Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:32 pm BST

PDB ID	:	2B81
Title	:	Crystal Structure of the Luciferase-like Monooxygenase from Bacillus cereus
Authors	:	Kim, Y.; Li, H.; Moy, S.; Collart, F.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2005-10-06
Resolution	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

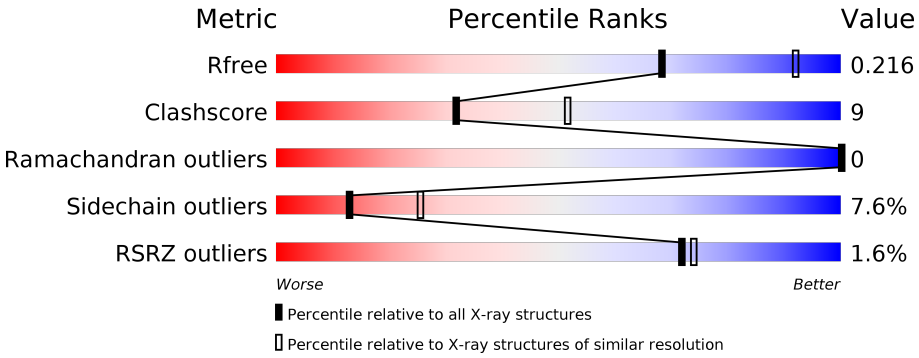
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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 <=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	323	80% 16%
1	B	323	82% 13%
1	C	323	79% 15%
1	D	323	77% 16% 5%

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
3	MES	A	2404	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12077 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 Luciferase-like monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	Se	0	14	0
			2690	1724	457	500	9			
1	B	318	Total	C	N	O	Se	0	12	0
			2690	1723	458	500	9			
1	C	320	Total	C	N	O	Se	0	9	0
			2670	1713	454	493	10			
1	D	318	Total	C	N	O	Se	0	13	0
			2698	1726	463	500	9			

There are 52 discrepancies between the modelled and reference sequences:

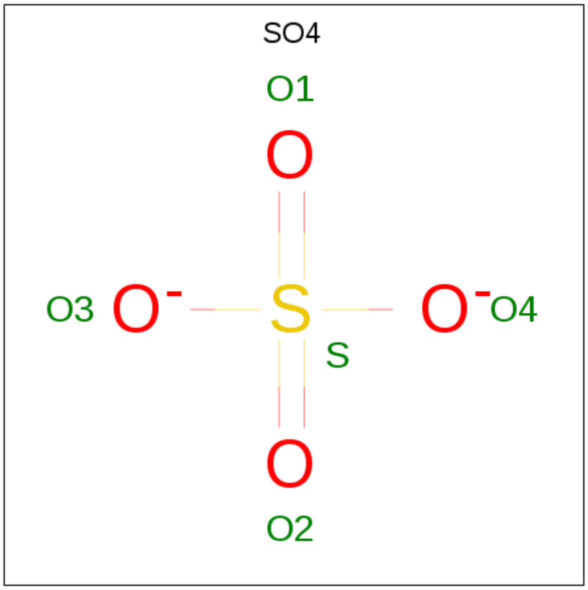
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP Q81B18
A	-1	ASN	-	CLONING ARTIFACT	UNP Q81B18
A	0	ALA	-	CLONING ARTIFACT	UNP Q81B18
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
A	4	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
A	16	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
A	40	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
A	81	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
A	82	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
A	128	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
A	204	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
A	215	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
A	250	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
B	-2	SER	-	CLONING ARTIFACT	UNP Q81B18
B	-1	ASN	-	CLONING ARTIFACT	UNP Q81B18
B	0	ALA	-	CLONING ARTIFACT	UNP Q81B18
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
B	4	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
B	16	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
B	40	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
B	81	MSE	MET	MODIFIED RESIDUE	UNP Q81B18

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
B	128	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
B	204	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
B	215	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
B	250	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
C	-2	SER	-	CLONING ARTIFACT	UNP Q81B18
C	-1	ASN	-	CLONING ARTIFACT	UNP Q81B18
C	0	ALA	-	CLONING ARTIFACT	UNP Q81B18
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
C	4	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
C	16	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
C	40	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
C	81	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
C	82	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
C	128	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
C	204	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
C	215	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
C	250	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
D	-2	SER	-	CLONING ARTIFACT	UNP Q81B18
D	-1	ASN	-	CLONING ARTIFACT	UNP Q81B18
D	0	ALA	-	CLONING ARTIFACT	UNP Q81B18
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
D	4	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
D	16	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
D	40	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
D	81	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
D	82	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
D	128	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
D	204	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
D	215	MSE	MET	MODIFIED RESIDUE	UNP Q81B18
D	250	MSE	MET	MODIFIED RESIDUE	UNP Q81B18

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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	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	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

Continued on next page...

Continued from previous page...

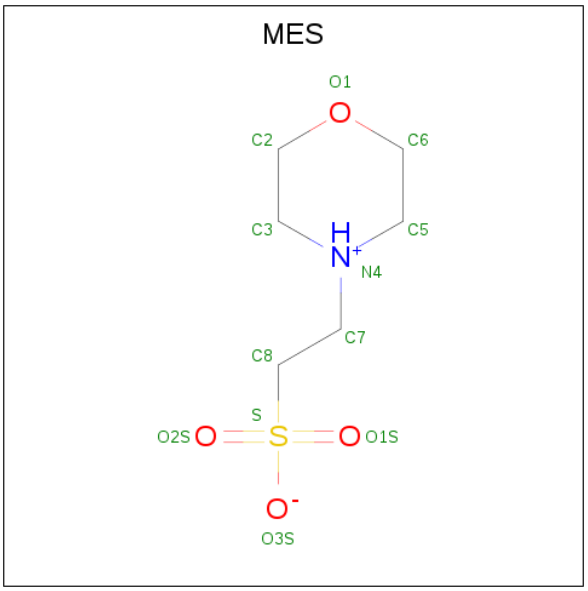
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0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

Continued on next page...

Continued from previous page...

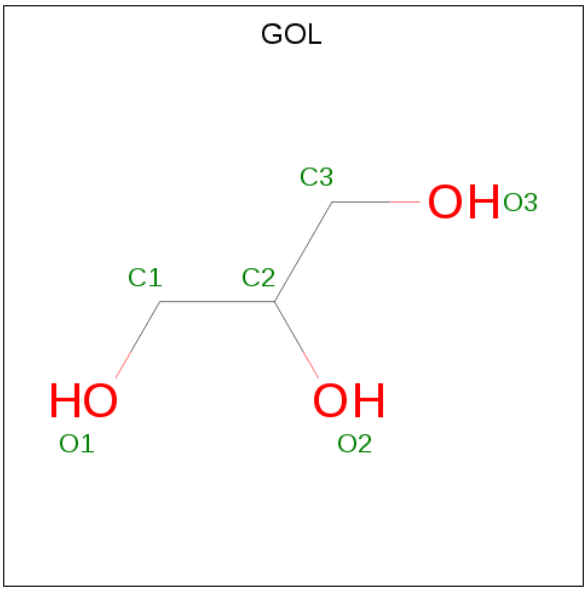
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 12 6 1 4 1	0	0
3	A	1	Total C N O S 12 6 1 4 1	0	0
3	B	1	Total C N O S 12 6 1 4 1	0	0
3	C	1	Total C N O S 12 6 1 4 1	0	0
3	D	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

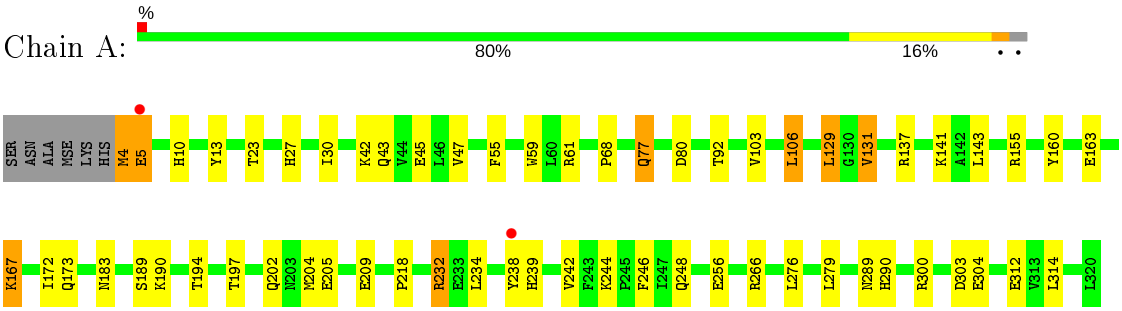
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	286	Total O 286 286	0	0
5	B	301	Total O 301 301	0	0
5	C	261	Total O 261 261	0	0
5	D	196	Total O 196 196	0	0

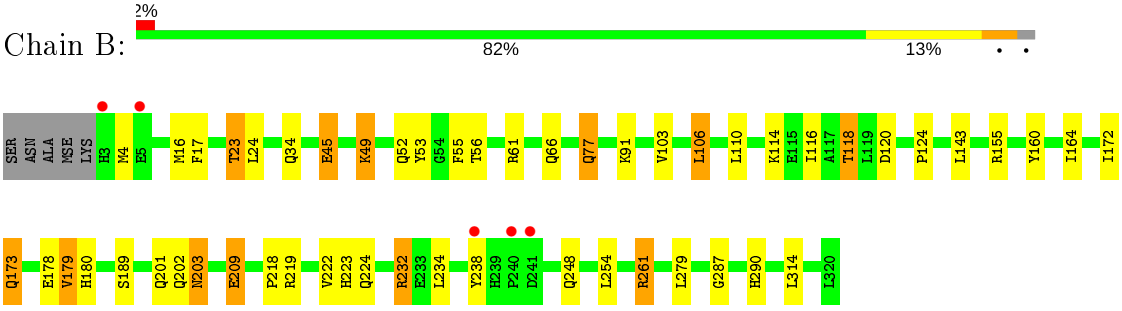
3 Residue-property plots (i)

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.

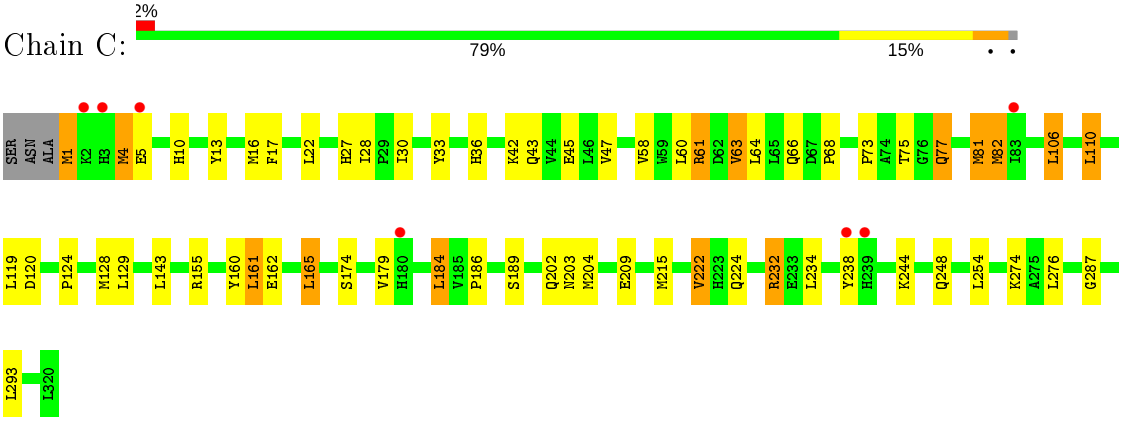
- Molecule 1: Luciferase-like monooxygenase



- Molecule 1: Luciferase-like monooxygenase

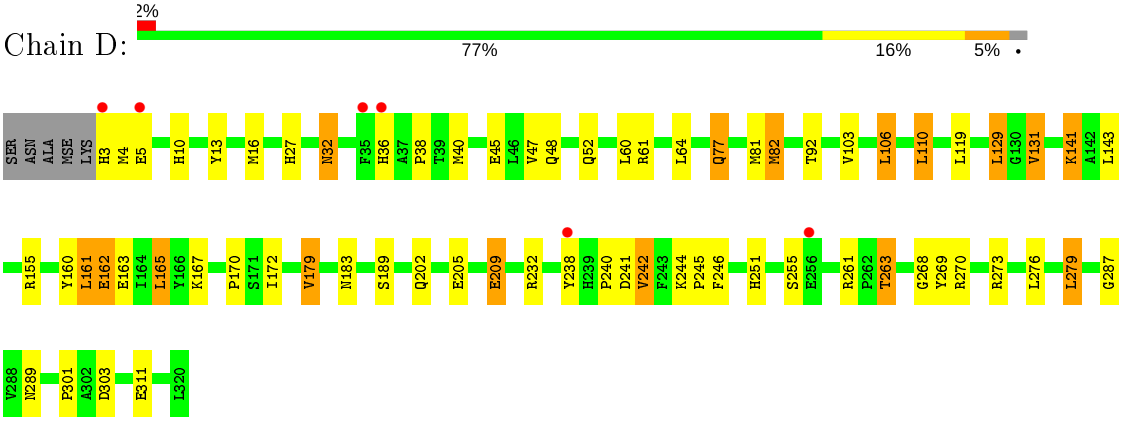


- Molecule 1: Luciferase-like monooxygenase



- Molecule 1: Luciferase-like monooxygenase

Chain D:


2%
77%
16%
5%
SER ASN ALA MSE LYS H3 M4 E5 H10 Y13 M16 H27 N32 F35 H36 A37 P38 T39 M40 E45 L46 V47 Q48 Q52 L60 R61 L64 Q77 M81 M82 T92 V103 L106 L110 L119 L129 G130 V131 K141 A142 L143
R155 Y160 L161 E162 E163 I164 L165 Y166 K167 P170 S171 I172 V179 N183 S189 Q202 E205 E209 R232 Y238 H239 P240 D241 V242 F243 K244 P245 F246 H251 S255 E256 R261 P262 T263 G268 Y269 R270 R273 L276 L279 G287
V288 N289 P301 A302 D303 E311 L320

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	138.47Å 159.94Å 172.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.81 – 2.50 47.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.81-2.50) 99.5 (47.81-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.183 , 0.218 0.181 , 0.216	Depositor DCC
R_{free} test set	13183 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12077	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, SO4, MES

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	0.58	0/2756	0.67	0/3719
1	B	0.58	0/2755	0.67	0/3718
1	C	0.57	0/2735	0.69	3/3689 (0.1%)
1	D	0.55	0/2762	0.62	0/3726
All	All	0.57	0/11008	0.66	3/14852 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	222	VAL	CB-CA-C	-6.00	100.01	111.40
1	C	61	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	61	ARG	NE-CZ-NH1	5.15	122.87	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	2690	0	2592	48	0
1	B	2690	0	2592	45	0
1	C	2670	0	2587	51	0
1	D	2698	0	2602	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	60	0	0	0	0
2	B	30	0	0	1	0
2	C	55	0	0	0	0
2	D	50	0	0	0	0
3	A	24	0	24	6	0
3	B	12	0	12	0	0
3	C	12	0	12	0	0
3	D	12	0	12	0	0
4	A	12	0	16	0	0
4	B	6	0	8	2	0
4	C	6	0	8	2	0
4	D	6	0	8	0	0
5	A	286	0	0	5	0
5	B	301	0	0	9	0
5	C	261	0	0	3	0
5	D	196	0	0	8	0
All	All	12077	0	10473	193	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 9.

All (193) 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:D:82:MSE:HA	1:D:82:MSE:HE3	1.37	1.04
1:A:80:ASP:H	1:B:118:THR:HG21	1.27	0.99
3:A:2404:MES:H62	1:C:68:PRO:HA	1.48	0.95
1:D:38:PRO:HG2	1:D:40:MSE:HE2	1.51	0.93
1:B:155:ARG:HH21	1:B:202:GLN:HE22	1.18	0.88
1:C:155:ARG:HH11	1:C:202:GLN:HE22	1.20	0.87
1:B:173[A]:GLN:NE2	1:B:178[A]:GLU:OE2	2.07	0.87
1:D:40:MSE:SE	5:D:2641:HOH:O	2.42	0.87
1:B:61:ARG:H	1:B:77:GLN:HE22	1.20	0.86
1:C:61:ARG:H	1:C:77:GLN:HE22	1.23	0.86
1:B:23:THR:HG22	1:B:290:HIS:HD1	1.40	0.86
1:D:246:PHE:H	1:D:289:ASN:HD22	1.21	0.85
1:D:10:HIS:HD2	1:D:13:TYR:H	1.24	0.84
1:D:82:MSE:HA	1:D:82:MSE:CE	2.09	0.82
1:A:10:HIS:HD2	1:A:13:TYR:H	1.25	0.82
1:C:30:ILE:H	1:C:43:GLN:HE22	1.27	0.82
1:A:163[A]:GLU:OE2	1:A:167:LYS:HE2	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:H	1:A:43:GLN:HE22	1.26	0.80
1:C:64:LEU:HD13	1:D:110:LEU:HD13	1.64	0.79
1:D:155:ARG:HE	1:D:202:GLN:HE22	1.28	0.79
1:C:1:MSE:N	1:C:4:MSE:HE3	1.97	0.79
1:A:246:PHE:H	1:A:289:ASN:HD22	1.31	0.78
1:C:215:MSE:SE	5:C:2714:HOH:O	2.50	0.78
1:A:42:LYS:HD2	1:A:45[B]:GLU:OE2	1.84	0.77
1:A:155:ARG:HH21	1:A:202:GLN:HE22	1.33	0.76
1:D:61:ARG:H	1:D:77:GLN:HE22	1.30	0.76
1:A:205[B]:GLU:HG3	1:A:238:TYR:OH	1.86	0.75
3:A:2404:MES:C6	1:C:68:PRO:HA	2.18	0.74
1:C:110:LEU:HD13	1:D:64:LEU:HD13	1.72	0.71
1:C:274:LYS:HZ1	4:C:2413:GOL:H2	1.53	0.71
1:C:1:MSE:H2	1:C:4:MSE:HE3	1.53	0.70
1:C:224:GLN:HE21	1:C:248:GLN:NE2	1.89	0.70
1:C:82:MSE:HE3	1:C:82:MSE:HA	1.73	0.70
1:C:204:MSE:HE3	1:C:234:LEU:CD1	2.22	0.70
1:A:239:HIS:O	1:A:242:VAL:HG12	1.92	0.69
1:C:28:ILE:HD13	1:C:58:VAL:HG13	1.73	0.69
1:D:38:PRO:HG2	1:D:40:MSE:CE	2.20	0.69
2:B:2421:SO4:O4	5:B:2654:HOH:O	2.09	0.69
1:C:215:MSE:CG	5:C:2714:HOH:O	2.42	0.68
1:B:23:THR:CG2	1:B:290:HIS:HD1	2.08	0.67
1:A:61:ARG:H	1:A:77:GLN:HE22	1.41	0.66
1:C:82:MSE:HE2	1:C:119:LEU:HD11	1.77	0.66
1:C:61:ARG:HD3	5:C:2460:HOH:O	1.95	0.66
1:C:10:HIS:HD2	1:C:13:TYR:H	1.45	0.65
1:A:239:HIS:HB2	1:A:242:VAL:HG11	1.77	0.65
1:A:10:HIS:CD2	1:A:13:TYR:H	2.12	0.64
1:C:42:LYS:HD2	1:C:45:GLU:OE1	1.97	0.64
1:C:27:HIS:CE1	1:C:61:ARG:HD2	2.33	0.64
1:A:42:LYS:CD	1:A:45[B]:GLU:OE2	2.45	0.64
1:C:204:MSE:HE3	1:C:234:LEU:HD12	1.78	0.63
1:D:61:ARG:CA	1:D:81:MSE:HE3	2.29	0.63
1:C:82:MSE:HE2	1:C:119:LEU:CD1	2.28	0.63
1:C:16:MSE:SE	1:C:128:MSE:HE3	2.48	0.62
1:D:129:LEU:HD22	1:D:131:VAL:HG23	1.82	0.62
1:B:261[A]:ARG:HE	1:B:261[A]:ARG:H	1.46	0.61
3:A:2404:MES:H22	1:C:73:PRO:HA	1.82	0.61
1:B:172:ILE:HB	1:B:179:VAL:HG13	1.81	0.61
1:A:256[A]:GLU:HG3	5:A:2772:HOH:O	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:MSE:CE	1:D:119:LEU:HD11	2.31	0.60
4:B:2412:GOL:H2	1:D:170:PRO:HA	1.83	0.60
1:B:232:ARG:NH2	1:B:287:GLY:O	2.34	0.60
1:C:10:HIS:CD2	1:C:13:TYR:H	2.19	0.60
1:C:60:LEU:O	1:C:81:MSE:HE1	2.02	0.60
1:A:239:HIS:HB2	1:A:242:VAL:CG1	2.31	0.60
1:B:222:VAL:CG2	5:B:2579:HOH:O	2.49	0.60
1:B:222:VAL:HG23	5:B:2579:HOH:O	2.02	0.60
1:A:61:ARG:HD3	5:A:2598:HOH:O	2.02	0.59
1:B:224:GLN:HE21	1:B:248:GLN:NE2	1.99	0.59
1:D:209[A]:GLU:HG2	1:D:238:TYR:CE2	2.38	0.59
1:B:23:THR:HG23	1:B:56:THR:OG1	2.03	0.58
1:A:204:MSE:HG2	1:A:234:LEU:HD12	1.87	0.56
1:D:232:ARG:NH2	1:D:287:GLY:O	2.38	0.56
1:A:303:ASP:OD2	1:A:304:GLU:N	2.40	0.55
1:D:269:TYR:CD1	1:D:279:LEU:HD11	2.42	0.55
1:A:59:TRP:HE1	1:A:290:HIS:HE1	1.56	0.54
1:C:232:ARG:NH2	1:C:287:GLY:O	2.40	0.54
1:D:82:MSE:HE1	1:D:119:LEU:CD1	2.37	0.54
1:A:163[B]:GLU:HB3	1:A:172:ILE:HD11	1.89	0.54
1:C:16:MSE:SE	1:C:17:PHE:CZ	3.11	0.54
1:C:66:GLN:NE2	1:D:183:ASN:HD22	2.06	0.54
1:D:263:THR:HG22	5:D:2509:HOH:O	2.08	0.53
1:C:204:MSE:HE3	1:C:234:LEU:HD11	1.90	0.53
1:A:27:HIS:HE1	1:A:61:ARG:HD2	1.74	0.53
1:B:49:LYS:HE2	5:B:2693:HOH:O	2.09	0.52
1:D:205:GLU:O	1:D:209[A]:GLU:HG3	2.10	0.52
1:C:209[A]:GLU:OE2	1:C:238:TYR:HB3	2.09	0.52
1:A:209[A]:GLU:HG2	1:A:238:TYR:CG	2.45	0.52
1:A:23:THR:OG1	1:A:290:HIS:HD2	1.93	0.52
1:B:106:LEU:HG	1:B:143:LEU:HD12	1.91	0.52
1:C:274:LYS:NZ	4:C:2413:GOL:H2	2.24	0.52
1:C:1:MSE:H3	1:C:4:MSE:HE3	1.73	0.52
1:D:82:MSE:HE2	1:D:119:LEU:HD11	1.92	0.51
1:A:137:ARG:HG2	5:A:2753:HOH:O	2.11	0.51
1:B:201:GLN:NE2	5:B:2669:HOH:O	2.42	0.51
1:B:201:GLN:HB3	5:B:2669:HOH:O	2.10	0.51
1:C:234:LEU:O	1:C:238:TYR:HD1	1.93	0.51
1:A:256[A]:GLU:HG2	1:A:300:ARG:HD2	1.91	0.51
3:A:2404:MES:H62	1:C:68:PRO:CA	2.31	0.51
1:A:246:PHE:H	1:A:289:ASN:ND2	2.05	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ILE:HD13	1:C:58:VAL:CG1	2.40	0.50
1:B:23:THR:CG2	1:B:56:THR:OG1	2.60	0.50
1:A:27:HIS:CE1	1:A:61:ARG:HD2	2.46	0.49
4:B:2412:GOL:H11	1:D:167:LYS:HE2	1.94	0.49
1:D:61:ARG:C	1:D:81:MSE:HE3	2.32	0.49
1:A:4:MSE:HG2	1:A:5:GLU:N	2.28	0.49
1:A:106:LEU:HG	1:A:143:LEU:HD12	1.94	0.48
1:D:32:ASN:H	1:D:32:ASN:HD22	1.60	0.48
1:A:141[A]:LYS:HD3	5:B:2615:HOH:O	2.13	0.48
1:D:82:MSE:HE1	1:D:119:LEU:HD11	1.94	0.48
1:A:183:ASN:HD22	1:B:66:GLN:NE2	2.10	0.48
1:D:45:GLU:HG3	5:D:2615:HOH:O	2.12	0.48
1:C:27:HIS:HE1	1:C:61:ARG:HD2	1.75	0.48
1:D:10:HIS:CD2	1:D:13:TYR:H	2.16	0.48
1:B:173[A]:GLN:HE21	1:B:178[A]:GLU:CD	2.17	0.48
1:B:209:GLU:HB2	1:B:238:TYR:CD1	2.48	0.48
1:D:47:VAL:HG12	1:D:92:THR:HG21	1.95	0.48
1:B:114:LYS:O	1:B:118:THR:CG2	2.62	0.47
1:C:209[A]:GLU:HB2	1:C:238:TYR:CD2	2.49	0.47
1:A:68:PRO:HB3	3:A:2404:MES:H51	1.97	0.47
1:D:106:LEU:HG	1:D:143:LEU:HD12	1.96	0.47
1:D:103:VAL:HG11	1:D:106:LEU:HD22	1.96	0.47
1:A:61:ARG:CD	5:A:2598:HOH:O	2.62	0.47
1:B:173[A]:GLN:HE21	1:B:178[A]:GLU:CG	2.26	0.47
1:C:106:LEU:HG	1:C:143:LEU:HD12	1.96	0.47
1:C:184:LEU:HD13	1:C:186:PRO:O	2.15	0.47
1:C:63:VAL:HG22	1:C:75:THR:HG22	1.96	0.47
1:D:52[B]:GLN:HB3	5:D:2491:HOH:O	2.14	0.47
1:A:232[A]:ARG:NH1	1:A:244:LYS:O	2.48	0.47
1:B:34:GLN:NE2	5:B:2541:HOH:O	2.46	0.47
1:D:141:LYS:HD2	1:D:141:LYS:HA	1.53	0.46
1:D:61:ARG:HA	1:D:81:MSE:HE3	1.95	0.46
1:B:45[B]:GLU:O	1:B:49:LYS:HG3	2.15	0.46
1:C:232:ARG:NH1	1:C:244:LYS:O	2.48	0.46
1:D:161:LEU:O	1:D:165:LEU:HB2	2.16	0.46
1:D:3:HIS:HD2	1:D:242:VAL:HG11	1.81	0.46
1:B:16:MSE:SE	1:B:17:PHE:CZ	3.19	0.45
1:B:4:MSE:H	1:B:4:MSE:SE	2.49	0.45
1:B:52[C]:GLN:HG2	1:B:53:TYR:N	2.32	0.45
1:A:4:MSE:CE	1:A:5:GLU:H	2.29	0.45
1:A:55:PHE:CZ	1:A:314:LEU:HD21	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:PHE:N	1:A:289:ASN:HD22	2.08	0.44
1:C:161:LEU:O	1:C:165:LEU:HB2	2.18	0.44
1:A:103:VAL:HG11	1:A:106:LEU:HD22	1.98	0.44
1:D:162:GLU:HG2	5:D:2592:HOH:O	2.17	0.44
1:D:163[A]:GLU:HG2	1:D:167:LYS:HD2	1.99	0.44
1:C:120:ASP:O	1:C:124:PRO:HA	2.17	0.44
1:C:82:MSE:CE	1:C:82:MSE:HA	2.46	0.44
1:D:172:ILE:HB	1:D:179:VAL:HG13	1.99	0.43
1:D:45:GLU:HA	1:D:48:GLN:HE21	1.83	0.43
1:D:255:SER:HB2	1:D:270:ARG:NH2	2.33	0.43
1:D:60:LEU:O	1:D:81:MSE:CE	2.67	0.43
1:B:103:VAL:HG11	1:B:106:LEU:HD22	2.00	0.43
1:C:60:LEU:C	1:C:81:MSE:HE1	2.37	0.43
1:A:30:ILE:H	1:A:43:GLN:NE2	2.05	0.43
1:B:155:ARG:HD3	1:B:202:GLN:NE2	2.33	0.43
1:B:222:VAL:HG22	5:B:2579:HOH:O	2.17	0.43
1:B:223:HIS:O	1:B:223:HIS:HD2	2.02	0.43
1:C:33:TYR:HB2	1:C:36:HIS:O	2.19	0.43
1:A:59:TRP:HE1	1:A:290:HIS:CE1	2.34	0.43
1:B:218:PRO:O	1:B:219:ARG:HD3	2.19	0.42
3:A:2404:MES:C5	1:C:68:PRO:HA	2.49	0.42
1:D:36:HIS:HD2	5:D:2625:HOH:O	2.02	0.42
1:B:178[A]:GLU:CG	1:B:180:HIS:CD2	3.02	0.42
1:D:311:GLU:HG2	5:D:2643:HOH:O	2.19	0.42
1:B:114:LYS:O	1:B:118:THR:HG23	2.19	0.42
1:A:218:PRO:HA	1:A:248:GLN:NE2	2.34	0.42
1:D:244:LYS:HA	1:D:245:PRO:HD3	1.88	0.42
1:B:55:PHE:CZ	1:B:314:LEU:HD21	2.55	0.42
1:D:82:MSE:CE	1:D:82:MSE:CA	2.86	0.42
1:D:232:ARG:NH1	1:D:244:LYS:O	2.53	0.41
1:C:60:LEU:HB2	1:C:81:MSE:CE	2.50	0.41
1:A:129:LEU:HD22	1:A:131:VAL:HG23	2.01	0.41
1:A:47:VAL:HG12	1:A:92:THR:HG21	2.02	0.41
1:B:116:ILE:HA	1:B:116:ILE:HD13	1.95	0.41
1:A:209[A]:GLU:HG2	1:A:238:TYR:CD1	2.56	0.41
1:C:28:ILE:HD11	1:C:47:VAL:CG2	2.51	0.41
1:A:129:LEU:O	1:A:194:THR:HA	2.20	0.41
1:A:256[B]:GLU:HG3	5:A:2764:HOH:O	2.20	0.41
1:D:16:MSE:SE	5:D:2640:HOH:O	2.88	0.41
1:D:27:HIS:HE1	1:D:61:ARG:HG3	1.86	0.41
1:B:155:ARG:HD3	1:B:202:GLN:HE22	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:PRO:O	1:D:241:ASP:HB2	2.21	0.41
1:B:203:ASN:HD22	1:B:203:ASN:C	2.24	0.41
1:A:30:ILE:N	1:A:43:GLN:HE22	2.06	0.40
1:B:234:LEU:O	1:B:238:TYR:HD2	2.04	0.40
1:A:4:MSE:HG2	1:A:5:GLU:HG3	2.03	0.40
1:B:110:LEU:HD13	1:B:164:ILE:HG12	2.03	0.40
1:D:251:HIS:O	1:D:268:GLY:HA3	2.22	0.40
1:B:120:ASP:O	1:B:124:PRO:HA	2.21	0.40
1:D:301:PRO:HB2	1:D:303[B]:ASP:OD1	2.22	0.40

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	329/323 (102%)	316 (96%)	13 (4%)	0	100	100
1	B	329/323 (102%)	319 (97%)	10 (3%)	0	100	100
1	C	327/323 (101%)	316 (97%)	11 (3%)	0	100	100
1	D	330/323 (102%)	320 (97%)	10 (3%)	0	100	100
All	All	1315/1292 (102%)	1271 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	286/267 (107%)	266 (93%)	20 (7%)	15 29
1	B	286/267 (107%)	264 (92%)	22 (8%)	13 25
1	C	284/267 (106%)	258 (91%)	26 (9%)	9 18
1	D	287/267 (108%)	260 (91%)	27 (9%)	8 17
All	All	1143/1068 (107%)	1048 (92%)	95 (8%)	13 22

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MSE
1	A	5	GLU
1	A	77	GLN
1	A	106	LEU
1	A	129	LEU
1	A	131	VAL
1	A	160	TYR
1	A	167	LYS
1	A	173[A]	GLN
1	A	173[B]	GLN
1	A	189[A]	SER
1	A	189[B]	SER
1	A	190	LYS
1	A	197	THR
1	A	232[A]	ARG
1	A	232[B]	ARG
1	A	266	ARG
1	A	276	LEU
1	A	279	LEU
1	A	312	GLU
1	B	23	THR
1	B	24	LEU
1	B	45[A]	GLU
1	B	45[B]	GLU
1	B	49	LYS
1	B	77	GLN
1	B	91	LYS
1	B	106	LEU
1	B	118	THR
1	B	160	TYR
1	B	173[A]	GLN
1	B	173[B]	GLN
1	B	179	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	189[A]	SER
1	B	189[B]	SER
1	B	203	ASN
1	B	209	GLU
1	B	232	ARG
1	B	254	LEU
1	B	261[A]	ARG
1	B	261[B]	ARG
1	B	279	LEU
1	C	1	MSE
1	C	4	MSE
1	C	5	GLU
1	C	22	LEU
1	C	63	VAL
1	C	77	GLN
1	C	81	MSE
1	C	82	MSE
1	C	106	LEU
1	C	110	LEU
1	C	129	LEU
1	C	160	TYR
1	C	161	LEU
1	C	162	GLU
1	C	165	LEU
1	C	174	SER
1	C	179	VAL
1	C	184	LEU
1	C	189[A]	SER
1	C	189[B]	SER
1	C	203	ASN
1	C	222	VAL
1	C	232	ARG
1	C	254	LEU
1	C	276	LEU
1	C	293	LEU
1	D	4	MSE
1	D	5	GLU
1	D	32	ASN
1	D	77	GLN
1	D	82	MSE
1	D	106	LEU
1	D	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	129	LEU
1	D	131	VAL
1	D	141	LYS
1	D	160	TYR
1	D	161	LEU
1	D	162	GLU
1	D	165	LEU
1	D	179	VAL
1	D	189[A]	SER
1	D	189[B]	SER
1	D	209[A]	GLU
1	D	209[B]	GLU
1	D	242	VAL
1	D	261[A]	ARG
1	D	261[B]	ARG
1	D	261[C]	ARG
1	D	263	THR
1	D	273	ARG
1	D	276	LEU
1	D	279	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	27	HIS
1	A	43	GLN
1	A	66	GLN
1	A	77	GLN
1	A	202	GLN
1	A	289	ASN
1	A	290	HIS
1	B	3	HIS
1	B	34	GLN
1	B	66	GLN
1	B	77	GLN
1	B	180	HIS
1	B	201	GLN
1	B	202	GLN
1	B	203	ASN
1	B	223	HIS
1	B	248	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	10	HIS
1	C	27	HIS
1	C	43	GLN
1	C	66	GLN
1	C	77	GLN
1	C	202	GLN
1	C	203	ASN
1	C	248	GLN
1	D	3	HIS
1	D	10	HIS
1	D	27	HIS
1	D	32	ASN
1	D	48	GLN
1	D	77	GLN
1	D	147	HIS
1	D	202	GLN
1	D	239	HIS
1	D	289	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

49 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	2457	-	4,4,4	0.10	0	6,6,6	0.48	0
2	SO4	A	2449	-	4,4,4	0.11	0	6,6,6	0.14	0
2	SO4	B	2458	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	C	2438	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	A	2446	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	D	2445	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	D	2451	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	C	2454	-	4,4,4	0.30	0	6,6,6	0.25	0
2	SO4	D	2441	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	A	2447	-	4,4,4	0.19	0	6,6,6	0.39	0
2	SO4	C	2439	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	A	2427	-	4,4,4	0.16	0	6,6,6	0.20	0
2	SO4	C	2437	-	4,4,4	0.11	0	6,6,6	0.37	0
2	SO4	B	2434	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	2433	-	4,4,4	0.16	0	6,6,6	0.14	0
3	MES	C	2401	-	12,12,12	2.22	1 (8%)	14,16,16	2.34	3 (21%)
2	SO4	D	2443	-	4,4,4	0.15	0	6,6,6	0.42	0
2	SO4	D	2425	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	C	2436	-	4,4,4	0.11	0	6,6,6	0.15	0
2	SO4	D	2435	-	4,4,4	0.11	0	6,6,6	0.33	0
2	SO4	C	2459	-	4,4,4	0.12	0	6,6,6	0.09	0
2	SO4	A	2448	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	A	2531	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	A	2426	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	D	2453	-	4,4,4	0.10	0	6,6,6	0.20	0
2	SO4	C	2456	-	4,4,4	0.17	0	6,6,6	0.21	0
4	GOL	C	2413	-	5,5,5	0.39	0	5,5,5	0.33	0
2	SO4	C	2452	-	4,4,4	0.17	0	6,6,6	0.06	0
3	MES	D	2402	-	12,12,12	2.28	1 (8%)	14,16,16	2.71	7 (50%)
4	GOL	D	2414	-	5,5,5	0.39	0	5,5,5	0.34	0
2	SO4	A	2428	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	A	2532	-	4,4,4	0.20	0	6,6,6	0.14	0
2	SO4	D	2424	-	4,4,4	0.13	0	6,6,6	0.23	0
2	SO4	B	2442	-	4,4,4	0.16	0	6,6,6	0.19	0
3	MES	B	2405	-	12,12,12	2.24	1 (8%)	14,16,16	2.40	5 (35%)
2	SO4	C	2444	-	4,4,4	0.15	0	6,6,6	0.20	0
2	SO4	A	2455	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	A	2530	-	4,4,4	0.19	0	6,6,6	0.25	0
4	GOL	A	2415	-	5,5,5	0.36	0	5,5,5	0.59	0
2	SO4	B	2421	-	4,4,4	0.16	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MES	A	2403	-	12,12,12	2.23	1 (8%)	14,16,16	2.64	6 (42%)
2	SO4	C	2450	-	4,4,4	0.13	0	6,6,6	0.24	0
2	SO4	C	2422	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	A	2429	-	4,4,4	0.16	0	6,6,6	0.35	0
4	GOL	B	2412	-	5,5,5	0.44	0	5,5,5	0.38	0
2	SO4	D	2440	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	D	2423	-	4,4,4	0.18	0	6,6,6	0.30	0
4	GOL	A	2411	-	5,5,5	0.50	0	5,5,5	0.42	0
3	MES	A	2404	-	12,12,12	2.07	1 (8%)	14,16,16	2.92	7 (50%)

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
4	GOL	D	2414	-	-	4/4/4/4	-
4	GOL	A	2415	-	-	4/4/4/4	-
4	GOL	C	2413	-	-	2/4/4/4	-
4	GOL	A	2411	-	-	2/4/4/4	-
4	GOL	B	2412	-	-	2/4/4/4	-
3	MES	B	2405	-	-	1/6/14/14	0/1/1/1
3	MES	C	2401	-	-	1/6/14/14	0/1/1/1
3	MES	A	2403	-	-	1/6/14/14	0/1/1/1
3	MES	D	2402	-	-	1/6/14/14	0/1/1/1
3	MES	A	2404	-	-	1/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2402	MES	C8-S	-7.56	1.66	1.77
3	B	2405	MES	C8-S	-7.37	1.67	1.77
3	A	2403	MES	C8-S	-7.33	1.67	1.77
3	C	2401	MES	C8-S	-7.28	1.67	1.77
3	A	2404	MES	C8-S	-6.83	1.67	1.77

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2403	MES	C5-N4-C3	7.49	125.68	108.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2401	MES	C5-N4-C3	7.24	125.13	108.83
3	B	2405	MES	C5-N4-C3	6.87	124.30	108.83
3	D	2402	MES	C5-N4-C3	5.14	120.39	108.83
3	A	2404	MES	C6-C5-N4	-4.60	103.12	110.10
3	D	2402	MES	C6-C5-N4	-4.57	103.18	110.10
3	A	2404	MES	C2-C3-N4	-4.51	103.27	110.10
3	A	2404	MES	C5-N4-C3	4.24	118.38	108.83
3	A	2404	MES	C7-N4-C3	3.79	120.94	111.23
3	A	2404	MES	C7-N4-C5	3.69	120.67	111.23
3	A	2404	MES	O3S-S-C8	3.68	111.72	105.77
3	D	2402	MES	C2-C3-N4	-3.65	104.57	110.10
3	D	2402	MES	C7-N4-C5	3.48	120.14	111.23
3	D	2402	MES	C7-N4-C3	3.21	119.45	111.23
3	A	2403	MES	O2S-S-C8	3.14	110.69	106.92
3	A	2403	MES	C2-C3-N4	2.92	114.53	110.10
3	C	2401	MES	C7-N4-C5	2.68	118.10	111.23
3	D	2402	MES	O1S-S-C8	2.67	110.13	106.92
3	B	2405	MES	C7-N4-C3	2.67	118.06	111.23
3	A	2404	MES	O1-C6-C5	-2.58	106.11	111.80
3	B	2405	MES	C7-N4-C5	2.50	117.63	111.23
3	B	2405	MES	O1S-S-C8	2.46	109.87	106.92
3	A	2403	MES	O3S-S-C8	2.45	109.73	105.77
3	B	2405	MES	O3S-S-C8	2.40	109.64	105.77
3	A	2403	MES	C7-N4-C3	2.33	117.18	111.23
3	A	2403	MES	C7-N4-C5	2.31	117.14	111.23
3	D	2402	MES	O3S-S-C8	2.28	109.46	105.77
3	C	2401	MES	C7-N4-C3	2.16	116.77	111.23

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2413	GOL	C1-C2-C3-O3
3	D	2402	MES	C8-C7-N4-C3
4	D	2414	GOL	C1-C2-C3-O3
4	A	2415	GOL	O1-C1-C2-O2
4	A	2415	GOL	O1-C1-C2-C3
4	B	2412	GOL	O1-C1-C2-O2
4	B	2412	GOL	O1-C1-C2-C3
3	A	2404	MES	C8-C7-N4-C3
4	D	2414	GOL	O1-C1-C2-C3
4	A	2415	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	2411	GOL	O1-C1-C2-C3
4	C	2413	GOL	O2-C2-C3-O3
4	D	2414	GOL	O2-C2-C3-O3
4	A	2415	GOL	O2-C2-C3-O3
3	C	2401	MES	C8-C7-N4-C3
3	A	2403	MES	C8-C7-N4-C5
4	D	2414	GOL	O1-C1-C2-O2
3	B	2405	MES	C8-C7-N4-C5
4	A	2411	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2413	GOL	2	0
2	B	2421	SO4	1	0
4	B	2412	GOL	2	0
3	A	2404	MES	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	308/323 (95%)	-0.48	2 (0%)	89 90	20, 29, 42, 65	0
1	B	309/323 (95%)	-0.48	5 (1%)	72 74	20, 28, 44, 81	0
1	C	310/323 (95%)	-0.38	7 (2%)	60 63	22, 31, 46, 100	0
1	D	309/323 (95%)	-0.22	6 (1%)	66 69	22, 37, 54, 83	0
All	All	1236/1292 (95%)	-0.39	20 (1%)	72 74	20, 31, 49, 100	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	HIS	5.4
1	B	3	HIS	5.2
1	C	3	HIS	5.0
1	B	5	GLU	3.5
1	C	238	TYR	3.3
1	A	238	TYR	3.3
1	B	238	TYR	3.3
1	C	5	GLU	3.2
1	D	36	HIS	3.2
1	D	238	TYR	3.1
1	C	2	LYS	2.7
1	B	241	ASP	2.7
1	C	180	HIS	2.6
1	A	5	GLU	2.6
1	D	35	PHE	2.4
1	D	5	GLU	2.4
1	C	239	HIS	2.3
1	C	83	ILE	2.3
1	D	256[A]	GLU	2.1
1	B	240	PRO	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. The B-factors column lists the minimum, median, 95^{th} 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
3	MES	D	2402	12/12	0.73	0.31	111,112,115,115	0
3	MES	A	2404	12/12	0.78	0.26	63,70,82,82	0
2	SO4	A	2448	5/5	0.79	0.27	102,102,102,103	0
2	SO4	A	2455	5/5	0.80	0.34	112,112,113,113	0
2	SO4	C	2459	5/5	0.84	0.45	125,125,126,126	0
2	SO4	A	2532	5/5	0.84	0.34	113,113,113,114	0
2	SO4	D	2425	5/5	0.86	0.29	99,99,99,99	1
2	SO4	A	2530	5/5	0.86	0.29	92,92,93,93	0
4	GOL	A	2415	6/6	0.86	0.23	69,69,70,71	0
4	GOL	B	2412	6/6	0.86	0.31	51,53,54,56	0
4	GOL	C	2413	6/6	0.86	0.17	68,69,69,70	0
2	SO4	B	2458	5/5	0.87	0.20	101,102,102,103	0
4	GOL	D	2414	6/6	0.87	0.24	52,54,54,54	0
2	SO4	C	2444	5/5	0.89	0.18	100,100,101,101	0
2	SO4	C	2436	5/5	0.90	0.30	94,94,94,94	0
2	SO4	A	2531	5/5	0.90	0.22	95,95,96,96	0
2	SO4	A	2449	5/5	0.90	0.20	105,105,105,106	0
2	SO4	C	2452	5/5	0.91	0.36	122,122,122,122	0
2	SO4	D	2453	5/5	0.91	0.27	98,98,99,99	0
4	GOL	A	2411	6/6	0.91	0.27	52,55,56,57	0
2	SO4	B	2442	5/5	0.91	0.26	85,85,86,86	0
2	SO4	C	2422	5/5	0.92	0.30	73,74,74,74	1
2	SO4	B	2433	5/5	0.92	0.21	99,99,100,100	0
2	SO4	C	2450	5/5	0.93	0.20	74,75,76,76	0
2	SO4	C	2454	5/5	0.93	0.13	65,67,68,68	0
2	SO4	C	2456	5/5	0.93	0.26	98,98,98,99	0
2	SO4	C	2439	5/5	0.93	0.28	97,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	2427	5/5	0.93	0.22	78,78,78,78	0
2	SO4	B	2457	5/5	0.94	0.23	67,68,68,70	0
2	SO4	C	2438	5/5	0.94	0.22	89,90,90,90	0
2	SO4	D	2445	5/5	0.94	0.36	116,116,116,116	0
2	SO4	D	2435	5/5	0.94	0.13	64,65,66,66	0
2	SO4	D	2440	5/5	0.94	0.49	96,96,96,97	0
2	SO4	C	2437	5/5	0.94	0.19	74,75,75,75	0
2	SO4	B	2434	5/5	0.94	0.34	92,93,93,93	0
2	SO4	A	2429	5/5	0.95	0.10	73,73,74,74	0
2	SO4	D	2443	5/5	0.95	0.11	71,71,72,72	0
3	MES	B	2405	12/12	0.95	0.14	58,62,66,66	0
2	SO4	A	2428	5/5	0.95	0.28	98,98,98,98	0
2	SO4	A	2447	5/5	0.95	0.16	73,73,73,73	0
2	SO4	D	2424	5/5	0.96	0.18	77,78,78,78	0
2	SO4	A	2446	5/5	0.96	0.17	72,73,74,74	0
3	MES	A	2403	12/12	0.97	0.13	51,55,57,58	0
3	MES	C	2401	12/12	0.97	0.14	45,53,58,58	0
2	SO4	D	2423	5/5	0.97	0.09	53,54,55,56	0
2	SO4	D	2441	5/5	0.97	0.23	81,81,82,82	0
2	SO4	A	2426	5/5	0.97	0.19	74,74,75,75	0
2	SO4	D	2451	5/5	0.98	0.13	59,61,61,62	0
2	SO4	B	2421	5/5	0.99	0.11	51,51,52,53	0

6.5 Other polymers

There are no such residues in this entry.