



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2026 – 09:16 am BST

PDB ID : 9F6C / pdb_00009f6c
Title : Cardiac myosin motor domain in the pre-powerstroke state co-crystallized with the inhibitor aficamten
Authors : Robert-Paganin, J.; Hartman, J.J.; Morgan, B.P.; Malik, F.I.; Houdusse, A.
Deposited on : 2024-05-01
Resolution : 2.33 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	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

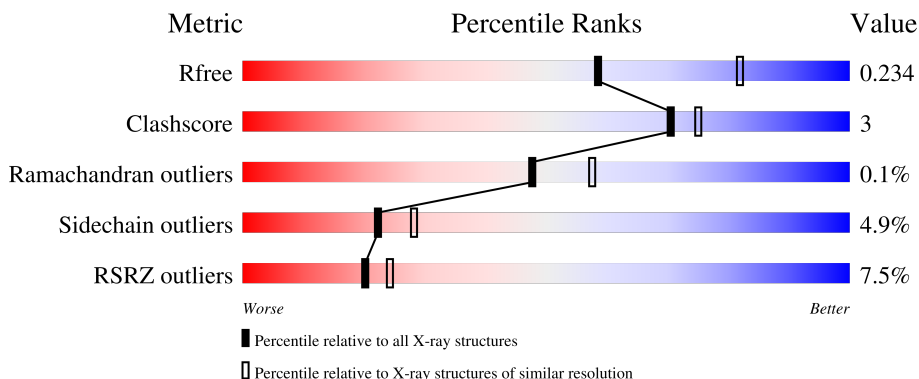
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	782	
1	B	782	

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
6	VO4	A	1005	-	-	X	-
6	VO4	B	804	-	-	X	-

2 Entry composition [i](#)

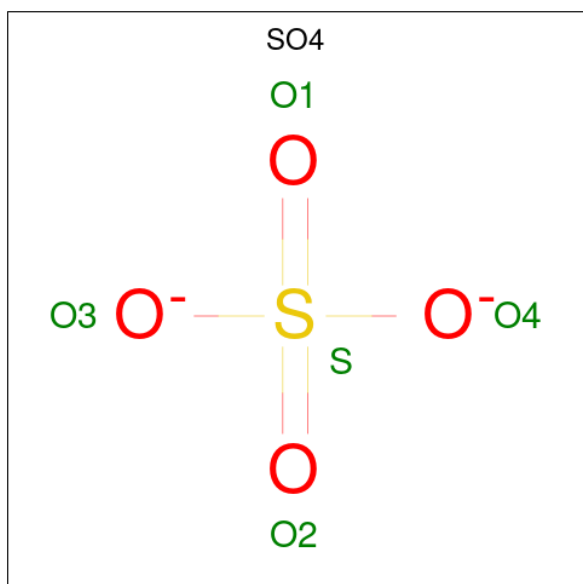
There are 7 unique types of molecules in this entry. The entry contains 11944 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	717	Total	C	N	O	S	1	2	0
			5794	3708	984	1072	30			
1	B	706	Total	C	N	O	S	1	1	0
			5699	3650	962	1056	31			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

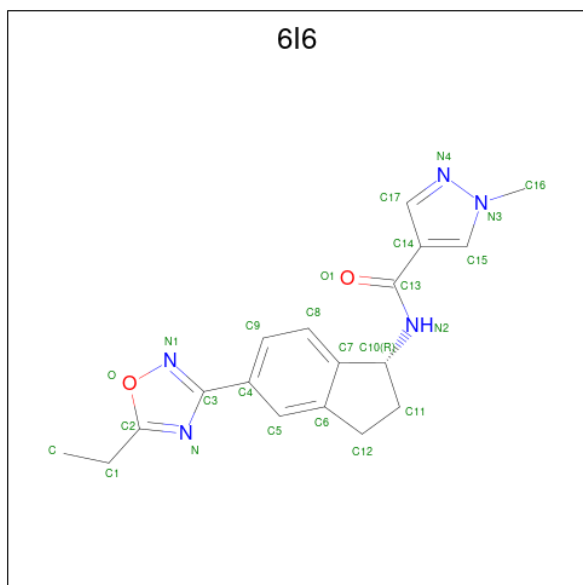
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

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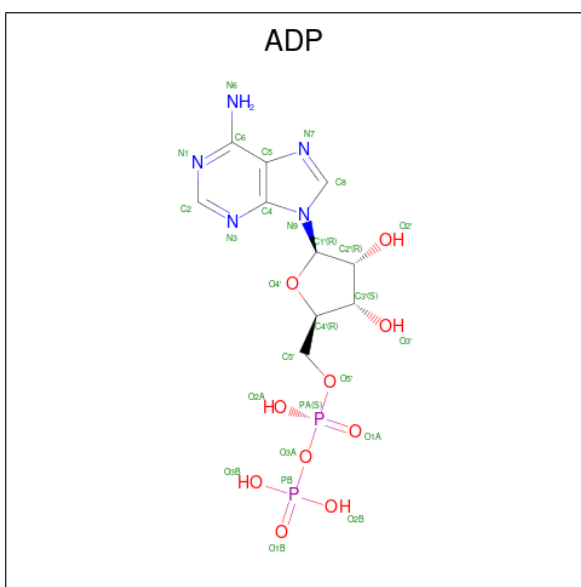
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is aficamten (CCD ID: 6I6) (formula: $C_{18}H_{19}N_5O_2$) (labeled as "Ligand of Interest" by depositor).



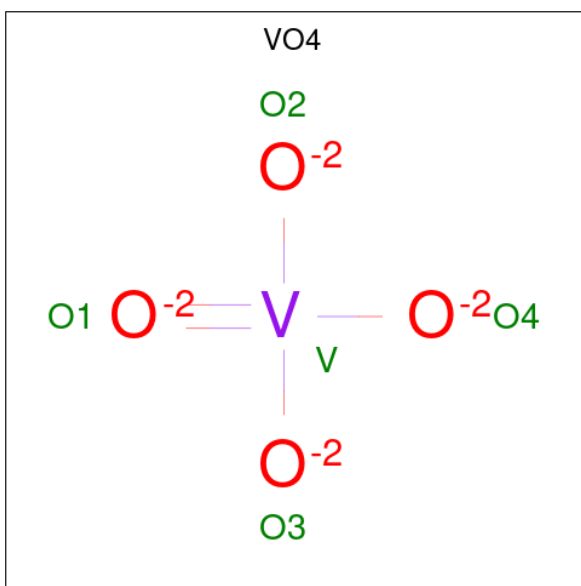
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	18	5	2		
4	B	1	Total	C	N	O	0	0
			25	18	5	2		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 6 is VANADATE ION (CCD ID: VO4) (formula: O_4V).



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

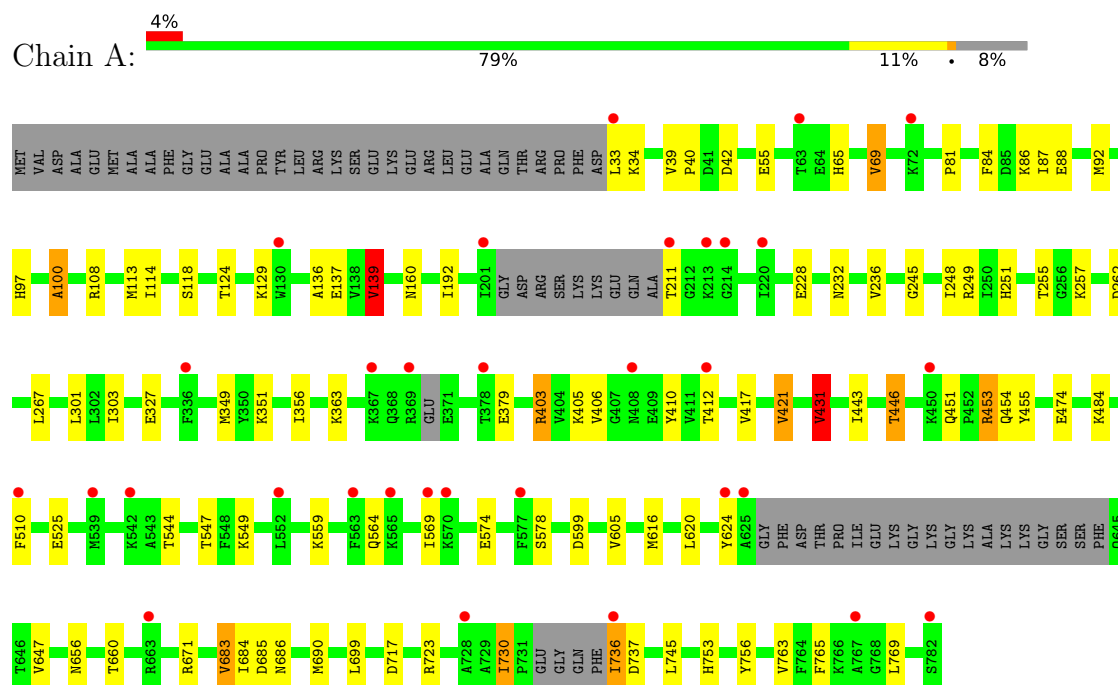
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	196	Total 196	O 196	0	0
7	B	134	Total 134	O 134	0	0

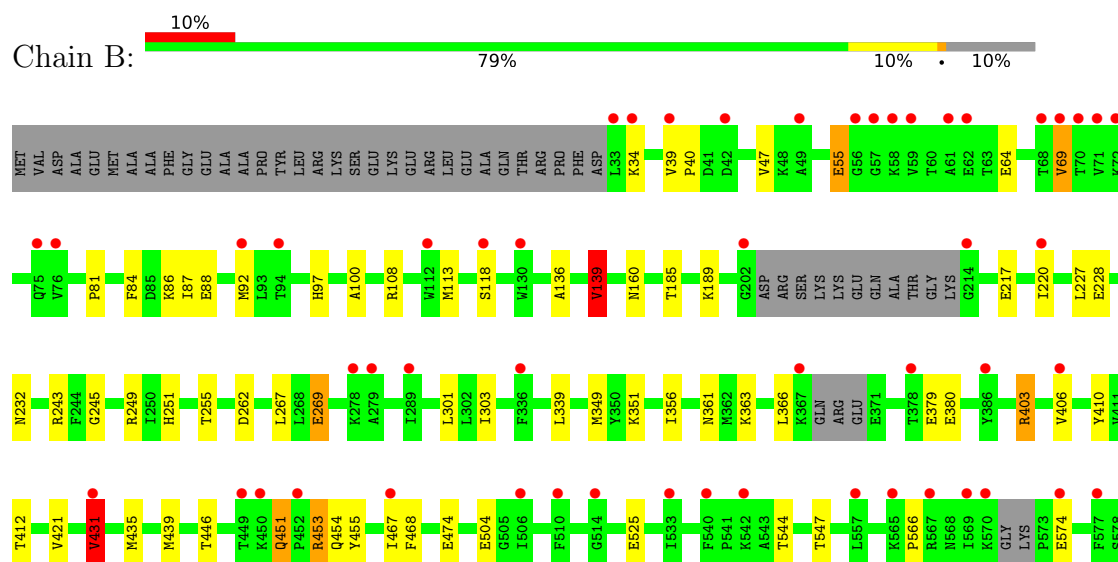
3 Residue-property plots [i](#)

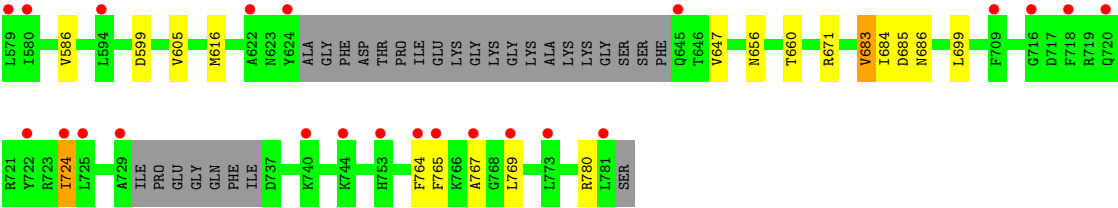
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

• Molecule 1: Myosin-7



• Molecule 1: Myosin-7





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.42Å 128.33Å 103.53Å 90.00° 91.47° 90.00°	Depositor
Resolution (Å)	46.60 – 2.33 46.60 – 2.33	Depositor EDS
% Data completeness (in resolution range)	67.2 (46.60-2.33) 67.3 (46.60-2.33)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.205 , 0.244 0.197 , 0.234	Depositor DCC
R_{free} test set	2562 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11944	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, 6I6, SO4, ADP, VO4, M3L

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	0.88	1/5890 (0.0%)	1.34	17/7939 (0.2%)
1	B	0.84	2/5793 (0.0%)	1.31	11/7807 (0.1%)
All	All	0.86	3/11683 (0.0%)	1.33	28/15746 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	599	ASP	CA-C	5.36	1.59	1.52
1	B	451	GLN	CA-C	5.35	1.59	1.53
1	A	690	MET	SD-CE	-5.15	1.66	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	685	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	65	HIS	N-CA-C	-6.88	104.41	114.39
1	A	42	ASP	CA-CB-CG	6.81	119.41	112.60
1	B	574	GLU	CB-CG-CD	6.78	124.12	112.60
1	A	736	ILE	CA-C-N	6.38	129.89	120.90
1	A	736	ILE	C-N-CA	6.38	129.89	120.90
1	B	431	VAL	N-CA-CB	6.34	120.08	110.58
1	A	574	GLU	CB-CG-CD	6.30	123.30	112.60
1	A	525	GLU	N-CA-C	6.27	121.06	113.41
1	B	525	GLU	N-CA-C	6.09	120.84	113.41
1	A	431	VAL	N-CA-CB	6.07	119.69	110.58
1	A	139	VAL	N-CA-CB	5.97	118.66	110.54
1	A	737	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	139	VAL	N-CA-CB	5.67	118.25	110.54
1	B	468	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	160	ASN	CA-CB-CG	-5.57	107.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ASN	CA-CB-CG	-5.46	107.14	112.60
1	A	717	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	269	GLU	CA-C-N	5.41	127.79	120.38
1	B	269	GLU	C-N-CA	5.41	127.79	120.38
1	A	683	VAL	N-CA-CB	5.36	117.42	110.99
1	B	683	VAL	N-CA-CB	5.34	117.40	110.99
1	B	685	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	566	PRO	N-CA-C	5.25	118.95	111.13
1	A	327	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	100	ALA	CA-C-N	5.11	126.95	120.72
1	A	100	ALA	C-N-CA	5.11	126.95	120.72
1	A	599	ASP	CA-CB-CG	5.08	117.68	112.60

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	5794	0	5778	38	0
1	B	5699	0	5671	38	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	25	0	0	2	0
4	B	25	0	0	1	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	5	0	0	2	0
6	B	5	0	0	3	0
7	A	196	0	0	2	0
7	B	134	0	0	0	0
All	All	11944	0	11473	79	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 3.

All (79) 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:B:504:GLU:HG2	1:B:764:PHE:HE1	1.49	0.78
1:B:504:GLU:HG2	1:B:764:PHE:CE1	2.31	0.66
1:B:339:LEU:O	1:B:446:THR:HG21	1.97	0.64
6:B:804:VO4:O1	6:B:804:VO4:V	1.56	0.62
6:B:804:VO4:V	6:B:804:VO4:O2	1.57	0.60
1:B:227:LEU:HD23	1:B:439:MET:HE3	1.84	0.60
6:A:1005:VO4:O2	6:A:1005:VO4:V	1.59	0.59
1:B:544:THR:HG22	1:B:547:THR:HG23	1.83	0.59
1:B:356:ILE:HD11	1:B:431:VAL:HG22	1.85	0.58
1:A:730:ILE:HD11	1:A:745:LEU:HD12	1.85	0.58
6:B:804:VO4:V	6:B:804:VO4:O4	1.59	0.57
6:A:1005:VO4:V	6:A:1005:VO4:O4	1.59	0.57
1:A:356:ILE:HD11	1:A:431:VAL:HG22	1.88	0.56
1:B:245:GLY:HA3	4:B:802:6I6:N1	2.21	0.56
1:A:559:LYS:HD3	1:B:55:GLU:CG	2.36	0.55
1:B:656:ASN:O	1:B:660:THR:HG23	2.06	0.54
1:B:47:VAL:HG22	1:B:64:GLU:HG2	1.88	0.54
1:B:84:PHE:HD1	1:B:87:ILE:HD12	1.72	0.54
1:B:301:LEU:HB2	1:B:303:ILE:HG12	1.89	0.54
1:A:84:PHE:HD1	1:A:87:ILE:HD12	1.73	0.53
1:A:301:LEU:HD22	1:A:351:LYS:HA	1.91	0.53
1:B:724:ILE:HG22	1:B:780:ARG:HG2	1.91	0.53
1:B:301:LEU:HD22	1:B:351:LYS:HA	1.91	0.53
1:A:403:ARG:HG2	1:A:410:TYR:CD1	2.44	0.52
1:B:108:ARG:NH1	1:B:113:MET:HB3	2.25	0.52
1:A:301:LEU:HB2	1:A:303:ILE:HG12	1.90	0.52
1:A:656:ASN:O	1:A:660:THR:HG23	2.08	0.52
1:A:192:ILE:HD11	1:A:248:ILE:HD13	1.92	0.52
1:A:245:GLY:HA3	4:A:1003:6I6:N1	2.24	0.52
1:B:403:ARG:HG2	1:B:410:TYR:CD1	2.45	0.52
1:A:765:PHE:HD1	1:A:769:LEU:HD23	1.74	0.52
1:A:88:GLU:HG2	1:A:108:ARG:HH21	1.76	0.51
1:B:88:GLU:HG2	1:B:108:ARG:HH21	1.75	0.51
1:B:39:VAL:HG11	1:B:69:VAL:HG11	1.93	0.50
1:B:765:PHE:HD1	1:B:769:LEU:HD23	1.77	0.50
1:B:39:VAL:HG13	1:B:40:PRO:HD2	1.94	0.49
1:A:97:HIS:CE1	1:A:100:ALA:HB2	2.48	0.48
1:A:443:ILE:O	1:A:446:THR:HG22	2.14	0.48
1:A:559:LYS:HD3	1:B:55:GLU:HG2	1.95	0.48
1:B:97:HIS:CE1	1:B:100:ALA:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:PRO:HD2	1:B:84:PHE:HD2	1.79	0.47
1:A:564[B]:GLN:HG3	1:A:578:SER:OG	2.14	0.46
1:A:684:ILE:HG22	1:A:686:ASN:HD22	1.80	0.46
1:A:39:VAL:HG11	1:A:69:VAL:HG11	1.98	0.46
1:B:467:ILE:HG22	1:B:586:VAL:HG22	1.98	0.46
1:A:108:ARG:HG2	1:A:113:MET:HE2	1.98	0.46
1:A:730:ILE:CD1	1:A:745:LEU:HD12	2.46	0.45
1:A:33:LEU:HD12	1:A:34:LYS:H	1.82	0.45
1:A:753:HIS:HA	1:A:756:TYR:CE2	2.51	0.45
1:A:81:PRO:HD2	1:A:84:PHE:HD2	1.82	0.45
1:B:251:HIS:HB3	1:B:453:ARG:HG2	1.98	0.45
1:A:474:GLU:HA	4:A:1003:6I6:O1	2.18	0.45
1:B:243:ARG:HD3	1:B:269:GLU:OE2	2.16	0.44
1:A:251:HIS:HB3	1:A:453:ARG:HG2	2.00	0.44
1:A:349:MET:HG2	1:A:616:MET:HE1	1.99	0.44
1:A:544:THR:HG22	1:A:547:THR:HG23	2.00	0.44
1:B:684:ILE:HG22	1:B:686:ASN:HD22	1.82	0.43
1:A:417:VAL:O	1:A:421:VAL:HG13	2.18	0.43
1:B:92[A]:MET:HE1	1:B:767:ALA:HB1	2.00	0.43
1:A:92:MET:HG2	7:A:1287:HOH:O	2.17	0.43
1:A:624:TYR:HD2	7:A:1290:HOH:O	2.01	0.43
1:B:349:MET:HG2	1:B:616:MET:HE1	2.00	0.43
1:A:136:ALA:HA	1:A:139:VAL:HG13	2.00	0.43
1:A:108:ARG:NH1	1:A:113:MET:HB3	2.34	0.43
1:A:723:ARG:HG3	1:A:730:ILE:HD12	2.00	0.43
1:B:228:GLU:O	1:B:232:ASN:HB2	2.20	0.42
1:B:81:PRO:HD2	1:B:84:PHE:CD2	2.54	0.42
1:A:39:VAL:HG13	1:A:40:PRO:HD2	2.02	0.41
1:A:249:ARG:HD3	1:A:262:ASP:OD1	2.21	0.41
1:B:185:THR:HG22	1:B:189:LYS:HE2	2.02	0.41
1:B:435:MET:HG3	1:B:616:MET:HE2	2.02	0.41
1:B:136:ALA:HA	1:B:139:VAL:HG13	2.02	0.41
1:B:249:ARG:HD3	1:B:262:ASP:OD1	2.21	0.41
1:B:435:MET:HG3	1:B:616:MET:CE	2.51	0.41
1:A:616:MET:O	1:A:620:LEU:HG	2.21	0.41
1:B:361:ASN:HB3	1:B:380:GLU:HG2	2.02	0.40
1:B:217:GLU:O	1:B:220:ILE:HG22	2.21	0.40
1:A:228:GLU:O	1:A:232:ASN:HB2	2.21	0.40
1:A:114:ILE:O	1:A:124:THR:HA	2.22	0.40

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	707/782 (90%)	686 (97%)	20 (3%)	1 (0%)	48	57
1	B	693/782 (89%)	677 (98%)	15 (2%)	1 (0%)	48	57
All	All	1400/1564 (90%)	1363 (97%)	35 (2%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	LEU
1	B	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	624/672 (93%)	590 (95%)	34 (5%)	20	24
1	B	614/672 (91%)	588 (96%)	26 (4%)	26	34
All	All	1238/1344 (92%)	1178 (95%)	60 (5%)	22	29

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	69	VAL
1	A	86	LYS
1	A	118	SER

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Mol	Chain	Res	Type
1	A	137	GLU
1	A	139	VAL
1	A	211	THR
1	A	236	VAL
1	A	255	THR
1	A	257	LYS
1	A	363	LYS
1	A	379	GLU
1	A	403	ARG
1	A	405	LYS
1	A	406	VAL
1	A	412	THR
1	A	421	VAL
1	A	431	VAL
1	A	446	THR
1	A	451	GLN
1	A	453	ARG
1	A	454	GLN
1	A	455	TYR
1	A	484	LYS
1	A	510	PHE
1	A	569	ILE
1	A	605	VAL
1	A	647	VAL
1	A	671	ARG
1	A	683	VAL
1	A	699	LEU
1	A	730	ILE
1	A	736	ILE
1	A	763	VAL
1	B	34	LYS
1	B	55	GLU
1	B	69	VAL
1	B	86	LYS
1	B	118	SER
1	B	139	VAL
1	B	255	THR
1	B	363	LYS
1	B	366	LEU
1	B	379	GLU
1	B	403	ARG
1	B	406	VAL

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Mol	Chain	Res	Type
1	B	412	THR
1	B	421	VAL
1	B	431	VAL
1	B	451	GLN
1	B	453	ARG
1	B	454	GLN
1	B	455	TYR
1	B	474	GLU
1	B	605	VAL
1	B	647	VAL
1	B	671	ARG
1	B	683	VAL
1	B	699	LEU
1	B	724	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	219	GLN
1	A	222	GLN
1	A	401	HIS
1	A	415	GLN
1	A	491	HIS
1	A	555	ASN
1	A	696	ASN
1	A	726	ASN
1	B	78	GLN
1	B	187	ASN
1	B	222	GLN
1	B	288	GLN
1	B	401	HIS
1	B	415	GLN
1	B	555	ASN
1	B	726	ASN
1	B	760	HIS

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	B	129	1	10,11,12	0.69	0	9,14,16	0.49	0
1	M3L	B	549	1	10,11,12	0.64	0	9,14,16	0.43	0
1	M3L	A	129	1	10,11,12	0.93	1 (10%)	9,14,16	0.46	0
1	M3L	A	549	1	10,11,12	0.82	1 (10%)	9,14,16	0.46	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	B	129	1	-	3/9/10/12	-
1	M3L	B	549	1	-	2/9/10/12	-
1	M3L	A	129	1	-	3/9/10/12	-
1	M3L	A	549	1	-	2/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	M3L	CB-CA	2.68	1.57	1.53
1	A	549	M3L	CB-CA	2.17	1.56	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	B	549	M3L	CA-CB-CG-CD
1	B	549	M3L	CE-CD-CG-CB
1	A	549	M3L	CE-CD-CG-CB
1	A	129	M3L	CD-CE-NZ-CM3
1	B	129	M3L	CD-CE-NZ-CM3
1	A	129	M3L	CD-CE-NZ-CM2
1	B	129	M3L	CD-CE-NZ-CM2
1	A	129	M3L	CD-CE-NZ-CM1
1	B	129	M3L	CD-CE-NZ-CM1

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
5	ADP	A	1004	6,3	27,29,29	0.50	0	42,45,45	0.48	0
4	6I6	B	802	-	28,28,28	0.34	0	37,40,40	0.48	0
4	6I6	A	1003	-	28,28,28	0.37	0	37,40,40	0.47	0
2	SO4	A	1001	-	4,4,4	0.30	0	6,6,6	0.13	0
5	ADP	B	803	6,3	27,29,29	0.65	1 (3%)	42,45,45	0.61	0
6	VO4	A	1005	5,3	0,4,4	-	-	-	-	-
6	VO4	B	804	5,3	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
5	ADP	B	803	6,3	-	3/16/32/32	0/3/3/3
5	ADP	A	1004	6,3	-	3/16/32/32	0/3/3/3
4	6I6	B	802	-	-	1/14/23/23	0/4/4/4
4	6I6	A	1003	-	-	1/14/23/23	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	803	ADP	PB-O3B	-2.45	1.45	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1004	ADP	PA-O3A-PB-O2B
5	B	803	ADP	PA-O3A-PB-O2B
4	A	1003	6I6	C-C1-C2-O
4	B	802	6I6	C-C1-C2-O
5	B	803	ADP	PA-O3A-PB-O1B
5	A	1004	ADP	PA-O3A-PB-O3B
5	B	803	ADP	PA-O3A-PB-O3B
5	A	1004	ADP	PA-O3A-PB-O1B

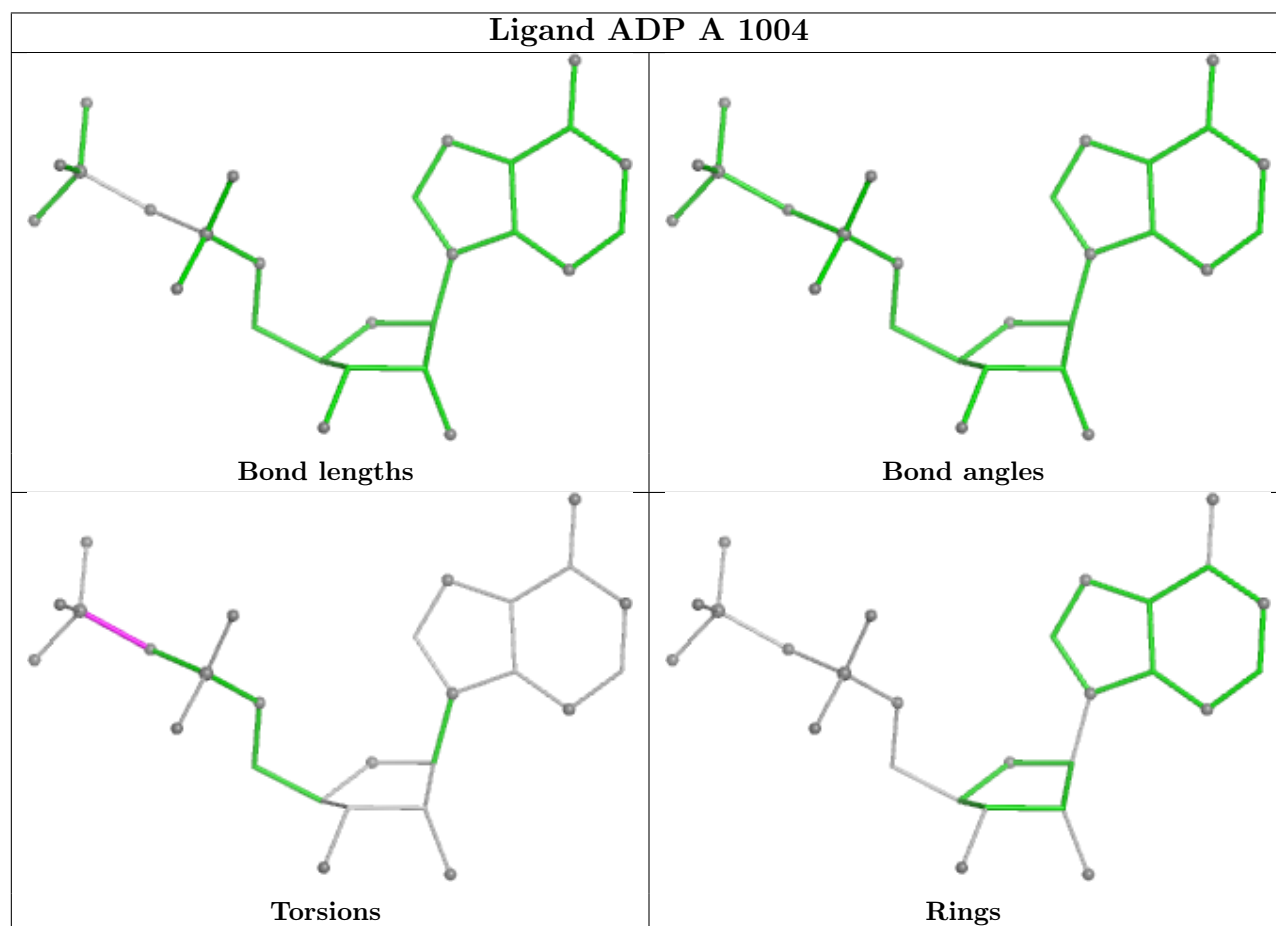
There are no ring outliers.

4 monomers are involved in 8 short contacts:

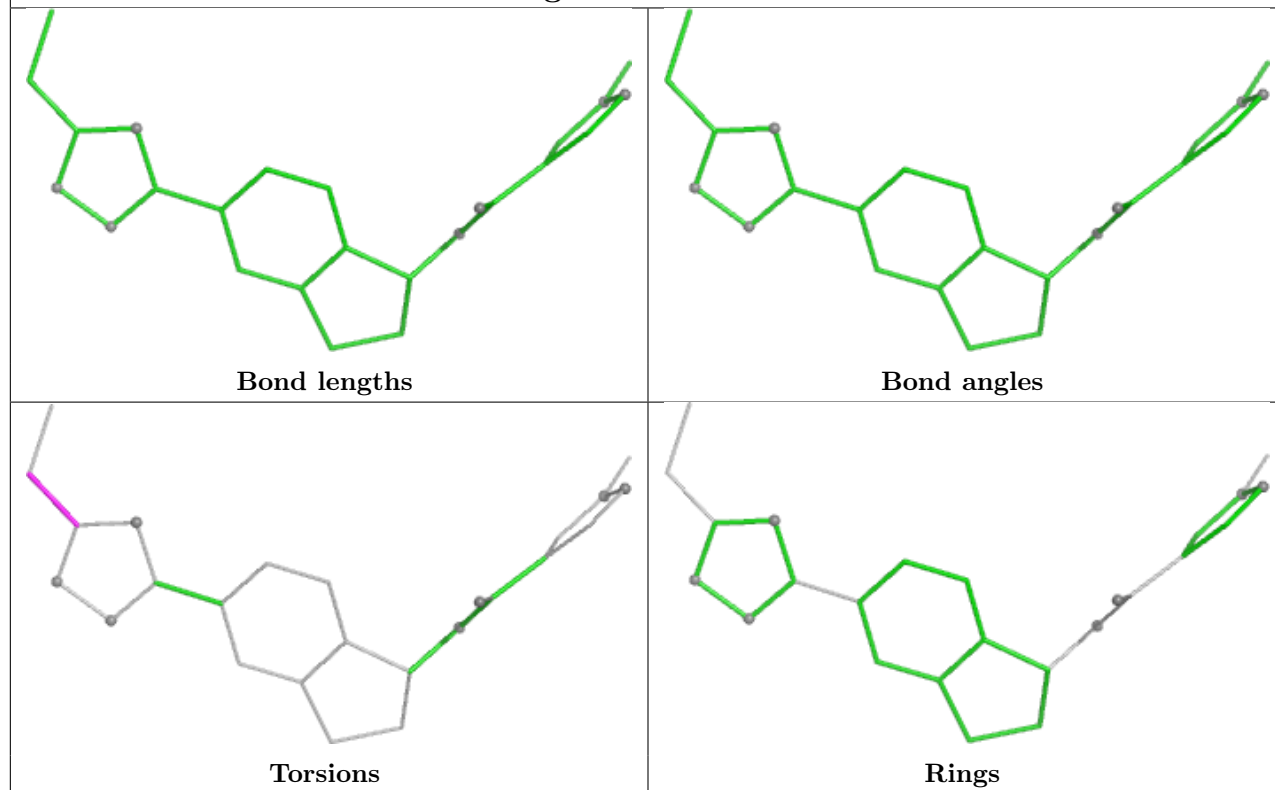
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	802	6I6	1	0
4	A	1003	6I6	2	0
6	A	1005	VO4	2	0
6	B	804	VO4	3	0

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

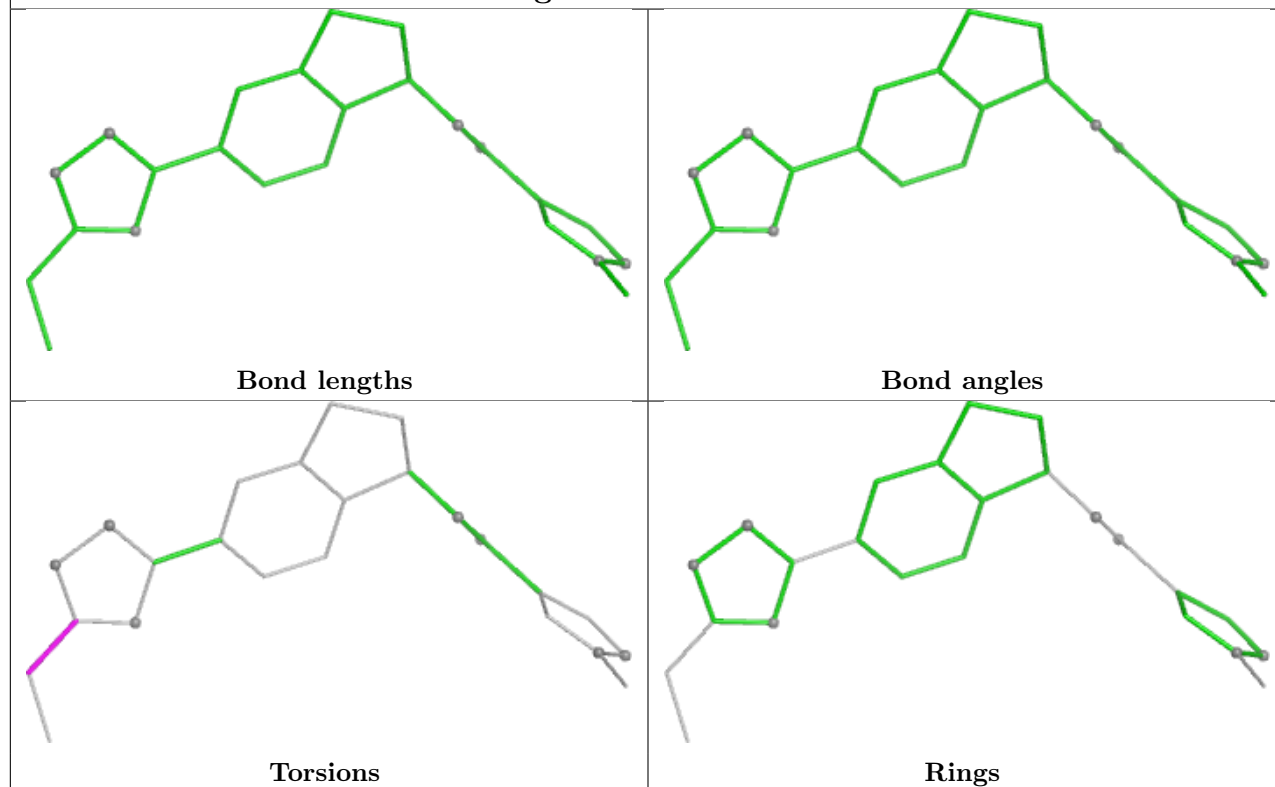
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

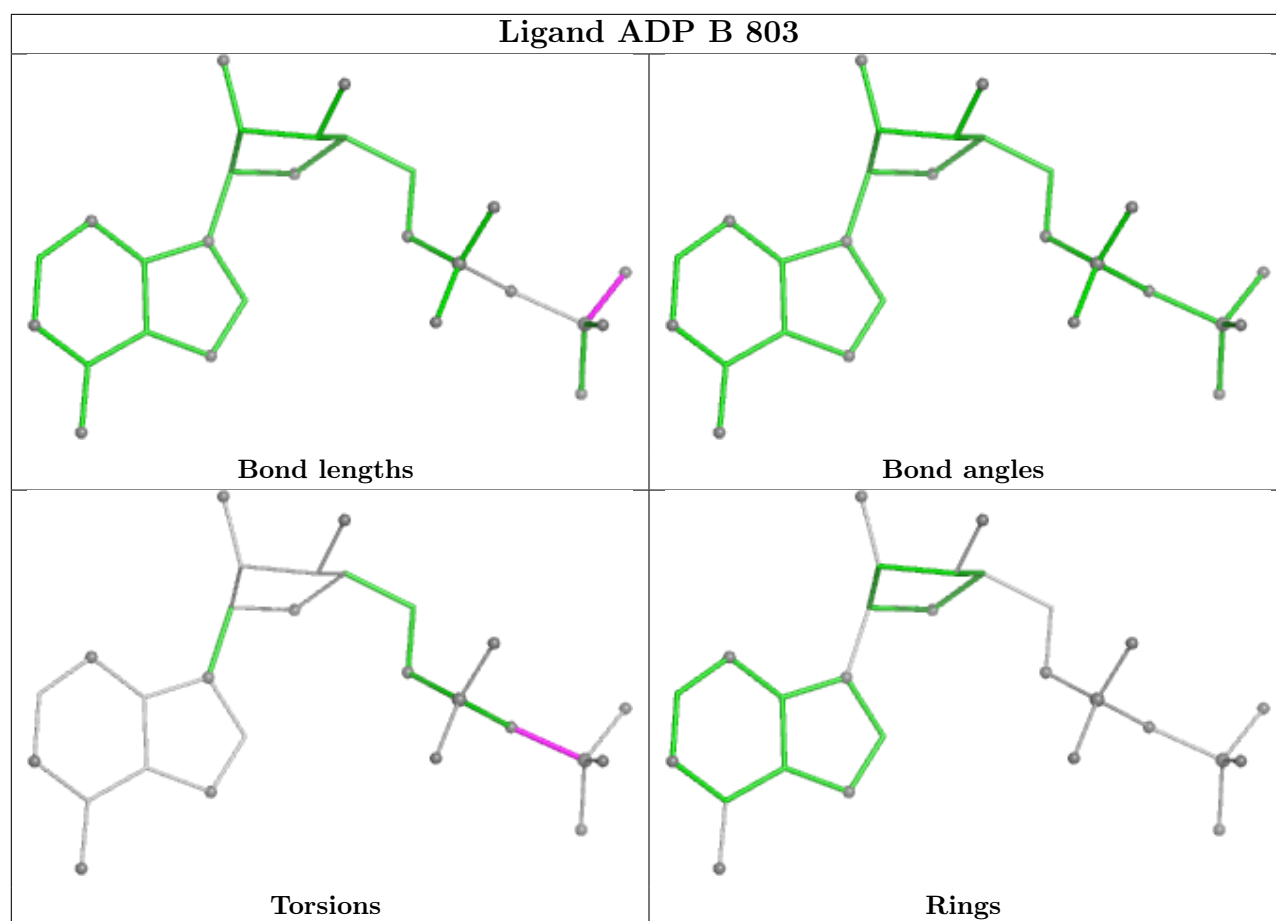


Ligand 6I6 B 802



Ligand 6I6 A 1003





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	715/782 (91%)	0.40	32 (4%)	38	44	33, 64, 102, 142	3 (0%)
1	B	704/782 (90%)	0.83	75 (10%)	11	13	33, 78, 122, 169	2 (0%)
All	All	1419/1564 (90%)	0.61	107 (7%)	20	24	33, 70, 114, 169	5 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	TRP	7.8
1	B	729	ALA	6.6
1	A	130	TRP	5.9
1	B	33	LEU	4.7
1	A	663[A]	ARG	4.5
1	A	736	ILE	4.5
1	B	467	ILE	4.4
1	B	202	GLY	4.4
1	B	724	ILE	4.4
1	B	336	PHE	4.4
1	A	625	ALA	4.2
1	B	781	LEU	4.0
1	B	767	ALA	3.6
1	B	570	LYS	3.6
1	B	709	PHE	3.5
1	B	39	VAL	3.5
1	B	624	TYR	3.5
1	A	565	LYS	3.4
1	B	57	GLY	3.4
1	B	764	PHE	3.4
1	B	70	THR	3.4
1	B	744	LYS	3.3
1	B	72	LYS	3.3
1	A	378	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	718	PHE	3.2
1	B	367	LYS	3.2
1	A	563	PHE	3.2
1	A	569	ILE	3.1
1	A	33	LEU	3.1
1	B	279	ALA	3.1
1	B	722	TYR	3.0
1	B	510	PHE	3.0
1	B	56	GLY	3.0
1	A	213	LYS	2.9
1	A	577	PHE	2.9
1	B	69	VAL	2.9
1	A	63	THR	2.9
1	B	59	VAL	2.8
1	B	214	GLY	2.8
1	B	92[A]	MET	2.8
1	A	450	LYS	2.8
1	B	68	THR	2.8
1	B	406	VAL	2.8
1	B	49	ALA	2.7
1	B	565	LYS	2.7
1	B	574	GLU	2.7
1	B	289	ILE	2.7
1	B	567	ARG	2.7
1	A	510	PHE	2.6
1	A	624	TYR	2.6
1	A	782	SER	2.6
1	B	533	ILE	2.6
1	A	211	THR	2.5
1	A	201	ILE	2.5
1	B	645	GLN	2.5
1	B	75	GLN	2.5
1	A	570	LYS	2.5
1	A	220	ILE	2.4
1	B	450	LYS	2.4
1	A	408	ASN	2.4
1	A	72	LYS	2.4
1	B	753	HIS	2.4
1	B	580	ILE	2.4
1	B	765	PHE	2.4
1	B	386	TYR	2.3
1	B	506	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	278	LYS	2.3
1	B	514	GLY	2.3
1	A	767	ALA	2.3
1	B	569	ILE	2.3
1	B	378	THR	2.3
1	A	369	ARG	2.3
1	B	220	ILE	2.3
1	B	740	LYS	2.3
1	A	728	ALA	2.2
1	B	112	TRP	2.2
1	A	552	LEU	2.2
1	B	71	VAL	2.2
1	B	58	LYS	2.2
1	B	622	ALA	2.2
1	A	336	PHE	2.2
1	B	61	ALA	2.2
1	B	76	VAL	2.2
1	B	34	LYS	2.2
1	A	412	THR	2.2
1	B	118	SER	2.2
1	B	579	LEU	2.1
1	B	94	THR	2.1
1	B	725	LEU	2.1
1	B	769	LEU	2.1
1	B	62	GLU	2.1
1	B	452	PRO	2.1
1	A	214	GLY	2.1
1	A	367	LYS	2.1
1	A	539	MET	2.1
1	B	42	ASP	2.1
1	B	431	VAL	2.1
1	B	540	PHE	2.1
1	A	542	LYS	2.1
1	B	542	LYS	2.1
1	B	557	LEU	2.1
1	B	720	GLN	2.1
1	B	716	GLY	2.1
1	B	449	THR	2.0
1	B	594	LEU	2.0
1	B	577	PHE	2.0
1	B	773	LEU	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($\text{\AA}^2$)	Q<0.9
1	M3L	A	549	12/13	0.86	0.18	71,79,96,96	0
1	M3L	B	129	12/13	0.89	0.13	73,77,85,86	0
1	M3L	A	129	12/13	0.94	0.12	57,60,68,69	0
1	M3L	B	549	12/13	0.95	0.13	80,89,107,109	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

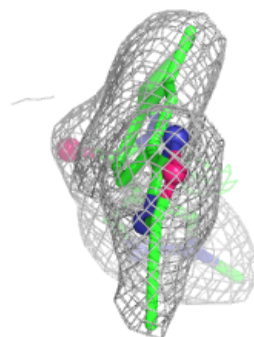
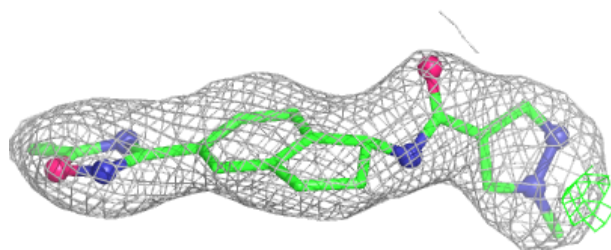
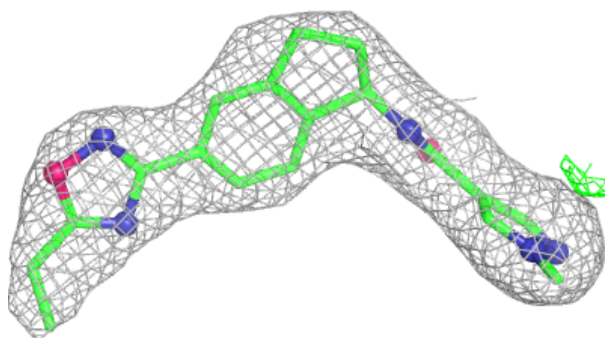
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1001	5/5	0.96	0.07	102,102,104,105	0
4	6I6	A	1003	25/25	0.97	0.07	47,55,62,64	0
4	6I6	B	802	25/25	0.97	0.06	45,49,57,57	0
5	ADP	B	803	27/27	0.97	0.07	47,62,67,72	0
5	ADP	A	1004	27/27	0.98	0.06	40,52,56,65	0
6	VO4	A	1005	5/5	0.98	0.06	43,48,53,61	0
6	VO4	B	804	5/5	0.98	0.07	50,52,58,65	0
3	MG	A	1002	1/1	0.99	0.07	53,53,53,53	0
3	MG	B	801	1/1	0.99	0.04	53,53,53,53	0

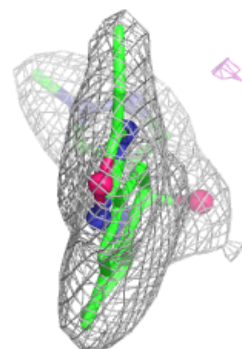
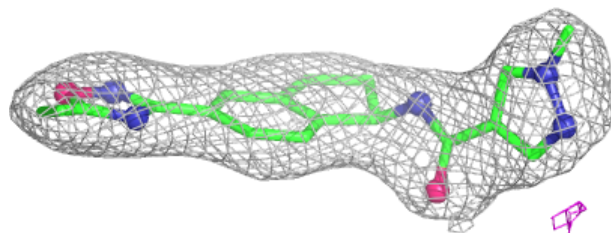
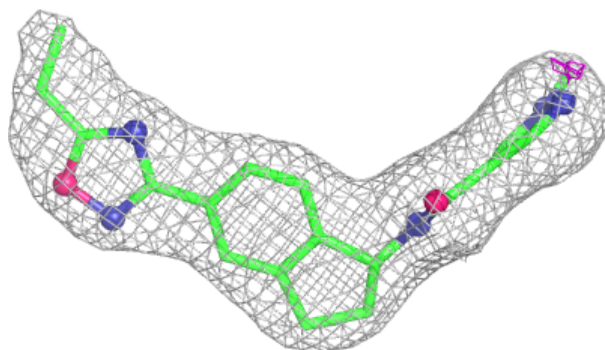
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 6I6 A 1003:

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

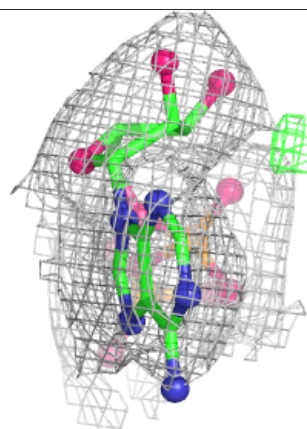
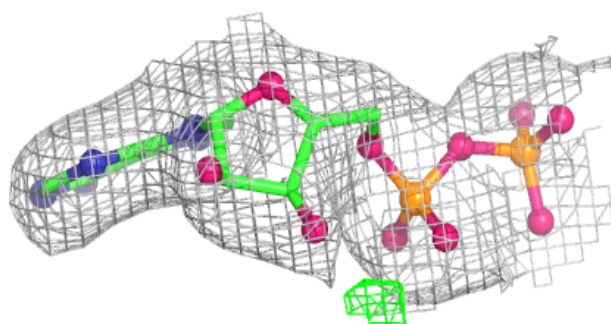
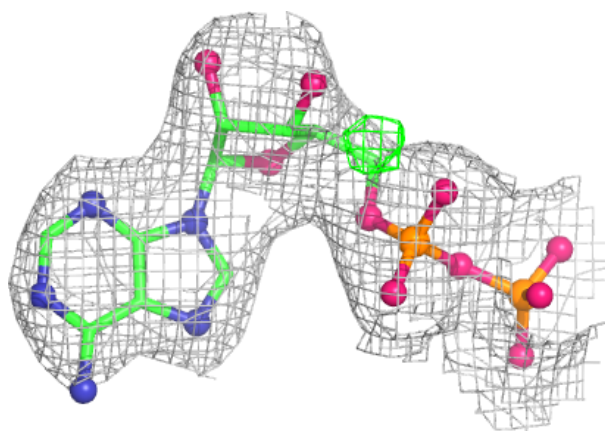
**Electron density around 6I6 B 802:**

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



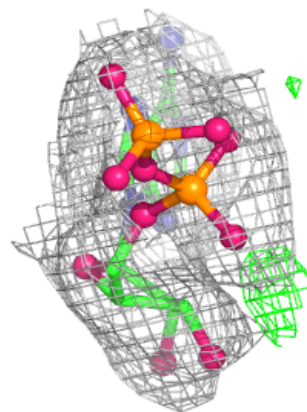
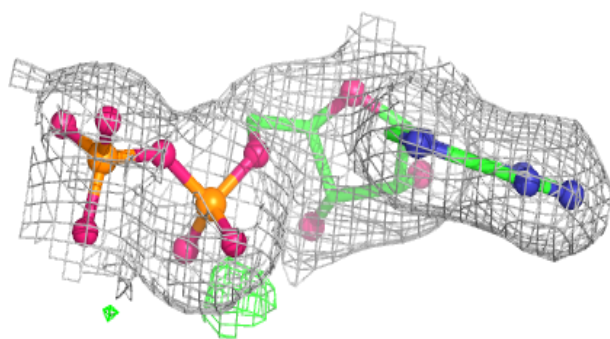
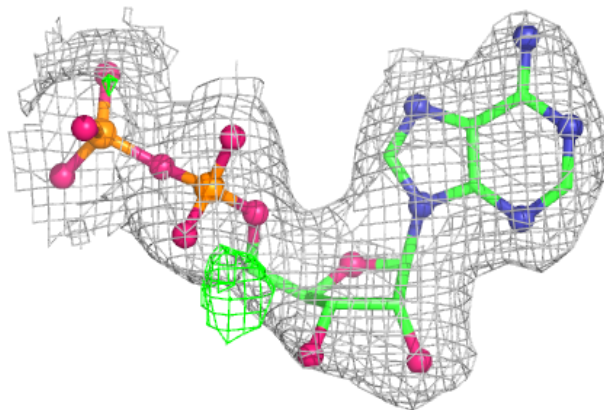
Electron density around ADP B 803:

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



Electron density around ADP A 1004:

$2mF_o-DF_c$ (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.