Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:45 am BST

PDB ID	:	4BYG
Title	:	ATPase crystal structure
Authors	:	Mattle, D.; Drachmann, N.D.; Liu, X.Y.; Pedersen, B.P.; Morth, J.P.; Wang, J.; Gourdon, P.; Nissen, P.
Deposited on	:	2013-07-19
Resolution	:	2.85 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 following versions of software and data (see references ⓘ) were used in the production of this report:

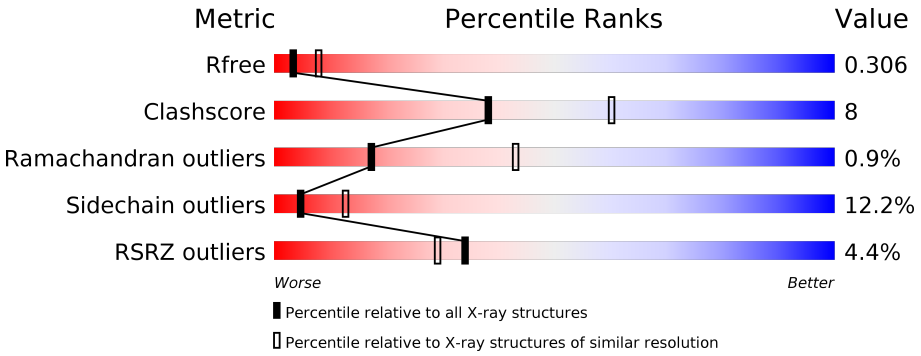
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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	736	4% 67% 21% • 10%

2 Entry composition

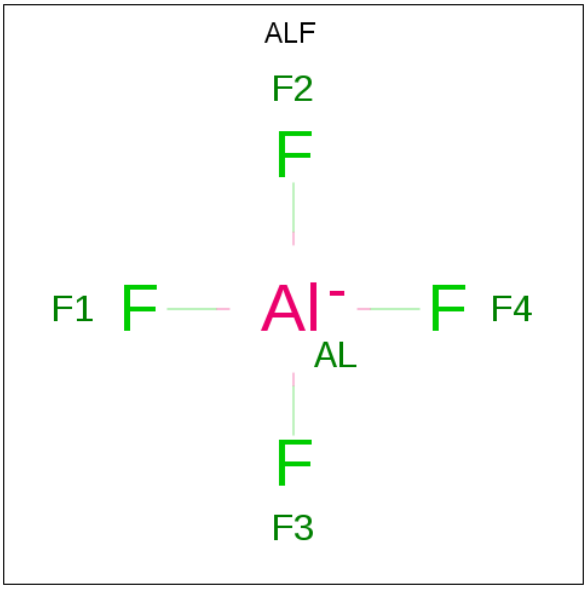
There are 6 unique types of molecules in this entry. The entry contains 5023 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 COPPER EFFLUX ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			

- Molecule 2 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Al	F	0	0
			5	1	4		

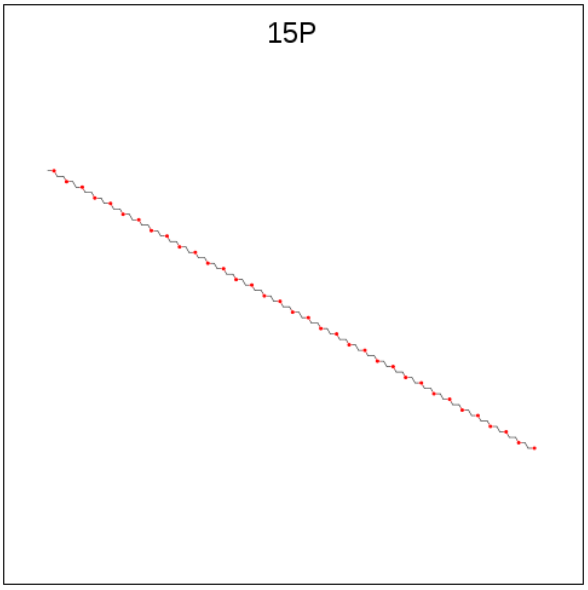
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: $C_{69}H_{140}O_{35}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 45 30 15	0	0

- Molecule 6 is water.

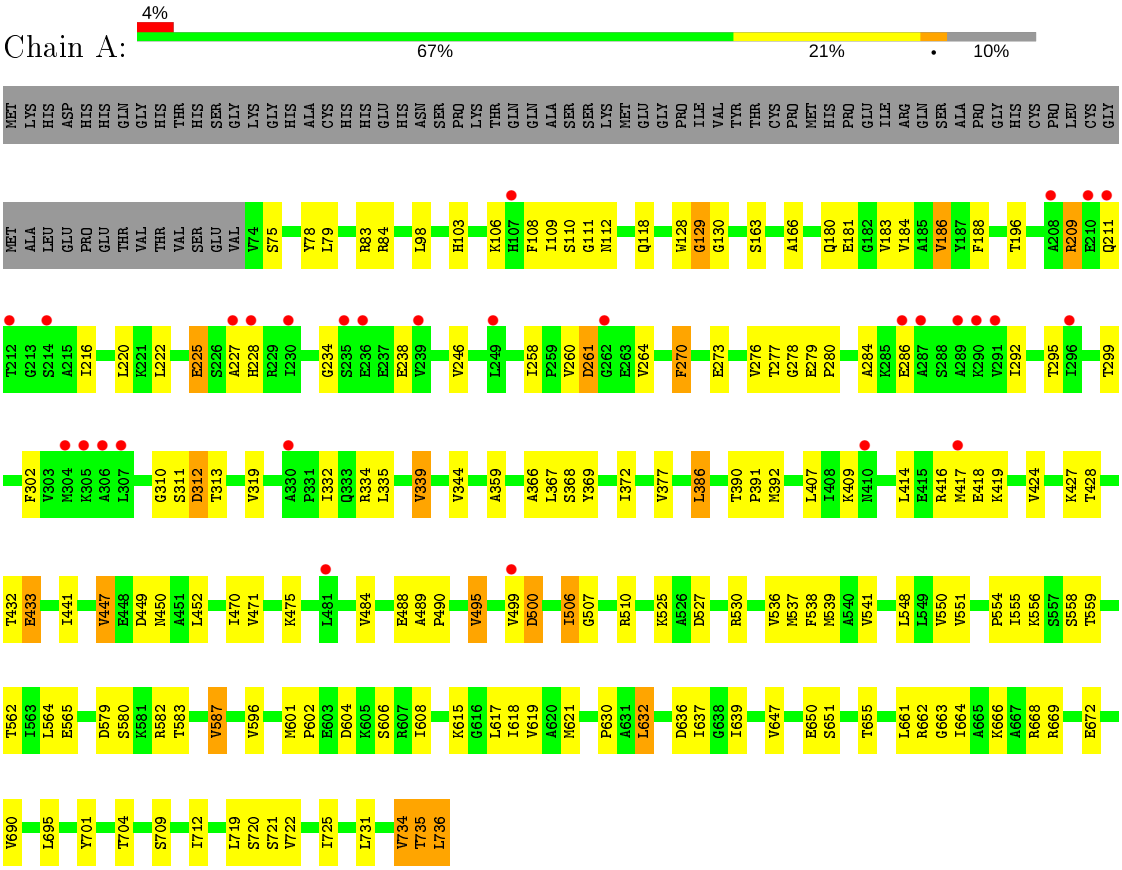
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	37	Total O 37 37	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: COPPER EFFLUX ATPASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.12Å 72.91Å 329.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.85 71.19 – 2.85	Depositor EDS
% Data completeness (in resolution range)	88.8 (14.98-2.85) 88.9 (71.19-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.86Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.232 , 0.287 0.242 , 0.306	Depositor DCC
R_{free} test set	1192 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5023	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: ALF, 15P, K, MG

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	0.24	0/5017	0.47	0/6812

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	734	VAL	Peptide

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	4934	0	5125	76	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	45	0	58	2	0
6	A	37	0	0	3	0
All	All	5023	0	5183	77	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 8.

All (77) 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:418:GLU:HG3	1:A:672:GLU:HG3	1.73	0.71
1:A:735:THR:HA	1:A:736:LEU:HB2	1.71	0.71
1:A:495:VAL:HG23	1:A:506:ILE:HG23	1.75	0.68
1:A:84:ARG:NH1	1:A:128:TRP:O	2.27	0.68
1:A:500:ASP:OD1	1:A:500:ASP:N	2.25	0.68
1:A:106:LYS:H	1:A:109:ILE:HD13	1.62	0.64
1:A:359:ALA:HA	1:A:366:ALA:HB1	1.82	0.62
1:A:419:LYS:HB3	1:A:618:ILE:HD13	1.82	0.60
1:A:427:LYS:HD2	1:A:587:VAL:HG11	1.83	0.60
1:A:536:VAL:HG22	1:A:550:VAL:HG12	1.84	0.59
1:A:261:ASP:HB3	1:A:292:ILE:HA	1.85	0.59
1:A:662:ARG:N	1:A:663:GLY:HA3	2.18	0.58
1:A:277:THR:O	6:A:2014:HOH:O	2.17	0.57
1:A:416:ARG:HB2	1:A:637:ILE:HD11	1.87	0.57
1:A:615:LYS:NZ	6:A:2031:HOH:O	2.39	0.55
1:A:409:LYS:NZ	1:A:650:GLU:OE1	2.39	0.55
1:A:386:LEU:H	1:A:386:LEU:HD12	1.71	0.55
1:A:417:MET:HG3	1:A:668:ARG:HA	1.90	0.54
1:A:428:THR:HA	1:A:432:THR:HG22	1.90	0.53
1:A:75:SER:HB3	1:A:78:TYR:HB3	1.90	0.53
1:A:78:TYR:HD2	1:A:79:LEU:HD12	1.74	0.53
1:A:447:VAL:HG22	1:A:450:ASN:HB2	1.90	0.53
1:A:621:MET:HG3	1:A:632:LEU:HD13	1.91	0.52
1:A:111:GLY:HA3	1:A:183:VAL:HG11	1.91	0.52
1:A:258:ILE:HD12	1:A:295:THR:HB	1.93	0.50
1:A:601:MET:HB3	1:A:602:PRO:HD2	1.92	0.50
1:A:98:LEU:HD23	1:A:118:GLN:HG3	1.93	0.50
1:A:735:THR:HG22	1:A:736:LEU:C	2.33	0.49
1:A:470:ILE:HG12	6:A:2026:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:VAL:HG12	1:A:499:VAL:HG22	1.94	0.49
1:A:556:LYS:HB2	1:A:559:THR:OG1	2.13	0.49
1:A:606:SER:HB2	1:A:630:PRO:HB2	1.94	0.48
1:A:112:ASN:ND2	5:A:1000:15P:O9	2.46	0.48
5:A:1000:15P:H242	5:A:1000:15P:H262	1.62	0.48
1:A:209:ARG:HH12	1:A:334:ARG:HH21	1.62	0.48
1:A:506:ILE:HB	1:A:539:MET:HG3	1.97	0.47
1:A:666:LYS:HG2	1:A:669:ARG:NH2	2.30	0.47
1:A:368:SER:O	1:A:372:ILE:HG12	2.14	0.47
1:A:186:VAL:HG13	1:A:188:PHE:H	1.80	0.47
1:A:276:VAL:O	1:A:278:GLY:N	2.43	0.47
1:A:441:ILE:HD11	1:A:452:LEU:HD13	1.96	0.46
1:A:270:PHE:HB3	1:A:284:ALA:HA	1.98	0.46
1:A:335:LEU:O	1:A:339:VAL:HG12	2.15	0.46
1:A:604:ASP:O	1:A:608:ILE:HG12	2.16	0.46
1:A:220:LEU:HG	1:A:319:VAL:HG12	1.98	0.46
1:A:225:GLU:HG2	1:A:225:GLU:H	1.51	0.46
1:A:129:GLY:HA3	1:A:130:GLY:HA3	1.54	0.45
1:A:447:VAL:HG23	1:A:450:ASN:H	1.82	0.45
1:A:103:HIS:CG	1:A:109:ILE:HG21	2.51	0.45
1:A:721:SER:O	1:A:725:ILE:HG12	2.17	0.45
1:A:166:ALA:HB1	1:A:184:VAL:HB	1.97	0.45
1:A:332:ILE:HG21	1:A:416:ARG:HD2	1.99	0.45
1:A:499:VAL:HA	1:A:500:ASP:HA	1.76	0.45
1:A:417:MET:HE2	1:A:637:ILE:HG21	1.99	0.45
1:A:731:LEU:O	1:A:734:VAL:HG22	2.17	0.45
1:A:111:GLY:HA3	1:A:183:VAL:HG21	1.99	0.44
1:A:163:SER:HB3	1:A:186:VAL:HG22	1.99	0.44
1:A:227:ALA:O	1:A:228:HIS:ND1	2.51	0.43
1:A:264:VAL:HG13	1:A:302:PHE:HB2	2.00	0.43
1:A:579:ASP:OD1	1:A:580:SER:N	2.42	0.43
1:A:277:THR:HG22	1:A:279:GLU:H	1.84	0.43
1:A:417:MET:HE1	1:A:639:ILE:HD11	2.00	0.42
1:A:366:ALA:O	1:A:367:LEU:HB2	2.19	0.42
1:A:390:THR:HB	1:A:391:PRO:HD3	2.01	0.42
1:A:310:GLY:O	1:A:313:THR:HG22	2.20	0.42
1:A:432:THR:OG1	1:A:554:PRO:O	2.34	0.42
1:A:471:VAL:O	1:A:475:LYS:HG3	2.19	0.42
1:A:489:ALA:HA	1:A:490:PRO:HD3	1.86	0.42
1:A:506:ILE:HD11	1:A:537:MET:HB3	2.02	0.42
1:A:279:GLU:HA	1:A:280:PRO:HD2	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:SER:O	1:A:562:THR:HG23	2.20	0.42
1:A:507:GLY:O	1:A:538:PHE:N	2.48	0.41
1:A:530:ARG:O	1:A:582:ARG:NH1	2.53	0.41
1:A:228:HIS:HD1	1:A:238:GLU:HG2	1.86	0.41
1:A:407:LEU:HB2	1:A:655:THR:HB	2.03	0.41
1:A:292:ILE:HD13	1:A:292:ILE:HA	1.97	0.40
1:A:433:GLU:HG2	1:A:433:GLU:H	1.53	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	661/736 (90%)	615 (93%)	40 (6%)	6 (1%)	17 43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	GLY
1	A	108	PHE
1	A	311	SER
1	A	312	ASP
1	A	299	THR
1	A	234	GLY

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	523/586 (89%)	459 (88%)	64 (12%)	5 13

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	110	SER
1	A	180	GLN
1	A	181	GLU
1	A	186	VAL
1	A	196	THR
1	A	209	ARG
1	A	211	GLN
1	A	216	ILE
1	A	222	LEU
1	A	225	GLU
1	A	246	VAL
1	A	260	VAL
1	A	261	ASP
1	A	270	PHE
1	A	273	GLU
1	A	286	GLU
1	A	312	ASP
1	A	339	VAL
1	A	344	VAL
1	A	369	TYR
1	A	377	VAL
1	A	386	LEU
1	A	392	MET
1	A	414	LEU
1	A	424	VAL
1	A	433	GLU
1	A	447	VAL
1	A	449	ASP
1	A	488	GLU
1	A	495	VAL
1	A	500	ASP
1	A	506	ILE
1	A	510	ARG
1	A	525	LYS
1	A	527	ASP

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Mol	Chain	Res	Type
1	A	541	VAL
1	A	548	LEU
1	A	551	VAL
1	A	555	ILE
1	A	564	LEU
1	A	565	GLU
1	A	583	THR
1	A	587	VAL
1	A	596	VAL
1	A	617	LEU
1	A	619	VAL
1	A	632	LEU
1	A	636	ASP
1	A	647	VAL
1	A	651	SER
1	A	661	LEU
1	A	664	ILE
1	A	690	VAL
1	A	695	LEU
1	A	701	TYR
1	A	704	THR
1	A	709	SER
1	A	712	ILE
1	A	719	LEU
1	A	720	SER
1	A	722	VAL
1	A	735	THR
1	A	736	LEU

Some 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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	ALF	A	995	3,6	0,4,4	0.00	-	-		
5	15P	A	1000	-	44,44,103	0.94	0	43,43,102	0.36	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	15P	A	1000	-	-	22/42/42/101	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1000	15P	C17-C18-O9-C19
5	A	1000	15P	C26-C25-O12-C24
5	A	1000	15P	O3-C7-C8-O4
5	A	1000	15P	O8-C17-C18-O9
5	A	1000	15P	O12-C25-C26-O13
5	A	1000	15P	O2-C5-C6-O3
5	A	1000	15P	O5-C10-C9-O4
5	A	1000	15P	O6-C13-C14-O7

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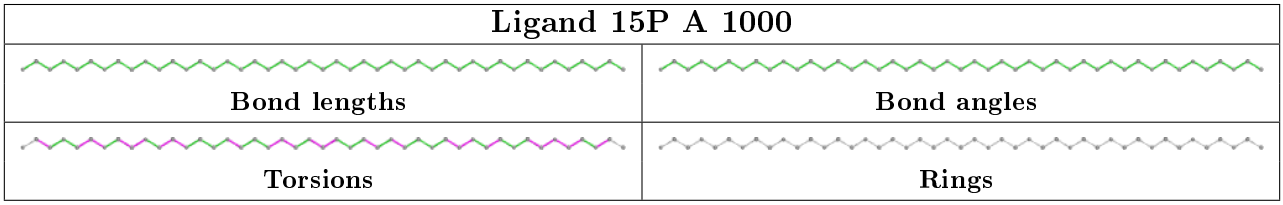
Mol	Chain	Res	Type	Atoms
5	A	1000	15P	O13-C27-C28-O14
5	A	1000	15P	C10-C9-O4-C8
5	A	1000	15P	O14-C29-C30-O15
5	A	1000	15P	O11-C23-C24-O12
5	A	1000	15P	C1-C2-O1-C3
5	A	1000	15P	C3-C4-O2-C5
5	A	1000	15P	C19-C20-O10-C21
5	A	1000	15P	O7-C15-C16-O8
5	A	1000	15P	C24-C23-O11-C22
5	A	1000	15P	C6-C5-O2-C4
5	A	1000	15P	C15-C16-O8-C17
5	A	1000	15P	O1-C3-C4-O2
5	A	1000	15P	C28-C27-O13-C26
5	A	1000	15P	C11-C12-O6-C13

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1000	15P	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 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.



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

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	663/736 (90%)	0.16	29 (4%) 34 29	29, 64, 152, 183	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	GLU	5.1
1	A	227	ALA	5.0
1	A	291	VAL	4.5
1	A	305	LYS	4.4
1	A	239	VAL	4.2
1	A	306	ALA	4.1
1	A	230	ILE	4.0
1	A	211	GLN	3.8
1	A	304	MET	3.7
1	A	262	GLY	3.3
1	A	214	SER	2.9
1	A	249	LEU	2.9
1	A	307	LEU	2.8
1	A	499	VAL	2.7
1	A	290	LYS	2.7
1	A	107	HIS	2.6
1	A	289	ALA	2.5
1	A	228	HIS	2.5
1	A	481	LEU	2.4
1	A	208	ALA	2.3
1	A	330	ALA	2.2
1	A	417	MET	2.2
1	A	410	ASN	2.2
1	A	287	ALA	2.2
1	A	286	GLU	2.2
1	A	212	THR	2.1
1	A	210	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	296	ILE	2.1
1	A	235	SER	2.1

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 carbohydrates in this entry.

6.4 Ligands (i)

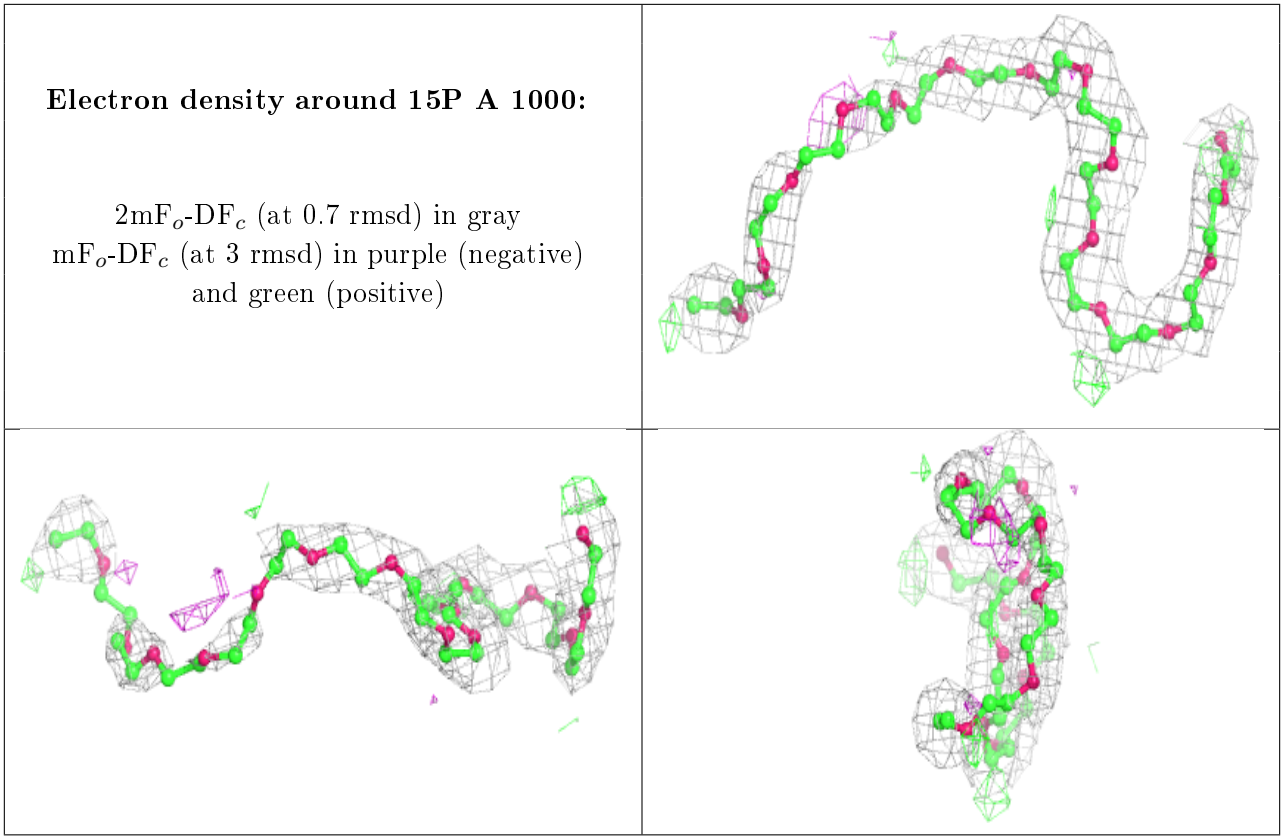
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	15P	A	1000	45/104	0.91	0.26	16,54,90,106	0
2	ALF	A	995	5/5	0.94	0.13	35,44,75,92	0
4	K	A	997	1/1	0.96	0.19	104,104,104,104	0
3	MG	A	996	1/1	0.99	0.10	68,68,68,68	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 15P A 1000:

$2mF_o$-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.