



Full wwPDB X-ray Structure Validation 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 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

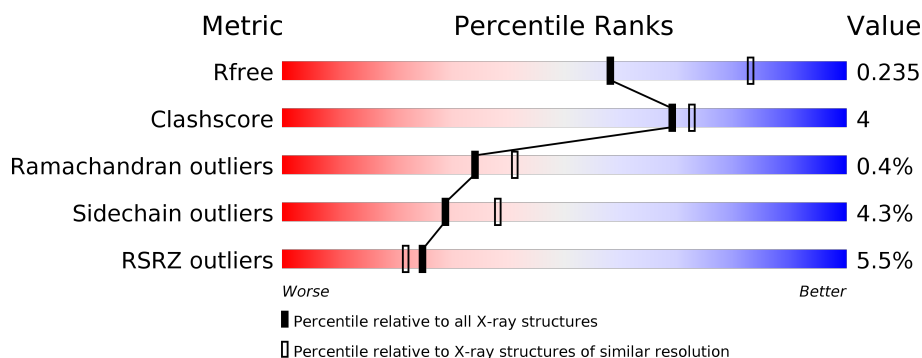
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.

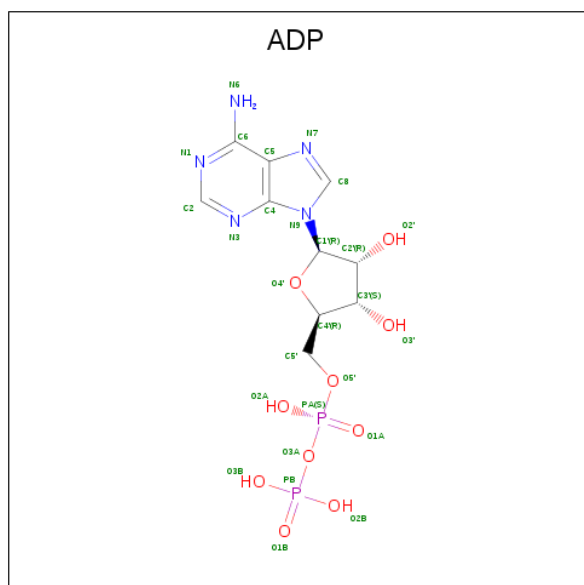
- Molecule 1 is a protein called Myosin-7.

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.

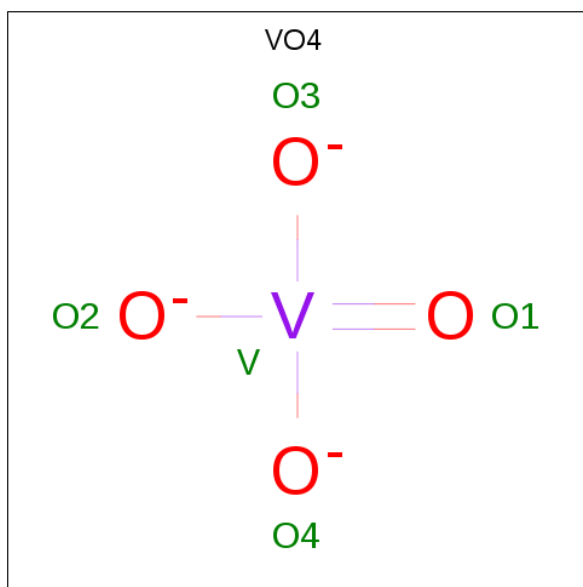
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	156	Total	C	N	O	S	0	0	0
			1234	778	203	243	10			
2	H	161	Total	C	N	O	S	0	0	0
			1275	804	209	252	10			

- 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).

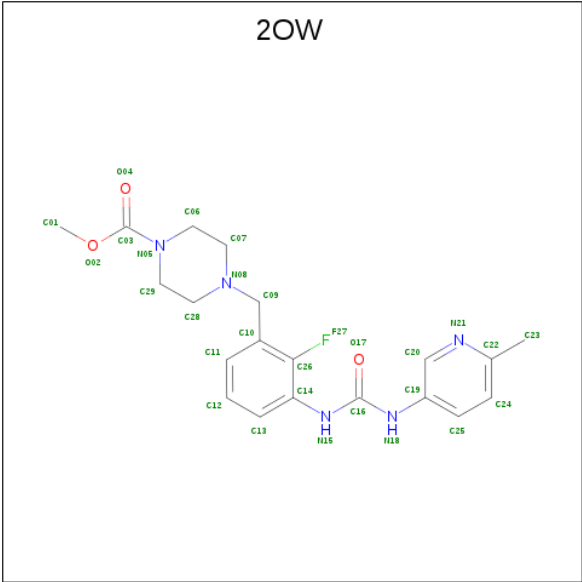


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	V	0	0
			5	4	1		
4	B	1	Total	O	V	0	0
			5	4	1		

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

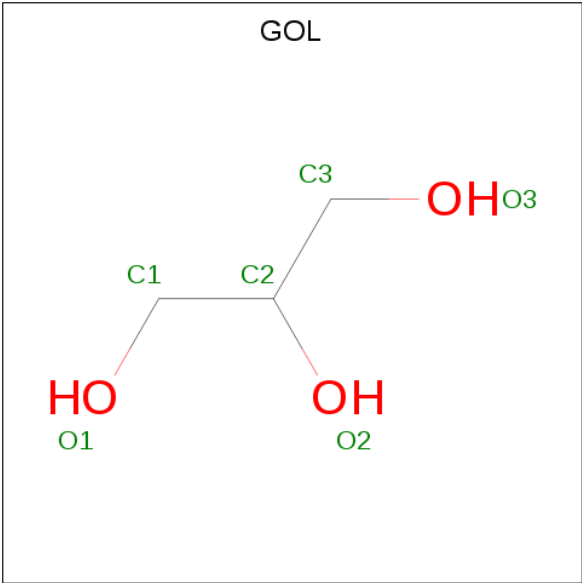
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- 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		

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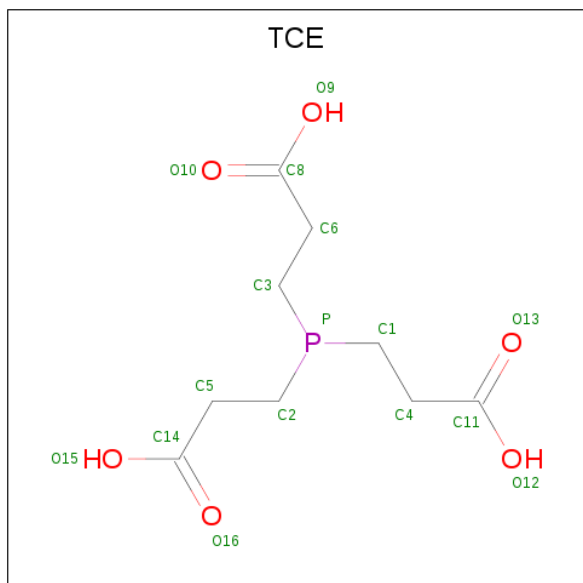
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total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

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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		

These plots are drawn for all protein, RNA and DNA 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.

Chain A:

Chain B:

4% 82% 9% 8%

MET VAL ASP ALA E5 F31 D42 L52 S53 R54 E55 G56 G57 K58 V59 E62 T63 E64 H65 G66 K67 T70 P81 K86 S111 S118 R143 G144 K145 K146 R147 S148 E149 S156 Q163 Y164 T167 Q172 S173 E179 I192 I198



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

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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.

All (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
1:B:513:PHE:H	7:B:908:GOL:H31	1.53	0.73
1:A:577:PHE:HE1	1:A:590:ILE:CD1	2.03	0.71
1:A:172:GLN:OE1	1:A:668:HIS:HE1	1.74	0.71
1:B:172:GLN:OE1	1:B:668:HIS:HE1	1.73	0.71
1:B:215:THR:HG22	1:B:218:ASP:H	1.56	0.70
1:A:660:THR:HG21	1:B:660:THR:HG21	0.72	0.70
1:A:277:LEU:HB3	7:A:912:GOL:H12	1.73	0.70
1:A:454:GLN:OE1	1:B:532:SER:HB3	1.92	0.69
1:A:660:THR:HG22	1:B:660:THR:CG2	2.13	0.69
1:B:504:GLU:HG2	1:B:764:PHE:HE1	1.58	0.67
1:B:216:LEU:O	1:B:220:ILE:HG13	1.94	0.67
1:B:145:LYS:HD3	1:B:149:GLU:HG3	1.77	0.65
1:A:143:ARG:CD	1:A:198:ILE:HD12	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LYS:HD2	1:B:163:GLN:HG3	1.79	0.65
1:A:577:PHE:HE1	1:A:590:ILE:HD11	1.61	0.64
2:G:49:GLU:H	2:G:123:GLN:NE2	1.96	0.64
2:H:49:GLU:H	2:H:123:GLN:NE2	1.96	0.64
1:B:795:VAL:HG12	1:B:799:MET:CE	2.29	0.63
7:B:911:GOL:H12	9:B:1053:HOH:O	1.99	0.62
4:A:902:VO4:O2	4:A:902:VO4:V	1.55	0.61
1:B:791:GLN:HG3	2:G:196:ILE:HG22	1.82	0.61
4:A:902:VO4:V	4:A:902:VO4:O1	1.58	0.61
1:A:513:PHE:H	7:A:906:GOL:H12	1.66	0.60
1:B:179:GLU:HB2	1:B:674:ILE:HD11	1.83	0.60
4:B:902:VO4:V	4:B:902:VO4:O3	1.58	0.60
4:B:902:VO4:V	4:B:902:VO4:O4	1.59	0.60
4:A:902:VO4:O4	4:A:902:VO4:V	1.59	0.60
1:A:143:ARG:HD2	1:A:198:ILE:HD12	1.84	0.59
1:A:192:ILE:HD11	1:A:248:ILE:HD13	1.84	0.59
1:A:532:SER:HB3	1:B:454:GLN:OE1	2.02	0.59
1:B:192:ILE:HD11	1:B:248:ILE:HD13	1.85	0.57
2:H:55:ILE:HD12	2:H:119:LEU:HD21	1.87	0.56
1:A:143:ARG:HD3	1:A:198:ILE:HD12	1.88	0.56
2:G:55:ILE:HD12	2:G:119:LEU:HD21	1.88	0.55
1:B:63:THR:HG22	1:B:65:HIS:H	1.71	0.54
1:B:795:VAL:HG12	1:B:799:MET:HE2	1.89	0.54
1:A:63:THR:HG22	1:A:65:HIS:H	1.71	0.54
1:B:791:GLN:CG	2:G:196:ILE:HG22	2.38	0.53
2:H:179:GLY:HA2	2:H:180:GLN:CB	2.39	0.53
1:A:484:LYS:HD3	1:A:655:LEU:HD22	1.91	0.53
2:H:93:GLN:OE1	7:H:203:GOL:H12	2.09	0.53
1:B:484:LYS:HD3	1:B:655:LEU:HD22	1.89	0.52
1:B:251:HIS:HB3	1:B:453[B]:ARG:HG2	1.91	0.52
2:H:93:GLN:NE2	7:H:202:GOL:H2	2.25	0.52
1:B:668:HIS:HD2	9:B:1124:HOH:O	1.93	0.51
1:A:17:ARG:HD2	7:A:909:GOL:H12	1.92	0.51
1:B:468:PHE:HB3	7:B:907:GOL:H32	1.93	0.51
2:H:157:LEU:HD23	2:H:187:ILE:HD13	1.92	0.51
1:A:577:PHE:CE1	1:A:590:ILE:CD1	2.90	0.51
1:A:616:MET:O	1:A:620:LEU:HG	2.12	0.50
2:G:154:GLY:HA2	2:G:187:ILE:HD12	1.94	0.50
1:A:712:ARG:HD2	9:A:1189:HOH:O	2.12	0.49
2:G:157:LEU:HD23	2:G:187:ILE:HD13	1.94	0.49
2:H:154:GLY:HA2	2:H:187:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:HIS:ND1	1:B:590:ILE:HG13	2.27	0.49
1:A:671:ARG:NH2	1:A:696:ASN:O	2.46	0.49
1:A:528:MET:SD	1:B:454:GLN:HG2	2.53	0.48
1:B:671:ARG:NH2	1:B:696:ASN:O	2.47	0.47
2:H:179:GLY:CA	2:H:180:GLN:HB2	2.44	0.47
1:B:616:MET:O	1:B:620:LEU:HG	2.14	0.47
1:A:146:LYS:HA	6:A:904:2OW:H6	1.96	0.47
2:H:93:GLN:HE22	7:H:202:GOL:H2	1.79	0.47
2:H:177:MET:O	2:H:180:GLN:HA	2.14	0.47
1:A:499:GLU:HG2	1:A:503[B]:LYS:HE3	1.96	0.47
1:B:504:GLU:HG2	1:B:764:PHE:CE1	2.45	0.47
1:B:54:ARG:HG3	1:B:59:VAL:HG22	1.98	0.46
1:A:86:LYS:HE2	1:A:111:SER:OG	2.15	0.46
1:B:770:LEU:HD23	6:B:904:2OW:H7	1.97	0.46
1:B:228:GLU:O	1:B:232:ASN:HB2	2.16	0.45
2:H:80:CYS:HB2	2:H:113:MET:HE1	1.98	0.45
1:B:86:LYS:HE2	1:B:111:SER:OG	2.17	0.45
1:B:235:THR:HA	1:B:280:GLU:HG2	1.99	0.45
1:B:143:ARG:HD3	1:B:198:ILE:HD12	1.98	0.45
1:B:164:TYR:HE1	6:B:904:2OW:C16	2.30	0.44
1:B:363:LYS:HB3	1:B:376:ASP:HB2	1.99	0.44
2:H:178:ALA:HA	2:H:179:GLY:HA2	1.79	0.44
1:A:52:LEU:HD11	1:A:62:GLU:HB2	1.99	0.44
1:B:52:LEU:HD11	1:B:62:GLU:HB2	1.99	0.44
1:B:795:VAL:HG12	1:B:799:MET:HE3	1.98	0.44
1:A:228:GLU:O	1:A:232:ASN:HB2	2.17	0.44
1:A:224:ASN:HD21	1:A:246:LYS:HE3	1.83	0.44
1:A:569:ILE:HG22	1:A:570:LYS:HE2	1.98	0.44
1:B:576:HIS:CG	1:B:590:ILE:HG13	2.53	0.43
1:A:656:ASN:O	1:A:660:THR:HG23	2.18	0.43
1:A:235:THR:HA	1:A:280:GLU:HG2	2.00	0.43
1:B:173:SER:HB3	1:B:665:THR:HG21	2.01	0.42
2:G:89:GLN:NE2	2:G:126:SER:HA	2.33	0.42
1:A:98:GLU:HB3	1:A:690:MET:HE3	2.01	0.42
2:H:75:ILE:HB	2:H:79:GLN:HG3	2.01	0.42
2:H:41:PHE:HB3	2:H:43:PRO:HD2	2.01	0.42
1:B:469:ASP:HB2	7:B:907:GOL:H2	2.01	0.42
1:A:54:ARG:HG3	1:A:59:VAL:HG22	2.01	0.42
2:G:49:GLU:H	2:G:123:GLN:HE21	1.67	0.42
1:B:167:THR:HG21	6:B:904:2OW:C10	2.50	0.41
1:A:513:PHE:H	7:A:906:GOL:C1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:PHE:O	1:A:440:VAL:HG23	2.20	0.41
1:B:436:PHE:O	1:B:440:VAL:HG23	2.21	0.41
1:B:494:PHE:HB3	7:B:908:GOL:H32	2.03	0.41
1:A:7:ALA:HB2	7:A:909:GOL:O2	2.21	0.40
1:B:243:ARG:HD2	1:B:272:ARG:NE	2.37	0.40
1:A:33:LEU:HG	1:A:78:GLN:HE22	1.85	0.40
1:A:97:HIS:CE1	1:A:100:ALA:HB2	2.57	0.40
1:A:388:MET:HB2	1:A:388:MET:HE2	2.02	0.40
1:A:715:TYR:HB3	1:A:738:SER:HB3	2.03	0.40
1:B:807:ARG:HG3	9:B:1301:HOH:O	2.22	0.40
1:B:798:ARG:HD3	2:G:85:ARG:O	2.22	0.40
1:A:243:ARG:HD2	1:A:272:ARG:NE	2.36	0.40
2:H:42:ASP:N	2:H:43:PRO:HD2	2.36	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	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

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	190	GLU
1	A	147	ARG

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Mol	Chain	Res	Type
1	A	267	LEU
1	B	267	LEU
1	B	807	ARG
2	H	180	GLN
1	B	148	SER
2	G	167	LYS

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

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	SER
1	A	237	ARG
1	A	243	ARG
1	A	318	THR
1	A	384	SER
1	A	437	ASN
1	A	578	SER
1	A	590	ILE
1	A	607	ASP
1	A	645	GLN
1	A	650	LEU
1	A	655	LEU
1	A	699	LEU
1	A	736	ILE
1	A	787	ARG

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Mol	Chain	Res	Type
1	A	800	GLU
1	B	67	LYS
1	B	118	SER
1	B	145	LYS
1	B	146	LYS
1	B	148	SER
1	B	149	GLU
1	B	156	SER
1	B	215	THR
1	B	237	ARG
1	B	243	ARG
1	B	267	LEU
1	B	313	ILE
1	B	327	GLU
1	B	376	ASP
1	B	384	SER
1	B	397	LYS
1	B	418	GLN
1	B	437	ASN
1	B	453[A]	ARG
1	B	453[B]	ARG
1	B	526	LYS
1	B	549	LYS
1	B	570	LYS
1	B	578	SER
1	B	607	ASP
1	B	655	LEU
1	B	665	THR
1	B	674	ILE
1	B	700	GLU
1	B	712	ARG
1	B	780	ARG
1	B	800	GLU
1	B	807	ARG
1	B	808	ARG
2	G	45	LYS
2	G	46	ILE
2	G	126	SER
2	G	149	ASN
2	G	151	THR
2	G	171	ASP
2	G	174	GLU

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Mol	Chain	Res	Type
2	G	190	GLU
2	H	42	ASP
2	H	45	LYS
2	H	46	ILE
2	H	57	GLU
2	H	79	GLN
2	H	126	SER
2	H	129	LYS
2	H	151	THR
2	H	164	LEU
2	H	171	ASP
2	H	174	GLU
2	H	175	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	78	GLN
1	A	224	ASN
1	A	668	HIS
1	B	492	HIS
1	B	656	ASN
1	B	668	HIS
2	G	89	GLN
2	G	123	GLN
2	G	149	ASN
2	H	123	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
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
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	-
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	-

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	904	2OW	C03-N05	8.67	1.49	1.35
6	B	904	2OW	C11-C10	8.65	1.54	1.39
6	B	904	2OW	C13-C14	8.58	1.54	1.39
6	A	904	2OW	C11-C10	8.54	1.54	1.39
6	B	904	2OW	O17-C16	8.38	1.40	1.23
6	B	904	2OW	C20-N21	8.22	1.51	1.34
6	A	904	2OW	C20-N21	8.09	1.51	1.34
6	B	904	2OW	C14-C26	8.08	1.52	1.38
6	A	904	2OW	C13-C14	8.07	1.53	1.39
6	A	904	2OW	C14-C26	7.93	1.52	1.38
6	B	904	2OW	C12-C11	7.74	1.55	1.38
6	A	904	2OW	O17-C16	7.73	1.39	1.23
6	A	904	2OW	C12-C11	7.69	1.55	1.38
6	B	904	2OW	C12-C13	7.62	1.55	1.38
6	A	904	2OW	C12-C13	7.28	1.54	1.38
6	B	904	2OW	C24-C22	7.16	1.55	1.39
6	A	904	2OW	C24-C22	7.00	1.55	1.39
6	A	904	2OW	C20-C19	6.77	1.51	1.39
6	B	904	2OW	C20-C19	6.72	1.51	1.39
6	B	904	2OW	O02-C03	5.60	1.44	1.34
6	B	904	2OW	C25-C24	5.47	1.48	1.38
6	A	904	2OW	C25-C24	5.15	1.48	1.38
6	B	904	2OW	C25-C19	5.08	1.47	1.39
6	B	904	2OW	C16-N15	4.95	1.47	1.37
6	B	904	2OW	C16-N18	4.88	1.47	1.37
6	A	904	2OW	O02-C03	4.88	1.42	1.34
6	A	904	2OW	C16-N15	4.49	1.46	1.37
6	A	904	2OW	C16-N18	4.37	1.46	1.37
6	A	904	2OW	C25-C19	3.89	1.45	1.39
6	B	904	2OW	C14-N15	3.62	1.48	1.41
6	B	904	2OW	C19-N18	3.45	1.48	1.41
6	A	904	2OW	C14-N15	3.40	1.48	1.41
6	B	904	2OW	C09-C10	3.18	1.56	1.51
6	A	904	2OW	C19-N18	3.12	1.48	1.41
6	A	904	2OW	C09-C10	3.07	1.56	1.51
3	A	901	ADP	PB-O3B	-2.48	1.45	1.54
8	B	914	TCE	P-C2	2.10	1.87	1.84

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
6	A	904	2OW	C19-N18-C16	-8.52	109.18	126.61
6	B	904	2OW	O17-C16-N15	-8.21	109.74	123.62
6	A	904	2OW	C14-N15-C16	-7.79	108.10	125.39
6	A	904	2OW	C09-C10-C26	-6.81	110.83	121.48
6	B	904	2OW	C14-N15-C16	-6.65	110.63	125.39
8	B	914	TCE	C1-P-C2	6.47	121.57	100.95
6	B	904	2OW	C19-N18-C16	-6.44	113.43	126.61
8	B	914	TCE	C1-P-C3	5.78	119.37	100.95
8	B	914	TCE	C3-P-C2	5.65	118.94	100.95
6	B	904	2OW	C20-N21-C22	5.38	123.68	117.45
6	A	904	2OW	C09-C10-C11	-4.79	110.66	120.11
6	A	904	2OW	C29-N05-C06	4.69	121.64	112.62
6	B	904	2OW	C13-C14-N15	-4.19	112.08	121.80
6	B	904	2OW	C25-C19-N18	-4.06	106.75	120.40
6	B	904	2OW	F27-C26-C14	-4.00	111.70	118.32
6	A	904	2OW	C24-C25-C19	-3.98	115.70	120.30
6	A	904	2OW	C25-C19-N18	-3.97	107.07	120.40
6	B	904	2OW	C09-C10-C11	-3.88	112.46	120.11
6	B	904	2OW	C26-C14-N15	-3.82	109.36	116.98
6	A	904	2OW	F27-C26-C10	-3.75	113.88	117.85
6	B	904	2OW	C14-C26-C10	-3.73	116.92	121.53
6	B	904	2OW	N18-C16-N15	-3.52	106.34	112.49
6	B	904	2OW	C28-C29-N05	3.50	117.94	110.44
6	B	904	2OW	C29-N05-C06	3.39	119.15	112.62
6	A	904	2OW	C13-C14-N15	-3.33	114.07	121.80
6	A	904	2OW	C14-C26-C10	-3.33	117.42	121.53
6	B	904	2OW	C09-C10-C26	-3.22	116.44	121.48
6	A	904	2OW	C10-C09-N08	-3.22	107.11	112.75
6	A	904	2OW	F27-C26-C14	-3.12	113.16	118.32
8	B	914	TCE	P-C1-C4	-3.08	110.06	113.67
6	A	904	2OW	C07-C06-N05	3.06	117.00	110.44
6	A	904	2OW	C28-C29-N05	3.05	116.97	110.44
8	B	914	TCE	P-C3-C6	-2.97	110.19	113.67
6	B	904	2OW	C12-C11-C10	-2.95	116.49	120.89
6	A	904	2OW	C25-C24-C22	-2.90	117.06	119.94
6	B	904	2OW	C07-C06-N05	2.89	116.62	110.44
6	A	904	2OW	C23-C22-N21	2.83	121.74	117.78
6	B	904	2OW	C11-C10-C26	2.67	118.38	116.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	904	2OW	C06-C07-N08	2.67	116.12	110.64
6	A	904	2OW	C13-C14-C26	2.52	121.52	117.80
3	B	901	ADP	O3B-PB-O2B	2.45	117.00	107.64
6	A	904	2OW	C20-C19-N18	-2.44	111.85	120.16
6	A	904	2OW	N18-C16-N15	-2.41	108.27	112.49
6	B	904	2OW	C10-C09-N08	-2.39	108.56	112.75
3	A	901	ADP	C5-C6-N6	2.39	123.98	120.35
6	B	904	2OW	C23-C22-N21	2.38	121.11	117.78
6	B	904	2OW	C29-C28-N08	2.36	115.49	110.64
6	A	904	2OW	C06-C07-N08	2.30	115.36	110.64
6	B	904	2OW	C11-C12-C13	-2.30	116.98	120.25
6	A	904	2OW	O02-C03-O04	-2.22	120.44	124.63
3	B	901	ADP	C5-C6-N6	2.21	123.70	120.35
6	B	904	2OW	C25-C24-C22	-2.20	117.75	119.94
6	B	904	2OW	O04-C03-N05	-2.12	120.77	124.32
6	B	904	2OW	C20-C19-N18	-2.07	113.09	120.16
6	A	904	2OW	C29-C28-N08	2.00	114.75	110.64
3	A	901	ADP	O5'-PA-O1A	2.00	116.89	109.07

There are no chirality outliers.

All (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
6	A	904	2OW	N05-C03-O02-C01
6	A	904	2OW	O02-C03-N05-C06
6	A	904	2OW	O02-C03-N05-C29
6	A	904	2OW	O04-C03-N05-C29
6	A	904	2OW	O17-C16-N15-C14
6	A	904	2OW	O17-C16-N18-C19
6	A	904	2OW	C20-C19-N18-C16
6	B	904	2OW	O04-C03-O02-C01
6	B	904	2OW	N05-C03-O02-C01
6	B	904	2OW	O17-C16-N15-C14
6	B	904	2OW	O17-C16-N18-C19
6	B	904	2OW	C20-C19-N18-C16
8	B	914	TCE	C5-C2-P-C3
8	B	914	TCE	P-C3-C6-C8

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Mol	Chain	Res	Type	Atoms
7	B	905	GOL	O1-C1-C2-C3
6	A	904	2OW	C10-C09-N08-C28
6	B	904	2OW	C10-C09-N08-C07
6	A	904	2OW	C10-C09-N08-C07
6	B	904	2OW	C10-C09-N08-C28
6	A	904	2OW	O04-C03-N05-C06
6	A	904	2OW	C26-C14-N15-C16
7	B	905	GOL	O1-C1-C2-O2
7	B	907	GOL	C1-C2-C3-O3
7	B	911	GOL	O1-C1-C2-C3
7	A	913	GOL	C1-C2-C3-O3
7	A	908	GOL	C1-C2-C3-O3
7	H	203	GOL	O1-C1-C2-C3
7	H	203	GOL	C1-C2-C3-O3
7	B	907	GOL	O2-C2-C3-O3
6	A	904	2OW	N15-C16-N18-C19
6	B	904	2OW	C13-C14-N15-C16
7	A	909	GOL	O1-C1-C2-O2
8	B	914	TCE	C4-C1-P-C2
7	A	917	GOL	O1-C1-C2-O2
7	A	913	GOL	O2-C2-C3-O3
6	A	904	2OW	C13-C14-N15-C16
6	B	904	2OW	N15-C16-N18-C19
3	B	901	ADP	PA-O3A-PB-O2B
7	H	203	GOL	O2-C2-C3-O3
8	B	914	TCE	P-C2-C5-C14
3	A	901	ADP	PA-O3A-PB-O3B
7	A	909	GOL	O2-C2-C3-O3
7	B	911	GOL	O1-C1-C2-O2
7	A	908	GOL	O2-C2-C3-O3
3	A	901	ADP	PA-O3A-PB-O1B
7	A	905	GOL	O1-C1-C2-O2
7	H	203	GOL	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 22 short contacts:

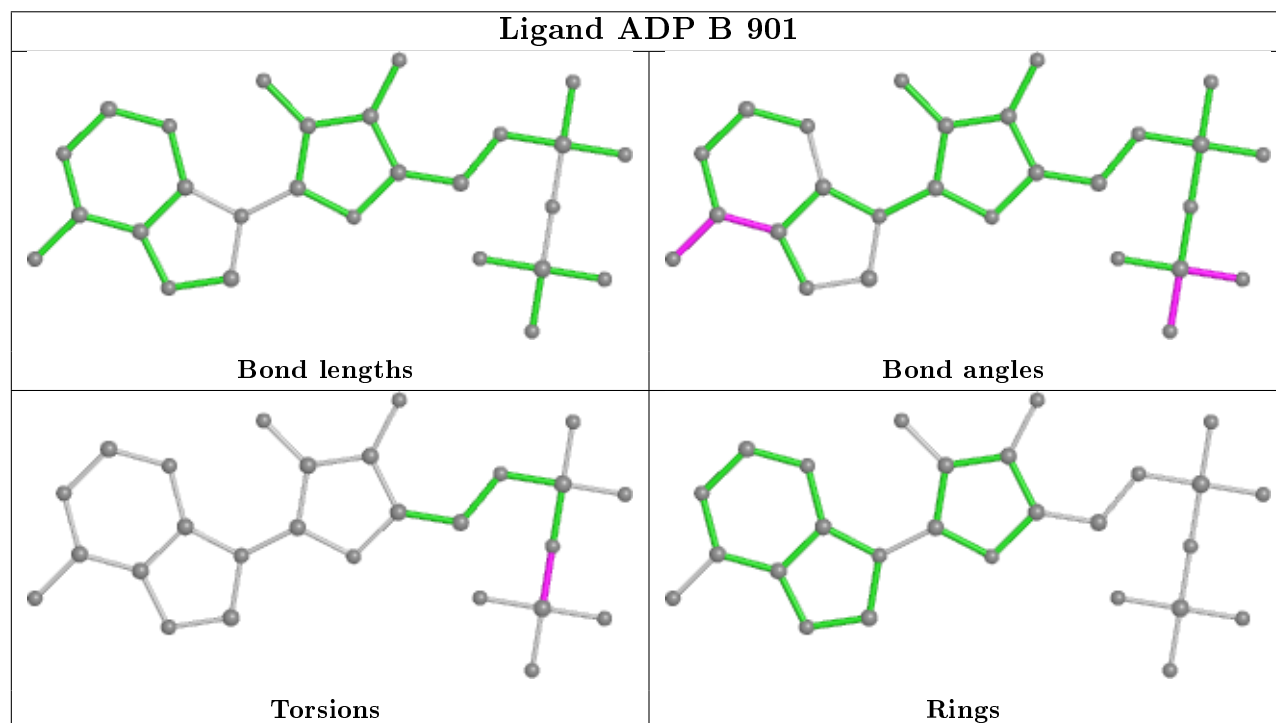
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	907	GOL	2	0
7	A	909	GOL	2	0
4	A	902	VO4	3	0
4	B	902	VO4	2	0

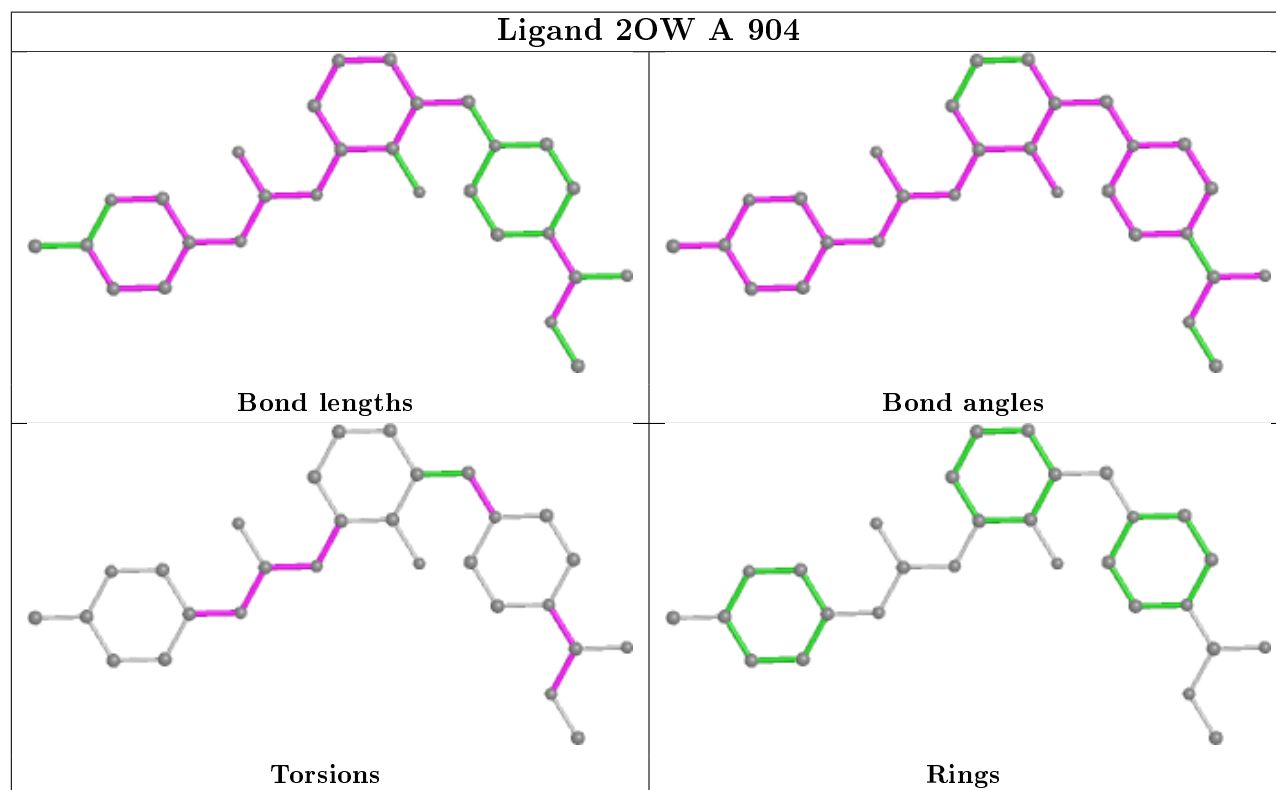
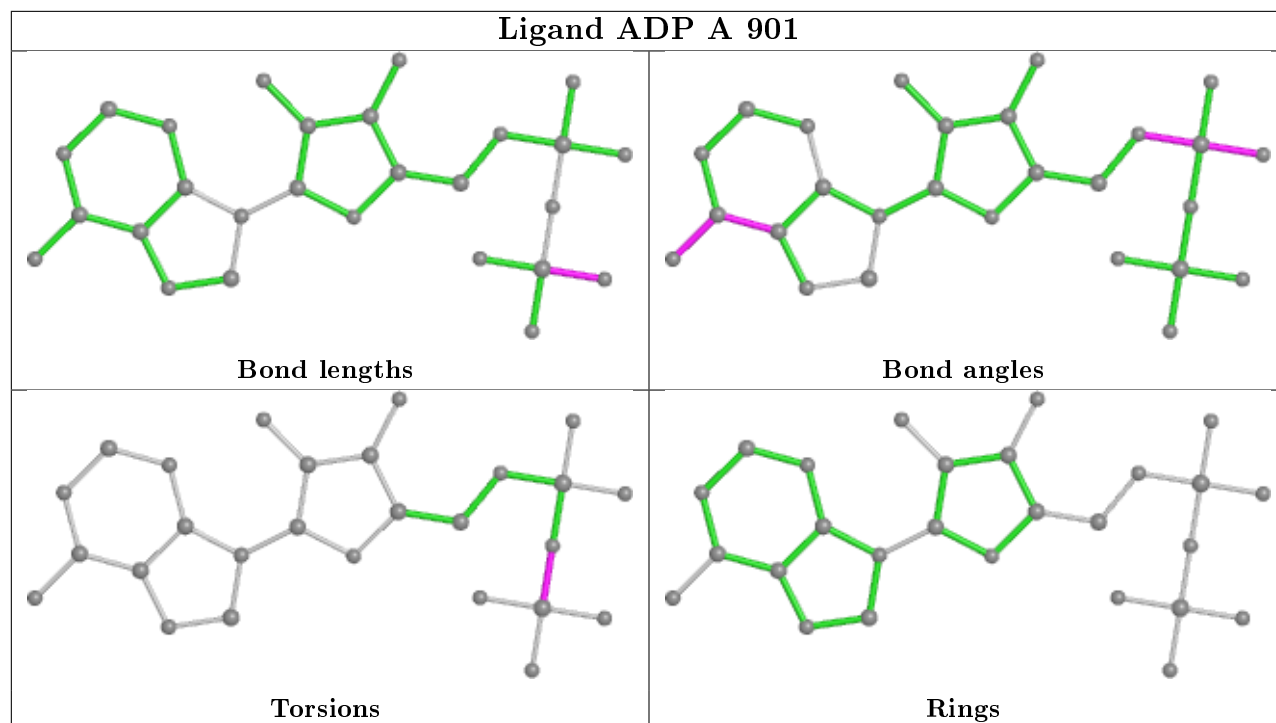
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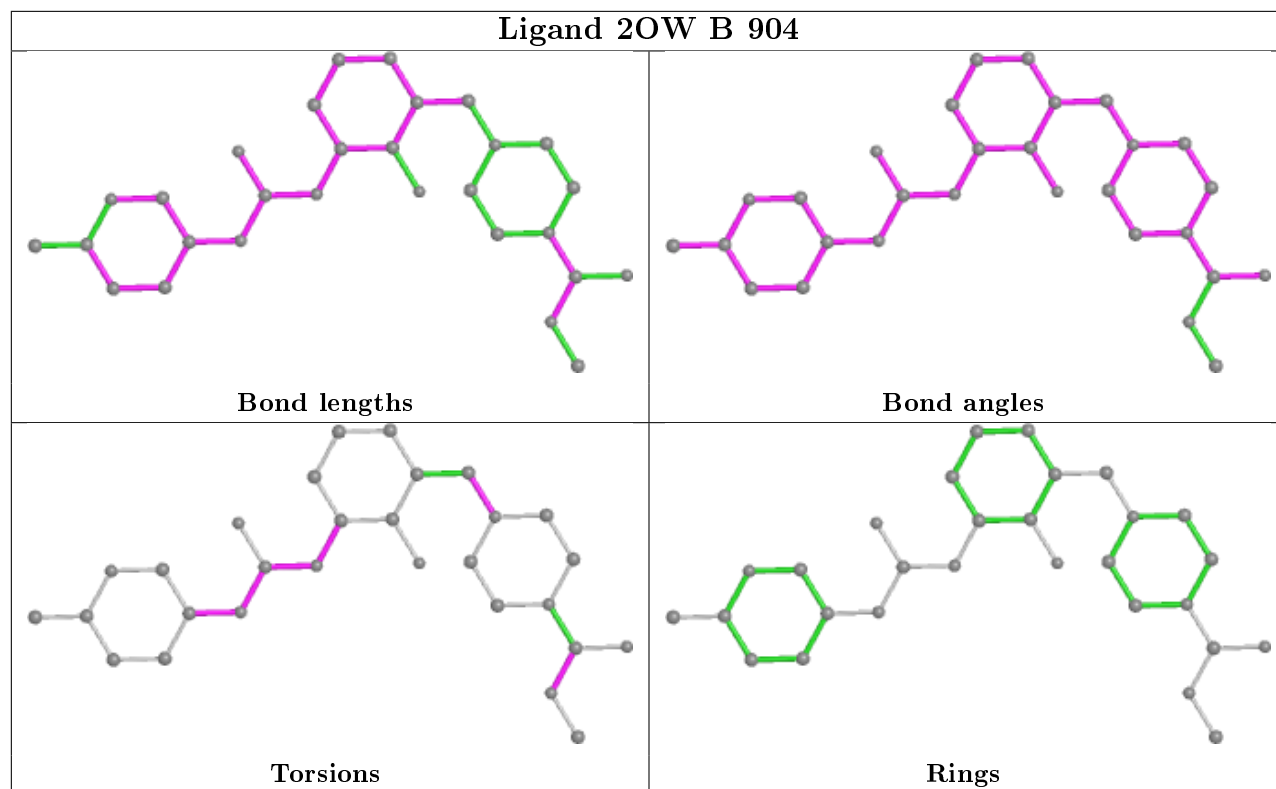
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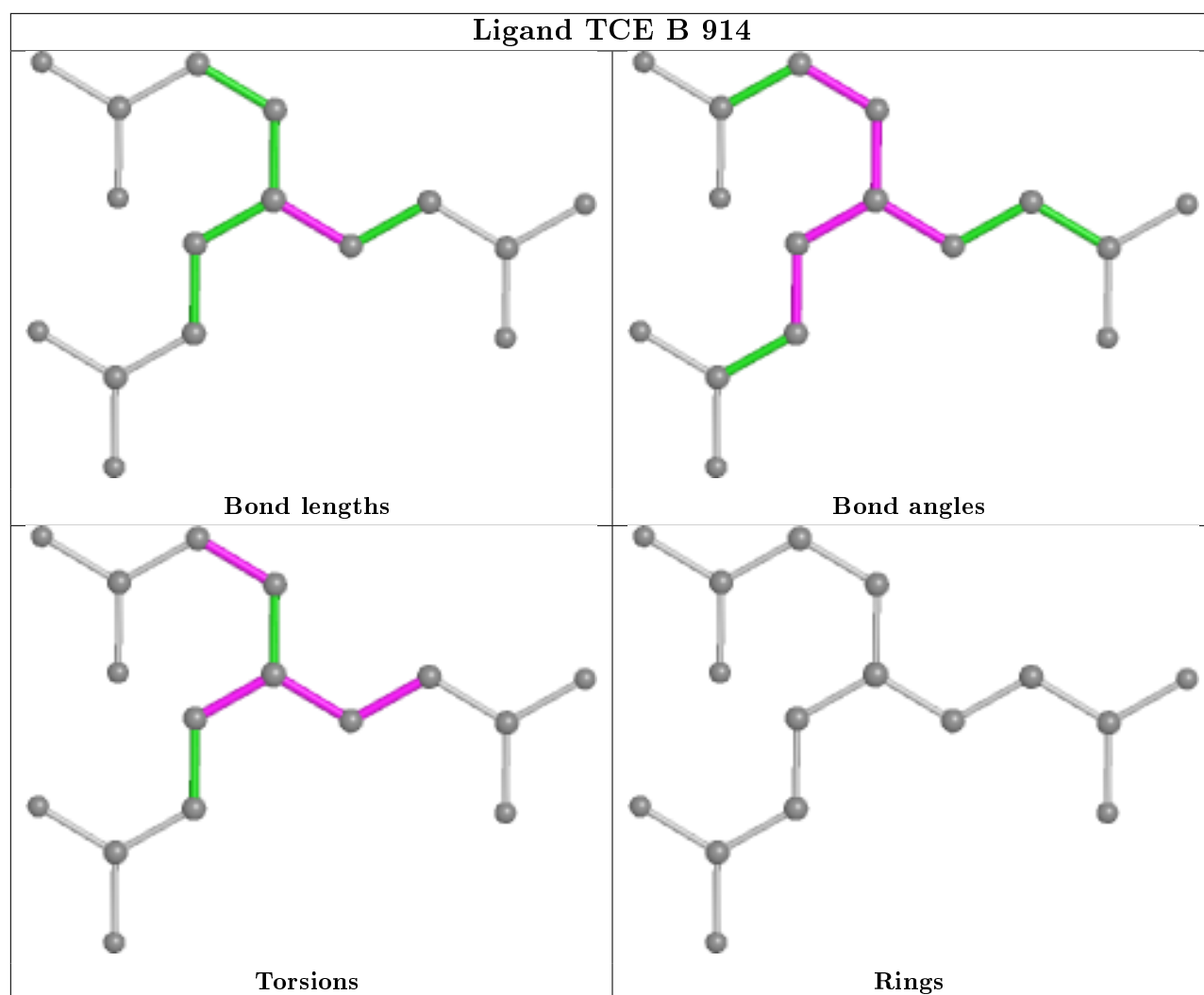
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	908	GOL	2	0
7	B	911	GOL	1	0
6	A	904	2OW	1	0
7	H	202	GOL	2	0
7	A	912	GOL	1	0
6	B	904	2OW	3	0
7	A	906	GOL	2	0
7	H	203	GOL	1	0

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

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	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%)

All (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
2	H	41	PHE	6.6
1	B	410	TYR	5.7
2	G	42	ASP	4.8
2	H	129	LYS	4.5
2	G	44	SER	4.5
1	B	67	LYS	4.5
1	B	55	GLU	4.5
1	A	356	ILE	4.3
2	G	128	ASN	4.3
2	G	186	CYS	4.3
2	G	52	PRO	4.3
2	G	130	ASP	4.2
1	A	55	GLU	4.1
2	G	185	GLY	4.0
1	A	569	ILE	3.9
1	A	732	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
2	G	182	ASP	3.8
1	B	65	HIS	3.8
2	G	129	LYS	3.8
1	B	371	GLU	3.8
1	B	42	ASP	3.7
1	B	58	LYS	3.6
2	G	184	ASN	3.6
2	G	131	THR	3.5
1	B	406	VAL	3.5
1	A	352	LEU	3.5
2	H	131	THR	3.5
2	H	130	ASP	3.4
1	B	66	GLY	3.3
1	A	58	LYS	3.3
1	A	736	ILE	3.2
2	G	110	SER	3.2
1	A	678	THR	3.2
1	A	130	TRP	3.2
1	B	369	ARG	3.2
1	A	530	ILE	3.1
1	B	353	THR	3.1
1	A	353	THR	3.1
2	G	153	MET	3.1
2	G	132	GLY	3.0
1	A	542	LYS	3.0
1	B	405	LYS	3.0
1	B	623	ASN	3.0
1	A	369	ARG	2.9
1	B	376	ASP	2.9
2	H	185	GLY	2.9
2	G	67	ARG	2.9
2	H	148	GLY	2.8
2	G	127	LYS	2.8
1	B	57	GLY	2.8
1	A	355	ALA	2.8
1	A	123	VAL	2.8
2	G	107	GLU	2.8
1	B	571	GLY	2.7
2	G	45	LYS	2.7
1	B	622	ALA	2.7
1	A	56	GLY	2.7
1	B	750	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	407	GLY	2.7
1	B	450	LYS	2.6
1	B	354	GLY	2.6
1	A	731	PRO	2.6
2	G	53	GLU	2.6
1	B	366	LEU	2.6
1	A	285	ILE	2.5
1	B	356	ILE	2.5
2	G	102	LYS	2.5
1	A	6	MET	2.4
1	A	450	LYS	2.4
1	B	56	GLY	2.4
1	B	81	PRO	2.4
1	A	148	SER	2.4
2	H	127	LYS	2.3
1	B	408	ASN	2.3
1	A	25	GLU	2.3
1	A	42	ASP	2.3
1	A	611	LYS	2.3
1	A	122	CYS	2.3
1	A	65	HIS	2.3
2	G	84	LEU	2.3
1	A	191	VAL	2.2
2	H	184	ASN	2.2
1	B	31	PHE	2.2
2	H	128	ASN	2.2
1	B	70	THR	2.2
1	B	355	ALA	2.2
1	A	21	LYS	2.2
1	B	673	ILE	2.2
1	B	64	GLU	2.2
2	G	124	HIS	2.2
1	B	570	LYS	2.2
1	B	799	MET	2.1
1	B	656	ASN	2.1
1	A	792	SER	2.1
1	A	541	PRO	2.0
1	B	803	LYS	2.0
2	H	46	ILE	2.0

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 [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
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

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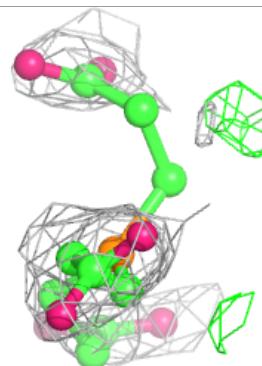
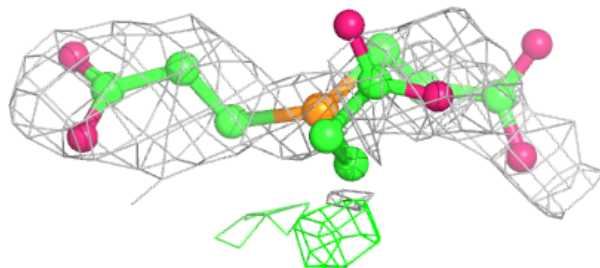
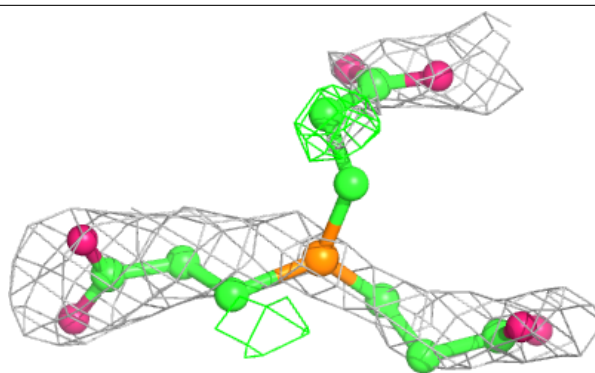
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	A	905	6/6	0.92	0.14	60,61,66,69	0
7	GOL	A	912	6/6	0.92	0.21	60,71,75,77	0
7	GOL	A	910	6/6	0.93	0.24	65,66,72,75	0
7	GOL	H	203	6/6	0.94	0.17	58,59,60,61	0
7	GOL	A	917	6/6	0.94	0.17	64,67,70,70	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.

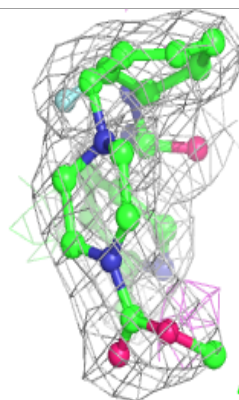
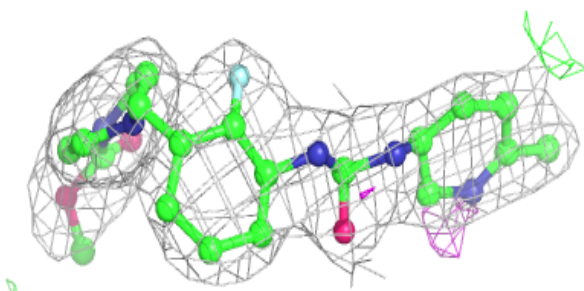
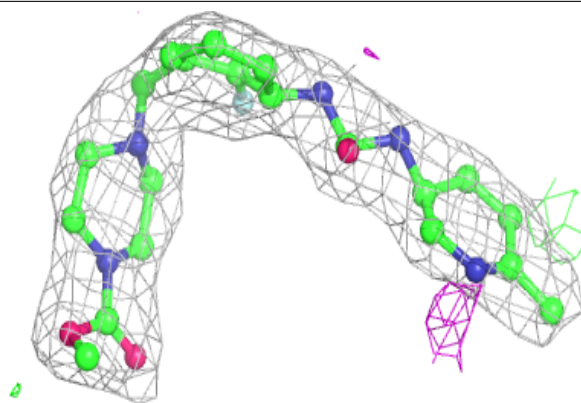
Electron density around TCE B 914:

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

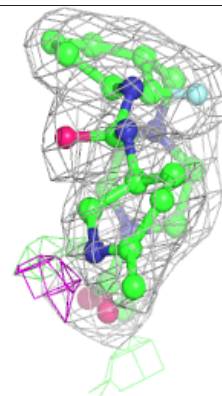
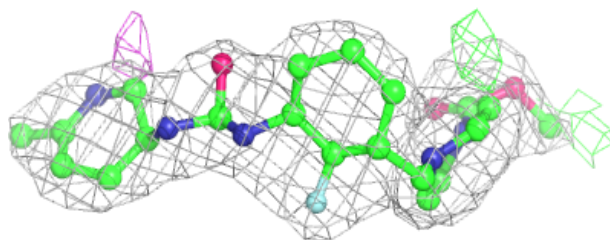
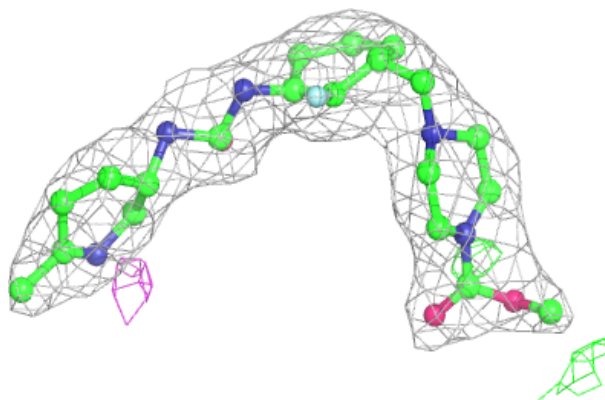


Electron density around 2OW B 904:

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

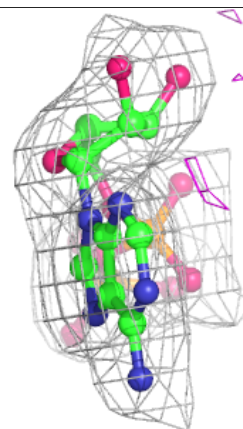
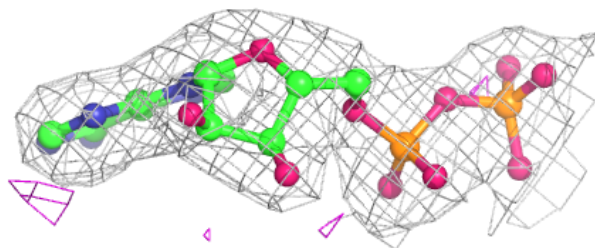
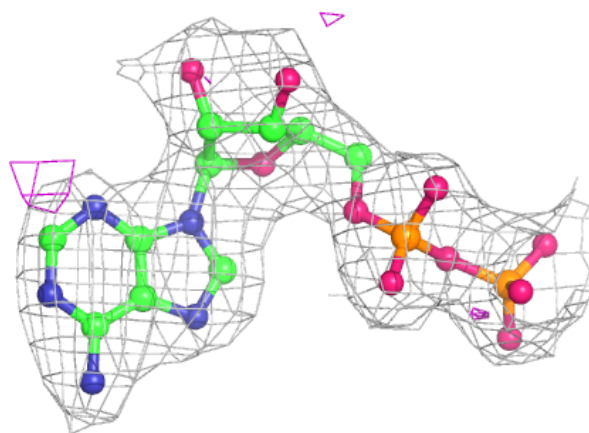
**Electron density around 2OW A 904:**

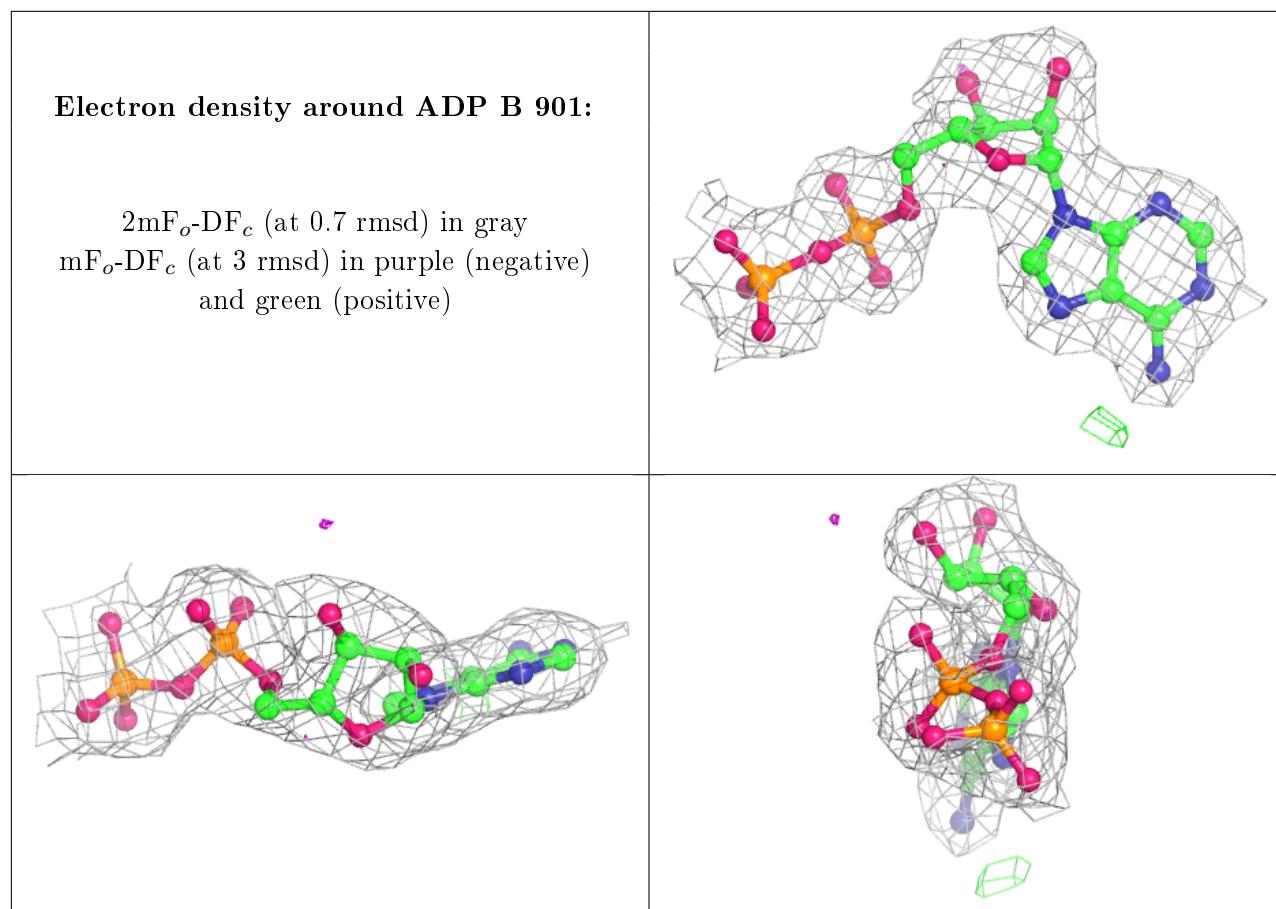
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.