



# Full wwPDB X-ray Structure Validation Report i

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 Full wwPDB X-ray Structure Validation 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 i symbol.

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The following versions of software and data (see [references](#) ①) 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

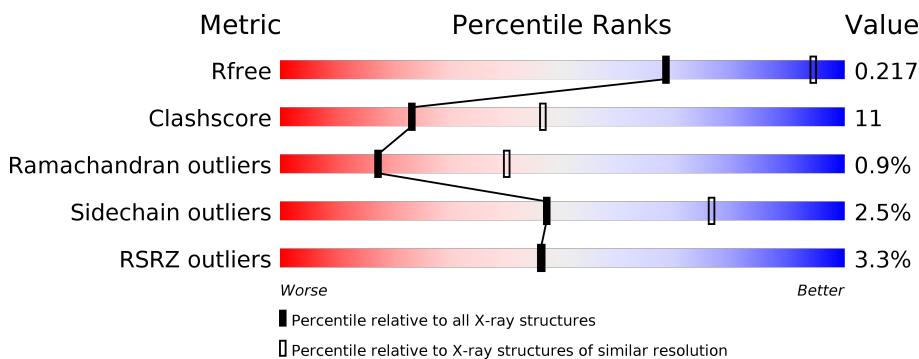
# 1 Overall quality at a glance

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 >=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.



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

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

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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

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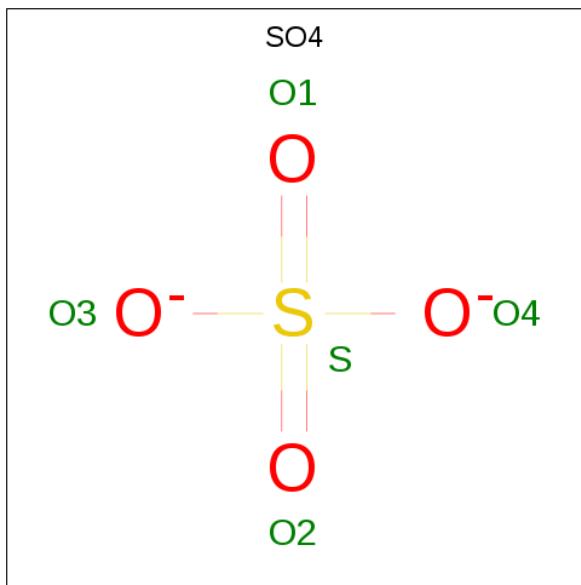
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP E9JES0
D	-19	MET	-	expression tag	UNP E9JES0
D	-18	GLY	-	expression tag	UNP E9JES0
D	-17	SER	-	expression tag	UNP E9JES0
D	-16	SER	-	expression tag	UNP E9JES0
D	-15	HIS	-	expression tag	UNP E9JES0
D	-14	HIS	-	expression tag	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

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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).



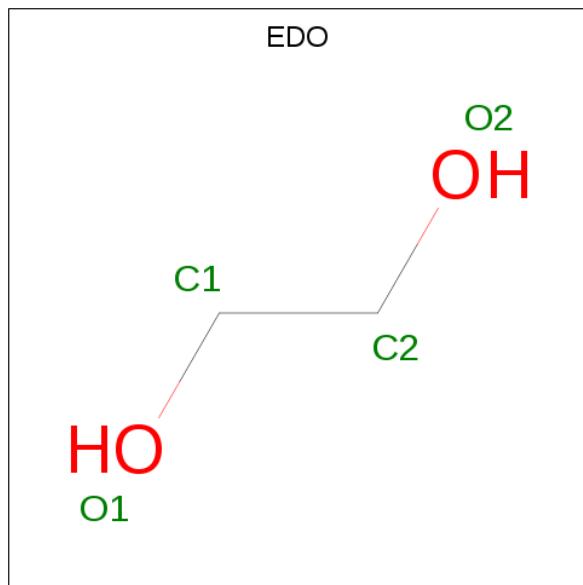
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

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

- 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 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

- 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

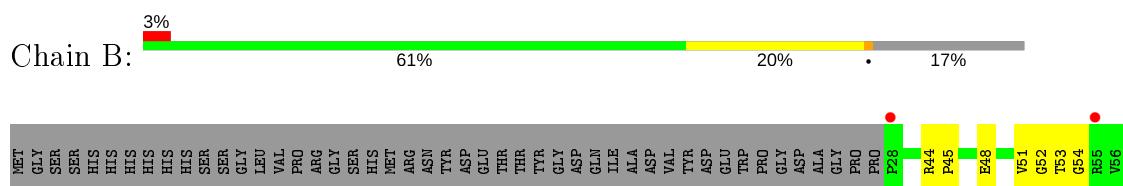
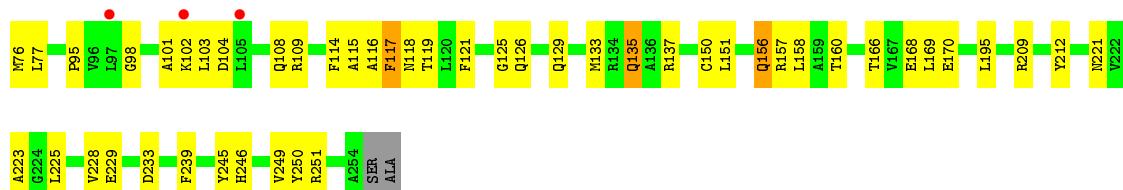
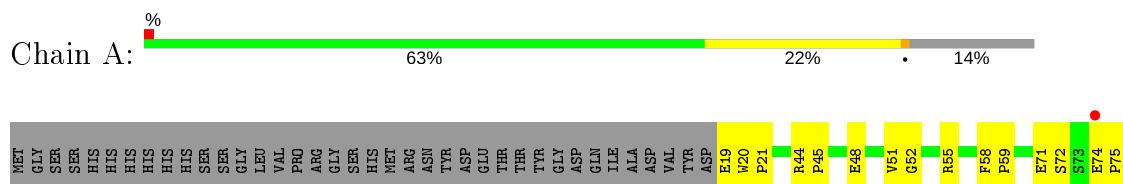
- Molecule 5 is water.

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

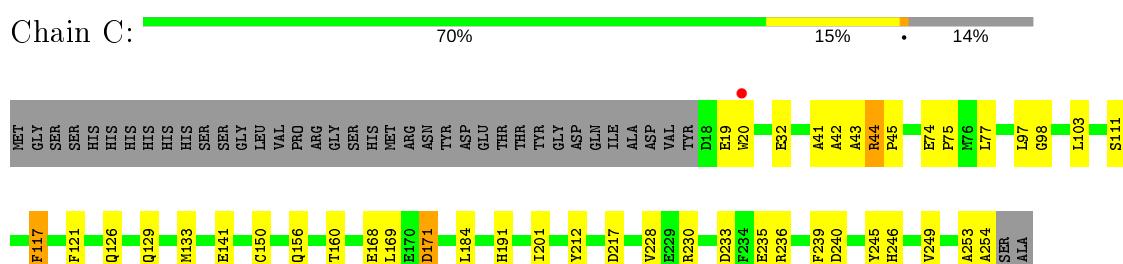
### 3 Residue-property plots

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.

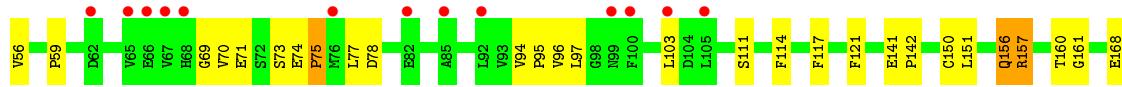
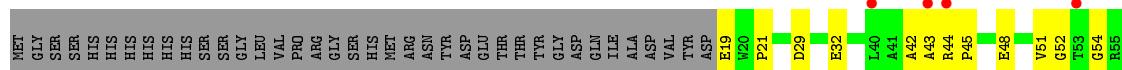
- Molecule 1: CcbJ



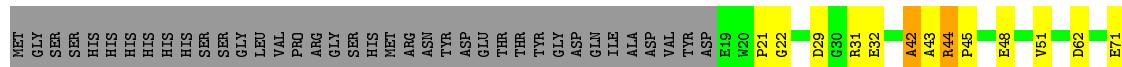
- Molecule 1: CcbJ



- Molecule 1: CcbJ



- Molecule 1: Ccb,J



- Molecule 1: CcbJ



## 4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ <sup>1</sup>	3.34 (at 2.69Å)	Xtriage
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	Xtriage
Anisotropy	0.227	Xtriage
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>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage'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  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality 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

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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.

All (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
1:D:51:VAL:CG2	1:D:69:GLY:CA	2.36	1.04
1:D:51:VAL:CG2	1:D:69:GLY:HA3	1.87	1.04
1:A:98:GLY:HA3	1:A:103:LEU:HD22	1.06	1.03
1:C:77:LEU:CD2	1:C:97:LEU:HB2	1.89	1.02
1:D:74:GLU:HG2	1:D:97:LEU:CD2	1.92	1.00
1:C:44:ARG:HD3	1:C:45:PRO:HD2	1.43	0.98
1:A:98:GLY:HA3	1:A:103:LEU:CD2	1.95	0.96
1:D:44:ARG:CG	1:D:45:PRO:HD2	1.94	0.95
1:D:44:ARG:HG3	1:D:45:PRO:CD	1.95	0.95
1:D:74:GLU:HG2	1:D:97:LEU:HD22	1.48	0.94
1:A:98:GLY:CA	1:A:103:LEU:HD22	1.97	0.91
1:F:98:GLY:HA3	1:F:103:LEU:CD2	2.00	0.90
1:D:74:GLU:CG	1:D:97:LEU:HD21	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LEU:HD23	1:D:97:LEU:HB2	1.56	0.88
1:D:77:LEU:CD2	1:D:97:LEU:HB2	2.06	0.86
1:C:42:ALA:O	1:C:44:ARG:N	2.09	0.85
1:C:44:ARG:CD	1:C:45:PRO:HD2	2.06	0.84
1:C:44:ARG:CG	1:C:45:PRO:HD3	2.09	0.82
1:F:98:GLY:CA	1:F:103:LEU:HD22	2.07	0.82
1:A:19:GLU:HB3	5:A:410:HOH:O	1.79	0.81
1:C:77:LEU:HD23	1:C:97:LEU:HB2	1.62	0.81
1:E:71:GLU:HB2	1:E:77:LEU:HD13	1.64	0.79
1:A:101:ALA:O	1:A:135:GLN:HG3	1.81	0.78
1:E:44:ARG:HG3	1:E:45:PRO:HD2	1.66	0.77
1:C:44:ARG:HD3	1:C:45:PRO:CD	2.15	0.77
1:C:44:ARG:CG	1:C:45:PRO:CD	2.63	0.77
1:D:74:GLU:CG	1:D:97:LEU:CD2	2.63	0.76
1:A:160:THR:HB	1:F:157:ARG:HH12	1.52	0.74
1:C:121:PHE:CE2	1:C:150:CYS:HB3	2.22	0.74
1:C:44:ARG:HG2	1:C:45:PRO:CD	2.18	0.73
1:F:48:GLU:HB2	1:F:114:PHE:CZ	2.23	0.73
1:B:99:ASN:O	1:B:103:LEU:HG	1.88	0.73
1:F:21:PRO:HG2	1:F:170:GLU:HG2	1.72	0.72
1:A:157:ARG:HH12	1:F:160:THR:HB	1.55	0.71
1:A:157:ARG:HH12	1:F:160:THR:CB	2.03	0.70
1:B:74:GLU:N	1:B:75:PRO:CD	2.53	0.70
1:E:121:PHE:CE2	1:E:150:CYS:HB3	2.27	0.70
1:C:77:LEU:HD22	1:C:97:LEU:HB2	1.72	0.69
1:B:100:PHE:HD2	1:B:100:PHE:H	1.41	0.69
1:B:171:ASP:N	1:B:171:ASP:OD1	2.25	0.68
1:A:126:GLN:N	2:A:302:SO4:O3	2.21	0.68
1:A:233:ASP:HB2	5:A:404:HOH:O	1.94	0.67
1:D:121:PHE:CE2	1:D:150:CYS:HB3	2.29	0.67
1:D:74:GLU:HG3	1:D:97:LEU:HD21	1.79	0.65
1:B:48:GLU:HB2	1:B:114:PHE:CZ	2.32	0.65
1:C:126:GLN:H	3:C:302:EDO:H22	1.61	0.65
1:D:51:VAL:HG21	1:D:69:GLY:C	2.16	0.65
1:D:48:GLU:HG3	1:D:114:PHE:CE1	2.32	0.64
1:C:44:ARG:CD	1:C:45:PRO:CD	2.76	0.64
1:D:51:VAL:CG2	1:D:69:GLY:C	2.66	0.64
1:D:71:GLU:HB3	1:D:77:LEU:HD13	1.79	0.64
1:E:48:GLU:OE1	1:E:51:VAL:HG23	1.99	0.62
1:C:42:ALA:C	1:C:44:ARG:H	2.02	0.62
1:D:48:GLU:HB2	1:D:114:PHE:CZ	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:GLU:HB2	1:F:142:PRO:HD2	1.82	0.60
1:E:77:LEU:HD23	1:E:97:LEU:HB2	1.83	0.60
1:B:228:VAL:CG1	1:B:251:ARG:HG2	2.31	0.60
1:C:74:GLU:N	1:C:75:PRO:HD2	2.17	0.60
1:C:160:THR:HB	1:D:157:ARG:HH12	1.66	0.59
1:D:73:SER:C	1:D:75:PRO:HD2	2.23	0.59
1:A:44:ARG:HB3	1:A:45:PRO:CD	2.33	0.58
1:E:74:GLU:N	1:E:75:PRO:CD	2.66	0.58
1:B:141:GLU:HB2	1:B:142:PRO:HD2	1.84	0.58
1:D:233:ASP:OD2	1:D:237:ARG:HD2	2.03	0.58
1:D:51:VAL:HG23	1:D:70:VAL:N	2.19	0.57
1:C:41:ALA:O	1:C:42:ALA:HB3	2.03	0.57
1:C:77:LEU:CD2	1:C:97:LEU:CB	2.75	0.57
1:F:21:PRO:HG2	1:F:170:GLU:CG	2.35	0.56
1:C:217:ASP:OD2	1:C:230:ARG:NH2	2.39	0.55
1:E:229:GLU:HG2	1:E:249:VAL:HB	1.88	0.55
1:B:229:GLU:HG2	1:B:249:VAL:HB	1.87	0.55
1:E:44:ARG:HD2	1:E:141:GLU:OE1	2.07	0.55
1:B:44:ARG:HB3	1:B:45:PRO:CD	2.37	0.55
1:D:239:PHE:CE1	1:D:246:HIS:HB3	2.42	0.55
1:D:74:GLU:N	1:D:75:PRO:CD	2.69	0.55
1:D:56:VAL:O	1:D:59:PRO:HD2	2.07	0.54
1:A:74:GLU:N	1:A:75:PRO:HD2	2.22	0.54
1:B:137:ARG:HD3	1:B:223:ALA:O	2.06	0.54
1:F:48:GLU:HB2	1:F:114:PHE:CE2	2.42	0.54
1:F:239:PHE:CE1	1:F:246:HIS:HB3	2.41	0.54
1:F:141:GLU:HB2	1:F:142:PRO:CD	2.37	0.54
1:B:73:SER:C	1:B:75:PRO:HD2	2.28	0.54
1:C:77:LEU:HD22	1:C:97:LEU:CB	2.36	0.54
1:B:100:PHE:HD2	1:B:100:PHE:N	2.05	0.54
1:B:226:GLU:HG2	1:B:253:ALA:HA	1.90	0.54
1:E:74:GLU:N	1:E:75:PRO:HD2	2.22	0.54
1:B:239:PHE:CE1	1:B:246:HIS:HB3	2.43	0.53
1:D:51:VAL:HG22	1:D:69:GLY:CA	2.35	0.53
1:B:141:GLU:HB2	1:B:142:PRO:CD	2.39	0.53
1:F:74:GLU:HB3	1:F:75:PRO:HD3	1.91	0.53
1:D:51:VAL:O	1:D:71:GLU:OE2	2.25	0.53
1:D:51:VAL:CG2	1:D:69:GLY:HA2	2.35	0.53
1:A:129:GLN:O	1:A:133:MET:HG3	2.10	0.52
1:C:44:ARG:CG	1:C:45:PRO:HD2	2.37	0.52
1:A:239:PHE:CE1	1:A:246:HIS:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:ARG:HD3	1:E:223:ALA:O	2.08	0.52
1:A:108:GLN:O	1:A:109:ARG:NH1	2.42	0.52
1:D:168:GLU:HG3	1:D:169:LEU:N	2.24	0.52
1:D:29:ASP:HA	1:D:32:GLU:OE1	2.10	0.52
1:C:171:ASP:N	1:C:171:ASP:OD1	2.44	0.51
1:A:151:LEU:C	1:A:151:LEU:HD12	2.30	0.51
1:A:229:GLU:HG2	1:A:249:VAL:HB	1.92	0.51
1:A:228:VAL:HG11	1:A:251:ARG:HD3	1.93	0.51
1:C:239:PHE:CE1	1:C:246:HIS:HB3	2.45	0.51
1:C:129:GLN:O	1:C:133:MET:HG3	2.10	0.51
1:E:73:SER:C	1:E:75:PRO:HD2	2.31	0.51
1:C:44:ARG:CB	1:C:45:PRO:CD	2.88	0.50
1:F:58:PHE:HB2	1:F:59:PRO:HD3	1.92	0.50
1:B:228:VAL:HG11	1:B:251:ARG:HG2	1.92	0.50
1:B:100:PHE:CD2	1:B:100:PHE:N	2.75	0.50
1:C:217:ASP:CG	1:C:230:ARG:HH22	2.15	0.50
1:A:20:TRP:HB3	1:A:21:PRO:HD2	1.93	0.50
1:A:51:VAL:HG12	1:A:71:GLU:HG2	1.94	0.50
1:E:42:ALA:O	1:E:43:ALA:C	2.50	0.50
1:E:77:LEU:CD2	1:E:97:LEU:HA	2.42	0.50
1:E:168:GLU:HG3	1:E:169:LEU:N	2.27	0.50
1:F:151:LEU:HD12	1:F:151:LEU:C	2.32	0.49
1:C:253:ALA:O	1:C:254:ALA:C	2.50	0.49
1:D:96:VAL:HG12	1:D:103:LEU:HD21	1.94	0.49
1:A:116:ALA:O	1:A:117:PHE:C	2.51	0.49
1:C:77:LEU:HD22	1:C:97:LEU:CA	2.42	0.49
1:B:156:GLN:HG2	1:B:158:LEU:HD21	1.95	0.49
1:B:228:VAL:HG13	1:B:251:ARG:HG2	1.95	0.49
1:C:32:GLU:N	1:C:32:GLU:OE1	2.42	0.49
1:B:238:ARG:HH12	1:D:237:ARG:HE	1.59	0.48
1:D:75:PRO:O	1:D:78:ASP:HB2	2.13	0.48
1:A:48:GLU:HB2	1:A:114:PHE:CZ	2.48	0.48
1:C:44:ARG:HH12	1:C:141:GLU:HB3	1.79	0.48
1:D:96:VAL:CG1	1:D:103:LEU:HD21	2.43	0.48
1:C:42:ALA:C	1:C:44:ARG:N	2.62	0.48
1:A:115:ALA:HB1	1:A:119:THR:HB	1.96	0.47
1:C:212:TYR:CZ	1:D:212:TYR:CZ	3.01	0.47
1:A:160:THR:CB	1:F:157:ARG:HH12	2.24	0.47
1:E:166:THR:HB	1:F:162:ASN:HB3	1.96	0.47
1:D:77:LEU:CD2	1:D:97:LEU:CB	2.87	0.47
1:B:52:GLY:C	1:B:54:GLY:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASP:OD1	1:B:87:HIS:HE1	1.97	0.47
1:D:199:GLY:HA2	1:E:201:ILE:HB	1.97	0.47
1:F:47:LEU:HD11	1:F:70:VAL:CG2	2.45	0.47
1:D:151:LEU:HD12	1:D:151:LEU:C	2.34	0.47
1:F:121:PHE:CE2	1:F:150:CYS:HB3	2.50	0.47
1:B:121:PHE:CE2	1:B:150:CYS:HB3	2.50	0.47
1:D:21:PRO:HG3	1:D:170:GLU:HG2	1.97	0.46
1:A:21:PRO:HG3	1:A:170:GLU:CG	2.45	0.46
1:C:168:GLU:HG3	1:C:169:LEU:N	2.31	0.46
1:D:44:ARG:HB3	1:D:111:SER:HB3	1.97	0.46
1:D:73:SER:C	1:D:75:PRO:CD	2.84	0.46
1:A:137:ARG:HD3	1:A:223:ALA:O	2.15	0.46
1:A:103:LEU:HG	1:A:104:ASP:N	2.30	0.46
1:E:117:PHE:O	1:E:118:ASN:HB2	2.16	0.46
1:F:115:ALA:HB1	1:F:119:THR:HB	1.97	0.46
1:F:168:GLU:HG3	1:F:169:LEU:N	2.31	0.45
1:C:235:GLU:O	1:C:236:ARG:HB2	2.16	0.45
1:B:184:LEU:HA	1:B:184:LEU:HD23	1.83	0.45
1:C:233:ASP:OD1	1:C:233:ASP:C	2.55	0.45
1:E:153:PRO:HB2	1:E:212:TYR:CE1	2.52	0.45
1:B:160:THR:HB	1:E:157:ARG:HH12	1.80	0.45
1:B:74:GLU:N	1:B:75:PRO:HD3	2.31	0.45
1:F:93:VAL:O	1:F:93:VAL:HG12	2.16	0.45
1:B:244:ARG:NH2	5:B:412:HOH:O	2.48	0.45
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.66	0.45
1:B:151:LEU:C	1:B:151:LEU:HD12	2.37	0.45
1:B:228:VAL:HG11	1:B:251:ARG:CD	2.47	0.45
1:F:20:TRP:HA	1:F:21:PRO:HD3	1.77	0.45
1:E:21:PRO:HG3	1:E:170:GLU:CD	2.36	0.44
1:F:74:GLU:N	1:F:75:PRO:HD2	2.32	0.44
1:F:87:HIS:ND1	1:F:88:PRO:HD2	2.32	0.44
1:A:156:GLN:HG2	1:A:158:LEU:HD21	1.99	0.44
1:B:74:GLU:N	1:B:75:PRO:HD2	2.31	0.44
1:A:212:TYR:CZ	1:F:212:TYR:CZ	3.06	0.44
1:B:71:GLU:O	1:B:97:LEU:HD12	2.17	0.44
1:C:77:LEU:HD22	1:C:97:LEU:HA	1.98	0.44
1:B:103:LEU:H	1:B:135:GLN:HE21	1.66	0.44
1:B:77:LEU:O	1:B:80:LEU:HB3	2.17	0.44
1:C:117:PHE:HE1	1:C:245:TYR:HH	1.64	0.44
1:A:221:ASN:ND2	5:A:418:HOH:O	2.43	0.44
1:C:228:VAL:HG22	1:C:249:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HG	1:A:104:ASP:H	1.83	0.43
1:C:184:LEU:HD21	1:D:239:PHE:CE2	2.52	0.43
1:A:121:PHE:CE2	1:A:150:CYS:HB3	2.54	0.43
1:B:156:GLN:HB3	1:B:158:LEU:HG	2.01	0.43
1:B:235:GLU:O	1:B:236:ARG:HB2	2.18	0.43
1:B:57:ALA:O	1:B:60:LEU:HB2	2.18	0.43
1:D:156:GLN:HE21	1:D:156:GLN:HB2	1.59	0.43
1:E:239:PHE:CE1	1:E:246:HIS:HB3	2.53	0.43
1:F:84:ALA:O	1:F:90:GLY:HA3	2.17	0.43
1:A:117:PHE:O	1:A:118:ASN:HB2	2.19	0.43
1:A:77:LEU:HD22	1:A:95:PRO:HB3	2.00	0.43
1:A:74:GLU:N	1:A:75:PRO:CD	2.82	0.43
1:A:102:LYS:O	1:A:103:LEU:HB2	2.19	0.43
1:A:58:PHE:HB2	1:A:59:PRO:HD3	2.01	0.43
1:B:228:VAL:HG11	1:B:251:ARG:HD3	2.00	0.43
1:B:48:GLU:HB2	1:B:114:PHE:CE2	2.54	0.43
1:D:56:VAL:C	1:D:59:PRO:HD2	2.39	0.43
1:D:217:ASP:OD2	1:D:230:ARG:NH2	2.52	0.42
1:E:48:GLU:HB2	1:E:114:PHE:CZ	2.54	0.42
1:D:191:HIS:CE1	1:D:205:PRO:HB3	2.54	0.42
1:D:42:ALA:C	1:D:44:ARG:N	2.71	0.42
1:A:195:LEU:HB3	1:B:201:ILE:HD13	2.00	0.42
1:D:42:ALA:O	1:D:43:ALA:C	2.58	0.42
1:E:156:GLN:HG2	1:E:158:LEU:HD21	2.00	0.42
1:A:55:ARG:O	1:A:59:PRO:HG2	2.19	0.42
1:F:103:LEU:O	1:F:135:GLN:NE2	2.53	0.42
1:A:157:ARG:NH1	1:F:160:THR:OG1	2.53	0.42
1:D:156:GLN:O	1:D:156:GLN:HG3	2.18	0.42
1:C:41:ALA:O	1:C:111:SER:CB	2.67	0.42
1:B:170:GLU:O	1:C:191:HIS:CE1	2.73	0.42
1:D:94:VAL:HA	1:D:95:PRO:HD3	1.83	0.42
1:B:116:ALA:O	1:B:117:PHE:C	2.57	0.41
1:F:179:SER:HB3	1:F:190:ALA:HB2	2.02	0.41
1:A:168:GLU:HG3	1:A:169:LEU:N	2.35	0.41
1:A:52:GLY:N	1:A:71:GLU:OE2	2.51	0.41
1:B:53:THR:HG22	1:B:79:LYS:HG2	2.02	0.41
1:E:87:HIS:HA	1:E:88:PRO:HD3	1.89	0.41
1:F:104:ASP:C	1:F:104:ASP:OD1	2.59	0.41
1:E:29:ASP:HA	1:E:32:GLU:OE1	2.20	0.41
1:A:125:GLY:HA2	1:A:209:ARG:HD3	2.02	0.41
1:A:151:LEU:HA	1:A:245:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ARG:HH22	1:E:62:ASP:CB	2.33	0.41
1:A:166:THR:HB	1:B:162:ASN:HB3	2.03	0.41
1:B:87:HIS:HA	1:B:88:PRO:HD3	1.91	0.41
1:C:98:GLY:HA3	1:C:103:LEU:HD11	2.03	0.41
1:B:199:GLY:HA2	1:C:201:ILE:HG13	2.02	0.41
1:E:184:LEU:HA	1:E:184:LEU:HD23	1.91	0.41
1:C:240:ASP:OD1	1:C:240:ASP:C	2.59	0.41
1:D:73:SER:O	1:D:74:GLU:C	2.60	0.41
1:B:77:LEU:HD23	1:B:77:LEU:HA	1.84	0.41
1:D:42:ALA:O	1:D:44:ARG:N	2.54	0.41
1:D:71:GLU:HG3	1:D:73:SER:H	1.86	0.41
1:D:160:THR:HG22	1:D:161:GLY:N	2.35	0.40
1:F:71:GLU:O	1:F:97:LEU:HD12	2.22	0.40
1:D:141:GLU:HB2	1:D:142:PRO:HD2	2.03	0.40
1:F:71:GLU:HB3	1:F:77:LEU:HD13	2.03	0.40
1:D:19:GLU:HG2	1:D:19:GLU:O	2.21	0.40
1:D:52:GLY:C	1:D:54:GLY:H	2.24	0.40
1:A:225:LEU:HB3	1:A:250:TYR:HB3	2.04	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1394/1656 (84%)	1338 (96%)	43 (3%)	13 (1%)	17   40

All (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
1	D	157	ARG
1	C	117	PHE
1	D	75	PRO
1	E	44	ARG
1	F	117	PHE
1	E	117	PHE
1	E	22	GLY
1	F	75	PRO

### 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

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	A	76	MET
1	A	135	GLN
1	A	156	GLN
1	B	51	VAL
1	B	100	PHE
1	B	157	ARG
1	B	171	ASP
1	B	191	HIS
1	B	196	SER
1	B	209	ARG
1	C	19	GLU
1	C	20	TRP
1	C	44	ARG
1	C	156	GLN
1	C	171	ASP
1	D	156	GLN
1	D	196	SER
1	D	209	ARG
1	E	156	GLN
1	E	171	ASP
1	E	196	SER
1	E	209	ARG
1	F	44	ARG
1	F	156	GLN
1	F	209	ARG
1	F	238	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
1	D	92	LEU	3.5
1	A	97	LEU	3.5
1	D	103	LEU	3.4
1	F	104	ASP	3.4
1	F	100	PHE	3.3
1	B	80	LEU	3.2
1	F	97	LEU	3.1
1	F	102	LYS	3.1
1	A	102	LYS	3.0
1	D	40	LEU	2.9
1	D	68	HIS	2.8
1	C	20	TRP	2.8
1	B	86	ALA	2.7
1	F	70	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	65	VAL	2.7
1	F	76	MET	2.6
1	B	55	ARG	2.6
1	F	107	GLU	2.6
1	E	103	LEU	2.6
1	D	100	PHE	2.6
1	D	62	ASP	2.6
1	D	76	MET	2.5
1	F	43	ALA	2.5
1	B	97	LEU	2.5
1	D	105	LEU	2.5
1	E	97	LEU	2.4
1	D	99	ASN	2.4
1	B	76	MET	2.3
1	B	28	PRO	2.2
1	D	53	THR	2.2
1	A	105	LEU	2.2
1	E	77	LEU	2.1
1	D	82	GLU	2.1
1	D	224	GLY	2.1
1	D	67	VAL	2.1
1	A	74	GLU	2.1
1	F	96	VAL	2.1
1	F	68	HIS	2.1
1	F	41	ALA	2.1
1	D	66	GLU	2.0
1	D	85	ALA	2.0
1	D	44	ARG	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<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.