



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2017 – 06:51 PM EST

PDB ID : 5LNH
Title : Structure of full length Unliganded CodY from Bacillus subtilis
Authors : Wilkinson, A.J.; Levdikov, V.M.; Blagova, E.V.
Deposited on : 2016-08-04
Resolution : 3.00 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028442

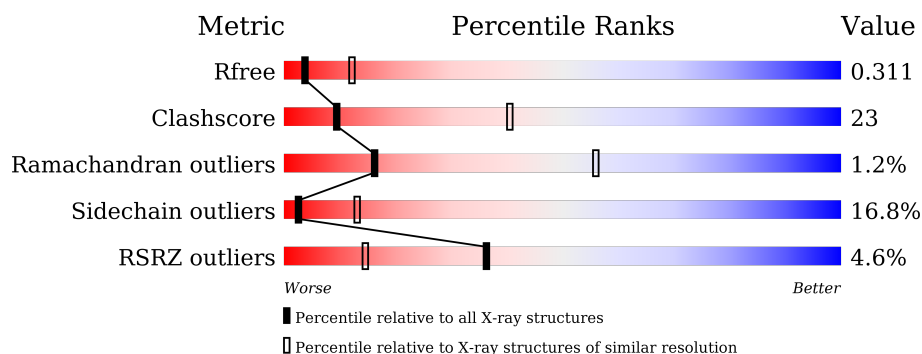
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	263	<div> <div>2%</div> <div> <div>52%</div> <div>36%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	263	<div> <div>2%</div> <div> <div>48%</div> <div>39%</div> <div>9%</div> <div>..</div> </div> </div>
1	C	263	<div> <div>4%</div> <div> <div>54%</div> <div>36%</div> <div>7%</div> <div>..</div> </div> </div>
1	D	263	<div> <div>12%</div> <div> <div>51%</div> <div>36%</div> <div>9%</div> <div>..</div> </div> </div>
1	E	263	<div> <div>2%</div> <div> <div>53%</div> <div>36%</div> <div>8%</div> <div>.</div> </div> </div>
1	F	263	<div> <div>5%</div> <div> <div>58%</div> <div>30%</div> <div>9%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	263	
1	H	263	
1	I	263	
1	K	263	

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	A	301	-	-	-	X
2	SO4	C	301	-	-	-	X
2	SO4	E	301	-	-	-	X
2	SO4	E	302	-	-	-	X
2	SO4	F	301	-	-	-	X
2	SO4	G	301	-	-	-	X
2	SO4	H	301	-	-	-	X
2	SO4	K	301	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20090 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 GTP-sensing transcriptional pleiotropic repressor CodY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	Se	0	0	0
			2002	1259	341	395	7			
1	B	255	Total	C	N	O	Se	0	0	0
			2002	1259	341	395	7			
1	C	255	Total	C	N	O	Se	0	0	0
			2002	1259	341	395	7			
1	D	255	Total	C	N	O	Se	0	0	0
			2002	1259	341	395	7			
1	E	255	Total	C	N	O	Se	0	0	0
			2002	1259	341	395	7			
1	F	255	Total	C	N	O	Se	0	0	0
			2002	1259	341	395	7			
1	G	255	Total	C	N	O	Se	0	0	0
			2002	1259	341	395	7			
1	H	255	Total	C	N	O	Se	0	0	0
			2002	1259	341	395	7			
1	I	255	Total	C	N	O	Se	0	0	0
			2002	1259	341	395	7			
1	K	255	Total	C	N	O	Se	0	0	0
			2002	1259	341	395	7			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	HIS	-	expression tag	UNP P39779
A	261	HIS	-	expression tag	UNP P39779
A	262	HIS	-	expression tag	UNP P39779
A	263	HIS	-	expression tag	UNP P39779
A	264	HIS	-	expression tag	UNP P39779
B	260	HIS	-	expression tag	UNP P39779
B	261	HIS	-	expression tag	UNP P39779
B	262	HIS	-	expression tag	UNP P39779
B	263	HIS	-	expression tag	UNP P39779

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	HIS	-	expression tag	UNP P39779
C	260	HIS	-	expression tag	UNP P39779
C	261	HIS	-	expression tag	UNP P39779
C	262	HIS	-	expression tag	UNP P39779
C	263	HIS	-	expression tag	UNP P39779
C	264	HIS	-	expression tag	UNP P39779
D	260	HIS	-	expression tag	UNP P39779
D	261	HIS	-	expression tag	UNP P39779
D	262	HIS	-	expression tag	UNP P39779
D	263	HIS	-	expression tag	UNP P39779
D	264	HIS	-	expression tag	UNP P39779
E	260	HIS	-	expression tag	UNP P39779
E	261	HIS	-	expression tag	UNP P39779
E	262	HIS	-	expression tag	UNP P39779
E	263	HIS	-	expression tag	UNP P39779
E	264	HIS	-	expression tag	UNP P39779
F	260	HIS	-	expression tag	UNP P39779
F	261	HIS	-	expression tag	UNP P39779
F	262	HIS	-	expression tag	UNP P39779
F	263	HIS	-	expression tag	UNP P39779
F	264	HIS	-	expression tag	UNP P39779
G	260	HIS	-	expression tag	UNP P39779
G	261	HIS	-	expression tag	UNP P39779
G	262	HIS	-	expression tag	UNP P39779
G	263	HIS	-	expression tag	UNP P39779
G	264	HIS	-	expression tag	UNP P39779
H	260	HIS	-	expression tag	UNP P39779
H	261	HIS	-	expression tag	UNP P39779
H	262	HIS	-	expression tag	UNP P39779
H	263	HIS	-	expression tag	UNP P39779
H	264	HIS	-	expression tag	UNP P39779
I	260	HIS	-	expression tag	UNP P39779
I	261	HIS	-	expression tag	UNP P39779
I	262	HIS	-	expression tag	UNP P39779
I	263	HIS	-	expression tag	UNP P39779
I	264	HIS	-	expression tag	UNP P39779
K	260	HIS	-	expression tag	UNP P39779
K	261	HIS	-	expression tag	UNP P39779
K	262	HIS	-	expression tag	UNP P39779
K	263	HIS	-	expression tag	UNP P39779
K	264	HIS	-	expression tag	UNP P39779

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

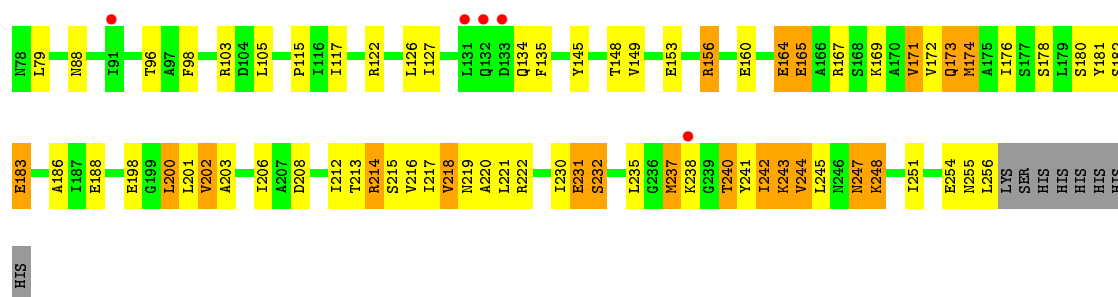


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

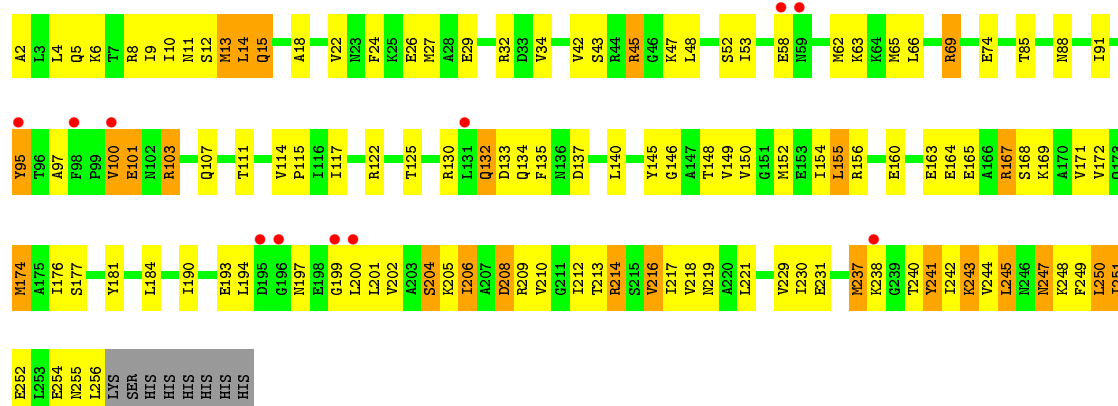
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	2	Total 2	O 2	0	0
3	C	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0
3	I	1	Total 1	O 1	0	0
3	K	1	Total 1	O 1	0	0

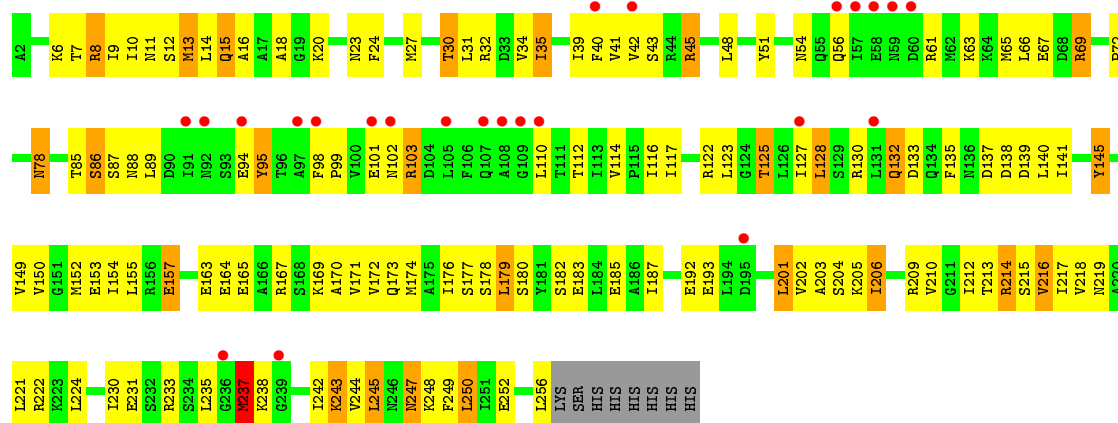




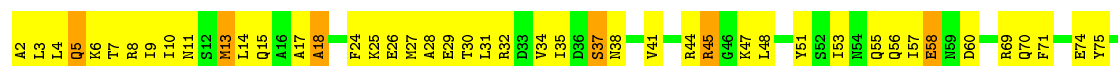
- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

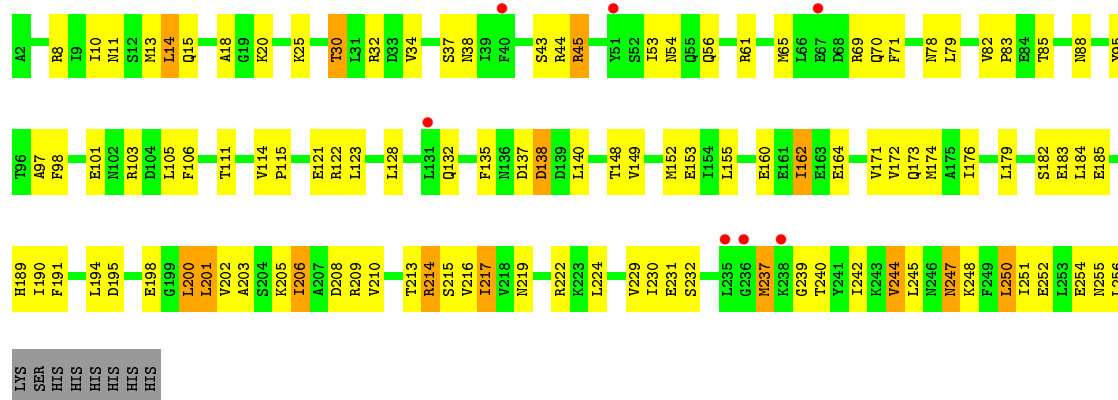


- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY



- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.87Å 110.55Å 257.41Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	46.68 – 3.00 46.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.68-3.00) 72.7 (46.66-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.279 0.272 , 0.311	Depositor DCC
R_{free} test set	2878 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20090	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.78	0/2015	0.88	1/2702 (0.0%)
1	B	1.37	21/2015 (1.0%)	1.16	15/2702 (0.6%)
1	C	0.70	4/2015 (0.2%)	0.77	2/2702 (0.1%)
1	D	0.96	10/2015 (0.5%)	0.83	2/2702 (0.1%)
1	E	1.00	5/2015 (0.2%)	0.85	2/2702 (0.1%)
1	F	0.98	15/2015 (0.7%)	0.79	0/2702
1	G	0.90	5/2015 (0.2%)	0.86	3/2702 (0.1%)
1	H	0.66	1/2015 (0.0%)	0.74	0/2702
1	I	0.68	0/2015	0.83	1/2702 (0.0%)
1	K	0.70	3/2015 (0.1%)	0.75	0/2702
All	All	0.90	64/20150 (0.3%)	0.85	26/27020 (0.1%)

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	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	8

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	LYS	CD-CE	25.69	2.15	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	ASP	CG-OD1	19.59	1.70	1.25
1	E	173	GLN	CD-NE2	17.84	1.77	1.32
1	D	234	SER	CB-OG	17.26	1.64	1.42
1	E	144	GLU	CD-OE2	16.55	1.43	1.25

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	ARG	NE-CZ-NH2	-19.90	110.35	120.30
1	B	214	ARG	NE-CZ-NH2	-19.79	110.41	120.30
1	D	233	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	B	214	ARG	NE-CZ-NH1	10.51	125.56	120.30
1	B	233	ARG	NE-CZ-NH1	-10.12	115.24	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	208	ASP	Sidechain
1	B	237	MSE	Peptide
1	C	237	MSE	Peptide
1	D	237	MSE	Peptide
1	E	237	MSE	Peptide

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	2002	0	2041	103	0
1	B	2002	0	2041	116	0
1	C	2002	0	2041	80	0
1	D	2002	0	2041	106	0
1	E	2002	0	2041	92	0
1	F	2002	0	2041	82	0
1	G	2002	0	2041	90	0
1	H	2002	0	2041	117	0
1	I	2002	0	2041	101	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2002	0	2041	82	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	E	10	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	K	5	0	0	0	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
All	All	20090	0	20410	914	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 914 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:F:243:LYS:CE	1:F:243:LYS:CD	1.74	1.63
1:E:20:LYS:CB	1:E:20:LYS:CG	1.77	1.58
1:D:158:LYS:CD	1:D:158:LYS:CE	1.76	1.58
1:F:243:LYS:NZ	1:F:243:LYS:CE	1.69	1.55
1:C:223:LYS:CE	1:C:223:LYS:NZ	1.69	1.54

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/263 (96%)	229 (90%)	19 (8%)	5 (2%)	9	41
1	B	253/263 (96%)	229 (90%)	22 (9%)	2 (1%)	24	66
1	C	253/263 (96%)	231 (91%)	18 (7%)	4 (2%)	12	48
1	D	253/263 (96%)	229 (90%)	20 (8%)	4 (2%)	12	48
1	E	253/263 (96%)	229 (90%)	21 (8%)	3 (1%)	16	56
1	F	253/263 (96%)	228 (90%)	22 (9%)	3 (1%)	16	56
1	G	253/263 (96%)	229 (90%)	21 (8%)	3 (1%)	16	56
1	H	253/263 (96%)	235 (93%)	16 (6%)	2 (1%)	24	66
1	I	253/263 (96%)	227 (90%)	23 (9%)	3 (1%)	16	56
1	K	253/263 (96%)	228 (90%)	23 (9%)	2 (1%)	24	66
All	All	2530/2630 (96%)	2294 (91%)	205 (8%)	31 (1%)	16	56

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ALA
1	A	237	MSE
1	B	18	ALA
1	B	237	MSE
1	C	18	ALA

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	221/222 (100%)	187 (85%)	34 (15%)	3	16
1	B	221/222 (100%)	184 (83%)	37 (17%)	3	13
1	C	221/222 (100%)	185 (84%)	36 (16%)	3	14
1	D	221/222 (100%)	192 (87%)	29 (13%)	5	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	221/222 (100%)	177 (80%)	44 (20%)	1	8
1	F	221/222 (100%)	191 (86%)	30 (14%)	5	20
1	G	221/222 (100%)	182 (82%)	39 (18%)	2	12
1	H	221/222 (100%)	179 (81%)	42 (19%)	2	10
1	I	221/222 (100%)	178 (80%)	43 (20%)	2	9
1	K	221/222 (100%)	184 (83%)	37 (17%)	3	13
All	All	2210/2220 (100%)	1839 (83%)	371 (17%)	2	13

5 of 371 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	214	ARG
1	F	247	ASN
1	K	44	ARG
1	E	234	SER
1	F	148	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	173	GLN
1	F	255	ASN
1	K	88	ASN
1	E	247	ASN
1	F	88	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 ⓘ

12 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	301	-	4,4,4	0.57	0	6,6,6	0.26	0
2	SO4	A	302	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	B	301	-	4,4,4	0.18	0	6,6,6	0.26	0
2	SO4	B	302	-	4,4,4	0.18	0	6,6,6	0.11	0
2	SO4	C	301	-	4,4,4	1.96	3 (75%)	6,6,6	0.74	0
2	SO4	E	301	-	4,4,4	0.96	0	6,6,6	0.42	0
2	SO4	E	302	-	4,4,4	0.40	0	6,6,6	0.14	0
2	SO4	F	301	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	G	301	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	H	301	-	4,4,4	0.83	0	6,6,6	0.12	0
2	SO4	I	301	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	K	301	-	4,4,4	1.21	0	6,6,6	0.20	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	301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	SO4	B	301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	302	-	-	0/0/0/0	0/0/0/0
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
2	SO4	E	301	-	-	0/0/0/0	0/0/0/0
2	SO4	E	302	-	-	0/0/0/0	0/0/0/0
2	SO4	F	301	-	-	0/0/0/0	0/0/0/0
2	SO4	G	301	-	-	0/0/0/0	0/0/0/0
2	SO4	H	301	-	-	0/0/0/0	0/0/0/0
2	SO4	I	301	-	-	0/0/0/0	0/0/0/0
2	SO4	K	301	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	SO4	O4-S	2.07	1.54	1.47
2	C	301	SO4	O3-S	2.10	1.55	1.47
2	C	301	SO4	O2-S	2.43	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	SO4	1	0
2	E	301	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	248/263 (94%)	0.27	4 (1%) 74 47	69, 86, 96, 106	0
1	B	248/263 (94%)	0.23	4 (1%) 74 47	69, 86, 96, 106	0
1	C	248/263 (94%)	0.25	10 (4%) 42 17	69, 86, 96, 106	0
1	D	248/263 (94%)	0.53	31 (12%) 5 2	69, 86, 96, 106	0
1	E	248/263 (94%)	0.15	6 (2%) 62 32	69, 86, 96, 106	0
1	F	248/263 (94%)	0.28	12 (4%) 34 14	69, 86, 96, 106	0
1	G	248/263 (94%)	0.24	11 (4%) 38 16	69, 86, 96, 106	0
1	H	248/263 (94%)	0.48	24 (9%) 10 4	69, 86, 96, 106	0
1	I	248/263 (94%)	0.17	5 (2%) 68 39	69, 86, 96, 106	0
1	K	248/263 (94%)	0.08	7 (2%) 56 27	69, 86, 96, 106	0
All	All	2480/2630 (94%)	0.27	114 (4%) 36 14	69, 86, 97, 106	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	THR	6.0
1	H	108	ALA	4.9
1	D	60	ASP	4.5
1	H	105	LEU	4.5
1	D	97	ALA	4.5

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(Å ²)	Q<0.9
2	SO4	F	301	5/5	0.42	0.64	7.60	180,180,180,181	0
2	SO4	K	301	5/5	0.72	0.41	5.76	184,185,185,185	0
2	SO4	A	301	5/5	0.78	0.50	4.92	157,158,158,159	0
2	SO4	H	301	5/5	0.58	0.47	4.63	173,174,174,174	0
2	SO4	C	301	5/5	0.78	0.36	3.99	148,149,149,150	0
2	SO4	E	302	5/5	0.66	0.44	3.72	198,199,199,199	0
2	SO4	G	301	5/5	0.79	0.36	2.47	140,140,141,141	0
2	SO4	E	301	5/5	0.86	0.31	2.23	160,160,160,160	0
2	SO4	B	301	5/5	0.84	0.36	1.84	143,143,144,144	0
2	SO4	I	301	5/5	0.90	0.27	0.30	148,148,148,149	0
2	SO4	A	302	5/5	0.75	0.16	-	160,160,160,160	0
2	SO4	B	302	5/5	0.86	0.16	-	162,162,163,163	0

6.5 Other polymers [i](#)

There are no such residues in this entry.