

Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 10:52 pm GMT

PDB ID	:	8B24
Title	:	Time-resolved structure of K+-dependent Na+-PPase from Thermotoga mar-
		itima 3600-seconds post reaction initiation with $Na+$
Authors	:	Strauss, J.; Vidilaseris, K.; Goldman, A.
Deposited on	:	2022-09-12
Resolution	:	4.53 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 4.53 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.



Motric	Whole archive	Similar resolution		
Wiethic	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	130704	1058 (5.28-3.80)		
Clashscore	141614	1126 (5.28-3.80)		
Ramachandran outliers	138981	1071 (5.26-3.80)		
Sidechain outliers	138945	1052 (5.26-3.80)		
RSRZ outliers	127900	1101 (5.30-3.70)		

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	20% 71%	25%	•••
1	В	735	14%	23%	•••



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10276 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	710	Total	С	Ν	0	\mathbf{S}	0	0	0
1	Π	/10	5076	3327	789	935	25	0	0	0
1	Р	705	Total	С	Ν	0	\mathbf{S}	0	4	0
1	D	705	5170	3389	811	943	27	0	4	0

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

Chain	Residue	Modelled	Actual	Actual Comment	
А	-8	MET	-	initiating methionine	UNP Q9S5X0
А	-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
А	-2	HIS	-	expression tag	UNP Q9S5X0
А	-1	HIS	-	expression tag	UNP Q9S5X0
А	0	HIS	-	expression tag	UNP Q9S5X0
А	1	HIS	-	expression tag	UNP Q9S5X0
А	353	LEU	VAL	engineered mutation	UNP Q9S5X0
А	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 DIPHOSPHATE (three-letter code: DPO) (formula: O₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	А	1	Total 9	O 7	Р 2	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	5	Total Mg 5 5	0	0
3	В	5	Total Mg 5 5	0	0

• Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total K 1 1	0	0

• Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	83.11Å 111.07Å 105.42Å	Depositor
a, b, c, α , β , γ	90.00° 108.90° 90.00°	Depositor
Bosolution(A)	99.74 - 4.53	Depositor
Resolution (A)	99.74 - 4.53	EDS
% Data completeness	56.3 (99.74-4.53)	Depositor
(in resolution range)	56.3(99.74-4.53)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.43 (at 4.47 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.326 , 0.361	Depositor
n, n_{free}	0.323 , 0.367	DCC
R_{free} test set	327 reflections $(5.42%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	287.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 353.1	EDS
L-test for twinning ²	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10276	wwPDB-VP
Average B, all atoms $(Å^2)$	389.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.35% 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: MG, DPO, K, PO4

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.28	0/5184	0.45	0/7093	
1	В	0.28	0/5280	0.47	0/7199	
All	All	0.28	0/10464	0.46	0/14292	

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	5076	0	4991	149	0
1	В	5170	0	5197	136	0
2	А	9	0	0	0	0
3	А	5	0	0	0	0
3	В	5	0	0	0	0
4	А	1	0	0	0	0
5	В	10	0	0	0	0
All	All	10276	0	10188	249	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 12.



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:576:GLU:HG3	1:B:602:ILE:HG13	1.66	0.76
1:A:540:LEU:HD22	1:B:535:LEU:HB3	1.67	0.76
1:A:247:SER:HA	1:A:707:LYS:HE3	1.66	0.75
1:A:340:THR:HG22	1:A:360:ILE:HD12	1.69	0.74
1:B:386:TYR:HA	1:B:391:THR:HB	1.69	0.74
1:B:194:GLY:O	1:B:198:THR:HG23	1.87	0.74
1:A:636:GLY:HA2	1:A:639:ILE:HD12	1.74	0.70
1:B:399:ILE:HA	1:B:680:PRO:HG3	1.73	0.70
1:A:639:ILE:HG12	1:B:539:MET:HG2	1.76	0.68
1:A:184:SER:HA	1:A:246:GLU:HG3	1.76	0.68
1:A:565:ALA:O	1:A:606:ASN:ND2	2.26	0.67
1:A:641:THR:HG22	1:A:706:ILE:HG12	1.76	0.67
1:B:138:LEU:HD13	1:B:295:LEU:HD23	1.77	0.66
1:B:308:VAL:HG21	1:B:324:SER:HB2	1.76	0.66
1:A:386:TYR:HA	1:A:391:THR:HB	1.79	0.65
1:B:95:MET:SD	1:B:96:LYS:N	2.70	0.64
1:A:350:LEU:HD22	1:A:358:GLY:HA2	1.79	0.64
1:A:538:ASN:ND2	1:B:535:LEU:O	2.30	0.64
1:B:115:ILE:HG23	1:B:487:LEU:HD11	1.79	0.64
1:B:366:ALA:HA	1:B:443:ALA:HA	1.81	0.63
1:A:444:ALA:HB2	1:A:508:PHE:HB3	1.81	0.62
1:A:553:ALA:HB2	1:B:421:THR:HG21	1.81	0.62
1:A:210:LYS:HA	1:A:215:LEU:O	2.00	0.62
1:B:138:LEU:HD12	1:B:298:LEU:HD22	1.82	0.62
1:A:535:LEU:O	1:B:538:ASN:ND2	2.32	0.61
1:B:50:LEU:HD11	1:B:95:MET:SD	2.40	0.61
1:A:511:LEU:HG	1:B:545:ILE:HD12	1.82	0.61
1:A:440:VAL:HG11	1:A:511:LEU:HD22	1.82	0.61
1:B:366:ALA:HB2	1:B:442:ILE:HG22	1.82	0.61
1:A:133:VAL:HG13	1:A:245:LEU:HB2	1.83	0.60
1:A:223:PRO:HA	1:A:596:TYR:CD1	2.35	0.60
1:A:7:PHE:HB3	1:A:295:LEU:HD13	1.83	0.60
1:A:220:PRO:HD3	1:A:473:MET:HA	1.83	0.60
1:A:358:GLY:O	1:A:361:SER:OG	2.18	0.60
1:A:223:PRO:HA	1:A:596:TYR:HD1	1.66	0.60
1:B:102:ASN:OD1	1:B:103:VAL:N	2.36	0.59
1:B:505:SER:HA	1:B:508:PHE:CE2	2.38	0.59
1:B:364:PHE:O	1:B:367:ILE:HG13	2.03	0.58
1:A:347:LEU:HB3	1:A:350:LEU:HD21	1.83	0.58
1:B:240:LEU:HD23	1:B:458:ASP:HB3	1.84	0.58

All (249) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:574:VAL:HG11	1:B:400:GLU:O	2.04	0.57
1:B:333:VAL:HG22	1:B:367:ILE:HG22	1.87	0.57
1:A:224:ALA:HB2	1:A:577:ILE:HD11	1.86	0.56
1:A:321:LEU:HD13	1:A:457:VAL:HG13	1.87	0.56
1:A:191:ARG:HH21	1:A:240:LEU:HA	1.70	0.56
1:A:643:LEU:O	1:A:647:MET:HG2	2.06	0.56
1:B:629:LEU:HD23	1:B:726:PHE:HB2	1.87	0.56
1:A:651:LEU:HD12	1:B:556:TYR:HD2	1.71	0.56
1:B:97:MET:HG2	1:B:128:VAL:HB	1.87	0.56
1:A:267:VAL:HA	1:A:275:VAL:O	2.05	0.56
1:A:492:ASN:ND2	1:A:660:ASP:OD2	2.39	0.56
1:A:381:GLU:HA	1:A:384:THR:HG22	1.88	0.55
1:A:79:ALA:HB1	1:A:179:TYR:HB2	1.89	0.55
1:A:401:GLY:O	1:A:405:VAL:HG23	2.05	0.55
1:A:578:ARG:NH1	1:B:399:ILE:O	2.33	0.55
1:A:252:ILE:HG12	1:A:445:LEU:HD13	1.87	0.55
1:B:539:MET:HE3	1:B:545:ILE:HA	1.89	0.55
1:B:216:PRO:HB2	1:B:219:ASP:HB2	1.89	0.55
1:A:407:SER:HB3	1:B:563:ILE:CG2	2.37	0.55
1:A:555:THR:HG23	1:A:702:LEU:HD22	1.88	0.54
1:B:293:PHE:HB3	1:B:445:LEU:HD21	1.88	0.54
1:B:526:ASP:HB3	1:B:534:VAL:HG22	1.89	0.54
1:A:414:MET:HB3	1:B:556:TYR:O	2.08	0.54
1:A:154:GLN:HA	1:A:157:ASN:HD21	1.74	0.53
1:A:32:THR:O	1:A:36:LYS:N	2.28	0.53
1:A:395:GLY:O	1:A:398:SER:OG	2.13	0.53
1:A:340:THR:HG21	1:A:360:ILE:HA	1.90	0.53
1:A:536:LEU:HD21	1:B:536:LEU:HD11	1.90	0.53
1:A:144:VAL:HG13	1:A:148:PHE:HD2	1.72	0.52
1:A:540:LEU:HD13	1:B:535:LEU:C	2.29	0.52
1:A:548:ALA:HB1	1:B:643:LEU:HD11	1.90	0.52
1:A:180:ALA:HB2	1:A:253:VAL:HG21	1.92	0.52
1:B:119:LEU:HD13	1:B:317:PRO:HB3	1.92	0.52
1:A:248:PHE:CZ	1:A:252:ILE:HD11	2.45	0.52
1:B:344:LEU:HB2	1:B:359:ALA:HB1	1.92	0.52
1:A:361:SER:HB2	1:A:435:ALA:HB2	1.92	0.52
1:B:82:LEU:O	1:B:86:MET:HG2	2.10	0.51
1:B:206:ASP:O	1:B:210:LYS:HG2	2.10	0.51
1:B:639:ILE:O	1:B:643:LEU:HG	2.10	0.51
1:A:519:PHE:O	1:A:522:ILE:HB	2.10	0.51
1:A:540:LEU:HD11	1:B:518:MET:HB3	1.93	0.51



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:700:PRO:O	1:B:704:ILE:HG12	2.11	0.51	
1:A:343:TYR:O	1:A:347:LEU:HG	2.11	0.51	
1:B:32:THR:OG1	1:B:110:ARG:NH1	2.43	0.51	
1:B:95:MET:SD	1:B:96:LYS:HG3	2.51	0.51	
1:A:138:LEU:HD13	1:A:295:LEU:HD23	1.92	0.51	
1:A:490:VAL:O	1:A:494:THR:HG23	2.11	0.50	
1:A:571:MET:HA	1:B:404:MET:SD	2.51	0.50	
1:A:647:MET:HG3	1:B:552:ALA:HB1	1.92	0.50	
1:A:362:PRO:O	1:A:366:ALA:N	2.31	0.50	
1:A:557:TYR:CD1	1:B:415:LYS:HA	2.46	0.50	
1:B:306:LEU:HD12	1:B:309:ILE:HD11	1.93	0.50	
1:A:415:LYS:HA	1:B:557:TYR:CD2	2.47	0.50	
1:A:519:PHE:CE1	1:A:535:LEU:HD21	2.46	0.50	
1:B:301:SER:HB3	1:B:453:THR:HG23	1.94	0.49	
1:B:337:ALA:HB2	1:B:363:TRP:CE2	2.47	0.49	
1:A:208:VAL:O	1:A:213:LEU:N	2.36	0.49	
1:A:639:ILE:O	1:A:643:LEU:HG	2.12	0.49	
1:A:82:LEU:HD23	1:A:144:VAL:HG23	1.94	0.49	
1:A:537:LEU:HB3	1:B:539:MET:H	1.76	0.49	
1:B:309:ILE:HG13	1:B:310:VAL:HG23	1.94	0.49	
1:B:548:ALA:HA	1:B:636:GLY:O	2.12	0.49	
1:A:80:PHE:HE2	1:A:185:ILE:HD12	1.77	0.49	
1:B:337:ALA:HB2	1:B:363:TRP:CZ2	2.48	0.49	
1:B:448:LEU:HD11	1:B:505:SER:HB2	1.93	0.49	
1:B:263:PHE:HB2	1:B:283:ILE:HG13	1.94	0.49	
1:A:86:MET:HB3	1:A:136:PHE:HB3	1.95	0.48	
1:A:563:ILE:O	1:A:567:THR:HG23	2.13	0.48	
1:B:544:VAL:HG22	1:B:632:GLU:HB3	1.95	0.48	
1:A:317:PRO:HG2	1:A:490:VAL:HG21	1.95	0.48	
1:A:344:LEU:HD23	1:A:358:GLY:HA3	1.95	0.48	
1:A:564:SER:HB2	1:B:411:SER:OG	2.12	0.48	
1:A:539:MET:HB2	1:B:537:LEU:HB3	1.96	0.48	
1:B:438:TYR:O	1:B:442:ILE:HG12	2.13	0.48	
1:B:38:ILE:HG23	1:B:473:MET:HE1	1.94	0.48	
1:A:133:VAL:HG13	1:A:245:LEU:HD12	1.96	0.48	
1:B:167:ILE:HD13	1:B:719:ILE:HG12	1.96	0.48	
1:B:52:HIS:NE2	1:B:601:GLU:HG2	2.29	0.48	
1:A:413:GLY:HA3	1:A:655:SER:HB2	1.96	0.48	
1:A:73:THR:HB	1:A:75:GLN:OE1	2.14	0.47	
1:A:539:MET:HE3	1:B:539:MET:HB2	1.96	0.47	
1:B:508:PHE:CD1	1:B:509:ALA:N	2.82	0.47	



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:256:ILE:HG23	1:B:287:ILE:HG23	1.96	0.47
1:A:321:LEU:HD22	1:A:457:VAL:HG22	1.97	0.47
1:A:359:ALA:O	1:A:362:PRO:HD2	2.13	0.47
1:A:537:LEU:HD23	1:B:539:MET:HB3	1.96	0.47
1:A:663:LYS:NZ	1:A:688:ASP:OD2	2.42	0.47
1:B:414:MET:O	1:B:417:VAL:HG22	2.15	0.47
1:A:95:MET:HA	1:A:237:VAL:HG11	1.97	0.47
1:A:698:VAL:O	1:A:702:LEU:HG	2.14	0.47
1:B:262:MET:HG3	1:B:519:PHE:HE2	1.78	0.47
1:B:282:THR:HA	1:B:347:LEU:HD22	1.96	0.47
1:A:535:LEU:HB3	1:B:540:LEU:HD12	1.97	0.47
1:B:158:LEU:HD23	1:B:280:LYS:HG2	1.97	0.47
1:A:195:GLY:HA2	1:A:198:THR:HG22	1.97	0.47
1:A:396:LYS:O	1:A:400:GLU:HG2	2.15	0.46
1:B:517:TYR:HB2	1:B:714:VAL:HG22	1.96	0.46
1:B:198:THR:HG22	1:B:231:GLY:CA	2.45	0.46
1:A:700:PRO:O	1:A:704:ILE:HG13	2.15	0.46
1:A:82:LEU:O	1:A:86:MET:HG2	2.15	0.46
1:B:199:LYS:HG3	1:B:693:PRO:HA	1.97	0.46
1:A:265:ILE:HG12	1:A:522:ILE:HG13	1.98	0.46
1:A:514:PHE:HE1	1:A:638:LEU:HB3	1.80	0.46
1:A:536:LEU:HD11	1:B:536:LEU:HD11	1.97	0.46
1:B:86:MET:HB3	1:B:136:PHE:HB3	1.97	0.46
1:B:332:THR:O	1:B:336:THR:OG1	2.16	0.46
1:A:258:LEU:HG	1:A:519:PHE:HE2	1.81	0.46
1:B:69:MET:HG2	1:B:74:TRP:HA	1.96	0.46
1:A:192:VAL:HG11	1:A:614:PRO:HG3	1.97	0.46
1:A:516:SER:HA	1:A:519:PHE:HB2	1.98	0.46
1:B:399:ILE:HG23	1:B:671:LEU:HD21	1.97	0.46
1:B:208:VAL:O	1:B:214:ASN:HA	2.16	0.46
1:B:643:LEU:O	1:B:647:MET:HG2	2.16	0.46
1:A:10:ILE:HG22	1:A:298:LEU:HD22	1.98	0.45
1:A:398:SER:HA	1:A:405:VAL:CG2	2.46	0.45
1:A:643:LEU:HD11	1:B:548:ALA:HB1	1.98	0.45
1:A:119:LEU:HD13	1:A:317:PRO:HB3	1.97	0.45
1:B:107:GLU:OE1	1:B:110:ARG:NH2	2.49	0.45
1:B:664:LYS:O	1:B:668:ALA:N	2.46	0.45
1:B:710:SER:O	1:B:714:VAL:HG23	2.16	0.45
1:A:60:VAL:O	1:A:64:ILE:HG12	2.17	0.45
1:A:208:VAL:HG21	1:A:574:VAL:HG13	1.98	0.45
1:A:29:PRO:HG2	1:A:107:GLU:OE1	2.16	0.45



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:209:GLY:O	1:A:215:LEU:HB2	2.17	0.45
1:A:522:ILE:HD12	1:A:527:ILE:HG13	1.98	0.45
1:A:558:PHE:HE1	1:A:614:PRO:HB3	1.82	0.45
1:B:575:ASP:HA	1:B:578:ARG:HE	1.82	0.44
1:A:538:ASN:HD21	1:A:540:LEU:HB2	1.82	0.44
1:A:154:GLN:HA	1:A:157:ASN:ND2	2.32	0.44
1:A:80:PHE:CE2	1:A:185:ILE:HD12	2.51	0.44
1:A:336:THR:HG22	1:A:363:TRP:HD1	1.82	0.44
1:A:349:GLY:O	1:A:352:VAL:HG22	2.17	0.44
1:A:448:LEU:HD13	1:A:505:SER:HB2	2.00	0.44
1:A:560:GLY:HA3	1:B:414:MET:HB2	1.99	0.44
1:A:567:THR:O	1:A:571:MET:N	2.39	0.44
1:B:573:MET:HB2	1:B:603:THR:HG22	2.00	0.44
1:A:207:LEU:O	1:A:211:THR:HB	2.18	0.44
1:A:537:LEU:N	1:B:538:ASN:OD1	2.51	0.44
1:A:222:ASN:HB3	1:A:225:THR:HG23	1.99	0.44
1:A:700:PRO:HA	1:A:703:ASP:OD2	2.18	0.44
1:A:191:ARG:HD3	1:A:700:PRO:HB2	2.00	0.43
1:A:446:GLY:HA2	1:A:449:SER:HB3	2.00	0.43
1:B:524:PRO:O	1:B:527:ILE:HG12	2.18	0.43
1:A:266:TYR:HB3	1:A:277:GLN:HB2	1.99	0.43
1:A:518:MET:HB2	1:B:540:LEU:HD11	1.99	0.43
1:B:233:ASN:O	1:B:237:VAL:HB	2.17	0.43
1:B:153:GLY:O	1:B:157:ASN:ND2	2.51	0.43
1:B:188:MET:HA	1:B:704:ILE:HG21	2.00	0.43
1:B:413:GLY:O	1:B:417:VAL:HG13	2.19	0.43
1:A:69:MET:HG2	1:A:74:TRP:HA	2.00	0.43
1:A:267:VAL:HG21	1:A:527:ILE:HG23	2.01	0.43
1:A:399:ILE:HD11	1:A:671:LEU:HD21	2.00	0.43
1:A:413:GLY:O	1:A:417:VAL:HG23	2.19	0.43
1:A:461:GLY:HA2	1:A:491:GLY:HA3	2.00	0.43
1:A:333:VAL:HG22	1:A:367:ILE:HG12	2.00	0.43
1:A:429:LEU:HD11	1:B:629:LEU:HD11	2.00	0.43
1:B:401:GLY:O	1:B:405:VAL:HG23	2.18	0.43
1:B:461:GLY:N	1:B:462:PRO:HD2	2.34	0.43
1:B:613:TYR:HB3	1:B:614:PRO:HD3	2.00	0.43
1:A:539:MET:HE1	1:A:639:ILE:HD13	2.00	0.42
1:B:517:TYR:CE1	1:B:717:VAL:HB	2.54	0.42
1:A:461:GLY:CA	1:A:491:GLY:HA3	2.49	0.42
1:B:151:TRP:CE3	1:B:152:MET:HG2	2.54	0.42
1:B:559:SER:OG	1:B:702:LEU:HD21	2.19	0.42



	hi o	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:50:LEU:HD21	1:A:92:ILE:HG12	2.02	0.42	
1:A:196:VAL:HA	1:A:566:VAL:HG22	2.02	0.42	
1:B:499:LYS:O	1:B:503:ILE:HG13	2.20	0.42	
1:A:418:PHE:HB3	1:A:419:PRO:HD3	2.01	0.42	
1:A:557:TYR:HD1	1:B:415:LYS:HA	1.85	0.42	
1:A:438:TYR:O	1:A:442:ILE:HG12	2.19	0.42	
1:A:210:LYS:HD3	1:A:217:GLU:HB2	2.02	0.42	
1:B:94:GLY:HA3	1:B:129:MET:SD	2.60	0.42	
1:A:513:LEU:HD13	1:A:710:SER:OG	2.19	0.41	
1:A:563:ILE:HB	1:B:411:SER:HB2	2.01	0.41	
1:A:645:GLY:HA3	1:A:706:ILE:HD11	2.02	0.41	
1:B:265:ILE:HG12	1:B:522:ILE:HD13	2.02	0.41	
1:B:510:ALA:HB1	1:B:642:VAL:HG22	2.02	0.41	
1:A:234:VAL:O	1:A:238:ALA:HB3	2.20	0.41	
1:A:503:ILE:HD13	1:A:703:ASP:HB3	2.02	0.41	
1:B:79:ALA:HB1	1:B:179:TYR:HB2	2.02	0.41	
1:B:541[A]:ASP:HB3	1:B:544:VAL:HG23	2.02	0.41	
1:A:160:ILE:HD11	1:A:168:ASN:HB2	2.02	0.41	
1:A:233:ASN:O	1:A:237:VAL:HB	2.21	0.41	
1:B:417:VAL:HA	1:B:650:ILE:HG21	2.02	0.41	
1:B:483:ILE:O	1:B:487:LEU:HD13	2.20	0.41	
1:B:396:LYS:O	1:B:399:ILE:HG12	2.20	0.41	
1:B:447:MET:SD	1:B:508:PHE:HE2	2.44	0.41	
1:B:237:VAL:HG23	1:B:462:PRO:HG3	2.03	0.41	
1:B:319:ARG:O	1:B:323:ILE:HG13	2.20	0.41	
1:B:370:ILE:HG23	1:B:450:PHE:HE1	1.86	0.41	
1:A:514:PHE:C	1:B:540:LEU:HD21	2.41	0.41	
1:A:536:LEU:HD11	1:B:536:LEU:HD21	2.02	0.41	
1:B:115:ILE:HG12	1:B:483:ILE:HG23	2.02	0.41	
1:A:476:LEU:HD12	1:A:476:LEU:HA	1.86	0.41	
1:B:252:ILE:HG23	1:B:290:PRO:HB2	2.03	0.41	
1:B:634:VAL:O	1:B:638:LEU:HG	2.21	0.41	
1:B:705:LEU:HA	1:B:708:ILE:HG22	2.02	0.41	
1:B:399:ILE:CG2	1:B:671:LEU:HD21	2.51	0.40	
1:B:508:PHE:HD1	1:B:509:ALA:N	2.20	0.40	
1:A:138:LEU:HD12	1:A:298:LEU:HD13	2.02	0.40	
1:A:540:LEU:HD21	1:B:518:MET:HB2	2.04	0.40	
1:A:544:VAL:HG22	1:A:632:GLU:HB3	2.02	0.40	
1:B:237:VAL:HG23	1:B:462:PRO:CG	2.51	0.40	
1:B:248:PHE:HZ	1:B:294:ALA:HB1	1.86	0.40	
1:B:693:PRO:O	1:B:697:THR:HB	2.21	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:HG	1:B:263:PHE:CD2	2.56	0.40
1:B:191:ARG:HA	1:B:191:ARG:HD3	1.72	0.40
1:A:53:GLU:O	1:A:57:ILE:HG12	2.22	0.40
1:B:418:PHE:HB3	1:B:419:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	706/735~(96%)	695~(98%)	11 (2%)	0	100	100
1	В	705/735~(96%)	696 (99%)	9 (1%)	0	100	100
All	All	1411/1470~(96%)	1391 (99%)	20 (1%)	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 side chain 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	Percen	tiles
1	А	500/575~(87%)	493~(99%)	7 (1%)	67	81
1	В	526/575~(92%)	520 (99%)	6 (1%)	73	85
All	All	1026/1150~(89%)	1013~(99%)	13 (1%)	69	82



Mol	Chain	Res	Type
1	А	25	VAL
1	А	164	TRP
1	А	191	ARG
1	А	361	SER
1	А	522	ILE
1	А	527	ILE
1	А	623	LEU
1	В	103	VAL
1	В	152	MET
1	В	191	ARG
1	В	487	LEU
1	В	508	PHE
1	В	579	ARG

All (13) residues with a non-rotameric sidechain are listed below:

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)

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mal	Tuno	Chain	Dec	Tink	B	ond leng	gths	B	ond ang	les
IVIOI	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	PO4	В	801	3	4,4,4	0.91	0	6,6,6	0.41	0
5	PO4	В	802	3	4,4,4	0.92	0	6,6,6	0.43	0
2	DPO	А	801	3,4	6,8,8	0.63	0	13,13,13	2.09	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DPO	А	801	3,4	-	0/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	801	DPO	P2-O4-P1	6.93	156.60	132.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 sufficient 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	<RSRZ $>$	#RSRZ>2		2	$OWAB(Å^2)$	Q<0.9
1	А	710/735~(96%)	0.86	149 (20%)	1	1	219, 383, 516, 644	0
1	В	705/735~(95%)	0.46	103~(14%)	2	3	215, 381, 531, 728	0
All	All	1415/1470~(96%)	0.66	252 (17%)	1	2	215, 382, 523, 728	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	320	GLU	13.6
1	В	211	THR	10.9
1	А	615	ALA	10.7
1	А	127	SER	10.4
1	А	314	SER	9.1
1	В	317	PRO	8.9
1	В	123	TYR	8.8
1	В	347	LEU	8.4
1	А	315	ASP	8.0
1	А	125	GLY	7.9
1	В	124	GLN	7.8
1	В	214	ASN	7.7
1	А	105	VAL	7.5
1	А	316	ASN	7.5
1	В	316	ASN	7.4
1	А	612	GLY	7.1
1	А	53	GLU	7.1
1	В	494	THR	6.8
1	А	123	TYR	6.5
1	В	490	VAL	6.4
1	В	423	THR	6.4
1	A	104	ARG	6.4
1	A	611	MET	6.2
1	В	87	SER	6.0



Mol	Chain	Res	Type	RSRZ
1	В	321	LEU	5.9
1	А	290	PRO	5.9
1	В	213	LEU	5.9
1	В	315	ASP	5.9
1	А	57	ILE	5.8
1	В	243	ASP	5.7
1	А	124	GLN	5.6
1	А	126	GLY	5.6
1	В	240	LEU	5.6
1	А	318	GLN	5.5
1	В	209	GLY	5.5
1	В	241	GLY	5.5
1	А	278	VAL	5.4
1	В	210	LYS	5.3
1	А	700	PRO	5.2
1	А	95	MET	5.1
1	А	614	PRO	5.1
1	А	106	ALA	5.1
1	В	489	ALA	5.0
1	В	419	PRO	5.0
1	В	318	GLN	5.0
1	А	91	GLY	5.0
1	А	670	ASN	4.9
1	А	188	MET	4.8
1	А	559	SER	4.8
1	А	563	ILE	4.7
1	А	128	VAL	4.6
1	А	243	ASP	4.6
1	А	610	GLN	4.6
1	А	562	LEU	4.5
1	В	324	SER	4.5
1	А	322	ASN	4.5
1	А	191	ARG	4.5
1	В	122	ALA	4.4
1	А	494	THR	4.4
1	А	618	ALA	4.4
1	В	212	GLU	4.4
1	А	270	ILE	4.4
1	А	271	GLY	4.3
1	А	58	PHE	4.3
1	А	282	THR	4.3
1	В	244	LEU	4.3



Mol	Chain	Res	Type	RSRZ
1	В	450	PHE	4.3
1	А	526	ASP	4.3
1	А	56	ALA	4.3
1	А	493	THR	4.2
1	А	94	GLY	4.2
1	А	279	PRO	4.2
1	В	703	ASP	4.1
1	А	401	GLY	4.1
1	А	674	TYR	4.1
1	А	386	TYR	4.1
1	В	426	LEU	4.0
1	А	145	TYR	4.0
1	А	308	VAL	4.0
1	А	497	ILE	4.0
1	В	614	PRO	4.0
1	В	247	SER	3.9
1	В	449	SER	3.9
1	А	699	GLY	3.9
1	А	122	ALA	3.9
1	В	488	ASP	3.9
1	В	191	ARG	3.9
1	А	703	ASP	3.9
1	В	245	LEU	3.9
1	А	131	LEU	3.9
1	В	346	ASP	3.8
1	В	127	SER	3.8
1	А	527	ILE	3.7
1	А	350	LEU	3.7
1	В	453	THR	3.7
1	А	496	ALA	3.7
1	А	681	HIS	3.7
1	В	236	ASP	3.7
1	В	563	ILE	3.6
1	А	501	PHE	3.6
1	A	678	SER	3.6
1	В	325	LEU	3.6
1	A	639	ILE	3.6
1	В	8	PHE	3.6
1	А	54	THR	3.6
1	A	17	PHE	3.6
1	В	323	ILE	3.5
1	В	542	ALA	3.5



Mol	Chain	Res	Type	RSRZ
1	В	57	ILE	3.5
1	А	671	LEU	3.5
1	А	698	VAL	3.5
1	А	167	ILE	3.5
1	А	545	ILE	3.5
1	А	347	LEU	3.5
1	А	119	LEU	3.5
1	А	558	PHE	3.4
1	А	317	PRO	3.4
1	А	348	GLN	3.4
1	А	102	ASN	3.4
1	А	248	PHE	3.4
1	А	286	LEU	3.4
1	В	418	PHE	3.3
1	В	246	GLU	3.3
1	А	319	ARG	3.3
1	А	101	ALA	3.3
1	В	314	SER	3.3
1	В	700	PRO	3.3
1	А	168	ASN	3.3
1	В	425	VAL	3.2
1	А	321	LEU	3.2
1	В	88	ALA	3.2
1	В	422	LEU	3.2
1	В	188	MET	3.2
1	В	524	PRO	3.2
1	А	283	ILE	3.1
1	В	493	THR	3.1
1	A	103	VAL	3.1
1	В	319	ARG	3.1
1	В	322	ASN	3.1
1	A	677	GLY	3.1
1	A	305	ILE	3.1
1	А	173	ALA	3.1
1	A	351	ASP	3.0
1	В	421	THR	3.0
1	А	172	PHE	3.0
1	A	457	VAL	3.0
1	А	93	VAL	3.0
1	В	525	SER	3.0
1	А	291	ILE	3.0
1	А	392	GLN	3.0



Mol	Chain	Res	Type	RSRZ
1	А	616	PHE	3.0
1	А	115	ILE	2.9
1	А	619	ILE	2.9
1	В	248	PHE	2.9
1	В	119	LEU	2.9
1	В	215	LEU	2.9
1	В	545	ILE	2.9
1	В	699	GLY	2.9
1	В	237	VAL	2.8
1	В	460	TYR	2.8
1	А	385	SER	2.8
1	В	308	VAL	2.8
1	В	184	SER	2.8
1	В	142	VAL	2.8
1	А	141	LEU	2.7
1	А	309	ILE	2.7
1	А	349	GLY	2.7
1	А	237	VAL	2.7
1	А	252	ILE	2.7
1	В	539	MET	2.7
1	А	144	VAL	2.7
1	В	31	GLY	2.7
1	В	497	ILE	2.7
1	А	512	SER	2.7
1	В	138	LEU	2.6
1	А	138	LEU	2.6
1	А	683	ALA	2.6
1	В	311	LYS	2.6
1	А	684	LEU	2.6
1	А	387	ARG	2.6
1	А	184	SER	2.6
1	А	511	LEU	2.6
1	В	242	ALA	2.6
1	A	133	VAL	2.6
1	В	561	TYR	2.5
1	А	166	GLY	2.5
1	A	260	SER	2.5
1	A	244	LEU	2.5
1	A	295	LEU	2.5
1	A	548	ALA	2.5
1	В	348[A]	GLN	2.5
1	А	524	PRO	2.5



Mol	Chain	Res	Type	RSRZ
1	В	457	VAL	2.5
1	В	187	ALA	2.5
1	В	310	VAL	2.5
1	А	523	SER	2.5
1	А	253	VAL	2.4
1	А	109	ALA	2.4
1	В	501	PHE	2.4
1	В	562	LEU	2.4
1	А	35	MET	2.4
1	А	525	SER	2.4
1	А	609	LYS	2.4
1	В	458	ASP	2.4
1	А	98	ALA	2.4
1	А	549	LEU	2.4
1	В	125	GLY	2.4
1	А	356	ARG	2.3
1	В	643	LEU	2.3
1	А	287	ILE	2.3
1	В	486	HIS	2.3
1	В	141	LEU	2.3
1	А	486	HIS	2.3
1	В	183	CYS	2.3
1	А	325	LEU	2.3
1	А	326	TRP	2.3
1	А	402	THR	2.3
1	А	306	LEU	2.3
1	А	294	ALA	2.3
1	B	447	MET	2.3
1	A	32	THR	2.3
1	A	500	GLY	2.2
1	В	491	GLY	2.2
1	B	53	GLU	2.2
1	B	305	ILE	2.2
1	А	87	SER	2.2
1	A	90	ALA	2.2
1	В	207	LEU	2.2
1	А	490	VAL	2.2
1	В	307	TYR	2.2
1	А	389	LYS	2.2
1	А	21	ASN	2.1
1	A	187	ALA	2.1
1	В	679	GLU	2.1



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Mol	Chain	Res	Type	RSRZ
1	А	4	ALA	2.1
1	А	285	ALA	2.1
1	В	376	ILE	2.1
1	А	400	GLU	2.1
1	А	256	ILE	2.1
1	В	238	ALA	2.1
1	А	107	GLU	2.1
1	А	60	VAL	2.1
1	В	192	VAL	2.1
1	В	618	ALA	2.1
1	В	239	GLY	2.0
1	А	393	PHE	2.0
1	А	450	PHE	2.0
1	В	454	SER	2.0
1	В	673	GLY	2.0
1	А	72	THR	2.0
1	А	557	TYR	2.0
1	А	307	TYR	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	$B-factors(Å^2)$	Q<0.9
3	MG	В	805	1/1	0.79	0.21	368,368,368,368	0
3	MG	В	803	1/1	0.82	0.19	352,352,352,352	0
5	PO4	В	802	5/5	0.85	0.14	406,406,406,406	0
3	MG	В	806	1/1	0.86	0.38	387,387,387,387	0
3	MG	А	803	1/1	0.86	0.13	472,472,472,472	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
5	PO4	В	801	5/5	0.89	0.09	389,389,389,389	0
3	MG	А	805	1/1	0.91	0.15	450,450,450,450	0
2	DPO	А	801	9/9	0.91	0.16	436,436,436,436	0
3	MG	А	804	1/1	0.93	0.18	440,440,440,440	0
4	K	А	807	1/1	0.93	0.13	331,331,331,331	0
3	MG	В	807	1/1	0.95	0.12	381,381,381,381	0
3	MG	А	802	1/1	0.95	0.06	474,474,474,474	0
3	MG	А	806	1/1	0.97	0.17	404,404,404,404	0
3	MG	В	804	1/1	0.97	0.10	379,379,379,379	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.

