



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 07:59 pm BST

PDB ID : 5N69
Title : Cardiac muscle myosin S1 fragment in the pre-powerstroke state co-crystallized with the activator Omecamtiv Mecarbil
Authors : Planelles-Herrero, V.J.; Hartman, J.J.; Robert-Paganin, J.; Malik, F.I.; Houdusse, A.
Deposited on : 2017-02-14
Resolution : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

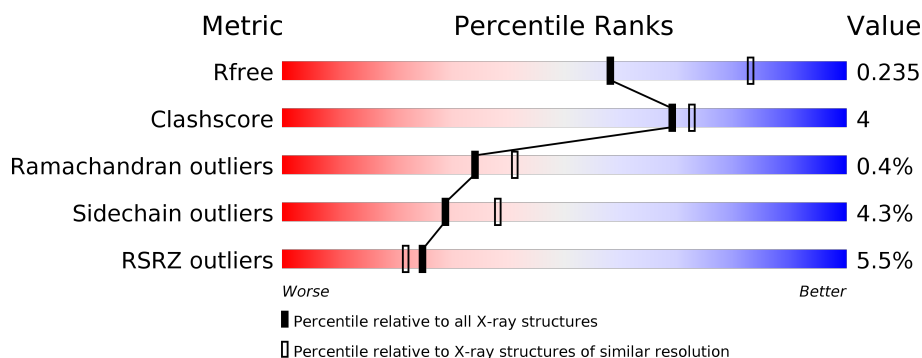
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	828	<div> <div>4%</div> <div>83%</div> <div>8%</div> <div>8%</div> </div>
1	B	828	<div> <div>4%</div> <div>82%</div> <div>9%</div> <div>8%</div> </div>
2	G	199	<div> <div>12%</div> <div>69%</div> <div>9%</div> <div>22%</div> </div>
2	H	199	<div> <div>6%</div> <div>65%</div> <div>14%</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	VO4	A	902	-	-	X	-
4	VO4	B	902	-	-	X	-
6	2OW	A	904	-	X	-	-
6	2OW	B	904	-	X	-	-
7	GOL	A	916	-	-	-	X
8	TCE	B	914	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 15990 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.

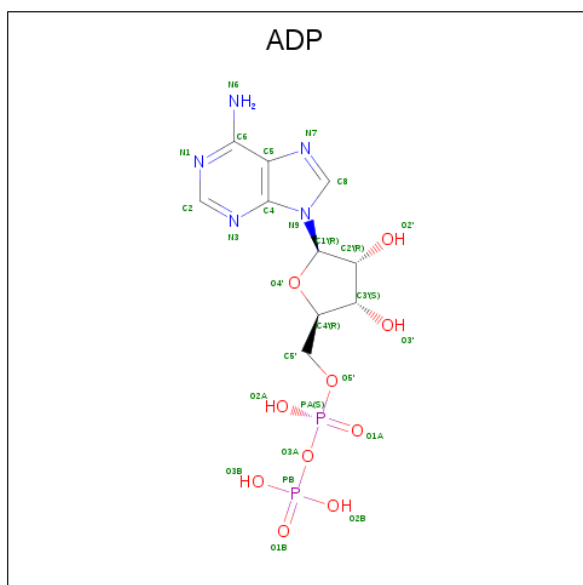
- Molecule 1 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	760	Total	C	N	O	S	0	3	0
			6164	3934	1057	1140	33			
1	B	765	Total	C	N	O	S	0	1	0
			6184	3950	1060	1142	32			

- Molecule 2 is a protein called Myosin light chain 3.

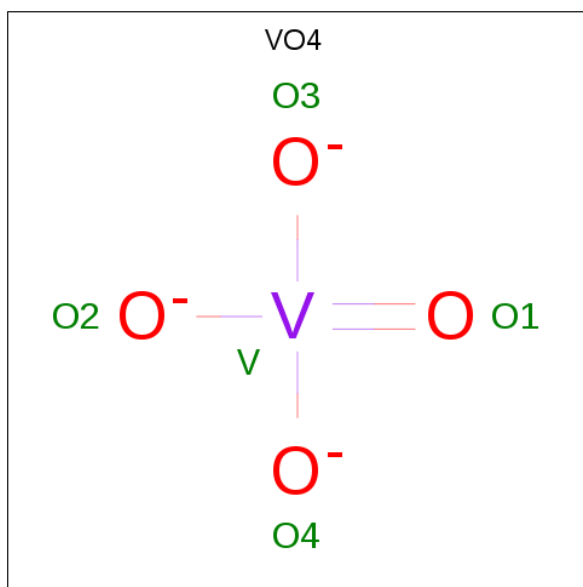
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	156	Total	C	N	O	S	0	0	0
			1234	778	203	243	10			
2	H	161	Total	C	N	O	S	0	0	0
			1275	804	209	252	10			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is VANADATE ION (three-letter code: VO4) (formula: O₄V).

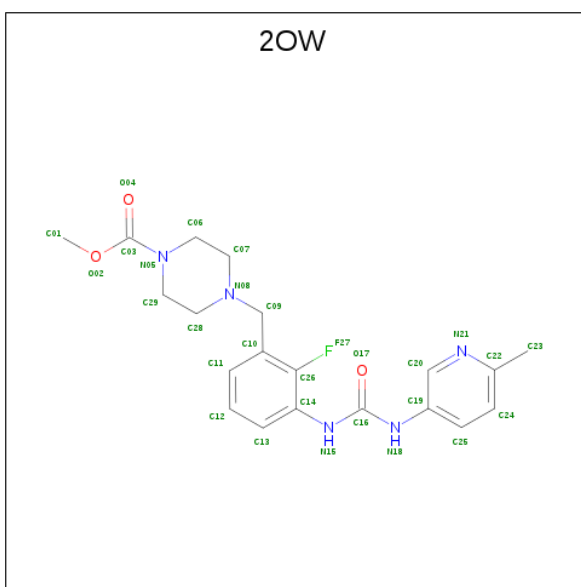


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	V	0	0
			5	4	1		
4	B	1	Total	O	V	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is methyl 4-(2-fluoro-3-{{(6-methylpyridin-3-yl)carbamoyl}amino}benzyl)piperazine-1-carboxylate (three-letter code: 2OW) (formula: C₂₀H₂₄FN₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			29	20	1	5	3		
6	B	1	Total	C	F	N	O	0	0
			29	20	1	5	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

Continued on next page...

Continued from previous page...

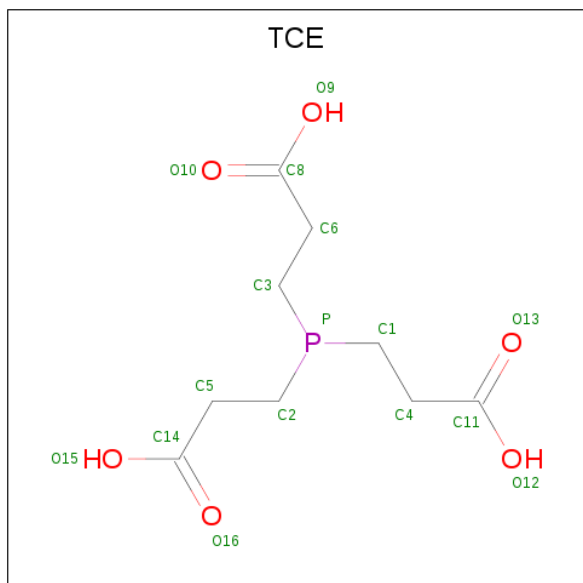
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			5	3	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		

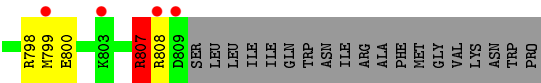
- Molecule 8 is 3,3',3''-phosphanetriyltripropanoic acid (three-letter code: TCE) (formula: $C_9H_{15}O_6P$).



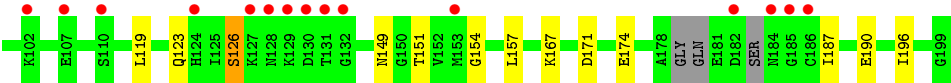
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	P	0	0
			16	9	6	1		

- Molecule 9 is water.

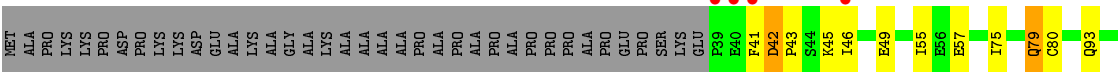
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	372	Total	O	0	0
			372	372		
9	B	343	Total	O	0	0
			343	343		
9	G	45	Total	O	0	0
			45	45		
9	H	84	Total	O	0	0
			84	84		



• Molecule 2: Myosin light chain 3



• Molecule 2: Myosin light chain 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.32Å 122.45Å 187.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.22 – 2.45 24.22 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.22-2.45) 99.3 (24.22-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.30	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.44Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.180 , 0.224 0.186 , 0.235	Depositor DCC
R_{free} test set	4145 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15990	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, ADP, VO4, M3L, TCE, 2OW

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	0.50	0/6275	0.69	2/8447 (0.0%)
1	B	0.49	0/6299	0.68	0/8479
2	G	0.47	0/1252	0.67	0/1678
2	H	0.50	0/1297	0.71	0/1741
All	All	0.49	0/15123	0.69	2/20345 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ALA	C-N-CA	6.02	136.74	121.70
1	A	449	THR	N-CA-C	-5.45	96.29	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6164	0	6153	44	0
1	B	6184	0	6183	50	0
2	G	1234	0	1213	9	0
2	H	1275	0	1252	16	0
3	A	27	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	0	0
4	A	5	0	0	3	0
4	B	5	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	29	0	24	1	0
6	B	29	0	24	3	0
7	A	78	0	104	5	0
7	B	54	0	72	5	0
7	H	17	0	21	3	0
8	B	16	0	12	0	0
9	A	372	0	0	1	0
9	B	343	0	0	3	0
9	G	45	0	0	0	0
9	H	84	0	0	0	0
All	All	15990	0	15082	113	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 4.

The worst 5 of 113 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:THR:CG2	1:B:660:THR:HG21	1.37	1.53
1:A:660:THR:HG21	1:B:660:THR:CG2	1.65	1.25
1:A:660:THR:CG2	1:B:660:THR:CG2	2.27	1.06
1:A:660:THR:HG22	1:B:660:THR:HG21	1.54	0.88
2:H:189:TYR:O	2:H:190:GLU:HB3	1.78	0.81

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	750/828 (91%)	724 (96%)	24 (3%)	2 (0%)	41	49
1	B	753/828 (91%)	730 (97%)	20 (3%)	3 (0%)	34	41
2	G	150/199 (75%)	144 (96%)	5 (3%)	1 (1%)	22	25
2	H	159/199 (80%)	156 (98%)	1 (1%)	2 (1%)	12	11
All	All	1812/2054 (88%)	1754 (97%)	50 (3%)	8 (0%)	34	41

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	190	GLU
1	A	147	ARG
1	A	267	LEU
1	B	267	LEU
1	B	807	ARG

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	664/715 (93%)	648 (98%)	16 (2%)	49	61
1	B	666/715 (93%)	632 (95%)	34 (5%)	24	31
2	G	135/165 (82%)	127 (94%)	8 (6%)	19	25
2	H	140/165 (85%)	128 (91%)	12 (9%)	10	11
All	All	1605/1760 (91%)	1535 (96%)	70 (4%)	29	37

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	397	LYS
1	B	578	SER
2	H	129	LYS
1	B	418	GLN
1	B	453[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	492	HIS
1	B	656	ASN
2	G	123	GLN
1	A	668	HIS
2	G	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	M3L	A	129	1	10,11,12	0.79	1 (10%)	9,14,16	0.93	1 (11%)
1	M3L	B	129	1	10,11,12	1.30	1 (10%)	9,14,16	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	M3L	A	129	1	-	0/9/10/12	-
1	M3L	B	129	1	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	M3L	CB-CA	3.94	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	M3L	CB-CA	2.10	1.56	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	M3L	CD-CE-NZ	2.38	125.95	116.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	GOL	H	201	-	3,4,5	0.02	0	1,4,5	0.02	0
7	GOL	A	905	-	5,5,5	0.11	0	5,5,5	0.70	0
7	GOL	B	907	-	5,5,5	0.09	0	5,5,5	0.24	0
7	GOL	A	909	-	5,5,5	0.21	0	5,5,5	0.67	0
7	GOL	B	910	-	5,5,5	0.04	0	5,5,5	0.22	0
3	ADP	B	901	5,4	24,29,29	0.69	0	29,45,45	0.88	2 (6%)
7	GOL	B	906	-	5,5,5	0.09	0	5,5,5	0.28	0
3	ADP	A	901	5,4	24,29,29	0.75	1 (4%)	29,45,45	0.90	2 (6%)
7	GOL	B	912	-	5,5,5	0.06	0	5,5,5	0.15	0
7	GOL	A	917	-	5,5,5	0.10	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	VO4	A	902	3,5	1,4,4	0.82	0	-		
7	GOL	B	909	-	5,5,5	0.08	0	5,5,5	0.28	0
4	VO4	B	902	3,5	1,4,4	0.58	0	-		
7	GOL	A	915	-	5,5,5	0.06	0	5,5,5	0.21	0
7	GOL	B	913	-	5,5,5	0.04	0	5,5,5	0.30	0
7	GOL	A	911	-	5,5,5	0.10	0	5,5,5	0.40	0
7	GOL	B	908	-	5,5,5	0.07	0	5,5,5	0.20	0
7	GOL	B	911	-	5,5,5	0.14	0	5,5,5	0.28	0
7	GOL	A	913	-	5,5,5	0.07	0	5,5,5	0.22	0
6	2OW	A	904	-	31,31,31	5.53	19 (61%)	41,42,42	4.12	25 (60%)
7	GOL	A	908	-	5,5,5	0.11	0	5,5,5	0.27	0
7	GOL	A	916	-	5,5,5	0.05	0	5,5,5	0.26	0
7	GOL	H	202	-	5,5,5	0.08	0	5,5,5	0.27	0
7	GOL	A	912	-	5,5,5	0.08	0	5,5,5	0.30	0
6	2OW	B	904	-	31,31,31	5.78	19 (61%)	41,42,42	3.84	27 (65%)
7	GOL	A	906	-	5,5,5	0.14	0	5,5,5	0.27	0
7	GOL	A	914	-	5,5,5	0.08	0	5,5,5	0.12	0
7	GOL	A	910	-	5,5,5	0.11	0	5,5,5	0.31	0
7	GOL	H	203	-	5,5,5	0.09	0	5,5,5	0.43	0
8	TCE	B	914	-	6,15,15	1.32	1 (16%)	9,18,18	3.75	5 (55%)
7	GOL	A	907	-	5,5,5	0.12	0	5,5,5	0.30	0
7	GOL	B	905	-	5,5,5	0.11	0	5,5,5	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	H	201	-	-	0/2/2/4	-
7	GOL	A	905	-	-	1/4/4/4	-
7	GOL	B	907	-	-	2/4/4/4	-
7	GOL	A	909	-	-	3/4/4/4	-
7	GOL	B	910	-	-	0/4/4/4	-
3	ADP	B	901	5,4	-	2/12/32/32	0/3/3/3
7	GOL	B	906	-	-	0/4/4/4	-
3	ADP	A	901	5,4	-	3/12/32/32	0/3/3/3
7	GOL	B	912	-	-	0/4/4/4	-
7	GOL	A	917	-	-	2/4/4/4	-
7	GOL	B	909	-	-	0/4/4/4	-
7	GOL	A	915	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	913	-	-	0/4/4/4	-
7	GOL	A	911	-	-	0/4/4/4	-
7	GOL	B	908	-	-	0/4/4/4	-
7	GOL	B	911	-	-	2/4/4/4	-
7	GOL	A	913	-	-	2/4/4/4	-
6	2OW	A	904	-	-	14/18/28/28	0/3/3/3
7	GOL	A	908	-	-	2/4/4/4	-
7	GOL	A	916	-	-	0/4/4/4	-
7	GOL	H	202	-	-	0/4/4/4	-
7	GOL	A	912	-	-	0/4/4/4	-
6	2OW	B	904	-	-	9/18/28/28	0/3/3/3
7	GOL	A	906	-	-	0/4/4/4	-
7	GOL	A	914	-	-	0/4/4/4	-
7	GOL	A	910	-	-	0/4/4/4	-
7	GOL	H	203	-	-	4/4/4/4	-
8	TCE	B	914	-	-	4/9/15/15	-
7	GOL	A	907	-	-	0/4/4/4	-
7	GOL	B	905	-	-	2/4/4/4	-

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	904	2OW	C10-C26	14.41	1.54	1.38
6	A	904	2OW	C10-C26	13.92	1.53	1.38
6	B	904	2OW	C03-N05	9.01	1.50	1.35
6	A	904	2OW	C03-N05	8.67	1.49	1.35
6	B	904	2OW	C11-C10	8.65	1.54	1.39

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	904	2OW	O17-C16-N18	-11.53	104.11	123.62
6	B	904	2OW	O17-C16-N18	-10.49	105.88	123.62
6	B	904	2OW	C19-C20-N21	-9.41	115.67	124.13
6	A	904	2OW	C19-C20-N21	-8.88	116.14	124.13
6	A	904	2OW	O17-C16-N15	-8.73	108.86	123.62

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

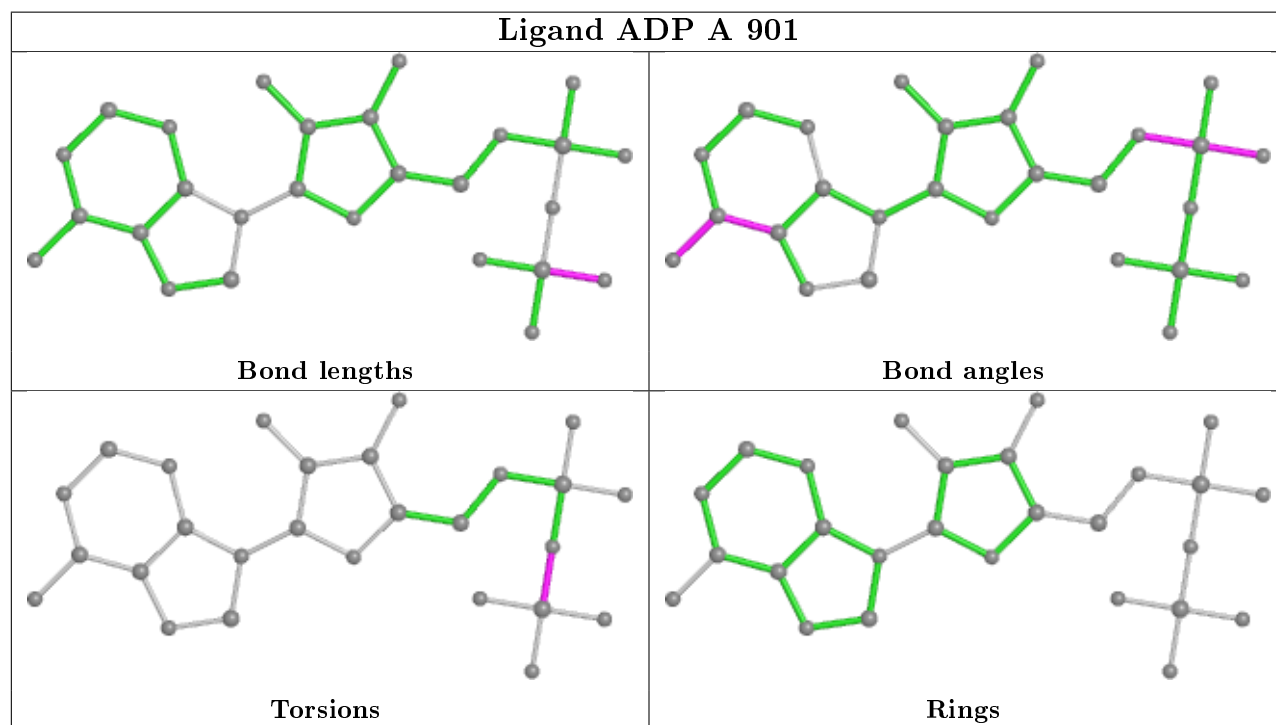
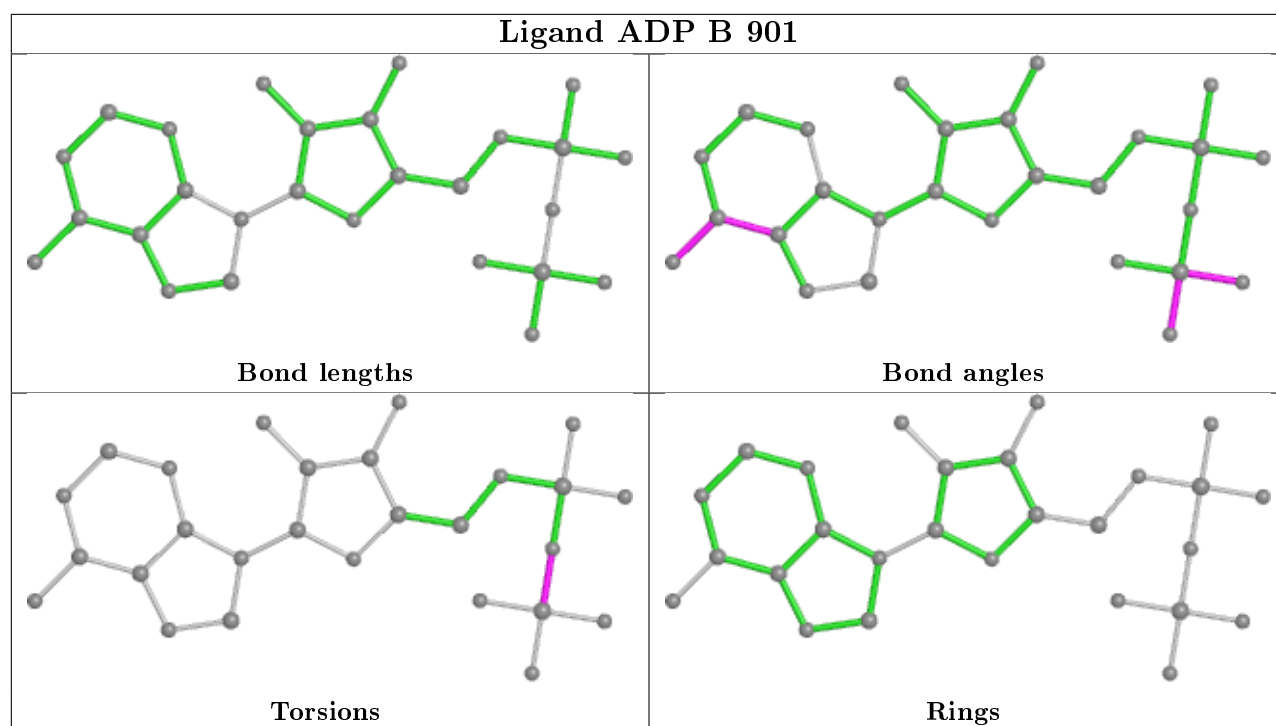
Mol	Chain	Res	Type	Atoms
7	A	909	GOL	O1-C1-C2-C3
3	B	901	ADP	PA-O3A-PB-O3B
3	A	901	ADP	PA-O3A-PB-O2B
7	A	917	GOL	O1-C1-C2-C3
6	A	904	2OW	O04-C03-O02-C01

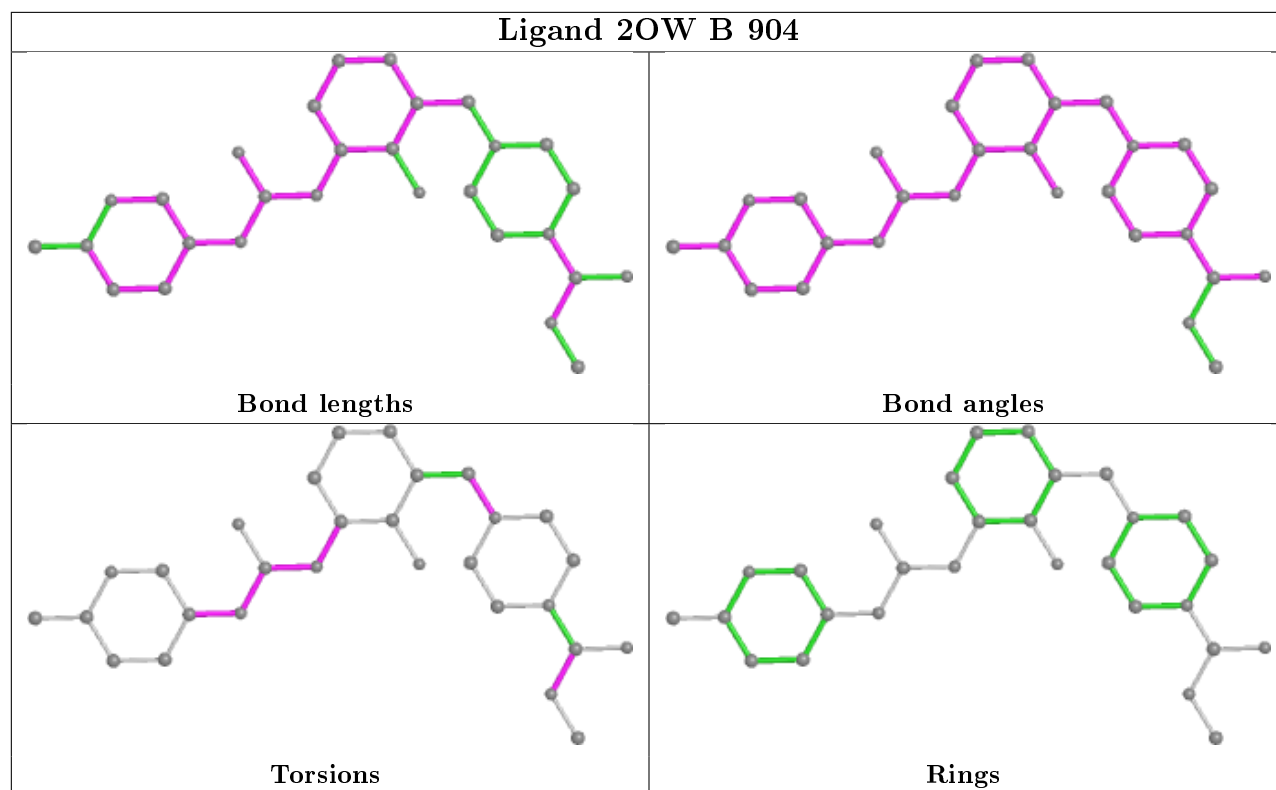
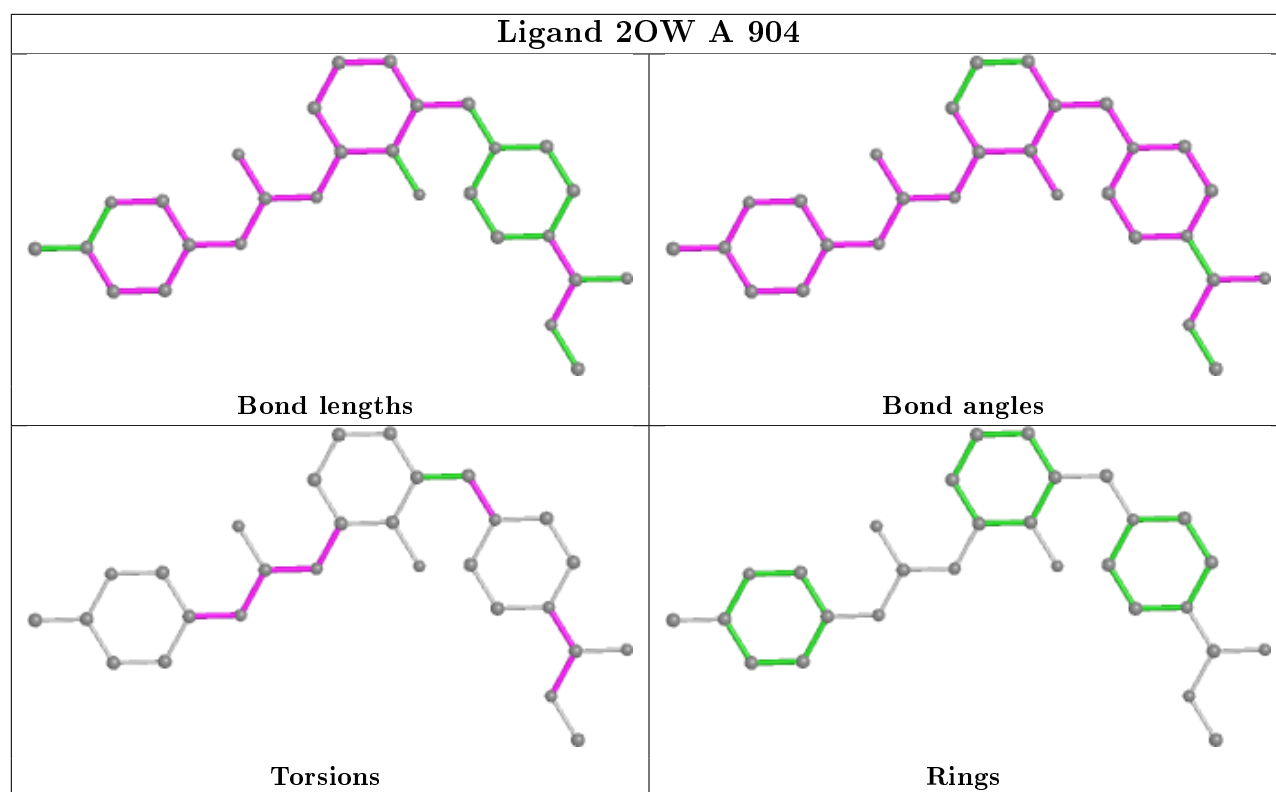
There are no ring outliers.

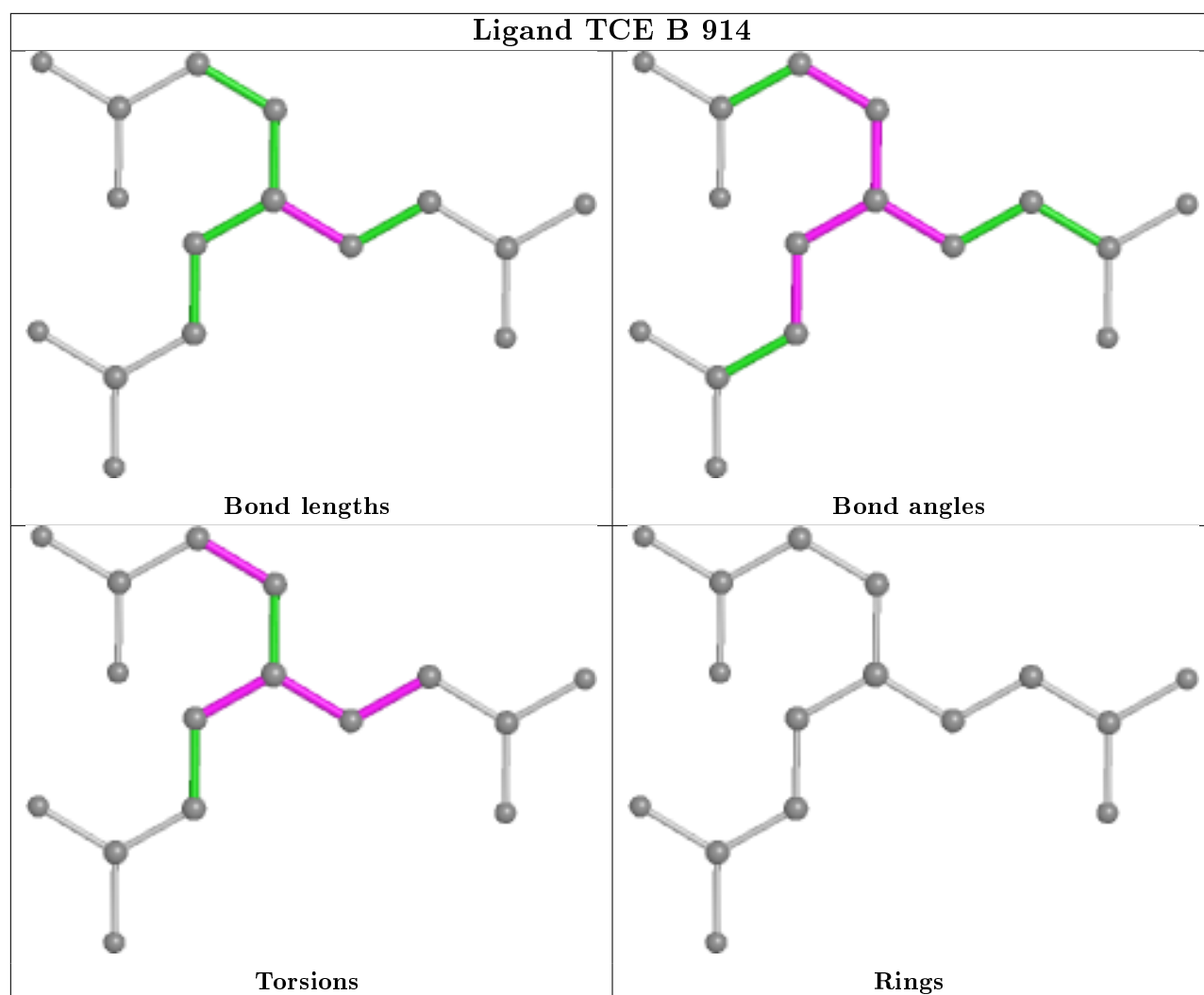
12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	907	GOL	2	0
7	A	909	GOL	2	0
4	A	902	VO4	3	0
4	B	902	VO4	2	0
7	B	908	GOL	2	0
7	B	911	GOL	1	0
6	A	904	2OW	1	0
7	H	202	GOL	2	0
7	A	912	GOL	1	0
6	B	904	2OW	3	0
7	A	906	GOL	2	0
7	H	203	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	759/828 (91%)	-0.07	30 (3%) 38 35	30, 48, 80, 130	2 (0%)
1	B	764/828 (92%)	-0.00	37 (4%) 30 28	31, 50, 87, 133	1 (0%)
2	G	156/199 (78%)	0.77	23 (14%) 2 1	57, 86, 137, 183	0
2	H	161/199 (80%)	0.14	12 (7%) 14 11	39, 55, 95, 139	0
All	All	1840/2054 (89%)	0.05	102 (5%) 25 22	30, 51, 95, 183	3 (0%)

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	809	ASP	8.9
2	G	41	PHE	8.6
1	B	808	ARG	8.0
2	H	39	PRO	7.4
2	H	40	GLU	7.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	M3L	B	129	12/13	0.96	0.20	39,43,47,48	0
1	M3L	A	129	12/13	0.97	0.16	44,47,50,51	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

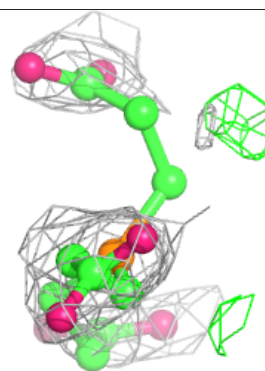
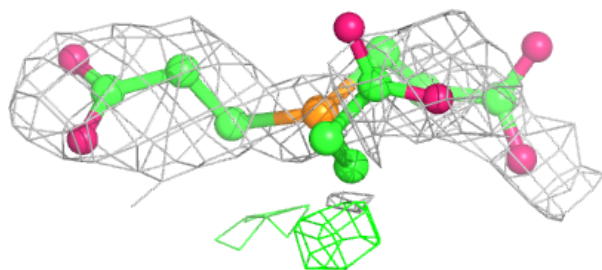
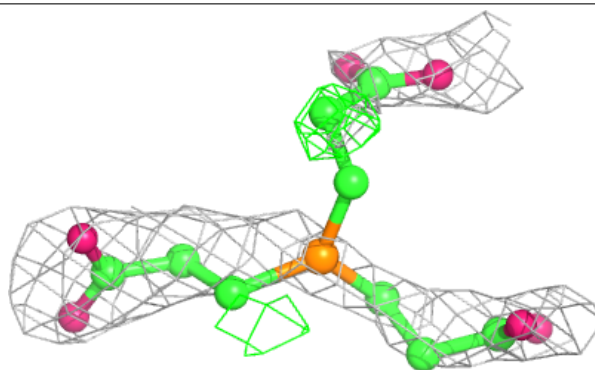
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	TCE	B	914	16/16	0.58	0.44	103,115,117,117	0
7	GOL	A	916	6/6	0.66	0.64	117,119,120,120	0
7	GOL	H	202	6/6	0.73	0.28	75,78,79,80	0
7	GOL	A	909	6/6	0.77	0.30	39,57,64,66	0
7	GOL	B	908	6/6	0.82	0.27	77,84,88,90	0
7	GOL	B	910	6/6	0.83	0.30	96,101,103,104	0
7	GOL	B	905	6/6	0.83	0.35	71,75,75,75	0
7	GOL	A	913	6/6	0.84	0.37	81,82,82,83	0
7	GOL	B	912	6/6	0.87	0.22	102,103,103,104	0
7	GOL	A	906	6/6	0.88	0.21	58,59,61,66	0
7	GOL	B	907	6/6	0.88	0.19	71,73,73,74	0
7	GOL	B	909	6/6	0.88	0.23	97,98,98,98	0
7	GOL	A	911	6/6	0.90	0.17	67,71,72,72	0
7	GOL	H	201	5/6	0.90	0.16	66,67,69,73	0
7	GOL	A	915	6/6	0.90	0.41	82,83,84,85	0
7	GOL	A	907	6/6	0.90	0.17	71,73,76,76	0
7	GOL	B	913	6/6	0.90	0.35	63,68,72,75	0
7	GOL	B	911	6/6	0.91	0.21	59,64,67,70	0
7	GOL	B	906	6/6	0.91	0.25	75,78,80,82	0
7	GOL	A	908	6/6	0.91	0.21	72,73,74,74	0
7	GOL	A	905	6/6	0.92	0.14	60,61,66,69	0
7	GOL	A	912	6/6	0.92	0.21	60,71,75,77	0
7	GOL	A	910	6/6	0.93	0.24	65,66,72,75	0
7	GOL	H	203	6/6	0.94	0.17	58,59,60,61	0
7	GOL	A	917	6/6	0.94	0.17	64,67,70,70	0
7	GOL	A	914	6/6	0.95	0.34	65,66,68,68	0
6	2OW	B	904	29/29	0.96	0.11	31,42,58,65	0
6	2OW	A	904	29/29	0.96	0.12	32,39,61,66	0
5	MG	B	903	1/1	0.97	0.16	43,43,43,43	0
3	ADP	A	901	27/27	0.98	0.09	32,41,45,46	0
3	ADP	B	901	27/27	0.98	0.12	35,40,43,45	0
4	VO4	A	902	5/5	0.99	0.11	38,38,41,45	0
4	VO4	B	902	5/5	0.99	0.14	39,41,45,47	0
5	MG	A	903	1/1	0.99	0.10	38,38,38,38	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.

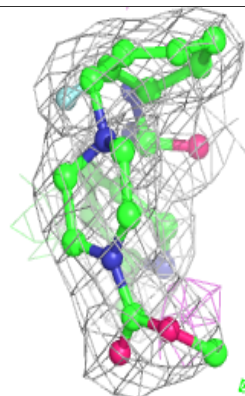
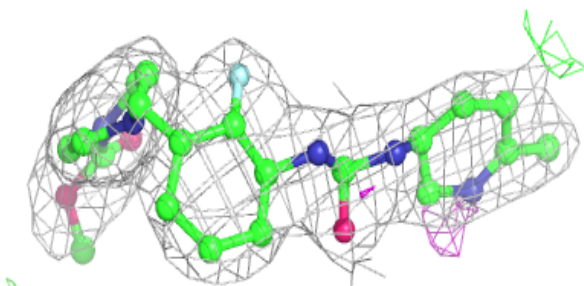
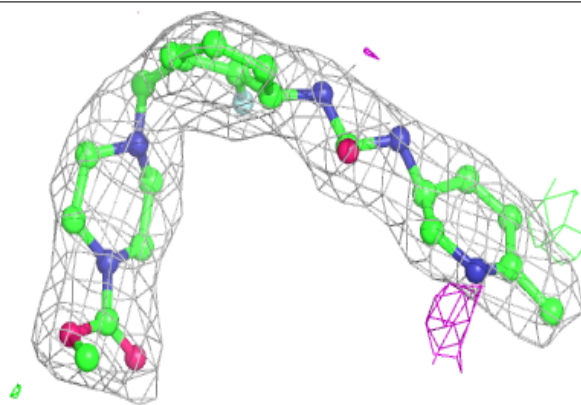
Electron density around TCE B 914:

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



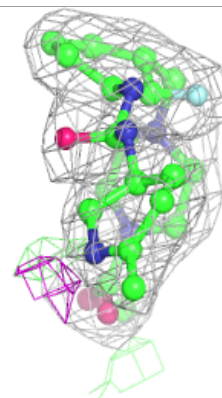
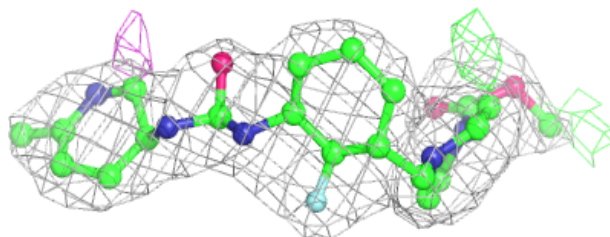
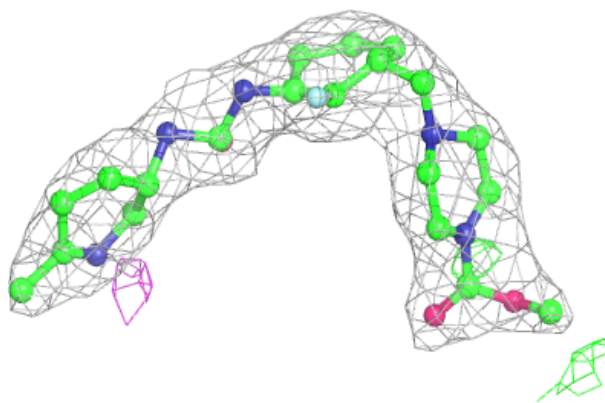
Electron density around 2OW B 904:

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

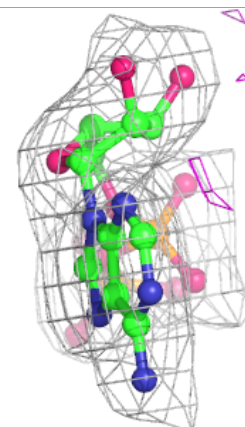
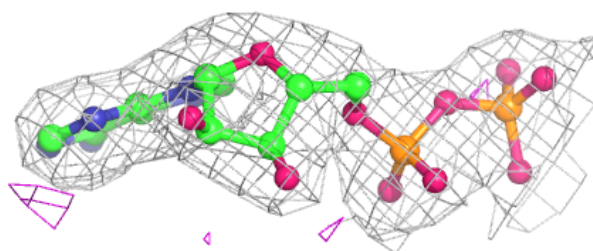
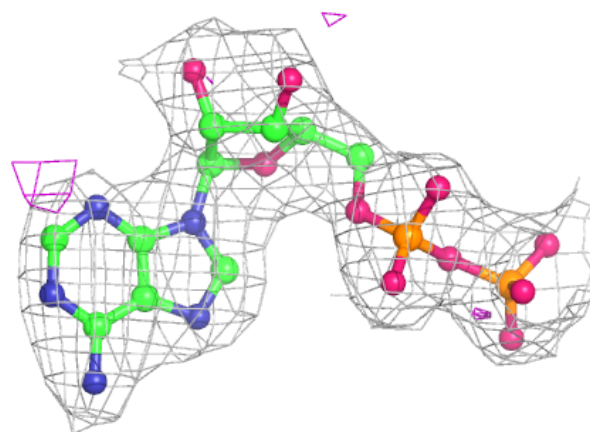


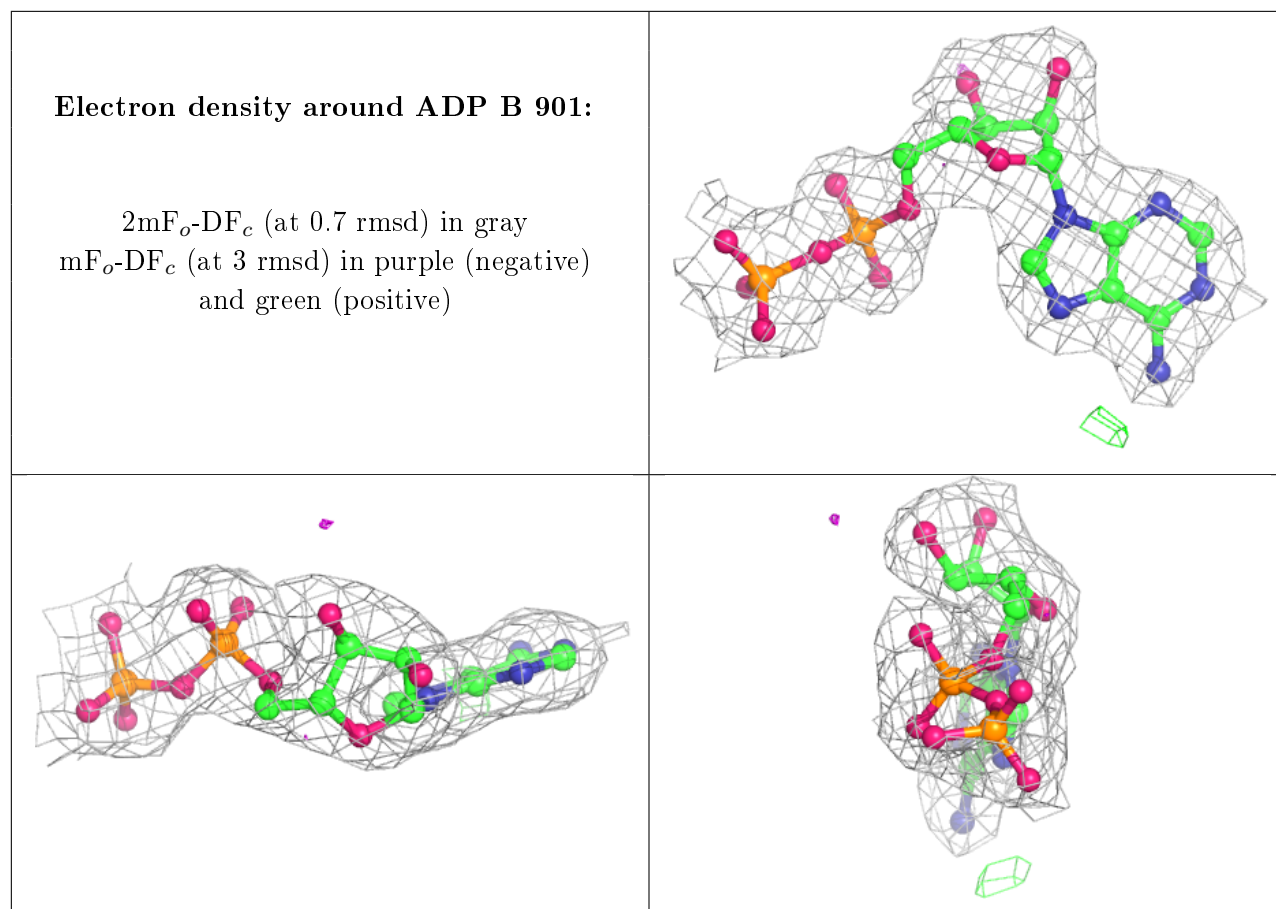
Electron density around 2OW A 904:

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

**Electron density around ADP A 901:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.