



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 01:18 PM BST

PDB ID : 3WEV
Title : Crystal structure of the Schiff base intermediate of L-Lys epsilon-oxidase from *Marinomonas mediterranea* with L-Lys
Authors : Okazaki, S.; Nakano, S.; Matsui, D.; Akaji, S.; Inagaki, K.; Asano, Y.
Deposited on : 2013-07-12
Resolution : 1.98 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 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 : 2.14.4.dev1
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) : 2.14.4.dev1

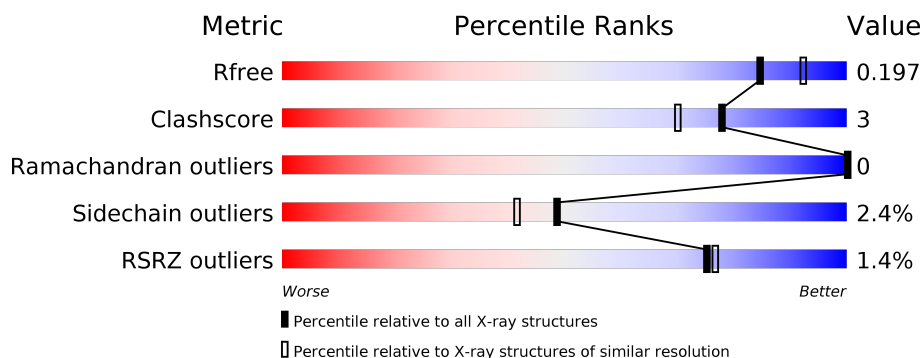
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 ≥ 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	LYS	B	801[A]	-	-	-	X

2 Entry composition [i](#)

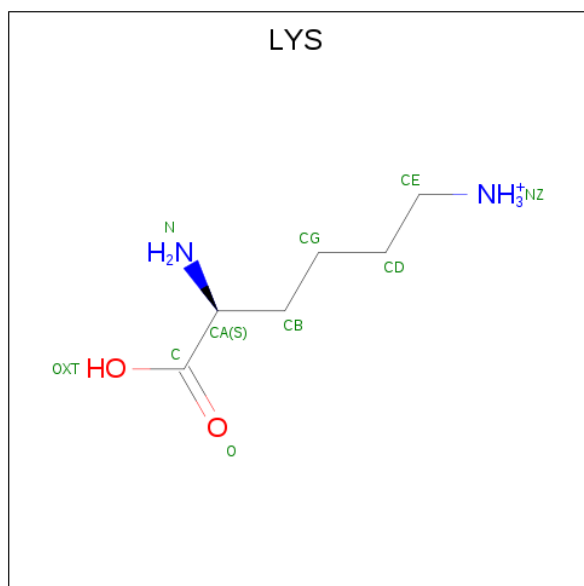
There are 6 unique types of molecules in this entry. The entry contains 12181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	680	Total	C	N	O	S	0	12	0
			5448	3422	910	1093	23			
1	B	681	Total	C	N	O	S	0	11	0
			5447	3416	907	1100	24			

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



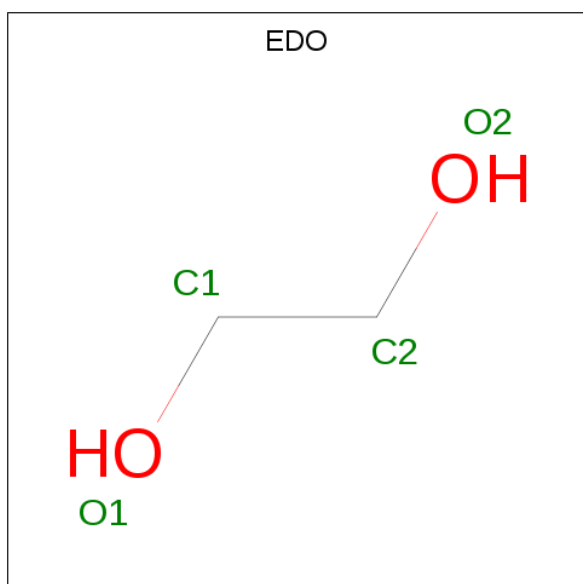
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	1
			10	6	2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



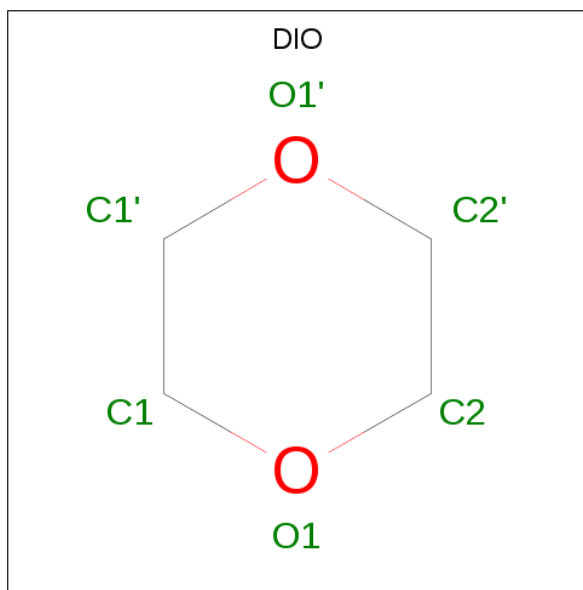
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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	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
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



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

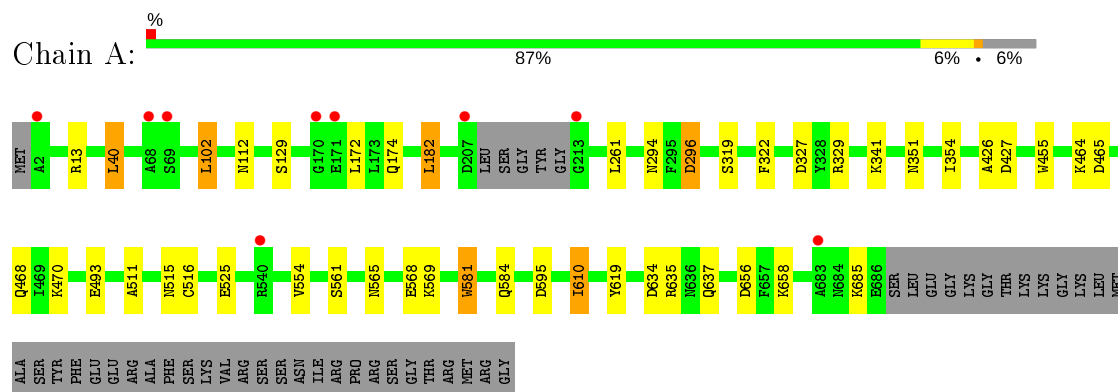
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	579	Total	O	0	6
			585	585		
6	B	600	Total	O	0	2
			602	602		

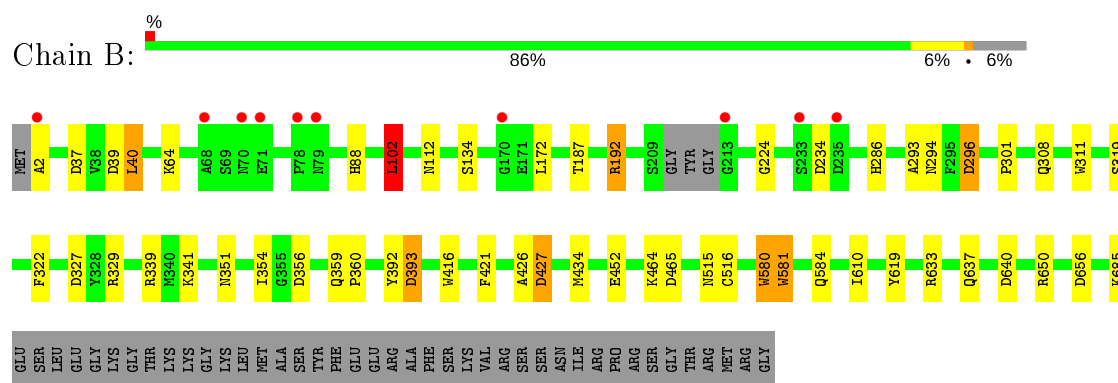
3 Residue-property plots [i](#)

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



• Molecule 1: L-lysine 6-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	194.99 Å 126.16 Å 70.86 Å 90.00° 99.03° 90.00°	Depositor
Resolution (Å)	46.86 – 1.98 46.86 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.86-1.98) 98.6 (46.86-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.98 (at 1.98 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.150 , 0.189 0.161 , 0.197	Depositor DCC
R_{free} test set	5745 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12181	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: TRQ, DIO, SO4, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.94	2/5568 (0.0%)	0.94	13/7580 (0.2%)
1	B	0.96	3/5550 (0.1%)	0.93	11/7557 (0.1%)
All	All	0.95	5/11118 (0.0%)	0.94	24/15137 (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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	525	GLU	CD-OE2	-6.60	1.18	1.25
1	B	416	TRP	CB-CG	-6.30	1.39	1.50
1	A	493	GLU	CD-OE1	-5.41	1.19	1.25
1	B	311	TRP	CG-CD1	5.02	1.43	1.36
1	B	452	GLU	CD-OE1	5.00	1.31	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	465	ASP	CB-CG-OD1	7.27	124.84	118.30
1	B	296	ASP	CB-CG-OD1	7.26	124.84	118.30
1	A	13[A]	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	13[B]	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	650	ARG	NE-CZ-NH2	-6.62	116.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	LEU	CB-CG-CD1	6.50	122.05	111.00
1	B	650	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	182	LEU	CB-CG-CD1	6.16	121.46	111.00
1	B	192	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	656	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	356	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	40	LEU	CB-CG-CD1	5.81	120.87	111.00
1	A	634	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	635	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	102	LEU	CB-CG-CD2	5.56	120.46	111.00
1	A	296	ASP	CB-CG-OD1	5.43	123.18	118.30
1	A	465	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	102	LEU	CB-CG-CD2	5.23	119.89	111.00
1	B	656	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	341	LYS	CD-CE-NZ	-5.17	99.81	111.70
1	B	356	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	102	LEU	CB-CG-CD1	5.08	119.63	111.00
1	B	465	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	580	TRP	Mainchain

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	5448	0	5094	27	0
1	B	5447	0	5065	31	0
2	A	10	0	11	3	0
2	B	10	0	9	1	0
3	A	15	0	0	0	0
3	B	10	0	0	1	0
4	A	24	0	36	0	0
4	B	24	0	36	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	8	2	0
6	A	585	0	0	10	0
6	B	602	0	0	10	0
All	All	12181	0	10259	61	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 3.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595[B]:ASP:OD1	6:A:1075[B]:HOH:O	1.57	1.19
1:B:351[A]:ASN:O	1:B:351[A]:ASN:OD1	1.72	1.08
1:A:685[B]:LYS:HA	1:A:685[B]:LYS:HE2	1.37	1.06
5:B:804:DIO:H1'2	6:B:1408:HOH:O	1.56	1.05
5:B:804:DIO:C1'	6:B:1408:HOH:O	2.21	0.80
1:A:327:ASP:OD1	6:A:1222:HOH:O	2.05	0.75
1:A:685[B]:LYS:CE	1:A:685[B]:LYS:HA	2.17	0.73
1:B:327:ASP:OD1	6:B:992:HOH:O	2.08	0.71
1:A:470:LYS:NZ	6:A:1458:HOH:O	2.16	0.66
1:A:595[B]:ASP:CG	6:A:1075[B]:HOH:O	2.16	0.66
1:B:351[A]:ASN:C	1:B:351[A]:ASN:OD1	2.35	0.64
1:B:341:LYS:HE2	6:B:1085:HOH:O	1.98	0.63
1:B:427[A]:ASP:N	1:B:427[A]:ASP:OD2	2.32	0.63
1:B:516:CYS:HA	1:B:581[A]:TRQ:HZ3	1.81	0.63
1:B:341:LYS:CE	6:B:1085:HOH:O	2.50	0.60
1:B:308[A]:GLN:HB2	6:B:1115:HOH:O	2.02	0.60
1:B:516:CYS:SG	1:B:581[A]:TRQ:HB3	2.43	0.58
1:A:464[A]:LYS:CE	6:A:1373:HOH:O	2.53	0.57
1:B:294:ASN:CG	1:B:426:ALA:HB2	2.25	0.56
1:A:174:GLN:OE1	6:A:1358:HOH:O	2.19	0.52
1:A:685[B]:LYS:CA	1:A:685[B]:LYS:HE2	2.19	0.52
1:A:329[A]:ARG:HD2	6:A:1222:HOH:O	2.09	0.52
1:A:296:ASP:OD1	1:A:329[B]:ARG:NH2	2.41	0.51
1:A:464[A]:LYS:NZ	1:A:468:GLN:OE1	2.43	0.51
1:B:580:TRP:HB3	1:B:581[A]:TRQ:CE3	2.40	0.51
1:A:511:ALA:HB2	1:A:619[A]:TYR:CE1	2.46	0.51
1:B:187:THR:HA	1:B:192:ARG:O	2.12	0.50
1:A:464[A]:LYS:HD3	6:A:1457:HOH:O	2.11	0.49
1:B:301:PRO:HB3	4:B:809:EDO:H12	1.94	0.49
1:B:359:GLN:HB3	1:B:360:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASN:HB2	1:A:354:ILE:HD11	1.95	0.48
1:A:516:CYS:SG	1:A:581:TRQ:HB3	2.54	0.47
1:B:319:SER:HA	1:B:322:PHE:CE1	2.51	0.46
1:A:319:SER:HA	1:A:322:PHE:CE2	2.50	0.46
1:B:286:HIS:HA	3:B:802:SO4:O2	2.17	0.45
1:B:64:LYS:HD2	1:B:434[A]:MET:HE1	2.00	0.44
1:B:392:TYR:O	1:B:393:ASP:HB2	2.18	0.44
1:B:112:ASN:HB2	1:B:354:ILE:HD11	2.00	0.44
1:B:2:ALA:N	6:B:1472:HOH:O	2.51	0.43
1:A:294:ASN:CG	1:A:426:ALA:HB2	2.38	0.43
1:A:511:ALA:HB2	1:A:619[A]:TYR:CZ	2.53	0.43
1:A:568:GLU:C	1:A:569:LYS:HG2	2.38	0.43
1:A:351:ASN:C	1:A:351:ASN:OD1	2.56	0.43
1:A:515:ASN:HB3	2:A:801:LYS:HG2	2.01	0.42
1:A:610[A]:ILE:N	1:A:610[A]:ILE:CD1	2.81	0.42
1:B:39:ASP:O	1:B:40:LEU:HB2	2.19	0.42
1:B:88:HIS:O	1:B:224:GLY:HA3	2.20	0.42
1:A:685[B]:LYS:CE	1:A:685[B]:LYS:CA	2.90	0.42
1:B:581[A]:TRQ:HZ3	2:B:801[A]:LYS:HE2	1.78	0.42
1:A:610[A]:ILE:CD1	1:A:610[A]:ILE:H	2.33	0.42
1:B:293:ALA:O	1:B:421:PHE:HA	2.20	0.41
1:B:234:ASP:OD1	1:B:234:ASP:C	2.58	0.41
1:B:296:ASP:OD1	1:B:329[B]:ARG:NH2	2.49	0.41
1:B:341:LYS:HE3	6:B:1085:HOH:O	2.17	0.41
1:B:515:ASN:HD21	4:B:805:EDO:C2	2.33	0.41
1:B:102:LEU:HD13	6:B:1403:HOH:O	2.20	0.41
1:A:581:TRQ:HZ3	2:A:801:LYS:HE2	1.83	0.40
1:B:37:ASP:HB2	6:B:1228:HOH:O	2.20	0.40
2:A:801:LYS:N	6:A:1157:HOH:O	2.55	0.40
1:A:426:ALA:HA	6:A:1376:HOH:O	2.22	0.40
1:B:619:TYR:CG	4:B:805:EDO:H21	2.56	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	687/726 (95%)	664 (97%)	23 (3%)	0	100	100
1	B	686/726 (94%)	662 (96%)	24 (4%)	0	100	100
All	All	1373/1452 (95%)	1326 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	602/627 (96%)	586 (97%)	16 (3%)	44	35
1	B	601/627 (96%)	587 (98%)	14 (2%)	50	44
All	All	1203/1254 (96%)	1173 (98%)	30 (2%)	49	39

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	102	LEU
1	A	129	SER
1	A	172	LEU
1	A	182	LEU
1	A	261	LEU
1	A	427	ASP
1	A	455	TRP
1	A	554	VAL
1	A	561	SER
1	A	565	ASN
1	A	584	GLN
1	A	610[A]	ILE
1	A	610[B]	ILE
1	A	637	GLN

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Mol	Chain	Res	Type
1	A	658	LYS
1	B	40	LEU
1	B	102	LEU
1	B	134	SER
1	B	172	LEU
1	B	393	ASP
1	B	427[A]	ASP
1	B	427[B]	ASP
1	B	464	LYS
1	B	584	GLN
1	B	610	ILE
1	B	633	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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	481	ASN
1	B	48	ASN
1	B	515	ASN
1	B	542	HIS
1	B	637	GLN
1	B	684	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	A	581	1,2	11,16,18	3.00	6 (54%)	11,22,26	2.26	5 (45%)
1	TRQ	B	581[A]	1,2	13,16,18	2.76	6 (46%)	14,22,26	19.79	10 (71%)
1	TRQ	B	581[B]	1	13,17,18	2.38	4 (30%)	14,24,26	3.26	4 (28%)

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	A	581	1,2	-	0/4/16/21	0/2/2/2
1	TRQ	B	581[A]	1,2	-	0/4/16/21	0/2/2/2
1	TRQ	B	581[B]	1	-	0/4/19/21	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	581	TRQ	O7-CZ2	5.98	1.31	1.22
1	A	581	TRQ	CE3-CZ3	5.21	1.41	1.33
1	B	581[B]	TRQ	CZ3-CE3	5.15	1.43	1.34
1	B	581[A]	TRQ	O6-CH2	-5.08	1.11	1.24
1	B	581[A]	TRQ	O7-CZ2	4.82	1.33	1.23
1	B	581[B]	TRQ	CH2-CZ2	-4.69	1.48	1.54
1	B	581[A]	TRQ	CZ3-CE3	4.20	1.41	1.34
1	A	581	TRQ	CD2-CE3	-3.72	1.36	1.44
1	B	581[A]	TRQ	CZ3-CH2	-3.10	1.37	1.45
1	B	581[A]	TRQ	CD2-CE3	-3.01	1.38	1.44
1	B	581[B]	TRQ	CD2-CE3	-2.91	1.38	1.44
1	B	581[A]	TRQ	CH2-CZ2	-2.90	1.50	1.54
1	A	581	TRQ	CH2-CZ2	2.89	1.47	1.39
1	B	581[B]	TRQ	CE2-CZ2	-2.20	1.47	1.50
1	A	581	TRQ	CB-CG	-2.14	1.48	1.51
1	A	581	TRQ	CD1-NE1	-2.10	1.33	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	581[A]	TRQ	O6-CH2-CZ2	-70.57	70.51	118.51
1	B	581[A]	TRQ	O6-CH2-CZ3	18.26	154.58	121.51
1	B	581[A]	TRQ	CZ2-CE2-NE1	10.34	136.45	119.94
1	B	581[B]	TRQ	CZ2-CE2-NE1	8.95	134.23	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	581[B]	TRQ	CG-CB-CA	-4.76	107.16	114.53
1	B	581[B]	TRQ	O7-CZ2-CE2	-4.34	117.25	121.84
1	A	581	TRQ	O7-CZ2-CH2	3.67	125.95	120.79
1	B	581[B]	TRQ	O7-CZ2-CH2	3.53	123.16	119.00
1	B	581[A]	TRQ	CD2-CE3-CZ3	3.51	125.33	121.09
1	B	581[A]	TRQ	CE3-CZ3-CH2	3.30	123.58	121.08
1	A	581	TRQ	CD2-CE3-CZ3	3.20	123.65	119.88
1	B	581[A]	TRQ	CZ3-CH2-CZ2	-3.14	114.42	118.72
1	A	581	TRQ	CB-CG-CD1	-3.03	124.22	127.97
1	B	581[A]	TRQ	CD2-CE2-NE1	-2.78	105.14	109.64
1	A	581	TRQ	CD2-CE2-NE1	-2.72	105.24	109.64
1	B	581[A]	TRQ	O7-CZ2-CE2	-2.69	118.99	121.84
1	A	581	TRQ	CG-CB-CA	-2.54	110.61	114.53
1	B	581[A]	TRQ	CE2-CD2-CE3	-2.08	116.56	119.15
1	B	581[A]	TRQ	CB-CG-CD1	-2.02	125.47	127.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	581	TRQ	2	0
1	B	581[A]	TRQ	4	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

20 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	LYS	A	801	1	5,9,9	1.11	0	4,10,10	2.10	2 (50%)
3	SO4	B	803	-	4,4,4	0.22	0	6,6,6	1.09	0
4	EDO	A	807	-	3,3,3	0.47	0	2,2,2	0.36	0
4	EDO	B	807	-	3,3,3	0.41	0	2,2,2	0.31	0
5	DIO	B	804	-	6,6,6	0.65	0	6,6,6	1.27	1 (16%)
4	EDO	A	806	-	3,3,3	0.72	0	2,2,2	0.57	0
4	EDO	A	810	-	3,3,3	0.56	0	2,2,2	0.63	0
4	EDO	B	810	-	3,3,3	0.44	0	2,2,2	0.70	0
4	EDO	A	809	-	3,3,3	0.66	0	2,2,2	0.25	0
4	EDO	B	805	-	3,3,3	0.40	0	2,2,2	0.90	0
3	SO4	A	803	-	4,4,4	0.09	0	6,6,6	0.39	0
3	SO4	A	804	-	4,4,4	0.48	0	6,6,6	0.61	0
4	EDO	A	805	-	3,3,3	0.31	0	2,2,2	0.16	0
3	SO4	A	802	-	4,4,4	0.71	0	6,6,6	0.71	0
2	LYS	B	801[A]	1	5,9,9	0.92	0	4,10,10	1.78	2 (50%)
3	SO4	B	802	-	4,4,4	0.22	0	6,6,6	0.52	0
4	EDO	B	808	-	3,3,3	0.33	0	2,2,2	1.31	0
4	EDO	A	808	-	3,3,3	0.33	0	2,2,2	1.18	0
4	EDO	B	806	-	3,3,3	0.31	0	2,2,2	0.21	0
4	EDO	B	809	-	3,3,3	0.29	0	2,2,2	0.67	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
2	LYS	A	801	1	-	1/5/9/9	-
4	EDO	A	807	-	-	1/1/1/1	-
4	EDO	B	807	-	-	1/1/1/1	-
5	DIO	B	804	-	-	-	0/1/1/1
4	EDO	A	806	-	-	1/1/1/1	-
4	EDO	A	810	-	-	1/1/1/1	-
4	EDO	B	810	-	-	0/1/1/1	-
4	EDO	A	809	-	-	0/1/1/1	-
4	EDO	B	805	-	-	1/1/1/1	-
4	EDO	A	805	-	-	0/1/1/1	-
2	LYS	B	801[A]	1	-	1/5/9/9	-
4	EDO	B	808	-	-	0/1/1/1	-
4	EDO	A	808	-	-	0/1/1/1	-
4	EDO	B	806	-	-	0/1/1/1	-
4	EDO	B	809	-	-	1/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	LYS	CG-CB-CA	3.17	123.33	113.35
2	B	801[A]	LYS	CG-CB-CA	2.70	121.85	113.35
5	B	804	DIO	C2-O1-C1	2.43	118.00	109.89
2	B	801[A]	LYS	CD-CE-NZ	2.27	129.05	112.78
2	A	801	LYS	CD-CE-NZ	2.21	128.61	112.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	EDO	O1-C1-C2-O2
4	B	805	EDO	O1-C1-C2-O2
2	B	801[A]	LYS	CA-CB-CG-CD
4	B	807	EDO	O1-C1-C2-O2
4	A	807	EDO	O1-C1-C2-O2
4	A	810	EDO	O1-C1-C2-O2
2	A	801	LYS	CE-CD-CG-CB
4	B	809	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	LYS	3	0
5	B	804	DIO	2	0
4	B	805	EDO	2	0
2	B	801[A]	LYS	1	0
3	B	802	SO4	1	0
4	B	809	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	580:TRP	C	581[B]:TRQ	N	1.67
1	A	580:TRP	C	581:TRQ	N	1.64

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	679/726 (93%)	-0.26	9 (1%) 77 78	10, 18, 35, 60	0
1	B	680/726 (93%)	-0.29	10 (1%) 73 75	11, 18, 35, 61	0
All	All	1359/1452 (93%)	-0.28	19 (1%) 75 77	10, 18, 35, 61	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	ALA	4.3
1	B	78	PRO	4.1
1	B	79	ASN	3.4
1	A	213	GLY	3.1
1	B	233	SER	2.7
1	B	170	GLY	2.6
1	B	213	GLY	2.6
1	A	683	ALA	2.5
1	A	68	ALA	2.4
1	B	235	ASP	2.4
1	B	70	ASN	2.3
1	B	71	GLU	2.2
1	A	2	ALA	2.2
1	A	540	ARG	2.1
1	A	170	GLY	2.1
1	A	207	ASP	2.1
1	A	171	GLU	2.1
1	B	2	ALA	2.0
1	A	69	SER	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	TRQ	A	581	15/17	0.96	0.13	13,16,24,29	0
1	TRQ	B	581[A]	15/17	0.97	0.12	11,13,16,17	15
1	TRQ	B	581[B]	16/17	0.97	0.12	11,11,12,12	16

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	LYS	B	801[A]	10/10	0.70	0.46	13,18,19,19	10
2	LYS	A	801	10/10	0.78	0.21	24,33,35,35	0
4	EDO	A	810	4/4	0.87	0.15	32,40,41,43	0
4	EDO	B	805	4/4	0.89	0.14	39,39,44,45	0
4	EDO	A	809	4/4	0.89	0.16	30,32,39,40	0
5	DIO	B	804	6/6	0.91	0.16	28,32,35,36	0
4	EDO	A	806	4/4	0.92	0.17	22,30,33,49	0
4	EDO	B	808	4/4	0.92	0.11	36,44,48,54	0
4	EDO	B	806	4/4	0.92	0.10	21,21,22,24	0
4	EDO	B	809	4/4	0.92	0.17	27,35,36,37	0
3	SO4	A	804	5/5	0.93	0.25	58,59,67,73	0
4	EDO	A	808	4/4	0.94	0.18	24,30,31,31	0
3	SO4	B	803	5/5	0.95	0.17	51,58,63,63	0
4	EDO	A	807	4/4	0.95	0.13	28,33,34,35	0
3	SO4	A	802	5/5	0.95	0.21	27,41,47,47	0
4	EDO	B	810	4/4	0.95	0.10	29,35,37,44	0
4	EDO	B	807	4/4	0.96	0.14	26,34,34,41	0
4	EDO	A	805	4/4	0.97	0.08	22,22,24,26	0
3	SO4	B	802	5/5	0.97	0.19	42,45,48,52	0
3	SO4	A	803	5/5	0.97	0.13	45,45,51,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.