



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 19, 2025 – 11:16 PM EDT

PDB ID : 4Q31
Title : The crystal structure of cystathione gamma lyase (CalE6) from *Micromonospora echinospora*
Authors : Tan, K.; Bigelow, L.; Jedrzejczak, R.; Babnigg, G.; Bingman, C.A.; Yen-namalli, R.M.; Singh, S.; Kharel, M.K.; Thorson, J.S.; Phillips Jr., G.N.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG); Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on : 2014-04-10
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

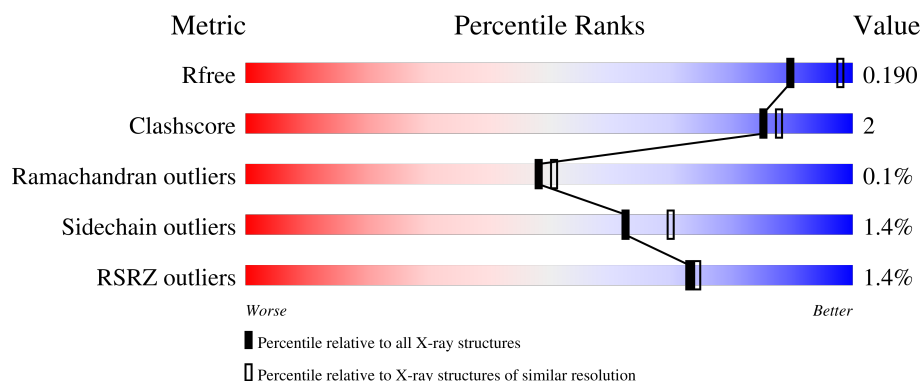
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

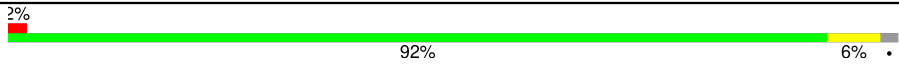
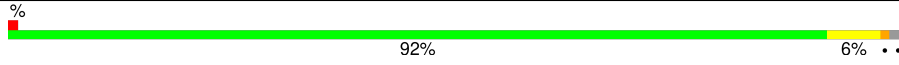
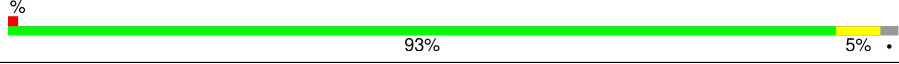
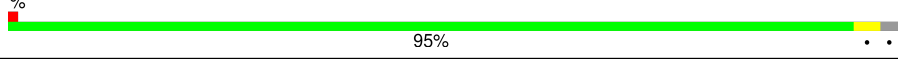
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	384	<div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> <div style="width: 2%;"></div> </div>
1	B	384	<div> <div style="width: 93%;"></div> <div style="width: 5%;"></div> <div style="width: 2%;"></div> </div>
1	C	384	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> </div>
1	D	384	<div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> <div style="width: 2%;"></div> </div>

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Validation Pipeline (wwPDB-VP) : 2.41.4

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Mol	Chain	Length	Quality of chain
1	E	384	
1	F	384	
1	G	384	
1	H	384	

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
4	GOL	D	407	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24719 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 cystathione gamma lyase CalE6.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	P	S	Se	0	1	0
			2844	1778	526	530	1	5	4			
1	B	378	Total	C	N	O	P	S	Se	0	1	0
			2851	1781	528	532	1	5	4			
1	C	379	Total	C	N	O	P	S	Se	0	0	0
			2827	1769	523	526	1	5	3			
1	D	376	Total	C	N	O	P	S	Se	0	1	0
			2817	1764	519	524	1	5	4			
1	E	376	Total	C	N	O	P	S	Se	0	0	0
			2813	1764	512	528	1	5	3			
1	F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	H	378	Total	C	N	O	P	S	Se	0	1	0
			2828	1770	520	529	1	5	3			

There are 32 discrepancies between the modelled and reference sequences:

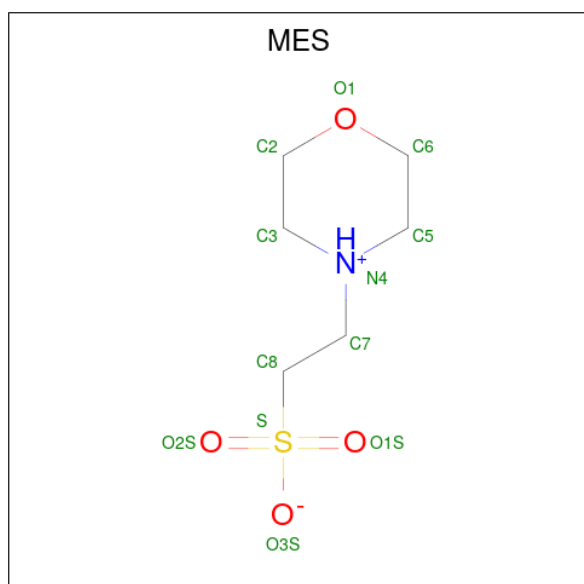
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8KNG3
A	-1	ASN	-	expression tag	UNP Q8KNG3
A	0	ALA	-	expression tag	UNP Q8KNG3
A	7	GLY	ASP	engineered mutation	UNP Q8KNG3
B	-2	SER	-	expression tag	UNP Q8KNG3
B	-1	ASN	-	expression tag	UNP Q8KNG3
B	0	ALA	-	expression tag	UNP Q8KNG3
B	7	GLY	ASP	engineered mutation	UNP Q8KNG3
C	-2	SER	-	expression tag	UNP Q8KNG3
C	-1	ASN	-	expression tag	UNP Q8KNG3
C	0	ALA	-	expression tag	UNP Q8KNG3
C	7	GLY	ASP	engineered mutation	UNP Q8KNG3
D	-2	SER	-	expression tag	UNP Q8KNG3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASN	-	expression tag	UNP Q8KNG3
D	0	ALA	-	expression tag	UNP Q8KNG3
D	7	GLY	ASP	engineered mutation	UNP Q8KNG3
E	-2	SER	-	expression tag	UNP Q8KNG3
E	-1	ASN	-	expression tag	UNP Q8KNG3
E	0	ALA	-	expression tag	UNP Q8KNG3
E	7	GLY	ASP	engineered mutation	UNP Q8KNG3
F	-2	SER	-	expression tag	UNP Q8KNG3
F	-1	ASN	-	expression tag	UNP Q8KNG3
F	0	ALA	-	expression tag	UNP Q8KNG3
F	7	GLY	ASP	engineered mutation	UNP Q8KNG3
G	-2	SER	-	expression tag	UNP Q8KNG3
G	-1	ASN	-	expression tag	UNP Q8KNG3
G	0	ALA	-	expression tag	UNP Q8KNG3
G	7	GLY	ASP	engineered mutation	UNP Q8KNG3
H	-2	SER	-	expression tag	UNP Q8KNG3
H	-1	ASN	-	expression tag	UNP Q8KNG3
H	0	ALA	-	expression tag	UNP Q8KNG3
H	7	GLY	ASP	engineered mutation	UNP Q8KNG3

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			11	6	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	1	Total	Cl	0	0
			1	1		
3	C	2	Total	Cl	0	0
			2	2		
3	D	2	Total	Cl	0	0
			2	2		
3	E	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	H	2	Total	Cl	0	0
			2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



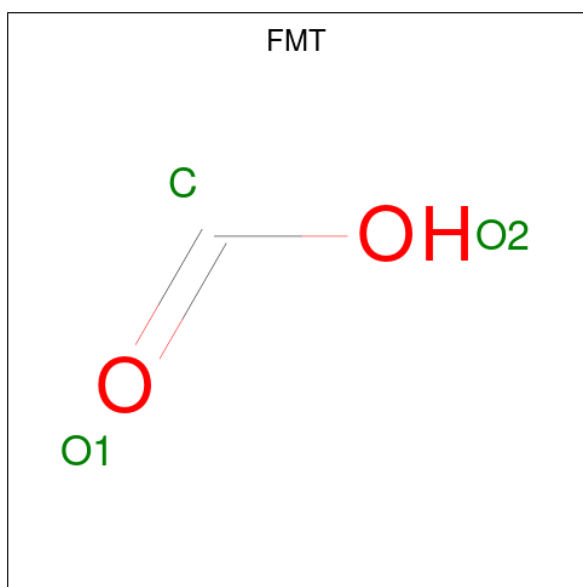
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	F	1	Total	C	O	0	0
			3	1	2		
5	G	1	Total	C	O	0	0
			3	1	2		
5	H	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	243	Total	O	0	0
			243	243		
6	B	228	Total	O	0	0
			228	228		
6	C	230	Total	O	0	0
			230	230		
6	D	215	Total	O	0	0
			215	215		
6	E	250	Total	O	0	0
			250	250		
6	F	204	Total	O	0	0
			204	204		
6	G	215	Total	O	0	0
			215	215		

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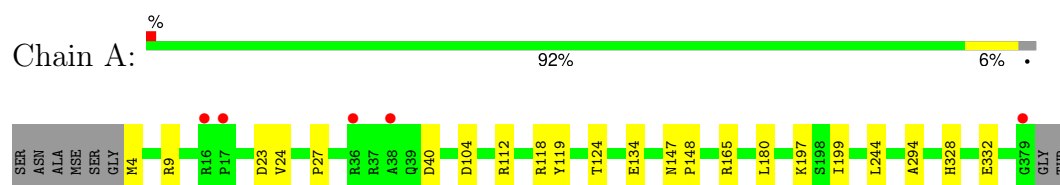
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	238	Total 238	O 238	0	0

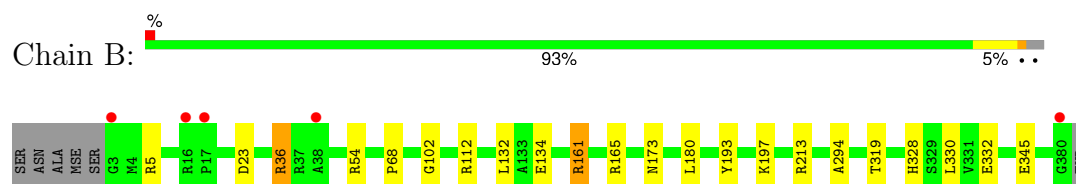
3 Residue-property plots [i](#)

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.

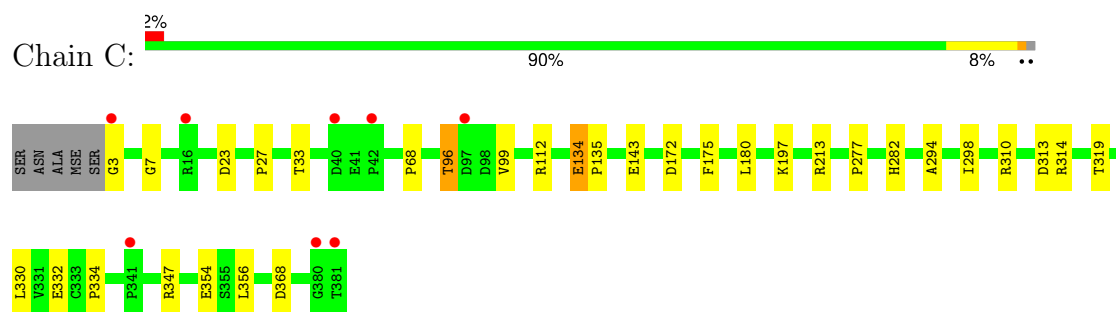
- Molecule 1: cystathione gamma lyase CalE6



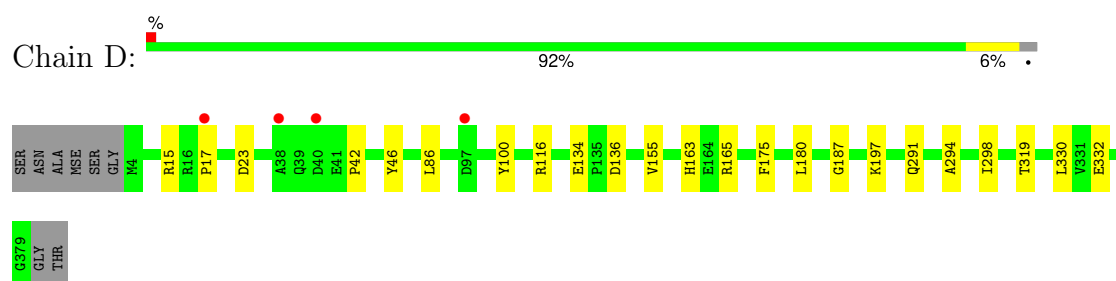
- Molecule 1: cystathione gamma lyase CalE6



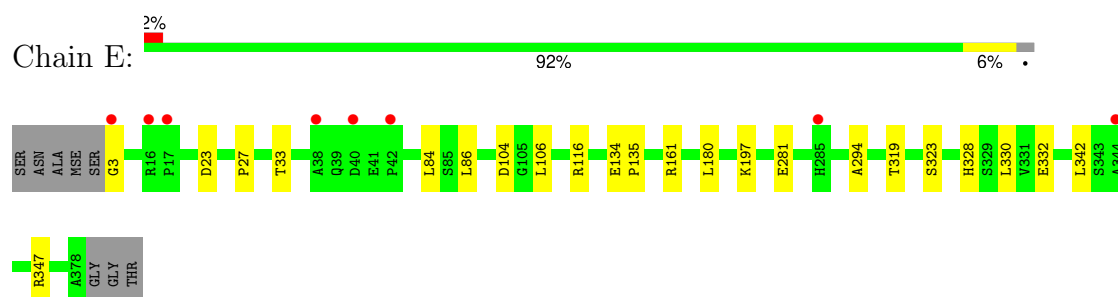
- Molecule 1: cystathione gamma lyase CalE6



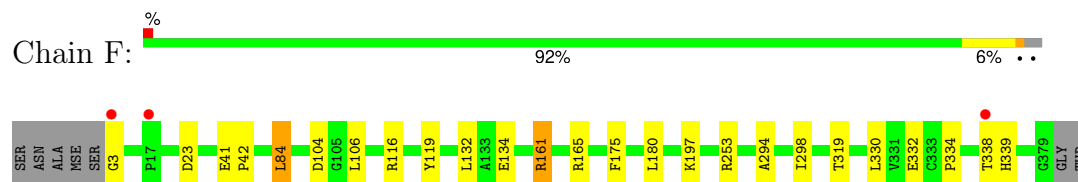
- Molecule 1: cystathione gamma lyase CalE6



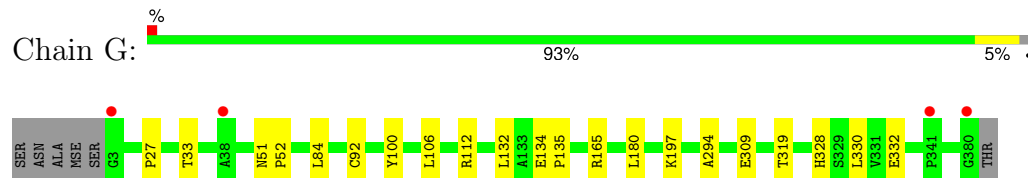
- Molecule 1: cystathione gamma lyase CalE6



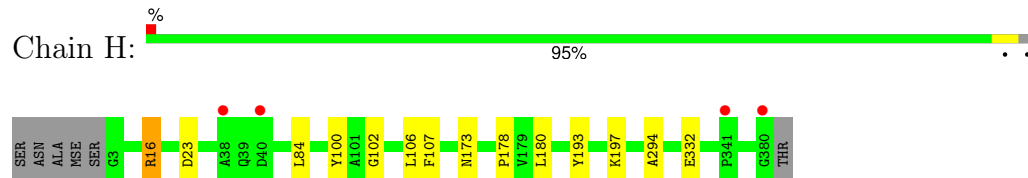
- Molecule 1: cystathione gamma lyase CalE6



- Molecule 1: cystathione gamma lyase CalE6



- Molecule 1: cystathione gamma lyase CalE6



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	146.85Å 146.98Å 349.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.97 – 2.10 33.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.97-2.10) 99.9 (33.97-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.152 , 0.191 0.152 , 0.190	Depositor DCC
R_{free} test set	11002 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24719	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.26% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, LLP, CL, GOL, FMT

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	0.36	0/2876	0.51	0/3916
1	B	0.37	0/2882	0.52	0/3922
1	C	0.37	0/2855	0.52	0/3890
1	D	0.35	0/2849	0.51	0/3884
1	E	0.37	0/2841	0.50	0/3871
1	F	0.36	0/2840	0.51	0/3871
1	G	0.35	0/2842	0.51	0/3874
1	H	0.36	0/2859	0.51	0/3894
All	All	0.36	0/22844	0.51	0/31122

There are no bond length outliers.

There are no bond angle outliers.

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	2844	0	2841	9	0
1	B	2851	0	2846	14	0
1	C	2827	0	2810	20	0
1	D	2817	0	2798	14	0
1	E	2813	0	2789	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2812	0	2786	14	0
1	G	2814	0	2786	10	0
1	H	2828	0	2811	8	0
2	A	12	0	12	0	0
2	B	12	0	12	1	0
2	C	12	0	12	1	0
2	D	12	0	12	1	0
2	E	12	0	12	0	0
2	F	11	0	12	0	0
2	G	12	0	12	2	0
2	H	12	0	12	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	1	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	2	0	0	0	0
4	A	24	0	32	1	0
4	B	36	0	48	1	0
4	C	6	0	8	0	0
4	D	24	0	32	5	0
4	E	24	0	32	1	0
4	F	18	0	24	1	0
4	G	30	0	40	1	0
4	H	6	0	8	0	0
5	A	3	0	1	0	0
5	C	3	0	1	0	0
5	F	3	0	1	0	0
5	G	3	0	1	0	0
5	H	3	0	1	0	0
6	A	243	0	0	0	0
6	B	228	0	0	2	0
6	C	230	0	0	2	0
6	D	215	0	0	0	0
6	E	250	0	0	2	0
6	F	204	0	0	1	0
6	G	215	0	0	0	0
6	H	238	0	0	1	0
All	All	24719	0	22792	96	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 2.

The worst 5 of 96 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:E:86:LEU:HB3	4:E:405:GOL:H11	1.75	0.67
1:F:134:GLU:O	1:F:165:ARG:NH1	2.28	0.67
1:C:3:GLY:N	6:C:644:HOH:O	2.29	0.65
1:F:338:THR:HG23	1:F:339:HIS:ND1	2.12	0.64
1:F:253:ARG:HD2	4:F:404:GOL:H11	1.83	0.61

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	373/384 (97%)	366 (98%)	7 (2%)	0	100	100
1	B	376/384 (98%)	364 (97%)	12 (3%)	0	100	100
1	C	376/384 (98%)	367 (98%)	9 (2%)	0	100	100
1	D	373/384 (97%)	363 (97%)	9 (2%)	1 (0%)	37	37
1	E	373/384 (97%)	366 (98%)	6 (2%)	1 (0%)	37	37
1	F	374/384 (97%)	367 (98%)	7 (2%)	0	100	100
1	G	375/384 (98%)	364 (97%)	11 (3%)	0	100	100
1	H	376/384 (98%)	365 (97%)	11 (3%)	0	100	100
All	All	2996/3072 (98%)	2922 (98%)	72 (2%)	2 (0%)	48	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	323	SER
1	D	42	PRO

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	292/293 (100%)	286 (98%)	6 (2%)	48	55
1	B	292/293 (100%)	287 (98%)	5 (2%)	56	63
1	C	286/293 (98%)	283 (99%)	3 (1%)	73	79
1	D	286/293 (98%)	284 (99%)	2 (1%)	81	87
1	E	286/293 (98%)	280 (98%)	6 (2%)	48	55
1	F	284/293 (97%)	280 (99%)	4 (1%)	62	70
1	G	285/293 (97%)	281 (99%)	4 (1%)	62	70
1	H	287/293 (98%)	284 (99%)	3 (1%)	73	79
All	All	2298/2344 (98%)	2265 (99%)	33 (1%)	62	70

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	328	HIS
1	G	332	GLU
1	H	332	GLU
1	C	96	THR
1	C	23	ASP

Sometimes 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 ⓘ

8 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	LLP	H	197	1	23,24,25	3.16	7 (30%)	25,32,34	1.52	5 (20%)
1	LLP	D	197	1	23,24,25	3.16	7 (30%)	25,32,34	1.33	4 (16%)
1	LLP	C	197	1	23,24,25	3.27	7 (30%)	25,32,34	1.41	3 (12%)
1	LLP	G	197	1	23,24,25	3.15	7 (30%)	25,32,34	1.34	6 (24%)
1	LLP	F	197	1	23,24,25	3.23	7 (30%)	25,32,34	1.36	4 (16%)
1	LLP	A	197	1	23,24,25	3.16	7 (30%)	25,32,34	1.40	5 (20%)
1	LLP	E	197	1	23,24,25	3.11	7 (30%)	25,32,34	1.30	4 (16%)
1	LLP	B	197	1	23,24,25	3.18	7 (30%)	25,32,34	1.32	5 (20%)

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	LLP	H	197	1	-	2/16/17/19	0/1/1/1
1	LLP	D	197	1	-	4/16/17/19	0/1/1/1
1	LLP	C	197	1	-	3/16/17/19	0/1/1/1
1	LLP	G	197	1	-	2/16/17/19	0/1/1/1
1	LLP	F	197	1	-	3/16/17/19	0/1/1/1
1	LLP	A	197	1	-	3/16/17/19	0/1/1/1
1	LLP	E	197	1	-	3/16/17/19	0/1/1/1
1	LLP	B	197	1	-	4/16/17/19	0/1/1/1

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	197	LLP	C2-N1	6.89	1.46	1.33
1	F	197	LLP	C2-N1	6.87	1.46	1.33
1	B	197	LLP	C2-N1	6.77	1.45	1.33
1	H	197	LLP	C2-N1	6.76	1.45	1.33
1	A	197	LLP	C2-N1	6.74	1.45	1.33

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	LLP	OP3-P-OP4	3.42	115.58	106.67
1	H	197	LLP	OP2-P-OP4	3.29	115.25	106.67
1	C	197	LLP	OP3-P-OP4	3.21	115.04	106.67
1	H	197	LLP	OP3-P-OP4	3.18	114.96	106.67
1	F	197	LLP	OP3-P-OP4	3.12	114.80	106.67

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	197	LLP	O-C-CA-CB
1	B	197	LLP	O-C-CA-CB
1	C	197	LLP	O-C-CA-CB
1	D	197	LLP	O-C-CA-CB
1	E	197	LLP	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 12 are monoatomic - leaving 41 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	$\# Z > 2$
4	GOL	B	407	-	5,5,5	0.38	0	5,5,5	0.35	0
4	GOL	G	407	-	5,5,5	0.33	0	5,5,5	0.40	0
5	FMT	A	408	-	2,2,2	0.68	0	1,1,1	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	404	-	5,5,5	0.32	0	5,5,5	0.27	0
4	GOL	A	405	-	5,5,5	0.32	0	5,5,5	0.25	0
4	GOL	B	405	-	5,5,5	0.41	0	5,5,5	0.28	0
4	GOL	E	403	-	5,5,5	0.38	0	5,5,5	0.32	0
4	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.22	0
4	GOL	G	403	-	5,5,5	0.39	0	5,5,5	0.41	0
2	MES	B	401	-	12,12,12	2.18	1 (8%)	15,16,16	2.14	7 (46%)
4	GOL	B	406	-	5,5,5	0.34	0	5,5,5	0.79	0
2	MES	E	401	-	12,12,12	2.14	1 (8%)	15,16,16	1.87	2 (13%)
4	GOL	D	407	-	5,5,5	0.43	0	5,5,5	0.49	0
2	MES	H	401	-	12,12,12	2.26	1 (8%)	15,16,16	1.74	3 (20%)
4	GOL	F	403	-	5,5,5	0.38	0	5,5,5	0.69	0
4	GOL	G	406	-	5,5,5	0.34	0	5,5,5	0.29	0
4	GOL	B	408	-	5,5,5	0.37	0	5,5,5	0.38	0
2	MES	D	401	-	12,12,12	2.19	1 (8%)	15,16,16	1.82	3 (20%)
5	FMT	F	406	-	2,2,2	0.64	0	1,1,1	0.09	0
4	GOL	D	405	-	5,5,5	0.37	0	5,5,5	0.38	0
4	GOL	B	404	-	5,5,5	0.36	0	5,5,5	0.47	0
4	GOL	D	406	-	5,5,5	0.36	0	5,5,5	0.34	0
4	GOL	G	404	-	5,5,5	0.35	0	5,5,5	0.30	0
4	GOL	E	404	-	5,5,5	0.40	0	5,5,5	0.26	0
4	GOL	A	407	-	5,5,5	0.44	0	5,5,5	0.52	0
5	FMT	G	408	-	2,2,2	0.71	0	1,1,1	0.22	0
5	FMT	C	405	-	2,2,2	0.69	0	1,1,1	0.15	0
4	GOL	G	405	-	5,5,5	0.43	0	5,5,5	0.19	0
4	GOL	F	404	-	5,5,5	0.45	0	5,5,5	0.41	0
2	MES	G	401	-	12,12,12	2.25	1 (8%)	15,16,16	1.86	3 (20%)
4	GOL	D	404	-	5,5,5	0.38	0	5,5,5	0.38	0
4	GOL	H	404	-	5,5,5	0.38	0	5,5,5	0.36	0
2	MES	A	401	-	12,12,12	2.04	1 (8%)	15,16,16	1.90	3 (20%)
4	GOL	F	405	-	5,5,5	0.34	0	5,5,5	0.40	0
4	GOL	E	405	-	5,5,5	0.43	0	5,5,5	0.36	0
5	FMT	H	405	-	2,2,2	0.69	0	1,1,1	0.22	0
2	MES	F	401	-	8,11,12	0.40	0	11,13,16	2.01	2 (18%)
4	GOL	A	406	-	5,5,5	0.32	0	5,5,5	0.44	0
4	GOL	E	406	-	5,5,5	0.42	0	5,5,5	0.14	0
2	MES	C	401	-	12,12,12	2.01	1 (8%)	15,16,16	1.86	4 (26%)
4	GOL	C	404	-	5,5,5	0.32	0	5,5,5	0.43	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
4	GOL	B	407	-	-	2/4/4/4	-
4	GOL	G	407	-	-	2/4/4/4	-
4	GOL	A	404	-	-	2/4/4/4	-
4	GOL	A	405	-	-	2/4/4/4	-
4	GOL	B	405	-	-	4/4/4/4	-
4	GOL	E	403	-	-	2/4/4/4	-
4	GOL	B	403	-	-	2/4/4/4	-
4	GOL	G	403	-	-	3/4/4/4	-
2	MES	B	401	-	-	1/6/14/14	0/1/1/1
4	GOL	B	406	-	-	2/4/4/4	-
2	MES	E	401	-	-	5/6/14/14	0/1/1/1
4	GOL	D	407	-	-	0/4/4/4	-
2	MES	H	401	-	-	1/6/14/14	0/1/1/1
4	GOL	F	403	-	-	0/4/4/4	-
4	GOL	G	406	-	-	1/4/4/4	-
4	GOL	B	408	-	-	2/4/4/4	-
2	MES	D	401	-	-	1/6/14/14	0/1/1/1
4	GOL	D	405	-	-	2/4/4/4	-
4	GOL	B	404	-	-	2/4/4/4	-
4	GOL	D	406	-	-	2/4/4/4	-
4	GOL	G	404	-	-	4/4/4/4	-
4	GOL	E	404	-	-	4/4/4/4	-
4	GOL	A	407	-	-	4/4/4/4	-
4	GOL	G	405	-	-	2/4/4/4	-
4	GOL	F	404	-	-	4/4/4/4	-
2	MES	G	401	-	-	1/6/14/14	0/1/1/1
4	GOL	D	404	-	-	0/4/4/4	-
4	GOL	H	404	-	-	2/4/4/4	-
2	MES	A	401	-	-	4/6/14/14	0/1/1/1
4	GOL	F	405	-	-	2/4/4/4	-
4	GOL	E	405	-	-	3/4/4/4	-
2	MES	F	401	-	-	4/5/13/14	0/1/1/1
4	GOL	A	406	-	-	2/4/4/4	-
4	GOL	E	406	-	-	4/4/4/4	-
2	MES	C	401	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	404	-	-	2/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	MES	C8-S	-7.53	1.67	1.77
2	G	401	MES	C8-S	-7.50	1.67	1.77
2	D	401	MES	C8-S	-7.16	1.67	1.77
2	B	401	MES	C8-S	-7.09	1.67	1.77
2	E	401	MES	C8-S	-6.97	1.67	1.77

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	MES	C5-N4-C3	5.61	120.93	108.84
2	F	401	MES	C5-N4-C3	5.45	120.57	108.84
2	B	401	MES	C5-N4-C3	4.94	119.47	108.84
2	A	401	MES	C5-N4-C3	4.80	119.17	108.84
2	D	401	MES	C5-N4-C3	4.73	119.03	108.84

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	MES	C7-C8-S-O1S
2	A	401	MES	C7-C8-S-O3S
2	B	401	MES	C8-C7-N4-C3
2	D	401	MES	C8-C7-N4-C3
2	E	401	MES	C8-C7-N4-C3

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	GOL	1	0
2	B	401	MES	1	0
4	D	407	GOL	4	0
2	H	401	MES	1	0
2	D	401	MES	1	0
4	D	406	GOL	1	0
4	A	407	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	405	GOL	1	0
4	F	404	GOL	1	0
2	G	401	MES	2	0
4	E	405	GOL	1	0
2	C	401	MES	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	372/384 (96%)	-0.63	5 (1%) 74 76	13, 24, 57, 90	0
1	B	374/384 (97%)	-0.64	5 (1%) 74 76	13, 24, 56, 72	0
1	C	375/384 (97%)	-0.55	8 (2%) 63 65	13, 24, 58, 81	0
1	D	372/384 (96%)	-0.55	4 (1%) 77 78	13, 23, 62, 82	0
1	E	372/384 (96%)	-0.60	8 (2%) 62 64	14, 23, 56, 88	0
1	F	373/384 (97%)	-0.55	3 (0%) 82 83	13, 24, 57, 74	0
1	G	374/384 (97%)	-0.60	4 (1%) 77 78	13, 26, 57, 71	0
1	H	374/384 (97%)	-0.63	4 (1%) 77 78	13, 24, 57, 76	1 (0%)
All	All	2986/3072 (97%)	-0.59	41 (1%) 73 74	13, 24, 58, 90	1 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	17	PRO	6.0
1	C	40	ASP	3.9
1	A	17	PRO	3.7
1	C	16	ARG	3.5
1	D	17	PRO	3.4

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

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	LLP	A	197	24/25	0.98	0.05	13,18,21,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LLP	B	197	24/25	0.98	0.04	10,17,22,23	0
1	LLP	C	197	24/25	0.98	0.04	13,18,22,25	0
1	LLP	E	197	24/25	0.98	0.05	13,16,20,21	0
1	LLP	F	197	24/25	0.98	0.06	15,18,25,29	0
1	LLP	D	197	24/25	0.99	0.04	12,19,22,22	0
1	LLP	G	197	24/25	0.99	0.04	13,19,22,23	0
1	LLP	H	197	24/25	0.99	0.05	13,18,22,23	0

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
5	FMT	A	408	3/3	0.70	0.22	57,57,60,61	0
4	GOL	B	408	6/6	0.76	0.17	71,74,75,76	0
4	GOL	G	404	6/6	0.77	0.18	48,56,63,64	0
4	GOL	B	406	6/6	0.78	0.18	37,59,63,64	0
4	GOL	B	403	6/6	0.81	0.14	55,59,60,62	0
4	GOL	B	407	6/6	0.82	0.16	36,58,61,63	0
4	GOL	F	404	6/6	0.82	0.16	41,50,53,54	0
4	GOL	E	405	6/6	0.83	0.18	54,58,60,63	0
4	GOL	D	407	6/6	0.83	0.18	49,55,57,57	0
4	GOL	G	406	6/6	0.84	0.16	65,67,67,69	0
4	GOL	D	405	6/6	0.84	0.16	55,58,65,66	0
4	GOL	A	405	6/6	0.85	0.18	33,53,57,58	0
4	GOL	E	406	6/6	0.85	0.14	44,50,54,60	0
4	GOL	G	407	6/6	0.85	0.14	61,64,65,66	0
4	GOL	A	407	6/6	0.85	0.16	39,51,53,54	0
5	FMT	H	405	3/3	0.85	0.15	47,47,47,48	0
4	GOL	A	406	6/6	0.87	0.12	45,47,52,52	0
3	CL	A	402	1/1	0.88	0.12	66,66,66,66	0
4	GOL	F	403	6/6	0.88	0.14	42,56,57,61	0
3	CL	A	403	1/1	0.88	0.13	53,53,53,53	0
3	CL	C	403	1/1	0.88	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	404	6/6	0.88	0.11	43,51,53,57	0
4	GOL	B	404	6/6	0.88	0.14	43,45,46,48	0
4	GOL	E	404	6/6	0.88	0.12	48,55,57,57	0
4	GOL	B	405	6/6	0.88	0.10	46,51,56,57	0
3	CL	H	403	1/1	0.89	0.12	52,52,52,52	0
4	GOL	G	405	6/6	0.89	0.13	39,47,50,50	0
4	GOL	D	406	6/6	0.89	0.12	46,56,61,64	0
4	GOL	H	404	6/6	0.90	0.10	40,49,53,54	0
4	GOL	D	404	6/6	0.90	0.11	41,47,48,50	0
5	FMT	G	408	3/3	0.90	0.12	43,43,46,46	0
4	GOL	F	405	6/6	0.90	0.11	44,50,51,52	0
3	CL	H	402	1/1	0.91	0.10	64,64,64,64	0
3	CL	E	402	1/1	0.91	0.10	56,56,56,56	0
3	CL	G	402	1/1	0.91	0.12	66,66,66,66	0
3	CL	F	402	1/1	0.92	0.11	60,60,60,60	0
2	MES	C	401	12/12	0.92	0.13	31,37,41,41	0
4	GOL	C	404	6/6	0.92	0.10	39,46,49,51	0
4	GOL	G	403	6/6	0.92	0.09	39,47,50,56	0
3	CL	D	402	1/1	0.92	0.14	61,61,61,61	0
3	CL	C	402	1/1	0.92	0.10	64,64,64,64	0
5	FMT	F	406	3/3	0.93	0.09	29,29,39,44	0
4	GOL	E	403	6/6	0.93	0.10	42,43,45,51	0
5	FMT	C	405	3/3	0.93	0.13	51,51,52,53	0
2	MES	D	401	12/12	0.94	0.11	31,38,45,45	0
2	MES	E	401	12/12	0.94	0.12	31,39,50,52	0
3	CL	B	402	1/1	0.94	0.12	67,67,67,67	0
2	MES	F	401	11/12	0.94	0.12	28,44,53,54	0
3	CL	D	403	1/1	0.95	0.09	64,64,64,64	0
2	MES	A	401	12/12	0.96	0.09	25,28,32,35	0
2	MES	B	401	12/12	0.96	0.09	29,32,36,39	0
2	MES	G	401	12/12	0.96	0.09	32,38,39,41	0
2	MES	H	401	12/12	0.98	0.06	26,29,38,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.