

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8B21
Title	:	Time-resolved structure of K+-dependent Na+-PPase from Thermotoga mar-
		itima 0-60-seconds post reaction initiation with $Na+$
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 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
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: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$			
R_{free}	130704	3163 (2.60-2.60)			
Clashscore	141614	3518 (2.60-2.60)			
Ramachandran outliers	138981	3455 (2.60-2.60)			
Sidechain outliers	138945	3455 (2.60-2.60)			
RSRZ outliers	127900	3104 (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 >=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	А	735	87%	10%	·
1	В	735	88%	9%	·

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
3	PEG	А	803	-	-	-	Х
3	PEG	В	801	-	-	-	Х
3	PEG	В	802	-	-	-	Х
3	PEG	В	804	-	-	-	Х
3	PEG	В	808	-	-	-	Х
4	PGE	А	804	-	-	-	Х
5	PG4	В	812	-	-	-	Х



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.

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

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

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

There are 24 discrepancies between the modelled and reference sequences:



• Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf
0	Λ	1	Total	С	Η	Ο	0	0
	1	38	12	25	1	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	А	1	Total	С	Η	Ο	0	0
5	11		17	4	10	3	Ŭ	Ŭ



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	Λ	1	Total C H	0	0	0	
5	A	1	17 4 10	3	0	0	
3	В	1	Total C H	Ο	0	0	
0	D	1	17 4 10	3	0	0	
ગ	В	1	Total C H	Ο	0	0	
0	D	1	17 4 10	3	0	0	
3	В	1	Total C H	Ο	0	0	
0	D	1	17 4 10	3	0	0	
3	В	1	Total C H	Ο	0	0	
0	D	1	17 4 10	3	0	0	
3	В	1	Total C H	Ο	0	0	
0	D	I	17 4 10	3	0	0	
3	В	1	Total C H	Ο	0	0	
	D	Ĩ	17 4 10	3	Ŭ		
3	В	1	Total C H	Ο	0	0	
	D	±	17 4 10	3	Ŭ		
3	В	1	Total C H	Ο	0	0	
	D	1	17 4 10	3	Ŭ		
3	В	1	Total C H	Ο	0	0	
0	D	1	17 4 10	3	0	0	
3	В	1	Total C H	Ο	0	0	
5 D		T	17 4 10	3	0	0	
3	В	1	Total C H	Ο	0	0	
		1	17 4 10	3	U		

• Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).





Mol	Chain	Residues	A	Ator	ns		ZeroOcc	AltConf
4 A	Δ	1	Total	С	Η	0	0	0
	Λ	I	24	6	14	4	0	
1	Δ Δ	1	Total	С	Η	Ο	0	0
4	Λ		24	6	14	4		0
1	Δ	1	Total	С	Η	0	0	0
4	A	L	24	6	14	4	0	0

• Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	A	Ator	\mathbf{ns}		ZeroOcc	AltConf	
5	Λ	1	Total	С	Η	Ο	0	0	
0	Л		31	8	18	5	0	U	
5	Δ	1	Total	С	Η	Ο	0	0	
0	Λ		31	8	18	5	0	U	
5	5 1	1	Total	С	Η	Ο	0	0	
0	Π		31	8	18	5	0	0	
5	В	1	Total	С	Η	Ο	0	0	
0	D	I	31	8	18	5			
5	В	1	Total	С	Η	Ο	0	0	
5	D	L	31	8	18	5	0	0	
5	В	1	Total	С	Η	O	0	0	
6	В	в 1	31	8	18	5	0	U	

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total O 1 1	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.



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

• Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump Chain B: 88% 9% .







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	84.02Å 110.05Å 107.41Å	Depositor
a, b, c, α , β , γ	90.00° 108.03° 90.00°	Depositor
Bosolution (Å)	102.13 - 2.59	Depositor
	102.13 - 2.59	EDS
% Data completeness	64.3 (102.13-2.59)	Depositor
(in resolution range)	64.3 (102.13-2.59)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.99 (at 2.58 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.220 , 0.236	Depositor
n, n_{free}	0.220 , 0.237	DCC
R_{free} test set	1757 reflections $(4.72%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	70.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.34 , 69.2	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	21562	wwPDB-VP
Average B, all atoms $(Å^2)$	72.0	wwPDB-VP

Xtriage'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.

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.



¹Intensities estimated from amplitudes.

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: PEG, PG4, PGE, LMT

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
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.27	0/5412	0.44	0/7373
1	В	0.28	0/5382	0.44	0/7338
All	All	0.28	0/10794	0.44	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 (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	А	5275	5302	5317	54	0
1	В	5227	5240	5206	44	0
2	А	13	25	25	0	0
3	А	14	20	20	0	0
3	В	77	110	110	0	0
4	А	30	42	42	0	0
5	А	39	54	54	0	0
5	В	39	54	54	1	0
6	B	1	0	0	0	0
All	All	10715	10847	10828	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including



hydrogen atoms). The all-atom clashscore for this structure is 4.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:421:THR:O	1:A:425:VAL:HG23	1.85	0.77
1:A:194:GLY:O	1:A:198:THR:HG23	1.89	0.73
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: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:259:ALA:HA	1:A:262:MET:HE2	1.83	0.61
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: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: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: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: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
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.94	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



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:A:651:LEU:C	1:A:651:LEU:HD23	2.36	0.46
1:A:30:GLU:CD	1:A:36:LYS:HG3	2.37	0.45
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:B:224:ALA:HA	1:B:573:MET:HE1	1.98	0.44
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:A:538:ASN:CG	1:B:536:LEU:HD12	2.38	0.44
1:A:639:ILE:HG13	1:B:539:MET:HG2	1.99	0.44
1:A:447:MET:HE2	1:A:505:SER:N	2.33	0.44
1:A:533:LEU:O	1:A:533:LEU:HD23	2.18	0.44
1:B:651:LEU:C	1:B:651:LEU:HD23	2.38	0.44
1:A:163:ASN:OD1	1:A:167:ILE:N	2.51	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: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
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:B:139:LEU:O	1:B:143:LEU:HG	2.21	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:310:VAL:HG12	1:B:310:VAL:O	2.21	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Perce	ntiles
1	А	722/735~(98%)	699~(97%)	23 (3%)	0	100	100
1	В	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	А	538/575~(94%)	536 (100%)	2~(0%)	91	97	
1	В	532/575~(92%)	529~(99%)	3~(1%)	86	95	
All	All	1070/1150~(93%)	1065 (100%)	5 (0%)	88	96	

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

Mol	Chain	Res	Type
1	А	17	PHE
1	А	508	PHE
1	В	17	PHE
1	В	477	ASP
1	В	508	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	Dec	Tink	Bo	Bond lengths			Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	PEG	В	805	-	$6,\!6,\!6$	1.00	0	$5,\!5,\!5$	0.63	0	
5	PG4	А	807	-	12,12,12	0.68	0	11,11,11	0.94	0	
3	PEG	В	802	-	6,6,6	0.90	0	$5,\!5,\!5$	0.62	0	
3	PEG	В	810	-	6,6,6	1.08	0	$5,\!5,\!5$	0.59	0	
4	PGE	А	808	-	9,9,9	1.20	1 (11%)	8,8,8	0.46	0	
5	PG4	А	806	-	12,12,12	0.68	0	11,11,11	0.94	0	
3	PEG	В	811	-	6,6,6	0.96	0	$5,\!5,\!5$	0.78	0	
2	LMT	А	801	-	12,12,36	0.30	0	$11,\!11,\!47$	0.40	0	
3	PEG	В	809	-	$6,\!6,\!6$	1.04	0	$5,\!5,\!5$	0.55	0	
3	PEG	А	803	-	$6,\!6,\!6$	1.05	0	$5,\!5,\!5$	0.62	0	
3	PEG	В	808	-	$6,\!6,\!6$	1.03	0	$5,\!5,\!5$	0.65	0	
3	PEG	В	804	-	$6,\!6,\!6$	1.16	0	$5,\!5,\!5$	0.58	0	
5	PG4	А	809	-	12,12,12	0.62	0	$11,\!11,\!11$	0.97	0	
5	PG4	В	814	-	$12,\!12,\!12$	0.67	0	$11,\!11,\!11$	0.92	0	
3	PEG	В	803	-	$6,\!6,\!6$	1.06	0	$5,\!5,\!5$	0.65	0	
4	PGE	А	804	-	$9,\!9,\!9$	1.20	1 (11%)	8,8,8	0.42	0	
5	PG4	В	812	-	12,12,12	0.73	0	11,11,11	0.90	0	
5	PG4	В	813	-	12,12,12	0.70	0	11,11,11	0.91	0	
4	PGE	А	805	-	9,9,9	1.19	2 (22%)	8,8,8	0.46	0	
3	PEG	В	807	-	6,6,6	0.90	0	$5,\!5,\!5$	0.65	0	
3	PEG	В	806	-	6,6,6	1.04	0	5, 5, 5	0.62	0	
3	PEG	А	802	-	6,6,6	0.93	0	5, 5, 5	0.65	0	
3	PEG	В	801	-	6,6,6	0.96	0	$5,\!5,\!5$	0.63	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	В	805	-	-	1/4/4/4	-
5	PG4	А	807	-	-	6/10/10/10	-
3	PEG	В	802	-	-	0/4/4/4	-
3	PEG	В	810	-	-	2/4/4/4	-
4	PGE	А	808	-	-	4/7/7/7	-
5	PG4	А	806	-	-	6/10/10/10	-
3	PEG	В	811	-	-	3/4/4/4	-
2	LMT	А	801	-	-	5/10/10/61	-
3	PEG	В	809	-	-	2/4/4/4	-
3	PEG	А	803	-	-	3/4/4/4	_



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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	А	804	PGE	C4-C3	2.19	1.60	1.49
4	А	808	PGE	C4-C3	2.15	1.60	1.49
4	А	805	PGE	C5-C6	2.05	1.60	1.49
4	А	805	PGE	C4-C3	2.04	1.59	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	812	PG4	O1-C1-C2-O2
5	В	812	PG4	O2-C3-C4-O3
5	А	809	PG4	O3-C5-C6-O4
4	А	804	PGE	O2-C3-C4-O3
5	А	809	PG4	O2-C3-C4-O3
5	В	813	PG4	O2-C3-C4-O3
5	В	813	PG4	O3-C5-C6-O4
3	В	803	PEG	O2-C3-C4-O4
3	В	807	PEG	O2-C3-C4-O4
3	В	808	PEG	O1-C1-C2-O2
3	В	809	PEG	O1-C1-C2-O2
3	В	811	PEG	O1-C1-C2-O2



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

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

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There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	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 then 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	$\langle RSRZ \rangle$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9
1	А	716/735~(97%)	1.08	106 (14%) 2	1	31, 69, 146, 181	1 (0%)
1	В	713/735~(97%)	0.96	96 (13%) 3	1	32, 76, 138, 175	0
All	All	1429/1470~(97%)	1.02	202 (14%) 2	1	31, 72, 143, 181	1 (0%)

All (202) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	В	596	TYR	10.5
1	А	596	TYR	8.2
1	А	119	LEU	7.5
1	В	119	LEU	7.2
1	А	123	TYR	7.2
1	В	207	LEU	6.8
1	А	476	LEU	6.6
1	А	230	VAL	6.2
1	А	474	CYS	6.1
1	В	595	ASP	5.8
1	А	115	ILE	5.8
1	А	594	PRO	5.7
1	В	115	ILE	5.6
1	В	233	ASN	5.5
1	В	210	LYS	5.5
1	А	116	GLY	5.4
1	А	475	GLU	5.2
1	В	211	THR	5.2
1	В	344	LEU	5.2
1	В	524	PRO	5.2
1	А	466	ASN	5.1
1	В	230	VAL	5.0
1	A	470	ILE	5.0
1	В	141	LEU	4.8



Mol	Chain	Res	Type	RSRZ
1	А	353	LEU	4.8
1	А	31	GLY	4.7
1	А	105	VAL	4.7
1	В	476	LEU	4.7
1	В	168	ASN	4.6
1	В	123	TYR	4.5
1	А	122	ALA	4.3
1	А	313	PRO	4.3
1	В	226	ILE	4.2
1	А	95	MET	4.1
1	А	487	LEU	4.1
1	А	223	PRO	4.1
1	В	197	TYR	4.0
1	В	114	LYS	4.0
1	А	189	PHE	4.0
1	A	406	ILE	4.0
1	В	466	ASN	4.0
1	В	353	LEU	3.9
1	А	98	ALA	3.8
1	А	463	ILE	3.8
1	В	7	PHE	3.7
1	А	473	MET	3.7
1	В	58	PHE	3.7
1	В	98	ALA	3.7
1	В	189	PHE	3.7
1	А	310	VAL	3.7
1	A	460	TYR	3.6
1	А	233	ASN	3.6
1	A	309	ILE	3.5
1	A	248	PHE	3.5
1	В	522	ILE	3.5
1	A	103	VAL	3.5
1	В	487	LEU	3.4
1	В	42	ILE	3.4
1	В	437	LEU	3.4
1	A	305	ILE	3.4
1	A	249	VAL	3.3
1	В	105	VAL	3.3
1	В	463	ILE	3.3
1	A	676	LYS	3.3
1	В	22	PHE	3.3
1	В	310	VAL	3.3



Mol	Chain	Res	Type	RSRZ
1	А	58	PHE	3.3
1	В	203	MET	3.3
1	А	690	VAL	3.3
1	А	659	TRP	3.2
1	В	326	TRP	3.2
1	В	708	ILE	3.2
1	В	102	ASN	3.2
1	В	30	GLU	3.1
1	А	120	LYS	3.1
1	А	371	PHE	3.1
1	А	469	GLY	3.1
1	А	127	SER	3.1
1	A	318	GLN	3.0
1	A	229	ASN	3.0
1	В	350	LEU	3.0
1	А	597	ASN	3.0
1	В	209	GLY	3.0
1	А	577	ILE	3.0
1	А	341	TYR	3.0
1	А	326	TRP	3.0
1	А	606	ASN	3.0
1	В	574	VAL	2.9
1	А	141	LEU	2.9
1	А	237	VAL	2.9
1	В	318	GLN	2.9
1	В	594	PRO	2.9
1	В	325	LEU	2.9
1	В	603	THR	2.8
1	A	131	LEU	2.8
1	В	313	PRO	2.8
1	В	157	ASN	2.8
1	В	347	LEU	2.8
1	В	103	VAL	2.8
1	А	167	ILE	2.7
1	А	128	VAL	2.7
1	В	158	LEU	2.7
1	В	371	PHE	2.7
1	А	30	GLU	2.7
1	В	346	ASP	2.7
1	В	572	LYS	2.7
1	А	549	LEU	2.7
1	А	166	GLY	2.7



Mol	Chain	Res	Type	RSRZ
1	А	492	ASN	2.7
1	А	542[A]	ALA	2.6
1	А	540	LEU	2.6
1	В	323	ILE	2.6
1	А	125	GLY	2.6
1	А	524	PRO	2.6
1	В	658	ALA	2.6
1	В	389	LYS	2.6
1	В	690	VAL	2.6
1	В	467	ALA	2.6
1	В	424	LEU	2.6
1	А	686	ILE	2.6
1	А	102	ASN	2.5
1	В	388	TYR	2.5
1	А	600	ILE	2.5
1	В	116	GLY	2.5
1	В	199	LYS	2.5
1	В	151	TRP	2.5
1	В	464	ALA	2.5
1	В	696	ASP	2.5
1	А	355	PHE	2.5
1	А	616	PHE	2.5
1	А	601	GLU	2.5
1	В	438	TYR	2.5
1	В	557	TYR	2.5
1	В	378	PHE	2.5
1	В	214	ASN	2.5
1	А	533	LEU	2.4
1	А	253	VAL	2.4
1	A	619	ILE	2.4
1	A	35	MET	2.4
1	В	495	ALA	2.4
1	A	42	ILE	2.4
1	А	277	GLN	2.4
1	A	467	ALA	2.4
1	А	138	LEU	2.4
1	В	428	ILE	2.4
1	В	460	TYR	2.4
1	А	611	MET	2.4
1	В	659	TRP	2.4
1	В	227	ALA	2.4
1	А	471	SER	2.4



Mol	Chain	Res	Type	RSRZ	
1	В	234	VAL	2.4	
1	В	643	LEU	2.4	
1	В	694	LEU	2.4	
1	В	106	ALA	2.3	
1	В	613	613 TYR		
1	А	437	LEU	2.3	
1	А	338	PHE	2.3	
1	В	662	ALA	2.3	
1	А	92	ILE	2.3	
1	А	158	LEU	2.3	
1	А	330	LEU	2.3	
1	А	220	PRO	2.2	
1	В	711	VAL	2.2	
1	A	392	GLN	2.2	
1	A	22	PHE	2.2	
1	В	107	GLU	2.2	
1	А	295	LEU	2.2	
1	А	579	ARG	2.2	
1	А	629	LEU	2.2	
1	А	3	VAL	2.2	
1	А	180	ALA	2.2	
1	В	305	ILE	2.2	
1	А	335	LEU	2.2	
1	В	237	VAL	2.2	
1	В	370	ILE	2.2	
1	А	298	LEU	2.2	
1	В	581	ALA	2.2	
1	А	608	LEU	2.2	
1	B	$22\overline{4}$	ALA	2.2	
1	А	257	ILE	2.2	
1	A	323	ILE	2.2	
1	В	95	MET	2.1	
1	А	252	ILE	2.1	
1	А	687	GLY	2.1	
1	В	212	GLU	2.1	
1	А	290	PRO	2.1	
1	В	124	GLN	2.1	
1	А	708	ILE	2.1	
1	В	309	ILE	2.1	
1	В	376	ILE	2.1	
1	A	684	LEU	2.1	
1	A	490	VAL	2.1	

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Mol	Chain	Res	Type	RSRZ
1	В	301	SER	2.1
1	А	491	GLY	2.1
1	А	545	ILE	2.1
1	А	628[A]	LEU	2.1
1	В	188	MET	2.0
1	В	511	LEU	2.0
1	А	643	LEU	2.0
1	А	172	PHE	2.0
1	В	410	LEU	2.0
1	В	470	ILE	2.0

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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	$B-factors(A^2)$	Q<0.9
5	PG4	А	807	13/13	0.52	0.23	33,33,93,93	0
3	PEG	В	809	7/7	0.54	0.40	33,33,74,74	0
3	PEG	В	804	7/7	0.56	0.42	31,31,70,70	0
3	PEG	В	805	7/7	0.58	0.36	31,31,89,89	0
5	PG4	А	806	13/13	0.65	0.34	33,33,85,85	0
3	PEG	В	803	7/7	0.65	0.39	33,33,77,77	0
3	PEG	А	803	7/7	0.68	0.55	33,33,73,73	0
4	PGE	А	804	10/10	0.70	0.74	33,33,71,71	0
4	PGE	А	808	10/10	0.70	0.38	33,33,80,80	0
3	PEG	В	802	7/7	0.70	0.66	31,31,76,76	0
3	PEG	В	811	7/7	0.70	0.34	33,33,77,77	0
5	PG4	В	814	13/13	0.70	0.16	33,33,87,87	0
2	LMT	А	801	13/35	0.73	0.27	12,12,69,69	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PG4	В	812	13/13	0.77	0.51	$33,\!33,\!79,\!79$	0
3	PEG	В	801	7/7	0.78	0.45	$31,\!31,\!73,\!73$	0
4	PGE	А	805	10/10	0.79	0.12	33,33,81,81	0
3	PEG	В	808	7/7	0.80	0.57	33,33,79,79	0
5	PG4	В	813	13/13	0.83	0.18	33,33,88,88	0
3	PEG	В	810	7/7	0.84	0.18	$33,\!33,\!78,\!78$	0
5	PG4	А	809	13/13	0.85	0.48	33,33,76,76	0
3	PEG	В	807	7/7	0.85	0.62	33,33,76,76	0
3	PEG	В	806	7/7	0.87	0.12	31,31,80,80	0
3	PEG	А	802	7/7	0.88	0.21	31,31,80,80	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.

