



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 02:48 pm BST

PDB ID : 4HGZ  
Title : Structure of the CcbJ Methyltransferase from *Streptomyces caelestis*  
Authors : Bauer, J.A.; Ondrovicova, G.; Kutejova, E.; Janata, J.  
Deposited on : 2012-10-09  
Resolution : 2.70 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](mailto: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

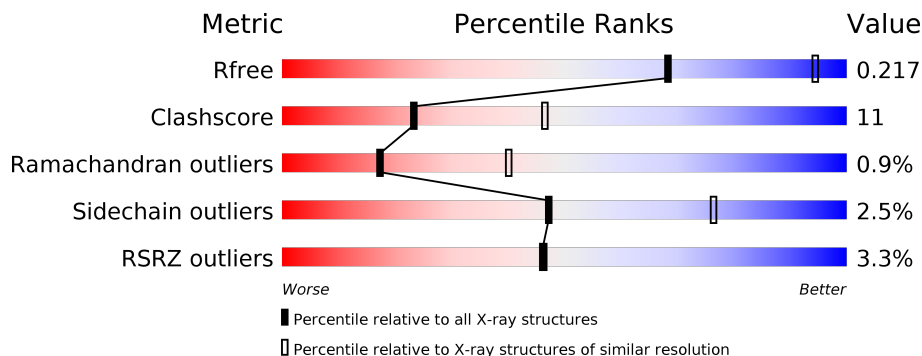
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	 % 63% 22% 14%
1	B	276	 3% 61% 20% 17%
1	C	276	 70% 15% 14%
1	D	276	 7% 66% 18% 15%
1	E	276	 % 69% 15% 14%
1	F	276	 4% 68% 16% 15%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	LI	C	301	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10930 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 CcbJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	236	Total 1801	C 1138	N 322	O 335	S 6	0	0	0
1	B	228	Total 1742	C 1099	N 313	O 324	S 6	0	0	0
1	C	237	Total 1809	C 1142	N 323	O 338	S 6	0	0	0
1	D	235	Total 1796	C 1135	N 321	O 334	S 6	0	0	0
1	E	236	Total 1801	C 1138	N 322	O 335	S 6	0	0	0
1	F	234	Total 1787	C 1130	N 320	O 331	S 6	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP E9JES0
A	-18	GLY	-	expression tag	UNP E9JES0
A	-17	SER	-	expression tag	UNP E9JES0
A	-16	SER	-	expression tag	UNP E9JES0
A	-15	HIS	-	expression tag	UNP E9JES0
A	-14	HIS	-	expression tag	UNP E9JES0
A	-13	HIS	-	expression tag	UNP E9JES0
A	-12	HIS	-	expression tag	UNP E9JES0
A	-11	HIS	-	expression tag	UNP E9JES0
A	-10	HIS	-	expression tag	UNP E9JES0
A	-9	SER	-	expression tag	UNP E9JES0
A	-8	SER	-	expression tag	UNP E9JES0
A	-7	GLY	-	expression tag	UNP E9JES0
A	-6	LEU	-	expression tag	UNP E9JES0
A	-5	VAL	-	expression tag	UNP E9JES0
A	-4	PRO	-	expression tag	UNP E9JES0
A	-3	ARG	-	expression tag	UNP E9JES0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP E9JES0
A	-1	SER	-	expression tag	UNP E9JES0
A	0	HIS	-	expression tag	UNP E9JES0
B	-19	MET	-	expression tag	UNP E9JES0
B	-18	GLY	-	expression tag	UNP E9JES0
B	-17	SER	-	expression tag	UNP E9JES0
B	-16	SER	-	expression tag	UNP E9JES0
B	-15	HIS	-	expression tag	UNP E9JES0
B	-14	HIS	-	expression tag	UNP E9JES0
B	-13	HIS	-	expression tag	UNP E9JES0
B	-12	HIS	-	expression tag	UNP E9JES0
B	-11	HIS	-	expression tag	UNP E9JES0
B	-10	HIS	-	expression tag	UNP E9JES0
B	-9	SER	-	expression tag	UNP E9JES0
B	-8	SER	-	expression tag	UNP E9JES0
B	-7	GLY	-	expression tag	UNP E9JES0
B	-6	LEU	-	expression tag	UNP E9JES0
B	-5	VAL	-	expression tag	UNP E9JES0
B	-4	PRO	-	expression tag	UNP E9JES0
B	-3	ARG	-	expression tag	UNP E9JES0
B	-2	GLY	-	expression tag	UNP E9JES0
B	-1	SER	-	expression tag	UNP E9JES0
B	0	HIS	-	expression tag	UNP E9JES0
C	-19	MET	-	expression tag	UNP E9JES0
C	-18	GLY	-	expression tag	UNP E9JES0
C	-17	SER	-	expression tag	UNP E9JES0
C	-16	SER	-	expression tag	UNP E9JES0
C	-15	HIS	-	expression tag	UNP E9JES0
C	-14	HIS	-	expression tag	UNP E9JES0
C	-13	HIS	-	expression tag	UNP E9JES0
C	-12	HIS	-	expression tag	UNP E9JES0
C	-11	HIS	-	expression tag	UNP E9JES0
C	-10	HIS	-	expression tag	UNP E9JES0
C	-9	SER	-	expression tag	UNP E9JES0
C	-8	SER	-	expression tag	UNP E9JES0
C	-7	GLY	-	expression tag	UNP E9JES0
C	-6	LEU	-	expression tag	UNP E9JES0
C	-5	VAL	-	expression tag	UNP E9JES0
C	-4	PRO	-	expression tag	UNP E9JES0
C	-3	ARG	-	expression tag	UNP E9JES0
C	-2	GLY	-	expression tag	UNP E9JES0
C	-1	SER	-	expression tag	UNP E9JES0

*Continued on next page...*

*Continued from previous page...*

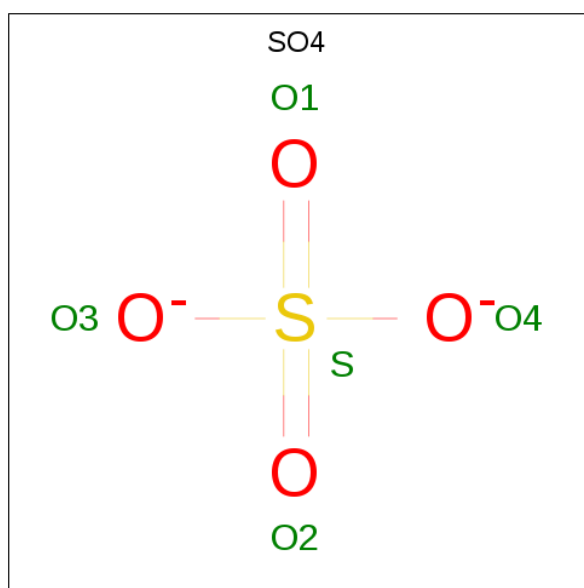
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP E9JES0
D	-19	MET	-	expression tag	UNP E9JES0
D	-18	GLY	-	expression tag	UNP E9JES0
D	-17	SER	-	expression tag	UNP E9JES0
D	-16	SER	-	expression tag	UNP E9JES0
D	-15	HIS	-	expression tag	UNP E9JES0
D	-14	HIS	-	expression tag	UNP E9JES0
D	-13	HIS	-	expression tag	UNP E9JES0
D	-12	HIS	-	expression tag	UNP E9JES0
D	-11	HIS	-	expression tag	UNP E9JES0
D	-10	HIS	-	expression tag	UNP E9JES0
D	-9	SER	-	expression tag	UNP E9JES0
D	-8	SER	-	expression tag	UNP E9JES0
D	-7	GLY	-	expression tag	UNP E9JES0
D	-6	LEU	-	expression tag	UNP E9JES0
D	-5	VAL	-	expression tag	UNP E9JES0
D	-4	PRO	-	expression tag	UNP E9JES0
D	-3	ARG	-	expression tag	UNP E9JES0
D	-2	GLY	-	expression tag	UNP E9JES0
D	-1	SER	-	expression tag	UNP E9JES0
D	0	HIS	-	expression tag	UNP E9JES0
E	-19	MET	-	expression tag	UNP E9JES0
E	-18	GLY	-	expression tag	UNP E9JES0
E	-17	SER	-	expression tag	UNP E9JES0
E	-16	SER	-	expression tag	UNP E9JES0
E	-15	HIS	-	expression tag	UNP E9JES0
E	-14	HIS	-	expression tag	UNP E9JES0
E	-13	HIS	-	expression tag	UNP E9JES0
E	-12	HIS	-	expression tag	UNP E9JES0
E	-11	HIS	-	expression tag	UNP E9JES0
E	-10	HIS	-	expression tag	UNP E9JES0
E	-9	SER	-	expression tag	UNP E9JES0
E	-8	SER	-	expression tag	UNP E9JES0
E	-7	GLY	-	expression tag	UNP E9JES0
E	-6	LEU	-	expression tag	UNP E9JES0
E	-5	VAL	-	expression tag	UNP E9JES0
E	-4	PRO	-	expression tag	UNP E9JES0
E	-3	ARG	-	expression tag	UNP E9JES0
E	-2	GLY	-	expression tag	UNP E9JES0
E	-1	SER	-	expression tag	UNP E9JES0
E	0	HIS	-	expression tag	UNP E9JES0
F	-19	MET	-	expression tag	UNP E9JES0

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP E9JES0
F	-17	SER	-	expression tag	UNP E9JES0
F	-16	SER	-	expression tag	UNP E9JES0
F	-15	HIS	-	expression tag	UNP E9JES0
F	-14	HIS	-	expression tag	UNP E9JES0
F	-13	HIS	-	expression tag	UNP E9JES0
F	-12	HIS	-	expression tag	UNP E9JES0
F	-11	HIS	-	expression tag	UNP E9JES0
F	-10	HIS	-	expression tag	UNP E9JES0
F	-9	SER	-	expression tag	UNP E9JES0
F	-8	SER	-	expression tag	UNP E9JES0
F	-7	GLY	-	expression tag	UNP E9JES0
F	-6	LEU	-	expression tag	UNP E9JES0
F	-5	VAL	-	expression tag	UNP E9JES0
F	-4	PRO	-	expression tag	UNP E9JES0
F	-3	ARG	-	expression tag	UNP E9JES0
F	-2	GLY	-	expression tag	UNP E9JES0
F	-1	SER	-	expression tag	UNP E9JES0
F	0	HIS	-	expression tag	UNP E9JES0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



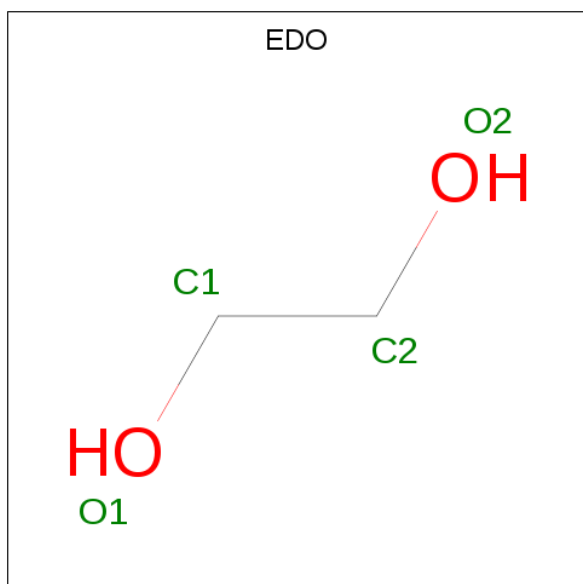
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is LITHIUM ION (three-letter code: LI) (formula: Li).



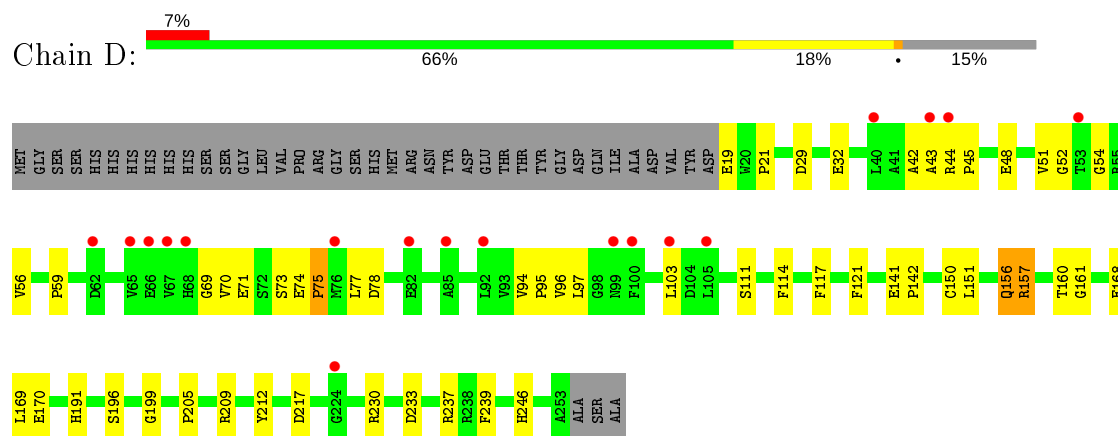
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Li 1 1	0	0
4	C	1	Total Li 1 1	0	0

- Molecule 5 is water.

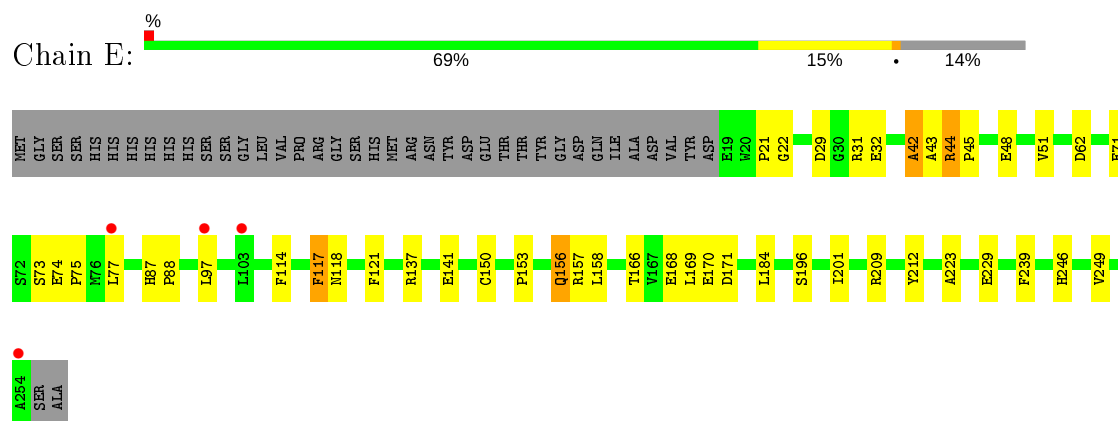
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	25	Total O 25 25	0	0
5	B	20	Total O 20 20	0	0
5	C	27	Total O 27 27	0	0
5	D	18	Total O 18 18	0	0
5	E	25	Total O 25 25	0	0
5	F	21	Total O 21 21	0	0



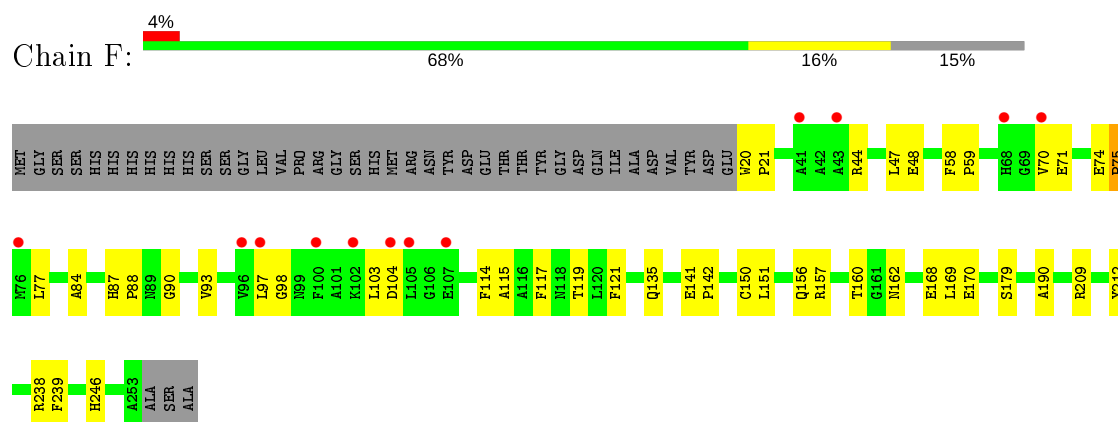
- Molecule 1: CcbJ



- Molecule 1: CcbJ



- Molecule 1: CcbJ



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.02Å 244.55Å 117.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.27 – 2.70 54.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (54.27-2.70) 99.8 (54.27-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.181 , 0.224 0.175 , 0.217	Depositor DCC
$R_{free}$ test set	3353 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtrriage
Anisotropy	0.227	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, SO4, LI

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	0.38	0/1841	0.55	0/2503
1	B	0.39	0/1777	0.55	0/2411
1	C	0.39	0/1849	0.54	0/2514
1	D	0.34	0/1836	0.53	0/2496
1	E	0.38	0/1841	0.55	0/2503
1	F	0.36	0/1827	0.52	0/2484
All	All	0.37	0/10971	0.54	0/14911

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1801	0	1767	47	0
1	B	1742	0	1721	46	0
1	C	1809	0	1771	45	0
1	D	1796	0	1762	59	0
1	E	1801	0	1767	27	0
1	F	1787	0	1756	34	0
2	A	15	0	0	1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	B	4	0	6	0	0
3	C	4	0	6	1	0
3	D	4	0	6	0	0
3	E	4	0	6	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	25	0	0	3	0
5	B	20	0	0	1	0
5	C	27	0	0	0	0
5	D	18	0	0	0	0
5	E	25	0	0	0	0
5	F	21	0	0	0	0
All	All	10930	0	10568	241	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 11.

The worst 5 of 241 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:98:GLY:HA3	1:F:103:LEU:HD22	1.21	1.18
1:D:51:VAL:HG21	1:D:69:GLY:HA3	1.16	1.14
1:D:51:VAL:HG21	1:D:69:GLY:CA	1.82	1.09
1:D:44:ARG:HG3	1:D:45:PRO:HD2	1.12	1.06
1:C:44:ARG:HG2	1:C:45:PRO:HD3	1.38	1.04

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	234/276 (85%)	228 (97%)	5 (2%)	1 (0%)	34	60
1	B	226/276 (82%)	217 (96%)	8 (4%)	1 (0%)	34	60
1	C	235/276 (85%)	226 (96%)	7 (3%)	2 (1%)	17	40
1	D	233/276 (84%)	221 (95%)	9 (4%)	3 (1%)	12	30
1	E	234/276 (85%)	223 (95%)	7 (3%)	4 (2%)	9	23
1	F	232/276 (84%)	223 (96%)	7 (3%)	2 (1%)	17	40
All	All	1394/1656 (84%)	1338 (96%)	43 (3%)	13 (1%)	17	40

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	ALA
1	A	117	PHE
1	B	117	PHE
1	E	42	ALA
1	D	117	PHE

### 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	183/217 (84%)	179 (98%)	4 (2%)	52	79
1	B	178/217 (82%)	171 (96%)	7 (4%)	32	61
1	C	184/217 (85%)	179 (97%)	5 (3%)	44	74
1	D	183/217 (84%)	180 (98%)	3 (2%)	62	85
1	E	183/217 (84%)	179 (98%)	4 (2%)	52	79
1	F	182/217 (84%)	178 (98%)	4 (2%)	52	79
All	All	1093/1302 (84%)	1066 (98%)	27 (2%)	47	76

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	171	ASP
1	F	156	GLN
1	C	44	ARG
1	B	51	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	156	GLN
1	F	156	GLN
1	D	156	GLN
1	B	156	GLN
1	E	156	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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
3	EDO	E	303	-	3,3,3	0.52	0	2,2,2	0.15	0
2	SO4	A	302	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	E	301	-	4,4,4	0.16	0	6,6,6	0.20	0
3	EDO	B	302	-	3,3,3	0.52	0	2,2,2	0.25	0
2	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	F	301	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	A	301	-	4,4,4	0.17	0	6,6,6	0.16	0
3	EDO	D	302	-	3,3,3	0.53	0	2,2,2	0.24	0
2	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	F	302	-	4,4,4	0.12	0	6,6,6	0.16	0
3	EDO	C	302	-	3,3,3	0.48	0	2,2,2	0.36	0
2	SO4	E	302	-	4,4,4	0.13	0	6,6,6	0.08	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
3	EDO	E	303	-	-	1/1/1/1	-
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	EDO	O1-C1-C2-O2
3	E	303	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	SO4	1	0
3	C	302	EDO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	236/276 (85%)	0.00	4 (1%) 70 72	30, 49, 96, 125	0
1	B	228/276 (82%)	0.17	8 (3%) 44 44	28, 53, 123, 167	0
1	C	237/276 (85%)	-0.04	1 (0%) 92 93	34, 51, 89, 140	0
1	D	235/276 (85%)	0.52	18 (7%) 13 11	27, 70, 137, 151	0
1	E	236/276 (85%)	0.11	4 (1%) 70 72	25, 51, 108, 132	0
1	F	234/276 (84%)	0.33	12 (5%) 28 26	29, 64, 130, 151	0
All	All	1406/1656 (84%)	0.18	47 (3%) 46 46	25, 55, 118, 167	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	105	LEU	4.3
1	B	103	LEU	4.2
1	E	254	ALA	4.0
1	B	102	LYS	4.0
1	D	43	ALA	3.8

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	LI	C	301	1/1	0.69	0.45	12,12,12,12	1
2	SO4	A	303	5/5	0.78	0.26	105,107,118,125	0
3	EDO	C	302	4/4	0.78	0.22	48,60,67,81	0
3	EDO	B	302	4/4	0.86	0.23	34,72,88,93	0
4	LI	D	301	1/1	0.88	0.50	2,2,2,2	1
2	SO4	A	301	5/5	0.91	0.17	54,65,98,109	0
2	SO4	B	301	5/5	0.92	0.13	89,93,102,112	0
2	SO4	E	302	5/5	0.92	0.23	84,107,125,137	0
2	SO4	E	301	5/5	0.93	0.13	46,79,108,109	0
2	SO4	F	301	5/5	0.93	0.14	61,73,94,106	0
3	EDO	E	303	4/4	0.93	0.20	39,57,72,84	0
3	EDO	D	302	4/4	0.94	0.15	53,55,82,85	0
2	SO4	A	302	5/5	0.95	0.23	71,80,89,98	0
2	SO4	F	302	5/5	0.96	0.15	69,78,82,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.