



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 10:26 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

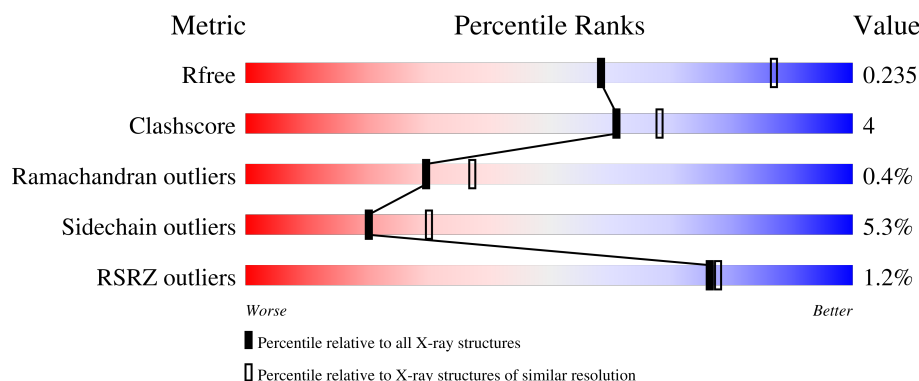
1 Overall quality at a glance

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	2% 79% 12% 8%
1	B	828	2% 79% 11% 8%
2	G	199	2% 65% 13% 22%
2	H	199	2% 61% 17% 19%

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.

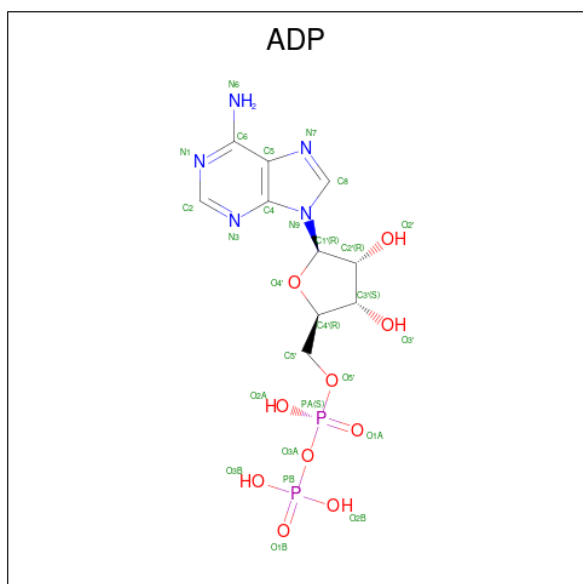
- Molecule 1 is a protein called Myosin-7.

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.

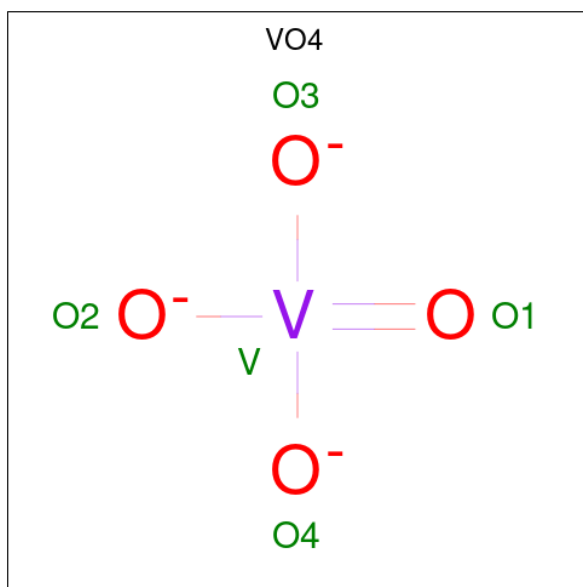
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	156	Total	C	N	O	S	0	0	0
			1234	778	203	243	10			
2	H	161	Total	C	N	O	S	0	0	0
			1275	804	209	252	10			

- 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: O_4V).

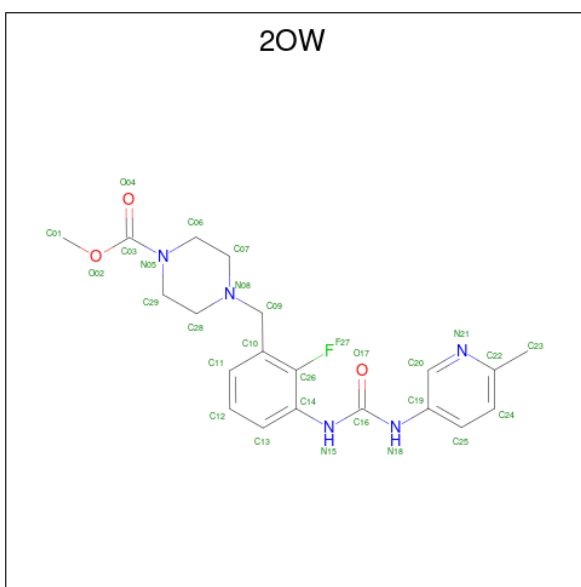


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O V	0	0
			5	4 1		
4	B	1	Total	O V	0	0
			5	4 1		

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

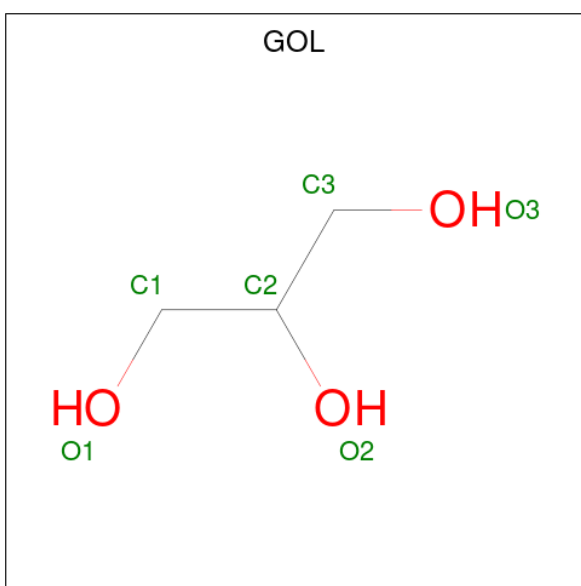
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is methyl 4-(2-fluoro-3-[(6-methylpyridin-3-yl)carbamoyl]amino}benzyl)piperazine-1-carboxylate (CCD ID: 2OW) (formula: $C_{20}H_{24}FN_5O_3$).



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: $C_3H_8O_3$).



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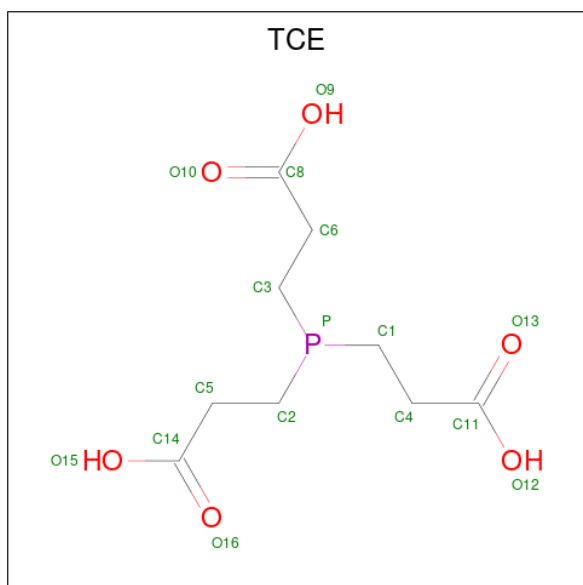
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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:

79% 12% 8%

Chain B:

Residue	Percentage (%)
MET	79%
VAL	11%
ASP	8%
ALA	2%

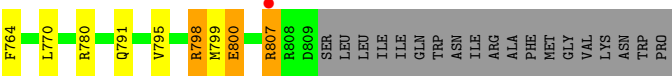
ARG
SER
LYS
GLY
GLN
THR
GLY
LYS
GLY
GLY
T215
L216
E217
D218
Q219
I220
I220
L227
E228
D228
N232
E274
K484
F494
Q498
K502
R503
E504
D512
F513
G514
M515
D516
E525
K526
S532
M539
K549
K570
H576
F577
S578
L579
I590
Q595
L604

D607
M616
L617
L620
M623
TYR
GLY
PHE
ASP
THR
PRO
ILE
GLU
LYS
GLY
LYS
GLY
LYS
ALA
LYS
LYS
GLY
SER
SER
PHE
Q645
L655
T660
M661
T685
H668
R671
T674
D695
M696
G697
E700
F731
GLU
GLN
PHE
ILE
D737

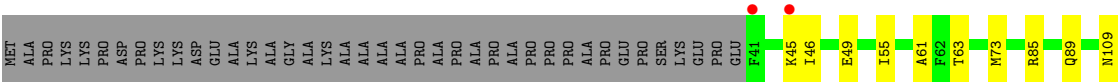
K405
V406
Q418
A423
M435
F436
N437
W438
M439
V440
R453
Q454
F468
D469
E474
K484
F494
Q498
K502
R503
E504
D512
F513
G514
M515
D516
E525
K526
S532
M539
K549
K570
H576
F577
S578
L579
I590
Q595
L604

ARG
SER
LYS
GLY
GLN
THR
GLY
LYS
GLY
GLY
T215
L216
E217
D218
Q219
I220
I220
L227
E228
D228
N232
E274
K484
F494
Q498
K502
R503
E504
D512
F513
G514
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K549
K570
H576
F577
S578
L579
I590
Q595
L604

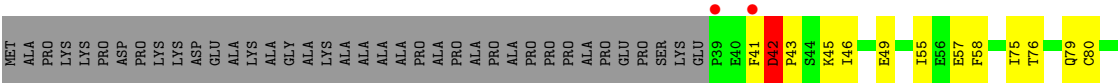
MET
VAL
ASP
ALA
E5
K21
K34
L52
S53
R54
V59
E62
T63
E64
H65
Q66
K67
T68
V69
K86
S111
S118
K129
R143
G144
K145
K146
R147
S148
E149
S156
Q163
Y164
T167
Q172
S173
E179
T192
I198
L201
GLY
ASP



● Molecule 2: Myosin light chain 3



● Molecule 2: Myosin light chain 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.32Å 122.45Å 187.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.22 – 2.45 24.22 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.22-2.45) 99.2 (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 [i](#)

5.1 Standard geometry [i](#)

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

The worst 5 of 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

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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

5 of 8 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	664/715 (93%)	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

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	655	LEU
2	G	171	ASP
1	B	671	ARG
2	G	45	LYS
2	H	45	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	656	ASN
1	B	791	GLN
2	H	128	ASN
1	B	726	ASN
2	G	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	M3L	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	904	2OW	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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	904	2OW	C19-N18-C16	-8.54	109.18	126.61

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

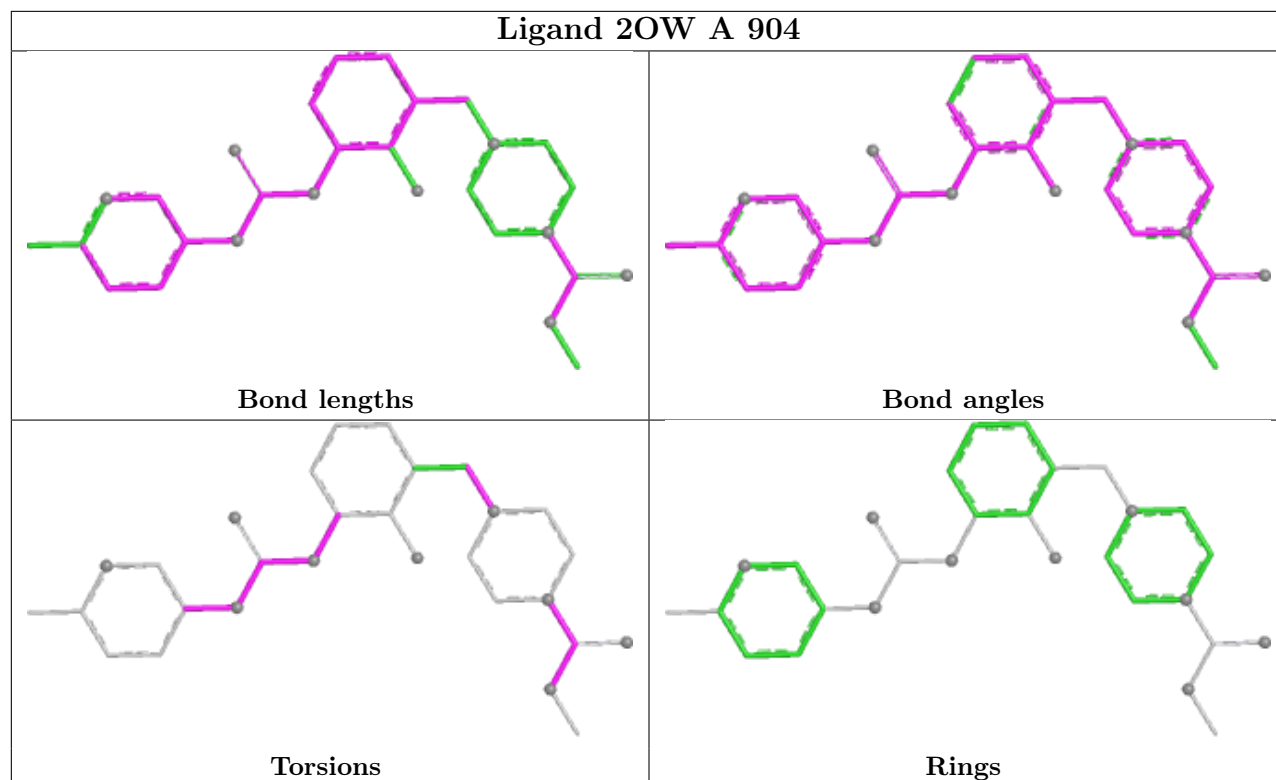
Mol	Chain	Res	Type	Atoms
3	A	901	ADP	PA-O3A-PB-O2B
3	B	901	ADP	PA-O3A-PB-O3B
6	A	904	2OW	O04-C03-O02-C01
6	A	904	2OW	N05-C03-O02-C01
6	A	904	2OW	O02-C03-N05-C06

There are no ring outliers.

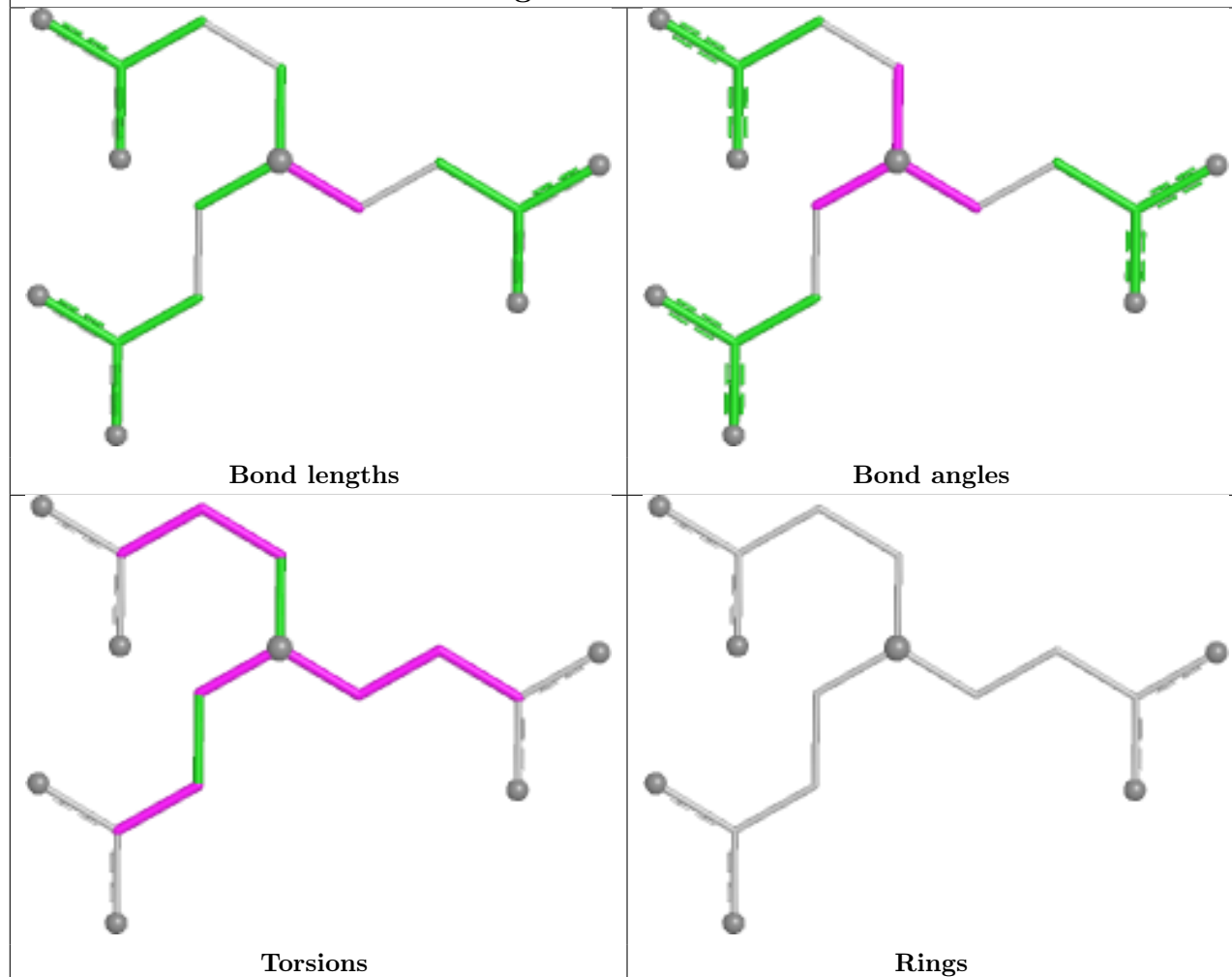
12 monomers are involved in 22 short contacts:

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

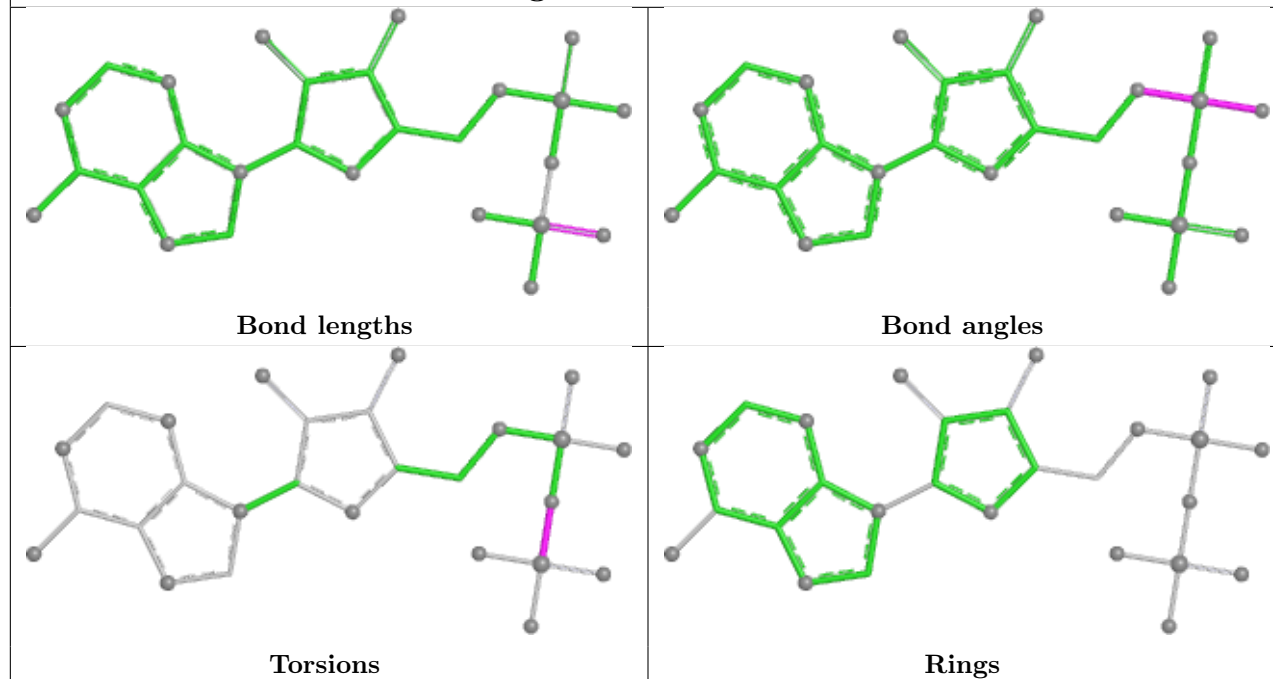
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

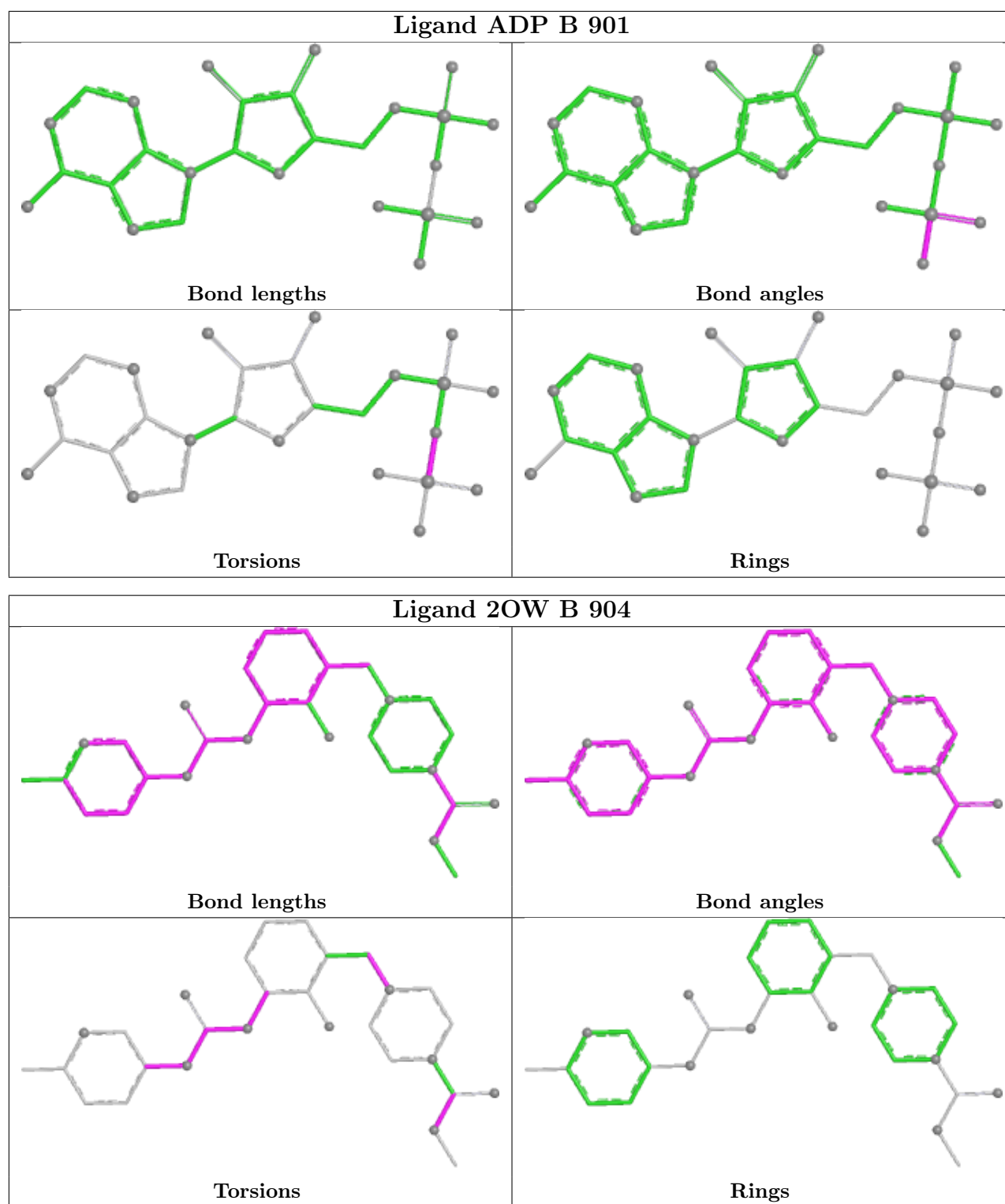


Ligand TCE B 914



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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	759/828 (91%)	-0.34	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%)

The worst 5 of 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

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 ⓘ

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.

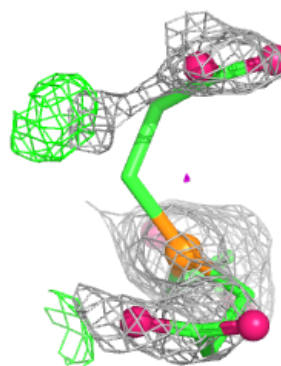
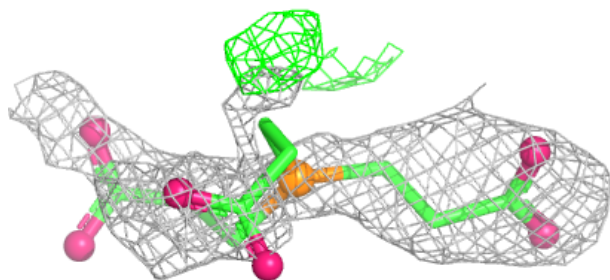
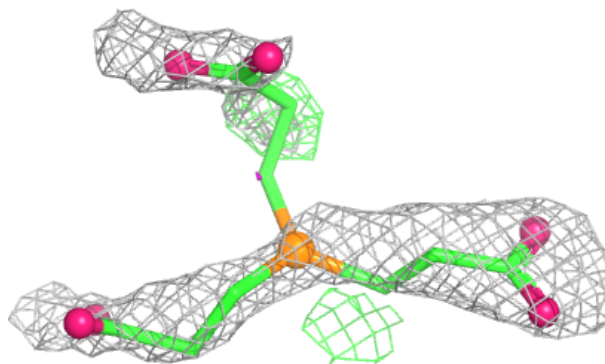
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	916	6/6	0.64	0.16	117,119,120,120	0
7	GOL	A	913	6/6	0.73	0.15	81,82,82,83	0
8	TCE	B	914	16/16	0.75	0.16	103,115,117,117	0
7	GOL	B	909	6/6	0.79	0.15	97,98,98,98	0
7	GOL	H	202	6/6	0.82	0.13	75,78,79,80	0
7	GOL	B	907	6/6	0.83	0.15	71,73,73,74	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
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.

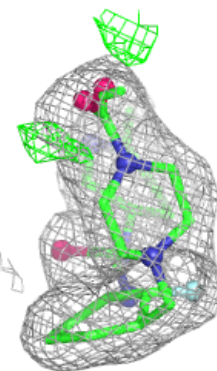
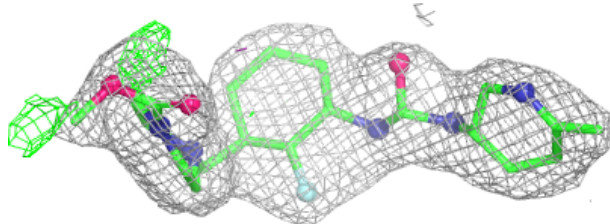
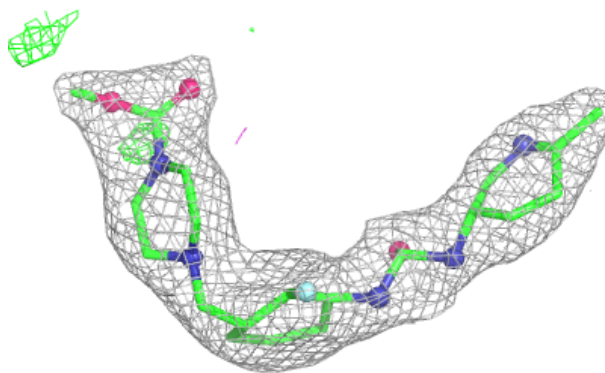
Electron density around TCE B 914:

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



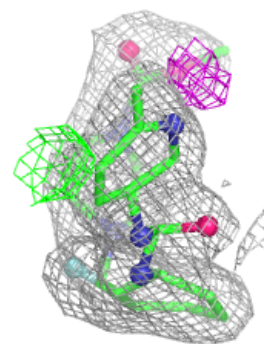
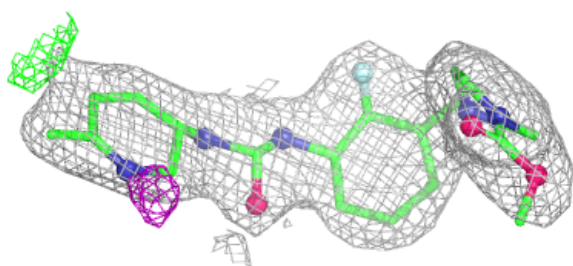
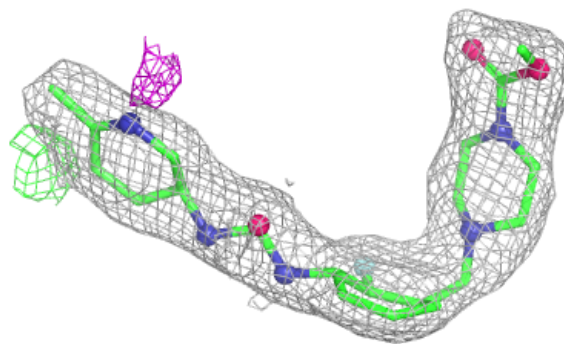
Electron density around 2OW A 904:

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

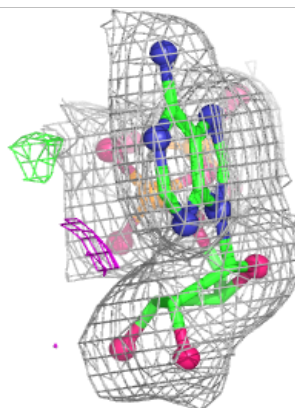
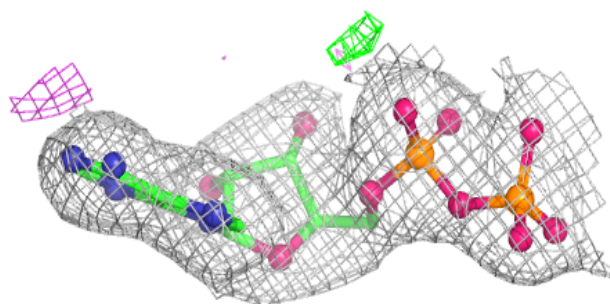
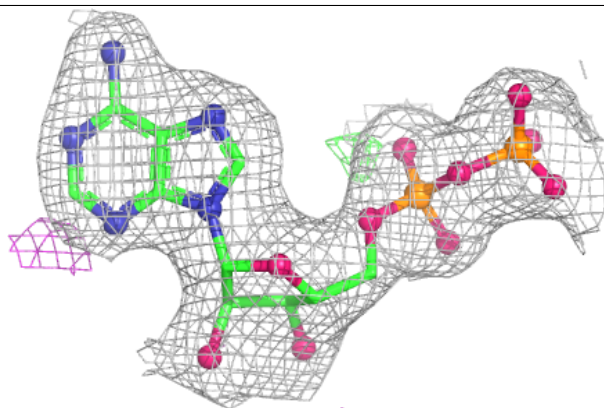


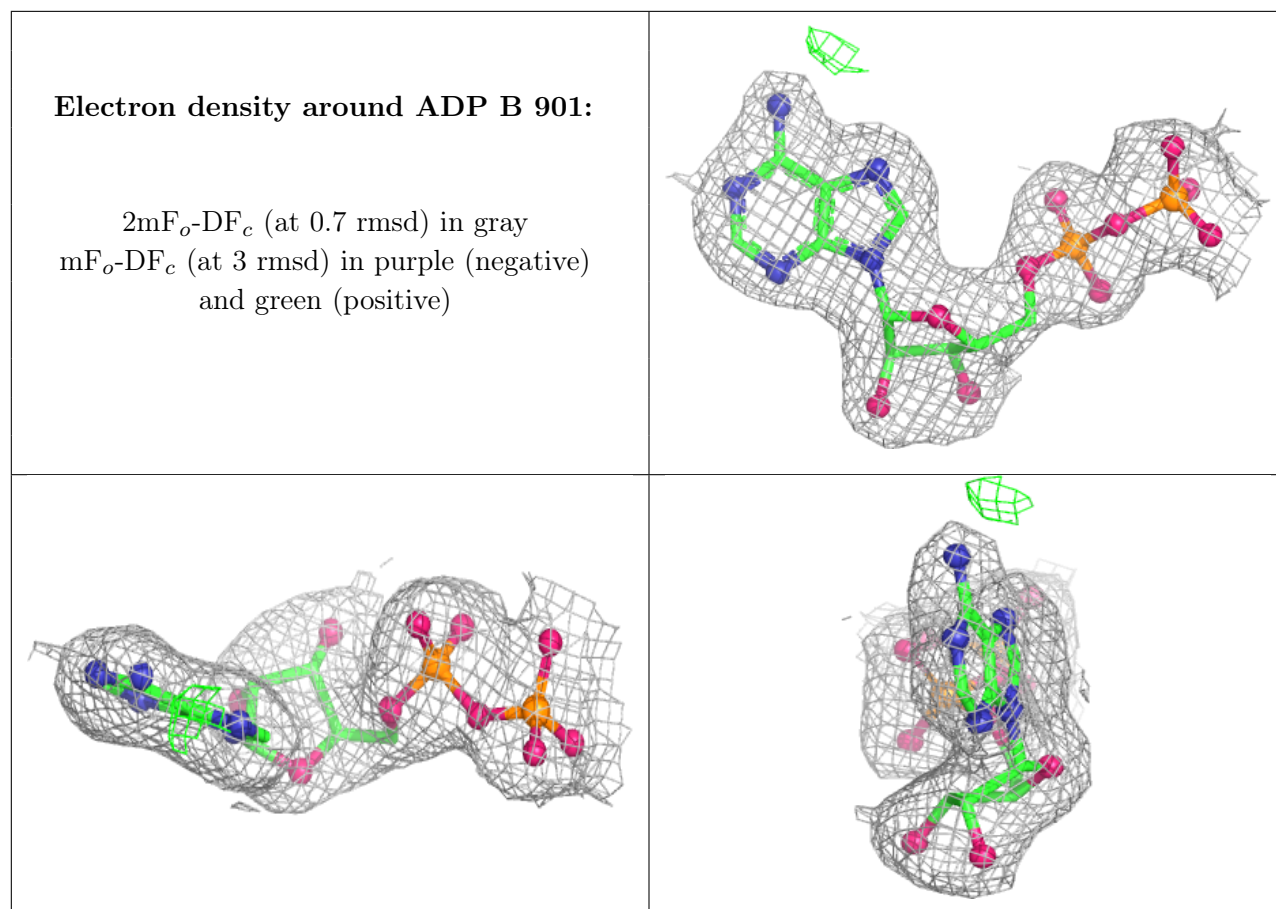
Electron density around 2OW B 904:

$2mF_o-DF_c$ (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)





6.5 Other polymers ⓘ

There are no such residues in this entry.