



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:09 AM UTC

PDB ID : 3WEU / pdb_00003weu
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

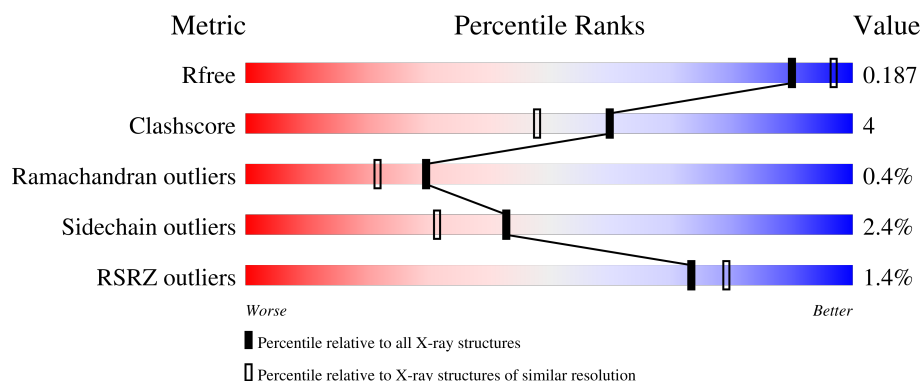
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	726	% 84% 9% 6%
1	B	726	% 83% 10% 6%

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
1	A	684	Total	C	N	O	S	0	6	0
			5430	3405	910	1092	23			
1	B	684	Total	C	N	O	S	0	20	0
			5553	3478	934	1118	23			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



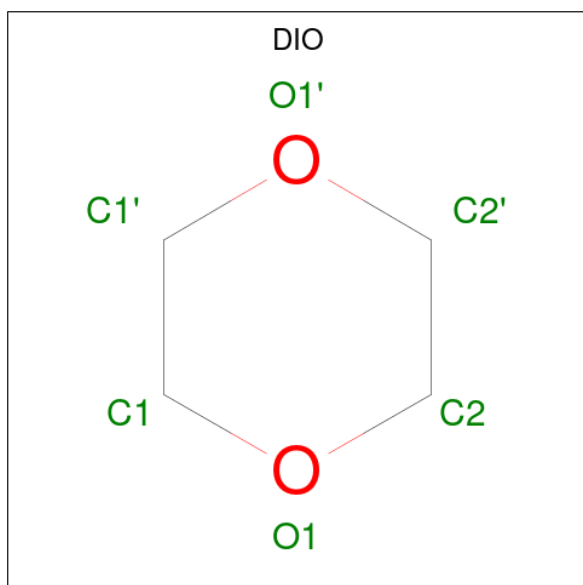
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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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 (CCD ID: DIO) (formula: $C_4H_8O_2$).



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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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	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	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		

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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		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 98.8 (47.54-1.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.143 , 0.178 0.155 , 0.187	Depositor DCC
R_{free} test set	3406 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12228	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CSD, DIO, TRQ, 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	1.27	11/5540 (0.2%)	1.12	15/7540 (0.2%)
1	B	1.24	12/5667 (0.2%)	1.08	9/7713 (0.1%)
All	All	1.25	23/11207 (0.2%)	1.10	24/15253 (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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	551	GLY	CA-C	6.94	1.61	1.51
1	B	445	LEU	C-O	-6.68	1.17	1.24
1	A	551	GLY	N-CA	6.36	1.54	1.45
1	B	384	ASN	CA-C	-6.18	1.47	1.53
1	B	230	VAL	CA-CB	-5.97	1.47	1.54
1	A	625	HIS	CA-CB	-5.84	1.45	1.53
1	B	222	SER	CA-C	-5.82	1.45	1.52
1	B	473	GLN	N-CA	5.66	1.54	1.47
1	B	555	PRO	N-CA	-5.55	1.40	1.47
1	A	514	PHE	C-O	-5.43	1.17	1.24
1	B	327	ASP	N-CA	-5.40	1.39	1.46
1	A	472	TYR	CA-CB	-5.39	1.46	1.53
1	A	573	PRO	CA-CB	-5.34	1.49	1.54
1	B	230	VAL	N-CA	-5.32	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	SER	N-CA	5.25	1.52	1.46
1	A	250	ASP	C-O	5.22	1.30	1.23
1	A	658	LYS	CA-C	-5.11	1.46	1.52
1	A	542	HIS	N-CA	-5.08	1.40	1.46
1	B	387	SER	C-O	-5.06	1.17	1.24
1	B	341	LYS	CA-CB	-5.05	1.45	1.53
1	B	683	ALA	N-CA	5.05	1.52	1.46
1	B	167	TYR	CA-C	-5.05	1.46	1.52
1	A	300	LEU	C-O	-5.04	1.19	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLY	CA-C-N	10.66	130.62	119.85
1	A	140	GLY	C-N-CA	10.66	130.62	119.85
1	B	425	PRO	CA-C-N	-6.63	112.18	122.59
1	B	425	PRO	C-N-CA	-6.63	112.18	122.59
1	A	426	ALA	N-CA-C	-6.31	100.16	109.81
1	A	325	GLN	N-CA-C	-6.19	104.99	112.54
1	B	480	VAL	CB-CA-C	-6.12	104.04	112.24
1	A	384	ASN	N-CA-C	5.96	117.16	107.32
1	A	550	ALA	O-C-N	-5.88	115.88	122.12
1	A	625	HIS	N-CA-C	5.68	119.79	112.41
1	B	480	VAL	N-CA-C	5.59	117.09	111.00
1	B	568	GLU	N-CA-C	5.53	118.23	111.82
1	B	573	PRO	O-C-N	5.50	123.74	121.15
1	A	158	ILE	N-CA-C	-5.41	103.65	108.95
1	B	426	ALA	N-CA-C	-5.37	101.19	109.52
1	A	425	PRO	CA-C-N	-5.28	113.58	123.03
1	A	425	PRO	C-N-CA	-5.28	113.58	123.03
1	B	468	GLN	N-CA-C	5.25	116.97	108.41
1	A	224	GLY	N-CA-C	5.12	117.50	110.69
1	A	550	ALA	CA-C-N	-5.11	111.40	121.41
1	A	550	ALA	C-N-CA	-5.11	111.40	121.41
1	A	426	ALA	CA-C-N	-5.06	112.99	121.39
1	A	426	ALA	C-N-CA	-5.06	112.99	121.39
1	B	401	LYS	N-CA-C	5.04	116.86	111.36

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	5078	37	0
1	B	5553	0	5169	58	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	10371	93	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 (93) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.70
1:A:638:ASN:CG	5:A:1362:HOH:O	2.37	0.68
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
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: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:B:351:ASN:OD1	1:B:351:ASN:C	2.46	0.57
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:324[B]:PHE:O	1:B:326:PHE:C	2.49	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: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:B:682:ASN:OD1	1:B:682:ASN:C	2.51	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:79:ASN:HA	1:B:233:SER:OG	2.13	0.49
1:B:516:CYS:SG	1:B:581:TRQ:HB3	2.53	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:98[B]:GLU:CD	2:B:801:SO4:O4	2.56	0.48
1:A:96:TRP:CG	1:A:97:TYR:H	2.32	0.47
1:B:448:CYS:N	1:B:449:PRO:CA	2.77	0.47
1:A:658:LYS:HB2	1:A:658:LYS:HE2	1.58	0.47
1:B:319:SER:HA	1:B:322:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:ILE:C	1:B:518:ILE:HD12	2.41	0.46
1:A:684:ASN:ND2	1:B:565[B]:ASN:OD1	2.49	0.46
1:B:448:CYS:N	1:B:449:PRO:C	2.73	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:A:351:ASN:OD1	1:A:351:ASN:C	2.59	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
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:234:ASP:OD1	1:B:234:ASP:C	2.60	0.43
1:A:434:MET:HB3	1:A:434:MET:HE2	1.84	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:A:550:ALA:O	1:A:551:GLY:C	2.60	0.43
1:B:98[B]:GLU:HB3	2:B:801:SO4:O4	2.18	0.42
1:B:377:MET:HA	1:B:378:PRO:C	2.43	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:A:6:HIS:HA	1:A:7:PRO:C	2.45	0.42
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:518:ILE:HD12	1:A:518:ILE:C	2.45	0.41
1:A:591:THR:HG23	1:A:610:ILE:HD12	2.03	0.41
1:A:172:LEU:CD2	1:A:201:PHE:HZ	2.34	0.41
1:B:331:GLY:C	1:B:339[A]:ARG:NH2	2.79	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:13[A]:ARG:HG3	1:B:59[A]:GLN:CD	2.46	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:A:294:ASN:CG	1:A:426:ALA:HB2	2.46	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

5.3.1 Protein backbone

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%)	30	22
1	B	700/726 (96%)	667 (95%)	30 (4%)	3 (0%)	30	22
All	All	1384/1452 (95%)	1326 (96%)	52 (4%)	6 (0%)	30	22

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

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%)	586 (98%)	12 (2%)	48	39
1	B	611/626 (98%)	591 (97%)	20 (3%)	33	20
All	All	1209/1252 (97%)	1177 (97%)	32 (3%)	43	28

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	486	GLU
1	A	554	VAL
1	A	584	GLN
1	A	610	ILE
1	A	633	ARG
1	A	658	LYS
1	A	686	GLU
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	486[A]	GLU
1	B	486[B]	GLU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	164	HIS
1	A	178	HIS
1	A	257	ASN
1	A	286	HIS
1	A	304	GLN
1	A	481	ASN

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Mol	Chain	Res	Type
1	A	542	HIS
1	A	608	GLN
1	A	637	GLN
1	A	684	ASN
1	B	48	ASN
1	B	286	HIS
1	B	471	HIS
1	B	481	ASN
1	B	542	HIS
1	B	608	GLN
1	B	637	GLN

5.3.3 RNA ⓘ

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	CSD	B	55	1	4,7,8	1.78	1 (25%)	1,8,10	4.08	1 (100%)
1	TRQ	B	581	1	16,17,18	1.91	2 (12%)	16,24,26	1.64	5 (31%)
1	TRQ	A	581	1	16,17,18	1.74	4 (25%)	16,24,26	2.01	3 (18%)
1	CSD	A	55	1	4,7,8	0.84	0	1,8,10	2.50	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	CSD	B	55	1	-	0/2/6/8	-
1	TRQ	B	581	1	-	0/5/19/21	0/2/2/2
1	TRQ	A	581	1	-	0/5/19/21	0/2/2/2
1	CSD	A	55	1	-	0/2/6/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	581	TRQ	CE2-NE1	-5.21	1.30	1.38
1	A	581	TRQ	CE2-NE1	-3.99	1.32	1.38
1	B	581	TRQ	CE3-CZ3	3.72	1.44	1.35
1	A	581	TRQ	CE3-CZ3	3.22	1.43	1.35
1	B	55	CSD	OD1-SG	-3.19	1.44	1.47
1	A	581	TRQ	O7-CZ2	2.96	1.30	1.23
1	A	581	TRQ	CH2-CZ2	-2.07	1.44	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	581	TRQ	O7-CZ2-CH2	5.94	125.96	118.39
1	B	55	CSD	OD1-SG-CB	-4.08	98.10	105.60
1	B	581	TRQ	O7-CZ2-CH2	2.89	122.07	118.39
1	B	581	TRQ	O6-CH2-CZ3	2.65	126.34	121.58
1	A	55	CSD	OD1-SG-CB	-2.50	101.00	105.60
1	B	581	TRQ	CE3-CZ3-CH2	-2.45	119.16	121.72
1	B	581	TRQ	O6-CH2-CZ2	-2.44	113.48	118.07
1	A	581	TRQ	CE3-CZ3-CH2	-2.41	119.20	121.72
1	A	581	TRQ	CG-CD1-NE1	2.23	112.09	109.22
1	B	581	TRQ	CE2-CD2-CG	-2.12	104.35	107.16

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
2	SO4	A	802	-	4,4,4	0.23	0	6,6,6	0.86	0
4	EDO	B	806	-	3,3,3	0.39	0	2,2,2	0.69	0
3	DIO	A	804	-	6,6,6	0.80	0	6,6,6	1.18	1 (16%)
2	SO4	A	801	-	4,4,4	0.94	0	6,6,6	0.64	0
2	SO4	B	802	-	4,4,4	0.23	0	6,6,6	0.42	0
4	EDO	B	811	-	3,3,3	0.49	0	2,2,2	0.37	0
4	EDO	A	810	-	3,3,3	0.38	0	2,2,2	0.72	0
2	SO4	B	803	-	4,4,4	0.35	0	6,6,6	0.93	0
4	EDO	A	811	-	3,3,3	0.30	0	2,2,2	1.10	0
4	EDO	B	810	-	3,3,3	0.35	0	2,2,2	1.05	0
4	EDO	B	808	-	3,3,3	0.42	0	2,2,2	0.34	0
4	EDO	B	809	-	3,3,3	0.53	0	2,2,2	0.62	0
4	EDO	B	812	-	3,3,3	0.41	0	2,2,2	0.48	0
2	SO4	A	803	-	4,4,4	0.55	0	6,6,6	0.71	0
4	EDO	A	813	-	3,3,3	0.43	0	2,2,2	1.15	0
4	EDO	A	812	-	3,3,3	0.56	0	2,2,2	0.29	0
4	EDO	B	805	-	3,3,3	0.15	0	2,2,2	1.21	0
4	EDO	A	808	-	3,3,3	0.53	0	2,2,2	0.66	0
4	EDO	A	807	-	3,3,3	0.48	0	2,2,2	0.36	0
4	EDO	A	806	-	3,3,3	0.43	0	2,2,2	0.25	0
3	DIO	B	804	-	6,6,6	0.65	0	6,6,6	0.66	0
4	EDO	B	813	-	3,3,3	0.47	0	2,2,2	0.67	0
2	SO4	B	801	-	4,4,4	1.03	0	6,6,6	0.67	0
4	EDO	A	805	-	3,3,3	0.33	0	2,2,2	0.56	0
4	EDO	A	809	-	3,3,3	0.38	0	2,2,2	0.72	0
4	EDO	B	807	-	3,3,3	0.12	0	2,2,2	0.45	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	806	-	-	0/1/1/1	-
3	DIO	A	804	-	-	-	0/1/1/1
4	EDO	B	811	-	-	1/1/1/1	-
4	EDO	A	810	-	-	1/1/1/1	-
4	EDO	A	811	-	-	0/1/1/1	-
4	EDO	B	810	-	-	0/1/1/1	-
4	EDO	B	808	-	-	0/1/1/1	-
4	EDO	B	812	-	-	0/1/1/1	-
4	EDO	B	809	-	-	0/1/1/1	-
4	EDO	A	813	-	-	1/1/1/1	-
4	EDO	A	812	-	-	1/1/1/1	-
4	EDO	B	805	-	-	0/1/1/1	-
4	EDO	A	808	-	-	0/1/1/1	-
4	EDO	A	807	-	-	0/1/1/1	-
4	EDO	A	806	-	-	0/1/1/1	-
3	DIO	B	804	-	-	-	0/1/1/1
4	EDO	B	813	-	-	1/1/1/1	-
4	EDO	A	805	-	-	0/1/1/1	-
4	EDO	A	809	-	-	0/1/1/1	-
4	EDO	B	807	-	-	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'	2.21	117.04	109.88

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	A	813	EDO	O1-C1-C2-O2
4	B	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	682/726 (93%)	-0.33	9 (1%) 75 80	6, 20, 37, 72	6 (0%)
1	B	682/726 (93%)	-0.35	10 (1%) 72 78	6, 19, 36, 82	20 (2%)
All	All	1364/1452 (93%)	-0.34	19 (1%) 73 79	6, 19, 37, 82	26 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	TYR	5.5
1	A	212	GLY	5.4
1	A	683	ALA	4.5
1	A	324	PHE	4.5
1	A	209	SER	3.9
1	A	551	GLY	3.1
1	A	685	LYS	3.0
1	A	213	GLY	2.8
1	B	683	ALA	2.8
1	B	324[A]	PHE	2.6
1	B	685	LYS	2.6
1	A	687	SER	2.5
1	B	210	GLY	2.3
1	B	78	PRO	2.2
1	B	325[A]	GLN	2.2
1	B	427	ASP	2.2
1	A	2	ALA	2.1
1	B	2	ALA	2.0
1	B	212	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	A	55	8/9	0.97	0.06	15,17,25,30	0
1	TRQ	B	581	16/17	0.97	0.05	12,14,19,22	0
1	CSD	B	55	8/9	0.98	0.04	15,17,24,27	0
1	TRQ	A	581	16/17	0.98	0.04	13,15,20,21	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	B	810	4/4	0.84	0.18	34,43,46,51	0
4	EDO	A	813	4/4	0.86	0.14	30,38,39,42	0
2	SO4	A	803	5/5	0.86	0.10	54,61,62,68	0
4	EDO	B	813	4/4	0.86	0.13	36,37,39,39	0
4	EDO	A	806	4/4	0.88	0.12	31,31,32,35	0
4	EDO	B	811	4/4	0.89	0.14	40,41,51,55	0
2	SO4	B	801	5/5	0.89	0.23	28,34,42,45	0
4	EDO	B	812	4/4	0.90	0.15	32,39,40,43	0
4	EDO	A	809	4/4	0.90	0.12	28,33,34,36	0
4	EDO	A	812	4/4	0.91	0.10	27,29,32,34	0
4	EDO	A	811	4/4	0.92	0.13	29,33,35,36	0
4	EDO	B	808	4/4	0.92	0.12	27,41,41,43	0
2	SO4	B	803	5/5	0.92	0.08	42,48,56,62	0
4	EDO	A	810	4/4	0.93	0.11	27,32,32,32	0
4	EDO	B	809	4/4	0.93	0.11	30,31,34,37	0
4	EDO	B	807	4/4	0.93	0.11	25,25,26,31	0
2	SO4	A	801	5/5	0.94	0.19	26,35,41,41	0
2	SO4	B	802	5/5	0.94	0.08	44,46,49,60	0
4	EDO	A	808	4/4	0.94	0.10	19,26,33,41	0
3	DIO	A	804	6/6	0.95	0.09	22,28,29,30	0
3	DIO	B	804	6/6	0.95	0.07	21,24,25,25	0
4	EDO	B	805	4/4	0.95	0.07	27,28,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	805	4/4	0.95	0.07	28,29,30,30	0
2	SO4	A	802	5/5	0.95	0.07	47,47,52,53	0
4	EDO	B	806	4/4	0.96	0.07	23,23,23,24	0
4	EDO	A	807	4/4	0.97	0.08	24,25,25,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.