Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:23 PM GMT

PDB ID	:	3TKQ
Title	:	Crystal structure of full-length human peroxiredoxin 4 with mixed conformation
Authors	:	Wang, X.; Wang, L.; Wang, X.; Sun, F.; Wang, C.-C.
Deposited on	:	2011-08-28
Resolution	:	2.22 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:

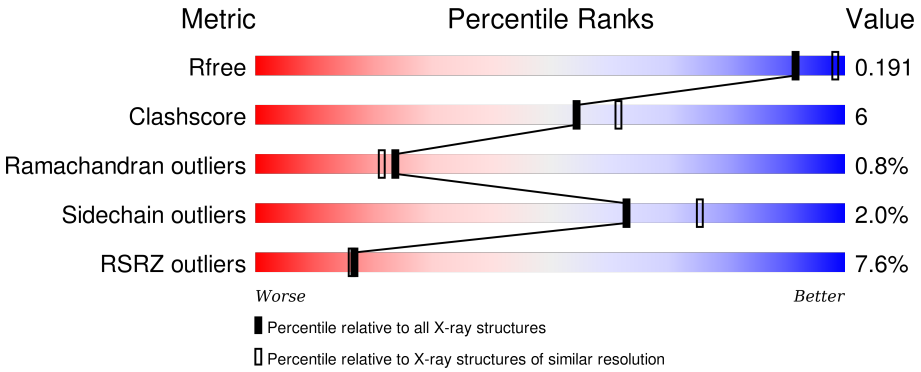
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.22 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	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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	246	14% 65% 11% • 22%
1	B	246	8% 65% 9% • 25%
1	C	246	2% 58% 8% • 33%
1	D	246	% 60% 6% • 33%
1	E	246	2% 57% 10% • 33%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7604 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-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	8	0
			1584	1030	259	291	4			
1	B	185	Total	C	N	O	S	0	8	0
			1540	999	253	284	4			
1	C	166	Total	C	N	O	S	0	8	0
			1407	913	232	259	3			
1	D	165	Total	C	N	O	S	0	1	0
			1339	866	223	248	2			
1	E	166	Total	C	N	O	S	0	7	0
			1398	908	231	256	3			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q13162
A	-10	ARG	-	EXPRESSION TAG	UNP Q13162
A	-9	GLY	-	EXPRESSION TAG	UNP Q13162
A	-8	SER	-	EXPRESSION TAG	UNP Q13162
A	-7	HIS	-	EXPRESSION TAG	UNP Q13162
A	-6	HIS	-	EXPRESSION TAG	UNP Q13162
A	-5	HIS	-	EXPRESSION TAG	UNP Q13162
A	-4	HIS	-	EXPRESSION TAG	UNP Q13162
A	-3	HIS	-	EXPRESSION TAG	UNP Q13162
A	-2	HIS	-	EXPRESSION TAG	UNP Q13162
A	-1	GLY	-	EXPRESSION TAG	UNP Q13162
A	0	SER	-	EXPRESSION TAG	UNP Q13162
B	-11	MET	-	EXPRESSION TAG	UNP Q13162
B	-10	ARG	-	EXPRESSION TAG	UNP Q13162
B	-9	GLY	-	EXPRESSION TAG	UNP Q13162
B	-8	SER	-	EXPRESSION TAG	UNP Q13162
B	-7	HIS	-	EXPRESSION TAG	UNP Q13162
B	-6	HIS	-	EXPRESSION TAG	UNP Q13162
B	-5	HIS	-	EXPRESSION TAG	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	EXPRESSION TAG	UNP Q13162
B	-3	HIS	-	EXPRESSION TAG	UNP Q13162
B	-2	HIS	-	EXPRESSION TAG	UNP Q13162
B	-1	GLY	-	EXPRESSION TAG	UNP Q13162
B	0	SER	-	EXPRESSION TAG	UNP Q13162
C	-11	MET	-	EXPRESSION TAG	UNP Q13162
C	-10	ARG	-	EXPRESSION TAG	UNP Q13162
C	-9	GLY	-	EXPRESSION TAG	UNP Q13162
C	-8	SER	-	EXPRESSION TAG	UNP Q13162
C	-7	HIS	-	EXPRESSION TAG	UNP Q13162
C	-6	HIS	-	EXPRESSION TAG	UNP Q13162
C	-5	HIS	-	EXPRESSION TAG	UNP Q13162
C	-4	HIS	-	EXPRESSION TAG	UNP Q13162
C	-3	HIS	-	EXPRESSION TAG	UNP Q13162
C	-2	HIS	-	EXPRESSION TAG	UNP Q13162
C	-1	GLY	-	EXPRESSION TAG	UNP Q13162
C	0	SER	-	EXPRESSION TAG	UNP Q13162
D	-11	MET	-	EXPRESSION TAG	UNP Q13162
D	-10	ARG	-	EXPRESSION TAG	UNP Q13162
D	-9	GLY	-	EXPRESSION TAG	UNP Q13162
D	-8	SER	-	EXPRESSION TAG	UNP Q13162
D	-7	HIS	-	EXPRESSION TAG	UNP Q13162
D	-6	HIS	-	EXPRESSION TAG	UNP Q13162
D	-5	HIS	-	EXPRESSION TAG	UNP Q13162
D	-4	HIS	-	EXPRESSION TAG	UNP Q13162
D	-3	HIS	-	EXPRESSION TAG	UNP Q13162
D	-2	HIS	-	EXPRESSION TAG	UNP Q13162
D	-1	GLY	-	EXPRESSION TAG	UNP Q13162
D	0	SER	-	EXPRESSION TAG	UNP Q13162
E	-11	MET	-	EXPRESSION TAG	UNP Q13162
E	-10	ARG	-	EXPRESSION TAG	UNP Q13162
E	-9	GLY	-	EXPRESSION TAG	UNP Q13162
E	-8	SER	-	EXPRESSION TAG	UNP Q13162
E	-7	HIS	-	EXPRESSION TAG	UNP Q13162
E	-6	HIS	-	EXPRESSION TAG	UNP Q13162
E	-5	HIS	-	EXPRESSION TAG	UNP Q13162
E	-4	HIS	-	EXPRESSION TAG	UNP Q13162
E	-3	HIS	-	EXPRESSION TAG	UNP Q13162
E	-2	HIS	-	EXPRESSION TAG	UNP Q13162
E	-1	GLY	-	EXPRESSION TAG	UNP Q13162
E	0	SER	-	EXPRESSION TAG	UNP Q13162

- Molecule 2 is water.

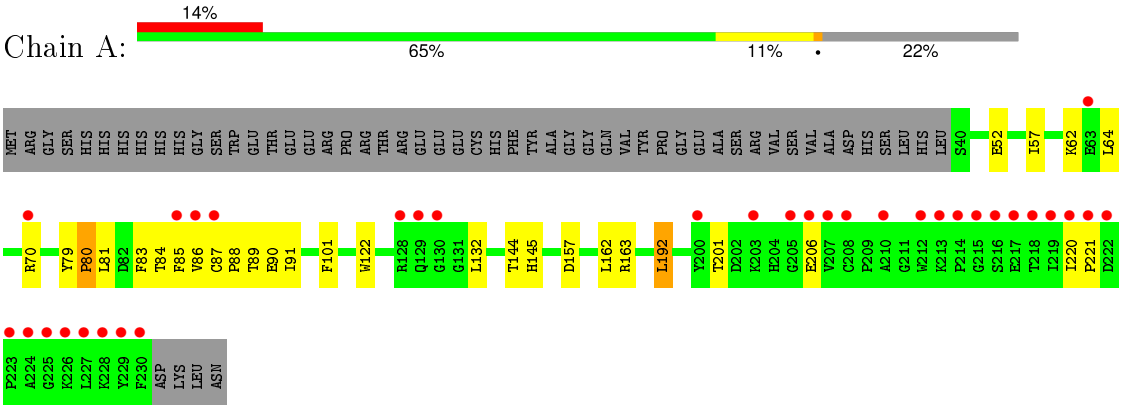
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	47	Total O 47 47	0	0
2	B	77	Total O 77 77	0	0
2	C	70	Total O 70 70	0	0
2	D	74	Total O 74 74	0	0
2	E	68	Total O 68 68	0	0

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.

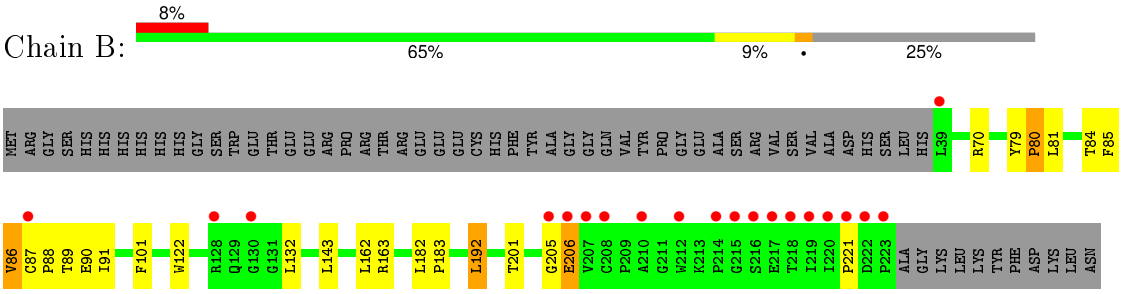
- Molecule 1: Peroxiredoxin-4

Chain A:



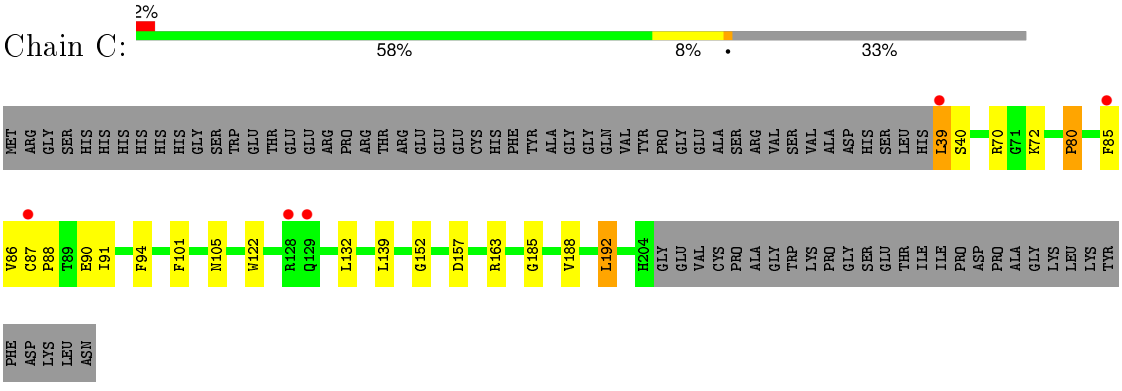
- Molecule 1: Peroxiredoxin-4

Chain B:



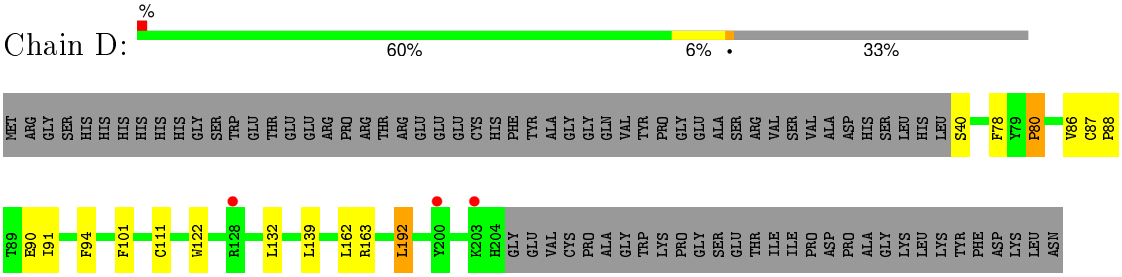
- Molecule 1: Peroxiredoxin-4

Chain C:



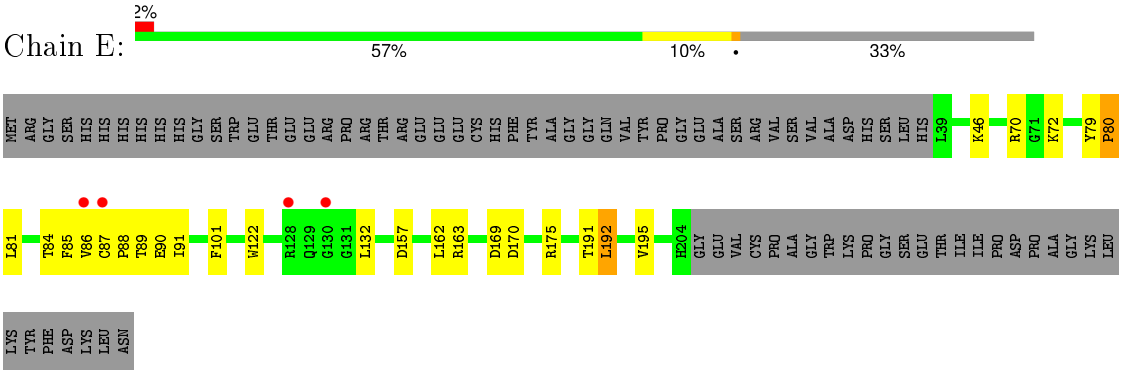
- Molecule 1: Peroxiredoxin-4

Chain D:



- Molecule 1: Peroxiredoxin-4

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.49Å 139.52Å 96.20Å 90.00° 103.38° 90.00°	Depositor
Resolution (Å)	38.86 – 2.22 38.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.86-2.22) 98.2 (38.86-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.186 , 0.224 0.184 , 0.191	Depositor DCC
R_{free} test set	3435 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 69604 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7604	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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

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	0.33	0/1631	0.50	0/2217
1	B	0.40	0/1585	0.55	0/2156
1	C	0.40	0/1443	0.56	0/1959
1	D	0.42	0/1375	0.57	0/1865
1	E	0.38	0/1434	0.55	0/1947
All	All	0.39	0/7468	0.55	0/10144

There are no bond length outliers.

There are no bond angle outliers.

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	1584	0	1565	22	0
1	B	1540	0	1525	20	0
1	C	1407	0	1394	18	0
1	D	1339	0	1329	12	0
1	E	1398	0	1388	21	0
2	A	47	0	0	0	0
2	B	77	0	0	1	0
2	C	70	0	0	1	0
2	D	74	0	0	1	0
2	E	68	0	0	1	0
All	All	7604	0	7201	93	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 6.

All (93) 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:D:80:PRO:HD2	1:D:87:CYS:SG	2.06	0.96
1:B:88[B]:PRO:HG3	1:B:122:TRP:HZ2	1.30	0.94
1:A:88[B]:PRO:HG3	1:A:122:TRP:HZ2	1.33	0.94
1:B:70:ARG:HD3	2:B:276:HOH:O	1.68	0.94
1:D:88:PRO:HG3	1:D:122:TRP:HZ2	1.36	0.90
1:A:80:PRO:HD2	1:A:87[B]:CYS:SG	2.19	0.83
1:A:88[B]:PRO:HG3	1:A:122:TRP:CZ2	2.13	0.83
1:B:88[B]:PRO:HG3	1:B:122:TRP:CZ2	2.13	0.81
1:B:87[B]:CYS:HB2	1:B:88[B]:PRO:HD3	1.64	0.80
1:C:80:PRO:HD2	1:C:87[B]:CYS:SG	2.22	0.79
1:C:88[B]:PRO:HG3	1:C:122:TRP:HZ2	1.49	0.77
1:E:88[B]:PRO:HG3	1:E:122:TRP:HZ2	1.49	0.77
1:D:88:PRO:HG3	1:D:122:TRP:CZ2	2.20	0.77
1:B:81:LEU:HB2	1:B:84[B]:THR:HG21	1.67	0.76
1:A:87[B]:CYS:HB2	1:A:88[B]:PRO:HD3	1.69	0.74
1:A:87[B]:CYS:O	1:A:91:ILE:HG13	1.88	0.73
1:B:80:PRO:HD2	1:B:87[B]:CYS:SG	2.29	0.71
1:A:86[B]:VAL:HB	1:A:163:ARG:NH2	2.05	0.71
1:E:88[B]:PRO:HG3	1:E:122:TRP:CZ2	2.25	0.70
1:E:87[B]:CYS:HB2	1:E:88[B]:PRO:HD3	1.71	0.70
1:C:39:LEU:HD13	1:C:40:SER:H	1.58	0.67
1:C:87[B]:CYS:O	1:C:91:ILE:HG13	1.94	0.66
1:B:87[B]:CYS:O	1:B:91:ILE:HG13	1.94	0.66
1:C:88[B]:PRO:HG3	1:C:122:TRP:CZ2	2.32	0.65
1:B:86[B]:VAL:HB	1:B:163:ARG:NH2	2.12	0.65
1:A:79:TYR:CD2	1:A:87[B]:CYS:HB3	2.33	0.64
1:D:40:SER:N	2:D:281:HOH:O	2.31	0.63
1:E:86[B]:VAL:HB	1:E:163:ARG:NH2	2.15	0.61
1:E:79:TYR:CD2	1:E:87[B]:CYS:HB3	2.36	0.61
1:C:86[B]:VAL:HB	1:C:163:ARG:NH2	2.16	0.60
1:E:87[B]:CYS:O	1:E:91:ILE:HG13	2.02	0.59
1:C:87[B]:CYS:HB2	1:C:88[B]:PRO:HD3	1.84	0.58
1:C:39:LEU:CD1	1:C:40:SER:H	2.17	0.56
1:D:87:CYS:HB2	1:D:88:PRO:HD3	1.87	0.55
1:D:101:PHE:CE2	1:D:192:LEU:HD13	2.42	0.54
1:B:81:LEU:HB2	1:B:84[B]:THR:CG2	2.37	0.54
1:B:79:TYR:CD2	1:B:87[B]:CYS:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:CYS:O	1:D:91:ILE:HG13	2.08	0.53
1:C:101:PHE:CE2	1:C:192:LEU:HD13	2.44	0.53
1:E:90:GLU:OE1	1:E:163:ARG:NH1	2.41	0.53
1:A:101:PHE:CE2	1:A:192:LEU:HD13	2.44	0.53
1:A:85[B]:PHE:O	1:A:88[B]:PRO:HD2	2.09	0.53
1:B:101:PHE:CE2	1:B:192:LEU:HD13	2.45	0.51
1:E:85[B]:PHE:O	1:E:88[B]:PRO:HD2	2.12	0.49
1:E:101:PHE:CE2	1:E:192:LEU:HD13	2.48	0.49
1:A:57:ILE:HD12	1:A:62:LYS:HB2	1.95	0.49
1:B:205:GLY:O	1:B:206:GLU:C	2.50	0.49
1:D:86:VAL:HB	1:D:163:ARG:NH2	2.28	0.48
1:D:90:GLU:O	1:D:94:PHE:HD2	1.97	0.47
1:A:144:THR:O	1:A:145:HIS:HB2	2.14	0.47
1:B:206:GLU:HA	1:B:221:PRO:HD3	1.95	0.47
1:D:78:PHE:HA	1:D:111:CYS:O	2.15	0.47
1:C:85[B]:PHE:O	1:C:88[B]:PRO:HD2	2.15	0.47
1:E:191:THR:O	1:E:195:VAL:HG23	2.15	0.46
1:E:70:ARG:HD3	2:E:278:HOH:O	2.14	0.46
1:A:83[A]:PHE:CZ	1:A:122:TRP:HA	2.49	0.46
1:E:72:LYS:O	1:E:170:ASP:HA	2.16	0.46
1:A:81:LEU:HB2	1:A:84[B]:THR:HG21	1.97	0.46
1:A:87[A]:CYS:HA	1:A:88[A]:PRO:HD3	1.81	0.46
1:E:80:PRO:HD2	1:E:87[B]:CYS:SG	2.56	0.46
1:B:89[B]:THR:OG1	1:B:90:GLU:N	2.49	0.46
1:B:87[B]:CYS:HB2	1:B:88[B]:PRO:CD	2.40	0.45
1:C:188:VAL:HG12	1:C:192:LEU:HD22	1.97	0.45
1:E:101:PHE:CZ	1:E:192:LEU:HD13	2.51	0.45
1:C:132:LEU:CD1	1:C:139:LEU:HD11	2.46	0.45
1:B:85[B]:PHE:O	1:B:88[B]:PRO:HD2	2.16	0.45
1:C:40:SER:HB2	1:C:152:GLY:HA3	1.99	0.44
1:C:72:LYS:HG2	1:C:105:ASN:OD1	2.17	0.44
1:C:90[B]:GLU:OE2	1:C:185:GLY:HA2	2.17	0.44
1:A:70:ARG:HA	1:A:70:ARG:HD2	1.82	0.44
1:E:87[B]:CYS:N	1:E:88[B]:PRO:CD	2.81	0.44
1:B:182:LEU:N	1:B:183:PRO:CD	2.80	0.44
1:D:80:PRO:CD	1:D:87:CYS:SG	2.92	0.44
1:A:81:LEU:O	1:A:84[B]:THR:OG1	2.23	0.44
1:A:86[B]:VAL:HB	1:A:163:ARG:CZ	2.49	0.43
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.85	0.43
1:E:81:LEU:HB2	1:E:84[B]:THR:HG21	1.99	0.43
1:A:201:THR:HG22	1:A:206:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:OE1	1:A:163:ARG:NH1	2.51	0.42
1:E:85[B]:PHE:C	1:E:88[B]:PRO:HD2	2.40	0.42
1:B:201:THR:HG22	1:B:206:GLU:O	2.19	0.42
1:B:132:LEU:HD23	1:B:132:LEU:HA	1.88	0.42
1:E:132:LEU:HA	1:E:132:LEU:HD23	1.86	0.42
1:C:90[B]:GLU:O	1:C:94:PHE:HD2	2.03	0.41
1:A:220:ILE:HA	1:A:221:PRO:HD3	1.75	0.41
1:D:132:LEU:CD1	1:D:139:LEU:HD11	2.51	0.41
1:C:70:ARG:HD2	1:C:70:ARG:HA	1.91	0.41
1:B:87[A]:CYS:HA	1:B:88[A]:PRO:HD3	1.79	0.41
1:E:89[B]:THR:OG1	1:E:90:GLU:N	2.53	0.40
1:A:52:GLU:HA	1:A:64:LEU:O	2.22	0.40
1:E:46:LYS:HA	1:E:46:LYS:HD2	1.86	0.40
1:C:70:ARG:HD3	2:C:247:HOH:O	2.21	0.40
1:E:169:ASP:OD2	1:E:175:ARG:HD3	2.22	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	197/246 (80%)	181 (92%)	13 (7%)	3 (2%)	13 9
1	B	191/246 (78%)	174 (91%)	15 (8%)	2 (1%)	19 16
1	C	172/246 (70%)	162 (94%)	9 (5%)	1 (1%)	30 29
1	D	164/246 (67%)	157 (96%)	6 (4%)	1 (1%)	30 29
1	E	171/246 (70%)	159 (93%)	11 (6%)	1 (1%)	30 29
All	All	895/1230 (73%)	833 (93%)	54 (6%)	8 (1%)	24 18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89[A]	THR
1	A	89[B]	THR
1	B	80	PRO
1	C	80	PRO
1	B	206	GLU
1	D	80	PRO
1	A	80	PRO
1	E	80	PRO

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	173/213 (81%)	170 (98%)	3 (2%)	68 80
1	B	170/213 (80%)	165 (97%)	5 (3%)	50 61
1	C	155/213 (73%)	152 (98%)	3 (2%)	65 77
1	D	147/213 (69%)	145 (99%)	2 (1%)	74 85
1	E	154/213 (72%)	151 (98%)	3 (2%)	65 77
All	All	799/1065 (75%)	783 (98%)	16 (2%)	63 75

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ASP
1	A	162	LEU
1	A	192	LEU
1	B	86[A]	VAL
1	B	86[B]	VAL
1	B	143	LEU
1	B	162	LEU
1	B	192	LEU
1	C	39	LEU
1	C	157	ASP
1	C	192	LEU
1	D	162	LEU

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Mol	Chain	Res	Type
1	D	192	LEU
1	E	157	ASP
1	E	162	LEU
1	E	192	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	204	HIS
1	C	204	HIS

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	191/246 (77%)	0.54	34 (17%)	2	2	36, 49, 81, 96	0
1	B	185/246 (75%)	0.38	20 (10%)	8	7	28, 39, 79, 101	0
1	C	166/246 (67%)	0.01	5 (3%)	54	53	29, 40, 59, 94	0
1	D	165/246 (67%)	-0.14	3 (1%)	71	70	31, 41, 59, 94	0
1	E	166/246 (67%)	-0.02	4 (2%)	62	61	31, 40, 62, 101	0
All	All	873/1230 (70%)	0.17	66 (7%)	17	16	28, 42, 75, 101	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	PRO	10.8
1	E	87[A]	CYS	7.8
1	B	222	ASP	7.4
1	A	87[A]	CYS	6.4
1	B	87[A]	CYS	6.0
1	B	128	ARG	5.4
1	B	214	PRO	5.2
1	B	221	PRO	5.1
1	B	220	ILE	5.1
1	A	220	ILE	4.9
1	E	128	ARG	4.9
1	A	212	TRP	4.8
1	A	128	ARG	4.8
1	A	206	GLU	4.7
1	C	87[A]	CYS	4.6
1	B	206	GLU	4.6
1	A	225	GLY	4.5
1	B	215	GLY	4.5
1	B	39	LEU	4.4
1	A	224	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	217	GLU	4.4
1	A	221	PRO	4.3
1	A	214	PRO	4.2
1	A	215	GLY	4.1
1	A	227	LEU	4.0
1	A	226	LYS	4.0
1	A	217	GLU	3.8
1	E	86[A]	VAL	3.6
1	B	212	TRP	3.5
1	B	210	ALA	3.5
1	A	216	SER	3.4
1	C	85[A]	PHE	3.4
1	B	218	THR	3.3
1	A	205	GLY	3.2
1	B	216	SER	3.2
1	A	208	CYS	3.1
1	B	219	ILE	3.1
1	B	208	CYS	3.0
1	C	128	ARG	3.0
1	A	228	LYS	3.0
1	A	222	ASP	3.0
1	A	218	THR	3.0
1	A	200	TYR	2.9
1	A	207	VAL	2.9
1	A	229	TYR	2.9
1	A	203	LYS	2.7
1	B	207	VAL	2.7
1	C	39	LEU	2.7
1	E	130	GLY	2.6
1	D	203	LYS	2.6
1	A	129	GLN	2.6
1	D	200	TYR	2.5
1	A	210	ALA	2.5
1	A	219	ILE	2.5
1	A	86[A]	VAL	2.3
1	A	130	GLY	2.3
1	A	63	GLU	2.2
1	A	85[A]	PHE	2.2
1	D	128	ARG	2.2
1	C	129	GLN	2.2
1	A	70	ARG	2.2
1	A	213	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	205	GLY	2.1
1	B	130	GLY	2.1
1	A	223	PRO	2.1
1	A	230	PHE	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.