



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 6QDJ / pdb_00006qdj
Title : Molecular features of the UNC-45 chaperone critical for binding and folding muscle myosin
Authors : Meinhart, A.; Clausen, T.; Arnese, R.
Deposited on : 2019-01-02
Resolution : 1.88 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

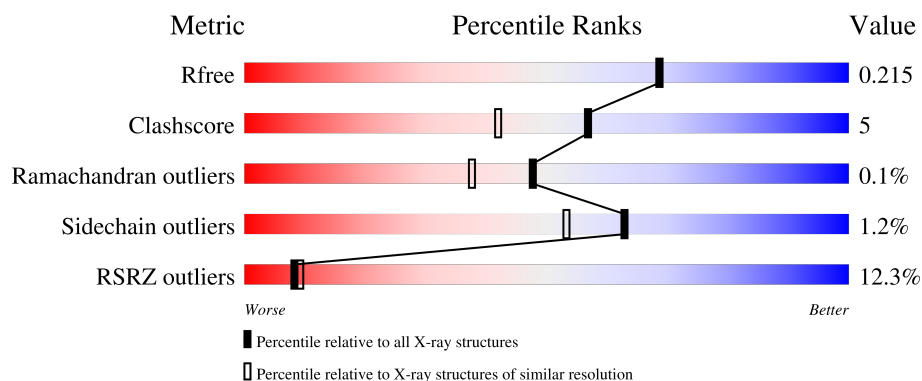
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	790	12% 86% 10% ..

2 Entry composition [i](#)

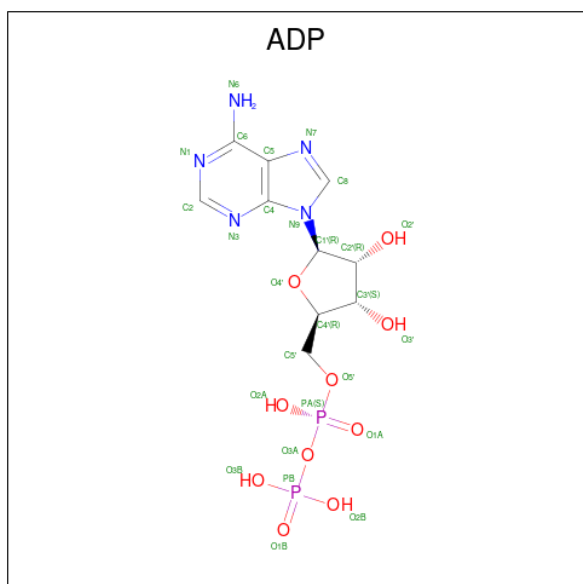
There are 8 unique types of molecules in this entry. The entry contains 6498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	758	6130	3896	1048	1144	42	0	1	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



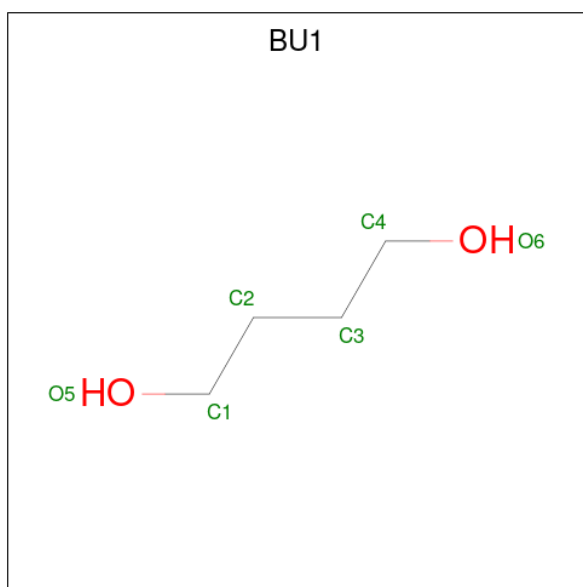
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



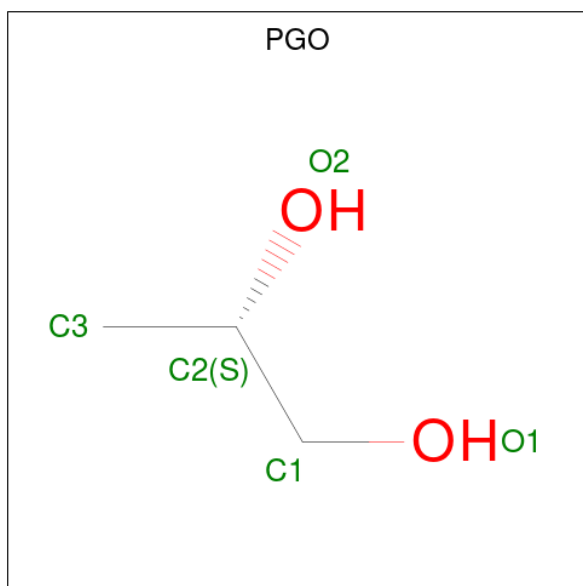
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1,4-BUTANEDIOL (CCD ID: BU1) (formula: $C_4H_{10}O_2$).



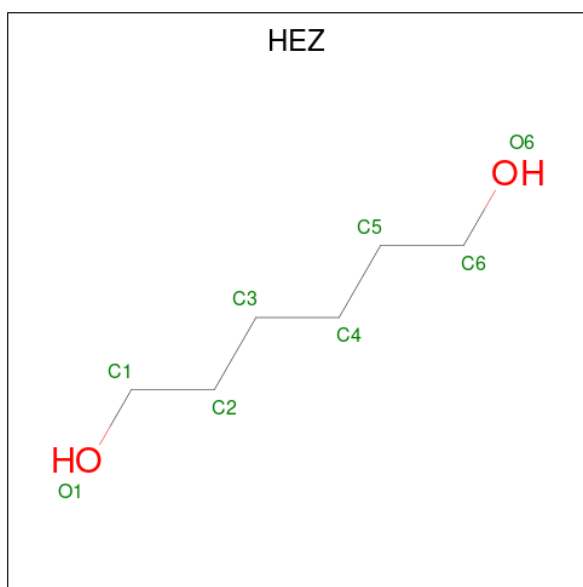
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: $C_3H_8O_2$).



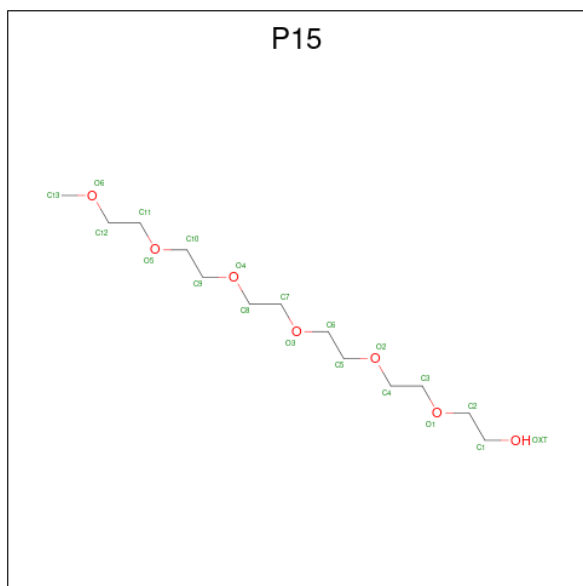
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			5	3	2		
5	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 6 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is 2,5,8,11,14,17-HEXAOXANONADECAN-19-OL (CCD ID: P15) (formula: $C_{13}H_{28}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			20	13	7		

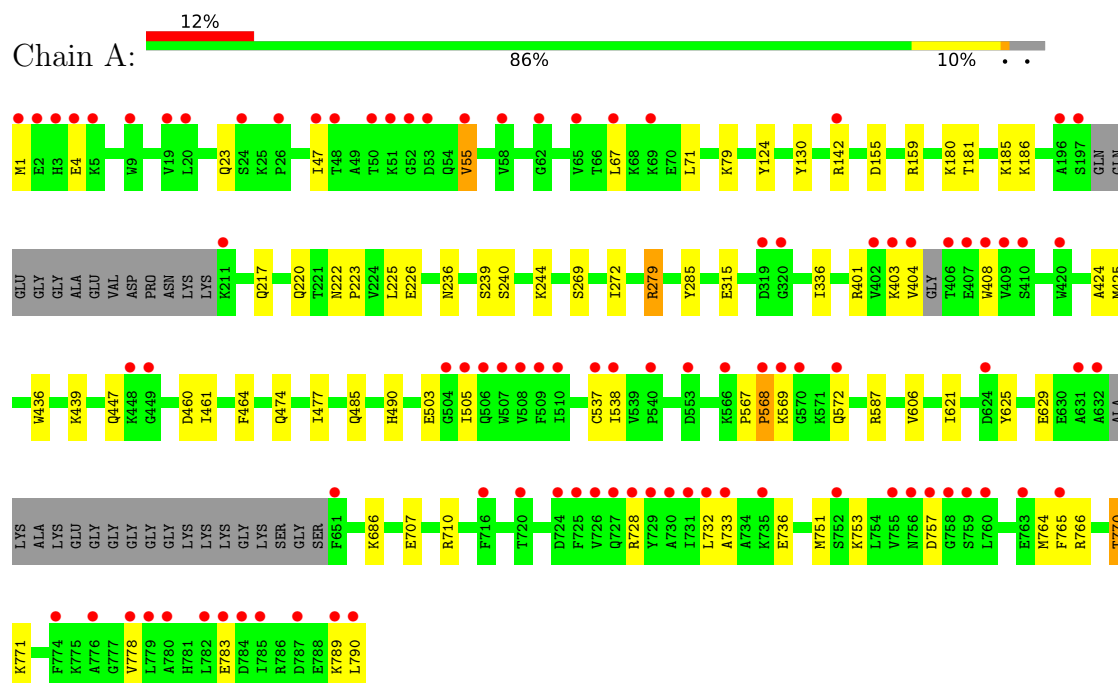
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	237	Total 237	O 237	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-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.11Å 111.96Å 84.74Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	84.03 – 1.88 84.03 – 1.88	Depositor EDS
% Data completeness (in resolution range)	94.4 (84.03-1.88) 94.4 (84.03-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.184 , 0.213 0.187 , 0.215	Depositor DCC
R_{free} test set	3811 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6498	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 5.60% 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: ADP, BU1, GOL, PGO, HEZ, P15

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	0.49	0/6261	0.61	0/8437

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 [i](#)

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	6130	0	6067	57	0
2	A	27	0	12	0	0
3	A	60	0	80	2	0
4	A	6	0	10	1	0
5	A	10	0	16	3	0
6	A	8	0	14	2	0
7	A	20	0	28	3	0
8	A	237	0	0	0	0
All	All	6498	0	6227	57	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 5.

All (57) 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:23:GLN:HG2	1:A:79:LYS:HA	1.70	0.73
1:A:272:ILE:HD11	7:A:816:P15:H71	1.76	0.66
1:A:753:LYS:NZ	1:A:757:ASP:OD2	2.28	0.66
1:A:503:GLU:OE2	1:A:770:THR:HG22	2.01	0.60
1:A:764:MET:HE2	1:A:778:VAL:HG22	1.84	0.60
1:A:770:THR:HG23	1:A:771:LYS:HG3	1.84	0.59
1:A:439:LYS:HE2	6:A:815:HEZ:H21	1.84	0.58
1:A:464:PHE:HE2	5:A:814:PGO:H33	1.68	0.58
1:A:765:PHE:O	1:A:766:ARG:HD2	2.03	0.58
1:A:568:PRO:HB3	1:A:572:GLN:O	2.05	0.57
1:A:47:ILE:HG23	1:A:55:VAL:HG23	1.85	0.57
1:A:279:ARG:HG2	1:A:285:TYR:CZ	2.40	0.56
1:A:485:GLN:OE1	5:A:814:PGO:H32	2.07	0.54
1:A:403:LYS:HB2	1:A:408:TRP:CZ3	2.42	0.53
1:A:220:GLN:O	1:A:223:PRO:HD2	2.08	0.53
1:A:707:GLU:CD	1:A:710:ARG:HH21	2.17	0.53
1:A:567:PRO:O	1:A:569:LYS:N	2.42	0.52
1:A:537:CYS:SG	1:A:538:ILE:HG23	2.49	0.52
1:A:728:ARG:HH21	1:A:783:GLU:CD	2.19	0.50
1:A:424:ALA:HB2	7:A:816:P15:H42	1.93	0.50
1:A:464:PHE:CE2	5:A:814:PGO:H33	2.47	0.49
1:A:436:TRP:HD1	6:A:815:HEZ:H32	1.78	0.48
1:A:751:MET:HE2	1:A:765:PHE:CG	2.48	0.48
1:A:142:ARG:HD3	1:A:142:ARG:HA	1.66	0.48
1:A:764:MET:HB3	1:A:778:VAL:HG21	1.95	0.48
1:A:732:LEU:HD23	1:A:789:LYS:HD2	1.95	0.47
1:A:733:ALA:HB2	1:A:753:LYS:HD3	1.96	0.47
1:A:67:LEU:HD22	1:A:71:LEU:HD12	1.96	0.47
1:A:728:ARG:NH2	1:A:783:GLU:OE1	2.39	0.47
1:A:401:ARG:HE	1:A:408:TRP:HB3	1.80	0.47
1:A:236:ASN:HB3	1:A:239:SER:HB2	1.97	0.47
1:A:279:ARG:HG3	1:A:315:GLU:O	2.15	0.46
1:A:461:ILE:HG13	3:A:807:GOL:C1	2.46	0.46
1:A:180:LYS:HB3	1:A:460:ASP:OD1	2.16	0.46
1:A:217:GLN:OE1	1:A:447:GLN:NE2	2.49	0.46
1:A:490:HIS:HB2	4:A:812:BU1:H12	1.97	0.46
1:A:461:ILE:HG13	3:A:807:GOL:H11	1.97	0.45
1:A:222:ASN:HB3	1:A:223:PRO:HD3	1.98	0.45
1:A:130:TYR:CD1	1:A:186:LYS:HD3	2.52	0.45
1:A:606:VAL:HG11	1:A:625:TYR:CD1	2.52	0.45
1:A:1:MET:HG3	1:A:4:GLU:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASP:O	1:A:159:ARG:HG2	2.18	0.44
1:A:244:LYS:HE2	1:A:244:LYS:HB3	1.87	0.44
1:A:220:GLN:HG3	1:A:336:ILE:HG21	2.00	0.43
1:A:240:SER:OG	1:A:244:LYS:NZ	2.47	0.43
1:A:269:SER:HB3	7:A:816:P15:H102	1.99	0.43
1:A:572:GLN:HB3	1:A:587:ARG:NH1	2.33	0.43
1:A:770:THR:CG2	1:A:771:LYS:HG3	2.49	0.43
1:A:505:ILE:HD13	1:A:505:ILE:HG21	1.69	0.42
1:A:124:TYR:CE2	1:A:686:LYS:HA	2.55	0.42
1:A:185:LYS:HE3	1:A:226:GLU:OE2	2.19	0.42
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.84	0.41
1:A:474:GLN:HA	1:A:477:ILE:HG22	2.02	0.41
1:A:736:GLU:OE1	1:A:736:GLU:N	2.44	0.41
1:A:764:MET:CE	1:A:778:VAL:HG22	2.50	0.41
1:A:425:MET:HE2	1:A:425:MET:HB2	1.80	0.41
1:A:751:MET:HE2	1:A:765:PHE:CD2	2.57	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	751/790 (95%)	734 (98%)	16 (2%)	1 (0%)	48 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	568	PRO

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	668/686 (97%)	660 (99%)	8 (1%)	63	53

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	181	THR
1	A	279	ARG
1	A	404	VAL
1	A	621	ILE
1	A	629	GLU
1	A	770	THR
1	A	790	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	220	GLN
1	A	486	GLN
1	A	628	GLN
1	A	698	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands 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	$\# Z > 2$
3	GOL	A	802	-	5,5,5	1.50	0	5,5,5	1.09	0
5	PGO	A	814	-	4,4,4	0.94	0	4,4,4	0.34	0
2	ADP	A	801	-	28,29,29	1.66	5 (17%)	43,45,45	1.76	9 (20%)
3	GOL	A	807	-	5,5,5	0.85	0	5,5,5	1.20	1 (20%)
7	P15	A	816	-	19,19,19	0.62	0	18,18,18	0.50	0
3	GOL	A	804	-	5,5,5	0.95	0	5,5,5	1.03	0
3	GOL	A	810	-	5,5,5	1.30	1 (20%)	5,5,5	1.03	0
4	BU1	A	812	-	5,5,5	0.63	0	4,4,4	0.17	0
5	PGO	A	813	-	4,4,4	0.75	0	4,4,4	0.85	0
3	GOL	A	806	-	5,5,5	1.15	0	5,5,5	1.25	1 (20%)
6	HEZ	A	815	-	7,7,7	0.41	0	6,6,6	0.25	0
3	GOL	A	803	-	5,5,5	1.11	0	5,5,5	0.68	0
3	GOL	A	805	-	5,5,5	1.47	1 (20%)	5,5,5	0.81	0
3	GOL	A	811	-	5,5,5	0.79	0	5,5,5	1.09	1 (20%)
3	GOL	A	809	-	5,5,5	1.68	2 (40%)	5,5,5	0.85	0
3	GOL	A	808	-	5,5,5	0.79	0	5,5,5	1.14	1 (20%)

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
3	GOL	A	802	-	-	3/4/4/4	-
5	PGO	A	814	-	-	0/2/2/2	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	801	-	-	2/16/32/32	0/3/3/3
3	GOL	A	807	-	-	2/4/4/4	-
7	P15	A	816	-	-	10/17/17/17	-
3	GOL	A	804	-	-	4/4/4/4	-
3	GOL	A	810	-	-	4/4/4/4	-
4	BU1	A	812	-	-	2/3/3/3	-
5	PGO	A	813	-	-	0/2/2/2	-
3	GOL	A	806	-	-	3/4/4/4	-
6	HEZ	A	815	-	-	2/5/5/5	-
3	GOL	A	803	-	-	4/4/4/4	-
3	GOL	A	805	-	-	2/4/4/4	-
3	GOL	A	811	-	-	4/4/4/4	-
3	GOL	A	809	-	-	0/4/4/4	-
3	GOL	A	808	-	-	4/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ADP	PA-O3A	4.73	1.64	1.59
2	A	801	ADP	C5-C4	4.63	1.47	1.39
3	A	809	GOL	C3-C2	2.80	1.62	1.51
3	A	810	GOL	C3-C2	2.66	1.61	1.51
2	A	801	ADP	C5-C6	2.48	1.47	1.41
2	A	801	ADP	C4-N9	-2.31	1.32	1.37
2	A	801	ADP	C8-N7	2.30	1.36	1.31
3	A	805	GOL	C1-C2	2.15	1.60	1.51
3	A	809	GOL	O3-C3	2.06	1.51	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ADP	N3-C2-N1	-4.60	121.61	128.58
2	A	801	ADP	C5-C4-N3	-4.28	120.82	126.72
2	A	801	ADP	N3-C4-N9	3.84	133.70	127.17
2	A	801	ADP	C4-N9-C8	3.55	109.47	105.74
2	A	801	ADP	C2-N3-C4	3.50	120.37	111.83
2	A	801	ADP	C2-N1-C6	2.82	123.36	118.73
2	A	801	ADP	C4-C5-N7	-2.53	107.69	110.58
3	A	806	GOL	C3-C2-C1	-2.33	103.24	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ADP	C6-C5-N7	2.28	136.48	132.09
3	A	807	GOL	C3-C2-C1	-2.18	103.78	111.80
3	A	808	GOL	C3-C2-C1	-2.17	103.82	111.80
3	A	811	GOL	C3-C2-C1	-2.14	103.94	111.80
2	A	801	ADP	C4-N9-C1'	-2.02	121.91	126.63

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O3B
3	A	803	GOL	O1-C1-C2-O2
3	A	803	GOL	O1-C1-C2-C3
3	A	803	GOL	C1-C2-C3-O3
3	A	804	GOL	O1-C1-C2-C3
3	A	806	GOL	O2-C2-C3-O3
3	A	807	GOL	O1-C1-C2-C3
3	A	808	GOL	O1-C1-C2-C3
3	A	810	GOL	O1-C1-C2-C3
3	A	811	GOL	O1-C1-C2-C3
3	A	811	GOL	C1-C2-C3-O3
7	A	816	P15	O5-C11-C12-O6
3	A	803	GOL	O2-C2-C3-O3
3	A	804	GOL	O1-C1-C2-O2
3	A	810	GOL	O1-C1-C2-O2
3	A	811	GOL	O1-C1-C2-O2
3	A	802	GOL	O1-C1-C2-C3
3	A	804	GOL	C1-C2-C3-O3
3	A	805	GOL	C1-C2-C3-O3
3	A	806	GOL	C1-C2-C3-O3
3	A	810	GOL	C1-C2-C3-O3
3	A	802	GOL	O1-C1-C2-O2
3	A	807	GOL	O1-C1-C2-O2
3	A	808	GOL	O1-C1-C2-O2
3	A	811	GOL	O2-C2-C3-O3
4	A	812	BU1	O5-C1-C2-C3
7	A	816	P15	O2-C5-C6-O3
6	A	815	HEZ	O1-C1-C2-C3
3	A	805	GOL	O2-C2-C3-O3
3	A	810	GOL	O2-C2-C3-O3
7	A	816	P15	O3-C7-C8-O4
3	A	804	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

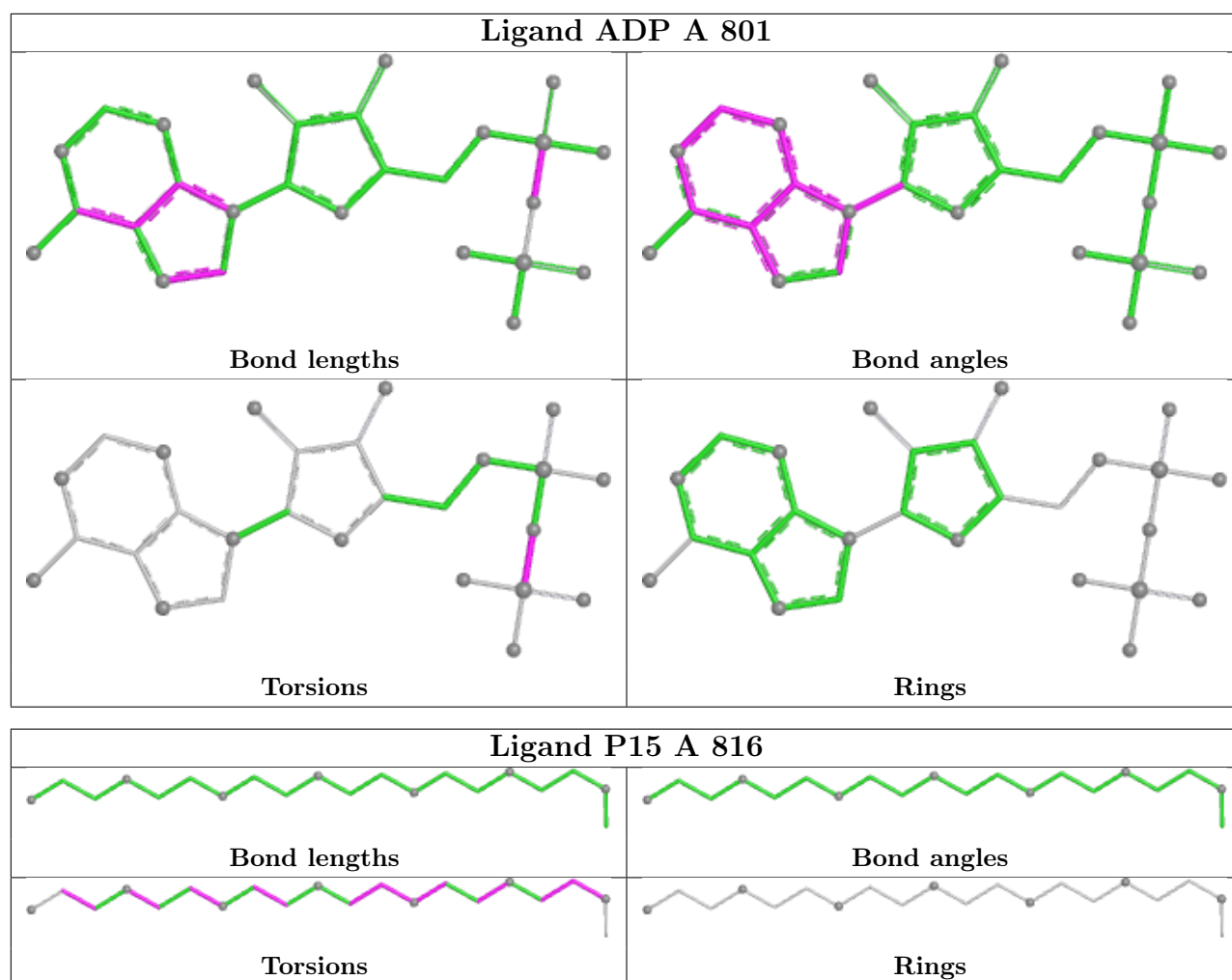
Mol	Chain	Res	Type	Atoms
3	A	806	GOL	O1-C1-C2-O2
7	A	816	P15	C7-C8-O4-C9
7	A	816	P15	C10-C9-O4-C8
7	A	816	P15	C9-C10-O5-C11
7	A	816	P15	C3-C4-O2-C5
7	A	816	P15	OXT-C1-C2-O1
7	A	816	P15	C4-C3-O1-C2
3	A	808	GOL	O2-C2-C3-O3
7	A	816	P15	C11-C12-O6-C13
4	A	812	BU1	C1-C2-C3-C4
3	A	802	GOL	O2-C2-C3-O3
3	A	808	GOL	C1-C2-C3-O3
2	A	801	ADP	PA-O3A-PB-O1B
6	A	815	HEZ	C2-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	814	PGO	3	0
3	A	807	GOL	2	0
7	A	816	P15	3	0
4	A	812	BU1	1	0
6	A	815	HEZ	2	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 ⓘ

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	758/790 (95%)	0.51	93 (12%) 8 9	17, 34, 66, 99	1 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	VAL	7.8
1	A	729	TYR	5.8
1	A	782	LEU	5.8
1	A	20	LEU	5.1
1	A	790	LEU	5.1
1	A	406	THR	4.7
1	A	507	TRP	4.6
1	A	197	SER	4.4
1	A	537	CYS	4.3
1	A	732	LEU	4.2
1	A	408	TRP	4.1
1	A	509	PHE	4.1
1	A	651	PHE	4.1
1	A	779	LEU	4.0
1	A	758	GLY	4.0
1	A	508	VAL	3.7
1	A	3	HIS	3.7
1	A	67	LEU	3.7
1	A	570	GLY	3.6
1	A	789	LYS	3.6
1	A	731	ILE	3.5
1	A	632	ALA	3.5
1	A	759	SER	3.5
1	A	760	LEU	3.4
1	A	448	LYS	3.3
1	A	774	PHE	3.3
1	A	720	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	505	ILE	3.3
1	A	403	LYS	3.2
1	A	407	GLU	3.2
1	A	778	VAL	3.1
1	A	1	MET	3.1
1	A	26	PRO	3.1
1	A	319	ASP	3.0
1	A	402	VAL	3.0
1	A	409	VAL	3.0
1	A	631	ALA	2.9
1	A	55	VAL	2.9
1	A	776	ALA	2.9
1	A	5	LYS	2.9
1	A	24	SER	2.9
1	A	52	GLY	2.9
1	A	69	LYS	2.8
1	A	538	ILE	2.8
1	A	211	LYS	2.8
1	A	58	VAL	2.8
1	A	50	THR	2.8
1	A	757	ASP	2.8
1	A	726	VAL	2.8
1	A	449	GLY	2.7
1	A	569	LYS	2.6
1	A	47	ILE	2.6
1	A	730	ALA	2.6
1	A	725	PHE	2.6
1	A	566	LYS	2.5
1	A	780	ALA	2.5
1	A	553	ASP	2.5
1	A	540	PRO	2.5
1	A	765	PHE	2.4
1	A	785	ILE	2.4
1	A	48	THR	2.4
1	A	504	GLY	2.4
1	A	51	LYS	2.4
1	A	755	VAL	2.4
1	A	783	GLU	2.3
1	A	196	ALA	2.3
1	A	320	GLY	2.3
1	A	19	VAL	2.3
1	A	506	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	65	VAL	2.3
1	A	735	LYS	2.3
1	A	9	TRP	2.2
1	A	4	GLU	2.2
1	A	510	ILE	2.2
1	A	142	ARG	2.2
1	A	716	PHE	2.2
1	A	724	ASP	2.2
1	A	727	GLN	2.1
1	A	2	GLU	2.1
1	A	733	ALA	2.1
1	A	624	ASP	2.1
1	A	728	ARG	2.1
1	A	572	GLN	2.1
1	A	784	ASP	2.1
1	A	787	ASP	2.1
1	A	410	SER	2.1
1	A	568	PRO	2.1
1	A	62	GLY	2.0
1	A	756	ASN	2.0
1	A	420	TRP	2.0
1	A	53	ASP	2.0
1	A	763	GLU	2.0
1	A	752	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

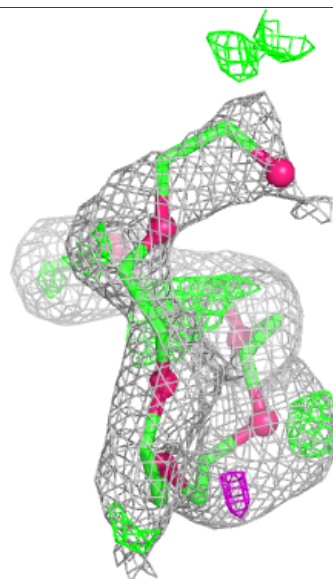
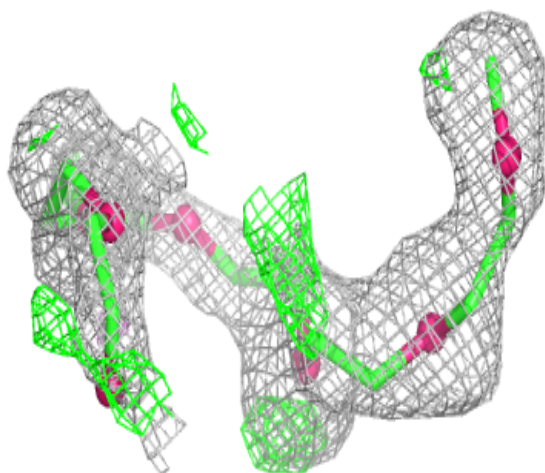
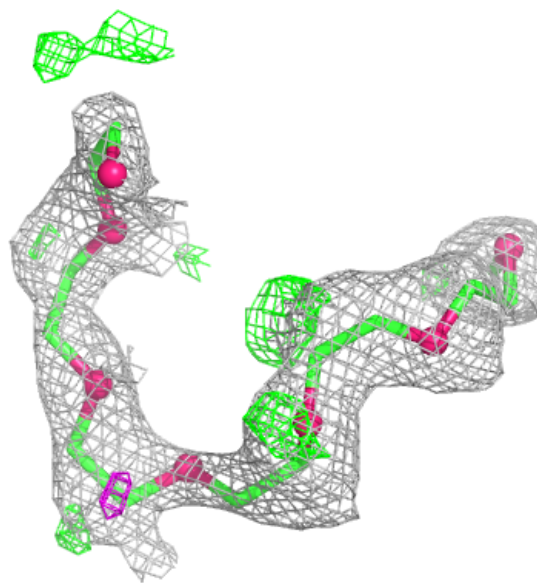
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

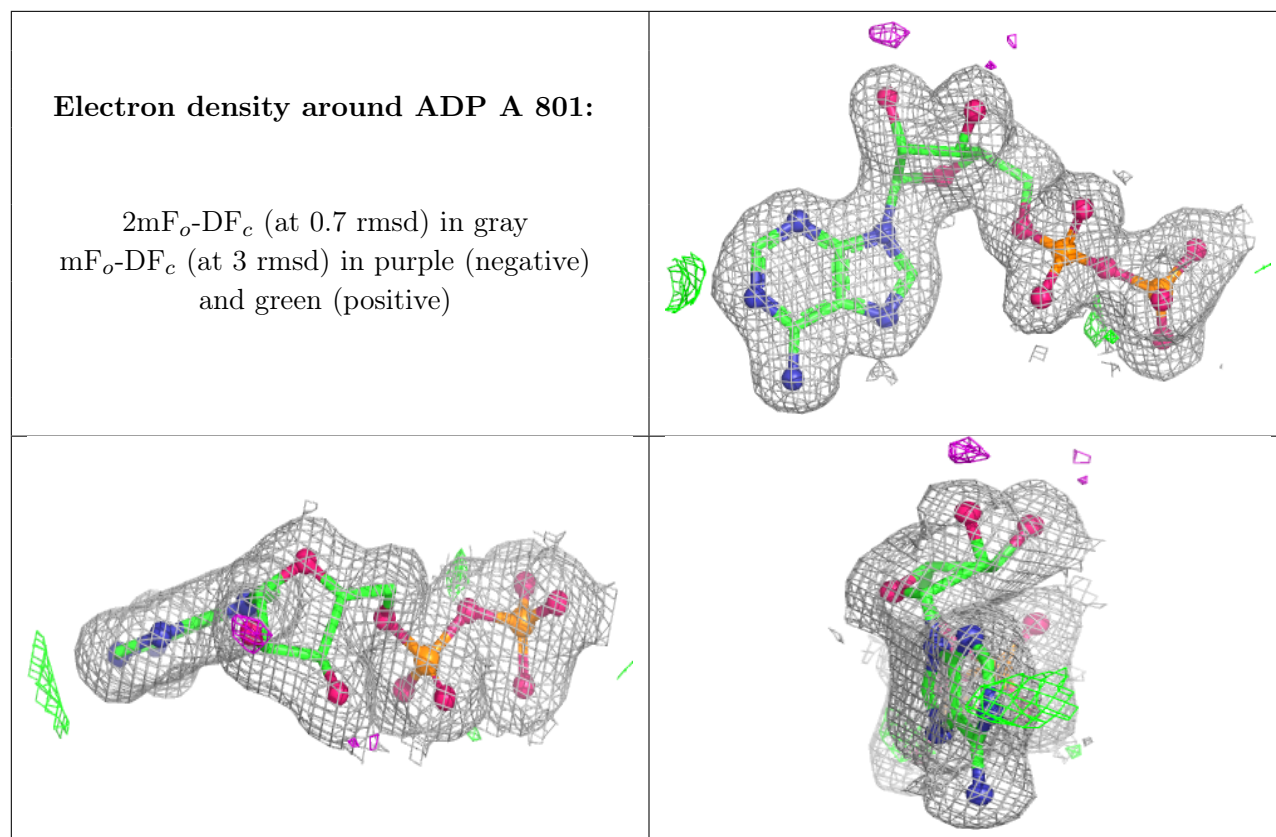
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	P15	A	816	20/20	0.76	0.23	49,57,71,71	0
3	GOL	A	811	6/6	0.79	0.16	33,43,47,57	0
6	HEZ	A	815	8/8	0.83	0.23	43,53,63,64	0
3	GOL	A	809	6/6	0.84	0.14	36,41,49,50	0
3	GOL	A	810	6/6	0.85	0.16	42,49,57,58	0
3	GOL	A	805	6/6	0.86	0.14	37,45,50,56	0
4	BU1	A	812	6/6	0.87	0.14	38,42,46,51	0
3	GOL	A	803	6/6	0.88	0.14	31,49,59,67	0
5	PGO	A	813	5/5	0.88	0.16	40,40,48,54	0
3	GOL	A	808	6/6	0.89	0.14	36,49,49,52	0
3	GOL	A	807	6/6	0.89	0.14	42,42,54,57	0
3	GOL	A	806	6/6	0.91	0.12	33,39,45,50	0
3	GOL	A	802	6/6	0.91	0.13	33,42,47,51	0
5	PGO	A	814	5/5	0.92	0.12	31,31,42,48	0
3	GOL	A	804	6/6	0.94	0.11	38,38,46,62	0
2	ADP	A	801	27/27	0.98	0.06	24,30,36,37	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 P15 A 816:

$2mF_o-DF_c$ (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.