



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 05:04 PM EDT

PDB ID : 2OXG  
Title : The SoxYZ Complex of Paracoccus pantotrophus  
Authors : Sauve, V.; Berks, B.C.; Hemmings, A.M.  
Deposited on : 2007-02-20  
Resolution : 1.40 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

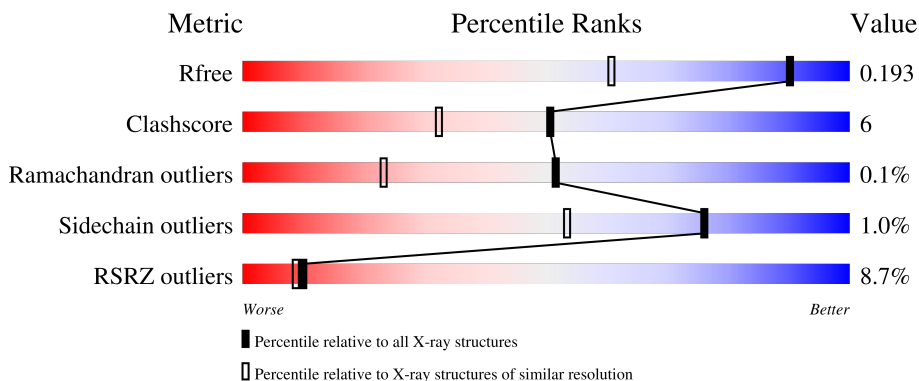
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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.



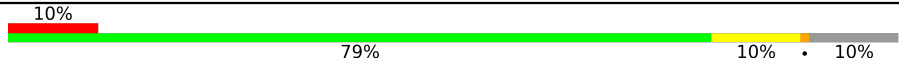

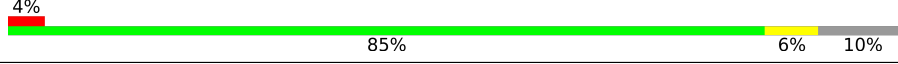
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	108	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 94%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div>
1	C	108	<div style="display: flex; align-items: center;"> <div style="width: 13%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div>
1	E	108	<div style="display: flex; align-items: center;"> <div style="width: 19%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	Z	108	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div>
2	B	124	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	D	124	 10% 79% 10% 10%
2	F	124	 5% 80% 10% 10%
2	Y	124	 4% 85% 6% 10%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7094 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 SoxZ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Z	108	Total 843	C 536	N 140	O 165	S 2	0	5	0
1	A	108	Total 834	C 528	N 138	O 166	S 2	0	4	0
1	C	101	Total 760	C 481	N 121	O 156	S 2	0	2	0
1	E	99	Total 750	C 476	N 118	O 154	S 2	0	3	0

- Molecule 2 is a protein called SoxY protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	Y	112	Total 777	C 482	N 137	O 155	S 3	0	2	0
2	B	110	Total 783	C 491	N 137	O 152	S 3	0	5	0
2	D	111	Total 788	C 490	N 135	O 160	S 3	0	5	0
2	F	112	Total 774	C 481	N 135	O 156	S 2	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	190	MET	-	cloning artifact	UNP Q9LCU9
Y	191	ARG	-	cloning artifact	UNP Q9LCU9
Y	192	GLY	-	cloning artifact	UNP Q9LCU9
Y	193	SER	-	cloning artifact	UNP Q9LCU9
Y	194	HIS	-	expression tag	UNP Q9LCU9
Y	195	HIS	-	expression tag	UNP Q9LCU9
Y	196	HIS	-	expression tag	UNP Q9LCU9
Y	197	HIS	-	expression tag	UNP Q9LCU9

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	198	HIS	-	expression tag	UNP Q9LCU9
Y	199	HIS	-	expression tag	UNP Q9LCU9
Y	200	GLY	-	cloning artifact	UNP Q9LCU9
Y	201	SER	-	cloning artifact	UNP Q9LCU9
B	-11	MET	-	cloning artifact	UNP Q9LCU9
B	-10	ARG	-	cloning artifact	UNP Q9LCU9
B	-9	GLY	-	cloning artifact	UNP Q9LCU9
B	-8	SER	-	cloning artifact	UNP Q9LCU9
B	-7	HIS	-	expression tag	UNP Q9LCU9
B	-6	HIS	-	expression tag	UNP Q9LCU9
B	-5	HIS	-	expression tag	UNP Q9LCU9
B	-4	HIS	-	expression tag	UNP Q9LCU9
B	-3	HIS	-	expression tag	UNP Q9LCU9
B	-2	HIS	-	expression tag	UNP Q9LCU9
B	-1	GLY	-	cloning artifact	UNP Q9LCU9
B	0	SER	-	cloning artifact	UNP Q9LCU9
D	190	MET	-	cloning artifact	UNP Q9LCU9
D	191	ARG	-	cloning artifact	UNP Q9LCU9
D	192	GLY	-	cloning artifact	UNP Q9LCU9
D	193	SER	-	cloning artifact	UNP Q9LCU9
D	194	HIS	-	expression tag	UNP Q9LCU9
D	195	HIS	-	expression tag	UNP Q9LCU9
D	196	HIS	-	expression tag	UNP Q9LCU9
D	197	HIS	-	expression tag	UNP Q9LCU9
D	198	HIS	-	expression tag	UNP Q9LCU9
D	199	HIS	-	expression tag	UNP Q9LCU9
D	200	GLY	-	cloning artifact	UNP Q9LCU9
D	201	SER	-	cloning artifact	UNP Q9LCU9
F	191	MET	-	cloning artifact	UNP Q9LCU9
F	192	ARG	-	cloning artifact	UNP Q9LCU9
F	193	GLY	-	cloning artifact	UNP Q9LCU9
F	194	SER	-	cloning artifact	UNP Q9LCU9
F	195	HIS	-	expression tag	UNP Q9LCU9
F	196	HIS	-	expression tag	UNP Q9LCU9
F	197	HIS	-	expression tag	UNP Q9LCU9
F	198	HIS	-	expression tag	UNP Q9LCU9
F	199	HIS	-	expression tag	UNP Q9LCU9
F	200	HIS	-	expression tag	UNP Q9LCU9
F	201	GLY	-	cloning artifact	UNP Q9LCU9
F	202	SER	-	cloning artifact	UNP Q9LCU9

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Z	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- 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	Y	1	Total C O 4 2 2	0	0

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

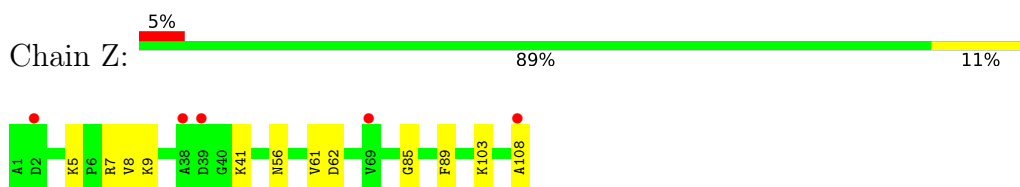
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Z	125	Total O 125 125	0	0
5	Y	105	Total O 105 105	0	0
5	A	126	Total O 126 126	0	0
5	B	105	Total O 105 105	0	0
5	C	65	Total O 65 65	0	0
5	D	91	Total O 91 91	0	0
5	E	57	Total O 57 57	0	0
5	F	80	Total O 80 80	0	0

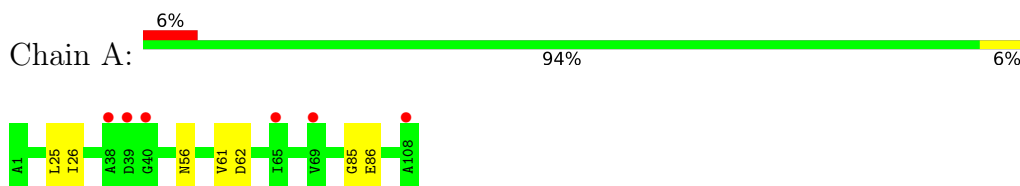
### 3 Residue-property plots [i](#)

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.

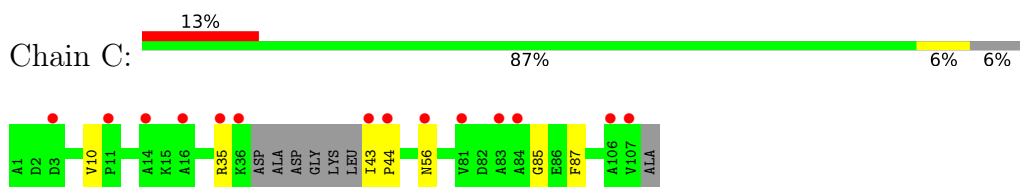
- Molecule 1: SoxZ protein



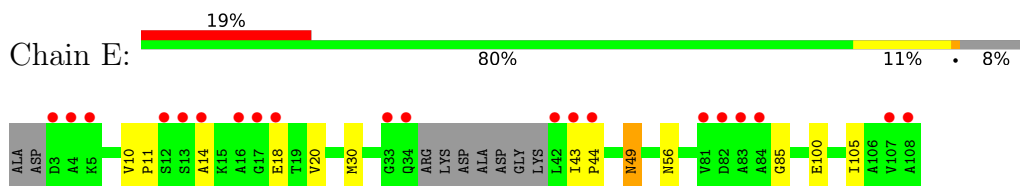
- Molecule 1: SoxZ protein



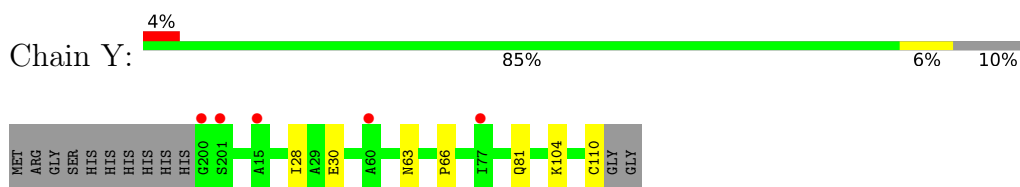
- Molecule 1: SoxZ protein



- Molecule 1: SoxZ protein

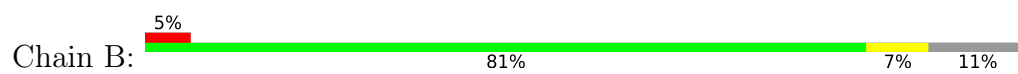


- Molecule 2: SoxY protein

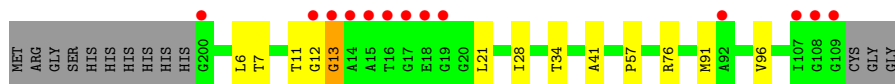
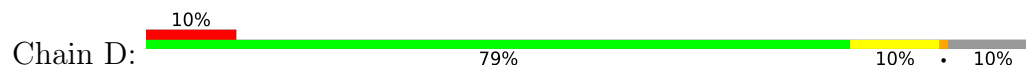


- Molecule 2: SoxY protein

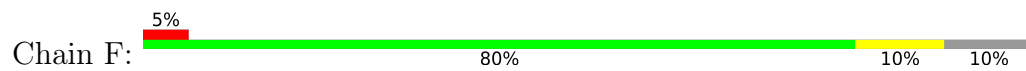




- Molecule 2: SoxY protein



- Molecule 2: SoxY protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	206.83Å 54.72Å 77.68Å 90.00° 98.68° 90.00°	Depositor
Resolution (Å)	50.00 – 1.40 31.54 – 1.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-1.40) 97.6 (31.54-1.40)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.40Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.168 , 0.194 0.166 , 0.193	Depositor DCC
$R_{free}$ test set	8301 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtrriage
Anisotropy	0.368	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7094	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8069e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, SO4

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	0.55	0/858	0.76	0/1167
1	C	0.48	0/783	0.67	0/1069
1	E	0.52	0/774	0.65	0/1055
1	Z	0.59	0/870	0.76	0/1182
2	B	0.54	0/805	0.71	0/1096
2	D	0.52	0/802	0.66	0/1095
2	F	0.56	0/783	0.66	0/1069
2	Y	0.53	0/793	0.66	0/1082
All	All	0.54	0/6468	0.69	0/8815

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	834	0	816	5	0
1	C	760	0	718	4	0
1	E	750	0	709	11	0
1	Z	843	0	840	13	0
2	B	783	0	822	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	788	0	802	16	0
2	F	774	0	785	9	0
2	Y	777	0	792	10	1
3	A	5	0	0	0	0
3	D	5	0	0	0	0
3	Z	5	0	0	0	0
4	B	8	0	12	3	0
4	F	4	0	6	0	0
4	Y	4	0	6	2	0
5	A	126	0	0	1	1
5	B	105	0	0	4	0
5	C	65	0	0	0	0
5	D	91	0	0	1	0
5	E	57	0	0	5	0
5	F	80	0	0	2	0
5	Y	105	0	0	1	0
5	Z	125	0	0	4	0
All	All	7094	0	6308	72	1

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 6.

All (72) 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)
2:Y:63[B]:ASN:ND2	2:D:13:GLY:HA2	1.31	1.42
2:Y:63[B]:ASN:ND2	2:D:13:GLY:CA	2.03	1.21
2:B:103:VAL:HG13	5:B:892:HOH:O	1.42	1.17
2:B:110:CYS:SG	4:B:806:EDO:O1	2.18	1.00
2:Y:63[B]:ASN:HD21	2:D:13:GLY:HA2	1.28	0.94
2:Y:63[B]:ASN:HD21	2:D:13:GLY:CA	1.75	0.92
2:Y:63[B]:ASN:HD22	2:D:13:GLY:CA	1.80	0.83
2:Y:63[B]:ASN:HD22	2:D:13:GLY:HA2	1.03	0.83
1:E:105:ILE:HD12	5:E:136:HOH:O	1.78	0.83
2:F:200:HIS:CG	2:F:201:GLY:H	2.00	0.81
1:Z:7:ARG:NH2	1:Z:9[A]:LYS:HE2	1.97	0.79
1:E:10:VAL:HG22	5:E:136:HOH:O	1.86	0.75
1:E:56:ASN:OD1	1:E:85:GLY:HA3	1.87	0.74
1:A:56:ASN:HD21	1:A:85:GLY:HA3	1.53	0.73
2:D:11[A]:THR:HG22	2:D:96:VAL:HG11	1.73	0.71
1:Z:56:ASN:HA	5:Z:870:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:GLU:HG2	5:B:869:HOH:O	1.94	0.67
2:F:200:HIS:CG	2:F:201:GLY:N	2.63	0.66
2:Y:63[B]:ASN:ND2	2:D:13:GLY:HA3	2.06	0.66
1:Z:8[B]:VAL:HG21	1:Z:103:LYS:HG3	1.77	0.65
2:Y:110:CYS:SG	4:Y:805:EDO:O1	2.38	0.65
2:F:6:LEU:HD12	2:F:57:PRO:HG2	1.78	0.65
1:E:100[B]:GLU:CD	5:E:138:HOH:O	2.37	0.62
2:Y:28:ILE:HD13	2:Y:104:LYS:HB2	1.84	0.60
1:Z:61[B]:VAL:HG12	1:Z:62:ASP:N	2.18	0.58
1:E:20:VAL:HG21	5:E:136:HOH:O	2.04	0.57
2:F:34:THR:O	2:F:34:THR:HG23	2.03	0.57
1:E:11:PRO:HD2	1:E:20:VAL:CG2	2.34	0.57
1:A:61[B]:VAL:HG12	1:A:62:ASP:N	2.20	0.57
2:B:110:CYS:HG	4:B:806:EDO:HO1	1.06	0.56
2:D:7:THR:O	2:D:11[B]:THR:HG23	2.05	0.56
1:Z:8[B]:VAL:CG2	1:Z:103:LYS:HE3	2.36	0.56
2:D:11[A]:THR:O	2:D:13:GLY:N	2.39	0.55
1:C:35:ARG:O	1:C:43:ILE:N	2.40	0.54
1:Z:8[B]:VAL:CG2	1:Z:103:LYS:HG3	2.38	0.53
1:Z:108:ALA:CB	5:Z:865:HOH:O	2.57	0.52
1:A:25[B]:LEU:HD13	1:A:26:ILE:N	2.25	0.51
1:Z:108:ALA:HB2	5:Z:865:HOH:O	2.11	0.50
1:E:14:ALA:HB1	1:E:18:GLU:HG2	1.94	0.50
1:Z:5:LYS:HE2	5:Z:925:HOH:O	2.11	0.49
1:A:56:ASN:ND2	1:A:86:GLU:H	2.10	0.49
1:A:56:ASN:ND2	1:A:85:GLY:HA3	2.25	0.49
1:Z:8[B]:VAL:HG22	1:Z:103:LYS:HE3	1.94	0.49
2:B:40[A]:LYS:HG2	2:B:72:ARG:HG3	1.94	0.48
2:F:39:VAL:HG12	5:F:862:HOH:O	2.12	0.48
1:E:11:PRO:HG2	1:E:20:VAL:HG23	1.96	0.48
1:Z:56:ASN:OD1	1:Z:85:GLY:HA3	2.14	0.48
2:D:6:LEU:HD12	2:D:57:PRO:HG2	1.96	0.47
2:D:34:THR:HG22	2:D:76:ARG:HD2	1.95	0.47
2:F:21:LEU:HD13	2:F:41:ALA:HB2	1.96	0.46
4:Y:805:EDO:H22	5:Y:833:HOH:O	2.16	0.46
1:E:30:MET:HB3	5:E:151:HOH:O	2.14	0.46
2:F:23:LEU:HB2	5:F:862:HOH:O	2.15	0.46
1:Z:8[A]:VAL:HG11	1:Z:89:PHE:CZ	2.51	0.46
2:B:80:ALA:HB2	2:B:110:CYS:HB2	1.98	0.45
2:Y:28:ILE:CD1	2:Y:104:LYS:HD2	2.47	0.45
1:E:49:ASN:C	1:E:49:ASN:HD22	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:VAL:HG11	1:C:87:PHE:CE1	2.52	0.45
2:D:11[A]:THR:HG21	5:D:891:HOH:O	2.16	0.44
1:C:43:ILE:HA	1:C:44:PRO:HD3	1.88	0.43
1:Z:61[B]:VAL:CG1	1:Z:62:ASP:N	2.82	0.43
2:D:34:THR:CG2	2:D:76:ARG:HD2	2.49	0.42
2:B:1:SER:N	5:B:896:HOH:O	2.53	0.42
2:F:22:THR:HB	2:F:40:LYS:HG2	2.01	0.42
1:C:56:ASN:OD1	1:C:85:GLY:HA3	2.18	0.41
1:E:43:ILE:HA	1:E:44:PRO:HD3	1.89	0.41
2:B:104:LYS:NZ	5:B:886:HOH:O	2.54	0.41
5:A:864:HOH:O	4:B:807:EDO:H12	2.19	0.41
2:D:11[A]:THR:O	2:D:12[A]:GLY:C	2.58	0.41
2:F:46:ALA:HA	2:F:62:PHE:O	2.21	0.41
2:B:34:THR:O	2:B:34:THR:HG23	2.21	0.41
2:D:21:LEU:HD13	2:D:41:ALA:HB2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:66:PRO:O	5:A:913:HOH:O[4_645]	2.19	0.01

## 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	110/108 (102%)	107 (97%)	3 (3%)	0	100	100
1	C	99/108 (92%)	97 (98%)	2 (2%)	0	100	100
1	E	98/108 (91%)	96 (98%)	2 (2%)	0	100	100
1	Z	111/108 (103%)	108 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	113/124 (91%)	111 (98%)	2 (2%)	0	100	100
2	D	114/124 (92%)	106 (93%)	7 (6%)	1 (1%)	17	3
2	F	110/124 (89%)	107 (97%)	3 (3%)	0	100	100
2	Y	112/124 (90%)	109 (97%)	3 (3%)	0	100	100
All	All	867/928 (93%)	841 (97%)	25 (3%)	1 (0%)	51	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	13	GLY

### 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	90/89 (101%)	90 (100%)	0	100	100
1	C	82/89 (92%)	82 (100%)	0	100	100
1	E	81/89 (91%)	80 (99%)	1 (1%)	71	47
1	Z	92/89 (103%)	91 (99%)	1 (1%)	73	50
2	B	78/85 (92%)	78 (100%)	0	100	100
2	D	78/85 (92%)	75 (96%)	3 (4%)	33	6
2	F	76/85 (89%)	76 (100%)	0	100	100
2	Y	77/85 (91%)	75 (97%)	2 (3%)	46	13
All	All	654/696 (94%)	647 (99%)	7 (1%)	76	50

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	41	LYS
2	Y	30	GLU
2	Y	81	GLN

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Mol	Chain	Res	Type
2	D	28	ILE
2	D	91[A]	MET
2	D	91[B]	MET
1	E	49	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	81	GLN
1	A	34	GLN
1	A	56	ASN
1	E	49	ASN
2	F	100	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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
3	SO4	D	801	-	4,4,4	0.16	0	6,6,6	0.11	0
4	EDO	B	806	-	3,3,3	0.72	0	2,2,2	0.28	0
4	EDO	B	807	-	3,3,3	0.56	0	2,2,2	0.19	0
4	EDO	F	804	-	3,3,3	0.67	0	2,2,2	0.19	0
3	SO4	Z	802	-	4,4,4	0.16	0	6,6,6	0.13	0
3	SO4	A	803	-	4,4,4	0.11	0	6,6,6	0.19	0
4	EDO	Y	805	-	3,3,3	0.55	0	2,2,2	0.11	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	804	-	-	0/1/1/1	-
4	EDO	Y	805	-	-	1/1/1/1	-
4	EDO	B	807	-	-	0/1/1/1	-
4	EDO	B	806	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	805	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	806	EDO	2	0
4	B	807	EDO	1	0
4	Y	805	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	108/108 (100%)	0.20	6 (5%) 24 22	8, 13, 26, 37	0
1	C	101/108 (93%)	0.66	14 (13%) 2 2	12, 22, 36, 39	0
1	E	99/108 (91%)	1.13	20 (20%) 1 0	13, 23, 38, 44	0
1	Z	108/108 (100%)	0.22	5 (4%) 32 32	9, 14, 26, 33	0
2	B	110/124 (88%)	-0.04	6 (5%) 25 23	9, 14, 23, 31	0
2	D	111/124 (89%)	0.37	13 (11%) 4 4	12, 19, 33, 43	0
2	F	112/124 (90%)	0.19	6 (5%) 25 24	10, 19, 26, 37	0
2	Y	112/124 (90%)	-0.02	5 (4%) 33 33	10, 15, 24, 35	0
All	All	861/928 (92%)	0.32	75 (8%) 10 9	8, 17, 33, 44	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	42	LEU	11.3
1	E	108	ALA	11.0
1	A	108	ALA	9.5
1	C	107	VAL	9.4
1	A	38	ALA	9.0
2	F	107	ILE	7.8
2	D	19	GLY	7.8
1	C	43	ILE	6.9
1	Z	108	ALA	6.5
1	E	43	ILE	6.5
1	E	107	VAL	6.2
1	E	4	ALA	6.0
2	D	15	ALA	5.8
2	D	14	ALA	5.5
1	E	3	ASP	5.4
1	C	36	LYS	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	Z	38	ALA	5.0
1	E	44	PRO	4.8
2	D	16	THR	4.7
2	D	18	GLU	4.7
1	C	83	ALA	4.6
1	E	16	ALA	4.5
2	F	200	HIS	4.3
1	E	83	ALA	4.3
1	E	17	GLY	4.2
2	F	109	GLY	4.2
1	E	34	GLN	4.0
1	C	16	ALA	3.9
1	A	39	ASP	3.9
1	C	14	ALA	3.8
1	C	44	PRO	3.6
1	C	106	ALA	3.5
1	E	82	ASP	3.5
1	C	35	ARG	3.3
2	B	110	CYS	3.2
1	C	11	PRO	3.2
2	D	13	GLY	3.1
1	C	84	ALA	3.0
2	D	17	GLY	3.0
2	F	108	GLY	3.0
1	E	33	GLY	2.9
2	Y	15	ALA	2.8
1	Z	69	VAL	2.8
1	E	84	ALA	2.7
2	D	109	GLY	2.7
1	E	5	LYS	2.6
1	C	3	ASP	2.6
2	F	201	GLY	2.5
1	E	14	ALA	2.5
1	A	40	GLY	2.5
1	E	18	GLU	2.5
1	A	69	VAL	2.5
2	B	59	VAL	2.5
2	Y	200	GLY	2.5
2	Y	201	SER	2.4
2	B	77	ILE	2.4
2	F	55	PRO	2.4
2	D	107	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	12[A]	GLY	2.3
2	D	108	GLY	2.3
2	B	49[A]	LEU	2.3
1	C	56	ASN	2.3
1	E	13	SER	2.2
1	E	81	VAL	2.2
2	D	92	ALA	2.1
2	B	60	ALA	2.1
1	A	65	ILE	2.1
2	B	30	GLU	2.1
2	D	200	GLY	2.1
1	Z	39	ASP	2.1
1	C	81	VAL	2.0
1	Z	2	ASP	2.0
1	E	12	SER	2.0
2	Y	77	ILE	2.0
2	Y	60	ALA	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	Y	805	4/4	0.84	0.20	28,31,32,32	0
3	SO4	A	803	5/5	0.86	0.25	42,43,45,47	0
3	SO4	D	801	5/5	0.88	0.26	57,57,57,58	0
4	EDO	B	806	4/4	0.90	0.11	23,26,28,30	0
4	EDO	B	807	4/4	0.92	0.10	26,31,33,38	0
3	SO4	Z	802	5/5	0.93	0.15	54,54,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	F	804	4/4	0.94	0.08	14,17,20,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.