



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:00 AM UTC

PDB ID : 8B21 / pdb\_00008b21  
Title : Time-resolved structure of K<sup>+</sup>-dependent Na<sup>+</sup>-PPase from *Thermotoga maritima* 0-60-seconds post reaction initiation with Na<sup>+</sup>  
Authors : Strauss, J.; Vidilaseris, K.; Goldman, A.  
Deposited on : 2022-09-12  
Resolution : 2.59 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

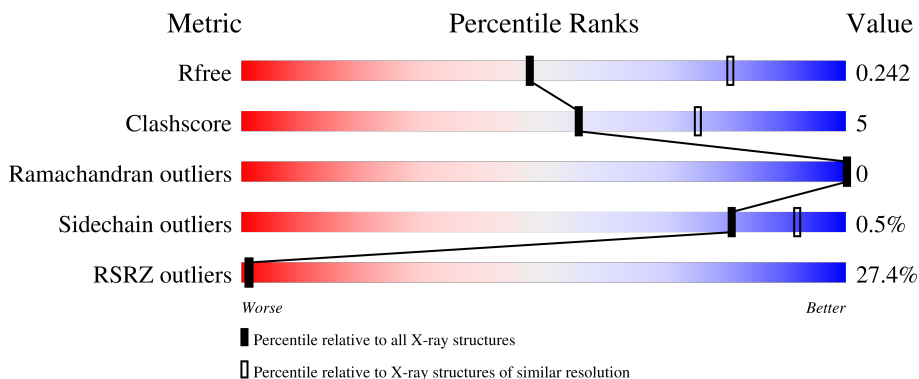
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


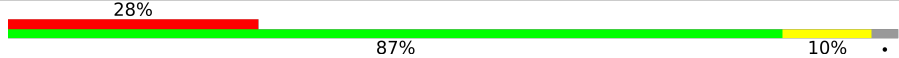
The reported resolution of this entry is 2.59 Å.

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))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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  $\geq 3$ , 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	735	
1	B	735	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21562 atoms, of which 10847 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.

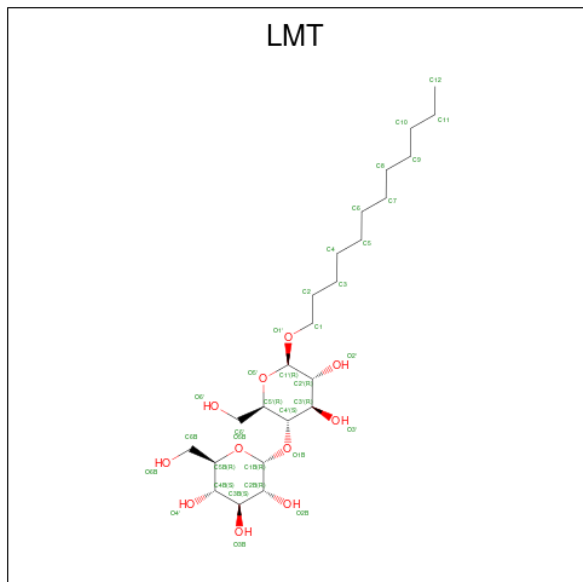
- Molecule 1 is a protein called K(+)-stimulated pyrophosphate-energized sodium pump.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	716	10577	3460	5302	832	956	27	1	10	0
1	B	713	10467	3427	5240	818	955	27	0	9	0

There are 24 discrepancies between the modelled and reference sequences:

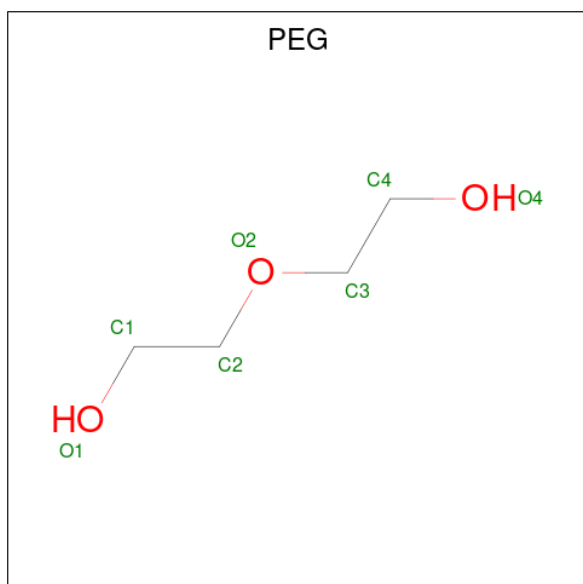
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP Q9S5X0
A	-7	ARG	-	expression tag	UNP Q9S5X0
A	-6	GLY	-	expression tag	UNP Q9S5X0
A	-5	SER	-	expression tag	UNP Q9S5X0
A	-4	HIS	-	expression tag	UNP Q9S5X0
A	-3	HIS	-	expression tag	UNP Q9S5X0
A	-2	HIS	-	expression tag	UNP Q9S5X0
A	-1	HIS	-	expression tag	UNP Q9S5X0
A	0	HIS	-	expression tag	UNP Q9S5X0
A	1	HIS	-	expression tag	UNP Q9S5X0
A	353	LEU	VAL	engineered mutation	UNP Q9S5X0
A	395	GLY	SER	engineered mutation	UNP Q9S5X0
B	-8	MET	-	initiating methionine	UNP Q9S5X0
B	-7	ARG	-	expression tag	UNP Q9S5X0
B	-6	GLY	-	expression tag	UNP Q9S5X0
B	-5	SER	-	expression tag	UNP Q9S5X0
B	-4	HIS	-	expression tag	UNP Q9S5X0
B	-3	HIS	-	expression tag	UNP Q9S5X0
B	-2	HIS	-	expression tag	UNP Q9S5X0
B	-1	HIS	-	expression tag	UNP Q9S5X0
B	0	HIS	-	expression tag	UNP Q9S5X0
B	1	HIS	-	expression tag	UNP Q9S5X0
B	353	LEU	VAL	engineered mutation	UNP Q9S5X0
B	395	GLY	SER	engineered mutation	UNP Q9S5X0

- Molecule 2 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	38	12	25	1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



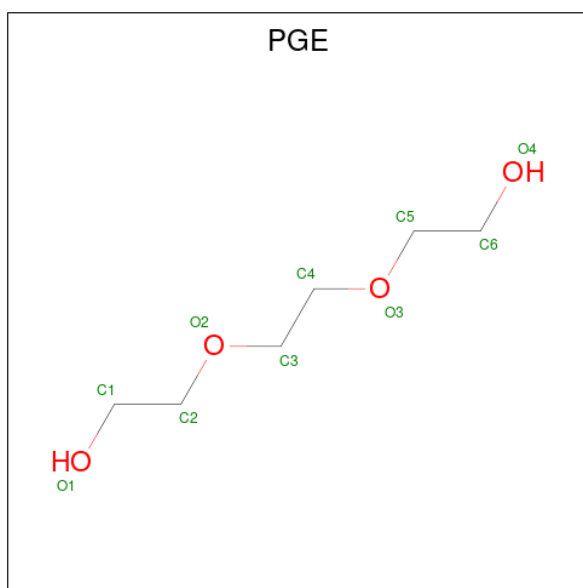
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	17	4	10	3	0	0

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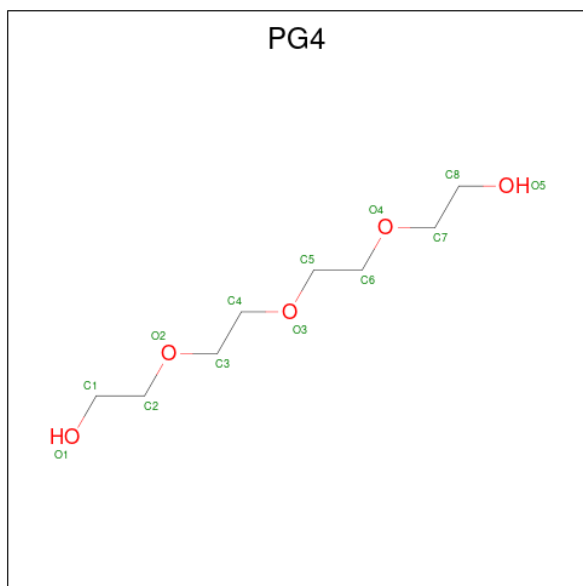
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			24	6	14	4		
4	A	1	Total	C	H	O	0	0
			24	6	14	4		
4	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			31	8	18	5		
5	A	1	Total	C	H	O	0	0
			31	8	18	5		
5	A	1	Total	C	H	O	0	0
			31	8	18	5		
5	B	1	Total	C	H	O	0	0
			31	8	18	5		
5	B	1	Total	C	H	O	0	0
			31	8	18	5		
5	B	1	Total	C	H	O	0	0
			31	8	18	5		

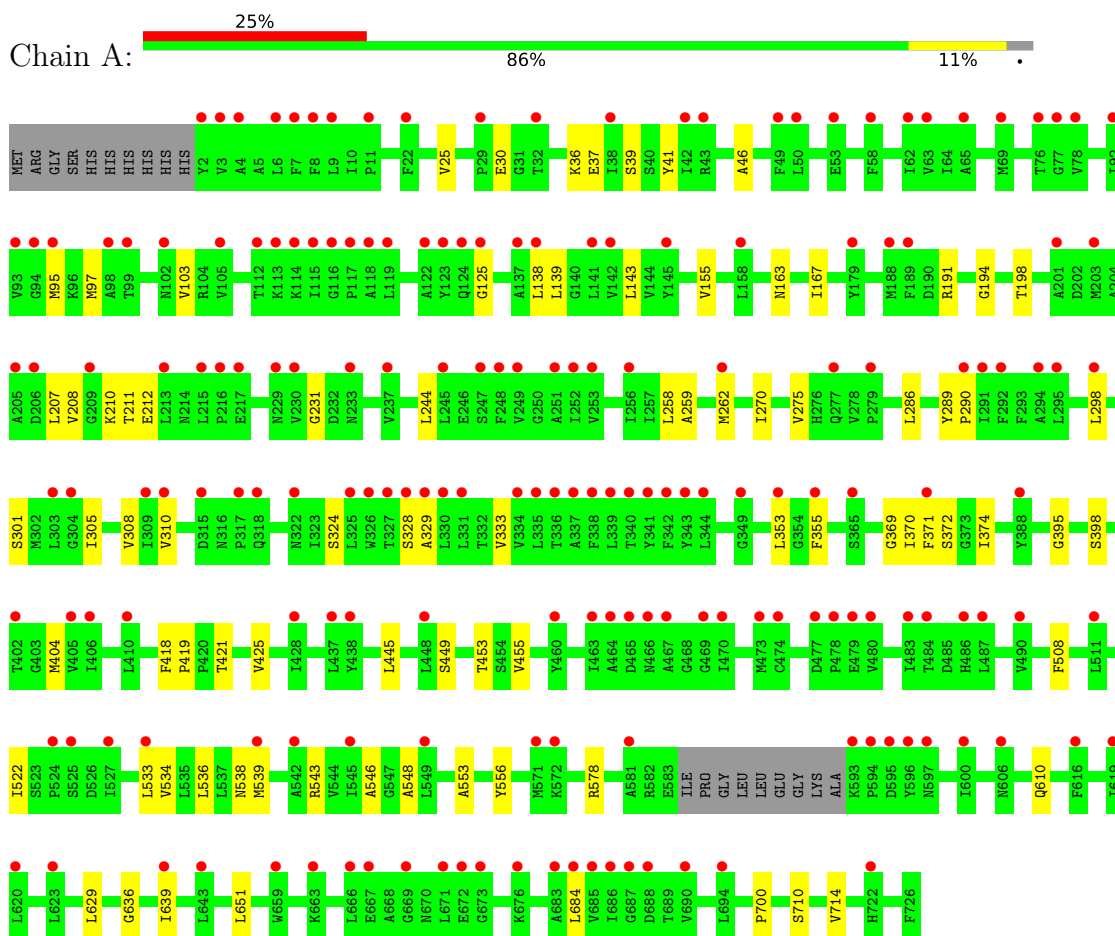
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	O	0	0
			1	1		

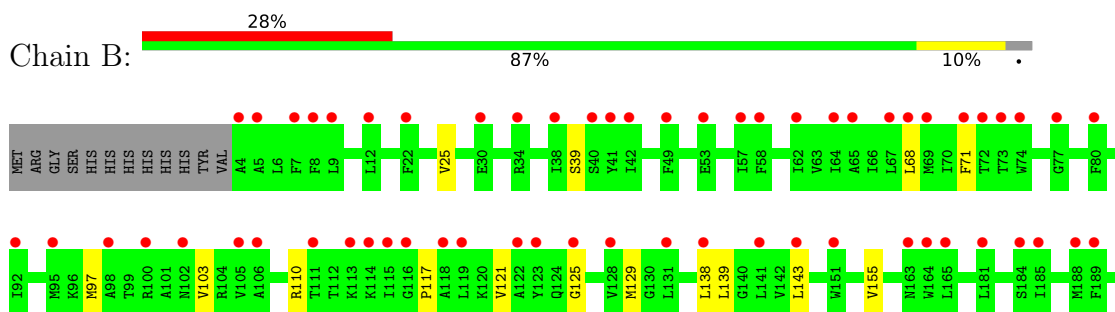
### 3 Residue-property plots

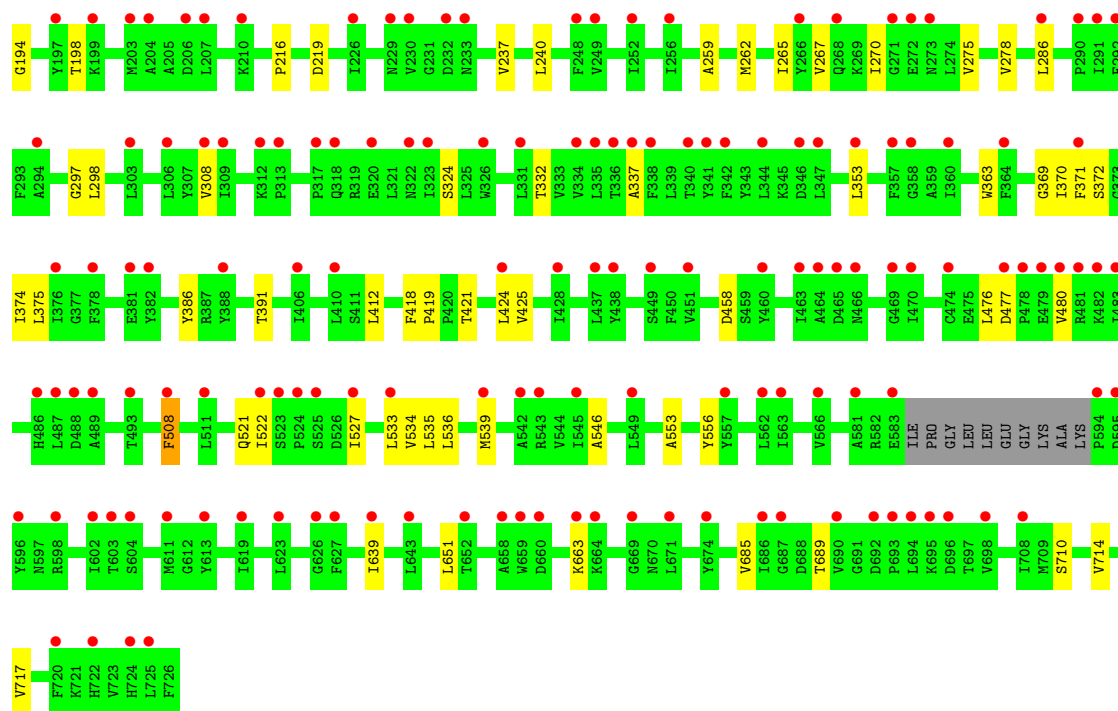
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: K(+)-stimulated pyrophosphate-energized sodium pump



- Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.02Å 110.05Å 107.41Å 90.00° 108.03° 90.00°	Depositor
Resolution (Å)	102.13 – 2.59 102.13 – 2.59	Depositor EDS
% Data completeness (in resolution range)	64.3 (102.13-2.59) 64.3 (102.13-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.220 , 0.236 0.227 , 0.242	Depositor DCC
$R_{free}$ test set	1760 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.3	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 85.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	21562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, PEG, PGE, PG4

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	0.17	0/5412	0.33	0/7373
1	B	0.17	0/5382	0.33	0/7338
All	All	0.17	0/10794	0.33	0/14711

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

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	5275	5302	5317	61	0
1	B	5227	5240	5206	49	0
2	A	13	25	25	0	0
3	A	14	20	20	0	0
3	B	77	110	110	0	0
4	A	30	42	42	0	0
5	A	39	54	54	0	0
5	B	39	54	54	1	0
6	B	1	0	0	0	0
All	All	10715	10847	10828	101	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 (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ALA:HA	1:A:262:MET:HE2	1.64	0.80
1:A:421:THR:O	1:A:425:VAL:HG23	1.85	0.77
1:B:25:VAL:HB	1:B:97:MET:HE1	1.68	0.74
1:A:25:VAL:HB	1:A:97:MET:HE1	1.68	0.73
1:A:194:GLY:O	1:A:198:THR:HG23	1.89	0.73
1:A:97:MET:HE3	1:A:125:GLY:HA2	1.72	0.72
1:A:328:SER:OG	1:A:453:THR:HG21	1.90	0.72
1:B:194:GLY:O	1:B:198:THR:HG23	1.91	0.70
1:A:270:ILE:HD12	1:A:275:VAL:HG21	1.77	0.67
1:A:262:MET:HE1	1:A:353:LEU:HD11	1.77	0.66
1:B:97:MET:HE3	1:B:125:GLY:HA2	1.77	0.66
1:A:556:TYR:HH	1:B:556:TYR:HH	1.41	0.65
1:A:536:LEU:HD11	1:B:536:LEU:HD11	1.79	0.64
1:B:278:VAL:HG21	1:B:353:LEU:HD21	1.80	0.62
1:A:425:VAL:HG13	1:B:546:ALA:HB1	1.81	0.62
1:B:522:ILE:HD12	1:B:534:VAL:HG11	1.81	0.62
1:A:522:ILE:HD13	1:A:534:VAL:HG11	1.84	0.59
1:B:270:ILE:HD12	1:B:275:VAL:HG21	1.84	0.59
1:B:476:LEU:HD23	1:B:480:VAL:HG11	1.85	0.58
1:A:262:MET:HE1	1:A:353:LEU:CD1	2.31	0.58
1:A:543[B]:ARG:NH1	1:A:629:LEU:O	2.36	0.58
1:B:308:VAL:HG21	1:B:324:SER:HB2	1.88	0.55
1:A:395:GLY:O	1:A:398:SER:OG	2.23	0.55
1:A:329:ALA:O	1:A:333:VAL:HG23	2.08	0.54
1:A:553:ALA:HB2	1:B:421:THR:HG21	1.88	0.53
1:A:421:THR:HG21	1:B:553:ALA:HB2	1.89	0.53
1:B:39:SER:HB2	1:B:103:VAL:CG2	2.40	0.52
1:B:375:LEU:HD21	5:B:812:PG4:H52	1.92	0.52
1:A:308:VAL:HG21	1:A:324:SER:HB2	1.91	0.51
1:A:301:SER:HB3	1:A:453:THR:HG23	1.93	0.50
1:A:651:LEU:C	1:A:651:LEU:HD23	2.36	0.50
1:B:522:ILE:CD1	1:B:534:VAL:HG11	2.42	0.49
1:B:533:LEU:O	1:B:533:LEU:HD23	2.12	0.49
1:B:259:ALA:HA	1:B:262:MET:HE2	1.94	0.49
1:A:30:GLU:CD	1:A:36:LYS:HG3	2.37	0.49
1:A:39:SER:HB2	1:A:103:VAL:CG2	2.42	0.49
1:A:522:ILE:CD1	1:A:534:VAL:HG11	2.42	0.49
1:A:548:ALA:HA	1:A:636:GLY:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ASN:CG	1:B:536:LEU:HD12	2.38	0.49
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.94	0.48
1:B:651:LEU:C	1:B:651:LEU:HD23	2.38	0.48
1:A:371:PHE:O	1:A:374:ILE:HG12	2.13	0.48
1:A:207:LEU:O	1:A:211:THR:HG23	2.14	0.48
1:B:110:ARG:HG3	1:B:480:VAL:HG21	1.94	0.47
1:A:138:LEU:HD12	1:A:298:LEU:HD22	1.95	0.47
1:A:212:GLU:OE1	1:A:578[B]:ARG:NH1	2.48	0.47
1:B:138:LEU:HD12	1:B:298:LEU:HD22	1.97	0.47
1:A:191:ARG:CZ	1:A:700:PRO:HB3	2.45	0.46
1:B:117:PRO:O	1:B:121:VAL:HG23	2.14	0.46
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.97	0.46
1:B:371:PHE:O	1:B:374:ILE:HG12	2.15	0.46
1:B:337:ALA:HB2	1:B:363:TRP:CZ2	2.51	0.46
1:B:68:LEU:O	1:B:71:PHE:O	2.34	0.46
1:A:353:LEU:HD22	1:A:355:PHE:CD1	2.50	0.46
1:B:297:GLY:HA2	1:B:332:THR:HG22	1.98	0.45
1:A:353:LEU:O	1:A:353:LEU:HD23	2.16	0.45
1:B:155:VAL:HG12	1:B:155:VAL:O	2.17	0.45
1:A:445:LEU:O	1:A:449:SER:N	2.49	0.45
1:B:265:ILE:HD13	1:B:535:LEU:HD11	1.99	0.45
1:A:207:LEU:O	1:A:211:THR:N	2.49	0.45
1:A:398:SER:HB3	1:A:684:LEU:HD21	1.99	0.45
1:A:353:LEU:HD22	1:A:355:PHE:CE1	2.52	0.44
1:B:216:PRO:HB2	1:B:219:ASP:HB2	1.99	0.44
1:B:412:LEU:C	1:B:412:LEU:HD23	2.42	0.44
1:A:639:ILE:HG13	1:B:539:MET:HG2	1.99	0.44
1:A:533:LEU:O	1:A:533:LEU:HD23	2.18	0.44
1:A:163:ASN:OD1	1:A:167:ILE:N	2.51	0.43
1:B:129:MET:HE2	1:B:237:VAL:O	2.18	0.43
1:A:546:ALA:HB1	1:B:425:VAL:HG13	2.01	0.43
1:B:267:VAL:HG21	1:B:527:ILE:HG12	2.00	0.43
1:A:30:GLU:OE2	1:A:36:LYS:HG3	2.18	0.43
1:A:155:VAL:HG12	1:A:155:VAL:O	2.18	0.43
1:A:46:ALA:HB1	1:A:95:MET:HE2	2.01	0.42
1:B:685:VAL:O	1:B:689:THR:HG23	2.20	0.42
1:A:305:ILE:HG13	1:A:453:THR:HG22	2.01	0.42
1:A:139:LEU:O	1:A:143:LEU:HG	2.20	0.42
1:A:710:SER:O	1:A:714:VAL:HG23	2.20	0.42
1:A:310:VAL:O	1:A:310:VAL:HG12	2.20	0.42
1:B:286:LEU:CD1	1:B:353:LEU:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:SER:O	1:B:714:VAL:HG23	2.20	0.42
1:A:208:VAL:HA	1:A:211:THR:OG1	2.20	0.42
1:B:240:LEU:HD23	1:B:458:ASP:HB3	2.02	0.42
1:A:258:LEU:O	1:A:262:MET:HG3	2.19	0.41
1:A:371:PHE:O	1:A:372:SER:C	2.62	0.41
1:A:369:GLY:O	1:A:370:ILE:C	2.63	0.41
1:B:139:LEU:O	1:B:143:LEU:HG	2.21	0.41
1:B:369:GLY:O	1:B:370:ILE:C	2.64	0.41
1:B:386:TYR:HA	1:B:391:THR:HB	2.03	0.41
1:B:521:GLN:HG2	1:B:717:VAL:HG21	2.02	0.41
1:B:424:LEU:HD22	1:B:508:PHE:CD1	2.56	0.41
1:B:371:PHE:O	1:B:372:SER:C	2.62	0.41
1:A:37:GLU:HG2	1:A:41:TYR:CZ	2.55	0.41
1:A:286:LEU:HD13	1:A:353:LEU:HD11	2.03	0.41
1:B:337:ALA:HB2	1:B:363:TRP:CE2	2.56	0.41
1:A:198:THR:HG22	1:A:231:GLY:CA	2.51	0.41
1:A:244:LEU:CD1	1:A:455:VAL:HG22	2.50	0.41
1:A:289:TYR:N	1:A:290:PRO:HD2	2.36	0.41
1:A:207:LEU:O	1:A:210:LYS:N	2.53	0.40
1:A:539:MET:HG2	1:B:639:ILE:HG13	2.04	0.40
1:A:30:GLU:OE1	1:A:36:LYS:HE2	2.21	0.40
1:B:663:LYS:HD2	1:B:685:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	722/735 (98%)	699 (97%)	23 (3%)	0	100	100
1	B	718/735 (98%)	696 (97%)	22 (3%)	0	100	100
All	All	1440/1470 (98%)	1395 (97%)	45 (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	538/575 (94%)	535 (99%)	3 (1%)	78	91
1	B	532/575 (92%)	530 (100%)	2 (0%)	84	93
All	All	1070/1150 (93%)	1065 (100%)	5 (0%)	81	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	404	MET
1	A	508	PHE
1	A	610	GLN
1	B	477	ASP
1	B	508	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	B	233	ASN
1	B	597	ASN
1	B	606	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

23 ligands 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
3	PEG	A	803	-	6,6,6	1.06	0	5,5,5	0.62	0
4	PGE	A	808	-	9,9,9	1.21	1 (11%)	8,8,8	0.46	0
5	PG4	A	807	-	12,12,12	0.69	0	11,11,11	0.93	0
3	PEG	B	805	-	6,6,6	1.01	0	5,5,5	0.63	0
3	PEG	B	810	-	6,6,6	1.09	0	5,5,5	0.58	0
5	PG4	A	809	-	12,12,12	0.63	0	11,11,11	0.95	0
3	PEG	B	801	-	6,6,6	0.97	0	5,5,5	0.62	0
3	PEG	B	804	-	6,6,6	1.17	0	5,5,5	0.57	0
5	PG4	B	814	-	12,12,12	0.68	0	11,11,11	0.91	0
3	PEG	B	811	-	6,6,6	0.98	0	5,5,5	0.78	0
2	LMT	A	801	-	12,12,36	0.30	0	11,11,47	0.40	0
5	PG4	B	812	-	12,12,12	0.74	0	11,11,11	0.89	0
3	PEG	B	808	-	6,6,6	1.04	0	5,5,5	0.64	0
3	PEG	B	806	-	6,6,6	1.05	0	5,5,5	0.61	0
5	PG4	A	806	-	12,12,12	0.69	0	11,11,11	0.93	0
4	PGE	A	804	-	9,9,9	1.21	1 (11%)	8,8,8	0.42	0
4	PGE	A	805	-	9,9,9	1.21	2 (22%)	8,8,8	0.46	0
3	PEG	B	802	-	6,6,6	0.91	0	5,5,5	0.62	0
3	PEG	B	809	-	6,6,6	1.05	0	5,5,5	0.54	0
3	PEG	B	807	-	6,6,6	0.91	0	5,5,5	0.65	0
3	PEG	A	802	-	6,6,6	0.93	0	5,5,5	0.65	0
3	PEG	B	803	-	6,6,6	1.07	0	5,5,5	0.65	0
5	PG4	B	813	-	12,12,12	0.72	0	11,11,11	0.90	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	803	-	-	3/4/4/4	-
4	PGE	A	808	-	-	4/7/7/7	-
5	PG4	A	807	-	-	7/10/10/10	-
3	PEG	B	805	-	-	1/4/4/4	-
3	PEG	B	810	-	-	2/4/4/4	-
5	PG4	A	809	-	-	7/10/10/10	-
3	PEG	B	801	-	-	0/4/4/4	-
3	PEG	B	804	-	-	1/4/4/4	-
5	PG4	B	814	-	-	5/10/10/10	-
3	PEG	B	811	-	-	3/4/4/4	-
2	LMT	A	801	-	-	5/10/10/61	-
5	PG4	B	812	-	-	6/10/10/10	-
3	PEG	B	808	-	-	3/4/4/4	-
3	PEG	B	806	-	-	1/4/4/4	-
5	PG4	A	806	-	-	6/10/10/10	-
4	PGE	A	804	-	-	4/7/7/7	-
4	PGE	A	805	-	-	2/7/7/7	-
3	PEG	B	802	-	-	0/4/4/4	-
3	PEG	B	809	-	-	2/4/4/4	-
3	PEG	B	807	-	-	3/4/4/4	-
3	PEG	A	802	-	-	1/4/4/4	-
3	PEG	B	803	-	-	3/4/4/4	-
5	PG4	B	813	-	-	6/10/10/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	804	PGE	C4-C3	2.24	1.60	1.49
4	A	808	PGE	C4-C3	2.20	1.60	1.49
4	A	805	PGE	C4-C3	2.08	1.59	1.49
4	A	805	PGE	C5-C6	2.07	1.60	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	812	PG4	O2-C3-C4-O3
5	A	809	PG4	O3-C5-C6-O4
5	B	812	PG4	O1-C1-C2-O2
4	A	804	PGE	O2-C3-C4-O3
5	A	809	PG4	O2-C3-C4-O3
5	B	813	PG4	O2-C3-C4-O3
3	B	803	PEG	O2-C3-C4-O4
3	B	807	PEG	O2-C3-C4-O4
3	B	808	PEG	O1-C1-C2-O2
3	B	809	PEG	O1-C1-C2-O2
3	B	811	PEG	O1-C1-C2-O2
4	A	808	PGE	O3-C5-C6-O4
5	A	809	PG4	O4-C7-C8-O5
5	B	813	PG4	O3-C5-C6-O4
3	A	803	PEG	O1-C1-C2-O2
3	A	803	PEG	O2-C3-C4-O4
3	B	808	PEG	O2-C3-C4-O4
3	B	809	PEG	O2-C3-C4-O4
4	A	805	PGE	O3-C5-C6-O4
5	B	814	PG4	O1-C1-C2-O2
5	B	814	PG4	O4-C7-C8-O5
5	A	807	PG4	O2-C3-C4-O3
5	A	806	PG4	O1-C1-C2-O2
2	A	801	LMT	C6-C7-C8-C9
5	B	812	PG4	O3-C5-C6-O4
4	A	808	PGE	O2-C3-C4-O3
3	B	807	PEG	O1-C1-C2-O2
3	B	810	PEG	O1-C1-C2-O2
5	B	813	PG4	O4-C7-C8-O5
2	A	801	LMT	C2-C3-C4-C5
3	B	811	PEG	O2-C3-C4-O4
4	A	808	PGE	O1-C1-C2-O2
5	A	807	PG4	O1-C1-C2-O2
5	A	809	PG4	O1-C1-C2-O2
5	A	806	PG4	O2-C3-C4-O3
5	A	807	PG4	O4-C7-C8-O5
4	A	804	PGE	C4-C3-O2-C2
3	A	802	PEG	C4-C3-O2-C2
5	B	814	PG4	O2-C3-C4-O3
3	B	806	PEG	C4-C3-O2-C2
5	B	813	PG4	C6-C5-O3-C4
3	B	810	PEG	O2-C3-C4-O4
5	B	812	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
3	B	805	PEG	C4-C3-O2-C2
5	A	807	PG4	C5-C6-O4-C7
5	A	806	PG4	O4-C7-C8-O5
3	B	803	PEG	C1-C2-O2-C3
4	A	804	PGE	O3-C5-C6-O4
5	B	812	PG4	O4-C7-C8-O5
3	B	811	PEG	C4-C3-O2-C2
5	A	806	PG4	C5-C6-O4-C7
5	B	813	PG4	C8-C7-O4-C6
5	A	806	PG4	C1-C2-O2-C3
4	A	804	PGE	C6-C5-O3-C4
5	A	809	PG4	C4-C3-O2-C2
4	A	808	PGE	C6-C5-O3-C4
3	A	803	PEG	C1-C2-O2-C3
5	B	812	PG4	C3-C4-O3-C5
5	B	814	PG4	O3-C5-C6-O4
5	B	813	PG4	O1-C1-C2-O2
5	A	806	PG4	C6-C5-O3-C4
2	A	801	LMT	C11-C10-C9-C8
3	B	803	PEG	O1-C1-C2-O2
5	A	809	PG4	C5-C6-O4-C7
3	B	807	PEG	C1-C2-O2-C3
2	A	801	LMT	O1'-C1-C2-C3
5	B	814	PG4	C4-C3-O2-C2
4	A	805	PGE	O1-C1-C2-O2
5	A	807	PG4	O3-C5-C6-O4
3	B	808	PEG	C1-C2-O2-C3
5	A	807	PG4	C3-C4-O3-C5
3	B	804	PEG	O2-C3-C4-O4
5	A	807	PG4	C1-C2-O2-C3
2	A	801	LMT	C9-C10-C11-C12
5	A	809	PG4	C3-C4-O3-C5

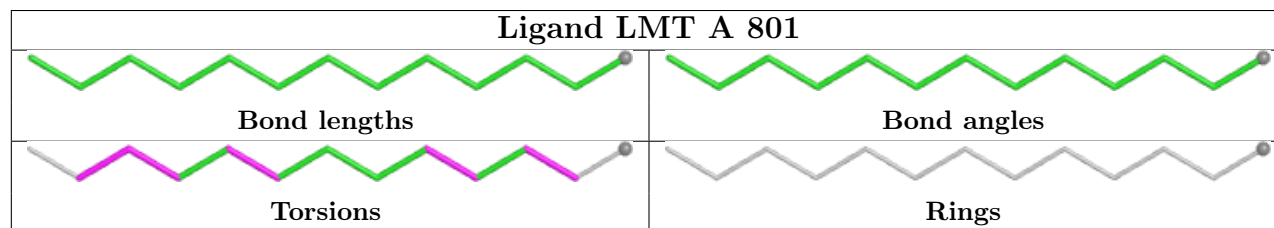
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	812	PG4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	716/735 (97%)	1.46	186 (25%) <b>1</b> <b>1</b>	20, 65, 137, 164	7 (0%)
1	B	713/735 (97%)	1.45	206 (28%) <b>1</b> <b>1</b>	23, 71, 130, 169	3 (0%)
All	All	1429/1470 (97%)	1.46	392 (27%) <b>1</b> <b>1</b>	20, 68, 134, 169	10 (0%)

All (392) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	487	LEU	10.2
1	A	248	PHE	9.1
1	B	119	LEU	8.9
1	B	207	LEU	8.5
1	B	141	LEU	8.2
1	A	686	ILE	8.0
1	A	98	ALA	7.6
1	A	123	TYR	7.3
1	A	659	TRP	7.0
1	A	95	MET	6.9
1	A	466	ASN	6.9
1	A	115	ILE	6.8
1	A	252	ILE	6.8
1	A	141	LEU	6.7
1	A	119	LEU	6.7
1	A	486	HIS	6.7
1	A	138	LEU	6.6
1	A	122	ALA	6.4
1	A	249	VAL	6.3
1	A	295	LEU	6.1
1	B	42	ILE	6.1
1	B	524	PRO	6.1
1	A	690	VAL	6.0
1	A	470	ILE	6.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	203	MET	5.9
1	A	406	ILE	5.9
1	A	594	PRO	5.9
1	A	463	ILE	5.8
1	B	694	LEU	5.8
1	B	639	ILE	5.7
1	A	545	ILE	5.6
1	B	466	ASN	5.5
1	B	696	ASP	5.4
1	B	226	ILE	5.4
1	B	487	LEU	5.4
1	B	9	LEU	5.3
1	A	3	VAL	5.2
1	A	474	CYS	5.2
1	B	542[A]	ALA	5.2
1	A	318	GLN	5.1
1	B	151	TRP	5.1
1	B	690	VAL	5.1
1	B	686	ILE	5.1
1	B	189	PHE	5.1
1	A	619	ILE	5.1
1	A	639	ILE	5.1
1	A	353	LEU	5.0
1	A	92	ILE	5.0
1	B	199	LYS	4.8
1	A	685	VAL	4.7
1	B	233	ASN	4.7
1	A	460	TYR	4.7
1	B	7	PHE	4.7
1	B	479	GLU	4.6
1	B	698	VAL	4.6
1	A	42	ILE	4.6
1	A	596	TYR	4.6
1	A	253	VAL	4.5
1	A	549	LEU	4.5
1	A	410	LEU	4.5
1	B	272	GLU	4.5
1	B	692	ASP	4.5
1	B	123	TYR	4.5
1	B	695	LYS	4.4
1	A	479	GLU	4.4
1	B	428	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	527	ILE	4.4
1	A	233	ASN	4.4
1	B	437	LEU	4.4
1	B	115	ILE	4.4
1	A	229	ASN	4.3
1	B	271	GLY	4.3
1	A	524	PRO	4.3
1	A	572	LYS	4.3
1	B	58	PHE	4.2
1	B	522	ILE	4.2
1	A	105	VAL	4.2
1	A	684	LEU	4.1
1	A	663	LYS	4.1
1	A	77	GLY	4.1
1	B	563	ILE	4.1
1	B	525	SER	4.0
1	A	7	PHE	4.0
1	B	248	PHE	4.0
1	B	290	PRO	4.0
1	B	410	LEU	4.0
1	A	8	PHE	3.9
1	A	483	ILE	3.9
1	B	185	ILE	3.9
1	B	323	ILE	3.9
1	A	542[A]	ALA	3.9
1	B	511	LEU	3.9
1	B	344	LEU	3.8
1	B	378	PHE	3.8
1	B	562	LEU	3.7
1	B	486	HIS	3.7
1	B	406	ILE	3.7
1	B	424	LEU	3.7
1	A	606	ASN	3.7
1	A	58	PHE	3.6
1	B	38	ILE	3.6
1	B	596	TYR	3.6
1	B	40	SER	3.6
1	B	92	ILE	3.6
1	B	294	ALA	3.6
1	A	672	GLU	3.5
1	A	142	VAL	3.5
1	A	343	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	438	TYR	3.5
1	A	277	GLN	3.5
1	B	477	ASP	3.5
1	A	2	TYR	3.5
1	B	465	ASP	3.5
1	B	181	LEU	3.5
1	B	523	SER	3.5
1	B	659	TRP	3.5
1	A	337	ALA	3.4
1	B	337	ALA	3.4
1	A	117	PRO	3.4
1	A	687	GLY	3.4
1	A	437	LEU	3.4
1	B	291	ILE	3.4
1	B	464	ALA	3.4
1	B	341	TYR	3.4
1	A	338	PHE	3.3
1	B	613	TYR	3.3
1	B	229	ASN	3.3
1	B	317	PRO	3.3
1	A	469	GLY	3.3
1	A	251	ALA	3.3
1	A	294	ALA	3.3
1	B	463	ILE	3.3
1	B	318	GLN	3.3
1	A	102	ASN	3.3
1	B	693	PRO	3.3
1	B	326	TRP	3.3
1	B	708	ILE	3.3
1	B	338	PHE	3.3
1	B	206	ASP	3.3
1	A	694	LEU	3.3
1	B	77	GLY	3.3
1	B	113	LYS	3.3
1	B	481	ARG	3.2
1	A	230	VAL	3.2
1	B	346	ASP	3.2
1	A	671	LEU	3.2
1	B	451	VAL	3.2
1	A	340	THR	3.2
1	A	315	ASP	3.2
1	B	595	ASP	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	335	LEU	3.2
1	B	41	TYR	3.2
1	A	336	THR	3.2
1	B	687	GLY	3.2
1	A	477	ASP	3.2
1	A	464	ALA	3.1
1	A	125	GLY	3.1
1	A	673	GLY	3.1
1	A	309	ILE	3.1
1	B	252	ILE	3.1
1	B	273	ASN	3.1
1	B	669	GLY	3.1
1	A	593	LYS	3.1
1	B	165	LEU	3.1
1	B	533	LEU	3.1
1	A	490	VAL	3.1
1	B	308	VAL	3.1
1	B	98	ALA	3.1
1	B	381	GLU	3.1
1	B	724	HIS	3.1
1	A	290	PRO	3.1
1	A	189	PHE	3.1
1	B	8	PHE	3.1
1	B	335	LEU	3.1
1	B	371	PHE	3.1
1	B	102	ASN	3.1
1	A	527	ILE	3.1
1	A	467	ALA	3.0
1	B	581	ALA	3.0
1	A	371	PHE	3.0
1	B	30	GLU	3.0
1	A	216	PRO	3.0
1	A	328	SER	3.0
1	A	114	LYS	3.0
1	B	322	ASN	3.0
1	A	118	ALA	3.0
1	A	237	VAL	3.0
1	A	217	GLU	2.9
1	B	493	THR	2.9
1	B	489	ALA	2.9
1	A	9	LEU	2.9
1	A	330	LEU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	184	SER	2.9
1	A	326	TRP	2.9
1	B	197	TYR	2.9
1	B	342	PHE	2.9
1	B	95	MET	2.9
1	A	484	THR	2.9
1	A	50	LEU	2.9
1	B	163	ASN	2.8
1	B	230	VAL	2.8
1	B	652	THR	2.8
1	A	215	LEU	2.8
1	B	347	LEU	2.8
1	B	643	LEU	2.8
1	B	188	MET	2.8
1	A	388	TYR	2.8
1	B	460	TYR	2.8
1	B	480	VAL	2.8
1	A	341	TYR	2.8
1	A	76	THR	2.8
1	B	336	THR	2.8
1	A	206	ASP	2.8
1	A	317	PRO	2.8
1	A	339	LEU	2.8
1	B	549	LEU	2.8
1	A	22	PHE	2.8
1	B	64	ILE	2.7
1	B	249	VAL	2.7
1	A	245	LEU	2.7
1	B	138	LEU	2.7
1	B	340	THR	2.7
1	A	539	MET	2.7
1	B	626	GLY	2.7
1	B	545	ILE	2.7
1	B	671	LEU	2.7
1	A	205	ALA	2.7
1	A	247	SER	2.7
1	B	566	VAL	2.7
1	A	438	TYR	2.7
1	B	65	ALA	2.7
1	A	124	GLN	2.7
1	B	100	ARG	2.7
1	A	93	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	581	ALA	2.6
1	A	428	ILE	2.6
1	A	473	MET	2.6
1	B	309	ILE	2.6
1	A	344	LEU	2.6
1	B	286	LEU	2.6
1	B	74	TRP	2.6
1	A	478	PRO	2.6
1	A	669	GLY	2.6
1	A	53	GLU	2.6
1	A	303	LEU	2.6
1	A	334	VAL	2.6
1	A	112	THR	2.6
1	A	209	GLY	2.5
1	B	69	MET	2.5
1	B	67	LEU	2.5
1	B	105	VAL	2.5
1	B	664	LYS	2.5
1	B	603	THR	2.5
1	A	331	LEU	2.5
1	A	310	VAL	2.5
1	B	5	ALA	2.5
1	A	688	ASP	2.5
1	B	164	TRP	2.5
1	B	114	LYS	2.5
1	B	4	ALA	2.5
1	B	469	GLY	2.5
1	B	557	TYR	2.5
1	A	38	ILE	2.5
1	A	62	ILE	2.5
1	B	62	ILE	2.5
1	A	298	LEU	2.5
1	A	676	LYS	2.5
1	B	320	GLU	2.4
1	B	376	ILE	2.4
1	A	355	PHE	2.4
1	B	594	PRO	2.4
1	A	600	ILE	2.4
1	B	360	ILE	2.4
1	B	488	ASP	2.4
1	A	145	TYR	2.4
1	A	213	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	448	LEU	2.4
1	A	342	PHE	2.4
1	B	508	PHE	2.4
1	A	78	VAL	2.4
1	A	597	ASN	2.4
1	A	65	ALA	2.4
1	A	402	THR	2.4
1	B	313	PRO	2.4
1	B	483	ILE	2.4
1	A	158	LEU	2.4
1	B	725	LEU	2.4
1	B	598	ARG	2.4
1	B	256	ILE	2.4
1	B	539	MET	2.4
1	A	201	ALA	2.4
1	B	106	ALA	2.4
1	B	204	ALA	2.4
1	A	29	PRO	2.3
1	A	99	THR	2.3
1	B	111	THR	2.3
1	A	43	ARG	2.3
1	A	291	ILE	2.3
1	B	306	LEU	2.3
1	B	474	CYS	2.3
1	A	292	PHE	2.3
1	B	357	PHE	2.3
1	A	304	GLY	2.3
1	A	349[A]	GLY	2.3
1	A	256	ILE	2.3
1	A	511	LEU	2.3
1	B	57	ILE	2.3
1	B	232	ASP	2.3
1	B	210	LYS	2.3
1	B	312	LYS	2.3
1	A	179	TYR	2.3
1	B	334	VAL	2.3
1	B	382	TYR	2.3
1	A	329	ALA	2.3
1	B	658	ALA	2.3
1	B	34	ARG	2.3
1	B	449	SER	2.3
1	B	68	LEU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	470	ILE	2.3
1	A	113	LYS	2.3
1	B	22	PHE	2.3
1	B	53	GLU	2.3
1	A	11	PRO	2.3
1	A	365	SER	2.3
1	A	525	SER	2.3
1	A	6	LEU	2.3
1	B	482	LYS	2.3
1	A	4	ALA	2.2
1	A	116	GLY	2.2
1	A	643	LEU	2.2
1	B	364	PHE	2.2
1	A	279	PRO	2.2
1	B	72	THR	2.2
1	B	125	GLY	2.2
1	B	131	LEU	2.2
1	B	543[A]	ARG	2.2
1	B	292	PHE	2.2
1	B	619	ILE	2.2
1	B	627	PHE	2.2
1	B	722[A]	HIS	2.2
1	B	266	TYR	2.2
1	A	405	VAL	2.1
1	A	480	VAL	2.1
1	A	137	ALA	2.1
1	A	722	HIS	2.1
1	A	188	MET	2.1
1	B	118	ALA	2.1
1	B	303	LEU	2.1
1	A	465	ASP	2.1
1	A	595	ASP	2.1
1	A	49	PHE	2.1
1	B	128	VAL	2.1
1	A	666	LEU	2.1
1	B	12	LEU	2.1
1	B	358	GLY	2.1
1	B	602	ILE	2.1
1	B	674	TYR	2.1
1	B	604	SER	2.1
1	B	478	PRO	2.1
1	B	49	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	80	PHE	2.1
1	B	611	MET	2.1
1	A	63	VAL	2.1
1	A	325	LEU	2.1
1	A	533	LEU	2.1
1	B	73	THR	2.1
1	B	116	GLY	2.1
1	B	143	LEU	2.1
1	B	388	TYR	2.1
1	A	571	MET	2.1
1	B	720	PHE	2.1
1	A	683	ALA	2.1
1	A	623	LEU	2.1
1	B	353	LEU	2.1
1	B	623	LEU	2.1
1	A	327	THR	2.1
1	B	583	GLU	2.1
1	B	660	ASP	2.1
1	B	268	GLN	2.0
1	A	616	PHE	2.0
1	B	122	ALA	2.0
1	A	620	LEU	2.0
1	B	331	LEU	2.0
1	A	94	GLY	2.0
1	A	667	GLU	2.0
1	A	32	THR	2.0
1	B	663	LYS	2.0
1	A	69	MET	2.0
1	A	203	MET	2.0
1	A	262	MET	2.0
1	B	71	PHE	2.0
1	A	322	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

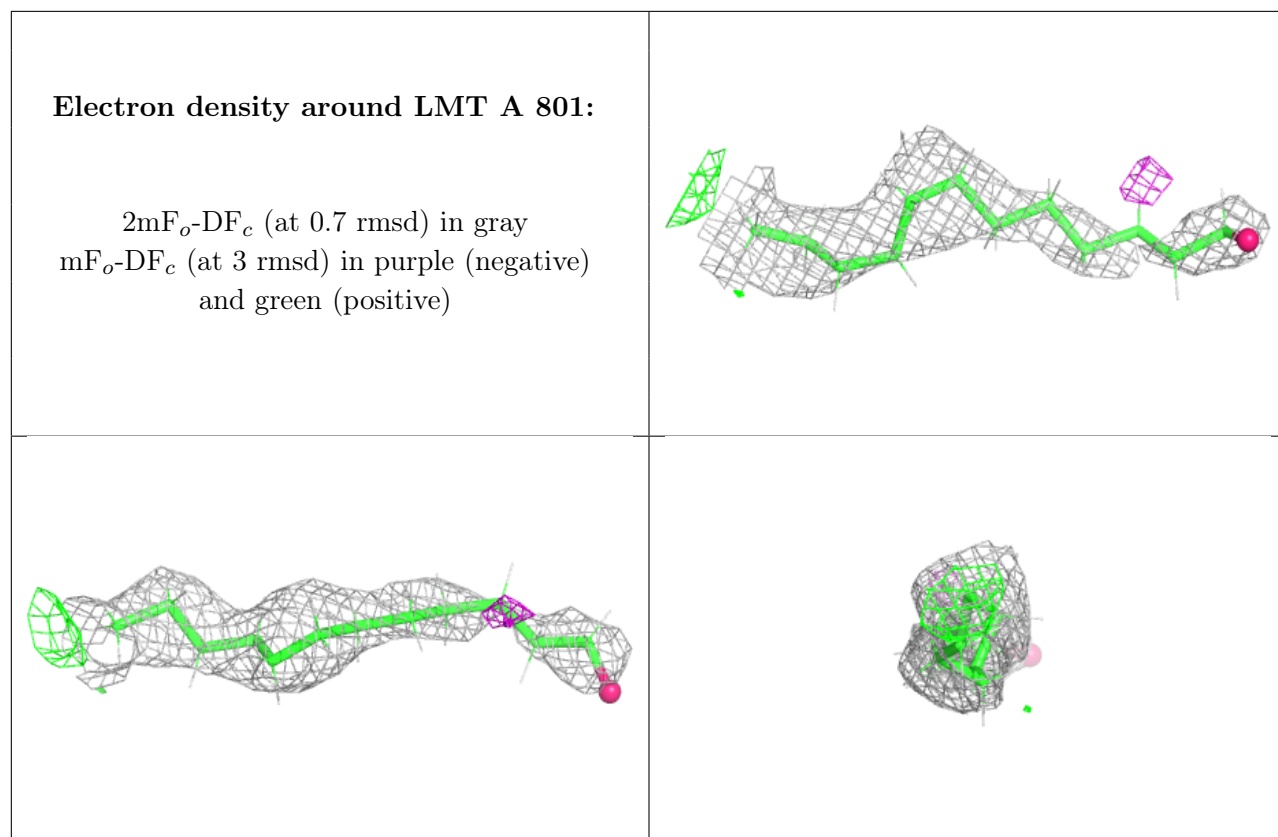
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PEG	B	803	7/7	0.41	0.19	33,33,77,77	0
3	PEG	B	808	7/7	0.54	0.25	33,33,79,79	0
5	PG4	A	807	13/13	0.56	0.17	33,33,93,93	0
3	PEG	B	809	7/7	0.63	0.16	33,33,74,74	0
3	PEG	B	811	7/7	0.64	0.16	33,33,77,77	0
5	PG4	B	813	13/13	0.67	0.16	33,33,88,88	0
5	PG4	B	814	13/13	0.67	0.15	33,33,87,87	0
5	PG4	A	806	13/13	0.71	0.21	33,33,85,85	0
3	PEG	B	810	7/7	0.74	0.13	33,33,78,78	0
3	PEG	B	805	7/7	0.74	0.13	31,31,89,89	0
4	PGE	A	808	10/10	0.75	0.15	33,33,80,80	0
3	PEG	A	803	7/7	0.76	0.15	33,33,73,73	0
3	PEG	B	801	7/7	0.80	0.21	31,31,73,73	0
3	PEG	B	804	7/7	0.80	0.16	31,31,70,70	0
2	LMT	A	801	13/35	0.81	0.20	12,12,69,69	0
3	PEG	B	802	7/7	0.81	0.10	31,31,76,76	0
4	PGE	A	805	10/10	0.83	0.10	33,33,81,81	0
3	PEG	B	807	7/7	0.83	0.17	33,33,76,76	0
5	PG4	B	812	13/13	0.84	0.14	33,33,79,79	0
3	PEG	B	806	7/7	0.84	0.13	31,31,80,80	0
5	PG4	A	809	13/13	0.84	0.15	33,33,76,76	0
3	PEG	A	802	7/7	0.87	0.11	31,31,80,80	0
4	PGE	A	804	10/10	0.87	0.18	33,33,71,71	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.