



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 10:28 AM EDT

PDB ID : 5N69 / pdb_00005n69
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

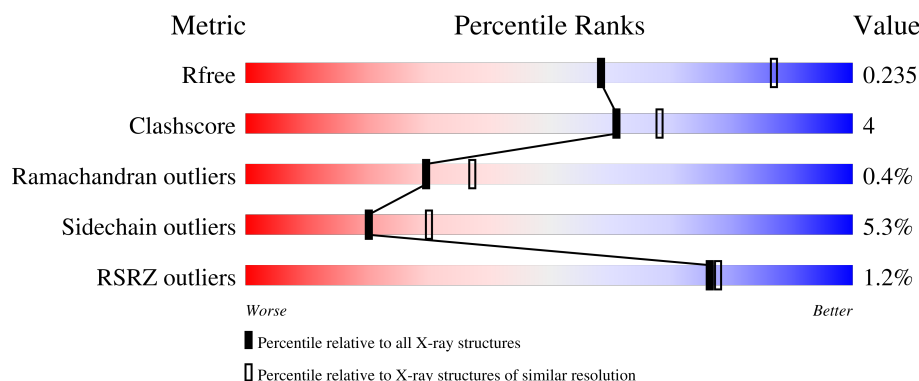
1 Overall quality at a glance

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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	828	
1	B	828	
2	G	199	
2	H	199	

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 criteria:

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	-	-

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.

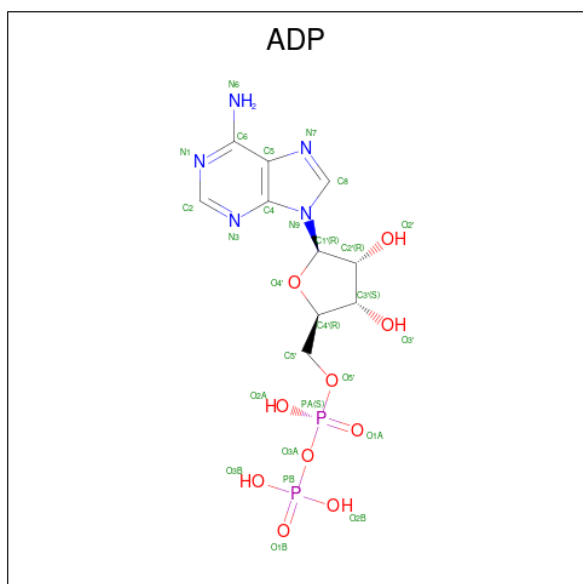
- Molecule 1 is a protein called Myosin-7.

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.

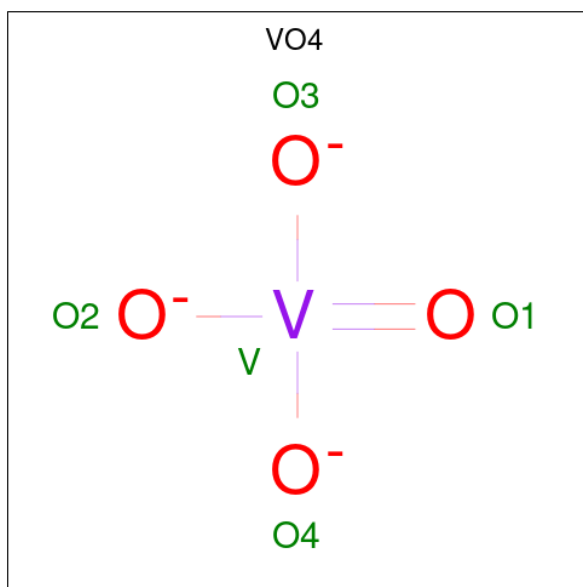
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	156	Total	C	N	O	S	0	0	0
			1234	778	203	243	10			
2	H	161	Total	C	N	O	S	0	0	0
			1275	804	209	252	10			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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 (CCD ID: VO4) (formula: O₄V).

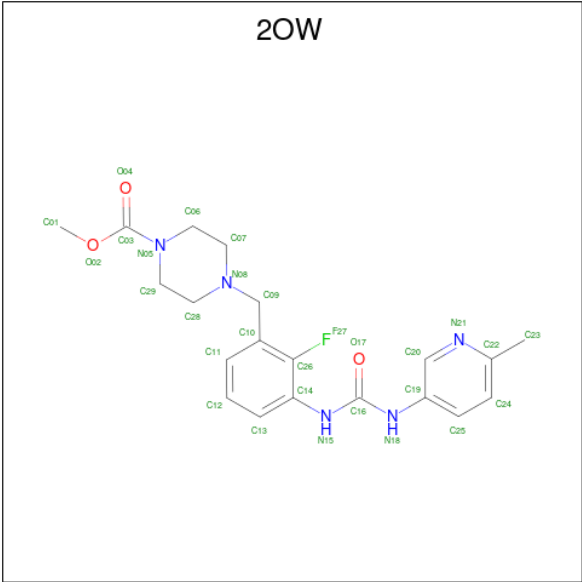


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O V	0	0
			5	4 1		
4	B	1	Total	O V	0	0
			5	4 1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

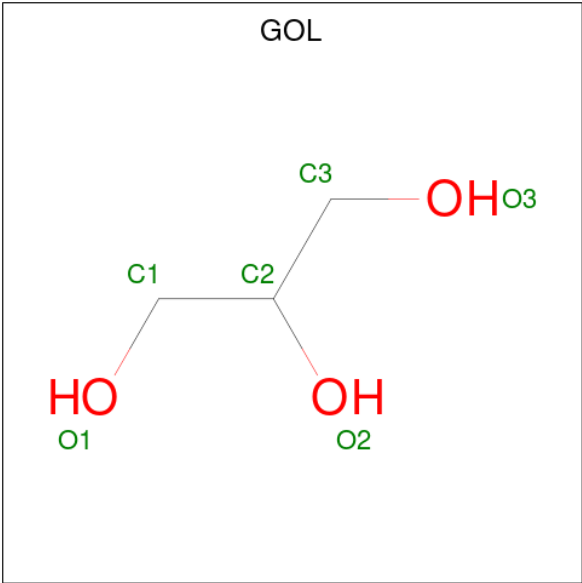
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is methyl 4-(2-fluoro-3-{{(6-methylpyridin-3-yl)carbamoyl}amino}benzyl)piperazine-1-carboxylate (CCD ID: 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 (CCD ID: 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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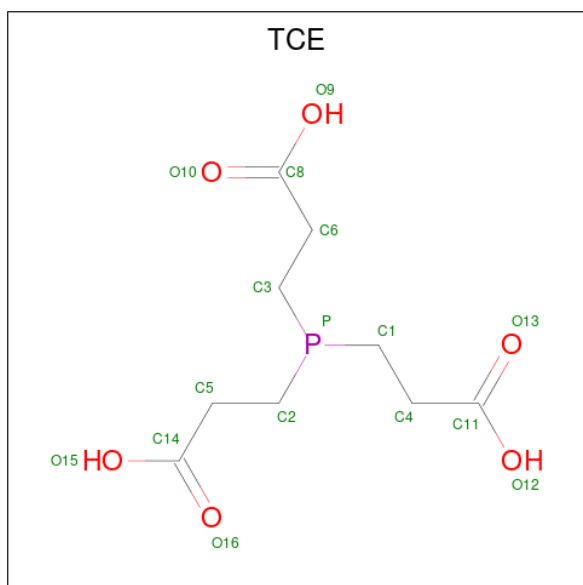
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	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		

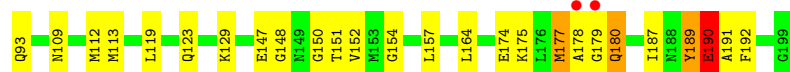
- Molecule 8 is 3,3',3''-phosphanetriyltripropanoic acid (CCD ID: TCE) (formula: C₉H₁₅O₆P).



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		



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) 99.2 (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 , 63.3	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, M3L, TCE, VO4, ADP, GOL, 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	0.86	2/6275 (0.0%)	1.38	21/8447 (0.2%)
1	B	0.84	0/6299	1.37	29/8479 (0.3%)
2	G	0.84	1/1252 (0.1%)	1.43	4/1678 (0.2%)
2	H	0.88	1/1297 (0.1%)	1.49	8/1741 (0.5%)
All	All	0.85	4/15123 (0.0%)	1.39	62/20345 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	PRO	CA-C	6.48	1.55	1.51
1	A	690	MET	SD-CE	-6.08	1.64	1.79
2	H	177	MET	SD-CE	-5.03	1.67	1.79
2	G	177	MET	SD-CE	-5.01	1.67	1.79

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	ILE	N-CA-CB	-9.25	102.04	112.21
1	A	7	ALA	CA-C-N	9.20	136.74	122.49
1	A	7	ALA	C-N-CA	9.20	136.74	122.49
1	A	449	THR	N-CA-C	-8.59	96.29	109.95
1	B	312	PHE	CA-CB-CG	7.57	121.36	113.80
1	B	468	PHE	CA-CB-CG	7.07	120.87	113.80
1	A	8	ALA	N-CA-C	-6.96	103.98	113.30
1	A	661	ASN	CA-CB-CG	6.88	119.48	112.60
1	B	685	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	468	PHE	CA-CB-CG	6.78	120.58	113.80
2	H	42	ASP	CA-CB-CG	6.69	119.29	112.60
1	B	661	ASN	CA-CB-CG	6.54	119.14	112.60
1	A	685	ASP	CA-CB-CG	6.51	119.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	148	GLY	CA-C-N	6.47	128.85	120.44
2	H	148	GLY	C-N-CA	6.47	128.85	120.44
1	A	700	GLU	CB-CG-CD	6.12	123.01	112.60
1	A	765	PHE	CA-CB-CG	6.04	119.84	113.80
2	G	61	ALA	CA-C-N	5.95	128.25	120.28
2	G	61	ALA	C-N-CA	5.95	128.25	120.28
1	A	573	PRO	CA-C-N	5.92	129.28	120.87
1	A	573	PRO	C-N-CA	5.92	129.28	120.87
1	A	310	TYR	CA-C-N	5.88	128.48	120.54
1	A	310	TYR	C-N-CA	5.88	128.48	120.54
1	B	502	LYS	CA-C-N	5.79	128.84	120.38
1	B	502	LYS	C-N-CA	5.79	128.84	120.38
2	H	150	GLY	N-CA-C	-5.75	107.25	115.64
1	B	310	TYR	CA-C-N	5.71	128.72	120.79
1	B	310	TYR	C-N-CA	5.71	128.72	120.79
2	H	109	ASN	CA-CB-CG	5.56	118.16	112.60
1	B	164	TYR	CA-C-N	5.55	127.66	120.44
1	B	164	TYR	C-N-CA	5.55	127.66	120.44
1	B	516	ASP	CA-CB-CG	5.52	118.12	112.60
2	G	109	ASN	CA-CB-CG	5.51	118.11	112.60
2	G	149	ASN	CA-CB-CG	5.44	118.04	112.60
2	H	191	ALA	N-CA-C	-5.41	105.04	111.69
1	A	85	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	512	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	358	HIS	CA-C-N	5.29	127.63	120.38
1	B	358	HIS	C-N-CA	5.29	127.63	120.38
1	A	311	ALA	CA-C-N	5.26	127.59	120.38
1	A	311	ALA	C-N-CA	5.26	127.59	120.38
1	B	700	GLU	CA-C-N	5.23	125.78	119.98
1	B	700	GLU	C-N-CA	5.23	125.78	119.98
1	B	353	THR	CA-C-N	5.15	125.67	120.00
1	B	353	THR	C-N-CA	5.15	125.67	120.00
1	A	516	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	700	GLU	CA-C-N	5.12	125.66	119.98
1	A	700	GLU	C-N-CA	5.12	125.66	119.98
2	H	189	TYR	N-CA-C	-5.11	103.41	110.35
2	H	58	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	164	TYR	CA-C-N	5.10	127.07	120.44
1	A	164	TYR	C-N-CA	5.10	127.07	120.44
1	B	617	LEU	CA-C-N	5.08	127.40	120.54
1	B	617	LEU	C-N-CA	5.08	127.40	120.54
1	B	696	ASN	CA-CB-CG	5.07	117.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	498	GLN	CA-C-N	5.06	127.07	120.28
1	B	498	GLN	C-N-CA	5.06	127.07	120.28
1	B	423	ALA	CA-C-N	5.05	127.01	120.44
1	B	423	ALA	C-N-CA	5.05	127.01	120.44
1	B	665	THR	N-CA-CB	-5.03	102.22	111.37
1	B	800	GLU	CB-CG-CD	5.02	121.13	112.60
1	B	525	GLU	N-CA-C	5.01	120.23	113.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6164	0	6153	50	0
1	B	6184	0	6183	53	0
2	G	1234	0	1213	12	0
2	H	1275	0	1252	18	0
3	A	27	0	12	0	0
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	126	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 (126) 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:A:660:THR:HG21	1:B:660:THR:HG21	0.72	0.70
1:B:215:THR:HG22	1:B:218:ASP:H	1.56	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:227:LEU:HD23	1:B:439:MET:HE3	1.77	0.66
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
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
1:A:227:LEU:HD23	1:A:439:MET:HE3	1.79	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
1:A:515:MET:HE2	1:A:697:GLY:HA3	1.81	0.62
7:B:911:GOL:H12	9:B:1053:HOH:O	1.99	0.62
1:B:795:VAL:HG12	1:B:799:MET:HE2	1.82	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:O3	4:B:902:VO4:V	1.58	0.60
4:B:902:VO4:V	4:B:902:VO4:O4	1.59	0.60
4:A:902:VO4:V	4:A:902:VO4:O4	1.59	0.60
1:A:143:ARG:HD2	1:A:198:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:102:LEU:HD22	1:A:690:MET:HE2	1.88	0.55
1:B:515:MET:HE2	1:B:697:GLY:HA3	1.88	0.55
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: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:76:THR:HG22	2:H:112:MET:HE1	1.91	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
1:B:435:MET:HG3	1:B:616:MET:HE1	1.92	0.51
2:H:157:LEU:HD23	2:H:187:ILE:HD13	1.92	0.51
1:A:46:PHE:HE2	1:A:690:MET:HE3	1.76	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
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
1:A:46:PHE:CE2	1:A:690:MET:HE3	2.50	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
2:H:177:MET:HE1	2:H:192:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:177:MET:HE1	2:G:192:PHE:CZ	2.50	0.46
2:G:63:THR:HA	2:G:73:MET:HE1	1.96	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
2:G:73:MET:HA	2:G:73:MET:HE2	1.97	0.45
1:B:228:GLU:O	1:B:232:ASN:HB2	2.16	0.45
1:A:359:PHE:CE1	1:A:388:MET:HE1	2.51	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: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:349:MET:HG2	1:A:616:MET:HE1	1.99	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
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:A:453:ARG:HG2	1:B:539:MET:HE1	2.01	0.42
2:H:80:CYS:HB2	2:H:113:MET:HE1	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:715:TYR:HB3	1:A:738:SER:HB3	2.03	0.40
1:B:798:ARG:HD3	2:G:85:ARG:O	2.22	0.40
1:B:807:ARG:HG3	9:B:1301:HOH: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%)	36	45
1	B	753/828 (91%)	730 (97%)	20 (3%)	3 (0%)	30	37
2	G	150/199 (75%)	144 (96%)	5 (3%)	1 (1%)	18	24
2	H	159/199 (80%)	156 (98%)	1 (1%)	2 (1%)	9	9
All	All	1812/2054 (88%)	1754 (97%)	50 (3%)	8 (0%)	30	37

All (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
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%)	639 (96%)	25 (4%)	29	43
1	B	666/715 (93%)	626 (94%)	40 (6%)	17	26
2	G	135/165 (82%)	126 (93%)	9 (7%)	15	20
2	H	140/165 (85%)	128 (91%)	12 (9%)	10	11
All	All	1605/1760 (91%)	1519 (95%)	86 (5%)	20	29

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	22	GLU
1	A	69	VAL
1	A	118	SER
1	A	237	ARG
1	A	281	ARG
1	A	318	THR
1	A	384	SER
1	A	418	GLN
1	A	437	ASN
1	A	474	GLU
1	A	578	SER
1	A	579	LEU
1	A	590	ILE
1	A	601	LEU
1	A	607	ASP
1	A	645	GLN
1	A	650	LEU
1	A	655	LEU
1	A	671	ARG
1	A	699	LEU
1	A	736	ILE
1	A	787	ARG
1	A	798	ARG

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Mol	Chain	Res	Type
1	A	800	GLU
1	B	21	LYS
1	B	34	LYS
1	B	67	LYS
1	B	69	VAL
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	267	LEU
1	B	281	ARG
1	B	313	ILE
1	B	327	GLU
1	B	376	ASP
1	B	384	SER
1	B	397	LYS
1	B	405	LYS
1	B	418	GLN
1	B	437	ASN
1	B	453[A]	ARG
1	B	453[B]	ARG
1	B	474	GLU
1	B	526	LYS
1	B	549	LYS
1	B	570	LYS
1	B	578	SER
1	B	579	LEU
1	B	595	GLN
1	B	601	LEU
1	B	607	ASP
1	B	655	LEU
1	B	665	THR
1	B	671	ARG
1	B	674	ILE
1	B	700	GLU
1	B	780	ARG
1	B	798	ARG
1	B	800	GLU
2	G	45	LYS

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Mol	Chain	Res	Type
2	G	46	ILE
2	G	149	ASN
2	G	151	THR
2	G	152	VAL
2	G	164	LEU
2	G	171	ASP
2	G	174	GLU
2	G	190	GLU
2	H	42	ASP
2	H	45	LYS
2	H	46	ILE
2	H	57	GLU
2	H	129	LYS
2	H	147	GLU
2	H	151	THR
2	H	152	VAL
2	H	164	LEU
2	H	174	GLU
2	H	175	LYS
2	H	190	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	78	GLN
1	A	187	ASN
1	A	224	ASN
1	A	401	HIS
1	A	651	HIS
1	A	656	ASN
1	A	668	HIS
1	A	720	GLN
1	A	726	ASN
1	A	755	GLN
1	B	187	ASN
1	B	401	HIS
1	B	651	HIS
1	B	656	ASN
1	B	668	HIS
1	B	726	ASN
1	B	791	GLN

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Mol	Chain	Res	Type
2	G	89	GLN
2	G	123	GLN
2	G	149	ASN
2	G	159	HIS
2	G	195	HIS
2	H	123	GLN
2	H	128	ASN
2	H	159	HIS

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	B	129	1	10,11,12	1.15	1 (10%)	9,14,16	0.70	0
1	M3L	A	129	1	10,11,12	0.73	0	9,14,16	1.03	1 (11%)

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	B	129	1	-	0/9/10/12	-
1	M3L	A	129	1	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	M3L	CB-CA	3.45	1.58	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	2.72	125.95	115.97

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 oligosaccharides 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	202	-	5,5,5	0.09	0	5,5,5	0.27	0
7	GOL	A	916	-	5,5,5	0.05	0	5,5,5	0.25	0
7	GOL	B	909	-	5,5,5	0.08	0	5,5,5	0.30	0
4	VO4	B	902	5,3	0,4,4	-	-	-		
7	GOL	B	905	-	5,5,5	0.11	0	5,5,5	0.18	0
7	GOL	B	906	-	5,5,5	0.09	0	5,5,5	0.28	0
7	GOL	B	907	-	5,5,5	0.09	0	5,5,5	0.24	0
7	GOL	B	908	-	5,5,5	0.08	0	5,5,5	0.20	0
6	2OW	A	904	-	31,31,31	5.34	19 (61%)	41,42,42	4.23	26 (63%)
7	GOL	B	911	-	5,5,5	0.15	0	5,5,5	0.28	0
8	TCE	B	914	-	12,15,15	1.38	1 (8%)	12,18,18	3.13	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	901	4,5	28,29,29	0.55	1 (3%)	43,45,45	0.60	1 (2%)
7	GOL	A	914	-	5,5,5	0.09	0	5,5,5	0.12	0
7	GOL	A	912	-	5,5,5	0.08	0	5,5,5	0.32	0
7	GOL	A	908	-	5,5,5	0.12	0	5,5,5	0.26	0
4	VO4	A	902	5,3	0,4,4	-	-	-	-	-
7	GOL	A	907	-	5,5,5	0.12	0	5,5,5	0.30	0
7	GOL	H	203	-	5,5,5	0.10	0	5,5,5	0.43	0
7	GOL	A	906	-	5,5,5	0.15	0	5,5,5	0.30	0
7	GOL	A	910	-	5,5,5	0.11	0	5,5,5	0.31	0
7	GOL	B	913	-	5,5,5	0.04	0	5,5,5	0.30	0
3	ADP	B	901	4,5	28,29,29	0.42	0	43,45,45	0.65	1 (2%)
7	GOL	A	917	-	5,5,5	0.10	0	5,5,5	0.31	0
7	GOL	H	201	-	4,4,5	0.47	0	4,4,5	0.74	0
7	GOL	A	905	-	5,5,5	0.11	0	5,5,5	0.74	0
7	GOL	A	915	-	5,5,5	0.06	0	5,5,5	0.20	0
7	GOL	B	912	-	5,5,5	0.06	0	5,5,5	0.14	0
7	GOL	A	909	-	5,5,5	0.22	0	5,5,5	0.69	0
7	GOL	A	911	-	5,5,5	0.10	0	5,5,5	0.40	0
7	GOL	B	910	-	5,5,5	0.05	0	5,5,5	0.23	0
6	2OW	B	904	-	31,31,31	5.59	19 (61%)	41,42,42	3.99	27 (65%)
7	GOL	A	913	-	5,5,5	0.08	0	5,5,5	0.21	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	202	-	-	0/4/4/4	-
7	GOL	A	916	-	-	0/4/4/4	-
7	GOL	B	909	-	-	0/4/4/4	-
7	GOL	B	905	-	-	2/4/4/4	-
7	GOL	B	906	-	-	0/4/4/4	-
7	GOL	B	907	-	-	2/4/4/4	-
7	GOL	B	908	-	-	0/4/4/4	-
6	2OW	A	904	-	-	14/18/28/28	0/3/3/3
7	GOL	B	911	-	-	2/4/4/4	-
8	TCE	B	914	-	-	10/15/15/15	-
3	ADP	A	901	4,5	-	3/16/32/32	0/3/3/3
7	GOL	A	914	-	-	0/4/4/4	-
7	GOL	A	912	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	908	-	-	2/4/4/4	-
7	GOL	A	907	-	-	0/4/4/4	-
7	GOL	H	203	-	-	4/4/4/4	-
7	GOL	A	906	-	-	0/4/4/4	-
7	GOL	A	910	-	-	0/4/4/4	-
7	GOL	B	913	-	-	0/4/4/4	-
3	ADP	B	901	4,5	-	2/16/32/32	0/3/3/3
7	GOL	A	917	-	-	2/4/4/4	-
7	GOL	H	201	-	-	0/2/2/4	-
7	GOL	A	905	-	-	1/4/4/4	-
7	GOL	A	915	-	-	0/4/4/4	-
7	GOL	B	912	-	-	0/4/4/4	-
7	GOL	A	909	-	-	3/4/4/4	-
7	GOL	A	911	-	-	0/4/4/4	-
7	GOL	B	910	-	-	0/4/4/4	-
6	2OW	B	904	-	-	9/18/28/28	0/3/3/3
7	GOL	A	913	-	-	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	C12-C11	9.54	1.55	1.38
6	A	904	2OW	C12-C11	9.47	1.55	1.38
6	B	904	2OW	C12-C13	9.39	1.55	1.38
6	B	904	2OW	C11-C10	9.01	1.54	1.39
6	A	904	2OW	C12-C13	8.97	1.54	1.38
6	B	904	2OW	C13-C14	8.93	1.54	1.39
6	A	904	2OW	C11-C10	8.90	1.54	1.39
6	B	904	2OW	C20-N21	8.50	1.51	1.34
6	B	904	2OW	C03-N05	8.43	1.50	1.35
6	A	904	2OW	C13-C14	8.40	1.53	1.39
6	A	904	2OW	C20-N21	8.36	1.51	1.34
6	B	904	2OW	O17-C16	8.28	1.40	1.23
6	A	904	2OW	C03-N05	8.11	1.49	1.35
6	B	904	2OW	C14-C26	8.06	1.52	1.38
6	B	904	2OW	C10-C26	8.04	1.54	1.38
6	A	904	2OW	C14-C26	7.92	1.52	1.38
6	A	904	2OW	C10-C26	7.76	1.53	1.38
6	A	904	2OW	O17-C16	7.64	1.39	1.23
6	B	904	2OW	C24-C22	7.23	1.55	1.39
6	A	904	2OW	C24-C22	7.07	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	904	2OW	C20-C19	6.97	1.51	1.39
6	B	904	2OW	C20-C19	6.92	1.51	1.39
6	B	904	2OW	C25-C24	6.12	1.48	1.38
6	B	904	2OW	O02-C03	5.78	1.44	1.34
6	A	904	2OW	C25-C24	5.76	1.48	1.38
6	B	904	2OW	C25-C19	5.08	1.47	1.39
6	A	904	2OW	O02-C03	5.04	1.42	1.34
6	B	904	2OW	C16-N15	4.69	1.47	1.37
6	B	904	2OW	C16-N18	4.62	1.47	1.37
6	A	904	2OW	C16-N15	4.25	1.46	1.37
6	A	904	2OW	C16-N18	4.14	1.46	1.37
6	A	904	2OW	C25-C19	3.88	1.45	1.39
6	B	904	2OW	C14-N15	3.52	1.48	1.41
6	B	904	2OW	C19-N18	3.46	1.48	1.41
6	A	904	2OW	C14-N15	3.30	1.48	1.41
6	A	904	2OW	C19-N18	3.13	1.48	1.41
6	B	904	2OW	C09-C10	3.03	1.56	1.51
6	A	904	2OW	C09-C10	2.92	1.56	1.51
3	A	901	ADP	PB-O3B	-2.56	1.45	1.54
8	B	914	TCE	P-C2	2.10	1.87	1.84

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	904	2OW	O17-C16-N18	-10.99	104.11	123.64
6	B	904	2OW	C19-C20-N21	-10.15	115.67	124.07
6	B	904	2OW	O17-C16-N18	-9.99	105.88	123.64
6	A	904	2OW	C19-C20-N21	-9.58	116.14	124.07
6	A	904	2OW	C19-N18-C16	-8.54	109.18	126.61
6	A	904	2OW	O17-C16-N15	-8.32	108.86	123.64
6	B	904	2OW	O02-C03-N05	8.28	118.27	111.61
6	A	904	2OW	O02-C03-N05	7.87	117.94	111.61
6	B	904	2OW	O17-C16-N15	-7.82	109.74	123.64
6	A	904	2OW	C14-N15-C16	-7.40	108.10	125.34
6	A	904	2OW	C09-C10-C26	-6.89	110.83	121.47
8	B	914	TCE	C1-P-C2	6.47	121.57	100.95
6	B	904	2OW	C19-N18-C16	-6.46	113.43	126.61
6	B	904	2OW	C14-N15-C16	-6.31	110.63	125.34
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	5.22	123.68	117.53
6	A	904	2OW	C09-C10-C11	-4.78	110.66	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	904	2OW	C29-N05-C06	4.39	121.64	112.68
6	B	904	2OW	C13-C14-N15	-4.20	112.08	121.82
6	B	904	2OW	F27-C26-C14	-4.13	111.70	118.28
6	B	904	2OW	C25-C19-N18	-4.07	106.75	120.41
6	A	904	2OW	C24-C25-C19	-3.99	115.70	120.30
6	A	904	2OW	C25-C19-N18	-3.97	107.07	120.41
6	B	904	2OW	C26-C14-N15	-3.91	109.36	117.02
6	B	904	2OW	C09-C10-C11	-3.87	112.46	120.12
6	B	904	2OW	C28-C29-N05	3.78	117.94	110.42
6	A	904	2OW	C13-C14-N15	-3.34	114.07	121.82
6	A	904	2OW	C07-C06-N05	3.31	117.00	110.42
6	A	904	2OW	C28-C29-N05	3.30	116.97	110.42
6	B	904	2OW	C09-C10-C26	-3.25	116.44	121.47
6	A	904	2OW	F27-C26-C14	-3.22	113.16	118.28
6	A	904	2OW	C10-C09-N08	-3.17	107.11	112.75
6	B	904	2OW	C29-N05-C06	3.17	119.15	112.68
6	B	904	2OW	N18-C16-N15	-3.16	106.34	112.44
6	B	904	2OW	C07-C06-N05	3.12	116.62	110.42
6	A	904	2OW	F27-C26-C10	-3.04	113.88	118.00
6	B	904	2OW	C12-C11-C10	-3.00	116.49	120.88
6	A	904	2OW	C25-C24-C22	-2.89	117.06	119.90
6	A	904	2OW	C13-C14-C26	2.73	121.52	117.72
6	A	904	2OW	C23-C22-N21	2.73	121.74	117.68
6	B	904	2OW	C06-C07-N08	2.71	116.12	110.65
6	B	904	2OW	C11-C10-C26	2.61	118.38	116.46
6	B	904	2OW	C11-C12-C13	-2.54	116.98	120.24
6	A	904	2OW	C20-C19-N18	-2.45	111.85	120.21
3	B	901	ADP	O3B-PB-O2B	2.45	117.00	107.80
6	B	904	2OW	C29-C28-N08	2.40	115.49	110.65
6	B	904	2OW	C10-C09-N08	-2.36	108.56	112.75
6	A	904	2OW	C06-C07-N08	2.34	115.36	110.65
6	B	904	2OW	C23-C22-N21	2.30	121.11	117.68
6	A	904	2OW	O02-C03-O04	-2.29	120.44	124.60
6	B	904	2OW	C25-C24-C22	-2.19	117.75	119.90
6	A	904	2OW	N18-C16-N15	-2.16	108.27	112.44
6	B	904	2OW	C20-C19-N18	-2.09	113.09	120.21
6	A	904	2OW	C29-C28-N08	2.03	114.75	110.65
6	B	904	2OW	O02-C03-O04	-2.03	120.92	124.60
6	A	904	2OW	C12-C11-C10	-2.01	117.94	120.88
3	A	901	ADP	O5'-PA-O1A	2.01	116.89	108.94

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ADP	PA-O3A-PB-O2B
3	B	901	ADP	PA-O3A-PB-O3B
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	C26-C14-N15-C16
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	C20-C19-N18-C16
7	A	909	GOL	O1-C1-C2-C3
7	A	917	GOL	O1-C1-C2-C3
7	B	905	GOL	O1-C1-C2-C3
8	B	914	TCE	C5-C2-P-C3
8	B	914	TCE	P-C3-C6-C8
6	A	904	2OW	O17-C16-N18-C19
6	B	904	2OW	O17-C16-N18-C19
6	A	904	2OW	C10-C09-N08-C28
6	B	904	2OW	C10-C09-N08-C07
6	A	904	2OW	O17-C16-N15-C14
6	B	904	2OW	O17-C16-N15-C14
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	O04-C03-N05-C29
7	B	905	GOL	O1-C1-C2-O2
8	B	914	TCE	C3-C6-C8-O10
8	B	914	TCE	C3-C6-C8-O9
7	A	908	GOL	C1-C2-C3-O3
7	A	913	GOL	C1-C2-C3-O3
7	B	907	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
7	A	909	GOL	O1-C1-C2-O2
6	B	904	2OW	C13-C14-N15-C16
7	B	911	GOL	O1-C1-C2-C3
7	A	913	GOL	O2-C2-C3-O3
7	A	917	GOL	O1-C1-C2-O2
8	B	914	TCE	C4-C1-P-C2

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Mol	Chain	Res	Type	Atoms
6	B	904	2OW	N15-C16-N18-C19
7	H	203	GOL	O2-C2-C3-O3
6	A	904	2OW	C13-C14-N15-C16
3	B	901	ADP	PA-O3A-PB-O2B
8	B	914	TCE	P-C2-C5-C14
8	B	914	TCE	O15-C14-C5-C2
8	B	914	TCE	O12-C11-C4-C1
8	B	914	TCE	O13-C11-C4-C1
8	B	914	TCE	O16-C14-C5-C2
7	A	908	GOL	O2-C2-C3-O3
7	A	909	GOL	O2-C2-C3-O3
3	A	901	ADP	PA-O3A-PB-O3B
7	A	905	GOL	O1-C1-C2-O2
7	B	911	GOL	O1-C1-C2-O2
7	H	203	GOL	O1-C1-C2-O2
3	A	901	ADP	PA-O3A-PB-O1B

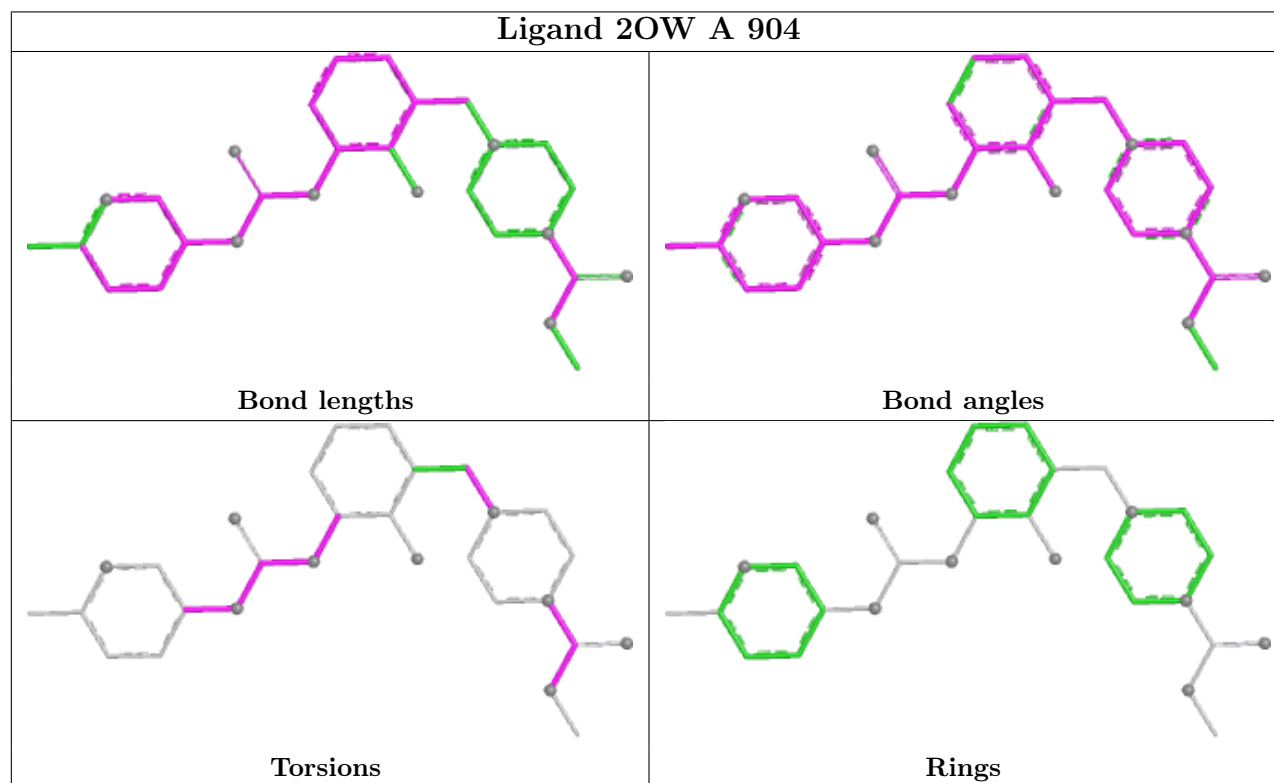
There are no ring outliers.

12 monomers are involved in 22 short contacts:

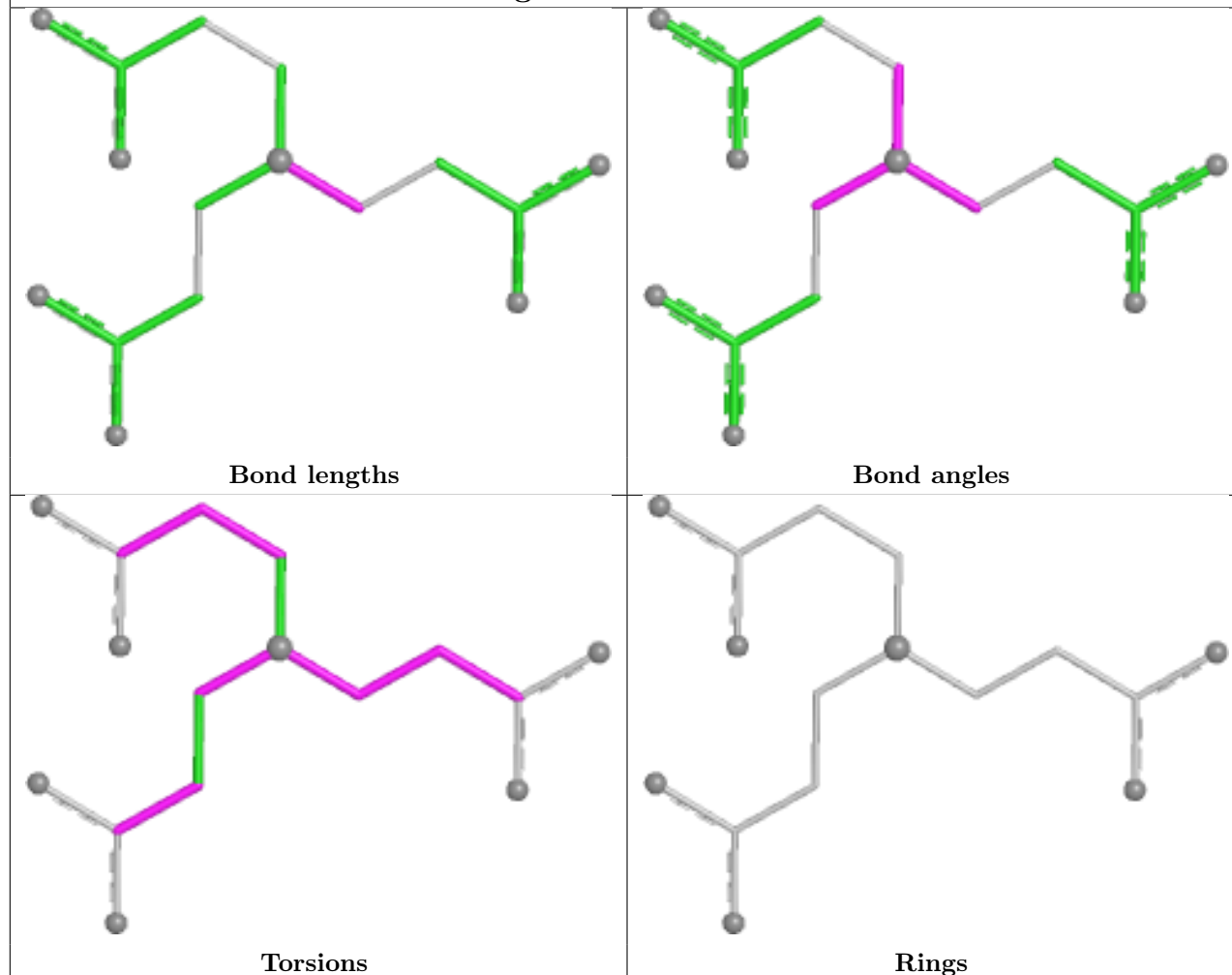
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	202	GOL	2	0
4	B	902	VO4	2	0
7	B	907	GOL	2	0
7	B	908	GOL	2	0
6	A	904	2OW	1	0
7	B	911	GOL	1	0
7	A	912	GOL	1	0
4	A	902	VO4	3	0
7	H	203	GOL	1	0
7	A	906	GOL	2	0
7	A	909	GOL	2	0
6	B	904	2OW	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

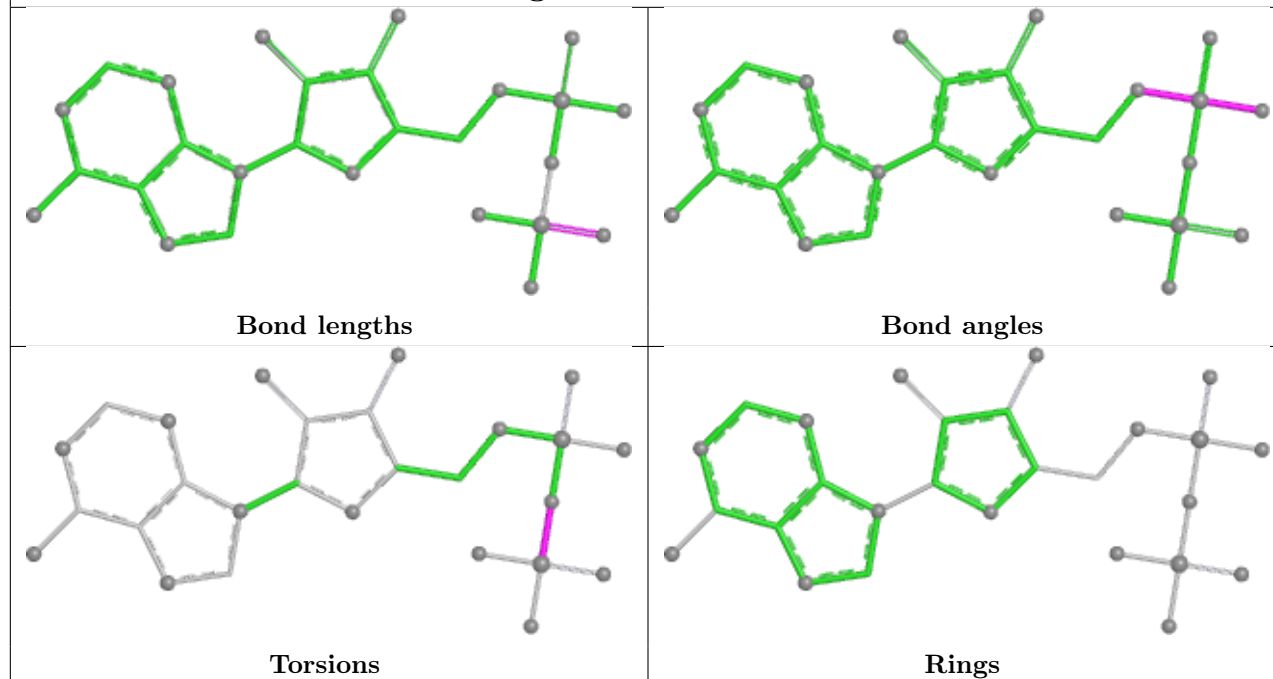
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

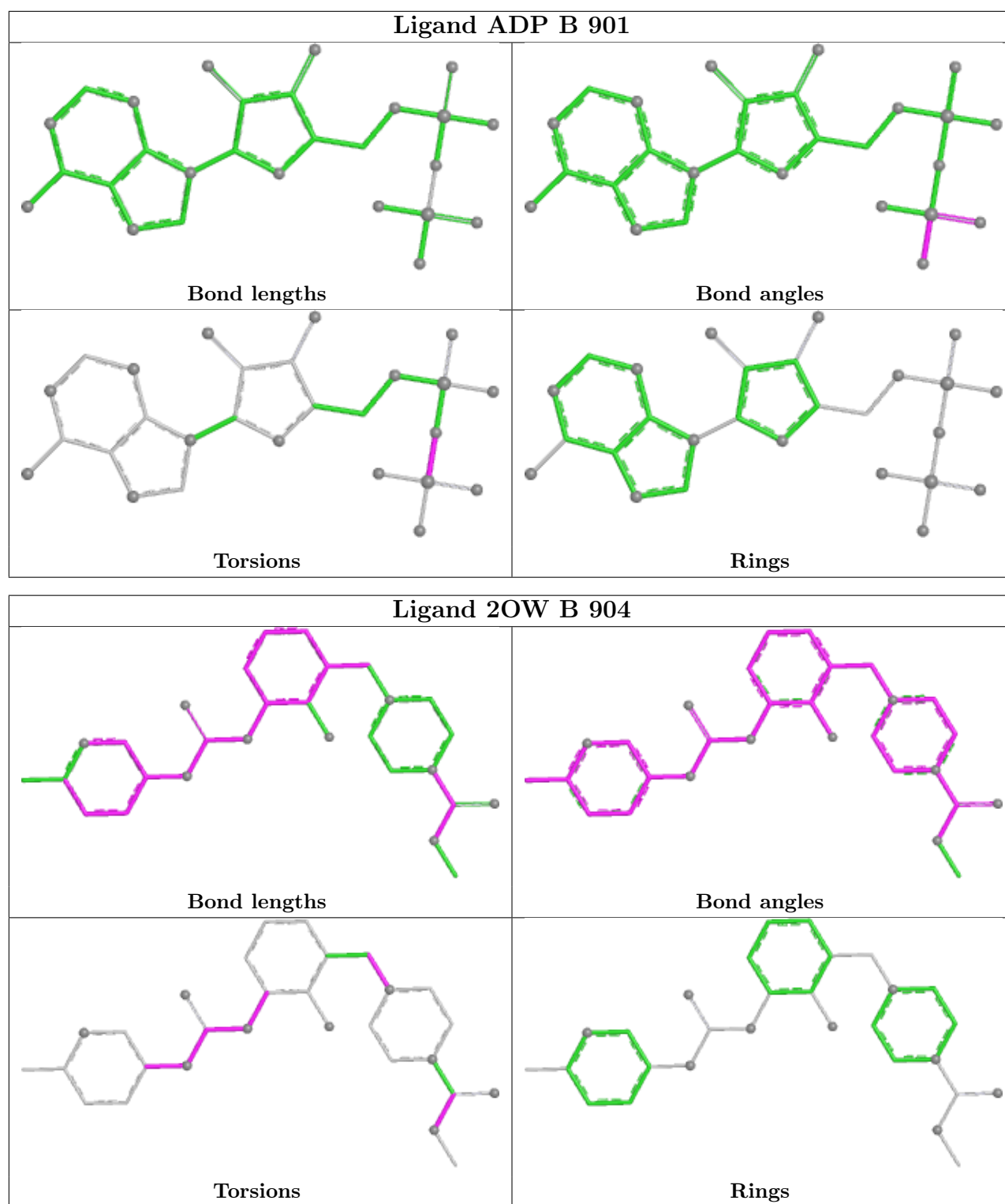


Ligand TCE B 914



Ligand ADP A 901





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.34	8 (1%) 78 79	25, 48, 80, 130	5 (0%)
1	B	764/828 (92%)	-0.34	6 (0%) 82 83	28, 50, 87, 133	2 (0%)
2	G	156/199 (78%)	0.38	4 (2%) 57 58	57, 86, 137, 183	0
2	H	161/199 (80%)	-0.16	4 (2%) 58 61	39, 55, 95, 139	0
All	All	1840/2054 (89%)	-0.26	22 (1%) 76 78	25, 51, 95, 183	7 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	ALA	8.5
2	G	178	ALA	3.2
1	A	736	ILE	2.9
1	B	145	LYS	2.9
1	A	622	ALA	2.9
1	A	404	VAL	2.8
1	B	201	ILE	2.7
1	A	4	ALA	2.6
1	B	807	ARG	2.6
1	A	130	TRP	2.4
2	H	179	GLY	2.4
1	A	6	MET	2.4
1	A	503[A]	LYS	2.4
1	B	406	VAL	2.3
2	G	199	GLY	2.2
2	H	41	PHE	2.2
2	H	39	PRO	2.2
2	G	41	PHE	2.1
1	B	54	ARG	2.1
2	H	178	ALA	2.0
1	B	146	LYS	2.0
2	G	45	LYS	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	0.95	0.07	39,43,47,48	0
1	M3L	A	129	12/13	0.96	0.08	44,47,50,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
7	GOL	A	916	6/6	0.64	0.16	117,119,120,120	0
7	GOL	A	913	6/6	0.73	0.15	81,82,82,83	0
8	TCE	B	914	16/16	0.75	0.16	103,115,117,117	0
7	GOL	B	909	6/6	0.79	0.15	97,98,98,98	0
7	GOL	H	202	6/6	0.82	0.13	75,78,79,80	0
7	GOL	B	907	6/6	0.83	0.15	71,73,73,74	0
7	GOL	A	906	6/6	0.83	0.14	58,59,61,66	0
7	GOL	B	913	6/6	0.83	0.14	63,68,72,75	0
7	GOL	A	907	6/6	0.83	0.16	71,73,76,76	0
7	GOL	B	905	6/6	0.83	0.16	71,75,75,75	0
7	GOL	B	908	6/6	0.84	0.18	77,84,88,90	0
7	GOL	H	201	5/6	0.84	0.13	66,67,69,73	0
7	GOL	A	909	6/6	0.84	0.17	39,57,64,66	0
7	GOL	B	912	6/6	0.84	0.13	102,103,103,104	0
7	GOL	A	914	6/6	0.85	0.13	65,66,68,68	0
7	GOL	A	915	6/6	0.85	0.13	82,83,84,85	0
7	GOL	B	906	6/6	0.87	0.16	75,78,80,82	0
7	GOL	A	911	6/6	0.87	0.12	67,71,72,72	0
7	GOL	A	908	6/6	0.87	0.15	72,73,74,74	0
7	GOL	A	905	6/6	0.89	0.10	60,61,66,69	0

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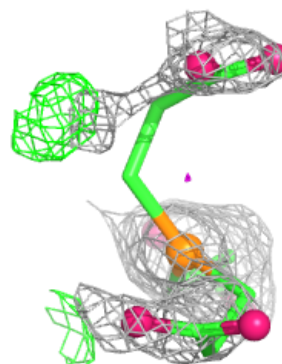
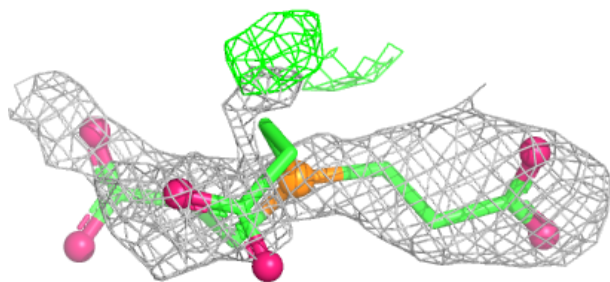
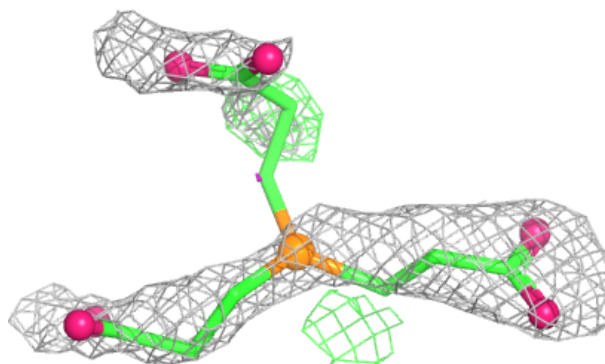
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	917	6/6	0.89	0.13	64,67,70,70	0
7	GOL	B	910	6/6	0.90	0.15	96,101,103,104	0
7	GOL	B	911	6/6	0.91	0.12	59,64,67,70	0
7	GOL	H	203	6/6	0.91	0.11	58,59,60,61	0
7	GOL	A	912	6/6	0.91	0.13	60,71,75,77	0
7	GOL	A	910	6/6	0.92	0.08	65,66,72,75	0
6	2OW	A	904	29/29	0.95	0.08	32,39,61,66	0
6	2OW	B	904	29/29	0.95	0.07	31,42,58,65	0
3	ADP	A	901	27/27	0.98	0.05	32,41,45,46	0
3	ADP	B	901	27/27	0.98	0.06	35,40,43,45	0
4	VO4	A	902	5/5	0.99	0.06	38,38,41,45	0
4	VO4	B	902	5/5	0.99	0.05	39,41,45,47	0
5	MG	A	903	1/1	0.99	0.05	38,38,38,38	0
5	MG	B	903	1/1	0.99	0.05	43,43,43,43	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.

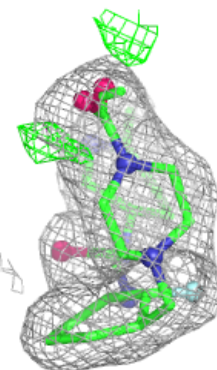
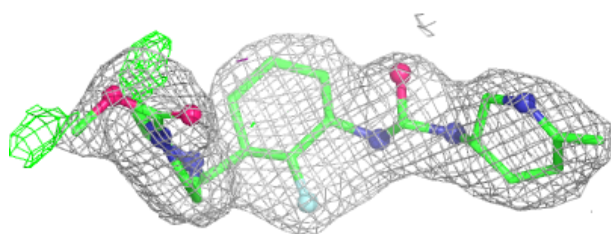
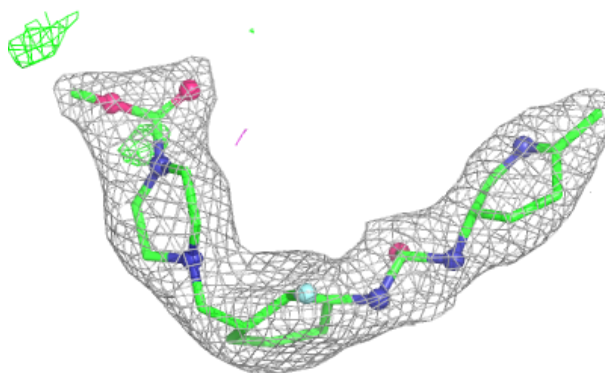
Electron density around TCE B 914:

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

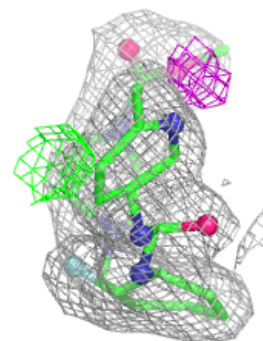
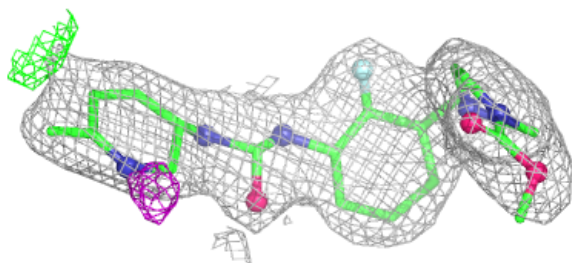
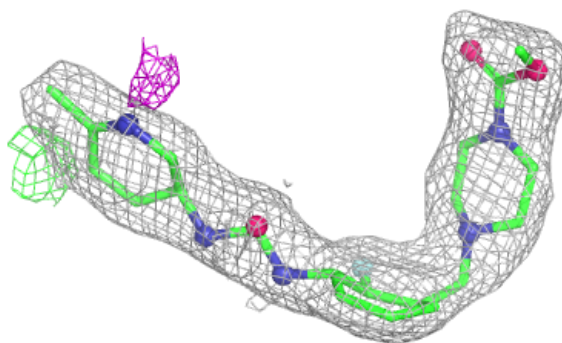


Electron density around 2OW A 904:

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

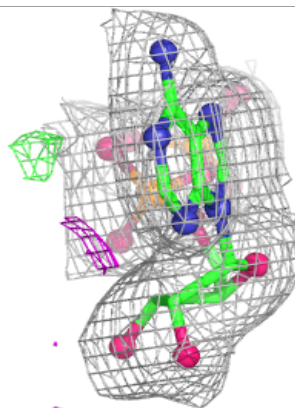
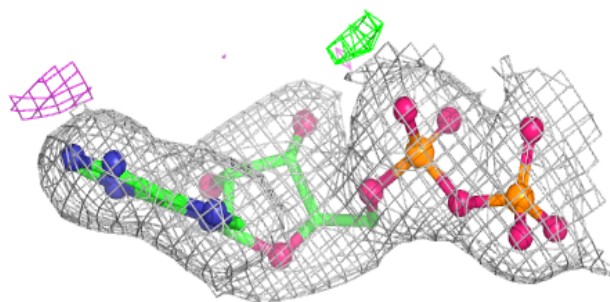
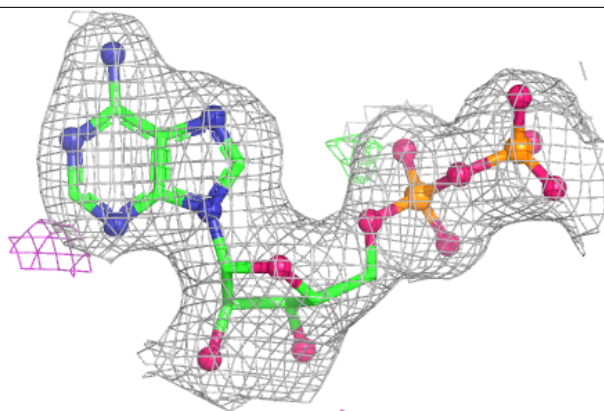
**Electron density around 2OW B 904:**

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

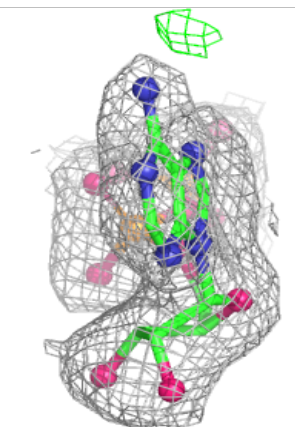
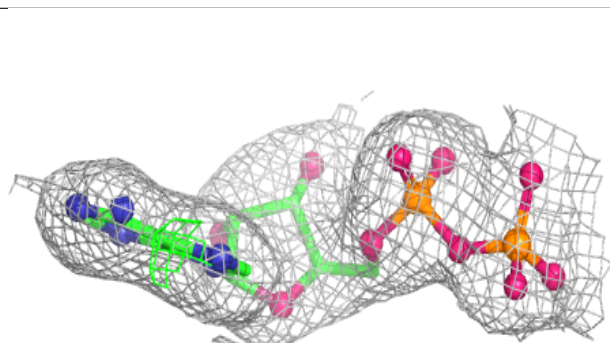
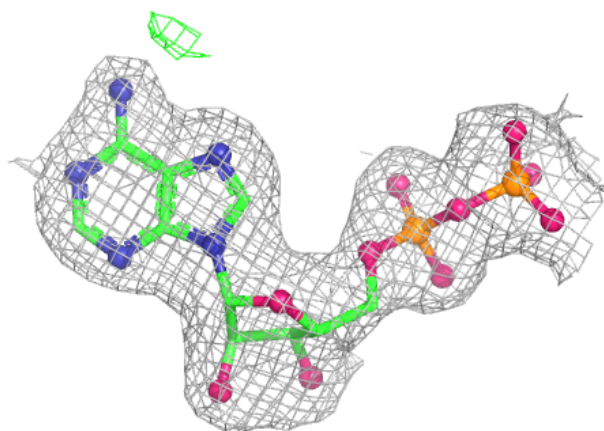


Electron density around ADP A 901:

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

**Electron density around ADP B 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 [i](#)

There are no such residues in this entry.