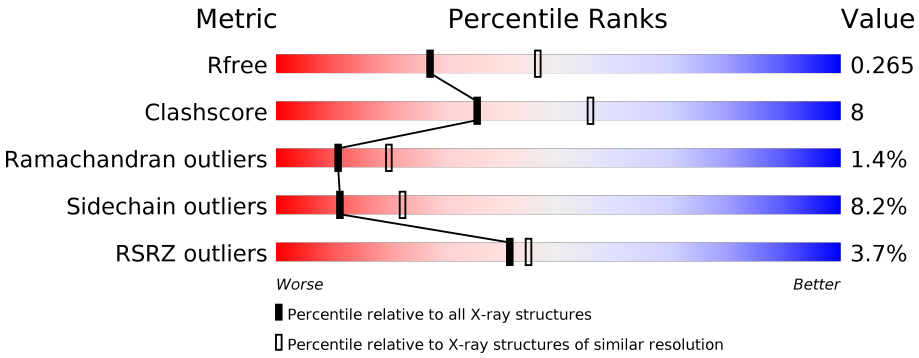
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	250	2% 74% 20%
1	B	250	5% 74% 18%
1	C	250	3% 75% 19%
1	D	250	4% 67% 26% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7778 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 Peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	1	0
			1984	1264	353	360	7			
1	B	240	Total	C	N	O	S	0	0	0
			1934	1236	344	347	7			
1	C	241	Total	C	N	O	S	0	0	0
			1948	1243	348	350	7			
1	D	236	Total	C	N	O	S	0	0	0
			1908	1220	338	343	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	VAL	engineered mutation	UNP Q9Y9L0
A	80	GLU	PHE	engineered mutation	UNP Q9Y9L0
A	81	ASP	SER	engineered mutation	UNP Q9Y9L0
A	83	SER	ILE	engineered mutation	UNP Q9Y9L0
A	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
A	210	SER	TRP	engineered mutation	UNP Q9Y9L0
B	23	ARG	VAL	engineered mutation	UNP Q9Y9L0
B	80	GLU	PHE	engineered mutation	UNP Q9Y9L0
B	81	ASP	SER	engineered mutation	UNP Q9Y9L0
B	83	SER	ILE	engineered mutation	UNP Q9Y9L0
B	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
B	210	SER	TRP	engineered mutation	UNP Q9Y9L0
C	23	ARG	VAL	engineered mutation	UNP Q9Y9L0
C	80	GLU	PHE	engineered mutation	UNP Q9Y9L0
C	81	ASP	SER	engineered mutation	UNP Q9Y9L0
C	83	SER	ILE	engineered mutation	UNP Q9Y9L0
C	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
C	210	SER	TRP	engineered mutation	UNP Q9Y9L0
D	23	ARG	VAL	engineered mutation	UNP Q9Y9L0
D	80	GLU	PHE	engineered mutation	UNP Q9Y9L0
D	81	ASP	SER	engineered mutation	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	83	SER	ILE	engineered mutation	UNP Q9Y9L0
D	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
D	210	SER	TRP	engineered mutation	UNP Q9Y9L0

- Molecule 2 is water.

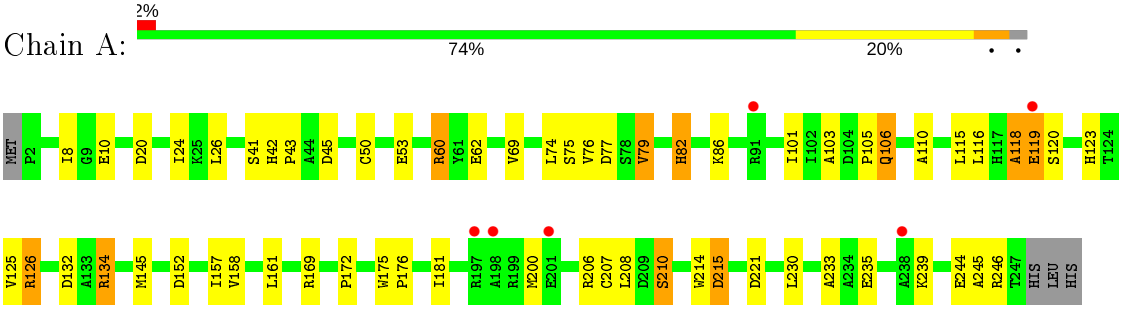
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	2	Total O 2 2	0	0

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 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.

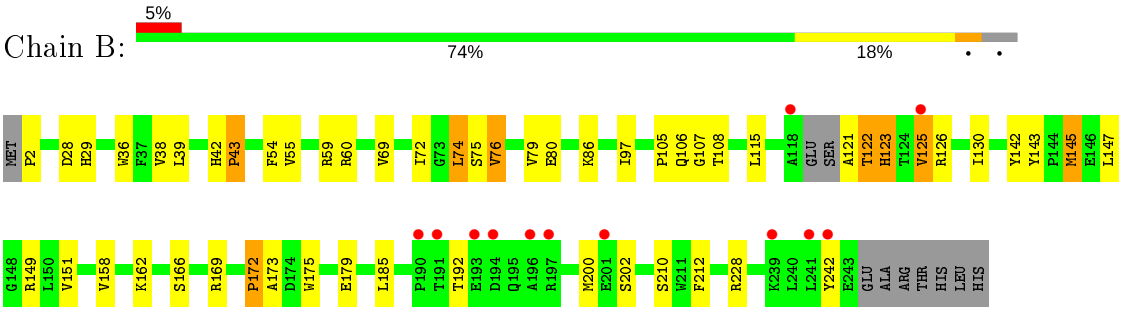
- Molecule 1: Peroxiredoxin

Chain A:



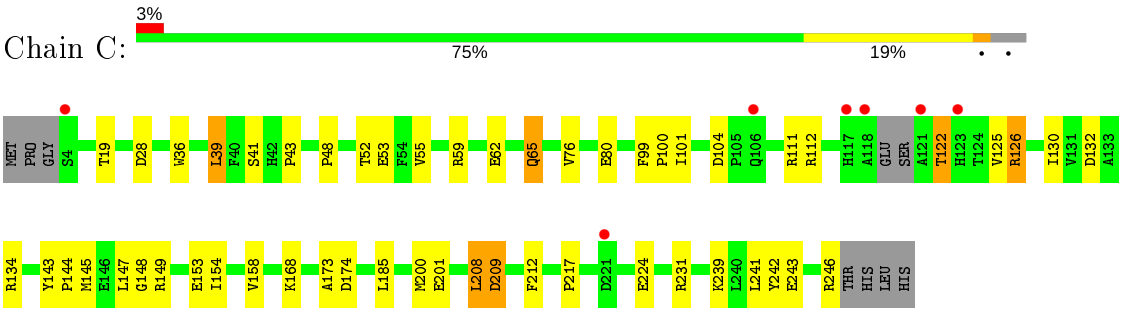
- Molecule 1: Peroxiredoxin

Chain B:



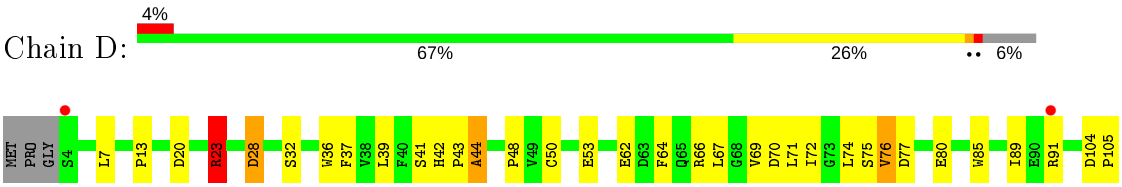
- Molecule 1: Peroxiredoxin

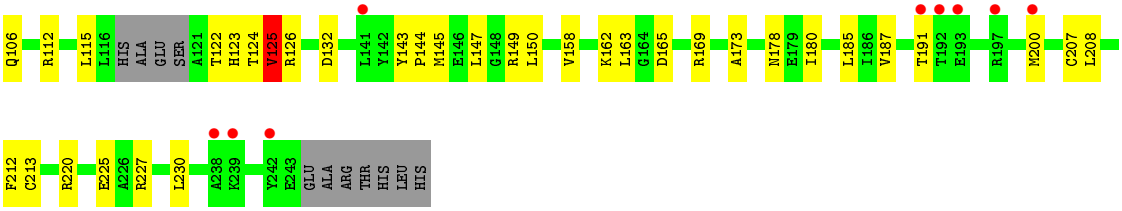
Chain C:



- Molecule 1: Peroxiredoxin

Chain D:




Q106
R112
L115
L116
HIS
ALA
GLU
SER
A121
T122
H123
T124
V125
R126
D132
L141
Y142
Y143
P144
M145
E146
L147
G148
R149
L150
V158
K162
L163
G164
D165
R169
A173
N178
E179
I180
L185
I186
V187
T191
T192
E193
R197
M200
C207
L208

F212
C213
R220
E225
A226
R227
L230
A238
K239
Y242
E243
GLU
ALA
ARG
THR
HIS
LEU
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.66Å 170.79Å 61.97Å 90.00° 114.00° 90.00°	Depositor
Resolution (Å)	36.33 – 2.51 36.33 – 2.51	Depositor EDS
% Data completeness (in resolution range)	84.2 (36.33-2.51) 84.2 (36.33-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.17 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.210 , 0.300 0.190 , 0.265	Depositor DCC
R_{free} test set	1433 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7778	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.59	0/2039	0.81	3/2770 (0.1%)
1	B	0.59	0/1985	0.81	3/2696 (0.1%)
1	C	0.61	0/1998	0.80	2/2713 (0.1%)
1	D	0.61	0/1957	0.82	4/2658 (0.2%)
All	All	0.60	0/7979	0.81	12/10837 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	C	149	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	149	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	149	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	60	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	D	23	ARG	NE-CZ-NH2	5.53	123.07	120.30
1	D	165	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	149	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	215	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	165	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	60	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	D	149	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ALA	Peptide
1	B	122	THR	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	1984	0	1963	36	0
1	B	1934	0	1915	27	0
1	C	1948	0	1928	36	0
1	D	1908	0	1892	41	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	7778	0	7698	126	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 8.

All (126) 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:A:118:ALA:HA	1:A:119:GLU:HB2	1.49	0.93
1:B:122:THR:N	1:B:123:HIS:HB2	1.86	0.88
1:C:53:GLU:OE1	1:C:126:ARG:NH1	2.06	0.88
1:D:36:TRP:CE2	1:D:132:ASP:HA	2.11	0.86
1:C:153:GLU:OE2	1:D:143:TYR:OH	1.97	0.81
1:A:200:MET:CE	1:A:210:SER:HA	2.11	0.80
1:D:36:TRP:CD2	1:D:132:ASP:HA	2.21	0.74
1:A:60:ARG:NE	1:A:152:ASP:OD1	2.21	0.73
1:C:126:ARG:HG2	1:C:143:TYR:O	1.88	0.73
1:A:118:ALA:CA	1:A:119:GLU:HB2	2.16	0.73
1:C:53:GLU:CD	1:C:126:ARG:HH12	1.93	0.70
1:B:172:PRO:HD2	1:B:175:TRP:HB2	1.74	0.69
1:D:69:VAL:HG21	1:D:158:VAL:HG11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:HIS:ND1	1:A:50:CYS:SG	2.71	0.63
1:C:126:ARG:HD3	1:C:145:MET:HA	1.81	0.62
1:C:174:ASP:HA	1:D:150:LEU:HD12	1.81	0.60
1:A:76:VAL:HG23	1:A:76:VAL:O	2.01	0.60
1:B:126:ARG:HB3	1:B:143:TYR:O	2.02	0.59
1:B:125:VAL:O	1:B:125:VAL:HG12	2.02	0.59
1:D:105:PRO:O	1:D:106:GLN:HB2	2.03	0.59
1:D:76:VAL:HA	1:D:104:ASP:O	2.04	0.58
1:D:132:ASP:C	1:D:132:ASP:OD1	2.43	0.56
1:A:200:MET:HE2	1:A:210:SER:HA	1.84	0.56
1:C:39:LEU:HD23	1:C:39:LEU:O	2.05	0.56
1:D:20:ASP:N	1:D:20:ASP:OD1	2.39	0.56
1:D:23:ARG:HG3	1:D:23:ARG:HH21	1.70	0.56
1:C:76:VAL:HG23	1:C:76:VAL:O	2.05	0.56
1:A:132:ASP:OD1	1:A:132:ASP:C	2.41	0.55
1:D:42:HIS:ND1	1:D:50:CYS:SG	2.75	0.55
1:C:224:GLU:OE1	1:C:231:ARG:NH2	2.38	0.55
1:D:64:PHE:CD2	1:D:71:LEU:HD21	2.42	0.55
1:B:158:VAL:O	1:B:162:LYS:HG3	2.06	0.55
1:C:130:ILE:HD11	1:C:154:ILE:HG23	1.89	0.55
1:C:173:ALA:HB2	1:D:53:GLU:HG2	1.87	0.55
1:A:45:ASP:OD1	1:A:75:SER:OG	2.23	0.54
1:C:132:ASP:OD2	1:C:134:ARG:NH1	2.40	0.54
1:D:67:LEU:O	1:D:162:LYS:HE2	2.07	0.54
1:C:43:PRO:O	1:C:76:VAL:HG22	2.07	0.54
1:C:125:VAL:HG23	1:C:125:VAL:O	2.07	0.54
1:A:76:VAL:CG2	1:A:76:VAL:O	2.56	0.54
1:D:23:ARG:CG	1:D:23:ARG:HH21	2.21	0.53
1:D:43:PRO:O	1:D:44:ALA:HB2	2.08	0.53
1:C:48:PRO:O	1:C:52:THR:HG23	2.09	0.53
1:A:41:SER:HB2	1:A:125:VAL:HG12	1.91	0.52
1:A:200:MET:HE1	1:A:210:SER:HA	1.91	0.52
1:B:43:PRO:O	1:B:76:VAL:HG22	2.10	0.51
1:A:132:ASP:OD2	1:A:134:ARG:NH1	2.41	0.51
1:D:74:LEU:C	1:D:74:LEU:HD13	2.30	0.50
1:B:39:LEU:HD12	1:B:72:ILE:HG23	1.93	0.49
1:D:41:SER:CB	1:D:74:LEU:HD12	2.42	0.49
1:B:74:LEU:HD22	1:B:75:SER:N	2.25	0.49
1:C:53:GLU:HG3	1:D:173:ALA:HB2	1.94	0.49
1:A:8:ILE:HD11	1:B:142:TYR:HB3	1.94	0.49
1:C:53:GLU:OE2	1:C:148:GLY:HA2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:VAL:CG2	1:D:158:VAL:HG11	2.41	0.49
1:A:69:VAL:HG21	1:A:158:VAL:HG11	1.95	0.48
1:D:123:HIS:HA	1:D:145:MET:HE3	1.94	0.48
1:A:118:ALA:CA	1:A:119:GLU:CB	2.91	0.48
1:C:36:TRP:CD2	1:C:132:ASP:HA	2.49	0.47
1:C:39:LEU:C	1:C:39:LEU:HD23	2.35	0.47
1:B:55:VAL:O	1:B:59:ARG:HG3	2.14	0.47
1:D:37:PHE:HA	1:D:70:ASP:O	2.14	0.47
1:A:43:PRO:O	1:A:76:VAL:HG22	2.14	0.47
1:C:76:VAL:HA	1:C:104:ASP:O	2.14	0.47
1:A:214:TRP:HH2	1:B:242:TYR:CD1	2.34	0.46
1:C:208:LEU:O	1:C:209:ASP:HB2	2.16	0.46
1:A:79:VAL:HG13	1:A:103:ALA:HB2	1.96	0.46
1:A:42:HIS:CE1	1:A:126:ARG:HH22	2.33	0.46
1:A:10:GLU:OE2	1:B:2:PRO:N	2.49	0.46
1:C:173:ALA:HB2	1:D:53:GLU:CG	2.46	0.46
1:D:169:ARG:HB3	1:D:185:LEU:HB3	1.98	0.45
1:A:110:ALA:HB3	1:A:116:LEU:CD2	2.46	0.45
1:C:19:THR:HA	1:C:101:ILE:O	2.17	0.45
1:D:28:ASP:N	1:D:28:ASP:OD1	2.50	0.45
1:B:42:HIS:NE2	1:B:54:PHE:HE1	2.15	0.45
1:C:122:THR:OG1	1:C:122:THR:O	2.28	0.45
1:B:151:VAL:HG12	1:B:151:VAL:O	2.15	0.45
1:A:172:PRO:HB3	1:A:181:ILE:HD11	1.98	0.45
1:A:244:GLU:HG3	1:A:244:GLU:O	2.16	0.45
1:D:23:ARG:NH2	1:D:23:ARG:HG3	2.28	0.44
1:A:157:ILE:HG12	1:B:147:LEU:HD21	2.00	0.44
1:A:206:ARG:HD2	1:B:242:TYR:CE2	2.53	0.44
1:C:241:LEU:HB2	1:D:180:ILE:HA	1.98	0.44
1:A:42:HIS:HE1	1:A:53:GLU:OE1	2.00	0.44
1:D:123:HIS:CA	1:D:145:MET:HE3	2.48	0.44
1:C:242:TYR:CE2	1:C:243:GLU:HG3	2.53	0.44
1:D:187:VAL:HG23	1:D:213:CYS:O	2.18	0.44
1:B:169:ARG:HB3	1:B:185:LEU:HB3	2.00	0.43
1:C:53:GLU:CG	1:D:173:ALA:HB2	2.48	0.43
1:B:105:PRO:C	1:B:107:GLY:H	2.22	0.43
1:B:200:MET:HA	1:B:200:MET:CE	2.49	0.43
1:B:86:LYS:HE2	1:B:97:ILE:HB	2.01	0.43
1:D:80:GLU:H	1:D:80:GLU:CD	2.22	0.42
1:A:214:TRP:HH2	1:B:242:TYR:CG	2.36	0.42
1:A:169:ARG:NE	1:A:215:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:HIS:HB3	1:A:145:MET:SD	2.59	0.42
1:B:126:ARG:HE	1:B:145:MET:HA	1.85	0.42
1:D:173:ALA:O	1:D:178:ASN:ND2	2.50	0.42
1:B:121:ALA:C	1:B:123:HIS:HB2	2.38	0.42
1:C:125:VAL:O	1:C:125:VAL:CG2	2.67	0.42
1:C:65:GLN:HA	1:C:65:GLN:OE1	2.20	0.42
1:D:39:LEU:HA	1:D:72:ILE:HG23	2.01	0.42
1:C:185:LEU:HD12	1:C:217:PRO:HD2	2.01	0.42
1:D:144:PRO:HG2	1:D:147:LEU:HB3	2.01	0.42
1:A:82:HIS:NE2	1:A:101:ILE:HG22	2.35	0.42
1:B:36:TRP:HB2	1:B:69:VAL:HG22	2.01	0.42
1:A:105:PRO:O	1:A:106:GLN:CB	2.68	0.42
1:B:172:PRO:O	1:B:173:ALA:C	2.58	0.42
1:D:74:LEU:HD13	1:D:75:SER:N	2.35	0.42
1:D:115:LEU:HB3	1:D:125:VAL:HA	2.01	0.42
1:B:28:ASP:O	1:B:29:HIS:C	2.56	0.41
1:C:112:ARG:O	1:C:112:ARG:HG3	2.20	0.41
1:C:99:PHE:HB2	1:C:100:PRO:HD2	2.02	0.41
1:D:200:MET:HE1	1:D:207:CYS:HB3	2.03	0.41
1:A:230:LEU:O	1:A:233:ALA:HB3	2.20	0.41
1:C:144:PRO:HD2	1:C:147:LEU:HD23	2.03	0.41
1:A:24:ILE:HD11	1:A:26:LEU:HD21	2.02	0.41
1:C:130:ILE:HG21	1:C:158:VAL:CG1	2.50	0.41
1:A:175:TRP:CD1	1:A:176:PRO:HA	2.56	0.40
1:C:153:GLU:OE1	1:C:153:GLU:HA	2.21	0.40
1:D:123:HIS:HA	1:D:145:MET:CE	2.51	0.40
1:B:38:VAL:HG22	1:B:130:ILE:HG12	2.02	0.40
1:D:124:THR:O	1:D:126:ARG:N	2.54	0.40
1:A:20:ASP:OD2	1:A:86:LYS:NZ	2.48	0.40
1:D:85:TRP:O	1:D:89:ILE:HG13	2.21	0.40
1:C:55:VAL:HG21	1:D:180:ILE:HD11	2.02	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	245/250 (98%)	218 (89%)	24 (10%)	3 (1%)	13 24
1	B	236/250 (94%)	211 (89%)	21 (9%)	4 (2%)	9 16
1	C	237/250 (95%)	218 (92%)	18 (8%)	1 (0%)	34 54
1	D	232/250 (93%)	212 (91%)	15 (6%)	5 (2%)	6 10
All	All	950/1000 (95%)	859 (90%)	78 (8%)	13 (1%)	11 20

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	A	120	SER
1	D	125	VAL
1	A	245	ALA
1	B	125	VAL
1	D	44	ALA
1	D	66	ARG
1	D	48	PRO
1	B	172	PRO
1	C	209	ASP
1	B	43	PRO
1	B	76	VAL
1	D	76	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	212/215 (99%)	195 (92%)	17 (8%)	12 23
1	B	206/215 (96%)	191 (93%)	15 (7%)	14 27
1	C	207/215 (96%)	190 (92%)	17 (8%)	11 22
1	D	204/215 (95%)	185 (91%)	19 (9%)	9 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	829/860 (96%)	761 (92%)	68 (8%)	11 22

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	74	LEU
1	A	77	ASP
1	A	79	VAL
1	A	82	HIS
1	A	106	GLN
1	A	115	LEU
1	A	126	ARG
1	A	134	ARG
1	A	161	LEU
1	A	207	CYS
1	A	208	LEU
1	A	210	SER
1	A	221	ASP
1	A	235	GLU
1	A	239	LYS
1	A	246	ARG
1	B	74	LEU
1	B	79	VAL
1	B	80	GLU
1	B	106	GLN
1	B	108	THR
1	B	115	LEU
1	B	123	HIS
1	B	145	MET
1	B	166	SER
1	B	179	GLU
1	B	192	THR
1	B	202	SER
1	B	210	SER
1	B	212	PHE
1	B	228	ARG
1	C	28	ASP
1	C	39	LEU
1	C	41	SER
1	C	59	ARG
1	C	62	GLU

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Mol	Chain	Res	Type
1	C	65	GLN
1	C	80	GLU
1	C	111	ARG
1	C	122	THR
1	C	126	ARG
1	C	168	LYS
1	C	200	MET
1	C	201	GLU
1	C	208	LEU
1	C	212	PHE
1	C	239	LYS
1	C	246	ARG
1	D	7	LEU
1	D	13	PRO
1	D	23	ARG
1	D	28	ASP
1	D	32	SER
1	D	62	GLU
1	D	77	ASP
1	D	91	ARG
1	D	112	ARG
1	D	122	THR
1	D	125	VAL
1	D	163	LEU
1	D	191	THR
1	D	208	LEU
1	D	212	PHE
1	D	220	ARG
1	D	225	GLU
1	D	227	ARG
1	D	230	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	B	92	HIS
1	B	204	GLN
1	D	195	GLN
1	D	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

There are no ligands in this entry.

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, 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	246/250 (98%)	-0.13	6 (2%) 59 62	21, 43, 77, 100	0
1	B	240/250 (96%)	-0.05	12 (5%) 28 30	21, 42, 82, 97	0
1	C	241/250 (96%)	-0.11	7 (2%) 51 55	24, 43, 73, 113	0
1	D	236/250 (94%)	-0.07	11 (4%) 31 33	19, 42, 76, 99	0
All	All	963/1000 (96%)	-0.09	36 (3%) 41 45	19, 42, 77, 113	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	ARG	5.3
1	B	242	TYR	4.5
1	C	123	HIS	4.3
1	B	191	THR	3.8
1	D	4	SER	3.8
1	D	192	THR	3.7
1	B	197	ARG	3.5
1	B	190	PRO	3.5
1	D	242	TYR	3.1
1	D	193	GLU	3.0
1	C	4	SER	2.9
1	B	201	GLU	2.8
1	A	201	GLU	2.8
1	D	197	ARG	2.8
1	C	117	HIS	2.8
1	B	118	ALA	2.8
1	A	119	GLU	2.7
1	B	196	ALA	2.7
1	D	91	ARG	2.6
1	D	191	THR	2.6
1	C	118	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	198	ALA	2.5
1	B	194	ASP	2.5
1	D	141	LEU	2.4
1	C	221	ASP	2.4
1	C	106	GLN	2.4
1	A	91	ARG	2.3
1	B	125	VAL	2.3
1	A	238	ALA	2.3
1	B	193	GLU	2.3
1	D	200	MET	2.2
1	B	241	LEU	2.2
1	B	239	LYS	2.1
1	C	121	ALA	2.0
1	D	238	ALA	2.0
1	D	239	LYS	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.