Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 12:22 PM JST

PDB ID	:	8JZI
Title	:	Mutant S-adenosylmethionine synthase from C. glutamicum
Authors	:	Lee, S.; Kim, K.J.
Deposited on	:	2023-07-05
Resolution	:	1.76 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.36
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)	:	2.36

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 1.76 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	Percentile Ranks	Value
Rfree		0.226
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.4%
RSRZ outliers		6.7%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
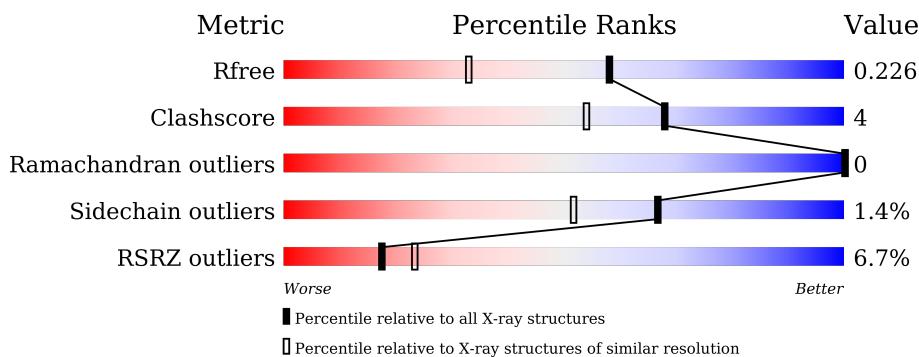
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	407	3% / 87% / 7% / 6%
1	B	407	5% / 84% / 9% / 7%
1	C	407	5% / 86% / 8% / 6%
1	D	407	11% / 88% / 6% / 6%
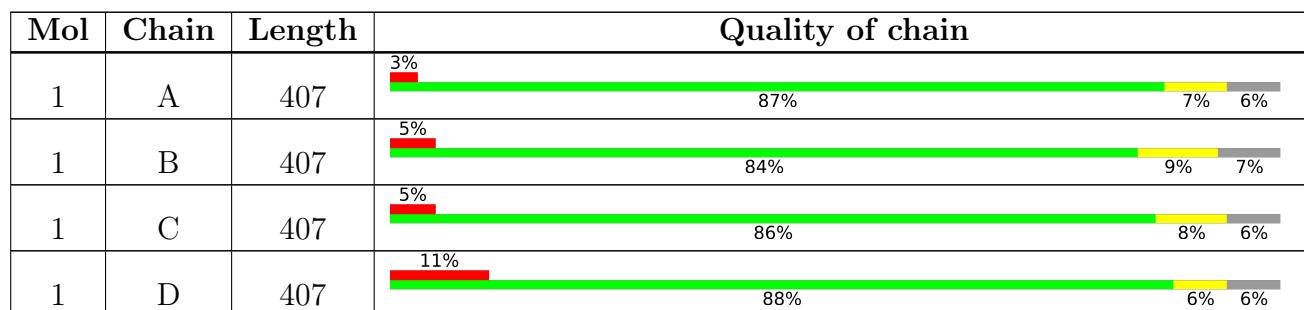
2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 12969 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 S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2933	1840	516	570	7			
1	B	380	Total	C	N	O	S	0	0	0
			2913	1829	510	567	7			
1	C	382	Total	C	N	O	S	0	0	0
			2918	1832	513	566	7			
1	D	383	Total	C	N	O	S	0	0	0
			2927	1837	515	568	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ALA	GLU	engineered mutation	UNP Q9K5E4
B	68	ALA	GLU	engineered mutation	UNP Q9K5E4
C	68	ALA	GLU	engineered mutation	UNP Q9K5E4
D	68	ALA	GLU	engineered mutation	UNP Q9K5E4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

GOL

C3

OH O3

C1 C2

HO OH

O1 O2
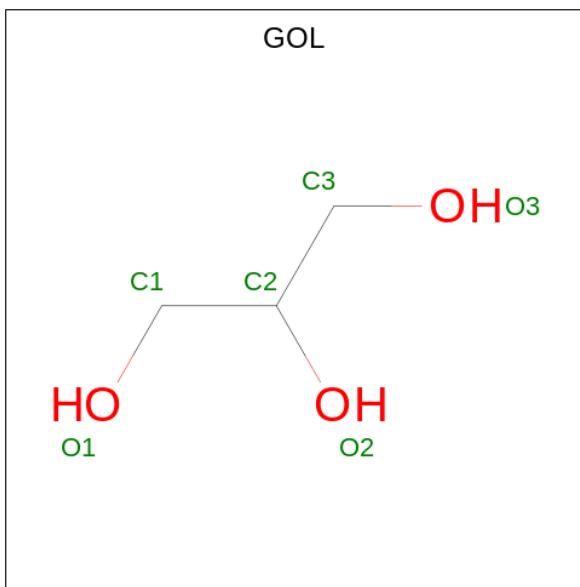
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0	0
2	D	1	Total 6	C 3	O 3	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

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PROTEIN DATA BANK

MES
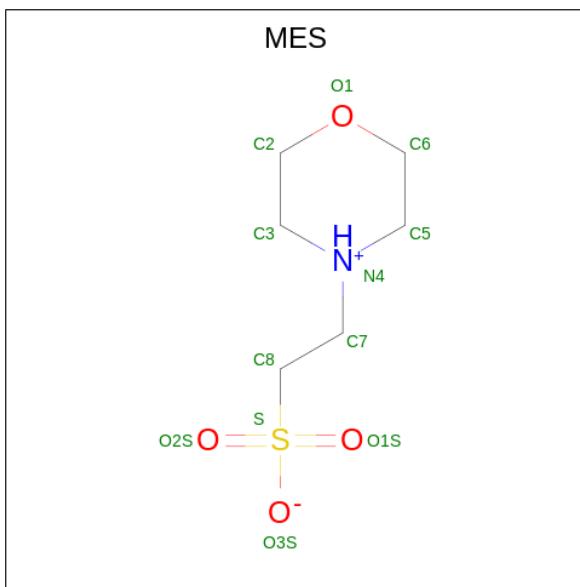
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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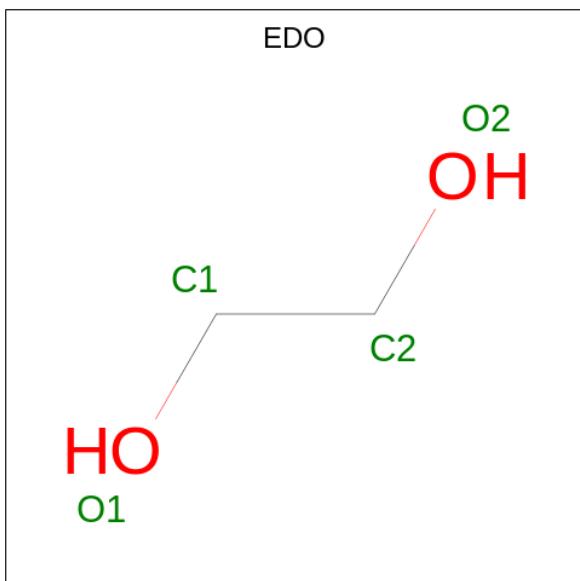
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total C O 4 2 2			0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	353	Total O 353 353		0	0
6	B	367	Total O 367 367		0	0
6	C	316	Total O 316 316		0	0
6	D	186	Total O 186 186		0	0

3 Residue-property plots ⓘ

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: S-adenosylmethionine synthase
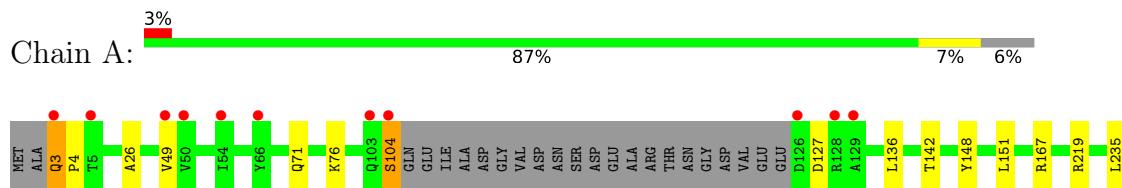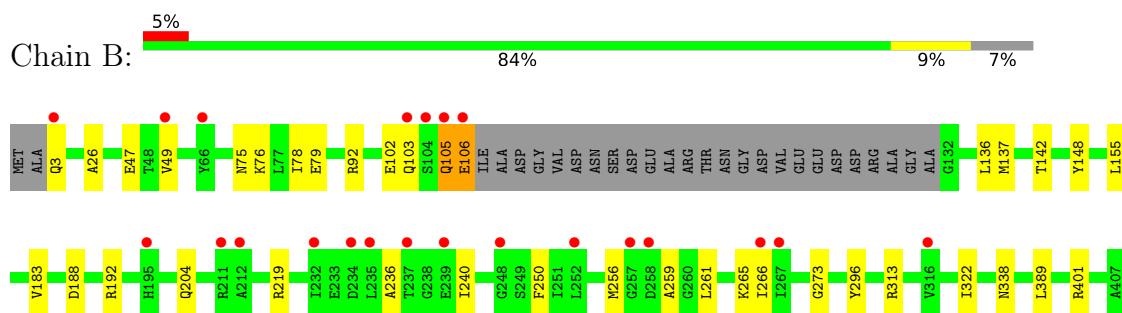
Chain A:

- Molecule 1: S-adenosylmethionine synthase

Chain B:

- Molecule 1: S-adenosylmethionine synthase

Chain C:

- Molecule 1: S-adenosylmethionine synthase

Chain D:
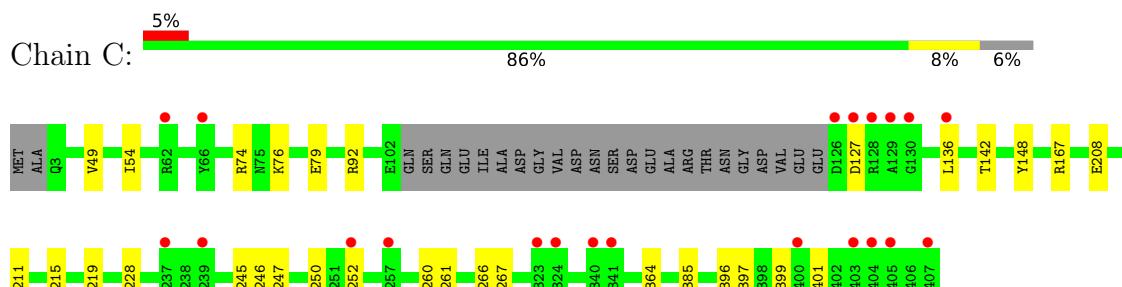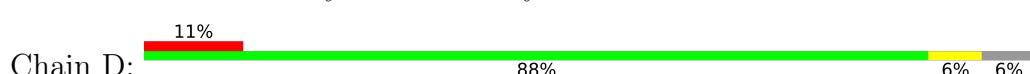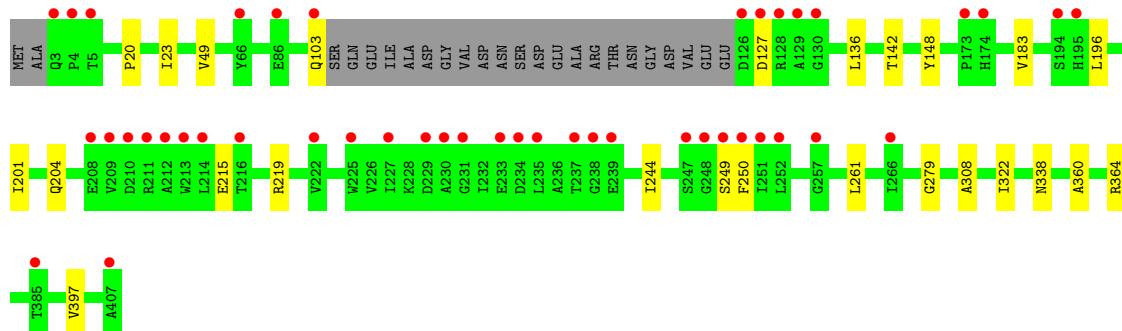
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.40Å　　125.44Å　　116.31Å 90.00°　　128.91°　　90.00°	Depositor
Resolution (Å)	31.55　–　1.76 31.53　–　1.76	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.55-1.76) 99.3 (31.53-1.76)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.36 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182　,　0.218 0.194　,　0.226	Depositor DCC
R_{free} test set	8140 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.0	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12969	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, NA, MES, GOL

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	0.78	0/2985	0.88	2/4055 (0.0%)
1	B	0.77	0/2965	0.91	5/4028 (0.1%)
1	C	0.78	0/2970	0.90	3/4035 (0.1%)
1	D	0.78	0/2979	0.89	0/4047
All	All	0.78	0/11899	0.89	10/16165 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	313	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	167	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	C	167	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	B	296	TYR	CB-CG-CD1	5.77	124.46	121.00
1	B	296	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	C	92	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	219	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	401	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	219	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	C	167	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2933	0	2908	23	0
1	B	2913	0	2890	24	0
1	C	2918	0	2895	33	0
1	D	2927	0	2903	17	0
2	A	12	0	16	4	0
2	B	12	0	16	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	12	0	13	1	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	B	4	0	6	1	0
6	A	353	0	0	3	0
6	B	367	0	0	6	0
6	C	316	0	0	12	0
6	D	186	0	0	0	0
All	All	12969	0	11663	88	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 (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:503:GOL:H32	6:B:710:HOH:O	1.60	0.99
1:A:49:VAL:HG21	1:B:49:VAL:HG21	1.50	0.92
1:A:104:SER:HB3	6:A:787:HOH:O	1.74	0.87
1:C:49:VAL:HG21	1:D:49:VAL:HG21	1.62	0.81
1:C:266:ILE:HG13	1:C:267:ILE:HD12	1.60	0.81
1:C:54:ILE:CG1	6:C:639:HOH:O	2.30	0.80
1:C:54:ILE:HG13	6:C:639:HOH:O	1.83	0.79
1:B:105:GLN:HG2	1:B:106:GLU:HG3	1.63	0.78
1:C:385:THR:HB	6:C:779:HOH:O	1.82	0.78
1:A:274:MET:SD	2:A:501:GOL:H32	2.26	0.76
1:C:267:ILE:HD13	1:D:279:GLY:HA2	1.72	0.71
1:A:127:ASP:OD1	1:A:364:ARG:NH1	2.23	0.70
1:A:260:GLY:C	1:A:261:LEU:HD12	2.14	0.68
1:A:104:SER:CB	6:A:787:HOH:O	2.35	0.64
1:A:151:LEU:HD21	1:A:235:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LEU:HG	6:C:783:HOH:O	1.98	0.63
1:C:266:ILE:CG1	1:C:267:ILE:HD12	2.27	0.62
1:A:127:ASP:HA	1:A:360:ALA:HB3	1.84	0.60
1:B:75:ASN:O	1:B:79:GLU:HG3	2.01	0.60
1:C:142:THR:O	1:C:148:TYR:HA	2.02	0.59
1:C:260:GLY:C	1:C:261:LEU:HD12	2.23	0.58
1:D:49:VAL:HG13	1:D:261:LEU:CD1	2.34	0.57
1:C:76:LYS:NZ	1:C:79:GLU:OE1	2.30	0.57
1:C:266:ILE:HG13	1:C:267:ILE:CD1	2.33	0.56
1:A:142:THR:O	1:A:148:TYR:HA	2.05	0.56
1:B:78:ILE:HD11	1:B:92:ARG:HG3	1.87	0.55
1:B:142:THR:O	1:B:148:TYR:HA	2.05	0.55
1:C:54:ILE:HD11	6:C:639:HOH:O	2.06	0.55
1:B:204:GLN:HA	1:B:250:PHE:O	2.06	0.55
1:D:49:VAL:HG13	1:D:261:LEU:HD12	1.89	0.55
1:A:252:LEU:HD22	1:A:252:LEU:N	2.21	0.55
1:C:228:LYS:HE2	6:C:874:HOH:O	2.07	0.55
1:D:142:THR:O	1:D:148:TYR:HA	2.07	0.54
5:B:502:EDO:C2	6:B:708:HOH:O	2.55	0.54
1:C:266:ILE:CG1	1:C:267:ILE:CD1	2.86	0.54
1:B:92:ARG:HD2	6:B:905:HOH:O	2.08	0.53
1:C:54:ILE:CD1	6:C:639:HOH:O	2.55	0.53
1:C:228:LYS:HD2	6:C:733:HOH:O	2.08	0.53
1:D:201:ILE:HB	1:D:244:ILE:HD13	1.90	0.53
1:C:267:ILE:HD12	1:C:267:ILE:N	2.22	0.53
1:D:308:ALA:HA	1:D:397:VAL:HG13	1.90	0.53
1:A:285:LYS:NZ	2:A:503:GOL:O2	2.37	0.52
1:C:245:ASN:N	1:C:246:PRO:CD	2.73	0.51
1:C:127:ASP:OD2	1:C:364:ARG:NH1	2.44	0.51
2:A:503:GOL:H31	1:B:265:LYS:NZ	2.26	0.50
1:A:3:GLN:N	1:A:4:PRO:CD	2.75	0.49
1:B:155:LEU:HD23	1:B:183:VAL:HG11	1.94	0.49
1:B:259:ALA:N	6:B:611:HOH:O	2.45	0.49
1:B:49:VAL:HG13	1:B:261:LEU:CD2	2.43	0.49
1:D:127:ASP:HA	1:D:360:ALA:HB3	1.94	0.49
1:C:211:ARG:HG2	6:C:616:HOH:O	2.13	0.48
1:B:49:VAL:HG13	1:B:261:LEU:HD23	1.95	0.47
1:A:261:LEU:HD12	1:A:261:LEU:N	2.29	0.47
1:C:397:VAL:O	1:C:401:ARG:HG2	2.14	0.47
3:A:502:MES:H22	6:A:676:HOH:O	2.15	0.47
1:A:26:ALA:HB1	1:A:76:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:GLU:O	1:D:219:ARG:HG3	2.15	0.47
1:B:188:ASP:OD2	1:B:192:ARG:NH1	2.48	0.46
1:D:20:PRO:HA	1:D:23:ILE:HD12	1.98	0.46
1:C:267:ILE:HD13	1:D:279:GLY:CA	2.43	0.45
1:D:127:ASP:OD2	1:D:364:ARG:NH1	2.50	0.45
1:D:204:GLN:HA	1:D:250:PHE:O	2.17	0.44
1:C:267:ILE:CD1	1:C:267:ILE:N	2.80	0.44
1:C:396:ARG:HD3	1:C:399:GLU:OE1	2.18	0.44
1:A:266:ILE:HD11	1:B:266:ILE:HD11	1.99	0.44
1:D:183:VAL:HG13	1:D:196:LEU:HD11	2.00	0.44
1:A:71:GLN:HG2	1:D:103:GLN:OE1	2.18	0.43
1:A:246:PRO:HG2	1:B:322:ILE:HB	2.01	0.43
1:C:76:LYS:HA	1:C:76:LYS:HD3	1.85	0.43
1:C:208:GLU:HG3	6:C:626:HOH:O	2.17	0.43
1:A:49:VAL:HG21	1:B:49:VAL:CG2	2.33	0.43
1:C:228:LYS:CE	6:C:874:HOH:O	2.66	0.43
1:C:247:SER:HB3	1:D:322:ILE:HG12	2.00	0.43
1:B:389:LEU:HD12	6:B:849:HOH:O	2.19	0.43
1:C:228:LYS:HE2	6:C:762:HOH:O	2.19	0.43
1:A:245:ASN:N	1:A:246:PRO:CD	2.82	0.43
1:A:243:LEU:HD21	6:B:902:HOH:O	2.19	0.43
1:B:236:ALA:O	1:B:240:ILE:HD11	2.19	0.43
1:B:105:GLN:HE22	1:C:74:ARG:HD2	1.84	0.42
1:B:102:GLU:O	1:B:103:GLN:HG3	2.19	0.42
1:A:261:LEU:HD11	1:B:47:GLU:HG3	2.01	0.42
1:A:276:ARG:HD2	1:B:273:GLY:O	2.19	0.42
1:B:26:ALA:HB1	1:B:76:LYS:HE3	2.00	0.42
1:B:192:ARG:NH1	1:B:192:ARG:HB2	2.34	0.42
1:C:215:GLU:O	1:C:219:ARG:HG3	2.21	0.41
1:D:183:VAL:HG13	1:D:196:LEU:CD1	2.51	0.41
1:A:251:ILE:HG22	1:A:252:LEU:HD22	2.02	0.41
1:C:266:ILE:HG12	1:C:267:ILE:CD1	2.51	0.41

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	380/407 (93%)	367 (97%)	13 (3%)	0	100	100
1	B	376/407 (92%)	361 (96%)	15 (4%)	0	100	100
1	C	378/407 (93%)	368 (97%)	10 (3%)	0	100	100
1	D	379/407 (93%)	366 (97%)	13 (3%)	0	100	100
All	All	1513/1628 (93%)	1462 (97%)	51 (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	308/327 (94%)	303 (98%)	5 (2%)	62	45
1	B	308/327 (94%)	301 (98%)	7 (2%)	50	28
1	C	306/327 (94%)	304 (99%)	2 (1%)	84	75
1	D	307/327 (94%)	304 (99%)	3 (1%)	76	63
All	All	1229/1308 (94%)	1212 (99%)	17 (1%)	67	52

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	104	SER
1	A	136	LEU
1	A	250	PHE
1	A	326	LYS
1	B	3	GLN
1	B	105	GLN
1	B	106	GLU

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Mol	Chain	Res	Type
1	B	136	LEU
1	B	137	MET
1	B	256	MET
1	B	338	ASN
1	C	136	LEU
1	C	250	PHE
1	D	136	LEU
1	D	249	SER
1	D	338	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	C	71	GLN

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#|Z| > 2$
2	GOL	B	503	-	5,5,5	0.32	0	5,5,5	0.35	0
2	GOL	A	501	-	5,5,5	0.17	0	5,5,5	1.25	1 (20%)
3	MES	A	502	-	12,12,12	0.78	0	14,16,16	0.76	1 (7%)
2	GOL	B	501	-	5,5,5	0.11	0	5,5,5	0.52	0
2	GOL	C	501	-	5,5,5	0.22	0	5,5,5	0.51	0
2	GOL	D	501	-	5,5,5	0.10	0	5,5,5	0.26	0
2	GOL	A	503	-	5,5,5	0.18	0	5,5,5	0.65	0
5	EDO	B	502	-	3,3,3	0.24	0	2,2,2	1.00	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	GOL	B	503	-	-	0/4/4/4	-
2	GOL	A	501	-	-	3/4/4/4	-
3	MES	A	502	-	-	3/6/14/14	0/1/1/1
2	GOL	B	501	-	-	2/4/4/4	-
2	GOL	C	501	-	-	1/4/4/4	-
2	GOL	D	501	-	-	2/4/4/4	-
2	GOL	A	503	-	-	4/4/4/4	-
5	EDO	B	502	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	GOL	O2-C2-C3	2.38	119.59	109.12
3	A	502	MES	O2S-S-C8	-2.19	104.27	106.92

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	GOL	O1-C1-C2-O2
2	A	503	GOL	O1-C1-C2-C3
2	A	503	GOL	C1-C2-C3-O3
2	B	501	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	502	MES	C7-C8-S-O2S
3	A	502	MES	C7-C8-S-O3S
2	A	501	GOL	O1-C1-C2-O2
2	B	501	GOL	O1-C1-C2-O2
2	A	501	GOL	O1-C1-C2-C3
2	D	501	GOL	O1-C1-C2-C3
2	A	503	GOL	O2-C2-C3-O3
2	A	501	GOL	O2-C2-C3-O3
2	D	501	GOL	O1-C1-C2-O2
5	B	502	EDO	O1-C1-C2-O2
3	A	502	MES	C7-C8-S-O1S
2	C	501	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	1	0
3	A	502	MES	1	0
2	A	503	GOL	3	0
5	B	502	EDO	1	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	384/407 (94%)	0.30	14 (3%)	42	49	9, 15, 32, 54	0
1	B	380/407 (93%)	0.39	22 (5%)	23	28	10, 16, 32, 81	0
1	C	382/407 (93%)	0.44	21 (5%)	25	31	10, 18, 37, 73	0
1	D	383/407 (94%)	0.81	45 (11%)	4	6	12, 22, 43, 61	0
All	All	1529/1628 (93%)	0.48	102 (6%)	17	23	9, 18, 37, 81	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	ARG	8.0
1	C	126	ASP	7.7
1	B	105	GLN	7.0
1	D	66	TYR	6.4
1	A	103	GLN	5.9
1	C	129	ALA	5.6
1	C	407	ALA	5.3
1	A	126	ASP	5.1
1	B	66	TYR	4.9
1	D	195	HIS	4.9
1	D	3	GLN	4.8
1	D	239	GLU	4.8
1	B	106	GLU	4.8
1	A	104	SER	4.7
1	D	126	ASP	4.7
1	D	209	VAL	4.6
1	A	3	GLN	4.5
1	D	234	ASP	4.3
1	D	212	ALA	4.2
1	D	213	TRP	4.2
1	A	66	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	235	LEU	4.1
1	A	407	ALA	4.0
1	D	5	THR	3.9
1	D	4	PRO	3.9
1	B	257	GLY	3.9
1	D	407	ALA	3.9
1	D	127	ASP	3.8
1	C	130	GLY	3.8
1	B	3	GLN	3.8
1	D	103	GLN	3.8
1	B	239	GLU	3.8
1	D	128	ARG	3.6
1	D	247	SER	3.5
1	A	129	ALA	3.5
1	C	404	LEU	3.5
1	B	211	ARG	3.5
1	C	323	GLY	3.4
1	D	214	LEU	3.4
1	C	127	ASP	3.3
1	C	341	GLY	3.2
1	C	257	GLY	3.2
1	D	231	GLY	3.1
1	C	252	LEU	3.1
1	D	225	TRP	3.1
1	D	210	ASP	3.0
1	C	66	TYR	3.0
1	C	405	LYS	3.0
1	D	227	ILE	2.9
1	D	249	SER	2.9
1	B	195	HIS	2.9
1	D	252	LEU	2.8
1	D	130	GLY	2.6
1	D	129	ALA	2.6
1	A	49	VAL	2.6
1	D	385	THR	2.5
1	D	86	GLU	2.5
1	D	248	GLY	2.5
1	C	340	GLU	2.5
1	D	250	PHE	2.5
1	D	211	ARG	2.5
1	D	266	ILE	2.5
1	D	238	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	230	ALA	2.5
1	B	232	ILE	2.5
1	A	128	ARG	2.4
1	B	316	VAL	2.4
1	B	267	ILE	2.4
1	A	238	GLY	2.4
1	A	340	GLU	2.3
1	D	257	GLY	2.3
1	D	237	THR	2.3
1	B	235	LEU	2.3
1	D	233	GLU	2.3
1	B	234	ASP	2.3
1	A	5	THR	2.3
1	B	252	LEU	2.3
1	D	208	GLU	2.3
1	B	258	ASP	2.3
1	B	104	SER	2.2
1	D	251	ILE	2.2
1	D	194	SER	2.2
1	D	216	THR	2.2
1	B	49	VAL	2.2
1	C	403	ALA	2.2
1	D	222	VAL	2.2
1	C	324	ARG	2.2
1	C	239	GLU	2.2
1	D	174	HIS	2.2
1	B	266	ILE	2.2
1	C	136	LEU	2.1
1	D	229	ASP	2.1
1	B	237	THR	2.1
1	D	173	PRO	2.1
1	C	400	LEU	2.1
1	A	54	ILE	2.1
1	C	62	ARG	2.1
1	A	50	VAL	2.1
1	B	103	GLN	2.1
1	B	212	ALA	2.1
1	C	237	THR	2.0
1	B	248	GLY	2.0

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

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

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	GOL	D	501	6/6	0.76	0.18	49,51,54,54	0
3	MES	A	502	12/12	0.80	0.25	28,48,51,52	0
2	GOL	A	503	6/6	0.87	0.17	25,27,33,35	0
5	EDO	B	502	4/4	0.90	0.14	25,28,30,33	0
2	GOL	B	503	6/6	0.92	0.15	16,20,21,25	0
2	GOL	B	501	6/6	0.92	0.11	22,26,30,31	0
2	GOL	A	501	6/6	0.93	0.13	21,24,25,25	0
4	NA	C	503	1/1	0.97	0.12	16,16,16,16	0
2	GOL	C	501	6/6	0.98	0.09	19,25,27,28	0
4	NA	A	504	1/1	0.98	0.16	8,8,8,8	0
4	NA	C	502	1/1	0.99	0.21	10,10,10,10	0
4	NA	A	505	1/1	1.00	0.14	6,6,6,6	0

6.5 Other polymers ⓘ

There are no such residues in this entry.