



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:20 PM UTC

PDB ID : 7B9C / pdb_00007b9c
Title : Structure of a minimal SF3B core in complex with spliceostatin A (form I)
Authors : Cretu, C.; Pena, V.
Deposited on : 2020-12-14
Resolution : 2.40 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

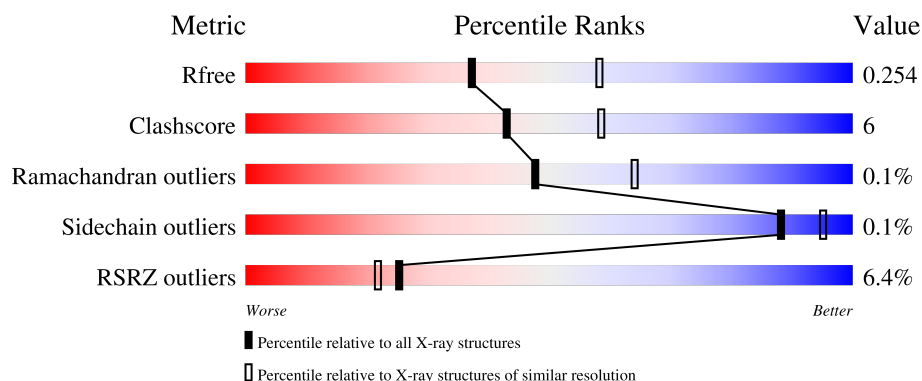
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	899	9% 78% 19% .
2	B	86	13% 78% 8% 14%
3	C	852	3% 84% 15% .
4	D	108	% 81% 15%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15067 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 Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	870	Total	C	N	O	S	0	1	0
			6880	4370	1177	1302	31			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q921M3
A	-8	ALA	-	expression tag	UNP Q921M3
A	-7	GLU	-	expression tag	UNP Q921M3
A	-6	PHE	-	expression tag	UNP Q921M3
A	-5	LYS	-	expression tag	UNP Q921M3
A	-4	GLY	-	expression tag	UNP Q921M3
A	-3	LEU	-	expression tag	UNP Q921M3
A	-2	ARG	-	expression tag	UNP Q921M3
A	-1	ARG	-	expression tag	UNP Q921M3
A	0	HIS	-	expression tag	UNP Q921M3
A	761	GLY	-	linker	UNP Q921M3
A	762	GLY	-	linker	UNP Q921M3
A	763	ASN	-	linker	UNP Q921M3
A	764	GLY	-	linker	UNP Q921M3
A	765	ASN	-	linker	UNP Q921M3
A	766	SER	-	linker	UNP Q921M3
A	767	GLY	-	linker	UNP Q921M3
A	?	-	GLU	deletion	UNP Q15393
A	?	-	ASP	deletion	UNP Q15393
A	?	-	PRO	deletion	UNP Q15393
A	?	-	THR	deletion	UNP Q15393
A	?	-	GLY	deletion	UNP Q15393
A	?	-	ASN	deletion	UNP Q15393
A	?	-	LYS	deletion	UNP Q15393
A	?	-	ALA	deletion	UNP Q15393
A	?	-	LEU	deletion	UNP Q15393
A	?	-	TRP	deletion	UNP Q15393

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q15393
A	?	-	ARG	deletion	UNP Q15393
A	?	-	GLY	deletion	UNP Q15393
A	?	-	LEU	deletion	UNP Q15393
A	?	-	LEU	deletion	UNP Q15393
A	?	-	ASN	deletion	UNP Q15393
A	?	-	GLY	deletion	UNP Q15393
A	?	-	ALA	deletion	UNP Q15393
A	1199	GLN	-	expression tag	UNP Q15393
A	1200	LEU	-	expression tag	UNP Q15393
A	1201	GLU	-	expression tag	UNP Q15393
A	1202	GLN	-	expression tag	UNP Q15393
A	1203	ASN	-	expression tag	UNP Q15393
A	1204	GLU	-	expression tag	UNP Q15393
A	1205	ALA	-	expression tag	UNP Q15393
A	1206	ALA	-	expression tag	UNP Q15393
A	1207	PHE	-	expression tag	UNP Q15393

- Molecule 2 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	74	Total	C	N	O	S	0	0	0
			607	384	106	112	5			

- Molecule 3 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	842	Total	C	N	O	S	0	0	0
			6707	4307	1152	1209	39			

- Molecule 4 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	92	Total	C	N	O	S	0	0	0
			693	424	122	134	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	GLY	-	expression tag	UNP Q7RTV0
D	-8	PRO	-	expression tag	UNP Q7RTV0
D	-7	LEU	-	expression tag	UNP Q7RTV0

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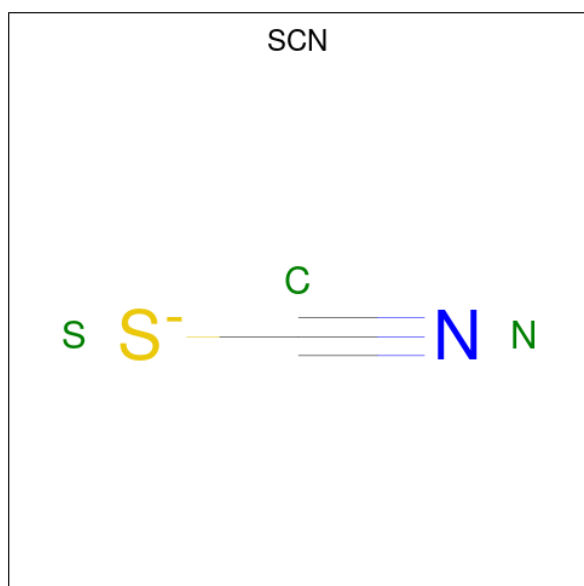
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q7RTV0
D	-5	SER	-	expression tag	UNP Q7RTV0
D	-4	PRO	-	expression tag	UNP Q7RTV0
D	-3	GLY	-	expression tag	UNP Q7RTV0
D	-2	SER	-	expression tag	UNP Q7RTV0
D	-1	ARG	-	expression tag	UNP Q7RTV0
D	0	ALA	-	expression tag	UNP Q7RTV0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

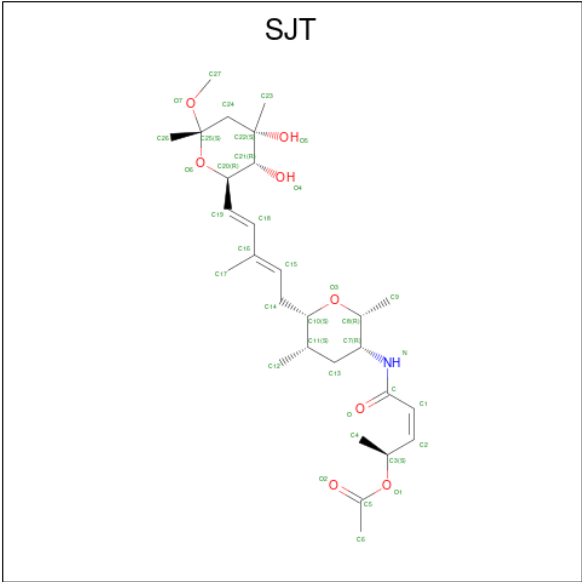
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	3	Total	Zn	0	0
			3	3		

- Molecule 6 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	S	0	0
			3	1	1	1		

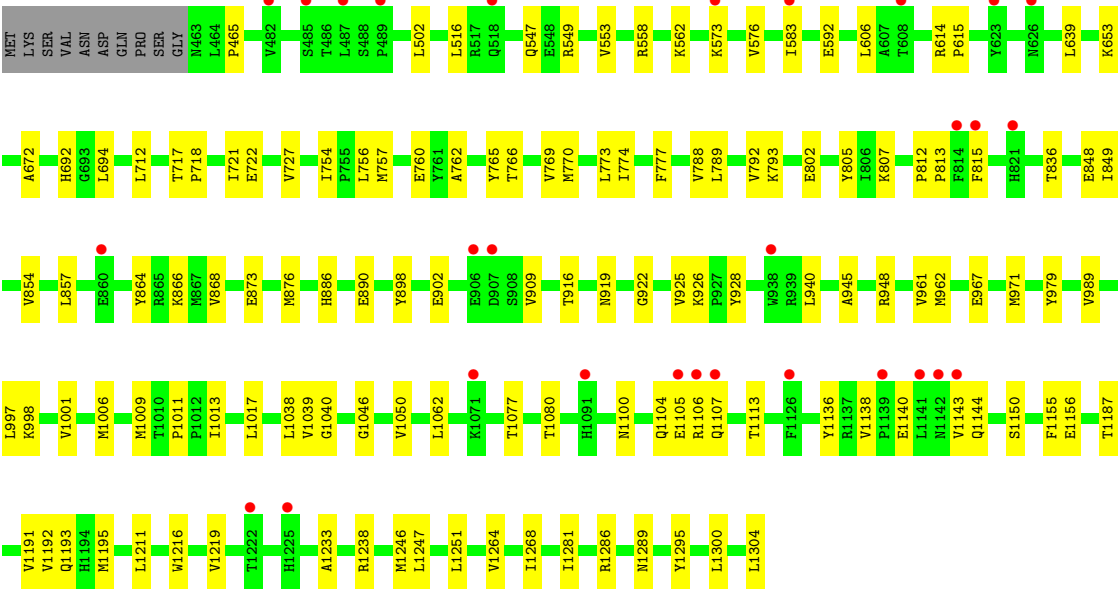
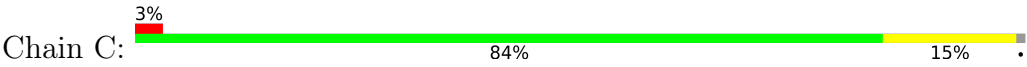
- Molecule 7 is spliceostatin A (form II) (CCD ID: SJT) (formula: C₂₈H₄₅NO₈) (labeled as "Ligand of Interest" by depositor).



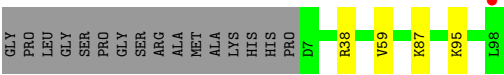
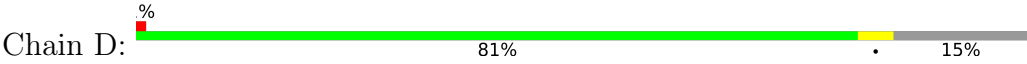
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			37	28	1	8		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	50	Total	O	0	0
			50	50		
8	B	4	Total	O	0	0
			4	4		
8	C	65	Total	O	0	0
			65	65		
8	D	18	Total	O	0	0
			18	18		



● Molecule 4: PHD finger-like domain-containing protein 5A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.57Å 111.07Å 248.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 2.40 49.75 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.75-2.40) 100.0 (49.75-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.216 , 0.248 0.223 , 0.254	Depositor DCC
R_{free} test set	6567 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15067	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: ZN, SJT, SCN

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	0/7032	0.36	0/9535
2	B	0.15	0/624	0.32	0/842
3	C	0.15	0/6835	0.34	0/9256
4	D	0.14	0/701	0.35	0/941
All	All	0.14	0/15192	0.35	0/20574

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	6880	0	6795	105	0
2	B	607	0	574	7	0
3	C	6707	0	6915	78	0
4	D	693	0	674	3	0
5	D	3	0	0	0	0
6	D	3	0	0	0	0
7	D	37	0	0	0	0
8	A	50	0	0	1	0
8	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	65	0	0	0	0
8	D	18	0	0	0	0
All	All	15067	0	14958	184	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 (184) 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)
3:C:1006:MET:HG2	3:C:1046:GLY:HA3	1.49	0.92
3:C:757:MET:HE3	3:C:762:ALA:HA	1.67	0.77
1:A:1112:VAL:HG13	1:A:1198:ALA:HA	1.68	0.75
3:C:1006:MET:HG3	3:C:1013:ILE:HG13	1.69	0.75
3:C:754:ILE:HA	3:C:757:MET:HE2	1.70	0.72
1:A:805:ASN:HB2	2:B:58:ASN:HB3	1.79	0.65
1:A:352:GLU:HB2	2:B:61:LYS:HE3	1.79	0.65
1:A:820:ALA:HA	1:A:823:MET:HE3	1.78	0.65
1:A:877:LEU:HD13	1:A:935:GLU:HG2	1.77	0.65
3:C:1192:VAL:HA	3:C:1195:MET:HE2	1.79	0.64
1:A:1006:GLN:OE1	3:C:1286:ARG:NH2	2.30	0.64
1:A:428:GLY:HA3	1:A:433:SER:HA	1.79	0.64
1:A:1182:THR:HG23	1:A:1185:GLU:H	1.63	0.63
3:C:866:LYS:HG3	3:C:909:VAL:HG11	1.80	0.63
3:C:1105:GLU:O	3:C:1107:GLN:N	2.31	0.63
1:A:10:ARG:NH1	1:A:57:GLU:OE2	2.32	0.63
3:C:919:ASN:HA	3:C:961:VAL:HG21	1.81	0.62
3:C:762:ALA:O	3:C:766:THR:HG23	2.00	0.62
3:C:573:LYS:HA	3:C:576:VAL:HG12	1.81	0.62
1:A:1049:LYS:NZ	3:C:1300:LEU:O	2.32	0.62
1:A:820:ALA:HB1	1:A:839:ALA:HB1	1.81	0.62
1:A:791:HIS:HE2	1:A:903:TRP:CG	2.18	0.60
1:A:947:GLU:HB3	1:A:963:VAL:HG12	1.84	0.60
1:A:1000:VAL:HG13	1:A:1012:VAL:HB	1.82	0.60
1:A:791:HIS:ND1	1:A:794:SER:HB3	2.17	0.60
3:C:945:ALA:HB1	3:C:989:VAL:HG21	1.84	0.60
3:C:807:LYS:HE3	3:C:848:GLU:HG3	1.85	0.59
1:A:240:GLY:HA3	1:A:246:SER:HB2	1.84	0.59
3:C:757:MET:HE1	3:C:765:TYR:HB3	1.85	0.58
1:A:412:ILE:HD13	1:A:1091:LEU:HD21	1.84	0.58
1:A:794:SER:OG	1:A:796:ASN:ND2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1195:MET:HE1	3:C:1211:LEU:HD13	1.85	0.57
3:C:864:TYR:O	3:C:868:VAL:HG23	2.03	0.57
1:A:888:ALA:HA	1:A:909:VAL:HG12	1.86	0.57
1:A:865:VAL:HG12	1:A:881:GLN:HA	1.86	0.57
1:A:867:ARG:HG3	1:A:876:THR:HG23	1.87	0.57
1:A:899:THR:HG21	1:A:904:TYR:HE1	1.70	0.57
3:C:766:THR:HA	3:C:769:VAL:HG22	1.86	0.56
1:A:1055:VAL:HB	1:A:1075:MET:HB3	1.86	0.56
3:C:922:GLY:O	3:C:925:VAL:HG12	2.05	0.56
3:C:1113:THR:HG23	3:C:1150:SER:HA	1.87	0.56
3:C:1138:VAL:HB	3:C:1143:VAL:HG11	1.86	0.56
3:C:1238:ARG:HA	3:C:1246:MET:HE3	1.86	0.56
3:C:979:TYR:CG	3:C:1011:PRO:HG3	2.42	0.55
3:C:549:ARG:NH1	3:C:592:GLU:OE1	2.31	0.55
1:A:910:ALA:HB2	1:A:948:VAL:HG13	1.89	0.55
3:C:793:LYS:HB2	3:C:836:THR:HG23	1.89	0.54
1:A:101:LYS:HD3	1:A:104:GLN:HB2	1.89	0.53
1:A:168:TYR:HB2	1:A:185:LEU:HB2	1.89	0.53
3:C:1062:LEU:HG	3:C:1077:THR:HG23	1.90	0.52
3:C:1187:THR:O	3:C:1191:VAL:HG23	2.09	0.51
1:A:1015:LYS:HD2	1:A:1022:ILE:HD13	1.91	0.51
1:A:120:PHE:HB2	1:A:133:SER:HB3	1.93	0.51
3:C:1193:GLN:HB2	3:C:1233:ALA:HA	1.93	0.51
3:C:940:LEU:O	3:C:948:ARG:HD3	2.11	0.51
3:C:802:GLU:HG3	3:C:805:TYR:H	1.76	0.51
1:A:926:TYR:CZ	1:A:942:LYS:HE2	2.46	0.50
1:A:239:PRO:HB3	1:A:294:LYS:HD3	1.93	0.50
1:A:131:MET:HE3	1:A:139:LYS:HB3	1.94	0.49
1:A:267:ILE:HD13	1:A:322:VAL:HG23	1.94	0.49
1:A:930:LEU:HG	1:A:934:GLY:HA2	1.94	0.49
1:A:175:VAL:HG11	1:A:181:MET:HG3	1.95	0.49
1:A:829:GLU:N	1:A:829:GLU:OE2	2.46	0.49
1:A:246:SER:O	1:A:246:SER:OG	2.28	0.49
3:C:815:PHE:HZ	3:C:849:ILE:HG23	1.77	0.49
1:A:808:THR:HG1	1:A:811:THR:HG1	1.60	0.49
3:C:962:MET:HE3	3:C:971:MET:HE1	1.95	0.48
1:A:816:LYS:NZ	1:A:845:GLU:O	2.44	0.48
1:A:416:ALA:HB3	1:A:418:GLU:HG3	1.95	0.48
3:C:672:ALA:HB2	3:C:712:LEU:HD23	1.96	0.48
1:A:328:LYS:HG3	1:A:372:GLU:HA	1.95	0.48
1:A:1091:LEU:HD11	1:A:1100:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD21	1:A:250:ILE:HD13	1.96	0.48
1:A:269:CYS:HB2	1:A:375:SER:HB3	1.96	0.48
1:A:440:HIS:HE2	1:A:1197:TYR:HE1	1.61	0.48
1:A:379:LEU:HD23	1:A:385:PHE:CE1	2.49	0.47
1:A:797:LEU:HG	1:A:871:PRO:HG3	1.95	0.47
3:C:465:PRO:HG2	3:C:502:LEU:HG	1.95	0.47
3:C:760:GLU:H	3:C:760:GLU:CD	2.21	0.47
4:D:59:VAL:HA	4:D:87:LYS:HD2	1.97	0.47
3:C:873:GLU:HG2	3:C:916:THR:OG1	2.15	0.47
1:A:875:ASN:OD1	1:A:875:ASN:N	2.46	0.47
1:A:896:PHE:HB2	1:A:899:THR:HG22	1.97	0.47
1:A:229:GLU:OE2	1:A:268:ARG:NH1	2.48	0.46
3:C:1264:VAL:O	3:C:1268:ILE:HG13	2.16	0.46
1:A:1077:TYR:HB2	1:A:1155:VAL:HG21	1.96	0.46
2:B:38:ASP:HB3	3:C:1281:ILE:HD11	1.97	0.46
3:C:553:VAL:HG21	3:C:592:GLU:HB3	1.98	0.46
1:A:185:LEU:HD21	1:A:235:LEU:HD21	1.97	0.46
1:A:833:GLU:HG3	1:A:834:LEU:N	2.31	0.46
1:A:1084:LEU:HD21	3:C:1304:LEU:HD12	1.96	0.46
3:C:854:VAL:O	3:C:857:LEU:HB2	2.16	0.46
1:A:1101:TYR:CZ	1:A:1109:GLY:HA3	2.51	0.46
3:C:547:GLN:HE21	4:D:95:LYS:HE2	1.80	0.46
3:C:606:LEU:HB2	3:C:639:LEU:HD13	1.98	0.45
3:C:1017:LEU:HD11	3:C:1039:VAL:HG13	1.98	0.45
3:C:1155:PHE:CD1	3:C:1195:MET:HG2	2.51	0.45
3:C:722:GLU:H	3:C:722:GLU:CD	2.24	0.45
3:C:1216:TRP:O	3:C:1219:VAL:HG22	2.15	0.45
3:C:1289:ASN:OD1	3:C:1295:TYR:N	2.44	0.45
1:A:819:MET:HA	1:A:822:GLU:HG2	1.99	0.45
1:A:373:PHE:HB3	1:A:385:PHE:CD2	2.52	0.45
1:A:1020:GLN:HB3	1:A:1022:ILE:HD11	1.99	0.45
1:A:260:ASN:HB3	1:A:264:GLN:HG2	1.99	0.45
2:B:11:LEU:HD12	2:B:11:LEU:HA	1.85	0.45
3:C:653:LYS:HG3	3:C:692:HIS:CE1	2.52	0.45
1:A:947:GLU:HG2	1:A:964:GLY:HA3	1.99	0.45
1:A:960:LEU:HD22	1:A:967:LEU:HD11	1.99	0.45
3:C:614:ARG:N	3:C:615:PRO:HD2	2.31	0.45
3:C:694:LEU:HD11	3:C:727:VAL:HG13	1.98	0.44
1:A:125:PRO:HG2	1:A:174:ASP:HA	1.99	0.44
1:A:1063:ASN:HB3	1:A:1066:VAL:HG22	1.99	0.44
3:C:774:ILE:O	3:C:777:PHE:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLY:HA2	1:A:132:ILE:HD11	1.99	0.44
1:A:327:LEU:HD12	1:A:327:LEU:N	2.33	0.44
3:C:1001:VAL:HG22	3:C:1009:MET:HG3	1.99	0.44
1:A:422:GLN:HB2	1:A:424:TYR:CE2	2.53	0.44
3:C:788:VAL:O	3:C:792:VAL:HG13	2.17	0.44
1:A:831:GLU:HB2	1:A:833:GLU:HG3	1.99	0.44
3:C:1136:TYR:CE1	3:C:1144:GLN:HB3	2.53	0.44
1:A:1027:ASP:OD1	1:A:1028:THR:N	2.50	0.43
3:C:516:LEU:HD11	3:C:558:ARG:HG3	2.00	0.43
3:C:562:LYS:HE2	3:C:562:LYS:HB2	1.82	0.43
1:A:328:LYS:CG	1:A:372:GLU:HA	2.49	0.43
1:A:1123:PHE:HE1	1:A:1190:LEU:HD23	1.83	0.43
1:A:96:LYS:HB2	1:A:98:MET:HG2	2.00	0.43
3:C:770:MET:HE1	3:C:773:LEU:HD23	2.00	0.43
3:C:1140:GLU:HB3	3:C:1143:VAL:HG12	2.00	0.43
1:A:258:TYR:CD1	1:A:322:VAL:HG21	2.54	0.43
1:A:1182:THR:HG22	1:A:1185:GLU:OE1	2.18	0.43
3:C:1100:ASN:O	3:C:1104:GLN:HG2	2.18	0.43
1:A:372:GLU:O	1:A:377:MET:HE1	2.18	0.43
1:A:1115:THR:OG1	1:A:1116:SER:N	2.52	0.43
3:C:926:LYS:NZ	3:C:967:GLU:OE1	2.49	0.43
1:A:990:ILE:HG23	1:A:1002:VAL:HG13	2.01	0.43
3:C:1247:LEU:O	3:C:1251:LEU:HG	2.19	0.43
1:A:23:SER:OG	1:A:29:GLU:OE1	2.35	0.42
1:A:807:TYR:CZ	1:A:857:ALA:HA	2.54	0.42
3:C:886:HIS:O	3:C:890:GLU:HG3	2.19	0.42
3:C:967:GLU:O	3:C:971:MET:HG2	2.19	0.42
1:A:270:PRO:HG3	1:A:379:LEU:HD21	2.00	0.42
1:A:310:ILE:HD11	1:A:333:VAL:HG22	1.99	0.42
1:A:187:MET:SD	2:B:73:LEU:HD22	2.60	0.42
3:C:925:VAL:HA	3:C:928:TYR:HD2	1.84	0.42
1:A:874:GLY:O	8:A:1301:HOH:O	2.20	0.42
1:A:10:ARG:HD2	1:A:55:THR:HG21	2.00	0.42
3:C:948:ARG:NH2	3:C:948:ARG:HB2	2.33	0.42
1:A:49:LYS:NZ	1:A:398:VAL:O	2.47	0.42
1:A:208:LEU:O	1:A:225:SER:HA	2.20	0.42
3:C:766:THR:O	3:C:770:MET:HB2	2.20	0.42
1:A:379:LEU:HD22	1:A:383:ASP:O	2.19	0.42
3:C:721:ILE:HD13	3:C:756:LEU:HB2	2.02	0.42
3:C:876:MET:HE2	3:C:876:MET:HB3	1.95	0.42
1:A:288:VAL:HG21	1:A:335:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:789:LEU:O	3:C:792:VAL:HG22	2.20	0.41
1:A:1147:SER:HB3	1:A:1151:PRO:HA	2.03	0.41
1:A:994:GLN:NE2	1:A:1036:ALA:O	2.49	0.41
1:A:1191:GLU:O	1:A:1195:THR:HG23	2.19	0.41
1:A:236:ILE:HB	1:A:249:LEU:HB2	2.01	0.41
1:A:255:TYR:CD1	1:A:268:ARG:HD3	2.55	0.41
2:B:11:LEU:HG	2:B:12:GLU:H	1.85	0.41
1:A:1028:THR:HG22	1:A:1070:LYS:HD2	2.02	0.41
1:A:1091:LEU:O	1:A:1092:ILE:HD13	2.21	0.41
1:A:894:CYS:HB3	1:A:954:PRO:HG3	2.02	0.41
3:C:998:LYS:HA	3:C:1038:LEU:HD13	2.03	0.41
1:A:866:ILE:HB	1:A:880:VAL:CG1	2.51	0.41
3:C:1017:LEU:HD22	3:C:1050:VAL:HG21	2.03	0.41
1:A:181:MET:HE3	1:A:212:GLU:HB2	2.03	0.41
1:A:886:GLU:OE1	1:A:926:TYR:OH	2.32	0.41
3:C:812:PRO:HB2	3:C:813:PRO:HD3	2.03	0.41
1:A:1173:LYS:HE3	1:A:1177:GLU:OE1	2.22	0.40
1:A:377:MET:HB2	1:A:385:PHE:HZ	1.86	0.40
1:A:929:LYS:HB2	1:A:929:LYS:HE2	1.85	0.40
2:B:72:MET:HE3	2:B:72:MET:HB3	1.96	0.40
3:C:717:THR:HA	3:C:718:PRO:HA	1.82	0.40
3:C:1040:GLY:HA2	3:C:1080:THR:HG23	2.04	0.40
1:A:86:ARG:HG2	1:A:106:THR:HA	2.02	0.40
1:A:384:THR:O	1:A:385:PHE:HB2	2.21	0.40
1:A:920:VAL:HG22	1:A:922:GLY:H	1.86	0.40
3:C:583:ILE:H	3:C:583:ILE:HG13	1.81	0.40
1:A:295:THR:OG1	1:A:298:MET:O	2.37	0.40
1:A:801:GLU:O	1:A:864:SER:HA	2.22	0.40
3:C:898:TYR:CZ	3:C:902:GLU:HG3	2.56	0.40
3:C:1156:GLU:O	4:D:38:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	867/899 (96%)	824 (95%)	43 (5%)	0	100	100
2	B	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
3	C	840/852 (99%)	822 (98%)	17 (2%)	1 (0%)	48	64
4	D	90/108 (83%)	86 (96%)	4 (4%)	0	100	100
All	All	1869/1945 (96%)	1801 (96%)	67 (4%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	1106	ARG

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	755/772 (98%)	755 (100%)	0	100	100
2	B	65/77 (84%)	65 (100%)	0	100	100
3	C	728/737 (99%)	727 (100%)	1 (0%)	88	95
4	D	79/90 (88%)	79 (100%)	0	100	100
All	All	1627/1676 (97%)	1626 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	997	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN

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Mol	Chain	Res	Type
1	A	218	ASN
1	A	394	ASN
1	A	411	GLN
1	A	844	ASN
3	C	547	GLN
3	C	682	HIS
3	C	1218	ASN

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 ⓘ

Of 5 ligands modelled in this entry, 3 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	$\# Z > 2$
7	SJT	D	105	4	38,38,38	0.20	0	51,55,55	0.60	1 (1%)
6	SCN	D	104	-	1,2,2	0.83	0	0,1,1	-	-

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
7	SJT	D	105	4	-	0/26/63/63	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	105	SJT	C2-C1-C	2.46	128.47	122.67

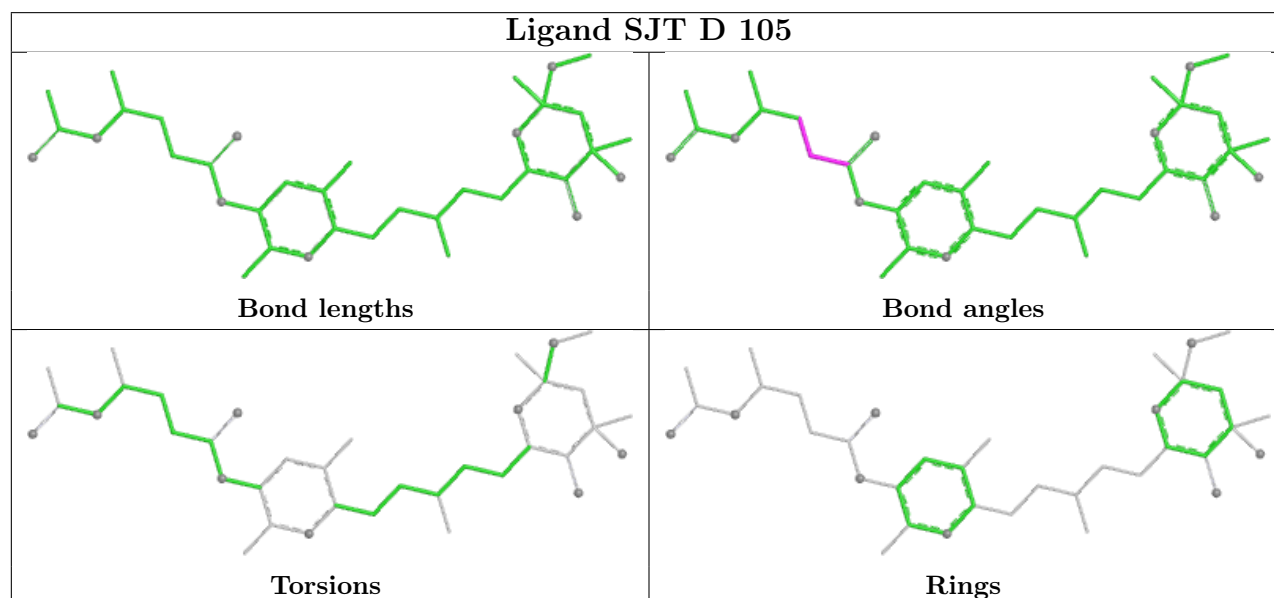
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	870/899 (96%)	0.78	79 (9%) 15 12	47, 74, 110, 150	1 (0%)
2	B	74/86 (86%)	0.85	11 (14%) 5 4	52, 65, 111, 121	0
3	C	842/852 (98%)	0.44	29 (3%) 48 44	50, 70, 96, 122	0
4	D	92/108 (85%)	0.13	1 (1%) 78 74	51, 59, 83, 96	0
All	All	1878/1945 (96%)	0.60	120 (6%) 25 22	47, 71, 104, 150	1 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	98	LEU	6.0
2	B	11	LEU	5.7
1	A	1066	VAL	5.0
1	A	428	GLY	4.7
2	B	14	LEU	4.7
3	C	938	TRP	4.6
1	A	773	VAL	4.5
2	B	13	HIS	4.5
1	A	0	HIS	4.3
1	A	148	ALA	4.3
1	A	835	ALA	4.2
1	A	1094	GLY	4.1
1	A	1198	ALA	3.9
1	A	278	LEU	3.9
1	A	384	THR	3.9
1	A	1197	TYR	3.6
1	A	824	VAL	3.6
1	A	1095	GLY	3.5
2	B	82	LYS	3.5
1	A	834	LEU	3.5
1	A	378	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	821	HIS	3.3
2	B	9	SER	3.3
3	C	1141	LEU	3.2
1	A	1	MET	3.1
1	A	224	TYR	3.1
1	A	379	LEU	3.1
2	B	15	GLN	3.0
1	A	826	ALA	3.0
3	C	1105	GLU	2.9
3	C	1107	GLN	2.9
3	C	1106	ARG	2.9
1	A	839	ALA	2.9
3	C	1143	VAL	2.8
1	A	373	PHE	2.8
3	C	482	VAL	2.8
1	A	1062	THR	2.8
1	A	385	PHE	2.8
3	C	1126	PHE	2.8
1	A	1117	HIS	2.7
1	A	1068	SER	2.7
1	A	-2	ARG	2.7
1	A	269	CYS	2.7
3	C	608	THR	2.7
1	A	366	ASP	2.6
1	A	440	HIS	2.6
1	A	343	LYS	2.6
1	A	1092	ILE	2.6
1	A	899	THR	2.6
1	A	874	GLY	2.6
1	A	914	ILE	2.6
1	A	427	CYS	2.6
1	A	827	ALA	2.6
3	C	1139	PRO	2.5
1	A	363	HIS	2.5
1	A	382	GLY	2.5
2	B	12	GLU	2.5
3	C	814	PHE	2.5
3	C	1142	ASN	2.5
1	A	-1	ARG	2.5
1	A	27[A]	GLN	2.5
1	A	836	ALA	2.5
3	C	1091	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	321	MET	2.5
1	A	320	ASP	2.4
1	A	842	PHE	2.4
1	A	1175	VAL	2.4
1	A	364	LEU	2.4
3	C	907	ASP	2.4
3	C	906	GLU	2.4
1	A	361	ILE	2.3
1	A	851	ILE	2.3
1	A	441	GLY	2.3
1	A	852	PHE	2.3
3	C	1071	LYS	2.3
2	B	18	TYR	2.3
3	C	626	ASN	2.3
3	C	1222	THR	2.3
1	A	900	GLY	2.3
3	C	487	LEU	2.3
3	C	815	PHE	2.3
3	C	623	TYR	2.3
3	C	485	SER	2.3
1	A	1093	PRO	2.3
1	A	1061	ASN	2.2
1	A	1063	ASN	2.2
1	A	47	THR	2.2
1	A	322	VAL	2.2
1	A	1195	THR	2.2
1	A	1128	MET	2.2
1	A	1116	SER	2.2
1	A	268	ARG	2.2
1	A	388	GLN	2.2
2	B	81	ASP	2.2
1	A	265	PRO	2.2
2	B	58	ASN	2.2
1	A	843	LEU	2.2
1	A	872	ILE	2.2
1	A	865	VAL	2.1
1	A	840	ALA	2.1
1	A	898	ASN	2.1
1	A	371	PRO	2.1
1	A	247	GLY	2.1
1	A	847	LEU	2.1
1	A	319	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	904	TYR	2.1
1	A	365	GLY	2.1
3	C	860	GLU	2.1
3	C	489	PRO	2.1
3	C	1225	HIS	2.1
1	A	922	GLY	2.1
2	B	17	LYS	2.1
3	C	518	GLN	2.0
1	A	774	PHE	2.0
1	A	1123	PHE	2.0
3	C	573	LYS	2.0
3	C	583	ILE	2.0
1	A	1096	SER	2.0
1	A	296	LYS	2.0
1	A	1193	ILE	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.

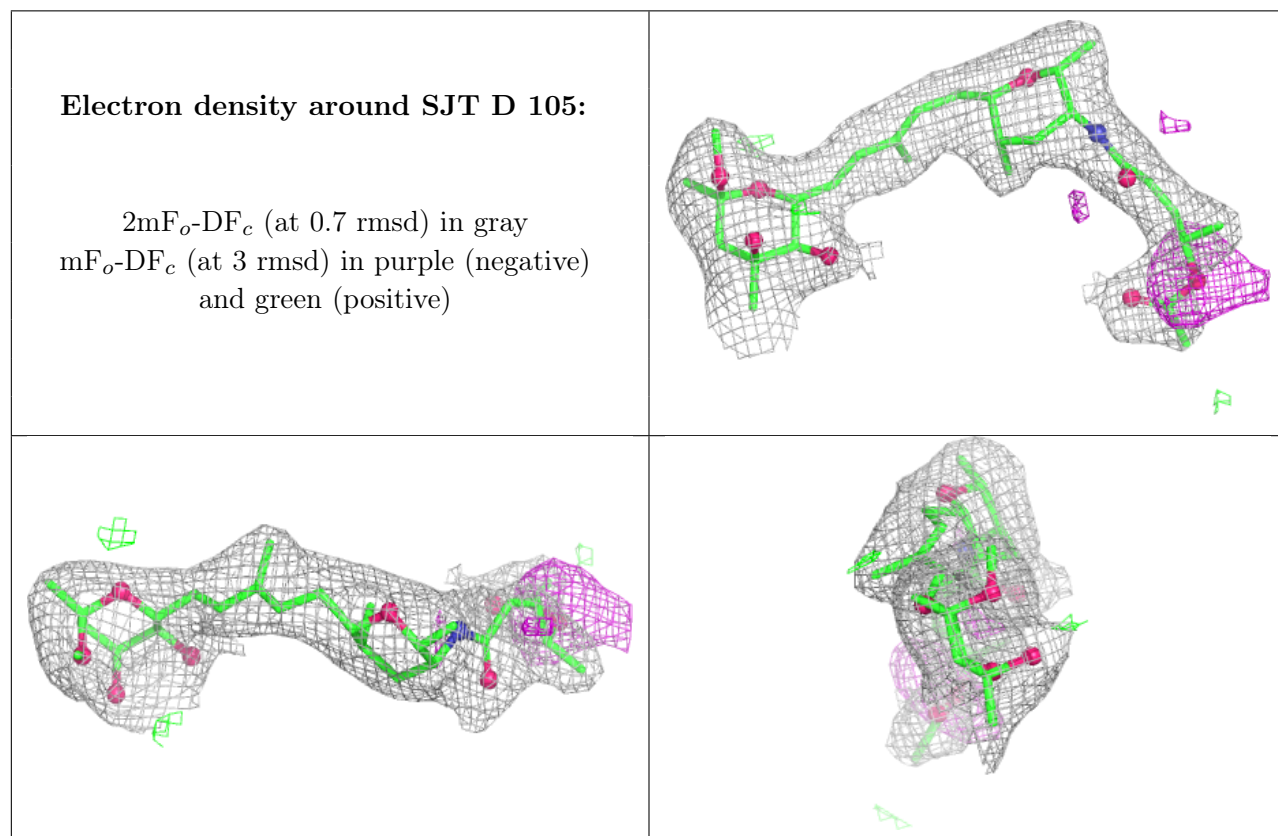
6.4 Ligands [i](#)

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
6	SCN	D	104	3/3	0.92	0.19	63,63,73,99	0
7	SJT	D	105	37/37	0.93	0.12	47,57,70,83	0
5	ZN	D	101	1/1	0.99	0.03	61,61,61,61	0
5	ZN	D	103	1/1	0.99	0.03	57,57,57,57	0
5	ZN	D	102	1/1	1.00	0.03	53,53,53,53	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 ⓘ

There are no such residues in this entry.