



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:24 AM UTC

PDB ID : 9HYO / pdb_00009hyo
Title : CRYSTAL STRUCTURE OF THE SMARCA2-VCB-COMPLEX WITH
PROTAC P4
Authors : Roy, M.J.
Deposited on : 2025-01-10
Resolution : 3.74 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

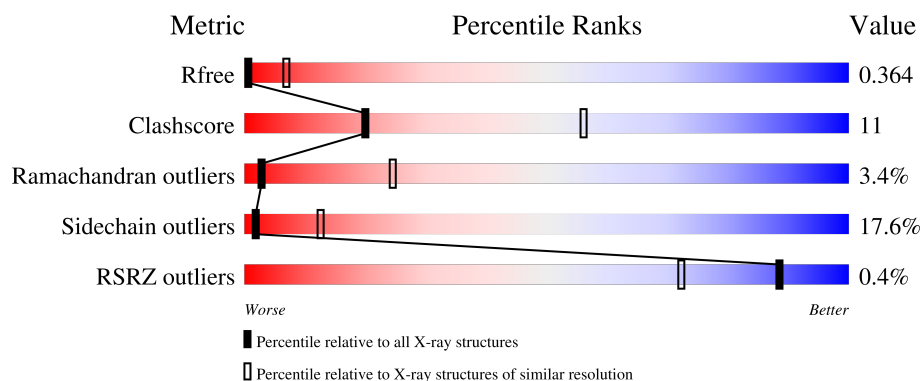
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.74 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	1234 (3.88-3.60)
Clashscore	190562	1274 (3.88-3.60)
Ramachandran outliers	187476	1226 (3.88-3.60)
Sidechain outliers	187428	1221 (3.88-3.60)
RSRZ outliers	180081	1233 (3.88-3.60)

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	123	<div> <div>%</div> <div> <div></div> <div>39%</div> <div>40%</div> <div>8%</div> <div>11%</div> </div> </div>
2	B	104	<div> <div>52%</div> <div>37%</div> <div>12%</div> </div>
3	C	97	<div> <div>56%</div> <div>30%</div> <div>10%</div> </div>
4	D	162	<div> <div>%</div> <div>55%</div> <div>30%</div> <div>6%</div> <div>8%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3688 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 Probable global transcription activator SNF2L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			899	572	158	166	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1371	SER	-	expression tag	UNP P51531
A	1372	MET	-	expression tag	UNP P51531

- 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
			803	510	137	152	4			

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	87	Total	C	N	O	S	0	0	0
			689	445	108	129	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	MET	-	initiating methionine	UNP Q15369

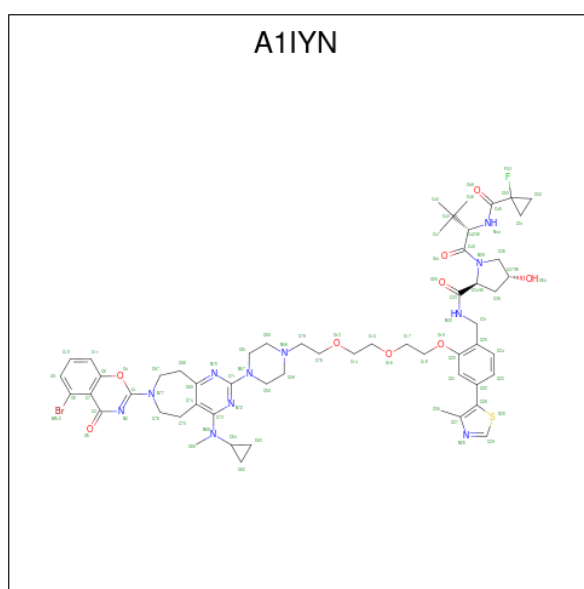
- Molecule 4 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	149	Total	C	N	O	S	0	0	0
			1215	772	222	219	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	52	GLY	-	expression tag	UNP P40337
D	53	SER	-	expression tag	UNP P40337

- Molecule 5 is (2 {S},4 {R})- {N}-[[2-[2-[2-[4-[7-(5-bromanyl-4-oxidanylidene-2,3-dihydro-1,3-benzoxazin-2-yl)-4-[cyclopropyl(methyl)amino]-5,6,8,9-tetrahydropyrimido[4,5-d]azepin-2-yl]piperazin-1-yl]ethoxy]ethoxy]ethoxy]-4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl]-1-[(2 {S})-2-[(1-fluoranylcyclopropyl)carbonylamino]-3,3-dimethyl-butanoyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: A1IYN) (formula: C₅₆H₇₁BrFN₁₁O₉S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	D	1	Total	Br	C	F	N	O	S	0	0
			79	1	56	1	11	9	1		

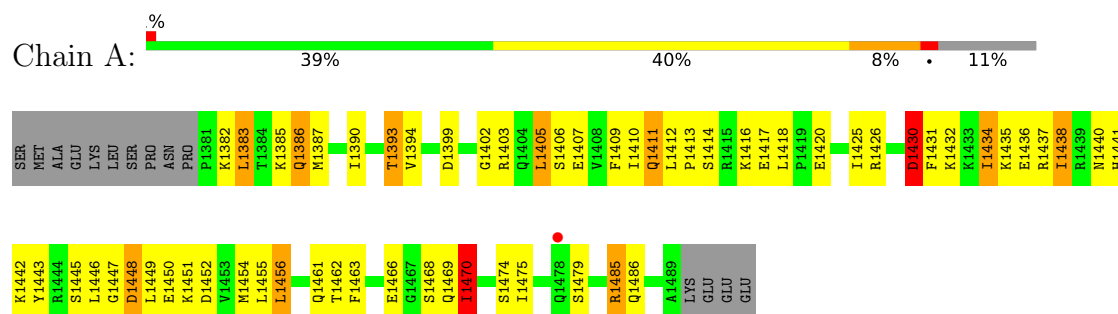
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	O	0	0
			2	2		
6	D	1	Total	O	0	0
			1	1		

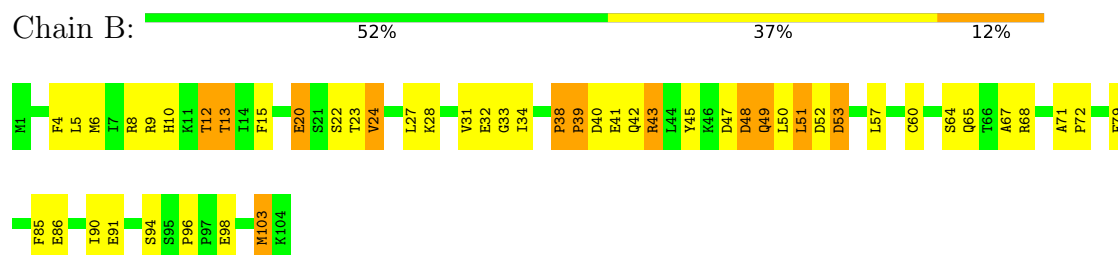
3 Residue-property plots [i](#)

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.

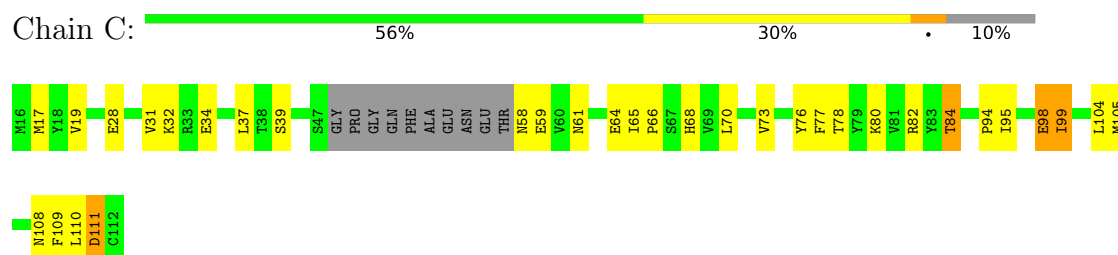
- Molecule 1: Probable global transcription activator SNF2L2



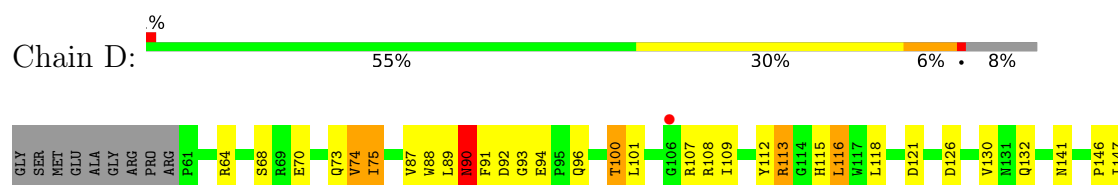
- Molecule 2: Elongin-B



- Molecule 3: Elongin-C



- Molecule 4: von Hippel-Lindau disease tumor suppressor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.52Å 64.10Å 89.48Å 90.00° 96.87° 90.00°	Depositor
Resolution (Å)	48.18 – 3.74 48.18 – 3.74	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.18-3.74) 98.6 (48.18-3.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.220 , 0.348 0.233 , 0.364	Depositor DCC
R_{free} test set	285 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	106.8	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3688	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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: A1IYN

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	0.84	0/913	1.69	26/1223 (2.1%)
2	B	0.98	1/819 (0.1%)	1.62	15/1108 (1.4%)
3	C	0.89	0/703	1.48	5/948 (0.5%)
4	D	0.93	0/1247	1.44	10/1702 (0.6%)
All	All	0.91	1/3682 (0.0%)	1.55	56/4981 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24	VAL	CA-C	5.07	1.59	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	GLU	CA-C-N	7.50	130.65	120.44
2	B	20	GLU	C-N-CA	7.50	130.65	120.44
2	B	23	THR	CA-C-N	7.15	129.82	120.60
2	B	23	THR	C-N-CA	7.15	129.82	120.60
1	A	1382	LYS	N-CA-C	-7.02	104.85	113.41
2	B	41	GLU	N-CA-C	-6.85	104.54	113.17
1	A	1399	ASP	CA-C-N	6.53	129.91	120.38
1	A	1399	ASP	C-N-CA	6.53	129.91	120.38
2	B	47	ASP	CA-C-N	6.51	133.97	121.54
2	B	47	ASP	C-N-CA	6.51	133.97	121.54
2	B	38	PRO	N-CA-C	6.49	118.61	110.70
4	D	191	HIS	N-CA-C	-6.36	101.63	109.65
1	A	1382	LYS	CA-C-N	6.32	129.08	120.54
1	A	1382	LYS	C-N-CA	6.32	129.08	120.54
4	D	150	ASN	CA-CB-CG	6.28	118.88	112.60
1	A	1399	ASP	CA-CB-CG	6.25	118.85	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1486	GLN	CA-C-N	6.24	128.55	120.44
1	A	1486	GLN	C-N-CA	6.24	128.55	120.44
3	C	111	ASP	CA-C-N	6.23	132.91	121.70
3	C	111	ASP	C-N-CA	6.23	132.91	121.70
2	B	52	ASP	CA-C-N	6.13	133.25	121.54
2	B	52	ASP	C-N-CA	6.13	133.25	121.54
2	B	91	GLU	CB-CG-CD	6.05	122.89	112.60
1	A	1479	SER	CA-C-N	6.05	128.75	120.46
1	A	1479	SER	C-N-CA	6.05	128.75	120.46
1	A	1434	ILE	N-CA-C	-6.03	105.84	111.45
1	A	1420	GLU	CA-C-N	6.00	128.56	120.65
1	A	1420	GLU	C-N-CA	6.00	128.56	120.65
4	D	121	ASP	CA-CB-CG	5.91	118.51	112.60
2	B	39	PRO	CA-C-N	5.90	132.80	121.54
2	B	39	PRO	C-N-CA	5.90	132.80	121.54
1	A	1430	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	1474	SER	CA-C-N	5.81	127.88	120.56
1	A	1474	SER	C-N-CA	5.81	127.88	120.56
1	A	1405	LEU	CA-C-N	5.77	128.81	120.38
1	A	1405	LEU	C-N-CA	5.77	128.81	120.38
2	B	49	GLN	CA-C-N	5.70	132.42	121.54
2	B	49	GLN	C-N-CA	5.70	132.42	121.54
1	A	1438	ILE	CA-C-N	5.42	127.85	120.54
1	A	1438	ILE	C-N-CA	5.42	127.85	120.54
1	A	1440	ASN	CA-C-N	5.34	131.75	121.54
1	A	1440	ASN	C-N-CA	5.34	131.75	121.54
4	D	157	THR	N-CA-C	-5.32	101.78	109.59
3	C	34	GLU	CA-C-N	5.21	127.69	120.29
3	C	34	GLU	C-N-CA	5.21	127.69	120.29
4	D	187	ASP	CA-C-N	5.21	129.40	120.71
4	D	187	ASP	C-N-CA	5.21	129.40	120.71
4	D	90	ASN	CA-C-N	5.14	131.37	121.54
4	D	90	ASN	C-N-CA	5.14	131.37	121.54
4	D	200	ARG	N-CA-C	-5.06	106.27	112.90
1	A	1470	ILE	CA-C-N	5.05	127.30	120.44
1	A	1470	ILE	C-N-CA	5.05	127.30	120.44
4	D	100	THR	N-CA-C	5.04	118.43	109.96
1	A	1393	THR	CA-C-N	5.04	126.91	120.56
1	A	1393	THR	C-N-CA	5.04	126.91	120.56
3	C	108	ASN	CA-CB-CG	5.01	117.61	112.60

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	899	0	931	26	0
2	B	803	0	796	26	0
3	C	689	0	686	14	0
4	D	1215	0	1209	27	0
5	D	79	0	0	3	0
6	B	2	0	0	0	0
6	D	1	0	0	0	0
All	All	3688	0	3622	83	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 11.

All (83) 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:1443:TYR:HB3	1:A:1448:ASP:HB3	1.74	0.68
1:A:1387:MET:HE1	1:A:1443:TYR:HB2	1.77	0.66
4:D:193:ASN:HB3	4:D:196:LYS:HB3	1.80	0.64
2:B:24:VAL:HB	2:B:53:ASP:HA	1.80	0.64
4:D:107:ARG:HH21	4:D:108:ARG:HH21	1.49	0.60
2:B:28:LYS:HD3	2:B:42:GLN:HB3	1.87	0.57
1:A:1410:ILE:HA	1:A:1431:PHE:HB2	1.86	0.57
4:D:180:ILE:HD12	4:D:184:LEU:HB2	1.87	0.56
1:A:1425:ILE:HD11	1:A:1463:PHE:HB2	1.88	0.56
2:B:43:ARG:HB2	2:B:85:PHE:CE1	2.41	0.56
2:B:96:PRO:HB3	3:C:99:ILE:HG22	1.87	0.56
2:B:24:VAL:HB	2:B:53:ASP:CA	2.37	0.55
1:A:1412:LEU:HB2	1:A:1430:ASP:HB3	1.89	0.54
2:B:31:VAL:C	2:B:33:GLY:H	2.17	0.53
3:C:104:LEU:HD22	4:D:166:VAL:HG21	1.92	0.52
4:D:73:GLN:H	4:D:141:ASN:HD21	1.56	0.52
1:A:1447:GLY:HA2	1:A:1485:ARG:HH12	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:HIS:H	2:B:90:ILE:HA	1.75	0.52
4:D:75:ILE:HD11	4:D:146:PRO:HB2	1.93	0.51
2:B:79:PHE:H	2:B:86:GLU:HG2	1.76	0.51
2:B:6:MET:HG3	2:B:72:PRO:HB2	1.91	0.50
3:C:80:LYS:O	3:C:84:THR:HB	2.12	0.50
2:B:94:SER:O	3:C:68:HIS:HB3	2.11	0.50
3:C:64:GLU:HG2	3:C:65:ILE:HG13	1.93	0.50
1:A:1409:PHE:HB3	1:A:1456:LEU:HD21	1.94	0.50
4:D:68:SER:HB2	4:D:70:GLU:CD	2.37	0.49
3:C:76:TYR:CE2	4:D:158:LEU:HB2	2.46	0.49
2:B:24:VAL:HA	2:B:27:LEU:HD12	1.93	0.49
4:D:109:ILE:HG23	5:D:301:A1IYN:C23	2.42	0.49
2:B:103:MET:HE2	4:D:169:LEU:HB2	1.94	0.49
2:B:27:LEU:HD11	2:B:57:LEU:HD21	1.95	0.49
3:C:98:GLU:H	3:C:98:GLU:CD	2.20	0.49
2:B:8:ARG:HB3	2:B:90:ILE:HG21	1.96	0.48
1:A:1386:GLN:HE21	1:A:1446:LEU:HD21	1.78	0.48
4:D:112:TYR:HB2	4:D:115:HIS:CD2	2.48	0.48
2:B:68:ARG:HB2	2:B:71:ALA:HB3	1.95	0.47
4:D:167:ARG:HD3	4:D:188:LEU:O	2.13	0.47
2:B:8:ARG:HG2	2:B:13:THR:HG23	1.97	0.47
1:A:1387:MET:HA	1:A:1390:ILE:HD12	1.96	0.47
1:A:1403:ARG:HH12	1:A:1405:LEU:HD23	1.79	0.47
4:D:171:LYS:HG2	4:D:172:PRO:HD2	1.97	0.47
4:D:178:LEU:HD12	4:D:180:ILE:HG12	1.95	0.47
3:C:109:PHE:HD1	3:C:110:LEU:HG	1.78	0.47
4:D:90:ASN:HB3	4:D:96:GLN:HE21	1.80	0.47
1:A:1443:TYR:CE2	1:A:1449:LEU:HD12	2.51	0.46
1:A:1468:SER:HB2	1:A:1470:ILE:HD12	1.98	0.46
2:B:39:PRO:HA	2:B:42:GLN:HB2	1.97	0.46
1:A:1409:PHE:HA	5:D:301:A1IYN:C10	2.46	0.46
2:B:9:ARG:HG2	2:B:10:HIS:HD2	1.81	0.46
4:D:108:ARG:O	4:D:109:ILE:HD13	2.16	0.46
2:B:4:PHE:CZ	3:C:82:ARG:HG2	2.52	0.45
2:B:57:LEU:HA	2:B:60:CYS:SG	2.57	0.45
2:B:45:TYR:HD2	2:B:48:ASP:HA	1.81	0.45
1:A:1412:LEU:HG	1:A:1413:PRO:HD2	1.98	0.45
2:B:12:THR:HA	3:C:28:GLU:HB2	1.98	0.45
1:A:1437:ARG:HG2	1:A:1442:LYS:HG3	2.00	0.44
2:B:32:GLU:CD	2:B:39:PRO:HD3	2.43	0.44
2:B:28:LYS:HD2	2:B:39:PRO:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:74:VAL:HB	4:D:109:ILE:HB	2.00	0.44
1:A:1452:ASP:O	1:A:1455:LEU:HB3	2.17	0.43
1:A:1468:SER:HA	4:D:94:GLU:HG2	1.99	0.43
1:A:1383:LEU:HA	1:A:1386:GLN:NE2	2.33	0.43
3:C:19:VAL:HG12	3:C:58:ASN:HA	1.99	0.43
4:D:165:VAL:O	4:D:169:LEU:HG	2.19	0.43
4:D:160:GLU:HG3	4:D:164:GLN:HE21	1.83	0.43
4:D:87:VAL:HB	4:D:118:LEU:HG	2.01	0.43
4:D:87:VAL:HA	4:D:96:GLN:O	2.19	0.42
1:A:1450:GLU:O	1:A:1454:MET:HG2	2.20	0.42
4:D:68:SER:HB3	4:D:113:ARG:HH21	1.85	0.42
3:C:39:SER:HB2	3:C:77:PHE:HZ	1.84	0.42
3:C:95:ILE:HB	4:D:165:VAL:HG21	2.01	0.42
1:A:1448:ASP:HA	1:A:1451:LYS:HD2	2.01	0.41
4:D:141:ASN:HA	4:D:147:ILE:HD11	2.02	0.41
1:A:1412:LEU:HD12	5:D:301:A1IYN:C9	2.49	0.41
2:B:15:PHE:HB2	3:C:31:VAL:HG12	2.03	0.41
1:A:1445:SER:HB3	1:A:1448:ASP:HB2	2.03	0.41
4:D:89:LEU:HD21	4:D:118:LEU:HD21	2.02	0.41
1:A:1411:GLN:HG2	1:A:1432:LYS:HD3	2.02	0.40
1:A:1414:SER:HB2	1:A:1417:GLU:HB2	2.03	0.40
4:D:88:TRP:HA	4:D:116:LEU:O	2.21	0.40
1:A:1383:LEU:HD12	1:A:1446:LEU:HG	2.03	0.40
1:A:1435:LYS:HA	1:A:1438:ILE:HD12	2.04	0.40
2:B:38:PRO:HA	2:B:39:PRO:HD3	1.95	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	107/123 (87%)	89 (83%)	15 (14%)	3 (3%)	4	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	102/104 (98%)	80 (78%)	16 (16%)	6 (6%)	1	15
3	C	83/97 (86%)	69 (83%)	12 (14%)	2 (2%)	4	29
4	D	147/162 (91%)	121 (82%)	22 (15%)	4 (3%)	4	27
All	All	439/486 (90%)	359 (82%)	65 (15%)	15 (3%)	3	24

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1441	HIS
2	B	40	ASP
2	B	48	ASP
2	B	51	LEU
2	B	67	ALA
2	B	53	ASP
4	D	91	PHE
4	D	93	GLY
4	D	158	LEU
4	D	154	PRO
1	A	1462	THR
2	B	22	SER
1	A	1402	GLY
3	C	66	PRO
3	C	94	PRO

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	102/115 (89%)	80 (78%)	22 (22%)	1	7
2	B	86/92 (94%)	73 (85%)	13 (15%)	3	16
3	C	78/86 (91%)	65 (83%)	13 (17%)	2	14
4	D	138/148 (93%)	115 (83%)	23 (17%)	2	14
All	All	404/441 (92%)	333 (82%)	71 (18%)	2	12

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1383	LEU
1	A	1385	LYS
1	A	1386	GLN
1	A	1393	THR
1	A	1394	VAL
1	A	1406	SER
1	A	1407	GLU
1	A	1411	GLN
1	A	1416	LYS
1	A	1418	LEU
1	A	1426	ARG
1	A	1430	ASP
1	A	1434	ILE
1	A	1436	GLU
1	A	1448	ASP
1	A	1456	LEU
1	A	1461	GLN
1	A	1466	GLU
1	A	1469	GLN
1	A	1470	ILE
1	A	1475	ILE
1	A	1485	ARG
2	B	5	LEU
2	B	12	THR
2	B	13	THR
2	B	20	GLU
2	B	34	ILE
2	B	43	ARG
2	B	49	GLN
2	B	50	LEU
2	B	51	LEU
2	B	64	SER
2	B	65	GLN
2	B	98	GLU
2	B	103	MET
3	C	17	MET
3	C	32	LYS
3	C	37	LEU
3	C	59	GLU
3	C	61	ASN
3	C	70	LEU
3	C	73	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	78	THR
3	C	84	THR
3	C	98	GLU
3	C	99	ILE
3	C	105	MET
3	C	111	ASP
4	D	64	ARG
4	D	74	VAL
4	D	75	ILE
4	D	90	ASN
4	D	92	ASP
4	D	100	THR
4	D	101	LEU
4	D	113	ARG
4	D	116	LEU
4	D	126	ASP
4	D	130	VAL
4	D	132	GLN
4	D	150	ASN
4	D	153	LEU
4	D	171	LYS
4	D	178	LEU
4	D	188	LEU
4	D	195	GLN
4	D	203	GLN
4	D	204	GLU
4	D	205	ARG
4	D	206	ILE
4	D	208	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1386	GLN
1	A	1396	ASN
1	A	1441	HIS
1	A	1461	GLN
1	A	1469	GLN
3	C	61	ASN
4	D	96	GLN
4	D	132	GLN
4	D	141	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	208	HIS
4	D	209	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 ⓘ

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	$\# Z > 2$
5	A1IYN	D	301	-	84,88,88	1.01	4 (4%)	106,129,129	1.49	7 (6%)

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	A1IYN	D	301	-	-	26/59/103/103	0/9/10/10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	A1IYN	C71-N57	5.30	1.46	1.35
5	D	301	A1IYN	C68-C69	4.04	1.53	1.51
5	D	301	A1IYN	C71-N70	3.58	1.41	1.34
5	D	301	A1IYN	C74-C73	2.62	1.46	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	301	A1IYN	C6-C7-C3	-7.61	116.68	122.93
5	D	301	A1IYN	C58-N57-C71	-6.78	108.26	121.67
5	D	301	A1IYN	C71-N70-C69	4.61	121.25	116.19
5	D	301	A1IYN	C61-N57-C71	-4.51	112.76	121.67
5	D	301	A1IYN	N72-C71-N70	-4.03	119.10	126.27
5	D	301	A1IYN	C74-C69-N70	-3.40	120.86	123.48
5	D	301	A1IYN	C71-N72-C73	3.01	120.98	114.97

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	301	A1IYN	C40-C42-C43-C45
5	D	301	A1IYN	C40-C42-C43-C46
5	D	301	A1IYN	C40-C42-C43-C47
5	D	301	A1IYN	O49-C48-C50-C51
5	D	301	A1IYN	C63-C64-N66-C73
5	D	301	A1IYN	C74-C73-N66-C64
5	D	301	A1IYN	C78-C79-N56-C59
5	D	301	A1IYN	O16-C17-C18-O19
5	D	301	A1IYN	N72-C71-N57-C58
5	D	301	A1IYN	C50-C48-N44-C42
5	D	301	A1IYN	N44-C42-C43-C47
5	D	301	A1IYN	N72-C73-N66-C65
5	D	301	A1IYN	O49-C48-N44-C42
5	D	301	A1IYN	N44-C42-C43-C45
5	D	301	A1IYN	N44-C42-C43-C46
5	D	301	A1IYN	C74-C73-N66-C65
5	D	301	A1IYN	C78-C79-N56-C60
5	D	301	A1IYN	C18-C17-O16-C15
5	D	301	A1IYN	C14-C15-O16-C17
5	D	301	A1IYN	C62-C64-N66-C73
5	D	301	A1IYN	C17-C18-O19-C20
5	D	301	A1IYN	C79-C78-O13-C14

Continued on next page...

Continued from previous page...

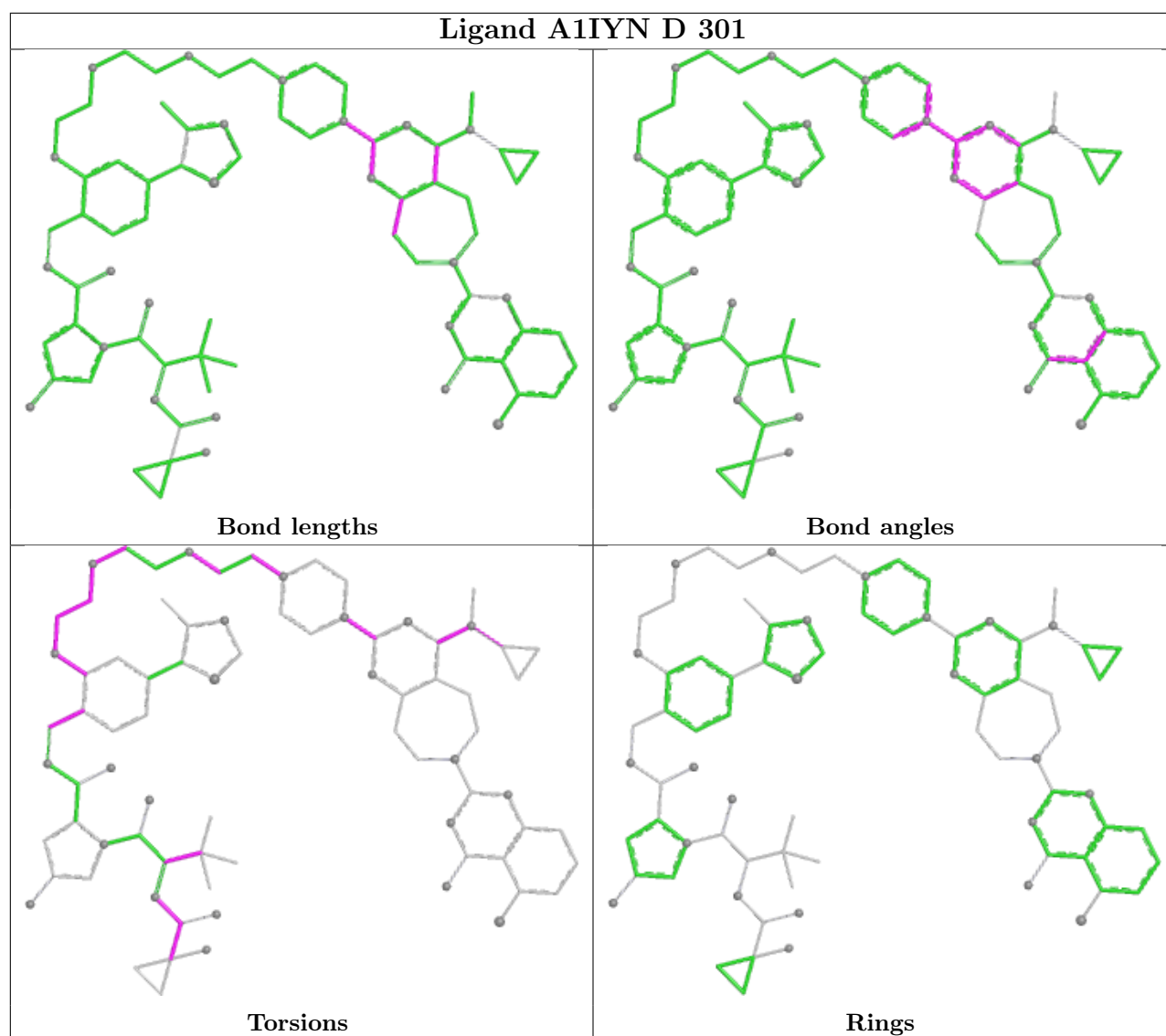
Mol	Chain	Res	Type	Atoms
5	D	301	A1IYN	C21-C20-O19-C18
5	D	301	A1IYN	C20-C25-C31-N32
5	D	301	A1IYN	C25-C20-O19-C18
5	D	301	A1IYN	N70-C71-N57-C61

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	301	A1IYN	3	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	109/123 (88%)	-0.17	1 (0%) 81 58	50, 61, 97, 116	0
2	B	104/104 (100%)	-0.49	0 100 100	43, 56, 81, 115	0
3	C	87/97 (89%)	-0.34	0 100 100	39, 57, 92, 113	0
4	D	149/162 (91%)	-0.28	1 (0%) 84 63	37, 52, 91, 111	0
All	All	449/486 (92%)	-0.31	2 (0%) 88 72	37, 57, 95, 116	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1478	GLN	3.6
4	D	106	GLY	2.3

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](#)

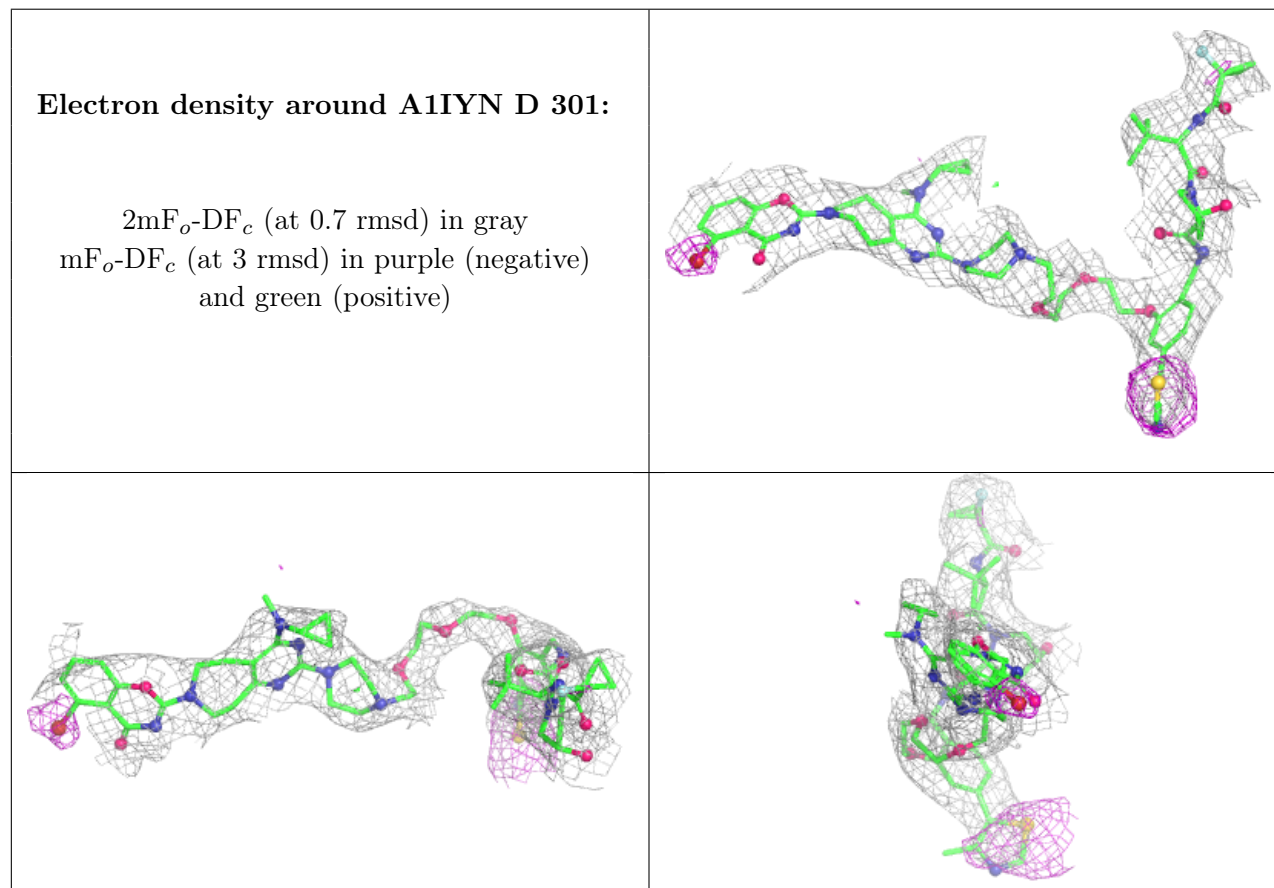
There are no oligosaccharides in this entry.

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(\AA^2)	Q<0.9
5	A1IYN	D	301	79/79	0.88	0.09	20,20,20,20	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.