



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:12 AM BST

PDB ID : 6LZK
Title : Aquifex aeolicus MutL ATPase domain with K252N mutation
Authors : Fukui, K.; Izuhara, K.; Yano, T.
Deposited on : 2020-02-19
Resolution : 3.16 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 : 2.14.6
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) : 2.14.6

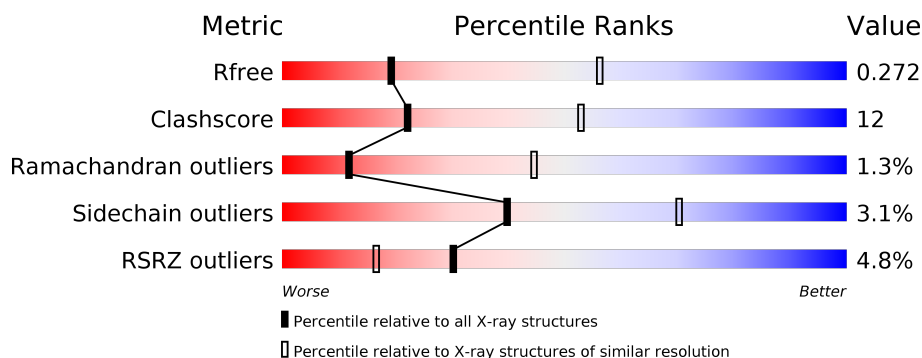
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	308	<div> <div>58%</div> <div>20%</div> <div>•</div> <div>20%</div> </div>
1	B	308	<div>4%</div> <div>61%</div> <div>17%</div> <div>•</div> <div>20%</div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6041 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 DNA mismatch repair protein MutL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			2035	1308	355	370	2			
1	B	247	Total	C	N	O	S	0	0	0
			2035	1308	355	370	2			
1	C	236	Total	C	N	O	S	0	0	0
			1950	1260	334	354	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O67518
A	245	ASN	LYS	engineered mutation	UNP O67518
B	1	MET	-	initiating methionine	UNP O67518
B	245	ASN	LYS	engineered mutation	UNP O67518
C	1	MET	-	initiating methionine	UNP O67518
C	245	ASN	LYS	engineered mutation	UNP O67518

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

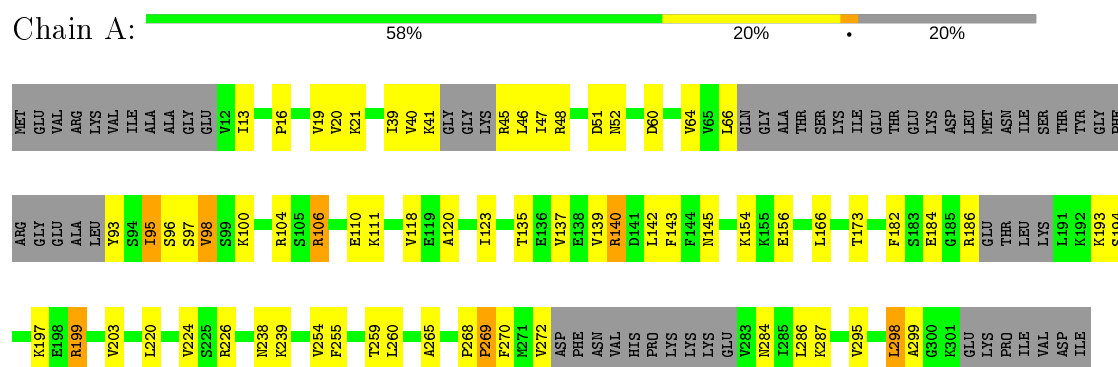
- Molecule 4 is water.

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

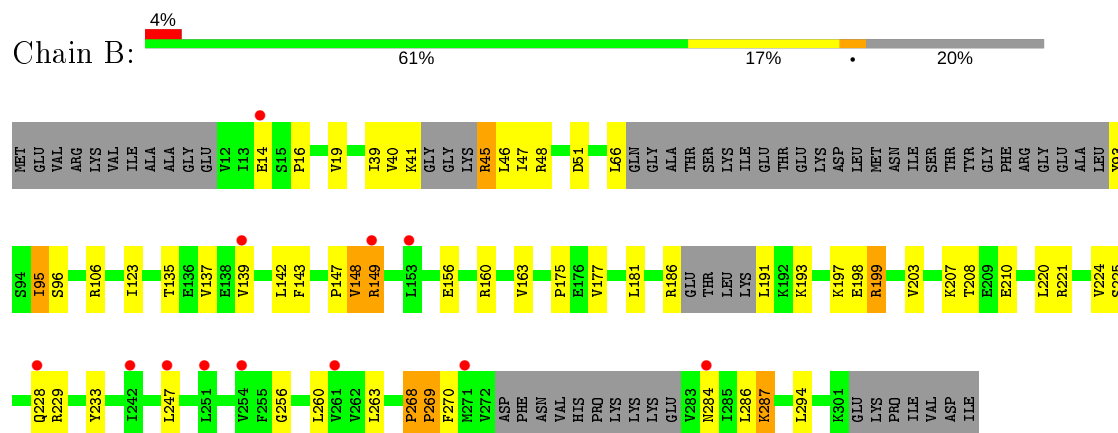
3 Residue-property plots [i](#)

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.

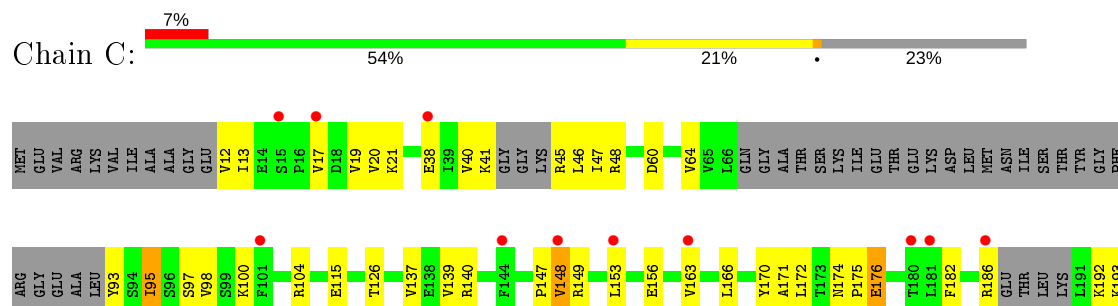
• Molecule 1: DNA mismatch repair protein MutL

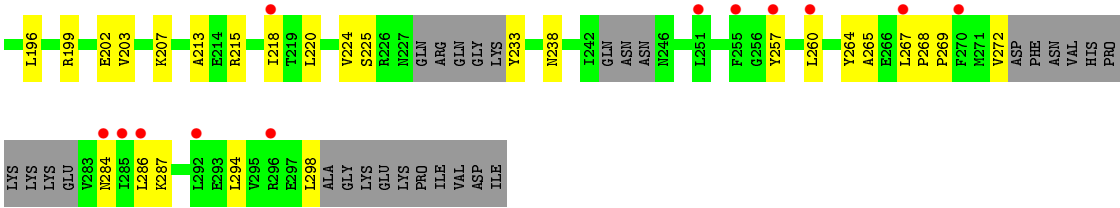


• Molecule 1: DNA mismatch repair protein MutL



• Molecule 1: DNA mismatch repair protein MutL





4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.90 Å 146.29 Å 175.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.36 – 3.16 42.36 – 3.16	Depositor EDS
% Data completeness (in resolution range)	92.3 (42.36-3.16) 92.3 (42.36-3.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.78 (at 3.19 Å)	Xtriage
Refinement program	PHENIX v1.10.1	Depositor
R, R_{free}	0.228 , 0.272 0.228 , 0.272	Depositor DCC
R_{free} test set	1832 reflections (6.89%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6041	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: NA, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/2061	0.57	0/2758
1	B	0.31	0/2061	0.58	0/2758
1	C	0.30	0/1974	0.57	0/2641
All	All	0.31	0/6096	0.57	0/8157

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	2
1	B	0	1
1	C	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	ILE	Peptide
1	A	98	VAL	Peptide
1	B	95	ILE	Peptide
1	C	95	ILE	Peptide
1	C	98	VAL	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	2035	0	2131	63	0
1	B	2035	0	2131	39	0
1	C	1950	0	2043	41	0
2	A	2	0	0	0	0
3	A	14	0	20	2	0
4	A	3	0	0	0	0
4	C	2	0	0	0	0
All	All	6041	0	6325	144	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 12.

All (144) 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:41:LYS:HD3	1:A:45:ARG:NH1	1.29	1.47
1:A:41:LYS:CD	1:A:45:ARG:HH12	1.44	1.30
1:A:41:LYS:CE	1:A:45:ARG:HH22	1.50	1.24
1:A:41:LYS:HE2	1:A:45:ARG:HH22	1.02	1.14
1:C:41:LYS:HB3	1:C:156:GLU:HG3	1.40	1.01
1:A:41:LYS:CE	1:A:45:ARG:NH2	2.24	1.00
1:A:41:LYS:HE2	1:A:45:ARG:NH2	1.85	0.89
1:A:41:LYS:NZ	1:A:45:ARG:NH2	2.24	0.86
1:B:16:PRO:HB3	1:B:47:ILE:HD11	1.59	0.84
1:A:41:LYS:HD3	1:A:45:ARG:CZ	2.10	0.81
1:B:40:VAL:HG22	1:B:46:LEU:HB3	1.66	0.78
1:A:41:LYS:HA	1:A:45:ARG:NH1	1.99	0.78
1:A:106:ARG:NH1	1:A:110:GLU:O	2.17	0.78
1:A:95:ILE:HA	1:A:97:SER:H	1.50	0.77
1:B:193:LYS:HE2	1:B:203:VAL:HG22	1.67	0.75
1:A:41:LYS:HD3	1:A:45:ARG:HH12	0.61	0.72
1:C:224:VAL:HA	1:C:260:LEU:O	1.90	0.71
1:A:193:LYS:HE2	1:A:203:VAL:HG22	1.75	0.69
1:A:41:LYS:CD	1:A:45:ARG:NH1	2.22	0.68
1:C:40:VAL:HG22	1:C:46:LEU:HB3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HB3	1:A:156:GLU:HB2	1.77	0.66
1:A:41:LYS:HZ3	1:A:45:ARG:NH2	1.94	0.66
1:B:147:PRO:O	1:B:148:VAL:HG12	1.96	0.65
1:C:95:ILE:HA	1:C:97:SER:H	1.63	0.63
1:A:41:LYS:CG	1:A:45:ARG:HH12	2.10	0.63
1:C:172:LEU:HD21	1:C:203:VAL:HG11	1.82	0.61
1:C:286:LEU:CD1	1:C:287:LYS:H	2.14	0.61
1:A:106:ARG:NH1	1:A:111:LYS:HA	2.16	0.61
1:B:210:GLU:OE2	1:B:221:ARG:NH2	2.24	0.59
1:A:51:ASP:HB3	1:A:135:THR:H	1.67	0.59
1:A:16:PRO:HB3	1:A:47:ILE:HD11	1.84	0.59
1:B:220:LEU:HD13	1:B:263:LEU:HD11	1.84	0.58
1:A:220:LEU:HD12	1:A:298:LEU:HD13	1.85	0.58
1:A:40:VAL:O	1:A:45:ARG:HA	2.02	0.58
1:C:147:PRO:O	1:C:148:VAL:HG12	2.03	0.57
1:A:184:GLU:N	1:A:184:GLU:OE1	2.36	0.57
1:B:270:PHE:HE2	1:B:287:LYS:HD3	1.69	0.57
1:B:224:VAL:HA	1:B:260:LEU:O	2.04	0.57
1:C:233:TYR:OH	1:C:257:TYR:O	2.22	0.57
1:A:41:LYS:CD	1:A:45:ARG:HH22	2.14	0.57
1:C:19:VAL:HG11	1:C:139:VAL:HG21	1.87	0.57
1:A:41:LYS:CB	1:A:45:ARG:HH12	2.18	0.56
1:A:19:VAL:HG11	1:A:139:VAL:HG21	1.87	0.56
1:A:95:ILE:CA	1:A:97:SER:H	2.19	0.56
1:B:41:LYS:HB3	1:B:156:GLU:HG3	1.87	0.55
1:C:286:LEU:HD12	1:C:287:LYS:H	1.71	0.55
1:A:226:ARG:HA	1:A:259:THR:HG22	1.88	0.54
1:A:48:ARG:HA	1:A:137:VAL:O	2.07	0.54
1:B:41:LYS:HG3	1:B:160:ARG:HB2	1.90	0.54
1:C:20:VAL:HG23	1:C:166:LEU:HD23	1.88	0.54
1:C:12:VAL:HG13	1:C:13:ILE:HG12	1.90	0.54
1:C:196:LEU:HD11	1:C:202:GLU:HG3	1.90	0.54
1:A:41:LYS:CA	1:A:45:ARG:NH1	2.71	0.54
1:B:225:SER:O	1:B:228:GLN:NE2	2.42	0.53
1:A:41:LYS:HA	1:A:45:ARG:CZ	2.39	0.52
1:A:60:ASP:O	1:A:64:VAL:HG13	2.10	0.52
1:B:181:LEU:HB3	1:B:191:LEU:HA	1.91	0.52
1:A:182:PHE:CE1	1:A:186:ARG:HB2	2.44	0.51
1:A:173:THR:HG23	1:A:239:LYS:HG2	1.91	0.51
1:A:182:PHE:HE1	1:A:186:ARG:HB2	1.75	0.51
1:B:268:PRO:HB2	1:B:269:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LYS:HD2	1:C:199:ARG:HE	1.74	0.51
1:A:269:PRO:HD2	1:A:270:PHE:CE2	2.46	0.51
1:C:220:LEU:HA	1:C:264:TYR:O	2.11	0.50
1:C:286:LEU:HD12	1:C:287:LYS:N	2.24	0.50
1:A:40:VAL:HG22	1:A:46:LEU:HB3	1.92	0.50
1:B:51:ASP:HB2	1:B:135:THR:O	2.12	0.50
1:A:41:LYS:CB	1:A:156:GLU:HB2	2.42	0.50
1:A:13:ILE:HG13	1:A:96:SER:HB2	1.94	0.49
1:A:100:LYS:HB3	1:A:140:ARG:O	2.12	0.49
1:B:177:VAL:O	1:B:199:ARG:NH2	2.45	0.49
1:A:41:LYS:CD	1:A:45:ARG:NH2	2.72	0.49
1:B:208:THR:OG1	1:B:224:VAL:N	2.46	0.49
1:A:295:VAL:O	1:A:298:LEU:HD23	2.13	0.48
1:A:270:PHE:HE1	1:A:287:LYS:HG2	1.79	0.48
1:B:51:ASP:HB3	1:B:135:THR:H	1.78	0.48
1:C:272:VAL:HA	1:C:284:ASN:HB3	1.95	0.48
1:C:170:TYR:O	1:C:174:ASN:ND2	2.46	0.48
1:C:175:PRO:HA	1:C:199:ARG:HH11	1.78	0.48
1:A:270:PHE:CD1	1:A:286:LEU:HA	2.49	0.48
1:A:39:ILE:HA	1:A:46:LEU:O	2.14	0.48
1:B:228:GLN:O	1:B:229:ARG:HG2	2.14	0.47
1:B:39:ILE:HA	1:B:46:LEU:O	2.14	0.47
1:A:41:LYS:CB	1:A:45:ARG:NH1	2.77	0.47
1:B:48:ARG:HA	1:B:137:VAL:O	2.14	0.47
1:C:41:LYS:HA	1:C:45:ARG:NH1	2.29	0.47
1:C:95:ILE:CA	1:C:97:SER:H	2.28	0.47
1:A:20:VAL:HG23	1:A:166:LEU:HD23	1.97	0.47
1:A:118:VAL:HG12	1:A:123:ILE:HA	1.96	0.47
1:B:142:LEU:HG	1:B:143:PHE:CD2	2.48	0.47
1:B:39:ILE:HD13	1:B:163:VAL:HG11	1.95	0.47
1:A:98:VAL:HG12	1:A:145:ASN:HD21	1.79	0.47
1:B:95:ILE:O	1:B:96:SER:HB3	2.15	0.47
1:C:47:ILE:HB	1:C:139:VAL:HB	1.96	0.47
1:C:149:ARG:O	1:C:153:LEU:HD13	2.15	0.47
1:C:100:LYS:HB3	1:C:140:ARG:O	2.15	0.46
1:C:176:GLU:CD	1:C:176:GLU:H	2.19	0.46
1:B:14:GLU:O	1:B:143:PHE:HE2	1.98	0.46
1:C:267:LEU:HD22	1:C:286:LEU:HD22	1.97	0.46
1:B:66:LEU:HD21	1:B:123:ILE:HD11	1.98	0.46
1:C:267:LEU:HD13	1:C:286:LEU:HD22	1.97	0.46
1:C:171:ALA:HB1	1:C:199:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LYS:O	1:C:225:SER:OG	2.17	0.46
1:B:45:ARG:HH21	1:B:47:ILE:HG13	1.81	0.46
1:C:238:ASN:N	1:C:265:ALA:O	2.48	0.46
1:B:41:LYS:CB	1:B:156:GLU:HG3	2.46	0.45
1:C:186:ARG:HH21	1:C:192:LYS:HD3	1.81	0.45
1:C:48:ARG:HA	1:C:137:VAL:O	2.16	0.45
1:A:154:LYS:N	1:A:154:LYS:HD2	2.30	0.45
1:A:272:VAL:HG23	1:A:284:ASN:HB3	1.99	0.45
1:C:213:ALA:HB2	1:C:298:LEU:HB3	1.98	0.45
3:A:403:PEG:H21	3:A:404:PEG:H11	1.99	0.45
1:A:224:VAL:HA	1:A:260:LEU:O	2.17	0.44
1:A:238:ASN:N	1:A:265:ALA:O	2.50	0.44
1:C:218:ILE:HG12	1:C:267:LEU:HD21	1.99	0.44
1:C:41:LYS:HD2	1:C:45:ARG:HH12	1.82	0.44
1:B:19:VAL:HG11	1:B:139:VAL:HG21	1.99	0.44
1:B:268:PRO:CB	1:B:269:PRO:HD3	2.48	0.44
1:B:149:ARG:HD3	1:B:149:ARG:HA	1.83	0.44
1:A:51:ASP:HB2	1:A:135:THR:O	2.18	0.44
1:C:284:ASN:N	1:C:284:ASN:OD1	2.51	0.43
1:C:17:VAL:HG23	1:C:163:VAL:HA	1.99	0.43
1:A:270:PHE:HD1	1:A:286:LEU:HA	1.84	0.43
1:C:215:ARG:HB2	1:C:294:LEU:HD21	2.01	0.43
1:A:194:SER:O	1:A:199:ARG:NH2	2.52	0.43
1:A:98:VAL:HG13	1:A:120:ALA:C	2.38	0.43
1:B:175:PRO:HA	1:B:199:ARG:NH1	2.34	0.42
1:C:115:GLU:O	1:C:126:THR:HA	2.19	0.42
1:A:142:LEU:HG	1:A:143:PHE:CD2	2.54	0.42
1:A:254:VAL:HG12	1:A:299:ALA:CB	2.49	0.42
1:A:95:ILE:HG23	1:A:98:VAL:HG23	2.00	0.42
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.87	0.42
1:A:226:ARG:NH2	1:A:255:PHE:O	2.53	0.42
1:B:294:LEU:HA	1:B:294:LEU:HD23	1.88	0.42
1:B:233:TYR:OH	1:B:256:GLY:O	2.30	0.42
1:B:284:ASN:N	1:B:284:ASN:OD1	2.51	0.41
1:B:41:LYS:HE2	1:B:45:ARG:HH12	1.86	0.41
1:C:60:ASP:O	1:C:64:VAL:HG13	2.20	0.41
1:A:45:ARG:N	3:A:404:PEG:HO4	2.18	0.41
1:B:40:VAL:O	1:B:45:ARG:HA	2.20	0.41
1:B:270:PHE:CD2	1:B:286:LEU:HA	2.56	0.41
1:B:197:LYS:HG3	1:B:198:GLU:H	1.85	0.40
1:A:118:VAL:HG12	1:A:123:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:HG3	1:C:182:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/308 (77%)	219 (92%)	15 (6%)	3 (1%)	12	44
1	B	237/308 (77%)	217 (92%)	17 (7%)	3 (1%)	12	44
1	C	222/308 (72%)	205 (92%)	14 (6%)	3 (1%)	11	43
All	All	696/924 (75%)	641 (92%)	46 (7%)	9 (1%)	12	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	VAL
1	B	269	PRO
1	C	148	VAL
1	A	268	PRO
1	A	269	PRO
1	C	269	PRO
1	B	268	PRO
1	A	140	ARG
1	C	268	PRO

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	227/278 (82%)	218 (96%)	9 (4%)	31	64
1	B	227/278 (82%)	219 (96%)	8 (4%)	36	67
1	C	219/278 (79%)	215 (98%)	4 (2%)	59	81
All	All	673/834 (81%)	652 (97%)	21 (3%)	40	70

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	52	ASN
1	A	66	LEU
1	A	93	TYR
1	A	104	ARG
1	A	106	ARG
1	A	197	LYS
1	A	199	ARG
1	A	298	LEU
1	B	45	ARG
1	B	93	TYR
1	B	106	ARG
1	B	149	ARG
1	B	186	ARG
1	B	199	ARG
1	B	207	LYS
1	B	287	LYS
1	C	21	LYS
1	C	93	TYR
1	C	104	ARG
1	C	176	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	PEG	A	403	-	6,6,6	0.42	0	5,5,5	0.49	0
3	PEG	A	404	-	6,6,6	0.41	0	5,5,5	0.47	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
3	PEG	A	403	-	-	2/4/4/4	-
3	PEG	A	404	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	PEG	O2-C3-C4-O4
3	A	403	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	A	404	PEG	O1-C1-C2-O2
3	A	403	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	PEG	1	0
3	A	404	PEG	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 ⓘ

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, 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	247/308 (80%)	0.06	0 100 100	37, 59, 96, 117	0
1	B	247/308 (80%)	0.46	12 (4%) 29 16	66, 102, 135, 174	0
1	C	236/308 (76%)	0.66	23 (9%) 7 4	51, 124, 161, 178	0
All	All	730/924 (79%)	0.39	35 (4%) 30 17	37, 94, 152, 178	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	270	PHE	4.0
1	C	260	LEU	3.4
1	B	14	GLU	3.2
1	C	285	ILE	3.2
1	C	148	VAL	3.2
1	C	17	VAL	3.1
1	C	15	SER	3.0
1	C	255	PHE	3.0
1	B	271	MET	2.9
1	C	186	ARG	2.9
1	B	251	LEU	2.9
1	B	153	LEU	2.7
1	C	267	LEU	2.7
1	C	218	ILE	2.7
1	C	257	TYR	2.5
1	B	228	GLN	2.5
1	C	181	LEU	2.5
1	B	284	ASN	2.4
1	C	180	THR	2.4
1	C	284	ASN	2.4
1	C	292	LEU	2.3
1	B	149	ARG	2.3
1	C	296	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	139	VAL	2.2
1	B	242	ILE	2.1
1	C	101	PHE	2.1
1	C	251	LEU	2.1
1	C	144	PHE	2.1
1	C	153	LEU	2.1
1	C	38	GLU	2.0
1	C	286	LEU	2.0
1	B	261	VAL	2.0
1	C	163	VAL	2.0
1	B	247	LEU	2.0
1	B	254	VAL	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, 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(\AA^2)	Q<0.9
3	PEG	A	404	7/7	0.70	0.30	96,98,107,110	0
3	PEG	A	403	7/7	0.84	0.32	76,87,94,95	0
2	NA	A	402	1/1	0.85	0.42	56,56,56,56	0
2	NA	A	401	1/1	0.86	0.37	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.