



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:02 PM EDT

PDB ID : 3ARX / pdb_00003arx
Title : Crystal Structure Analysis of Chitinase A from *Vibrio harveyi* with novel inhibitors - complex structure with Propentofylline
Authors : Pantoom, S.; Vetter, I.R.; Prinz, H.; Suginta, W.
Deposited on : 2010-12-09
Resolution : 1.16 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

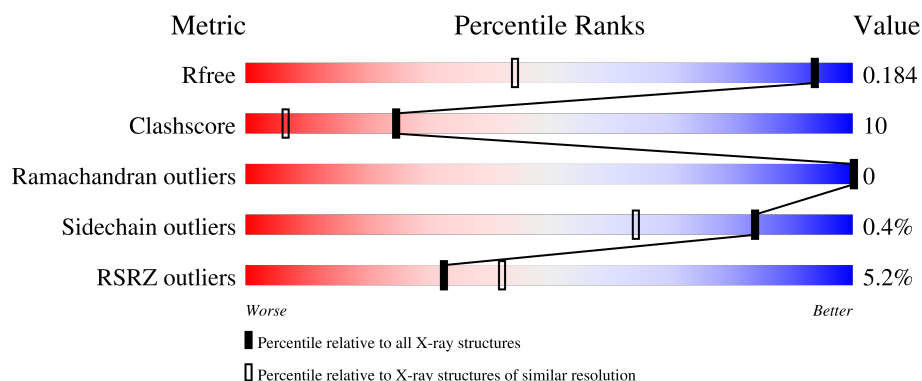
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.16 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	1256 (1.18-1.14)
Clashscore	190562	1272 (1.18-1.14)
Ramachandran outliers	187476	1246 (1.18-1.14)
Sidechain outliers	187428	1246 (1.18-1.14)
RSRZ outliers	180081	1255 (1.18-1.14)

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	584	5% 74% 23% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	POY	A	607[A]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	POY	A	607[B]	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5759 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.

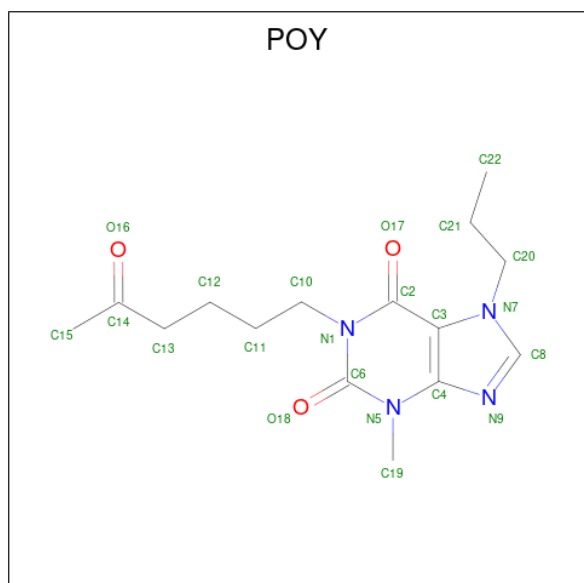
- Molecule 1 is a protein called Chitinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	575	4588	2931	728	900	29	0	34	0

There are 8 discrepancies between the modelled and reference sequences:

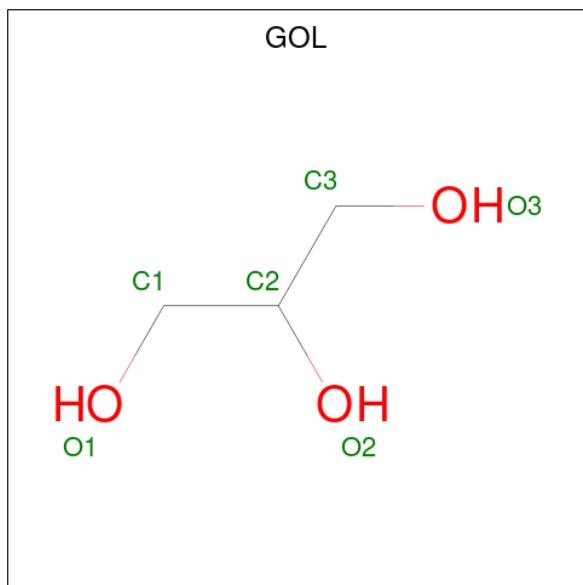
Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ARG	-	expression tag	UNP Q9AMP1
A	599	SER	-	expression tag	UNP Q9AMP1
A	600	HIS	-	expression tag	UNP Q9AMP1
A	601	HIS	-	expression tag	UNP Q9AMP1
A	602	HIS	-	expression tag	UNP Q9AMP1
A	603	HIS	-	expression tag	UNP Q9AMP1
A	604	HIS	-	expression tag	UNP Q9AMP1
A	605	HIS	-	expression tag	UNP Q9AMP1

- Molecule 2 is 3-methyl-1-(5-oxohexyl)-7-propyl-3,7-dihydro-1H-purine-2,6-dione (CCD ID: POY) (formula: C₁₅H₂₂N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	15	4	3		
2	A	1	Total	C	N	O	0	1
			44	30	8	6		

- 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		

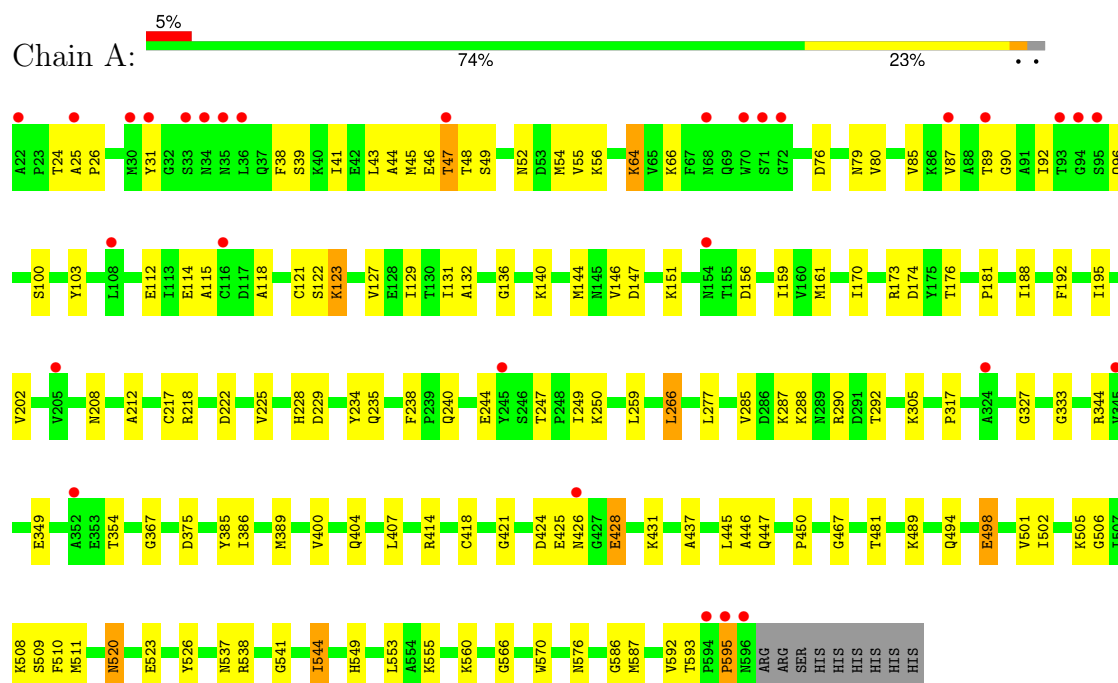
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1099	Total	O	0	0
			1099	1099		

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: Chitinase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.11Å 50.93Å 93.17Å 90.00° 99.45° 90.00°	Depositor
Resolution (Å)	40.66 – 1.16 40.66 – 1.16	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.66-1.16) 98.4 (40.66-1.16)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.16Å)	Xtriage
Refinement program	REFMAC 5.6.0093	Depositor
R, R_{free}	0.161 , 0.185 0.160 , 0.184	Depositor DCC
R_{free} test set	10234 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.4	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	0.98	EDS
Total number of atoms	5759	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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: GOL, POY

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	1.98	100/4796 (2.1%)	1.45	21/6525 (0.3%)

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	ASP	C-O	-8.29	1.14	1.23
1	A	44	ALA	CA-C	-7.57	1.43	1.52
1	A	494	GLN	CA-CB	-7.32	1.41	1.53
1	A	96	GLN	CA-C	-7.29	1.43	1.52
1	A	181	PRO	CA-C	-7.14	1.46	1.52
1	A	129	ILE	CA-CB	6.93	1.63	1.54
1	A	24	THR	CA-C	6.87	1.61	1.52
1	A	509	SER	CA-C	-6.80	1.43	1.52
1	A	385	TYR	CA-C	-6.75	1.44	1.52
1	A	447	GLN	CA-CB	-6.75	1.42	1.53
1	A	118	ALA	CA-C	-6.69	1.43	1.52
1	A	195	ILE	CA-CB	-6.69	1.46	1.54
1	A	317	PRO	CA-C	-6.69	1.44	1.52
1	A	45	MET	CA-C	6.57	1.61	1.52
1	A	121	CYS	CA-C	-6.54	1.44	1.52
1	A	92	ILE	N-CA	-6.53	1.38	1.46
1	A	76	ASP	N-CA	-6.41	1.38	1.46
1	A	287	LYS	N-CA	-6.36	1.38	1.46
1	A	131	ILE	CA-CB	-6.31	1.45	1.53
1	A	64	LYS	CA-C	-6.31	1.45	1.52
1	A	136	GLY	CA-C	6.29	1.60	1.51
1	A	421	GLY	C-O	6.29	1.31	1.23
1	A	39	SER	C-O	6.18	1.31	1.23
1	A	509	SER	C-O	6.17	1.32	1.24
1	A	501	VAL	N-CA	6.11	1.53	1.46
1	A	266	LEU	C-O	6.09	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	TYR	CA-C	6.07	1.61	1.52
1	A	238	PHE	C-O	-5.99	1.16	1.24
1	A	123	LYS	CB-CG	-5.96	1.34	1.52
1	A	112	GLU	CA-C	-5.94	1.45	1.52
1	A	202	VAL	CA-CB	5.86	1.63	1.54
1	A	240	GLN	CA-C	-5.86	1.44	1.52
1	A	333	GLY	C-N	5.82	1.41	1.33
1	A	52	ASN	C-N	-5.81	1.25	1.33
1	A	238	PHE	CA-C	5.79	1.59	1.52
1	A	526	TYR	C-O	5.78	1.30	1.23
1	A	247	THR	CA-C	5.75	1.59	1.53
1	A	537	ASN	N-CA	5.75	1.53	1.46
1	A	45	MET	C-O	5.74	1.31	1.23
1	A	147	ASP	CA-C	-5.74	1.46	1.53
1	A	354	THR	CA-CB	5.65	1.61	1.54
1	A	502	ILE	C-O	5.63	1.29	1.24
1	A	176	THR	C-N	-5.60	1.26	1.33
1	A	66	LYS	C-O	-5.59	1.17	1.23
1	A	520	ASN	CA-C	-5.55	1.45	1.53
1	A	523	GLU	CB-CG	-5.55	1.35	1.52
1	A	526	TYR	CA-C	-5.54	1.45	1.52
1	A	100	SER	N-CA	5.53	1.52	1.46
1	A	259	LEU	C-O	5.51	1.30	1.24
1	A	400	VAL	C-O	5.51	1.31	1.24
1	A	510	PHE	CA-C	-5.50	1.45	1.52
1	A	481	THR	C-O	5.49	1.31	1.24
1	A	445	LEU	C-O	5.48	1.30	1.24
1	A	146	VAL	C-O	5.47	1.30	1.24
1	A	118	ALA	C-O	5.47	1.31	1.24
1	A	505	LYS	C-O	5.47	1.30	1.24
1	A	555	LYS	CA-C	-5.47	1.45	1.52
1	A	375	ASP	C-N	5.46	1.41	1.34
1	A	489	LYS	C-N	-5.46	1.27	1.33
1	A	250	LYS	CA-C	5.45	1.60	1.52
1	A	170	ILE	CA-CB	-5.44	1.48	1.54
1	A	595	PRO	C-O	5.43	1.30	1.23
1	A	450	PRO	C-O	5.42	1.29	1.23
1	A	43	LEU	N-CA	5.41	1.52	1.46
1	A	292	THR	CA-C	5.39	1.59	1.52
1	A	234	TYR	N-CA	5.38	1.52	1.46
1	A	509	SER	CB-OG	-5.37	1.31	1.42
1	A	400	VAL	CA-C	5.37	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	ALA	N-CA	5.33	1.53	1.46
1	A	48	THR	C-O	5.30	1.29	1.24
1	A	327	GLY	CA-C	-5.29	1.48	1.52
1	A	344	ARG	CZ-NH2	5.28	1.40	1.33
1	A	26	PRO	C-O	-5.23	1.17	1.23
1	A	498	GLU	C-O	5.23	1.30	1.23
1	A	112	GLU	N-CA	5.22	1.52	1.46
1	A	47	THR	C-O	5.20	1.30	1.23
1	A	349	GLU	C-O	5.19	1.30	1.24
1	A	41	ILE	CA-C	-5.17	1.46	1.52
1	A	54	MET	C-N	-5.17	1.27	1.33
1	A	249	ILE	N-CA	5.16	1.52	1.46
1	A	80	VAL	CA-CB	5.15	1.61	1.54
1	A	222	ASP	C-O	-5.14	1.17	1.23
1	A	144	MET	C-O	5.12	1.29	1.23
1	A	217	CYS	N-CA	-5.12	1.39	1.46
1	A	386	ILE	C-O	5.10	1.29	1.24
1	A	418	CYS	CA-C	-5.10	1.46	1.52
1	A	156	ASP	CG-OD1	5.08	1.35	1.25
1	A	560	LYS	C-N	-5.07	1.27	1.33
1	A	541	GLY	N-CA	5.07	1.52	1.45
1	A	127	VAL	CA-CB	-5.05	1.47	1.55
1	A	122	SER	CA-C	5.05	1.58	1.52
1	A	467	GLY	N-CA	5.05	1.52	1.45
1	A	235	GLN	C-O	5.05	1.30	1.23
1	A	506	GLY	CA-C	-5.04	1.46	1.52
1	A	85	VAL	N-CA	-5.03	1.40	1.46
1	A	544	ILE	N-CA	5.03	1.52	1.46
1	A	173	ARG	CD-NE	5.02	1.53	1.46
1	A	225	VAL	C-O	5.02	1.30	1.24
1	A	49[A]	SER	C-N	-5.01	1.27	1.33
1	A	49[B]	SER	C-N	-5.01	1.27	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	MET	N-CA-C	13.57	130.58	113.88
1	A	45	MET	CA-C-O	7.69	127.93	119.24
1	A	538	ARG	NE-CZ-NH1	-7.01	114.49	121.50
1	A	31	TYR	N-CA-C	-6.05	104.60	112.23
1	A	159[A]	ILE	CA-CB-CG2	-5.94	100.40	110.50
1	A	159[B]	ILE	CA-CB-CG2	-5.94	100.40	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	508	LYS	CG-CD-CE	-5.93	97.67	111.30
1	A	290	ARG	NE-CZ-NH2	-5.88	113.91	119.20
1	A	132	ALA	CA-C-O	5.87	127.74	121.05
1	A	218	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	A	446	ALA	CA-C-O	-5.63	113.50	119.97
1	A	114	GLU	N-CA-CB	-5.55	101.59	111.08
1	A	404	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	A	38	PHE	CA-C-O	-5.48	114.91	121.11
1	A	38	PHE	CA-CB-CG	-5.44	108.36	113.80
1	A	55	VAL	CA-C-O	5.29	125.61	120.27
1	A	249	ILE	N-CA-C	-5.17	100.67	108.12
1	A	115	ALA	O-C-N	5.09	129.36	123.30
1	A	576	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	238	PHE	O-C-N	5.04	125.92	121.19
1	A	566	GLY	CA-C-O	5.01	124.37	120.91

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	4588	0	4406	73	2
2	A	66	0	66	26	0
3	A	6	0	8	1	0
4	A	1099	0	0	35	7
All	All	5759	0	4480	90	7

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 10.

All (90) 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:305:LYS:HD2	4:A:904:HOH:O	1.28	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:607[A]:POY:H15	4:A:1276:HOH:O	1.27	1.26
2:A:607[A]:POY:H10	4:A:949:HOH:O	1.43	1.19
1:A:151:LYS:HE2	4:A:1236:HOH:O	1.41	1.19
1:A:498:GLU:OE1	2:A:607[B]:POY:H15B	1.44	1.15
1:A:229:ASP:HA	2:A:607[A]:POY:H15B	1.33	1.08
2:A:607[B]:POY:H20	2:A:607[B]:POY:O17	1.53	1.05
2:A:607[A]:POY:H8	2:A:607[A]:POY:H22A	1.39	1.04
1:A:511[B]:MET:SD	1:A:544:ILE:CD1	2.48	1.01
1:A:511[B]:MET:SD	1:A:544:ILE:HD12	2.02	1.00
2:A:607[A]:POY:C15	4:A:1276:HOH:O	1.89	1.00
1:A:511[B]:MET:HE1	1:A:544:ILE:HD11	1.44	0.99
2:A:607[A]:POY:O16	4:A:1595:HOH:O	1.82	0.97
1:A:87[A]:VAL:HG21	1:A:103:TYR:CE1	2.02	0.93
2:A:606:POY:O16	4:A:1235:HOH:O	1.87	0.93
1:A:511[B]:MET:HE1	1:A:544:ILE:CD1	2.04	0.87
1:A:151:LYS:HE3	4:A:1133:HOH:O	1.74	0.86
1:A:87[A]:VAL:CG2	1:A:103:TYR:CE1	2.59	0.85
1:A:212:ALA:HB1	2:A:607[A]:POY:H15A	1.57	0.85
1:A:192[A]:PHE:HZ	1:A:570[A]:TRP:CZ3	1.95	0.84
1:A:511[B]:MET:CE	1:A:544:ILE:CD1	2.57	0.82
1:A:87[A]:VAL:CG2	1:A:103:TYR:HE1	1.94	0.81
1:A:174:ASP:OD1	4:A:1230:HOH:O	1.98	0.79
1:A:244[A]:GLU:OE2	4:A:730:HOH:O	1.99	0.79
1:A:277:LEU:CD1	2:A:607[B]:POY:H22	2.12	0.79
1:A:79:ASN:OD1	1:A:89[B]:THR:HG22	1.83	0.78
1:A:277:LEU:HD12	2:A:607[B]:POY:H22	1.65	0.78
1:A:192[A]:PHE:HZ	1:A:570[A]:TRP:HZ3	1.31	0.76
1:A:511[B]:MET:CE	1:A:544:ILE:HD11	2.14	0.76
2:A:607[A]:POY:O18	2:A:607[A]:POY:C11	2.34	0.76
1:A:192[A]:PHE:CZ	1:A:570[A]:TRP:CZ3	2.74	0.75
2:A:607[B]:POY:O17	2:A:607[B]:POY:C20	2.32	0.75
1:A:389[B]:MET:HE3	4:A:1218:HOH:O	1.87	0.74
1:A:229:ASP:HB2	2:A:607[A]:POY:H13A	1.70	0.72
1:A:192[A]:PHE:HE2	1:A:570[A]:TRP:HH2	1.38	0.72
2:A:606:POY:C14	4:A:1235:HOH:O	2.37	0.71
1:A:192[A]:PHE:CZ	1:A:570[A]:TRP:HZ3	2.08	0.71
1:A:123:LYS:HD3	4:A:1084:HOH:O	1.89	0.70
1:A:511[B]:MET:SD	1:A:544:ILE:HD13	2.32	0.68
2:A:607[A]:POY:H22A	2:A:607[A]:POY:C8	2.22	0.65
1:A:123:LYS:CD	4:A:1084:HOH:O	2.46	0.62
2:A:607[A]:POY:O18	2:A:607[A]:POY:H11	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASP:OD1	1:A:428[A]:GLU:HG3	2.01	0.61
1:A:414:ARG:HD2	4:A:895:HOH:O	2.02	0.60
1:A:192[A]:PHE:CE2	1:A:570[A]:TRP:HH2	2.17	0.60
1:A:595:PRO:HA	4:A:1668:HOH:O	2.00	0.60
1:A:431:LYS:HE3	4:A:823:HOH:O	2.02	0.59
1:A:592[B]:VAL:HG12	1:A:593:THR:N	2.16	0.59
1:A:192[A]:PHE:CE2	1:A:570[A]:TRP:CH2	2.89	0.59
1:A:161:MET:CE	1:A:587[A]:MET:HG3	2.33	0.58
1:A:288:LYS:HB3	4:A:767:HOH:O	2.04	0.56
1:A:151:LYS:CE	4:A:1133:HOH:O	2.44	0.55
1:A:87[A]:VAL:HG23	1:A:103:TYR:HE1	1.71	0.54
1:A:229:ASP:CA	2:A:607[A]:POY:H15B	2.22	0.53
1:A:208[A]:ASN:OD1	4:A:1126:HOH:O	2.19	0.52
1:A:89[B]:THR:HG21	4:A:892:HOH:O	2.09	0.52
1:A:367:GLY:HA3	2:A:606:POY:H15	1.92	0.52
1:A:140:LYS:HD3	4:A:718:HOH:O	2.09	0.52
1:A:285:VAL:HG13	4:A:1575:HOH:O	2.10	0.50
1:A:288:LYS:HE3	4:A:639:HOH:O	2.10	0.50
1:A:89[A]:THR:HG22	1:A:90:GLY:N	2.26	0.50
1:A:47:THR:HG23	4:A:1104:HOH:O	2.12	0.49
2:A:607[A]:POY:H15A	4:A:1276:HOH:O	1.85	0.48
1:A:431:LYS:HE2	4:A:661:HOH:O	2.14	0.48
1:A:47:THR:CG2	4:A:1104:HOH:O	2.61	0.47
1:A:288:LYS:HD2	4:A:1088:HOH:O	2.14	0.47
2:A:607[A]:POY:O18	2:A:607[A]:POY:H11A	2.13	0.47
1:A:87[B]:VAL:HG13	4:A:1554:HOH:O	2.14	0.47
1:A:277:LEU:HD11	2:A:607[B]:POY:H22	1.91	0.46
1:A:549:HIS:CE1	1:A:553:LEU:HD11	2.50	0.46
1:A:592[B]:VAL:CG1	1:A:593:THR:N	2.79	0.45
1:A:586:GLY:HA3	4:A:1462:HOH:O	2.16	0.45
1:A:192[A]:PHE:CZ	1:A:570[A]:TRP:CH2	3.04	0.44
1:A:424:ASP:OD2	1:A:428[A]:GLU:CD	2.61	0.44
1:A:228[A]:HIS:CE1	2:A:607[A]:POY:O18	2.71	0.44
1:A:425:GLU:CD	1:A:425:GLU:H	2.26	0.43
1:A:188:ILE:HD12	1:A:266:LEU:HD21	2.00	0.43
1:A:87[A]:VAL:CG2	1:A:103:TYR:CD1	3.00	0.43
3:A:3500:GOL:H11	4:A:696:HOH:O	2.19	0.43
2:A:607[A]:POY:H8	2:A:607[A]:POY:C22	2.22	0.42
1:A:407[A]:LEU:HA	1:A:437:ALA:HB3	2.02	0.42
2:A:607[A]:POY:C8	2:A:607[A]:POY:C22	2.88	0.41
1:A:305:LYS:HE3	4:A:10:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:MET:HE1	1:A:587[A]:MET:HG3	2.03	0.41
1:A:426:ASN:HB2	1:A:428[A]:GLU:HG3	2.03	0.40
1:A:56:LYS:HD2	4:A:989:HOH:O	2.20	0.40
1:A:79:ASN:OD1	1:A:89[B]:THR:CG2	2.64	0.40
1:A:46:GLU:N	4:A:732:HOH:O	1.63	0.40

All (7) 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)
4:A:1073:HOH:O	4:A:1196:HOH:O[1_565]	1.63	0.57
4:A:1196:HOH:O	4:A:1234:HOH:O[1_545]	1.70	0.50
4:A:1191:HOH:O	4:A:1227:HOH:O[2_545]	1.78	0.42
4:A:963:HOH:O	4:A:1226:HOH:O[2_545]	1.83	0.37
1:A:520:ASN:ND2	4:A:1147:HOH:O[1_565]	1.94	0.26
1:A:244[A]:GLU:OE2	4:A:779:HOH:O[2_556]	2.08	0.12
4:A:1225:HOH:O	4:A:1516:HOH:O[2_556]	2.15	0.05

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	607/584 (104%)	588 (97%)	19 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	494/469 (105%)	491 (99%)	3 (1%)	78	53

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	A	428[A]	GLU
1	A	428[B]	GLU

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	52	ASN
1	A	145	ASN
1	A	221	ASN
1	A	447	GLN
1	A	515	ASN
1	A	529	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	3500	-	5,5,5	0.85	0	5,5,5	0.71	0
2	POY	A	606	-	23,23,23	1.94	8 (34%)	32,32,32	2.17	11 (34%)
2	POY	A	607[A]	-	23,23,23	1.17	3 (13%)	32,32,32	3.18	16 (50%)
2	POY	A	607[B]	-	23,23,23	1.79	4 (17%)	32,32,32	5.09	19 (59%)

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	3500	-	-	0/4/4/4	-
2	POY	A	606	-	-	3/10/10/10	0/2/2/2
2	POY	A	607[A]	-	-	6/10/10/10	0/2/2/2
2	POY	A	607[B]	-	-	6/10/10/10	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	607[B]	POY	C3-N7	-5.45	1.28	1.39
2	A	606	POY	C8-N7	4.12	1.43	1.36
2	A	606	POY	C3-N7	-3.23	1.32	1.39
2	A	607[B]	POY	C15-C14	3.16	1.61	1.49
2	A	607[B]	POY	C2-N1	-3.12	1.34	1.40
2	A	606	POY	C15-C14	-3.03	1.39	1.49
2	A	607[A]	POY	C2-N1	2.74	1.45	1.40
2	A	607[B]	POY	C13-C14	2.73	1.58	1.50
2	A	606	POY	C10-N1	2.63	1.53	1.47
2	A	606	POY	C19-N5	2.62	1.51	1.47
2	A	606	POY	C6-N1	2.51	1.43	1.38
2	A	606	POY	C2-N1	-2.37	1.36	1.40
2	A	607[A]	POY	C10-N1	2.37	1.52	1.47
2	A	606	POY	O16-C14	2.19	1.29	1.21
2	A	607[A]	POY	C13-C14	2.01	1.56	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	607[B]	POY	C20-N7-C3	-15.99	102.66	128.85
2	A	607[B]	POY	C8-N7-C3	11.67	113.17	105.86
2	A	607[B]	POY	C20-N7-C8	10.61	144.14	126.71
2	A	607[B]	POY	N7-C8-N9	-10.07	103.02	113.52
2	A	607[A]	POY	C8-N7-C3	8.90	111.43	105.86
2	A	607[B]	POY	N5-C4-N9	6.31	136.19	126.27
2	A	607[A]	POY	C2-C3-N7	6.15	137.12	131.54
2	A	607[A]	POY	C2-N1-C6	-5.97	118.28	125.62
2	A	607[A]	POY	N7-C8-N9	-5.52	107.77	113.52
2	A	607[B]	POY	N1-C6-N5	5.25	123.19	116.72
2	A	607[B]	POY	C2-N1-C6	-5.11	119.33	125.62
2	A	606	POY	C19-N5-C6	4.87	125.82	117.33
2	A	606	POY	C8-N7-C3	4.42	108.63	105.86
2	A	607[A]	POY	C10-N1-C2	4.40	123.41	117.18
2	A	607[B]	POY	C22-C21-C20	-4.24	92.31	111.76
2	A	607[A]	POY	C3-C2-N1	4.08	119.90	112.23
2	A	607[B]	POY	C2-C3-N7	-4.02	127.90	131.54
2	A	606	POY	C2-N1-C6	-3.91	120.80	125.62
2	A	606	POY	C20-N7-C3	-3.86	122.54	128.85
2	A	607[A]	POY	N1-C6-N5	3.68	121.25	116.72
2	A	607[A]	POY	C20-N7-C8	-3.54	120.90	126.71
2	A	607[A]	POY	C21-C20-N7	-3.33	107.51	112.47
2	A	607[B]	POY	C3-C4-N5	-3.23	116.83	121.74
2	A	607[B]	POY	C8-N9-C4	3.19	110.64	102.98
2	A	607[B]	POY	C19-N5-C6	3.19	122.89	117.33
2	A	606	POY	N1-C6-N5	3.17	120.62	116.72
2	A	606	POY	C11-C12-C13	-3.07	101.85	113.13
2	A	606	POY	C19-N5-C4	-3.03	116.28	120.75
2	A	607[B]	POY	O18-C6-N1	-3.03	117.90	121.98
2	A	607[A]	POY	O18-C6-N1	-3.03	117.91	121.98
2	A	607[B]	POY	C10-N1-C6	2.97	122.03	117.64
2	A	606	POY	C2-C3-N7	2.95	134.21	131.54
2	A	607[A]	POY	C19-N5-C6	2.87	122.34	117.33
2	A	607[A]	POY	C19-N5-C4	-2.75	116.70	120.75
2	A	607[A]	POY	O17-C2-C3	-2.75	120.75	126.38
2	A	607[A]	POY	N5-C4-N9	2.70	130.51	126.27
2	A	607[B]	POY	C3-C4-N9	-2.66	106.82	112.10
2	A	607[B]	POY	C11-C10-N1	2.63	118.59	112.36
2	A	607[A]	POY	C2-C3-C4	-2.53	119.74	122.92
2	A	606	POY	N7-C8-N9	-2.39	111.03	113.52
2	A	606	POY	C3-C2-N1	2.36	116.68	112.23
2	A	607[B]	POY	C2-C3-C4	2.29	125.80	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	607[B]	POY	C3-C2-N1	2.21	116.38	112.23
2	A	606	POY	C4-C3-N7	-2.20	102.89	104.96
2	A	607[A]	POY	C8-N9-C4	2.11	108.04	102.98
2	A	607[B]	POY	C12-C11-C10	-2.04	103.90	113.17

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	606	POY	C12-C13-C14-C15
2	A	606	POY	C12-C13-C14-O16
2	A	607[A]	POY	C11-C10-N1-C2
2	A	607[A]	POY	C11-C10-N1-C6
2	A	607[B]	POY	N7-C20-C21-C22
2	A	607[B]	POY	C12-C13-C14-C15
2	A	607[B]	POY	C10-C11-C12-C13
2	A	607[B]	POY	C11-C12-C13-C14
2	A	607[A]	POY	C21-C20-N7-C3
2	A	607[B]	POY	C21-C20-N7-C3
2	A	607[B]	POY	C12-C13-C14-O16
2	A	607[A]	POY	N7-C20-C21-C22
2	A	607[A]	POY	C21-C20-N7-C8
2	A	606	POY	N1-C10-C11-C12
2	A	607[A]	POY	C10-C11-C12-C13

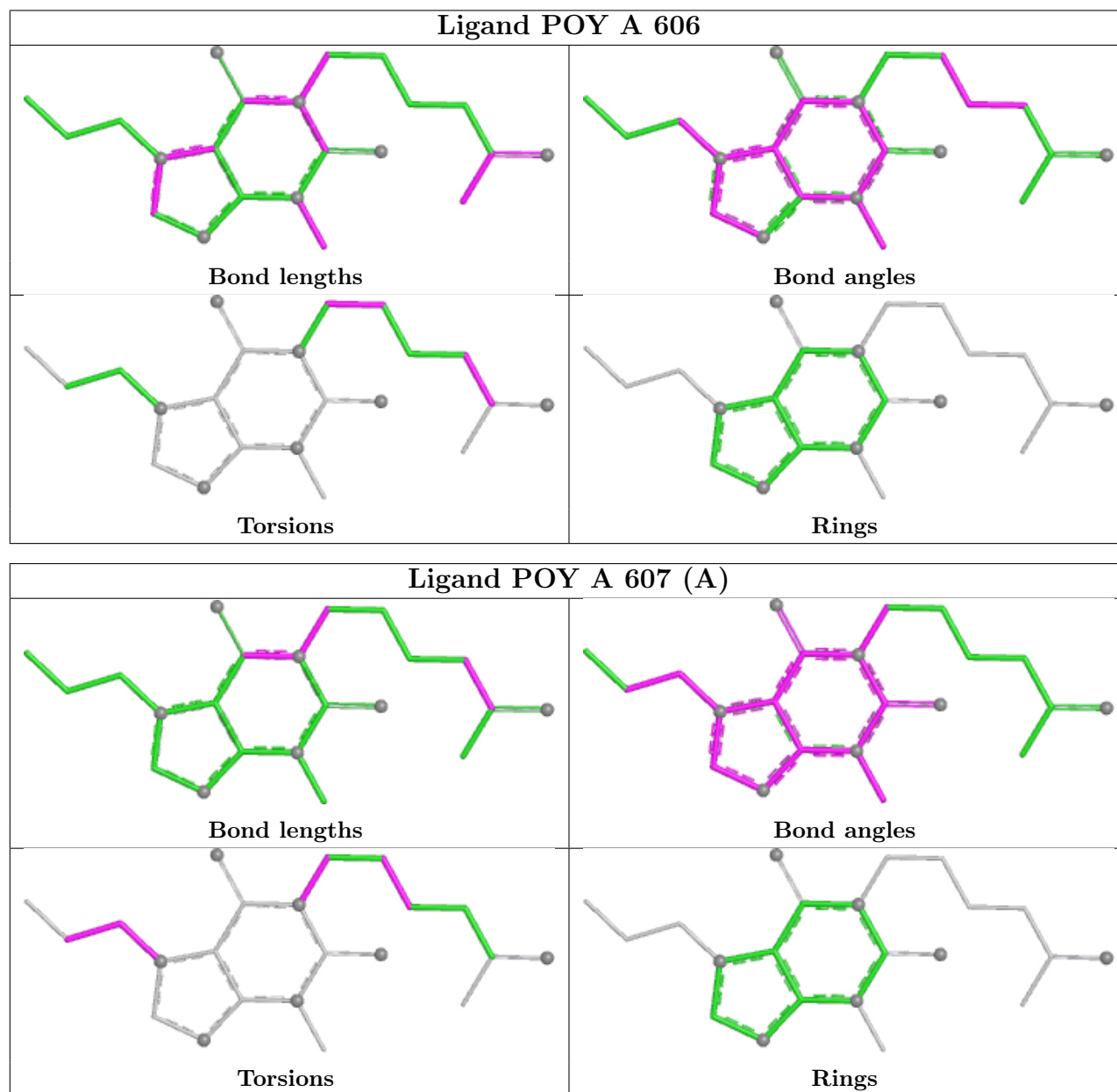
There are no ring outliers.

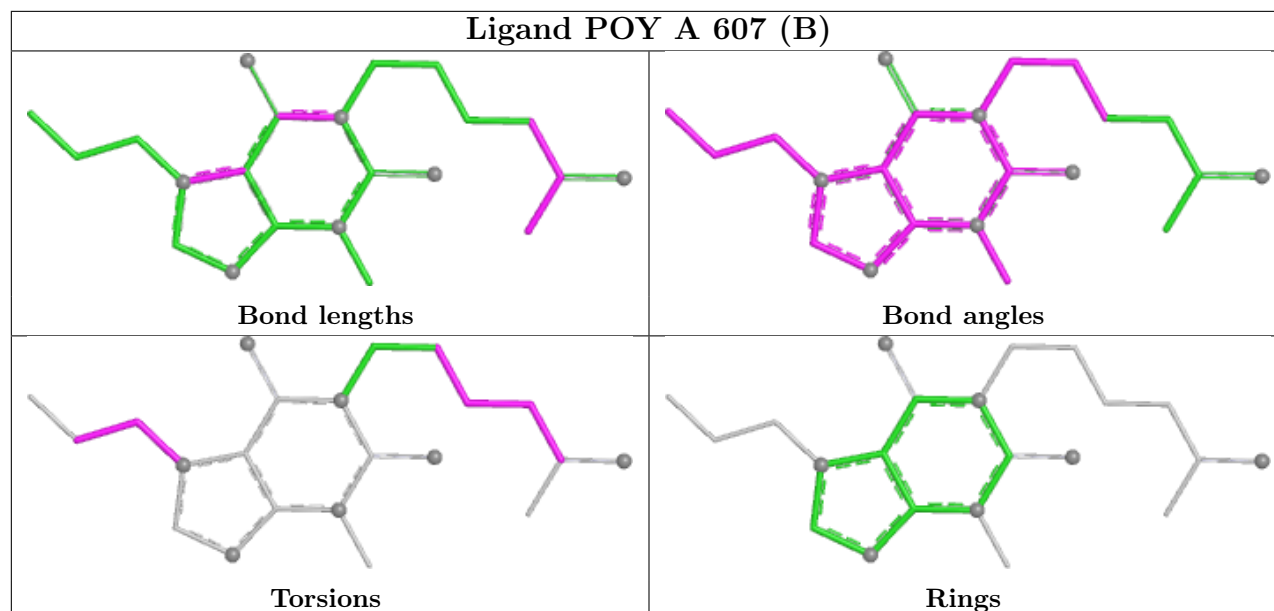
4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3500	GOL	1	0
2	A	606	POY	3	0
2	A	607[A]	POY	17	0
2	A	607[B]	POY	6	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	575/584 (98%)	0.41	30 (5%)	33 42	4, 12, 23, 64	34 (5%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	ASN	4.7
1	A	596	ASN	4.5
1	A	70	TRP	4.3
1	A	116	CYS	3.8
1	A	34	ASN	3.7
1	A	93	THR	3.3
1	A	71	SER	3.1
1	A	72	GLY	2.9
1	A	31	TYR	2.8
1	A	352	ALA	2.8
1	A	595	PRO	2.7
1	A	94	GLY	2.7
1	A	33	SER	2.6
1	A	36	LEU	2.5
1	A	87[A]	VAL	2.5
1	A	89[A]	THR	2.5
1	A	22	ALA	2.5
1	A	25	ALA	2.5
1	A	594	PRO	2.4
1	A	95[A]	SER	2.4
1	A	30	MET	2.3
1	A	108	LEU	2.3
1	A	426	ASN	2.2
1	A	154	ASN	2.2
1	A	68	ASN	2.1
1	A	345	VAL	2.1
1	A	245	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	205[A]	VAL	2.1
1	A	47	THR	2.1
1	A	324	ALA	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](#)

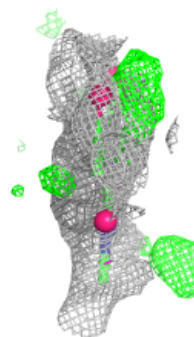
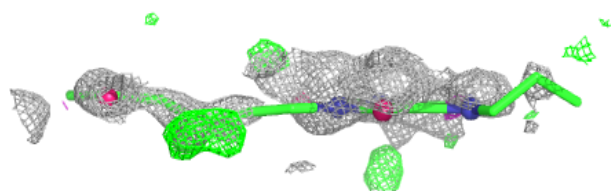
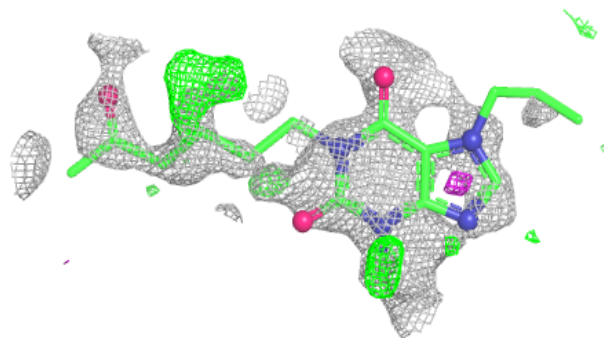
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	POY	A	607[A]	22/22	0.73	0.23	23,48,56,62	22
2	POY	A	607[B]	22/22	0.73	0.23	8,16,21,23	22
2	POY	A	606	22/22	0.90	0.10	12,19,22,24	0
3	GOL	A	3500	6/6	0.94	0.08	16,19,20,21	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.

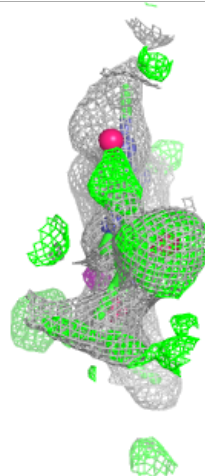
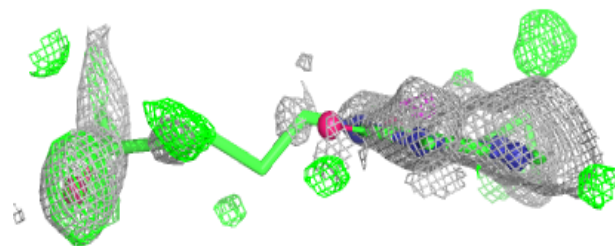
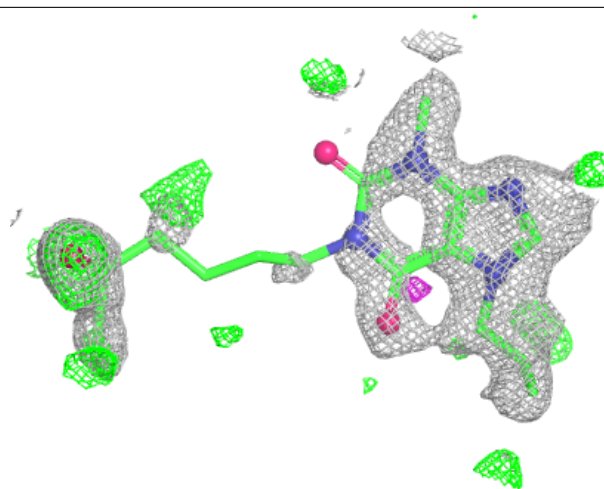
Electron density around POY A 607 (A):

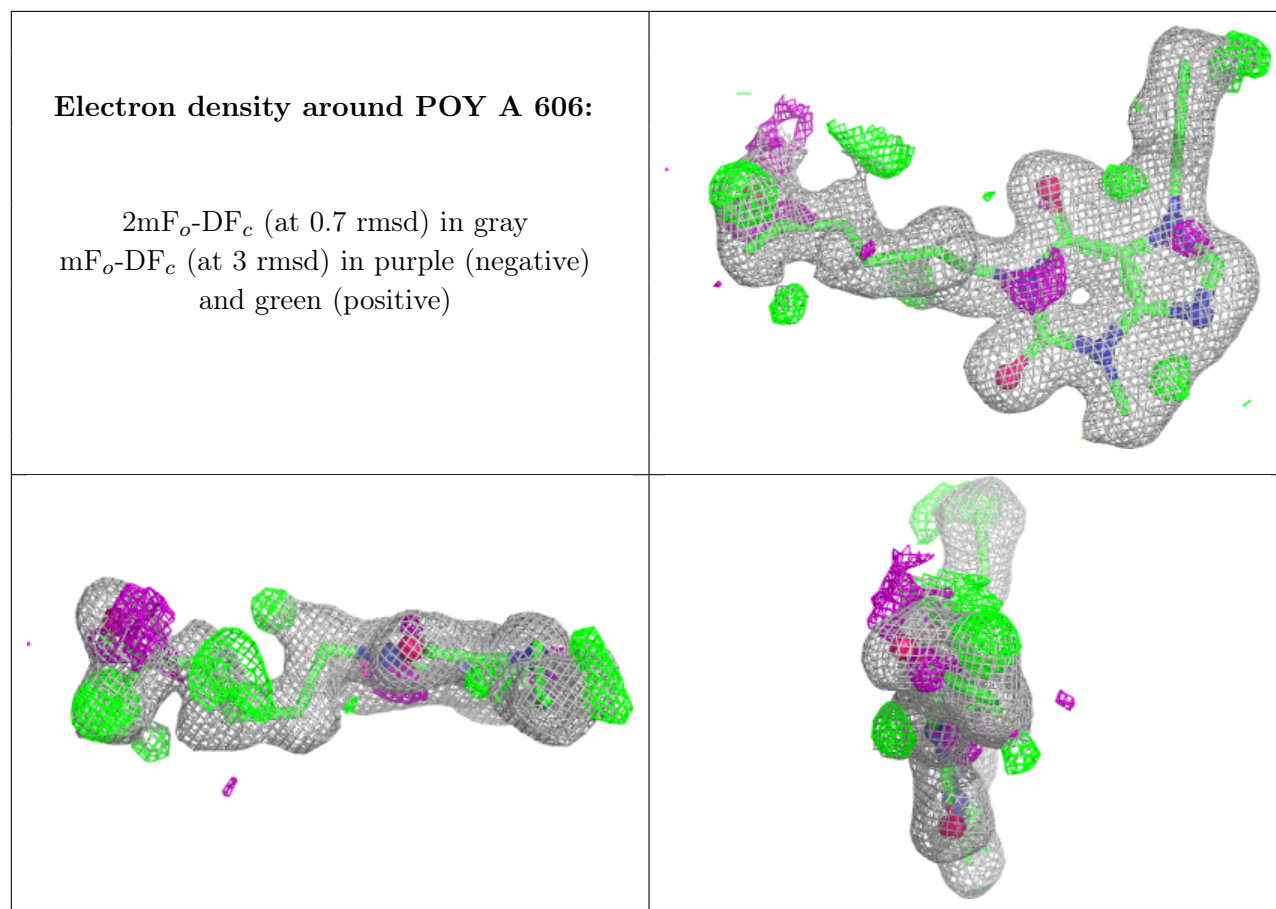
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around POY A 607 (B):

$2mF_o-DF_c$ (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.