



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:39 PM GMT

PDB ID : 3P8U
Title : Crystal structure of mEosFP in its green state
Authors : Adam, V.; Nienhaus, G.U.; Bourgeois, D.
Deposited on : 2010-10-15
Resolution : 2.25 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

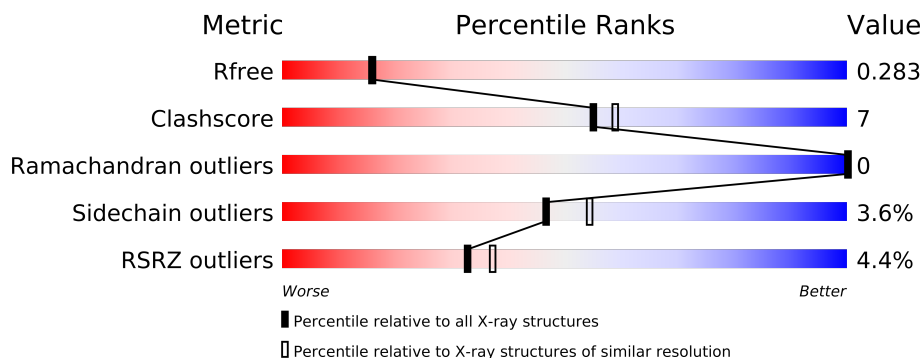
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.25 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}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	230	
1	B	230	
1	C	230	
1	D	230	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO3	A	1000	-	X
2	SO3	D	1000	-	X
3	SO4	A	1010	-	X
3	SO4	A	1040	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	B	1040	-	X
3	SO4	C	1040	-	X
3	SO4	D	1040	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7773 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Green to red photoconvertible GPF-like protein EosFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	7	0
			1822	1163	310	337	12			
1	B	220	Total	C	N	O	S	0	6	0
			1812	1156	310	335	11			
1	C	223	Total	C	N	O	S	0	5	0
			1837	1171	317	337	12			
1	D	221	Total	C	N	O	S	0	7	0
			1829	1168	312	337	12			

There are 44 discrepancies between the modelled and reference sequences:

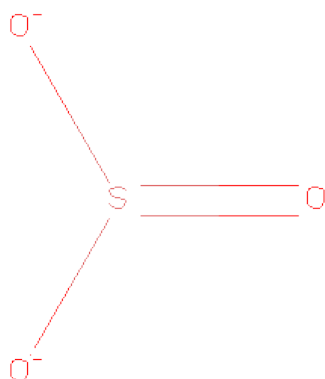
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
A	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
A	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
A	123	THR	VAL	ENGINEERED MUTATION	UNP Q5S6Z9
A	158	HIS	THR	ENGINEERED MUTATION	UNP Q5S6Z9
B	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
B	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
B	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
B	123	THR	VAL	ENGINEERED MUTATION	UNP Q5S6Z9

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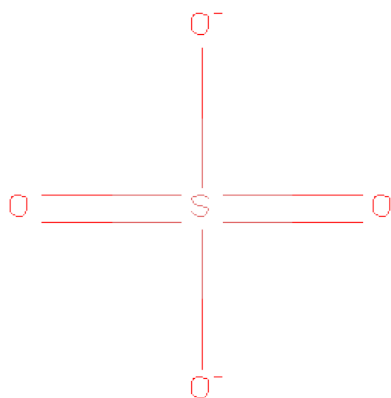
Chain	Residue	Modelled	Actual	Comment	Reference
B	158	HIS	THR	ENGINEERED MUTATION	UNP Q5S6Z9
C	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
C	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
C	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
C	123	THR	VAL	ENGINEERED MUTATION	UNP Q5S6Z9
C	158	HIS	THR	ENGINEERED MUTATION	UNP Q5S6Z9
D	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
D	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
D	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
D	123	THR	VAL	ENGINEERED MUTATION	UNP Q5S6Z9
D	158	HIS	THR	ENGINEERED MUTATION	UNP Q5S6Z9

- Molecule 2 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 4 3 1	0	0
2	A	1	Total O S 4 3 1	0	0
2	B	1	Total O S 4 3 1	0	0
2	D	1	Total O S 4 3 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	65	Total	O	0	0
			65	65		
4	C	95	Total	O	0	0
			95	95		
4	D	143	Total	O	0	0
			143	143		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.45Å 96.82Å 140.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 2.25 48.41 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.41-2.25) 99.5 (48.41-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.232 , 0.284 0.234 , 0.283	Depositor DCC
R_{free} test set	2817 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 56342 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7773	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 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CR8, SO3, 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	0.29	0/1866	0.62	0/2514
1	B	0.27	0/1850	0.60	0/2493
1	C	0.33	0/1874	0.66	0/2525
1	D	0.33	0/1870	0.70	2/2518 (0.1%)
All	All	0.31	0/7460	0.65	2/10050 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	D	66	ARG	NE-CZ-NH1	5.47	123.03	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1822	0	1756	26	0
1	B	1812	0	1739	21	0
1	C	1837	0	1761	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1829	0	1765	31	0
2	A	8	0	0	1	0
2	B	4	0	0	0	0
2	D	4	0	0	1	0
3	A	20	0	0	2	0
3	B	20	0	0	0	0
3	C	15	0	0	1	0
3	D	20	0	0	1	0
4	A	79	0	0	0	0
4	B	65	0	0	0	0
4	C	95	0	0	4	0
4	D	143	0	0	1	0
All	All	7773	0	7021	97	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (97) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:13[A]:ARG:HG3	1:B:13[A]:ARG:HH11	1.03	1.13
1:D:13[B]:ARG:HG2	1:D:13[B]:ARG:HH11	1.15	1.06
1:B:13[A]:ARG:CG	1:B:13[A]:ARG:HH11	1.74	0.99
1:B:13[A]:ARG:HG3	1:B:13[A]:ARG:NH1	1.78	0.95
1:D:13[B]:ARG:CG	1:D:13[B]:ARG:HH11	1.78	0.94
1:D:13[B]:ARG:NH1	1:D:13[B]:ARG:HG2	1.83	0.84
4:C:2055:HOH:O	1:D:100:ILE:HD11	1.82	0.77
1:C:65:ASN:O	1:C:87:TYR:OH	2.04	0.76
1:D:195[B]:CYS:SG	2:D:1000:SO3:S	2.85	0.75
1:C:201:HIS:NE2	4:C:2257:HOH:O	2.26	0.67
1:A:159:MET:O	1:A:170:ARG:NH2	2.29	0.65
1:D:148:VAL:HG22	1:D:186:LEU:HD22	1.82	0.62
1:A:145:LYS:HD2	1:A:189:TYR:OH	2.01	0.60
1:D:218:SER:HB2	1:D:223:ASN:HA	1.84	0.59
1:D:40:MET:HB2	1:D:64:CR8:H10	1.84	0.59
1:B:13[A]:ARG:NH1	1:B:13[A]:ARG:CG	2.47	0.58
1:D:13[B]:ARG:NH1	1:D:15:GLU:OE2	2.36	0.57
1:A:145:LYS:HD2	1:A:189:TYR:CZ	2.40	0.57
1:B:93:LEU:HD23	1:B:93:LEU:N	2.21	0.56
1:B:64:CR8:H2	1:B:196:ILE:HB	1.88	0.56
1:D:12:LEU:HD23	1:D:12:LEU:C	2.26	0.55
1:B:102:ILE:HD12	1:B:103:ALA:N	2.21	0.55
1:D:66:ARG:HG2	1:D:79:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:13[A]:ARG:HG2	1:C:13[A]:ARG:HH11	1.71	0.55
1:B:76:GLN:NE2	1:B:81:GLN:OE1	2.37	0.55
1:B:15:GLU:HG2	1:B:24:VAL:HG22	1.89	0.54
1:A:195[B]:CYS:SG	2:A:1000:SO3:S	3.06	0.54
1:B:87:TYR:CE1	1:B:107:ILE:HD12	2.43	0.52
1:C:198:ILE:HD12	4:C:2190:HOH:O	2.09	0.52
1:A:148:VAL:HG22	1:A:186:LEU:HD22	1.92	0.52
1:A:198:ILE:HG23	1:A:208:VAL:HG13	1.91	0.52
1:A:4:ILE:HG13	1:A:109:MET:HE1	1.91	0.52
1:C:196:ILE:HD11	1:C:210:LEU:HD21	1.92	0.51
1:A:145:LYS:CD	1:A:189:TYR:OH	2.58	0.51
1:B:13[B]:ARG:CZ	1:B:15:GLU:OE2	2.59	0.50
1:B:102:ILE:HD12	1:B:102:ILE:C	2.31	0.50
1:C:65:ASN:O	1:C:65:ASN:OD1	2.29	0.50
1:D:64:CR8:H2	1:D:196:ILE:HB	1.95	0.49
1:D:91:ARG:HD3	1:D:173:PHE:CD2	2.48	0.49
1:A:167:ALA:HB1	3:C:1040:SO4:O1	2.12	0.49
1:C:65:ASN:OD1	1:C:67:VAL:HB	2.13	0.49
1:A:158:HIS:ND1	1:A:170:ARG:NH1	2.60	0.49
1:A:55:ASP:HB3	1:A:161:LEU:HD21	1.96	0.48
1:A:40:MET:HB2	1:A:64:CR8:H10	1.95	0.48
1:A:145:LYS:O	1:A:155:GLY:HA2	2.14	0.47
1:C:2:SER:O	1:C:3:ALA:HB3	2.13	0.47
1:D:196:ILE:HG22	4:D:2017:HOH:O	2.13	0.47
1:D:17:ASN:ND2	3:D:1020:SO4:O2	2.46	0.47
1:D:137:LEU:HD21	1:D:164:GLU:HG2	1.97	0.47
1:C:13[A]:ARG:HG2	1:C:13[A]:ARG:NH1	2.29	0.46
1:B:91:ARG:HG2	1:B:93:LEU:CD2	2.45	0.46
1:A:150[A]:ASP:CG	3:A:1040:SO4:O3	2.54	0.46
1:D:19:ASN:HD21	1:D:125:PHE:HB2	1.80	0.46
1:A:10:ILE:HG21	1:A:40:MET:CE	2.45	0.46
1:C:5:LYS:NZ	1:C:112:ASP:HB3	2.31	0.46
1:D:67:VAL:HG11	1:D:114:PHE:CZ	2.51	0.45
1:D:93:LEU:HB2	1:D:101:CYS:HB2	1.97	0.45
1:D:123:THR:OG1	1:D:124:ASN:N	2.49	0.45
1:D:163:LEU:HD11	1:D:169:TYR:HB2	1.99	0.45
1:C:206:ASN:N	1:C:206:ASN:HD22	2.14	0.45
1:D:125:PHE:CE1	1:D:131:VAL:HG21	2.51	0.45
1:C:178:LYS:HD2	4:C:2229:HOH:O	2.17	0.45
1:D:218:SER:H	1:D:223:ASN:HB3	1.81	0.45
1:A:148:VAL:HG11	1:A:186:LEU:HD13	1.99	0.45
1:C:64:CR8:H6	1:C:64:CR8:N15	2.31	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:67:VAL:HG11	1:C:114:PHE:CZ	2.52	0.44
1:A:140:GLU:HG3	1:C:189:TYR:CE1	2.52	0.44
1:A:13[B]:ARG:HH11	1:A:24:VAL:HG11	1.82	0.44
1:A:67:VAL:HG12	1:A:68:PHE:N	2.32	0.44
1:C:102:ILE:HD13	1:D:123:THR:HG21	1.99	0.44
1:D:8:MET:HE2	1:D:112:ASP:C	2.39	0.43
1:A:13[B]:ARG:NH1	1:A:24:VAL:HG11	2.33	0.43
1:B:142:SER:OG	1:B:194:HIS:HB2	2.19	0.43
1:A:93:LEU:N	1:A:93:LEU:HD12	2.34	0.43
1:D:145:LYS:O	1:D:155:GLY:HA2	2.18	0.43
1:A:65:ASN:OD1	1:A:67:VAL:HB	2.19	0.43
1:D:87:TYR:CE1	1:D:107:ILE:HD12	2.54	0.42
1:C:40:MET:SD	1:C:42:LEU:HD21	2.59	0.42
1:B:52:PHE:CE1	1:B:57:LEU:HD11	2.54	0.42
1:D:16:GLY:HA3	1:D:120:PHE:O	2.19	0.42
1:C:57:LEU:O	1:C:60:ALA:HB3	2.19	0.42
1:B:12:LEU:HD23	1:B:12:LEU:C	2.40	0.42
1:C:66:ARG:HB2	1:C:66:ARG:CZ	2.50	0.42
1:A:148:VAL:CG2	1:A:186:LEU:HD22	2.50	0.41
1:C:144:GLU:CD	1:C:146:MET:HE2	2.40	0.41
1:A:17:ASN:HA	1:A:21:HIS:O	2.20	0.41
1:A:57:LEU:O	1:A:60:ALA:HB3	2.19	0.41
1:B:87:TYR:CZ	1:B:107:ILE:HD12	2.55	0.41
1:B:40:MET:HB2	1:B:64:CR8:H10	2.03	0.41
1:B:198:ILE:HG23	1:B:208:VAL:HG13	2.03	0.41
1:D:83:PHE:HB3	1:D:84:PRO:HA	2.02	0.41
1:B:93:LEU:HB3	1:B:171:CYS:SG	2.62	0.40
1:A:202:ASP:OD1	1:A:202:ASP:C	2.59	0.40
1:B:13[A]:ARG:NH1	1:B:26:ASP:OD1	2.54	0.40
1:C:102:ILE:HD13	1:D:123:THR:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	225/230 (98%)	220 (98%)	5 (2%)	0	100	100
1	B	223/230 (97%)	216 (97%)	7 (3%)	0	100	100
1	C	225/230 (98%)	222 (99%)	3 (1%)	0	100	100
1	D	225/230 (98%)	221 (98%)	4 (2%)	0	100	100
All	All	898/920 (98%)	879 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	196/197 (100%)	190 (97%)	6 (3%)	52	61
1	B	194/197 (98%)	188 (97%)	6 (3%)	52	61
1	C	196/197 (100%)	190 (97%)	6 (3%)	52	61
1	D	196/197 (100%)	185 (94%)	11 (6%)	30	30
All	All	782/788 (99%)	753 (96%)	29 (4%)	47	53

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	67	VAL
1	A	73	ASP
1	A	100	ILE
1	A	104	ARG
1	A	203	LYS
1	B	13[A]	ARG
1	B	13[B]	ARG
1	B	93	LEU
1	B	102	ILE
1	B	145	LYS
1	B	172	ASP
1	C	66	ARG
1	C	102	ILE

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Mol	Chain	Res	Type
1	C	106	ASP
1	C	128	ASN
1	C	145	LYS
1	C	200	SER
1	D	1	MET
1	D	13[A]	ARG
1	D	13[B]	ARG
1	D	66	ARG
1	D	135	LYS
1	D	145	LYS
1	D	150	ASP
1	D	185	LYS
1	D	194	HIS
1	D	203	LYS
1	D	222	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	74	HIS
1	B	124	ASN
1	C	74	HIS
1	C	166	ASN
1	C	206	ASN
1	C	213	HIS
1	D	74	HIS
1	D	133	GLN
1	D	166	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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
1	CR8	A	64	1	27,27,28	3.04	11 (40%)	29,37,39	2.39	9 (31%)
1	CR8	B	64	1	27,27,28	3.96	10 (37%)	29,37,39	2.18	6 (20%)
1	CR8	C	64	1	27,27,28	3.17	15 (55%)	29,37,39	2.20	12 (41%)
1	CR8	D	64	1	27,27,28	3.54	14 (51%)	29,37,39	2.13	8 (27%)

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
1	CR8	A	64	1	-	0/9/25/26	0/3/3/3
1	CR8	B	64	1	-	1/9/25/26	0/3/3/3
1	CR8	C	64	1	-	0/9/25/26	0/3/3/3
1	CR8	D	64	1	-	0/9/25/26	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	CR8	O19-C	16.30	1.22	1.11
1	D	64	CR8	O19-C	11.24	1.19	1.11
1	C	64	CR8	O19-C	9.07	1.17	1.11
1	A	64	CR8	O19-C	8.09	1.16	1.11
1	C	64	CR8	C21-N22	-5.73	1.30	1.38
1	D	64	CR8	C21-N22	-5.48	1.31	1.38
1	D	64	CR8	C8-C7	5.29	1.48	1.36
1	B	64	CR8	C8-C7	5.28	1.47	1.36
1	A	64	CR8	C8-C7	5.23	1.47	1.36
1	D	64	CR8	C14-N13	-5.10	1.31	1.36
1	A	64	CR8	C21-N22	-5.05	1.31	1.38
1	B	64	CR8	C21-N22	-4.95	1.31	1.38
1	D	64	CR8	C9-C12	-4.76	1.32	1.40
1	A	64	CR8	C4-C1	-4.74	1.35	1.46
1	C	64	CR8	C14-N13	-4.67	1.31	1.36
1	D	64	CR8	C12-N13	-4.49	1.26	1.36
1	A	64	CR8	C14-N13	-4.49	1.31	1.36
1	D	64	CR8	C4-C1	-4.36	1.36	1.46
1	C	64	CR8	C9-C12	-4.23	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	CR8	C4-C1	-4.23	1.36	1.46
1	C	64	CR8	C4-C1	-4.20	1.36	1.46
1	C	64	CR8	C8-C7	3.96	1.45	1.36
1	C	64	CR8	C12-N13	-3.93	1.28	1.36
1	A	64	CR8	C9-N15	-3.86	1.30	1.39
1	A	64	CR8	C9-C12	-3.85	1.34	1.40
1	B	64	CR8	C12-N13	-3.79	1.28	1.36
1	B	64	CR8	C2-C1	-3.70	1.37	1.46
1	A	64	CR8	C2-C1	-3.64	1.37	1.46
1	C	64	CR8	C9-N15	-3.62	1.31	1.39
1	A	64	CR8	C12-N13	-3.45	1.29	1.36
1	D	64	CR8	C2-C1	-3.38	1.38	1.46
1	B	64	CR8	C9-C12	-3.21	1.35	1.40
1	D	64	CR8	C9-N15	-3.20	1.32	1.39
1	B	64	CR8	C14-N13	-3.03	1.33	1.36
1	B	64	CR8	C9-N15	-2.95	1.32	1.39
1	C	64	CR8	C20-C21	2.89	1.52	1.49
1	A	64	CR8	C9-C8	2.81	1.49	1.39
1	D	64	CR8	C9-C8	2.73	1.49	1.39
1	C	64	CR8	C2-C1	-2.63	1.40	1.46
1	B	64	CR8	C9-C8	2.55	1.48	1.39
1	D	64	CR8	C17-N13	-2.45	1.43	1.48
1	C	64	CR8	C17-N13	-2.34	1.43	1.48
1	D	64	CR8	C10-N11	-2.31	1.30	1.34
1	C	64	CR8	C6-C7	-2.30	1.35	1.41
1	A	64	CR8	C14-C16	-2.30	1.46	1.50
1	C	64	CR8	C10-N11	-2.29	1.30	1.34
1	C	64	CR8	C9-C8	2.26	1.47	1.39
1	D	64	CR8	C10-N22	-2.20	1.31	1.34
1	D	64	CR8	C6-C7	-2.16	1.36	1.41
1	C	64	CR8	C10-N22	-2.05	1.31	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	CR8	C9-C12-N13	7.71	113.73	104.65
1	D	64	CR8	C9-C12-N13	7.53	113.51	104.65
1	B	64	CR8	C9-C12-N13	7.30	113.24	104.65
1	C	64	CR8	C9-C12-N13	6.43	112.22	104.65
1	A	64	CR8	C12-N13-C14	-6.30	103.61	111.94
1	B	64	CR8	C12-N13-C14	-5.66	104.47	111.94
1	D	64	CR8	C12-N13-C14	-4.61	105.85	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	CR8	C12-N13-C14	-4.53	105.95	111.94
1	C	64	CR8	C20-C21-N22	3.22	130.11	122.94
1	D	64	CR8	C16-C14-N15	2.92	129.86	124.27
1	C	64	CR8	C20-C21-C23	-2.77	125.72	130.62
1	A	64	CR8	C20-C16-C14	2.69	114.08	111.18
1	C	64	CR8	C4-C5-C7	-2.65	119.62	121.92
1	D	64	CR8	C20-C21-C23	-2.62	125.99	130.62
1	C	64	CR8	C6-C7-C5	2.54	120.97	115.23
1	C	64	CR8	C2-C6-C7	-2.51	119.73	121.92
1	A	64	CR8	C9-C8-C7	2.49	134.02	128.63
1	A	64	CR8	C2-C6-C7	-2.48	119.76	121.92
1	A	64	CR8	C5-C7-C8	-2.40	116.02	122.34
1	A	64	CR8	C20-C21-C23	-2.37	126.44	130.62
1	B	64	CR8	C4-C1-C2	2.31	120.73	116.66
1	D	64	CR8	C20-C21-N22	2.30	128.08	122.94
1	C	64	CR8	N22-C10-N11	-2.29	106.36	111.49
1	A	64	CR8	C17-N13-C12	2.27	128.55	124.24
1	C	64	CR8	C5-C7-C8	-2.21	116.52	122.34
1	C	64	CR8	C16-C14-N15	2.16	128.40	124.27
1	B	64	CR8	C21-C20-C16	-2.15	108.81	113.19
1	B	64	CR8	C17-N13-C14	2.14	129.63	126.62
1	D	64	CR8	C5-C4-C1	-2.10	118.13	121.17
1	C	64	CR8	C21-C20-C16	2.09	117.43	113.19
1	C	64	CR8	C23-N11-C10	2.08	108.94	105.76
1	B	64	CR8	C20-C16-N	-2.07	102.43	112.09
1	D	64	CR8	C4-C1-C2	2.06	120.28	116.66
1	D	64	CR8	C9-C8-C7	2.04	133.04	128.63
1	A	64	CR8	C23-N11-C10	2.04	108.87	105.76

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	64	CR8	C16-C20-C21-N22

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

19 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	SO3	A	1000	-	3,3,3	1.11	0	2,3,3	0.54	0
3	SO4	A	1010	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	A	1020	-	4,4,4	0.23	0	6,6,6	0.15	0
3	SO4	A	1030	-	4,4,4	0.19	0	6,6,6	0.07	0
3	SO4	A	1040	-	4,4,4	0.20	0	6,6,6	0.10	0
2	SO3	A	227	-	3,3,3	0.99	0	2,3,3	0.56	0
2	SO3	B	1000	-	3,3,3	1.34	0	2,3,3	0.60	0
3	SO4	B	1010	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	B	1020	-	4,4,4	0.20	0	6,6,6	0.09	0
3	SO4	B	1030	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	B	1040	-	4,4,4	0.21	0	6,6,6	0.10	0
3	SO4	C	1020	-	4,4,4	0.21	0	6,6,6	0.14	0
3	SO4	C	1030	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	C	1040	-	4,4,4	0.21	0	6,6,6	0.25	0
2	SO3	D	1000	-	3,3,3	1.12	0	2,3,3	0.57	0
3	SO4	D	1010	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	D	1020	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	D	1030	-	4,4,4	0.21	0	6,6,6	0.18	0
3	SO4	D	1040	-	4,4,4	0.22	0	6,6,6	0.07	0

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	SO3	A	1000	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1010	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1020	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1030	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1040	-	-	0/0/0/0	0/0/0/0
2	SO3	A	227	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO3	B	1000	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1010	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1020	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1030	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1040	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1020	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1030	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1040	-	-	0/0/0/0	0/0/0/0
2	SO3	D	1000	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1010	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1020	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1030	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1040	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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	221/230 (96%)	0.27	7 (3%) 45 52	29, 42, 52, 63	0
1	B	220/230 (95%)	0.69	22 (10%) 8 9	30, 46, 60, 71	0
1	C	223/230 (96%)	0.32	5 (2%) 59 65	25, 38, 52, 63	0
1	D	221/230 (96%)	0.16	4 (1%) 65 72	16, 32, 42, 59	0
All	All	885/920 (96%)	0.36	38 (4%) 33 39	16, 39, 57, 71	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13[A]	ARG	4.8
1	B	3	ALA	4.3
1	B	2	SER	4.0
1	B	182	LYS	3.9
1	B	115	TYR	3.9
1	B	114	PHE	3.5
1	B	28[A]	ASP	3.5
1	B	111	GLY	3.4
1	B	84	PRO	3.2
1	D	94	THR	3.1
1	A	13[A]	ARG	3.1
1	C	28[A]	ASP	3.1
1	C	42	LEU	2.8
1	A	28[A]	ASP	2.8
1	D	13[A]	ARG	2.7
1	B	94	THR	2.6
1	A	223	ASN	2.5
1	B	4	ILE	2.5
1	A	93	LEU	2.4
1	B	10	ILE	2.4
1	C	203	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	15	GLU	2.4
1	B	11	ASN	2.3
1	B	171	CYS	2.3
1	B	45	LYS	2.3
1	B	183	GLY	2.2
1	B	203	LYS	2.2
1	C	13[A]	ARG	2.2
1	B	100	ILE	2.2
1	D	98	GLY	2.2
1	D	100	ILE	2.1
1	B	200	SER	2.1
1	B	47	GLY	2.1
1	A	100	ILE	2.1
1	A	170	ARG	2.0
1	C	166	ASN	2.0
1	B	204	ASP	2.0
1	A	195[A]	CYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CR8	D	64	25/26	0.11	-0.58	14,19,21,22	0
1	CR8	A	64	25/26	0.12	-0.66	22,28,32,32	0
1	CR8	C	64	25/26	0.10	-1.01	19,24,32,33	0
1	CR8	B	64	25/26	0.10	-1.23	35,38,41,41	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO3	D	1000	4/4	0.26	9.89	57,57,57,57	4
3	SO4	A	1040	5/5	0.22	5.73	55,55,55,55	5
3	SO4	B	1040	5/5	0.34	5.71	62,62,62,63	5
3	SO4	A	1010	5/5	0.31	5.51	68,68,68,68	5
3	SO4	D	1040	5/5	0.27	5.22	61,62,62,62	5
2	SO3	A	1000	4/4	0.34	4.73	60,61,61,61	4
3	SO4	C	1040	5/5	0.29	2.93	43,43,44,44	5
3	SO4	C	1030	5/5	0.39	1.43	57,57,57,57	5
3	SO4	D	1010	5/5	0.20	1.37	61,61,61,61	5
2	SO3	B	1000	4/4	0.18	0.60	59,59,59,59	4
3	SO4	B	1030	5/5	0.25	0.43	57,57,58,58	5
3	SO4	A	1030	5/5	0.18	0.38	41,41,41,41	5
3	SO4	A	1020	5/5	0.14	-0.08	90,90,90,90	0
3	SO4	B	1010	5/5	0.27	-0.21	45,46,46,46	5
3	SO4	D	1030	5/5	0.14	-0.31	40,40,40,40	5
3	SO4	D	1020	5/5	0.11	-1.01	71,71,71,72	0
3	SO4	C	1020	5/5	0.10	-1.38	70,70,70,70	0
3	SO4	B	1020	5/5	0.11	-1.57	86,86,87,87	0
2	SO3	A	227	4/4	0.10	-1.74	64,64,64,64	4

6.5 Other polymers ⓘ

There are no such residues in this entry.