



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:20 AM UTC

PDB ID : 8QYU / pdb_00008qyu
Title : Beta-cardiac myosin S1 fragment in the pre-powerstroke state complexed to Omecamtiv mecarbil
Authors : Robert-Paganin, J.; Kikuti, C.; Auguin, D.; Rety, S.; David, A.; Houdusse, A.
Deposited on : 2023-10-26
Resolution : 1.96 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

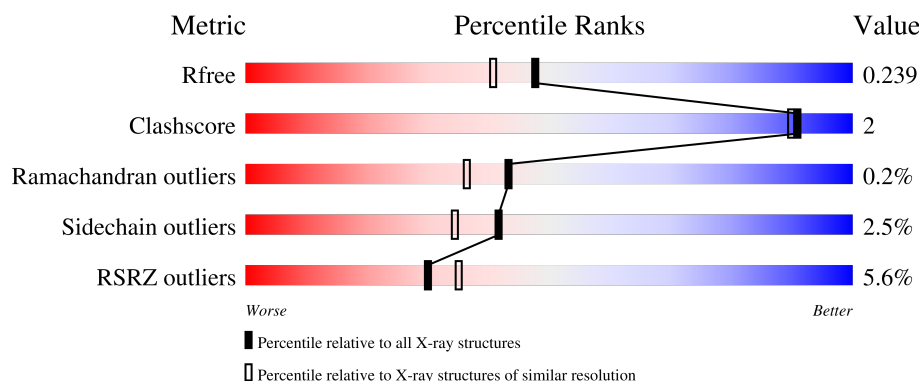
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	810	4% 88% 6% • 5%
1	B	810	4% 86% 6% • 7%
2	G	199	11% 66% 5% 30%
2	H	199	5% 72% 6% 22%

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	B	902	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 15636 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.

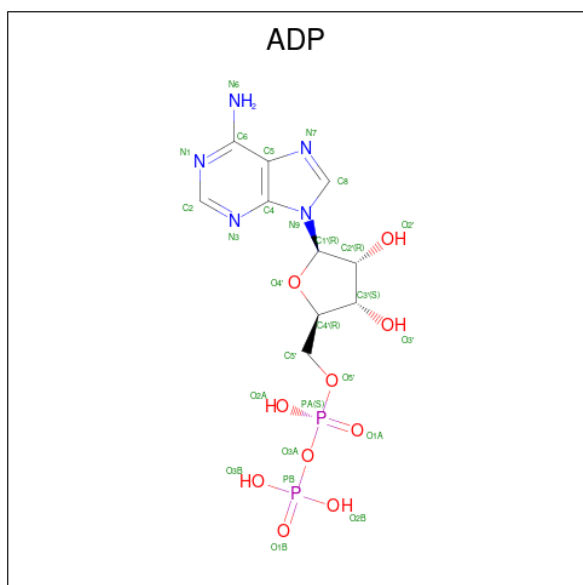
- Molecule 1 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	768	Total	C	N	O	S	0	2	0
			6224	3976	1064	1151	33			
1	B	756	Total	C	N	O	S	0	3	0
			6127	3927	1039	1128	33			

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

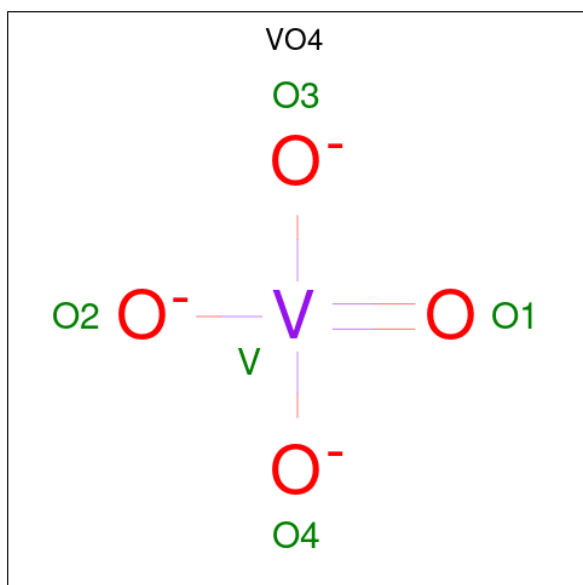
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	140	Total	C	N	O	S	0	0	0
			1117	710	182	215	10			
2	H	155	Total	C	N	O	S	0	1	0
			1231	776	205	240	10			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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: O_4V) (labeled as "Ligand of Interest" by depositor).



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) (labeled as "Ligand of Interest" by depositor).

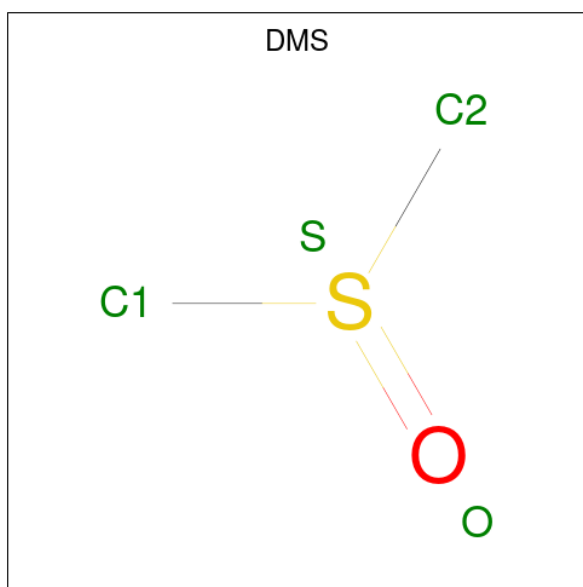
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



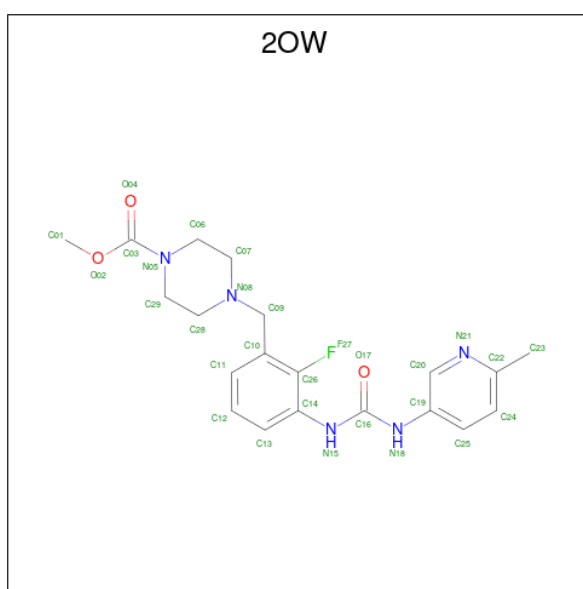
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 8 is methyl 4-(2-fluoro-3-{[(6-methylpyridin-3-yl)carbamoyl]amino}benzyl)piperazine-1-carboxylate (CCD ID: 2OW) (formula: $C_{20}H_{24}FN_5O_3$) (labeled as "Ligand of Interest" by depositor).



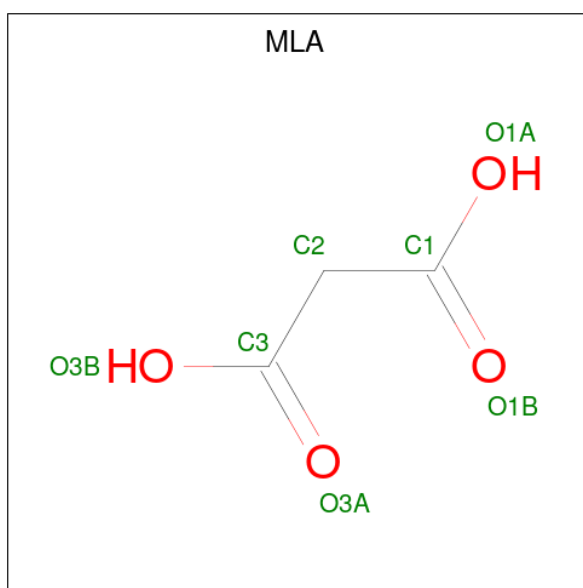
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	F	N	O	0
			29	20	1	5	3	0
8	B	1	Total	C	F	N	O	0
			29	20	1	5	3	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

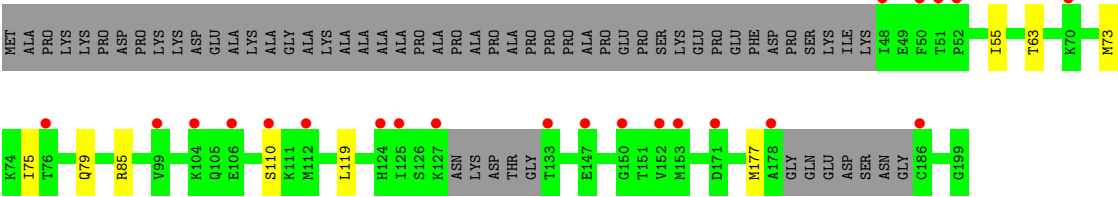
- Molecule 10 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



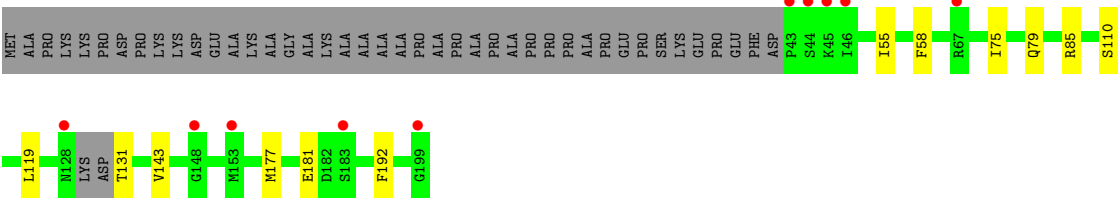
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	366	Total 366	O 366	0	0
11	B	324	Total 324	O 324	0	0
11	G	17	Total 17	O 17	0	0
11	H	62	Total 62	O 62	0	0



• 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	98.00Å 122.50Å 187.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.63 – 1.96 22.63 – 1.96	Depositor EDS
% Data completeness (in resolution range)	57.2 (22.63-1.96) 57.3 (22.63-1.96)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.96Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.191 , 0.235 0.193 , 0.239	Depositor DCC
R_{free} test set	4645 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15636	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: 2OW, ADP, MLA, FMT, DMS, M3L, GOL, MG, VO4

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	0.87	1/6328 (0.0%)	1.30	11/8525 (0.1%)
1	B	0.86	0/6231	1.30	19/8394 (0.2%)
2	G	0.82	1/1134 (0.1%)	1.42	0/1520
2	H	0.84	0/1253	1.40	1/1679 (0.1%)
All	All	0.86	2/14946 (0.0%)	1.32	31/20118 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	MET	SD-CE	-5.95	1.64	1.79
2	G	177	MET	SD-CE	-5.30	1.66	1.79

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	ILE	N-CA-CB	-10.03	101.18	112.21
1	B	736	ILE	CA-C-N	6.04	129.34	120.82
1	B	736	ILE	C-N-CA	6.04	129.34	120.82
1	B	281	ARG	CB-CG-CD	-6.04	97.41	111.30
1	A	766	LYS	N-CA-C	-5.99	101.61	110.48
1	B	148	SER	CA-C-N	5.97	130.69	120.72
1	B	148	SER	C-N-CA	5.97	130.69	120.72
2	H	58	PHE	CA-CB-CG	5.89	119.69	113.80
1	B	200	ALA	CA-C-N	5.83	132.19	121.70
1	B	200	ALA	C-N-CA	5.83	132.19	121.70
1	B	660	THR	CA-C-N	5.67	128.20	120.54
1	B	660	THR	C-N-CA	5.67	128.20	120.54
1	B	554	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	766	LYS	N-CA-C	-5.54	102.28	110.48
1	B	525	GLU	N-CA-C	5.43	120.06	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ASP	CA-C-N	5.40	127.52	120.28
1	A	218	ASP	C-N-CA	5.40	127.52	120.28
1	B	468	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	310	TYR	CA-C-N	5.24	127.25	120.44
1	B	310	TYR	C-N-CA	5.24	127.25	120.44
1	B	313	ILE	CA-CB-CG2	5.19	119.33	110.50
1	A	590	ILE	N-CA-CB	-5.16	104.23	112.07
1	A	468	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	469	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	358	HIS	CA-C-N	5.07	127.07	120.28
1	A	358	HIS	C-N-CA	5.07	127.07	120.28
1	B	765	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	525	GLU	N-CA-C	5.05	119.59	113.38
1	A	765	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	573	PRO	CA-C-N	5.03	128.01	120.87
1	A	573	PRO	C-N-CA	5.03	128.01	120.87

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	6224	0	6213	20	0
1	B	6127	0	6129	20	0
2	G	1117	0	1106	5	0
2	H	1231	0	1221	7	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	5	0	0	1	0
4	B	5	0	0	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	2	0	0
6	B	6	0	3	0	0
7	A	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	4	0	6	0	0
8	A	29	0	24	0	0
8	B	29	0	24	0	0
9	B	12	0	16	0	0
10	B	7	0	2	0	0
11	A	366	0	0	1	0
11	B	324	0	0	1	0
11	G	17	0	0	0	0
11	H	62	0	0	0	0
All	All	15636	0	14788	51	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 2.

All (51) 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)
2:G:55:ILE:HD12	2:G:119:LEU:HD21	1.68	0.76
2:H:55:ILE:HD12	2:H:119:LEU:HD21	1.68	0.75
2:H:75:ILE:HB	2:H:79:GLN:HG3	1.76	0.68
4:B:902:VO4:O4	4:B:902:VO4:V	1.54	0.65
4:A:902:VO4:V	4:A:902:VO4:O4	1.54	0.63
2:G:75:ILE:HB	2:G:79:GLN:HG3	1.81	0.62
4:B:902:VO4:V	4:B:902:VO4:O2	1.57	0.62
1:A:227:LEU:HD23	1:A:439:MET:HE3	1.83	0.60
1:B:227:LEU:HD23	1:B:439:MET:HE3	1.84	0.60
4:B:902:VO4:V	4:B:902:VO4:O3	1.59	0.59
1:A:196:ALA:HB2	1:A:220:ILE:HD11	1.86	0.58
1:A:515:MET:HE2	1:A:697:GLY:HA3	1.86	0.56
1:B:281:ARG:HD3	11:B:1103:HOH:O	2.07	0.54
1:A:660:THR:HG21	1:B:660:THR:OG1	2.09	0.53
1:A:781:LEU:HD22	2:H:143:VAL:HG11	1.91	0.51
1:A:657:LYS:HG2	1:B:657:LYS:HG2	1.93	0.51
1:B:27:GLN:HG3	1:B:28:THR:HG23	1.94	0.50
1:B:798:ARG:HD3	2:G:85:ARG:O	2.10	0.50
1:A:454:GLN:HG2	1:B:536:GLU:OE2	2.12	0.49
1:A:512:ASP:HA	7:A:905:DMS:H12	1.94	0.49
1:B:24:LEU:HA	1:B:27:GLN:HG2	1.94	0.48
2:H:177:MET:HE1	2:H:192:PHE:CE1	2.48	0.48
1:A:401:HIS:HB3	1:A:412:THR:HB	1.96	0.47
1:B:59:VAL:HG23	1:B:73:GLU:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:901:ADP:O1B	4:B:902:VO4:O3	2.33	0.47
2:G:63:THR:HG22	2:G:73:MET:SD	2.55	0.46
1:B:114:ILE:O	1:B:124:THR:HA	2.16	0.46
1:A:715:TYR:HB3	1:A:738:SER:HB3	1.97	0.46
1:B:196:ALA:HB2	1:B:220:ILE:HD11	1.99	0.45
1:B:339:LEU:HD13	1:B:443:ILE:HG12	1.98	0.45
1:B:401:HIS:HB3	1:B:412:THR:HB	1.98	0.45
1:A:185:THR:HG22	1:A:189:LYS:HE2	1.99	0.44
1:B:715:TYR:HB3	1:B:738:SER:HB3	1.99	0.44
1:A:403:ARG:HB3	1:A:410:TYR:HB3	2.00	0.43
1:A:712:ARG:HG3	1:A:762:LYS:HD3	2.00	0.43
1:B:238:ASN:HB3	1:B:241:SER:HB2	1.99	0.43
1:A:443:ILE:O	1:A:446:THR:HG22	2.19	0.43
1:A:435:MET:HG3	1:A:616:MET:CE	2.49	0.42
1:B:515:MET:HE2	1:B:697:GLY:HA3	2.00	0.42
1:B:234:LYS:HG2	1:B:239:ASP:HA	2.02	0.42
1:A:114:ILE:O	1:A:124:THR:HA	2.20	0.41
1:A:238:ASN:HB3	1:A:241:SER:HB2	2.01	0.41
2:H:75:ILE:HB	2:H:79:GLN:CG	2.49	0.41
1:A:81:PRO:HB2	11:A:1240:HOH:O	2.19	0.41
1:B:657:LYS:O	1:B:660:THR:HB	2.21	0.41
2:H:177:MET:HE1	2:H:192:PHE:CZ	2.55	0.41
1:A:234:LYS:HG2	1:A:239:ASP:HA	2.02	0.41
1:B:435:MET:HG3	1:B:616:MET:CE	2.51	0.41
2:G:75:ILE:HB	2:G:79:GLN:CG	2.50	0.41
1:A:798:ARG:HD3	2:H:85:ARG:O	2.21	0.41
1:B:243:ARG:HD3	1:B:269:GLU:OE1	2.22	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	760/810 (94%)	739 (97%)	19 (2%)	2 (0%)	36	28
1	B	743/810 (92%)	726 (98%)	16 (2%)	1 (0%)	48	41
2	G	134/199 (67%)	132 (98%)	2 (2%)	0	100	100
2	H	152/199 (76%)	149 (98%)	3 (2%)	0	100	100
All	All	1789/2018 (89%)	1746 (98%)	40 (2%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	570	LYS
1	B	267	LEU
1	A	267	LEU

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	669/698 (96%)	650 (97%)	19 (3%)	38	30
1	B	660/698 (95%)	643 (97%)	17 (3%)	40	33
2	G	122/165 (74%)	121 (99%)	1 (1%)	73	74
2	H	135/165 (82%)	132 (98%)	3 (2%)	45	40
All	All	1586/1726 (92%)	1546 (98%)	40 (2%)	42	34

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	59	VAL
1	A	146	LYS
1	A	157	ILE
1	A	260	SER
1	A	267	LEU
1	A	271	SER
1	A	294	LYS

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Mol	Chain	Res	Type
1	A	384	SER
1	A	453	ARG
1	A	474	GLU
1	A	570	LYS
1	A	590	ILE
1	A	652	ARG
1	A	663	ARG
1	A	690	MET
1	A	712	ARG
1	A	738	SER
1	A	798	ARG
1	B	71	VAL
1	B	157	ILE
1	B	260	SER
1	B	267	LEU
1	B	271	SER
1	B	294	LYS
1	B	313	ILE
1	B	384	SER
1	B	397	LYS
1	B	453	ARG
1	B	474	GLU
1	B	503	LYS
1	B	570	LYS
1	B	663	ARG
1	B	671	ARG
1	B	738	SER
1	B	798	ARG
2	G	110	SER
2	H	110	SER
2	H	131	THR
2	H	181	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	222	GLN
1	A	306	ASN
1	A	401	HIS
1	A	437	ASN
1	A	492	HIS

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Mol	Chain	Res	Type
1	A	562	ASN
1	A	564	GLN
1	A	791	GLN
1	B	27	GLN
1	B	187	ASN
1	B	222	GLN
1	B	306	ASN
1	B	401	HIS
1	B	437	ASN
1	B	555	ASN
1	B	562	ASN
1	B	711	ASN
1	B	791	GLN
2	G	105	GLN
2	G	109	ASN
2	H	105	GLN
2	H	109	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	0.82	1 (10%)	9,14,16	0.70	0
1	M3L	B	549	1	10,11,12	0.61	0	9,14,16	0.65	0
1	M3L	B	129	1	10,11,12	0.93	1 (10%)	9,14,16	0.78	1 (11%)
1	M3L	A	549	1	10,11,12	0.95	1 (10%)	9,14,16	0.55	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	549	1	-	1/9/10/12	-
1	M3L	B	129	1	-	0/9/10/12	-
1	M3L	A	549	1	-	1/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	549	M3L	CB-CA	2.80	1.57	1.53
1	B	129	M3L	CB-CA	2.59	1.57	1.53
1	A	129	M3L	CB-CA	2.35	1.57	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	M3L	CD-CE-NZ	2.25	124.22	115.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	549	M3L	CA-CB-CG-CD
1	A	549	M3L	CA-CB-CG-CD

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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z > 2$
6	FMT	B	904	-	2,2,2	1.16	0	1,1,1	1.12	0
7	DMS	B	906	-	3,3,3	0.32	0	3,3,3	0.83	0
6	FMT	A	904	-	2,2,2	1.15	0	1,1,1	1.20	0
7	DMS	A	907	-	3,3,3	0.58	0	3,3,3	0.48	0
4	VO4	B	902	3,5	0,4,4	-	-	-	-	-
10	MLA	B	909	-	6,6,6	1.24	0	7,7,7	1.50	3 (42%)
6	FMT	B	905	-	2,2,2	1.07	0	1,1,1	1.19	0
3	ADP	B	901	5,4	28,29,29	0.35	0	43,45,45	0.51	0
7	DMS	A	905	-	3,3,3	0.27	0	3,3,3	0.40	0
8	2OW	A	908	-	31,31,31	0.31	0	41,42,42	0.58	0
8	2OW	B	910	-	31,31,31	0.43	0	41,42,42	0.52	0
3	ADP	A	901	5,4	28,29,29	0.35	0	43,45,45	0.44	0
9	GOL	B	908	-	5,5,5	0.12	0	5,5,5	0.22	0
7	DMS	A	906	-	3,3,3	0.40	0	3,3,3	0.76	0
9	GOL	B	907	-	5,5,5	0.03	0	5,5,5	0.14	0
4	VO4	A	902	3,5	0,4,4	-	-	-	-	-

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
10	MLA	B	909	-	-	2/4/4/4	-
8	2OW	A	908	-	-	5/18/28/28	1/3/3/3
3	ADP	B	901	5,4	-	2/16/32/32	0/3/3/3
8	2OW	B	910	-	-	6/18/28/28	1/3/3/3
3	ADP	A	901	5,4	-	3/16/32/32	0/3/3/3
9	GOL	B	908	-	-	0/4/4/4	-
9	GOL	B	907	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	909	MLA	C3-C2-C1	-2.36	104.61	112.95
10	B	909	MLA	O3B-C3-C2	2.26	121.50	114.51
10	B	909	MLA	O3A-C3-C2	-2.02	116.37	122.11

There are no chirality outliers.

All (18) 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
8	A	908	2OW	O04-C03-O02-C01
8	A	908	2OW	N05-C03-O02-C01
8	A	908	2OW	C26-C14-N15-C16
8	B	910	2OW	N05-C03-O02-C01
8	B	910	2OW	C26-C14-N15-C16
8	B	910	2OW	O04-C03-O02-C01
8	A	908	2OW	C10-C09-N08-C07
8	A	908	2OW	C10-C09-N08-C28
10	B	909	MLA	O1B-C1-C2-C3
8	B	910	2OW	C10-C09-N08-C07
8	B	910	2OW	C10-C09-N08-C28
10	B	909	MLA	O1A-C1-C2-C3
3	A	901	ADP	PA-O3A-PB-O1B
3	A	901	ADP	PA-O3A-PB-O3B
3	B	901	ADP	PA-O3A-PB-O2B
8	B	910	2OW	C13-C14-N15-C16

All (2) ring outliers are listed below:

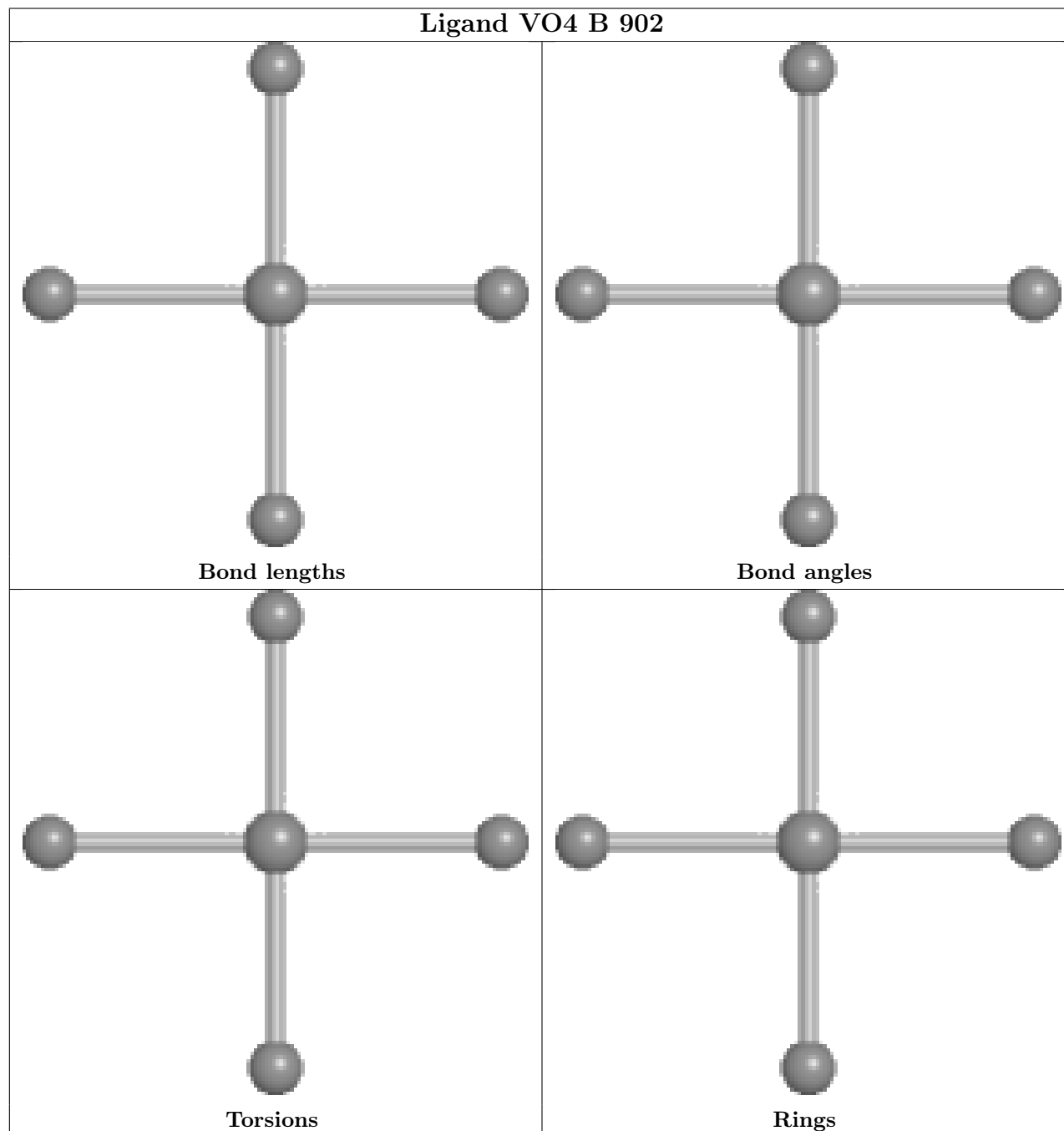
Mol	Chain	Res	Type	Atoms
8	B	910	2OW	C06-C07-C28-C29-N05-N08
8	A	908	2OW	C06-C07-C28-C29-N05-N08

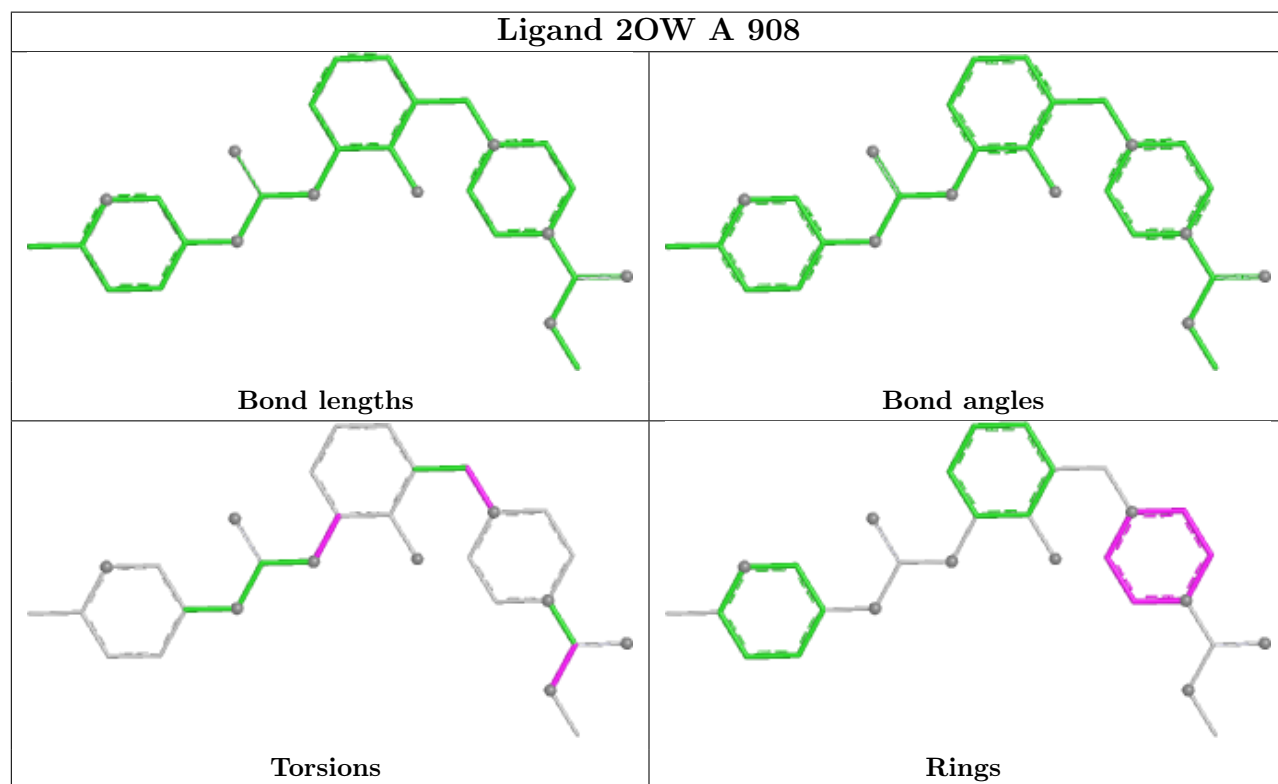
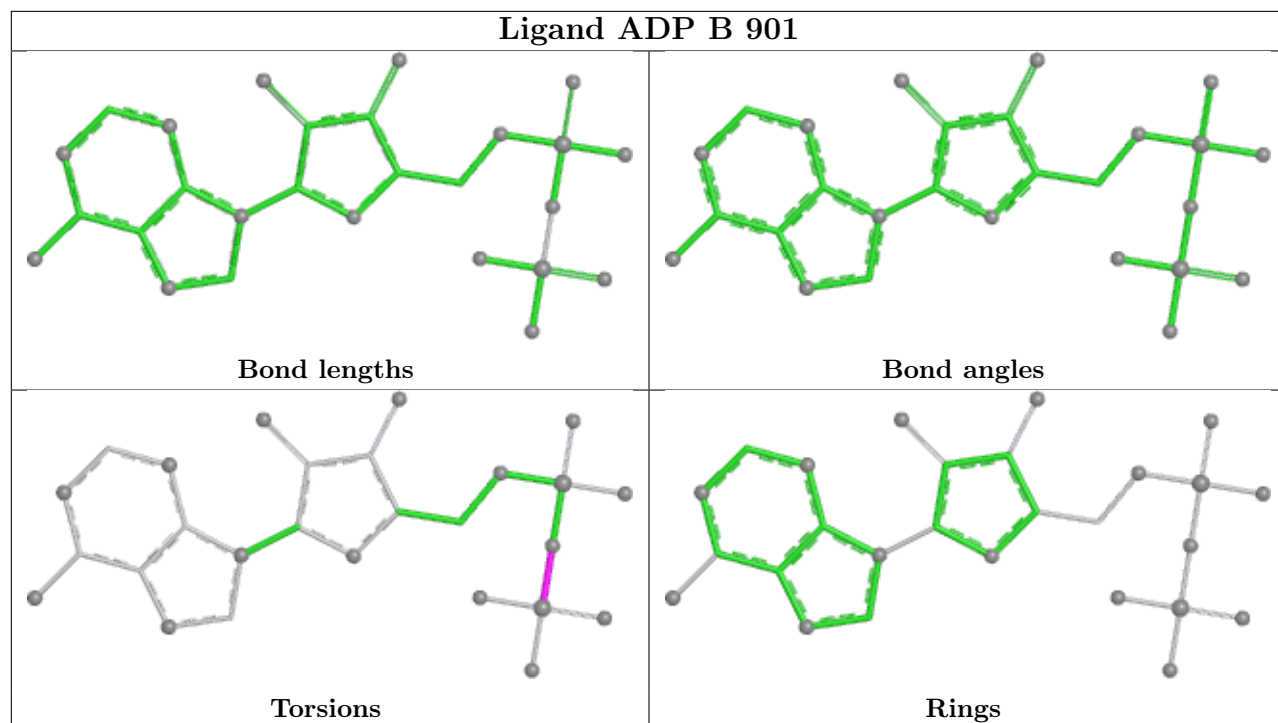
4 monomers are involved in 6 short contacts:

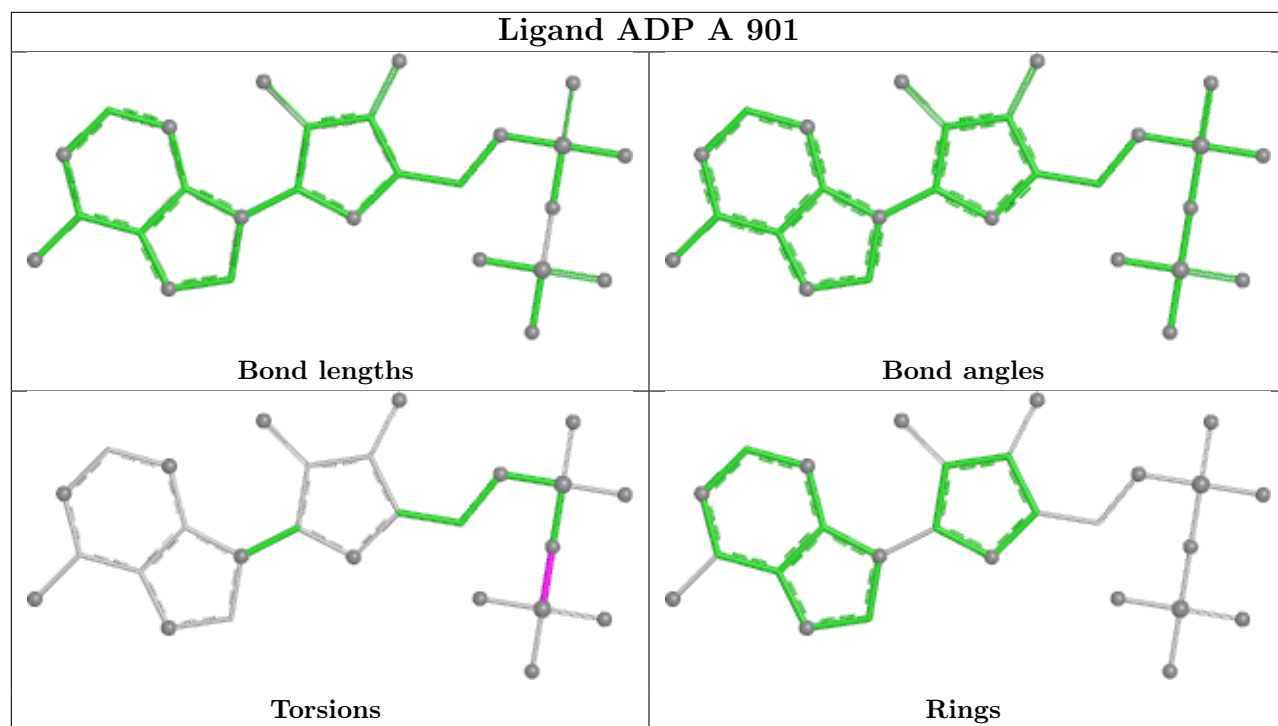
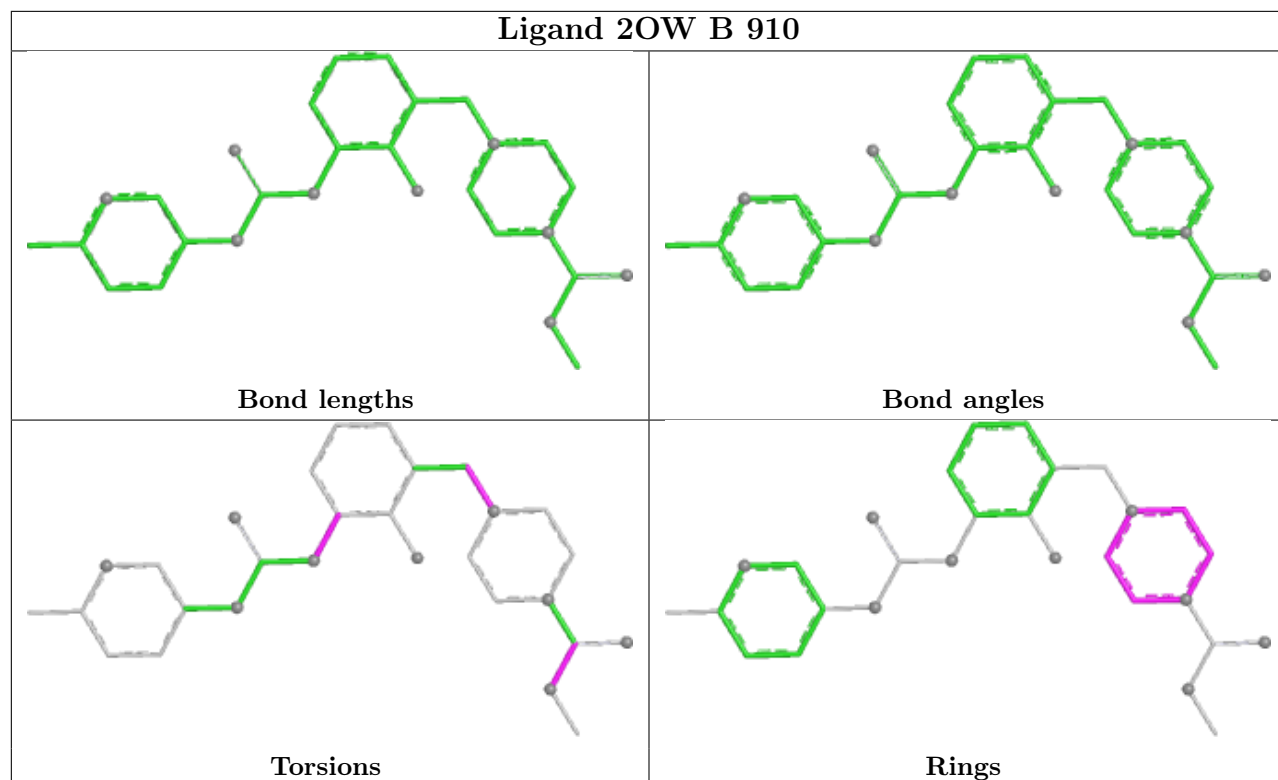
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	902	VO4	4	0
3	B	901	ADP	1	0
7	A	905	DMS	1	0
4	A	902	VO4	1	0

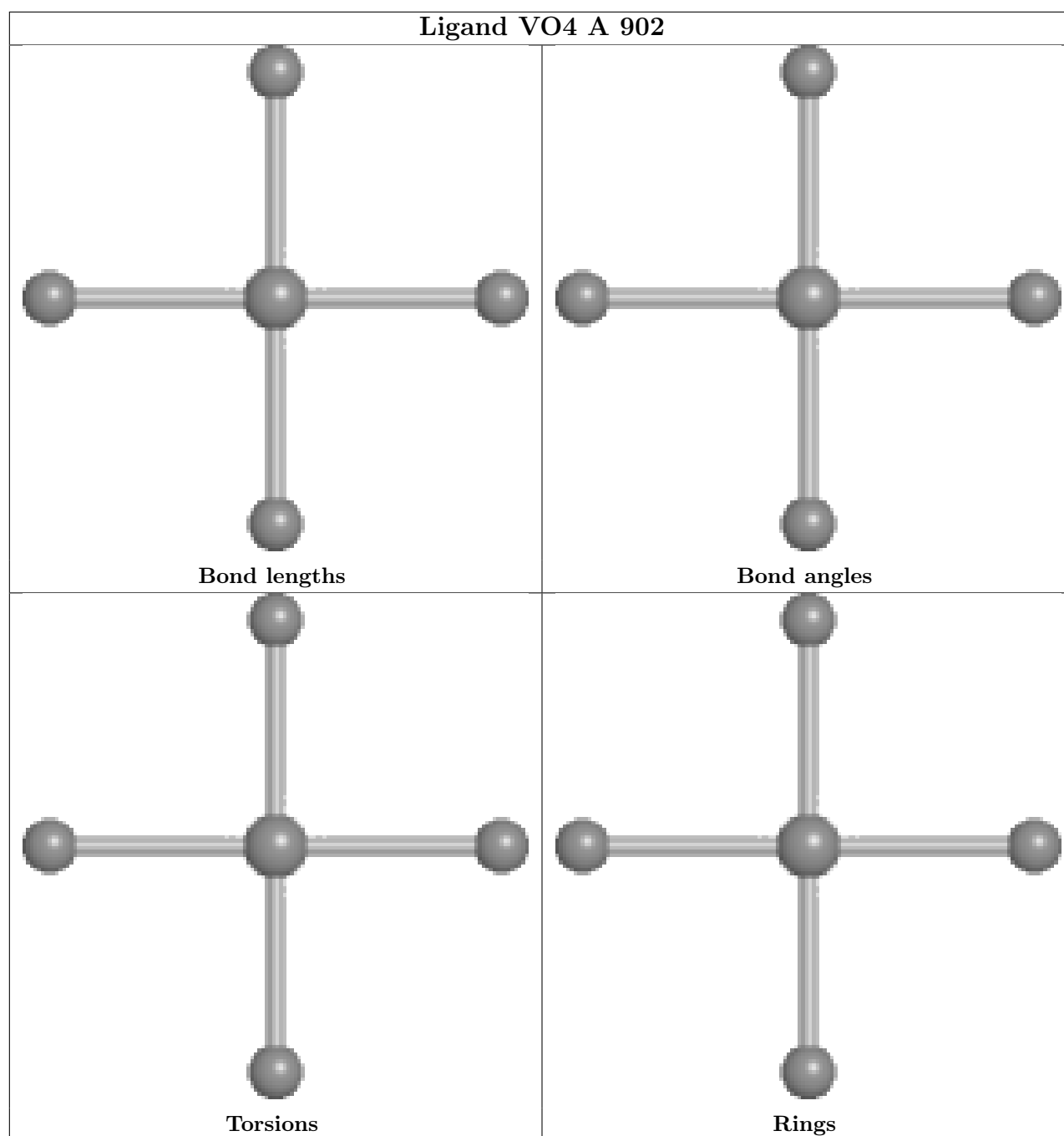
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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	766/810 (94%)	0.05	33 (4%)	40	46	12, 31, 64, 99	3 (0%)
1	B	754/810 (93%)	0.13	36 (4%)	35	41	12, 33, 67, 112	3 (0%)
2	G	140/199 (70%)	1.24	22 (15%)	5	5	39, 62, 94, 125	0
2	H	155/199 (77%)	0.39	10 (6%)	25	28	24, 40, 70, 92	1 (0%)
All	All	1815/2018 (89%)	0.21	101 (5%)	30	35	12, 34, 72, 125	7 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	ILE	5.9
2	G	48	ILE	5.8
2	H	43	PRO	5.3
1	B	57	GLY	5.2
1	A	622	ALA	4.2
1	B	130[A]	TRP	3.9
1	B	622	ALA	3.8
1	A	70	THR	3.8
1	A	571	GLY	3.7
2	G	178	ALA	3.7
1	A	21	LYS	3.7
1	A	569	ILE	3.7
2	G	50	PHE	3.7
1	B	410	TYR	3.6
1	A	220	ILE	3.6
1	B	804	LEU	3.6
1	B	70	THR	3.5
1	B	54	ARG	3.5
1	B	366	LEU	3.5
1	B	63	THR	3.5
2	G	99	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	805	LEU	3.4
1	A	810	SER	3.3
1	B	411	VAL	3.3
1	B	806	GLU	3.3
1	B	735	PHE	3.3
2	H	128	ASN	3.3
1	A	130[A]	TRP	3.2
1	A	69	VAL	3.1
1	A	410	TYR	3.1
1	A	404	VAL	3.0
1	A	4	ALA	3.0
2	G	51	THR	3.0
1	B	67	LYS	3.0
1	B	71	VAL	3.0
2	H	183	SER	3.0
1	B	802	LYS	3.0
1	B	731	PRO	3.0
2	H	153	MET	2.9
2	H	45	LYS	2.9
1	A	663	ARG	2.9
1	B	72	LYS	2.8
1	A	413	LYS	2.8
1	B	570	LYS	2.8
1	A	653	GLU	2.8
1	A	53	SER	2.8
2	G	147	GLU	2.8
2	G	124	HIS	2.8
1	A	3	ASP	2.8
2	G	133	THR	2.7
1	A	645	GLN	2.7
1	A	570	LYS	2.7
1	A	657	LYS	2.7
2	G	127	LYS	2.7
2	G	150	GLY	2.6
2	G	76	THR	2.6
1	A	67	LYS	2.6
1	B	728	ALA	2.6
1	B	569	ILE	2.6
2	G	186	CYS	2.5
1	A	20	GLU	2.5
1	A	408	ASN	2.5
1	A	54	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	52	PRO	2.5
1	B	422	TYR	2.5
1	B	68	THR	2.4
1	B	42	ASP	2.4
2	G	152	VAL	2.4
1	B	50	THR	2.4
2	H	46	ILE	2.4
2	H	44	SER	2.4
1	B	407	GLY	2.3
1	B	663	ARG	2.3
2	G	104	LYS	2.3
1	B	417	VAL	2.3
2	G	70	LYS	2.3
1	B	31	PHE	2.2
1	B	409	GLU	2.2
2	G	112	MET	2.2
1	A	201	ILE	2.1
2	G	125	ILE	2.1
1	A	60	THR	2.1
1	B	58	LYS	2.1
1	A	5	GLU	2.1
2	G	153	MET	2.1
2	G	171	ASP	2.1
1	A	19	SER	2.1
2	G	110	SER	2.1
1	B	69	VAL	2.1
1	A	58	LYS	2.1
2	H	199	GLY	2.1
1	A	539	MET	2.1
2	H	67[A]	ARG	2.1
1	A	62	GLU	2.0
2	G	106	GLU	2.0
1	B	148	SER	2.0
1	A	57	GLY	2.0
2	H	148	GLY	2.0
1	B	406	VAL	2.0
1	A	65	HIS	2.0
1	B	408	ASN	2.0

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

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	A	129	12/13	0.94	0.08	21,29,33,33	0
1	M3L	A	549	12/13	0.95	0.09	22,36,51,52	0
1	M3L	B	129	12/13	0.95	0.07	19,28,32,36	0
1	M3L	B	549	12/13	0.95	0.11	20,26,39,45	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

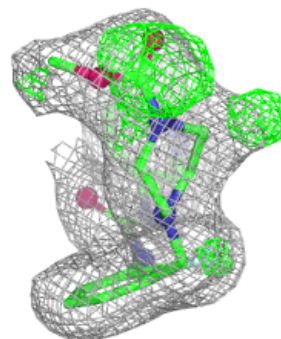
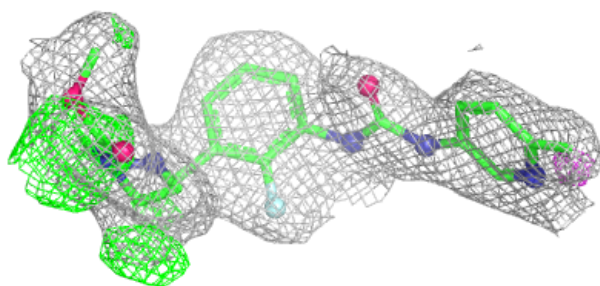
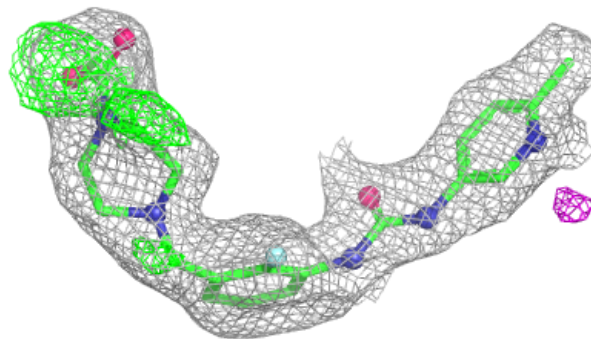
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	MLA	B	909	7/7	0.77	0.17	34,46,55,61	0
7	DMS	A	907	4/4	0.87	0.17	37,41,49,57	0
9	GOL	B	907	6/6	0.87	0.15	56,61,66,68	0
6	FMT	B	904	3/3	0.87	0.14	53,53,55,56	0
9	GOL	B	908	6/6	0.88	0.15	57,63,67,69	0
6	FMT	B	905	3/3	0.89	0.13	55,55,57,59	0
8	2OW	A	908	29/29	0.90	0.09	15,24,36,39	0
7	DMS	A	905	4/4	0.90	0.12	14,33,46,51	0
8	2OW	B	910	29/29	0.91	0.08	9,25,36,39	0
6	FMT	A	904	3/3	0.93	0.10	42,42,42,46	0
7	DMS	A	906	4/4	0.94	0.14	18,52,57,60	0
7	DMS	B	906	4/4	0.96	0.09	44,54,56,56	0
3	ADP	B	901	27/27	0.98	0.05	17,23,30,35	0
4	VO4	B	902	5/5	0.98	0.07	16,20,26,30	0
4	VO4	A	902	5/5	0.99	0.05	19,21,25,35	0
3	ADP	A	901	27/27	0.99	0.04	15,22,28,29	0
5	MG	A	903	1/1	0.99	0.03	22,22,22,22	0
5	MG	B	903	1/1	0.99	0.03	17,17,17,17	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.

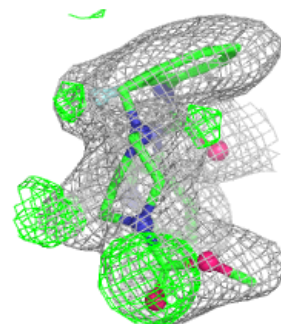
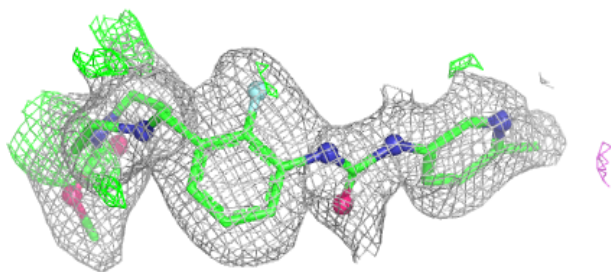
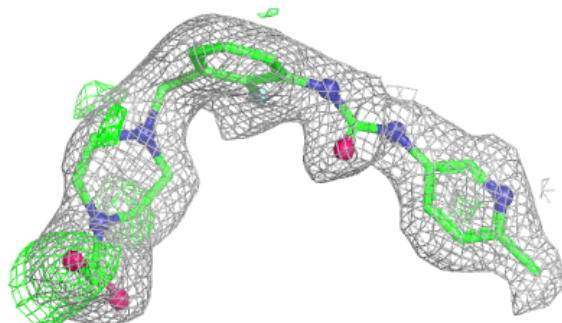
Electron density around 2OW A 908:

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



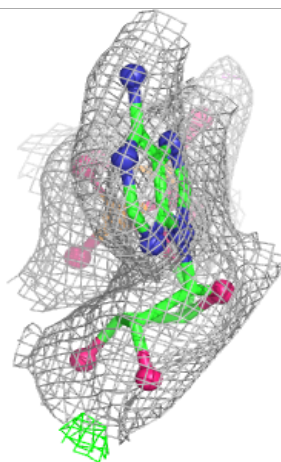
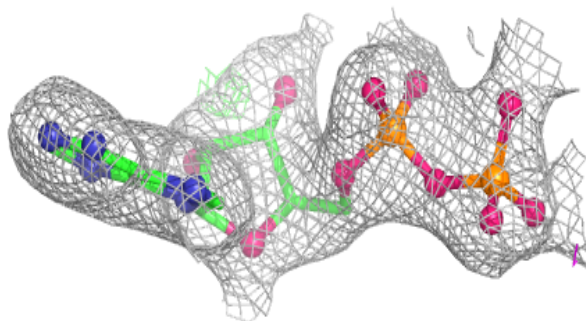
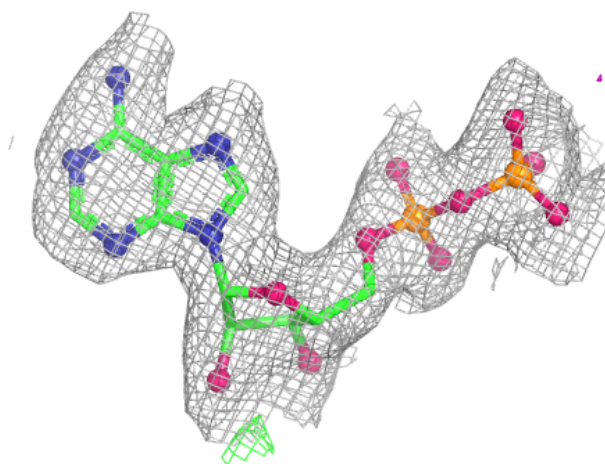
Electron density around 2OW B 910:

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



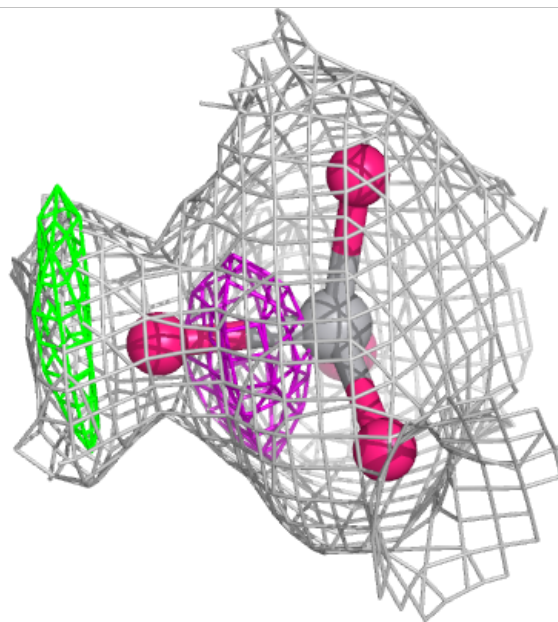
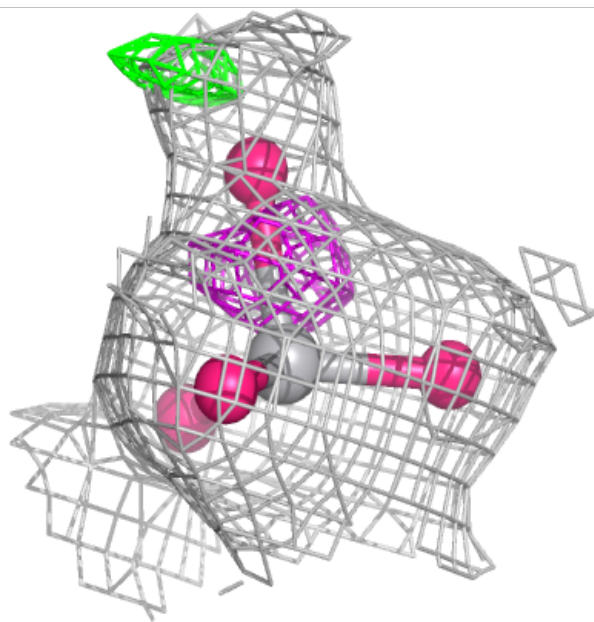
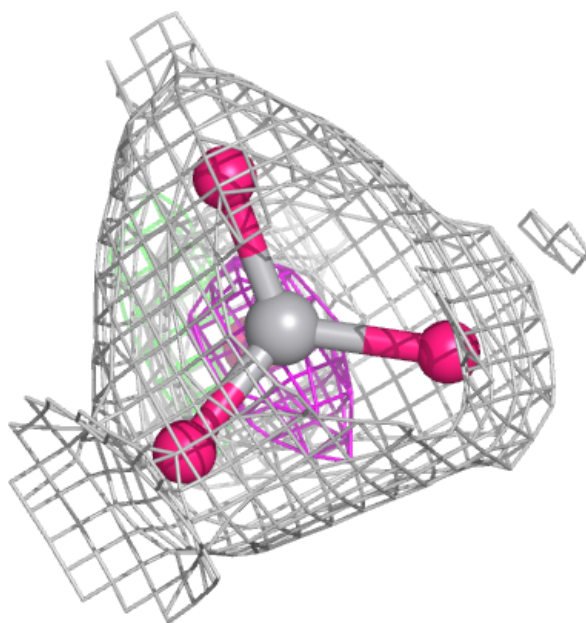
Electron density around ADP B 901:

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



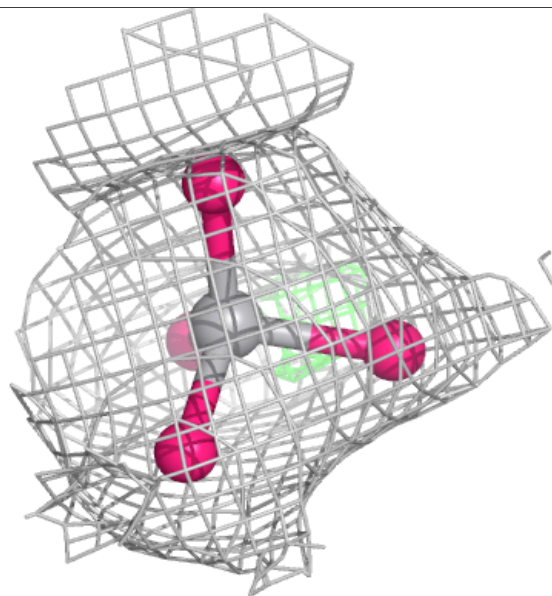
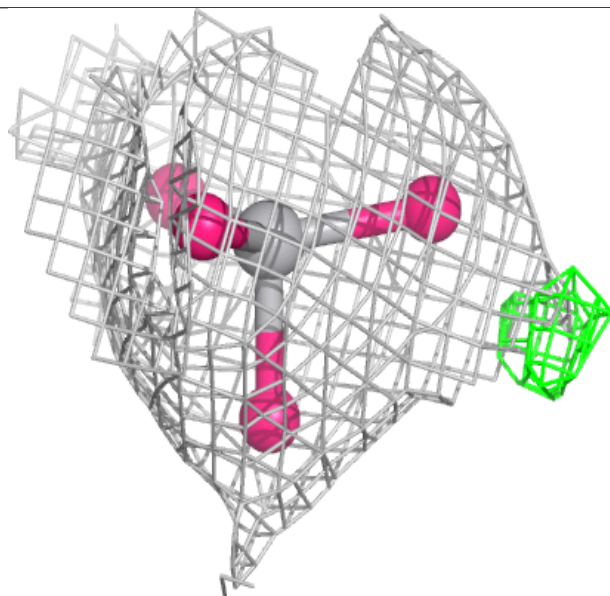
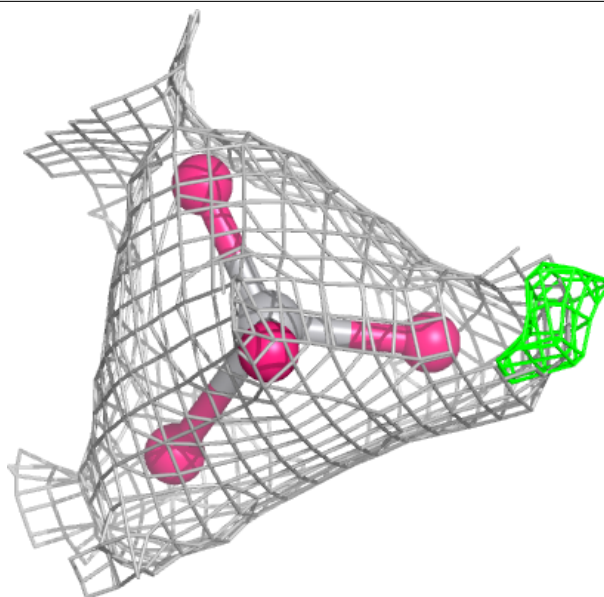
Electron density around VO4 B 902:

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



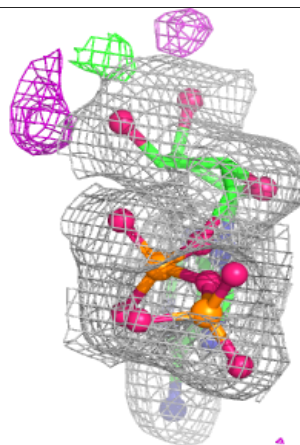
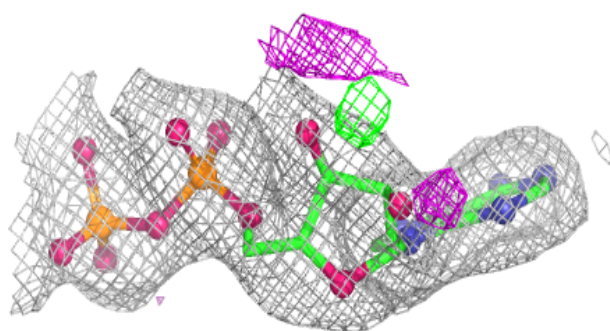
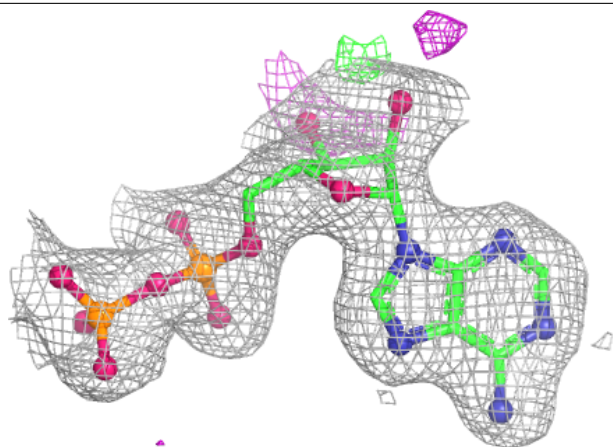
Electron density around VO4 A 902:

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



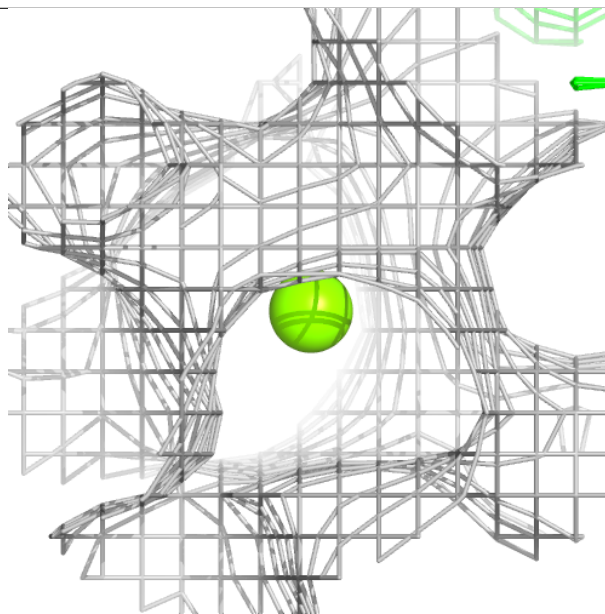
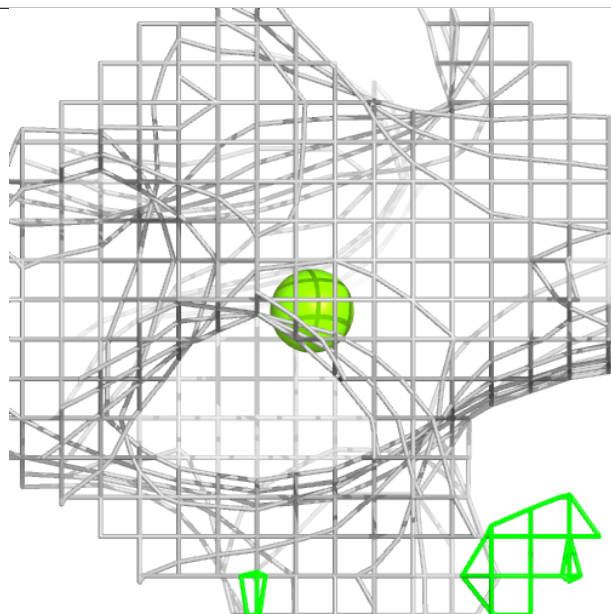
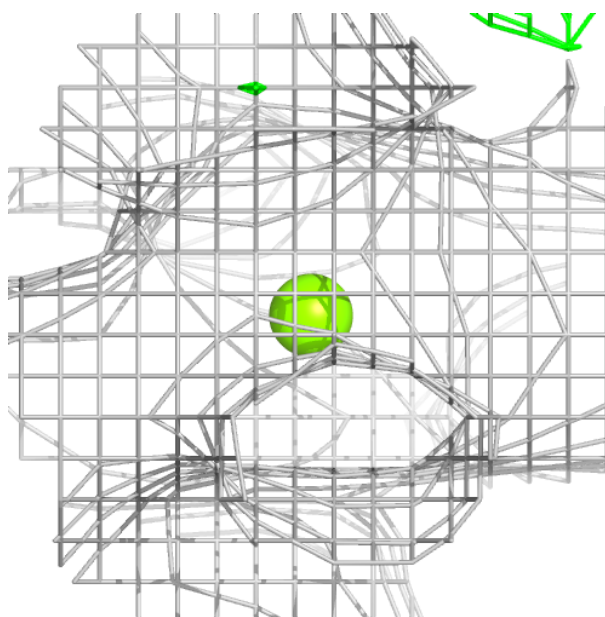
Electron density around ADP A 901:

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



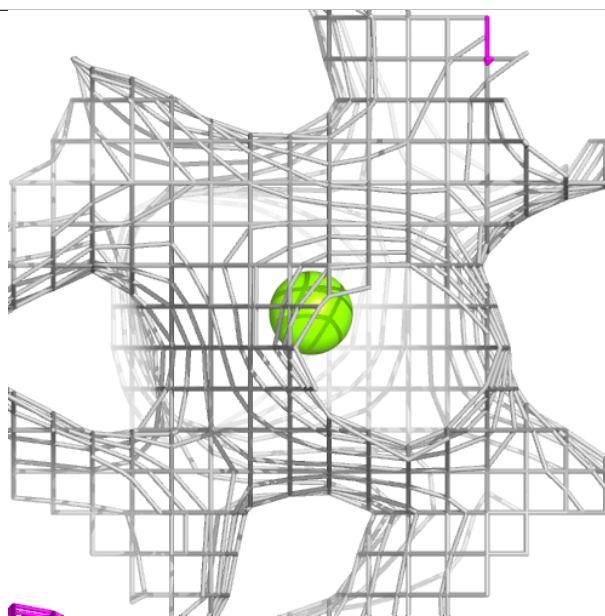
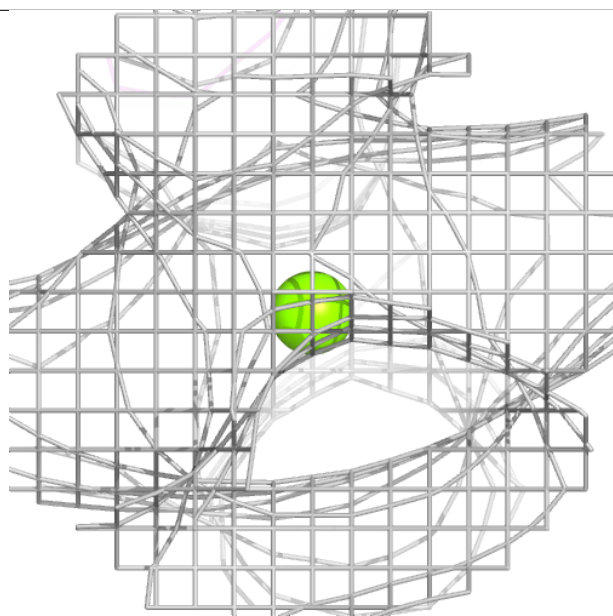
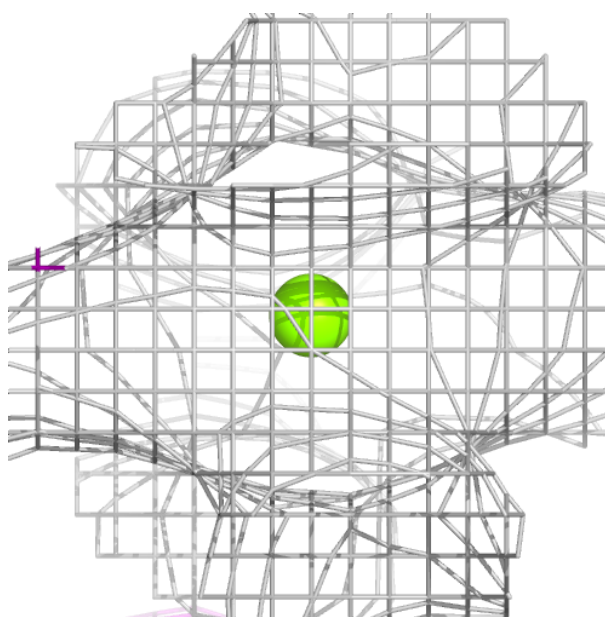
Electron density around MG A 903:

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



Electron density around MG B 903:

$2mF_o-DF_c$ (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.