



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:05 PM UTC

PDB ID : 3TMR / pdb_00003tmr
Title : IrisFP, planar chromophore
Authors : Adam, V.; Carpentier, P.; Roy, A.; Field, M.; Bourgeois, D.
Deposited on : 2011-08-31
Resolution : 2.00 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

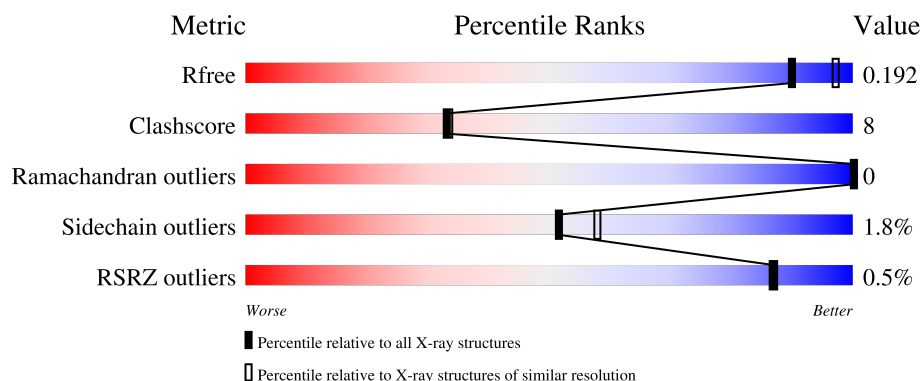
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

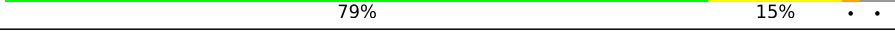
The reported resolution of this entry is 2.00 Å.

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	230	
1	B	230	
1	C	230	
1	D	230	

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	B	230	-	-	X	-
2	SO4	B	231	-	-	X	-
3	SO3	A	228	-	-	X	-
3	SO3	C	228	-	-	X	-
3	SO3	D	229	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8177 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 Green to red photoconvertible GPF-like protein EosFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	3	4	0
			1808	1150	309	337	12			
1	B	221	Total	C	N	O	S	1	3	0
			1792	1141	305	335	11			
1	C	221	Total	C	N	O	S	1	2	0
			1787	1138	305	332	12			
1	D	221	Total	C	N	O	S	2	3	0
			1790	1140	305	333	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	173	SER	PHE	engineered mutation	UNP Q5S6Z9
A	191	LEU	PHE	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	173	SER	PHE	engineered mutation	UNP Q5S6Z9

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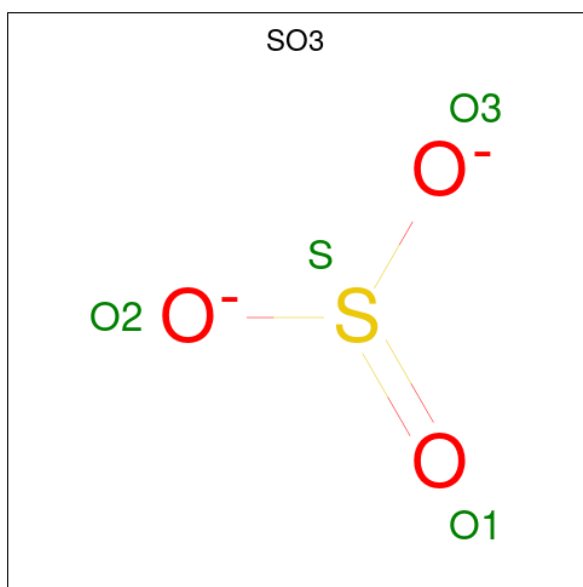
Chain	Residue	Modelled	Actual	Comment	Reference
B	191	LEU	PHE	engineered mutation	UNP Q5S6Z9
C	-5	HIS	-	expression tag	UNP Q5S6Z9
C	-4	HIS	-	expression tag	UNP Q5S6Z9
C	-3	HIS	-	expression tag	UNP Q5S6Z9
C	-2	HIS	-	expression tag	UNP Q5S6Z9
C	-1	HIS	-	expression tag	UNP Q5S6Z9
C	0	HIS	-	expression tag	UNP Q5S6Z9
C	64	CR8	HIS	chromophore	UNP Q5S6Z9
C	64	CR8	TYR	chromophore	UNP Q5S6Z9
C	64	CR8	GLY	chromophore	UNP Q5S6Z9
C	173	SER	PHE	engineered mutation	UNP Q5S6Z9
C	191	LEU	PHE	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	173	SER	PHE	engineered mutation	UNP Q5S6Z9
D	191	LEU	PHE	engineered mutation	UNP Q5S6Z9

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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	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	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	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
2	C	1	Total O S 5 4 1	0	0
2	C	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	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

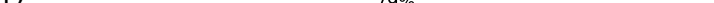
- Molecule 3 is SULFITE ION (CCD ID: SO3) (formula: O₃S).

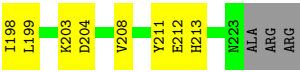
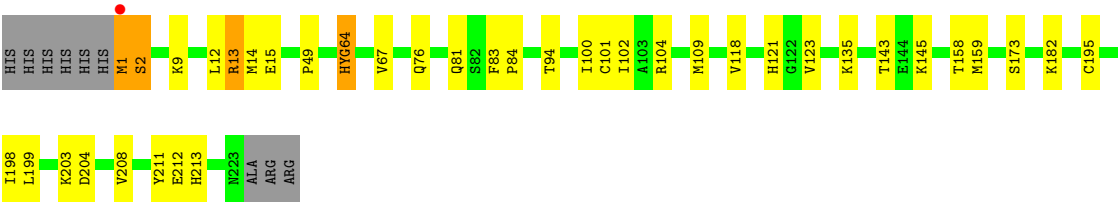


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			4	3	1		
3	B	1	Total	O	S	0	0
			4	3	1		
3	C	1	Total	O	S	0	0
			4	3	1		
3	D	1	Total	O	S	0	0
			4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	224	Total	O	0	0
			224	224		
4	B	256	Total	O	0	0
			256	256		
4	C	219	Total	O	0	0
			219	219		
4	D	190	Total	O	0	0
			190	190		

Chain D:  79% 15% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.84Å 96.51Å 140.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.98 – 2.00 12.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (12.98-2.00) 94.7 (12.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.157 , 0.195 0.153 , 0.192	Depositor DCC
R_{free} test set	3728 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8177	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CR8, SO4, SO3

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	0.39	0/1838	0.71	0/2478
1	B	0.41	0/1821	0.71	0/2455
1	C	0.38	0/1813	0.70	0/2444
1	D	0.36	0/1819	0.72	0/2452
All	All	0.39	0/7291	0.71	0/9829

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1808	0	1730	31	0
1	B	1792	0	1719	22	0
1	C	1787	0	1715	28	0
1	D	1790	0	1720	36	0
2	A	15	0	0	0	0
2	B	30	0	0	2	2
2	C	25	0	0	1	0
2	D	25	0	0	2	0
3	A	4	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	1	0
3	C	4	0	0	6	0
3	D	4	0	0	5	0
4	A	224	0	0	5	3
4	B	256	0	0	3	0
4	C	219	0	0	3	1
4	D	190	0	0	1	0
All	All	8177	0	6884	111	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (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:B:195:CYS:SG	3:B:229:SO3:S	2.36	1.23
1:A:195[A]:CYS:SG	3:A:228:SO3:S	2.47	1.13
1:C:195[A]:CYS:SG	3:C:228:SO3:S	2.54	1.04
1:D:195[A]:CYS:SG	3:D:229:SO3:S	2.56	1.03
1:B:183:GLY:N	2:B:230:SO4:O2	1.96	0.97
1:C:13:ARG:NH2	4:C:1219:HOH:O	2.00	0.94
1:C:13:ARG:NH1	1:C:15:GLU:OE2	2.13	0.82
1:A:13:ARG:NH1	1:A:15:GLU:OE2	2.12	0.81
1:A:13:ARG:HD3	1:A:26:ASP:OD1	1.87	0.74
1:A:5:LYS:NZ	1:A:112:ASP:HB3	2.03	0.73
1:B:158:THR:OG1	1:D:158:THR:HG23	1.89	0.72
1:A:211:TYR:HE2	3:A:228:SO3:O3	1.73	0.72
2:D:1225:SO4:O1	4:D:846:HOH:O	2.08	0.71
1:B:2:SER:HB2	4:B:1248:HOH:O	1.94	0.68
1:B:182:LYS:HG3	2:B:230:SO4:O3	1.94	0.67
1:D:1:MET:N	1:D:2:SER:HB3	2.09	0.67
1:D:182:LYS:HG3	2:D:1227:SO4:O4	1.95	0.67
4:C:1113:HOH:O	1:D:104:ARG:HD2	1.95	0.65
1:C:7:ASP:OD1	1:C:32:LYS:NZ	2.30	0.65
1:D:1:MET:N	1:D:2:SER:CB	2.59	0.65
1:A:159:MET:HE2	1:A:173:SER:HB2	1.79	0.64
1:D:76:GLN:NE2	1:D:81:GLN:HG3	2.12	0.64
1:A:158:THR:HG23	1:A:170:ARG:CZ	2.28	0.63
1:D:1:MET:H3	1:D:2:SER:CB	2.11	0.63
1:A:195[B]:CYS:HB3	3:A:228:SO3:S	2.39	0.62
1:D:13:ARG:NH1	1:D:15:GLU:OE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:H2	1:D:2:SER:HB3	1.66	0.61
1:A:5:LYS:HZ2	1:A:112:ASP:HB3	1.65	0.60
4:B:1270:HOH:O	1:D:195[B]:CYS:SG	2.56	0.60
1:C:195[B]:CYS:SG	3:C:228:SO3:S	3.00	0.60
1:D:83:PHE:CD2	1:D:109:MET:HE2	2.36	0.59
1:A:78:TYR:HE1	4:A:661:HOH:O	1.84	0.59
1:C:197:GLU:CB	3:C:228:SO3:O1	2.51	0.59
1:D:83:PHE:HB3	1:D:109:MET:CE	2.32	0.59
1:B:159:MET:HE2	1:B:173:SER:HB2	1.84	0.59
1:C:158:THR:HG23	1:C:170:ARG:CZ	2.36	0.56
1:C:197:GLU:HB2	3:C:228:SO3:O1	2.06	0.56
1:B:41:ASP:OD1	1:B:209:LYS:HE3	2.06	0.55
1:D:195[A]:CYS:SG	3:D:229:SO3:O1	2.63	0.55
1:A:211:TYR:CE2	3:A:228:SO3:O3	2.56	0.55
1:C:85:LYS:CG	1:C:180:LYS:HG2	2.37	0.55
1:D:198:ILE:HG23	1:D:208:VAL:HG13	1.88	0.54
1:C:83:PHE:HB3	1:C:84:PRO:HA	1.90	0.54
1:C:182:LYS:HG3	2:C:1227:SO4:O1	2.08	0.54
1:C:159:MET:HE2	1:C:173:SER:HB2	1.90	0.53
1:A:5:LYS:HZ1	1:A:112:ASP:HB3	1.72	0.53
1:A:64:CR8:H23	1:A:212:GLU:HB2	1.91	0.53
1:C:67:VAL:HG21	1:C:83:PHE:CE1	2.44	0.53
1:B:158:THR:HG23	1:B:170:ARG:CZ	2.39	0.52
1:D:67:VAL:HG21	1:D:83:PHE:CE1	2.44	0.52
1:B:10:ILE:HD12	4:B:982:HOH:O	2.09	0.52
1:D:76:GLN:HE22	1:D:81:GLN:HG3	1.75	0.51
1:A:12:LEU:C	1:A:12:LEU:HD23	2.35	0.51
1:A:83:PHE:HB3	1:A:84:PRO:HA	1.91	0.51
1:C:64:CR8:H23	1:C:212:GLU:HB2	1.92	0.50
1:D:212:GLU:HG2	1:D:213:HIS:N	2.27	0.50
1:A:2:SER:O	1:A:3:ALA:HB3	2.11	0.50
1:C:85:LYS:HG2	1:C:180:LYS:HG2	1.95	0.49
1:C:101:CYS:HA	1:C:121:HIS:O	2.11	0.49
1:C:198:ILE:HG23	1:C:208:VAL:HG13	1.95	0.49
1:A:13:ARG:CD	1:A:26:ASP:OD1	2.56	0.48
1:A:149:ARG:NH2	4:A:859:HOH:O	2.46	0.48
1:B:212:GLU:HG2	1:B:213:HIS:N	2.28	0.48
1:D:211:TYR:CE2	3:D:229:SO3:O1	2.67	0.47
1:C:87:TYR:CZ	1:C:107:ILE:HD12	2.50	0.47
1:A:32:LYS:NZ	4:A:929:HOH:O	2.33	0.47
1:C:195[A]:CYS:SG	3:C:228:SO3:O2	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ILE:HD12	1:D:102:ILE:C	2.38	0.47
1:A:159:MET:CE	1:A:173:SER:HB2	2.45	0.47
1:D:159:MET:HE2	1:D:173:SER:HB2	1.97	0.46
1:B:145:LYS:NZ	1:D:143:THR:H	2.13	0.46
1:D:1:MET:H3	1:D:2:SER:HB2	1.79	0.46
1:C:94:THR:HG23	1:C:100:ILE:CD1	2.45	0.46
1:D:94:THR:HA	1:D:100:ILE:HD13	1.98	0.46
1:C:197:GLU:HB3	3:C:228:SO3:O1	2.15	0.45
1:B:110:GLU:HG3	1:B:115:TYR:CE1	2.52	0.45
1:B:143:THR:H	1:D:145:LYS:NZ	2.15	0.45
1:A:0:HIS:HD2	1:A:1:MET:O	2.01	0.44
1:A:64:CR8:H10	4:A:727:HOH:O	2.17	0.44
1:A:87:TYR:CZ	1:A:107:ILE:HD12	2.53	0.44
1:C:90:GLU:HB3	1:D:123:VAL:HB	2.00	0.44
1:A:190:HIS:C	1:A:191:LEU:HD12	2.43	0.44
1:B:220:LEU:HB2	1:D:195[B]:CYS:HB2	2.00	0.44
1:A:140:GLU:HB3	1:C:189:TYR:CE2	2.53	0.43
1:D:83:PHE:HB3	1:D:84:PRO:HA	1.99	0.43
1:A:49:PRO:HB3	1:A:204:ASP:HB3	2.00	0.43
1:C:67:VAL:HG11	1:C:114:PHE:CZ	2.54	0.43
1:D:64:CR8:H23	1:D:212:GLU:HB2	2.00	0.43
1:B:87:TYR:CZ	1:B:107:ILE:HD12	2.54	0.42
1:D:14:MET:HA	1:D:118:VAL:O	2.19	0.42
1:A:195[A]:CYS:SG	3:A:228:SO3:O3	2.76	0.42
1:D:12:LEU:C	1:D:12:LEU:HD23	2.44	0.42
1:A:149:ARG:NH1	4:A:288:HOH:O	2.50	0.42
1:B:102:ILE:C	1:B:102:ILE:HD12	2.45	0.42
1:B:158:THR:HG23	1:B:170:ARG:NH1	2.34	0.42
1:D:101:CYS:HA	1:D:121:HIS:O	2.20	0.42
1:B:83:PHE:HB3	1:B:84:PRO:HA	2.02	0.41
1:B:163:LEU:HD11	1:B:169:TYR:HB2	2.01	0.41
1:C:85:LYS:HG3	1:C:180:LYS:HG2	2.02	0.41
1:A:212:GLU:HG2	1:A:213:HIS:N	2.36	0.41
1:C:222:ASP:O	1:C:223:ASN:C	2.63	0.41
1:D:195[B]:CYS:SG	3:D:229:SO3:S	3.19	0.41
1:D:199:LEU:HD11	1:D:211:TYR:HB2	2.03	0.41
1:A:101:CYS:HA	1:A:121:HIS:O	2.21	0.41
1:B:14:MET:HA	1:B:118:VAL:O	2.21	0.40
1:D:195[B]:CYS:HB3	3:D:229:SO3:S	2.60	0.40
1:A:143:THR:H	1:C:145:LYS:NZ	2.20	0.40
1:B:159:MET:CE	1:B:173:SER:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LYS:HE2	1:B:203:LYS:HB3	1.95	0.40
1:C:40:MET:HE3	4:C:729:HOH:O	2.20	0.40
1:D:49:PRO:HB3	1:D:204:ASP:HB3	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:SO4:O1	4:A:661:HOH:O[3_544]	1.59	0.61
2:B:231:SO4:O3	4:A:382:HOH:O[3_544]	1.61	0.59
4:A:904:HOH:O	4:C:1199:HOH:O[4_455]	2.17	0.03

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	221/230 (96%)	219 (99%)	2 (1%)	0	100	100
1	B	219/230 (95%)	219 (100%)	0	0	100	100
1	C	218/230 (95%)	217 (100%)	1 (0%)	0	100	100
1	D	219/230 (95%)	217 (99%)	2 (1%)	0	100	100
All	All	877/920 (95%)	872 (99%)	5 (1%)	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	194/197 (98%)	193 (100%)	1 (0%)	81	87
1	B	192/197 (98%)	189 (98%)	3 (2%)	55	62
1	C	191/197 (97%)	187 (98%)	4 (2%)	47	52
1	D	192/197 (98%)	186 (97%)	6 (3%)	35	37
All	All	769/788 (98%)	755 (98%)	14 (2%)	51	58

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	LYS
1	B	67	VAL
1	B	110	GLU
1	B	180	LYS
1	C	13	ARG
1	C	67	VAL
1	C	180	LYS
1	C	181	GLU
1	D	1	MET
1	D	2	SER
1	D	9	LYS
1	D	13	ARG
1	D	135	LYS
1	D	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	B	206	ASN
1	C	11	ASN
1	C	22	HIS
1	C	81	GLN
1	D	76	GLN
1	D	166	ASN

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
1	CR8	C	64	1	25,27,28	1.73	6 (24%)	24,37,39	1.19	1 (4%)
1	CR8	B	64	1	25,27,28	1.71	6 (24%)	24,37,39	1.33	2 (8%)
1	CR8	D	64	1	25,27,28	1.74	5 (20%)	24,37,39	1.36	2 (8%)
1	CR8	A	64	1	25,27,28	1.77	6 (24%)	24,37,39	1.27	1 (4%)

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	C	64	1	-	5/12/25/26	0/3/3/3
1	CR8	B	64	1	-	6/12/25/26	0/3/3/3
1	CR8	D	64	1	-	6/12/25/26	0/3/3/3
1	CR8	A	64	1	-	6/12/25/26	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	CR8	C8-C7	4.04	1.49	1.39
1	D	64	CR8	C8-C7	4.00	1.49	1.39
1	D	64	CR8	C1-N2	3.95	1.38	1.32
1	B	64	CR8	C8-C7	3.86	1.48	1.39
1	C	64	CR8	C8-C7	3.85	1.48	1.39
1	A	64	CR8	C1-N2	3.69	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	CR8	C1-N2	3.69	1.37	1.32
1	A	64	CR8	C8-CA2	3.61	1.49	1.40
1	C	64	CR8	C1-N2	3.54	1.37	1.32
1	B	64	CR8	C8-CA2	3.54	1.48	1.40
1	D	64	CR8	C8-CA2	3.52	1.48	1.40
1	C	64	CR8	C8-CA2	3.45	1.48	1.40
1	B	64	CR8	C4-C11	-2.70	1.39	1.46
1	C	64	CR8	C4-C11	-2.67	1.39	1.46
1	A	64	CR8	C4-C11	-2.62	1.39	1.46
1	D	64	CR8	C4-C11	-2.59	1.39	1.46
1	D	64	CR8	C12-C11	-2.41	1.40	1.46
1	B	64	CR8	C12-C11	-2.34	1.40	1.46
1	C	64	CR8	C12-C11	-2.29	1.40	1.46
1	A	64	CR8	C12-C11	-2.26	1.40	1.46
1	C	64	CR8	C6-C12	2.08	1.40	1.35
1	A	64	CR8	C6-C12	2.05	1.40	1.35
1	B	64	CR8	C6-C12	2.00	1.40	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	CR8	C12-C6-C7	-2.79	119.46	122.10
1	A	64	CR8	C12-C6-C7	-2.61	119.63	122.10
1	D	64	CR8	C12-C6-C7	-2.50	119.74	122.10
1	B	64	CR8	C12-C6-C7	-2.47	119.76	122.10
1	D	64	CR8	CA1-C20-C21	-2.30	109.41	113.23
1	B	64	CR8	C4-C11-C12	2.05	120.47	116.67

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	CR8	C3-CA3-N3-C2
1	A	64	CR8	C3-CA3-N3-C1
1	A	64	CR8	CA1-C20-C21-N22
1	A	64	CR8	CA1-C20-C21-C23
1	B	64	CR8	C3-CA3-N3-C2
1	B	64	CR8	C3-CA3-N3-C1
1	B	64	CR8	CA1-C20-C21-N22
1	B	64	CR8	CA1-C20-C21-C23
1	C	64	CR8	C3-CA3-N3-C2
1	C	64	CR8	CA1-C20-C21-N22

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Mol	Chain	Res	Type	Atoms
1	C	64	CR8	CA1-C20-C21-C23
1	D	64	CR8	C3-CA3-N3-C2
1	D	64	CR8	C3-CA3-N3-C1
1	D	64	CR8	CA1-C20-C21-N22
1	D	64	CR8	CA1-C20-C21-C23
1	C	64	CR8	C3-CA3-N3-C1
1	A	64	CR8	C5-C7-C8-CA2
1	A	64	CR8	C6-C7-C8-CA2
1	B	64	CR8	C5-C7-C8-CA2
1	B	64	CR8	C6-C7-C8-CA2
1	C	64	CR8	C6-C7-C8-CA2
1	D	64	CR8	C5-C7-C8-CA2
1	D	64	CR8	C6-C7-C8-CA2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	64	CR8	1	0
1	D	64	CR8	1	0
1	A	64	CR8	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 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	B	227	-	4,4,4	0.25	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO3	A	228	-	1,3,3	8.90	1 (100%)	0,3,3	-	-
3	SO3	B	229	-	1,3,3	8.72	1 (100%)	0,3,3	-	-
2	SO4	B	230	-	4,4,4	0.33	0	6,6,6	0.25	0
2	SO4	D	227	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	C	1224	-	4,4,4	0.27	0	6,6,6	0.11	0
2	SO4	C	1227	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	D	1227	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	D	228	-	4,4,4	0.26	0	6,6,6	0.15	0
2	SO4	A	1224	-	4,4,4	0.29	0	6,6,6	0.22	0
2	SO4	B	231	-	4,4,4	0.43	0	6,6,6	0.38	0
2	SO4	B	1224	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	C	227	-	4,4,4	0.26	0	6,6,6	0.14	0
3	SO3	D	229	-	1,3,3	8.39	1 (100%)	0,3,3	-	-
2	SO4	C	1226	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	D	1226	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	C	1225	-	4,4,4	0.25	0	6,6,6	0.16	0
3	SO3	C	228	-	1,3,3	8.32	1 (100%)	0,3,3	-	-
2	SO4	B	1225	-	4,4,4	0.23	0	6,6,6	0.23	0
2	SO4	A	227	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	B	228	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	A	1225	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	D	1225	-	4,4,4	0.26	0	6,6,6	0.07	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	228	SO3	O1-S	8.90	1.82	1.44
3	B	229	SO3	O1-S	8.72	1.81	1.44
3	D	229	SO3	O1-S	8.39	1.80	1.44
3	C	228	SO3	O1-S	8.32	1.80	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	228	SO3	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	229	SO3	1	0
2	B	230	SO4	2	0
2	C	1227	SO4	1	0
2	D	1227	SO4	1	0
2	B	231	SO4	0	2
3	D	229	SO3	5	0
3	C	228	SO3	6	0
2	D	1225	SO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.72	0 100 100	13, 22, 39, 68	6 (2%)
1	B	220/230 (95%)	-0.85	3 (1%) 73 73	12, 20, 35, 63	5 (2%)
1	C	220/230 (95%)	-0.72	0 100 100	15, 23, 41, 64	4 (1%)
1	D	220/230 (95%)	-0.60	1 (0%) 87 87	16, 26, 45, 104	6 (2%)
All	All	881/920 (95%)	-0.72	4 (0%) 87 87	12, 23, 41, 104	21 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.0
1	B	1	MET	2.8
1	B	223	ASN	2.6
1	B	222	ASP	2.1

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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CR8	A	64	25/26	0.97	0.04	15,18,22,27	0
1	CR8	B	64	25/26	0.97	0.05	11,16,19,22	0
1	CR8	C	64	25/26	0.97	0.04	16,18,22,23	0
1	CR8	D	64	25/26	0.97	0.05	19,22,26,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	231	5/5	0.78	0.24	26,50,57,79	0
2	SO4	C	1226	5/5	0.82	0.12	34,44,56,56	5
2	SO4	C	227	5/5	0.82	0.17	55,71,89,92	0
2	SO4	C	1227	5/5	0.83	0.08	48,49,61,66	5
2	SO4	B	230	5/5	0.83	0.17	54,62,84,89	0
2	SO4	D	1226	5/5	0.83	0.13	40,44,60,63	5
2	SO4	D	1227	5/5	0.83	0.10	54,54,73,74	5
2	SO4	C	1225	5/5	0.85	0.10	57,58,61,67	0
2	SO4	A	227	5/5	0.85	0.20	44,62,84,87	0
2	SO4	B	1224	5/5	0.87	0.10	54,55,67,78	0
2	SO4	D	227	5/5	0.87	0.12	60,69,84,87	0
2	SO4	A	1225	5/5	0.88	0.08	42,46,55,61	5
2	SO4	B	228	5/5	0.89	0.17	49,60,88,95	0
3	SO3	C	228	4/4	0.89	0.29	45,49,55,65	0
3	SO3	A	228	4/4	0.90	0.33	45,45,58,64	0
3	SO3	B	229	4/4	0.90	0.32	38,38,44,68	0
2	SO4	D	1225	5/5	0.90	0.14	47,56,66,70	0
3	SO3	D	229	4/4	0.90	0.32	41,54,56,58	0
2	SO4	B	1225	5/5	0.92	0.08	27,36,45,46	5
2	SO4	A	1224	5/5	0.92	0.12	43,46,58,58	0
2	SO4	B	227	5/5	0.97	0.07	34,39,41,46	0
2	SO4	C	1224	5/5	0.98	0.07	35,40,45,53	0
2	SO4	D	228	5/5	0.98	0.05	31,39,42,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.