



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:53 pm BST

PDB ID : 3GZB  
Title : Crystal structure of putative SnoaL-like polyketide cyclase (YP\_001182657.1) from *Shewanella putrefaciens* CN-32 at 1.44 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2009-04-06  
Resolution : 1.44 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 ⓘ symbol.

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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

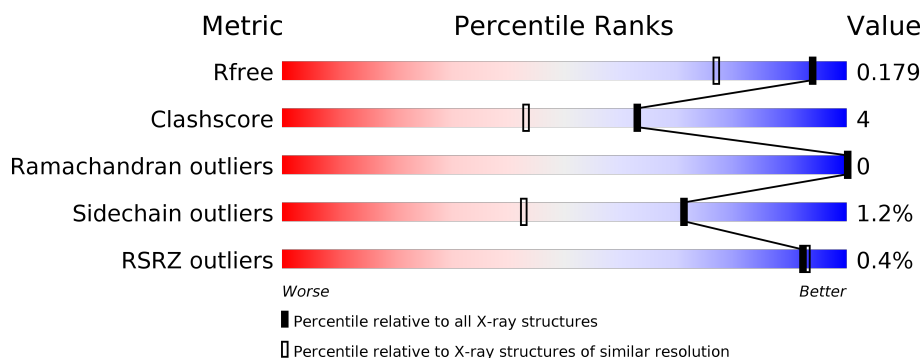
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.44 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	154	<div> <div style="width: 93%;"></div> <div style="width: 7%;"></div> </div>
1	B	154	<div> <div style="width: 81%;"></div> <div style="width: 8%;"></div> <div style="width: 11%;"></div> </div>
1	C	154	<div> <div style="width: 92%;"></div> <div style="width: 7%;"></div> <div style="width: 1%;"></div> </div>
1	D	154	<div> <div style="width: 81%;"></div> <div style="width: 8%;"></div> <div style="width: 11%;"></div> </div>
1	E	154	<div> <div style="width: 91%;"></div> <div style="width: 8%;"></div> <div style="width: 1%;"></div> </div>
1	F	154	<div> <div style="width: 84%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> <div style="width: 11%;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	154	 88%12%
1	H	154	 80%9%11%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12036 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 Putative SnoaL-like polyketide cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	Se	0	18	0
			1339	867	221	240	11			
1	B	137	Total	C	N	O	Se	0	10	0
			1169	752	195	214	8			
1	C	154	Total	C	N	O	Se	0	15	0
			1317	849	223	235	10			
1	D	137	Total	C	N	O	Se	0	14	0
			1199	771	200	219	9			
1	E	154	Total	C	N	O	Se	0	15	0
			1313	849	216	239	9			
1	F	137	Total	C	N	O	Se	0	12	0
			1175	758	194	216	7			
1	G	154	Total	C	N	O	Se	0	16	0
			1323	854	220	239	10			
1	H	137	Total	C	N	O	Se	0	14	0
			1195	769	201	217	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP A4Y4H5
B	0	GLY	-	LEADER SEQUENCE	UNP A4Y4H5
C	0	GLY	-	LEADER SEQUENCE	UNP A4Y4H5
D	0	GLY	-	LEADER SEQUENCE	UNP A4Y4H5
E	0	GLY	-	LEADER SEQUENCE	UNP A4Y4H5
F	0	GLY	-	LEADER SEQUENCE	UNP A4Y4H5
G	0	GLY	-	LEADER SEQUENCE	UNP A4Y4H5
H	0	GLY	-	LEADER SEQUENCE	UNP A4Y4H5

- Molecule 2 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	1
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 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
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	265	Total O 266 266	0	3
5	B	207	Total O 209 209	0	3
5	C	213	Total O 218 218	0	6
5	D	172	Total O 174 174	0	6

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	220	Total 224	O 224	0	4
5	F	208	Total 211	O 211	0	3
5	G	259	Total 261	O 261	0	3
5	H	189	Total 191	O 191	0	2

### 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: Putative SnoaL-like polyketide cyclase

Chain A: 



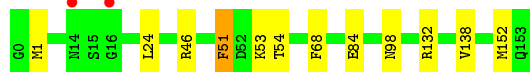
- Molecule 1: Putative SnoaL-like polyketide cyclase

Chain B: 




- Molecule 1: Putative SnoaL-like polyketide cyclase

Chain C: 




- Molecule 1: Putative SnoaL-like polyketide cyclase

Chain D: 




- Molecule 1: Putative SnoaL-like polyketide cyclase

Chain E: 




- Molecule 1: Putative SnoaL-like polyketide cyclase

Chain F:  84% 11%




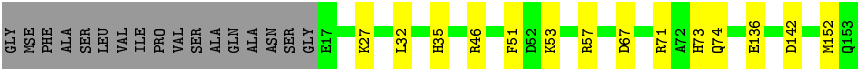
• Molecule 1: Putative SnoaL-like polyketide cyclase

Chain G:  88% 12%



• Molecule 1: Putative SnoaL-like polyketide cyclase

Chain H:  80% 9% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.24Å 89.94Å 94.32Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	47.14 – 1.44 47.16 – 1.44	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.14-1.44) 99.2 (47.16-1.44)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.5.0053, PHENIX	Depositor
R, $R_{free}$	0.151 , 0.174 0.159 , 0.179	Depositor DCC
$R_{free}$ test set	13577 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -l,k,h 0.014 for -h,-l,-k 0.005 for -h,l,k 0.126 for -k,-h,-l 0.125 for k,h,-l 0.006 for -l,-h,k 0.006 for -k,l,-h 0.005 for l,h,k 0.005 for k,-l,-h 0.127 for h,-k,-l 0.012 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, MPD, 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	0.77	0/1416	0.86	1/1888 (0.1%)
1	B	0.85	2/1217 (0.2%)	0.82	0/1624
1	C	0.73	0/1381	0.82	1/1842 (0.1%)
1	D	0.69	0/1262	0.78	0/1683
1	E	0.72	0/1377	0.82	2/1839 (0.1%)
1	F	0.84	0/1229	0.87	1/1641 (0.1%)
1	G	0.79	0/1391	0.84	1/1858 (0.1%)
1	H	0.78	0/1255	0.87	1/1674 (0.1%)
All	All	0.77	2/10528 (0.0%)	0.84	7/14049 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	MSE	CG-SE	-6.14	1.74	1.95
1	B	136	GLU	CG-CD	5.31	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	E	139	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	51	PHE	CB-CG-CD1	5.29	124.50	120.80
1	E	51	PHE	CB-CG-CD1	5.28	124.50	120.80
1	A	64	PHE	CB-CG-CD1	5.19	124.43	120.80
1	H	142	ASP	CB-CG-OD1	5.18	122.96	118.30
1	G	63	ARG	NE-CZ-NH2	-5.10	117.75	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	1339	0	1382	12	0
1	B	1169	0	1169	8	0
1	C	1317	0	1349	10	0
1	D	1199	0	1208	8	0
1	E	1313	0	1342	14	0
1	F	1175	0	1178	5	0
1	G	1323	0	1352	19	0
1	H	1195	0	1211	12	0
2	A	16	0	28	0	0
2	C	24	0	42	0	0
2	E	24	0	42	3	0
2	G	24	0	42	2	0
3	A	8	0	14	0	0
3	B	8	0	14	0	0
3	D	8	0	14	0	0
3	F	16	0	28	2	0
3	H	8	0	14	0	0
4	A	12	0	18	0	0
4	B	24	0	36	1	0
4	C	8	0	12	0	0
4	D	16	0	24	2	0
4	E	16	0	24	1	0
4	F	12	0	18	2	0
4	G	20	0	30	3	0
4	H	8	0	12	2	0
5	A	266	0	0	6	0
5	B	209	0	0	3	0
5	C	218	0	0	5	0
5	D	174	0	0	1	0
5	E	224	0	0	7	0
5	F	211	0	0	1	0
5	G	261	0	0	7	0
5	H	191	0	0	5	0
All	All	12036	0	10603	89	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 (89) 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:133[A]:ARG:HD2	5:A:420:HOH:O	1.75	0.85
1:H:67[B]:ASP:OD2	1:H:71:ARG:NH1	2.08	0.84
1:A:98:ASN:ND2	5:A:266:HOH:O	2.13	0.80
1:C:98:ASN:ND2	5:C:404[A]:HOH:O	2.13	0.80
1:D:67[A]:ASP:OD2	1:D:71:ARG:NH1	2.16	0.78
1:G:73[B]:HIS:CD2	5:G:259:HOH:O	2.40	0.75
2:G:154:MRD:O4	2:G:154:MRD:H1C1	1.92	0.69
1:E:34[B]:GLU:HG3	5:E:340:HOH:O	1.92	0.69
4:E:158:EDO:H12	5:E:255:HOH:O	1.91	0.68
1:H:152[A]:MSE:HA	1:H:152[A]:MSE:HE2	1.75	0.68
2:E:155:MRD:O4	2:E:155:MRD:H1C2	1.94	0.67
1:G:84:GLU:HG2	5:G:283:HOH:O	1.95	0.67
1:A:152[B]:MSE:HE1	5:A:448:HOH:O	1.94	0.66
1:E:95:MSE:SE	1:G:1[A]:MSE:HE1	2.46	0.66
1:C:152[B]:MSE:HE3	5:C:302:HOH:O	1.97	0.64
1:B:46[A]:ARG:HD2	5:B:303:HOH:O	1.98	0.64
1:C:24:LEU:HD13	1:C:132[A]:ARG:NH2	2.13	0.64
1:G:98:ASN:ND2	5:G:283:HOH:O	2.29	0.63
4:G:159:EDO:H22	5:G:359:HOH:O	1.98	0.63
1:E:7[B]:ILE:HD11	1:E:12:GLN:NE2	2.14	0.62
1:B:126[B]:LYS:NZ	5:B:350:HOH:O	2.32	0.61
1:F:32[A]:LEU:HD21	4:F:156:EDO:C1	2.31	0.61
1:D:51:PHE:CE2	1:D:53[A]:LYS:HG2	2.36	0.60
2:G:154:MRD:O4	2:G:154:MRD:C1	2.50	0.60
1:C:84:GLU:HG2	5:C:404[A]:HOH:O	2.03	0.58
1:G:152[B]:MSE:HE3	5:G:303:HOH:O	2.03	0.58
1:H:74[B]:GLN:HG2	5:H:247:HOH:O	2.03	0.57
1:D:32:LEU:HD21	4:D:155:EDO:C1	2.36	0.56
1:A:53[A]:LYS:HD2	5:A:439:HOH:O	2.05	0.56
1:H:35[A]:HIS:NE2	1:H:73:HIS:ND1	2.38	0.56
1:E:98:ASN:OD1	5:E:304:HOH:O	2.18	0.55
1:B:71:ARG:HG3	5:B:332:HOH:O	2.06	0.55
1:H:32[A]:LEU:HD21	4:H:155:EDO:C2	2.36	0.55
1:E:152:MSE:HE2	1:E:152:MSE:HA	1.89	0.55
1:G:132:ARG:HE	4:G:159:EDO:HO1	1.52	0.54
1:C:53[B]:LYS:HG3	1:C:138:VAL:HG13	1.90	0.53
1:G:84:GLU:CG	5:G:283:HOH:O	2.52	0.53
1:A:148:ASP:O	1:A:152[B]:MSE:HE2	2.10	0.52
1:H:51:PHE:CE2	1:H:53[A]:LYS:HG2	2.45	0.52
3:F:155[A]:MPD:O2	3:F:155[A]:MPD:H52	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:155:MRD:O4	2:E:155:MRD:C1	2.58	0.51
1:E:84:GLU:HG2	5:E:304:HOH:O	2.11	0.51
1:C:132[A]:ARG:NH2	5:C:328:HOH:O	2.44	0.50
1:E:34[B]:GLU:CG	5:E:340:HOH:O	2.54	0.50
1:A:84:GLU:HG2	5:A:266:HOH:O	2.12	0.50
1:G:128:ASP:HB3	1:G:133[B]:ARG:HB3	1.94	0.50
1:G:35:HIS:HE2	1:G:73[B]:HIS:HD1	1.59	0.50
1:G:5[A]:LEU:HG	1:G:7[A]:ILE:CD1	2.42	0.49
1:E:5[A]:LEU:CD1	1:G:7[A]:ILE:HG13	2.42	0.49
1:E:1[B]:MSE:HG3	1:G:81:PHE:O	2.13	0.48
1:G:5[A]:LEU:HG	1:G:7[A]:ILE:HD11	1.95	0.48
1:F:32[A]:LEU:HD21	4:F:156:EDO:H12	1.96	0.48
1:A:83:ILE:HG21	1:C:1[A]:MSE:HE3	1.95	0.48
1:E:46[A]:ARG:NH1	5:E:331:HOH:O	2.43	0.48
1:E:84:GLU:CG	5:E:304:HOH:O	2.62	0.48
1:F:51:PHE:CE2	1:F:53:LYS:HG3	2.49	0.48
1:E:83:ILE:HD13	1:G:1[B]:MSE:HE3	1.95	0.47
1:A:84:GLU:CG	5:A:266:HOH:O	2.63	0.47
1:H:32[A]:LEU:HD21	4:H:155:EDO:H21	1.96	0.47
1:B:35[B]:HIS:NE2	1:B:73:HIS:ND1	2.39	0.47
1:D:32:LEU:HD21	4:D:155:EDO:H12	1.97	0.47
1:H:35[A]:HIS:CE1	1:H:73:HIS:HD1	2.29	0.47
1:D:35[A]:HIS:CE1	1:D:73:HIS:HD1	2.32	0.46
1:H:136:GLU:CD	5:H:233:HOH:O	2.53	0.46
1:B:32:LEU:HD21	4:B:157:EDO:C2	2.45	0.46
1:E:1[A]:MSE:HE3	1:G:83:ILE:HG21	1.98	0.46
1:G:132:ARG:NE	4:G:159:EDO:O1	2.33	0.46
1:B:77:LEU:O	1:B:78[B]:GLU:HG2	2.16	0.45
1:D:91[B]:SER:OG	1:D:126[B]:LYS:HE2	2.16	0.45
1:G:7[B]:ILE:HD11	1:G:12:GLN:OE1	2.15	0.45
1:A:128:ASP:HB3	1:A:133[A]:ARG:HB3	1.99	0.44
1:C:46[A]:ARG:HG2	5:C:255[A]:HOH:O	2.18	0.44
1:G:46[A]:ARG:NH1	5:G:375:HOH:O	2.50	0.44
1:A:149:GLN:HA	1:A:152[B]:MSE:CE	2.49	0.43
1:D:77:LEU:O	1:D:78[B]:GLU:HG2	2.19	0.43
1:C:24:LEU:HD13	1:C:132[A]:ARG:CZ	2.48	0.43
1:H:57[A]:ARG:CD	5:H:354:HOH:O	2.67	0.42
1:H:46[B]:ARG:NH1	5:H:349:HOH:O	2.52	0.42
2:E:155:MRD:H1C2	2:E:155:MRD:HA	1.84	0.42
1:H:27[B]:LYS:HE3	5:H:308:HOH:O	2.18	0.41
3:F:155[A]:MPD:O2	3:F:155[A]:MPD:C5	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLN:HA	1:A:152[B]:MSE:HE3	2.02	0.41
1:F:74[A]:GLN:HG2	5:F:311:HOH:O	2.19	0.41
1:B:151:ALA:O	1:B:152[A]:MSE:HE2	2.21	0.41
1:B:35[B]:HIS:CE1	1:B:73:HIS:HD1	2.30	0.41
1:F:34[B]:GLU:CG	1:F:36:ASP:HB2	2.52	0.40
1:E:1[B]:MSE:SE	1:G:81:PHE:HD2	2.54	0.40
1:D:152[B]:MSE:HE3	5:D:320:HOH:O	2.20	0.40
1:A:83:ILE:HD13	1:C:1[A]:MSE:CE	2.51	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	171/154 (111%)	171 (100%)	0	0	100	100
1	B	145/154 (94%)	145 (100%)	0	0	100	100
1	C	167/154 (108%)	167 (100%)	0	0	100	100
1	D	150/154 (97%)	150 (100%)	0	0	100	100
1	E	167/154 (108%)	167 (100%)	0	0	100	100
1	F	147/154 (96%)	147 (100%)	0	0	100	100
1	G	168/154 (109%)	168 (100%)	0	0	100	100
1	H	149/154 (97%)	149 (100%)	0	0	100	100
All	All	1264/1232 (103%)	1264 (100%)	0	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	151/124 (122%)	150 (99%)	1 (1%)	84	64
1	B	128/124 (103%)	127 (99%)	1 (1%)	81	61
1	C	146/124 (118%)	143 (98%)	3 (2%)	53	19
1	D	133/124 (107%)	131 (98%)	2 (2%)	65	34
1	E	146/124 (118%)	144 (99%)	2 (1%)	67	37
1	F	129/124 (104%)	128 (99%)	1 (1%)	81	61
1	G	148/124 (119%)	145 (98%)	3 (2%)	55	21
1	H	133/124 (107%)	133 (100%)	0	100	100
All	All	1114/992 (112%)	1101 (99%)	13 (1%)	71	43

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	PHE
1	B	54	THR
1	C	51	PHE
1	C	54	THR
1	C	68	PHE
1	D	74[A]	GLN
1	D	74[B]	GLN
1	E	51	PHE
1	E	68	PHE
1	F	53	LYS
1	G	51	PHE
1	G	54	THR
1	G	68	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN

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Mol	Chain	Res	Type
1	C	74	GLN
1	E	74	GLN
1	G	74	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

46 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	F	157	-	3,3,3	0.32	0	2,2,2	0.18	0
4	EDO	B	158	-	3,3,3	0.81	0	2,2,2	0.63	0
3	MPD	A	155	-	7,7,7	0.36	0	9,10,10	0.55	0
4	EDO	D	156	-	3,3,3	0.31	0	2,2,2	0.67	0
3	MPD	F	154	-	7,7,7	0.40	0	9,10,10	0.49	0
4	EDO	A	158	-	3,3,3	0.55	0	2,2,2	1.09	0
4	EDO	G	158	-	3,3,3	0.39	0	2,2,2	0.80	0
2	MRD	G	154	-	7,7,7	0.29	0	9,10,10	0.63	0
3	MPD	F	155[A]	-	7,7,7	0.92	1 (14%)	9,10,10	1.35	1 (11%)
2	MRD	E	155	-	7,7,7	0.16	0	9,10,10	0.34	0
4	EDO	H	156	-	3,3,3	0.30	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MRD	C	156	-	7,7,7	0.32	0	9,10,10	0.34	0
4	EDO	E	160	-	3,3,3	0.59	0	2,2,2	0.24	0
4	EDO	B	157	-	3,3,3	0.31	0	2,2,2	0.57	0
2	MRD	G	156	-	7,7,7	0.43	0	9,10,10	0.73	0
3	MPD	B	154	-	7,7,7	0.33	0	9,10,10	0.60	0
4	EDO	B	156	-	3,3,3	0.22	0	2,2,2	0.37	0
4	EDO	B	160	-	3,3,3	0.48	0	2,2,2	0.39	0
4	EDO	D	155	-	3,3,3	0.34	0	2,2,2	0.10	0
3	MPD	H	154	-	7,7,7	0.43	0	9,10,10	0.68	0
4	EDO	D	157	-	3,3,3	0.52	0	2,2,2	0.27	0
4	EDO	B	159	-	3,3,3	0.47	0	2,2,2	0.21	0
4	EDO	E	158	-	3,3,3	0.23	0	2,2,2	0.80	0
4	EDO	F	158	-	3,3,3	0.76	0	2,2,2	0.22	0
4	EDO	G	160	-	3,3,3	0.58	0	2,2,2	0.17	0
2	MRD	G	155	-	7,7,7	0.46	0	9,10,10	1.16	1 (11%)
4	EDO	C	158	-	3,3,3	0.50	0	2,2,2	0.39	0
4	EDO	C	157	-	3,3,3	0.85	0	2,2,2	0.44	0
4	EDO	E	157	-	3,3,3	0.49	0	2,2,2	0.42	0
4	EDO	F	156	-	3,3,3	0.25	0	2,2,2	0.52	0
4	EDO	A	157	-	3,3,3	0.43	0	2,2,2	0.57	0
4	EDO	G	159	-	3,3,3	0.51	0	2,2,2	0.39	0
4	EDO	G	161	-	3,3,3	0.51	0	2,2,2	0.46	0
4	EDO	D	158	-	3,3,3	0.34	0	2,2,2	0.75	0
3	MPD	D	154	-	7,7,7	0.30	0	9,10,10	0.64	0
2	MRD	E	156	-	7,7,7	0.63	0	9,10,10	1.04	1 (11%)
2	MRD	C	155	-	7,7,7	0.57	0	9,10,10	1.12	0
4	EDO	G	157	-	3,3,3	0.89	0	2,2,2	0.65	0
4	EDO	H	155	-	3,3,3	0.39	0	2,2,2	0.13	0
2	MRD	C	154	-	7,7,7	0.39	0	9,10,10	0.66	0
2	MRD	A	154	-	7,7,7	0.48	0	9,10,10	1.05	0
4	EDO	B	155	-	3,3,3	0.48	0	2,2,2	0.72	0
4	EDO	A	159	-	3,3,3	0.40	0	2,2,2	0.61	0
2	MRD	E	154	-	7,7,7	0.44	0	9,10,10	0.23	0
4	EDO	E	159	-	3,3,3	0.41	0	2,2,2	0.48	0
2	MRD	A	156	-	7,7,7	0.22	0	9,10,10	0.41	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	EDO	F	157	-	-	0/1/1/1	-
4	EDO	B	158	-	-	1/1/1/1	-
3	MPD	A	155	-	-	0/5/5/5	-
4	EDO	D	156	-	-	1/1/1/1	-
3	MPD	F	154	-	-	0/5/5/5	-
4	EDO	A	158	-	-	0/1/1/1	-
4	EDO	G	158	-	-	0/1/1/1	-
2	MRD	G	154	-	-	0/5/5/5	-
3	MPD	F	155[A]	-	-	2/5/5/5	-
2	MRD	E	155	-	-	0/5/5/5	-
4	EDO	H	156	-	-	0/1/1/1	-
2	MRD	C	156	-	-	0/5/5/5	-
4	EDO	E	160	-	-	0/1/1/1	-
4	EDO	B	157	-	-	1/1/1/1	-
2	MRD	G	156	-	-	0/5/5/5	-
3	MPD	B	154	-	-	0/5/5/5	-
4	EDO	B	156	-	-	0/1/1/1	-
4	EDO	B	160	-	-	0/1/1/1	-
4	EDO	D	155	-	-	0/1/1/1	-
3	MPD	H	154	-	-	0/5/5/5	-
4	EDO	D	157	-	-	0/1/1/1	-
4	EDO	B	159	-	-	0/1/1/1	-
4	EDO	E	158	-	-	1/1/1/1	-
4	EDO	F	158	-	-	1/1/1/1	-
4	EDO	G	160	-	-	0/1/1/1	-
2	MRD	G	155	-	-	0/5/5/5	-
4	EDO	C	158	-	-	0/1/1/1	-
4	EDO	C	157	-	-	0/1/1/1	-
4	EDO	E	157	-	-	0/1/1/1	-
4	EDO	F	156	-	-	1/1/1/1	-
4	EDO	A	157	-	-	0/1/1/1	-
4	EDO	G	159	-	-	0/1/1/1	-
4	EDO	G	161	-	-	1/1/1/1	-
4	EDO	D	158	-	-	0/1/1/1	-
3	MPD	D	154	-	-	0/5/5/5	-
2	MRD	E	156	-	-	0/5/5/5	-
2	MRD	C	155	-	-	0/5/5/5	-
4	EDO	G	157	-	-	0/1/1/1	-
4	EDO	H	155	-	-	0/1/1/1	-
2	MRD	C	154	-	-	0/5/5/5	-
2	MRD	A	154	-	-	0/5/5/5	-
4	EDO	B	155	-	-	0/1/1/1	-
4	EDO	A	159	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MRD	E	154	-	-	0/5/5/5	-
4	EDO	E	159	-	-	0/1/1/1	-
2	MRD	A	156	-	-	0/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	155[A]	MPD	CM-C2	2.05	1.58	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	155[A]	MPD	O2-C2-C1	-3.00	98.47	108.08
2	G	155	MRD	O2-C2-C3	-2.41	100.73	109.80
2	E	156	MRD	O4-C4-C5	2.13	118.58	109.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	158	EDO	O1-C1-C2-O2
4	B	158	EDO	O1-C1-C2-O2
3	F	155[A]	MPD	C2-C3-C4-O4
4	G	161	EDO	O1-C1-C2-O2
4	D	156	EDO	O1-C1-C2-O2
4	B	157	EDO	O1-C1-C2-O2
4	F	156	EDO	O1-C1-C2-O2
3	F	155[A]	MPD	C2-C3-C4-C5
4	E	158	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	154	MRD	2	0
3	F	155[A]	MPD	2	0
2	E	155	MRD	3	0
4	B	157	EDO	1	0
4	D	155	EDO	2	0
4	E	158	EDO	1	0
4	F	156	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	159	EDO	3	0
4	H	155	EDO	2	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	146/154 (94%)	-0.25	0 100 100	8, 12, 19, 28	0
1	B	130/154 (84%)	-0.19	1 (0%) 86 86	7, 12, 27, 39	0
1	C	146/154 (94%)	-0.30	2 (1%) 75 75	9, 15, 25, 43	0
1	D	130/154 (84%)	-0.30	0 100 100	10, 15, 29, 37	0
1	E	146/154 (94%)	-0.28	1 (0%) 87 88	9, 14, 24, 43	0
1	F	130/154 (84%)	-0.33	0 100 100	9, 13, 22, 36	0
1	G	146/154 (94%)	-0.21	0 100 100	8, 11, 20, 36	0
1	H	130/154 (84%)	-0.20	0 100 100	8, 13, 26, 38	0
All	All	1104/1232 (89%)	-0.26	4 (0%) 92 93	7, 13, 24, 43	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	16	GLY	2.8
1	C	14	ASN	2.3
1	B	107	GLN	2.1
1	C	16	GLY	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 ⓘ

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	EDO	F	158	4/4	0.63	0.18	29,33,42,45	0
4	EDO	B	158	4/4	0.66	0.13	29,36,36,38	0
3	MPD	F	155[A]	8/8	0.67	0.20	12,18,20,29	8
4	EDO	C	157	4/4	0.77	0.12	26,30,32,33	0
4	EDO	E	157	4/4	0.78	0.14	22,28,33,33	0
2	MRD	A	156	8/8	0.79	0.17	30,39,43,43	0
4	EDO	G	157	4/4	0.83	0.10	24,26,28,28	0
4	EDO	A	158	4/4	0.83	0.12	23,27,29,30	0
2	MRD	G	154	8/8	0.87	0.14	27,36,37,45	0
4	EDO	G	161	4/4	0.89	0.14	25,36,40,45	0
2	MRD	E	155	8/8	0.89	0.17	27,34,40,46	0
4	EDO	G	159	4/4	0.89	0.12	41,41,42,43	0
3	MPD	H	154	8/8	0.90	0.11	20,22,25,26	0
4	EDO	B	159	4/4	0.90	0.17	36,37,41,45	0
2	MRD	C	156	8/8	0.90	0.16	31,40,44,44	0
3	MPD	D	154	8/8	0.91	0.10	23,26,32,33	0
2	MRD	C	155	8/8	0.91	0.11	17,23,33,34	0
4	EDO	D	155	4/4	0.91	0.14	27,33,34,35	0
2	MRD	E	154	8/8	0.91	0.08	21,24,28,33	0
3	MPD	A	155	8/8	0.91	0.09	22,25,27,32	0
3	MPD	B	154	8/8	0.92	0.09	21,23,28,28	0
3	MPD	F	154	8/8	0.92	0.08	18,19,21,23	0
4	EDO	B	155	4/4	0.93	0.10	25,25,29,32	0
4	EDO	E	158	4/4	0.93	0.12	26,32,32,45	0
2	MRD	C	154	8/8	0.93	0.09	22,24,27,35	0
4	EDO	A	157	4/4	0.94	0.08	26,29,39,44	0
4	EDO	D	157	4/4	0.94	0.12	22,44,44,47	0
4	EDO	F	157	4/4	0.94	0.15	23,31,35,38	0
2	MRD	A	154	8/8	0.94	0.09	14,18,27,28	0
4	EDO	D	158	4/4	0.94	0.11	29,35,38,47	0
4	EDO	B	160	4/4	0.94	0.12	25,42,43,44	0
2	MRD	E	156	8/8	0.94	0.10	14,20,27,28	0
4	EDO	D	156	4/4	0.95	0.10	29,38,42,43	0
4	EDO	F	156	4/4	0.95	0.18	23,25,28,33	0
4	EDO	E	160	4/4	0.95	0.10	18,38,44,46	0
2	MRD	G	155	8/8	0.95	0.10	13,18,23,29	0
4	EDO	E	159	4/4	0.95	0.11	27,31,37,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	157	4/4	0.95	0.20	27,28,28,35	0
4	EDO	B	156	4/4	0.96	0.10	22,27,34,36	0
4	EDO	G	158	4/4	0.96	0.12	23,26,35,37	0
4	EDO	A	159	4/4	0.96	0.09	17,37,40,44	0
4	EDO	G	160	4/4	0.96	0.12	16,26,37,43	0
4	EDO	H	155	4/4	0.96	0.12	24,25,27,28	0
4	EDO	H	156	4/4	0.96	0.12	24,28,35,37	0
4	EDO	C	158	4/4	0.97	0.07	27,34,40,50	0
2	MRD	G	156	8/8	0.97	0.07	18,20,22,34	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.