Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 12:22 PM JST

PDB ID	:	8JZH
Title	:	C. glutamicum S-adenosylmethionine synthase
Authors	:	Lee, S.; Kim, K.J.
Deposited on	:	2023-07-05
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

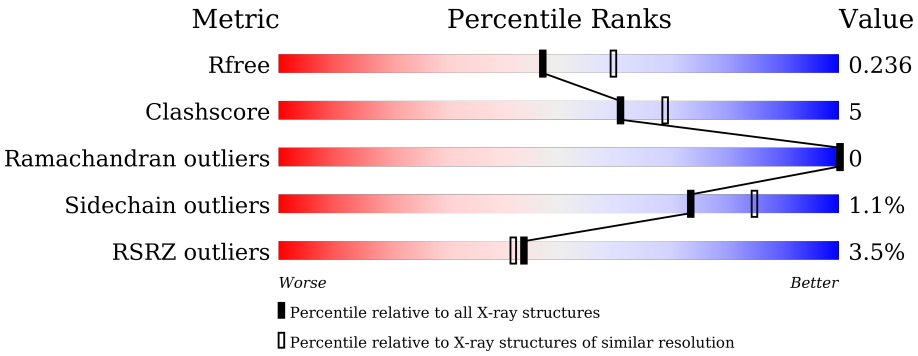
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	412	2% 86% 8% 6%
1	B	412	2% 87% 7% • 6%
1	C	412	6% 81% 13% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9681 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.

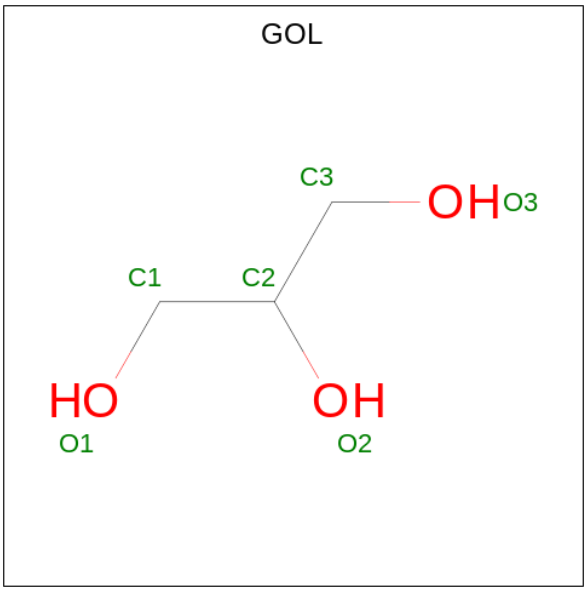
- Molecule 1 is a protein called S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2977	1867	521	582	7			
1	B	389	Total	C	N	O	S	0	0	0
			2989	1874	526	582	7			
1	C	386	Total	C	N	O	S	0	0	0
			2958	1852	519	580	7			

There are 15 discrepancies between the modelled and reference sequences:

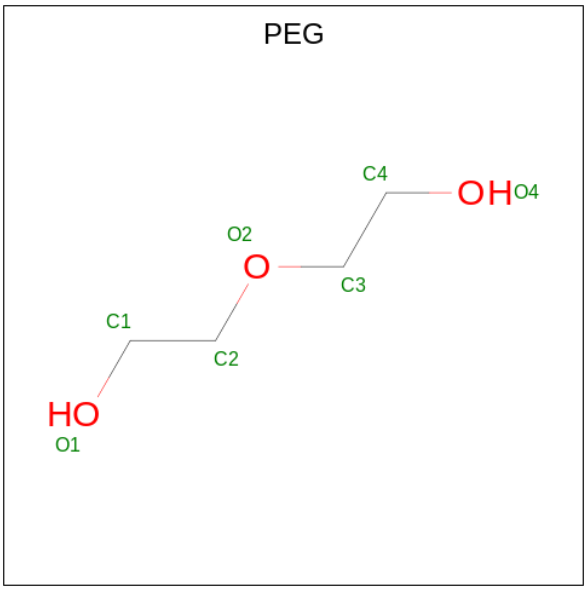
Chain	Residue	Modelled	Actual	Comment	Reference
A	408	LEU	-	expression tag	UNP Q9K5E4
A	409	GLU	-	expression tag	UNP Q9K5E4
A	410	HIS	-	expression tag	UNP Q9K5E4
A	411	HIS	-	expression tag	UNP Q9K5E4
A	412	HIS	-	expression tag	UNP Q9K5E4
B	408	LEU	-	expression tag	UNP Q9K5E4
B	409	GLU	-	expression tag	UNP Q9K5E4
B	410	HIS	-	expression tag	UNP Q9K5E4
B	411	HIS	-	expression tag	UNP Q9K5E4
B	412	HIS	-	expression tag	UNP Q9K5E4
C	408	LEU	-	expression tag	UNP Q9K5E4
C	409	GLU	-	expression tag	UNP Q9K5E4
C	410	HIS	-	expression tag	UNP Q9K5E4
C	411	HIS	-	expression tag	UNP Q9K5E4
C	412	HIS	-	expression tag	UNP Q9K5E4

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



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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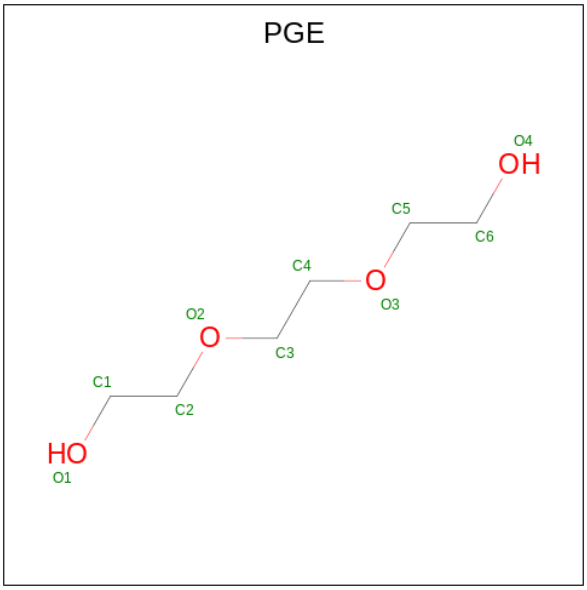
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	2	Total Na 2 2	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 10 6 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 10 6 4	0	0

- Molecule 6 is water.

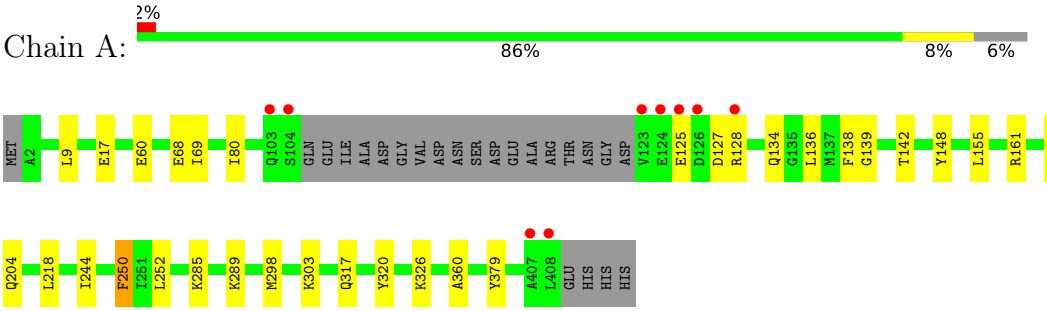
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	263	Total O 263 263	0	0
6	B	192	Total O 192 192	0	0
6	C	212	Total O 212 212	0	0

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.

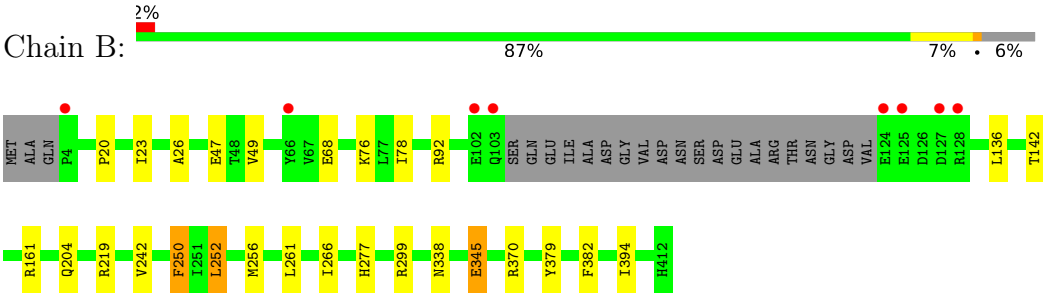
• Molecule 1: S-adenosylmethionine synthase

Chain A:



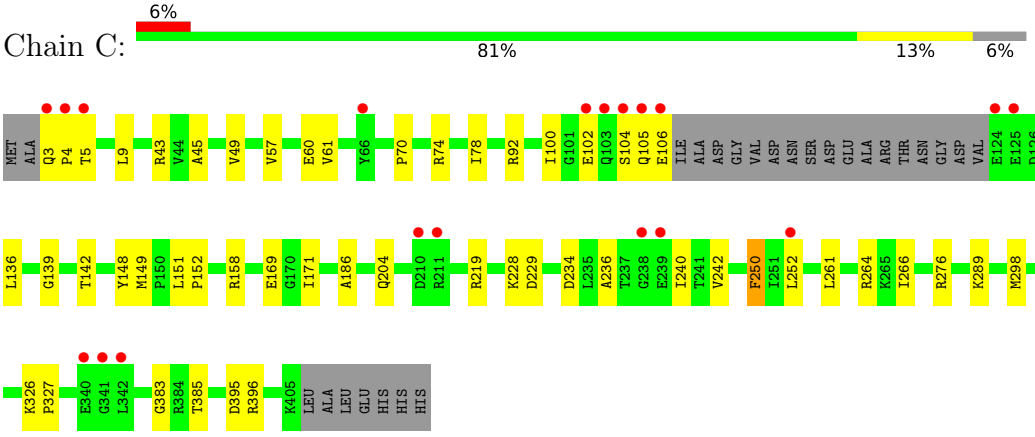
• Molecule 1: S-adenosylmethionine synthase

Chain B:



• Molecule 1: S-adenosylmethionine synthase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	129.15Å 203.89Å 144.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.20 29.47 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.48-2.20) 98.7 (29.47-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.77 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.183 , 0.229 0.197 , 0.236	Depositor DCC
R_{free} test set	4851 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9681	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GOL, NA, PEG, PGE

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	0.70	1/3029 (0.0%)	0.77	0/4116
1	B	0.74	0/3044	0.91	2/4135 (0.0%)
1	C	0.60	0/3010	0.68	0/4089
All	All	0.68	1/9083 (0.0%)	0.79	2/12340 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	GLU	CD-OE1	6.01	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	370	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	B	370	ARG	NE-CZ-NH2	-5.70	117.45	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	2977	0	2948	21	0
1	B	2989	0	2949	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2958	0	2917	39	0
2	A	12	0	16	1	0
2	B	6	0	8	0	0
3	A	35	0	50	6	0
3	B	14	0	20	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	B	10	0	14	0	0
5	C	10	0	14	3	0
6	A	263	0	0	2	0
6	B	192	0	0	3	0
6	C	212	0	0	0	0
All	All	9681	0	8936	81	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 5.

All (81) 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:49:VAL:HG21	1:C:49:VAL:HG21	1.50	0.93
1:A:303:LYS:HZ1	3:A:505:PEG:H31	1.35	0.92
1:B:345:GLU:OE2	6:B:601:HOH:O	1.93	0.84
1:C:326:LYS:HD2	1:C:327:PRO:HD2	1.71	0.70
1:B:161:ARG:HH11	1:B:379:TYR:HB3	1.55	0.70
1:A:303:LYS:NZ	3:A:505:PEG:H31	2.06	0.70
1:C:252:LEU:HD23	1:C:252:LEU:H	1.60	0.65
1:A:142:THR:O	1:A:148:TYR:HA	1.97	0.64
3:A:506:PEG:H21	6:A:719:HOH:O	1.97	0.63
1:C:142:THR:O	1:C:148:TYR:HA	1.99	0.63
1:A:127:ASP:HA	1:A:360:ALA:HB3	1.81	0.62
1:A:125:GLU:HA	1:A:128:ARG:NE	2.16	0.61
1:A:125:GLU:O	1:A:128:ARG:HG2	2.01	0.60
1:A:303:LYS:HZ1	3:A:505:PEG:C3	2.11	0.60
1:A:161:ARG:HG3	3:A:506:PEG:H12	1.83	0.60
1:C:105:GLN:O	1:C:106:GLU:C	2.41	0.58
1:A:161:ARG:HG2	1:A:379:TYR:CD1	2.39	0.57
1:C:43:ARG:HB3	1:C:106:GLU:HG3	1.86	0.57
1:A:138:PHE:CE1	1:A:317:GLN:HB2	2.40	0.57
1:B:219:ARG:HD3	1:B:242:VAL:HG21	1.88	0.56
1:A:69:ILE:HD12	3:A:507:PEG:H41	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ARG:CB	1:C:106:GLU:HG3	2.38	0.54
1:B:142:THR:O	1:B:148:TYR:HA	2.07	0.54
1:A:204:GLN:HA	1:A:250:PHE:O	2.07	0.54
1:C:236:ALA:HA	1:C:240:ILE:HD11	1.91	0.53
1:B:78:ILE:HD11	1:B:92:ARG:HG3	1.90	0.53
1:A:155:LEU:HD23	1:A:183:VAL:HG11	1.92	0.51
1:A:161:ARG:HG2	1:A:379:TYR:CG	2.45	0.51
1:A:285:LYS:HB3	1:A:289:LYS:HG3	1.90	0.51
1:B:68:GLU:HG3	6:B:763:HOH:O	2.11	0.51
1:B:219:ARG:HG3	6:B:767:HOH:O	2.11	0.50
1:C:49:VAL:HG13	1:C:261:LEU:CD2	2.41	0.50
1:C:261:LEU:HB2	1:C:264:ARG:HG3	1.93	0.50
1:C:74:ARG:O	1:C:78:ILE:HG12	2.12	0.50
1:B:345:GLU:HB2	1:C:5:THR:OG1	2.12	0.49
1:C:169:GLU:HB2	1:C:171:ILE:HD13	1.94	0.49
1:B:252:LEU:HD21	1:B:256:MET:CE	2.42	0.49
2:A:502:GOL:H12	1:C:228:LYS:HB3	1.95	0.49
1:C:3:GLN:NE2	1:C:4:PRO:HD2	2.28	0.49
1:C:78:ILE:HD11	1:C:92:ARG:HG3	1.94	0.48
1:C:385:THR:HG21	5:C:501:PGE:H62	1.95	0.48
1:A:17:GLU:HG3	1:A:80:ILE:HG23	1.96	0.48
1:B:47:GLU:HB3	1:C:261:LEU:HD11	1.95	0.48
1:B:49:VAL:HG13	1:B:261:LEU:HD23	1.95	0.48
1:C:9:LEU:HD23	1:C:186:ALA:HA	1.96	0.48
1:C:49:VAL:HG22	1:C:261:LEU:HD22	1.96	0.47
1:B:161:ARG:NH1	1:B:379:TYR:HB3	2.25	0.47
1:C:60:GLU:HB3	1:C:104:SER:HB3	1.96	0.47
1:A:218:LEU:HB2	1:A:244:ILE:HD13	1.97	0.47
1:B:204:GLN:HA	1:B:250:PHE:O	2.14	0.47
1:C:395:ASP:O	1:C:396:ARG:HD2	2.16	0.46
1:C:70:PRO:O	1:C:74:ARG:HG3	2.16	0.46
1:A:9:LEU:HD23	1:A:186:ALA:HA	1.97	0.46
1:C:45:ALA:HB2	1:C:289:LYS:HE2	1.98	0.46
1:C:151:LEU:HB3	1:C:152:PRO:HD3	1.98	0.46
1:A:134:GLN:HA	1:A:320:TYR:O	2.17	0.45
1:C:61:VAL:O	1:C:102:GLU:HA	2.17	0.45
1:C:158:ARG:HH12	5:C:501:PGE:H32	1.81	0.45
1:C:149:MET:HG3	1:C:383:GLY:HA3	1.97	0.45
1:C:276:ARG:HD3	1:C:315:GLU:OE2	2.17	0.45
1:A:68:GLU:HB3	6:A:790:HOH:O	2.16	0.44
1:B:219:ARG:HD2	1:B:219:ARG:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ILE:HD12	1:B:277:HIS:CE1	2.52	0.44
1:B:299:ARG:HG2	1:B:382:PHE:CD1	2.52	0.43
1:B:338:ASN:OD1	1:B:338:ASN:N	2.49	0.43
1:C:3:GLN:HG3	1:C:4:PRO:HD2	2.00	0.43
1:C:204:GLN:HA	1:C:250:PHE:O	2.19	0.43
1:B:49:VAL:HG13	1:B:261:LEU:CD2	2.49	0.43
1:C:229:ASP:HB3	5:C:501:PGE:H32	2.01	0.43
1:B:20:PRO:HA	1:B:23:ILE:HD12	2.02	0.42
1:C:57:VAL:HG12	1:C:100:ILE:HD11	2.02	0.42
1:C:139:GLY:HA3	1:C:298:MET:HB3	2.01	0.42
1:A:139:GLY:HA3	1:A:298:MET:HB3	2.00	0.42
1:B:26:ALA:HB1	1:B:76:LYS:HE2	2.02	0.42
1:B:394:ILE:HG13	1:B:394:ILE:O	2.19	0.41
1:B:266:ILE:HD11	1:C:266:ILE:HD11	2.03	0.41
1:C:219:ARG:NH2	1:C:242:VAL:HB	2.36	0.41
1:C:234:ASP:OD1	1:C:234:ASP:N	2.54	0.41
1:B:157:HIS:HB3	1:B:161:ARG:HH12	1.85	0.41
1:C:3:GLN:CD	1:C:4:PRO:HD2	2.41	0.41
1:C:49:VAL:HG13	1:C:261:LEU:HD23	2.02	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	385/412 (93%)	376 (98%)	9 (2%)	0	100	100
1	B	385/412 (93%)	373 (97%)	12 (3%)	0	100	100
1	C	382/412 (93%)	369 (97%)	13 (3%)	0	100	100
All	All	1152/1236 (93%)	1118 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	314/333 (94%)	310 (99%)	4 (1%)	69 81
1	B	315/333 (95%)	311 (99%)	4 (1%)	69 81
1	C	312/333 (94%)	310 (99%)	2 (1%)	86 93
All	All	941/999 (94%)	931 (99%)	10 (1%)	73 85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	250	PHE
1	A	252	LEU
1	A	326	LYS
1	B	136	LEU
1	B	250	PHE
1	B	252	LEU
1	B	345	GLU
1	C	136	LEU
1	C	250	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	71	GLN
1	C	190	GLN
1	C	221	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	0.12	0	5,5,5	0.57	0
2	GOL	A	502	-	5,5,5	0.08	0	5,5,5	0.35	0
3	PEG	A	506	-	6,6,6	0.19	0	5,5,5	0.27	0
5	PGE	C	501	-	9,9,9	0.35	0	8,8,8	0.56	0
3	PEG	A	503	-	6,6,6	0.48	0	5,5,5	0.20	0
5	PGE	B	501	-	9,9,9	0.28	0	8,8,8	0.12	0
3	PEG	B	502	-	6,6,6	0.24	0	5,5,5	0.20	0
3	PEG	A	504	-	6,6,6	0.33	0	5,5,5	0.24	0
3	PEG	B	504	-	6,6,6	0.48	0	5,5,5	0.39	0
3	PEG	A	505	-	6,6,6	0.32	0	5,5,5	0.30	0
3	PEG	A	507	-	6,6,6	0.56	0	5,5,5	0.58	0
2	GOL	A	501	-	5,5,5	0.17	0	5,5,5	0.35	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	-	-	1/4/4/4	-
2	GOL	A	502	-	-	1/4/4/4	-
3	PEG	A	506	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	C	501	-	-	3/7/7/7	-
3	PEG	A	503	-	-	1/4/4/4	-
5	PGE	B	501	-	-	5/7/7/7	-
3	PEG	B	502	-	-	1/4/4/4	-
3	PEG	A	504	-	-	3/4/4/4	-
3	PEG	B	504	-	-	2/4/4/4	-
3	PEG	A	505	-	-	2/4/4/4	-
3	PEG	A	507	-	-	2/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
3	A	505	PEG	O1-C1-C2-O2
3	A	507	PEG	O2-C3-C4-O4
5	B	501	PGE	O1-C1-C2-O2
3	A	504	PEG	O1-C1-C2-O2
3	A	506	PEG	O2-C3-C4-O4
5	B	501	PGE	O3-C5-C6-O4
3	B	504	PEG	O2-C3-C4-O4
2	A	501	GOL	O1-C1-C2-O2
3	A	503	PEG	O1-C1-C2-O2
3	A	504	PEG	O2-C3-C4-O4
3	A	505	PEG	O2-C3-C4-O4
3	B	502	PEG	O1-C1-C2-O2
3	A	506	PEG	O1-C1-C2-O2
5	C	501	PGE	O1-C1-C2-O2
5	C	501	PGE	O3-C5-C6-O4
3	A	504	PEG	C4-C3-O2-C2
3	A	507	PEG	C4-C3-O2-C2
5	B	501	PGE	C4-C3-O2-C2
3	A	506	PEG	C1-C2-O2-C3
5	B	501	PGE	C6-C5-O3-C4
5	C	501	PGE	C3-C4-O3-C5
3	B	504	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
2	B	503	GOL	C1-C2-C3-O3
2	A	502	GOL	O1-C1-C2-C3
5	B	501	PGE	O2-C3-C4-O3

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	GOL	1	0
3	A	506	PEG	2	0
5	C	501	PGE	3	0
3	A	505	PEG	3	0
3	A	507	PEG	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, 95^{th} 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	389/412 (94%)	-0.25	9 (2%)	60	58	24, 34, 60, 156	0
1	B	389/412 (94%)	-0.22	8 (2%)	63	61	28, 39, 67, 115	0
1	C	386/412 (93%)	-0.09	24 (6%)	20	19	28, 39, 71, 125	0
All	All	1164/1236 (94%)	-0.19	41 (3%)	44	42	24, 38, 68, 156	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	VAL	9.0
1	C	128	ARG	7.1
1	A	125	GLU	7.0
1	A	124	GLU	6.6
1	B	124	GLU	5.9
1	A	408	LEU	5.5
1	C	124	GLU	5.0
1	B	128	ARG	5.0
1	C	3	GLN	4.8
1	C	125	GLU	4.5
1	A	126	ASP	4.4
1	B	102	GLU	3.9
1	B	4	PRO	3.9
1	A	407	ALA	3.4
1	C	105	GLN	3.4
1	C	106	GLU	3.4
1	A	104	SER	3.2
1	C	129	ALA	3.2
1	B	66	TYR	3.0
1	C	103	GLN	3.0
1	C	341	GLY	3.0
1	C	104	SER	2.9
1	B	127	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	4	PRO	2.8
1	B	103	GLN	2.8
1	B	125	GLU	2.7
1	C	340	GLU	2.7
1	C	211	ARG	2.7
1	A	128	ARG	2.6
1	C	252	LEU	2.5
1	C	342	LEU	2.5
1	C	127	ASP	2.5
1	C	238	GLY	2.5
1	C	210	ASP	2.4
1	C	5	THR	2.3
1	C	66	TYR	2.3
1	C	239	GLU	2.2
1	C	301	VAL	2.2
1	C	316	VAL	2.2
1	A	103	GLN	2.1
1	C	102	GLU	2.1

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, 95^{th} 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
3	PEG	B	504	7/7	0.71	0.29	74,80,84,94	0
3	PEG	A	505	7/7	0.72	0.17	69,73,78,87	0
3	PEG	A	506	7/7	0.76	0.23	61,73,86,87	0
3	PEG	A	503	7/7	0.77	0.16	58,71,77,82	0
4	NA	B	505	1/1	0.77	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGE	B	501	10/10	0.77	0.21	70,81,84,86	0
3	PEG	A	507	7/7	0.79	0.19	43,53,57,59	0
3	PEG	A	504	7/7	0.79	0.17	50,58,63,64	0
4	NA	B	506	1/1	0.82	0.21	32,32,32,32	0
2	GOL	B	503	6/6	0.85	0.18	48,59,61,68	0
2	GOL	A	502	6/6	0.85	0.18	38,42,52,57	0
4	NA	A	508	1/1	0.90	0.23	25,25,25,25	0
3	PEG	B	502	7/7	0.91	0.12	53,55,61,62	0
2	GOL	A	501	6/6	0.91	0.08	40,51,54,55	0
5	PGE	C	501	10/10	0.91	0.13	43,50,61,65	0

6.5 Other polymers (i)

There are no such residues in this entry.