



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:47 pm BST

PDB ID : 3C3P
Title : Crystal structure of a methyltransferase (NP_951602.1) from *Geobacter sulfurreducens* at 1.90 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-01-28
Resolution : 1.90 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

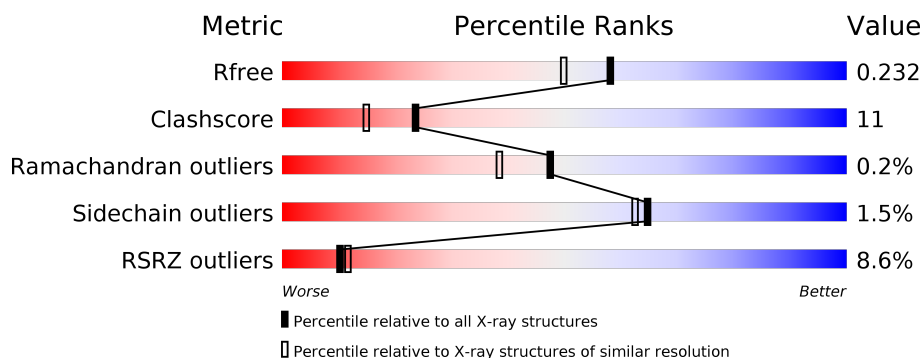
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. 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	210	<div> <div>9%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	B	210	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>• 10%</div> </div> </div>
1	C	210	<div> <div>10%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 7%</div> </div> </div>

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
3	EDO	A	212	-	-	-	X
3	EDO	A	214	-	-	-	X
3	EDO	A	215	-	-	-	X
3	EDO	A	216	-	-	-	X
3	EDO	B	211	-	-	-	X
3	EDO	C	213	-	-	-	X
3	EDO	C	219	-	-	-	X
3	EDO	C	221	-	-	-	X
4	PEG	A	220	-	-	-	X
4	PEG	B	215	-	-	-	X
4	PEG	B	217	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4997 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 Methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	Se	0	15	0
			1595	1015	292	279	3	6			
1	B	190	Total	C	N	O	S	Se	0	8	0
			1507	959	273	267	3	5			
1	C	195	Total	C	N	O	S	Se	0	9	0
			1539	982	279	270	3	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q74FR2
B	0	GLY	-	LEADER SEQUENCE	UNP Q74FR2
C	0	GLY	-	LEADER SEQUENCE	UNP Q74FR2

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



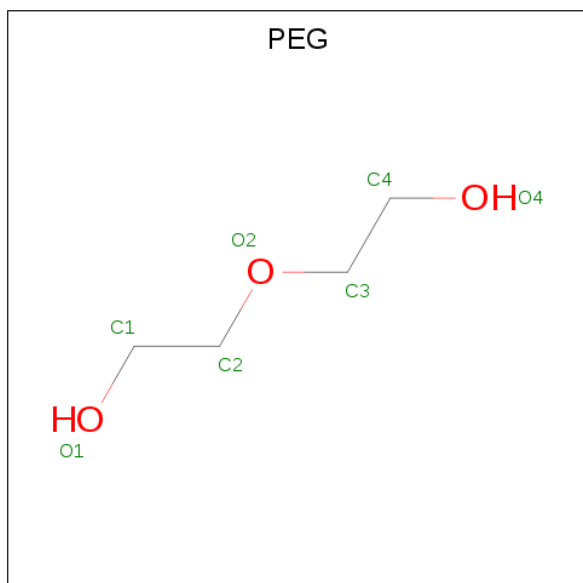
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0

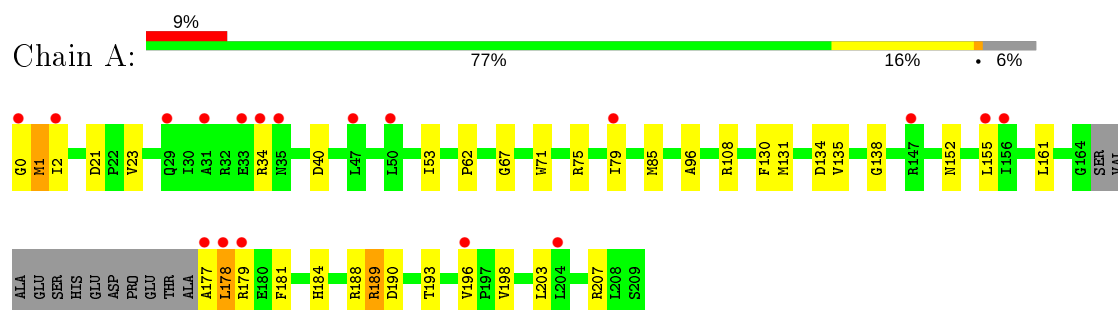
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	57	Total O 57 57	0	0
5	B	69	Total O 69 69	0	0
5	C	69	Total O 69 69	0	0

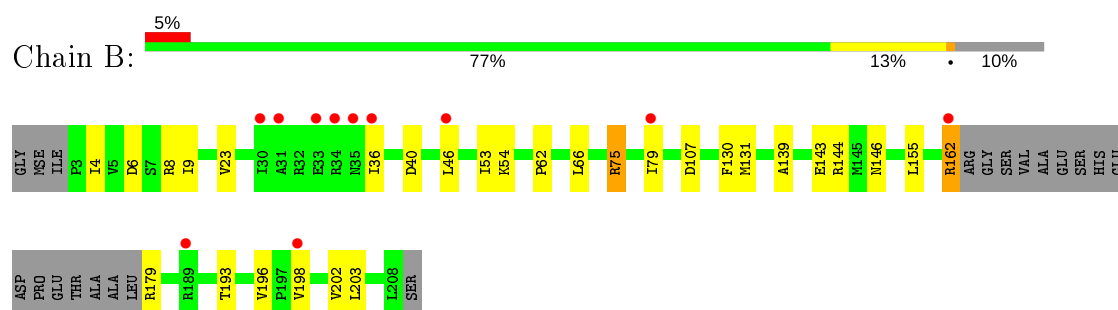
3 Residue-property plots [i](#)

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.

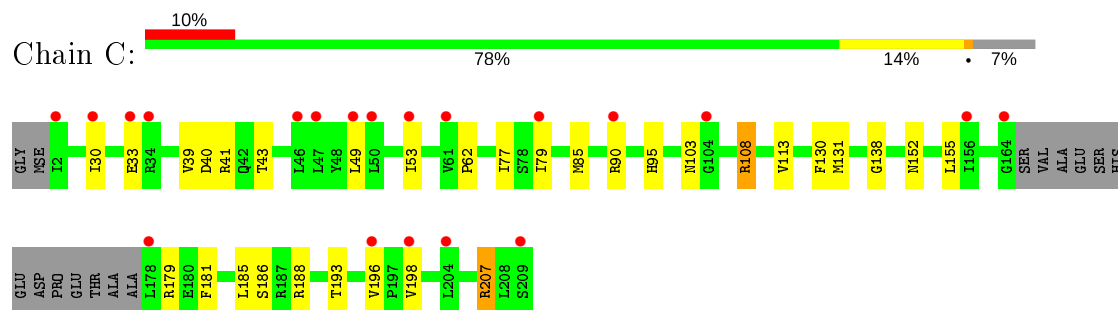
• Molecule 1: Methyltransferase



• Molecule 1: Methyltransferase



• Molecule 1: Methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.88Å 76.04Å 85.17Å 90.00° 118.27° 90.00°	Depositor
Resolution (Å)	28.32 – 1.90 28.32 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.32-1.90) 99.9 (28.32-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.4.0067, PHENIX	Depositor
R, R_{free}	0.199 , 0.232 0.201 , 0.232	Depositor DCC
R_{free} test set	3515 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4997	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, CL

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	0.64	0/1655	0.94	1/2232 (0.0%)
1	B	0.69	0/1547	1.01	5/2092 (0.2%)
1	C	0.68	0/1582	1.01	7/2138 (0.3%)
All	All	0.67	0/4784	0.99	13/6462 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	B	75	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	C	207	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	C	207	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	40	ASP	CB-CG-OD1	6.54	124.18	118.30
1	C	188	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	C	85	MSE	CG-SE-CE	-5.67	86.44	98.90
1	B	144	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	40	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	40	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	144	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	C	108	ARG	N-CA-CB	-5.20	101.24	110.60
1	C	41	ARG	NE-CZ-NH1	-5.09	117.76	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	1595	0	1650	48	0
1	B	1507	0	1535	37	0
1	C	1539	0	1581	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	48	1	0
3	B	12	0	18	2	0
3	C	52	0	78	0	0
4	A	21	0	30	0	0
4	B	35	0	50	0	0
4	C	7	0	10	0	0
5	A	57	0	0	0	0
5	B	69	0	0	0	0
5	C	69	0	0	0	0
All	All	4997	0	5000	110	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 (110) 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:B:131:MSE:CE	1:B:155:LEU:HD11	1.34	1.56
1:A:131:MSE:CE	1:A:155[A]:LEU:HD11	1.55	1.35
1:C:131:MSE:CE	1:C:155[A]:LEU:HD11	1.60	1.31
1:A:1:MSE:CE	1:A:1:MSE:H	1.55	1.20
1:B:131:MSE:HE3	1:B:155:LEU:CD1	1.77	1.15
1:B:131:MSE:CE	1:B:155:LEU:CD1	2.25	1.14
1:C:131:MSE:HE3	1:C:155[A]:LEU:HD11	1.25	1.08
1:A:34[B]:ARG:HH11	1:A:34[B]:ARG:HG2	1.14	1.08
1:B:131:MSE:HE1	1:B:155:LEU:HD11	1.33	1.08
1:A:131:MSE:HE3	1:A:155[A]:LEU:HD11	1.30	1.06
1:C:196[B]:VAL:HG12	1:C:198[B]:VAL:HG23	1.37	1.04
1:A:161:LEU:O	1:A:177:ALA:HB1	1.57	1.03
1:A:196[B]:VAL:HG12	1:A:198[B]:VAL:HG13	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196[B]:VAL:HG12	1:B:198[B]:VAL:HG23	1.42	1.02
1:A:1:MSE:H	1:A:1:MSE:HE3	1.24	1.00
1:A:34[B]:ARG:CG	1:A:34[B]:ARG:HH11	1.78	0.95
1:C:131:MSE:HE1	1:C:155[A]:LEU:HD21	1.47	0.94
1:B:131:MSE:HE3	1:B:155:LEU:HD11	0.93	0.92
1:A:189[A]:ARG:HG3	1:A:189[A]:ARG:HH11	1.33	0.91
1:A:2:ILE:HG21	1:A:177:ALA:HB2	1.50	0.91
1:B:196[B]:VAL:CG1	1:B:198[B]:VAL:HG23	2.03	0.88
1:A:1:MSE:HE2	1:A:1:MSE:H	1.36	0.88
1:A:189[A]:ARG:CG	1:A:189[A]:ARG:HH11	1.86	0.87
1:C:131:MSE:CE	1:C:155[A]:LEU:CD1	2.52	0.86
1:A:1:MSE:CE	1:A:1:MSE:N	2.37	0.86
1:A:131:MSE:HE2	1:A:155[A]:LEU:HD11	1.55	0.85
1:C:131:MSE:HE3	1:C:155[A]:LEU:CD1	2.07	0.84
1:C:131:MSE:HE2	1:C:155[A]:LEU:HD11	1.60	0.82
1:A:178:LEU:O	1:A:179[B]:ARG:HD3	1.79	0.82
1:A:79[B]:ILE:HG12	1:A:108:ARG:NH2	1.97	0.80
1:A:196[B]:VAL:CG1	1:A:198[B]:VAL:HG13	2.10	0.79
1:A:131:MSE:CE	1:A:155[A]:LEU:CD1	2.51	0.79
1:A:34[B]:ARG:HG2	1:A:34[B]:ARG:NH1	1.92	0.78
1:A:1:MSE:N	1:A:1:MSE:HE2	1.97	0.77
1:C:196[B]:VAL:CG1	1:C:198[B]:VAL:HG23	2.12	0.76
1:C:90:ARG:HG2	1:C:113:VAL:HG21	1.68	0.76
1:C:185:LEU:HG	1:C:193[A]:THR:HG21	1.68	0.76
1:A:131:MSE:HE3	1:A:155[A]:LEU:CD1	2.12	0.75
1:A:134[B]:ASP:OD1	1:A:135:VAL:HG23	1.89	0.71
1:B:79:ILE:HD11	1:B:107:ASP:CG	2.13	0.69
1:B:131:MSE:HE1	1:B:155:LEU:CD1	2.09	0.69
1:A:196[B]:VAL:HG13	1:B:196[B]:VAL:CG1	2.23	0.69
1:A:196[B]:VAL:CG1	1:B:196[B]:VAL:HG13	2.28	0.63
1:A:196[B]:VAL:HG13	1:B:196[B]:VAL:HG13	1.81	0.63
1:A:53:ILE:HD11	1:B:53[B]:ILE:HD11	1.79	0.63
1:A:1:MSE:N	1:A:1:MSE:HE3	2.07	0.62
1:B:79:ILE:CD1	1:B:107:ASP:CG	2.67	0.62
1:B:79:ILE:HD13	1:B:107:ASP:OD2	2.00	0.62
1:C:196[B]:VAL:HG12	1:C:198[B]:VAL:CG2	2.22	0.61
1:A:193:THR:HG21	1:A:203:LEU:HD11	1.82	0.60
1:B:79:ILE:CD1	1:B:107:ASP:OD2	2.49	0.60
1:B:4:ILE:HD11	1:B:162:ARG:HB2	1.83	0.59
1:A:189[A]:ARG:NH1	1:A:189[A]:ARG:HG3	2.14	0.59
1:C:49:LEU:HD21	1:C:53[A]:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186[B]:SER:HA	1:C:193[B]:THR:HG21	1.84	0.59
1:A:131:MSE:HE1	1:A:155[A]:LEU:HD11	1.76	0.58
1:A:71:TRP:O	1:A:75:ARG:HG3	2.04	0.58
1:B:54:LYS:HZ3	3:B:212:EDO:C1	2.16	0.57
1:A:131:MSE:HE1	1:A:155[A]:LEU:HD21	1.87	0.57
1:A:177:ALA:HB3	1:B:9:ILE:CD1	2.36	0.56
1:A:34[B]:ARG:CG	1:A:34[B]:ARG:NH1	2.49	0.56
1:B:62:PRO:HD2	1:B:130:PHE:O	2.05	0.56
1:C:131:MSE:HE1	1:C:155[A]:LEU:CD2	2.28	0.56
1:A:189[A]:ARG:CG	1:A:189[A]:ARG:NH1	2.56	0.54
1:C:131:MSE:CE	1:C:155[A]:LEU:HD21	2.30	0.53
1:B:46:LEU:HD22	1:B:198[A]:VAL:HG11	1.91	0.52
1:A:152:ASN:HA	1:A:207:ARG:O	2.10	0.52
1:B:196[A]:VAL:HG23	1:B:198[A]:VAL:HG12	1.92	0.52
1:C:77:ILE:HD11	1:C:108:ARG:HG2	1.92	0.52
1:A:0:GLY:CA	1:A:1:MSE:HE2	2.40	0.51
1:C:138:GLY:HA3	1:C:181:PHE:CD1	2.47	0.50
1:A:193:THR:CG2	1:A:203:LEU:HD11	2.41	0.50
1:B:198[A]:VAL:HG13	1:B:202:VAL:HG23	1.94	0.49
1:B:23:VAL:HG13	3:B:211:EDO:H12	1.93	0.49
1:C:196[B]:VAL:CG1	1:C:198[B]:VAL:CG2	2.88	0.49
1:B:139:ALA:O	1:B:143:GLU:HG2	2.13	0.48
1:C:62:PRO:HD2	1:C:130:PHE:O	2.14	0.48
1:C:79:ILE:HG12	1:C:108:ARG:NH2	2.29	0.48
1:A:138:GLY:HA3	1:A:181:PHE:CD1	2.49	0.47
1:C:30:ILE:HA	1:C:33:GLU:HG2	1.96	0.47
1:B:36:ILE:HD12	1:B:66:LEU:HD21	1.96	0.47
1:C:49:LEU:CD2	1:C:53[A]:ILE:HD11	2.44	0.46
1:C:30:ILE:CD1	1:C:95:HIS:NE2	2.79	0.46
1:A:193:THR:CG2	1:A:203:LEU:CD1	2.94	0.46
1:C:186[B]:SER:HA	1:C:193[B]:THR:CG2	2.46	0.46
1:A:138:GLY:HA3	1:A:181:PHE:CG	2.51	0.46
1:A:21:ASP:OD1	1:A:23:VAL:HG23	2.16	0.45
1:C:39:VAL:HG13	1:C:43:THR:HB	1.98	0.45
1:A:184:HIS:NE2	1:A:188:ARG:HD2	2.33	0.44
1:A:67:GLY:HA3	1:A:96:ALA:HB2	2.00	0.44
1:A:62:PRO:HD2	1:A:130:PHE:O	2.16	0.44
1:A:178:LEU:O	1:A:179[B]:ARG:CD	2.59	0.44
1:B:79:ILE:HD11	1:B:107:ASP:OD2	2.16	0.44
3:A:214:EDO:H11	1:B:193:THR:O	2.18	0.43
1:C:77:ILE:CD1	1:C:108:ARG:HG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:HD23	1:B:203:LEU:C	2.38	0.43
1:B:6:ASP:OD2	1:B:8:ARG:HB2	2.18	0.43
1:C:138:GLY:HA3	1:C:181:PHE:CG	2.54	0.42
1:C:30:ILE:HD12	1:C:95:HIS:NE2	2.35	0.42
1:C:108:ARG:HB2	1:C:108:ARG:HE	1.67	0.41
1:B:196[B]:VAL:HG11	1:B:198[B]:VAL:HG23	1.98	0.41
1:B:46:LEU:CD2	1:B:198[A]:VAL:HG11	2.50	0.41
1:C:152:ASN:HA	1:C:207:ARG:O	2.20	0.41
1:B:198[A]:VAL:HG13	1:B:202:VAL:CG2	2.50	0.41
1:A:188:ARG:HB3	1:A:190:ASP:OD1	2.21	0.40
1:A:196[B]:VAL:HG13	1:B:196[B]:VAL:HG11	2.00	0.40
1:B:196[B]:VAL:CG1	1:B:198[B]:VAL:CG2	2.87	0.40
1:B:179[B]:ARG:HB2	1:B:179[B]:ARG:HE	1.55	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	209/210 (100%)	203 (97%)	5 (2%)	1 (0%)	29	18
1	B	193/210 (92%)	189 (98%)	4 (2%)	0	100	100
1	C	200/210 (95%)	193 (96%)	7 (4%)	0	100	100
All	All	602/630 (96%)	585 (97%)	16 (3%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	LEU

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	170/168 (101%)	166 (98%)	4 (2%)	49	43
1	B	160/168 (95%)	156 (98%)	4 (2%)	47	41
1	C	163/168 (97%)	162 (99%)	1 (1%)	86	87
All	All	493/504 (98%)	484 (98%)	9 (2%)	65	55

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	85	MSE
1	A	189[A]	ARG
1	A	189[B]	ARG
1	B	75	ARG
1	B	146[A]	ASN
1	B	146[B]	ASN
1	B	162	ARG
1	C	179	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

Of 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 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	$\# Z > 2$
4	PEG	B	218	-	6,6,6	0.32	0	5,5,5	1.21	1 (20%)
3	EDO	A	216	-	3,3,3	0.45	0	2,2,2	0.35	0
4	PEG	B	216	-	6,6,6	0.47	0	5,5,5	0.44	0
3	EDO	A	212	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	C	222	-	3,3,3	0.49	0	2,2,2	0.25	0
3	EDO	C	210	-	3,3,3	0.48	0	2,2,2	0.39	0
3	EDO	B	212	-	3,3,3	0.04	0	2,2,2	0.91	0
3	EDO	C	211	-	3,3,3	0.44	0	2,2,2	0.23	0
3	EDO	A	211	-	3,3,3	0.34	0	2,2,2	0.44	0
3	EDO	C	217	-	3,3,3	0.56	0	2,2,2	0.13	0
3	EDO	B	213	-	3,3,3	0.38	0	2,2,2	0.04	0
3	EDO	C	221	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	C	213	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	C	215	-	3,3,3	0.36	0	2,2,2	0.89	0
3	EDO	C	218	-	3,3,3	0.71	0	2,2,2	0.37	0
4	PEG	B	215	-	6,6,6	0.60	0	5,5,5	0.74	0
3	EDO	B	211	-	3,3,3	0.47	0	2,2,2	0.09	0
3	EDO	C	216	-	3,3,3	0.64	0	2,2,2	0.14	0
3	EDO	C	219	-	3,3,3	0.43	0	2,2,2	0.57	0
3	EDO	A	213	-	3,3,3	0.40	0	2,2,2	0.42	0
4	PEG	A	221	-	6,6,6	0.60	0	5,5,5	0.53	0
4	PEG	A	219	-	6,6,6	0.40	0	5,5,5	0.38	0
4	PEG	B	217	-	6,6,6	0.55	0	5,5,5	0.43	0
3	EDO	C	214	-	3,3,3	0.42	0	2,2,2	0.35	0
4	PEG	C	223	-	6,6,6	0.42	0	5,5,5	0.38	0
3	EDO	A	215	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	A	218	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EDO	C	212	-	3,3,3	0.43	0	2,2,2	0.41	0
3	EDO	A	217	-	3,3,3	0.51	0	2,2,2	0.25	0
4	PEG	B	214	-	6,6,6	0.35	0	5,5,5	0.74	0
4	PEG	A	220	-	6,6,6	0.50	0	5,5,5	0.18	0
3	EDO	A	214	-	3,3,3	0.31	0	2,2,2	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	220	-	3,3,3	0.54	0	2,2,2	0.26	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
4	PEG	B	218	-	-	3/4/4/4	-
3	EDO	A	216	-	-	0/1/1/1	-
4	PEG	B	216	-	-	1/4/4/4	-
3	EDO	A	212	-	-	0/1/1/1	-
3	EDO	C	222	-	-	1/1/1/1	-
3	EDO	C	210	-	-	1/1/1/1	-
3	EDO	B	212	-	-	0/1/1/1	-
3	EDO	C	211	-	-	1/1/1/1	-
3	EDO	A	211	-	-	0/1/1/1	-
3	EDO	C	217	-	-	0/1/1/1	-
3	EDO	B	213	-	-	1/1/1/1	-
3	EDO	C	221	-	-	1/1/1/1	-
3	EDO	C	213	-	-	0/1/1/1	-
3	EDO	C	215	-	-	1/1/1/1	-
3	EDO	C	218	-	-	1/1/1/1	-
4	PEG	B	215	-	-	3/4/4/4	-
3	EDO	B	211	-	-	1/1/1/1	-
3	EDO	C	216	-	-	1/1/1/1	-
3	EDO	C	219	-	-	1/1/1/1	-
3	EDO	A	213	-	-	1/1/1/1	-
4	PEG	A	221	-	-	3/4/4/4	-
4	PEG	A	219	-	-	1/4/4/4	-
4	PEG	B	217	-	-	2/4/4/4	-
3	EDO	C	214	-	-	1/1/1/1	-
4	PEG	C	223	-	-	3/4/4/4	-
3	EDO	A	215	-	-	1/1/1/1	-
3	EDO	A	218	-	-	1/1/1/1	-
3	EDO	C	212	-	-	1/1/1/1	-
3	EDO	A	217	-	-	1/1/1/1	-
4	PEG	B	214	-	-	2/4/4/4	-
4	PEG	A	220	-	-	2/4/4/4	-
3	EDO	A	214	-	-	1/1/1/1	-
3	EDO	C	220	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	218	PEG	O2-C2-C1	-2.44	99.33	110.07

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	215	PEG	C1-C2-O2-C3
4	B	218	PEG	O2-C3-C4-O4
4	C	223	PEG	O2-C3-C4-O4
4	B	218	PEG	O1-C1-C2-O2
4	B	215	PEG	O1-C1-C2-O2
4	B	217	PEG	O2-C3-C4-O4
4	B	215	PEG	O2-C3-C4-O4
4	B	214	PEG	O1-C1-C2-O2
4	B	214	PEG	O2-C3-C4-O4
3	C	222	EDO	O1-C1-C2-O2
3	C	215	EDO	O1-C1-C2-O2
3	C	218	EDO	O1-C1-C2-O2
3	A	213	EDO	O1-C1-C2-O2
3	A	215	EDO	O1-C1-C2-O2
3	C	212	EDO	O1-C1-C2-O2
3	A	214	EDO	O1-C1-C2-O2
3	C	220	EDO	O1-C1-C2-O2
4	B	217	PEG	O1-C1-C2-O2
3	C	221	EDO	O1-C1-C2-O2
3	C	211	EDO	O1-C1-C2-O2
3	C	214	EDO	O1-C1-C2-O2
3	A	218	EDO	O1-C1-C2-O2
4	A	221	PEG	C1-C2-O2-C3
4	C	223	PEG	C1-C2-O2-C3
3	C	219	EDO	O1-C1-C2-O2
4	B	218	PEG	C1-C2-O2-C3
4	A	219	PEG	C1-C2-O2-C3
4	A	220	PEG	C1-C2-O2-C3
3	C	216	EDO	O1-C1-C2-O2
4	A	221	PEG	O1-C1-C2-O2
4	B	216	PEG	C4-C3-O2-C2
3	B	213	EDO	O1-C1-C2-O2
4	A	220	PEG	C4-C3-O2-C2
4	A	221	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	C	210	EDO	O1-C1-C2-O2
3	B	211	EDO	O1-C1-C2-O2
3	A	217	EDO	O1-C1-C2-O2
4	C	223	PEG	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	212	EDO	1	0
3	B	211	EDO	1	0
3	A	214	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	192/210 (91%)	0.49	18 (9%) 8 9	25, 34, 48, 71	0
1	B	185/210 (88%)	0.22	11 (5%) 22 25	23, 33, 47, 59	0
1	C	190/210 (90%)	0.49	20 (10%) 6 7	22, 33, 49, 57	0
All	All	567/630 (90%)	0.40	49 (8%) 10 12	22, 33, 49, 71	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	178	LEU	7.3
1	A	0	GLY	7.2
1	A	177	ALA	7.0
1	A	178	LEU	5.7
1	A	29[A]	GLN	4.8
1	C	209	SER	4.4
1	C	46	LEU	4.1
1	A	33	GLU	4.1
1	C	30	ILE	3.8
1	C	50	LEU	3.7
1	B	35	ASN	3.6
1	B	189	ARG	3.5
1	C	2	ILE	3.4
1	B	33	GLU	3.4
1	C	90	ARG	3.4
1	A	35	ASN	3.3
1	A	79[A]	ILE	3.2
1	C	47	LEU	3.2
1	C	79	ILE	3.1
1	C	204	LEU	3.1
1	B	31	ALA	3.0
1	B	34	ARG	2.9
1	B	36	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	34[A]	ARG	2.8
1	C	33	GLU	2.8
1	A	147	ARG	2.7
1	C	104	GLY	2.7
1	C	196[A]	VAL	2.7
1	B	30	ILE	2.7
1	A	155[A]	LEU	2.7
1	B	198[A]	VAL	2.6
1	A	179[A]	ARG	2.6
1	A	2	ILE	2.6
1	B	79	ILE	2.6
1	A	156	ILE	2.5
1	C	156	ILE	2.5
1	C	164	GLY	2.5
1	C	61	VAL	2.3
1	A	47	LEU	2.3
1	C	198[A]	VAL	2.3
1	B	162	ARG	2.3
1	A	31	ALA	2.2
1	A	196[A]	VAL	2.2
1	C	49	LEU	2.2
1	C	34	ARG	2.2
1	A	50	LEU	2.2
1	B	46	LEU	2.1
1	C	53[A]	ILE	2.1
1	A	204	LEU	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	216	4/4	0.26	0.60	88,88,88,88	0
3	EDO	C	211	4/4	0.39	0.38	64,64,64,64	0
4	PEG	A	220	7/7	0.49	0.57	85,85,85,85	0
4	PEG	B	217	7/7	0.51	0.42	65,67,68,69	0
3	EDO	C	219	4/4	0.57	0.57	57,59,59,59	0
4	PEG	A	221	7/7	0.57	0.39	63,64,65,65	0
3	EDO	C	221	4/4	0.58	0.47	81,81,81,81	0
3	EDO	C	222	4/4	0.60	0.33	66,66,66,66	0
3	EDO	C	213	4/4	0.61	0.49	68,68,68,69	0
3	EDO	B	213	4/4	0.63	0.26	61,61,62,62	0
3	EDO	B	211	4/4	0.64	0.46	63,63,63,64	0
4	PEG	B	215	7/7	0.65	0.46	47,50,51,51	0
3	EDO	C	216	4/4	0.65	0.17	53,53,53,53	0
4	PEG	C	223	7/7	0.66	0.18	61,62,65,66	0
3	EDO	A	215	4/4	0.67	0.41	63,64,64,64	0
3	EDO	A	214	4/4	0.71	0.43	49,49,50,51	0
3	EDO	A	212	4/4	0.75	0.51	53,53,53,54	0
3	EDO	C	218	4/4	0.75	0.32	21,28,30,33	0
3	EDO	C	220	4/4	0.79	0.38	52,54,54,56	0
4	PEG	B	218	7/7	0.81	0.48	46,47,48,48	0
3	EDO	C	217	4/4	0.81	0.27	39,40,40,41	0
3	EDO	A	218	4/4	0.81	0.22	39,42,42,42	0
3	EDO	C	210	4/4	0.82	0.42	38,41,41,43	0
3	EDO	C	212	4/4	0.84	0.54	76,76,77,77	0
4	PEG	A	219	7/7	0.85	0.18	66,66,67,67	0
4	PEG	B	216	7/7	0.85	0.24	52,52,53,53	0
4	PEG	B	214	7/7	0.85	0.15	53,54,56,56	0
3	EDO	B	212	4/4	0.86	0.26	38,40,41,44	0
3	EDO	C	214	4/4	0.87	0.30	56,56,56,56	0
3	EDO	C	215	4/4	0.88	0.32	52,53,53,54	0
3	EDO	A	211	4/4	0.88	0.13	57,57,57,57	0
3	EDO	A	213	4/4	0.88	0.41	54,54,54,54	0
3	EDO	A	217	4/4	0.90	0.26	53,55,55,55	0
2	CL	B	210	1/1	0.93	0.11	79,79,79,79	0
2	CL	A	210	1/1	0.97	0.04	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.