



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 02:43 PM EDT

PDB ID : 2IFU
Title : Crystal Structure of a Gamma-SNAP from *Danio rerio*
Authors : Bitto, E.; Wesenberg, G.E.; Phillips Jr., G.N.; McCoy, J.G.; Bingman, C.A.;
Center for Eukaryotic Structural Genomics (CESG)
Deposited on : unknown
Resolution : 2.60 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

<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 : rb-20030345
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) : rb-20030345

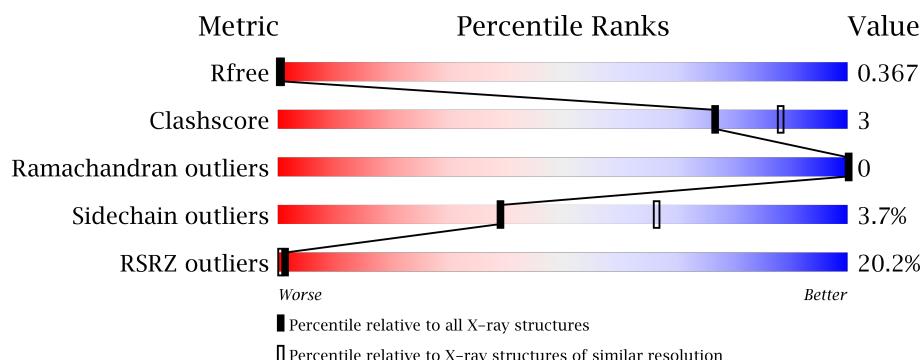
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	307	<div> <div>12%</div> <div>80%</div> <div>8%</div> <div>10%</div> </div>
1	B	307	<div> <div>4%</div> <div>78%</div> <div>10%</div> <div>10%</div> </div>
1	C	307	<div> <div>18%</div> <div>79%</div> <div>8%</div> <div>11%</div> </div>
1	D	307	<div> <div>35%</div> <div>79%</div> <div>8%</div> <div>12%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8758 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 gamma-snap.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	Se	0	2	0
			2181	1373	372	419	5	12			
1	B	275	Total	C	N	O	S	Se	0	1	0
			2176	1369	372	419	5	11			
1	C	272	Total	C	N	O	S	Se	0	0	0
			2152	1354	368	415	5	10			
1	D	270	Total	C	N	O	S	Se	0	0	0
			2135	1342	365	413	5	10			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	CLONING ARTIFACT	UNP Q5BJK3
A	0	ILE	-	CLONING ARTIFACT	UNP Q5BJK3
A	1	ALA	MET	CLONING ARTIFACT	UNP Q5BJK3
A	24	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
A	82	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
A	83	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
A	90	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
A	103	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
A	115	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
A	124	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
A	182	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
A	186	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
A	261	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
B	-1	ALA	-	CLONING ARTIFACT	UNP Q5BJK3
B	0	ILE	-	CLONING ARTIFACT	UNP Q5BJK3
B	1	ALA	MET	CLONING ARTIFACT	UNP Q5BJK3
B	24	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
B	82	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
B	83	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
B	90	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
B	103	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	115	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
B	124	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
B	182	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
B	186	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
B	261	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
C	-1	ALA	-	CLONING ARTIFACT	UNP Q5BJK3
C	0	ILE	-	CLONING ARTIFACT	UNP Q5BJK3
C	1	ALA	MET	CLONING ARTIFACT	UNP Q5BJK3
C	24	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
C	82	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
C	83	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
C	90	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
C	103	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
C	115	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
C	124	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
C	182	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
C	186	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
C	261	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
D	-1	ALA	-	CLONING ARTIFACT	UNP Q5BJK3
D	0	ILE	-	CLONING ARTIFACT	UNP Q5BJK3
D	1	ALA	MET	CLONING ARTIFACT	UNP Q5BJK3
D	24	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
D	82	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
D	83	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
D	90	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
D	103	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
D	115	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
D	124	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
D	182	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
D	186	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3
D	261	MSE	MET	MODIFIED RESIDUE	UNP Q5BJK3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	17	Total	O	0	0
			17	17		

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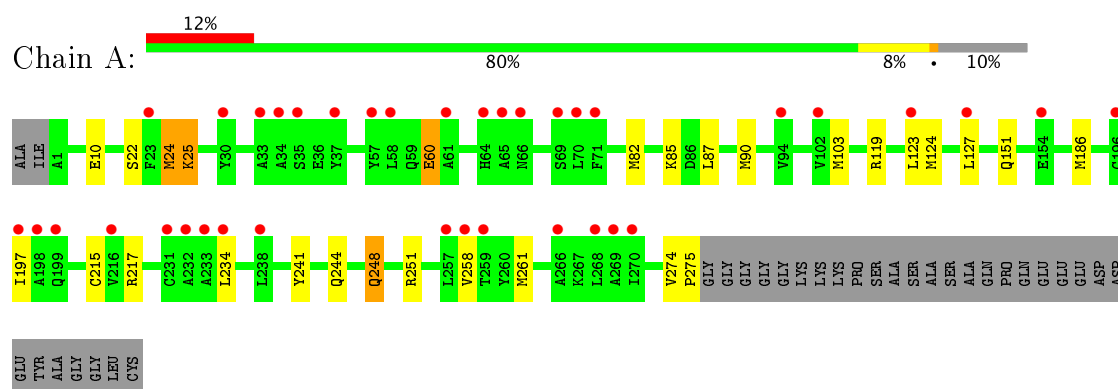
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	6	Total	O	0	0
			6	6		

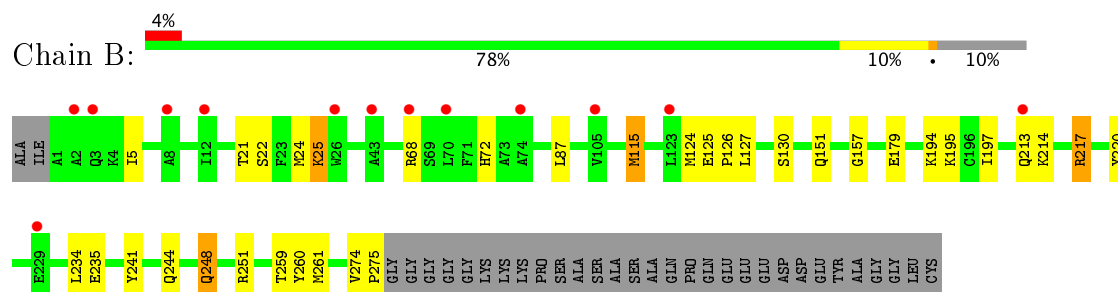
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

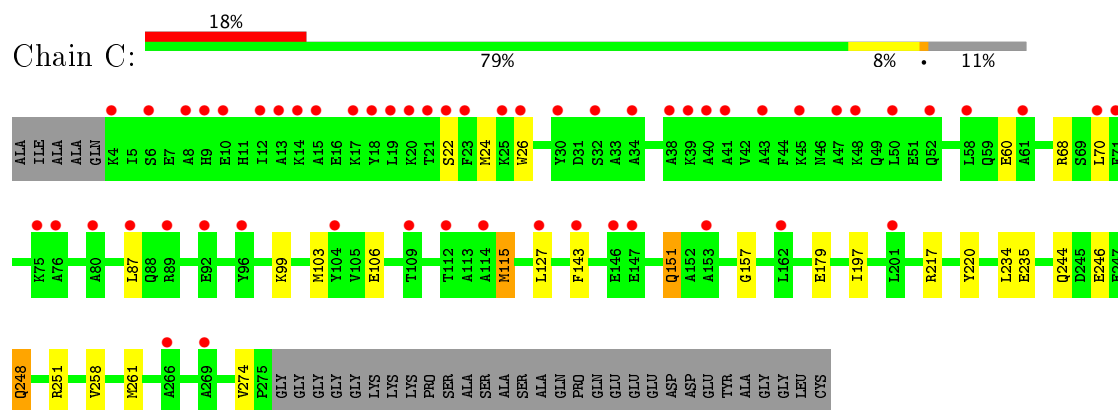
- Molecule 1: gamma-snap



- Molecule 1: gamma-snap

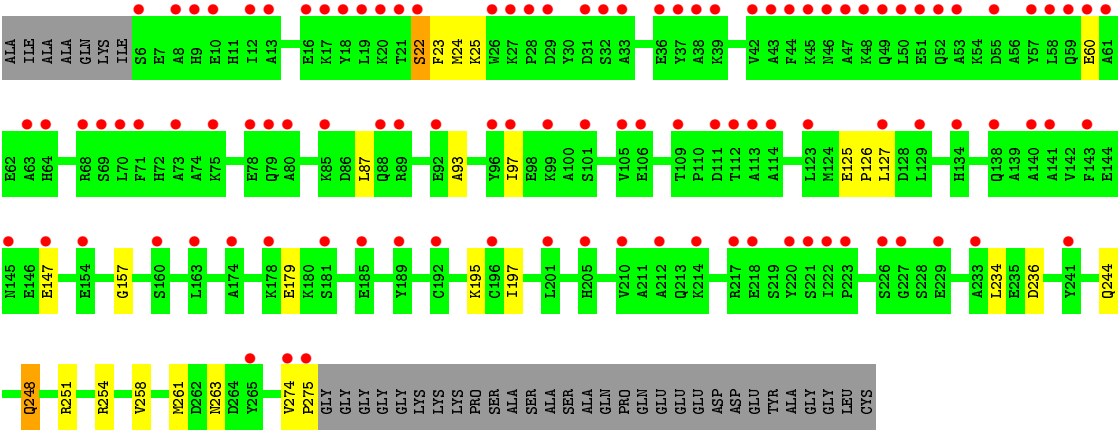


- Molecule 1: gamma-snap



- Molecule 1: gamma-snap

Chain D: 35% 79% 8% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.38 Å 90.81 Å 264.17 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.05 – 2.60 40.05 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (40.05-2.60) 96.1 (40.05-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.239 , 0.261 0.361 , 0.367	Depositor DCC
R_{free} test set	3044 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	8758	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: 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	1.00	6/2213 (0.3%)	0.86	3/2959 (0.1%)
1	B	0.90	6/2206 (0.3%)	0.92	4/2952 (0.1%)
1	C	0.57	1/2179 (0.0%)	0.64	2/2916 (0.1%)
1	D	0.42	0/2162	0.55	0/2894
All	All	0.76	13/8760 (0.1%)	0.76	9/11721 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	TYR	CE2-CZ	-8.19	1.27	1.38
1	A	215	CYS	CB-SG	-7.34	1.69	1.82
1	A	103	MSE	CG-SE	-6.44	1.73	1.95
1	A	60	GLU	CB-CG	-6.21	1.40	1.52
1	B	115[A]	MSE	SE-CE	5.98	2.30	1.95
1	B	115[B]	MSE	SE-CE	5.98	2.30	1.95
1	B	241	TYR	CG-CD2	-5.83	1.31	1.39
1	C	115	MSE	SE-CE	5.78	2.29	1.95
1	B	241	TYR	CE1-CZ	-5.73	1.31	1.38
1	A	10	GLU	CD-OE2	5.52	1.31	1.25
1	A	241	TYR	CE1-CZ	-5.32	1.31	1.38
1	A	241	TYR	CG-CD2	-5.31	1.32	1.39
1	B	241	TYR	CG-CD1	-5.30	1.32	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	ARG	NE-CZ-NH2	15.91	128.25	120.30
1	B	217	ARG	NE-CZ-NH1	-13.78	113.41	120.30
1	A	217	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	217	ARG	NE-CZ-NH1	7.76	124.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	ARG	CD-NE-CZ	7.76	134.47	123.60
1	C	217	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	217	ARG	CD-NE-CZ	5.13	130.78	123.60
1	B	68	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	217	ARG	NE-CZ-NH1	5.04	122.82	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	2181	0	2171	15	0
1	B	2176	0	2162	17	1
1	C	2152	0	2132	14	0
1	D	2135	0	2108	17	1
2	A	15	0	0	0	0
2	B	20	0	0	1	0
2	C	10	0	0	0	0
2	D	5	0	0	0	0
3	A	41	0	0	0	0
3	B	17	0	0	0	0
3	C	6	0	0	0	0
All	All	8758	0	8573	60	1

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 (60) 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:186:MSE:CE	1:A:186:MSE:SE	2.17	1.43
1:B:115[B]:MSE:CE	1:B:115[B]:MSE:SE	2.20	1.39
1:A:24:MSE:SE	1:A:24:MSE:CE	2.23	1.34
1:C:115:MSE:CE	1:C:115:MSE:SE	2.29	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115[A]:MSE:CE	1:B:115[A]:MSE:SE	2.30	1.28
1:A:82[A]:MSE:SE	1:A:119:ARG:HH21	1.87	1.07
1:A:90:MSE:HE2	1:A:123:LEU:HB2	1.40	1.03
1:C:220:TYR:OH	1:C:235:GLU:OE2	1.90	0.88
1:A:85:LYS:HD2	1:A:123:LEU:HD13	1.58	0.84
1:B:244:GLN:HE21	1:B:275:PRO:HG2	1.46	0.80
1:A:82[A]:MSE:SE	1:A:119:ARG:NH2	2.69	0.71
1:B:260:TYR:OH	1:D:251:ARG:HA	1.89	0.70
1:A:248:GLN:HG2	1:A:251:ARG:NH2	2.11	0.65
1:A:244:GLN:HE21	1:A:275:PRO:HG2	1.62	0.64
1:C:248:GLN:HG2	1:C:251:ARG:HH22	1.61	0.64
1:A:248:GLN:HG2	1:A:251:ARG:HH22	1.63	0.64
1:D:248:GLN:HG2	1:D:251:ARG:NH2	2.13	0.63
1:C:248:GLN:HG2	1:C:251:ARG:NH2	2.14	0.63
1:A:90:MSE:HE2	1:A:123:LEU:CB	2.24	0.60
1:B:72:HIS:ND1	2:B:308:SO4:O3	2.33	0.60
1:D:248:GLN:HG2	1:D:251:ARG:HH22	1.66	0.60
1:A:25:LYS:HG3	1:A:25:LYS:O	2.03	0.58
1:D:197:ILE:HA	1:D:234:LEU:HD21	1.87	0.57
1:B:25:LYS:O	1:B:25:LYS:HG3	2.04	0.57
1:A:197:ILE:HA	1:A:234:LEU:HD21	1.87	0.56
1:B:197:ILE:HA	1:B:234:LEU:HD21	1.87	0.56
1:D:244:GLN:HE21	1:D:275:PRO:HG2	1.72	0.54
1:B:157:GLY:HA2	1:B:179:GLU:OE2	2.08	0.53
1:A:244:GLN:HA	1:A:274:VAL:HG23	1.92	0.51
1:B:248:GLN:HG2	1:B:251:ARG:NH2	2.28	0.49
1:C:70:LEU:HD13	1:C:106:GLU:HB3	1.95	0.48
1:B:244:GLN:HA	1:B:274:VAL:HG23	1.94	0.48
1:B:248:GLN:HG2	1:B:251:ARG:HH22	1.79	0.47
1:B:259:THR:HB	1:D:254:ARG:HG2	1.96	0.47
1:D:244:GLN:HA	1:D:274:VAL:HG23	1.96	0.46
1:D:93:ALA:O	1:D:97:ILE:HG12	2.15	0.46
1:C:157:GLY:HA2	1:C:179:GLU:OE2	2.17	0.44
1:D:24:MSE:HB2	1:D:24:MSE:HE3	1.91	0.44
1:C:244:GLN:HA	1:C:274:VAL:HG23	1.99	0.44
1:D:195:LYS:HD3	1:D:195:LYS:HA	1.89	0.44
1:D:263:ASN:HD22	1:D:263:ASN:N	2.15	0.43
1:C:143:PHE:CG	1:C:151:GLN:HB3	2.54	0.43
1:B:115[A]:MSE:HE3	1:B:115[A]:MSE:HB3	1.99	0.43
1:C:197:ILE:HA	1:C:234:LEU:HD21	2.01	0.43
1:C:68:ARG:NH1	1:D:236:ASP:OD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:SER:OG	1:D:23:PHE:N	2.51	0.43
1:C:258:VAL:O	1:C:261:MSE:HG2	2.18	0.42
1:A:85:LYS:HD2	1:A:123:LEU:CD1	2.40	0.42
1:C:99:LYS:O	1:C:103:MSE:HG3	2.19	0.42
1:B:220:TYR:OH	1:B:235:GLU:OE2	2.29	0.42
1:B:194:LYS:O	1:B:261:MSE:HE1	2.20	0.42
1:D:258:VAL:O	1:D:261:MSE:HG2	2.18	0.42
1:B:125:GLU:HB2	1:B:126:PRO:HD3	2.02	0.41
1:D:25:LYS:O	1:D:25:LYS:HG3	2.21	0.41
1:A:258:VAL:O	1:A:261:MSE:HG2	2.21	0.41
1:B:195:LYS:HD3	1:B:195:LYS:HA	1.86	0.41
1:D:125:GLU:HB2	1:D:126:PRO:HD3	2.03	0.40
1:C:246:GLU:HG3	1:C:274:VAL:HG12	2.03	0.40
1:C:22:SER:C	1:C:24:MSE:H	2.24	0.40
1:D:157:GLY:HA2	1:D:179:GLU:OE2	2.22	0.40

All (1) 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:5:ILE:CG2	1:D:147:GLU:OE2[4_445]	2.17	0.03

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	275/307 (90%)	267 (97%)	8 (3%)	0	100	100
1	B	274/307 (89%)	267 (97%)	7 (3%)	0	100	100
1	C	270/307 (88%)	261 (97%)	9 (3%)	0	100	100
1	D	268/307 (87%)	262 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1087/1228 (88%)	1057 (97%)	30 (3%)	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	225/233 (97%)	216 (96%)	9 (4%)	36	64
1	B	224/233 (96%)	211 (94%)	13 (6%)	23	46
1	C	222/233 (95%)	216 (97%)	6 (3%)	50	77
1	D	220/233 (94%)	215 (98%)	5 (2%)	56	81
All	All	891/932 (96%)	858 (96%)	33 (4%)	39	66

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	24	MSE
1	A	25	LYS
1	A	60	GLU
1	A	87	LEU
1	A	124	MSE
1	A	127	LEU
1	A	151	GLN
1	A	248	GLN
1	B	21	THR
1	B	22	SER
1	B	24	MSE
1	B	25	LYS
1	B	87	LEU
1	B	124	MSE
1	B	127	LEU
1	B	130	SER

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Mol	Chain	Res	Type
1	B	151	GLN
1	B	213	GLN
1	B	214	LYS
1	B	217	ARG
1	B	248	GLN
1	C	26	TRP
1	C	60	GLU
1	C	87	LEU
1	C	127	LEU
1	C	151	GLN
1	C	248	GLN
1	D	22	SER
1	D	60	GLU
1	D	87	LEU
1	D	127	LEU
1	D	248	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	52	GLN
1	A	138	GLN
1	A	213	GLN
1	A	244	GLN
1	A	263	ASN
1	B	49	GLN
1	B	52	GLN
1	B	138	GLN
1	B	151	GLN
1	B	213	GLN
1	B	244	GLN
1	B	263	ASN
1	C	49	GLN
1	C	52	GLN
1	C	138	GLN
1	C	151	GLN
1	C	166	GLN
1	C	213	GLN
1	C	244	GLN
1	C	263	ASN
1	D	49	GLN

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Mol	Chain	Res	Type
1	D	52	GLN
1	D	107	ASN
1	D	138	GLN
1	D	213	GLN
1	D	244	GLN
1	D	263	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 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	306	-	4,4,4	0.26	0	6,6,6	0.90	0
2	SO4	A	307	-	4,4,4	0.26	0	6,6,6	0.70	0
2	SO4	A	308	-	4,4,4	0.22	0	6,6,6	0.39	0
2	SO4	B	306	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	B	307	-	4,4,4	0.27	0	6,6,6	0.83	0
2	SO4	B	308	-	4,4,4	0.40	0	6,6,6	0.92	0
2	SO4	B	309	-	4,4,4	0.23	0	6,6,6	0.31	0
2	SO4	C	306	-	4,4,4	0.24	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	307	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	D	306	-	4,4,4	0.14	0	6,6,6	0.19	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	306	-	-	0/0/0/0	0/0/0/0
2	SO4	A	307	-	-	0/0/0/0	0/0/0/0
2	SO4	A	308	-	-	0/0/0/0	0/0/0/0
2	SO4	B	306	-	-	0/0/0/0	0/0/0/0
2	SO4	B	307	-	-	0/0/0/0	0/0/0/0
2	SO4	B	308	-	-	0/0/0/0	0/0/0/0
2	SO4	B	309	-	-	0/0/0/0	0/0/0/0
2	SO4	C	306	-	-	0/0/0/0	0/0/0/0
2	SO4	C	307	-	-	0/0/0/0	0/0/0/0
2	SO4	D	306	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	308	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

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	265/307 (86%)	1.11	37 (13%) 3 2	57, 70, 77, 86	0
1	B	265/307 (86%)	0.71	13 (4%) 30 24	55, 69, 78, 88	0
1	C	262/307 (85%)	1.19	55 (20%) 1 0	59, 69, 76, 84	0
1	D	260/307 (84%)	1.87	107 (41%) 0 0	60, 71, 76, 85	0
All	All	1052/1228 (85%)	1.22	212 (20%) 1 0	55, 70, 77, 88	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	48	LYS	8.9
1	D	26	TRP	6.7
1	D	185	GLU	6.7
1	C	17	LYS	6.6
1	D	61	ALA	6.3
1	D	192	CYS	6.0
1	D	47	ALA	5.9
1	D	71	PHE	5.8
1	D	9	HIS	5.8
1	D	50	LEU	5.6
1	D	31	ASP	5.5
1	D	43	ALA	5.5
1	B	2	ALA	5.4
1	D	201	LEU	5.4
1	D	105	VAL	5.3
1	C	13	ALA	5.3
1	D	78	GLU	5.2
1	C	20	LYS	5.1
1	D	6	SER	5.1
1	D	96	TYR	5.1
1	C	6	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	19	LEU	4.9
1	C	32	SER	4.9
1	D	12	ILE	4.9
1	D	223	PRO	4.9
1	C	19	LEU	4.8
1	C	34	ALA	4.8
1	C	40	ALA	4.8
1	D	217	ARG	4.8
1	C	10	GLU	4.7
1	C	15	ALA	4.7
1	D	227	GLY	4.7
1	D	46	ASN	4.5
1	D	141	ALA	4.5
1	C	8	ALA	4.5
1	B	3	GLN	4.4
1	D	42	VAL	4.4
1	D	38	ALA	4.3
1	C	43	ALA	4.3
1	C	147	GLU	4.2
1	D	147	GLU	4.0
1	D	73	ALA	4.0
1	D	221	SER	4.0
1	D	44	PHE	3.9
1	D	68	ARG	3.9
1	D	45	LYS	3.9
1	D	8	ALA	3.9
1	D	123	LEU	3.8
1	D	79	GLN	3.8
1	D	212	ALA	3.8
1	D	89	ARG	3.7
1	D	59	GLN	3.7
1	C	30	TYR	3.7
1	B	8	ALA	3.6
1	C	41	ALA	3.6
1	D	106	GLU	3.6
1	D	37	TYR	3.6
1	D	29	ASP	3.5
1	C	14	LYS	3.5
1	C	89	ARG	3.5
1	D	97	ILE	3.4
1	D	39	LYS	3.4
1	D	70	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	80	ALA	3.3
1	D	80	ALA	3.3
1	D	28	PRO	3.2
1	D	101	SER	3.2
1	C	45	LYS	3.2
1	C	38	ALA	3.2
1	D	145	ASN	3.2
1	C	21	THR	3.2
1	D	205	HIS	3.2
1	C	71	PHE	3.2
1	C	50	LEU	3.2
1	C	47	ALA	3.1
1	D	143	PHE	3.1
1	D	17	LYS	3.1
1	C	26	TRP	3.1
1	D	218	GLU	3.1
1	D	109	THR	3.1
1	D	226	SER	3.0
1	D	88	GLN	3.0
1	C	52	GLN	3.0
1	D	111	ASP	3.0
1	D	36	GLU	2.9
1	C	112	THR	2.9
1	D	52	GLN	2.9
1	D	181	SER	2.9
1	C	109	THR	2.9
1	D	214	LYS	2.9
1	D	57	TYR	2.9
1	C	70	LEU	2.9
1	D	55	ASP	2.9
1	D	69	SER	2.8
1	C	23	PHE	2.8
1	A	198	ALA	2.8
1	C	39	LYS	2.8
1	D	154	GLU	2.8
1	C	87	LEU	2.8
1	D	22	SER	2.8
1	A	123	LEU	2.8
1	D	27	LYS	2.8
1	D	33	ALA	2.8
1	D	92	GLU	2.8
1	A	127	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	20	LYS	2.8
1	D	220	TYR	2.8
1	D	174	ALA	2.7
1	D	16	GLU	2.7
1	D	265	TYR	2.7
1	C	22	SER	2.7
1	A	197	ILE	2.7
1	D	49	GLN	2.7
1	C	61	ALA	2.6
1	D	134	HIS	2.6
1	D	63	ALA	2.6
1	D	138	GLN	2.6
1	A	58	LEU	2.6
1	A	270	ILE	2.6
1	D	64	HIS	2.6
1	D	140	ALA	2.6
1	D	10	GLU	2.6
1	A	266	ALA	2.5
1	C	4	LYS	2.5
1	A	69	SER	2.5
1	C	76	ALA	2.5
1	C	96	TYR	2.5
1	C	12	ILE	2.5
1	D	275	PRO	2.5
1	C	146	GLU	2.4
1	D	114	ALA	2.4
1	D	229	GLU	2.4
1	B	213	GLN	2.4
1	C	48	LYS	2.4
1	D	112	THR	2.4
1	B	68	ARG	2.4
1	B	229	GLU	2.4
1	C	58	LEU	2.4
1	A	35	SER	2.4
1	A	30	TYR	2.4
1	A	269	ALA	2.4
1	D	196	CYS	2.4
1	A	71	PHE	2.4
1	A	65	ALA	2.4
1	B	43	ALA	2.4
1	A	23	PHE	2.3
1	D	58	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	153	ALA	2.3
1	D	210	VAL	2.3
1	D	51	GLU	2.3
1	A	64	HIS	2.3
1	A	268	LEU	2.3
1	D	13	ALA	2.3
1	D	53	ALA	2.3
1	A	34	ALA	2.3
1	A	258	VAL	2.3
1	D	113	ALA	2.3
1	C	75	LYS	2.3
1	D	75	LYS	2.3
1	A	257	LEU	2.3
1	C	114	ALA	2.3
1	A	259	THR	2.2
1	D	189	TYR	2.2
1	A	61	ALA	2.2
1	C	18	TYR	2.2
1	C	9	HIS	2.2
1	C	127	LEU	2.2
1	D	32	SER	2.2
1	D	127	LEU	2.2
1	C	269	ALA	2.2
1	D	99	LYS	2.2
1	D	178	LYS	2.2
1	B	123	LEU	2.2
1	C	25	LYS	2.2
1	D	21	THR	2.2
1	B	12	ILE	2.2
1	B	26	TRP	2.2
1	D	60	GLU	2.2
1	B	70	LEU	2.2
1	C	162	LEU	2.2
1	B	74	ALA	2.2
1	A	154	GLU	2.1
1	A	232	ALA	2.1
1	C	266	ALA	2.1
1	A	231	CYS	2.1
1	D	85	LYS	2.1
1	B	105	VAL	2.1
1	D	241	TYR	2.1
1	A	70	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	2.1
1	A	233	ALA	2.1
1	D	233	ALA	2.1
1	A	216	VAL	2.1
1	C	104	TYR	2.1
1	C	143	PHE	2.1
1	A	102	VAL	2.1
1	D	129	LEU	2.1
1	A	94	VAL	2.1
1	A	37	TYR	2.1
1	D	160	SER	2.1
1	A	234	LEU	2.1
1	D	274	VAL	2.1
1	A	66	ASN	2.1
1	C	201	LEU	2.0
1	D	222	ILE	2.0
1	C	92	GLU	2.0
1	A	199	GLN	2.0
1	A	57	TYR	2.0
1	A	33	ALA	2.0
1	A	196	CYS	2.0
1	D	163	LEU	2.0
1	D	18	TYR	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 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(\AA^2)	Q<0.9
2	SO4	D	306	5/5	0.83	0.28	1.89	159,159,159,159	0
2	SO4	A	308	5/5	0.73	0.28	-0.14	113,114,115,116	0
2	SO4	C	306	5/5	0.72	0.24	-0.98	125,125,126,127	0
2	SO4	B	307	5/5	0.81	0.15	-1.41	96,100,101,102	0
2	SO4	B	308	5/5	0.93	0.16	-1.48	67,73,77,79	0
2	SO4	A	306	5/5	0.91	0.17	-1.82	72,74,76,77	0
2	SO4	B	306	5/5	0.83	0.14	-2.54	120,121,121,121	0
2	SO4	C	307	5/5	0.81	0.20	-	139,139,140,140	0
2	SO4	B	309	5/5	0.72	0.17	-	123,123,123,123	0
2	SO4	A	307	5/5	0.93	0.13	-	73,79,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.