



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 06:37 AM EDT

PDB ID : 6PSP
Title : Adenylate kinase from Methanococcus igneus - AP5A bound form
Authors : Moon, S.; Kim, J.; Bae, E.; Phillips Jr., G.N.
Deposited on : 2019-07-13
Resolution : 2.25 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 ⓘ 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 ⓘ](#)) 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

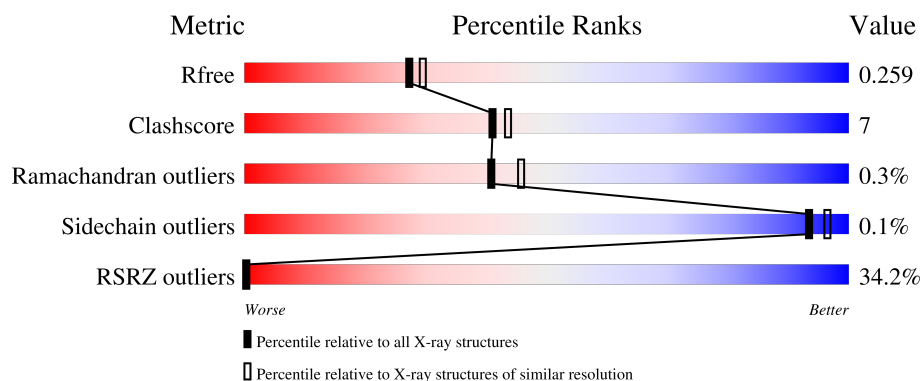
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 $\leq 5\%$. 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	200	<div> <div>30%</div> <div>82%</div> <div>13%</div> <div>.</div> </div>
1	B	200	<div> <div>20%</div> <div>82%</div> <div>13%</div> <div>.</div> </div>
1	C	200	<div> <div>34%</div> <div>75%</div> <div>20%</div> <div>.</div> </div>
1	D	200	<div> <div>30%</div> <div>84%</div> <div>10%</div> <div>.</div> </div>
1	E	200	<div> <div>38%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	200	<div><div></div><div>44%</div><div></div><div>76%</div><div></div><div>20%</div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18757 atoms, of which 9450 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 Adenylate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	191	Total	C	H	N	O	S	0	0	0
			3038	934	1551	256	289	8			
1	B	191	Total	C	H	N	O	S	0	0	0
			3038	934	1551	256	289	8			
1	C	191	Total	C	H	N	O	S	0	0	0
			3038	934	1551	256	289	8			
1	D	191	Total	C	H	N	O	S	0	0	0
			3038	934	1551	256	289	8			
1	E	191	Total	C	H	N	O	S	0	0	0
			3038	934	1551	256	289	8			
1	F	191	Total	C	H	N	O	S	0	0	0
			3038	934	1551	256	289	8			

There are 48 discrepancies between the modelled and reference sequences:

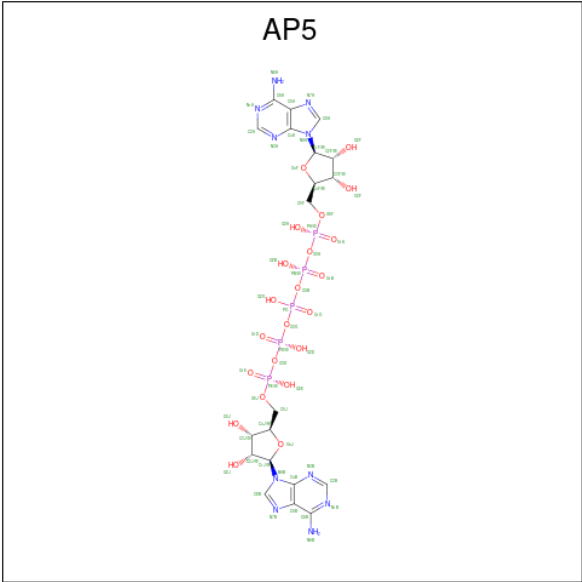
Chain	Residue	Modelled	Actual	Comment	Reference
A	193	LEU	-	expression tag	UNP P43408
A	194	GLU	-	expression tag	UNP P43408
A	195	HIS	-	expression tag	UNP P43408
A	196	HIS	-	expression tag	UNP P43408
A	197	HIS	-	expression tag	UNP P43408
A	198	HIS	-	expression tag	UNP P43408
A	199	HIS	-	expression tag	UNP P43408
A	200	HIS	-	expression tag	UNP P43408
B	193	LEU	-	expression tag	UNP P43408
B	194	GLU	-	expression tag	UNP P43408
B	195	HIS	-	expression tag	UNP P43408
B	196	HIS	-	expression tag	UNP P43408
B	197	HIS	-	expression tag	UNP P43408
B	198	HIS	-	expression tag	UNP P43408
B	199	HIS	-	expression tag	UNP P43408
B	200	HIS	-	expression tag	UNP P43408
C	193	LEU	-	expression tag	UNP P43408

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	194	GLU	-	expression tag	UNP P43408
C	195	HIS	-	expression tag	UNP P43408
C	196	HIS	-	expression tag	UNP P43408
C	197	HIS	-	expression tag	UNP P43408
C	198	HIS	-	expression tag	UNP P43408
C	199	HIS	-	expression tag	UNP P43408
C	200	HIS	-	expression tag	UNP P43408
D	193	LEU	-	expression tag	UNP P43408
D	194	GLU	-	expression tag	UNP P43408
D	195	HIS	-	expression tag	UNP P43408
D	196	HIS	-	expression tag	UNP P43408
D	197	HIS	-	expression tag	UNP P43408
D	198	HIS	-	expression tag	UNP P43408
D	199	HIS	-	expression tag	UNP P43408
D	200	HIS	-	expression tag	UNP P43408
E	193	LEU	-	expression tag	UNP P43408
E	194	GLU	-	expression tag	UNP P43408
E	195	HIS	-	expression tag	UNP P43408
E	196	HIS	-	expression tag	UNP P43408
E	197	HIS	-	expression tag	UNP P43408
E	198	HIS	-	expression tag	UNP P43408
E	199	HIS	-	expression tag	UNP P43408
E	200	HIS	-	expression tag	UNP P43408
F	193	LEU	-	expression tag	UNP P43408
F	194	GLU	-	expression tag	UNP P43408
F	195	HIS	-	expression tag	UNP P43408
F	196	HIS	-	expression tag	UNP P43408
F	197	HIS	-	expression tag	UNP P43408
F	198	HIS	-	expression tag	UNP P43408
F	199	HIS	-	expression tag	UNP P43408
F	200	HIS	-	expression tag	UNP P43408

- Molecule 2 is BIS(ADENOSINE)-5'-PENTAPHOSPHATE (three-letter code: AP5) (formula: C₂₀H₂₉N₁₀O₂₂P₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 81	C 20	H 24	N 10	O 22	P 5	0	0
2	B	1	Total 81	C 20	H 24	N 10	O 22	P 5	0	0
2	C	1	Total 81	C 20	H 24	N 10	O 22	P 5	0	0
2	D	1	Total 81	C 20	H 24	N 10	O 22	P 5	0	0
2	E	1	Total 81	C 20	H 24	N 10	O 22	P 5	0	0
2	F	1	Total 81	C 20	H 24	N 10	O 22	P 5	0	0

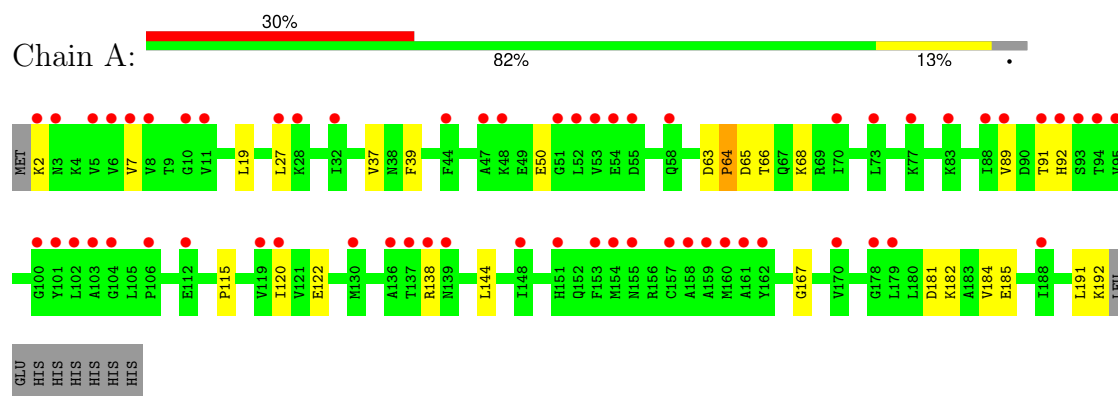
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	13	Total	O	0	0
			13	13		
3	C	10	Total	O	0	0
			10	10		
3	D	5	Total	O	0	0
			5	5		
3	E	5	Total	O	0	0
			5	5		
3	F	7	Total	O	0	0
			7	7		

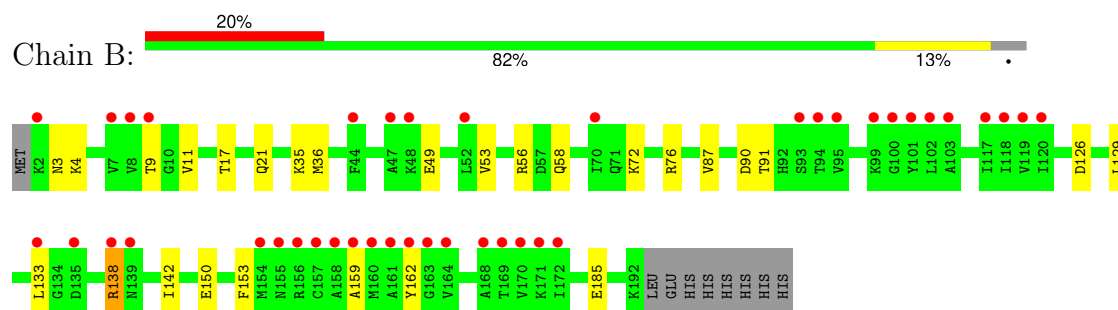
3 Residue-property plots [i](#)

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.

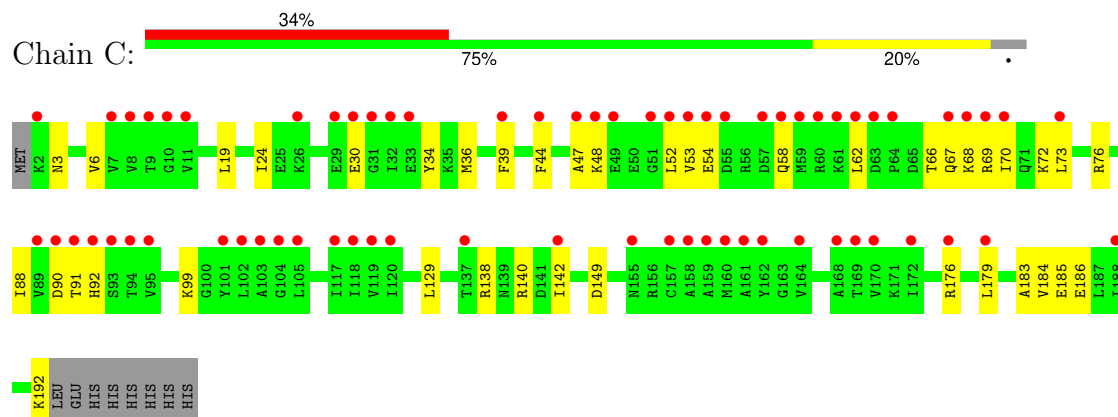
• Molecule 1: Adenylate kinase



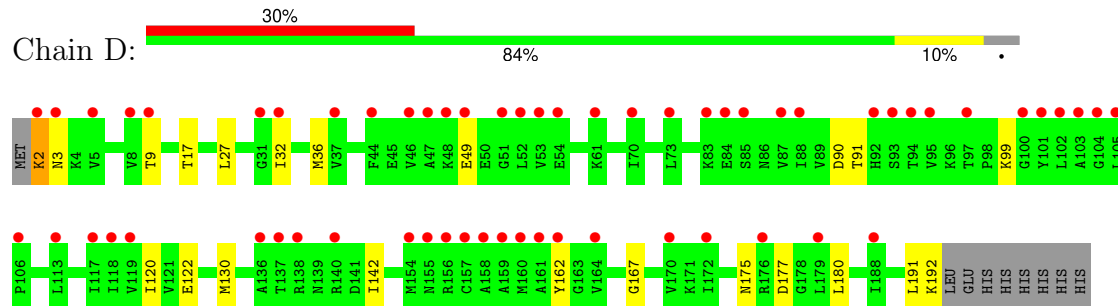
• Molecule 1: Adenylate kinase



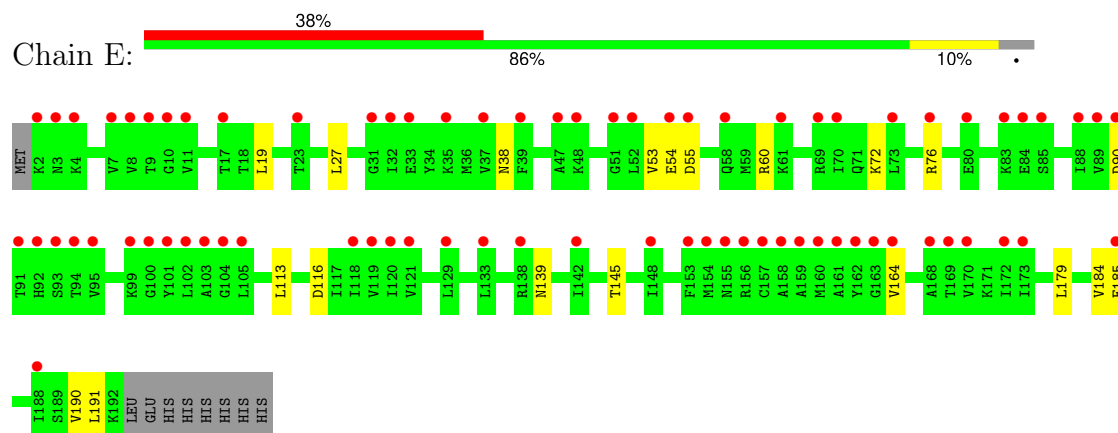
• Molecule 1: Adenylate kinase



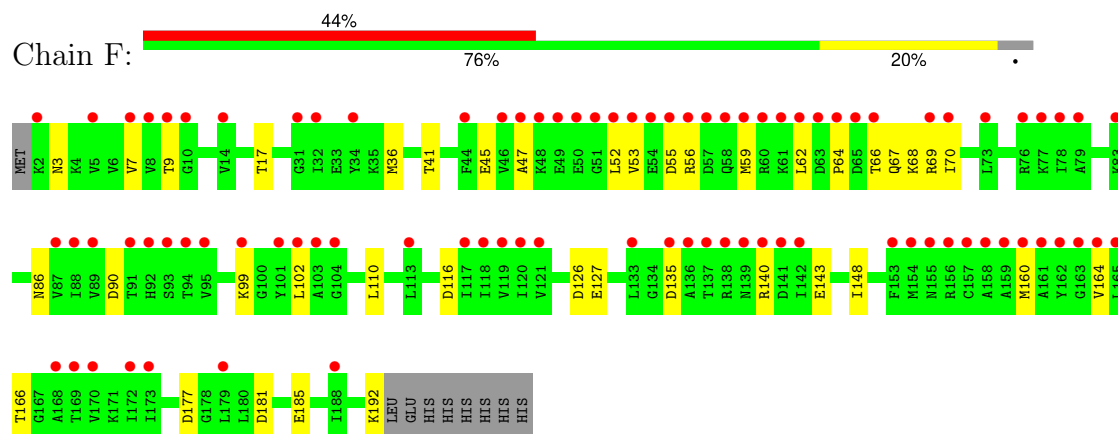
- Molecule 1: Adenylate kinase



- Molecule 1: Adenylate kinase



- Molecule 1: Adenylate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.44Å 122.63Å 83.72Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	33.19 – 2.25 33.19 – 2.25	Depositor EDS
% Data completeness (in resolution range)	80.4 (33.19-2.25) 80.4 (33.19-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.215 , 0.256 0.216 , 0.259	Depositor DCC
R_{free} test set	1977 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18757	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AP5

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	0.66	1/1501 (0.1%)	0.76	0/2021
1	B	0.86	3/1501 (0.2%)	0.93	2/2021 (0.1%)
1	C	0.84	1/1501 (0.1%)	0.91	1/2021 (0.0%)
1	D	0.61	1/1501 (0.1%)	0.74	1/2021 (0.0%)
1	E	0.68	1/1501 (0.1%)	0.81	2/2021 (0.1%)
1	F	0.66	0/1501	0.80	2/2021 (0.1%)
All	All	0.73	7/9006 (0.1%)	0.83	8/12126 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	185	GLU	CG-CD	6.80	1.62	1.51
1	B	150	GLU	CD-OE2	6.41	1.32	1.25
1	C	185	GLU	CG-CD	5.73	1.60	1.51
1	D	2	LYS	CE-NZ	-5.73	1.34	1.49
1	B	11	VAL	CB-CG2	5.63	1.64	1.52
1	A	64	PRO	N-CD	-5.39	1.40	1.47
1	B	4	LYS	CD-CE	5.20	1.64	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	116	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	56	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	E	113	LEU	CB-CG-CD2	5.24	119.91	111.00
1	F	102	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	B	138	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	D	130	MET	CB-CG-SD	5.10	127.69	112.40
1	C	176	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	F	116	ASP	CB-CG-OD1	5.05	122.84	118.30

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	1487	1551	1550	19	0
1	B	1487	1551	1550	16	0
1	C	1487	1551	1550	36	0
1	D	1487	1551	1550	17	0
1	E	1487	1551	1550	15	0
1	F	1487	1551	1550	35	0
2	A	57	24	24	3	0
2	B	57	24	24	1	0
2	C	57	24	24	4	0
2	D	57	24	24	4	0
2	E	57	24	24	0	0
2	F	57	24	24	0	0
3	A	3	0	0	1	0
3	B	13	0	0	0	0
3	C	10	0	0	6	0
3	D	5	0	0	1	0
3	E	5	0	0	6	0
3	F	7	0	0	4	0
All	All	9307	9450	9444	132	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 7.

All (132) 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:C:186:GLU:N	3:C:402:HOH:O	1.85	1.06
1:C:69:ARG:O	3:C:401:HOH:O	1.84	0.94
1:F:41:THR:OG1	1:F:56:ARG:NH1	2.03	0.90
1:F:41:THR:OG1	1:F:56:ARG:NH2	2.10	0.85
1:E:55:ASP:N	3:E:402:HOH:O	2.01	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ASN:O	3:E:401:HOH:O	1.99	0.81
1:F:140:ARG:NE	3:F:401:HOH:O	1.88	0.80
1:C:149:ASP:OD2	3:C:403:HOH:O	2.03	0.76
1:D:2:LYS:O	1:D:2:LYS:HG3	1.86	0.73
1:A:167:GLY:O	1:C:68:LYS:NZ	2.19	0.73
1:C:140:ARG:NH2	2:C:300:AP5:O1G	2.22	0.72
1:F:66:THR:HG23	1:F:69:ARG:NH2	2.03	0.72
1:F:53:VAL:HG13	1:F:62:LEU:HD11	1.70	0.72
1:F:41:THR:OG1	1:F:56:ARG:CZ	2.37	0.72
1:A:192:LYS:O	1:C:99:LYS:NZ	2.23	0.70
1:F:192:LYS:O	3:F:402:HOH:O	2.09	0.70
1:C:44:PHE:HA	1:C:47:ALA:HB3	1.77	0.67
1:F:36:MET:CE	1:F:90:ASP:OD2	2.44	0.66
1:D:167:GLY:O	1:F:68:LYS:NZ	2.23	0.65
1:F:135:ASP:OD2	1:F:140:ARG:NH2	2.30	0.65
1:F:36:MET:HE3	1:F:90:ASP:OD2	1.97	0.64
1:F:3:ASN:HA	1:F:86:ASN:OD1	1.96	0.64
1:A:2:LYS:O	1:A:2:LYS:HG3	1.96	0.64
1:A:50:GLU:OE1	3:A:401:HOH:O	2.14	0.63
2:D:300:AP5:O2A	3:D:401:HOH:O	2.15	0.63
1:B:36:MET:HE3	1:B:90:ASP:OD2	1.99	0.63
1:C:138:ARG:NH1	2:C:300:AP5:O3A	2.32	0.62
1:F:41:THR:CB	1:F:56:ARG:HH22	2.15	0.59
1:C:54:GLU:N	1:C:58:GLN:OE1	2.35	0.59
1:F:53:VAL:HB	1:F:55:ASP:O	2.02	0.59
1:C:39:PHE:HB2	1:C:91:THR:HB	1.85	0.58
1:C:44:PHE:HE1	1:C:48:LYS:HB2	1.69	0.58
1:C:44:PHE:CE1	1:C:48:LYS:HB2	2.39	0.57
1:F:67:GLN:O	1:F:70:ILE:N	2.37	0.57
1:F:127:GLU:OE2	1:F:177:ASP:HB2	2.06	0.56
1:F:66:THR:HG23	1:F:69:ARG:HH22	1.70	0.55
1:A:2:LYS:O	1:A:2:LYS:CG	2.54	0.55
1:D:192:LYS:O	1:F:99:LYS:NZ	2.40	0.54
1:A:181:ASP:O	1:A:185:GLU:OE1	2.25	0.54
1:A:138:ARG:NH1	2:A:300:AP5:O1A	2.40	0.54
1:C:183:ALA:C	3:C:402:HOH:O	2.47	0.53
1:D:27:LEU:HD11	1:D:191:LEU:HD12	1.91	0.53
1:C:92:HIS:CE1	2:C:300:AP5:O1B	2.63	0.52
1:E:27:LEU:HD11	1:E:191:LEU:HD12	1.92	0.52
1:F:64:PRO:HA	3:F:403:HOH:O	2.09	0.52
1:B:53:VAL:HA	1:B:58:GLN:OE1	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LEU:O	1:B:133:LEU:HG	2.09	0.51
1:C:66:THR:HG23	1:C:69:ARG:HH21	1.75	0.51
1:C:19:LEU:HD12	1:C:184:VAL:HG22	1.92	0.51
1:A:63:ASP:OD2	1:A:65:ASP:HB2	2.10	0.51
1:B:36:MET:CE	1:B:90:ASP:OD2	2.59	0.50
1:E:53:VAL:HB	3:E:402:HOH:O	2.12	0.49
1:D:27:LEU:HB3	1:D:32:ILE:HB	1.94	0.49
1:C:36:MET:CE	1:C:90:ASP:OD2	2.60	0.49
1:B:138:ARG:NH1	2:B:300:AP5:O1A	2.44	0.49
1:A:64:PRO:O	1:A:68:LYS:HE2	2.13	0.49
1:D:142:ILE:HG13	1:D:142:ILE:O	2.12	0.49
1:A:63:ASP:HB3	1:A:66:THR:HB	1.93	0.49
1:E:72:LYS:HE2	1:E:76:ARG:HH11	1.78	0.48
1:C:72:LYS:HE2	1:C:76:ARG:HH11	1.78	0.48
1:C:184:VAL:C	3:C:402:HOH:O	2.51	0.48
1:B:49:GLU:O	1:B:49:GLU:HG2	2.12	0.48
1:F:66:THR:HA	1:F:69:ARG:HH21	1.79	0.48
1:C:34:TYR:CD2	1:C:88:ILE:HG13	2.49	0.48
1:C:179:LEU:HD21	1:E:179:LEU:HD21	1.96	0.48
1:F:181:ASP:O	1:F:185:GLU:HG2	2.14	0.47
1:B:142:ILE:O	1:B:142:ILE:HG13	2.13	0.47
1:E:54:GLU:N	3:E:402:HOH:O	2.47	0.47
1:C:73:LEU:HG	3:C:401:HOH:O	2.14	0.47
1:A:120:ILE:HG22	1:A:122:GLU:HG3	1.97	0.47
1:C:30:GLU:OE1	1:C:192:LYS:NZ	2.48	0.47
1:C:72:LYS:HE2	1:C:76:ARG:NH1	2.30	0.47
1:F:17:THR:HG23	1:F:36:MET:HE1	1.96	0.47
1:D:2:LYS:O	1:D:2:LYS:CG	2.59	0.47
1:F:135:ASP:CB	1:F:140:ARG:HH12	2.27	0.47
1:A:144:LEU:HD22	1:F:126:ASP:HB3	1.97	0.47
1:D:180:LEU:HB2	2:D:300:AP5:N6B	2.29	0.47
1:F:47:ALA:HB1	1:F:53:VAL:HG22	1.97	0.47
1:B:17:THR:HG23	1:B:36:MET:HE1	1.97	0.47
1:C:53:VAL:CG1	1:C:62:LEU:HD11	2.45	0.46
1:C:24:ILE:CD1	1:C:36:MET:HB2	2.46	0.46
1:F:67:GLN:HG3	3:F:403:HOH:O	2.15	0.46
1:B:72:LYS:HE2	1:B:76:ARG:HH11	1.80	0.46
1:E:55:ASP:O	3:E:402:HOH:O	2.20	0.45
2:A:300:AP5:O1E	2:A:300:AP5:O2D	2.34	0.45
2:A:300:AP5:O2D	2:A:300:AP5:O2G	2.34	0.45
1:B:126:ASP:OD1	1:E:145:THR:OG1	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ASN:ND2	2:D:300:AP5:N7B	2.60	0.45
1:C:36:MET:HE3	1:C:90:ASP:OD2	2.16	0.45
1:F:7:VAL:HG12	1:F:9:THR:HG23	1.97	0.45
1:B:133:LEU:HD23	1:B:142:ILE:HG22	1.99	0.45
1:A:19:LEU:HD12	1:A:184:VAL:HG22	1.98	0.45
1:A:27:LEU:HD11	1:A:191:LEU:HD12	1.98	0.45
1:B:9:THR:HA	1:B:91:THR:O	2.16	0.45
1:C:67:GLN:O	1:C:70:ILE:N	2.50	0.45
1:C:52:LEU:HD13	1:C:66:THR:CG2	2.47	0.44
1:F:160:MET:O	1:F:164:VAL:HG23	2.16	0.44
1:C:48:LYS:NZ	1:C:54:GLU:HA	2.33	0.44
1:D:177:ASP:HA	2:D:300:AP5:N1B	2.33	0.44
1:A:37:VAL:O	1:A:89:VAL:HA	2.17	0.44
1:D:17:THR:HG23	1:D:36:MET:HE1	2.00	0.44
1:B:159:ALA:HA	1:B:162:TYR:CD2	2.53	0.43
1:F:143:GLU:HG3	1:F:148:ILE:HG13	1.99	0.43
1:C:138:ARG:HD2	2:C:300:AP5:O1G	2.18	0.43
1:F:41:THR:O	1:F:45:GLU:HG3	2.18	0.43
1:F:52:LEU:HD13	1:F:66:THR:HG21	2.00	0.43
1:A:182:LYS:HA	1:A:185:GLU:OE1	2.18	0.43
1:D:9:THR:HA	1:D:91:THR:O	2.18	0.43
1:D:49:GLU:O	1:D:49:GLU:HG2	2.18	0.43
1:A:39:PHE:HB2	1:A:91:THR:HB	2.01	0.42
1:C:6:VAL:O	1:C:88:ILE:HA	2.19	0.42
1:D:120:ILE:HG22	1:D:122:GLU:HG3	1.99	0.42
1:F:135:ASP:HB3	1:F:140:ARG:NH1	2.34	0.42
1:C:53:VAL:HG13	1:C:62:LEU:HD11	2.01	0.42
1:B:21:GLN:HG2	1:B:36:MET:SD	2.60	0.42
1:C:129:LEU:HD12	1:C:129:LEU:O	2.20	0.41
1:F:64:PRO:O	1:F:68:LYS:HE2	2.20	0.41
1:E:38:ASN:HA	1:E:90:ASP:HB2	2.02	0.41
1:C:142:ILE:O	1:C:142:ILE:HG13	2.19	0.41
1:D:162:TYR:HE1	1:E:164:VAL:HG13	1.85	0.41
1:A:91:THR:OG1	1:A:92:HIS:N	2.50	0.41
1:F:110:LEU:HD21	1:F:166:THR:HG23	2.03	0.41
1:D:99:LYS:NZ	1:E:190:VAL:O	2.38	0.41
1:A:7:VAL:HG23	1:A:115:PRO:HB3	2.02	0.41
1:B:35:LYS:O	1:B:87:VAL:HA	2.21	0.41
1:E:60:ARG:NH2	3:E:401:HOH:O	2.43	0.41
1:F:53:VAL:HG21	1:F:59:MET:CG	2.51	0.41
1:E:19:LEU:HD12	1:E:184:VAL:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:VAL:O	1:E:190:VAL:CG1	2.69	0.40
1:D:36:MET:HE3	1:D:90:ASP:OD2	2.21	0.40
1:C:34:TYR:HD2	1:C:88:ILE:HG13	1.85	0.40
1:B:153:PHE:C	1:B:153:PHE:CD1	2.95	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	189/200 (94%)	182 (96%)	7 (4%)	0	100	100
1	B	189/200 (94%)	180 (95%)	8 (4%)	1 (0%)	29	29
1	C	189/200 (94%)	179 (95%)	9 (5%)	1 (0%)	29	29
1	D	189/200 (94%)	181 (96%)	7 (4%)	1 (0%)	29	29
1	E	189/200 (94%)	182 (96%)	7 (4%)	0	100	100
1	F	189/200 (94%)	181 (96%)	8 (4%)	0	100	100
All	All	1134/1200 (94%)	1085 (96%)	46 (4%)	3 (0%)	41	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	ASN
1	C	3	ASN
1	D	3	ASN

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	166/175 (95%)	166 (100%)	0	100	100
1	B	166/175 (95%)	165 (99%)	1 (1%)	86	91
1	C	166/175 (95%)	166 (100%)	0	100	100
1	D	166/175 (95%)	166 (100%)	0	100	100
1	E	166/175 (95%)	166 (100%)	0	100	100
1	F	166/175 (95%)	166 (100%)	0	100	100
All	All	996/1050 (95%)	995 (100%)	1 (0%)	93	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	185	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	3	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
2	AP5	D	300	-	54,62,62	1.39	9 (16%)	61,98,98	1.70	13 (21%)
2	AP5	E	300	-	54,62,62	1.33	6 (11%)	61,98,98	1.58	9 (14%)
2	AP5	A	300	-	54,62,62	1.48	9 (16%)	61,98,98	1.57	8 (13%)
2	AP5	B	300	-	54,62,62	2.13	7 (12%)	61,98,98	2.34	21 (34%)
2	AP5	F	300	-	54,62,62	1.47	8 (14%)	61,98,98	1.76	16 (26%)
2	AP5	C	300	-	54,62,62	1.83	11 (20%)	61,98,98	2.34	22 (36%)

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	AP5	D	300	-	-	9/36/76/76	0/6/6/6
2	AP5	E	300	-	-	13/36/76/76	0/6/6/6
2	AP5	A	300	-	-	20/36/76/76	0/6/6/6
2	AP5	B	300	-	-	10/36/76/76	0/6/6/6
2	AP5	F	300	-	-	9/36/76/76	0/6/6/6
2	AP5	C	300	-	-	8/36/76/76	0/6/6/6

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	AP5	PG-O3B	8.88	1.69	1.59
2	B	300	AP5	O4J-C1J	6.74	1.49	1.40
2	C	300	AP5	PA-O3A	5.62	1.65	1.59
2	B	300	AP5	PG-O3G	5.39	1.65	1.59
2	C	300	AP5	O4J-C1J	5.19	1.47	1.40
2	B	300	AP5	PD-O3G	5.14	1.65	1.59
2	A	300	AP5	PB-O3B	5.01	1.64	1.59
2	F	300	AP5	PG-O3B	4.99	1.64	1.59
2	C	300	AP5	PB-O3A	4.97	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	300	AP5	PD-O3G	4.38	1.64	1.59
2	A	300	AP5	PG-O3B	4.23	1.64	1.59
2	D	300	AP5	PB-O3B	4.17	1.64	1.59
2	A	300	AP5	PA-O3A	4.06	1.63	1.59
2	F	300	AP5	PD-O3D	3.97	1.63	1.59
2	F	300	AP5	PB-O3B	3.86	1.63	1.59
2	D	300	AP5	PD-O3G	3.65	1.63	1.59
2	C	300	AP5	PD-O3D	3.65	1.63	1.59
2	E	300	AP5	PG-O3B	3.62	1.63	1.59
2	D	300	AP5	PG-O3B	3.60	1.63	1.59
2	B	300	AP5	PE-O3D	3.52	1.63	1.59
2	C	300	AP5	C8A-N7A	3.27	1.40	1.34
2	B	300	AP5	C2B-N3B	3.08	1.36	1.32
2	C	300	AP5	C2A-N3A	2.95	1.36	1.32
2	E	300	AP5	PB-O3A	2.94	1.62	1.59
2	C	300	AP5	PG-O3B	2.91	1.62	1.59
2	A	300	AP5	PE-O3D	2.83	1.62	1.59
2	F	300	AP5	PA-O3A	2.79	1.62	1.59
2	D	300	AP5	PB-O3A	2.74	1.62	1.59
2	E	300	AP5	PG-O3G	2.66	1.62	1.59
2	F	300	AP5	PE-O3D	2.58	1.62	1.59
2	A	300	AP5	O4J-C1J	2.57	1.44	1.40
2	D	300	AP5	PA-O3A	2.52	1.62	1.59
2	C	300	AP5	PE-O3D	2.47	1.62	1.59
2	F	300	AP5	O4J-C1J	2.45	1.44	1.40
2	F	300	AP5	O4F-C1F	2.42	1.44	1.40
2	A	300	AP5	PD-O3G	2.37	1.62	1.59
2	D	300	AP5	O4J-C1J	2.28	1.43	1.40
2	F	300	AP5	PB-O3A	2.23	1.61	1.59
2	A	300	AP5	PG-O3G	2.23	1.61	1.59
2	C	300	AP5	C2B-N3B	2.23	1.35	1.32
2	A	300	AP5	O4F-C1F	2.21	1.43	1.40
2	E	300	AP5	PE-O3D	2.20	1.61	1.59
2	A	300	AP5	C2A-N3A	2.17	1.35	1.32
2	D	300	AP5	PE-O3D	2.14	1.61	1.59
2	C	300	AP5	C6A-C5A	2.14	1.51	1.43
2	E	300	AP5	O4F-C1F	2.13	1.43	1.40
2	D	300	AP5	C2A-N3A	2.08	1.35	1.32
2	B	300	AP5	PB-O3B	2.07	1.61	1.59
2	C	300	AP5	PB-O3B	2.05	1.61	1.59
2	D	300	AP5	PG-O3G	2.05	1.61	1.59

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	AP5	O2A-PA-O3A	-6.75	89.02	107.27
2	B	300	AP5	O2D-PD-O3D	6.29	124.28	107.27
2	B	300	AP5	O3G-PD-O1D	-6.18	92.12	110.70
2	C	300	AP5	O3A-PA-O1A	-5.89	92.98	110.70
2	C	300	AP5	O4F-C1F-N9A	5.59	116.16	108.75
2	C	300	AP5	O2D-PD-O3D	5.45	121.99	107.27
2	C	300	AP5	O3B-PB-O1B	-5.41	94.43	110.70
2	D	300	AP5	N3B-C2B-N1B	-4.92	121.99	128.67
2	A	300	AP5	C1J-N9B-C4B	-4.60	118.55	126.64
2	C	300	AP5	C1F-N9A-C4A	-4.57	118.61	126.64
2	E	300	AP5	N3A-C2A-N1A	-4.52	122.53	128.67
2	F	300	AP5	N3B-C2B-N1B	-4.51	122.55	128.67
2	C	300	AP5	C4A-C5A-N7A	-4.49	104.60	109.34
2	F	300	AP5	O2D-PD-O3G	4.34	119.02	107.27
2	F	300	AP5	N3A-C2A-N1A	-4.28	122.86	128.67
2	B	300	AP5	O4J-C1J-N9B	-4.22	103.14	108.75
2	A	300	AP5	N3B-C2B-N1B	-4.22	122.94	128.67
2	B	300	AP5	N3B-C2B-N1B	-4.20	122.97	128.67
2	D	300	AP5	C1J-N9B-C4B	-4.03	119.57	126.64
2	B	300	AP5	C2J-C3J-C4J	4.01	110.35	102.61
2	B	300	AP5	N3A-C2A-N1A	-3.99	123.26	128.67
2	E	300	AP5	N3B-C2B-N1B	-3.97	123.29	128.67
2	B	300	AP5	C4J-O4J-C1J	3.95	113.55	109.92
2	A	300	AP5	O4J-C1J-N9B	3.89	113.91	108.75
2	C	300	AP5	C5A-C6A-N6A	3.89	126.24	120.31
2	E	300	AP5	O4J-C1J-N9B	-3.88	103.60	108.75
2	D	300	AP5	N3A-C2A-N1A	-3.73	123.61	128.67
2	D	300	AP5	O2D-PD-O3G	3.72	117.33	107.27
2	A	300	AP5	C4B-C5B-N7B	-3.56	105.57	109.34
2	C	300	AP5	O2E-PE-O1E	3.49	128.69	112.44
2	D	300	AP5	O2B-PB-O3B	3.48	116.68	107.27
2	F	300	AP5	O2B-PB-O3B	3.47	116.64	107.27
2	C	300	AP5	O2A-PA-O1A	3.42	128.37	112.44
2	E	300	AP5	C4J-O4J-C1J	-3.42	106.80	109.92
2	A	300	AP5	N3A-C2A-N1A	-3.41	124.05	128.67
2	C	300	AP5	O3G-PD-O1D	-3.28	100.84	110.70
2	E	300	AP5	O2D-PD-O3G	3.28	116.13	107.27
2	C	300	AP5	C2J-C3J-C4J	3.22	108.84	102.61
2	B	300	AP5	O2G-PG-O3B	3.17	115.84	107.27
2	B	300	AP5	C5B-C6B-N6B	-3.17	115.48	120.31
2	C	300	AP5	O2G-PG-O3G	3.16	115.81	107.27
2	F	300	AP5	C1F-N9A-C4A	-3.13	121.14	126.64
2	D	300	AP5	O3G-PD-O1D	-3.08	101.44	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	AP5	C5F-C4F-C3F	-3.02	104.33	115.21
2	C	300	AP5	N3A-C2A-N1A	-2.97	124.64	128.67
2	C	300	AP5	O2B-PB-O3B	2.96	115.28	107.27
2	E	300	AP5	C1F-N9A-C4A	-2.96	121.44	126.64
2	C	300	AP5	C4F-O4F-C1F	2.84	112.53	109.92
2	F	300	AP5	O3G-PG-O1G	-2.80	102.29	110.70
2	D	300	AP5	O4J-C1J-N9B	2.77	112.42	108.75
2	B	300	AP5	O2F-C2F-C3F	-2.74	103.02	111.82
2	B	300	AP5	O5J-C5J-C4J	-2.72	99.74	108.99
2	F	300	AP5	O3D-PD-O1D	-2.70	102.58	110.70
2	F	300	AP5	O2E-PE-O1E	2.67	124.88	112.44
2	B	300	AP5	O2B-PB-O1B	2.65	124.78	112.44
2	D	300	AP5	O2E-PE-O1E	2.65	124.76	112.44
2	C	300	AP5	O2B-PB-O1B	2.60	124.54	112.44
2	A	300	AP5	C4A-C5A-N7A	-2.50	106.70	109.34
2	D	300	AP5	O4F-C4F-C3F	2.49	110.10	105.15
2	A	300	AP5	O3A-PB-O1B	-2.48	103.25	110.70
2	F	300	AP5	C4A-C5A-N7A	-2.44	106.76	109.34
2	B	300	AP5	O2A-PA-O1A	2.42	123.72	112.44
2	C	300	AP5	O2G-PG-O3B	-2.41	100.75	107.27
2	B	300	AP5	O4J-C4J-C3J	-2.40	100.39	105.15
2	B	300	AP5	O4F-C4F-C5F	2.38	116.95	109.33
2	B	300	AP5	O5J-PE-O1E	-2.38	99.52	108.94
2	C	300	AP5	C4B-C5B-N7B	-2.34	106.86	109.34
2	B	300	AP5	O3G-PG-O1G	2.33	117.71	110.70
2	A	300	AP5	C5B-C6B-N6B	2.32	123.85	120.31
2	F	300	AP5	O2A-PA-O3A	-2.32	101.01	107.27
2	F	300	AP5	C4B-C5B-N7B	-2.29	106.92	109.34
2	E	300	AP5	C1J-N9B-C4B	-2.22	122.74	126.64
2	D	300	AP5	O4F-C1F-N9A	-2.19	105.84	108.75
2	D	300	AP5	O5F-PA-O1A	-2.19	100.25	108.94
2	F	300	AP5	O2D-PD-O3D	2.18	113.17	107.27
2	B	300	AP5	N6B-C6B-N1B	2.18	122.99	118.33
2	F	300	AP5	O4F-C4F-C5F	2.13	116.15	109.33
2	C	300	AP5	O3B-PG-O1G	2.11	117.05	110.70
2	C	300	AP5	C1J-N9B-C4B	-2.08	122.98	126.64
2	D	300	AP5	O2D-PD-O3D	2.07	112.87	107.27
2	C	300	AP5	N3B-C2B-N1B	-2.07	125.87	128.67
2	F	300	AP5	O4F-C4F-C3F	2.06	109.25	105.15
2	D	300	AP5	C5F-C4F-C3F	-2.05	107.82	115.21
2	F	300	AP5	C5F-C4F-C3F	-2.05	107.82	115.21
2	B	300	AP5	O3J-C3J-C4J	-2.05	105.20	111.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	300	AP5	O2B-PB-O1B	2.05	121.96	112.44
2	F	300	AP5	O4J-C4J-C3J	2.04	109.20	105.15
2	E	300	AP5	N6B-C6B-N1B	2.02	122.64	118.33
2	C	300	AP5	C5B-C6B-N6B	-2.00	117.26	120.31

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	AP5	C5F-O5F-PA-O1A
2	A	300	AP5	C5F-O5F-PA-O3A
2	A	300	AP5	C5J-O5J-PE-O3D
2	A	300	AP5	C5J-O5J-PE-O1E
2	A	300	AP5	C5J-O5J-PE-O2E
2	A	300	AP5	O4F-C4F-C5F-O5F
2	A	300	AP5	C3F-C4F-C5F-O5F
2	B	300	AP5	C5F-O5F-PA-O3A
2	B	300	AP5	O4F-C4F-C5F-O5F
2	B	300	AP5	C3F-C4F-C5F-O5F
2	D	300	AP5	C5J-O5J-PE-O2E
2	E	300	AP5	C5F-O5F-PA-O1A
2	E	300	AP5	C5F-O5F-PA-O3A
2	E	300	AP5	C5J-O5J-PE-O3D
2	E	300	AP5	C5J-O5J-PE-O1E
2	E	300	AP5	C5J-O5J-PE-O2E
2	E	300	AP5	O4F-C4F-C5F-O5F
2	E	300	AP5	C3F-C4F-C5F-O5F
2	F	300	AP5	C5J-O5J-PE-O3D
2	F	300	AP5	C5J-O5J-PE-O1E
2	F	300	AP5	C5J-O5J-PE-O2E
2	F	300	AP5	O4F-C4F-C5F-O5F
2	F	300	AP5	C3F-C4F-C5F-O5F
2	A	300	AP5	O4J-C4J-C5J-O5J
2	A	300	AP5	C3J-C4J-C5J-O5J
2	D	300	AP5	O4J-C4J-C5J-O5J
2	D	300	AP5	C3J-C4J-C5J-O5J
2	F	300	AP5	O4J-C4J-C5J-O5J
2	F	300	AP5	C3J-C4J-C5J-O5J
2	B	300	AP5	PB-O3A-PA-O5F
2	D	300	AP5	PB-O3A-PA-O5F
2	F	300	AP5	PB-O3A-PA-O5F
2	C	300	AP5	O4F-C4F-C5F-O5F

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	300	AP5	PB-O3A-PA-O1A
2	A	300	AP5	PA-O3A-PB-O1B
2	A	300	AP5	PG-O3B-PB-O2B
2	A	300	AP5	PE-O3D-PD-O2D
2	C	300	AP5	PD-O3G-PG-O2G
2	D	300	AP5	PD-O3G-PG-O1G
2	E	300	AP5	PD-O3G-PG-O2G
2	A	300	AP5	C5F-O5F-PA-O2A
2	B	300	AP5	C5F-O5F-PA-O1A
2	B	300	AP5	C5F-O5F-PA-O2A
2	B	300	AP5	C5J-O5J-PE-O3D
2	B	300	AP5	C5J-O5J-PE-O1E
2	B	300	AP5	C5J-O5J-PE-O2E
2	C	300	AP5	C5F-O5F-PA-O3A
2	C	300	AP5	C5J-O5J-PE-O1E
2	D	300	AP5	C5J-O5J-PE-O3D
2	D	300	AP5	C5J-O5J-PE-O1E
2	A	300	AP5	PA-O3A-PB-O2B
2	A	300	AP5	PG-O3B-PB-O1B
2	A	300	AP5	PD-O3G-PG-O2G
2	D	300	AP5	PD-O3G-PG-O2G
2	D	300	AP5	PG-O3G-PD-O2D
2	A	300	AP5	PD-O3G-PG-O1G
2	A	300	AP5	PE-O3D-PD-O1D
2	C	300	AP5	PD-O3G-PG-O1G
2	E	300	AP5	PB-O3A-PA-O5F
2	E	300	AP5	PD-O3D-PE-O5J
2	C	300	AP5	C3F-C4F-C5F-O5F
2	A	300	AP5	PB-O3A-PA-O2A
2	C	300	AP5	PA-O3A-PB-O1B
2	E	300	AP5	PD-O3G-PG-O1G
2	B	300	AP5	PB-O3A-PA-O2A
2	C	300	AP5	PA-O3A-PB-O2B
2	E	300	AP5	PE-O3D-PD-O1D
2	E	300	AP5	PE-O3D-PD-O2D
2	F	300	AP5	PB-O3A-PA-O2A

There are no ring outliers.

4 monomers are involved in 12 short contacts:

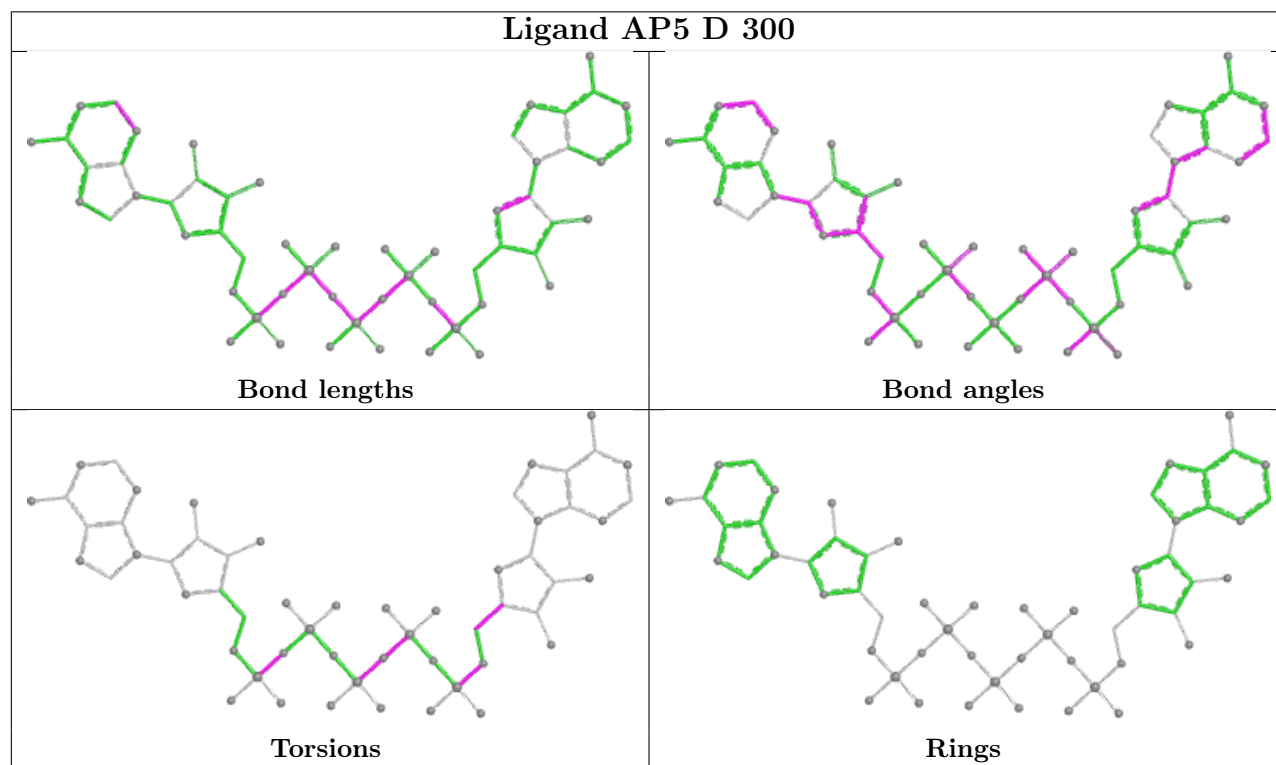
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	300	AP5	4	0

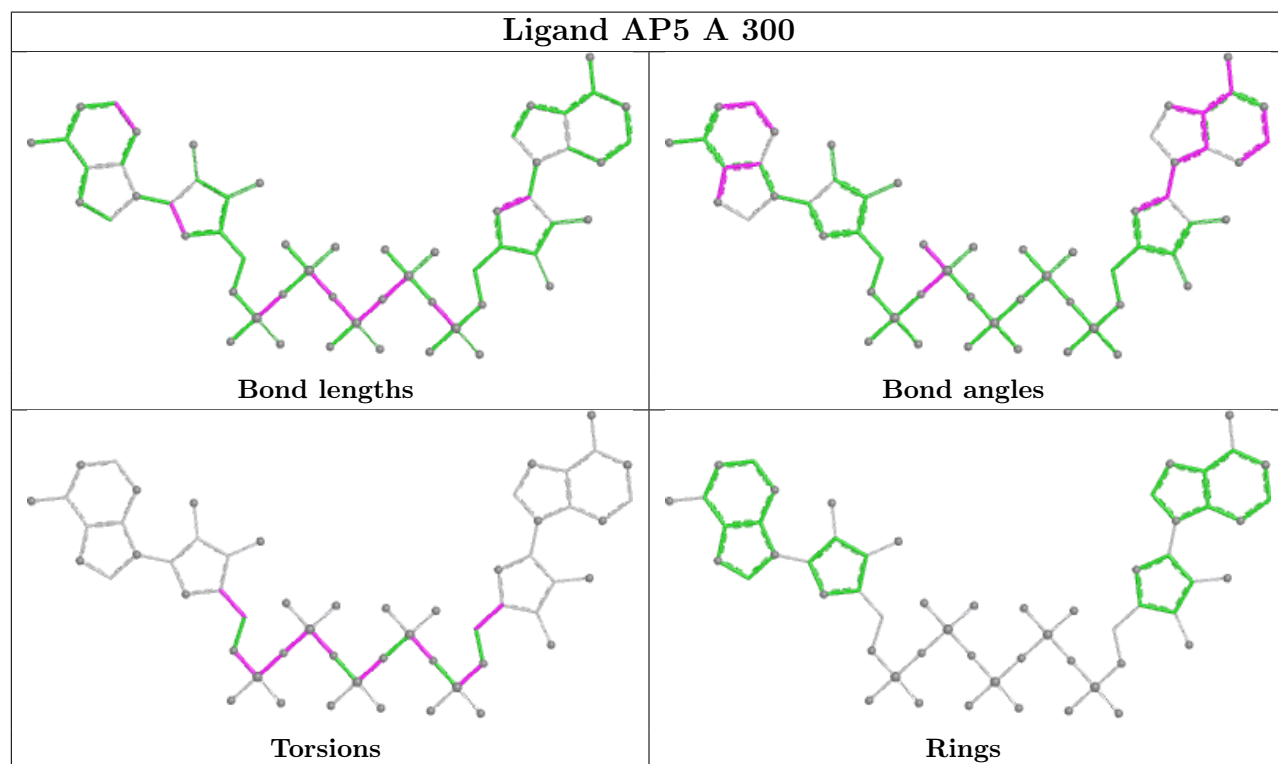
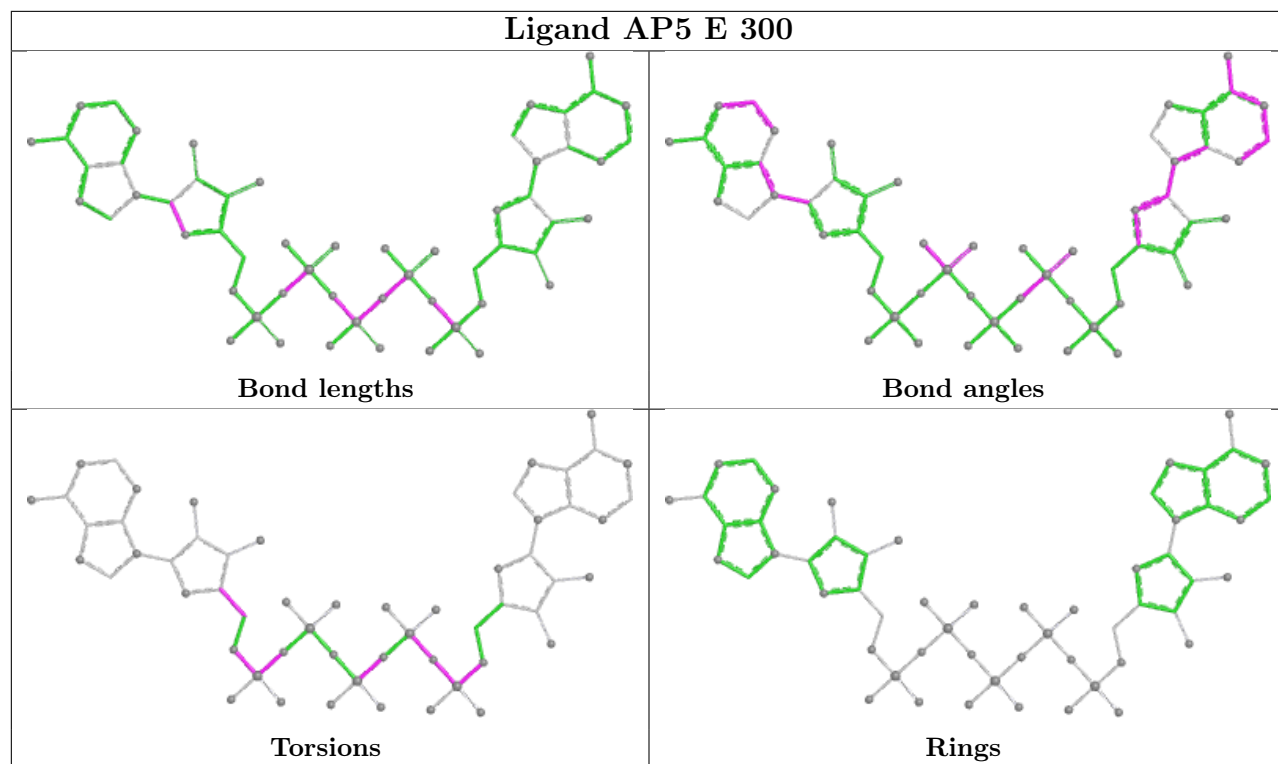
Continued on next page...

Continued from previous page...

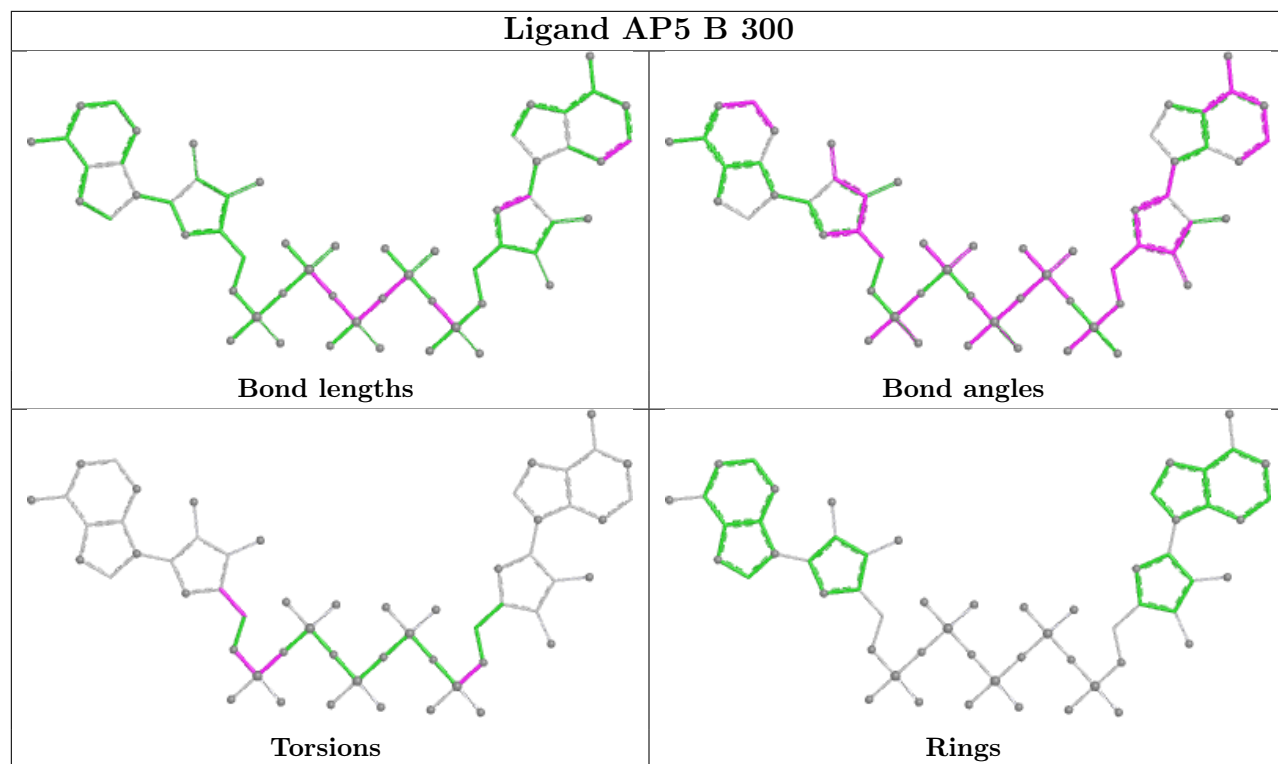
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	AP5	3	0
2	B	300	AP5	1	0
2	C	300	AP5	4	0

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.

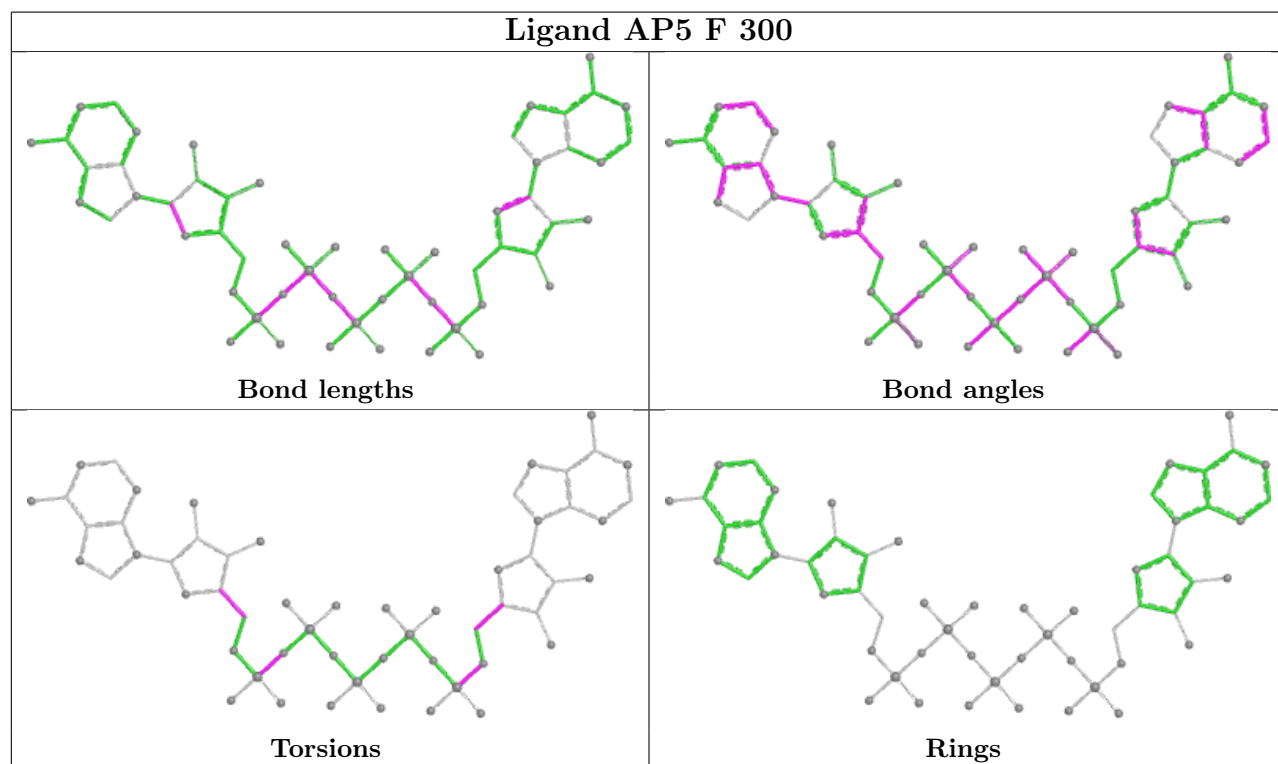


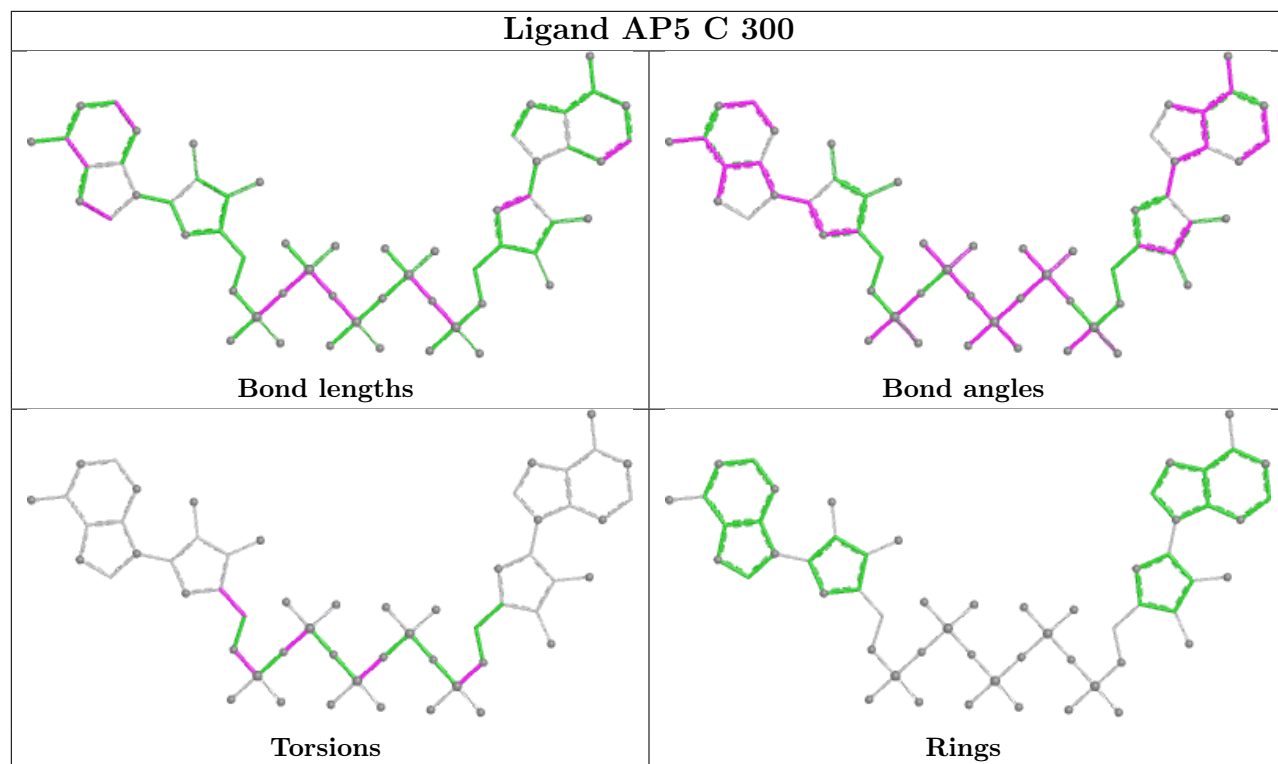


Ligand AP5 B 300



Ligand AP5 F 300





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, 95th 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 ²)	Q<0.9
1	A	191/200 (95%)	1.50	60 (31%) 0 0	48, 78, 111, 126	0
1	B	191/200 (95%)	1.12	41 (21%) 0 0	45, 58, 76, 94	0
1	C	191/200 (95%)	1.77	68 (35%) 0 0	46, 69, 112, 147	0
1	D	191/200 (95%)	1.50	60 (31%) 0 0	60, 86, 114, 124	0
1	E	191/200 (95%)	1.78	75 (39%) 0 0	58, 81, 109, 123	0
1	F	191/200 (95%)	2.20	88 (46%) 0 0	63, 90, 130, 162	0
All	All	1146/1200 (95%)	1.64	392 (34%) 0 0	45, 78, 116, 162	0

All (392) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	52	LEU	10.9
1	E	2	LYS	9.9
1	F	64	PRO	9.7
1	C	64	PRO	9.6
1	F	51	GLY	8.4
1	F	57	ASP	8.2
1	C	47	ALA	7.9
1	F	48	LYS	7.5
1	F	54	GLU	7.4
1	F	47	ALA	7.4
1	F	159	ALA	7.0
1	F	55	ASP	6.7
1	F	157	CYS	6.6
1	A	94	THR	6.4
1	D	2	LYS	6.3
1	D	52	LEU	6.3
1	C	62	LEU	6.2
1	F	44	PHE	6.0
1	F	56	ARG	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	61	LYS	5.9
1	E	159	ALA	5.8
1	D	157	CYS	5.7
1	E	161	ALA	5.6
1	F	58	GLN	5.5
1	C	54	GLU	5.5
1	E	157	CYS	5.5
1	F	140	ARG	5.4
1	D	158	ALA	5.3
1	A	103	ALA	5.2
1	F	59	MET	5.2
1	A	95	VAL	5.1
1	B	159	ALA	5.1
1	F	136	ALA	5.1
1	A	2	LYS	5.0
1	F	50	GLU	5.0
1	A	93	SER	4.9
1	F	141	ASP	4.9
1	D	159	ALA	4.9
1	A	157	CYS	4.9
1	E	51	GLY	4.8
1	C	61	LYS	4.8
1	F	52	LEU	4.8
1	F	53	VAL	4.8
1	C	157	CYS	4.8
1	D	161	ALA	4.8
1	C	48	LYS	4.8
1	F	46	VAL	4.8
1	B	160	MET	4.7
1	E	138	ARG	4.7
1	D	85	SER	4.7
1	E	160	MET	4.7
1	F	60	ARG	4.7
1	D	32	ILE	4.6
1	F	103	ALA	4.6
1	F	160	MET	4.6
1	B	118	ILE	4.6
1	C	158	ALA	4.6
1	D	48	LYS	4.6
1	C	63	ASP	4.6
1	B	52	LEU	4.6
1	F	158	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	10	GLY	4.5
1	F	78	ILE	4.5
1	F	161	ALA	4.5
1	A	154	MET	4.4
1	E	162	TYR	4.4
1	F	8	VAL	4.4
1	D	162	TYR	4.4
1	F	92	HIS	4.4
1	F	142	ILE	4.4
1	C	53	VAL	4.3
1	F	93	SER	4.3
1	A	101	TYR	4.3
1	B	119	VAL	4.3
1	C	32	ILE	4.3
1	D	103	ALA	4.3
1	E	158	ALA	4.3
1	A	83	LYS	4.3
1	A	54	GLU	4.3
1	F	5	VAL	4.2
1	C	2	LYS	4.2
1	E	94	THR	4.2
1	E	70	ILE	4.2
1	A	155	ASN	4.2
1	F	155	ASN	4.2
1	E	93	SER	4.2
1	B	158	ALA	4.2
1	C	10	GLY	4.1
1	A	52	LEU	4.1
1	A	158	ALA	4.1
1	C	92	HIS	4.1
1	D	93	SER	4.1
1	C	93	SER	4.1
1	B	157	CYS	4.0
1	F	138	ARG	4.0
1	E	52	LEU	4.0
1	A	161	ALA	4.0
1	E	54	GLU	4.0
1	C	57	ASP	4.0
1	F	9	THR	4.0
1	E	164	VAL	4.0
1	C	59	MET	4.0
1	F	119	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	155	ASN	3.9
1	D	47	ALA	3.9
1	C	31	GLY	3.9
1	E	103	ALA	3.9
1	F	102	LEU	3.9
1	A	162	TYR	3.9
1	F	94	THR	3.9
1	B	170	VAL	3.9
1	E	154	MET	3.9
1	E	3	ASN	3.8
1	A	92	HIS	3.8
1	C	94	THR	3.8
1	D	160	MET	3.8
1	F	99	LYS	3.8
1	E	118	ILE	3.8
1	E	185	GLU	3.8
1	C	51	GLY	3.7
1	C	162	TYR	3.7
1	D	138	ARG	3.7
1	F	91	THR	3.7
1	F	62	LEU	3.7
1	B	164	VAL	3.7
1	F	162	TYR	3.7
1	F	120	ILE	3.7
1	A	102	LEU	3.7
1	E	101	TYR	3.7
1	C	170	VAL	3.7
1	E	119	VAL	3.7
1	B	162	TYR	3.6
1	F	10	GLY	3.6
1	C	161	ALA	3.6
1	D	70	ILE	3.6
1	C	142	ILE	3.6
1	E	142	ILE	3.6
1	A	32	ILE	3.6
1	E	163	GLY	3.6
1	F	95	VAL	3.6
1	A	138	ARG	3.6
1	C	159	ALA	3.5
1	C	103	ALA	3.5
1	E	133	LEU	3.5
1	E	9	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	102	LEU	3.5
1	B	168	ALA	3.5
1	B	93	SER	3.5
1	C	7	VAL	3.4
1	C	67	GLN	3.4
1	C	102	LEU	3.4
1	C	30	GLU	3.4
1	A	28	LYS	3.4
1	F	70	ILE	3.4
1	B	154	MET	3.4
1	E	170	VAL	3.4
1	F	170	VAL	3.4
1	D	155	ASN	3.4
1	E	8	VAL	3.3
1	F	163	GLY	3.3
1	B	161	ALA	3.3
1	B	7	VAL	3.3
1	E	48	LYS	3.3
1	E	23	THR	3.3
1	A	159	ALA	3.3
1	C	118	ILE	3.3
1	D	46	VAL	3.3
1	E	4	LYS	3.3
1	D	3	ASN	3.3
1	C	91	THR	3.3
1	D	84	GLU	3.3
1	C	68	LYS	3.3
1	E	11	VAL	3.3
1	B	169	THR	3.3
1	E	102	LEU	3.2
1	B	117	ILE	3.2
1	F	7	VAL	3.2
1	F	135	ASP	3.2
1	E	83	LYS	3.2
1	C	11	VAL	3.2
1	E	69	ARG	3.2
1	D	92	HIS	3.1
1	C	95	VAL	3.1
1	C	58	GLN	3.1
1	D	104	GLY	3.1
1	A	55	ASP	3.1
1	F	63	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	153	PHE	3.1
1	F	137	THR	3.1
1	B	138	ARG	3.1
1	A	5	VAL	3.0
1	E	95	VAL	3.0
1	F	104	GLY	3.0
1	E	92	HIS	3.0
1	A	100	GLY	3.0
1	E	35	LYS	3.0
1	C	33	GLU	3.0
1	A	91	THR	3.0
1	A	160	MET	3.0
1	A	48	LYS	3.0
1	C	44	PHE	3.0
1	B	95	VAL	3.0
1	A	130	MET	3.0
1	F	66	THR	3.0
1	F	169	THR	3.0
1	C	104	GLY	2.9
1	A	73	LEU	2.9
1	D	137	THR	2.9
1	E	47	ALA	2.9
1	E	100	GLY	2.9
1	B	172	ILE	2.9
1	F	32	ILE	2.9
1	C	49	GLU	2.9
1	F	133	LEU	2.9
1	C	119	VAL	2.9
1	B	139	ASN	2.9
1	D	101	TYR	2.9
1	D	49	GLU	2.9
1	C	9	THR	2.9
1	D	9	THR	2.9
1	D	154	MET	2.9
1	D	188	ILE	2.8
1	F	118	ILE	2.8
1	A	53	VAL	2.8
1	F	65	ASP	2.8
1	A	51	GLY	2.8
1	B	120	ILE	2.8
1	A	7	VAL	2.8
1	F	121	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	179	LEU	2.8
1	E	91	THR	2.8
1	D	95	VAL	2.8
1	F	154	MET	2.8
1	B	9	THR	2.8
1	E	153	PHE	2.8
1	B	47	ALA	2.8
1	B	155	ASN	2.8
1	B	8	VAL	2.7
1	B	163	GLY	2.7
1	E	85	SER	2.7
1	E	105	LEU	2.7
1	F	113	LEU	2.7
1	D	170	VAL	2.7
1	E	129	LEU	2.7
1	F	139	ASN	2.7
1	A	89	VAL	2.7
1	E	148	ILE	2.7
1	C	60	ARG	2.7
1	D	87	VAL	2.7
1	D	179	LEU	2.7
1	E	73	LEU	2.7
1	E	84	GLU	2.7
1	C	164	VAL	2.7
1	F	89	VAL	2.7
1	C	160	MET	2.7
1	E	76	ARG	2.7
1	C	55	ASP	2.7
1	B	101	TYR	2.7
1	C	155	ASN	2.6
1	F	49	GLU	2.6
1	A	137	THR	2.6
1	B	102	LEU	2.6
1	D	51	GLY	2.6
1	D	54	GLU	2.6
1	A	27	LEU	2.6
1	B	99	LYS	2.6
1	D	8	VAL	2.6
1	F	14	VAL	2.6
1	C	70	ILE	2.6
1	D	118	ILE	2.6
1	E	55	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	73	LEU	2.6
1	E	7	VAL	2.6
1	D	136	ALA	2.6
1	F	173	ILE	2.6
1	D	31	GLY	2.6
1	F	172	ILE	2.6
1	A	44	PHE	2.6
1	F	101	TYR	2.6
1	A	139	ASN	2.6
1	D	106	PRO	2.5
1	A	8	VAL	2.5
1	B	2	LYS	2.5
1	F	156	ARG	2.5
1	B	94	THR	2.5
1	E	120	ILE	2.5
1	C	90	ASP	2.5
1	C	105	LEU	2.5
1	D	5	VAL	2.5
1	E	88	ILE	2.5
1	F	77	LYS	2.5
1	D	105	LEU	2.5
1	E	61	LYS	2.5
1	E	58	GLN	2.5
1	A	170	VAL	2.4
1	C	101	TYR	2.4
1	E	33	GLU	2.4
1	A	47	ALA	2.4
1	A	6	VAL	2.4
1	C	8	VAL	2.4
1	E	80	GLU	2.4
1	B	48	LYS	2.4
1	F	2	LYS	2.4
1	A	11	VAL	2.4
1	C	26	LYS	2.4
1	D	97	THR	2.4
1	C	120	ILE	2.4
1	C	188	ILE	2.4
1	D	117	ILE	2.4
1	C	69	ARG	2.4
1	D	156	ARG	2.4
1	E	104	GLY	2.4
1	F	188	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	76	ARG	2.4
1	A	112	GLU	2.4
1	F	164	VAL	2.4
1	A	3	ASN	2.4
1	A	77	LYS	2.3
1	A	106	PRO	2.3
1	D	37	VAL	2.3
1	C	117	ILE	2.3
1	E	188	ILE	2.3
1	C	169	THR	2.3
1	D	94	THR	2.3
1	D	83	LYS	2.3
1	E	31	GLY	2.3
1	B	156	ARG	2.3
1	F	69	ARG	2.3
1	C	29	GLU	2.3
1	E	17	THR	2.3
1	F	179	LEU	2.3
1	B	100	GLY	2.3
1	D	176	ARG	2.3
1	D	113	LEU	2.3
1	F	73	LEU	2.3
1	A	178	GLY	2.3
1	C	176	ARG	2.3
1	E	39	PHE	2.3
1	E	99	LYS	2.3
1	E	172	ILE	2.3
1	C	179	LEU	2.2
1	A	10	GLY	2.2
1	E	32	ILE	2.2
1	A	151	HIS	2.2
1	D	53	VAL	2.2
1	E	156	ARG	2.2
1	A	188	ILE	2.2
1	E	173	ILE	2.2
1	C	89	VAL	2.2
1	D	164	VAL	2.2
1	D	44	PHE	2.2
1	A	88	ILE	2.2
1	E	37	VAL	2.2
1	E	89	VAL	2.2
1	E	169	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	79	ALA	2.2
1	E	121	VAL	2.2
1	F	31	GLY	2.2
1	F	87	VAL	2.2
1	B	103	ALA	2.2
1	D	61	LYS	2.2
1	F	168	ALA	2.2
1	F	117	ILE	2.2
1	B	133	LEU	2.1
1	F	34	TYR	2.1
1	C	172	ILE	2.1
1	C	73	LEU	2.1
1	A	119	VAL	2.1
1	C	137	THR	2.1
1	C	168	ALA	2.1
1	D	119	VAL	2.1
1	F	153	PHE	2.1
1	B	70	ILE	2.1
1	C	39	PHE	2.1
1	D	140	ARG	2.1
1	A	58	GLN	2.1
1	A	136	ALA	2.1
1	A	120	ILE	2.1
1	F	88	ILE	2.1
1	D	100	GLY	2.1
1	B	44	PHE	2.1
1	A	148	ILE	2.0
1	B	171	LYS	2.0
1	B	135	ASP	2.0
1	E	90	ASP	2.0
1	F	83	LYS	2.0
1	A	70	ILE	2.0
1	D	172	ILE	2.0
1	E	168	ALA	2.0
1	D	88	ILE	2.0
1	F	165	LEU	2.0
1	A	104	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

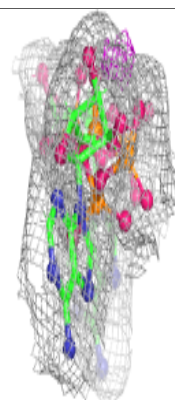
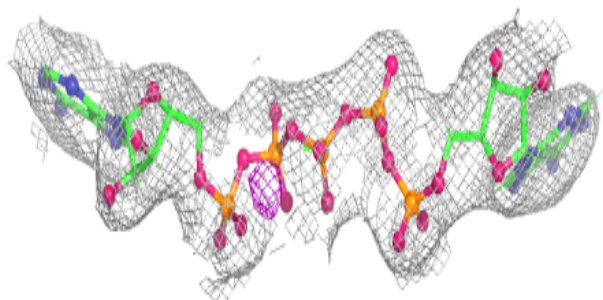
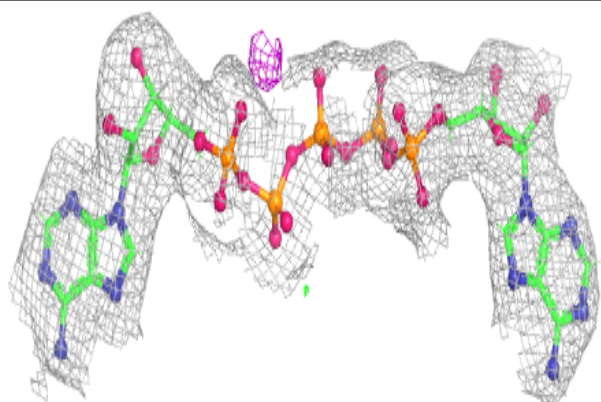
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AP5	D	300	57/57	0.91	0.16	62,84,89,92	0
2	AP5	E	300	57/57	0.91	0.22	62,78,83,87	0
2	AP5	F	300	57/57	0.91	0.16	62,88,100,103	0
2	AP5	B	300	57/57	0.94	0.15	46,51,62,62	0
2	AP5	A	300	57/57	0.94	0.16	62,72,81,88	0
2	AP5	C	300	57/57	0.95	0.22	56,62,71,73	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.

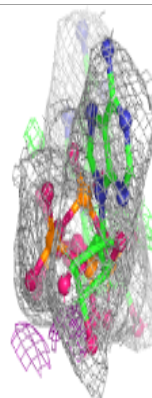
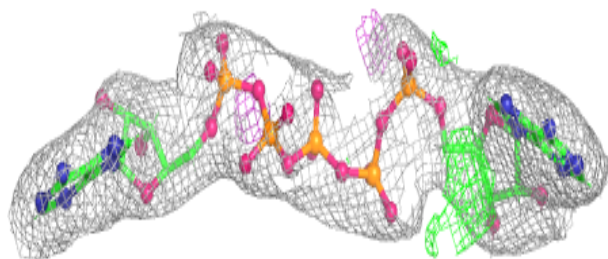
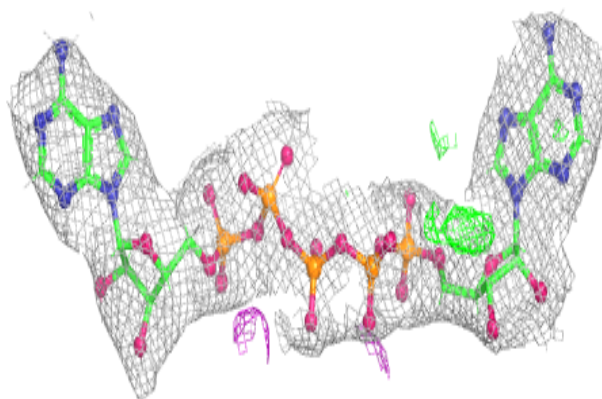
Electron density around AP5 D 300:

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

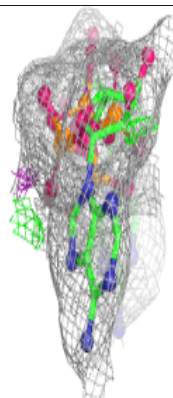
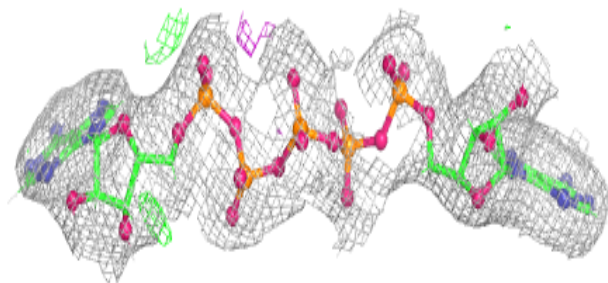
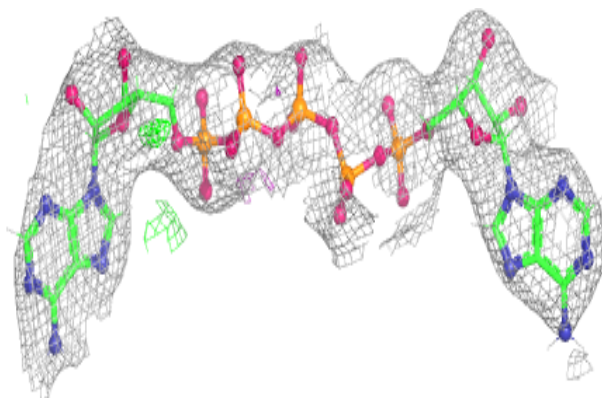


Electron density around AP5 E 300:

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

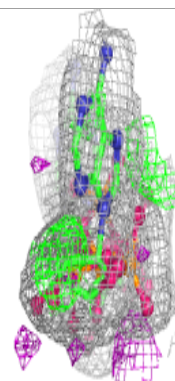
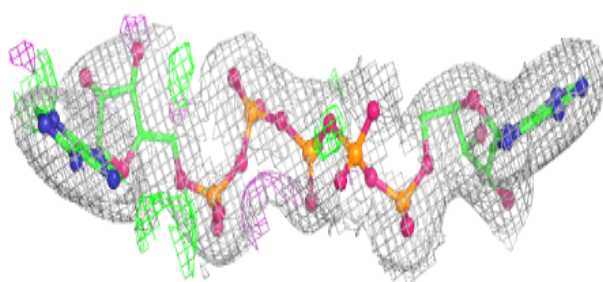
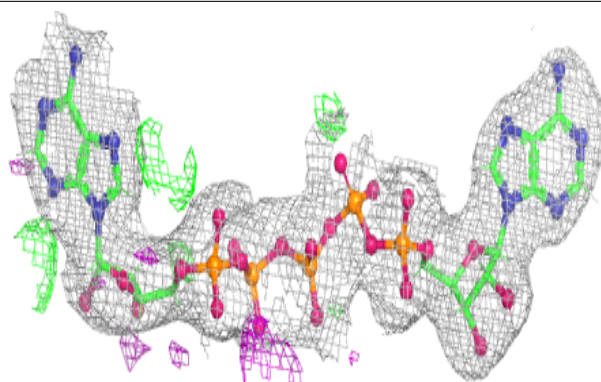
**Electron density around AP5 F 300:**

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

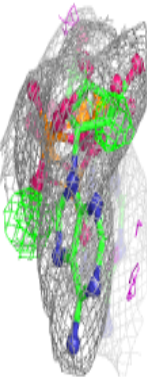
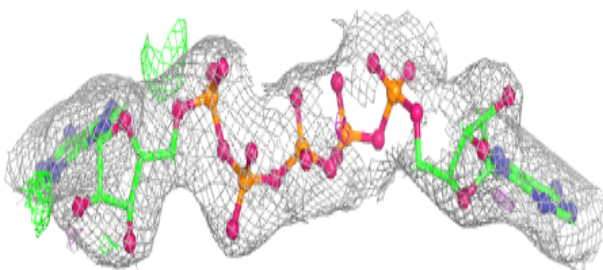
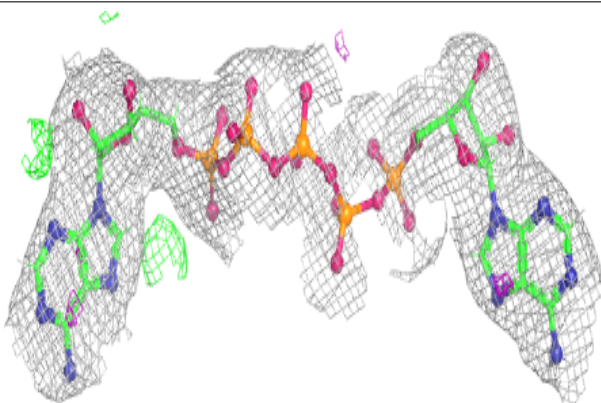


Electron density around AP5 B 300:

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

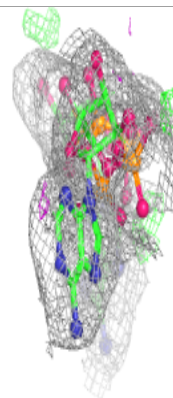
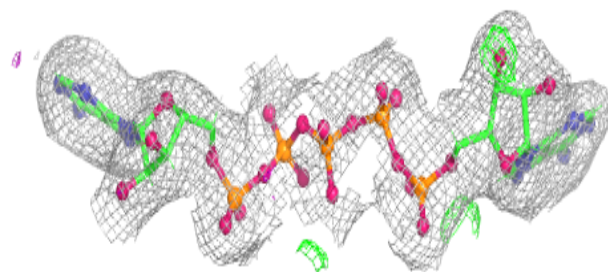
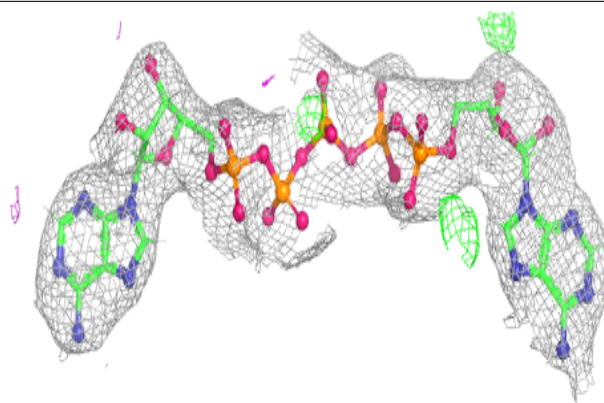
**Electron density around AP5 A 300:**

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



Electron density around AP5 C 300:

$2mF_o-DF_c$ (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.