Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 01:19 pm BST

PDB ID	:	8BJH
Title	:	chimera of the inactive ExoY Nucleotidyl Cyclase domain from Vibrio nigripulchritudo MARTX toxin, with the double mutation K3528M and K3535I, fused to a proline-Rich-Domain (PRD) and profilin, bound to Latrunculin B-ADP-Mg-actin
Authors	:	Teixeira-Nunes, M.; Renault, L.; Retailleau, P.
Deposited on	:	2022-11-04
Resolution	:	1.69 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 (i) 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 (1)) were used in the production of this report:

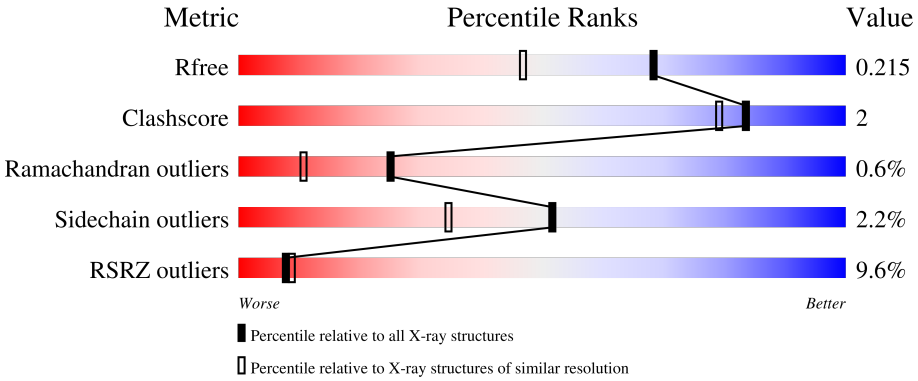
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	375	5% 94%
2	B	591	11% 77% 7% 15%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7980 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 Actin, alpha skeletal muscle, intermediate form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	13	0
			2948	1881	493	553	21			

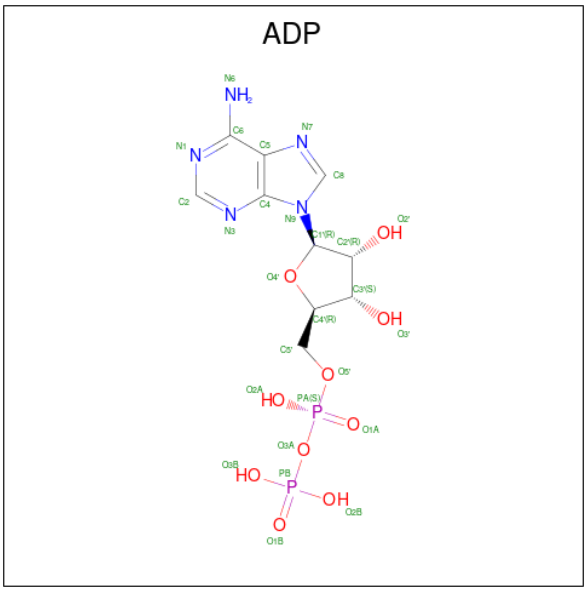
- Molecule 2 is a protein called Putative Adenylate cyclase,Profilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	502	Total	C	N	O	S	0	12	0
			3952	2500	655	781	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	451	GLY	-	expression tag	UNP A0A6N3LUE9
B	452	PRO	-	expression tag	UNP A0A6N3LUE9
B	453	GLY	-	expression tag	UNP A0A6N3LUE9
B	454	SER	-	expression tag	UNP A0A6N3LUE9
B	528	MET	LYS	engineered mutation	UNP A0A6N3LUE9
B	535	ILE	LYS	engineered mutation	UNP A0A6N3LUE9
B	897	PRO	-	linker	UNP A0A6N3LUE9
B	898	PRO	-	linker	UNP A0A6N3LUE9
B	899	PRO	-	linker	UNP A0A6N3LUE9
B	900	PRO	-	linker	UNP A0A6N3LUE9
B	901	GLY	-	linker	UNP A0A6N3LUE9
B	902	GLY	-	linker	UNP A0A6N3LUE9

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

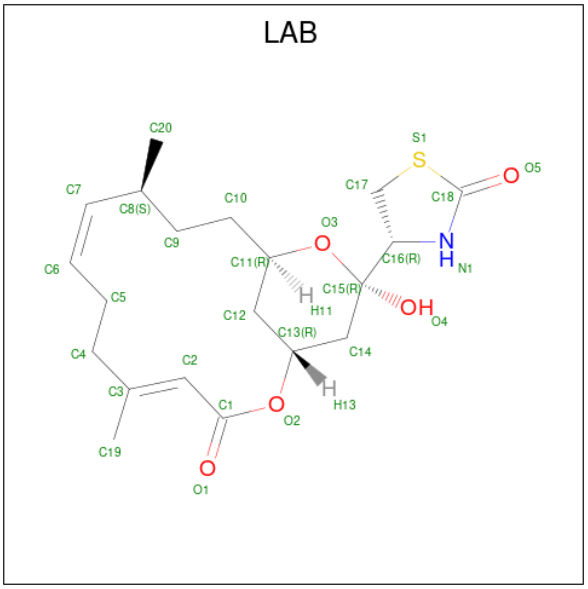


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

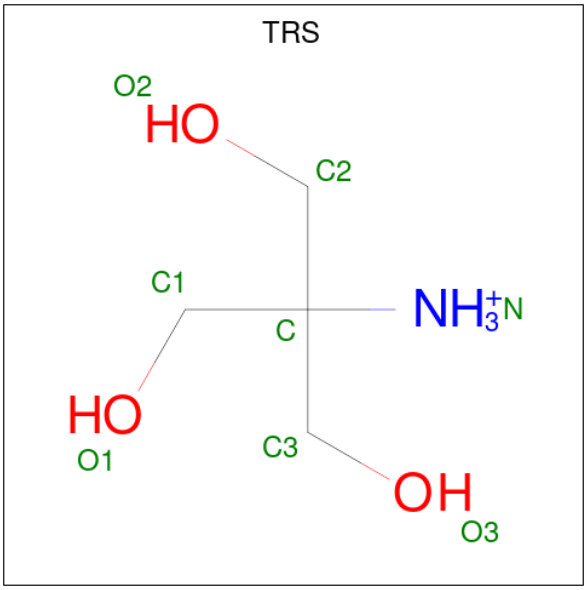
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is LATRUNCULIN B (three-letter code: LAB) (formula: $C_{20}H_{29}NO_5S$) (labeled as "Ligand of Interest" by depositor).



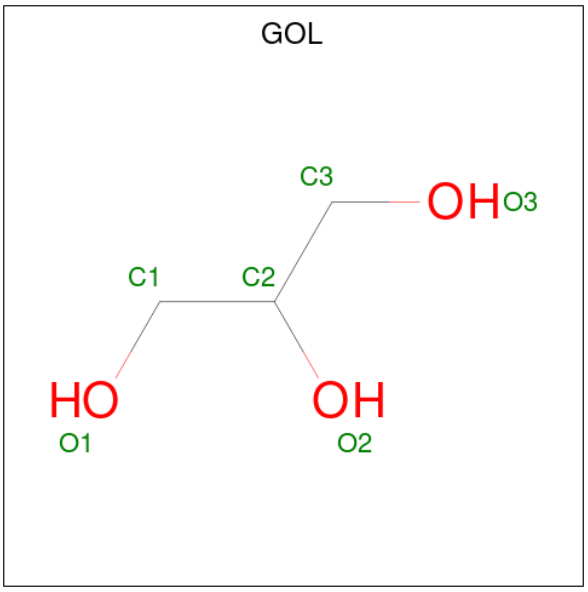
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



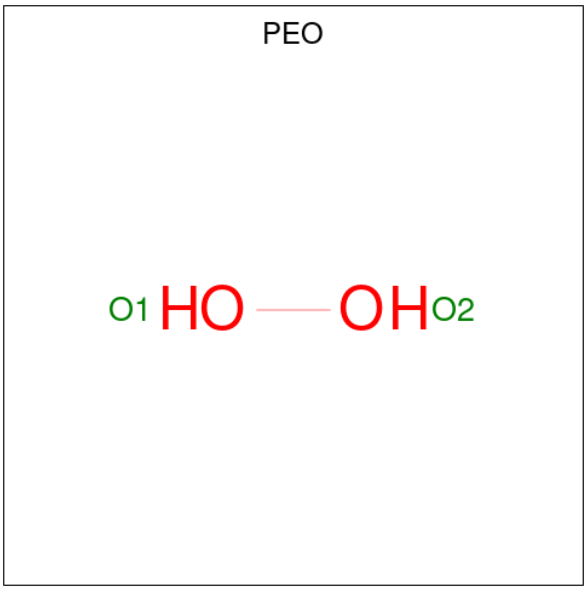
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 2 2	0	0

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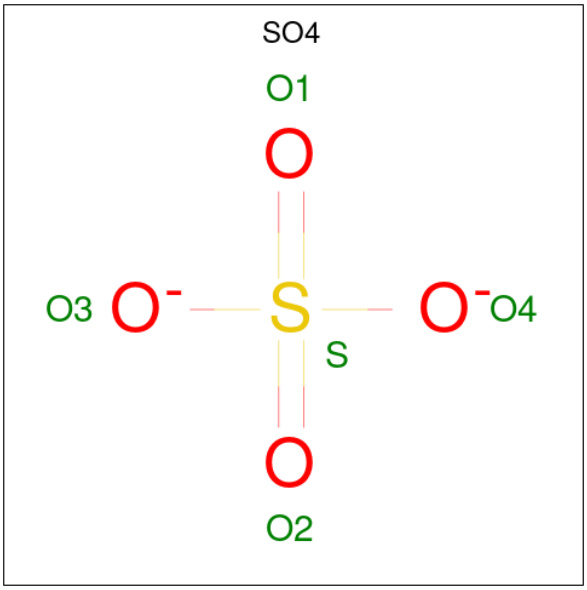
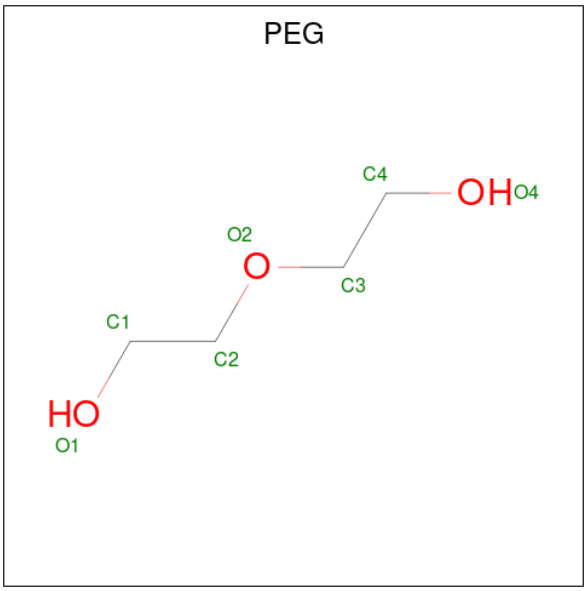
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 11 is water.

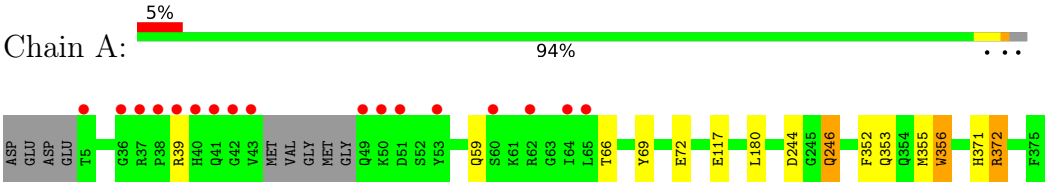
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	415	Total	O	0	0
			415	415		
11	B	543	Total	O	0	0
			543	543		

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.

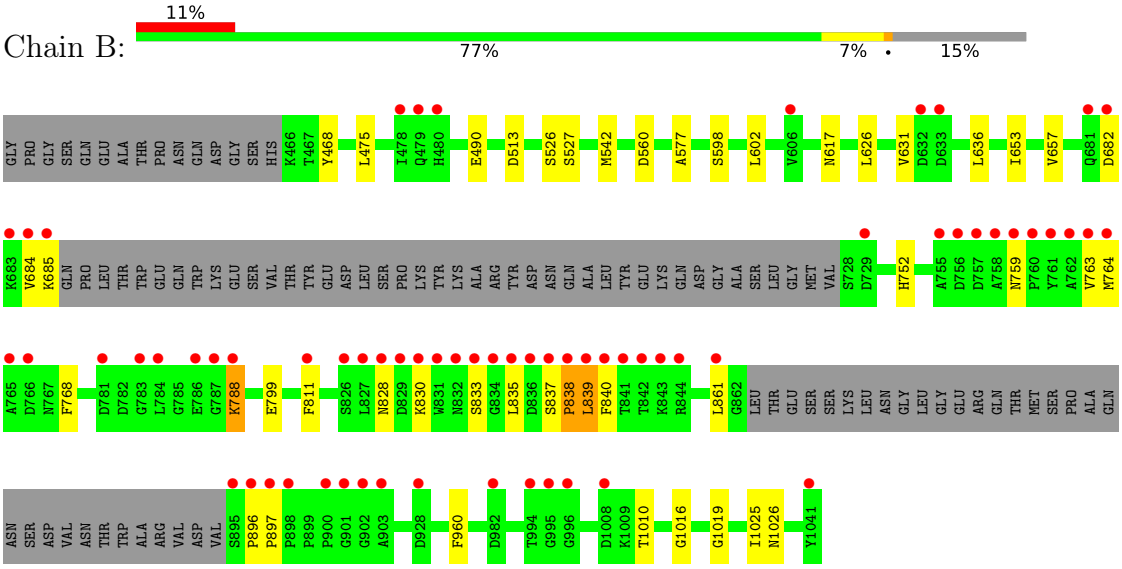
• Molecule 1: Actin, alpha skeletal muscle, intermediate form

Chain A:



• Molecule 2: Putative Adenylate cyclase,Profilin-1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.74Å 62.83Å 93.58Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	93.57 – 1.69 93.57 – 1.69	Depositor EDS
% Data completeness (in resolution range)	76.5 (93.57-1.69) 76.5 (93.57-1.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 1.69Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.178 , 0.212 0.182 , 0.215	Depositor DCC
R_{free} test set	4009 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7980	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PEO, PEG, SO4, TRS, MG, LAB, ADP, GOL

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	0.44	0/3053	0.56	0/4133
2	B	0.39	0/4065	0.55	0/5504
All	All	0.41	0/7118	0.56	0/9637

There are no bond length outliers.

There are no bond angle outliers.

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	2948	0	2954	9	0
2	B	3952	0	3899	23	0
3	A	27	0	12	0	0
4	A	1	0	0	0	0
5	A	27	0	29	0	0
6	A	8	0	12	0	0
6	B	8	0	12	0	0
7	A	6	0	8	0	0
7	B	12	0	16	2	0
8	A	10	0	0	3	0
8	B	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	10	0	0	1	0
10	B	7	0	10	0	0
11	A	415	0	0	0	0
11	B	543	0	0	1	0
All	All	7980	0	6952	34	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 (34) 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)
8:B:1207:PEO:O1	8:B:1207:PEO:O2	1.53	1.26
8:A:409:PEO:O1	8:A:409:PEO:O2	1.53	1.25
8:A:408:PEO:O1	8:A:408:PEO:O2	1.53	1.25
8:A:406:PEO:O1	8:A:406:PEO:O2	1.58	1.22
2:B:617:ASN:HB2	7:B:1205:GOL:H11	1.72	0.71
1:A:353:GLN:HA	1:A:356[B]:TRP:CD1	2.25	0.70
1:A:353:GLN:HA	1:A:356[B]:TRP:HD1	1.58	0.68
2:B:468:TYR:HE1	2:B:788:LYS:HZ3	1.44	0.66
1:A:372:ARG:HG3	2:B:1026:ASN:OD1	1.99	0.63
1:A:117:GLU:OE2	1:A:371[B]:HIS:NE2	2.25	0.61
2:B:468:TYR:HE1	2:B:788:LYS:NZ	2.05	0.54
1:A:244:ASP:OD1	1:A:246[A]:GLN:HB2	2.09	0.52
2:B:490[A]:GLU:HG2	9:B:1202:SO4:O3	2.11	0.51
2:B:602:LEU:HD21	2:B:626:LEU:HD12	1.93	0.49
2:B:617:ASN:HB2	7:B:1205:GOL:C1	2.40	0.49
1:A:39:ARG:HG2	1:A:66:THR:HG23	1.94	0.49
2:B:598:SER:HB3	11:B:1314:HOH:O	2.13	0.47
2:B:577:ALA:HB1	2:B:653:ILE:HG23	1.97	0.46
1:A:69:TYR:HB2	1:A:72:GLU:HG3	1.97	0.45
2:B:838:PRO:HB2	2:B:839:LEU:HD23	1.98	0.45
2:B:527:SER:OG	2:B:752:HIS:NE2	2.45	0.45
2:B:631:VAL:HB	2:B:636:LEU:HD12	1.99	0.44
2:B:468:TYR:HB3	2:B:475:LEU:HB2	1.99	0.44
1:A:59:GLN:HE21	2:B:684:VAL:HG12	1.83	0.43
2:B:684:VAL:HG23	2:B:685:LYS:HD2	2.01	0.43
2:B:861:LEU:O	2:B:1019:GLY:HA2	2.19	0.42
2:B:1016:GLY:HA3	2:B:1025:ILE:HD11	2.02	0.42
2:B:764:MET:SD	2:B:768:PHE:HD2	2.43	0.41
2:B:837:SER:HA	2:B:838:PRO:HD3	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352[B]:PHE:HD1	1:A:355:MET:SD	2.44	0.41
2:B:764:MET:SD	2:B:768:PHE:CD2	3.13	0.41
2:B:799[A]:GLU:H	2:B:799[A]:GLU:CD	2.24	0.41
2:B:811:PHE:CD2	2:B:840:PHE:HZ	2.39	0.41
2:B:896:PRO:HA	2:B:897:PRO:HD3	1.97	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	375/375 (100%)	368 (98%)	7 (2%)	0	100 100
2	B	508/591 (86%)	484 (95%)	19 (4%)	5 (1%)	15 4
All	All	883/966 (91%)	852 (96%)	26 (3%)	5 (1%)	25 11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	835	LEU
2	B	763	VAL
2	B	833	SER
2	B	759	ASN
2	B	838	PRO

5.3.2 Protein sidechains (i)

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	324/318 (102%)	318 (98%)	6 (2%)	57 41
2	B	440/504 (87%)	428 (97%)	12 (3%)	44 26
All	All	764/822 (93%)	746 (98%)	18 (2%)	52 31

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LEU
1	A	246[A]	GLN
1	A	246[B]	GLN
1	A	356[A]	TRP
1	A	356[B]	TRP
1	A	372	ARG
2	B	513	ASP
2	B	526	SER
2	B	542	MET
2	B	560	ASP
2	B	657	VAL
2	B	682	ASP
2	B	788	LYS
2	B	828	ASN
2	B	830	LYS
2	B	839	LEU
2	B	960	PHE
2	B	1010	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#\|Z\| > 2$
8	PEO	A	409	-	1,1,1	1.00	0	-		
8	PEO	A	407	-	1,1,1	0.79	0	-		
5	LAB	A	403	-	28,29,29	0.32	0	30,41,41	0.73	1 (3%)
8	PEO	B	1209	-	1,1,1	0.52	0	-		
6	TRS	A	404	-	7,7,7	0.22	0	9,9,9	0.27	0
6	TRS	B	1203	-	7,7,7	0.16	0	9,9,9	0.25	0
3	ADP	A	401	4	24,29,29	0.75	0	29,45,45	0.83	1 (3%)
8	PEO	B	1207	-	1,1,1	1.09	0	-		
8	PEO	B	1208	-	1,1,1	0.83	0	-		
8	PEO	A	406	-	1,1,1	1.49	0	-		
7	GOL	B	1204	-	5,5,5	0.05	0	5,5,5	0.22	0
9	SO4	B	1201	-	4,4,4	0.16	0	6,6,6	0.13	0
7	GOL	A	405	-	5,5,5	0.05	0	5,5,5	0.26	0
8	PEO	A	410	-	1,1,1	0.34	0	-		
7	GOL	B	1205	-	5,5,5	0.08	0	5,5,5	0.23	0
9	SO4	B	1202	-	4,4,4	0.27	0	6,6,6	0.39	0
8	PEO	A	408	-	1,1,1	1.05	0	-		
10	PEG	B	1206	-	6,6,6	0.23	0	5,5,5	0.04	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
5	LAB	A	403	-	-	4/21/49/49	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TRS	A	404	-	-	0/9/9/9	-
6	TRS	B	1203	-	-	0/9/9/9	-
3	ADP	A	401	4	-	0/12/32/32	0/3/3/3
7	GOL	B	1204	-	-	0/4/4/4	-
7	GOL	A	405	-	-	0/4/4/4	-
7	GOL	B	1205	-	-	0/4/4/4	-
10	PEG	B	1206	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	ADP	C5-C6-N6	2.14	123.61	120.35
5	A	403	LAB	C3-C2-C1	2.10	132.65	127.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	403	LAB	O3-C15-C16-C17
10	B	1206	PEG	O2-C3-C4-O4
10	B	1206	PEG	O1-C1-C2-O2
10	B	1206	PEG	C1-C2-O2-C3
10	B	1206	PEG	C4-C3-O2-C2
5	A	403	LAB	O2-C1-C2-C3
5	A	403	LAB	C11-C10-C9-C8
5	A	403	LAB	O1-C1-C2-C3

There are no ring outliers.

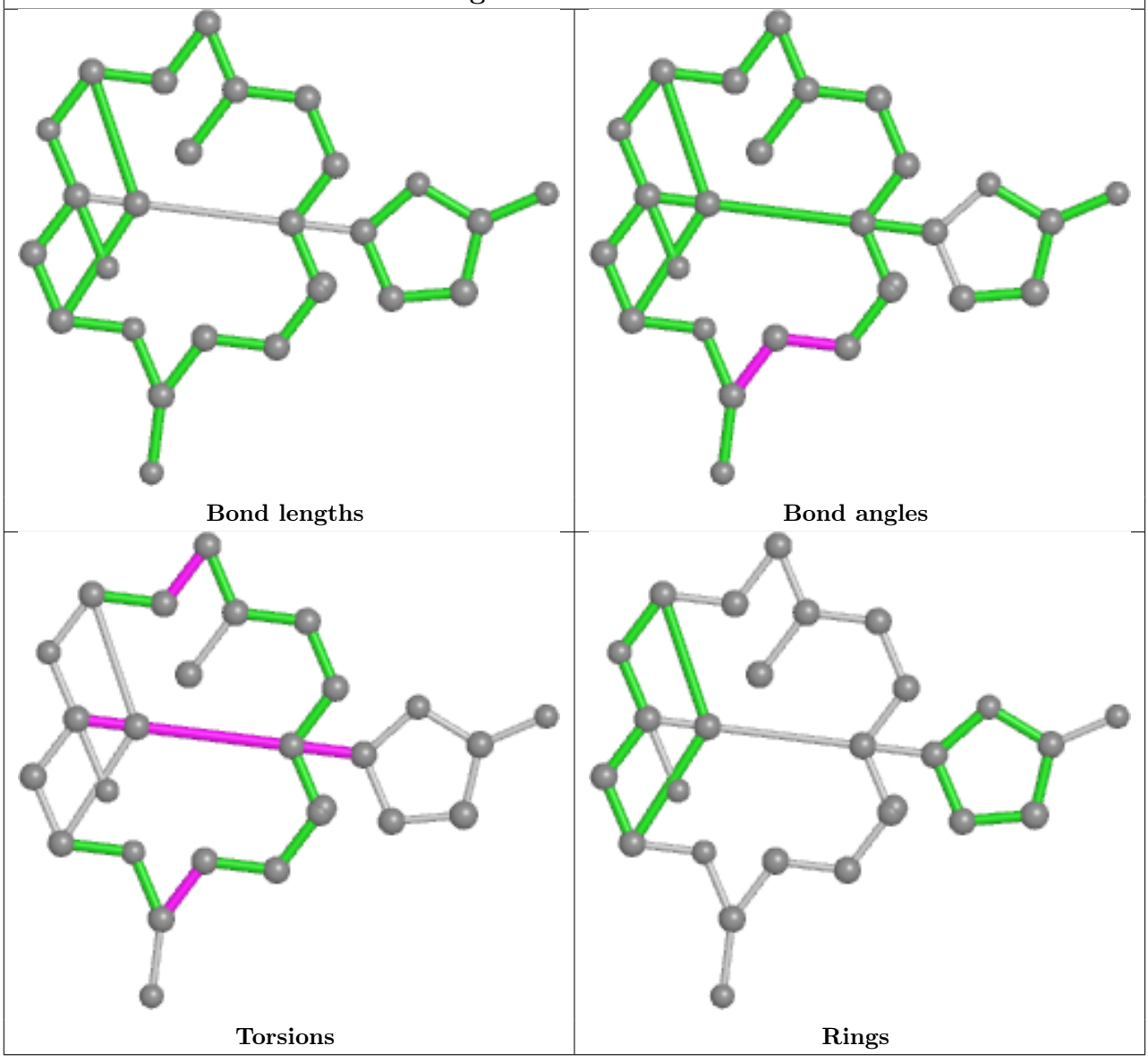
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	409	PEO	1	0
8	B	1207	PEO	1	0
8	A	406	PEO	1	0
7	B	1205	GOL	2	0
9	B	1202	SO4	1	0
8	A	408	PEO	1	0

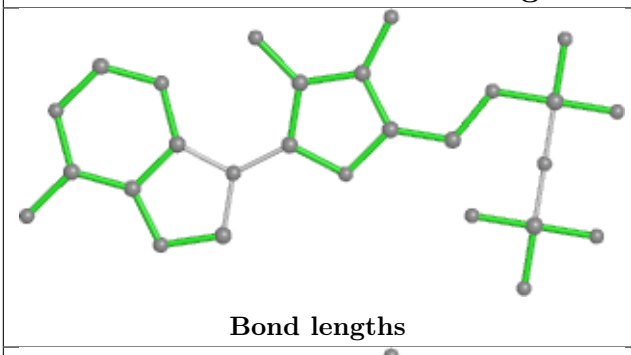
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

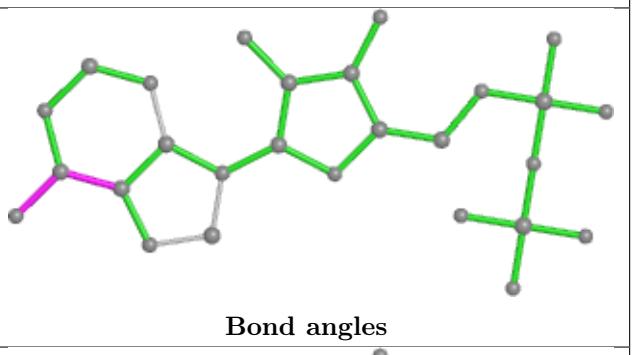
Ligand LAB A 403



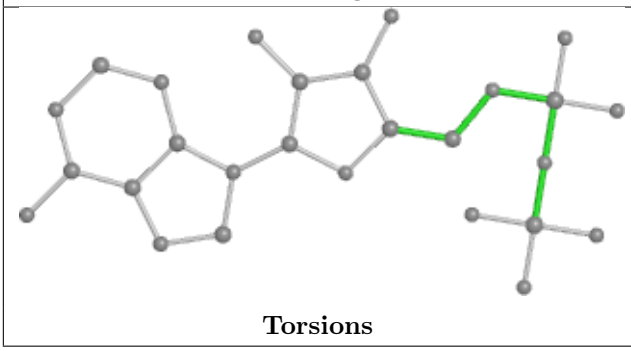
Ligand ADP A 401



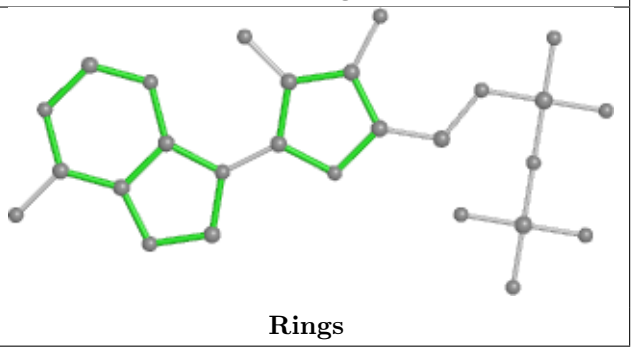
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	366/375 (97%)	0.12	17 (4%) 32 36	16, 25, 51, 90	0
2	B	502/591 (84%)	0.70	66 (13%) 3 3	20, 32, 77, 93	0
All	All	868/966 (89%)	0.45	83 (9%) 8 9	16, 29, 69, 93	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	759	ASN	13.3
2	B	760	PRO	12.8
2	B	762	ALA	12.4
2	B	684	VAL	11.8
2	B	836	ASP	10.8
2	B	761	TYR	10.5
2	B	763	VAL	10.4
2	B	840	PHE	10.0
2	B	835	LEU	9.8
2	B	839	LEU	9.2
2	B	842	THR	9.1
1	A	42	GLY	9.1
2	B	995	GLY	8.8
2	B	902	GLY	8.3
2	B	901	GLY	8.2
2	B	757	ASP	8.2
2	B	683	LYS	7.9
2	B	758	ALA	7.9
1	A	43	VAL	7.4
2	B	827	LEU	7.2
1	A	41	GLN	6.9
2	B	841	THR	6.8
2	B	843	LYS	6.7
2	B	903	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
2	B	685	LYS	6.3
2	B	765	ALA	6.1
2	B	833	SER	5.6
2	B	837	SER	5.5
2	B	682	ASP	5.3
2	B	755	ALA	5.1
2	B	828	ASN	5.0
2	B	480	HIS	4.7
1	A	49	GLN	4.5
2	B	832	ASN	4.3
2	B	831	TRP	4.2
1	A	40	HIS	4.2
2	B	681	GLN	4.2
1	A	38	PRO	4.2
2	B	834	GLY	4.1
2	B	830	LYS	3.9
2	B	838	PRO	3.8
1	A	5	THR	3.7
1	A	51	ASP	3.7
2	B	479	GLN	3.7
2	B	895	SER	3.6
2	B	900	PRO	3.6
2	B	844	ARG	3.5
2	B	896	PRO	3.4
2	B	786	GLU	3.4
1	A	53	TYR	3.4
1	A	39	ARG	3.3
2	B	729	ASP	3.2
1	A	64	ILE	3.1
2	B	478	ILE	3.0
2	B	994	THR	3.0
2	B	632	ASP	3.0
2	B	788	LYS	2.9
2	B	766	ASP	2.9
2	B	787	GLY	2.9
1	A	50	LYS	2.8
2	B	764	MET	2.7
2	B	1041	TYR	2.7
2	B	781	ASP	2.7
1	A	36	GLY	2.7
2	B	811	PHE	2.7
1	A	65	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	897	PRO	2.7
2	B	633	ASP	2.5
2	B	756	ASP	2.5
2	B	928	ASP	2.4
1	A	60	SER	2.4
1	A	62	ARG	2.3
2	B	606	VAL	2.3
2	B	996	GLY	2.3
2	B	783	GLY	2.2
2	B	898	PRO	2.2
1	A	37	ARG	2.2
2	B	784	LEU	2.2
2	B	861	LEU	2.2
2	B	982	ASP	2.1
2	B	826	SER	2.1
2	B	1008	ASP	2.1
2	B	829	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PEO	B	1208	2/2	0.42	0.17	64,64,64,64	0
7	GOL	A	405	6/6	0.50	0.19	64,65,65,65	0
10	PEG	B	1206	7/7	0.67	0.13	51,51,52,52	0
8	PEO	B	1209	2/2	0.72	0.21	66,66,66,66	0
7	GOL	B	1204	6/6	0.76	0.13	70,70,70,71	0
7	GOL	B	1205	6/6	0.79	0.21	51,51,52,52	0

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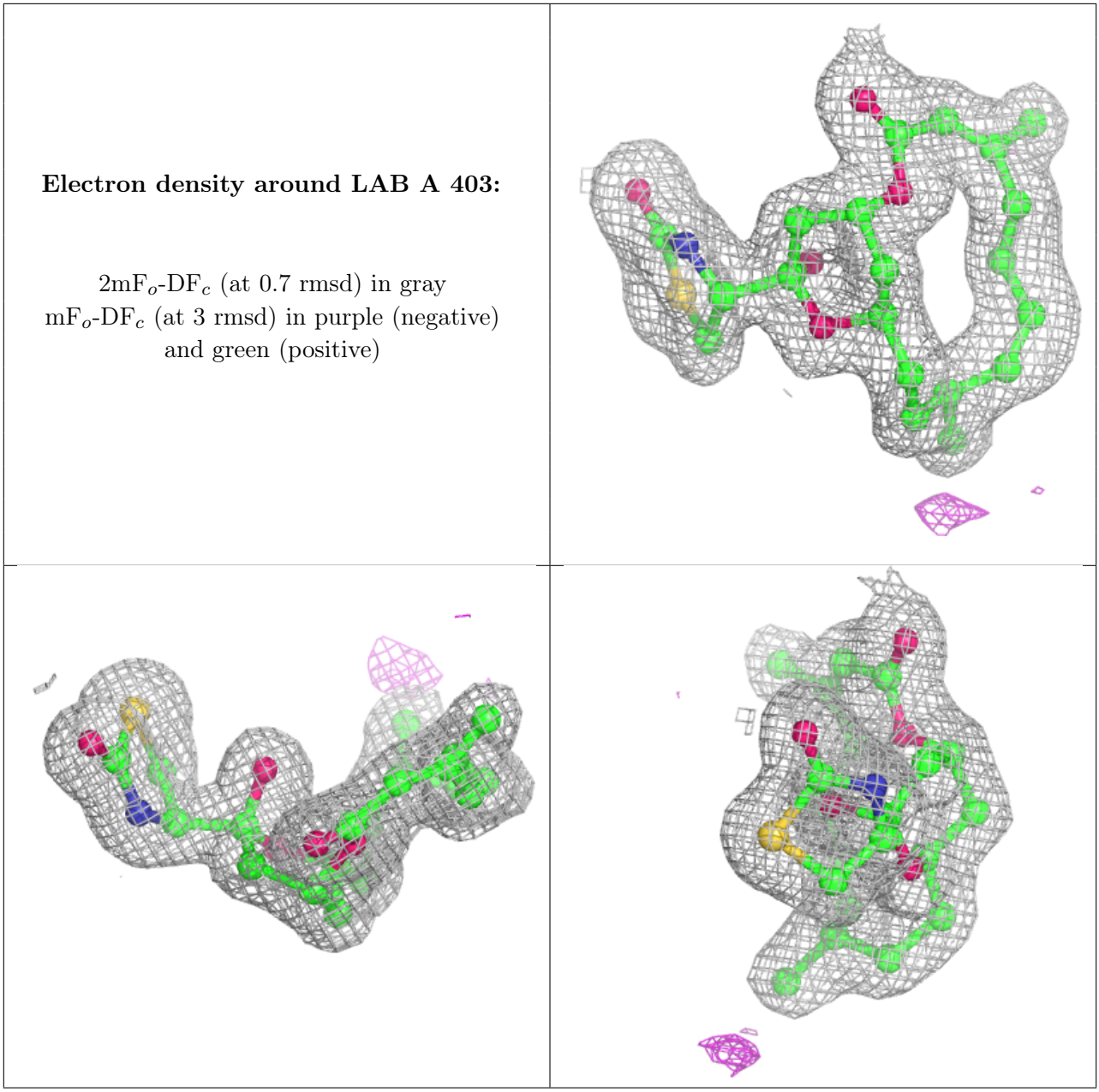
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PEO	A	408	2/2	0.81	0.12	47,47,47,47	0
8	PEO	B	1207	2/2	0.82	0.30	48,48,48,48	0
6	TRS	B	1203	8/8	0.83	0.15	42,42,42,43	0
9	SO4	B	1201	5/5	0.85	0.18	82,82,83,83	0
8	PEO	A	409	2/2	0.86	0.16	47,47,47,47	0
8	PEO	A	410	2/2	0.89	0.12	54,54,54,54	0
8	PEO	A	406	2/2	0.89	0.11	38,38,38,39	0
8	PEO	A	407	2/2	0.89	0.22	37,37,37,37	0
6	TRS	A	404	8/8	0.90	0.13	29,30,31,31	0
5	LAB	A	403	27/27	0.95	0.08	25,27,29,29	0
9	SO4	B	1202	5/5	0.98	0.13	33,34,34,35	0
3	ADP	A	401	27/27	0.98	0.08	18,20,22,23	0
4	MG	A	402	1/1	0.99	0.07	20,20,20,20	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.

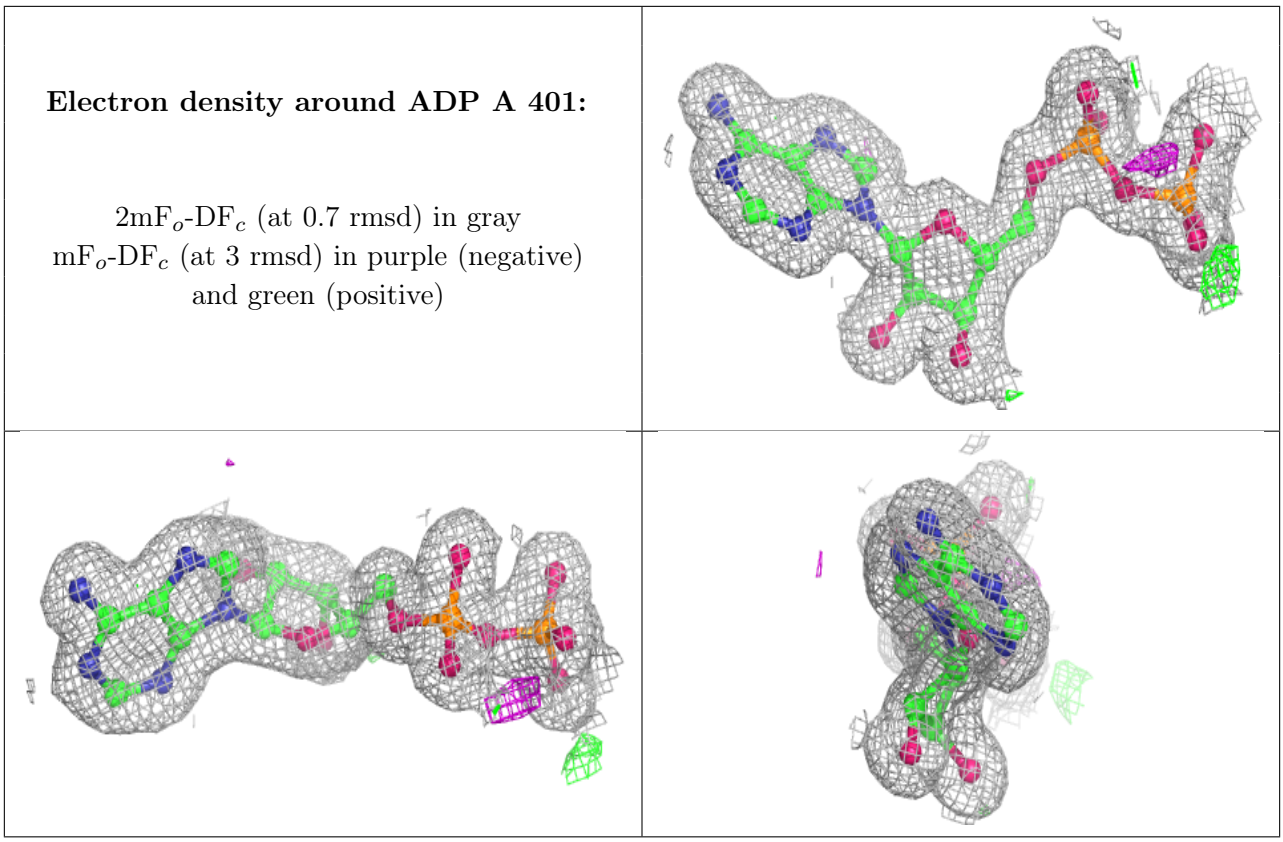
Electron density around LAB A 403:

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



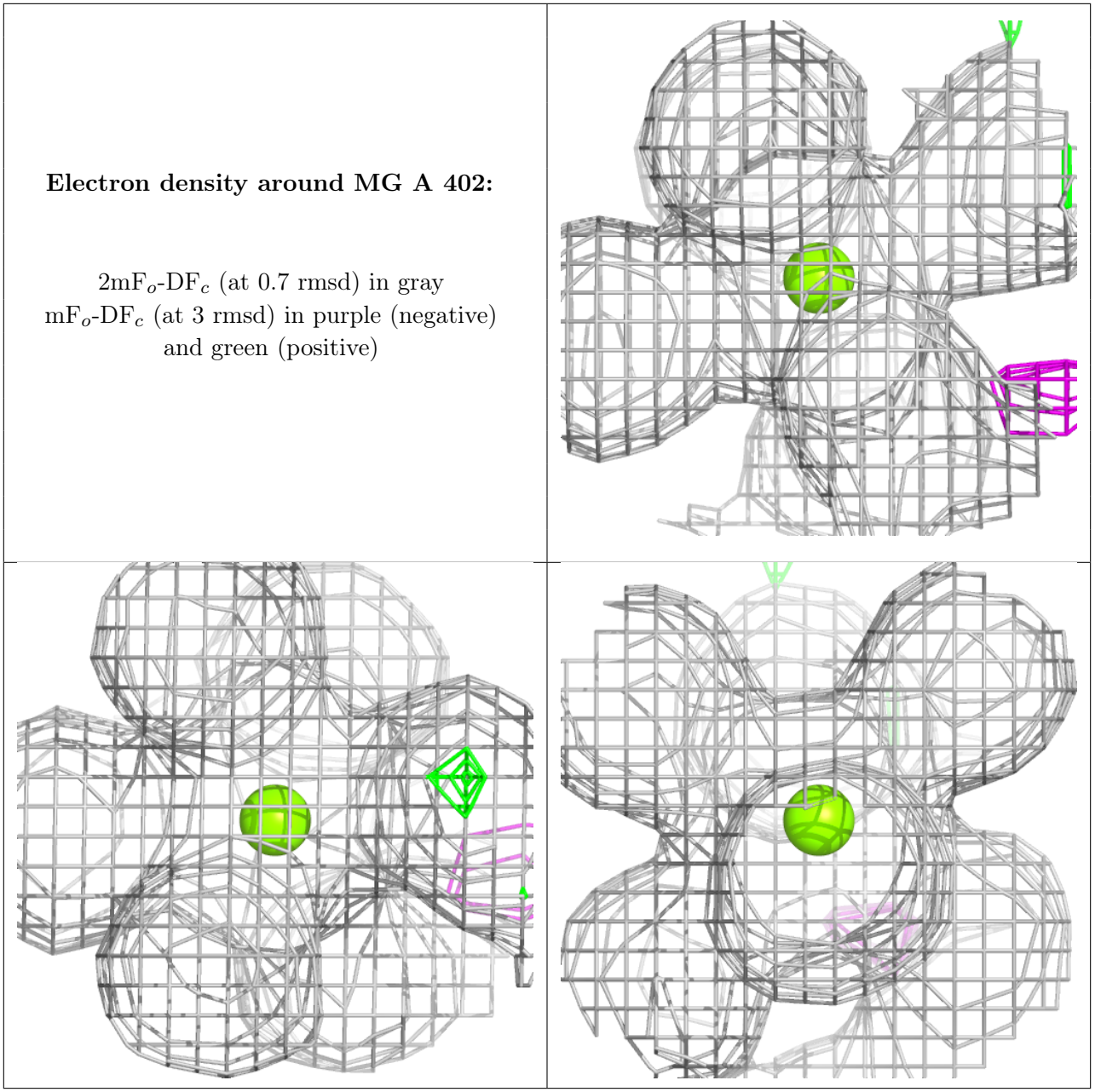
Electron density around ADP A 401:

$2mF_o$-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 402:

$2mF_o$-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.