Full wwPDB X-ray Structure Validation Report (i)

Sep 4, 2023 – 08:52 PM EDT

PDB ID	:	3TJF
Title	:	Crystal Structure of human peroxiredoxin IV C51A mutant in reduced form
Authors	:	Cao, Z.; Tavender, T.J.; Roszak, A.W.; Cogdell, R.J.; Bulleid, N.J.
Deposited on	:	2011-08-24
Resolution	:	2.04 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 (i) 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 (1)) were used in the production of this report:

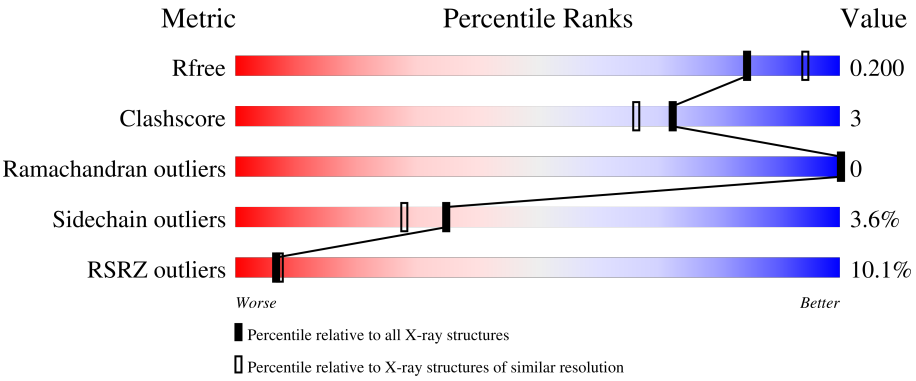
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	254	8% 68% 7% • 23%
1	B	254	5% 71% 5% 23%
1	C	254	8% 69% 8% • 23%
1	D	254	7% 70% 6% 24%
1	E	254	10% 69% 7% • 23%

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	SO4	D	463	-	-	-	X
2	SO4	D	464	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8896 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	195	Total	C	N	O	S	0	6	0
			1598	1036	261	298	3			
1	B	195	Total	C	N	O	S	0	6	0
			1601	1038	263	297	3			
1	C	196	Total	C	N	O	S	0	7	0
			1617	1047	265	302	3			
1	D	194	Total	C	N	O	S	0	7	0
			1597	1035	262	297	3			
1	E	196	Total	C	N	O	S	0	8	0
			1614	1046	262	303	3			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	expression tag	UNP Q13162
A	19	GLY	-	expression tag	UNP Q13162
A	20	SER	-	expression tag	UNP Q13162
A	21	SER	-	expression tag	UNP Q13162
A	22	HIS	-	expression tag	UNP Q13162
A	23	HIS	-	expression tag	UNP Q13162
A	24	HIS	-	expression tag	UNP Q13162
A	25	HIS	-	expression tag	UNP Q13162
A	26	HIS	-	expression tag	UNP Q13162
A	27	HIS	-	expression tag	UNP Q13162
A	28	SER	-	expression tag	UNP Q13162
A	29	GLN	-	expression tag	UNP Q13162
A	30	ASP	-	expression tag	UNP Q13162
A	31	PRO	-	expression tag	UNP Q13162
A	32	LEU	-	expression tag	UNP Q13162
A	33	VAL	-	expression tag	UNP Q13162
A	34	PRO	-	expression tag	UNP Q13162
A	35	ARG	-	expression tag	UNP Q13162
A	36	GLY	-	expression tag	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
A	37	SER	-	expression tag	UNP Q13162
A	51	ALA	CYS	engineered mutation	UNP Q13162
B	18	MET	-	expression tag	UNP Q13162
B	19	GLY	-	expression tag	UNP Q13162
B	20	SER	-	expression tag	UNP Q13162
B	21	SER	-	expression tag	UNP Q13162
B	22	HIS	-	expression tag	UNP Q13162
B	23	HIS	-	expression tag	UNP Q13162
B	24	HIS	-	expression tag	UNP Q13162
B	25	HIS	-	expression tag	UNP Q13162
B	26	HIS	-	expression tag	UNP Q13162
B	27	HIS	-	expression tag	UNP Q13162
B	28	SER	-	expression tag	UNP Q13162
B	29	GLN	-	expression tag	UNP Q13162
B	30	ASP	-	expression tag	UNP Q13162
B	31	PRO	-	expression tag	UNP Q13162
B	32	LEU	-	expression tag	UNP Q13162
B	33	VAL	-	expression tag	UNP Q13162
B	34	PRO	-	expression tag	UNP Q13162
B	35	ARG	-	expression tag	UNP Q13162
B	36	GLY	-	expression tag	UNP Q13162
B	37	SER	-	expression tag	UNP Q13162
B	51	ALA	CYS	engineered mutation	UNP Q13162
C	18	MET	-	expression tag	UNP Q13162
C	19	GLY	-	expression tag	UNP Q13162
C	20	SER	-	expression tag	UNP Q13162
C	21	SER	-	expression tag	UNP Q13162
C	22	HIS	-	expression tag	UNP Q13162
C	23	HIS	-	expression tag	UNP Q13162
C	24	HIS	-	expression tag	UNP Q13162
C	25	HIS	-	expression tag	UNP Q13162
C	26	HIS	-	expression tag	UNP Q13162
C	27	HIS	-	expression tag	UNP Q13162
C	28	SER	-	expression tag	UNP Q13162
C	29	GLN	-	expression tag	UNP Q13162
C	30	ASP	-	expression tag	UNP Q13162
C	31	PRO	-	expression tag	UNP Q13162
C	32	LEU	-	expression tag	UNP Q13162
C	33	VAL	-	expression tag	UNP Q13162
C	34	PRO	-	expression tag	UNP Q13162
C	35	ARG	-	expression tag	UNP Q13162
C	36	GLY	-	expression tag	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
C	37	SER	-	expression tag	UNP Q13162
C	51	ALA	CYS	engineered mutation	UNP Q13162
D	18	MET	-	expression tag	UNP Q13162
D	19	GLY	-	expression tag	UNP Q13162
D	20	SER	-	expression tag	UNP Q13162
D	21	SER	-	expression tag	UNP Q13162
D	22	HIS	-	expression tag	UNP Q13162
D	23	HIS	-	expression tag	UNP Q13162
D	24	HIS	-	expression tag	UNP Q13162
D	25	HIS	-	expression tag	UNP Q13162
D	26	HIS	-	expression tag	UNP Q13162
D	27	HIS	-	expression tag	UNP Q13162
D	28	SER	-	expression tag	UNP Q13162
D	29	GLN	-	expression tag	UNP Q13162
D	30	ASP	-	expression tag	UNP Q13162
D	31	PRO	-	expression tag	UNP Q13162
D	32	LEU	-	expression tag	UNP Q13162
D	33	VAL	-	expression tag	UNP Q13162
D	34	PRO	-	expression tag	UNP Q13162
D	35	ARG	-	expression tag	UNP Q13162
D	36	GLY	-	expression tag	UNP Q13162
D	37	SER	-	expression tag	UNP Q13162
D	51	ALA	CYS	engineered mutation	UNP Q13162
E	18	MET	-	expression tag	UNP Q13162
E	19	GLY	-	expression tag	UNP Q13162
E	20	SER	-	expression tag	UNP Q13162
E	21	SER	-	expression tag	UNP Q13162
E	22	HIS	-	expression tag	UNP Q13162
E	23	HIS	-	expression tag	UNP Q13162
E	24	HIS	-	expression tag	UNP Q13162
E	25	HIS	-	expression tag	UNP Q13162
E	26	HIS	-	expression tag	UNP Q13162
E	27	HIS	-	expression tag	UNP Q13162
E	28	SER	-	expression tag	UNP Q13162
E	29	GLN	-	expression tag	UNP Q13162
E	30	ASP	-	expression tag	UNP Q13162
E	31	PRO	-	expression tag	UNP Q13162
E	32	LEU	-	expression tag	UNP Q13162
E	33	VAL	-	expression tag	UNP Q13162
E	34	PRO	-	expression tag	UNP Q13162
E	35	ARG	-	expression tag	UNP Q13162
E	36	GLY	-	expression tag	UNP Q13162

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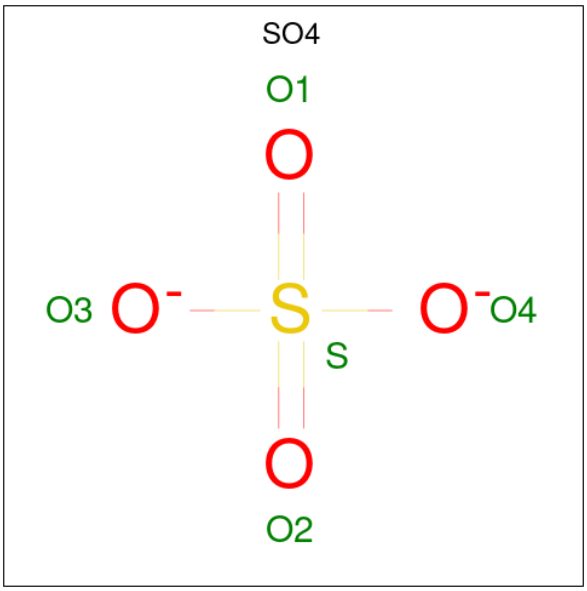
Chain	Residue	Modelled	Actual	Comment	Reference
E	37	SER	-	expression tag	UNP Q13162
E	51	ALA	CYS	engineered mutation	UNP Q13162

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

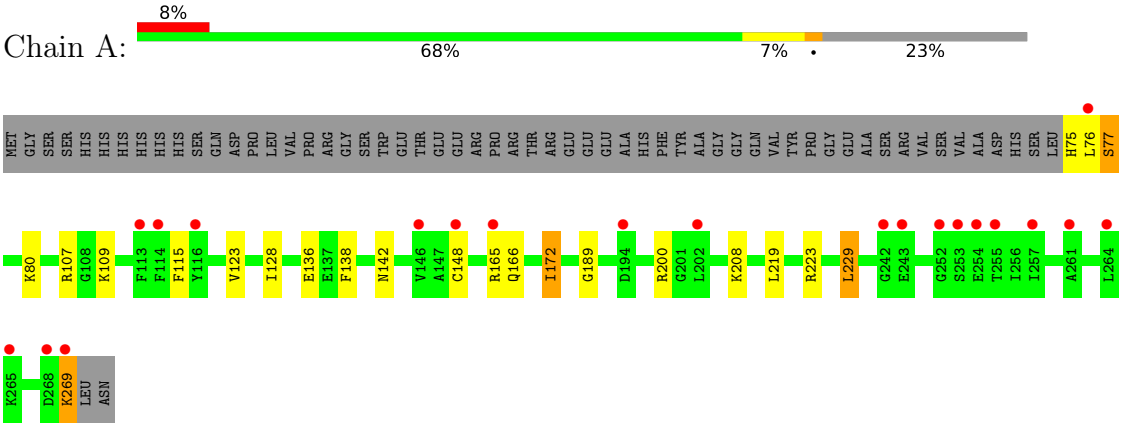
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	149	Total O 149 149	0	0
3	B	175	Total O 175 175	0	0
3	C	147	Total O 147 147	0	0
3	D	162	Total O 162 162	0	0
3	E	161	Total O 161 161	0	0

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.

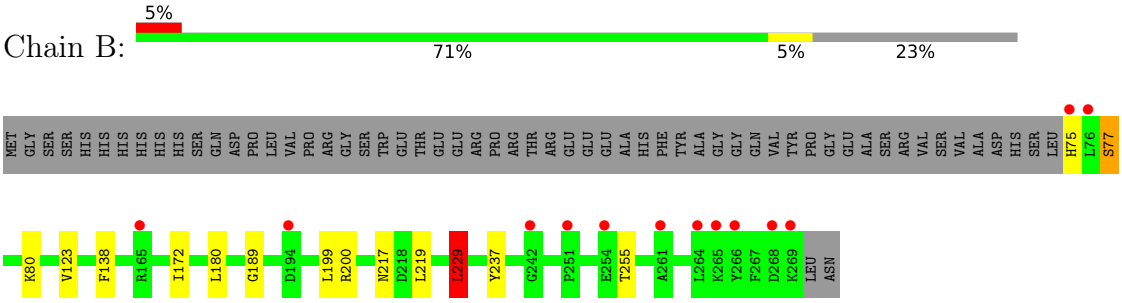
• Molecule 1: Peroxiredoxin-4

Chain A:



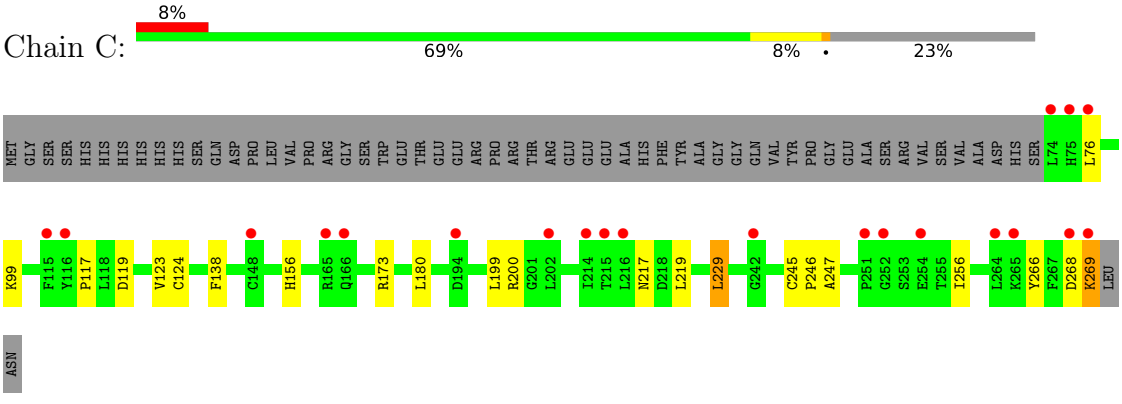
• Molecule 1: Peroxiredoxin-4

Chain B:



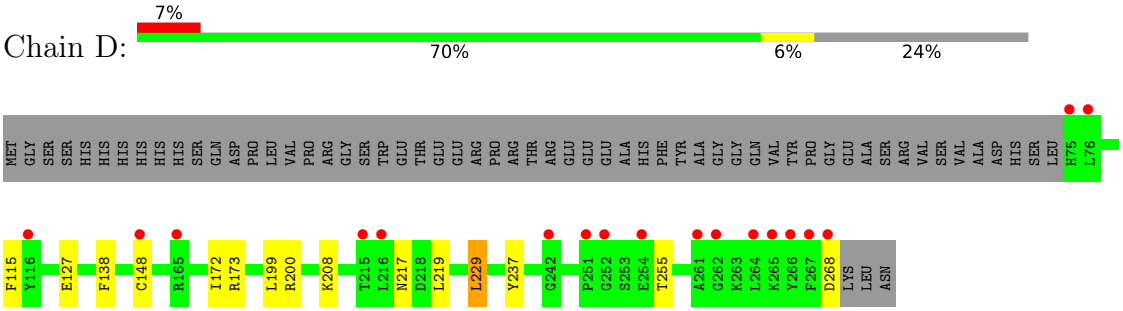
• Molecule 1: Peroxiredoxin-4

Chain C:



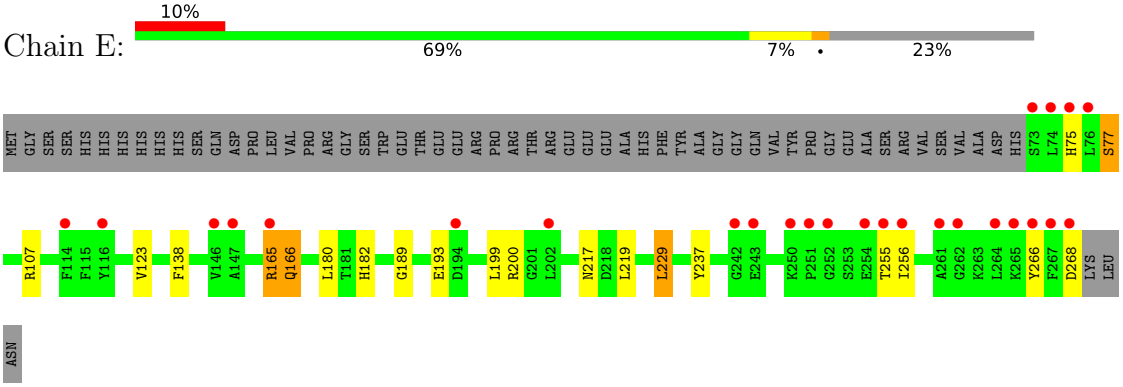
• Molecule 1: Peroxiredoxin-4

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	108.35Å 138.85Å 96.24Å 90.00° 103.97° 90.00°	Depositor
Resolution (Å)	28.77 – 2.04 28.77 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.77-2.04) 99.3 (28.77-2.04)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.160 , 0.197 0.161 , 0.200	Depositor DCC
R_{free} test set	4344 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 56.6	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	0.97	EDS
Total number of atoms	8896	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: SO4

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	0.78	0/1658	0.74	1/2249 (0.0%)
1	B	0.75	0/1658	0.74	1/2248 (0.0%)
1	C	0.65	0/1674	0.66	0/2271
1	D	0.76	0/1656	0.73	1/2245 (0.0%)
1	E	0.80	0/1680	0.77	2/2280 (0.1%)
All	All	0.75	0/8326	0.73	5/11293 (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	E	107	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	173	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	E	180	LEU	CA-CB-CG	5.11	127.04	115.30
1	B	229	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	107	ARG	NE-CZ-NH2	-5.03	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	1598	0	1588	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1601	0	1594	9	0
1	C	1617	0	1603	12	0
1	D	1597	0	1587	5	0
1	E	1614	0	1603	15	0
2	A	20	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
2	E	10	0	0	0	0
3	A	149	0	0	3	0
3	B	175	0	0	0	0
3	C	147	0	0	3	0
3	D	162	0	0	1	0
3	E	161	0	0	2	0
All	All	8896	0	7975	54	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 3.

All (54) 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:165:ARG:HG3	1:A:166[A]:GLN:HE21	1.44	0.82
1:E:166[A]:GLN:NE2	1:E:166[A]:GLN:HA	1.92	0.82
1:E:166[A]:GLN:HA	1:E:166[A]:GLN:HE21	1.44	0.81
1:A:136[B]:GLU:HG2	3:A:352:HOH:O	1.85	0.75
1:A:269:LYS:HE3	1:A:269:LYS:HA	1.69	0.74
1:C:119:ASP:OD2	1:C:156:HIS:HD2	1.74	0.69
1:E:166[A]:GLN:HE21	1:E:166[A]:GLN:CA	2.09	0.65
1:C:173:ARG:HD3	3:C:357:HOH:O	1.97	0.63
1:A:75:HIS:CE1	3:A:408:HOH:O	2.52	0.63
1:A:138:PHE:CE2	1:A:229:LEU:HD13	2.37	0.59
1:D:138:PHE:CE2	1:D:229:LEU:HD13	2.39	0.58
1:E:166[A]:GLN:NE2	1:E:166[A]:GLN:CA	2.66	0.56
1:A:208:LYS:HE3	3:A:364:HOH:O	2.07	0.55
1:E:193[B]:GLU:HG3	3:E:381:HOH:O	2.08	0.53
1:E:138:PHE:CZ	1:E:229:LEU:HD13	2.45	0.52
1:B:138:PHE:CE2	1:B:229:LEU:HD13	2.45	0.52
1:E:123:VAL:HB	1:E:200:ARG:NH2	2.26	0.51
1:E:165:ARG:HG2	1:E:166[B]:GLN:HG3	1.93	0.51
1:A:269:LYS:HA	1:A:269:LYS:CE	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ARG:CD	3:C:357:HOH:O	2.56	0.50
1:E:77:SER:HB2	1:E:189:GLY:HA3	1.94	0.49
1:C:123:VAL:HB	1:C:200:ARG:NH2	2.28	0.48
1:B:138:PHE:CZ	1:B:229:LEU:HD13	2.48	0.48
1:C:200:ARG:HB2	1:C:217:ASN:HB2	1.96	0.47
1:C:99:LYS:HE2	3:C:413:HOH:O	2.15	0.47
1:D:237:TYR:CE1	1:D:255:THR:HG21	2.50	0.47
1:C:245:CYS:HA	1:C:246:PRO:HD3	1.79	0.46
1:A:77:SER:HB2	1:A:189:GLY:HA3	1.97	0.46
1:C:138:PHE:CE2	1:C:229:LEU:HD13	2.51	0.46
1:A:200:ARG:HB3	1:A:223:ARG:CZ	2.46	0.45
1:A:80:LYS:HZ3	1:B:75:HIS:N	2.15	0.45
1:C:117:PRO:HD2	1:C:124:CYS:SG	2.57	0.45
1:A:123:VAL:HB	1:A:200:ARG:NH2	2.32	0.45
1:A:128:ILE:HG22	1:A:172:ILE:CD1	2.47	0.44
1:B:200:ARG:HB2	1:B:217:ASN:HB2	1.99	0.44
1:C:268:ASP:O	1:C:269:LYS:HD2	2.17	0.44
3:D:381:HOH:O	1:E:182:HIS:NE2	2.35	0.44
1:E:75:HIS:NE2	3:E:459:HOH:O	2.36	0.44
1:E:237:TYR:CE1	1:E:255:THR:HG21	2.53	0.44
1:A:138:PHE:CZ	1:A:229:LEU:HD13	2.53	0.43
1:D:200:ARG:HB2	1:D:217:ASN:HB2	1.99	0.43
1:B:237:TYR:CE1	1:B:255:THR:HG21	2.54	0.43
1:E:200:ARG:HB2	1:E:217:ASN:HB2	2.00	0.43
1:B:77:SER:HB2	1:B:189:GLY:CA	2.49	0.42
1:E:138:PHE:CE2	1:E:229:LEU:HD13	2.55	0.42
1:A:109:LYS:HG2	1:A:142:ASN:OD1	2.19	0.41
1:A:115:PHE:HA	1:A:148:CYS:O	2.20	0.41
1:D:115:PHE:HA	1:D:148:CYS:O	2.20	0.41
1:B:123:VAL:HB	1:B:200:ARG:NH2	2.36	0.41
1:A:75:HIS:HB2	1:B:80:LYS:HG2	2.03	0.41
1:C:247:ALA:HB2	1:D:127:GLU:HA	2.03	0.41
1:E:256:ILE:HG12	1:E:266:TYR:CG	2.56	0.41
1:C:256:ILE:HG12	1:C:266:TYR:CG	2.55	0.41
1:B:77:SER:HB2	1:B:189:GLY:HA3	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	199/254 (78%)	192 (96%)	7 (4%)	0	100	100
1	B	199/254 (78%)	192 (96%)	7 (4%)	0	100	100
1	C	201/254 (79%)	195 (97%)	6 (3%)	0	100	100
1	D	198/254 (78%)	191 (96%)	7 (4%)	0	100	100
1	E	202/254 (80%)	194 (96%)	8 (4%)	0	100	100
All	All	999/1270 (79%)	964 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	176/220 (80%)	170 (97%)	6 (3%)	37	30
1	B	176/220 (80%)	170 (97%)	6 (3%)	37	30
1	C	178/220 (81%)	172 (97%)	6 (3%)	37	30
1	D	176/220 (80%)	168 (96%)	8 (4%)	27	20
1	E	179/220 (81%)	171 (96%)	8 (4%)	27	20
All	All	885/1100 (80%)	851 (96%)	34 (4%)	35	26

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	77	SER
1	A	172	ILE
1	A	219	LEU
1	A	229	LEU
1	A	269	LYS
1	B	77	SER
1	B	172	ILE
1	B	180	LEU
1	B	199	LEU
1	B	219	LEU
1	B	229	LEU
1	C	76	LEU
1	C	180	LEU
1	C	199	LEU
1	C	219	LEU
1	C	229	LEU
1	C	269	LYS
1	D	172	ILE
1	D	199	LEU
1	D	208[A]	LYS
1	D	208[B]	LYS
1	D	219	LEU
1	D	229	LEU
1	D	268[A]	ASP
1	D	268[B]	ASP
1	E	77	SER
1	E	165	ARG
1	E	166[A]	GLN
1	E	166[B]	GLN
1	E	199	LEU
1	E	219	LEU
1	E	229	LEU
1	E	268	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	236	GLN
1	C	156	HIS
1	C	241	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

15 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	SO4	C	448	-	4,4,4	0.12	0	6,6,6	0.20	0
2	SO4	D	463	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	A	450	-	4,4,4	0.19	0	6,6,6	0.18	0
2	SO4	C	612	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	B	476	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	D	462	-	4,4,4	0.11	0	6,6,6	0.18	0
2	SO4	D	464	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	E	462	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	B	477	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	A	449	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	E	461	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	452	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	A	451	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	C	447	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	B	475	-	4,4,4	0.19	0	6,6,6	0.20	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

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	195/254 (76%)	0.39	21 (10%)	5 6	23, 33, 54, 71	0
1	B	195/254 (76%)	0.19	13 (6%)	17 19	24, 34, 60, 77	0
1	C	196/254 (77%)	0.42	21 (10%)	6 6	30, 40, 59, 75	0
1	D	194/254 (76%)	0.21	18 (9%)	8 9	25, 34, 60, 70	1 (0%)
1	E	196/254 (77%)	0.49	26 (13%)	3 2	24, 36, 61, 79	0
All	All	976/1270 (76%)	0.34	99 (10%)	7 7	23, 36, 60, 79	1 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	74	LEU	6.3
1	B	76	LEU	6.2
1	A	76	LEU	6.2
1	E	265	LYS	5.8
1	C	74	LEU	5.5
1	E	76	LEU	5.3
1	B	269	LYS	5.1
1	C	76	LEU	5.1
1	D	268[A]	ASP	5.0
1	E	73	SER	4.9
1	C	265	LYS	4.8
1	A	254[A]	GLU	4.6
1	D	265	LYS	4.4
1	A	264	LEU	4.4
1	A	242	GLY	4.4
1	B	268	ASP	4.4
1	A	165	ARG	4.3
1	E	266	TYR	4.3
1	D	242	GLY	4.2
1	B	254[A]	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	268	ASP	4.0
1	E	75	HIS	4.0
1	C	269	LYS	3.8
1	B	242	GLY	3.7
1	B	75	HIS	3.7
1	D	264	LEU	3.7
1	D	254[A]	GLU	3.6
1	A	268	ASP	3.6
1	C	268	ASP	3.6
1	C	252	GLY	3.6
1	D	76	LEU	3.6
1	D	165	ARG	3.5
1	E	252	GLY	3.4
1	D	251	PRO	3.3
1	E	255	THR	3.3
1	E	264	LEU	3.3
1	E	254[A]	GLU	3.3
1	E	251	PRO	3.3
1	C	194[A]	ASP	3.2
1	C	165	ARG	3.2
1	C	242	GLY	3.2
1	A	269	LYS	3.2
1	A	252	GLY	3.1
1	D	252	GLY	3.1
1	C	254[A]	GLU	3.1
1	A	265	LYS	3.1
1	A	261	ALA	3.0
1	E	243	GLU	3.0
1	C	202	LEU	3.0
1	B	165	ARG	3.0
1	D	75	HIS	2.9
1	B	265	LYS	2.9
1	D	262	GLY	2.9
1	B	194[A]	ASP	2.9
1	B	264	LEU	2.9
1	E	262	GLY	2.7
1	A	116	TYR	2.7
1	E	256	ILE	2.6
1	E	242	GLY	2.6
1	B	251	PRO	2.6
1	E	261	ALA	2.6
1	E	114	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	116	TYR	2.6
1	A	202	LEU	2.6
1	B	261	ALA	2.5
1	B	266	TYR	2.5
1	D	116	TYR	2.5
1	D	266	TYR	2.5
1	C	214	ILE	2.5
1	E	146	VAL	2.5
1	C	264	LEU	2.5
1	A	114	PHE	2.5
1	C	166[A]	GLN	2.4
1	E	147	ALA	2.4
1	E	165	ARG	2.4
1	C	148	CYS	2.3
1	E	267	PHE	2.3
1	E	250	LYS	2.3
1	C	116	TYR	2.2
1	A	255	THR	2.2
1	C	115	PHE	2.2
1	D	215	THR	2.2
1	A	148	CYS	2.2
1	D	261	ALA	2.2
1	A	257	ILE	2.2
1	E	194[A]	ASP	2.2
1	D	148	CYS	2.2
1	A	243	GLU	2.1
1	C	215	THR	2.1
1	A	146	VAL	2.1
1	C	216	LEU	2.1
1	C	251	PRO	2.1
1	A	194[A]	ASP	2.1
1	D	216	LEU	2.1
1	E	202	LEU	2.1
1	A	113	PHE	2.1
1	D	267	PHE	2.1
1	A	253	SER	2.0
1	C	75	HIS	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 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
2	SO4	C	612	5/5	0.47	0.35	143,143,144,145	0
2	SO4	A	450	5/5	0.64	0.36	110,110,111,113	0
2	SO4	B	476	5/5	0.71	0.21	116,117,118,119	0
2	SO4	B	477	5/5	0.72	0.28	120,120,121,123	0
2	SO4	D	464	5/5	0.75	0.46	154,154,155,156	0
2	SO4	B	475	5/5	0.76	0.27	101,101,102,104	0
2	SO4	D	463	5/5	0.80	0.44	131,131,132,132	0
2	SO4	C	448	5/5	0.80	0.36	152,153,154,155	0
2	SO4	A	451	5/5	0.82	0.48	109,110,111,112	0
2	SO4	E	461	5/5	0.85	0.36	124,124,126,127	0
2	SO4	A	452	5/5	0.88	0.25	107,107,109,110	0
2	SO4	E	462	5/5	0.88	0.19	118,119,119,120	0
2	SO4	A	449	5/5	0.90	0.16	105,106,106,107	0
2	SO4	C	447	5/5	0.90	0.16	106,107,108,108	0
2	SO4	D	462	5/5	0.93	0.15	105,105,106,107	0

6.5 Other polymers (i)

There are no such residues in this entry.