



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 09:22 am GMT

PDB ID : 3TMT
Title : IrisFP, distorted 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

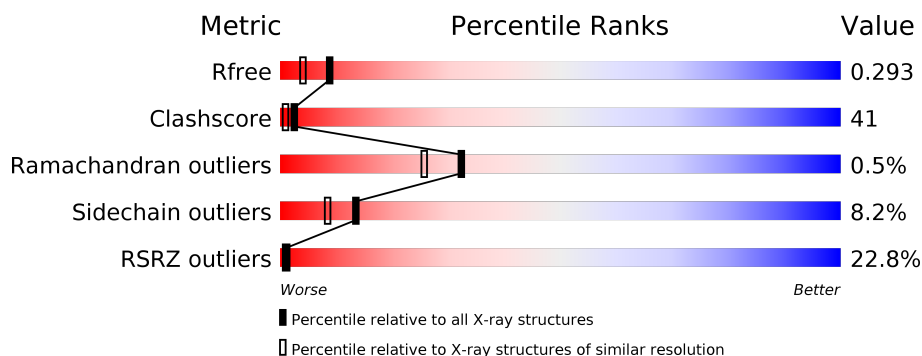
1 Overall quality at a glance

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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>24%</div> <div>42%</div> <div>47%</div> <div>7%</div> <div>• •</div> </div>
1	B	230	<div> <div>10%</div> <div>48%</div> <div>45%</div> <div>• •</div> </div>
1	C	230	<div> <div>27%</div> <div>42%</div> <div>48%</div> <div>5%</div> <div>•</div> </div>
1	D	230	<div> <div>26%</div> <div>42%</div> <div>46%</div> <div>7%</div> <div>• •</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	1225	-	-	X	-
2	SO4	B	227	-	-	X	-
2	SO4	C	1225	-	-	-	X
2	SO4	C	1226	-	-	X	-
2	SO4	D	1225	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9939 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	220	Total	C	N	O	S	1	2	0
			1779	1133	304	331	11			
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:

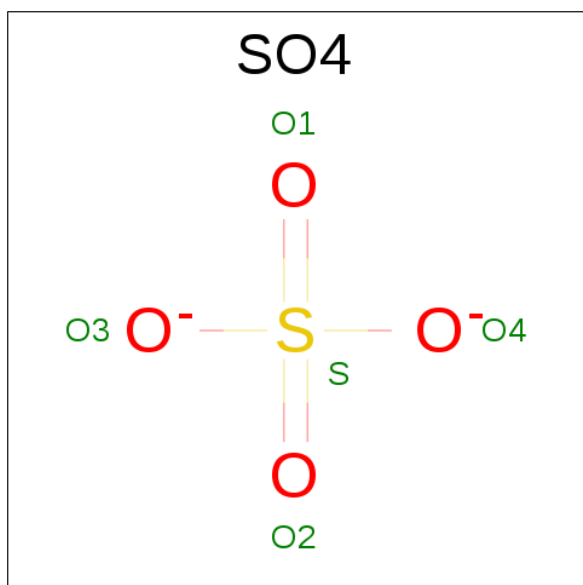
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
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 (three-letter code: 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	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
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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	679	Total O 679 679	0	0
3	B	555	Total O 555 555	0	0
3	C	660	Total O 660 660	0	0

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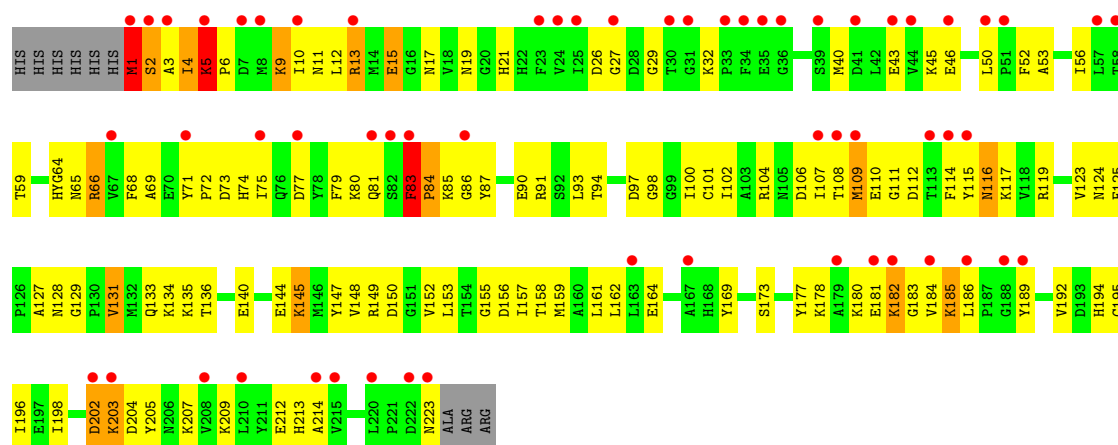
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	791	Total 791	O 791	0	0

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 24% 42% 47% 7%
- HIS H1S H1S H1S H1S H0 M1 S2 A3 I4 K5 P6 D7 P8 N11 L12 R13 M14 E15 V18 N19 R22 F23 V24 I25 D26 G27 D28 G29 T30 G31 K32 P33 F34 E35 K37 Q38 S39 M40 D41 L42 F43 V44 K45 E46 P49 L50 F51 F52 A53 F54 D55 I56

- Chain B:
-
- 10% 48% 45%
- HIS HIS HIS HIS HIS HIS M1 S2 A3 I4 K5 M8 K9 N10 N11 N12 H21 H22 F23 V24 I25 T30 G31 Q38 Q39 M40 D41 L42 E43 V44 G47 G48 L49 P50 L50 P51 F54 D55 I56 L57 F61 HYG64 N65 R66 V67 F68 A69 E70 Y71 P72 I75 O76 K77
- Y78 F79 K80 F83 P84 K85 G86 Y87 S88 W89 E90 K91 S92 G98 G99 I100 C101 R104 M105 D106 I107 T108 M109 E110 F114 Y115 N116 K117 V118 R119 E120 H121 G122 V123 M124 F125 Y126 A127 N128 V131 K134 K135 T136 L137 K138 T143 E144 K145 M146 R149 Y150
- G155 D156 I157 M158 M159 A160 L161 L162 L163 L164 E165 G166 M166 Y169 R170 S173 T176 Y177 K180 E181 E182 G183 P187 G188 Y189 V192 D193 H194 C195 I196 E197 I198 L199 K203 K209 L210 E211 E212 H213 A214 V215 A216 L220 P221 D222 N223 ALA ARG ARG

- [illegible]



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 – 1.99	Depositor EDS
% Data completeness (in resolution range)	83.9 (12.98-2.00) 82.8 (12.98-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.295 , 0.295 0.293 , 0.293	Depositor DCC
R_{free} test set	3246 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	2.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9939	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CR8, 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	0.85	13/1838 (0.7%)	0.83	10/2478 (0.4%)
1	B	0.41	0/1821	0.60	0/2455
1	C	0.61	2/1805 (0.1%)	0.63	1/2434 (0.0%)
1	D	0.69	6/1819 (0.3%)	0.71	4/2452 (0.2%)
All	All	0.66	21/7283 (0.3%)	0.70	15/9819 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	2
All	All	0	4

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	SER	CB-OG	-15.59	1.22	1.42
1	A	221	PRO	CA-CB	-10.25	1.33	1.53
1	C	4	ILE	CB-CG2	-9.66	1.23	1.52
1	A	1	MET	C-O	-9.53	1.05	1.23
1	A	3	ALA	C-O	-8.81	1.06	1.23

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	MET	CG-SD-CE	9.53	115.45	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	LEU	CA-CB-CG	9.19	136.44	115.30
1	A	3	ALA	N-CA-CB	8.49	121.99	110.10
1	A	2	SER	N-CA-C	7.64	131.63	111.00
1	D	5	LYS	CD-CE-NZ	6.71	127.13	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	PRO	Peptide
1	C	2	SER	Peptide
1	D	1	MET	Peptide
1	D	83	PHE	Peptide

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	1808	0	1740	153	0
1	B	1792	0	1729	139	1
1	C	1779	0	1714	144	1
1	D	1790	0	1730	144	0
2	A	20	0	0	1	0
2	B	15	0	0	5	0
2	C	25	0	0	4	0
2	D	25	0	0	1	0
3	A	679	0	0	79	5
3	B	555	0	0	67	6
3	C	660	0	0	66	3
3	D	791	0	0	68	5
All	All	9939	0	6913	574	11

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 41.

The worst 5 of 574 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:135:LYS:NZ	3:A:723:HOH:O	1.86	1.06
2:B:1225:SO4:O4	3:B:595:HOH:O	1.75	1.03
1:B:5:LYS:NZ	3:B:662:HOH:O	1.83	1.03
1:C:197:GLU:OE2	3:C:1385:HOH:O	1.80	0.99
1:D:212:GLU:OE1	3:D:2145:HOH:O	1.81	0.97

The worst 5 of 11 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)
1:B:128:ASN:ND2	3:B:322:HOH:O[3_554]	1.89	0.31
3:A:3106:HOH:O	3:D:2715:HOH:O[4_445]	1.99	0.21
3:B:2380:HOH:O	3:D:2944:HOH:O[3_554]	2.02	0.18
3:A:453:HOH:O	3:B:301:HOH:O[3_554]	2.04	0.16
3:C:1436:HOH:O	3:D:2068:HOH:O[2_555]	2.05	0.15

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	223/230 (97%)	210 (94%)	11 (5%)	2 (1%)	20	12
1	B	221/230 (96%)	218 (99%)	3 (1%)	0	100	100
1	C	219/230 (95%)	211 (96%)	8 (4%)	0	100	100
1	D	221/230 (96%)	212 (96%)	7 (3%)	2 (1%)	20	12
All	All	884/920 (96%)	851 (96%)	29 (3%)	4 (0%)	32	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PRO
1	A	222	ASP

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Mol	Chain	Res	Type
1	D	84	PRO
1	D	131	VAL

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%)	174 (90%)	20 (10%)	8	4
1	B	192/197 (98%)	180 (94%)	12 (6%)	21	15
1	C	190/197 (96%)	174 (92%)	16 (8%)	13	8
1	D	192/197 (98%)	177 (92%)	15 (8%)	15	9
All	All	768/788 (98%)	705 (92%)	63 (8%)	13	8

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	145	LYS
1	C	32	LYS
1	D	145	LYS
1	B	166	ASN
1	B	203	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	GLN

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	A	64	1	18,27,28	1.87	4 (22%)	16,37,39	1.48	2 (12%)
1	CR8	B	64	1	18,27,28	1.95	6 (33%)	16,37,39	1.46	3 (18%)
1	CR8	C	64	1	18,27,28	1.81	3 (16%)	16,37,39	1.32	2 (12%)
1	CR8	D	64	1	18,27,28	1.86	4 (22%)	16,37,39	1.48	2 (12%)

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	-	0/8/25/26	0/3/3/3
1	CR8	B	64	1	-	0/8/25/26	0/3/3/3
1	CR8	C	64	1	-	0/8/25/26	0/3/3/3
1	CR8	D	64	1	-	0/8/25/26	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	CR8	C4-C1	-2.97	1.38	1.46
1	D	64	CR8	C4-C1	-2.97	1.38	1.46
1	C	64	CR8	C2-C1	-2.94	1.39	1.46
1	B	64	CR8	C2-C1	-2.89	1.39	1.46
1	A	64	CR8	C4-C1	-2.74	1.39	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	CR8	C2-C6-C7	-3.62	118.87	121.95
1	C	64	CR8	C4-C5-C7	-3.05	119.36	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	CR8	O19-C-C17	-2.68	117.87	126.26
1	C	64	CR8	C2-C6-C7	-2.32	119.98	121.95
1	B	64	CR8	C2-C6-C7	-2.23	120.06	121.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	64	CR8	8	0
1	B	64	CR8	6	0
1	C	64	CR8	4	0
1	D	64	CR8	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

17 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	A	1224	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	A	1225	-	4,4,4	0.11	0	6,6,6	0.16	0
2	SO4	A	227	-	4,4,4	0.18	0	6,6,6	0.08	0
2	SO4	A	228	-	4,4,4	0.19	0	6,6,6	0.14	0
2	SO4	B	1224	-	4,4,4	0.20	0	6,6,6	0.10	0
2	SO4	B	1225	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	227	-	4,4,4	0.20	0	6,6,6	0.36	0
2	SO4	C	1224	-	4,4,4	0.16	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	1225	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	C	1226	-	4,4,4	0.12	0	6,6,6	0.11	0
2	SO4	C	1227	-	4,4,4	0.16	0	6,6,6	0.05	0
2	SO4	C	227	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	D	1225	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	D	1226	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	D	1227	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	D	227	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	D	228	-	4,4,4	0.16	0	6,6,6	0.13	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	SO4	A	1224	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1225	-	-	0/0/0/0	0/0/0/0
2	SO4	A	227	-	-	0/0/0/0	0/0/0/0
2	SO4	A	228	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1224	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1225	-	-	0/0/0/0	0/0/0/0
2	SO4	B	227	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1224	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1225	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1226	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1227	-	-	0/0/0/0	0/0/0/0
2	SO4	C	227	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1225	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1226	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1227	-	-	0/0/0/0	0/0/0/0
2	SO4	D	227	-	-	0/0/0/0	0/0/0/0
2	SO4	D	228	-	-	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.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	227	SO4	1	0
2	B	1224	SO4	1	0
2	B	1225	SO4	2	0
2	B	227	SO4	2	0
2	C	1224	SO4	1	0
2	C	1226	SO4	3	0
2	D	1226	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%)	1.44	56 (25%) 1 1	12, 20, 30, 38	2 (0%)
1	B	220/230 (95%)	1.21	24 (10%) 6 6	11, 18, 26, 40	1 (0%)
1	C	219/230 (95%)	1.58	62 (28%) 1 1	14, 21, 30, 37	2 (0%)
1	D	220/230 (95%)	1.56	59 (26%) 1 1	13, 22, 34, 49	3 (1%)
All	All	880/920 (95%)	1.45	201 (22%) 1 1	11, 20, 31, 49	8 (0%)

The worst 5 of 201 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	SER	6.5
1	B	1	MET	6.0
1	C	10	ILE	4.5
1	C	81	GLN	4.5
1	A	222	ASP	4.4

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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CR8	B	64	25/26	0.89	0.19	-	11,17,21,23	0
1	CR8	D	64	25/26	0.86	0.18	-	11,19,25,27	0
1	CR8	A	64	25/26	0.87	0.18	-	9,18,26,34	0
1	CR8	C	64	25/26	0.84	0.21	-	6,17,24,32	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	C	1225	5/5	0.87	0.34	5.78	23,23,39,51	0
2	SO4	D	1225	5/5	0.89	0.29	2.17	29,30,35,37	0
2	SO4	A	1224	5/5	0.82	0.24	1.71	21,30,35,46	0
2	SO4	B	1224	5/5	0.75	0.36	1.56	34,40,51,62	0
2	SO4	D	228	5/5	0.89	0.24	1.53	28,28,33,41	0
2	SO4	C	1224	5/5	0.86	0.24	0.05	22,27,39,49	0
2	SO4	A	227	5/5	0.92	0.16	-1.78	29,30,36,38	0
2	SO4	C	227	5/5	0.64	0.33	-	36,38,55,74	0
2	SO4	B	1225	5/5	0.89	0.21	-	8,13,20,27	5
2	SO4	A	1225	5/5	0.72	0.28	-	11,11,22,35	5
2	SO4	C	1226	5/5	0.69	0.35	-	25,25,29,40	5
2	SO4	C	1227	5/5	0.82	0.22	-	24,27,39,45	5
2	SO4	B	227	5/5	0.82	0.25	-	17,26,28,42	0
2	SO4	D	1226	5/5	0.51	0.37	-	29,36,44,51	5
2	SO4	A	228	5/5	0.70	0.35	-	31,34,54,59	0
2	SO4	D	1227	5/5	0.83	0.31	-	18,27,33,39	5
2	SO4	D	227	5/5	0.89	0.34	-	32,35,45,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.