



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:01 PM UTC

PDB ID : 3DDE / pdb\_00003dde  
Title : Crystal structure of a domain of unknown function with a heme oxygenase-like fold (sden\_3740) from shewanella denitrificans os217 at 2.30 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2008-06-05  
Resolution : 2.30 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.

The types of validation reports are described at

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

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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

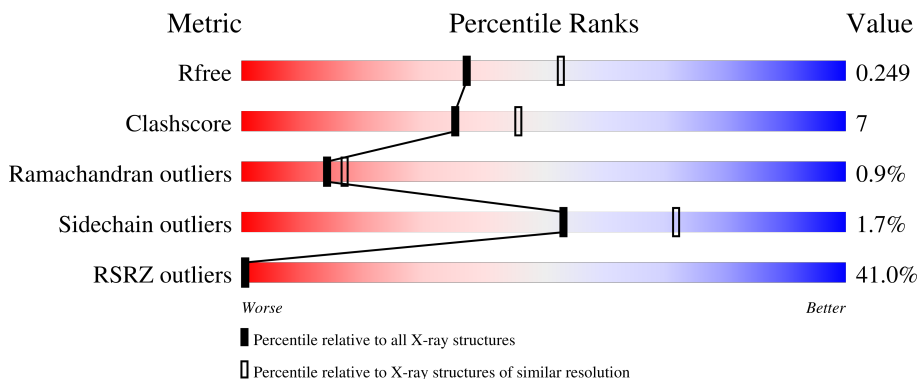
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	239	<p>60% (Poor fit), 80% (0 outliers), 15% (1 outlier), 5% (2 outliers), 0% (3+ outliers), 0% (Not modelled)</p>
1	B	239	<p>17% (Poor fit), 87% (0 outliers), 9% (1 outlier), 5% (2 outliers), 0% (3+ outliers), 0% (Not modelled)</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3753 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.

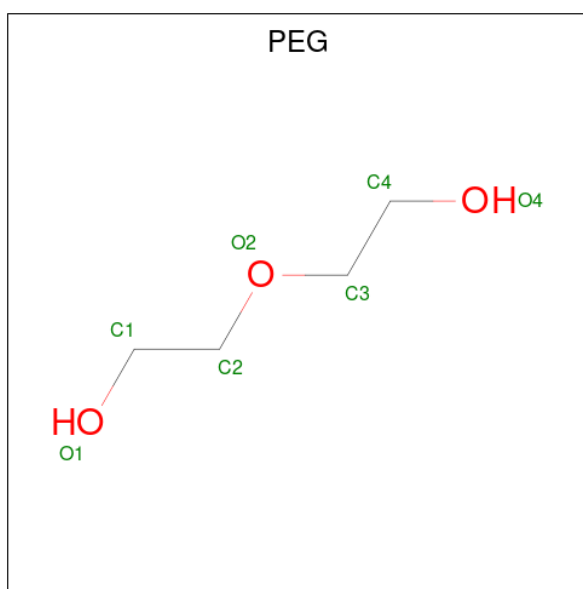
- Molecule 1 is a protein called TENA/THI-4 protein, Domain of Unknown Function with a Heme Oxygenase-like Fold.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	232	1823	1174	294	345	2	8	0	7	0
1	B	231	1817	1167	291	349	2	8	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q12HR3
B	0	GLY	-	expression tag	UNP Q12HR3

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



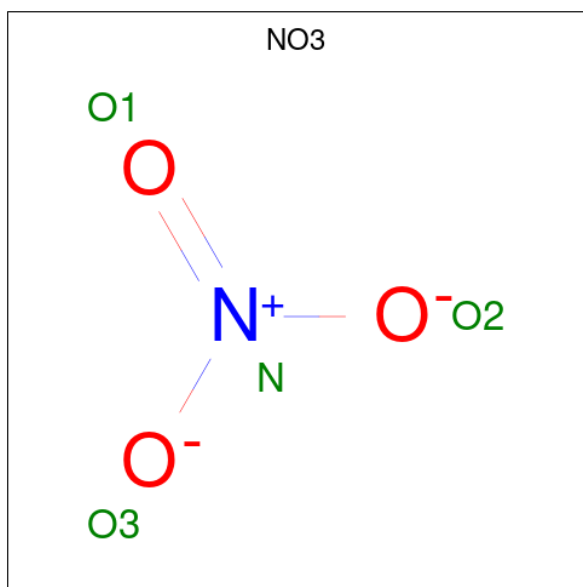
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	7	4	3	0	0

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

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO<sub>3</sub>).



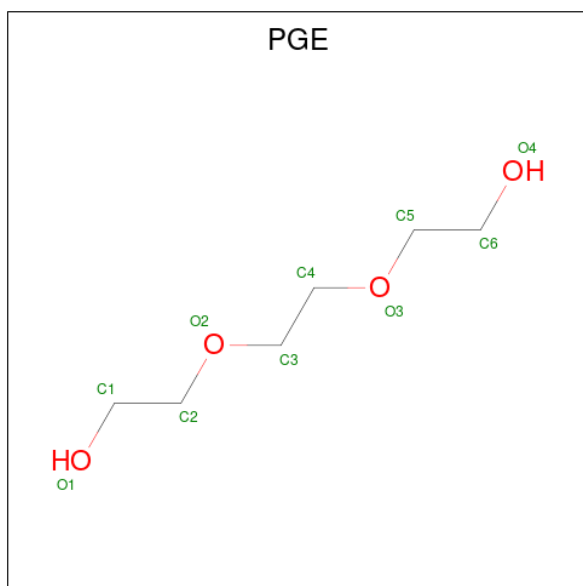
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

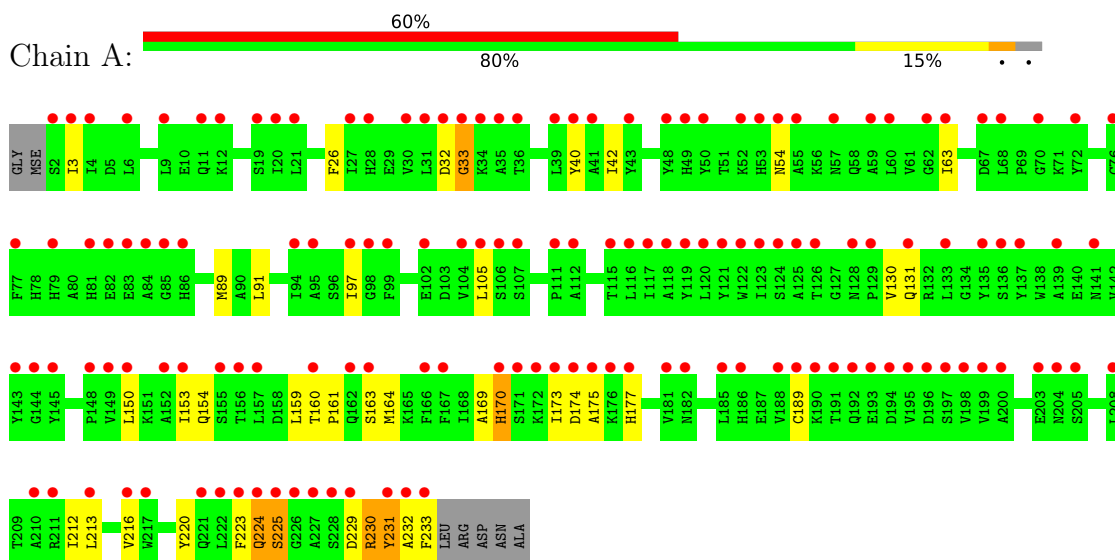
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total 30	O 30	0	0
6	B	44	Total 44	O 44	0	0

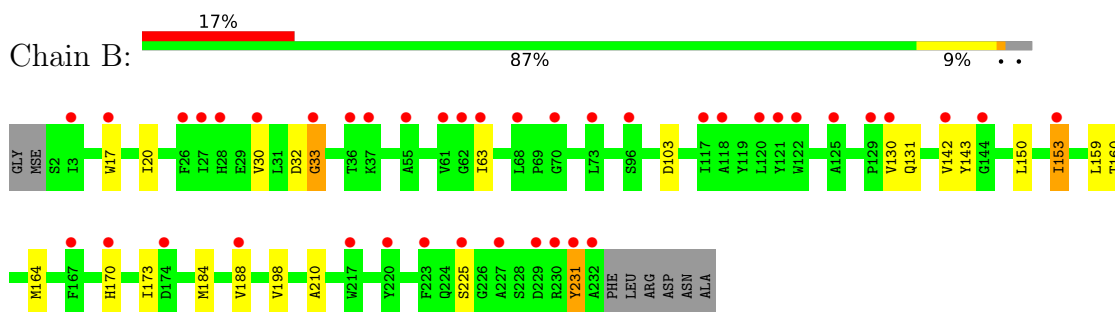
### 3 Residue-property plots i

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: TENA/THI-4 protein, Domain of Unknown Function with a Heme Oxygenase-like Fold



- Molecule 1: TENA/THI-4 protein, Domain of Unknown Function with a Heme Oxygenase-like Fold



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.81Å 66.00Å 84.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.17 – 2.30 29.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.17-2.30) 99.3 (29.17-2.30)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, $R_{free}$	0.220 , 0.253 0.221 , 0.249	Depositor DCC
$R_{free}$ test set	1206 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	3753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PGE, NO3, PEG

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	0.73	2/1873 (0.1%)	0.96	4/2544 (0.2%)
1	B	0.72	0/1856	0.96	2/2521 (0.1%)
All	All	0.72	2/3729 (0.1%)	0.96	6/5065 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	PHE	C-O	6.87	1.37	1.23
1	A	154	GLN	CD-OE1	5.81	1.34	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	N-CA-C	8.18	120.80	109.18
1	A	131	GLN	N-CA-C	6.75	119.47	111.71
1	B	131	GLN	N-CA-C	6.45	119.13	111.71
1	A	175	ALA	N-CA-C	-5.94	105.87	113.23
1	B	160	THR	N-CA-C	-5.72	103.44	110.31
1	A	54	ASN	N-CA-C	5.43	117.27	111.36

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	1823	0	1719	31	0
1	B	1817	0	1707	23	0
2	A	14	0	20	0	0
2	B	7	0	10	0	0
3	B	4	0	0	0	0
4	B	4	0	6	0	0
5	B	10	0	14	0	0
6	A	30	0	0	0	0
6	B	44	0	0	0	0
All	All	3753	0	3476	53	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 7.

All (53) 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:32[B]:ASP:O	1:B:33[B]:GLY:C	2.10	0.94
1:B:32[B]:ASP:O	1:B:33[B]:GLY:O	1.92	0.85
1:A:42:ILE:HG22	1:A:216:VAL:HG13	1.69	0.73
1:A:170:HIS:O	1:A:174:ASP:CB	2.38	0.72
1:A:32[B]:ASP:O	1:A:33[B]:GLY:O	2.08	0.71
1:A:32[B]:ASP:O	1:A:33[B]:GLY:C	2.41	0.63
1:A:173:ILE:O	1:A:173:ILE:HG22	1.99	0.62
1:B:159:LEU:HD12	1:B:164:MSE:HE2	1.81	0.62
1:B:103:ASP:HB3	1:B:231:TYR:CZ	2.35	0.61
1:B:32[B]:ASP:CG	1:B:33[B]:GLY:H	2.08	0.61
1:B:173:ILE:H	1:B:173:ILE:HD12	1.66	0.61
1:B:159:LEU:HB2	1:B:164:MSE:HE1	1.85	0.59
1:A:42:ILE:CG2	1:A:216:VAL:HG13	2.34	0.58
1:A:150:LEU:O	1:A:153:ILE:HG22	2.04	0.57
1:A:91:LEU:HD21	1:A:105:LEU:HD21	1.87	0.56
1:A:220:TYR:O	1:A:223:PHE:HB3	2.07	0.55
1:A:159:LEU:HD22	1:A:163:SER:HB2	1.89	0.54
1:B:32[B]:ASP:CG	1:B:33[B]:GLY:N	2.62	0.54
1:A:89[A]:MSE:HE1	1:A:169:ALA:HB2	1.90	0.54
1:B:159:LEU:HB2	1:B:164:MSE:CE	2.37	0.54
1:A:159:LEU:HD22	1:A:163:SER:CB	2.38	0.54
1:A:173:ILE:HD12	1:A:173:ILE:N	2.23	0.53
1:B:170:HIS:HA	1:B:173:ILE:HD13	1.91	0.53
1:B:159:LEU:CD1	1:B:164:MSE:HE2	2.40	0.52
1:A:224:GLN:O	1:A:225:SER:OG	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:CD1	1:B:63:ILE:HD12	2.42	0.49
1:A:91:LEU:CD2	1:A:105:LEU:HD21	2.42	0.49
1:B:173:ILE:HD12	1:B:173:ILE:N	2.27	0.49
1:B:17:TRP:CZ2	1:B:142:VAL:HG23	2.47	0.49
1:B:150:LEU:O	1:B:153:ILE:HG22	2.13	0.48
1:A:224:GLN:O	1:A:225:SER:CB	2.62	0.48
1:B:20:ILE:CD1	1:B:210:ALA:HB2	2.45	0.47
1:B:159:LEU:HD12	1:B:164:MSE:CE	2.45	0.46
1:A:26:PHE:CD2	1:A:213:LEU:HD22	2.51	0.46
1:B:142:VAL:HG13	1:B:143:TYR:N	2.31	0.45
1:A:173:ILE:O	1:A:173:ILE:CG2	2.64	0.45
1:B:142:VAL:CG1	1:B:143:TYR:N	2.80	0.44
1:B:20:ILE:HD13	1:B:210:ALA:HB2	1.98	0.44
1:B:130:VAL:HG12	1:B:198:VAL:CG2	2.49	0.43
1:A:160:THR:HB	1:A:161:PRO:HD2	2.01	0.43
1:A:159:LEU:HD13	1:A:164:MSE:CE	2.48	0.43
1:A:3:ILE:HG22	1:A:189:CYS:O	2.18	0.43
1:A:231:TYR:CD2	1:A:231:TYR:N	2.85	0.43
1:A:223:PHE:HZ	1:A:232:ALA:HB2	1.85	0.42
1:A:229:ASP:O	1:A:229:ASP:OD1	2.38	0.42
1:A:174:ASP:HA	1:A:177:HIS:HB2	2.02	0.42
1:B:30:VAL:HG13	1:B:153:ILE:HD12	2.02	0.41
1:A:40:TYR:HD2	1:A:97:ILE:HD13	1.83	0.41
1:A:89[B]:MSE:HA	1:A:89[B]:MSE:HE2	2.02	0.41
1:A:229:ASP:C	1:A:230:ARG:HG3	2.46	0.41
1:A:159:LEU:HB2	1:A:164:MSE:HE1	2.02	0.41
1:A:212:ILE:O	1:A:216:VAL:HG23	2.21	0.41
1:B:184:MSE:O	1:B:188:VAL:HG22	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	237/239 (99%)	224 (94%)	10 (4%)	3 (1%)	9	10
1	B	235/239 (98%)	224 (95%)	8 (3%)	3 (1%)	9	10
All	All	472/478 (99%)	448 (95%)	18 (4%)	6 (1%)	14	10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33[A]	GLY
1	A	33[B]	GLY
1	A	225	SER
1	B	33[A]	GLY
1	B	33[B]	GLY
1	B	225	SER

### 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	186/197 (94%)	182 (98%)	4 (2%)	45	65
1	B	185/197 (94%)	183 (99%)	2 (1%)	65	81
All	All	371/394 (94%)	365 (98%)	6 (2%)	53	73

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	VAL
1	A	170	HIS
1	A	224	GLN
1	A	231	TYR
1	B	153	ILE
1	B	231	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	182	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	B	240	-	3,3,3	0.54	0	2,2,2	0.15	0
2	PEG	B	242	-	6,6,6	0.49	0	5,5,5	0.25	0
2	PEG	A	240	-	6,6,6	0.57	0	5,5,5	0.19	0
3	NO3	B	239	-	1,3,3	3.43	1 (100%)	0,3,3	-	-
5	PGE	B	241	-	9,9,9	0.53	0	8,8,8	0.30	0
2	PEG	A	239	-	6,6,6	0.64	0	5,5,5	0.21	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	B	240	-	-	1/1/1/1	-
2	PEG	B	242	-	-	2/4/4/4	-
2	PEG	A	239	-	-	2/4/4/4	-
2	PEG	A	240	-	-	2/4/4/4	-
5	PGE	B	241	-	-	3/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	239	NO3	O1-N	3.43	1.41	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	239	PEG	O2-C3-C4-O4
5	B	241	PGE	O2-C3-C4-O3
2	A	239	PEG	O1-C1-C2-O2
2	B	242	PEG	O1-C1-C2-O2
5	B	241	PGE	O1-C1-C2-O2
5	B	241	PGE	O3-C5-C6-O4
2	A	240	PEG	O1-C1-C2-O2
2	A	240	PEG	C1-C2-O2-C3
2	B	242	PEG	O2-C3-C4-O4
4	B	240	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	225/239 (94%)	2.35	143 (63%) <b>0</b> <b>0</b>	25, 52, 61, 72	6 (2%)
1	B	224/239 (93%)	1.33	41 (18%) <b>3</b> <b>4</b>	25, 52, 63, 73	5 (2%)
All	All	449/478 (93%)	1.84	184 (40%) <b>0</b> <b>0</b>	25, 52, 63, 73	11 (2%)

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33[A]	GLY	5.6
1	A	227	ALA	4.9
1	A	185	LEU	4.6
1	A	233	PHE	4.5
1	A	112	ALA	4.5
1	A	119	TYR	4.4
1	A	174	ASP	4.4
1	A	175	ALA	4.3
1	A	162	GLN	4.3
1	A	122	TRP	4.3
1	A	222	LEU	4.2
1	A	231	TYR	4.2
1	A	228	SER	4.1
1	A	104	VAL	3.9
1	A	186	HIS	3.9
1	A	188	VAL	3.9
1	A	105	LEU	3.8
1	B	3	ILE	3.8
1	A	125	ALA	3.8
1	B	231	TYR	3.8
1	A	223	PHE	3.8
1	B	33[A]	GLY	3.8
1	A	170	HIS	3.7
1	A	217	TRP	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	150	LEU	3.7
1	A	208	LEU	3.6
1	B	26	PHE	3.6
1	A	198	VAL	3.6
1	A	129	PRO	3.5
1	A	9	LEU	3.5
1	A	123	ILE	3.4
1	A	225	SER	3.4
1	A	192	GLN	3.4
1	A	121	TYR	3.4
1	B	61	VAL	3.4
1	B	232	ALA	3.3
1	A	60	LEU	3.3
1	A	135	TYR	3.3
1	A	99	PHE	3.3
1	A	63	ILE	3.3
1	A	137	TYR	3.3
1	A	59	ALA	3.2
1	B	125	ALA	3.2
1	A	173	ILE	3.2
1	A	118	ALA	3.2
1	A	97	ILE	3.2
1	A	177	HIS	3.1
1	A	43	TYR	3.1
1	A	133	LEU	3.1
1	A	54	ASN	3.1
1	A	199	VAL	3.1
1	A	131	GLN	3.1
1	A	143	TYR	3.0
1	A	4	ILE	3.0
1	A	28	HIS	3.0
1	A	172	LYS	3.0
1	A	116	LEU	3.0
1	A	120	LEU	3.0
1	A	126	THR	3.0
1	B	223	PHE	3.0
1	A	144	GLY	3.0
1	A	41	ALA	2.9
1	B	28	HIS	2.9
1	A	124	SER	2.9
1	A	182	ASN	2.9
1	A	3	ILE	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	27	ILE	2.9
1	A	139	ALA	2.8
1	B	217	TRP	2.8
1	A	128	ASN	2.8
1	B	73	LEU	2.8
1	A	21	LEU	2.8
1	A	232	ALA	2.8
1	A	39	LEU	2.8
1	A	77	PHE	2.8
1	A	19	SER	2.7
1	A	197	SER	2.7
1	A	189	CYS	2.7
1	A	157	LEU	2.7
1	A	160	THR	2.7
1	A	117	ILE	2.7
1	A	153	ILE	2.7
1	A	190	LYS	2.7
1	A	6	LEU	2.7
1	A	76	CYS	2.7
1	B	167	PHE	2.7
1	A	30	VAL	2.7
1	A	115	THR	2.7
1	A	191	THR	2.7
1	B	220	TYR	2.6
1	B	188	VAL	2.6
1	A	106	SER	2.6
1	B	96	SER	2.6
1	B	70	GLY	2.6
1	A	148	PRO	2.6
1	A	20	ILE	2.6
1	A	107	SER	2.6
1	B	129	PRO	2.6
1	A	72	TYR	2.6
1	B	170	HIS	2.6
1	B	120	LEU	2.5
1	A	166	PHE	2.5
1	A	2	SER	2.5
1	A	195	VAL	2.5
1	B	37	LYS	2.5
1	A	145	TYR	2.5
1	A	226	GLY	2.5
1	B	225	SER	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	27	ILE	2.5
1	A	204	ASN	2.5
1	B	122	TRP	2.5
1	A	210	ALA	2.4
1	A	35	ALA	2.4
1	A	55	ALA	2.4
1	A	167	PHE	2.4
1	A	48	TYR	2.4
1	A	102	GLU	2.4
1	A	229	ASP	2.4
1	A	156	THR	2.4
1	A	163	SER	2.4
1	B	117	ILE	2.4
1	A	211	ARG	2.4
1	B	121	TYR	2.3
1	A	84	ALA	2.3
1	A	205	SER	2.3
1	A	81	HIS	2.3
1	A	50	TYR	2.3
1	A	152	ALA	2.3
1	A	203	GLU	2.3
1	A	111	PRO	2.3
1	A	40	TYR	2.3
1	A	36	THR	2.3
1	A	181	VAL	2.3
1	A	68	LEU	2.3
1	A	95	ALA	2.3
1	A	224	GLN	2.3
1	A	94	ILE	2.3
1	B	63	ILE	2.3
1	A	194	ASP	2.2
1	A	70	GLY	2.2
1	B	62	GLY	2.2
1	A	31	LEU	2.2
1	A	57	ASN	2.2
1	B	144	GLY	2.2
1	A	82	GLU	2.2
1	B	227	ALA	2.2
1	B	229	ASP	2.2
1	A	171	SER	2.2
1	B	230	ARG	2.2
1	A	176	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	221	GLN	2.2
1	B	55	ALA	2.2
1	A	213	LEU	2.1
1	A	32[A]	ASP	2.1
1	B	130	VAL	2.1
1	B	142	VAL	2.1
1	A	79	HIS	2.1
1	A	86[A]	HIS	2.1
1	A	136	SER	2.1
1	A	34[A]	LYS	2.1
1	B	68	LEU	2.1
1	B	30	VAL	2.1
1	A	98	GLY	2.1
1	A	193	GLU	2.1
1	A	141	ASN	2.1
1	A	11	GLN	2.1
1	B	17	TRP	2.1
1	A	85	GLY	2.1
1	A	83	GLU	2.1
1	B	174	ASP	2.1
1	A	216	VAL	2.1
1	A	62	GLY	2.1
1	A	52	LYS	2.0
1	B	36	THR	2.0
1	A	67	ASP	2.0
1	A	196	ASP	2.0
1	A	149	VAL	2.0
1	A	12[A]	LYS	2.0
1	A	155	SER	2.0
1	A	200	ALA	2.0
1	B	118	ALA	2.0
1	A	49	HIS	2.0
1	A	53	HIS	2.0
1	B	153	ILE	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 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, 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
2	PEG	A	240	7/7	0.71	0.20	57,58,58,59	7
2	PEG	A	239	7/7	0.75	0.20	65,65,66,66	0
5	PGE	B	241	10/10	0.76	0.22	70,70,71,72	0
4	EDO	B	240	4/4	0.77	0.18	58,58,58,58	0
2	PEG	B	242	7/7	0.85	0.19	48,49,49,50	0
3	NO3	B	239	4/4	0.90	0.17	50,51,51,53	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.