



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:36 PM UTC

PDB ID : 1HFA / pdb_00001hfa
Title : CALM-N N-terminal domain of clathrin assembly lymphoid myeloid leukaemia protein, PI(4,5)P2 complex
Authors : Ford, M.G.J.; Evans, P.R.; McMahon, H.T.
Deposited on : 2000-11-30
Resolution : 2.00 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

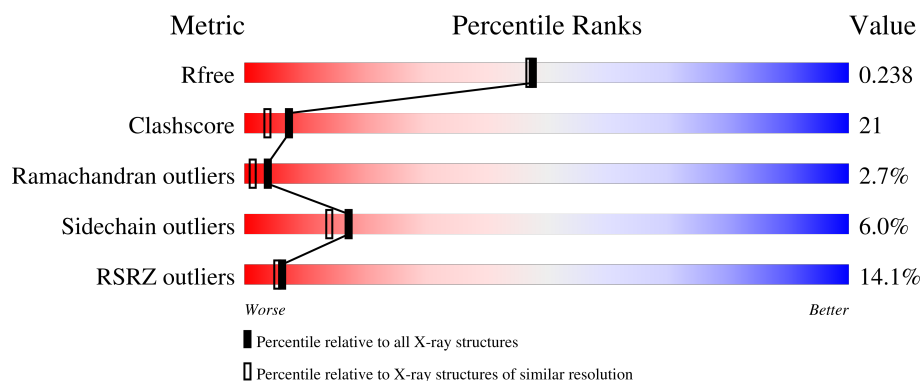
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	289	

2 Entry composition [i](#)

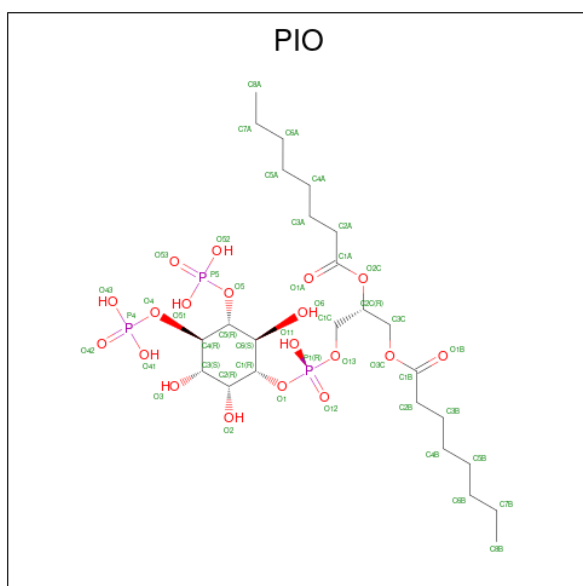
There are 3 unique types of molecules in this entry. The entry contains 2266 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CLATHRIN ASSEMBLY PROTEIN SHORT FORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2114	1345	363	393	13	0	0	0

- Molecule 2 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	24	6	15	3	0	0

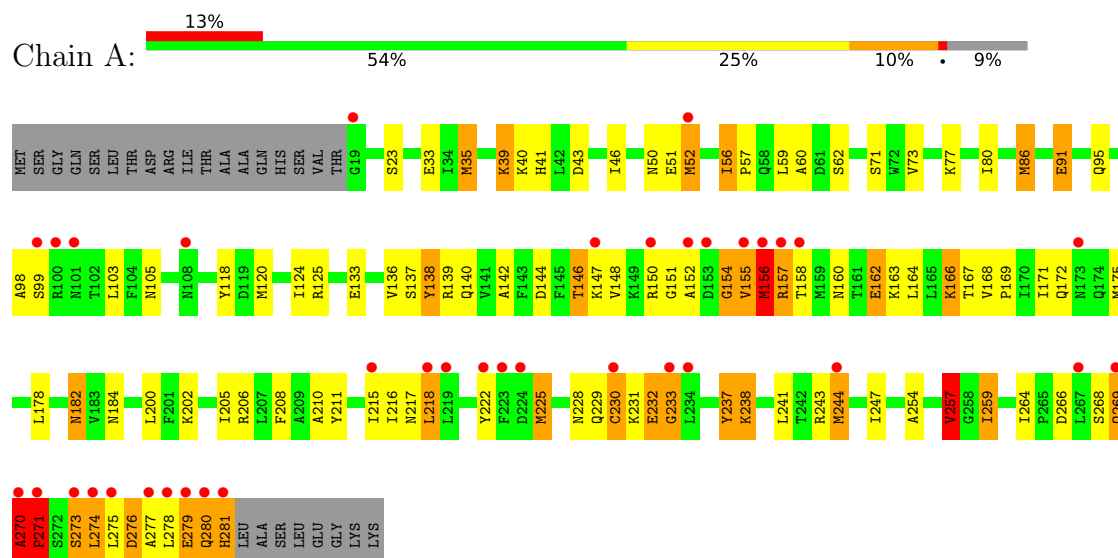
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		

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: CLATHRIN ASSEMBLY PROTEIN SHORT FORM



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.72Å 77.72Å 122.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.94 – 2.00 65.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (65.94-2.00) 99.9 (65.59-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.197 , 0.230 0.209 , 0.238	Depositor DCC
R_{free} test set	1322 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2266	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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: PIO

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	2.02	37/2150 (1.7%)	1.63	28/2896 (1.0%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	MET	SD-CE	-28.91	1.07	1.79
1	A	56	ILE	CA-CB	-15.89	1.43	1.53
1	A	52	MET	SD-CE	15.56	2.18	1.79
1	A	156	MET	SD-CE	-11.71	1.50	1.79
1	A	35	MET	SD-CE	-11.04	1.51	1.79
1	A	120	MET	SD-CE	-9.93	1.54	1.79
1	A	175	MET	SD-CE	-9.61	1.55	1.79
1	A	264	ILE	CA-CB	-8.25	1.43	1.54
1	A	146	THR	CA-CB	8.18	1.67	1.53
1	A	171	ILE	CA-CB	-8.03	1.44	1.54
1	A	225	MET	SD-CE	-7.86	1.59	1.79
1	A	184	ASN	CA-C	-7.51	1.43	1.52
1	A	80	ILE	CA-C	7.29	1.61	1.52
1	A	257	VAL	C-O	-7.04	1.14	1.24
1	A	244	MET	SD-CE	-6.93	1.62	1.79
1	A	91	GLU	C-O	-6.71	1.15	1.24
1	A	175	MET	CA-C	-6.41	1.44	1.52
1	A	211	TYR	CA-C	6.37	1.61	1.52
1	A	46	ILE	CA-C	6.35	1.60	1.52
1	A	200	LEU	N-CA	-6.33	1.38	1.46
1	A	172	GLN	CA-C	-5.78	1.45	1.52
1	A	71	SER	CA-CB	-5.71	1.45	1.53
1	A	39	LYS	CA-C	5.68	1.60	1.52
1	A	52	MET	C-O	-5.62	1.16	1.24
1	A	215	ILE	CA-CB	-5.61	1.47	1.54
1	A	124	ILE	CA-CB	-5.57	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	ASP	C-O	-5.45	1.17	1.24
1	A	259	ILE	N-CA	5.42	1.52	1.46
1	A	59	LEU	C-O	-5.39	1.18	1.24
1	A	138	TYR	C-O	-5.33	1.17	1.24
1	A	95	GLN	N-CA	5.21	1.52	1.46
1	A	184	ASN	C-O	-5.21	1.17	1.23
1	A	210	ALA	CA-CB	-5.14	1.44	1.53
1	A	125	ARG	C-O	5.13	1.30	1.24
1	A	206	ARG	CG-CD	-5.09	1.37	1.52
1	A	50	ASN	C-O	-5.05	1.17	1.24
1	A	125	ARG	CA-CB	5.03	1.61	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	GLU	N-CA-C	-8.21	101.92	111.03
1	A	268	SER	N-CA-C	-8.06	92.84	107.60
1	A	103	LEU	N-CA-CB	-7.85	104.28	111.59
1	A	178	LEU	N-CA-C	-7.81	102.71	111.07
1	A	142	ALA	N-CA-C	7.20	121.64	112.86
1	A	140	GLN	N-CA-C	6.76	118.65	111.28
1	A	277	ALA	N-CA-C	-6.74	105.17	113.19
1	A	206	ARG	CA-CB-CG	-6.73	100.64	114.10
1	A	157	ARG	N-CA-C	6.70	118.38	111.14
1	A	276	ASP	N-CA-C	-6.22	104.06	113.89
1	A	279	GLU	N-CA-C	-6.22	105.79	113.19
1	A	270	ALA	N-CA-C	6.13	123.35	109.81
1	A	86	MET	CG-SD-CE	-6.12	87.44	100.90
1	A	237	TYR	N-CA-C	-6.07	104.73	111.71
1	A	271	PRO	CB-CA-C	-6.03	101.62	111.56
1	A	118	TYR	CB-CA-C	-5.68	101.36	110.79
1	A	148	VAL	N-CA-C	5.60	116.16	110.05
1	A	182	ASN	CB-CA-C	-5.52	104.06	111.89
1	A	238	LYS	N-CA-C	-5.49	105.20	111.07
1	A	280	GLN	N-CA-CB	5.45	117.32	110.45
1	A	182	ASN	N-CA-C	5.37	118.80	111.39
1	A	205	ILE	N-CA-C	5.22	115.99	110.72
1	A	60	ALA	N-CA-C	5.20	117.62	111.33
1	A	154	GLY	N-CA-C	5.18	125.46	113.18
1	A	167	THR	N-CA-C	5.11	116.66	111.14
1	A	133	GLU	N-CA-CB	-5.10	102.37	110.28
1	A	152	ALA	N-CA-C	-5.09	108.33	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	GLU	CA-CB-CG	-5.04	104.03	114.10

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	2114	0	2137	88	0
2	A	24	0	9	1	0
3	A	128	0	0	7	1
All	All	2266	0	2146	88	1

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 21.

All (88) 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:86:MET:CE	1:A:86:MET:CG	2.08	1.32
1:A:52:MET:CE	1:A:52:MET:SD	2.18	1.31
1:A:86:MET:CE	1:A:86:MET:SD	1.07	1.17
1:A:208:PHE:HE1	1:A:244:MET:HE1	1.06	1.10
1:A:208:PHE:CE1	1:A:244:MET:HE1	1.88	1.08
1:A:86:MET:SD	1:A:86:MET:HE1	1.67	1.04
1:A:86:MET:SD	1:A:86:MET:HE2	1.67	1.04
1:A:86:MET:SD	1:A:86:MET:HE3	1.67	1.03
1:A:39:LYS:NZ	1:A:43:ASP:OD2	2.07	0.88
1:A:144:ASP:OD1	1:A:146:THR:OG1	1.97	0.82
1:A:164:LEU:HD22	1:A:217:ASN:ND2	1.93	0.81
1:A:208:PHE:CE1	1:A:244:MET:CE	2.67	0.77
1:A:244:MET:HE3	1:A:244:MET:HA	1.66	0.76
1:A:270:ALA:N	1:A:271:PRO:HD3	2.02	0.74
1:A:243:ARG:O	1:A:247:ILE:HG13	1.89	0.73
1:A:225:MET:HE2	1:A:230:CYS:HA	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HG	1:A:274:LEU:O	1.89	0.72
1:A:86:MET:HE3	1:A:86:MET:CB	2.21	0.70
1:A:91:GLU:OE2	1:A:138:TYR:OH	2.08	0.69
1:A:237:TYR:CE1	1:A:241:LEU:HD11	2.27	0.69
1:A:225:MET:CE	1:A:230:CYS:HA	2.23	0.69
1:A:269:GLN:HE21	1:A:269:GLN:HA	1.59	0.66
1:A:155:VAL:O	1:A:156:MET:C	2.34	0.66
1:A:269:GLN:HE21	1:A:269:GLN:CA	2.07	0.66
1:A:229:GLN:O	1:A:231:LYS:N	2.28	0.66
1:A:279:GLU:O	1:A:279:GLU:HG2	1.98	0.63
1:A:160:ASN:OD1	1:A:162:GLU:N	2.31	0.63
1:A:257:VAL:CG1	1:A:257:VAL:O	2.45	0.63
1:A:40:LYS:NZ	2:A:300:PIO:O53	2.23	0.62
1:A:86:MET:CG	1:A:86:MET:HE2	2.05	0.62
1:A:86:MET:HE2	1:A:86:MET:HG3	1.80	0.62
1:A:86:MET:HE3	1:A:86:MET:HB2	1.82	0.62
1:A:229:GLN:C	1:A:231:LYS:H	2.07	0.62
1:A:147:LYS:HE3	3:A:2079:HOH:O	1.99	0.61
1:A:269:GLN:O	1:A:269:GLN:HG3	2.01	0.61
1:A:86:MET:CG	1:A:86:MET:HE3	2.05	0.60
1:A:105:ASN:ND2	1:A:105:ASN:C	2.59	0.60
1:A:168:VAL:N	1:A:169:PRO:CD	2.64	0.59
1:A:105:ASN:ND2	1:A:105:ASN:O	2.34	0.58
1:A:163:LYS:O	1:A:166:LYS:HB2	2.03	0.58
1:A:105:ASN:C	1:A:105:ASN:HD22	2.11	0.57
1:A:151:GLY:O	1:A:157:ARG:HD2	2.04	0.57
1:A:276:ASP:C	1:A:278:LEU:H	2.12	0.57
1:A:273:SER:O	1:A:275:LEU:N	2.38	0.56
1:A:99:SER:HB2	3:A:2045:HOH:O	2.05	0.55
1:A:40:LYS:HE3	1:A:41:HIS:CE1	2.42	0.54
1:A:147:LYS:CE	3:A:2079:HOH:O	2.55	0.54
1:A:225:MET:HE3	1:A:230:CYS:N	2.22	0.54
1:A:86:MET:CE	1:A:86:MET:HG3	2.24	0.54
1:A:154:GLY:O	1:A:157:ARG:N	2.38	0.54
1:A:273:SER:C	1:A:275:LEU:H	2.16	0.54
1:A:229:GLN:C	1:A:231:LYS:N	2.65	0.53
1:A:278:LEU:C	1:A:280:GLN:N	2.64	0.52
1:A:279:GLU:C	1:A:281:HIS:H	2.17	0.52
1:A:164:LEU:CD2	1:A:217:ASN:ND2	2.69	0.50
1:A:244:MET:CE	1:A:244:MET:HA	2.40	0.50
1:A:274:LEU:O	1:A:274:LEU:CG	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:MET:HE3	1:A:229:GLN:C	2.37	0.49
1:A:276:ASP:C	1:A:278:LEU:N	2.68	0.49
1:A:162:GLU:HG2	1:A:163:LYS:N	2.27	0.48
1:A:222:TYR:HE1	1:A:276:ASP:HB2	1.78	0.48
1:A:225:MET:HG2	1:A:230:CYS:SG	2.53	0.48
1:A:237:TYR:HE1	1:A:241:LEU:HD11	1.77	0.48
1:A:56:ILE:HB	1:A:57:PRO:HD3	1.96	0.48
1:A:228:ASN:O	1:A:231:LYS:HB3	2.14	0.47
1:A:275:LEU:HG	3:A:2125:HOH:O	2.13	0.47
1:A:278:LEU:C	1:A:280:GLN:H	2.22	0.47
1:A:160:ASN:OD1	1:A:160:ASN:C	2.57	0.47
1:A:158:THR:O	1:A:158:THR:HG22	2.14	0.47
1:A:160:ASN:ND2	3:A:2087:HOH:O	2.47	0.46
1:A:73:VAL:HG12	1:A:77:LYS:HD2	1.98	0.46
1:A:222:TYR:CE1	1:A:276:ASP:HB2	2.50	0.45
1:A:51:GLU:HB3	3:A:2016:HOH:O	2.16	0.45
1:A:154:GLY:O	1:A:155:VAL:C	2.58	0.45
1:A:257:VAL:O	1:A:257:VAL:HG13	2.16	0.45
1:A:98:ALA:O	1:A:139:ARG:NH1	2.49	0.45
1:A:273:SER:C	1:A:275:LEU:N	2.74	0.45
1:A:232:GLU:O	1:A:233:GLY:C	2.59	0.44
1:A:269:GLN:C	1:A:271:PRO:HD3	2.43	0.43
1:A:225:MET:HB2	1:A:229:GLN:OE1	2.19	0.43
1:A:237:TYR:O	1:A:238:LYS:C	2.62	0.43
1:A:254:ALA:HB1	1:A:259:ILE:HD12	2.01	0.43
1:A:33:GLU:HG2	1:A:35:MET:HG2	2.02	0.41
1:A:144:ASP:CG	1:A:146:THR:OG1	2.63	0.40
1:A:150:ARG:NH2	3:A:2085:HOH:O	2.54	0.40
1:A:86:MET:CE	1:A:86:MET:CB	2.81	0.40
1:A:164:LEU:HG	1:A:218:LEU:CD1	2.52	0.40
1:A:270:ALA:N	1:A:271:PRO:CD	2.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2044:HOH:O	3:A:2044:HOH:O[7_556]	2.03	0.17

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	261/289 (90%)	241 (92%)	13 (5%)	7 (3%)	4 1

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	A	270	ALA
1	A	230	CYS
1	A	273	SER
1	A	274	LEU
1	A	233	GLY
1	A	271	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	235/256 (92%)	221 (94%)	14 (6%)	17 14

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	62	SER
1	A	136	VAL
1	A	137	SER

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Mol	Chain	Res	Type
1	A	156	MET
1	A	162	GLU
1	A	166	LYS
1	A	182	ASN
1	A	202	LYS
1	A	216	ILE
1	A	218	LEU
1	A	257	VAL
1	A	269	GLN
1	A	281	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	95	GLN
1	A	101	ASN
1	A	116	GLN
1	A	212	ASN
1	A	269	GLN

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](#)

1 ligand is 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
2	PIO	A	300	-	24,24,47	2.09	7 (29%)	39,39,65	1.52	7 (17%)

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
2	PIO	A	300	-	-	0/15/39/68	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	PIO	P1-O1	4.19	1.66	1.59
2	A	300	PIO	P1-O12	4.18	1.63	1.50
2	A	300	PIO	P4-O42	4.09	1.63	1.50
2	A	300	PIO	P5-O53	3.58	1.61	1.50
2	A	300	PIO	P4-O4	2.57	1.64	1.59
2	A	300	PIO	P1-O13	2.38	1.63	1.54
2	A	300	PIO	P1-O11	2.33	1.63	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	PIO	C5-C6-C1	3.81	116.83	109.11
2	A	300	PIO	O43-P4-O41	3.25	119.99	107.80
2	A	300	PIO	C2-C3-C4	3.05	116.61	109.68
2	A	300	PIO	O1-C1-C6	2.76	114.58	108.73
2	A	300	PIO	O5-C5-C4	2.56	114.20	108.76
2	A	300	PIO	O3-C3-C2	-2.53	104.41	110.38
2	A	300	PIO	O11-P1-O12	2.24	119.55	110.83

There are no chirality outliers.

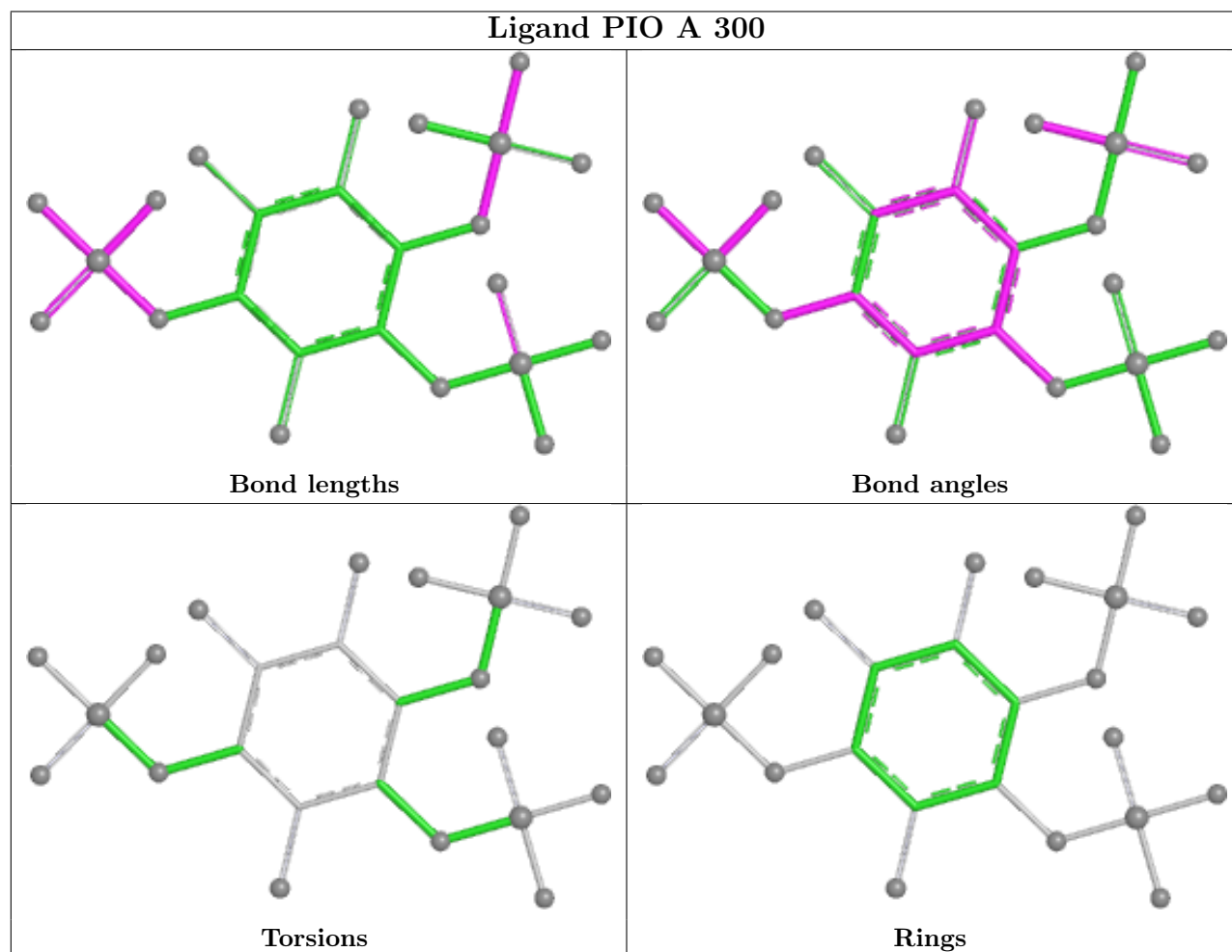
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	PIO	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 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	263/289 (91%)	0.67	37 (14%) 6 5	24, 41, 85, 124	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	TYR	6.5
1	A	275	LEU	5.3
1	A	277	ALA	5.2
1	A	281	HIS	4.6
1	A	150	ARG	4.5
1	A	278	LEU	4.5
1	A	218	LEU	4.4
1	A	279	GLU	4.0
1	A	52	MET	3.7
1	A	270	ALA	3.7
1	A	230	CYS	3.6
1	A	99	SER	3.6
1	A	219	LEU	3.5
1	A	19	GLY	3.4
1	A	153	ASP	3.3
1	A	224	ASP	3.3
1	A	234	LEU	3.3
1	A	274	LEU	3.2
1	A	267	LEU	3.0
1	A	152	ALA	2.8
1	A	158	THR	2.8
1	A	100	ARG	2.7
1	A	147	LYS	2.7
1	A	280	GLN	2.6
1	A	156	MET	2.5
1	A	215	ILE	2.4
1	A	157	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	244	MET	2.3
1	A	155	VAL	2.3
1	A	101	ASN	2.3
1	A	269	GLN	2.2
1	A	271	PRO	2.2
1	A	233	GLY	2.2
1	A	173	ASN	2.2
1	A	108	ASN	2.1
1	A	223	PHE	2.1
1	A	273	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

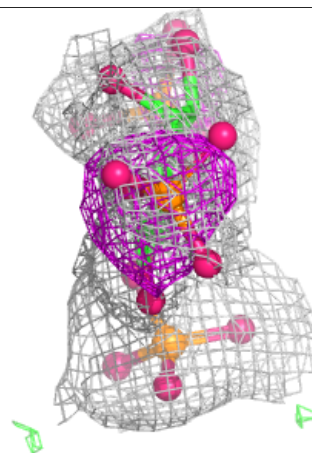
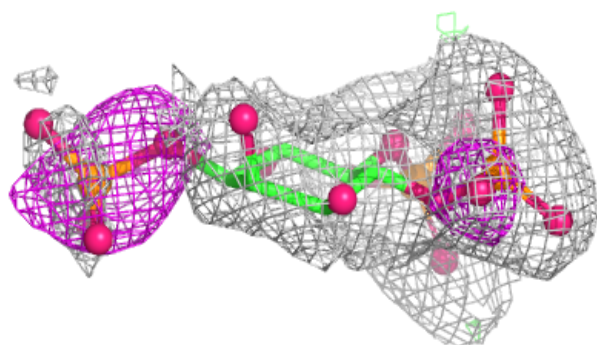
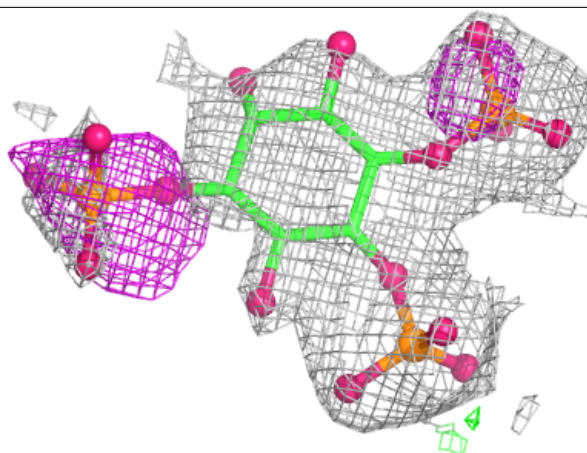
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PIO	A	300	24/47	0.77	0.11	64,84,103,105	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 PIO A 300:

$2mF_o-DF_c$ (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.