



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 03:03 AM EDT

PDB ID : 3C9T  
Title : AaThiL complexed with AMPPCP and TMP  
Authors : McCulloch, K.M.; Kinsland, C.; Begley, T.P.; Ealick, S.E.  
Deposited on : 2008-02-18  
Resolution : 2.60 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

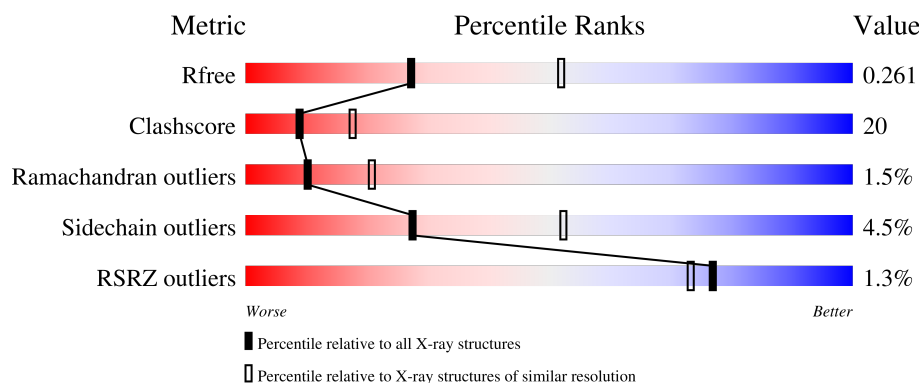
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	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  $\geq 3$ , 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	342	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 15%, yellow 37%, green 55%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>55%</span> <span>32%</span> <span>10%</span> </div> </div>
1	B	342	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 15%, yellow 30%, green 57%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>57%</span> <span>30%</span> <span>10%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5011 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 Thiamine monophosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2432	1562	404	457	9			
1	B	309	Total	C	N	O	S	0	0	0
			2449	1574	406	460	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	EXPRESSION TAG	UNP O67883
A	-34	GLY	-	EXPRESSION TAG	UNP O67883
A	-33	SER	-	EXPRESSION TAG	UNP O67883
A	-32	HIS	-	EXPRESSION TAG	UNP O67883
A	-31	HIS	-	EXPRESSION TAG	UNP O67883
A	-30	HIS	-	EXPRESSION TAG	UNP O67883
A	-29	HIS	-	EXPRESSION TAG	UNP O67883
A	-28	HIS	-	EXPRESSION TAG	UNP O67883
A	-27	HIS	-	EXPRESSION TAG	UNP O67883
A	-26	ASP	-	EXPRESSION TAG	UNP O67883
A	-25	ILE	-	EXPRESSION TAG	UNP O67883
A	-24	THR	-	EXPRESSION TAG	UNP O67883
A	-23	SER	-	EXPRESSION TAG	UNP O67883
A	-22	LEU	-	EXPRESSION TAG	UNP O67883
A	-21	TYR	-	EXPRESSION TAG	UNP O67883
A	-20	LYS	-	EXPRESSION TAG	UNP O67883
A	-19	LYS	-	EXPRESSION TAG	UNP O67883
A	-18	ALA	-	EXPRESSION TAG	UNP O67883
A	-17	GLY	-	EXPRESSION TAG	UNP O67883
A	-16	SER	-	EXPRESSION TAG	UNP O67883
A	-15	ALA	-	EXPRESSION TAG	UNP O67883
A	-14	ALA	-	EXPRESSION TAG	UNP O67883
A	-13	ALA	-	EXPRESSION TAG	UNP O67883
A	-12	VAL	-	EXPRESSION TAG	UNP O67883
A	-11	LEU	-	EXPRESSION TAG	UNP O67883

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLU	-	EXPRESSION TAG	UNP O67883
A	-9	GLU	-	EXPRESSION TAG	UNP O67883
A	-8	ASN	-	EXPRESSION TAG	UNP O67883
A	-7	LEU	-	EXPRESSION TAG	UNP O67883
A	-6	TYR	-	EXPRESSION TAG	UNP O67883
A	-5	PHE	-	EXPRESSION TAG	UNP O67883
A	-4	GLN	-	EXPRESSION TAG	UNP O67883
A	-3	GLY	-	EXPRESSION TAG	UNP O67883
A	-2	SER	-	EXPRESSION TAG	UNP O67883
A	-1	PHE	-	EXPRESSION TAG	UNP O67883
A	0	THR	-	EXPRESSION TAG	UNP O67883
B	-35	MET	-	EXPRESSION TAG	UNP O67883
B	-34	GLY	-	EXPRESSION TAG	UNP O67883
B	-33	SER	-	EXPRESSION TAG	UNP O67883
B	-32	HIS	-	EXPRESSION TAG	UNP O67883
B	-31	HIS	-	EXPRESSION TAG	UNP O67883
B	-30	HIS	-	EXPRESSION TAG	UNP O67883
B	-29	HIS	-	EXPRESSION TAG	UNP O67883
B	-28	HIS	-	EXPRESSION TAG	UNP O67883
B	-27	HIS	-	EXPRESSION TAG	UNP O67883
B	-26	ASP	-	EXPRESSION TAG	UNP O67883
B	-25	ILE	-	EXPRESSION TAG	UNP O67883
B	-24	THR	-	EXPRESSION TAG	UNP O67883
B	-23	SER	-	EXPRESSION TAG	UNP O67883
B	-22	LEU	-	EXPRESSION TAG	UNP O67883
B	-21	TYR	-	EXPRESSION TAG	UNP O67883
B	-20	LYS	-	EXPRESSION TAG	UNP O67883
B	-19	LYS	-	EXPRESSION TAG	UNP O67883
B	-18	ALA	-	EXPRESSION TAG	UNP O67883
B	-17	GLY	-	EXPRESSION TAG	UNP O67883
B	-16	SER	-	EXPRESSION TAG	UNP O67883
B	-15	ALA	-	EXPRESSION TAG	UNP O67883
B	-14	ALA	-	EXPRESSION TAG	UNP O67883
B	-13	ALA	-	EXPRESSION TAG	UNP O67883
B	-12	VAL	-	EXPRESSION TAG	UNP O67883
B	-11	LEU	-	EXPRESSION TAG	UNP O67883
B	-10	GLU	-	EXPRESSION TAG	UNP O67883
B	-9	GLU	-	EXPRESSION TAG	UNP O67883
B	-8	ASN	-	EXPRESSION TAG	UNP O67883
B	-7	LEU	-	EXPRESSION TAG	UNP O67883
B	-6	TYR	-	EXPRESSION TAG	UNP O67883
B	-5	PHE	-	EXPRESSION TAG	UNP O67883

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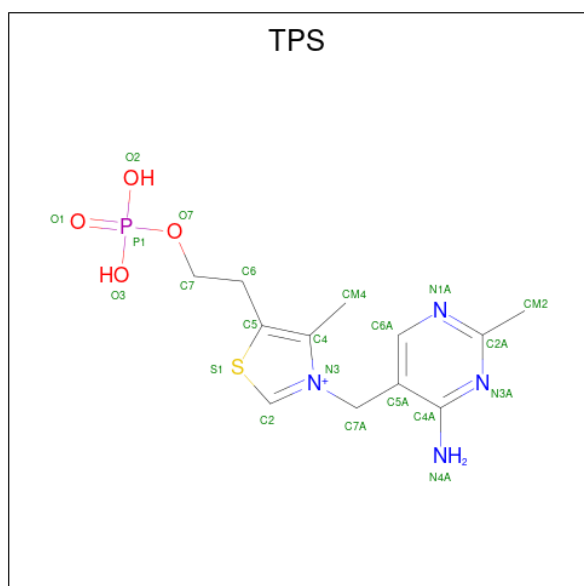
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLN	-	EXPRESSION TAG	UNP O67883
B	-3	GLY	-	EXPRESSION TAG	UNP O67883
B	-2	SER	-	EXPRESSION TAG	UNP O67883
B	-1	PHE	-	EXPRESSION TAG	UNP O67883
B	0	THR	-	EXPRESSION TAG	UNP O67883

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

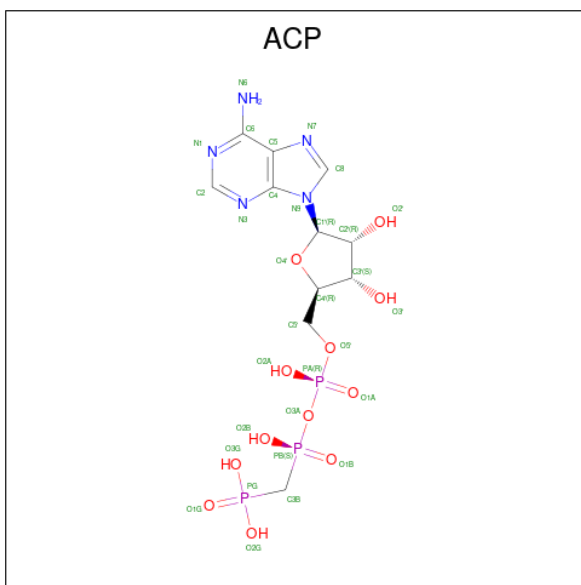
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Mg 5 5	0	0
2	B	5	Total Mg 5 5	0	0

- Molecule 3 is THIAMIN PHOSPHATE (three-letter code: TPS) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>4</sub>PS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 22 12 4 4 1 1	0	0
3	B	1	Total C N O P S 22 12 4 4 1 1	0	0

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
4	B	1	Total 31	C 11	N 5	O 12	P 3	0	0

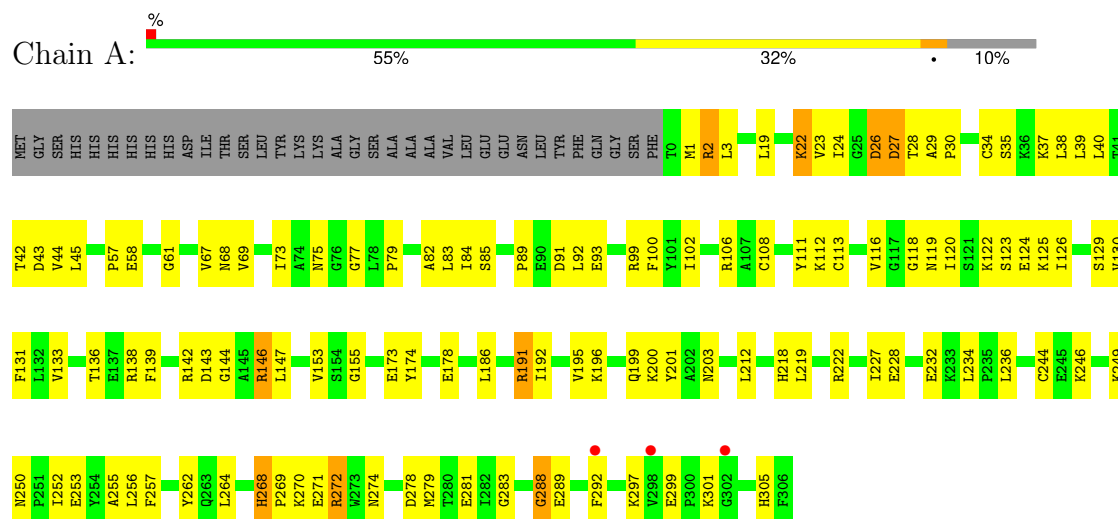
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0
5	B	6	Total O 6 6	0	0

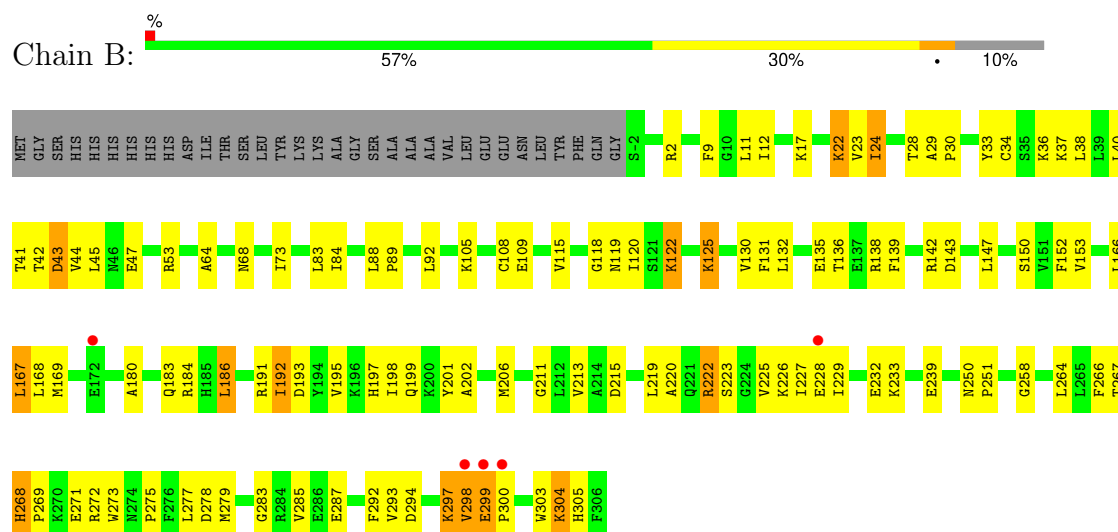
### 3 Residue-property plots

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

#### • Molecule 1: Thiamine monophosphate kinase



#### • Molecule 1: Thiamine monophosphate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.75Å 66.84Å 196.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.65 – 2.60 46.83 – 2.13	Depositor EDS
% Data completeness (in resolution range)	86.8 (31.65-2.60) 86.5 (46.83-2.13)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.14Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.213 , 0.270 0.207 , 0.261	Depositor DCC
$R_{free}$ test set	4406 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPS, MG, ACP

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	0.39	0/2481	0.64	1/3346 (0.0%)
1	B	0.39	0/2499	0.62	0/3370
All	All	0.39	0/4980	0.63	1/6716 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	GLY	N-CA-C	5.05	125.71	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2432	0	2448	115	0
1	B	2449	0	2462	104	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	22	0	16	0	0
3	B	22	0	16	0	0
4	A	31	0	14	0	0
4	B	31	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	0	0	0
5	B	6	0	0	0	0
All	All	5011	0	4970	202	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 20.

All (202) 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:28:THR:HB	1:A:75:ASN:HD22	1.05	1.15
1:A:28:THR:HG21	1:A:39:LEU:HB3	1.43	1.00
1:A:142:ARG:HG3	1:A:222:ARG:HG2	1.43	0.96
1:B:22:LYS:H	1:B:22:LYS:HE2	1.30	0.93
1:A:219:LEU:HD22	1:A:227:ILE:HD11	1.48	0.93
1:A:28:THR:HB	1:A:75:ASN:ND2	1.86	0.90
1:B:201:TYR:HB3	1:B:272:ARG:HD2	1.54	0.90
1:A:196:LYS:HG3	1:A:200:LYS:HE3	1.55	0.88
1:B:125:LYS:HB3	1:B:125:LYS:NZ	1.91	0.86
1:B:180:ALA:O	1:B:183:GLN:HB3	1.78	0.83
1:A:102:ILE:O	1:A:106:ARG:HG2	1.86	0.75
1:A:26:ASP:HB3	1:A:142:ARG:HG2	1.68	0.73
1:B:299:GLU:HB2	1:B:300:PRO:CA	2.19	0.72
1:A:22:LYS:HD2	1:A:23:VAL:H	1.55	0.71
1:A:28:THR:CG2	1:A:39:LEU:HB3	2.19	0.71
1:A:91:ASP:O	1:B:2:ARG:HG3	1.93	0.68
1:A:28:THR:CB	1:A:75:ASN:HD22	1.96	0.67
1:B:225:VAL:HG21	1:B:285:VAL:HG13	1.76	0.67
1:B:191:ARG:NH1	1:B:193:ASP:OD1	2.27	0.67
1:A:153:VAL:HA	1:A:264:LEU:O	1.93	0.67
1:B:28:THR:HG22	1:B:41:THR:HB	1.76	0.66
1:A:173:GLU:OE2	1:A:173:GLU:HA	1.96	0.66
1:B:299:GLU:HB2	1:B:300:PRO:HA	1.78	0.66
1:A:28:THR:HG21	1:A:39:LEU:CB	2.21	0.65
1:A:131:PHE:HB2	1:B:131:PHE:CD1	2.32	0.64
1:A:40:LEU:CD2	1:A:133:VAL:HG22	2.27	0.64
1:B:73:ILE:HG12	1:B:192:ILE:HA	1.78	0.64
1:A:28:THR:H	1:A:75:ASN:HD21	1.43	0.64
1:B:22:LYS:H	1:B:22:LYS:CE	2.07	0.64
1:B:299:GLU:H	1:B:299:GLU:CD	2.01	0.64
1:A:67:VAL:HG23	1:A:262:TYR:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:N	1:A:37:LYS:HD2	2.14	0.63
1:B:125:LYS:HB3	1:B:125:LYS:HZ3	1.64	0.63
1:A:27:ASP:CG	1:A:142:ARG:HH21	2.02	0.62
1:B:64:ALA:O	1:B:130:VAL:HG11	1.99	0.62
1:B:125:LYS:HB3	1:B:125:LYS:HZ2	1.64	0.62
1:A:67:VAL:HG23	1:A:262:TYR:CZ	2.35	0.61
1:A:108:CYS:HB3	1:A:113:CYS:O	2.00	0.61
1:B:303:TRP:HE1	1:B:305:HIS:CE1	2.19	0.60
1:A:270:LYS:HD3	1:A:281:GLU:OE1	2.02	0.60
1:B:37:LYS:O	1:B:136:THR:HG22	2.02	0.60
1:B:297:LYS:HG3	1:B:298:VAL:N	2.17	0.60
1:B:192:ILE:HD13	1:B:192:ILE:O	2.01	0.60
1:A:83:LEU:HD21	1:A:116:VAL:HG23	1.84	0.59
1:B:191:ARG:HH11	1:B:191:ARG:HA	1.67	0.59
1:A:69:VAL:O	1:A:73:ILE:HG12	2.03	0.59
1:B:36:LYS:HG2	1:B:136:THR:O	2.03	0.59
1:A:28:THR:CG2	1:A:29:ALA:N	2.66	0.58
1:A:83:LEU:HD11	1:B:40:LEU:HB3	1.85	0.58
1:A:131:PHE:HB2	1:B:131:PHE:CG	2.39	0.58
1:B:138:ARG:HD3	1:B:199:GLN:O	2.03	0.57
1:B:47:GLU:OE2	1:B:53:ARG:HB2	2.04	0.57
1:B:299:GLU:HB2	1:B:300:PRO:C	2.25	0.57
1:B:206:MET:CE	1:B:215:ASP:HB3	2.34	0.57
1:B:226:LYS:HE3	1:B:292:PHE:CD1	2.40	0.57
1:B:228:GLU:O	1:B:283:GLY:HA3	2.05	0.56
1:B:30:PRO:HG3	1:B:139:PHE:CE1	2.41	0.56
1:B:273:TRP:CZ2	1:B:275:PRO:HB3	2.40	0.56
1:A:174:TYR:HB3	1:A:178:GLU:HB2	1.86	0.56
1:A:27:ASP:H	1:A:142:ARG:NH2	2.04	0.56
1:B:184:ARG:HH12	1:B:239:GLU:CG	2.18	0.56
1:B:150:SER:HB2	1:B:152:PHE:CE1	2.42	0.55
1:A:201:TYR:CD2	1:A:272:ARG:HG3	2.42	0.55
1:A:250:ASN:HD21	1:A:252:ILE:HB	1.71	0.55
1:B:206:MET:HE2	1:B:215:ASP:HB3	1.88	0.55
1:B:213:VAL:HG11	1:B:298:VAL:HG11	1.87	0.55
1:A:228:GLU:O	1:A:283:GLY:HA3	2.07	0.54
1:A:40:LEU:HD23	1:A:133:VAL:HG22	1.90	0.54
1:A:68:ASN:HD22	1:A:130:VAL:HG12	1.73	0.54
1:A:228:GLU:OE2	1:A:292:PHE:HB2	2.08	0.54
1:A:234:LEU:O	1:A:236:LEU:HD22	2.07	0.54
1:B:269:PRO:HB2	1:B:271:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PHE:CD2	1:A:301:LYS:HB2	2.43	0.53
1:A:305:HIS:HD2	1:B:122:LYS:HD2	1.73	0.53
1:B:147:LEU:HD11	1:B:287:GLU:N	2.22	0.53
1:A:119:ASN:HB2	1:B:42:THR:HG23	1.91	0.53
1:A:22:LYS:HD2	1:A:22:LYS:H	1.74	0.52
1:A:28:THR:HG22	1:A:29:ALA:N	2.24	0.52
1:A:28:THR:N	1:A:75:ASN:HD21	2.07	0.52
1:A:92:LEU:HD13	1:A:126:ILE:HD11	1.92	0.52
1:B:197:HIS:NE2	1:B:268:HIS:HE1	2.07	0.52
1:A:244:CYS:HB3	1:A:249:LYS:O	2.10	0.52
1:B:68:ASN:ND2	1:B:132:LEU:HB2	2.25	0.52
1:B:213:VAL:HG11	1:B:298:VAL:CG1	2.40	0.51
1:B:250:ASN:HD22	1:B:251:PRO:HD2	1.76	0.51
1:A:28:THR:N	1:A:75:ASN:ND2	2.59	0.51
1:A:93:GLU:H	1:A:93:GLU:CD	2.14	0.51
1:A:292:PHE:CE2	1:A:297:LYS:HB2	2.46	0.50
1:A:28:THR:H	1:A:75:ASN:ND2	2.07	0.50
1:A:44:VAL:HG22	1:A:129:SER:HA	1.92	0.50
1:A:30:PRO:HB3	1:A:139:PHE:CD1	2.46	0.50
1:A:271:GLU:H	1:A:271:GLU:CD	2.13	0.50
1:A:122:LYS:H	1:B:305:HIS:CD2	2.30	0.50
1:A:26:ASP:CB	1:A:142:ARG:HG2	2.40	0.49
1:A:3:LEU:HD22	1:B:92:LEU:HB3	1.94	0.49
1:A:124:GLU:O	1:A:125:LYS:HD2	2.11	0.49
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.78	0.49
1:A:22:LYS:HD2	1:A:23:VAL:N	2.25	0.49
1:A:26:ASP:O	1:A:28:THR:N	2.45	0.49
1:A:85:SER:HB3	1:A:129:SER:HB3	1.94	0.49
1:A:131:PHE:CD1	1:B:83:LEU:HD12	2.48	0.49
1:A:200:LYS:HB2	1:A:201:TYR:CD1	2.47	0.49
1:B:105:LYS:HE2	1:B:109:GLU:OE2	2.11	0.49
1:A:144:GLY:O	1:A:203:ASN:HB3	2.12	0.49
1:B:227:ILE:HG22	1:B:229:ILE:HG13	1.94	0.49
1:B:293:VAL:HB	1:B:298:VAL:HG21	1.94	0.48
1:A:269:PRO:HB3	1:A:271:GLU:OE1	2.13	0.48
1:B:297:LYS:O	1:B:298:VAL:HB	2.14	0.48
1:B:226:LYS:HE3	1:B:292:PHE:CE1	2.48	0.48
1:B:269:PRO:HD2	1:B:272:ARG:NH2	2.28	0.48
1:B:125:LYS:NZ	1:B:125:LYS:CB	2.70	0.48
1:A:69:VAL:HG13	1:A:79:PRO:CG	2.44	0.48
1:A:218:HIS:O	1:A:222:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:VAL:O	1:B:294:ASP:HB2	2.14	0.47
1:A:131:PHE:CB	1:B:131:PHE:CD1	2.96	0.47
1:A:305:HIS:CD2	1:B:122:LYS:H	2.31	0.47
1:A:111:TYR:O	1:A:112:LYS:HB2	2.14	0.47
1:B:152:PHE:HB2	1:B:266:PHE:CE1	2.49	0.47
1:B:299:GLU:CD	1:B:299:GLU:N	2.66	0.47
1:A:34:CYS:O	1:A:35:SER:HB2	2.15	0.47
1:B:152:PHE:CE1	1:B:268:HIS:CD2	3.03	0.47
1:A:143:ASP:HB3	1:A:222:ARG:HG3	1.97	0.47
1:A:192:ILE:O	1:A:195:VAL:HG23	2.14	0.47
1:A:73:ILE:HG21	1:A:191:ARG:O	2.15	0.47
1:A:42:THR:HG23	1:B:119:ASN:HB2	1.97	0.47
1:B:166:LEU:HA	1:B:169:MET:HE3	1.97	0.47
1:A:61:GLY:HA2	1:A:100:PHE:CE1	2.50	0.46
1:A:212:LEU:HD23	1:A:256:LEU:HD23	1.98	0.46
1:B:152:PHE:CD2	1:B:279:MET:HG2	2.50	0.46
1:A:22:LYS:NZ	1:A:23:VAL:HG13	2.31	0.45
1:B:30:PRO:HG3	1:B:139:PHE:CD1	2.52	0.45
1:B:33:TYR:HB3	1:B:38:LEU:HD13	1.99	0.45
1:B:142:ARG:HB2	1:B:219:LEU:HD22	1.98	0.45
1:A:234:LEU:HD23	1:A:255:ALA:CB	2.48	0.45
1:B:153:VAL:HA	1:B:264:LEU:O	2.17	0.44
1:B:143:ASP:HB3	1:B:222:ARG:HD3	1.97	0.44
1:A:58:GLU:OE2	1:A:99:ARG:NH2	2.50	0.44
1:A:22:LYS:CD	1:A:23:VAL:HG13	2.48	0.44
1:A:191:ARG:HH22	1:A:278:ASP:CG	2.20	0.44
1:A:196:LYS:HA	1:A:196:LYS:HD2	1.72	0.44
1:B:34:CYS:C	1:B:36:LYS:H	2.21	0.44
1:B:43:ASP:HB2	1:B:68:ASN:OD1	2.17	0.44
1:B:120:ILE:HG12	4:B:307:ACP:N7	2.33	0.44
1:B:143:ASP:O	1:B:223:SER:HA	2.16	0.44
1:B:191:ARG:HH12	1:B:193:ASP:CG	2.20	0.44
1:B:269:PRO:CD	1:B:272:ARG:NH2	2.81	0.44
1:B:23:VAL:O	1:B:24:ILE:HB	2.17	0.44
1:B:250:ASN:HD22	1:B:251:PRO:CD	2.31	0.44
1:A:299:GLU:O	1:A:299:GLU:HG3	2.18	0.44
1:B:167:LEU:HD21	1:B:186:LEU:HD13	2.00	0.44
1:B:192:ILE:O	1:B:195:VAL:HG23	2.18	0.44
1:B:277:LEU:C	1:B:279:MET:H	2.21	0.44
1:B:108:CYS:SG	1:B:115:VAL:HG23	2.58	0.44
1:A:268:HIS:C	1:A:268:HIS:HD1	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LYS:HD3	1:B:135:GLU:HG2	2.00	0.44
1:A:89:PRO:HA	1:A:123:SER:O	2.18	0.43
1:B:269:PRO:CB	1:B:271:GLU:HG2	2.48	0.43
1:A:27:ASP:HA	4:B:307:ACP:O1B	2.18	0.43
1:B:269:PRO:CD	1:B:272:ARG:HH21	2.32	0.43
1:A:138:ARG:HD3	1:A:199:GLN:O	2.19	0.43
1:A:69:VAL:HG13	1:A:79:PRO:HG2	2.01	0.43
1:A:2:ARG:N	1:A:2:ARG:HD2	2.33	0.43
1:A:155:GLY:HA2	1:A:278:ASP:OD2	2.18	0.43
1:A:28:THR:CB	1:A:75:ASN:ND2	2.68	0.42
1:A:246:LYS:O	1:A:246:LYS:HG2	2.19	0.42
1:A:234:LEU:HD23	1:A:255:ALA:HB1	2.00	0.42
1:B:211:GLY:HA2	1:B:258:GLY:O	2.19	0.42
1:B:84:ILE:O	1:B:118:GLY:HA3	2.19	0.42
1:B:150:SER:HB2	1:B:152:PHE:HE1	1.83	0.42
1:B:233:LYS:O	1:B:233:LYS:HG2	2.19	0.42
1:A:274:ASN:HB3	1:A:279:MET:HE3	2.01	0.42
1:B:297:LYS:O	1:B:298:VAL:CB	2.68	0.42
1:A:58:GLU:CD	1:A:99:ARG:HE	2.23	0.42
1:A:82:ALA:HA	1:A:131:PHE:O	2.19	0.42
1:B:9:PHE:CE2	1:B:304:LYS:HD2	2.54	0.42
1:B:17:LYS:HD3	1:B:17:LYS:C	2.40	0.42
1:A:77:GLY:HA2	1:A:136:THR:HB	2.02	0.42
1:A:92:LEU:CD1	1:A:126:ILE:HD11	2.49	0.42
1:A:120:ILE:HD13	1:B:12:ILE:HD11	2.02	0.42
1:B:239:GLU:H	1:B:239:GLU:CD	2.22	0.42
1:A:201:TYR:HB3	1:A:272:ARG:CG	2.50	0.41
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.93	0.41
1:A:57:PRO:HG2	1:A:58:GLU:OE2	2.20	0.41
1:B:220:ALA:HB2	1:B:227:ILE:HG12	2.00	0.41
1:A:19:LEU:HD21	1:B:115:VAL:CG1	2.50	0.41
1:A:29:ALA:HB3	1:A:40:LEU:HB2	2.02	0.41
1:A:44:VAL:CG1	1:A:45:LEU:N	2.83	0.41
1:B:44:VAL:HG12	1:B:45:LEU:N	2.36	0.41
1:A:23:VAL:HG23	1:A:24:ILE:N	2.35	0.41
1:A:147:LEU:H	1:A:147:LEU:CD2	2.34	0.41
1:B:88:LEU:HA	1:B:89:PRO:HD3	1.90	0.41
1:B:198:ILE:HA	1:B:202:ALA:HB2	2.02	0.41
1:A:22:LYS:HD3	1:A:23:VAL:HG13	2.03	0.41
1:A:85:SER:OG	1:B:44:VAL:CG2	2.68	0.41
1:A:84:ILE:O	1:A:118:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LYS:HE2	1:B:136:THR:C	2.41	0.41
1:A:26:ASP:HB3	1:A:142:ARG:CG	2.44	0.41
1:A:116:VAL:HB	1:B:29:ALA:HB1	2.01	0.41
1:B:150:SER:O	1:B:267:THR:HA	2.21	0.41
1:B:184:ARG:HH12	1:B:239:GLU:HG3	1.84	0.41
1:A:3:LEU:HD21	1:B:88:LEU:HD13	2.02	0.40
1:A:73:ILE:HG23	1:A:195:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/342 (89%)	284 (93%)	18 (6%)	3 (1%)	15	32
1	B	307/342 (90%)	284 (92%)	17 (6%)	6 (2%)	7	14
All	All	612/684 (90%)	568 (93%)	35 (6%)	9 (2%)	10	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	289	GLU
1	B	24	ILE
1	B	297	LYS
1	B	299	GLU
1	A	288	GLY
1	B	304	LYS
1	B	298	VAL
1	B	278	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/291 (90%)	251 (95%)	12 (5%)	27	51
1	B	265/291 (91%)	253 (96%)	12 (4%)	27	52
All	All	528/582 (91%)	504 (96%)	24 (4%)	27	52

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	22	LYS
1	A	26	ASP
1	A	43	ASP
1	A	146	ARG
1	A	186	LEU
1	A	191	ARG
1	A	232	GLU
1	A	253	GLU
1	A	268	HIS
1	A	272	ARG
1	B	11	LEU
1	B	22	LYS
1	B	43	ASP
1	B	122	LYS
1	B	125	LYS
1	B	167	LEU
1	B	168	LEU
1	B	186	LEU
1	B	192	ILE
1	B	222	ARG
1	B	232	GLU
1	B	268	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	46	ASN
1	A	75	ASN
1	A	119	ASN
1	A	183	GLN
1	A	199	GLN
1	A	203	ASN
1	A	221	GLN
1	A	238	ASN
1	A	305	HIS
1	B	46	ASN
1	B	218	HIS
1	B	221	GLN
1	B	250	ASN
1	B	268	HIS
1	B	305	HIS

### 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, 10 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACP	B	307	2	27,33,33	2.14	5 (18%)	33,52,52	2.50	16 (48%)
4	ACP	A	307	2	27,33,33	2.18	7 (25%)	33,52,52	2.49	16 (48%)
3	TPS	A	308	2	20,23,23	2.16	7 (35%)	25,33,33	1.22	2 (8%)
3	TPS	B	308	2	20,23,23	2.30	5 (25%)	25,33,33	1.30	2 (8%)

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	ACP	B	307	2	-	3/15/38/38	0/3/3/3
4	ACP	A	307	2	-	3/15/38/38	0/3/3/3
3	TPS	A	308	2	-	1/10/11/11	0/2/2/2
3	TPS	B	308	2	-	2/10/11/11	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	307	ACP	PB-O3A	7.56	1.66	1.58
4	B	307	ACP	PB-O3A	7.04	1.66	1.58
3	B	308	TPS	C6-C5	-6.01	1.47	1.51
3	A	308	TPS	C6-C5	-4.94	1.48	1.51
3	B	308	TPS	C7A-N3	4.09	1.56	1.48
3	A	308	TPS	C7A-N3	3.86	1.55	1.48
4	B	307	ACP	PG-O2G	-3.67	1.46	1.55
4	A	307	ACP	PB-O2B	-3.65	1.47	1.56
3	B	308	TPS	C2A-N1A	3.63	1.39	1.34
4	B	307	ACP	PB-O2B	-3.61	1.47	1.56
4	B	307	ACP	C2-N3	3.41	1.37	1.32
3	B	308	TPS	C5A-C4A	3.40	1.48	1.42
3	A	308	TPS	C2A-N1A	3.31	1.39	1.34
3	A	308	TPS	C5A-C4A	3.20	1.48	1.42
4	A	307	ACP	PG-O2G	-3.05	1.48	1.55
3	B	308	TPS	C4A-N3A	2.99	1.39	1.35
4	A	307	ACP	PA-O3A	2.69	1.62	1.59
4	A	307	ACP	C2-N3	2.61	1.36	1.32
3	A	308	TPS	C4A-N3A	2.60	1.38	1.35
4	B	307	ACP	C4-N3	2.54	1.39	1.35
4	A	307	ACP	C4-N3	2.45	1.39	1.35
3	A	308	TPS	C2A-N3A	-2.44	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	308	TPS	C7A-C5A	2.13	1.55	1.51
4	A	307	ACP	O4'-C1'	2.03	1.43	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	307	ACP	O5'-C5'-C4'	7.11	133.21	108.99
4	A	307	ACP	O5'-C5'-C4'	6.58	131.41	108.99
4	A	307	ACP	PB-O3A-PA	4.51	147.08	132.37
4	A	307	ACP	O3G-PG-C3B	-4.31	95.94	106.40
4	B	307	ACP	PB-O3A-PA	4.26	146.29	132.37
4	B	307	ACP	N3-C2-N1	-4.25	122.91	128.67
4	A	307	ACP	N3-C2-N1	-4.16	123.03	128.67
4	B	307	ACP	C5'-C4'-C3'	-3.74	101.77	115.21
4	B	307	ACP	O4'-C4'-C5'	3.66	121.06	109.33
4	B	307	ACP	O3G-PG-C3B	-3.47	97.99	106.40
4	A	307	ACP	O4'-C4'-C5'	3.29	119.87	109.33
4	A	307	ACP	C5'-C4'-C3'	-3.24	103.55	115.21
4	A	307	ACP	O1B-PB-C3B	-3.20	100.64	109.05
4	A	307	ACP	O2B-PB-C3B	3.04	119.33	106.73
4	A	307	ACP	O2G-PG-C3B	2.92	113.49	106.40
4	B	307	ACP	C4-C5-N7	2.86	112.35	109.34
3	B	308	TPS	C5-C4-N3	2.76	113.09	107.57
4	B	307	ACP	C6-C5-C4	-2.68	112.68	117.90
3	A	308	TPS	C5-C4-N3	2.67	112.91	107.57
4	B	307	ACP	O2A-PA-O5'	2.66	119.64	107.57
4	A	307	ACP	C4-C5-N7	2.65	112.14	109.34
4	A	307	ACP	C6-C5-C4	-2.62	112.81	117.90
4	B	307	ACP	O2B-PB-C3B	2.60	117.52	106.73
4	B	307	ACP	C4'-O4'-C1'	-2.59	107.55	109.92
4	A	307	ACP	C1'-N9-C4	-2.57	122.13	126.64
4	B	307	ACP	O4'-C4'-C3'	2.54	110.19	105.15
4	A	307	ACP	C4'-O4'-C1'	-2.51	107.62	109.92
4	B	307	ACP	O2G-PG-C3B	2.49	112.44	106.40
4	B	307	ACP	C1'-N9-C4	-2.48	122.29	126.64
4	B	307	ACP	O1B-PB-C3B	-2.38	102.78	109.05
4	A	307	ACP	O2A-PA-O5'	2.36	118.27	107.57
4	A	307	ACP	O5'-PA-O1A	-2.22	100.13	108.94
3	A	308	TPS	CM2-C2A-N3A	2.11	120.29	117.13
3	B	308	TPS	CM2-C2A-N3A	2.09	120.25	117.13
4	A	307	ACP	O3G-PG-O2G	2.02	113.70	107.96
4	B	307	ACP	O4'-C1'-N9	2.01	111.42	108.75

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	308	TPS	C4-C5-C6-C7
3	B	308	TPS	C4-C5-C6-C7
4	A	307	ACP	O4'-C4'-C5'-O5'
4	A	307	ACP	C3'-C4'-C5'-O5'
4	B	307	ACP	O4'-C4'-C5'-O5'
4	B	307	ACP	C3'-C4'-C5'-O5'
4	A	307	ACP	PB-O3A-PA-O5'
4	B	307	ACP	PB-O3A-PA-O5'
3	B	308	TPS	C5A-C7A-N3-C4

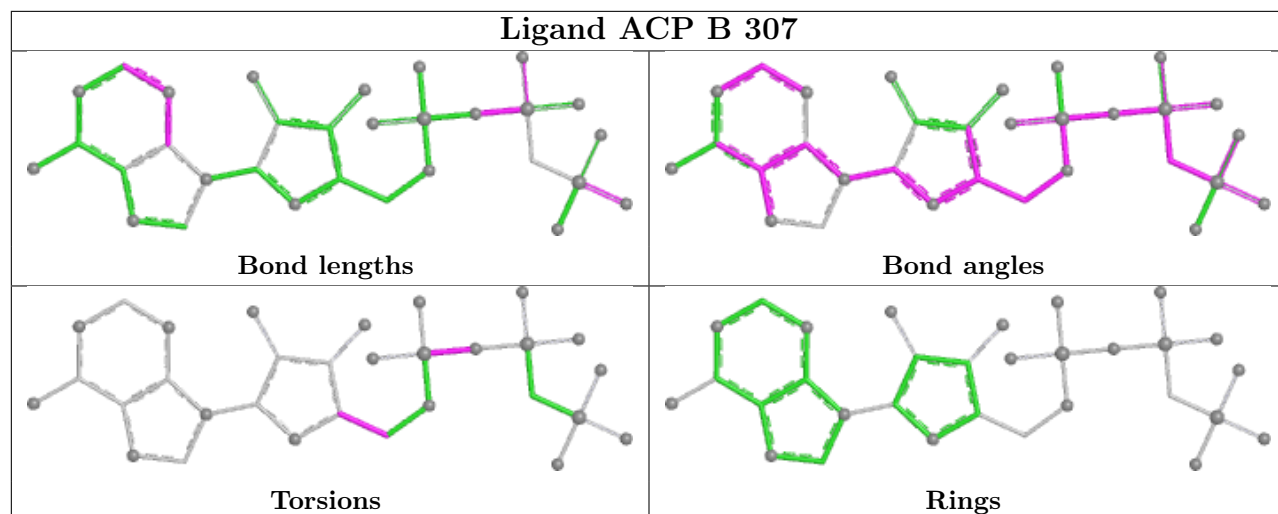
There are no ring outliers.

1 monomer is involved in 2 short contacts:

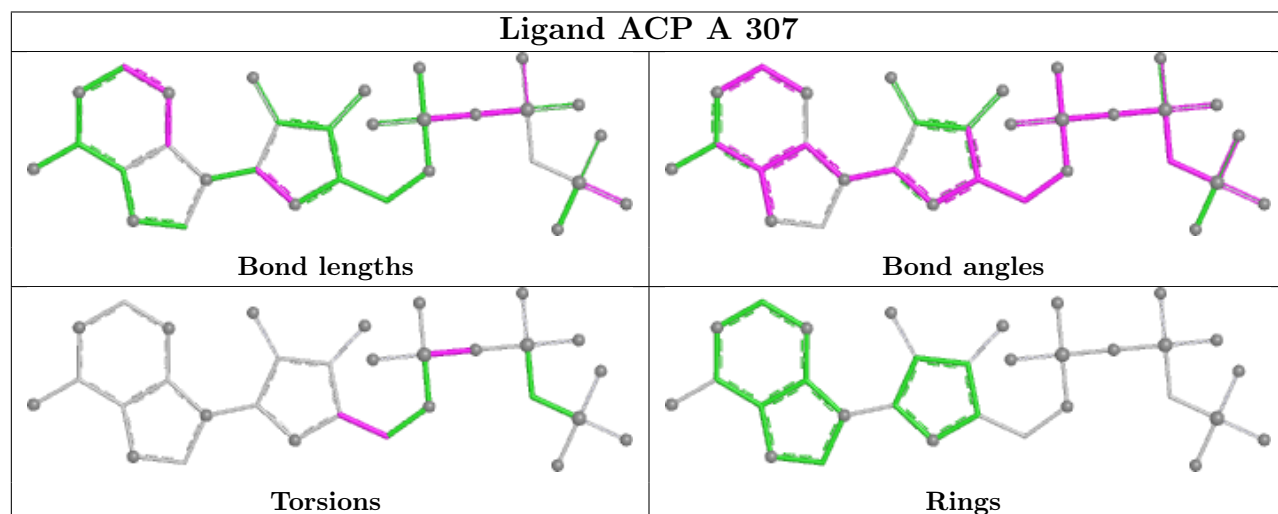
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	307	ACP	2	0

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.

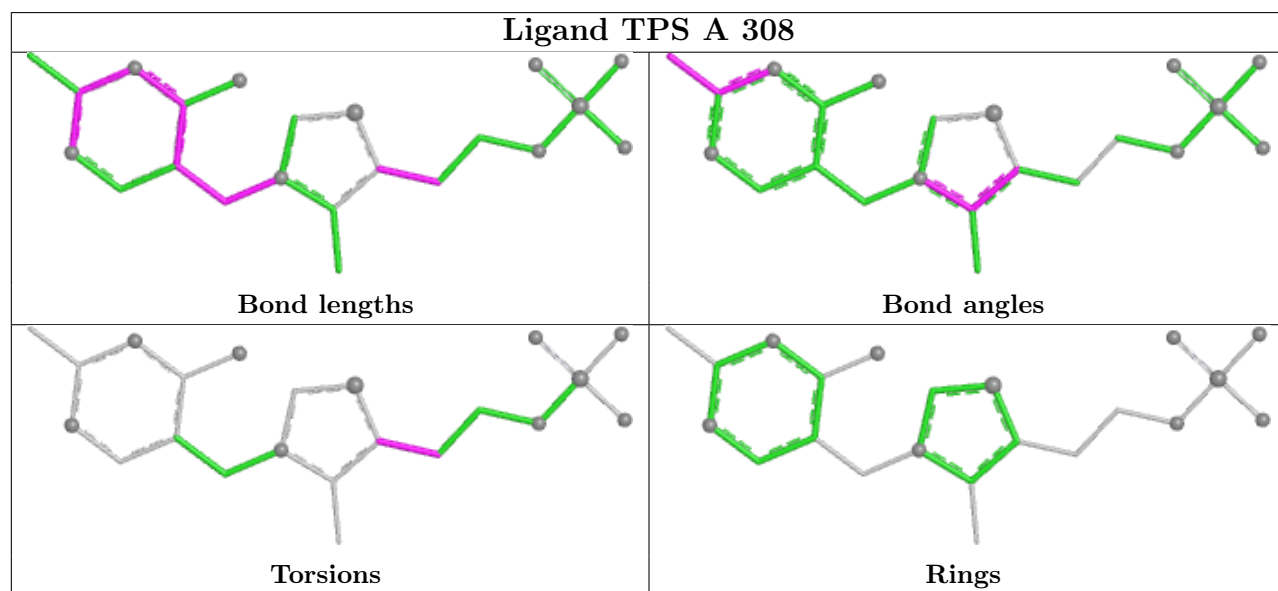
## Ligand ACP B 307

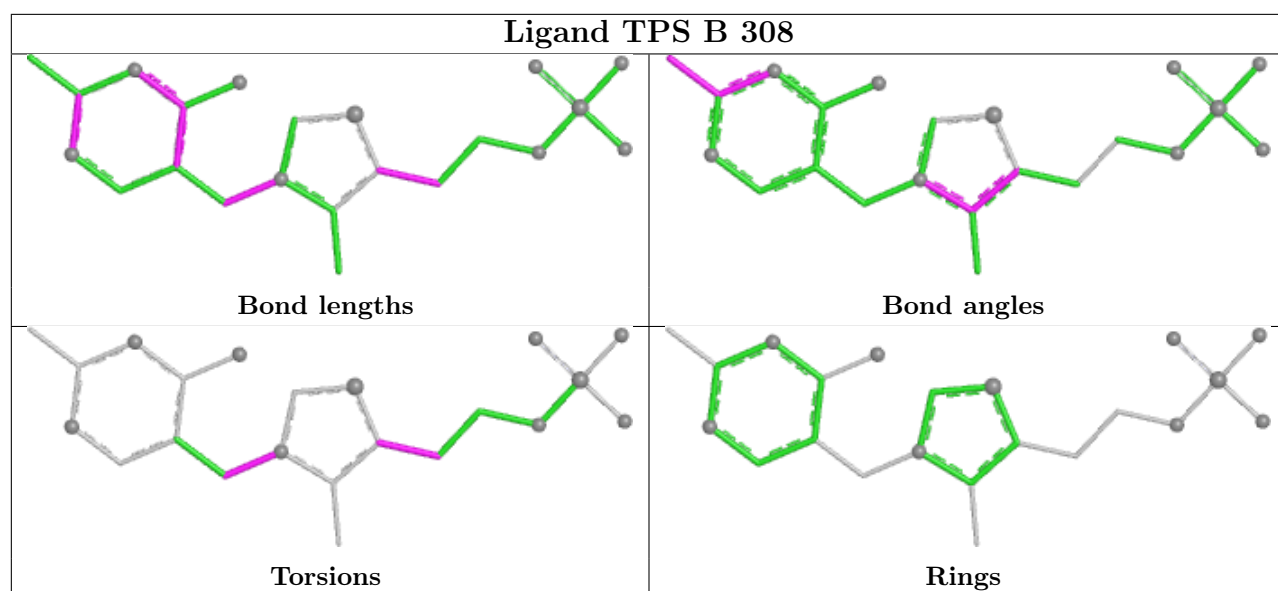


## Ligand ACP A 307



## Ligand TPS A 308





## 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<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	307/342 (89%)	-0.12	3 (0%) 82 80	35, 53, 77, 96	1 (0%)
1	B	309/342 (90%)	-0.09	5 (1%) 72 68	35, 55, 81, 97	1 (0%)
All	All	616/684 (90%)	-0.10	8 (1%) 77 73	35, 54, 80, 97	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PRO	3.3
1	B	299	GLU	3.3
1	A	302	GLY	2.4
1	B	298	VAL	2.3
1	B	172	GLU	2.2
1	A	298	VAL	2.1
1	A	292	PHE	2.0
1	B	228	GLU	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.

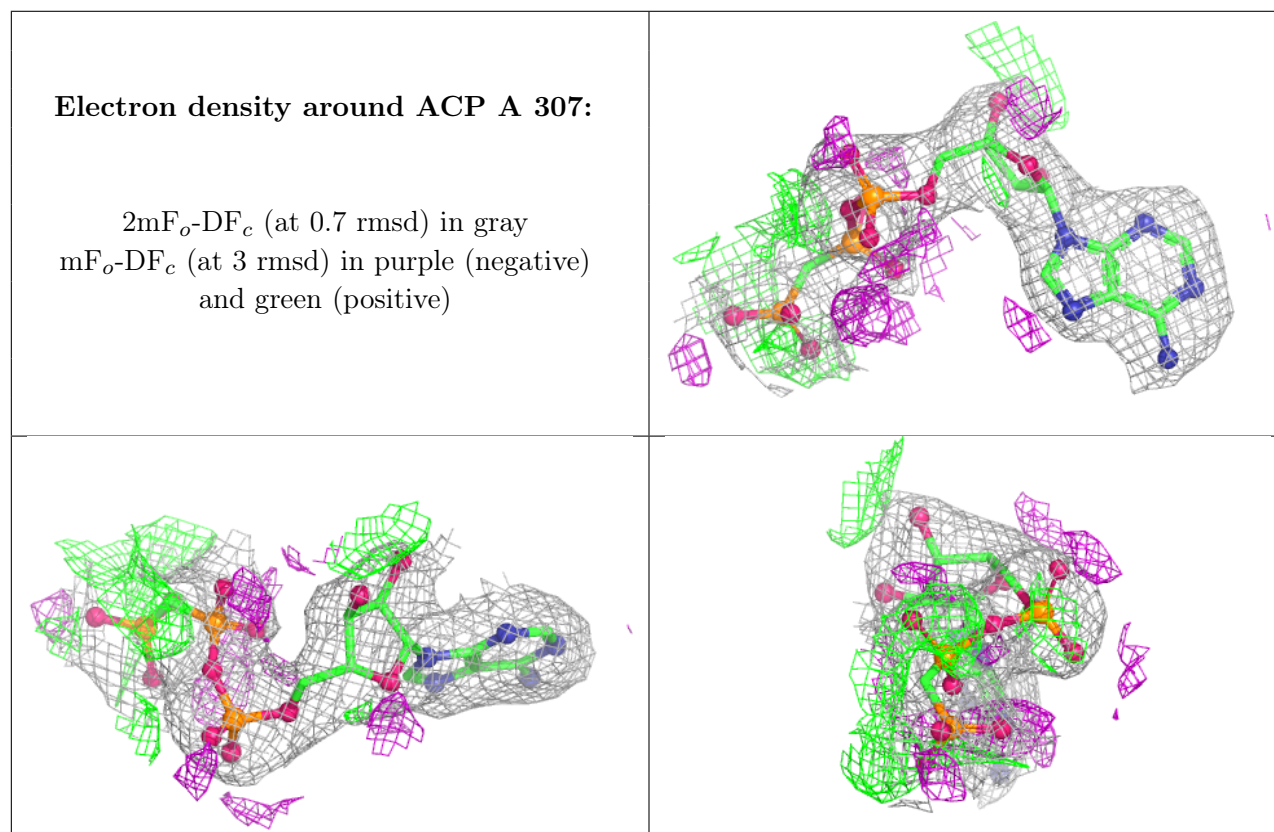
### 6.4 Ligands [i](#)

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
2	MG	A	312	1/1	0.89	0.29	40,40,40,40	0
2	MG	B	312	1/1	0.94	0.28	29,29,29,29	0
2	MG	B	313	1/1	0.94	0.28	27,27,27,27	0
2	MG	B	314	1/1	0.94	0.26	35,35,35,35	0
4	ACP	A	307	31/31	0.95	0.18	44,54,64,65	0
4	ACP	B	307	31/31	0.95	0.18	39,49,64,65	0
2	MG	A	309	1/1	0.96	0.29	25,25,25,25	0
2	MG	A	313	1/1	0.96	0.26	25,25,25,25	0
3	TPS	B	308	22/22	0.96	0.17	46,51,57,58	0
2	MG	B	310	1/1	0.96	0.26	30,30,30,30	0
2	MG	A	310	1/1	0.96	0.34	32,32,32,32	0
3	TPS	A	308	22/22	0.97	0.18	47,52,56,60	0
2	MG	B	311	1/1	0.97	0.28	25,25,25,25	0
2	MG	A	314	1/1	0.99	0.23	25,25,25,25	0

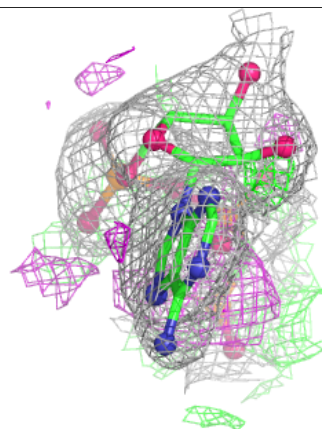
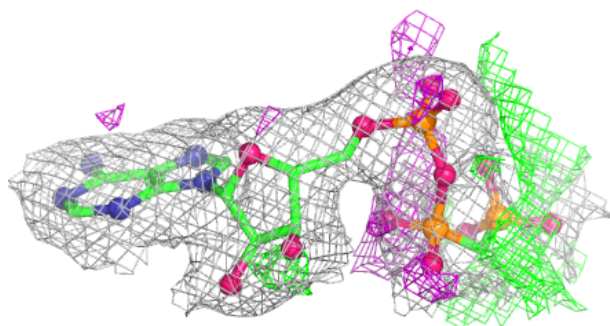
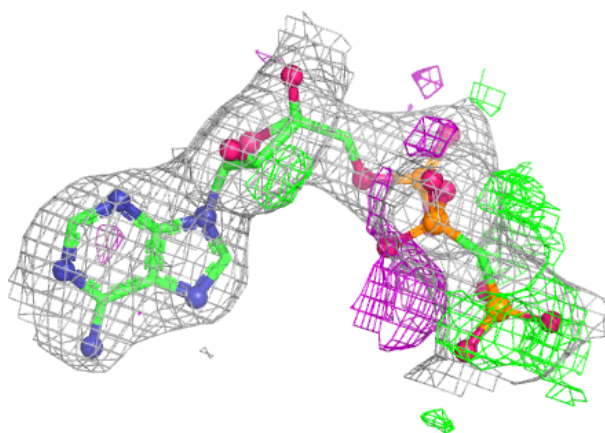
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



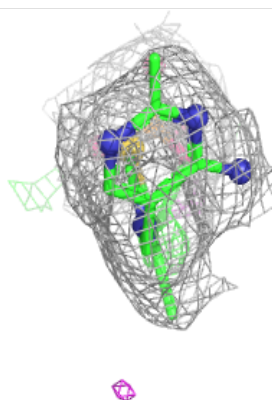
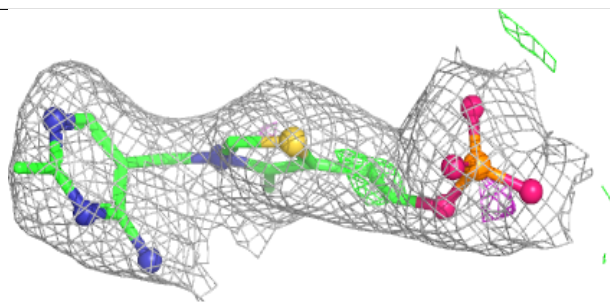
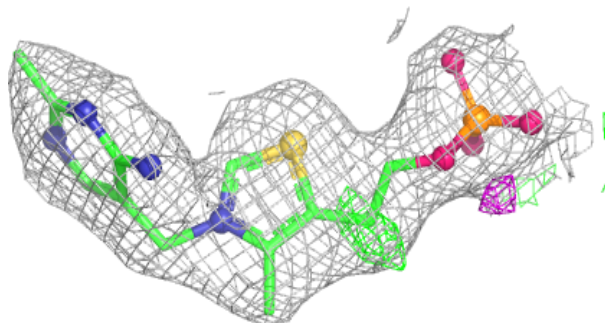


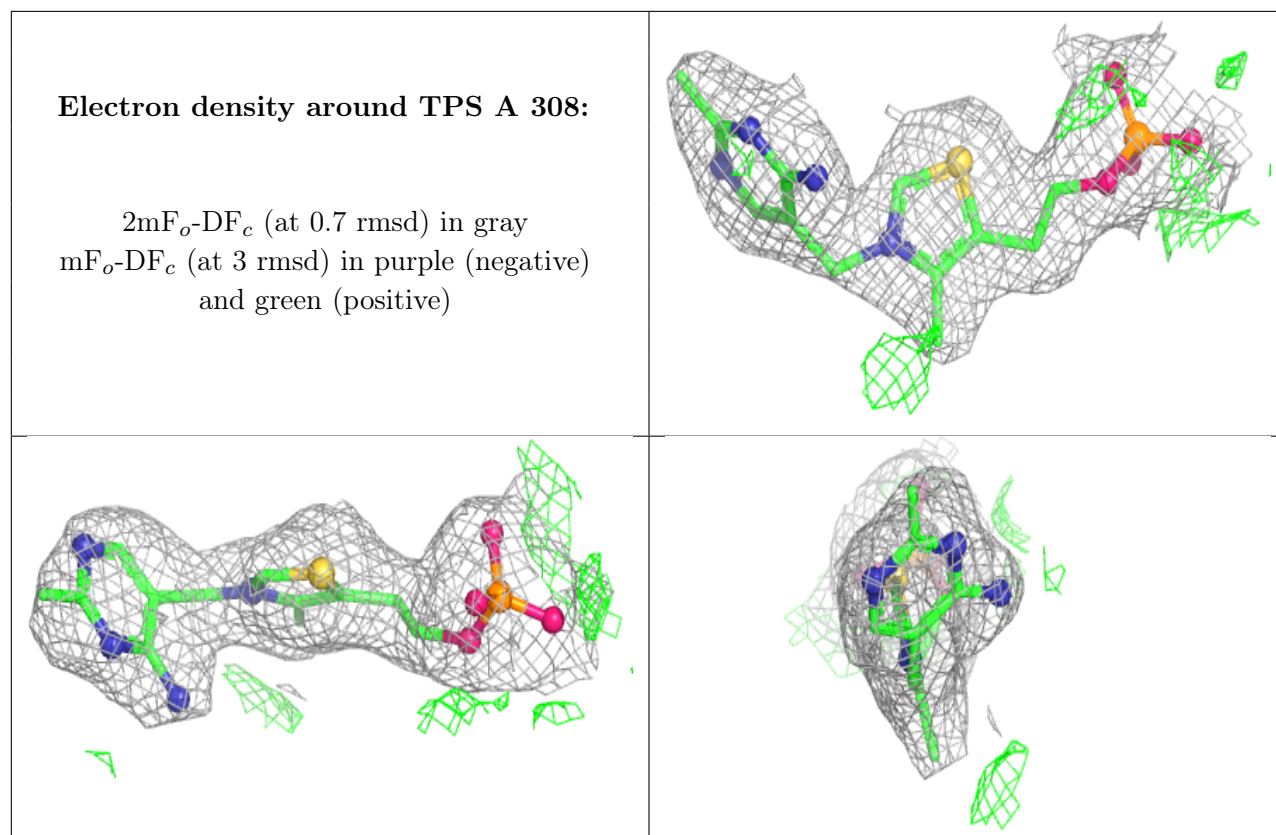
**Electron density around ACP B 307:**

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

**Electron density around TPS B 308:**

$2mF_o-DF_c$  (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.