Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 05:32 AM EDT

PDB ID	:	3TKS
Title	:	Crystal structure of full-length human peroxiredoxin 4 in three different redox states
Authors	:	Wang, X.; Wang, L.; Wang, X.; Sun, F.; Wang, C.-C.
Deposited on	:	2011-08-28
Resolution	:	2.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

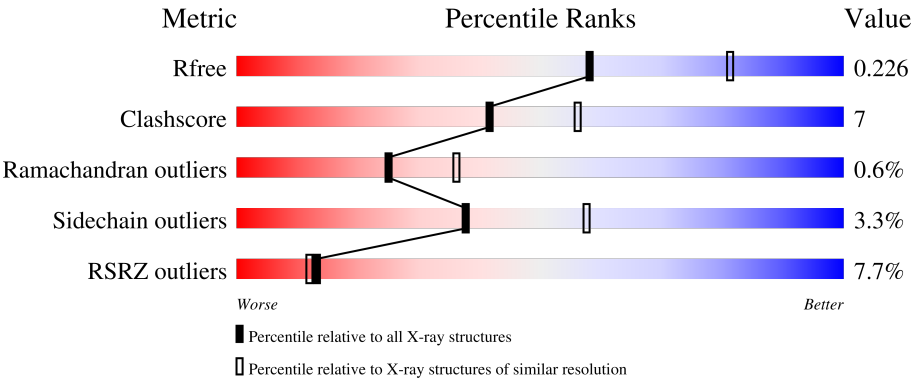
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	2% 68% 11% • 20%
1	B	246	4% 59% 20% • 20%
2	C	246	8% 67% 12% • 20%
2	D	246	7% 65% 14% • 20%
3	E	246	10% 70% 9% • 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSO	B	87	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8468 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	197	Total	C	N	O	S	0	4	0
			1605	1040	267	295	3			
1	B	197	Total	C	N	O	S	0	3	0
			1600	1035	267	295	3			

There are 24 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
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

- Molecule 2 is a protein called Peroxiredoxin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	197	Total	C	N	O	S	0	3	0
			1594	1031	264	296	3			
2	D	197	Total	C	N	O	S	0	4	0
			1598	1034	265	296	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

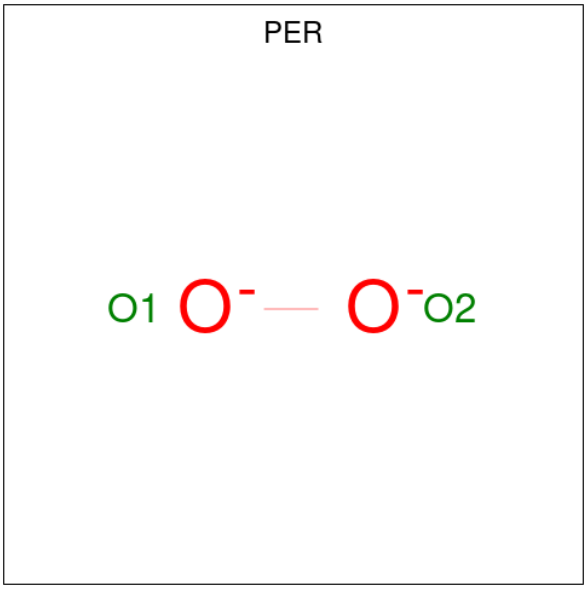
- Molecule 3 is a protein called Peroxiredoxin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	197	Total	C	N	O	S	0	2	0
			1590	1029	264	294	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 4 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 2 2	0	0
4	C	1	Total O 2 2	0	0
4	D	1	Total O 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	108	Total O 108 108	0	0

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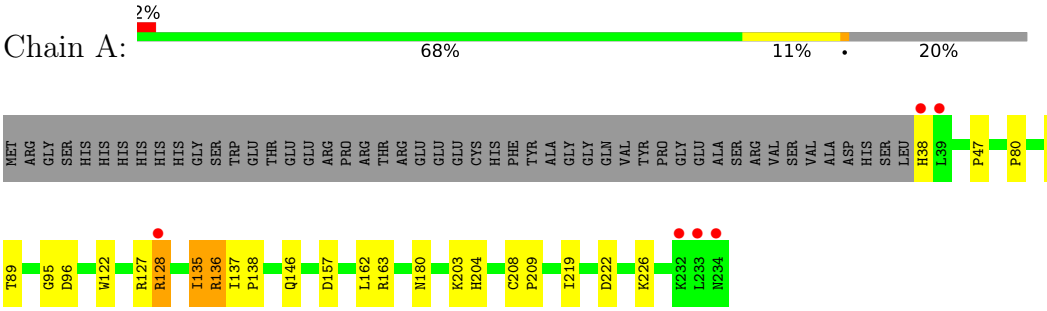
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	100	Total O 100 100	0	0
5	C	117	Total O 117 117	0	0
5	D	99	Total O 99 99	0	0
5	E	51	Total O 51 51	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

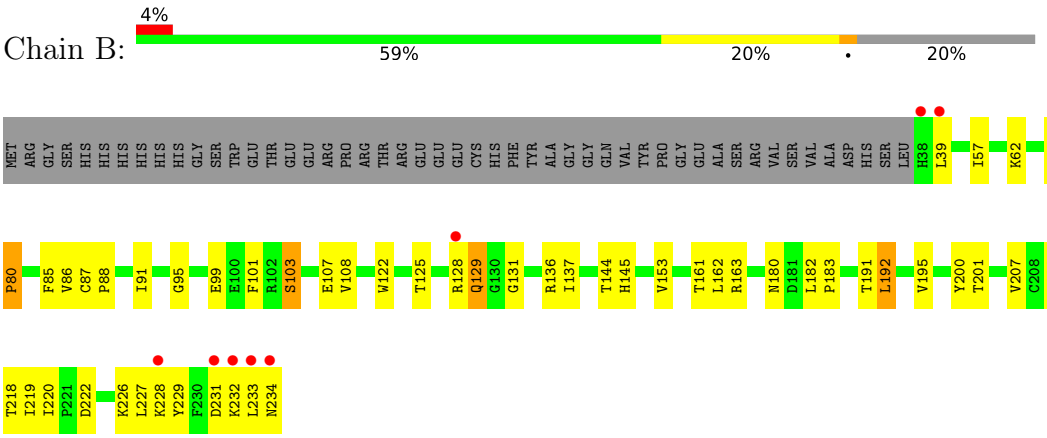
• Molecule 1: Peroxiredoxin-4

Chain A:



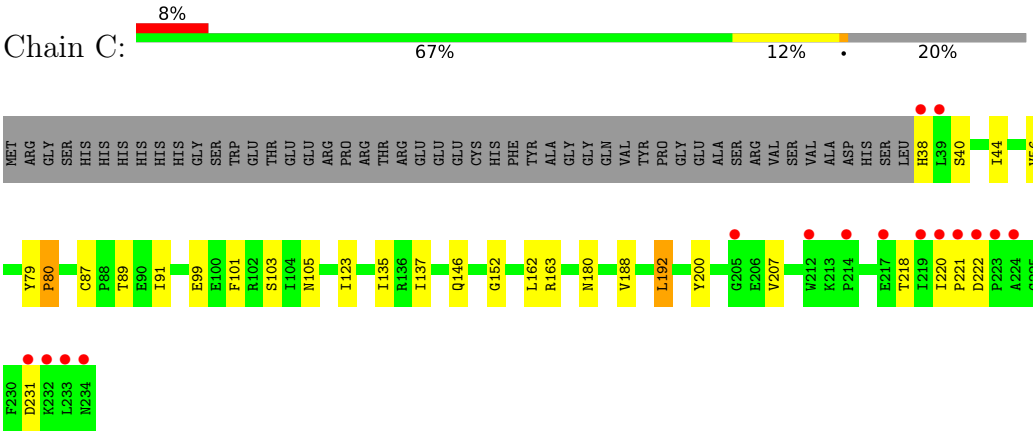
• Molecule 1: Peroxiredoxin-4

Chain B:



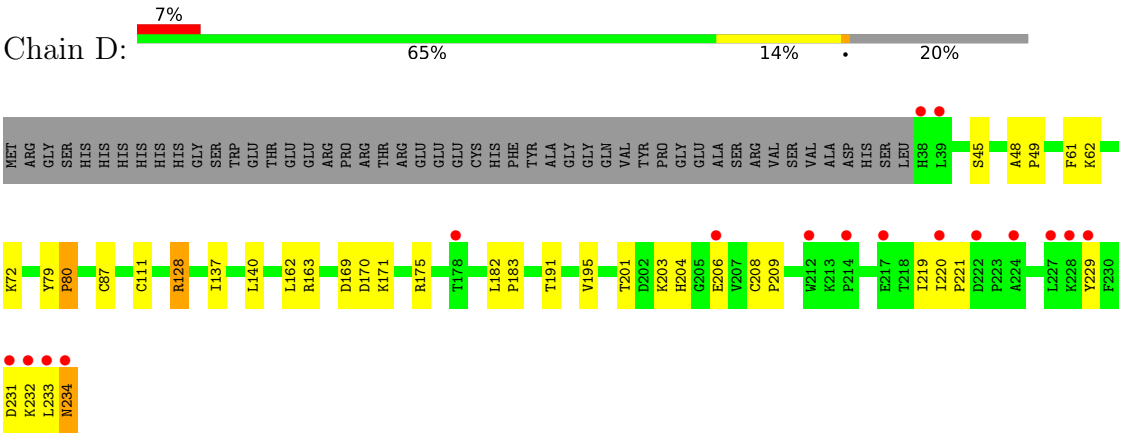
• Molecule 2: Peroxiredoxin-4

Chain C:



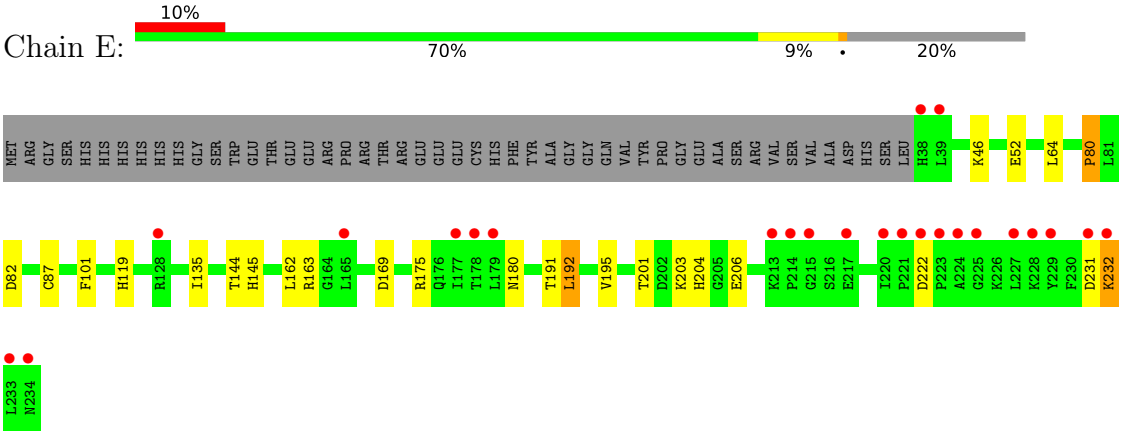
• Molecule 2: Peroxiredoxin-4

Chain D:



• Molecule 3: 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	183.18Å 140.10Å 61.50Å 90.00° 102.48° 90.00°	Depositor
Resolution (Å)	30.52 – 2.40 35.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.52-2.40) 97.1 (35.03-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.183 , 0.232 0.179 , 0.226	Depositor DCC
R_{free} test set	2895 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8468	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.44	0/1651	0.56	0/2236
1	B	0.42	0/1640	0.55	0/2222
2	C	0.43	0/1637	0.57	0/2219
2	D	0.43	0/1644	0.56	0/2231
3	E	0.37	0/1638	0.52	0/2221
All	All	0.42	0/8210	0.55	0/11129

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	1605	0	1605	26	0
1	B	1600	0	1590	33	0
2	C	1594	0	1584	18	0
2	D	1598	0	1584	21	0
3	E	1590	0	1576	13	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	108	0	0	1	0
5	B	100	0	0	3	0
5	C	117	0	0	2	0
5	D	99	0	0	0	0
5	E	51	0	0	1	0
All	All	8468	0	7939	111	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 7.

All (111) 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:136[A]:ARG:H	1:A:136[A]:ARG:HD2	1.09	1.15
1:B:80:PRO:HD2	1:B:87:CSO:OD	1.75	0.85
2:C:80:PRO:HD2	2:C:87:CSD:OD1	1.78	0.83
1:B:91:ILE:HG23	1:B:137[B]:ILE:HD11	1.61	0.82
1:B:233:LEU:O	1:B:234:ASN:O	1.96	0.82
1:A:95:GLY:HA3	1:A:136[A]:ARG:NH1	1.96	0.80
2:D:80:PRO:HD2	2:D:87:CSD:OD1	1.81	0.80
1:A:80:PRO:HD2	1:A:87:CSO:OD	1.82	0.79
2:D:233:LEU:O	2:D:234:ASN:HB2	1.86	0.75
2:C:79:TYR:HB2	2:C:87:CSD:OD1	1.87	0.74
1:A:38:HIS:NE2	1:A:146[A]:GLN:NE2	2.35	0.73
1:A:136[A]:ARG:H	1:A:136[A]:ARG:CD	1.92	0.73
1:A:88:PRO:HG3	1:A:122:TRP:HZ2	1.57	0.70
1:B:85:PHE:O	1:B:88:PRO:HD2	1.91	0.70
1:A:87:CSO:HB3	1:A:88:PRO:HD3	1.73	0.69
2:C:101:PHE:CE2	2:C:192:LEU:HD13	2.28	0.69
1:B:201:THR:HG23	5:B:241:HOH:O	1.93	0.68
1:A:127:ARG:H	1:A:128:ARG:NH2	1.92	0.67
3:E:135:ILE:HD12	5:E:284:HOH:O	1.99	0.63
1:A:95:GLY:HA3	1:A:136[A]:ARG:HH11	1.61	0.62
1:A:86:VAL:HB	1:A:163:ARG:NH2	2.14	0.62
2:D:79:TYR:HB2	2:D:87:CSD:OD1	2.00	0.61
2:C:200:TYR:CE1	2:C:218:THR:HG21	2.36	0.61
2:C:163:ARG:HB2	2:C:180:ASN:HB2	1.81	0.61
1:B:86:VAL:HB	1:B:163:ARG:NH2	2.16	0.60
2:C:188:VAL:HG12	2:C:192:LEU:HD22	1.83	0.59
1:A:127:ARG:HG3	1:A:128:ARG:HH21	1.69	0.57
1:B:87:CSO:HB3	1:B:88:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PRO:HD2	1:B:87:CSO:HD	1.68	0.56
1:B:128:ARG:HB2	1:B:129:GLN:NE2	2.20	0.56
3:E:201:THR:HG22	3:E:206:GLU:O	2.05	0.56
1:A:135:ILE:HD12	1:A:136[A]:ARG:NH1	2.20	0.55
1:B:88:PRO:HG3	1:B:122:TRP:HZ2	1.72	0.55
3:E:231:ASP:O	3:E:232:LYS:HG2	2.06	0.55
1:B:108:VAL:O	1:B:137[A]:ILE:HG23	2.07	0.55
3:E:163:ARG:HB2	3:E:180:ASN:HB2	1.89	0.55
2:C:207:VAL:HG13	2:C:221:PRO:HG3	1.88	0.54
1:A:96:ASP:OD1	1:A:136[A]:ARG:NH2	2.41	0.54
1:A:88:PRO:HG3	1:A:122:TRP:CZ2	2.41	0.53
2:D:111:CYS:HB2	2:D:140:LEU:HB3	1.91	0.52
2:D:231:ASP:C	2:D:233:LEU:H	2.12	0.52
1:A:47:PRO:HB3	5:A:321:HOH:O	2.10	0.52
2:D:128:ARG:HB3	2:D:128:ARG:NH1	2.24	0.51
1:B:191:THR:O	1:B:195:VAL:HG23	2.12	0.50
2:C:101:PHE:CZ	2:C:192:LEU:HD13	2.46	0.50
1:A:137:ILE:HG22	1:A:138:PRO:O	2.11	0.50
2:C:91:ILE:HG23	2:C:137:ILE:HD11	1.94	0.50
2:D:219:ILE:HG12	2:D:229:TYR:CG	2.46	0.50
1:B:99:GLU:O	1:B:103:SER:HB3	2.12	0.50
2:D:169:ASP:OD2	2:D:175:ARG:HD3	2.12	0.50
1:B:222:ASP:O	1:B:226:LYS:HB3	2.12	0.50
1:B:228:LYS:O	1:B:232:LYS:HD3	2.12	0.49
1:A:163:ARG:HB2	1:A:180:ASN:HB2	1.94	0.49
3:E:191:THR:O	3:E:195:VAL:HG23	2.13	0.48
1:A:135:ILE:CD1	1:A:136[A]:ARG:NH1	2.77	0.47
1:A:128:ARG:H	1:A:128:ARG:NE	2.12	0.47
1:A:85:PHE:O	1:A:88:PRO:HD2	2.15	0.47
2:C:99:GLU:O	2:C:103[B]:SER:HB3	2.15	0.47
3:E:80:PRO:HD2	3:E:87:CYS:SG	2.54	0.47
2:C:40:SER:HB2	2:C:152:GLY:HA3	1.97	0.47
2:C:135:ILE:HD12	5:C:291:HOH:O	2.14	0.47
1:B:128:ARG:HB2	1:B:129:GLN:HE21	1.79	0.47
3:E:101:PHE:CE2	3:E:192:LEU:HD13	2.50	0.47
2:D:201:THR:HG22	2:D:206:GLU:O	2.15	0.46
2:D:231:ASP:O	2:D:233:LEU:N	2.45	0.46
2:C:38:HIS:NE2	2:C:146:GLN:NE2	2.59	0.46
1:B:57:ILE:HD12	1:B:62:LYS:HB2	1.97	0.46
2:D:128:ARG:HB3	2:D:128:ARG:HH11	1.80	0.45
1:B:207:VAL:O	1:B:209:PRO:HD3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:TYR:CE1	1:B:218:THR:HG21	2.51	0.45
2:D:72:LYS:O	2:D:170:ASP:HA	2.17	0.45
3:E:52:GLU:HA	3:E:64:LEU:O	2.17	0.45
1:B:233:LEU:O	1:B:234:ASN:C	2.53	0.44
3:E:169:ASP:OD2	3:E:175:ARG:HD3	2.17	0.44
2:C:220:ILE:HA	2:C:221:PRO:HD3	1.75	0.44
2:D:208:CYS:HA	2:D:209:PRO:HD3	1.86	0.44
1:B:72:LYS:HD3	1:B:107:GLU:HG2	2.00	0.44
1:B:87:CSO:O	1:B:91:ILE:HG13	2.18	0.44
1:B:125:THR:HG22	1:B:131:GLY:HA3	2.00	0.44
3:E:101:PHE:CZ	3:E:192:LEU:HD13	2.53	0.43
1:B:144:THR:O	1:B:145:HIS:HB2	2.19	0.43
2:C:137:ILE:O	2:C:137:ILE:HG13	2.18	0.43
2:D:48:ALA:O	2:D:49:PRO:C	2.56	0.43
1:A:222:ASP:O	1:A:226:LYS:HB3	2.19	0.43
2:D:182:LEU:N	2:D:183:PRO:CD	2.81	0.43
1:B:220:ILE:HD12	5:B:271:HOH:O	2.19	0.43
2:D:61:PHE:O	2:D:62:LYS:HD3	2.18	0.43
2:D:220:ILE:HA	2:D:221:PRO:HD3	1.83	0.42
1:A:209:PRO:HG3	1:A:219:ILE:HG13	2.00	0.42
1:B:219:ILE:HG12	1:B:229:TYR:CG	2.54	0.42
2:D:182:LEU:N	2:D:183:PRO:HD3	2.34	0.42
1:B:95:GLY:N	1:B:137[A]:ILE:HD11	2.34	0.42
1:B:182:LEU:N	1:B:183:PRO:CD	2.83	0.42
2:C:56:VAL:HG11	2:C:123:ILE:HD12	2.00	0.42
2:D:191:THR:O	2:D:195:VAL:HG23	2.19	0.42
2:C:70:ARG:HD3	5:C:424:HOH:O	2.20	0.42
1:A:208:CYS:HA	1:A:209:PRO:HD3	1.90	0.42
1:A:38:HIS:CD2	1:A:146[A]:GLN:HE22	2.31	0.42
1:B:227:LEU:O	1:B:231:ASP:HB3	2.20	0.42
3:E:203:LYS:HD2	3:E:204:HIS:CE1	2.55	0.42
1:B:101:PHE:CE2	1:B:192:LEU:HD13	2.55	0.41
3:E:144:THR:O	3:E:145:HIS:HB2	2.20	0.41
1:B:163:ARG:HB2	1:B:180:ASN:HB2	2.03	0.41
2:C:72:LYS:HG2	2:C:105:ASN:OD1	2.20	0.41
1:A:203:LYS:HG2	1:A:204:HIS:CE1	2.56	0.41
2:D:87:CSD:OD1	2:D:163:ARG:NH1	2.50	0.41
2:D:203:LYS:HD3	2:D:204:HIS:NE2	2.35	0.40
3:E:82:ASP:OD2	3:E:119:HIS:ND1	2.51	0.40
1:B:153:VAL:O	1:B:161:THR:HA	2.22	0.40
1:B:70:ARG:HD3	5:B:286:HOH:O	2.20	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	198/246 (80%)	192 (97%)	6 (3%)	0	100	100
1	B	197/246 (80%)	190 (96%)	6 (3%)	1 (0%)	29	41
2	C	197/246 (80%)	190 (96%)	6 (3%)	1 (0%)	29	41
2	D	198/246 (80%)	189 (96%)	7 (4%)	2 (1%)	15	23
3	E	197/246 (80%)	188 (95%)	7 (4%)	2 (1%)	15	23
All	All	987/1230 (80%)	949 (96%)	32 (3%)	6 (1%)	25	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	PRO
2	C	80	PRO
2	D	80	PRO
2	D	232	LYS
3	E	232	LYS
3	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	175/212 (82%)	167 (95%)	8 (5%)	27	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	173/212 (82%)	166 (96%)	7 (4%)	31 49
2	C	173/212 (82%)	167 (96%)	6 (4%)	36 55
2	D	173/212 (82%)	167 (96%)	6 (4%)	36 55
3	E	173/213 (81%)	169 (98%)	4 (2%)	50 70
All	All	867/1061 (82%)	836 (96%)	31 (4%)	38 54

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	THR
1	A	128	ARG
1	A	135	ILE
1	A	136[A]	ARG
1	A	136[B]	ARG
1	A	157[A]	ASP
1	A	157[B]	ASP
1	A	162	LEU
1	B	39	LEU
1	B	103	SER
1	B	129	GLN
1	B	136[A]	ARG
1	B	136[B]	ARG
1	B	162	LEU
1	B	192	LEU
2	C	44	ILE
2	C	89	THR
2	C	162	LEU
2	C	192	LEU
2	C	222	ASP
2	C	231	ASP
2	D	45	SER
2	D	128	ARG
2	D	137	ILE
2	D	162	LEU
2	D	171	LYS
2	D	234	ASN
3	E	46	LYS
3	E	162	LEU
3	E	192	LEU
3	E	222	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	B	129	GLN
3	E	145	HIS
3	E	204	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CSD	C	87	2	3,7,8	1.08	0	1,8,10	0.88	0
1	CSO	A	87	1	3,6,7	0.62	0	0,6,8	-	-
2	CSD	D	87	2	3,7,8	1.10	0	1,8,10	0.35	0
1	CSO	B	87	1	3,6,7	0.62	0	0,6,8	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSD	C	87	2	-	0/2/6/8	-
1	CSO	A	87	1	-	0/1/5/7	-
2	CSD	D	87	2	-	0/2/6/8	-
1	CSO	B	87	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	87	CSD	2	0
1	A	87	CSO	2	0
2	D	87	CSD	3	0
1	B	87	CSO	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
4	PER	C	235	-	0,1,1	-	-	-		
4	PER	A	235	-	0,1,1	-	-	-		
4	PER	D	235	-	0,1,1	-	-	-		

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	196/246 (79%)	-0.17	6 (3%) 49 47	21, 33, 49, 74	0
1	B	196/246 (79%)	0.11	9 (4%) 32 31	21, 35, 56, 76	0
2	C	196/246 (79%)	0.12	20 (10%) 6 6	19, 31, 85, 106	0
2	D	196/246 (79%)	0.09	17 (8%) 10 9	20, 31, 77, 98	0
3	E	197/246 (80%)	0.48	24 (12%) 4 3	27, 45, 92, 108	0
All	All	981/1230 (79%)	0.13	76 (7%) 13 12	19, 35, 76, 108	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	LEU	7.2
2	C	232	LYS	6.9
3	E	233	LEU	6.1
2	C	233	LEU	6.0
2	D	232	LYS	5.9
1	B	232	LYS	5.8
3	E	38	HIS	5.7
2	D	38	HIS	5.6
3	E	234	ASN	5.5
1	B	38	HIS	5.3
1	B	39	LEU	5.2
2	D	233	LEU	5.2
3	E	232	LYS	5.2
2	D	234	ASN	5.0
2	D	231	ASP	4.9
2	C	227	LEU	4.8
1	A	233	LEU	4.7
2	C	234	ASN	4.7
2	C	231	ASP	4.6
3	E	231	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	C	228	LYS	4.6
2	C	39	LEU	4.4
2	D	39	LEU	4.2
2	D	228	LYS	4.2
2	D	227	LEU	4.1
3	E	227	LEU	4.0
3	E	229	TYR	4.0
1	B	234	ASN	3.8
2	C	221	PRO	3.7
2	D	224	ALA	3.7
2	C	38	HIS	3.7
2	D	214	PRO	3.6
1	A	39	LEU	3.6
2	C	229	TYR	3.5
1	A	38	HIS	3.5
3	E	178	THR	3.3
1	B	231	ASP	3.3
2	C	222	ASP	3.3
3	E	228	LYS	3.3
1	A	234	ASN	3.2
3	E	217	GLU	3.1
3	E	39	LEU	3.1
2	D	220	ILE	3.1
2	C	226	LYS	3.0
2	C	214	PRO	3.0
3	E	177	ILE	3.0
1	B	128	ARG	2.9
2	D	217	GLU	2.9
2	C	205	GLY	2.8
3	E	213	LYS	2.7
2	C	212	TRP	2.7
3	E	214	PRO	2.7
1	A	232	LYS	2.7
3	E	224	ALA	2.7
3	E	128	ARG	2.7
1	B	228	LYS	2.6
3	E	221	PRO	2.5
3	E	220	ILE	2.5
1	B	216	SER	2.5
3	E	223	PRO	2.5
1	A	128	ARG	2.4
2	D	222	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	165	LEU	2.4
2	D	206	GLU	2.3
2	C	224	ALA	2.3
3	E	179	LEU	2.3
3	E	215	GLY	2.3
2	D	178	THR	2.2
2	D	229	TYR	2.2
2	C	220	ILE	2.2
3	E	225	GLY	2.2
3	E	222	ASP	2.1
2	C	223	PRO	2.1
2	D	212	TRP	2.1
2	C	217	GLU	2.1
2	C	219	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
1	CSO	B	87	7/8	0.90	0.19	44,47,47,48	0
1	CSO	A	87	7/8	0.96	0.12	40,43,43,44	0
2	CSD	C	87	8/9	0.97	0.12	34,35,36,36	0
2	CSD	D	87	8/9	0.98	0.10	30,30,32,34	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	PER	C	235	2/2	0.87	0.21	50,50,50,51	0
4	PER	A	235	2/2	0.90	0.20	56,56,56,56	0
4	PER	D	235	2/2	0.96	0.12	40,40,40,41	0

6.5 Other polymers (i)

There are no such residues in this entry.