



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:47 PM UTC

PDB ID : 2OQM / pdb_00002oqm
Title : Crystal structure of a dinb family member protein (sden_0562) from she-
wanella denitrificans at 1.83 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-01-31
Resolution : 1.83 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

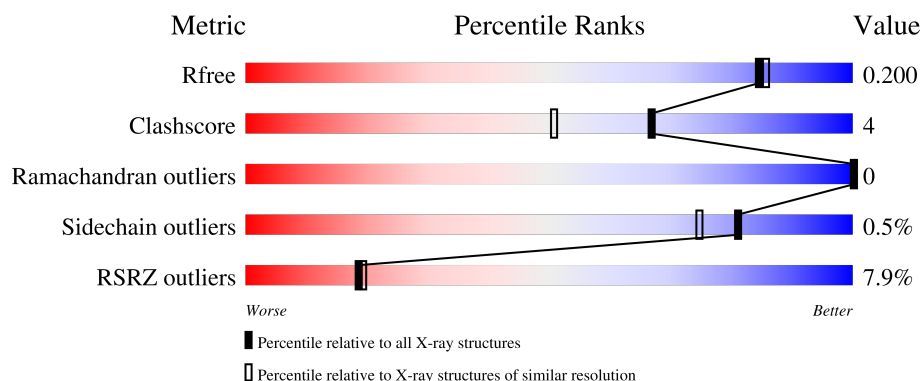
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 of 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	192	3% 83% 10% 6%
1	B	192	2% 88% 5% 7%
1	C	192	18% 90% 7%
1	D	192	6% 85% 7% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	177	-	-	X	-
3	FMT	A	186	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6349 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 Hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	Se	0	6	0
			1445	929	244	267	1	4			
1	B	178	Total	C	N	O	S	Se	0	3	0
			1405	906	231	263	1	4			
1	C	179	Total	C	N	O	S	Se	0	4	0
			1409	908	232	264	1	4			
1	D	178	Total	C	N	O	S	Se	0	2	0
			1396	899	232	260	1	4			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	expression tag	UNP Q12RS4
A	-17	GLY	-	expression tag	UNP Q12RS4
A	-16	SER	-	expression tag	UNP Q12RS4
A	-15	ASP	-	expression tag	UNP Q12RS4
A	-14	LYS	-	expression tag	UNP Q12RS4
A	-13	ILE	-	expression tag	UNP Q12RS4
A	-12	HIS	-	expression tag	UNP Q12RS4
A	-11	HIS	-	expression tag	UNP Q12RS4
A	-10	HIS	-	expression tag	UNP Q12RS4
A	-9	HIS	-	expression tag	UNP Q12RS4
A	-8	HIS	-	expression tag	UNP Q12RS4
A	-7	HIS	-	expression tag	UNP Q12RS4
A	-6	GLU	-	expression tag	UNP Q12RS4
A	-5	ASN	-	expression tag	UNP Q12RS4
A	-4	LEU	-	expression tag	UNP Q12RS4
A	-3	TYR	-	expression tag	UNP Q12RS4
A	-2	PHE	-	expression tag	UNP Q12RS4
A	-1	GLN	-	expression tag	UNP Q12RS4
A	0	GLY	-	expression tag	UNP Q12RS4
A	1	MSE	MET	modified residue	UNP Q12RS4
A	13	MSE	MET	modified residue	UNP Q12RS4

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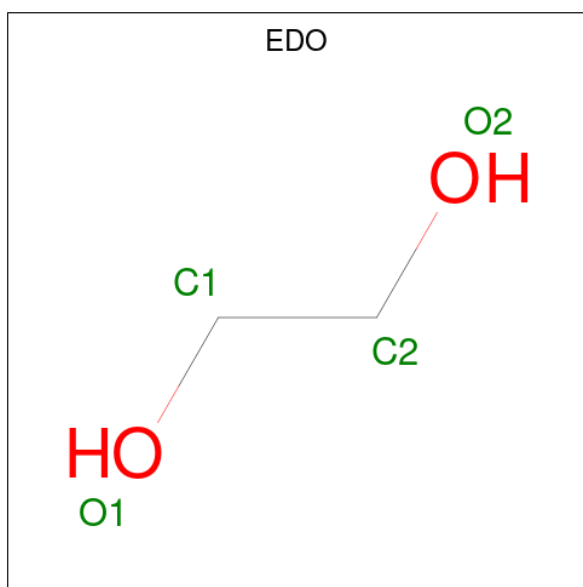
Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MSE	MET	modified residue	UNP Q12RS4
A	166	MSE	MET	modified residue	UNP Q12RS4
B	-18	MSE	-	expression tag	UNP Q12RS4
B	-17	GLY	-	expression tag	UNP Q12RS4
B	-16	SER	-	expression tag	UNP Q12RS4
B	-15	ASP	-	expression tag	UNP Q12RS4
B	-14	LYS	-	expression tag	UNP Q12RS4
B	-13	ILE	-	expression tag	UNP Q12RS4
B	-12	HIS	-	expression tag	UNP Q12RS4
B	-11	HIS	-	expression tag	UNP Q12RS4
B	-10	HIS	-	expression tag	UNP Q12RS4
B	-9	HIS	-	expression tag	UNP Q12RS4
B	-8	HIS	-	expression tag	UNP Q12RS4
B	-7	HIS	-	expression tag	UNP Q12RS4
B	-6	GLU	-	expression tag	UNP Q12RS4
B	-5	ASN	-	expression tag	UNP Q12RS4
B	-4	LEU	-	expression tag	UNP Q12RS4
B	-3	TYR	-	expression tag	UNP Q12RS4
B	-2	PHE	-	expression tag	UNP Q12RS4
B	-1	GLN	-	expression tag	UNP Q12RS4
B	0	GLY	-	expression tag	UNP Q12RS4
B	1	MSE	MET	modified residue	UNP Q12RS4
B	13	MSE	MET	modified residue	UNP Q12RS4
B	35	MSE	MET	modified residue	UNP Q12RS4
B	166	MSE	MET	modified residue	UNP Q12RS4
C	-18	MSE	-	expression tag	UNP Q12RS4
C	-17	GLY	-	expression tag	UNP Q12RS4
C	-16	SER	-	expression tag	UNP Q12RS4
C	-15	ASP	-	expression tag	UNP Q12RS4
C	-14	LYS	-	expression tag	UNP Q12RS4
C	-13	ILE	-	expression tag	UNP Q12RS4
C	-12	HIS	-	expression tag	UNP Q12RS4
C	-11	HIS	-	expression tag	UNP Q12RS4
C	-10	HIS	-	expression tag	UNP Q12RS4
C	-9	HIS	-	expression tag	UNP Q12RS4
C	-8	HIS	-	expression tag	UNP Q12RS4
C	-7	HIS	-	expression tag	UNP Q12RS4
C	-6	GLU	-	expression tag	UNP Q12RS4
C	-5	ASN	-	expression tag	UNP Q12RS4
C	-4	LEU	-	expression tag	UNP Q12RS4
C	-3	TYR	-	expression tag	UNP Q12RS4
C	-2	PHE	-	expression tag	UNP Q12RS4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLN	-	expression tag	UNP Q12RS4
C	0	GLY	-	expression tag	UNP Q12RS4
C	1	MSE	MET	modified residue	UNP Q12RS4
C	13	MSE	MET	modified residue	UNP Q12RS4
C	35	MSE	MET	modified residue	UNP Q12RS4
C	166	MSE	MET	modified residue	UNP Q12RS4
D	-18	MSE	-	expression tag	UNP Q12RS4
D	-17	GLY	-	expression tag	UNP Q12RS4
D	-16	SER	-	expression tag	UNP Q12RS4
D	-15	ASP	-	expression tag	UNP Q12RS4
D	-14	LYS	-	expression tag	UNP Q12RS4
D	-13	ILE	-	expression tag	UNP Q12RS4
D	-12	HIS	-	expression tag	UNP Q12RS4
D	-11	HIS	-	expression tag	UNP Q12RS4
D	-10	HIS	-	expression tag	UNP Q12RS4
D	-9	HIS	-	expression tag	UNP Q12RS4
D	-8	HIS	-	expression tag	UNP Q12RS4
D	-7	HIS	-	expression tag	UNP Q12RS4
D	-6	GLU	-	expression tag	UNP Q12RS4
D	-5	ASN	-	expression tag	UNP Q12RS4
D	-4	LEU	-	expression tag	UNP Q12RS4
D	-3	TYR	-	expression tag	UNP Q12RS4
D	-2	PHE	-	expression tag	UNP Q12RS4
D	-1	GLN	-	expression tag	UNP Q12RS4
D	0	GLY	-	expression tag	UNP Q12RS4
D	1	MSE	MET	modified residue	UNP Q12RS4
D	13	MSE	MET	modified residue	UNP Q12RS4
D	35	MSE	MET	modified residue	UNP Q12RS4
D	166	MSE	MET	modified residue	UNP Q12RS4

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



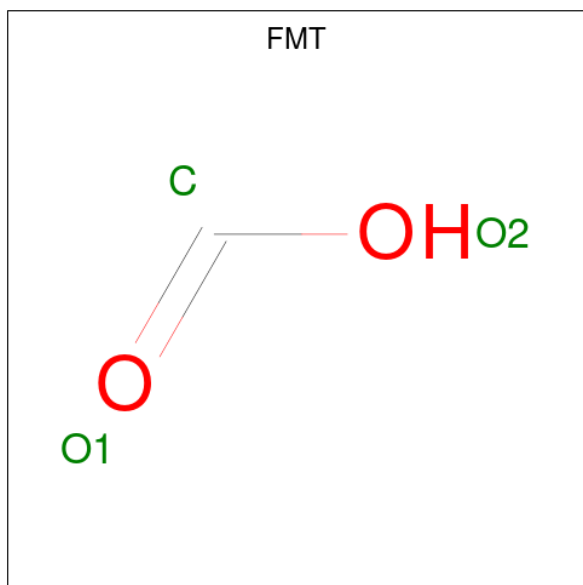
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total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

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

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0

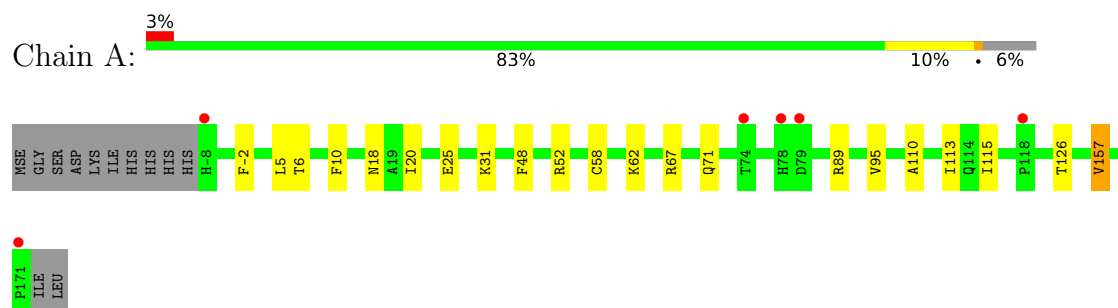
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	146	Total 150	O 150	0	4
5	B	162	Total 162	O 162	0	0
5	C	103	Total 104	O 104	0	1
5	D	134	Total 137	O 137	0	3

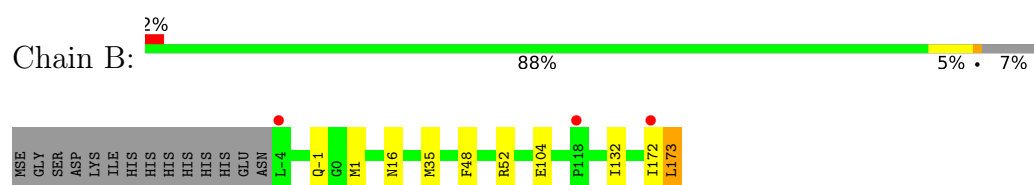
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

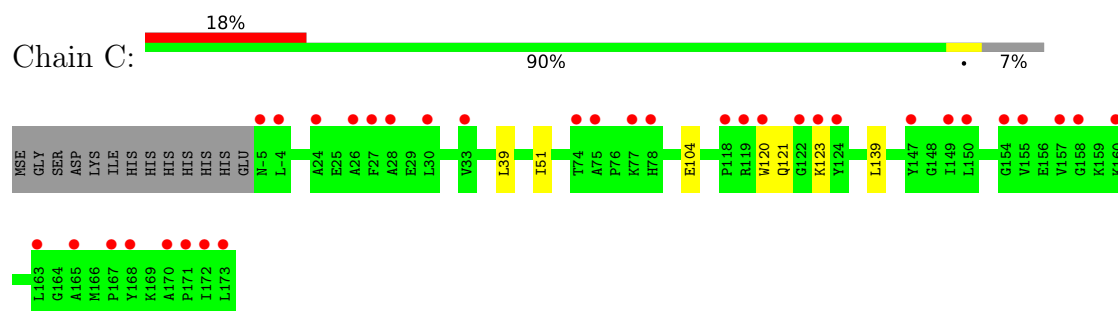
- Molecule 1: Hypothetical protein



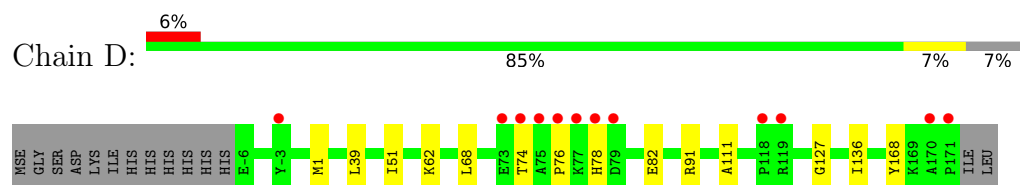
- Molecule 1: Hypothetical protein



- Molecule 1: Hypothetical protein



- Molecule 1: Hypothetical protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.44Å 71.72Å 93.49Å 90.00° 107.35° 90.00°	Depositor
Resolution (Å)	45.22 – 1.83 45.22 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.22-1.83) 98.4 (45.22-1.83)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.157 , 0.196 0.164 , 0.200	Depositor DCC
R_{free} test set	3437 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6349	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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: CL, FMT, EDO

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	1.00	0/1488	0.88	0/2006
1	B	1.02	1/1438 (0.1%)	0.92	0/1943
1	C	0.86	0/1439	0.89	0/1945
1	D	1.01	1/1426 (0.1%)	0.93	0/1927
All	All	0.97	2/5791 (0.0%)	0.91	0/7821

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	MSE	SE-CE	-9.69	1.66	1.95
1	B	35	MSE	SE-CE	-5.38	1.79	1.95

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	1445	0	1444	22	0
1	B	1405	0	1387	8	0
1	C	1409	0	1379	6	0
1	D	1396	0	1374	9	0
2	A	16	0	24	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	24	0	36	0	0
2	C	8	0	12	1	0
2	D	20	0	30	0	0
3	A	27	0	10	1	0
3	B	18	0	6	2	0
3	C	15	0	5	0	0
3	D	12	0	4	1	0
4	D	1	0	0	0	0
5	A	150	0	0	2	0
5	B	162	0	0	0	0
5	C	104	0	0	2	0
5	D	137	0	0	2	0
All	All	6349	0	5711	43	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 4.

All (43) 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:A:18[B]:ASN:HD21	2:A:177:EDO:C1	2.03	0.71
1:A:18[B]:ASN:HD21	2:A:177:EDO:H12	1.58	0.68
1:A:18[B]:ASN:HD22	2:A:177:EDO:H21	1.60	0.66
1:A:18[B]:ASN:ND2	2:A:177:EDO:H21	2.11	0.66
1:A:52:ARG:HD3	5:A:295:HOH:O	1.96	0.64
1:D:74:THR:CB	5:D:251:HOH:O	2.46	0.63
1:B:173:LEU:HD12	1:B:173:LEU:O	2.00	0.62
1:C:123:LYS:HB3	1:D:168:TYR:HB3	1.87	0.55
1:D:78:HIS:HB3	5:D:311:HOH:O	2.06	0.55
2:A:176:EDO:H22	1:B:132:ILE:HG23	1.88	0.54
1:A:18[B]:ASN:ND2	2:A:177:EDO:C2	2.70	0.54
1:B:48:PHE:HB3	1:B:52:ARG:HB2	1.90	0.53
1:A:31:LYS:HD2	5:C:257:HOH:O	2.08	0.52
1:A:71:GLN:OE1	3:A:179:FMT:H	2.10	0.52
1:D:111:ALA:O	3:D:183:FMT:H	2.11	0.51
1:A:20:ILE:HG23	1:A:157:VAL:HG11	1.93	0.50
1:A:-2:PHE:CE1	1:B:1:MSE:HE2	2.46	0.50
1:A:5:LEU:HD22	2:A:176:EDO:H12	1.93	0.50
1:C:104:GLU:HG3	5:C:249:HOH:O	2.10	0.50
1:A:18[B]:ASN:ND2	2:A:177:EDO:C1	2.75	0.49
1:A:25:GLU:OE2	1:A:89:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:TRP:CD1	1:C:120:TRP:N	2.80	0.49
1:B:1:GLN:HG2	1:B:104[B]:GLU:HG3	1.96	0.48
2:C:175:EDO:H21	1:D:136:ILE:HG21	1.94	0.48
1:A:89:ARG:HD2	2:A:177:EDO:H12	1.95	0.47
1:A:67:ARG:HB3	1:A:115:ILE:HD12	1.97	0.47
1:A:110:ALA:O	1:A:113:ILE:HG22	2.14	0.47
1:A:6:THR:O	1:A:10:PHE:HB2	2.16	0.46
1:A:62:LYS:NZ	5:A:272:HOH:O	2.47	0.46
1:D:82:GLU:OE2	1:D:91:ARG:HD2	2.15	0.46
1:A:58:CYS:HB3	1:A:95:VAL:HG21	1.99	0.45
1:A:126:THR:HG21	2:A:174:EDO:H11	1.98	0.45
1:C:120:TRP:O	1:C:121:GLN:C	2.61	0.44
1:A:48:PHE:HB3	1:A:52:ARG:HB2	2.01	0.43
1:D:39:LEU:HB3	1:D:51:ILE:HG13	2.00	0.43
1:A:2:PHE:CD1	1:B:1:MSE:HE2	2.54	0.43
1:D:62:LYS:NZ	1:D:76:PRO:O	2.46	0.42
1:C:39:LEU:O	1:C:51:ILE:HG13	2.20	0.41
1:B:16:ASN:OD1	3:B:183:FMT:C	2.69	0.41
3:B:180:FMT:H	3:B:185:FMT:O1	2.20	0.41
1:C:139:LEU:C	1:C:139:LEU:HD13	2.46	0.40
1:D:68:LEU:HD21	1:D:127:GLY:O	2.21	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	184/192 (96%)	182 (99%)	2 (1%)	0	100	100
1	B	179/192 (93%)	176 (98%)	3 (2%)	0	100	100
1	C	181/192 (94%)	179 (99%)	2 (1%)	0	100	100
1	D	178/192 (93%)	174 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	722/768 (94%)	711 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/155 (97%)	149 (99%)	1 (1%)	76	68
1	B	143/155 (92%)	141 (99%)	2 (1%)	59	45
1	C	142/155 (92%)	142 (100%)	0	100	100
1	D	142/155 (92%)	142 (100%)	0	100	100
All	All	577/620 (93%)	574 (100%)	3 (0%)	81	75

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	VAL
1	B	172	ILE
1	B	173	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	117	GLN
1	D	47	GLN
1	D	121	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 1 is monoatomic - leaving 41 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	$\# Z > 2$
2	EDO	B	178	-	3,3,3	0.42	0	2,2,2	0.16	0
2	EDO	D	176	-	3,3,3	0.54	0	2,2,2	0.43	0
3	FMT	B	184	-	2,2,2	0.62	0	1,1,1	0.60	0
3	FMT	B	183	-	2,2,2	0.70	0	1,1,1	0.06	0
2	EDO	B	177	-	3,3,3	0.63	0	2,2,2	0.28	0
3	FMT	A	185	-	2,2,2	0.74	0	1,1,1	0.40	0
3	FMT	D	181	-	2,2,2	0.65	0	1,1,1	0.24	0
3	FMT	A	184	-	2,2,2	0.64	0	1,1,1	0.24	0
3	FMT	A	178	-	2,2,2	0.62	0	1,1,1	0.32	0
3	FMT	A	183	-	2,2,2	0.65	0	1,1,1	0.24	0
3	FMT	A	181	-	2,2,2	0.69	0	1,1,1	0.28	0
2	EDO	B	174	-	3,3,3	0.46	0	2,2,2	0.56	0
2	EDO	D	175	-	3,3,3	0.49	0	2,2,2	0.71	0
2	EDO	A	176	-	3,3,3	0.30	0	2,2,2	0.33	0
3	FMT	A	182	-	2,2,2	0.60	0	1,1,1	0.38	0
3	FMT	B	182	-	2,2,2	0.67	0	1,1,1	0.32	0
2	EDO	A	174	-	3,3,3	0.49	0	2,2,2	0.14	0
2	EDO	A	175	-	3,3,3	0.51	0	2,2,2	0.17	0
2	EDO	C	174	-	3,3,3	0.47	0	2,2,2	0.07	0
2	EDO	D	178	-	3,3,3	0.86	0	2,2,2	0.60	0
3	FMT	C	177	-	2,2,2	0.90	0	1,1,1	0.04	0
2	EDO	A	177	-	3,3,3	0.65	0	2,2,2	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	D	177	-	3,3,3	0.62	0	2,2,2	0.12	0
3	FMT	D	180	-	2,2,2	0.71	0	1,1,1	0.18	0
3	FMT	D	182	-	2,2,2	0.58	0	1,1,1	0.50	0
3	FMT	C	178	-	2,2,2	0.67	0	1,1,1	0.32	0
2	EDO	B	176	-	3,3,3	0.61	0	2,2,2	0.07	0
3	FMT	B	185	-	2,2,2	0.68	0	1,1,1	0.10	0
3	FMT	D	183	-	2,2,2	1.12	0	1,1,1	1.08	0
3	FMT	B	181	-	2,2,2	0.72	0	1,1,1	0.41	0
3	FMT	A	186	-	2,2,2	2.93	2 (100%)	1,1,1	2.15	1 (100%)
3	FMT	B	180	-	2,2,2	0.87	0	1,1,1	0.39	0
3	FMT	A	179	-	2,2,2	0.76	0	1,1,1	0.75	0
3	FMT	C	176	-	2,2,2	0.62	0	1,1,1	0.33	0
2	EDO	C	175	-	3,3,3	0.55	0	2,2,2	0.70	0
3	FMT	C	180	-	2,2,2	0.59	0	1,1,1	0.36	0
2	EDO	B	175	-	3,3,3	0.30	0	2,2,2	0.57	0
3	FMT	A	180	-	2,2,2	0.66	0	1,1,1	0.30	0
3	FMT	C	179	-	2,2,2	0.62	0	1,1,1	0.66	0
2	EDO	D	179	-	3,3,3	0.56	0	2,2,2	0.29	0
2	EDO	B	179	-	3,3,3	0.66	0	2,2,2	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	175	-	-	0/1/1/1	-
2	EDO	B	178	-	-	1/1/1/1	-
2	EDO	D	176	-	-	1/1/1/1	-
2	EDO	A	177	-	-	0/1/1/1	-
2	EDO	A	176	-	-	0/1/1/1	-
2	EDO	D	177	-	-	0/1/1/1	-
2	EDO	B	177	-	-	0/1/1/1	-
2	EDO	A	174	-	-	1/1/1/1	-
2	EDO	A	175	-	-	1/1/1/1	-
2	EDO	C	174	-	-	0/1/1/1	-
2	EDO	C	175	-	-	1/1/1/1	-
2	EDO	D	178	-	-	0/1/1/1	-
2	EDO	B	175	-	-	0/1/1/1	-
2	EDO	B	176	-	-	1/1/1/1	-
2	EDO	D	179	-	-	0/1/1/1	-
2	EDO	B	179	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	174	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	186	FMT	O1-C	3.42	1.41	1.22
3	A	186	FMT	O2-C	2.35	1.40	1.28

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	186	FMT	O2-C-O1	-2.15	103.59	126.59

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	176	EDO	O1-C1-C2-O2
2	B	174	EDO	O1-C1-C2-O2
2	C	175	EDO	O1-C1-C2-O2
2	B	178	EDO	O1-C1-C2-O2
2	A	174	EDO	O1-C1-C2-O2
2	B	176	EDO	O1-C1-C2-O2
2	A	175	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	183	FMT	1	0
2	A	176	EDO	2	0
2	A	174	EDO	1	0
2	A	177	EDO	7	0
3	B	185	FMT	1	0
3	D	183	FMT	1	0
3	B	180	FMT	1	0
3	A	179	FMT	1	0
2	C	175	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, 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	176/192 (91%)	0.27	6 (3%)	48	52	14, 28, 47, 64	6 (3%)
1	B	174/192 (90%)	0.18	3 (1%)	69	77	16, 28, 44, 54	3 (1%)
1	C	175/192 (91%)	1.20	34 (19%)	3	3	15, 28, 48, 52	4 (2%)
1	D	174/192 (90%)	0.26	12 (6%)	23	24	15, 28, 51, 62	2 (1%)
All	All	699/768 (91%)	0.48	55 (7%)	18	19	14, 28, 49, 64	15 (2%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	76	PRO	4.3
1	D	78	HIS	4.3
1	C	120	TRP	4.3
1	C	172	ILE	4.2
1	A	171	PRO	4.2
1	D	74	THR	4.0
1	D	75	ALA	3.7
1	D	79	ASP	3.6
1	C	118	PRO	3.6
1	C	75	ALA	3.3
1	C	-5	ASN	3.3
1	D	171	PRO	3.2
1	C	173	LEU	3.1
1	D	118	PRO	3.0
1	D	119	ARG	3.0
1	C	26	ALA	3.0
1	C	28	ALA	3.0
1	C	154	GLY	2.9
1	C	147	TYR	2.8
1	C	171	PRO	2.8
1	C	124	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	170	ALA	2.8
1	C	27	PHE	2.8
1	D	77	LYS	2.7
1	B	118	PRO	2.6
1	B	172	ILE	2.6
1	A	78	HIS	2.6
1	C	167	PRO	2.6
1	C	-4	LEU	2.6
1	A	-8	HIS	2.5
1	C	123	LYS	2.5
1	C	33	VAL	2.5
1	C	158	GLY	2.4
1	C	165	ALA	2.4
1	C	119	ARG	2.4
1	B	-4	LEU	2.3
1	C	157	VAL	2.3
1	C	30	LEU	2.3
1	C	78	HIS	2.3
1	A	74	THR	2.3
1	C	77	LYS	2.3
1	C	170	ALA	2.2
1	D	73	GLU	2.2
1	A	79	ASP	2.2
1	C	160	LYS	2.2
1	C	74	THR	2.2
1	A	118	PRO	2.2
1	D	-3	TYR	2.2
1	C	150	LEU	2.2
1	C	168	TYR	2.1
1	C	122	GLY	2.1
1	C	24	ALA	2.1
1	C	155	VAL	2.1
1	C	163	LEU	2.1
1	C	149	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	FMT	B	185	3/3	0.69	0.20	72,72,72,72	0
3	FMT	C	176	3/3	0.73	0.20	75,75,77,77	0
3	FMT	C	179	3/3	0.74	0.17	69,69,70,70	0
3	FMT	A	184	3/3	0.79	0.18	62,62,64,65	0
2	EDO	A	177	4/4	0.80	0.16	54,58,59,61	0
3	FMT	D	182	3/3	0.80	0.20	62,62,66,67	0
2	EDO	D	177	4/4	0.81	0.17	47,60,62,66	0
3	FMT	A	181	3/3	0.82	0.18	53,53,56,58	0
3	FMT	B	184	3/3	0.82	0.18	75,75,76,76	0
3	FMT	D	181	3/3	0.83	0.17	61,61,62,63	0
3	FMT	A	186	3/3	0.85	0.21	77,77,78,78	0
3	FMT	D	183	3/3	0.85	0.14	65,65,66,67	0
3	FMT	B	180	3/3	0.86	0.15	40,40,47,48	0
3	FMT	C	177	3/3	0.86	0.18	45,45,52,53	0
3	FMT	A	183	3/3	0.87	0.18	59,59,61,61	0
2	EDO	D	179	4/4	0.87	0.15	37,41,43,49	0
3	FMT	A	180	3/3	0.88	0.14	57,57,57,58	0
3	FMT	A	179	3/3	0.88	0.12	64,64,65,65	0
2	EDO	A	175	4/4	0.89	0.14	44,45,53,54	0
3	FMT	A	182	3/3	0.89	0.14	51,51,52,53	0
3	FMT	C	180	3/3	0.90	0.18	44,44,52,57	0
3	FMT	C	178	3/3	0.90	0.14	61,61,62,63	0
2	EDO	B	179	4/4	0.91	0.17	33,37,40,45	0
3	FMT	B	183	3/3	0.91	0.20	47,47,47,48	0
3	FMT	A	185	3/3	0.91	0.16	49,49,49,50	0
2	EDO	A	174	4/4	0.91	0.12	39,50,55,59	0
2	EDO	D	178	4/4	0.92	0.13	26,30,39,42	0
2	EDO	B	178	4/4	0.92	0.11	38,39,43,46	0
2	EDO	B	174	4/4	0.92	0.11	35,49,50,50	0
3	FMT	B	182	3/3	0.92	0.16	42,42,51,56	0
2	EDO	B	175	4/4	0.92	0.17	26,30,32,34	0
3	FMT	A	178	3/3	0.94	0.10	40,40,44,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	B	176	4/4	0.94	0.15	29,29,33,35	0
3	FMT	D	180	3/3	0.95	0.10	51,51,51,52	0
2	EDO	B	177	4/4	0.95	0.09	28,29,30,34	0
3	FMT	B	181	3/3	0.96	0.09	52,52,52,53	0
2	EDO	C	175	4/4	0.96	0.10	27,32,34,39	0
2	EDO	C	174	4/4	0.97	0.12	30,36,37,41	0
2	EDO	D	175	4/4	0.97	0.09	22,29,29,32	0
2	EDO	D	176	4/4	0.97	0.14	25,28,33,39	0
2	EDO	A	176	4/4	0.98	0.14	22,27,32,36	0
4	CL	D	174	1/1	0.98	0.09	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.