Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2021 – 05:14 pm BST

PDB ID	:	7B9C
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 following versions of software and data (see references ⓘ) were used in the production of this report:

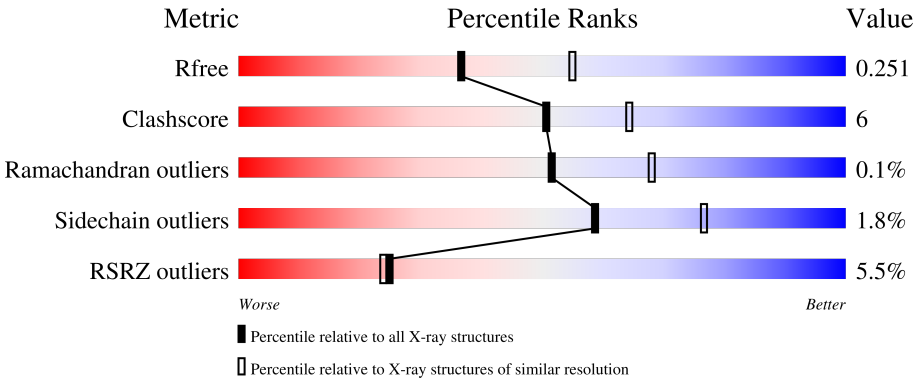
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

1 Overall quality at a glance (i)

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	8% 78% 19%
2	B	86	21% 78% 8% 14%
3	C	852	83% 16%
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
			Total	C	N	O	S			
1	A	870	6880	4370	1177	1302	31	0	1	0

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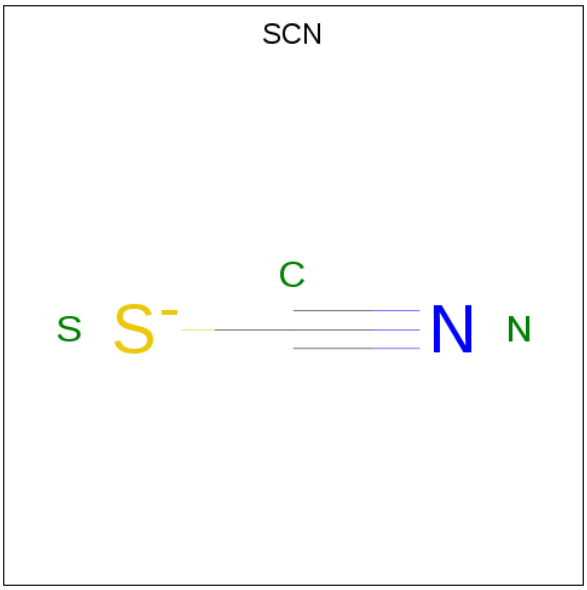
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q7RTV0
D	-5	SER	-	expression tag	UNP Q7RTV0
D	-4	PRO	-	expression tag	UNP Q7RTV0
D	-3	GLY	-	expression tag	UNP Q7RTV0
D	-2	SER	-	expression tag	UNP Q7RTV0
D	-1	ARG	-	expression tag	UNP Q7RTV0
D	0	ALA	-	expression tag	UNP Q7RTV0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

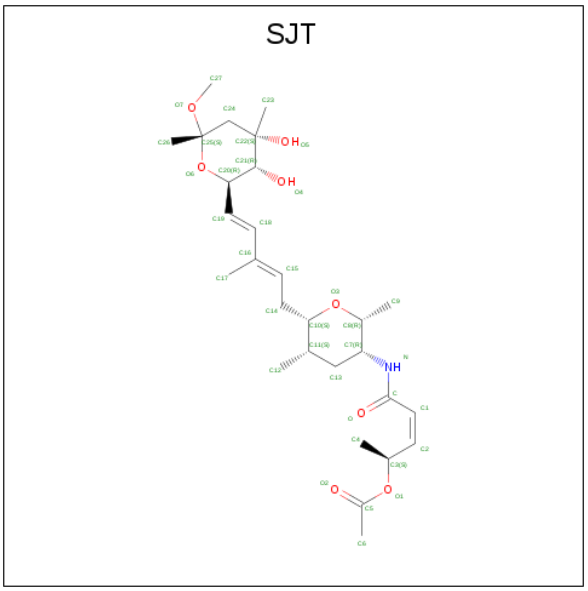
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	D	3	3	3	0	0

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 7 is spliceostatin A (form II) (three-letter code: SJT) (formula: $C_{28}H_{45}NO_8$) (labeled as "Ligand of Interest" by depositor).



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

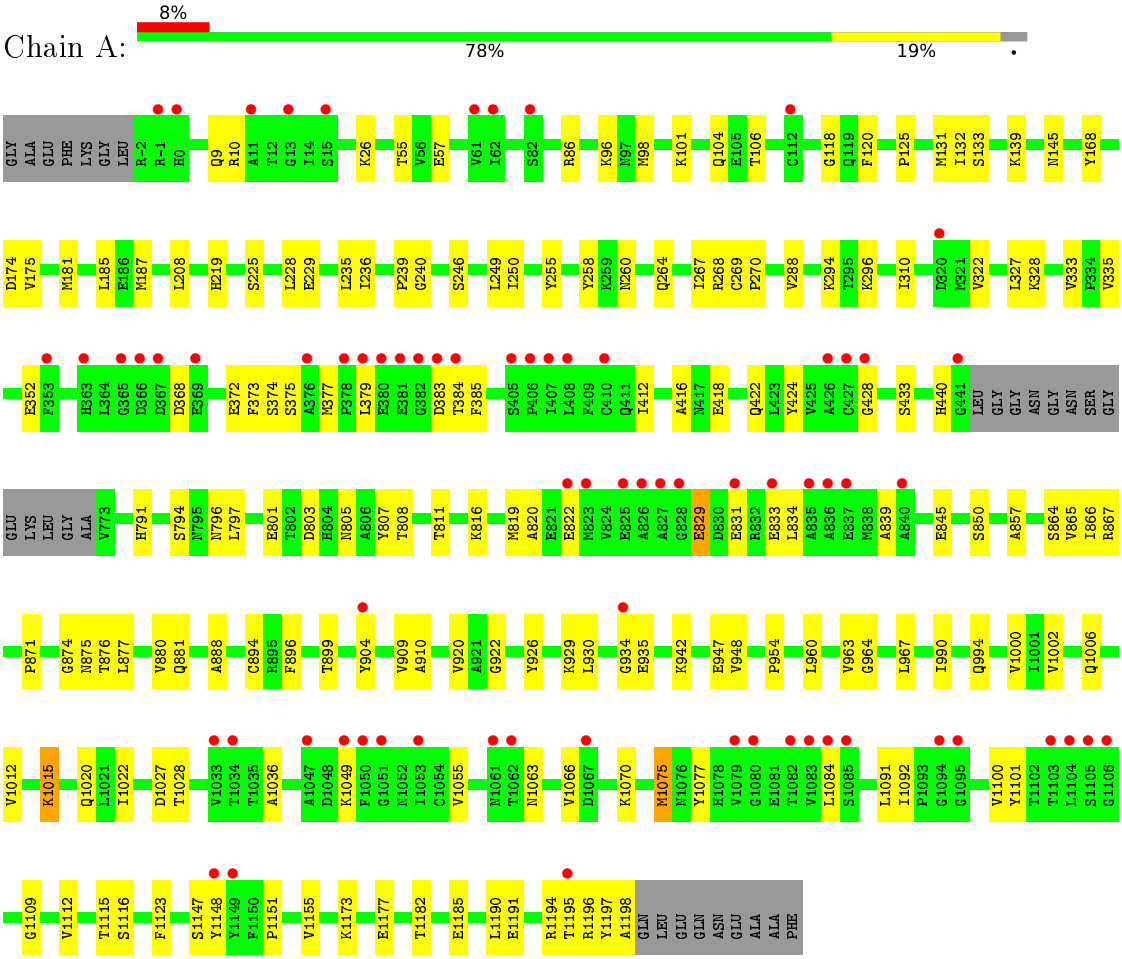
- Molecule 8 is water.

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

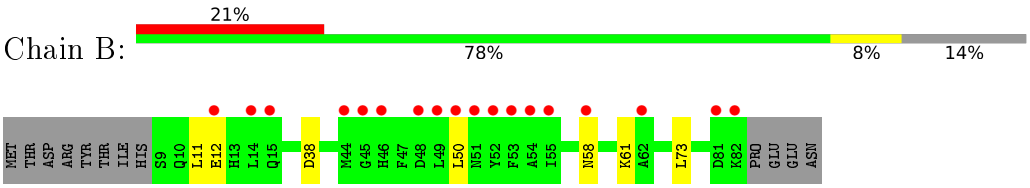
3 Residue-property plots (i)

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: Splicing factor 3B subunit 3

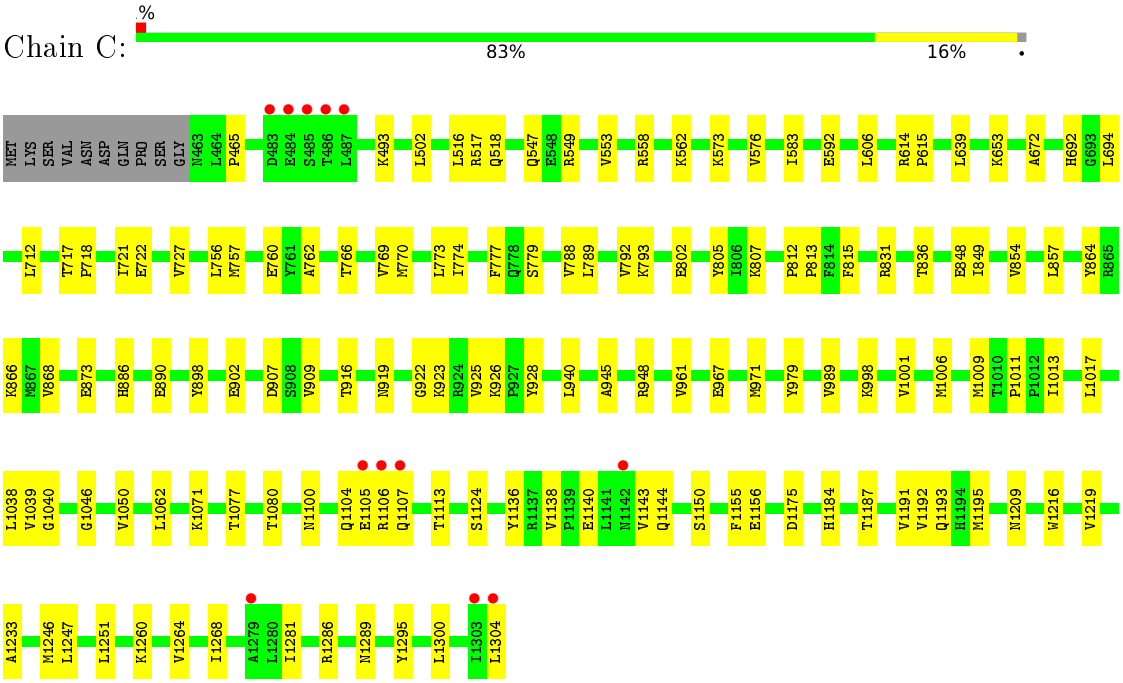


- Molecule 2: Splicing factor 3B subunit 5



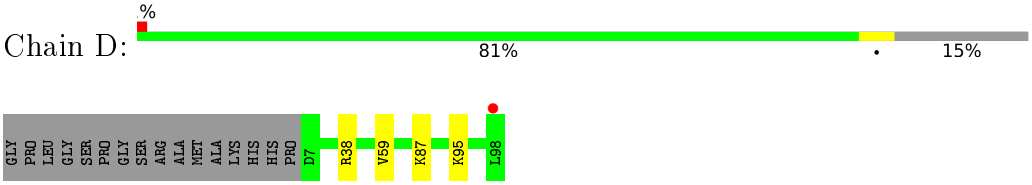
- Molecule 3: Splicing factor 3B subunit 1

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.75-2.40) 99.6 (49.75-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.216 , 0.248 0.219 , 0.251	Depositor DCC
R_{free} test set	6567 reflections (4.93%)	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 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SJT, ZN, 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	0.27	0/7032	0.46	0/9535
2	B	0.26	0/624	0.41	0/842
3	C	0.25	0/6835	0.41	0/9256
4	D	0.26	0/701	0.46	0/941
All	All	0.26	0/15192	0.44	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

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	97	0
2	B	607	0	574	6	0
3	C	6707	0	6915	73	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	170	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 (170) 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
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
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:877:LEU:HD13	1:A:935:GLU:HG2	1.77	0.65
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: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
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
3:C:864:TYR:O	3:C:868:VAL:HG23	2.03	0.57
3:C:757:MET:HE3	3:C:762:ALA:HA	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1192:VAL:HA	3:C:1195:MET:HE2	1.85	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: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: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
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:770:MET:HE3	3:C:773:LEU:HB3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:816:LYS:NZ	1:A:845:GLU:O	2.44	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: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
3:C:926:LYS:NZ	3:C:967:GLU:OE1	2.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:760:GLU:H	3:C:760:GLU:CD	2.21	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:1115:THR:OG1	1:A:1116:SER:N	2.52	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: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
3:C:1195:MET:HE2	3:C:1195:MET:HB2	1.78	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:808:THR:OG1	1:A:811:THR:OG1	2.34	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
1:A:288:VAL:HG21	1:A:335:VAL:HG13	2.02	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:717:THR:HA	3:C:718:PRO:HA	1.82	0.40
3:C:722:GLU:H	3:C:722:GLU:CD	2.24	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: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 (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	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%)	51 68
4	D	90/108 (83%)	86 (96%)	4 (4%)	0	100 100
All	All	1869/1945 (96%)	1801 (96%)	67 (4%)	1 (0%)	51 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	1106	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	755/772 (98%)	740 (98%)	15 (2%)	55	74
2	B	65/77 (84%)	64 (98%)	1 (2%)	65	80
3	C	728/737 (99%)	714 (98%)	14 (2%)	57	75
4	D	79/90 (88%)	79 (100%)	0	100	100
All	All	1627/1676 (97%)	1597 (98%)	30 (2%)	59	76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	26	LYS
1	A	145	ASN
1	A	219	HIS
1	A	296	LYS
1	A	368	ASP
1	A	374	SER
1	A	803	ASP
1	A	829	GLU
1	A	850	SER
1	A	1015	LYS
1	A	1075	MET
1	A	1148	TYR
1	A	1194	ARG
1	A	1196	ARG
2	B	50	LEU
3	C	493	LYS
3	C	517	ARG
3	C	518	GLN
3	C	779	SER
3	C	831	ARG

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Mol	Chain	Res	Type
3	C	907	ASP
3	C	923	LYS
3	C	1071	LYS
3	C	1124	SER
3	C	1175	ASP
3	C	1184	HIS
3	C	1209	ASN
3	C	1246	MET
3	C	1260	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
3	C	547	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 monosaccharides 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	$\#\|Z\|>2$
6	SCN	D	104	-	1,2,2	0.85	0	0,1,1	0.00	-
7	SJT	D	105	4	37,38,38	0.19	0	42,55,55	0.57	1 (2%)

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(^{o})	Ideal(^{o})
7	D	105	SJT	C2-C1-C	2.31	128.47	122.69

There are no chirality outliers.

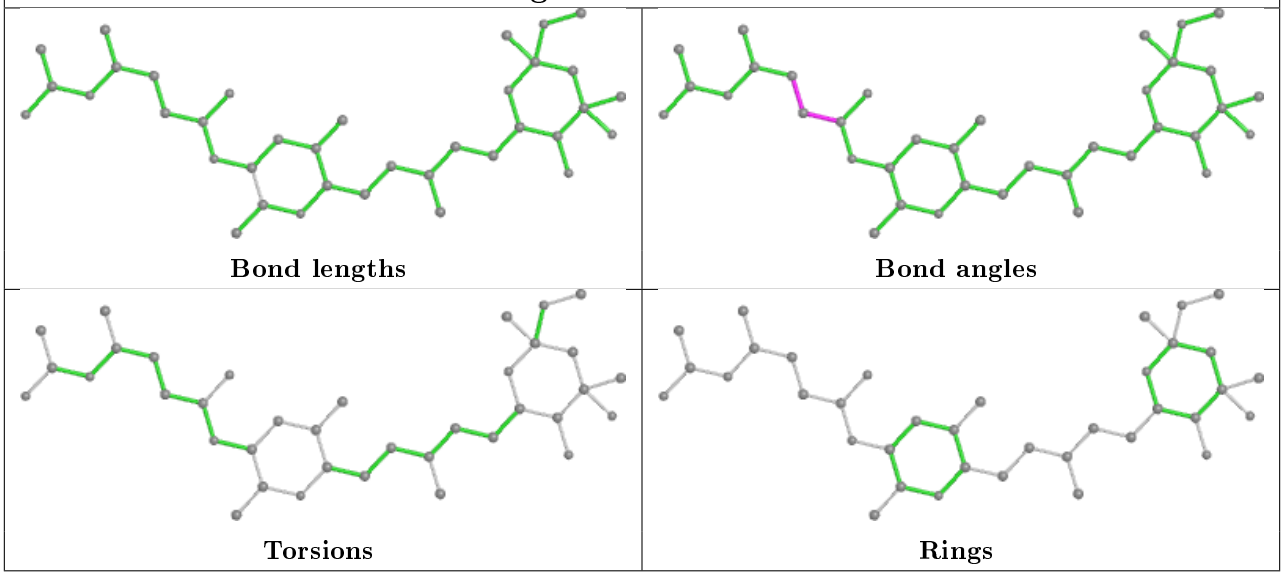
There are no torsion outliers.

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 then 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.

Ligand SJT D 105



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.52	72 (8%) 11 10	47, 74, 110, 150	0
2	B	74/86 (86%)	0.89	18 (24%) 0 0	52, 65, 111, 121	0
3	C	842/852 (98%)	-0.06	12 (1%) 75 73	50, 70, 96, 122	0
4	D	92/108 (85%)	0.01	1 (1%) 80 79	51, 59, 83, 96	0
All	All	1878/1945 (96%)	0.25	103 (5%) 25 24	47, 71, 104, 150	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	GLY	6.4
3	C	1107	GLN	5.9
1	A	381	GLU	4.9
1	A	380	GLU	4.6
4	D	98	LEU	4.6
1	A	384	THR	4.6
1	A	379	LEU	4.5
1	A	826	ALA	4.3
1	A	827	ALA	4.1
1	A	836	ALA	3.9
1	A	828	GLY	3.9
3	C	487	LEU	3.8
3	C	1106	ARG	3.8
1	A	383	ASP	3.8
1	A	428	GLY	3.8
1	A	1094	GLY	3.8
2	B	82	LYS	3.6
1	A	1095	GLY	3.6
1	A	1104	LEU	3.6
1	A	1083	VAL	3.6
1	A	1082	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	52	TYR	3.4
3	C	1304	LEU	3.2
3	C	485	SER	3.2
2	B	14	LEU	3.2
1	A	1084	LEU	3.2
1	A	427	CYS	3.2
1	A	833	GLU	3.1
1	A	408	LEU	3.1
1	A	406	PRO	3.1
1	A	831	GLU	3.0
1	A	407	ILE	3.0
2	B	49	LEU	2.9
2	B	81	ASP	2.9
1	A	378	PRO	2.9
1	A	1047	ALA	2.9
2	B	55	ILE	2.9
1	A	904	TYR	2.9
1	A	320	ASP	2.8
1	A	365	GLY	2.8
1	A	1105	SER	2.8
1	A	823	MET	2.8
2	B	44	MET	2.8
1	A	835	ALA	2.8
1	A	1149	TYR	2.8
1	A	353	PHE	2.7
1	A	405	SER	2.7
3	C	1105	GLU	2.7
3	C	1279	ALA	2.6
2	B	45	GLY	2.6
1	A	1148	TYR	2.6
1	A	1062	THR	2.6
1	A	441	GLY	2.6
3	C	483	ASP	2.6
1	A	376	ALA	2.5
1	A	1053	ILE	2.5
1	A	61	VAL	2.5
1	A	1103	THR	2.5
1	A	1050	PHE	2.5
2	B	54	ALA	2.5
2	B	15	GLN	2.4
1	A	367	ASP	2.4
1	A	1080	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	51	ASN	2.4
2	B	53	PHE	2.4
1	A	1085	SER	2.4
1	A	0	HIS	2.4
2	B	50	LEU	2.4
1	A	837	GLU	2.4
1	A	825	GLU	2.4
1	A	363	HIS	2.3
2	B	46	HIS	2.3
1	A	112	CYS	2.3
1	A	1067	ASP	2.3
1	A	62	ILE	2.3
1	A	410	CYS	2.3
1	A	1034	THR	2.3
1	A	13	GLY	2.3
2	B	48	ASP	2.3
1	A	1079	VAL	2.2
1	A	366	ASP	2.2
2	B	58	ASN	2.2
1	A	1051	GLY	2.2
3	C	1142	ASN	2.2
1	A	822	GLU	2.2
1	A	1106	GLY	2.2
3	C	1303	ILE	2.2
1	A	1061	ASN	2.2
1	A	1195	THR	2.2
1	A	-1	ARG	2.2
1	A	1049	LYS	2.1
1	A	1033	VAL	2.1
1	A	426	ALA	2.1
1	A	369	GLU	2.1
2	B	12	GLU	2.1
3	C	484	GLU	2.1
3	C	486	THR	2.1
1	A	11	ALA	2.0
2	B	62	ALA	2.0
1	A	934	GLY	2.0
1	A	15	SER	2.0
1	A	82	SER	2.0
1	A	840	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 monosaccharides in this entry.

6.4 Ligands (i)

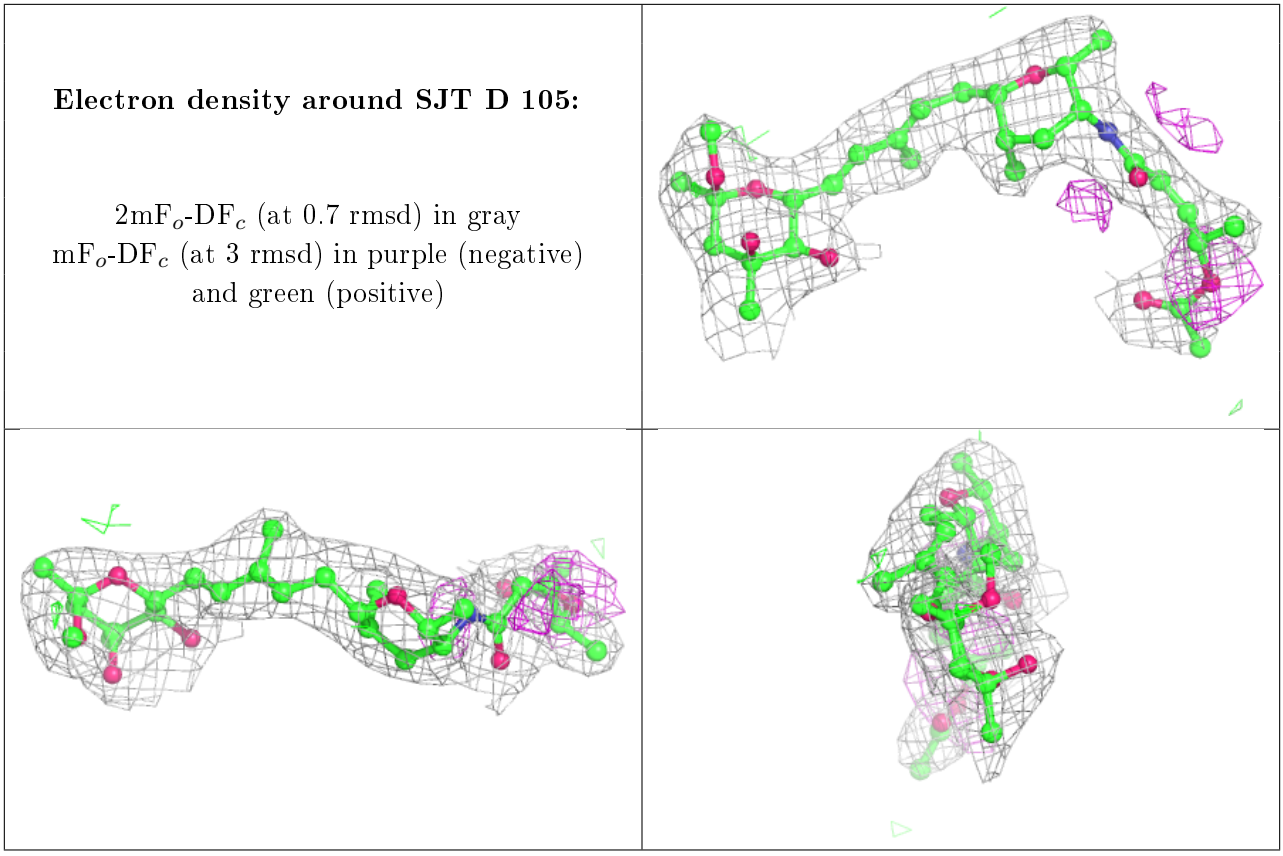
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
7	SJT	D	105	37/37	0.93	0.18	47,57,70,83	0
6	SCN	D	104	3/3	0.94	0.24	63,63,73,99	0
5	ZN	D	101	1/1	0.98	0.17	61,61,61,61	0
5	ZN	D	103	1/1	0.99	0.17	57,57,57,57	0
5	ZN	D	102	1/1	1.00	0.18	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.

Electron density around SJT D 105:

$2mF_o$-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.