



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:14 PM UTC

PDB ID : 8YMB / pdb_00008ymb
Title : The crystal structure of SHD931 in complex with Brd4-BD2 and VCB
Authors : Huang, W.X.; Chen, Y.H.; Li, C.G.; Ding, K.
Deposited on : 2024-03-08
Resolution : 2.95 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

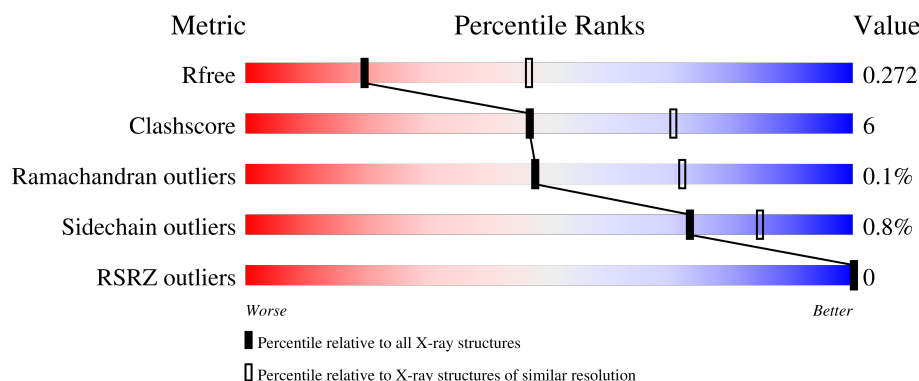
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	128	
1	F	128	
2	B	122	
2	G	122	
3	C	98	

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Mol	Chain	Length	Quality of chain
3	H	98	 77% 12% 11%
4	D	161	 85% 6% 8%
4	I	161	 67% 21% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7153 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 Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			831	532	134	154	11			
1	F	109	Total	C	N	O	S	0	0	0
			834	534	137	152	11			

- Molecule 2 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			798	507	132	155	4			
2	G	104	Total	C	N	O	S	0	0	0
			801	509	136	152	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q15370
B	-2	SER	-	expression tag	UNP Q15370
B	-1	GLY	-	expression tag	UNP Q15370
B	0	SER	-	expression tag	UNP Q15370
G	-3	GLY	-	expression tag	UNP Q15370
G	-2	SER	-	expression tag	UNP Q15370
G	-1	GLY	-	expression tag	UNP Q15370
G	0	SER	-	expression tag	UNP Q15370

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	88	Total	C	N	O	S	0	0	0
			695	448	112	129	6			
3	H	87	Total	C	N	O	S	0	0	0
			686	443	108	129	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	15	GLY	-	expression tag	UNP Q15369
C	16	SER	-	expression tag	UNP Q15369
H	15	GLY	-	expression tag	UNP Q15369
H	16	SER	-	expression tag	UNP Q15369

- Molecule 4 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	148	Total	C	N	O	S	0	0	0
			1191	757	216	216	2			
4	I	142	Total	C	N	O	S	0	0	0
			1156	737	211	206	2			

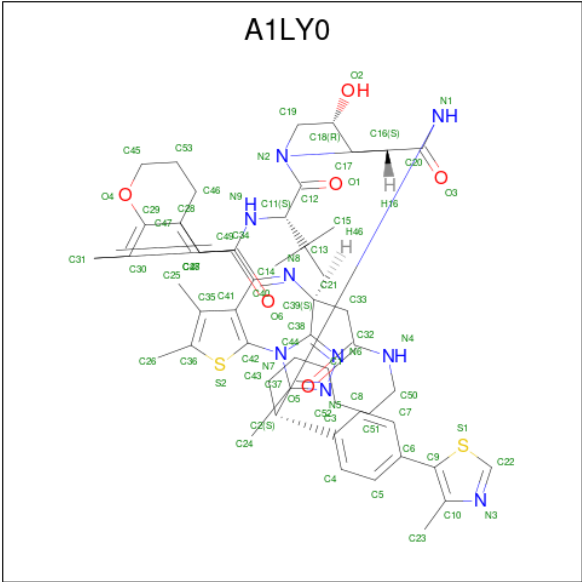
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	53	GLY	-	expression tag	UNP P40337
D	54	SER	-	expression tag	UNP P40337
I	53	GLY	-	expression tag	UNP P40337
I	54	SER	-	expression tag	UNP P40337

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		
5	D	3	Total	Cl	0	0
			3	3		
5	G	1	Total	Cl	0	0
			1	1		
5	H	1	Total	Cl	0	0
			1	1		
5	I	1	Total	Cl	0	0
			1	1		

- Molecule 6 is SHD931 (CCD ID: A1LY0) (formula: C₅₃H₆₇N₉O₆S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			70	53	9	6	2		
6	I	1	Total	C	N	O	S	0	0
			70	53	9	6	2		

- Molecule 7 is water.

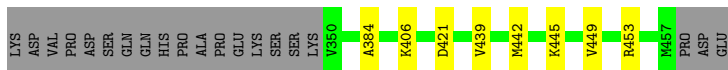
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		
7	C	1	Total	O	0	0
			1	1		
7	D	4	Total	O	0	0
			4	4		
7	F	1	Total	O	0	0
			1	1		
7	G	2	Total	O	0	0
			2	2		
7	H	2	Total	O	0	0
			2	2		
7	I	2	Total	O	0	0
			2	2		

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: Bromodomain-containing protein 4

Chain A: 



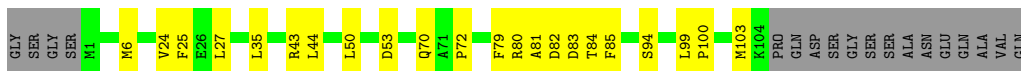
- Molecule 1: Bromodomain-containing protein 4

Chain F: 



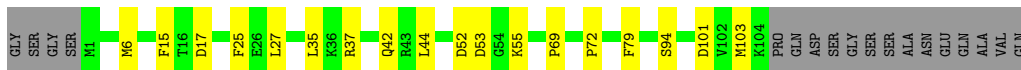
- Molecule 2: Elongin-B

Chain B: 



- Molecule 2: Elongin-B

Chain G: 



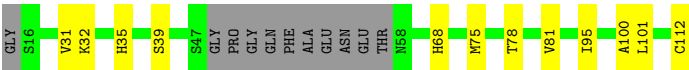
- Molecule 3: Elongin-C

Chain C: 

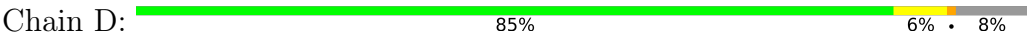


- Molecule 3: Elongin-C

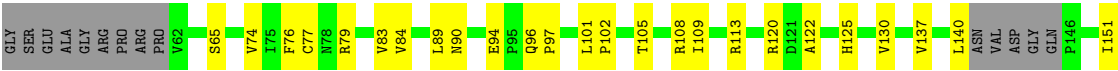
Chain H: 



- Molecule 4: von Hippel-Lindau disease tumor suppressor



- Molecule 4: von Hippel-Lindau disease tumor suppressor



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	84.06Å 84.39Å 382.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.84 – 2.95 47.84 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.84-2.95) 98.4 (47.84-2.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.240 , 0.270 0.241 , 0.272	Depositor DCC
R_{free} test set	2005 reflections (6.85%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.427 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7153	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, A1LY0

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	0.14	0/852	0.26	0/1153
1	F	0.16	0/856	0.29	0/1159
2	B	0.46	0/814	0.52	0/1104
2	G	0.10	0/817	0.30	0/1107
3	C	0.10	0/709	0.25	0/958
3	H	0.09	0/700	0.24	0/946
4	D	0.10	0/1223	0.26	0/1671
4	I	0.10	0/1186	0.25	0/1617
All	All	0.19	0/7157	0.30	0/9715

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	831	0	763	6	0
1	F	834	0	764	7	0
2	B	798	0	781	17	0
2	G	801	0	792	15	0
3	C	695	0	696	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	686	0	682	10	0
4	D	1191	0	1168	10	0
4	I	1156	0	1148	22	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
5	D	3	0	0	1	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
6	D	70	0	0	1	0
6	I	70	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	4	0	0	0	0
7	F	1	0	0	0	0
7	G	2	0	0	0	0
7	H	2	0	0	0	0
7	I	2	0	0	0	0
All	All	7153	0	6794	79	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 6.

All (79) 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)
4:I:90:ASN:HD21	4:I:94:GLU:HB3	1.56	0.69
2:G:103:MET:HE1	3:H:100:ALA:HB3	1.76	0.68
2:G:6:MET:HG3	2:G:72:PRO:HB2	1.81	0.62
4:I:84:VAL:HG11	4:I:151:ILE:HD13	1.82	0.62
4:D:108:ARG:NH1	5:D:302:CL:CL	2.62	0.61
2:B:25:PHE:HB2	2:B:53:ASP:HB3	1.83	0.60
3:C:101:LEU:HD11	4:D:178:LEU:HD22	1.85	0.58
4:I:204:GLU:O	4:I:208:HIS:ND1	2.36	0.58
2:G:35:LEU:HD23	2:G:79:PHE:HZ	1.68	0.57
2:B:6:MET:HG3	2:B:72:PRO:HB2	1.86	0.56
4:D:186:GLU:N	4:D:186:GLU:OE1	2.39	0.56
2:B:24:VAL:HG13	2:B:44:LEU:HD12	1.88	0.56
1:A:439:VAL:HA	1:A:442:MET:HE2	1.86	0.56
2:B:99:LEU:HD23	2:B:100:PRO:O	2.07	0.55
4:I:180:ILE:HB	4:I:184:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:37:ARG:O	2:G:42:GLN:NE2	2.39	0.54
4:I:77:CYS:HB3	4:I:79:ARG:NH1	2.23	0.53
2:G:52:ASP:H	2:G:55:LYS:HE2	1.73	0.53
2:G:27:LEU:HD23	2:G:44:LEU:HD13	1.91	0.52
2:B:84:THR:OG1	2:B:85:PHE:N	2.42	0.51
3:C:95:ILE:HB	4:D:165:VAL:HG21	1.93	0.51
2:G:25:PHE:HB2	2:G:53:ASP:HB3	1.92	0.51
2:B:81:ALA:O	2:B:83:ASP:N	2.44	0.50
3:H:39:SER:HA	3:H:112:CYS:HB3	1.93	0.50
4:I:90:ASN:HD22	4:I:96:GLN:NE2	2.09	0.50
2:B:100:PRO:HD2	2:B:103:MET:SD	2.51	0.50
2:B:80:ARG:HA	2:B:85:PHE:HA	1.93	0.50
2:B:94:SER:OG	3:C:68:HIS:ND1	2.31	0.50
4:I:76:PHE:HB3	4:I:101:LEU:HD11	1.92	0.49
1:A:406:LYS:NZ	1:A:421:ASP:OD2	2.34	0.48
2:B:43:ARG:HD3	2:B:50:LEU:HD11	1.95	0.48
1:A:442:MET:HE1	6:D:304:A1LY0:C28	2.43	0.48
3:H:95:ILE:HB	4:I:165:VAL:HG21	1.94	0.48
1:A:384:ALA:HA	4:D:108:ARG:O	2.13	0.48
2:G:94:SER:OG	3:H:68:HIS:ND1	2.28	0.48
4:I:113:ARG:HD3	4:I:140:LEU:HG	1.95	0.48
2:B:70:GLN:OE1	2:B:70:GLN:N	2.36	0.48
4:D:84:VAL:HG11	4:D:151:ILE:HD13	1.96	0.48
4:D:204:GLU:O	4:D:208:HIS:ND1	2.47	0.47
3:C:57:THR:OG1	3:C:58:ASN:N	2.46	0.47
2:G:69:PRO:HB3	3:H:78:THR:HG22	1.95	0.47
4:I:90:ASN:HD22	4:I:96:GLN:HE21	1.60	0.47
4:D:90:ASN:HD21	4:D:94:GLU:HB3	1.79	0.47
4:I:65:SER:OG	4:I:89:LEU:O	2.33	0.47
4:I:170:VAL:HG21	4:I:178:LEU:HD11	1.96	0.47
2:G:15:PHE:HB2	3:H:31:VAL:HG12	1.97	0.47
4:D:208:HIS:HD2	2:G:101:ASP:HA	1.80	0.46
2:G:35:LEU:HD23	2:G:79:PHE:CZ	2.49	0.46
1:F:372:TYR:HA	1:F:442:MET:HE3	1.98	0.46
3:C:63:ARG:NH2	4:I:96:GLN:HE22	2.14	0.45
4:I:102:PRO:O	4:I:105:THR:OG1	2.33	0.45
3:C:44:ALA:O	4:I:194:VAL:HG23	2.15	0.45
4:I:120:ARG:NH2	4:I:125:HIS:O	2.50	0.45
1:F:384:ALA:HA	4:I:108:ARG:O	2.17	0.45
4:I:83:VAL:HB	4:I:122:ALA:HB3	1.98	0.44
1:F:369:HIS:ND1	1:F:372:TYR:OH	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:17:ASP:OD1	3:H:32:LYS:NZ	2.51	0.44
4:I:74:VAL:O	4:I:109:ILE:N	2.47	0.44
2:B:27:LEU:HD23	2:B:44:LEU:HD13	2.00	0.44
3:C:101:LEU:HD21	4:D:178:LEU:HD13	1.99	0.44
3:C:109:PHE:HZ	4:I:97:PRO:HB2	1.83	0.44
1:F:441:ALA:O	1:F:445:LYS:HG2	2.18	0.44
3:C:39:SER:HA	3:C:112:CYS:HB3	2.00	0.44
3:C:16:SER:OG	3:C:17:MET:N	2.51	0.43
3:H:101:LEU:HD11	4:I:178:LEU:HD22	2.00	0.43
3:C:79:TYR:OH	3:C:91:PRO:O	2.34	0.43
2:G:103:MET:HE2	4:I:169:LEU:HD12	2.01	0.42
2:B:70:GLN:H	2:B:70:GLN:CD	2.26	0.42
1:A:445:LYS:HD3	1:A:445:LYS:HA	1.80	0.42
3:H:35:HIS:CE1	3:H:81:VAL:HG11	2.55	0.42
2:B:35:LEU:HD23	2:B:79:PHE:CZ	2.55	0.42
2:B:35:LEU:HD23	2:B:79:PHE:HZ	1.85	0.42
1:F:402:THR:O	1:F:406:LYS:HG3	2.20	0.41
1:A:449:VAL:HG13	1:A:453:ARG:NH1	2.36	0.40
1:F:440:VAL:O	1:F:444:ARG:HG3	2.21	0.40
2:B:84:THR:OG1	5:B:201:CL:CL	2.76	0.40
2:B:81:ALA:N	2:B:84:THR:O	2.54	0.40
1:F:381:ASP:HB3	1:F:384:ALA:HB3	2.03	0.40
2:G:6:MET:SD	3:H:75:MET:HE2	2.61	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	106/128 (83%)	106 (100%)	0	0	100	100
1	F	107/128 (84%)	107 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	102/122 (84%)	97 (95%)	4 (4%)	1 (1%)	12	32
2	G	102/122 (84%)	97 (95%)	5 (5%)	0	100	100
3	C	84/98 (86%)	84 (100%)	0	0	100	100
3	H	83/98 (85%)	82 (99%)	1 (1%)	0	100	100
4	D	146/161 (91%)	141 (97%)	5 (3%)	0	100	100
4	I	138/161 (86%)	133 (96%)	5 (4%)	0	100	100
All	All	868/1018 (85%)	847 (98%)	20 (2%)	1 (0%)	48	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	82	ASP

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	83/113 (74%)	83 (100%)	0	100	100
1	F	82/113 (73%)	81 (99%)	1 (1%)	63	79
2	B	86/105 (82%)	86 (100%)	0	100	100
2	G	86/105 (82%)	86 (100%)	0	100	100
3	C	79/86 (92%)	78 (99%)	1 (1%)	61	78
3	H	78/86 (91%)	78 (100%)	0	100	100
4	D	133/147 (90%)	131 (98%)	2 (2%)	57	76
4	I	130/147 (88%)	128 (98%)	2 (2%)	57	76
All	All	757/902 (84%)	751 (99%)	6 (1%)	73	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	47	SER

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Mol	Chain	Res	Type
4	D	130	VAL
4	D	186	GLU
1	F	361	LEU
4	I	130	VAL
4	I	137	VAL

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

Mol	Chain	Res	Type
1	A	433	ASN
3	C	108	ASN
1	F	396	HIS
3	H	108	ASN
4	I	96	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](#)

Of 10 ligands modelled in this entry, 8 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
6	A1LY0	I	302	-	72,77,77	1.72	15 (20%)	95,111,111	2.27	31 (32%)
6	A1LY0	D	304	-	72,77,77	1.72	14 (19%)	95,111,111	2.29	35 (36%)

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
6	A1LY0	I	302	-	-	10/61/89/89	0/6/8/8
6	A1LY0	D	304	-	-	13/61/89/89	0/6/8/8

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	302	A1LY0	C10-N3	5.49	1.45	1.38
6	D	304	A1LY0	C10-N3	5.33	1.45	1.38
6	I	302	A1LY0	C37-N5	3.99	1.36	1.31
6	D	304	A1LY0	C37-N5	3.94	1.36	1.31
6	I	302	A1LY0	C38-N6	3.37	1.35	1.32
6	D	304	A1LY0	C3-C2	3.33	1.56	1.52
6	D	304	A1LY0	C20-N1	3.32	1.41	1.34
6	D	304	A1LY0	C38-N6	3.29	1.35	1.32
6	I	302	A1LY0	C20-N1	3.15	1.40	1.34
6	I	302	A1LY0	C3-C2	3.11	1.56	1.52
6	D	304	A1LY0	C33-C32	3.07	1.58	1.51
6	I	302	A1LY0	C16-C20	3.07	1.60	1.52
6	D	304	A1LY0	N5-N6	-2.83	1.33	1.39
6	D	304	A1LY0	C41-C42	2.80	1.44	1.38
6	I	302	A1LY0	N5-N6	-2.72	1.33	1.39
6	I	302	A1LY0	C33-C32	2.72	1.57	1.51
6	I	302	A1LY0	C41-C42	2.72	1.44	1.38
6	D	304	A1LY0	C16-C20	2.70	1.59	1.52
6	I	302	A1LY0	C48-C49	2.65	1.56	1.51
6	D	304	A1LY0	C11-C12	-2.63	1.49	1.53
6	D	304	A1LY0	C48-C49	2.62	1.56	1.51
6	I	302	A1LY0	C43-C2	-2.45	1.50	1.53
6	I	302	A1LY0	C11-C12	-2.45	1.50	1.53
6	D	304	A1LY0	C39-N8	-2.36	1.45	1.47
6	I	302	A1LY0	C51-C50	2.33	1.60	1.51
6	D	304	A1LY0	C9-S1	2.29	1.79	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	304	A1LY0	C51-C50	2.28	1.60	1.51
6	I	302	A1LY0	C9-S1	2.13	1.78	1.73
6	I	302	A1LY0	C7-C8	2.03	1.42	1.38

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	302	A1LY0	C22-S1-C9	8.36	93.34	88.96
6	D	304	A1LY0	C22-S1-C9	7.85	93.07	88.96
6	I	302	A1LY0	C10-C9-S1	-7.61	104.98	109.64
6	D	304	A1LY0	C10-C9-S1	-7.44	105.08	109.64
6	D	304	A1LY0	C34-C40-N8	-5.49	111.00	117.30
6	I	302	A1LY0	C5-C6-C7	-5.04	112.15	118.57
6	D	304	A1LY0	C5-C6-C7	-4.99	112.22	118.57
6	I	302	A1LY0	C6-C9-C10	4.96	137.54	130.81
6	D	304	A1LY0	C24-C37-N5	-4.70	118.62	125.96
6	I	302	A1LY0	C24-C37-N5	-4.61	118.76	125.96
6	D	304	A1LY0	C6-C9-C10	4.42	136.81	130.81
6	I	302	A1LY0	C34-C40-N8	-4.23	112.45	117.30
6	I	302	A1LY0	S1-C22-N3	-4.21	112.47	116.08
6	D	304	A1LY0	S1-C22-N3	-4.12	112.54	116.08
6	I	302	A1LY0	C2-N1-C20	3.94	128.45	122.98
6	D	304	A1LY0	C4-C3-C8	-3.91	113.46	118.30
6	I	302	A1LY0	C4-C3-C8	-3.81	113.59	118.30
6	D	304	A1LY0	C2-N1-C20	3.74	128.17	122.98
6	D	304	A1LY0	C31-C34-C27	-3.34	114.33	118.57
6	D	304	A1LY0	C30-C31-C34	3.26	124.28	120.80
6	I	302	A1LY0	C31-C34-C27	-3.13	114.58	118.57
6	D	304	A1LY0	C13-C11-C12	-3.09	109.11	113.23
6	I	302	A1LY0	C8-C7-C6	3.07	124.08	120.80
6	D	304	A1LY0	C30-C29-C28	-3.06	115.69	120.16
6	D	304	A1LY0	C8-C7-C6	3.05	124.06	120.80
6	D	304	A1LY0	C5-C6-C9	3.00	125.62	120.84
6	I	302	A1LY0	N7-C38-N6	2.99	112.97	109.44
6	I	302	A1LY0	C30-C29-C28	-2.99	115.80	120.16
6	I	302	A1LY0	C30-C31-C34	2.93	123.93	120.80
6	D	304	A1LY0	N7-C38-N6	2.87	112.83	109.44
6	D	304	A1LY0	C9-C10-N3	2.84	117.73	114.99
6	I	302	A1LY0	C4-C5-C6	2.80	123.79	120.80
6	I	302	A1LY0	C8-C3-C2	2.78	126.43	120.79
6	I	302	A1LY0	C9-C10-N3	2.78	117.67	114.99
6	I	302	A1LY0	C5-C6-C9	2.69	125.12	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	304	A1LY0	C4-C5-C6	2.69	123.67	120.80
6	D	304	A1LY0	C8-C3-C2	2.68	126.24	120.79
6	I	302	A1LY0	C48-C49-N9	2.66	120.55	115.86
6	I	302	A1LY0	C38-C39-N8	2.59	111.06	106.80
6	I	302	A1LY0	C13-C11-C12	-2.56	109.82	113.23
6	D	304	A1LY0	C11-N9-C49	2.56	127.01	121.98
6	I	302	A1LY0	C38-N6-N5	-2.55	104.91	107.82
6	I	302	A1LY0	C24-C37-N7	2.55	130.21	124.90
6	D	304	A1LY0	C17-C16-C20	-2.49	106.59	111.36
6	D	304	A1LY0	C24-C37-N7	2.47	130.04	124.90
6	D	304	A1LY0	C38-C39-N8	2.45	110.83	106.80
6	I	302	A1LY0	C3-C2-N1	-2.43	107.93	112.07
6	D	304	A1LY0	C17-C18-C19	-2.41	100.49	103.18
6	D	304	A1LY0	C5-C4-C3	2.31	123.49	121.18
6	D	304	A1LY0	C38-N6-N5	-2.30	105.20	107.82
6	I	302	A1LY0	C11-N9-C49	2.29	126.48	121.98
6	D	304	A1LY0	C33-C32-N4	2.28	119.49	115.97
6	I	302	A1LY0	C5-C4-C3	2.27	123.45	121.18
6	D	304	A1LY0	C27-C28-C29	2.25	122.30	119.73
6	I	302	A1LY0	C17-C16-C20	-2.25	107.05	111.36
6	D	304	A1LY0	O5-C32-N4	-2.24	118.64	123.03
6	D	304	A1LY0	C48-C49-N9	2.23	119.79	115.86
6	D	304	A1LY0	C3-C2-N1	-2.21	108.30	112.07
6	I	302	A1LY0	O5-C32-N4	-2.21	118.69	123.03
6	I	302	A1LY0	O2-C18-C19	-2.15	105.96	110.33
6	D	304	A1LY0	C27-C34-C40	2.13	124.24	120.74
6	I	302	A1LY0	C17-C18-C19	-2.12	100.82	103.18
6	D	304	A1LY0	C43-C2-N1	2.07	112.09	109.56
6	D	304	A1LY0	C34-C40-C41	2.05	121.46	118.75
6	D	304	A1LY0	C21-C13-C11	2.04	113.88	109.71
6	I	302	A1LY0	C21-C13-C11	2.00	113.81	109.71

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	302	A1LY0	C47-C46-C53-C45
6	I	302	A1LY0	C52-C1-C44-C43
6	I	302	A1LY0	C30-C29-O4-C45
6	I	302	A1LY0	C28-C29-O4-C45
6	D	304	A1LY0	C47-C46-C53-C45
6	D	304	A1LY0	C28-C29-O4-C45

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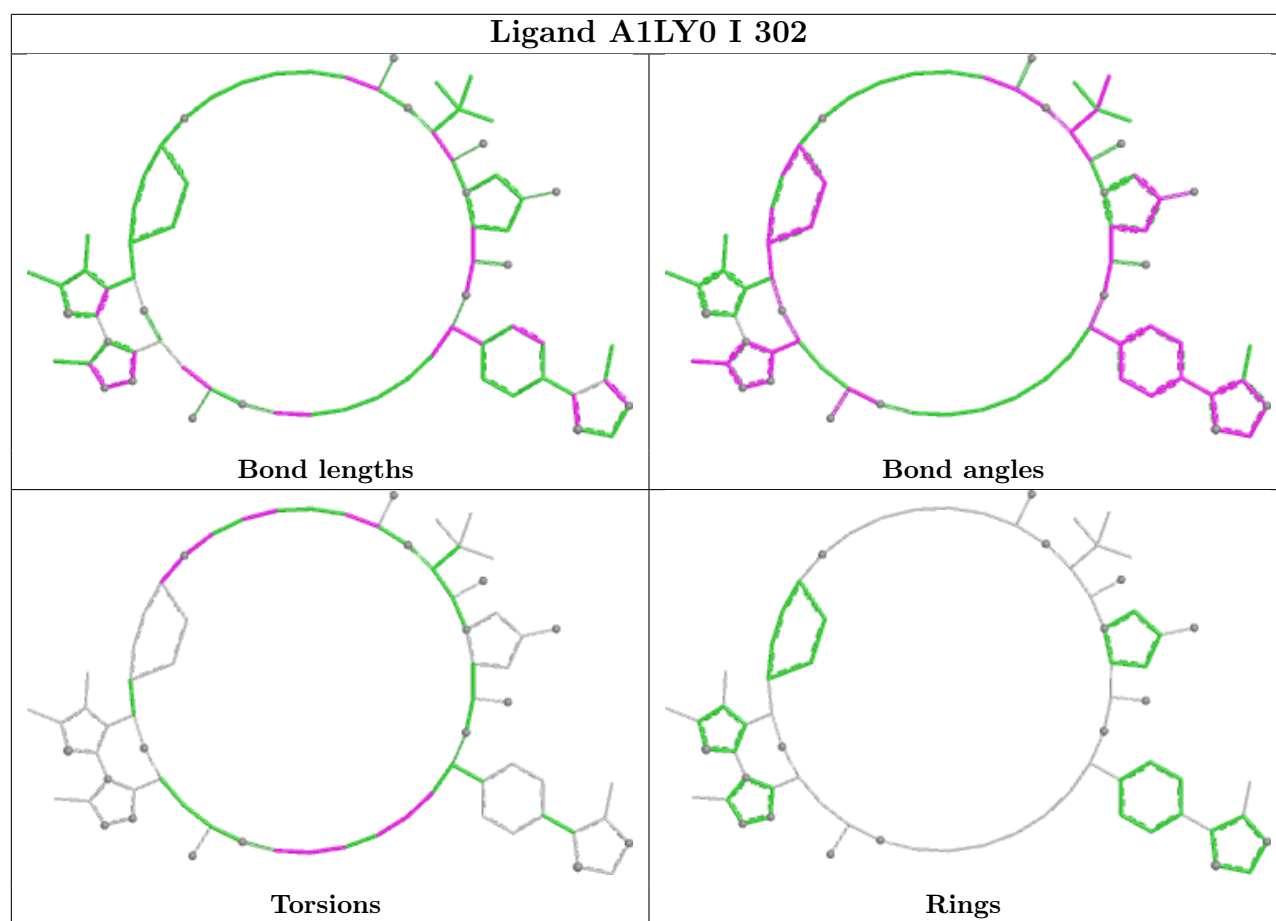
Mol	Chain	Res	Type	Atoms
6	D	304	A1LY0	C30-C29-O4-C45
6	D	304	A1LY0	C52-C1-C44-C43
6	I	302	A1LY0	C47-C48-C49-O6
6	I	302	A1LY0	C47-C48-C49-N9
6	D	304	A1LY0	N4-C50-C51-C52
6	D	304	A1LY0	C47-C48-C49-N9
6	D	304	A1LY0	C47-C48-C49-O6
6	I	302	A1LY0	C50-C51-C52-C1
6	D	304	A1LY0	C50-C51-C52-C1
6	I	302	A1LY0	C53-C45-O4-C29
6	D	304	A1LY0	C2-C43-C44-C1
6	D	304	A1LY0	C53-C45-O4-C29
6	I	302	A1LY0	C2-C43-C44-C1
6	I	302	A1LY0	N4-C50-C51-C52
6	D	304	A1LY0	N9-C11-C13-C21
6	D	304	A1LY0	N9-C11-C13-C15
6	D	304	A1LY0	C53-C46-C47-C48

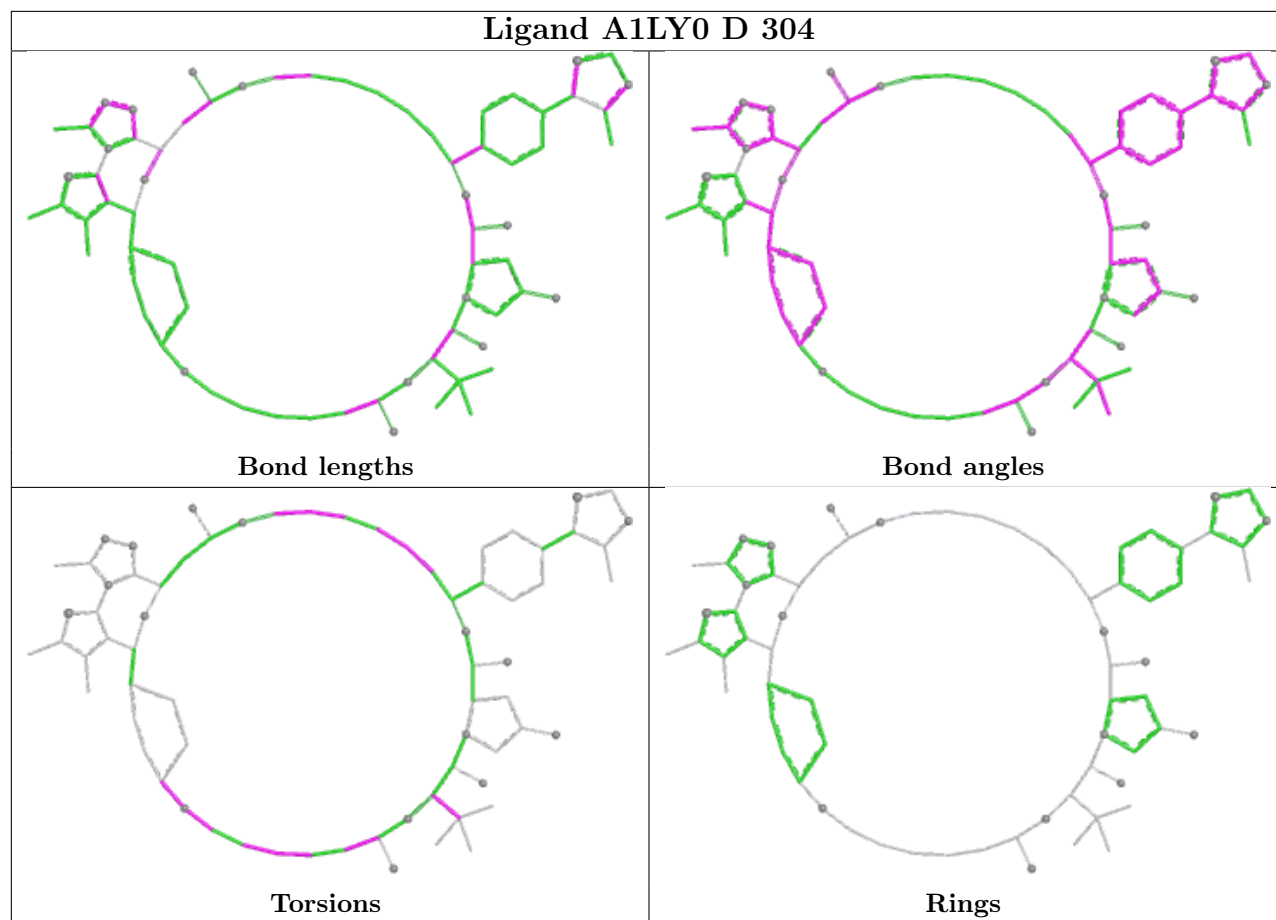
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	304	A1LY0	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 [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	108/128 (84%)	-0.91	0 100 100	70, 87, 115, 124	0
1	F	109/128 (85%)	-0.92	0 100 100	69, 85, 111, 125	0
2	B	104/122 (85%)	-0.95	0 100 100	58, 78, 97, 103	0
2	G	104/122 (85%)	-0.94	0 100 100	56, 75, 90, 96	0
3	C	88/98 (89%)	-0.96	0 100 100	52, 63, 89, 99	0
3	H	87/98 (88%)	-0.99	0 100 100	54, 63, 86, 99	0
4	D	148/161 (91%)	-1.04	0 100 100	51, 72, 100, 122	0
4	I	142/161 (88%)	-1.04	0 100 100	49, 72, 93, 105	0
All	All	890/1018 (87%)	-0.97	0 100 100	49, 76, 103, 125	0

There are no RSRZ outliers to report.

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](#)

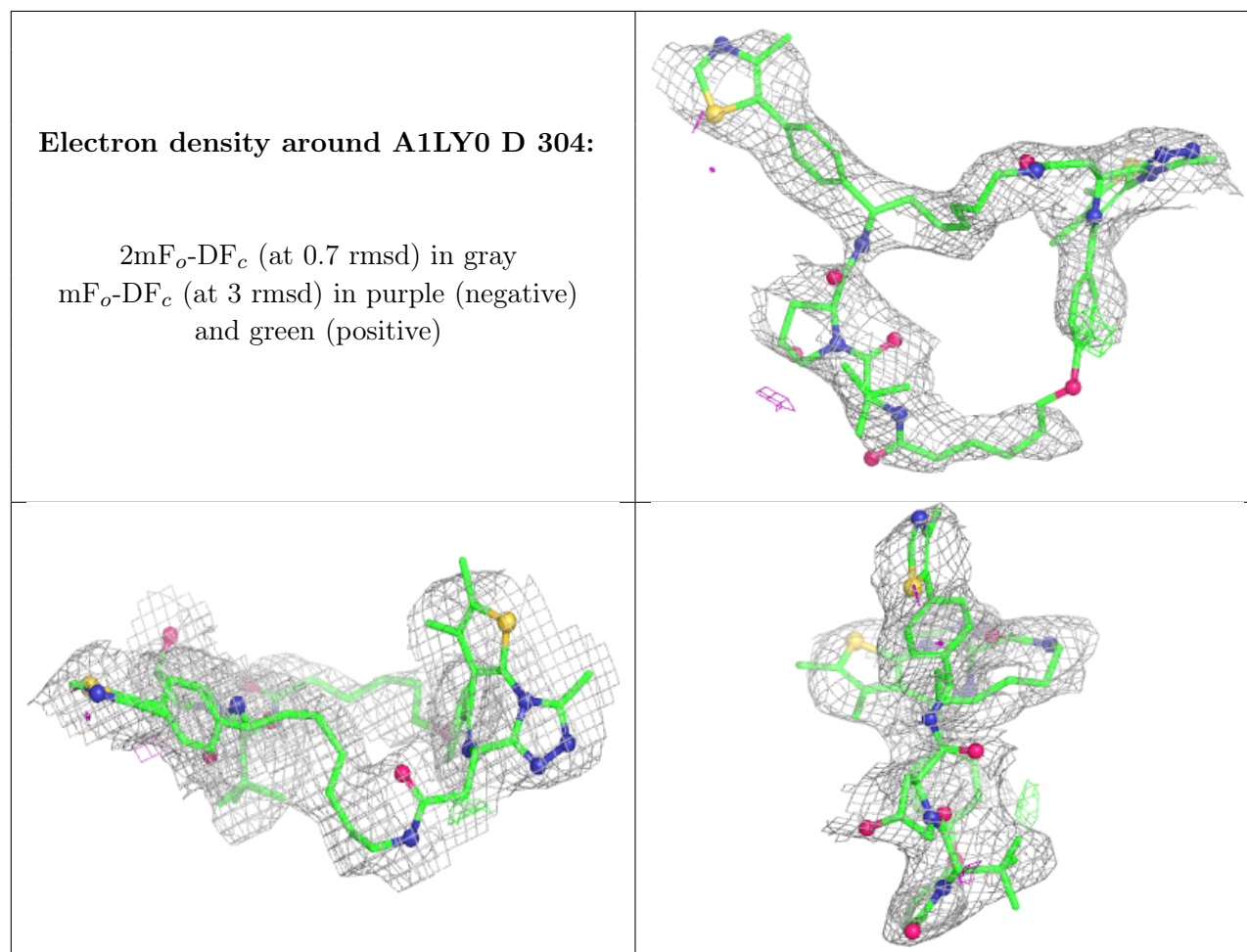
There are no oligosaccharides in this entry.

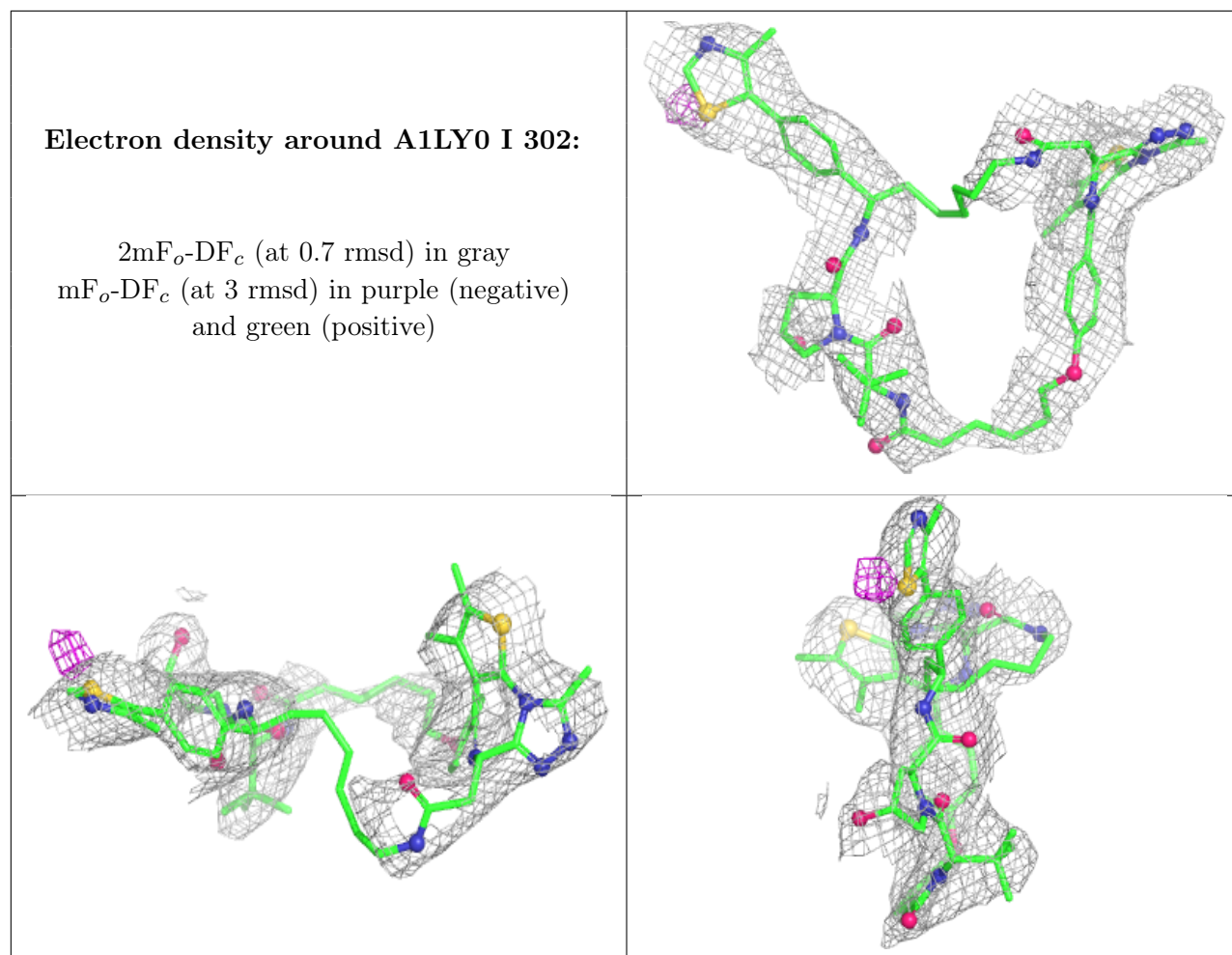
6.4 Ligands [i](#)

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	CL	G	201	1/1	0.96	0.10	100,100,100,100	0
5	CL	D	303	1/1	0.97	0.04	90,90,90,90	0
5	CL	A	501	1/1	0.97	0.06	101,101,101,101	0
5	CL	H	201	1/1	0.97	0.08	101,101,101,101	0
5	CL	D	302	1/1	0.98	0.06	79,79,79,79	0
5	CL	B	201	1/1	0.99	0.03	84,84,84,84	0
5	CL	I	301	1/1	0.99	0.03	83,83,83,83	0
6	A1LY0	D	304	70/70	0.99	0.06	61,75,83,91	0
6	A1LY0	I	302	70/70	0.99	0.06	64,77,87,91	0
5	CL	D	301	1/1	1.00	0.02	82,82,82,82	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.