WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 29, 2024 – 06:56 PM EDT

PDB ID	:	4E1J
Title	:	Crystal structure of glycerol kinase in complex with glycerol from Sinorhizobium meliloti 1021
Authors	:	Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; Lafleur, J.; Siedel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2012-03-06
Resolution	:	2.33 Å(reported)

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

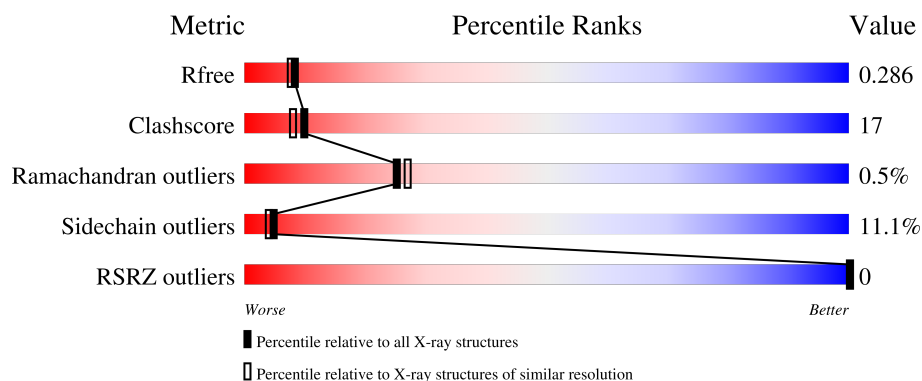|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.33 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		0.286
Clashscore		17
Ramachandran outliers		0.5%
Sidechain outliers		11.1%
RSRZ outliers		0

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$_{free}$	164625	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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	520	72% 18% 6% ·
1	B	520	65% 23% 6% 7%
1	C	520	68% 25% · ·
1	D	520	60% 21% · 16%

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 14333 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 Glycerol kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	Se	0	0	0
			3754	2382	650	706	8	8			
1	B	484	Total	C	N	O	S	Se	0	0	0
			3678	2332	642	688	8	8			
1	C	503	Total	C	N	O	S	Se	0	0	0
			3774	2387	654	716	8	9			
1	D	437	Total	C	N	O	S	Se	0	0	0
			3009	1875	533	587	8	6			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP O86033
A	2	HIS	-	expression tag	UNP O86033
A	3	HIS	-	expression tag	UNP O86033
A	4	HIS	-	expression tag	UNP O86033
A	5	HIS	-	expression tag	UNP O86033
A	6	HIS	-	expression tag	UNP O86033
A	7	HIS	-	expression tag	UNP O86033
A	8	SER	-	expression tag	UNP O86033
A	9	SER	-	expression tag	UNP O86033
A	10	GLY	-	expression tag	UNP O86033
A	11	VAL	-	expression tag	UNP O86033
A	12	ASP	-	expression tag	UNP O86033
A	13	LEU	-	expression tag	UNP O86033
A	14	GLY	-	expression tag	UNP O86033
A	15	THR	-	expression tag	UNP O86033
A	16	GLU	-	expression tag	UNP O86033
A	17	ASN	-	expression tag	UNP O86033
A	18	LEU	-	expression tag	UNP O86033
A	19	TYR	-	expression tag	UNP O86033
A	20	PHE	-	expression tag	UNP O86033
A	21	GLN	-	expression tag	UNP O86033

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	-	expression tag	UNP O86033
A	23	MSE	-	expression tag	UNP O86033
B	1	MSE	-	expression tag	UNP O86033
B	2	HIS	-	expression tag	UNP O86033
B	3	HIS	-	expression tag	UNP O86033
B	4	HIS	-	expression tag	UNP O86033
B	5	HIS	-	expression tag	UNP O86033
B	6	HIS	-	expression tag	UNP O86033
B	7	HIS	-	expression tag	UNP O86033
B	8	SER	-	expression tag	UNP O86033
B	9	SER	-	expression tag	UNP O86033
B	10	GLY	-	expression tag	UNP O86033
B	11	VAL	-	expression tag	UNP O86033
B	12	ASP	-	expression tag	UNP O86033
B	13	LEU	-	expression tag	UNP O86033
B	14	GLY	-	expression tag	UNP O86033
B	15	THR	-	expression tag	UNP O86033
B	16	GLU	-	expression tag	UNP O86033
B	17	ASN	-	expression tag	UNP O86033
B	18	LEU	-	expression tag	UNP O86033
B	19	TYR	-	expression tag	UNP O86033
B	20	PHE	-	expression tag	UNP O86033
B	21	GLN	-	expression tag	UNP O86033
B	22	SER	-	expression tag	UNP O86033
B	23	MSE	-	expression tag	UNP O86033
C	1	MSE	-	expression tag	UNP O86033
C	2	HIS	-	expression tag	UNP O86033
C	3	HIS	-	expression tag	UNP O86033
C	4	HIS	-	expression tag	UNP O86033
C	5	HIS	-	expression tag	UNP O86033
C	6	HIS	-	expression tag	UNP O86033
C	7	HIS	-	expression tag	UNP O86033
C	8	SER	-	expression tag	UNP O86033
C	9	SER	-	expression tag	UNP O86033
C	10	GLY	-	expression tag	UNP O86033
C	11	VAL	-	expression tag	UNP O86033
C	12	ASP	-	expression tag	UNP O86033
C	13	LEU	-	expression tag	UNP O86033
C	14	GLY	-	expression tag	UNP O86033
C	15	THR	-	expression tag	UNP O86033
C	16	GLU	-	expression tag	UNP O86033
C	17	ASN	-	expression tag	UNP O86033

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	LEU	-	expression tag	UNP O86033
C	19	TYR	-	expression tag	UNP O86033
C	20	PHE	-	expression tag	UNP O86033
C	21	GLN	-	expression tag	UNP O86033
C	22	SER	-	expression tag	UNP O86033
C	23	MSE	-	expression tag	UNP O86033
D	1	MSE	-	expression tag	UNP O86033
D	2	HIS	-	expression tag	UNP O86033
D	3	HIS	-	expression tag	UNP O86033
D	4	HIS	-	expression tag	UNP O86033
D	5	HIS	-	expression tag	UNP O86033
D	6	HIS	-	expression tag	UNP O86033
D	7	HIS	-	expression tag	UNP O86033
D	8	SER	-	expression tag	UNP O86033
D	9	SER	-	expression tag	UNP O86033
D	10	GLY	-	expression tag	UNP O86033
D	11	VAL	-	expression tag	UNP O86033
D	12	ASP	-	expression tag	UNP O86033
D	13	LEU	-	expression tag	UNP O86033
D	14	GLY	-	expression tag	UNP O86033
D	15	THR	-	expression tag	UNP O86033
D	16	GLU	-	expression tag	UNP O86033
D	17	ASN	-	expression tag	UNP O86033
D	18	LEU	-	expression tag	UNP O86033
D	19	TYR	-	expression tag	UNP O86033
D	20	PHE	-	expression tag	UNP O86033
D	21	GLN	-	expression tag	UNP O86033
D	22	SER	-	expression tag	UNP O86033
D	23	MSE	-	expression tag	UNP O86033

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

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total 21	O 21	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	28	Total 28	O 28	0	0
5	C	24	Total 24	O 24	0	0
5	D	24	Total 24	O 24	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.
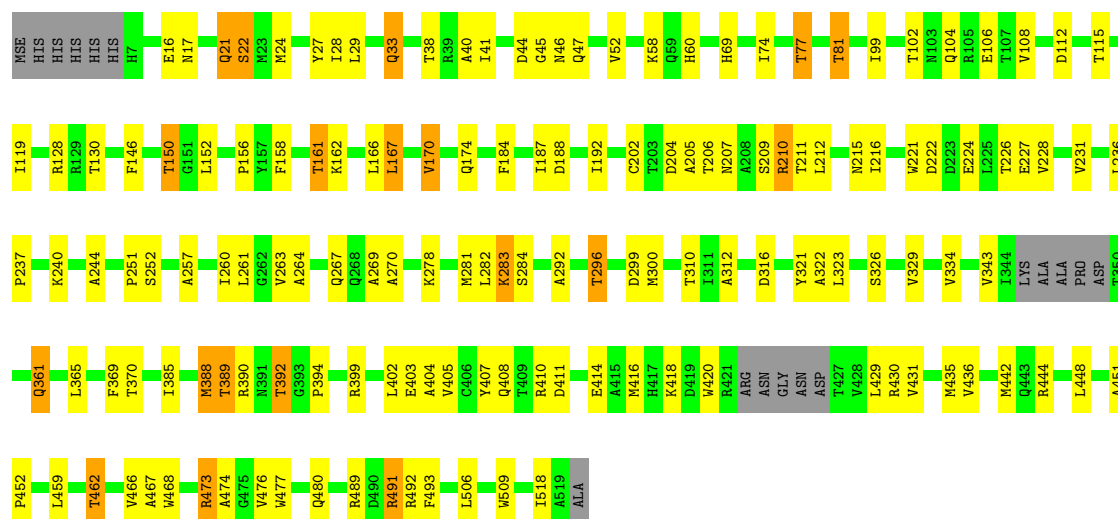
• Molecule 1: Glycerol kinase
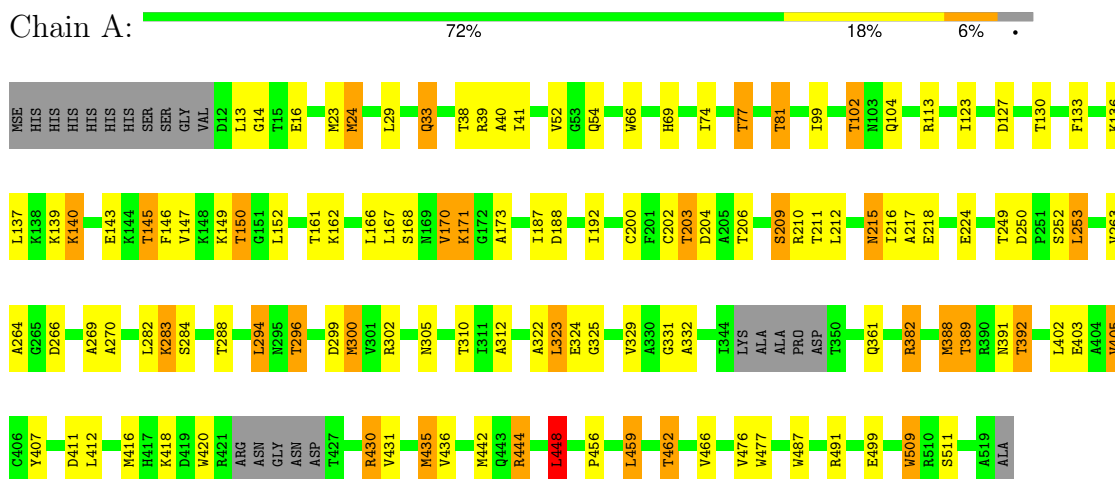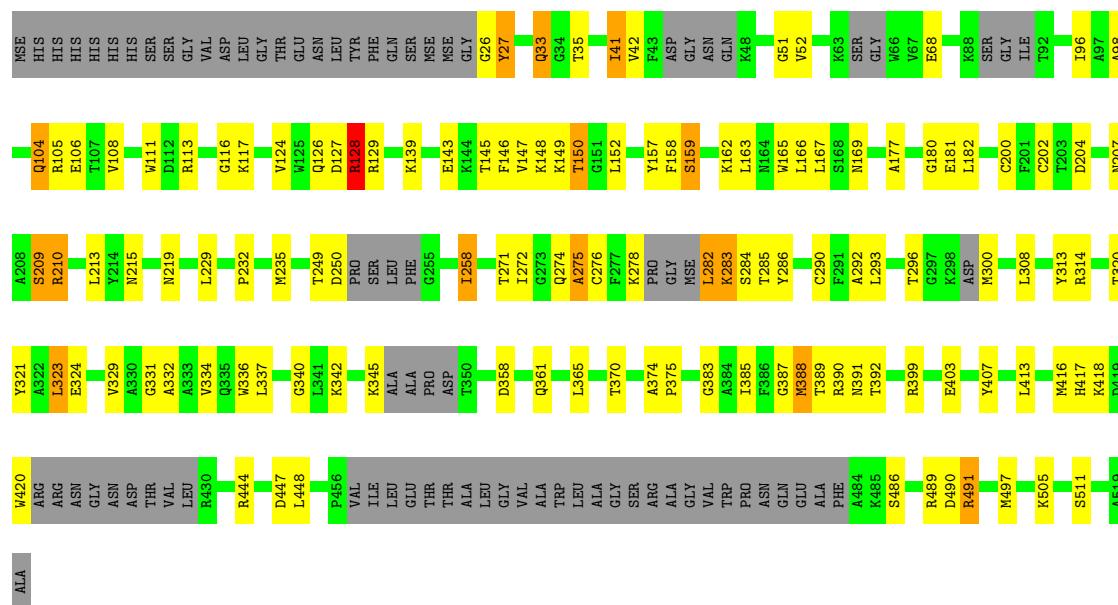
Chain A:

• Molecule 1: Glycerol kinase
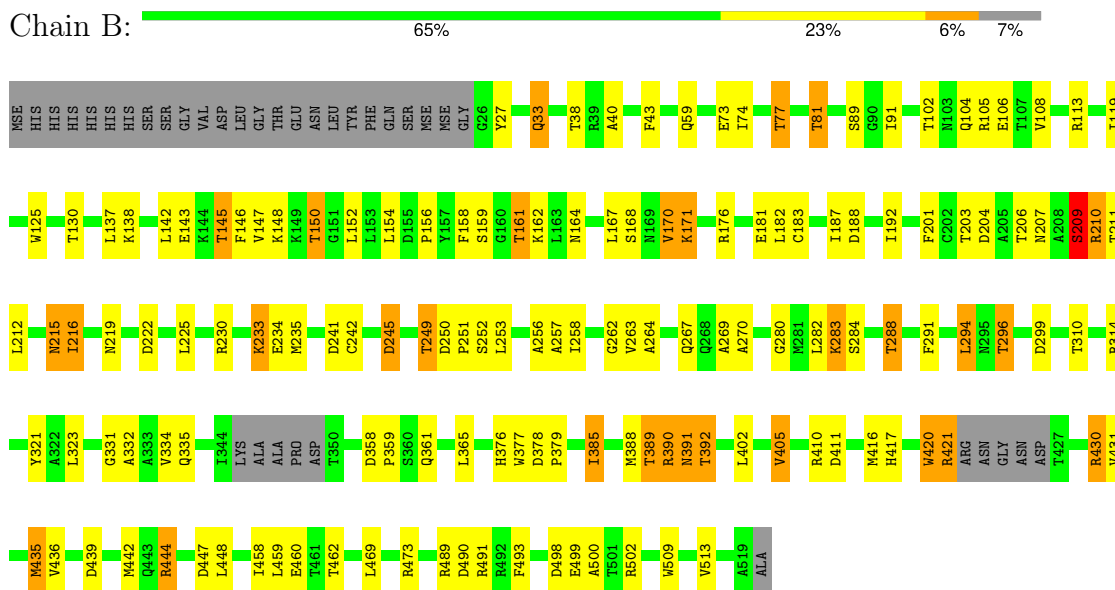
Chain B:

• Molecule 1: Glycerol kinase

Chain C:

● Molecule 1: Glycerol kinase

Chain D:

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.22Å 101.97Å 107.55Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	47.57 – 2.33 47.57 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.57-2.33) 99.8 (47.57-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.230 , 0.290 0.229 , 0.286	Depositor DCC
R_{free} test set	4303 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.4	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14333	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, 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	0.87	0/3824	0.88	5/5191 (0.1%)
1	B	0.88	1/3748 (0.0%)	0.87	3/5085 (0.1%)
1	C	0.75	0/3844	0.80	1/5220 (0.0%)
1	D	0.59	0/3057	0.71	1/4169 (0.0%)
All	All	0.79	1/14473 (0.0%)	0.82	10/19665 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	SER	CB-OG	-5.24	1.35	1.42

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	241	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	448	LEU	CB-CG-CD1	5.60	120.51	111.00
1	A	209	SER	CB-CA-C	-5.43	99.78	110.10
1	B	430	ARG	NE-CZ-NH1	5.42	123.01	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3754	0	3611	122	0
1	B	3678	0	3575	136	0
1	C	3774	0	3582	120	0
1	D	3009	0	2539	101	0
2	A	6	0	8	0	0
2	B	6	0	8	2	0
2	C	6	0	7	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	C	1	0	0	0	0
5	A	21	0	0	2	0
5	B	28	0	0	3	0
5	C	24	0	0	1	0
5	D	24	0	0	1	0
All	All	14333	0	13330	473	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 17.

The worst 5 of 473 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:171:LYS:HE2	1:B:171:LYS:H	1.07	1.11
1:B:282:LEU:CD1	1:B:416:MSE:HE1	1.80	1.11
1:C:402:LEU:O	1:C:405:VAL:HG12	1.52	1.10
1:D:361:GLN:HE22	1:D:392:THR:HG22	1.07	1.09
1:A:402:LEU:O	1:A:405:VAL:HG12	1.54	1.08

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/520 (95%)	466 (95%)	25 (5%)	1 (0%)	44	51
1	B	478/520 (92%)	458 (96%)	19 (4%)	1 (0%)	44	51
1	C	497/520 (96%)	470 (95%)	26 (5%)	1 (0%)	44	51
1	D	417/520 (80%)	370 (89%)	40 (10%)	7 (2%)	7	5
All	All	1884/2080 (91%)	1764 (94%)	110 (6%)	10 (0%)	25	27

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	MSE
1	C	518	ILE
1	D	52	VAL
1	D	417	HIS
1	B	499	GLU

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	371/405 (92%)	331 (89%)	40 (11%)	5	4
1	B	367/405 (91%)	320 (87%)	47 (13%)	3	3
1	C	368/405 (91%)	331 (90%)	37 (10%)	6	5
1	D	242/405 (60%)	217 (90%)	25 (10%)	6	5
All	All	1348/1620 (83%)	1199 (89%)	149 (11%)	5	4

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	444	ARG
1	D	388	MSE
1	C	466	VAL
1	D	159	SER
1	B	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	391	ASN
1	D	361	GLN
1	B	496	HIS
1	D	215	ASN
1	B	443	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	A	601	-	5,5,5	0.26	0	5,5,5	0.66	0
2	GOL	C	602	-	5,5,5	0.53	0	5,5,5	2.11	2 (40%)
2	GOL	B	601	-	5,5,5	0.64	0	5,5,5	0.49	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	A	601	-	-	0/4/4/4	-
2	GOL	C	602	-	-	2/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-

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	C	602	GOL	O2-C2-C1	3.18	122.33	109.18
2	C	602	GOL	O2-C2-C3	2.27	118.58	109.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	GOL	C1-C2-C3-O3
2	C	602	GOL	O1-C1-C2-C3
2	C	602	GOL	C1-C2-C3-O3
2	B	601	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	GOL	1	0
2	B	601	GOL	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	488/520 (93%)	-1.13	0	100	100	24, 39, 57, 64	0
1	B	476/520 (91%)	-1.14	0	100	100	25, 38, 55, 66	0
1	C	493/520 (94%)	-0.92	0	100	100	30, 50, 69, 73	0
1	D	430/520 (82%)	-0.59	0	100	100	42, 81, 105, 111	0
All	All	1887/2080 (90%)	-0.95	0	100	100	24, 47, 93, 111	0

There are no RSRZ outliers to report.

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
3	NA	C	603	1/1	0.97	0.12	37,37,37,37	0
2	GOL	C	602	6/6	0.98	0.06	34,37,41,44	0
2	GOL	A	601	6/6	0.99	0.03	25,28,29,30	0
3	NA	A	602	1/1	0.99	0.10	56,56,56,56	0

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	601	6/6	0.99	0.03	26,28,31,32	0
4	CL	C	601	1/1	0.99	0.05	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.