



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:53 AM BST

PDB ID : 3WEU  
Title : Crystal structure of the L-Lys epsilon-oxidase from *Marinomonas mediterranea*  
Authors : Okazaki, S.; Nakano, S.; Matsui, D.; Akaji, S.; Inagaki, K.; Asano, Y.  
Deposited on : 2013-07-12  
Resolution : 1.93 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 : 2.13.1  
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) : 2.13.1

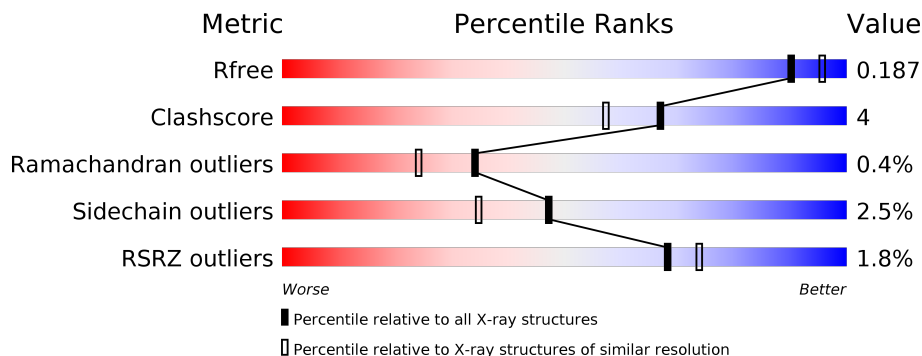
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	726	
1	B	726	

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	SO4	A	802	-	-	X	-
2	SO4	B	801	-	-	X	-

## 2 Entry composition [i](#)

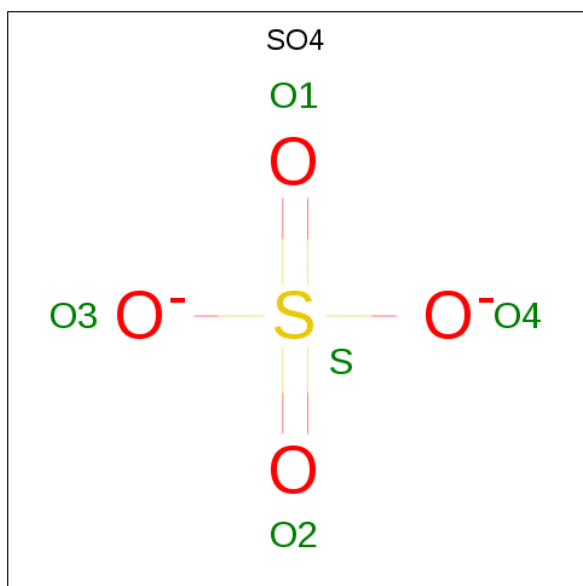
There are 5 unique types of molecules in this entry. The entry contains 12228 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lysine 6-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	684	Total 5430	C 3405	N 910	O 1092	S 23	0	6	0
1	B	684	Total 5553	C 3478	N 934	O 1118	S 23	0	20	0

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



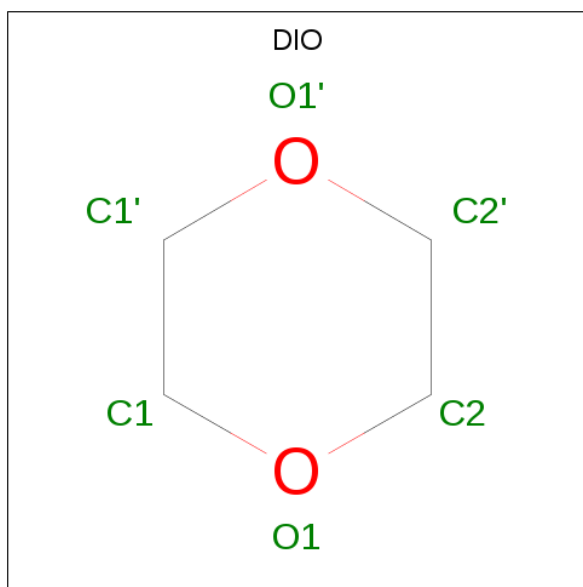
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

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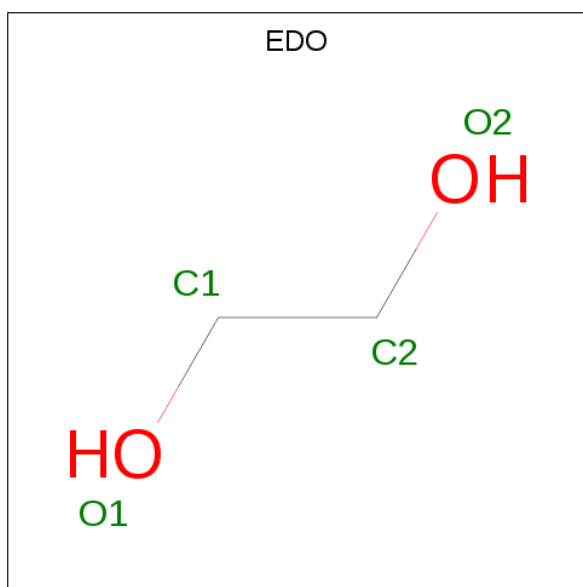
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	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 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	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	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		


- Molecule 5 is water.

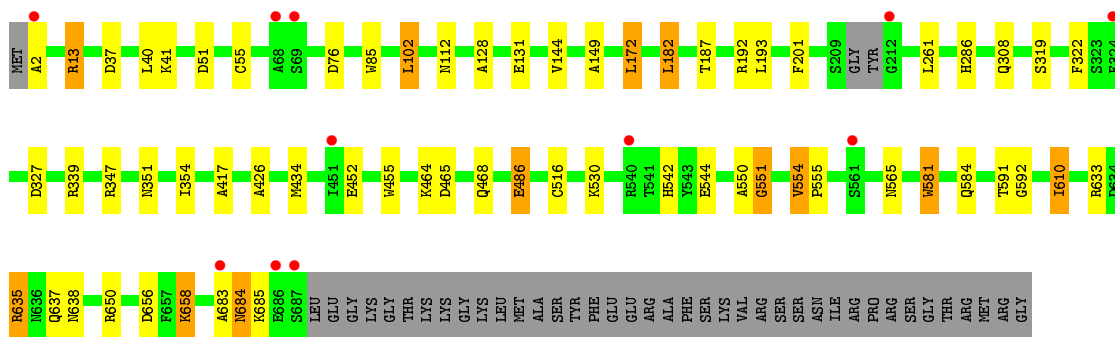
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	548	Total	O	0	2
			550	550		
5	B	580	Total	O	0	1
			581	581		

### 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.

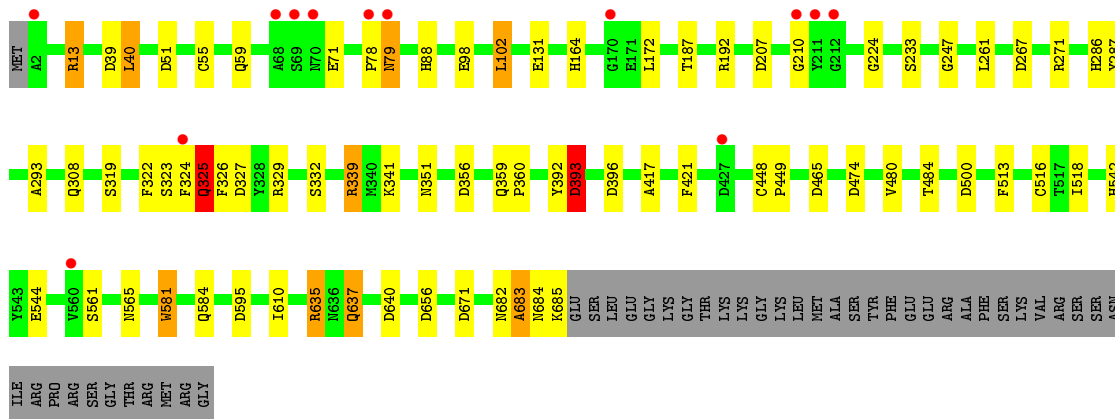
- Molecule 1: L-lysine 6-oxidase

Chain A: 



- Molecule 1: L-lysine 6-oxidase

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.09Å 125.75Å 70.59Å 90.00° 99.22° 90.00°	Depositor
Resolution (Å)	47.54 – 1.93 47.54 – 1.93	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.54-1.93) 98.4 (47.54-1.93)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.19 (at 1.92Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.143 , 0.178 0.155 , 0.187	Depositor DCC
$R_{free}$ test set	1996 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: TRQ, CSD, DIO, 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	1.01	3/5540 (0.1%)	1.00	20/7540 (0.3%)
1	B	1.00	1/5667 (0.0%)	0.98	17/7713 (0.2%)
All	All	1.01	4/11207 (0.0%)	0.99	37/15253 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	551	GLY	CA-C	6.13	1.61	1.51
1	A	551	GLY	N-CA	5.70	1.54	1.46
1	B	393	ASP	CB-CG	-5.54	1.40	1.51
1	A	486	GLU	CD-OE1	5.02	1.31	1.25

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339[A]	ARG	NE-CZ-NH2	-9.67	115.46	120.30
1	B	339[B]	ARG	NE-CZ-NH2	-9.67	115.46	120.30
1	A	37	ASP	CB-CG-OD1	8.48	125.93	118.30
1	A	182	LEU	CB-CG-CD1	8.11	124.80	111.00
1	A	656	ASP	CB-CG-OD2	-7.49	111.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	656	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	102	LEU	CB-CG-CD1	6.52	122.08	111.00
1	B	339[A]	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	339[B]	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	102	LEU	CB-CG-CD1	6.24	121.60	111.00
1	A	465	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	51	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	102	LEU	CB-CG-CD2	6.00	121.21	111.00
1	B	356	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	465	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	347	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	513	PHE	CB-CG-CD1	5.73	124.81	120.80
1	A	37	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	51	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	650	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	500	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	635[A]	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	635[B]	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	356	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	530	LYS	CD-CE-NZ	-5.47	99.12	111.70
1	A	13[A]	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	13[B]	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	76	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	474	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	550	ALA	C-N-CA	-5.19	111.40	122.30
1	B	671	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	635[A]	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	635[B]	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	396	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	41	LYS	CD-CE-NZ	-5.02	100.16	111.70
1	B	595[A]	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	595[B]	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	551	GLY	Peptide
1	B	325[B]	GLN	Peptide

## 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	5430	0	5077	31	0
1	B	5553	0	5168	54	0
2	A	15	0	0	2	0
2	B	15	0	0	3	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	36	0	54	0	0
4	B	36	0	54	0	0
5	A	550	0	0	10	0
5	B	581	0	0	9	0
All	All	12228	0	10369	83	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 (83) 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:324[B]:PHE:O	1:B:326:PHE:N	1.79	1.12
1:B:323:SER:O	1:B:324[B]:PHE:CD1	2.10	1.05
1:B:324[B]:PHE:O	1:B:326:PHE:O	1.79	1.00
1:B:131:GLU:OE1	5:B:1280:HOH:O	1.80	0.99
1:B:324[B]:PHE:CE2	1:B:325[B]:GLN:HG3	1.98	0.97
1:A:638:ASN:HB3	5:A:1362:HOH:O	1.75	0.85
1:B:329[B]:ARG:NH1	5:B:1359:HOH:O	1.94	0.83
1:A:592:GLY:O	1:A:635[A]:ARG:NH2	2.12	0.82
1:B:324[B]:PHE:CD2	1:B:325[B]:GLN:N	2.49	0.81
1:B:323:SER:O	1:B:324[B]:PHE:CG	2.34	0.80
1:B:164[A]:HIS:HE1	1:B:480:VAL:O	1.67	0.77
1:A:638:ASN:CB	5:A:1362:HOH:O	2.31	0.77
1:A:327:ASP:OD1	5:A:1237:HOH:O	2.04	0.74
1:B:164[A]:HIS:CE1	1:B:480:VAL:O	2.41	0.74
1:B:682:ASN:O	1:B:683:ALA:HB3	1.90	0.71
1:B:637:GLN:OE1	5:B:1435:HOH:O	2.13	0.66
1:A:308[A]:GLN:HB2	5:A:1091:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:ASN:O	1:B:683:ALA:CB	2.43	0.65
1:B:78:PRO:O	1:B:79:ASN:HB2	1.98	0.64
1:A:638:ASN:CG	5:A:1362:HOH:O	2.37	0.63
1:B:13[A]:ARG:HG3	1:B:59[A]:GLN:HB3	1.80	0.63
1:A:339[A]:ARG:NH1	1:A:417:ALA:O	2.32	0.62
1:B:308[A]:GLN:HB2	5:B:1122:HOH:O	1.99	0.62
1:A:464[A]:LYS:NZ	1:A:468:GLN:OE1	2.34	0.59
1:A:308[B]:GLN:OE1	5:A:1136:HOH:O	2.17	0.57
1:A:434:MET:CE	5:A:1436:HOH:O	2.53	0.57
1:B:78:PRO:O	1:B:79:ASN:CB	2.53	0.57
1:B:339[A]:ARG:HB3	1:B:417:ALA:HA	1.86	0.56
1:B:565[B]:ASN:ND2	5:B:1443:HOH:O	2.30	0.56
1:B:341:LYS:CE	5:B:1089:HOH:O	2.53	0.55
1:B:341:LYS:HE3	5:B:1089:HOH:O	2.05	0.55
1:B:324[B]:PHE:CG	1:B:325[B]:GLN:N	2.75	0.54
1:B:267:ASP:OD1	1:B:271[B]:ARG:HD3	2.08	0.53
1:A:2:ALA:N	5:A:1432:HOH:O	2.42	0.53
1:B:351:ASN:OD1	1:B:351:ASN:C	2.46	0.53
1:A:516:CYS:SG	1:A:581:TRQ:HB3	2.50	0.52
1:A:565:ASN:OD1	1:B:684:ASN:OD1	2.28	0.52
1:A:13[A]:ARG:NH2	1:A:452:GLU:OE2	2.32	0.52
1:B:286:HIS:HA	2:B:802:SO4:O2	2.10	0.51
1:B:359:GLN:HB3	1:B:360:PRO:HD2	1.94	0.49
1:B:324[B]:PHE:O	1:B:326:PHE:C	2.49	0.49
1:B:516:CYS:SG	1:B:581:TRQ:HB3	2.53	0.49
1:B:79:ASN:HA	1:B:233:SER:OG	2.13	0.49
1:A:464[A]:LYS:CE	5:A:1411:HOH:O	2.61	0.49
1:B:635[A]:ARG:HB3	1:B:635[A]:ARG:HH11	1.78	0.48
1:A:187:THR:HA	1:A:192:ARG:O	2.13	0.48
1:A:286:HIS:HA	2:A:802:SO4:O2	2.13	0.48
1:B:448:CYS:N	1:B:449:PRO:CA	2.77	0.47
1:B:682:ASN:C	1:B:682:ASN:OD1	2.51	0.47
1:B:319:SER:HA	1:B:322:PHE:CE1	2.50	0.47
1:A:658:LYS:HE2	1:A:658:LYS:HB2	1.58	0.47
1:A:684:ASN:ND2	1:B:565[B]:ASN:OD1	2.49	0.46
1:B:327:ASP:OD1	5:B:992:HOH:O	2.21	0.46
1:B:332:SER:O	1:B:339[A]:ARG:NH2	2.47	0.45
1:B:13[B]:ARG:HA	1:B:247:GLY:O	2.17	0.45
1:B:88:HIS:O	1:B:224:GLY:HA3	2.17	0.45
1:B:271[B]:ARG:HD2	1:B:287:TYR:OH	2.16	0.45
1:B:13[A]:ARG:HG3	1:B:59[A]:GLN:CB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LYS:HE2	5:B:1089:HOH:O	2.17	0.44
1:A:426:ALA:HA	5:A:1414:HOH:O	2.17	0.44
1:B:207[B]:ASP:HB3	1:B:210:GLY:H	1.83	0.43
1:B:98[B]:GLU:CD	2:B:801:SO4:O4	2.56	0.43
1:A:286:HIS:HD2	2:A:802:SO4:O1	2.01	0.43
1:B:13[A]:ARG:CG	1:B:59[A]:GLN:HB3	2.47	0.43
1:B:392:TYR:O	1:B:393:ASP:HB2	2.19	0.43
1:B:98[B]:GLU:HB3	2:B:801:SO4:O4	2.18	0.42
1:A:319:SER:HA	1:A:322:PHE:CE2	2.54	0.42
1:B:39:ASP:O	1:B:40:LEU:HB2	2.18	0.42
1:A:112:ASN:HB2	1:A:354:ILE:HD11	2.01	0.42
1:B:518:ILE:HD12	1:B:518:ILE:C	2.41	0.41
1:A:128:ALA:HB3	1:A:131:GLU:HG3	2.01	0.41
1:B:542:HIS:CE1	1:B:544:GLU:CG	3.03	0.41
1:B:187:THR:HA	1:B:192:ARG:O	2.21	0.41
1:A:591:THR:HG23	1:A:610:ILE:HD12	2.03	0.41
1:B:448:CYS:N	1:B:449:PRO:C	2.73	0.41
1:A:172:LEU:CD2	1:A:201:PHE:HZ	2.34	0.41
1:A:351:ASN:C	1:A:351:ASN:OD1	2.59	0.41
1:A:85:TRP:CD2	1:A:193:LEU:HB2	2.56	0.41
1:A:554:VAL:HA	1:A:555:PRO:HD3	1.87	0.41
1:B:293:ALA:O	1:B:421:PHE:HA	2.22	0.40
1:A:144:VAL:HG22	1:A:149:ALA:HB3	2.03	0.40
1:A:542:HIS:CE1	1:A:544:GLU:CG	3.04	0.40
1:B:13[A]:ARG:HA	1:B:247:GLY:O	2.22	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	684/726 (94%)	659 (96%)	22 (3%)	3 (0%)	34 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	700/726 (96%)	667 (95%)	30 (4%)	3 (0%)	34 24
All	All	1384/1452 (95%)	1326 (96%)	52 (4%)	6 (0%)	34 24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	683	ALA
1	A	684	ASN
1	B	325[A]	GLN
1	B	325[B]	GLN
1	B	683	ALA
1	A	685	LYS

### 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	598/626 (96%)	585 (98%)	13 (2%)	52 39
1	B	611/626 (98%)	592 (97%)	19 (3%)	40 26
All	All	1209/1252 (97%)	1177 (97%)	32 (3%)	47 32

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	102	LEU
1	A	172	LEU
1	A	182	LEU
1	A	261	LEU
1	A	455	TRP
1	A	486	GLU
1	A	554	VAL
1	A	584	GLN
1	A	610	ILE

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Mol	Chain	Res	Type
1	A	633	ARG
1	A	637	GLN
1	A	658	LYS
1	B	13[A]	ARG
1	B	13[B]	ARG
1	B	40	LEU
1	B	71	GLU
1	B	79	ASN
1	B	102	LEU
1	B	172	LEU
1	B	261[A]	LEU
1	B	261[B]	LEU
1	B	393	ASP
1	B	484	THR
1	B	561	SER
1	B	584	GLN
1	B	610	ILE
1	B	635[A]	ARG
1	B	635[B]	ARG
1	B	637	GLN
1	B	640	ASP
1	B	685	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	286	HIS
1	A	542	HIS
1	A	684	ASN
1	B	48	ASN
1	B	286	HIS
1	B	542	HIS
1	B	637	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.



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

4 non-standard protein/DNA/RNA residues 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
1	TRQ	B	581	1	13,17,18	3.02	4 (30%)	14,24,26	3.35	7 (50%)
1	TRQ	A	581	1	13,17,18	3.21	5 (38%)	14,24,26	3.41	6 (42%)
1	CSD	B	55	1	3,7,8	0.88	0	1,8,10	3.91	1 (100%)
1	CSD	A	55	1	3,7,8	0.40	0	1,8,10	2.38	1 (100%)

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
1	TRQ	B	581	1	-	0/4/19/21	0/2/2/2
1	TRQ	A	581	1	-	0/4/19/21	0/2/2/2
1	CSD	B	55	1	-	0/2/6/8	-
1	CSD	A	55	1	-	0/2/6/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	581	TRQ	CH2-CZ2	-8.97	1.44	1.54
1	B	581	TRQ	CH2-CZ2	-7.37	1.45	1.54
1	B	581	TRQ	CZ3-CE3	5.55	1.44	1.34
1	A	581	TRQ	CZ3-CE3	4.88	1.43	1.34
1	B	581	TRQ	CE2-CZ2	-4.29	1.44	1.50
1	A	581	TRQ	O7-CZ2	3.20	1.30	1.23
1	A	581	TRQ	CE2-CZ2	-2.66	1.46	1.50
1	A	581	TRQ	CD2-CE3	-2.50	1.39	1.44
1	B	581	TRQ	CD2-CE3	-2.27	1.40	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	581	TRQ	O6-CH2-CZ2	-7.39	113.48	118.51
1	B	581	TRQ	CZ2-CE2-NE1	7.27	131.55	119.94
1	A	581	TRQ	CZ2-CE2-NE1	7.22	131.46	119.94
1	A	581	TRQ	O7-CZ2-CH2	5.91	125.96	119.00
1	A	581	TRQ	O7-CZ2-CE2	-5.47	116.05	121.84
1	A	581	TRQ	O6-CH2-CZ2	-5.05	115.08	118.51
1	B	55	CSD	OD1-SG-CB	-3.91	98.10	105.54
1	B	581	TRQ	O7-CZ2-CE2	-3.90	117.71	121.84
1	B	581	TRQ	CB-CA-C	-3.14	105.58	111.47
1	B	581	TRQ	O6-CH2-CZ3	2.67	126.34	121.51
1	B	581	TRQ	O7-CZ2-CH2	2.61	122.07	119.00
1	B	581	TRQ	CE3-CZ3-CH2	-2.53	119.16	121.08
1	A	581	TRQ	CE3-CZ3-CH2	-2.48	119.20	121.08
1	A	55	CSD	OD1-SG-CB	-2.38	101.00	105.54
1	A	581	TRQ	CB-CA-C	-2.15	107.44	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	581	TRQ	1	0
1	A	581	TRQ	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

26 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	A	806	-	3,3,3	0.44	0	2,2,2	0.20	0
4	EDO	A	810	-	3,3,3	0.38	0	2,2,2	0.70	0
4	EDO	A	807	-	3,3,3	0.48	0	2,2,2	0.39	0
2	SO4	B	803	-	4,4,4	0.25	0	6,6,6	0.94	0
4	EDO	A	812	-	3,3,3	0.58	0	2,2,2	0.34	0
4	EDO	A	808	-	3,3,3	0.57	0	2,2,2	0.64	0
4	EDO	B	808	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	B	805	-	3,3,3	0.14	0	2,2,2	1.22	0
4	EDO	A	811	-	3,3,3	0.29	0	2,2,2	1.10	0
2	SO4	A	803	-	4,4,4	0.46	0	6,6,6	0.85	0
3	DIO	A	804	-	6,6,6	0.77	0	6,6,6	1.14	1 (16%)
3	DIO	B	804	-	6,6,6	0.65	0	6,6,6	0.64	0
4	EDO	B	807	-	3,3,3	0.12	0	2,2,2	0.54	0
4	EDO	B	809	-	3,3,3	0.54	0	2,2,2	0.59	0
4	EDO	B	806	-	3,3,3	0.40	0	2,2,2	0.67	0
4	EDO	A	813	-	3,3,3	0.43	0	2,2,2	1.16	0
2	SO4	A	802	-	4,4,4	0.17	0	6,6,6	0.84	0
4	EDO	A	805	-	3,3,3	0.37	0	2,2,2	0.54	0
2	SO4	A	801	-	4,4,4	0.89	0	6,6,6	0.70	0
4	EDO	B	813	-	3,3,3	0.48	0	2,2,2	0.71	0
4	EDO	B	812	-	3,3,3	0.42	0	2,2,2	0.45	0
4	EDO	A	809	-	3,3,3	0.39	0	2,2,2	0.71	0
2	SO4	B	802	-	4,4,4	0.15	0	6,6,6	0.45	0
4	EDO	B	810	-	3,3,3	0.36	0	2,2,2	1.04	0
4	EDO	B	811	-	3,3,3	0.50	0	2,2,2	0.33	0
2	SO4	B	801	-	4,4,4	0.99	0	6,6,6	0.68	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	813	-	-	1/1/1/1	-
4	EDO	A	806	-	-	0/1/1/1	-
3	DIO	A	804	-	-	-	0/1/1/1
3	DIO	B	804	-	-	-	0/1/1/1
4	EDO	B	810	-	-	0/1/1/1	-
4	EDO	A	810	-	-	1/1/1/1	-
4	EDO	B	811	-	-	1/1/1/1	-
4	EDO	B	807	-	-	0/1/1/1	-
4	EDO	A	807	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	809	-	-	0/1/1/1	-
4	EDO	B	806	-	-	0/1/1/1	-
4	EDO	A	813	-	-	1/1/1/1	-
4	EDO	A	812	-	-	1/1/1/1	-
4	EDO	B	812	-	-	0/1/1/1	-
4	EDO	A	805	-	-	0/1/1/1	-
4	EDO	A	808	-	-	0/1/1/1	-
4	EDO	B	808	-	-	0/1/1/1	-
4	EDO	B	805	-	-	0/1/1/1	-
4	EDO	A	809	-	-	0/1/1/1	-
4	EDO	A	811	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	DIO	C2'-O1'-C1'	2.14	117.04	109.89

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	810	EDO	O1-C1-C2-O2
4	B	811	EDO	O1-C1-C2-O2
4	A	812	EDO	O1-C1-C2-O2
4	B	813	EDO	O1-C1-C2-O2
4	A	813	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
2	A	802	SO4	2	0
2	B	802	SO4	1	0
2	B	801	SO4	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	682/726 (93%)	-0.34	11 (1%) 72 77	12, 20, 37, 72	0
1	B	682/726 (93%)	-0.42	13 (1%) 66 72	12, 19, 37, 82	0
All	All	1364/1452 (93%)	-0.38	24 (1%) 68 74	12, 19, 37, 82	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	TYR	4.6
1	B	324[A]	PHE	4.2
1	B	79	ASN	3.6
1	B	68	ALA	3.4
1	A	212	GLY	3.4
1	A	687	SER	3.3
1	A	68	ALA	3.2
1	A	683	ALA	3.1
1	B	170	GLY	2.8
1	B	2	ALA	2.8
1	B	78	PRO	2.6
1	A	2	ALA	2.4
1	A	561	SER	2.3
1	B	210	GLY	2.3
1	A	69	SER	2.3
1	B	212	GLY	2.1
1	A	324	PHE	2.1
1	A	451	ILE	2.1
1	A	686	GLU	2.1
1	A	540	ARG	2.1
1	B	69	SER	2.1
1	B	560	VAL	2.1
1	B	70	ASN	2.0
1	B	427	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TRQ	B	581	16/17	0.97	0.08	12,14,19,22	0
1	TRQ	A	581	16/17	0.98	0.14	13,15,20,21	0
1	CSD	A	55	8/9	0.98	0.08	15,17,25,30	0
1	CSD	B	55	8/9	0.99	0.05	15,17,24,27	0

## 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	B	811	4/4	0.88	0.13	40,41,51,55	0
4	EDO	A	813	4/4	0.90	0.11	30,38,39,42	0
4	EDO	B	813	4/4	0.90	0.13	36,37,39,39	0
4	EDO	A	806	4/4	0.90	0.11	31,31,32,35	0
4	EDO	B	808	4/4	0.91	0.12	27,41,41,43	0
4	EDO	B	810	4/4	0.92	0.08	34,43,46,51	0
2	SO4	A	803	5/5	0.93	0.17	54,61,62,68	0
4	EDO	B	812	4/4	0.93	0.14	32,39,40,43	0
4	EDO	A	809	4/4	0.93	0.13	28,33,34,36	0
4	EDO	B	809	4/4	0.93	0.13	30,31,34,37	0
2	SO4	B	803	5/5	0.93	0.13	42,48,56,62	0
4	EDO	B	807	4/4	0.94	0.12	25,25,26,31	0
4	EDO	A	812	4/4	0.94	0.14	27,29,32,34	0
2	SO4	B	801	5/5	0.94	0.22	28,34,42,45	0
4	EDO	A	808	4/4	0.95	0.14	19,26,33,41	0
4	EDO	A	811	4/4	0.95	0.17	29,33,35,36	0
3	DIO	B	804	6/6	0.96	0.07	21,24,25,25	0
4	EDO	B	805	4/4	0.96	0.08	27,28,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	801	5/5	0.96	0.16	26,35,41,41	0
3	DIO	A	804	6/6	0.97	0.06	22,28,29,30	0
4	EDO	A	805	4/4	0.97	0.19	28,29,30,30	0
4	EDO	A	810	4/4	0.97	0.09	27,32,32,32	0
2	SO4	B	802	5/5	0.98	0.16	44,46,49,60	0
2	SO4	A	802	5/5	0.98	0.16	47,47,52,53	0
4	EDO	B	806	4/4	0.98	0.11	23,23,23,24	0
4	EDO	A	807	4/4	0.98	0.08	24,25,25,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.