



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:26 AM UTC

PDB ID : 4BYG / pdb_00004byg
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

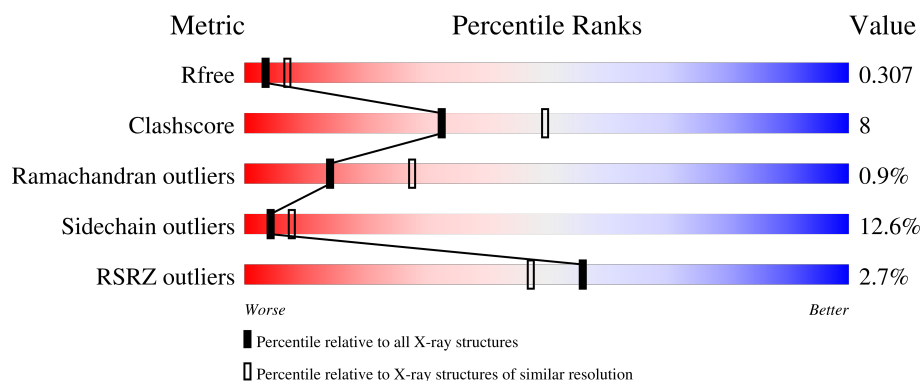
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	736	

2 Entry composition [i](#)

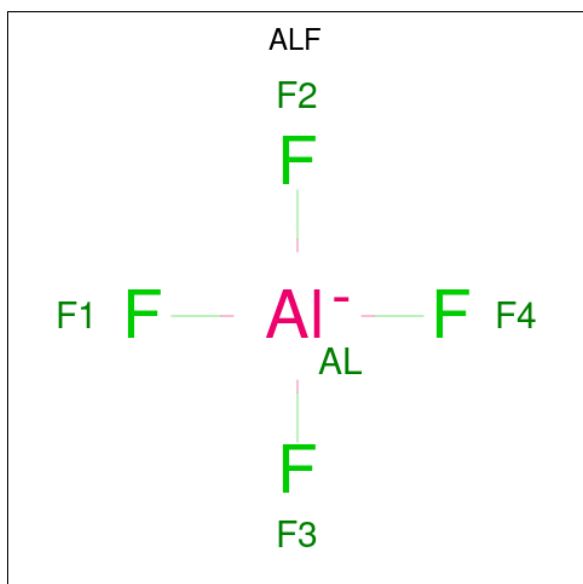
There are 6 unique types of molecules in this entry. The entry contains 5023 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: ALF) (formula: AlF_4).



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

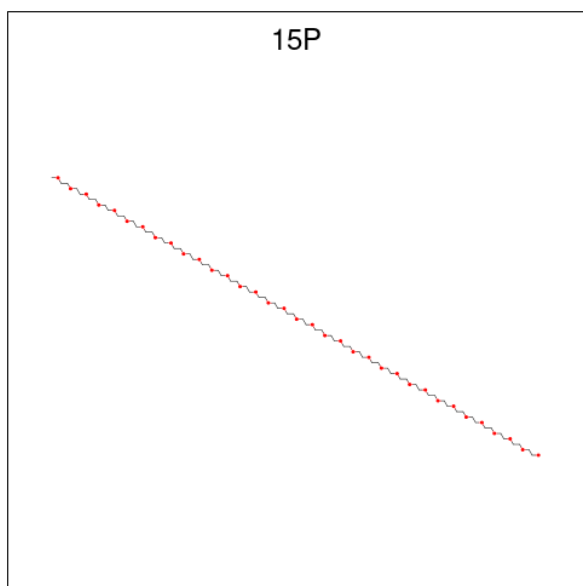
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is POTASSIUM ION (CCD ID: 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) (CCD ID: 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

4 Data and refinement statistics

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 14.98 – 2.85	Depositor EDS
% Data completeness (in resolution range)	88.8 (14.98-2.85) 88.1 (14.98-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.86Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.232 , 0.287 0.243 , 0.307	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)	0.30 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

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: K, ALF, 15P, 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	0.35	0/5017	0.83	7/6812 (0.1%)

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.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	362	GLY	CA-C-N	9.11	129.04	120.03
1	A	362	GLY	C-N-CA	9.11	129.04	120.03
1	A	734	VAL	N-CA-C	7.86	118.65	108.12
1	A	735	THR	N-CA-C	-7.62	97.65	109.76
1	A	664	ILE	N-CA-C	-6.98	105.98	112.96
1	A	662	ARG	N-CA-C	5.52	117.73	111.11
1	A	687	ILE	N-CA-C	5.35	116.72	110.62

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	79	0
2	A	5	0	0	0	0
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	80	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 (80) 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:430:THR:HA	1:A:641:MET:HE2	1.71	0.72
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:N	1:A:500:ASP:OD1	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:HD12	1:A:386:LEU:H	1.71	0.55
1:A:417:MET:HG3	1:A:668:ARG:HA	1.90	0.54
1:A:735:THR:HG22	1:A:736:LEU:C	2.33	0.54
1:A:428:THR:HA	1:A:432:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:470:ILE:HG12	6:A:2026:HOH:O	2.13	0.49
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:H	1:A:225:GLU:HG2	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	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:451:ALA:HB1	1:A:539:MET:HE1	2.03	0.41
1:A:292:ILE:HA	1:A:292:ILE:HD13	1.97	0.40
1:A:417:MET:HE1	1:A:639:ILE:HD11	2.03	0.40
1:A:433:GLU:H	1:A:433:GLU:HG2	1.53	0.40
1:A:310:GLY:C	1:A:312:ASP:H	2.29	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	661/736 (90%)	615 (93%)	40 (6%)	6 (1%)	14 28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	GLY
1	A	108	PHE
1	A	311	SER

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Mol	Chain	Res	Type
1	A	312	ASP
1	A	299	THR
1	A	234	GLY

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	523/586 (89%)	457 (87%)	66 (13%)	4 8

All (66) 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	186	VAL
1	A	196	THR
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	286	GLU
1	A	312	ASP
1	A	315	LEU
1	A	327	ARG
1	A	332	ILE
1	A	339	VAL
1	A	344	VAL
1	A	347	VAL
1	A	377	VAL
1	A	386	LEU
1	A	392	MET

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Mol	Chain	Res	Type
1	A	412	GLU
1	A	414	LEU
1	A	424	VAL
1	A	433	GLU
1	A	447	VAL
1	A	449	ASP
1	A	484	VAL
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
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	607	ARG
1	A	617	LEU
1	A	619	VAL
1	A	632	LEU
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	706	LEU
1	A	709	SER
1	A	712	ILE
1	A	719	LEU
1	A	720	SER
1	A	722	VAL
1	A	735	THR

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Mol	Chain	Res	Type
1	A	736	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	A	464	HIS
1	A	513	GLN
1	A	515	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

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	6,3	4,4,4	1.37	0	-		
5	15P	A	1000	-	44,44,103	0.95	0	43,43,102	0.35	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	O12-C25-C26-O13
5	A	1000	15P	O3-C7-C8-O4
5	A	1000	15P	O8-C17-C18-O9
5	A	1000	15P	O2-C5-C6-O3
5	A	1000	15P	O5-C10-C9-O4
5	A	1000	15P	O6-C13-C14-O7
5	A	1000	15P	O13-C27-C28-O14
5	A	1000	15P	O14-C29-C30-O15
5	A	1000	15P	C10-C9-O4-C8
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	C24-C23-O11-C22
5	A	1000	15P	O7-C15-C16-O8
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	C11-C12-O6-C13
5	A	1000	15P	C28-C27-O13-C26

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 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 15P A 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	663/736 (90%)	-0.17	18 (2%)	56 47	29, 64, 152, 183	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ILE	3.5
1	A	239	VAL	3.3
1	A	111	GLY	3.2
1	A	287	ALA	3.0
1	A	214	SER	2.9
1	A	247	GLY	2.7
1	A	362	GLY	2.6
1	A	215	ALA	2.6
1	A	489	ALA	2.6
1	A	103	HIS	2.4
1	A	105	LEU	2.4
1	A	108	PHE	2.3
1	A	230	ILE	2.3
1	A	702	PRO	2.1
1	A	465	PRO	2.1
1	A	104	GLY	2.1
1	A	492	GLY	2.0
1	A	363	PRO	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](#)

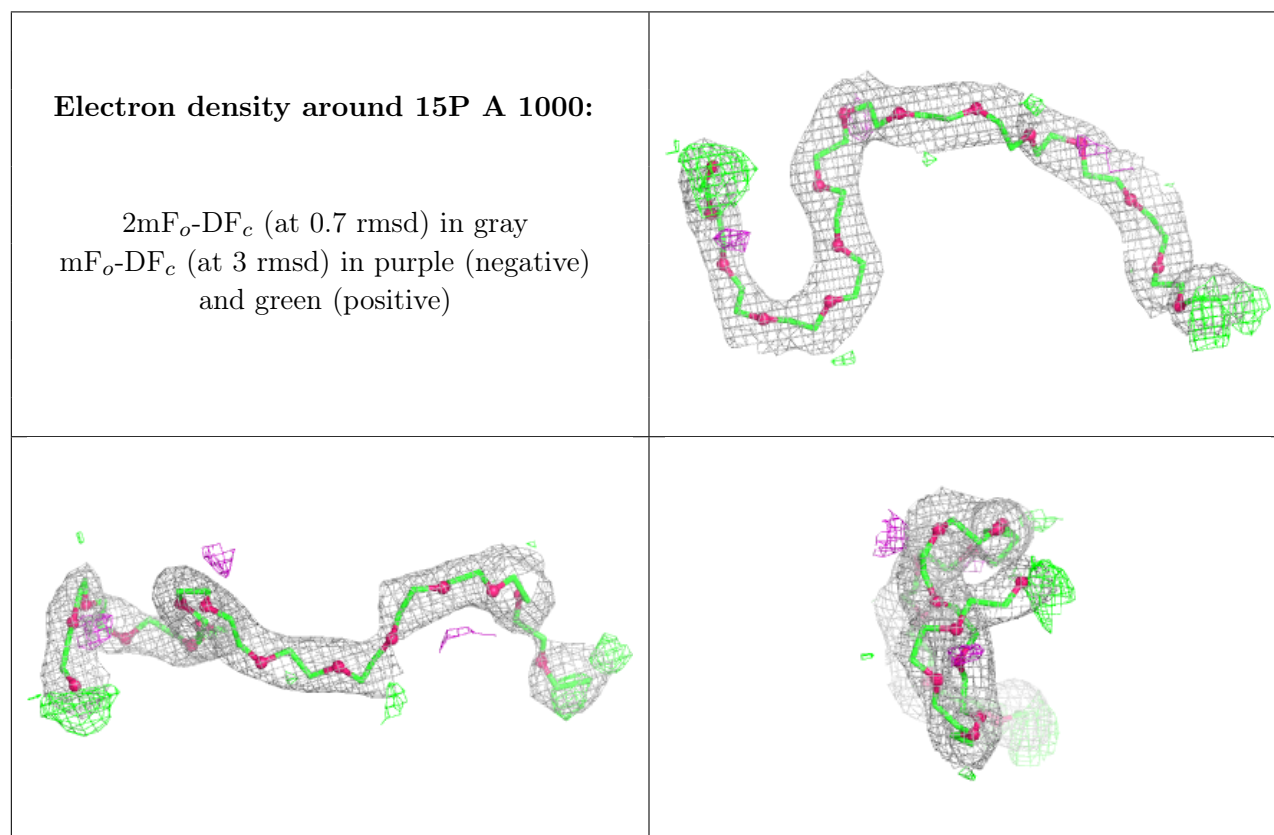
There are no oligosaccharides in this entry.

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
5	15P	A	1000	45/104	0.88	0.10	16,54,90,106	0
4	K	A	997	1/1	0.90	0.09	104,104,104,104	0
2	ALF	A	995	5/5	0.93	0.08	35,44,75,92	0
3	MG	A	996	1/1	0.99	0.02	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.