



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:47 pm BST

PDB ID : 3SEQ
Title : Crystal structure of C176A mutant of glutamine-dependent NAD⁺ synthetase from *M. tuberculosis* in complex with AMPCPP and NaAD⁺
Authors : Chuenchor, W.; Gerratana, B.
Deposited on : 2011-06-10
Resolution : 2.73 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 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 : 2.11
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) : 2.11

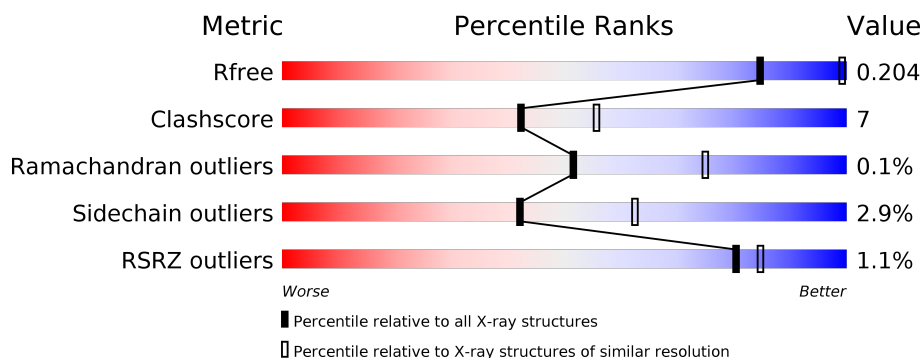
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 on 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	680	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 83%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>83% 13% . .</div>
1	B	680	<div> <div style="width: 83%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>83% 13% . .</div>
1	C	680	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 80%; background-color: green;"></div> <div style="width: 15%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>80% 15% . .</div>
1	D	680	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 81%; background-color: green;"></div> <div style="width: 14%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>81% 14% . .</div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20820 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.

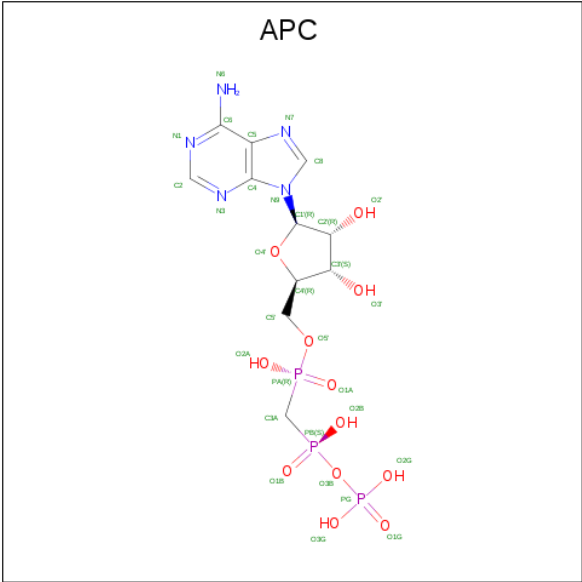
- Molecule 1 is a protein called Glutamine-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5102	3234	905	948	15			
1	B	658	Total	C	N	O	S	0	0	0
			5063	3215	894	939	15			
1	C	650	Total	C	N	O	S	0	0	0
			4992	3171	885	921	15			
1	D	650	Total	C	N	O	S	0	0	0
			5002	3174	887	926	15			

There are 8 discrepancies between the modelled and reference sequences:

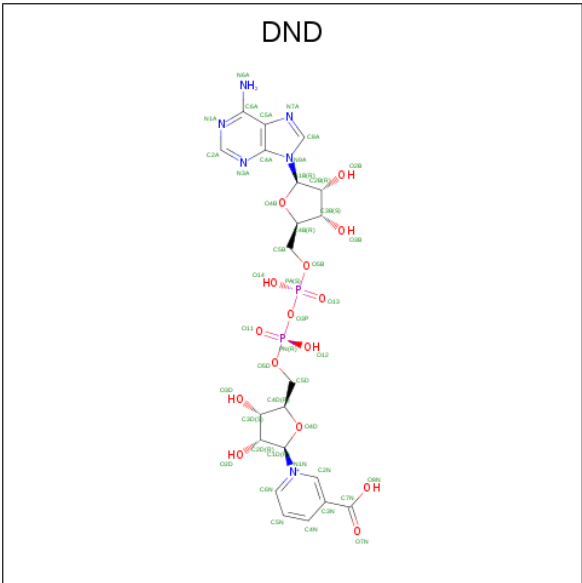
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P0A5L6
A	176	ALA	CYS	engineered mutation	UNP P0A5L6
B	0	SER	-	expression tag	UNP P0A5L6
B	176	ALA	CYS	engineered mutation	UNP P0A5L6
C	0	SER	-	expression tag	UNP P0A5L6
C	176	ALA	CYS	engineered mutation	UNP P0A5L6
D	0	SER	-	expression tag	UNP P0A5L6
D	176	ALA	CYS	engineered mutation	UNP P0A5L6

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

- Molecule 3 is NICOTINIC ACID ADENINE DINUCLEOTIDE (three-letter code: DND) (formula: C₂₁H₂₇N₆O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	6	15	2		

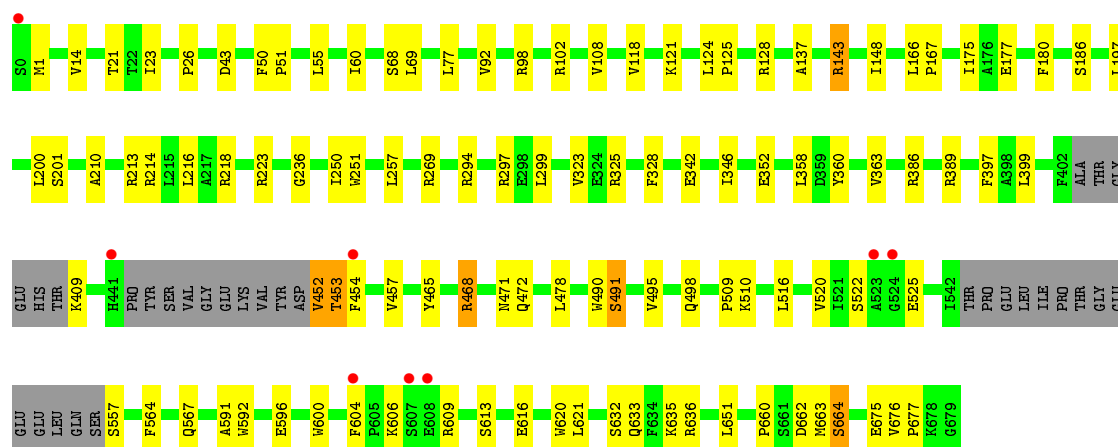
- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



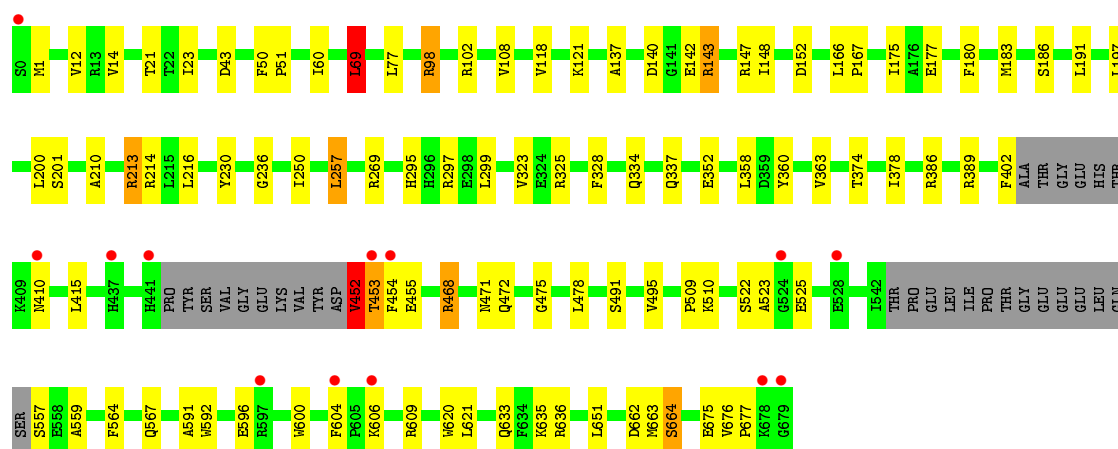
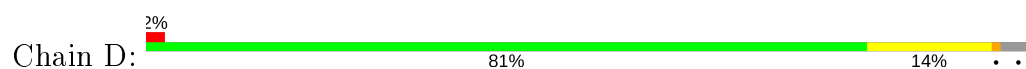
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	96	Total	O	0	0
			96	96		
5	B	92	Total	O	0	0
			92	92		
5	C	73	Total	O	0	0
			73	73		
5	D	88	Total	O	0	0
			88	88		



• Molecule 1: Glutamine-dependent NAD(+) synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.17Å 178.17Å 214.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.09 – 2.73 40.09 – 2.73	Depositor EDS
% Data completeness (in resolution range)	96.3 (40.09-2.73) 91.5 (40.09-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.163 , 0.212 0.155 , 0.204	Depositor DCC
R_{free} test set	4400 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	1.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20820	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% 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: GOL, DND, APC

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	0.61	0/5222	0.73	2/7099 (0.0%)
1	B	0.62	0/5183	0.72	2/7049 (0.0%)
1	C	0.61	0/5108	0.71	2/6941 (0.0%)
1	D	0.62	0/5118	0.73	2/6955 (0.0%)
All	All	0.61	0/20631	0.72	8/28044 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	294	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	294	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	213	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	A	69	LEU	CA-CB-CG	-5.69	102.22	115.30
1	D	69	LEU	CA-CB-CG	-5.62	102.37	115.30
1	C	223	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	69	LEU	CA-CB-CG	-5.15	103.46	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	452	VAL	Peptide
1	D	452	VAL	Peptide

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	5102	0	4976	69	1
1	B	5063	0	4930	69	0
1	C	4992	0	4868	75	0
1	D	5002	0	4878	74	1
2	A	31	0	14	2	0
2	B	31	0	14	2	0
2	C	31	0	14	3	0
2	D	31	0	14	1	0
3	A	44	0	25	4	0
3	B	44	0	25	1	0
3	C	44	0	25	2	0
3	D	44	0	25	2	0
4	B	6	0	8	1	0
4	D	6	0	8	0	0
5	A	96	0	0	6	0
5	B	92	0	0	2	0
5	C	73	0	0	2	0
5	D	88	0	0	4	0
All	All	20820	0	19824	276	1

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 (276) 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:D:98:ARG:HH11	1:D:98:ARG:HG2	1.29	0.96
1:D:633:GLN:OE1	1:D:636:ARG:NH1	2.04	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HH11	1:B:98:ARG:HG2	1.37	0.90
1:A:98:ARG:HG2	1:A:98:ARG:HH11	1.35	0.88
1:A:633:GLN:OE1	1:A:636:ARG:NH1	2.06	0.88
1:B:451:ASP:HB3	1:B:453:THR:H	1.40	0.87
1:A:468:ARG:NH2	1:D:495:VAL:O	2.08	0.87
1:C:98:ARG:HG2	1:C:98:ARG:HH11	1.38	0.86
1:C:633:GLN:OE1	1:C:636:ARG:NH1	2.07	0.86
1:B:633:GLN:OE1	1:B:636:ARG:NH1	2.10	0.84
1:B:468:ARG:NH2	1:C:495:VAL:O	2.11	0.83
1:D:143:ARG:HH11	1:D:143:ARG:HG2	1.43	0.83
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.44	0.83
1:B:495:VAL:O	1:C:468:ARG:NH2	2.13	0.82
2:D:680:APC:H3A1	2:D:680:APC:H3'	1.68	0.76
1:A:606:LYS:HA	1:A:609:ARG:HD3	1.66	0.75
1:B:363:VAL:HG13	1:B:478:LEU:HD13	1.68	0.75
1:B:135:GLN:OE1	4:B:682:GOL:O2	2.03	0.75
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.52	0.75
1:D:606:LYS:HA	1:D:609:ARG:HD3	1.68	0.74
1:A:495:VAL:O	1:D:468:ARG:NH2	2.21	0.73
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.53	0.73
1:A:102:ARG:HD3	1:A:137:ALA:HB2	1.71	0.73
1:B:102:ARG:HD3	1:B:137:ALA:HB2	1.70	0.73
1:B:606:LYS:HA	1:B:609:ARG:HD3	1.69	0.73
1:A:363:VAL:HG13	1:A:478:LEU:HD13	1.71	0.72
1:D:452:VAL:N	1:D:454:PHE:HB3	2.04	0.72
1:A:468:ARG:NH1	1:A:471:ASN:OD1	2.24	0.71
1:A:252:GLU:OE2	5:A:725:HOH:O	2.08	0.71
1:A:297:ARG:NH2	1:B:142:GLU:OE2	2.23	0.70
1:C:606:LYS:HA	1:C:609:ARG:HD3	1.72	0.70
1:D:363:VAL:HG13	1:D:478:LEU:HD13	1.74	0.70
1:D:102:ARG:HD3	1:D:137:ALA:HB2	1.73	0.70
1:D:525:GLU:HB2	5:D:728:HOH:O	1.90	0.69
1:B:468:ARG:NH1	1:B:471:ASN:OD1	2.25	0.69
1:C:363:VAL:HG13	1:C:478:LEU:HD13	1.73	0.69
1:B:525:GLU:OE1	1:B:525:GLU:HA	1.94	0.67
1:C:468:ARG:NH1	1:C:471:ASN:OD1	2.26	0.66
1:D:525:GLU:OE1	1:D:525:GLU:HA	1.96	0.65
1:A:451:ASP:HB3	1:A:453:THR:H	1.60	0.65
1:A:525:GLU:OE1	1:A:525:GLU:HA	1.95	0.64
1:D:468:ARG:NH1	1:D:471:ASN:OD1	2.27	0.64
1:C:525:GLU:OE1	1:C:525:GLU:HA	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:HD3	1:C:137:ALA:HB2	1.81	0.63
1:D:143:ARG:HG2	1:D:143:ARG:NH1	2.14	0.61
1:A:98:ARG:NH1	1:A:98:ARG:HG2	2.11	0.60
1:C:297:ARG:NH2	1:D:142:GLU:OE2	2.34	0.60
1:A:636:ARG:HD3	1:A:651:LEU:HB3	1.84	0.60
1:C:98:ARG:NH1	1:C:98:ARG:HG2	2.12	0.59
1:B:636:ARG:HD3	1:B:651:LEU:HB3	1.84	0.59
1:C:452:VAL:N	1:C:454:PHE:H	2.01	0.58
1:B:451:ASP:HB3	1:B:453:THR:N	2.13	0.58
1:D:21:THR:O	1:D:236:GLY:HA3	2.03	0.58
1:D:567:GLN:OE1	1:D:567:GLN:HA	2.04	0.58
1:C:323:VAL:HG12	1:C:591:ALA:HB2	1.85	0.58
1:C:121:LYS:HD2	1:C:175:ILE:HG22	1.86	0.58
1:B:472:GLN:HB2	1:C:453:THR:HG21	1.84	0.58
1:C:632:SER:OG	1:C:636:ARG:NH2	2.37	0.58
2:C:680:APC:H3A1	2:C:680:APC:H3'	1.85	0.57
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.13	0.57
1:B:98:ARG:NH1	1:B:98:ARG:HG2	2.14	0.57
1:D:98:ARG:NH1	1:D:98:ARG:HG2	2.07	0.57
1:D:186:SER:HB2	1:D:197:LEU:HD13	1.87	0.57
1:A:186:SER:HB2	1:A:197:LEU:HD13	1.87	0.56
1:D:23:ILE:HB	1:D:60:ILE:HG22	1.87	0.56
1:B:43:ASP:OD2	1:B:269:ARG:NH2	2.38	0.56
1:A:567:GLN:OE1	1:A:567:GLN:HA	2.06	0.56
1:C:636:ARG:HD3	1:C:651:LEU:HB3	1.88	0.56
1:A:210:ALA:HA	1:A:213:ARG:HD2	1.89	0.55
1:C:21:THR:O	1:C:236:GLY:HA3	2.06	0.55
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.20	0.55
1:A:510:LYS:HD2	1:A:564:PHE:CD2	2.42	0.55
1:A:453:THR:HG21	1:D:472:GLN:HB2	1.88	0.55
1:B:453:THR:HG21	1:C:472:GLN:HB2	1.88	0.54
1:D:523:ALA:HB3	5:D:728:HOH:O	2.07	0.54
1:A:14:VAL:HG23	1:A:250:ILE:HD13	1.90	0.54
1:B:632:SER:OG	1:B:636:ARG:NH2	2.41	0.54
1:C:186:SER:HB2	1:C:197:LEU:HD13	1.90	0.54
1:A:389:ARG:CD	5:A:753:HOH:O	2.56	0.54
1:A:604:PHE:O	1:A:609:ARG:HD2	2.08	0.54
1:B:77:LEU:HD11	1:B:108:VAL:HG11	1.89	0.54
1:A:389:ARG:HD3	5:A:753:HOH:O	2.07	0.54
1:C:14:VAL:HG23	1:C:250:ILE:HD13	1.90	0.54
1:C:143:ARG:HG2	1:C:143:ARG:NH1	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:VAL:HG12	1:B:591:ALA:HB2	1.90	0.53
1:C:23:ILE:HB	1:C:60:ILE:HG22	1.90	0.53
1:D:510:LYS:HD2	1:D:564:PHE:CD2	2.43	0.53
2:A:680:APC:H3A2	2:A:680:APC:O2G	2.09	0.53
1:C:210:ALA:O	1:C:214:ARG:HG3	2.08	0.53
1:A:23:ILE:HB	1:A:60:ILE:HG22	1.90	0.53
1:D:604:PHE:O	1:D:609:ARG:HD2	2.09	0.53
1:B:23:ILE:HB	1:B:60:ILE:HG22	1.91	0.53
1:A:200:LEU:N	1:A:200:LEU:HD12	2.23	0.53
1:D:620:TRP:CE3	1:D:620:TRP:HA	2.43	0.52
1:C:620:TRP:CE3	1:C:620:TRP:HA	2.44	0.52
1:D:323:VAL:HG12	1:D:591:ALA:HB2	1.91	0.52
1:D:98:ARG:HH11	1:D:98:ARG:CG	2.10	0.52
1:A:121:LYS:HD2	1:A:175:ILE:HG22	1.91	0.52
1:B:21:THR:O	1:B:236:GLY:HA3	2.10	0.52
1:C:77:LEU:HD11	1:C:108:VAL:HG11	1.92	0.51
1:C:43:ASP:OD2	1:C:269:ARG:NH2	2.41	0.51
1:C:210:ALA:HA	1:C:213:ARG:HD2	1.91	0.51
1:A:180:PHE:CD2	1:A:216:LEU:CD1	2.93	0.51
2:B:680:APC:O2G	2:B:680:APC:H3A2	2.11	0.51
1:C:200:LEU:N	1:C:200:LEU:HD12	2.26	0.51
1:C:218:ARG:HG3	1:C:251:TRP:CZ3	2.44	0.51
1:D:636:ARG:HD3	1:D:651:LEU:HB3	1.92	0.51
1:B:662:ASP:N	1:B:662:ASP:OD1	2.43	0.51
1:A:472:GLN:HB2	1:D:453:THR:HG21	1.92	0.51
1:C:510:LYS:HD2	1:C:564:PHE:CD2	2.45	0.51
1:C:662:ASP:N	1:C:662:ASP:OD1	2.44	0.51
1:C:567:GLN:OE1	1:C:567:GLN:HA	2.11	0.51
1:D:210:ALA:O	1:D:214:ARG:HG3	2.11	0.51
1:B:50:PHE:HB3	1:B:51:PRO:CD	2.41	0.50
1:D:200:LEU:N	1:D:200:LEU:HD12	2.27	0.50
1:B:402:PHE:HD2	1:B:458:GLN:NE2	2.10	0.50
1:D:43:ASP:OD2	1:D:269:ARG:NH2	2.41	0.50
1:D:210:ALA:HA	1:D:213:ARG:HD2	1.93	0.50
1:A:210:ALA:O	1:A:214:ARG:HG3	2.11	0.50
1:B:510:LYS:HD2	1:B:564:PHE:CD2	2.47	0.50
1:A:21:THR:O	1:A:236:GLY:HA3	2.11	0.50
1:B:121:LYS:HD2	1:B:175:ILE:HG22	1.92	0.50
1:D:1:MET:HB3	1:D:675:GLU:OE1	2.11	0.50
1:B:174:GLU:HG2	5:B:694:HOH:O	2.11	0.49
1:B:441:HIS:HE2	1:B:451:ASP:HB2	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:THR:HG23	1:D:415:LEU:HD22	1.94	0.49
1:B:186:SER:HB2	1:B:197:LEU:HD13	1.95	0.49
1:A:451:ASP:HB3	1:A:453:THR:N	2.27	0.49
1:A:620:TRP:CE3	1:A:620:TRP:HA	2.47	0.49
1:D:328:PHE:CG	1:D:509:PRO:HG3	2.47	0.49
1:C:360:TYR:HB3	1:C:389:ARG:HD2	1.94	0.49
1:D:600:TRP:CD2	1:D:609:ARG:HG2	2.47	0.49
1:A:126:THR:OG1	1:A:133:ARG:HB2	2.12	0.49
1:B:180:PHE:CD2	1:B:216:LEU:CD1	2.96	0.49
1:C:1:MET:HB3	1:C:675:GLU:OE1	2.13	0.49
1:B:200:LEU:N	1:B:200:LEU:HD12	2.29	0.48
1:B:620:TRP:CE3	1:B:620:TRP:HA	2.49	0.48
1:A:69:LEU:HG	1:A:69:LEU:O	2.11	0.48
1:B:210:ALA:O	1:B:214:ARG:HG3	2.14	0.48
1:C:633:GLN:HA	1:C:636:ARG:NH1	2.28	0.48
1:B:360:TYR:HB3	1:B:389:ARG:HD2	1.94	0.48
1:B:604:PHE:O	1:B:609:ARG:HD2	2.14	0.48
1:D:147:ARG:NH1	1:D:152:ASP:OD2	2.45	0.47
1:B:510:LYS:HE3	1:B:564:PHE:CE2	2.49	0.47
1:C:180:PHE:CD2	1:C:216:LEU:CD1	2.98	0.47
1:A:1:MET:HB3	1:A:675:GLU:OE1	2.15	0.47
1:B:348:VAL:O	1:B:352:GLU:HG3	2.13	0.47
1:D:12:VAL:HG13	1:D:12:VAL:O	2.12	0.47
1:A:633:GLN:HA	1:A:636:ARG:NH1	2.30	0.47
1:C:121:LYS:HD2	1:C:175:ILE:CG2	2.44	0.47
1:C:635:LYS:NZ	3:C:681:DND:O11	2.39	0.47
1:D:510:LYS:HE3	1:D:564:PHE:CE2	2.49	0.47
1:B:52:GLU:HB2	1:B:201:SER:C	2.35	0.47
1:A:200:LEU:H	1:A:200:LEU:HD12	1.80	0.47
1:A:435:MET:SD	1:A:457:VAL:HG13	2.54	0.47
1:A:468:ARG:HA	1:A:468:ARG:HD3	1.51	0.47
1:D:77:LEU:HD11	1:D:108:VAL:HG11	1.97	0.47
1:B:468:ARG:HD3	1:B:468:ARG:HA	1.45	0.47
3:B:681:DND:N6A	1:C:358:LEU:HD21	2.30	0.47
1:D:183:MET:HB3	5:D:707:HOH:O	2.15	0.46
1:C:328:PHE:CG	1:C:509:PRO:HG3	2.50	0.46
1:D:118:VAL:HG21	1:D:148:ILE:CD1	2.46	0.46
1:D:180:PHE:CD2	1:D:216:LEU:CD1	2.98	0.46
1:C:490:TRP:CZ2	1:C:557:SER:HA	2.51	0.46
1:D:635:LYS:NZ	3:D:681:DND:O11	2.47	0.46
1:A:118:VAL:HG21	1:A:148:ILE:CD1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HD2	1:A:175:ILE:CG2	2.46	0.46
1:B:567:GLN:OE1	1:B:567:GLN:HA	2.15	0.46
1:A:328:PHE:CG	1:A:509:PRO:HG3	2.52	0.45
1:B:210:ALA:HA	1:B:213:ARG:HD2	1.98	0.45
1:C:124:LEU:HA	1:C:125:PRO:HD2	1.85	0.45
1:D:374:THR:HG23	1:D:415:LEU:CD2	2.46	0.45
1:B:445:VAL:HG23	1:B:445:VAL:O	2.16	0.45
1:D:328:PHE:CD2	1:D:509:PRO:HG3	2.51	0.45
1:A:43:ASP:OD2	1:A:269:ARG:NH2	2.44	0.45
1:D:14:VAL:HG23	1:D:250:ILE:HD13	1.99	0.45
1:B:140:ASP:HB2	1:D:295:HIS:ND1	2.31	0.45
2:A:680:APC:O2A	3:A:681:DND:C7N	2.65	0.45
1:B:325:ARG:HB3	1:B:592:TRP:CZ2	2.52	0.45
1:B:126:THR:OG1	1:B:133:ARG:HB2	2.16	0.44
1:B:351:LEU:O	1:B:355:LEU:HG	2.17	0.44
1:B:88:LEU:N	1:B:89:PRO:CD	2.81	0.44
1:D:452:VAL:N	1:D:455:GLU:H	2.15	0.44
1:A:180:PHE:CD2	1:A:216:LEU:HD13	2.52	0.44
1:D:557:SER:C	1:D:559:ALA:N	2.71	0.44
1:A:514:GLN:HE21	1:A:518:ARG:HH21	1.65	0.44
1:C:166:LEU:N	1:C:167:PRO:HD3	2.32	0.44
1:C:26:PRO:HA	1:C:55:LEU:O	2.17	0.44
1:A:600:TRP:CD2	1:A:609:ARG:HG2	2.52	0.44
1:C:490:TRP:NE1	3:C:681:DND:H13	2.33	0.44
1:D:50:PHE:HB3	1:D:51:PRO:CD	2.48	0.44
1:A:510:LYS:HE3	1:A:564:PHE:CE2	2.52	0.44
1:C:510:LYS:HE3	1:C:564:PHE:CE2	2.52	0.44
1:A:77:LEU:HD11	1:A:108:VAL:HG11	2.00	0.44
1:C:468:ARG:HA	1:C:468:ARG:HD3	1.46	0.44
1:B:328:PHE:CG	1:B:509:PRO:HG3	2.52	0.44
1:A:662:ASP:N	1:A:662:ASP:OD1	2.50	0.44
1:D:360:TYR:HB3	1:D:389:ARG:HD2	2.00	0.44
1:D:69:LEU:O	1:D:69:LEU:HG	2.15	0.44
1:C:491:SER:HB3	1:C:498:GLN:HB2	2.01	0.43
1:C:663:MET:HG2	1:C:664:SER:O	2.18	0.43
1:A:323:VAL:HG12	1:A:591:ALA:HB2	2.01	0.43
1:A:348:VAL:O	1:A:352:GLU:HG3	2.18	0.43
1:D:600:TRP:CE2	1:D:609:ARG:HG2	2.54	0.43
1:B:12:VAL:HG13	1:B:12:VAL:O	2.18	0.43
1:A:102:ARG:HB3	5:A:699:HOH:O	2.18	0.43
1:B:471:ASN:HB2	1:C:453:THR:HG23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:PHE:HB3	1:C:51:PRO:CD	2.48	0.43
1:B:121:LYS:HD2	1:B:175:ILE:CG2	2.49	0.43
1:D:402:PHE:HD2	1:D:454:PHE:CZ	2.37	0.43
1:C:660:PRO:HG3	1:D:60:ILE:HA	1.99	0.43
1:D:633:GLN:HA	1:D:636:ARG:NH1	2.34	0.43
1:A:166:LEU:N	1:A:167:PRO:HD3	2.34	0.43
1:B:118:VAL:HG21	1:B:148:ILE:CD1	2.48	0.43
1:D:325:ARG:HB3	1:D:592:TRP:CZ2	2.54	0.43
1:C:180:PHE:CD2	1:C:216:LEU:HD13	2.54	0.43
1:C:604:PHE:O	1:C:609:ARG:HD2	2.19	0.43
1:A:558:GLU:CD	1:A:563:PRO:HA	2.39	0.43
1:D:166:LEU:N	1:D:167:PRO:HD3	2.34	0.43
1:D:180:PHE:CD2	1:D:216:LEU:HD13	2.52	0.43
1:C:92:VAL:CG1	1:C:200:LEU:HD11	2.49	0.42
1:C:399:LEU:N	2:C:680:APC:N1	2.55	0.42
1:C:352:GLU:OE2	1:C:386:ARG:HD3	2.19	0.42
1:A:342:GLU:O	1:A:346:ILE:HG13	2.19	0.42
1:A:449:VAL:O	1:A:449:VAL:HG12	2.19	0.42
1:B:14:VAL:HG23	1:B:250:ILE:HD13	2.02	0.42
1:D:121:LYS:HD2	1:D:175:ILE:HG22	2.01	0.42
1:A:490:TRP:NE1	3:A:681:DND:H13	2.34	0.42
3:A:681:DND:N6A	1:D:358:LEU:HD21	2.33	0.42
1:C:128:ARG:HH11	1:C:128:ARG:HD2	1.71	0.42
1:D:663:MET:HG2	1:D:664:SER:O	2.20	0.42
1:D:621:LEU:HA	5:D:722:HOH:O	2.19	0.42
1:B:435:MET:HG3	1:C:465:TYR:CE1	2.54	0.42
1:C:600:TRP:CD2	1:C:609:ARG:HG2	2.55	0.42
1:A:389:ARG:HD2	5:A:753:HOH:O	2.19	0.42
1:A:23:ILE:HB	1:A:60:ILE:CG2	2.50	0.42
1:B:51:PRO:O	1:B:54:THR:OG1	2.36	0.42
1:B:600:TRP:CD2	1:B:609:ARG:HG2	2.55	0.42
1:D:378:ILE:HD13	1:D:378:ILE:HA	1.91	0.42
1:B:534:LEU:HA	1:B:534:LEU:HD23	1.78	0.41
1:A:660:PRO:HG3	1:B:60:ILE:HA	2.02	0.41
3:A:681:DND:O2B	1:D:475:GLY:O	2.37	0.41
1:D:525:GLU:CA	1:D:525:GLU:OE1	2.65	0.41
1:C:218:ARG:HG3	1:C:251:TRP:CE3	2.55	0.41
1:D:257:LEU:HA	1:D:257:LEU:HD12	1.76	0.41
1:C:118:VAL:HG21	1:C:148:ILE:CD1	2.50	0.41
1:B:69:LEU:HG	1:B:69:LEU:O	2.18	0.41
1:A:445:VAL:O	1:A:445:VAL:CG1	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:PRO:HD2	5:C:796:HOH:O	2.20	0.41
1:C:452:VAL:C	1:C:454:PHE:N	2.72	0.41
1:B:182:PRO:HG2	1:D:191:LEU:HD21	2.02	0.41
1:D:662:ASP:OD1	1:D:662:ASP:N	2.54	0.41
1:C:453:THR:O	1:C:457:VAL:HG23	2.21	0.41
2:B:680:APC:H5'2	2:B:680:APC:H3A2	1.73	0.41
1:C:397:PHE:O	2:C:680:APC:H2	2.21	0.41
1:C:516:LEU:O	1:C:520:VAL:HG23	2.20	0.41
1:A:13:ARG:HB3	1:A:45:ALA:HA	2.03	0.41
1:C:92:VAL:HG11	1:C:200:LEU:HD11	2.02	0.41
1:B:423:PHE:CG	1:B:424:SER:N	2.89	0.41
1:B:295:HIS:ND1	1:D:140:ASP:HB2	2.36	0.41
1:D:230:TYR:C	1:D:230:TYR:CD1	2.94	0.41
1:D:676:VAL:HA	1:D:677:PRO:HD3	1.97	0.41
1:A:124:LEU:HA	1:A:125:PRO:HD2	1.89	0.40
1:B:146:ILE:HD13	1:B:146:ILE:HG21	1.88	0.40
1:A:358:LEU:HD21	3:D:681:DND:N6A	2.37	0.40
1:B:223:ARG:HD3	5:B:753:HOH:O	2.20	0.40
1:A:174:GLU:HG2	5:A:756:HOH:O	2.21	0.40
1:C:613:SER:OG	1:C:616:GLU:HG3	2.20	0.40
1:C:676:VAL:HA	1:C:677:PRO:HD3	1.96	0.40
1:D:352:GLU:OE2	1:D:386:ARG:HB2	2.22	0.40
1:B:600:TRP:CE2	1:B:609:ARG:HG2	2.57	0.40
1:C:325:ARG:HB3	1:C:592:TRP:CZ2	2.56	0.40
1:A:218:ARG:HG3	1:A:251:TRP:CZ3	2.57	0.40
1:A:360:TYR:HB3	1:A:389:ARG:HD2	2.02	0.40
1:C:342:GLU:O	1:C:346:ILE:HG13	2.21	0.40
1:C:621:LEU:HA	5:C:784:HOH:O	2.21	0.40

All (1) 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)
1:A:142:GLU:OE2	1:D:297:ARG:NH2[8_555]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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	655/680 (96%)	631 (96%)	24 (4%)	0	100	100
1	B	652/680 (96%)	626 (96%)	25 (4%)	1 (0%)	47	69
1	C	642/680 (94%)	618 (96%)	23 (4%)	1 (0%)	47	69
1	D	642/680 (94%)	621 (97%)	20 (3%)	1 (0%)	47	69
All	All	2591/2720 (95%)	2496 (96%)	92 (4%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	177	GLU
1	D	177	GLU
1	B	177	GLU

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	525/548 (96%)	506 (96%)	19 (4%)	35	55
1	B	517/548 (94%)	505 (98%)	12 (2%)	50	70
1	C	509/548 (93%)	496 (97%)	13 (3%)	46	66
1	D	512/548 (93%)	496 (97%)	16 (3%)	40	60
All	All	2063/2192 (94%)	2003 (97%)	60 (3%)	42	62

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	68	SER
1	A	69	LEU
1	A	98	ARG
1	A	143	ARG
1	A	201	SER
1	A	257	LEU
1	A	299	LEU
1	A	334	GLN
1	A	337	GLN
1	A	445	VAL
1	A	451	ASP
1	A	453	THR
1	A	468	ARG
1	A	491	SER
1	A	518	ARG
1	A	522	SER
1	A	543	THR
1	A	664	SER
1	B	5	SER
1	B	68	SER
1	B	98	ARG
1	B	143	ARG
1	B	201	SER
1	B	257	LEU
1	B	299	LEU
1	B	453	THR
1	B	468	ARG
1	B	491	SER
1	B	522	SER
1	B	664	SER
1	C	68	SER
1	C	69	LEU
1	C	143	ARG
1	C	201	SER
1	C	257	LEU
1	C	299	LEU
1	C	409	LYS
1	C	453	THR
1	C	468	ARG
1	C	491	SER
1	C	522	SER
1	C	596	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	664	SER
1	D	69	LEU
1	D	98	ARG
1	D	143	ARG
1	D	201	SER
1	D	257	LEU
1	D	299	LEU
1	D	334	GLN
1	D	337	GLN
1	D	410	ASN
1	D	452	VAL
1	D	453	THR
1	D	468	ARG
1	D	491	SER
1	D	522	SER
1	D	596	GLU
1	D	664	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	514	GLN
1	B	514	GLN
1	B	515	HIS
1	C	345	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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	B	682	-	5,5,5	0.40	0	5,5,5	0.17	0
3	DND	C	681	-	40,48,48	1.04	2 (5%)	47,73,73	1.28	4 (8%)
2	APC	A	680	-	27,33,33	1.33	3 (11%)	31,52,52	1.44	4 (12%)
4	GOL	D	682	-	5,5,5	0.78	0	5,5,5	0.42	0
2	APC	C	680	-	27,33,33	1.45	4 (14%)	31,52,52	1.57	8 (25%)
3	DND	D	681	-	40,48,48	1.05	2 (5%)	47,73,73	1.27	3 (6%)
3	DND	B	681	-	40,48,48	1.19	3 (7%)	47,73,73	1.21	2 (4%)
3	DND	A	681	-	40,48,48	1.11	3 (7%)	47,73,73	1.26	3 (6%)
2	APC	B	680	-	27,33,33	1.51	5 (18%)	31,52,52	1.37	3 (9%)
2	APC	D	680	-	27,33,33	1.52	3 (11%)	31,52,52	1.48	5 (16%)

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	B	682	-	-	4/4/4/4	-
3	DND	C	681	-	-	8/22/62/62	0/5/5/5
2	APC	A	680	-	-	4/15/38/38	0/3/3/3
4	GOL	D	682	-	-	0/4/4/4	-
2	APC	C	680	-	-	6/15/38/38	0/3/3/3
3	DND	D	681	-	-	10/22/62/62	0/5/5/5
3	DND	B	681	-	-	8/22/62/62	0/5/5/5
3	DND	A	681	-	-	8/22/62/62	0/5/5/5
2	APC	B	680	-	-	10/15/38/38	0/3/3/3
2	APC	D	680	-	-	7/15/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	681	DND	C3N-C7N	5.45	1.52	1.47
3	D	681	DND	C3N-C7N	4.60	1.51	1.47
3	A	681	DND	C3N-C7N	4.50	1.51	1.47
2	D	680	APC	PB-O3B	4.40	1.63	1.58
2	C	680	APC	PB-O3B	4.30	1.63	1.58
3	C	681	DND	C3N-C7N	4.23	1.51	1.47
2	B	680	APC	PB-O3B	4.14	1.63	1.58
2	D	680	APC	PA-O5'	3.83	1.63	1.57
2	A	680	APC	PB-O3B	3.62	1.62	1.58
2	B	680	APC	PA-O5'	3.52	1.62	1.57
2	A	680	APC	PA-O5'	3.38	1.62	1.57
2	C	680	APC	PA-O5'	3.31	1.62	1.57
3	A	681	DND	O4B-C1B	2.65	1.44	1.41
2	D	680	APC	O4'-C1'	2.50	1.44	1.41
3	A	681	DND	O4D-C1D	2.45	1.44	1.41
3	B	681	DND	O4B-C1B	2.41	1.44	1.41
2	B	680	APC	O4'-C1'	2.32	1.44	1.41
3	C	681	DND	O4B-C1B	2.31	1.44	1.41
3	D	681	DND	O4B-C1B	2.26	1.44	1.41
2	A	680	APC	PA-O2A	-2.25	1.51	1.56
3	B	681	DND	C2A-N3A	2.24	1.35	1.32
2	B	680	APC	C2-N3	2.18	1.35	1.32
2	C	680	APC	PA-O2A	-2.10	1.51	1.56
2	C	680	APC	O4'-C1'	2.05	1.43	1.41
2	B	680	APC	PA-O2A	-2.00	1.51	1.56

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	681	DND	N3A-C2A-N1A	-5.66	119.84	128.68
3	A	681	DND	N3A-C2A-N1A	-4.98	120.89	128.68
3	C	681	DND	N3A-C2A-N1A	-4.89	121.03	128.68
3	B	681	DND	N3A-C2A-N1A	-4.77	121.22	128.68
2	A	680	APC	N3-C2-N1	-4.12	122.24	128.68
2	D	680	APC	N3-C2-N1	-3.96	122.49	128.68
2	B	680	APC	N3-C2-N1	-3.80	122.73	128.68
2	C	680	APC	N3-C2-N1	-3.74	122.84	128.68
3	B	681	DND	C3D-C2D-C1D	3.52	106.28	100.98
2	C	680	APC	O5'-C5'-C4'	3.34	120.49	108.99
3	A	681	DND	C3D-C2D-C1D	3.30	105.94	100.98
2	A	680	APC	O2B-PB-O1B	3.25	120.93	110.07
2	C	680	APC	O1A-PA-C3A	2.96	116.91	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	680	APC	O2B-PB-O1B	2.85	119.57	110.07
2	A	680	APC	C3'-C2'-C1'	2.61	104.92	100.98
2	C	680	APC	O2B-PB-O1B	2.57	118.65	110.07
3	C	681	DND	C6N-N1N-C2N	-2.53	119.67	121.97
2	B	680	APC	O5'-C5'-C4'	2.45	117.43	108.99
2	D	680	APC	O1B-PB-C3A	-2.39	102.76	109.07
3	C	681	DND	C3D-C2D-C1D	2.38	104.56	100.98
2	C	680	APC	O4'-C4'-C5'	2.35	117.12	109.37
2	D	680	APC	O2A-PA-O1A	2.34	117.89	110.07
3	D	681	DND	C3D-C2D-C1D	2.32	104.47	100.98
3	C	681	DND	O2D-C2D-C3D	-2.31	104.36	111.82
3	A	681	DND	C6N-N1N-C2N	-2.29	119.89	121.97
2	D	680	APC	O3G-PG-O2G	2.23	116.16	107.64
2	C	680	APC	O2A-PA-O1A	2.17	117.32	110.07
2	C	680	APC	N6-C6-N1	2.13	122.99	118.57
2	C	680	APC	PG-O3B-PB	-2.08	125.28	132.62
2	A	680	APC	O3G-PG-O2G	2.02	115.34	107.64
3	D	681	DND	O4D-C4D-C3D	2.01	109.10	105.11
2	D	680	APC	O2B-PB-O1B	2.01	116.80	110.07

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	682	GOL	O1-C1-C2-C3
3	C	681	DND	C5D-O5D-PN-O3P
3	C	681	DND	PN-O3P-PA-O5B
3	C	681	DND	C3D-C4D-C5D-O5D
2	A	680	APC	PB-C3A-PA-O1A
2	C	680	APC	PA-C3A-PB-O1B
2	C	680	APC	PA-C3A-PB-O2B
2	C	680	APC	PA-C3A-PB-O3B
2	C	680	APC	PB-C3A-PA-O1A
3	D	681	DND	C5D-O5D-PN-O11
3	D	681	DND	O4D-C1D-N1N-C6N
3	D	681	DND	O4D-C1D-N1N-C2N
3	D	681	DND	C2D-C1D-N1N-C6N
3	D	681	DND	C2D-C1D-N1N-C2N
3	B	681	DND	PN-O3P-PA-O5B
3	B	681	DND	O4D-C1D-N1N-C6N
3	B	681	DND	O4D-C1D-N1N-C2N
3	B	681	DND	C2D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	681	DND	C2D-C1D-N1N-C2N
3	A	681	DND	C5D-O5D-PN-O11
3	A	681	DND	O4D-C1D-N1N-C6N
2	B	680	APC	PB-O3B-PG-O2G
2	B	680	APC	PB-C3A-PA-O1A
2	B	680	APC	PB-C3A-PA-O2A
2	B	680	APC	C5'-O5'-PA-O1A
2	B	680	APC	C5'-O5'-PA-C3A
2	D	680	APC	PA-C3A-PB-O1B
2	D	680	APC	PA-C3A-PB-O2B
2	D	680	APC	PA-C3A-PB-O3B
2	D	680	APC	C5'-O5'-PA-O1A
3	A	681	DND	O4D-C4D-C5D-O5D
3	A	681	DND	C3D-C4D-C5D-O5D
2	B	680	APC	O4'-C4'-C5'-O5'
2	B	680	APC	C3'-C4'-C5'-O5'
3	C	681	DND	O4D-C4D-C5D-O5D
2	C	680	APC	O4'-C4'-C5'-O5'
2	C	680	APC	C3'-C4'-C5'-O5'
4	B	682	GOL	C1-C2-C3-O3
4	B	682	GOL	O1-C1-C2-O2
4	B	682	GOL	O2-C2-C3-O3
2	A	680	APC	C5'-O5'-PA-C3A
3	D	681	DND	PN-O3P-PA-O5B
3	A	681	DND	PN-O3P-PA-O5B
3	B	681	DND	O4D-C4D-C5D-O5D
3	D	681	DND	C5D-O5D-PN-O3P
3	A	681	DND	C5D-O5D-PN-O3P
3	C	681	DND	C4B-C5B-O5B-PA
3	D	681	DND	C4B-C5B-O5B-PA
3	B	681	DND	C4B-C5B-O5B-PA
3	A	681	DND	C4B-C5B-O5B-PA
3	C	681	DND	C5D-O5D-PN-O11
3	C	681	DND	C5D-O5D-PN-O12
3	D	681	DND	C5D-O5D-PN-O12
2	A	680	APC	PB-C3A-PA-O2A
3	D	681	DND	O4D-C4D-C5D-O5D
2	D	680	APC	PB-C3A-PA-O1A
2	B	680	APC	C5'-O5'-PA-O2A
2	D	680	APC	C5'-O5'-PA-O2A
2	B	680	APC	PB-O3B-PG-O1G
2	B	680	APC	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

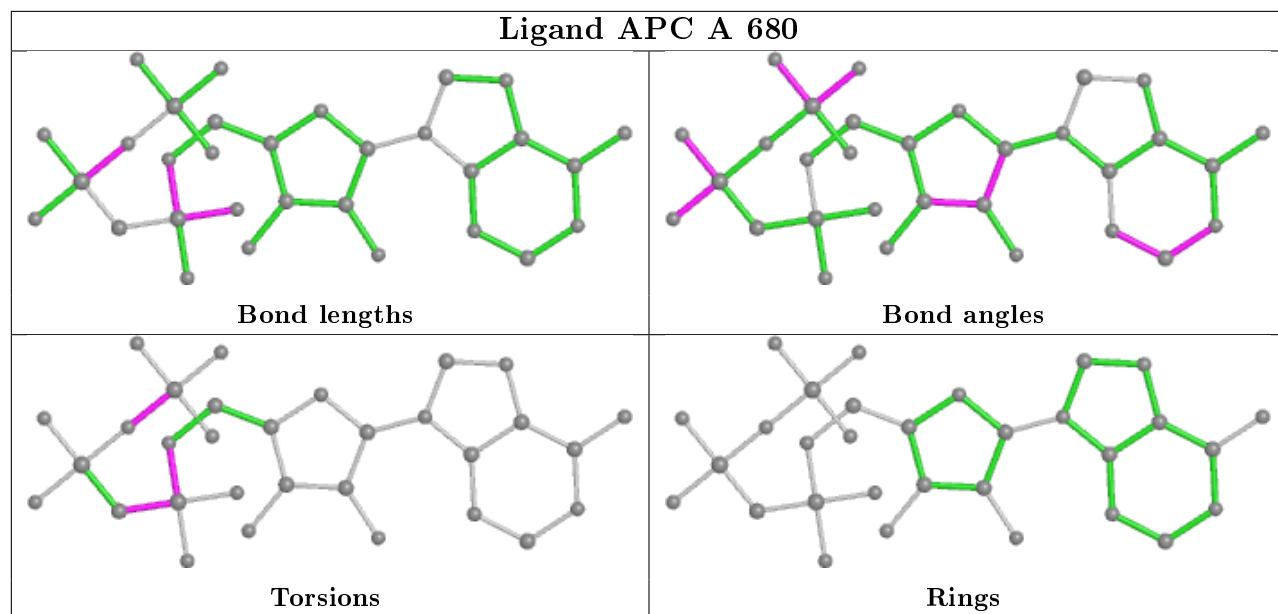
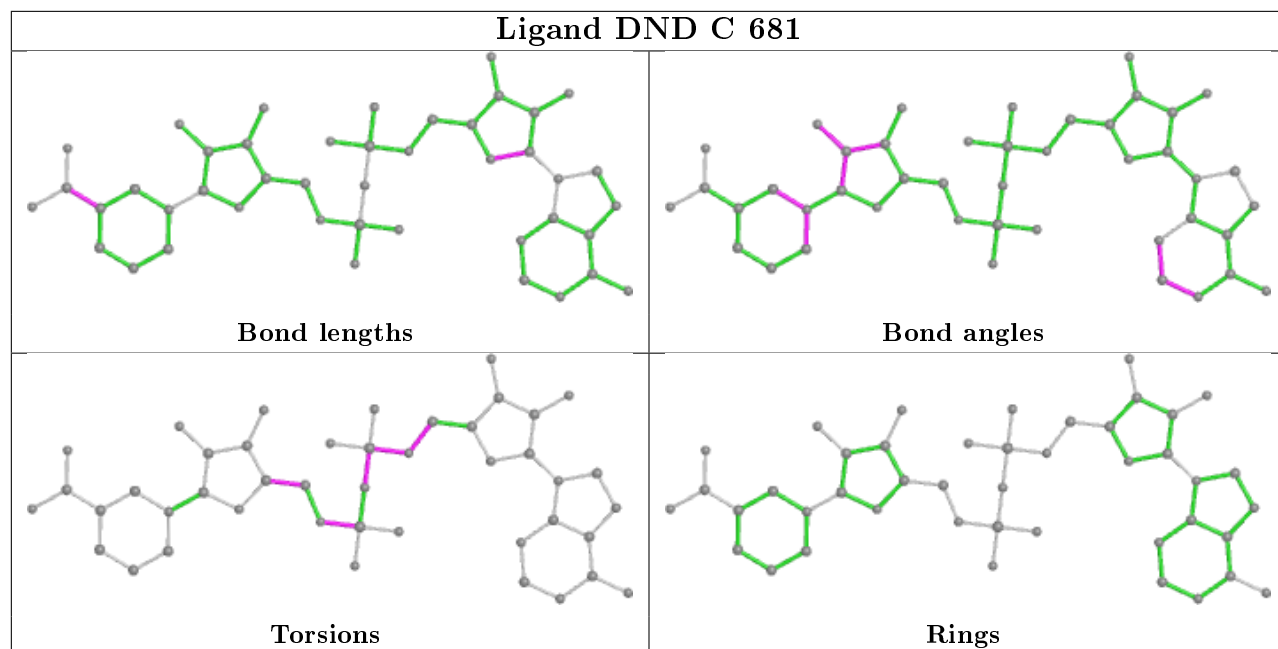
Mol	Chain	Res	Type	Atoms
3	B	681	DND	C3D-C4D-C5D-O5D
3	C	681	DND	C5B-O5B-PA-O13
2	A	680	APC	PB-O3B-PG-O1G
3	A	681	DND	C3B-C4B-C5B-O5B
2	D	680	APC	C4'-C5'-O5'-PA

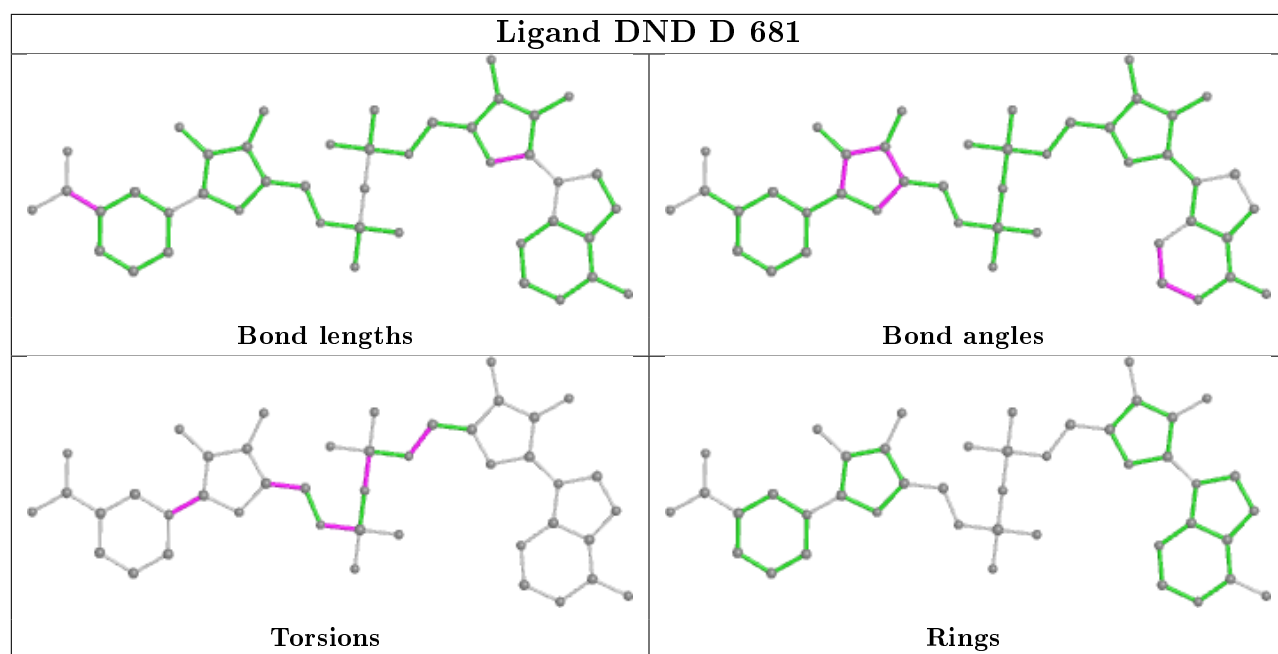
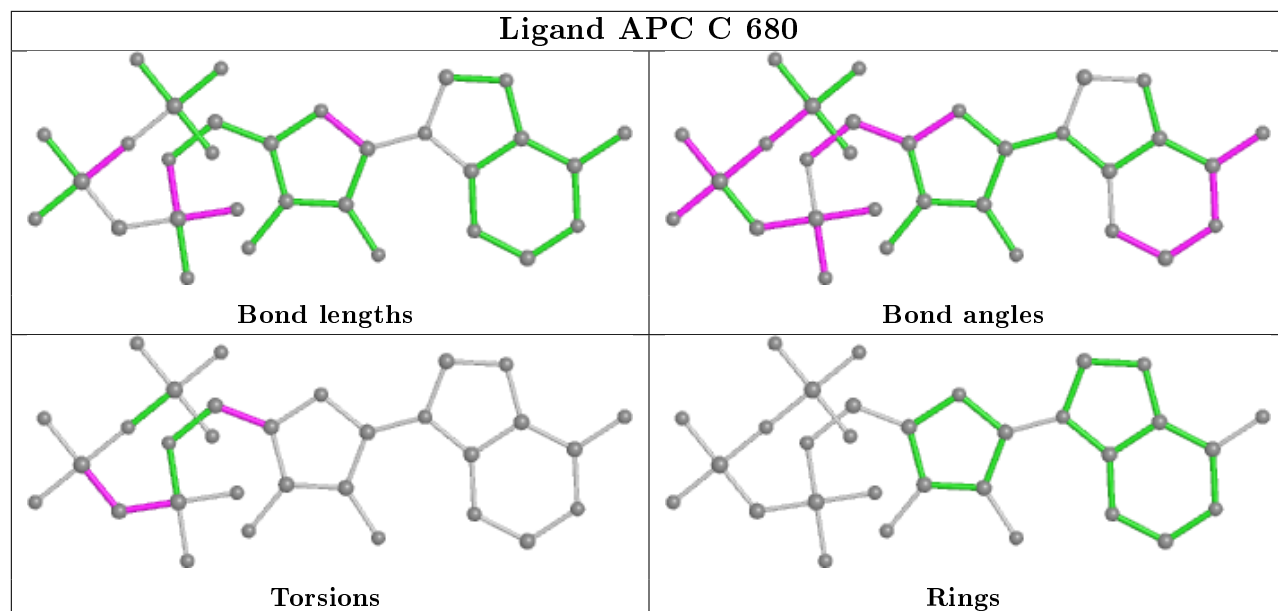
There are no ring outliers.

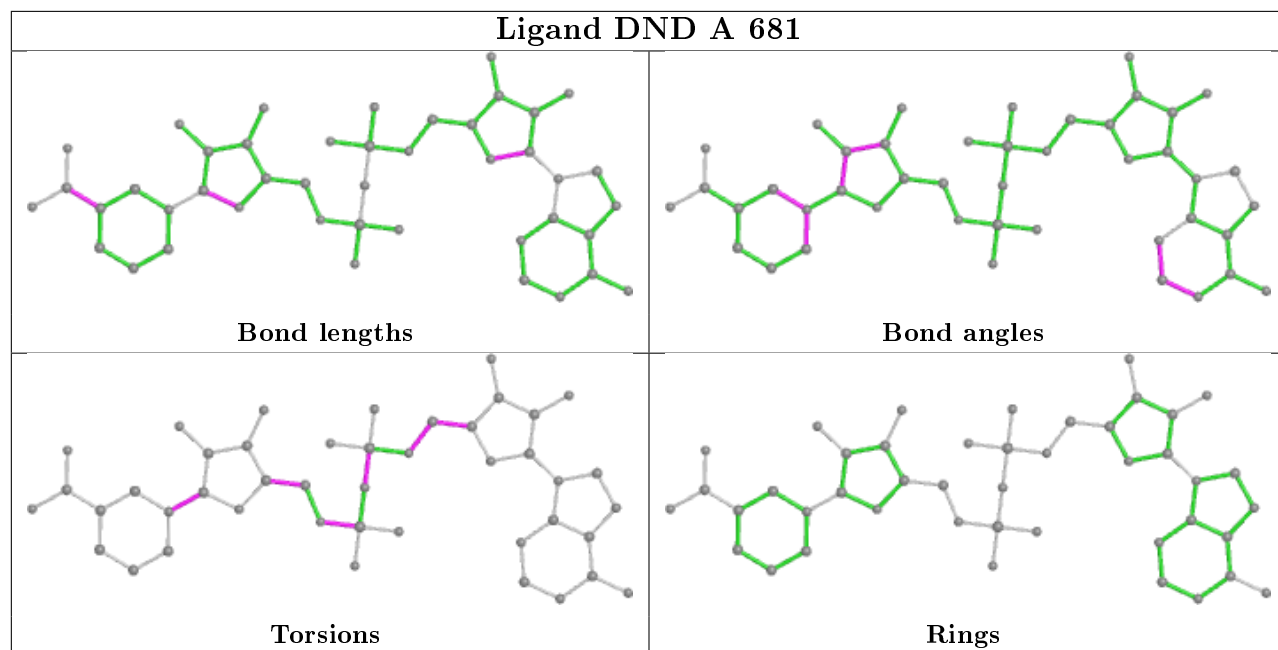
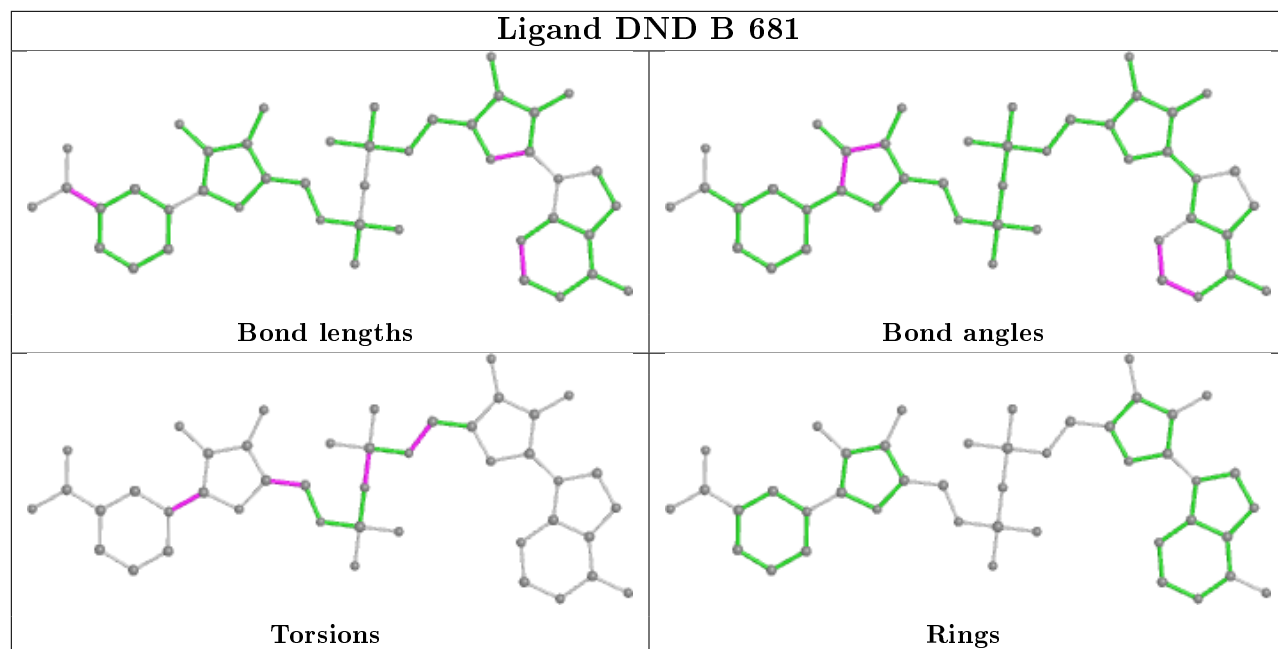
9 monomers are involved in 17 short contacts:

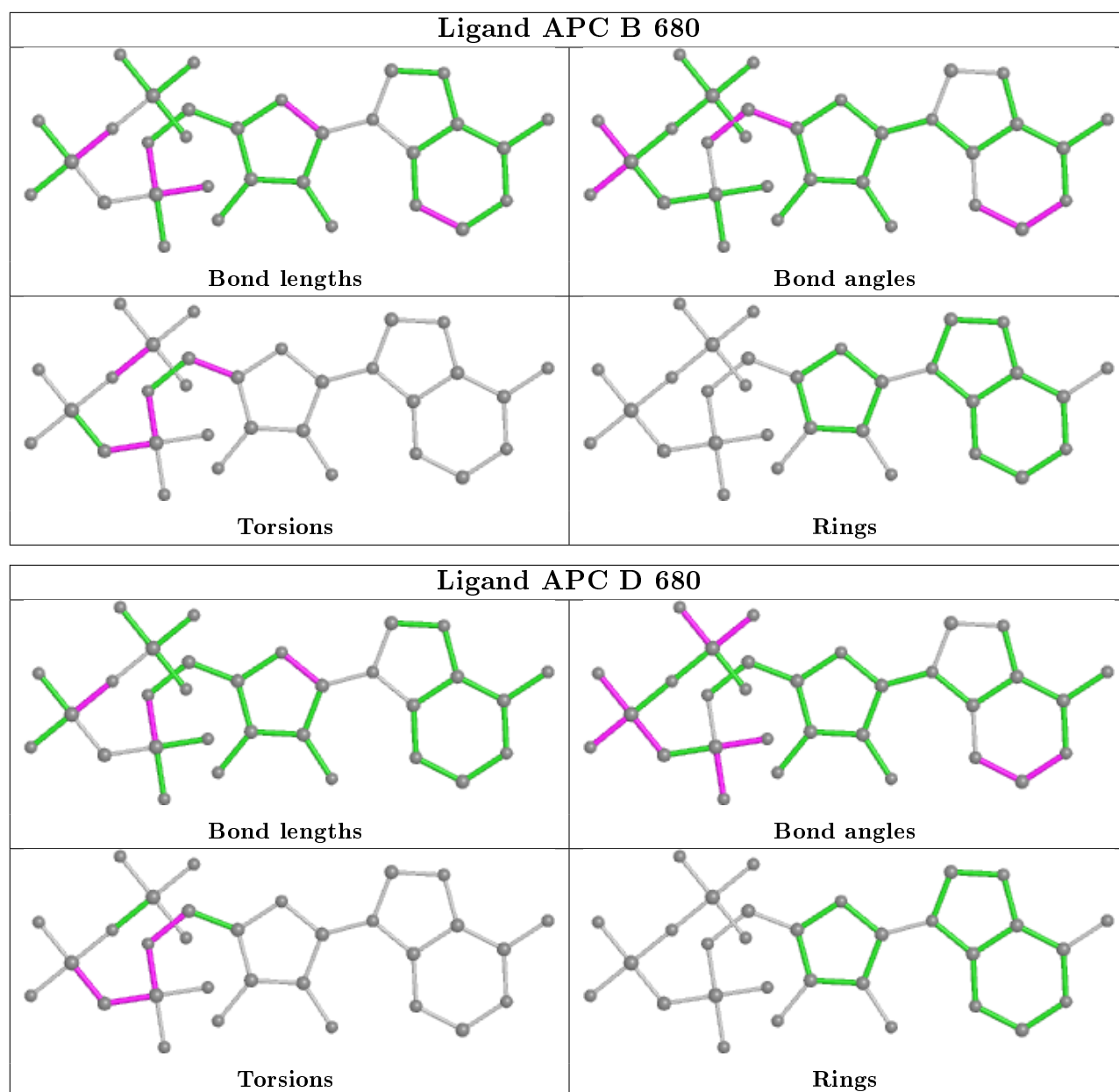
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	682	GOL	1	0
3	C	681	DND	2	0
2	A	680	APC	2	0
2	C	680	APC	3	0
3	D	681	DND	2	0
3	B	681	DND	1	0
3	A	681	DND	4	0
2	B	680	APC	2	0
2	D	680	APC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 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	661/680 (97%)	-0.54	5 (0%) 86 89	13, 30, 56, 87	0
1	B	658/680 (96%)	-0.56	3 (0%) 91 93	14, 30, 55, 87	0
1	C	650/680 (95%)	-0.50	8 (1%) 79 83	17, 32, 56, 89	0
1	D	650/680 (95%)	-0.52	13 (2%) 65 72	14, 30, 55, 90	0
All	All	2619/2720 (96%)	-0.53	29 (1%) 80 85	13, 31, 56, 90	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	SER	5.4
1	C	0	SER	3.9
1	D	441	HIS	3.5
1	C	454	PHE	3.3
1	B	0	SER	3.3
1	D	437	HIS	3.2
1	C	441	HIS	3.1
1	D	0	SER	3.0
1	A	524	GLY	2.8
1	D	454	PHE	2.7
1	C	607	SER	2.7
1	D	678	LYS	2.7
1	D	410	ASN	2.5
1	A	450	TYR	2.5
1	D	528	GLU	2.5
1	C	523	ALA	2.5
1	D	524	GLY	2.5
1	A	449	VAL	2.5
1	C	604	PHE	2.4
1	D	604	PHE	2.3
1	A	529	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	608	GLU	2.2
1	D	453	THR	2.2
1	D	606	LYS	2.1
1	D	679	GLY	2.1
1	B	608	GLU	2.1
1	D	597	ARG	2.1
1	B	523	ALA	2.0
1	C	524	GLY	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 carbohydrates in this entry.

6.4 Ligands [i](#)

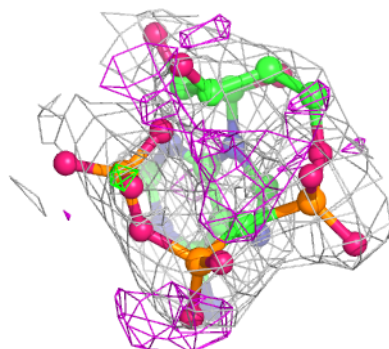
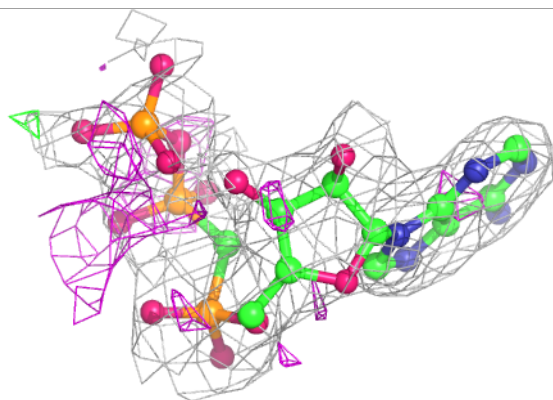
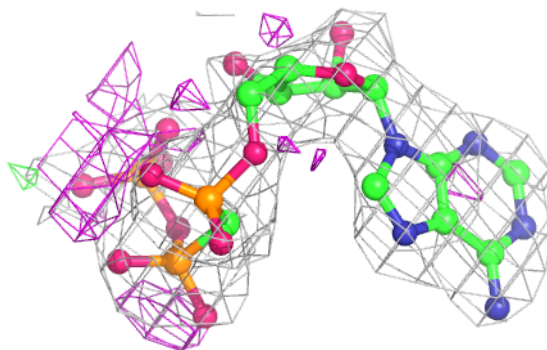
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	D	682	6/6	0.67	0.35	36,68,74,81	0
2	APC	D	680	31/31	0.92	0.16	41,63,114,119	0
2	APC	C	680	31/31	0.94	0.13	37,61,103,140	0
3	DND	B	681	44/44	0.94	0.20	27,79,151,156	0
3	DND	C	681	44/44	0.94	0.23	39,73,144,154	0
3	DND	D	681	44/44	0.95	0.21	27,65,132,135	0
4	GOL	B	682	6/6	0.95	0.18	38,48,57,60	0
3	DND	A	681	44/44	0.95	0.19	31,59,121,140	0
2	APC	B	680	31/31	0.95	0.14	38,59,112,160	0
2	APC	A	680	31/31	0.95	0.14	32,59,102,161	0

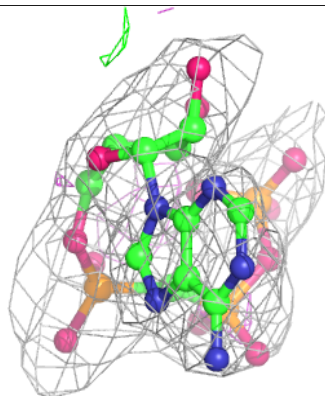
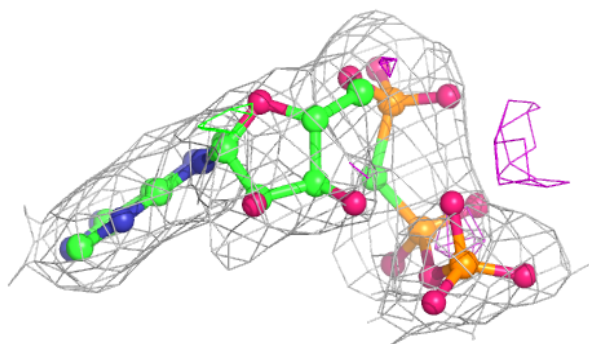
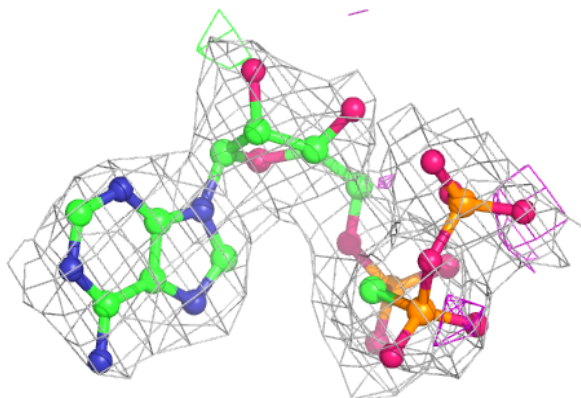
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around APC D 680:

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

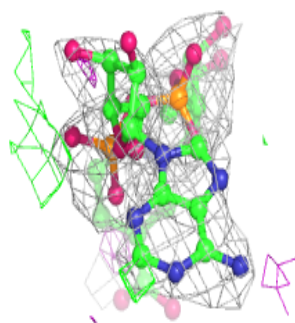
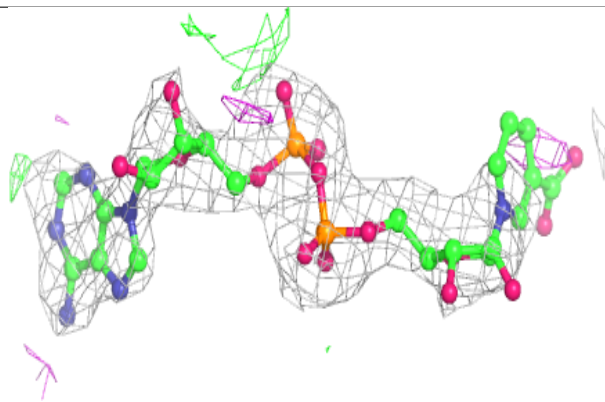
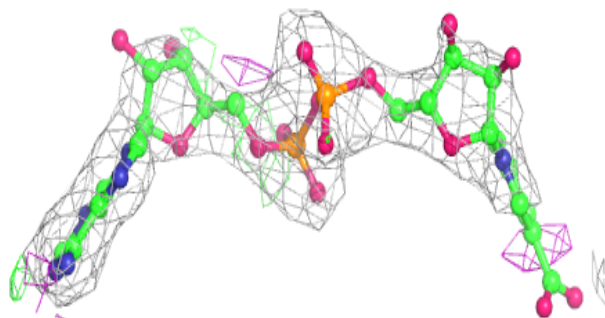
**Electron density around APC C 680:**

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

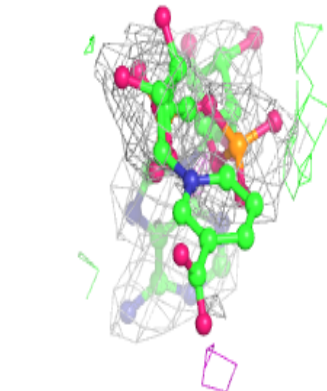
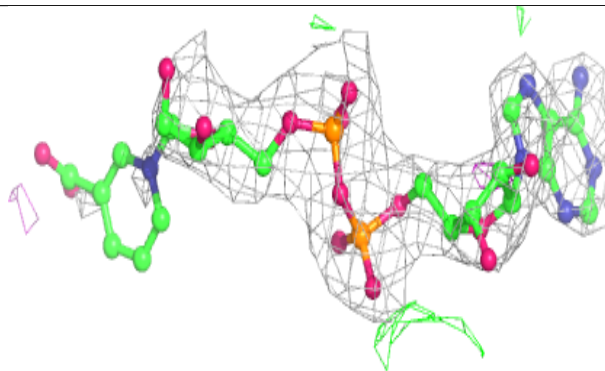
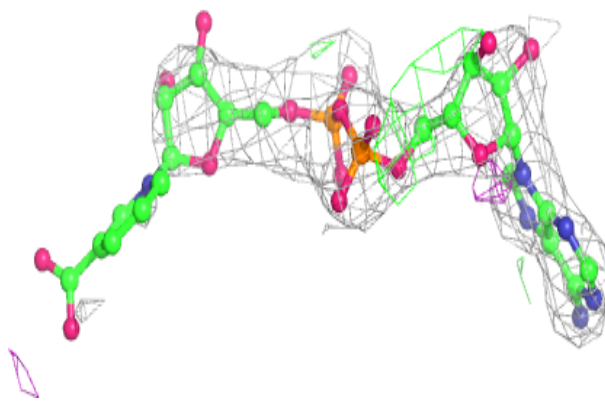


Electron density around DND B 681:

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

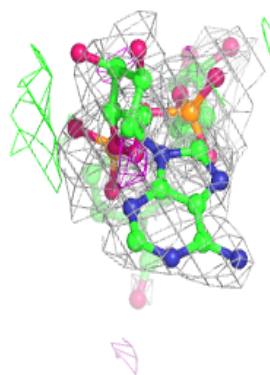
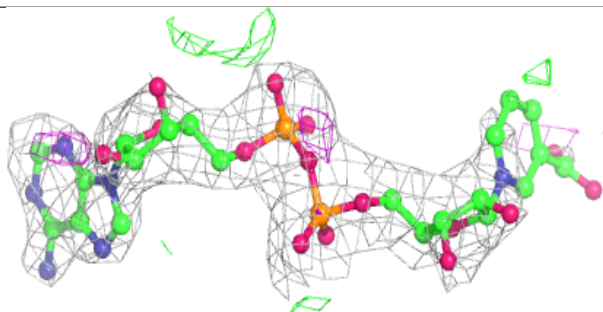
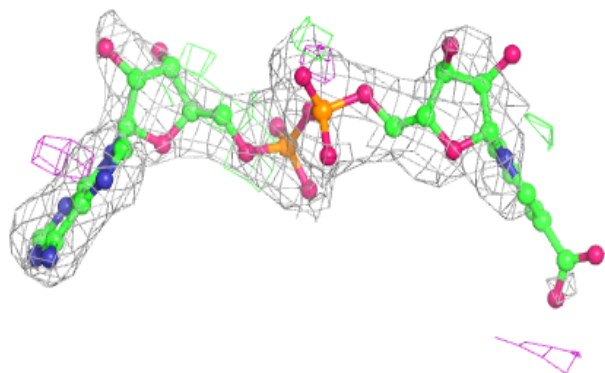
**Electron density around DND C 681:**

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

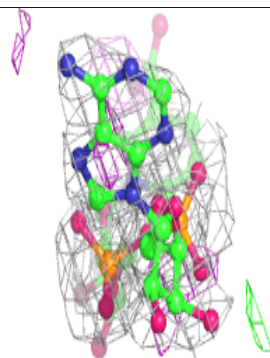
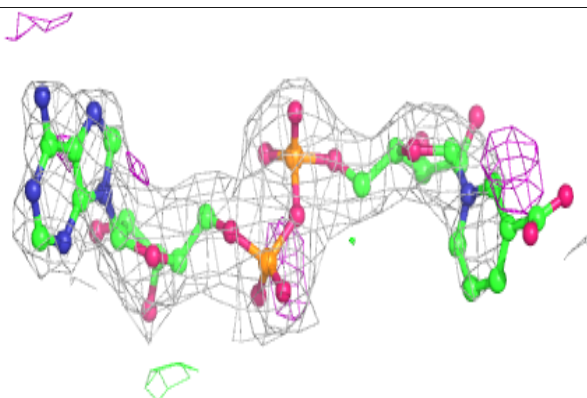
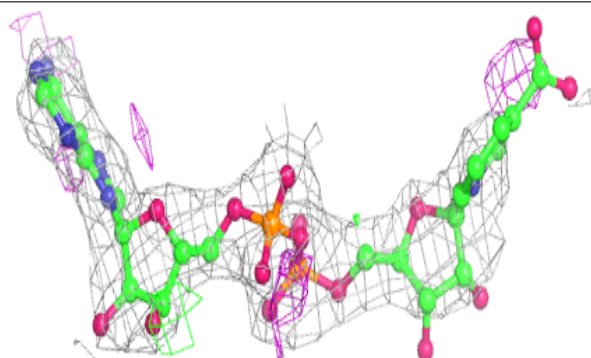


Electron density around DND D 681:

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

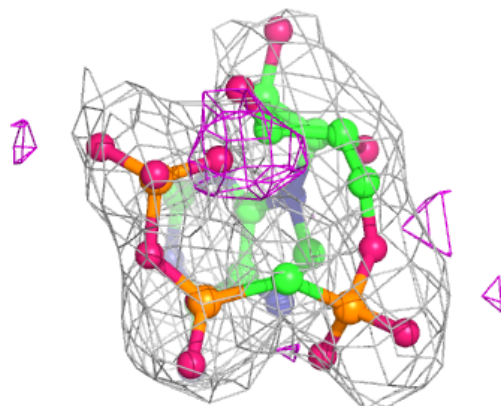
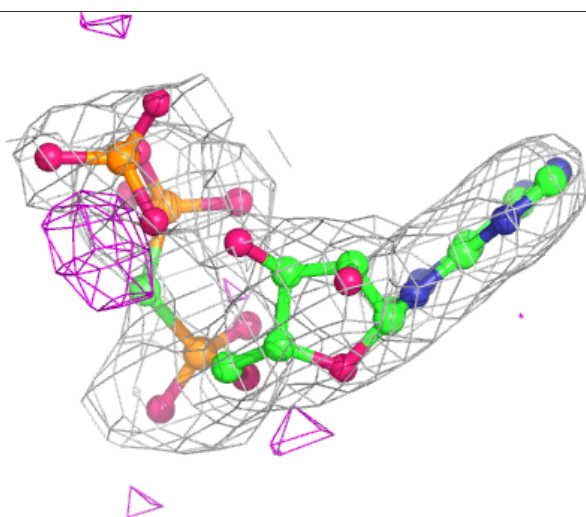
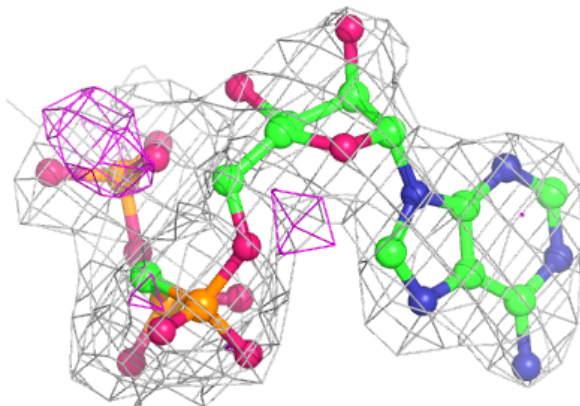
**Electron density around DND A 681:**

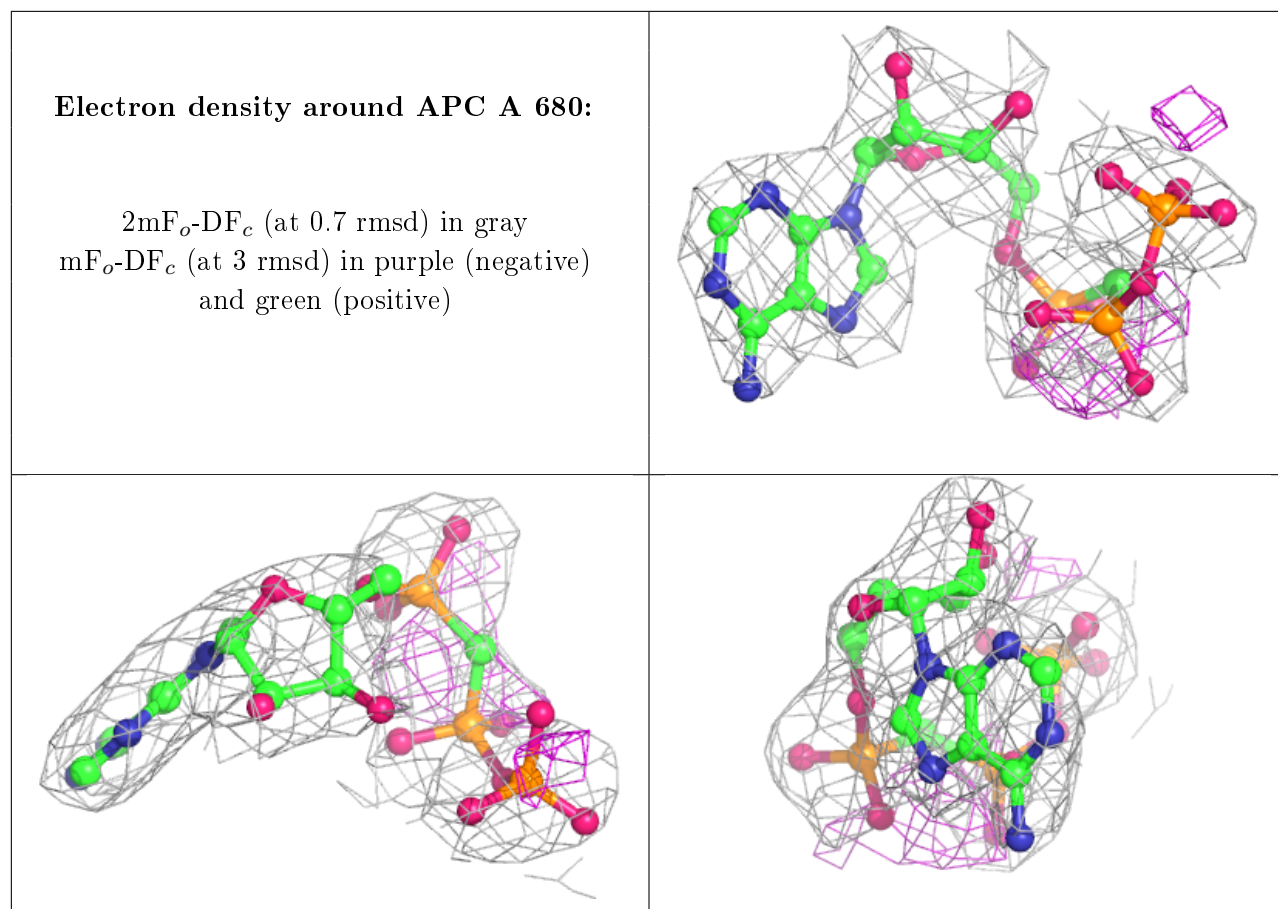
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around APC B 680:

$2mF_o-DF_c$ (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.