



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 03:35 PM EDT

PDB ID : 6M96  
Title : ATP-bound conformation of the WzmWzt O antigen ABC transporter  
Authors : Caffalette, C.A.; Zimmer, J.  
Deposited on : 2018-08-22  
Resolution : 2.05 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

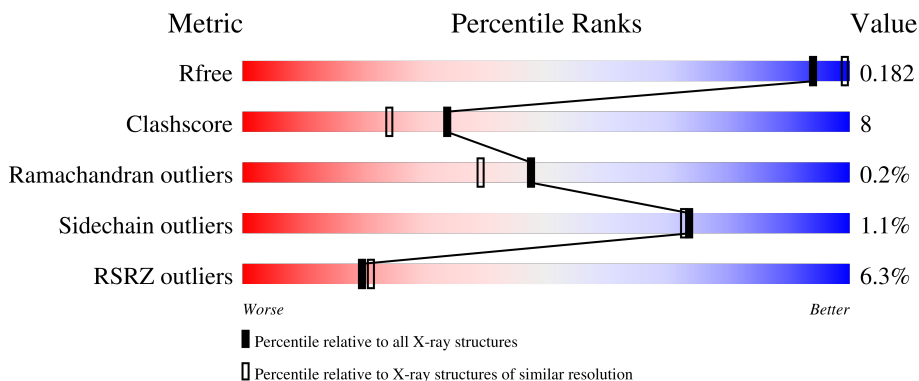
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.05 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))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	244	
2	B	256	

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 4982 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ABC transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	238	1949	1267	319	356	7	0	10	0

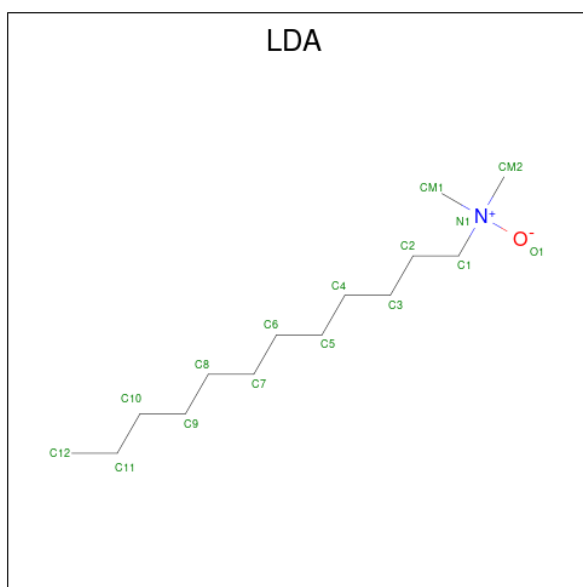
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O67181
A	1	GLY	-	expression tag	UNP O67181
A	167	GLN	GLU	engineered mutation	UNP O67181
A	236	LYS	-	expression tag	UNP O67181
A	237	LEU	-	expression tag	UNP O67181
A	238	HIS	-	expression tag	UNP O67181
A	239	HIS	-	expression tag	UNP O67181
A	240	HIS	-	expression tag	UNP O67181
A	241	HIS	-	expression tag	UNP O67181
A	242	HIS	-	expression tag	UNP O67181
A	243	HIS	-	expression tag	UNP O67181

- Molecule 2 is a protein called Transport permease protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	256	2281	1613	313	350	5	0	27	0

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 4 4	0	0
3	B	1	Total C N O 13 11 1 1	0	0
3	B	1	Total C N O 16 14 1 1	0	0
3	B	1	Total C N O 16 14 1 1	0	0
3	B	1	Total C N O 16 14 1 1	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C N O 16 14 1 1	0	0
3	B	1	Total C N O 8 6 1 1	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 4 4	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C N O 12 10 1 1	0	0
3	B	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			9	7	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C			0	0
			8	8				
3	B	1	Total	C			0	0
			4	4				
3	B	1	Total	C			0	0
			5	5				
3	B	1	Total	C			0	0
			3	3				
3	B	1	Total	C			0	0
			3	3				
3	B	1	Total	C			0	0
			5	5				
3	B	1	Total	C			0	0
			8	8				
3	B	1	Total	C			0	0
			9	9				
3	B	1	Total	C			0	0
			5	5				
3	B	1	Total	C			0	0
			3	3				
3	B	1	Total	C			0	0
			5	5				
3	B	1	Total	C			0	0
			3	3				
3	B	1	Total	C			0	0
			4	4				
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C			0	0
			4	4				
3	B	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



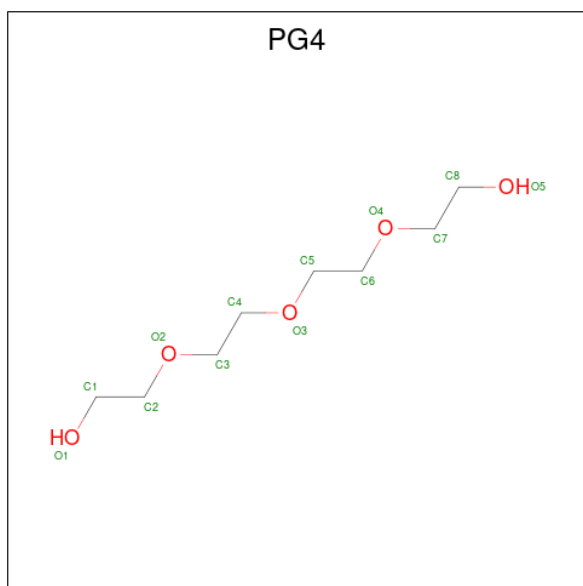
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	10	5	13	3	0	0

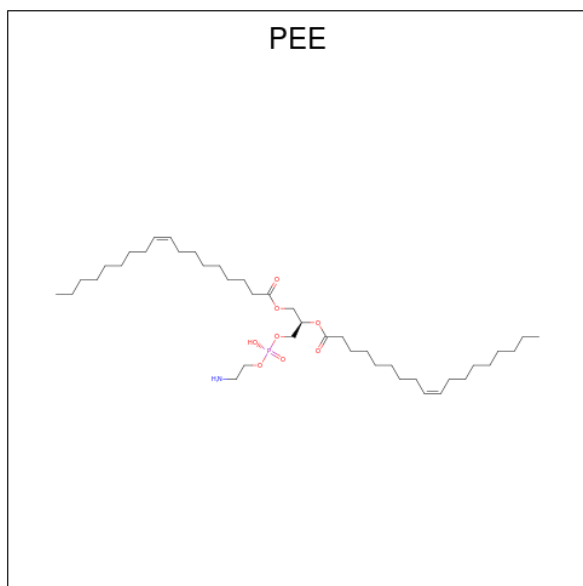
- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	13	8	5	0	0
6	A	1	10	6	4	0	0

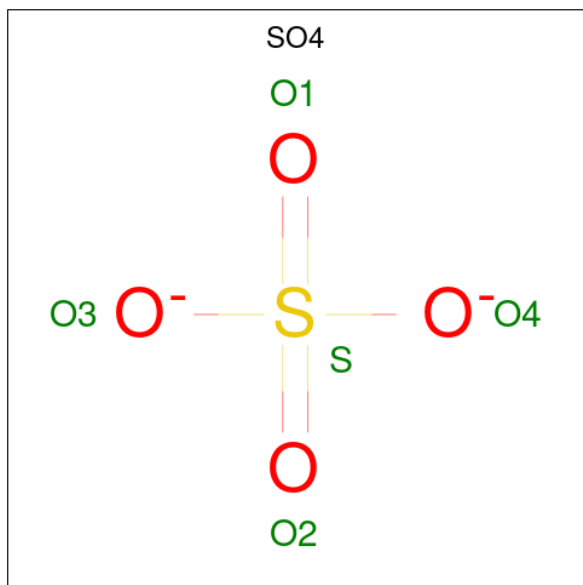
- Molecule 7 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE)

(formula: C<sub>41</sub>H<sub>78</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	9	3	1	4	1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).

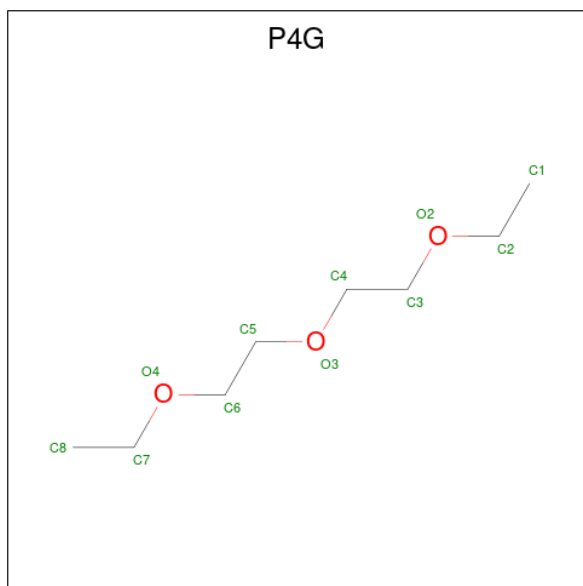


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
8	B	1	5	4	1	0	0

- Molecule 9 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G)



(formula: C<sub>8</sub>H<sub>18</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C O	0	0
			9	6 3		

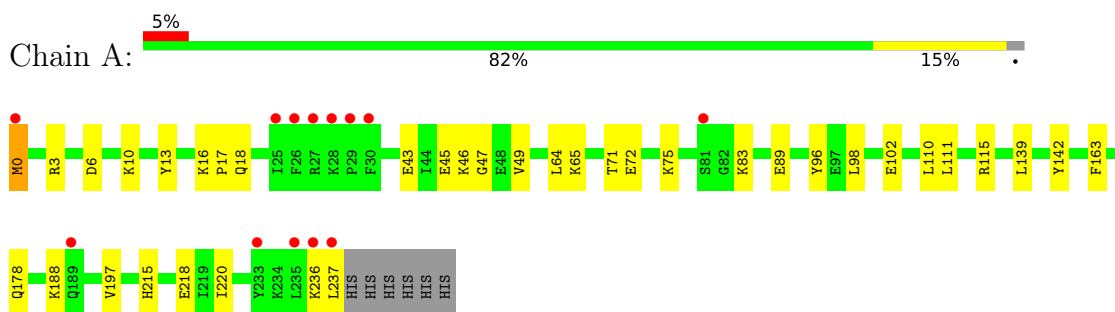
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	232	Total	O	0	0
			232	232		
10	B	139	Total	O	0	0
			139	139		

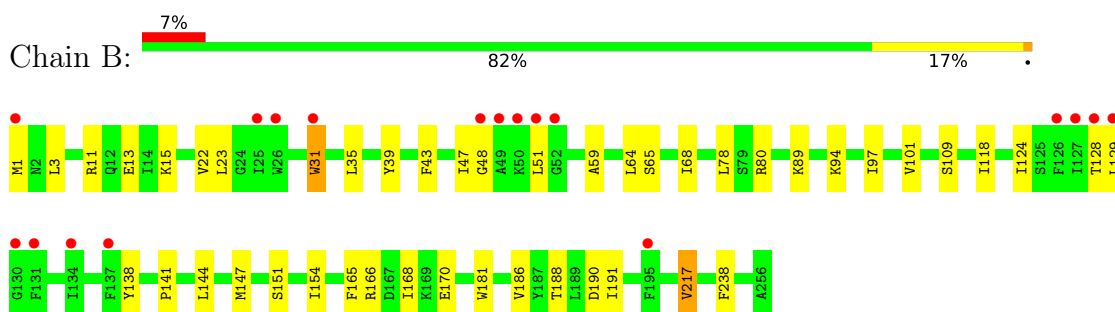
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ABC transporter



- Molecule 2: Transport permease protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.75Å 144.75Å 201.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.88 – 2.05 24.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.88-2.05) 100.0 (24.88-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.04Å)	Xtrriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, $R_{free}$	0.164 , 0.182 0.164 , 0.182	Depositor DCC
$R_{free}$ test set	4011 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 78.1	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	0.97	EDS
Total number of atoms	4982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: ATP, PG4, GOL, LDA, P4G, SO4, PEE

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	0.46	0/2015	0.59	0/2707
2	B	0.39	0/2444	0.50	0/3334
All	All	0.42	0/4459	0.54	0/6041

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	1949	0	2036	35	0
2	B	2281	0	2470	46	0
3	A	4	0	7	0	0
3	B	252	0	451	15	0
4	A	36	0	46	1	0
4	B	12	0	16	0	0
5	A	31	0	12	0	0
6	A	23	0	31	2	0
7	A	9	0	7	1	0
8	B	5	0	0	0	0
9	B	9	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	232	0	0	11	9
10	B	139	0	0	4	6
All	All	4982	0	5089	82	10

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 8.

All (82) 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:13:TYR:O	10:A:401:HOH:O	1.95	0.84
2:B:109[A]:SER:OG	10:B:401:HOH:O	1.97	0.83
1:A:65:LYS:HB3	1:A:71[B]:THR:HG23	1.61	0.81
1:A:215:HIS:O	10:A:402:HOH:O	2.02	0.77
1:A:65:LYS:NZ	10:A:405:HOH:O	2.18	0.77
2:B:124:ILE:HD13	3:B:313:LDA:H91	1.69	0.74
3:B:302:LDA:H62	3:B:315:LDA:H81	1.77	0.67
1:A:178:GLN:NE2	10:A:409:HOH:O	2.27	0.67
2:B:128:THR:OG1	10:B:402:HOH:O	2.14	0.65
2:B:190:ASP:OD2	3:B:315:LDA:HM11	1.94	0.65
1:A:46:LYS:NZ	10:A:411:HOH:O	2.30	0.65
2:B:1:MET:HG3	2:B:3:LEU:H	1.63	0.63
1:A:218:GLU:HB2	10:A:402:HOH:O	1.99	0.62
2:B:188:THR:O	2:B:191[B]:ILE:HG13	2.00	0.61
1:A:72[B]:GLU:OE2	10:A:403:HOH:O	2.15	0.59
2:B:97:ILE:HD11	2:B:101[B]:VAL:HG21	1.85	0.58
1:A:115:ARG:NH1	2:B:11:ARG:HH21	2.03	0.56
1:A:64:LEU:HD11	1:A:197:VAL:HG21	1.88	0.55
1:A:72[B]:GLU:OE1	10:A:404:HOH:O	2.18	0.55
2:B:31[A]:TRP:HA	2:B:31[A]:TRP:CE3	2.41	0.55
1:A:115:ARG:HH12	2:B:11:ARG:HH21	1.55	0.55
2:B:65[B]:SER:HA	2:B:68[B]:ILE:HG12	1.89	0.55
2:B:48:GLY:HA2	2:B:51:LEU:O	2.07	0.54
2:B:144:LEU:HA	2:B:147:MET:HE3	1.89	0.54
3:B:304:LDA:H102	3:B:315:LDA:HM23	1.89	0.53
2:B:31[A]:TRP:HA	2:B:31[A]:TRP:HE3	1.73	0.53
2:B:43:PHE:O	2:B:47[A]:ILE:HG13	2.08	0.53
2:B:170:GLU:HG3	9:B:335:P4G:H62	1.90	0.52
1:A:10:LYS:HE2	7:A:311:PEE:H11	1.91	0.52
1:A:71[A]:THR:OG1	10:A:406:HOH:O	2.19	0.51
2:B:11:ARG:HD3	2:B:15:LYS:HZ3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:MET:SD	1:A:3:ARG:HG3	2.51	0.51
2:B:59:ALA:HB1	3:B:304:LDA:H32	1.94	0.50
1:A:139[B]:LEU:HD12	1:A:142:TYR:CD2	2.46	0.50
2:B:217[A]:VAL:HG12	3:B:304:LDA:H21	1.95	0.49
2:B:181:TRP:CZ3	2:B:186[A]:VAL:HG21	2.48	0.48
2:B:13:GLU:HG2	2:B:109[A]:SER:HB2	1.95	0.48
1:A:49:VAL:CG2	1:A:188[B]:LYS:HD2	2.43	0.48
2:B:1:MET:HG3	2:B:3:LEU:N	2.29	0.48
1:A:115:ARG:NH2	2:B:11:ARG:HH21	2.13	0.47
3:B:306:LDA:HM23	3:B:306:LDA:H21	1.76	0.47
1:A:17:PRO:HB2	2:B:165:PHE:CE2	2.50	0.47
2:B:166:ARG:HH12	9:B:335:P4G:H32	1.79	0.47
3:B:302:LDA:HM11	3:B:302:LDA:H21	1.60	0.47
1:A:220:ILE:HG23	10:A:402:HOH:O	2.14	0.46
1:A:83:LYS:HD2	1:A:111:LEU:O	2.15	0.46
2:B:1:MET:N	10:B:405:HOH:O	2.46	0.46
1:A:188[B]:LYS:HD3	6:A:309:PG4:H62	1.99	0.45
2:B:65[B]:SER:HA	2:B:68[B]:ILE:CG1	2.46	0.45
2:B:39:TYR:HB2	2:B:64:LEU:HD21	1.98	0.45
2:B:129:LEU:HD21	3:B:304:LDA:O1	2.17	0.45
2:B:138:TYR:O	2:B:141:PRO:HD2	2.16	0.45
1:A:16:LYS:HD2	1:A:18:GLN:HB2	1.98	0.45
1:A:110:LEU:HD21	2:B:97:ILE:HD12	1.99	0.45
3:B:304:LDA:HM12	3:B:304:LDA:H22	1.68	0.45
1:A:0:MET:HG3	1:A:3:ARG:NE	2.31	0.44
1:A:43:GLU:HG2	1:A:45[B]:GLU:OE2	2.17	0.44
2:B:78[A]:LEU:HD11	2:B:154:ILE:HG22	1.99	0.44
3:B:314:LDA:H21	3:B:314:LDA:HM23	1.77	0.44
2:B:78[B]:LEU:CD1	2:B:151:SER:HA	2.48	0.43
1:A:98:LEU:HD22	1:A:102[B]:GLU:OE1	2.18	0.43
2:B:11:ARG:HH11	2:B:15:LYS:HZ3	1.67	0.43
2:B:35:LEU:HD12	2:B:35:LEU:HA	1.87	0.43
1:A:236:LYS:O	1:A:237:LEU:HD12	2.19	0.43
3:B:303:LDA:HM23	3:B:303:LDA:H22	1.73	0.43
1:A:96:TYR:HA	1:A:139[B]:LEU:HB3	2.00	0.42
2:B:118:ILE:HD12	2:B:118:ILE:HA	1.93	0.42
1:A:75:LYS:HD2	6:A:310:PG4:H22	2.01	0.42
1:A:115:ARG:CZ	2:B:11:ARG:HH21	2.31	0.42
2:B:128:THR:C	2:B:129:LEU:HD12	2.39	0.42
1:A:115:ARG:HH22	2:B:11:ARG:HH21	1.67	0.42
2:B:22[B]:VAL:HG12	2:B:23:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ARG:NH1	10:B:401:HOH:O	2.40	0.42
2:B:165:PHE:O	2:B:168:ILE:HG12	2.19	0.42
2:B:238:PHE:CE1	3:B:311:LDA:H112	2.54	0.42
2:B:191[B]:ILE:CG2	3:B:315:LDA:H32	2.51	0.41
3:B:312:LDA:H11	3:B:312:LDA:H42	1.93	0.41
1:A:89:GLU:HG3	2:B:94:LYS:O	2.21	0.41
4:A:305:GOL:H31	10:A:613:HOH:O	2.20	0.41
1:A:3:ARG:HG2	1:A:43:GLU:OE2	2.21	0.41
1:A:47:GLY:O	1:A:188[A]:LYS:HE3	2.20	0.41
2:B:31[B]:TRP:CE3	2:B:31[B]:TRP:HA	2.56	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:480:HOH:O	10:A:480:HOH:O[12_566]	1.87	0.33
10:A:608:HOH:O	10:A:608:HOH:O[10_667]	1.99	0.21
10:B:492:HOH:O	10:B:492:HOH:O[10_667]	1.99	0.21
10:A:450:HOH:O	10:B:508:HOH:O[8_567]	2.04	0.16
10:A:504:HOH:O	10:A:504:HOH:O[12_566]	2.07	0.13
10:A:559:HOH:O	10:B:474:HOH:O[8_567]	2.09	0.11
10:A:596:HOH:O	10:B:526:HOH:O[8_567]	2.10	0.10
10:A:520:HOH:O	10:B:508:HOH:O[8_567]	2.12	0.08
10:A:547:HOH:O	10:A:615:HOH:O[10_667]	2.12	0.08
10:A:592:HOH:O	10:B:514:HOH:O[10_667]	2.19	0.01

## 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	246/244 (101%)	239 (97%)	6 (2%)	1 (0%)	34 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	282/256 (110%)	278 (99%)	4 (1%)	0	100	100
All	All	528/500 (106%)	517 (98%)	10 (2%)	1 (0%)	47	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASP

### 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	217/213 (102%)	215 (99%)	2 (1%)	78	79
2	B	265/237 (112%)	260 (98%)	5 (2%)	57	53
All	All	482/450 (107%)	475 (98%)	7 (2%)	73	62

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	163	PHE
2	B	31[A]	TRP
2	B	31[B]	TRP
2	B	89	LYS
2	B	217[A]	VAL
2	B	217[B]	VAL

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](#)

46 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
4	GOL	A	304	-	5,5,5	1.11	1 (20%)	5,5,5	0.93	0
3	LDA	B	307	-	4,7,15	3.50	1 (25%)	6,9,17	0.63	0
3	LDA	B	302	-	12,15,15	2.05	1 (8%)	14,17,17	0.71	0
3	LDA	B	325	-	2,2,15	0.31	0	0,1,17	-	-
3	LDA	B	305	-	7,7,15	0.29	0	6,6,17	0.46	0
8	SO4	B	334	-	4,4,4	0.20	0	6,6,6	0.81	0
3	LDA	B	310	-	3,3,15	0.37	0	2,2,17	0.63	0
6	PG4	A	309	-	12,12,12	0.53	0	11,11,11	0.28	0
3	LDA	B	326	-	3,3,15	0.35	0	0,1,17	-	-
3	LDA	B	312	-	8,11,15	2.54	1 (12%)	10,13,17	0.63	0
3	LDA	B	303	-	12,15,15	2.05	1 (8%)	14,17,17	0.66	0
3	LDA	B	316	-	7,7,15	0.29	0	6,6,17	0.43	0
4	GOL	A	306	-	5,5,5	0.69	0	5,5,5	1.11	0
3	LDA	B	315	-	12,15,15	2.09	1 (8%)	14,17,17	0.56	0
3	LDA	B	331	-	4,4,15	6.39	2 (50%)	6,6,17	0.26	0
3	LDA	B	308	-	5,5,15	0.31	0	4,4,17	0.31	0
3	LDA	B	317	-	3,3,15	0.38	0	2,2,17	0.62	0
7	PEE	A	311	-	8,8,50	0.98	0	9,10,55	0.48	0
3	LDA	B	327	-	2,2,15	0.30	0	0,1,17	-	-
3	LDA	B	304	-	12,15,15	2.00	1 (8%)	14,17,17	0.82	0
3	LDA	B	313	-	9,9,15	0.26	0	8,8,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ATP	A	308	-	26,33,33	0.99	2 (7%)	31,52,52	1.35	2 (6%)
4	GOL	A	307	-	5,5,5	0.94	0	5,5,5	1.02	0
6	PG4	A	310	-	9,9,12	0.50	0	8,8,11	0.29	0
3	LDA	B	306	-	12,15,15	2.06	1 (8%)	14,17,17	0.49	0
4	GOL	B	333	-	5,5,5	0.89	0	5,5,5	1.15	0
3	LDA	B	321	-	4,4,15	0.31	0	3,3,17	0.40	0
3	LDA	B	301	-	9,12,15	2.39	1 (11%)	11,14,17	0.71	0
3	LDA	B	328	-	3,3,15	0.39	0	2,2,17	0.64	0
3	LDA	B	318	-	4,4,15	0.35	0	3,3,17	0.31	0
3	LDA	B	319	-	2,2,15	0.31	0	0,1,17	-	-
3	LDA	B	329	-	12,15,15	2.13	1 (8%)	14,17,17	0.46	0
3	LDA	B	320	-	2,2,15	0.24	0	0,1,17	-	-
4	GOL	A	302	-	5,5,5	0.82	0	5,5,5	0.99	0
4	GOL	A	305	-	5,5,5	1.34	1 (20%)	5,5,5	1.02	0
3	LDA	B	311	-	5,5,15	0.27	0	4,4,17	0.39	0
4	GOL	B	332	-	5,5,5	0.91	0	5,5,5	0.91	0
3	LDA	B	330	-	3,3,15	0.40	0	2,2,17	0.59	0
3	LDA	B	324	-	4,4,15	0.32	0	3,3,17	0.32	0
3	LDA	B	322	-	7,7,15	0.26	0	6,6,17	0.62	0
3	LDA	B	314	-	5,8,15	3.21	1 (20%)	7,10,17	0.30	0
3	LDA	A	301	-	3,3,15	0.34	0	2,2,17	0.67	0
4	GOL	A	303	-	5,5,5	0.98	0	5,5,5	1.03	0
9	P4G	B	335	-	8,8,10	0.55	0	7,7,9	0.27	0
3	LDA	B	309	-	5,5,15	0.30	0	4,4,17	0.39	0
3	LDA	B	323	-	8,8,15	0.28	0	7,7,17	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	304	-	-	2/4/4/4	-
3	LDA	B	307	-	-	2/5/5/13	-
3	LDA	B	302	-	-	6/13/13/13	-
3	LDA	B	305	-	-	1/5/5/13	-
3	LDA	B	310	-	-	1/1/1/13	-
6	PG4	A	309	-	-	5/10/10/10	-
3	LDA	B	312	-	-	7/9/9/13	-
3	LDA	B	303	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	B	316	-	-	1/5/5/13	-
4	GOL	A	306	-	-	0/4/4/4	-
3	LDA	B	315	-	-	4/13/13/13	-
3	LDA	B	308	-	-	1/3/3/13	-
3	LDA	B	317	-	-	0/1/1/13	-
7	PEE	A	311	-	-	2/8/8/54	-
3	LDA	B	304	-	-	5/13/13/13	-
3	LDA	B	313	-	-	6/7/7/13	-
5	ATP	A	308	-	-	1/18/38/38	0/3/3/3
4	GOL	A	307	-	-	2/4/4/4	-
6	PG4	A	310	-	-	4/7/7/10	-
3	LDA	B	306	-	-	3/13/13/13	-
4	GOL	B	333	-	-	2/4/4/4	-
3	LDA	B	321	-	-	0/2/2/13	-
3	LDA	B	301	-	-	1/10/10/13	-
3	LDA	B	328	-	-	0/1/1/13	-
3	LDA	B	318	-	-	0/2/2/13	-
3	LDA	B	329	-	-	5/13/13/13	-
4	GOL	A	302	-	-	2/4/4/4	-
4	GOL	A	305	-	-	0/4/4/4	-
3	LDA	B	311	-	-	1/3/3/13	-
4	GOL	B	332	-	-	0/4/4/4	-
3	LDA	B	330	-	-	1/1/1/13	-
3	LDA	B	324	-	-	0/2/2/13	-
3	LDA	B	322	-	-	1/5/5/13	-
3	LDA	B	314	-	-	0/6/6/13	-
3	LDA	A	301	-	-	1/1/1/13	-
4	GOL	A	303	-	-	3/4/4/4	-
9	P4G	B	335	-	-	2/6/6/8	-
3	LDA	B	309	-	-	3/3/3/13	-
3	LDA	B	323	-	-	1/6/6/13	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	331	LDA	O1-N1	-12.56	1.25	1.42
3	B	329	LDA	O1-N1	-7.29	1.25	1.42
3	B	315	LDA	O1-N1	-7.19	1.25	1.42
3	B	314	LDA	O1-N1	-7.15	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	312	LDA	O1-N1	-7.14	1.25	1.42
3	B	301	LDA	O1-N1	-7.12	1.25	1.42
3	B	302	LDA	O1-N1	-7.07	1.25	1.42
3	B	303	LDA	O1-N1	-7.07	1.25	1.42
3	B	306	LDA	O1-N1	-7.06	1.25	1.42
3	B	307	LDA	O1-N1	-6.98	1.25	1.42
3	B	304	LDA	O1-N1	-6.88	1.26	1.42
5	A	308	ATP	O4'-C1'	2.89	1.45	1.41
4	A	305	GOL	O2-C2	-2.53	1.35	1.43
4	A	304	GOL	O2-C2	-2.20	1.36	1.43
3	B	331	LDA	C1-N1	-2.13	1.45	1.48
5	A	308	ATP	C5-C4	2.04	1.46	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	308	ATP	N3-C2-N1	-4.13	122.22	128.68
5	A	308	ATP	C2-N1-C6	2.59	123.18	118.75

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	LDA	C2-C1-N1-CM2
3	B	303	LDA	C2-C1-N1-O1
3	B	303	LDA	C2-C1-N1-CM1
3	B	303	LDA	C2-C1-N1-CM2
3	B	312	LDA	C2-C1-N1-O1
3	B	312	LDA	C2-C1-N1-CM1
3	B	312	LDA	C2-C1-N1-CM2
3	B	329	LDA	C2-C1-N1-O1
3	B	329	LDA	C2-C1-N1-CM2
3	B	329	LDA	N1-C1-C2-C3
4	A	303	GOL	C1-C2-C3-O3
4	A	304	GOL	O1-C1-C2-O2
4	A	304	GOL	O1-C1-C2-C3
4	A	307	GOL	C1-C2-C3-O3
4	B	333	GOL	O1-C1-C2-C3
3	B	329	LDA	C7-C8-C9-C10
3	B	304	LDA	C1-C2-C3-C4
6	A	309	PG4	O2-C3-C4-O3
4	A	307	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	310	PG4	O1-C1-C2-O2
9	B	335	P4G	O3-C5-C6-O4
7	A	311	PEE	C4-O4P-P-O3P
3	B	315	LDA	C6-C7-C8-C9
3	B	302	LDA	C4-C5-C6-C7
3	B	312	LDA	C3-C4-C5-C6
4	A	302	GOL	C1-C2-C3-O3
4	A	303	GOL	O1-C1-C2-C3
3	B	304	LDA	C5-C6-C7-C8
3	B	302	LDA	C3-C4-C5-C6
3	B	302	LDA	C2-C3-C4-C5
4	A	303	GOL	O2-C2-C3-O3
4	B	333	GOL	O1-C1-C2-O2
3	B	303	LDA	C1-C2-C3-C4
3	B	306	LDA	C1-C2-C3-C4
3	B	313	LDA	C3-C4-C5-C6
3	B	313	LDA	C6-C7-C8-C9
3	B	303	LDA	C3-C4-C5-C6
3	B	305	LDA	C5-C6-C7-C8
3	B	313	LDA	C1-C2-C3-C4
4	A	302	GOL	O2-C2-C3-O3
3	B	316	LDA	C9-C10-C11-C12
3	B	307	LDA	C1-C2-C3-C4
3	B	306	LDA	C9-C10-C11-C12
3	B	313	LDA	C5-C6-C7-C8
3	B	315	LDA	C7-C8-C9-C10
3	B	307	LDA	N1-C1-C2-C3
3	B	309	LDA	C7-C8-C9-C10
6	A	309	PG4	C5-C6-O4-C7
3	B	315	LDA	C4-C5-C6-C7
3	B	313	LDA	C2-C3-C4-C5
3	B	303	LDA	C5-C6-C7-C8
3	B	302	LDA	C1-C2-C3-C4
3	B	303	LDA	C9-C10-C11-C12
3	B	309	LDA	C11-C10-C9-C8
3	B	302	LDA	C7-C8-C9-C10
6	A	309	PG4	C4-C3-O2-C2
3	B	329	LDA	C2-C1-N1-CM1
3	B	309	LDA	C9-C10-C11-C12
3	B	308	LDA	C7-C8-C9-C10
7	A	311	PEE	C4-O4P-P-O1P
3	B	323	LDA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
9	B	335	P4G	C3-C4-O3-C5
3	B	303	LDA	C4-C5-C6-C7
3	B	313	LDA	C7-C8-C9-C10
6	A	310	PG4	O2-C3-C4-O3
3	A	301	LDA	C9-C10-C11-C12
3	B	310	LDA	C9-C10-C11-C12
3	B	330	LDA	C9-C10-C11-C12
3	B	303	LDA	C6-C7-C8-C9
3	B	312	LDA	C1-C2-C3-C4
3	B	304	LDA	C4-C5-C6-C7
3	B	312	LDA	C5-C6-C7-C8
6	A	309	PG4	C1-C2-O2-C3
6	A	309	PG4	O3-C5-C6-O4
3	B	306	LDA	C7-C8-C9-C10
3	B	302	LDA	C5-C6-C7-C8
3	B	315	LDA	C5-C6-C7-C8
3	B	304	LDA	C6-C7-C8-C9
6	A	310	PG4	O3-C5-C6-O4
3	B	312	LDA	C2-C3-C4-C5
5	A	308	ATP	PA-O3A-PB-O2B
6	A	310	PG4	C3-C4-O3-C5
3	B	311	LDA	C9-C10-C11-C12
3	B	322	LDA	C7-C8-C9-C10
3	B	304	LDA	C7-C8-C9-C10

There are no ring outliers.

14 monomers are involved in 21 short contacts:

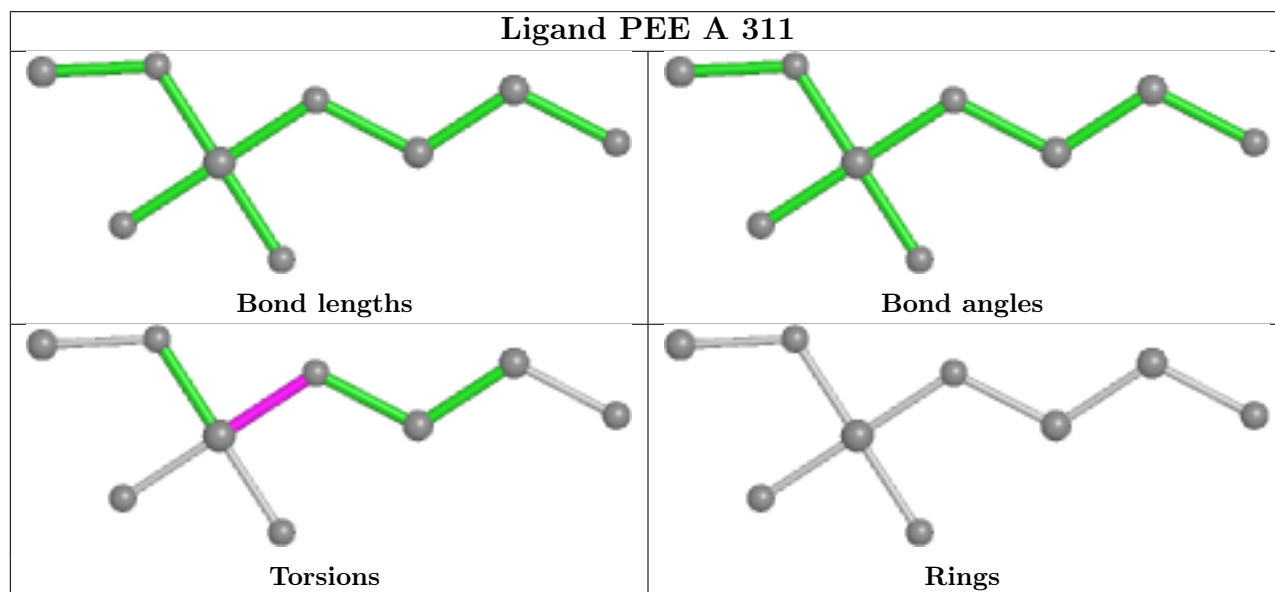
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	LDA	2	0
6	A	309	PG4	1	0
3	B	312	LDA	1	0
3	B	303	LDA	1	0
3	B	315	LDA	4	0
7	A	311	PEE	1	0
3	B	304	LDA	5	0
3	B	313	LDA	1	0
6	A	310	PG4	1	0
3	B	306	LDA	1	0
4	A	305	GOL	1	0
3	B	311	LDA	1	0
3	B	314	LDA	1	0

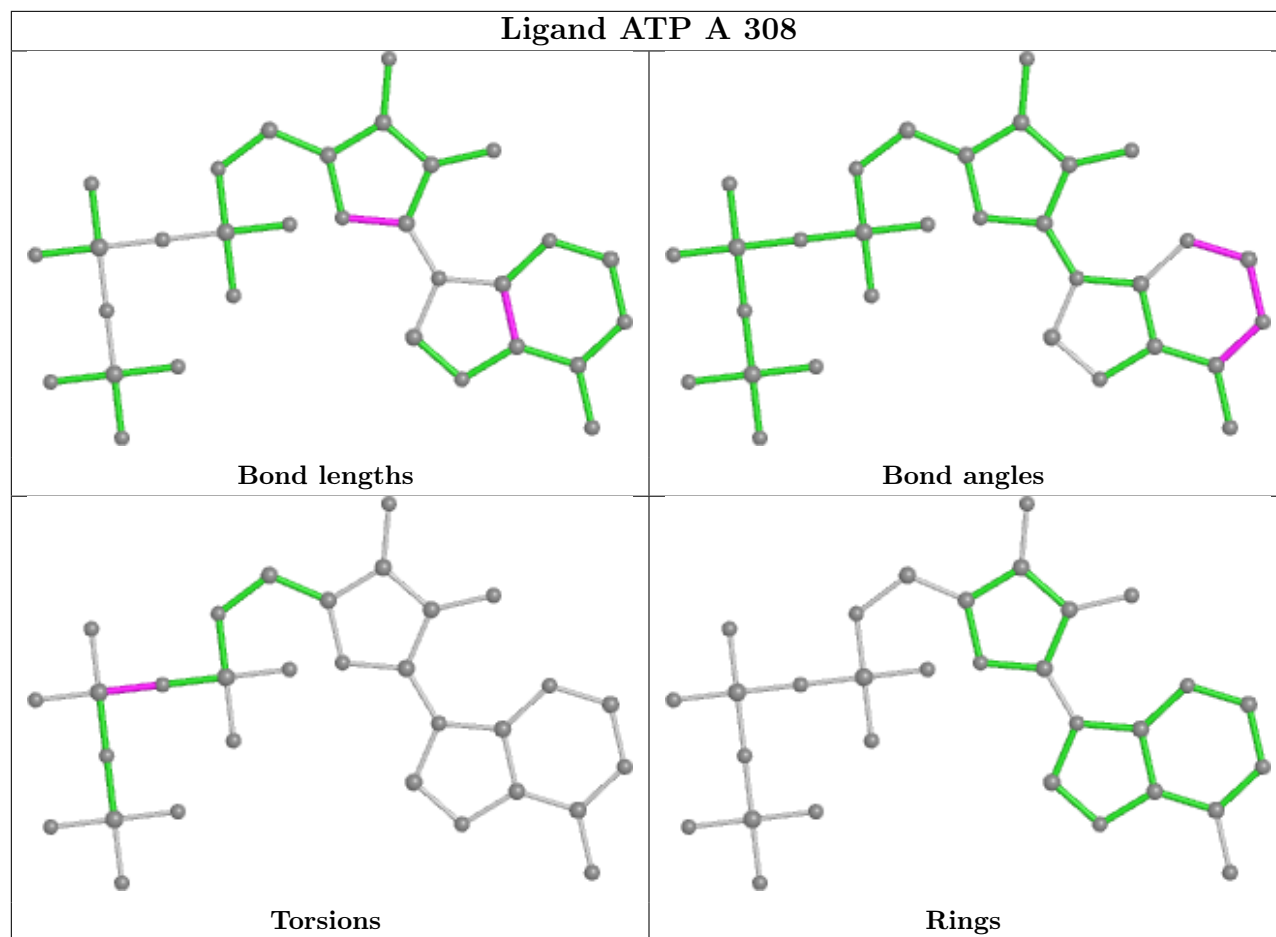
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	335	P4G	2	0

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	238/244 (97%)	-0.13	13 (5%) 25 27	28, 40, 77, 133	0
2	B	256/256 (100%)	-0.18	18 (7%) 16 18	30, 46, 82, 132	0
All	All	494/500 (98%)	-0.16	31 (6%) 20 21	28, 43, 82, 133	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	131	PHE	6.5
1	A	26	PHE	5.7
1	A	237	LEU	5.5
2	B	51	LEU	5.4
1	A	0	MET	4.9
1	A	233	TYR	4.5
2	B	49	ALA	4.4
2	B	127	ILE	4.3
2	B	50	LYS	4.2
1	A	27	ARG	4.2
2	B	1	MET	4.1
1	A	236	LYS	3.9
2	B	52	GLY	3.9
2	B	137	PHE	3.9
2	B	126	PHE	3.8
2	B	130	GLY	3.8
1	A	25	ILE	3.7
2	B	134	ILE	3.4
1	A	189	GLN	3.2
2	B	195	PHE	3.0
1	A	28	LYS	3.0
2	B	31[A]	TRP	3.0
1	A	30	PHE	2.9
1	A	29	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	48	GLY	2.8
2	B	129	LEU	2.5
2	B	26	TRP	2.4
1	A	81	SER	2.3
2	B	128	THR	2.2
1	A	235	LEU	2.1
2	B	25	ILE	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 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<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	LDA	B	318	5/16	0.50	0.36	67,79,82,83	0
3	LDA	B	312	12/16	0.63	0.37	81,101,121,123	0
3	LDA	B	324	5/16	0.63	0.25	69,76,81,81	0
3	LDA	B	314	9/16	0.64	0.29	76,94,109,116	0
3	LDA	B	331	5/16	0.64	0.30	119,123,124,124	0
3	LDA	B	325	3/16	0.71	0.22	76,76,78,78	0
3	LDA	B	313	10/16	0.72	0.30	79,85,87,88	0
3	LDA	B	329	16/16	0.73	0.26	64,88,115,118	0
3	LDA	B	309	6/16	0.74	0.28	62,75,78,79	0
3	LDA	B	330	4/16	0.75	0.20	88,90,92,92	0
3	LDA	B	307	8/16	0.75	0.39	97,117,122,122	0
4	GOL	A	307	6/6	0.77	0.19	80,90,93,100	0
6	PG4	A	309	13/13	0.77	0.19	64,83,96,96	0
3	LDA	B	302	16/16	0.78	0.20	58,78,91,94	0
3	LDA	B	308	6/16	0.79	0.29	67,71,76,79	0
3	LDA	B	321	5/16	0.80	0.31	81,83,86,86	0

*Continued on next page...*

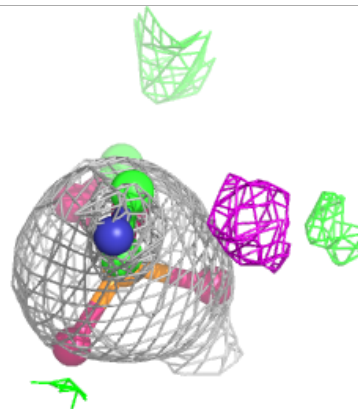
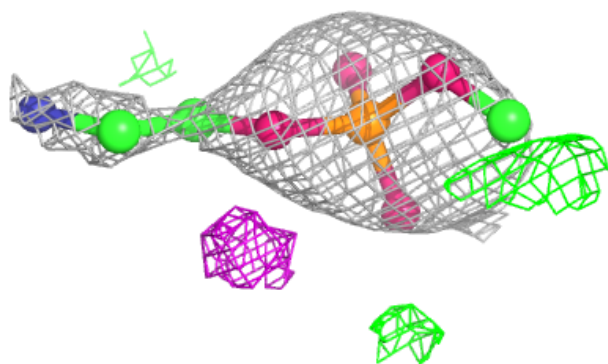
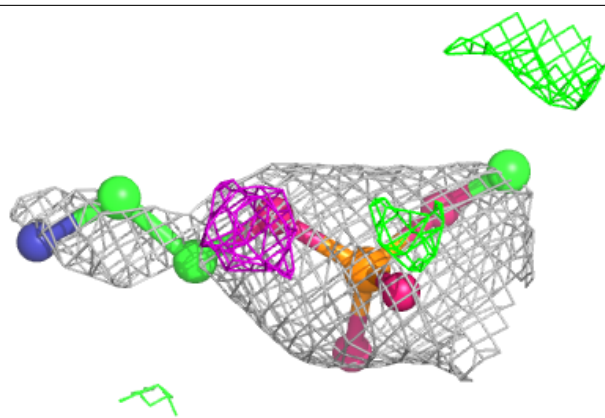
*Continued from previous page...*

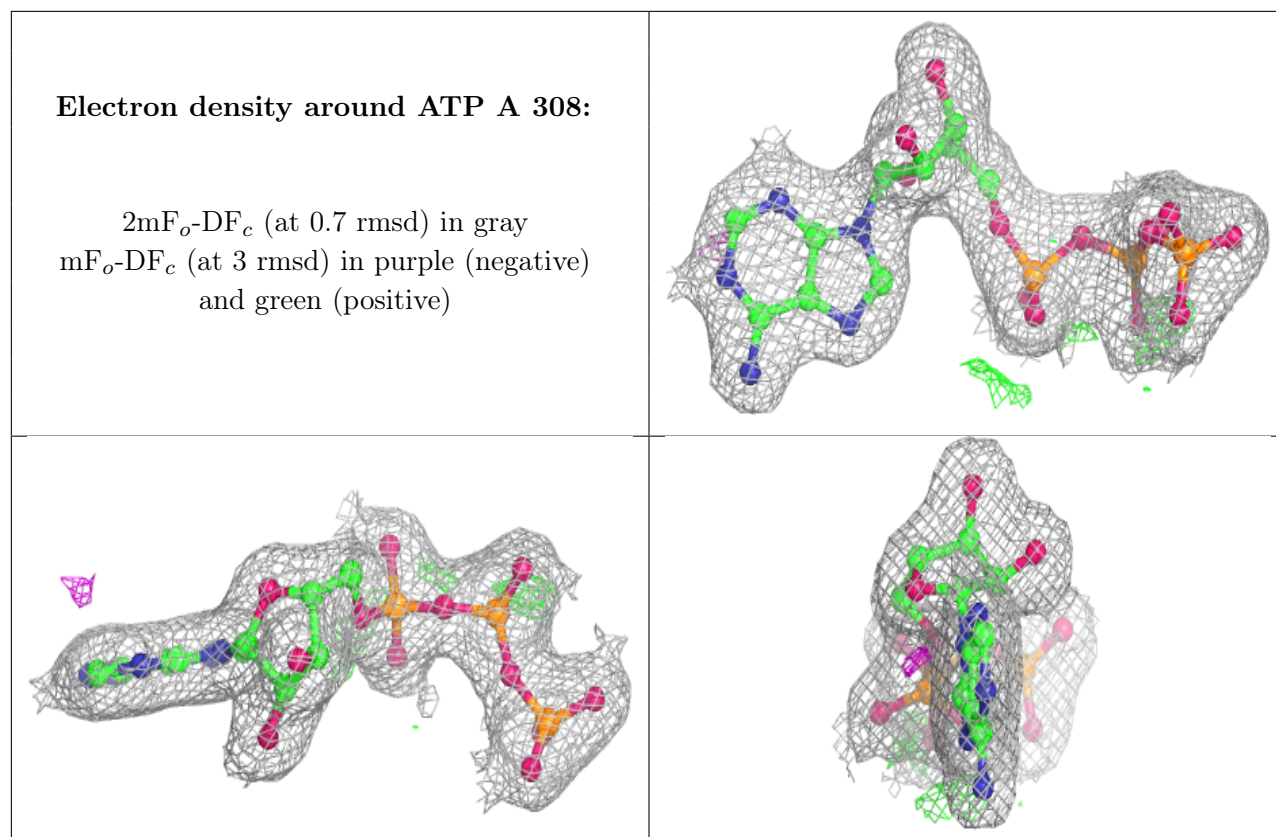
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LDA	B	306	16/16	0.81	0.17	73,80,116,117	0
6	PG4	A	310	10/13	0.81	0.17	60,73,86,87	0
3	LDA	B	316	8/16	0.82	0.33	75,80,86,87	0
3	LDA	B	323	9/16	0.82	0.22	69,74,82,82	0
3	LDA	B	328	4/16	0.82	0.14	69,70,73,78	0
3	LDA	B	311	6/16	0.83	0.23	73,76,79,80	0
3	LDA	B	322	8/16	0.83	0.25	64,68,73,76	0
3	LDA	B	305	8/16	0.83	0.14	67,72,73,76	0
3	LDA	B	310	4/16	0.84	0.21	70,79,79,81	0
3	LDA	B	326	5/16	0.85	0.24	77,81,84,84	0
3	LDA	B	315	16/16	0.87	0.28	71,84,96,98	0
9	P4G	B	335	9/11	0.87	0.14	84,88,93,94	0
3	LDA	B	304	16/16	0.88	0.24	26,46,61,66	0
4	GOL	A	305	6/6	0.89	0.21	72,79,82,85	0
4	GOL	A	306	6/6	0.89	0.16	69,73,80,82	0
3	LDA	B	317	4/16	0.89	0.41	47,61,71,80	0
3	LDA	B	303	16/16	0.90	0.14	56,71,84,88	0
3	LDA	B	301	13/16	0.90	0.15	62,68,76,77	0
4	GOL	A	303	6/6	0.91	0.13	63,69,74,74	0
4	GOL	B	333	6/6	0.92	0.13	55,57,66,66	0
3	LDA	B	327	3/16	0.92	0.22	66,66,75,77	0
7	PEE	A	311	9/51	0.93	0.19	100,105,110,110	0
3	LDA	A	301	4/16	0.93	0.43	84,86,87,89	0
4	GOL	A	304	6/6	0.94	0.14	61,82,88,97	0
3	LDA	B	319	3/16	0.94	0.10	56,56,67,74	0
3	LDA	B	320	3/16	0.94	0.12	62,62,63,74	0
4	GOL	A	302	6/6	0.96	0.16	41,71,76,88	0
4	GOL	B	332	6/6	0.97	0.10	37,42,48,51	0
8	SO4	B	334	5/5	0.99	0.09	49,50,52,64	0
5	ATP	A	308	31/31	0.99	0.07	26,28,31,32	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.

**Electron density around PEE A 311:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.