



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2021 – 05:07 pm BST

PDB ID : 7OMF
Title : Structure of a minimal SF3B core in complex with sudemycin D6 (form I)
Authors : Cretu, C.; Pena, V.
Deposited on : 2021-05-21
Resolution : 3.00 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

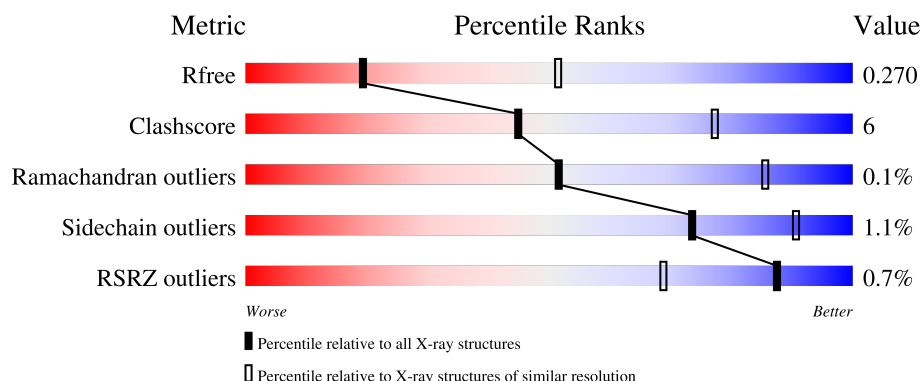
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	
2	B	86	
3	C	852	
4	D	108	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14852 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	869	Total	C	N	O	S	0	0	0
			6870	4364	1175	1300	31			

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q15393
A	-8	ALA	-	expression tag	UNP Q15393
A	-7	GLU	-	expression tag	UNP Q15393
A	-6	PHE	-	expression tag	UNP Q15393
A	-5	LYS	-	expression tag	UNP Q15393
A	-4	GLY	-	expression tag	UNP Q15393
A	-3	LEU	-	expression tag	UNP Q15393
A	-2	ARG	-	expression tag	UNP Q15393
A	-1	ARG	-	expression tag	UNP Q15393
A	0	HIS	-	expression tag	UNP Q15393
A	761	GLY	-	linker	UNP Q15393
A	762	GLY	-	linker	UNP Q15393
A	763	ASN	-	linker	UNP Q15393
A	764	GLY	-	linker	UNP Q15393
A	765	ASN	-	linker	UNP Q15393
A	766	SER	-	linker	UNP Q15393
A	767	GLY	-	linker	UNP Q15393
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	1200	ASP	-	expression tag	UNP Q15393
A	1201	TYR	-	expression tag	UNP Q15393
A	1202	LYS	-	expression tag	UNP Q15393
A	1203	ASP	-	expression tag	UNP Q15393
A	1204	ASP	-	expression tag	UNP Q15393
A	1205	ASP	-	expression tag	UNP Q15393
A	1206	ASP	-	expression tag	UNP Q15393
A	1207	LYS	-	expression tag	UNP Q15393

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	65	Total	C	N	O	S	0	0	0
			535	340	93	97	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	93	Total	C	N	O	S	0	0	0
			700	429	123	135	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
D	-6	GLY	-	expression tag	UNP Q7RTV0

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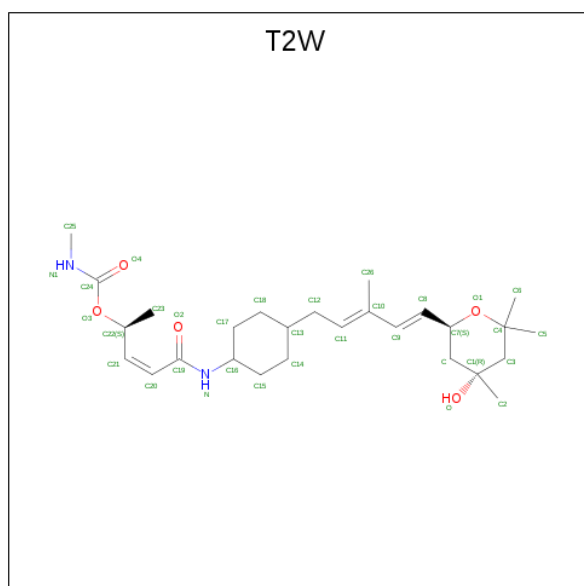
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	SER	-	expression tag	UNP Q7RTV0
D	-4	PRO	-	expression tag	UNP Q7RTV0
D	-3	GLY	-	expression tag	UNP Q7RTV0
D	-2	SER	-	expression tag	UNP Q7RTV0
D	-1	ARG	-	expression tag	UNP Q7RTV0
D	0	ALA	-	expression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

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

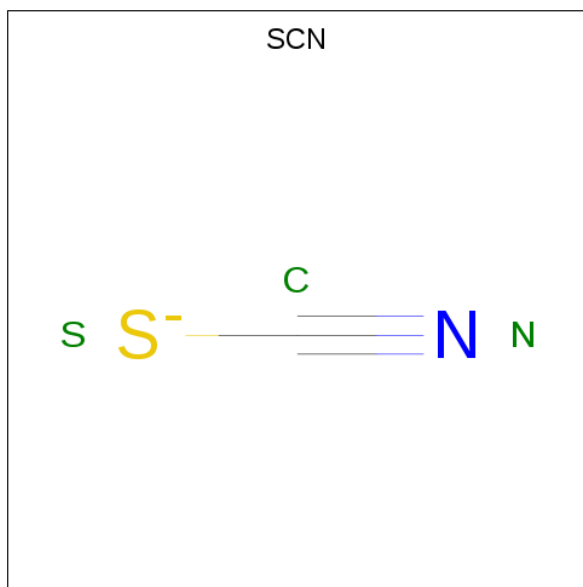
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	3	Total Zn 3 3	0	0

- Molecule 6 is [({Z},2 {S})-5-[[4-[(2 {E},4 {E})-3-methyl-5-[(2 {S},4 {R})-4,6,6-trimethyl-4-oxidanyl-oxan-2-yl]penta-2,4-dienyl]cyclohexyl]amino]-5-oxidanylidene-pent-3-en-2-yl] {N}-methylcarbamate (three-letter code: T2W) (formula:) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C N O 34 27 2 5	0	0

- Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

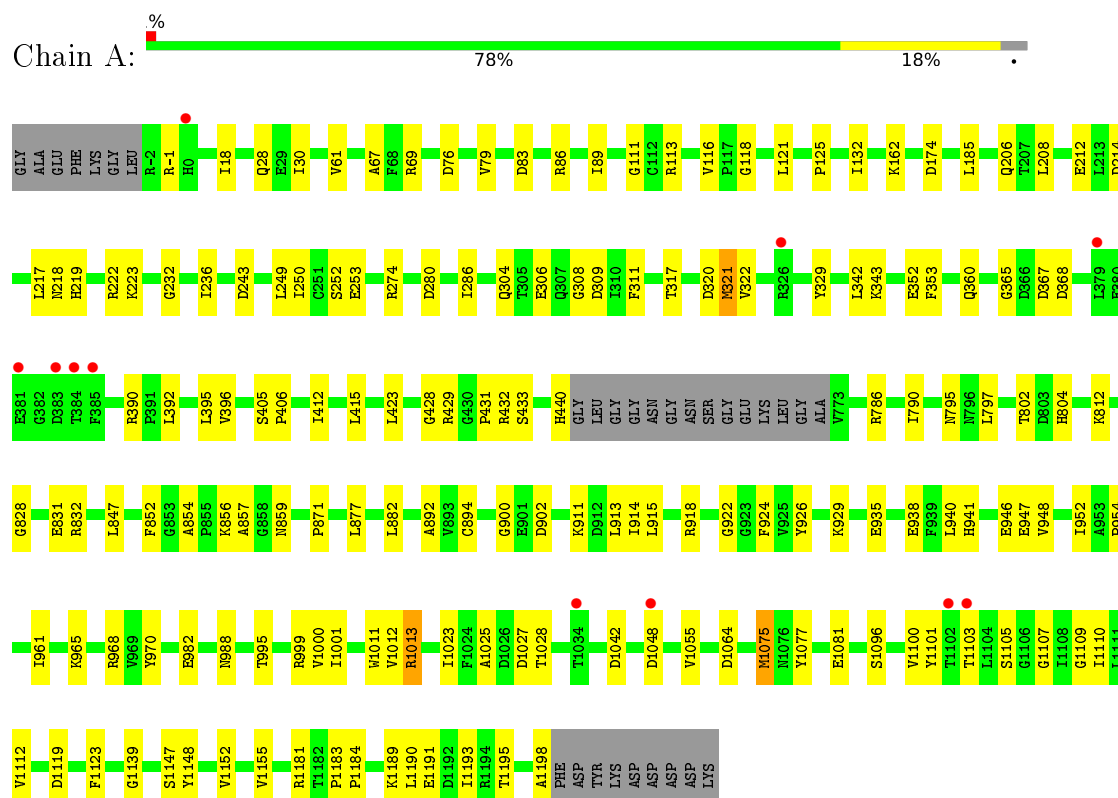


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	S	0	0
			3	1	1	1		

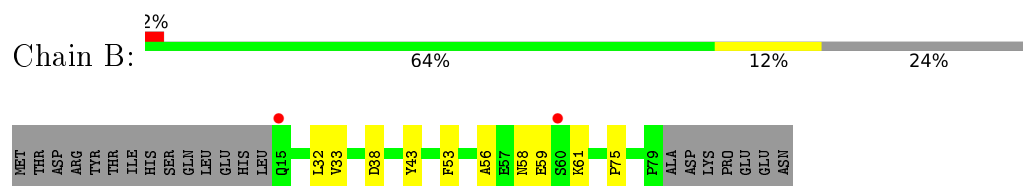
3 Residue-property plots

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.

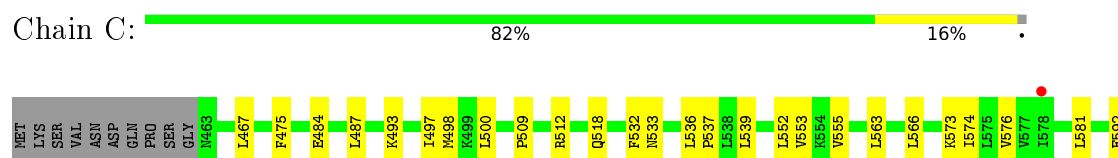
• Molecule 1: Splicing factor 3B subunit 3

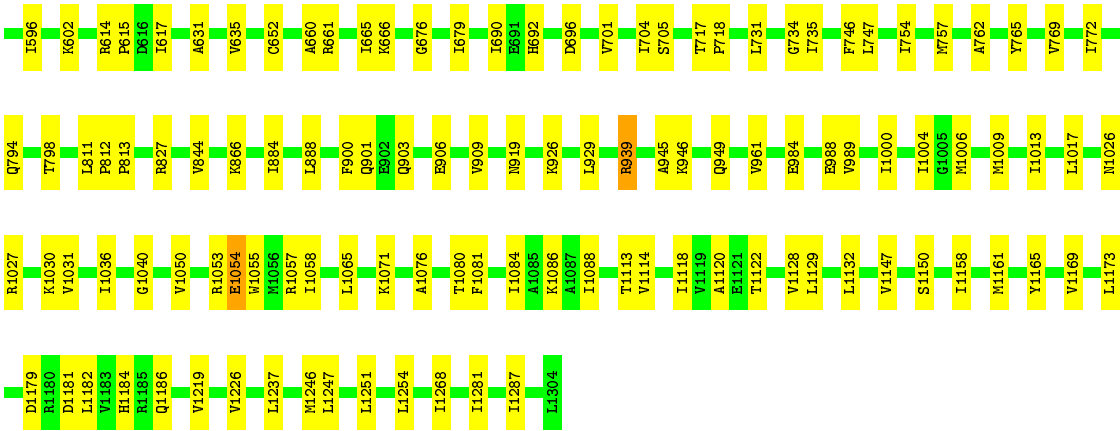


• Molecule 2: Splicing factor 3B subunit 5

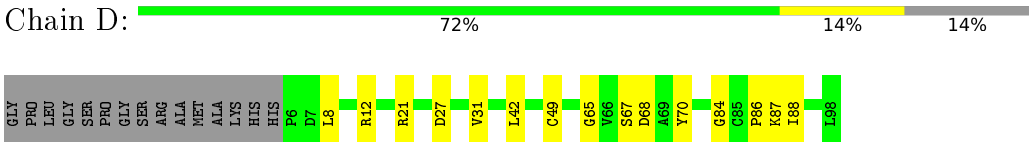


• Molecule 3: Splicing factor 3B subunit 1





● 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	106.36Å 109.85Å 253.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 3.00 49.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.03-3.00) 99.6 (49.03-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.232 , 0.266 0.234 , 0.270	Depositor DCC
R_{free} test set	3288 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	114.2	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14852	wwPDB-VP
Average B, all atoms (Å ²)	112.0	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: SCN, T2W, ZN

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	0/7019	0.52	0/9518
2	B	0.28	0/551	0.48	0/744
3	C	0.26	0/6835	0.47	0/9256
4	D	0.27	0/709	0.55	0/952
All	All	0.27	0/15114	0.50	0/20470

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	6870	0	6784	98	0
2	B	535	0	504	7	0
3	C	6707	0	6915	85	0
4	D	700	0	682	9	0
5	D	3	0	0	0	0
6	D	34	0	0	0	0
7	D	3	0	0	0	0
All	All	14852	0	14885	193	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 (193) 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:866:LYS:HG3	3:C:909:VAL:HG11	1.58	0.85
3:C:1219:VAL:HG21	3:C:1268:ILE:HD11	1.60	0.82
3:C:665:ILE:HG23	3:C:690:ILE:HD11	1.66	0.77
1:A:1011:TRP:HB2	1:A:1025:ALA:HB3	1.68	0.73
1:A:280:ASP:HB2	1:A:857:ALA:HB1	1.70	0.71
3:C:484:GLU:HA	3:C:487:LEU:HD23	1.73	0.70
1:A:79:VAL:HG12	1:A:121:LEU:HD21	1.75	0.69
3:C:900:PHE:O	3:C:939:ARG:NH2	2.24	0.69
3:C:553:VAL:HG21	3:C:592:GLU:HB3	1.74	0.68
1:A:797:LEU:HD13	1:A:871:PRO:HG3	1.76	0.67
3:C:661:ARG:NH1	3:C:696:ASP:OD2	2.21	0.66
1:A:1103:THR:HG22	1:A:1105:SER:H	1.61	0.65
1:A:786:ARG:NH1	1:A:802:THR:O	2.30	0.64
3:C:1113:THR:HG23	3:C:1150:SER:HA	1.79	0.64
1:A:320:ASP:OD1	1:A:321:MET:N	2.31	0.64
3:C:1055:TRP:HB3	3:C:1088:ILE:HD11	1.78	0.64
3:C:1054:GLU:HA	3:C:1057:ARG:HD3	1.81	0.63
3:C:536:LEU:HD11	3:C:574:ILE:HD13	1.81	0.62
4:D:49:CYS:HB3	4:D:87:LYS:HD3	1.82	0.62
3:C:1186:GLN:HB2	3:C:1226:VAL:HG12	1.82	0.61
1:A:428:GLY:HA3	1:A:433:SER:HA	1.83	0.61
1:A:854:ALA:HB3	1:A:856:LYS:HE3	1.84	0.59
1:A:79:VAL:HG22	1:A:89:ILE:HG12	1.85	0.59
1:A:18:ILE:HD12	1:A:67:ALA:HB2	1.84	0.59
1:A:1191:GLU:O	1:A:1195:THR:HG23	2.03	0.59
3:C:617:ILE:HG22	3:C:660:ALA:HA	1.84	0.58
3:C:1120:ALA:HB2	3:C:1128:VAL:HG11	1.85	0.58
3:C:945:ALA:HB1	3:C:989:VAL:HG21	1.84	0.58
1:A:352:GLU:HB2	2:B:61:LYS:HE3	1.86	0.58
1:A:86:ARG:NH1	1:A:1139:GLY:O	2.37	0.58
3:C:1036:ILE:HD11	3:C:1065:LEU:HD13	1.85	0.58
3:C:731:LEU:O	3:C:735:ILE:HG12	2.03	0.58
3:C:509:PRO:HG3	3:C:512:ARG:HH21	1.69	0.57
3:C:563:LEU:HB3	3:C:566:LEU:HB2	1.85	0.57
1:A:61:VAL:HB	1:A:83:ASP:HB3	1.87	0.57
1:A:412:ILE:HG12	1:A:423:LEU:HG	1.86	0.57
1:A:232:GLY:HA2	1:A:252:SER:HA	1.86	0.56
1:A:429:ARG:NH2	2:B:59:GLU:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:VAL:HB	1:A:1075:MET:HB3	1.86	0.56
1:A:1119:ASP:OD1	1:A:1189:LYS:NZ	2.38	0.56
3:C:1086:LYS:HD3	3:C:1122:THR:HG22	1.86	0.56
1:A:1027:ASP:OD1	1:A:1028:THR:N	2.39	0.56
1:A:947:GLU:HG2	1:A:948:VAL:H	1.71	0.56
3:C:901:GLN:HA	3:C:939:ARG:HH21	1.71	0.56
1:A:1077:TYR:HB2	1:A:1155:VAL:HG21	1.86	0.55
3:C:665:ILE:HD13	3:C:705:SER:HB3	1.88	0.55
3:C:919:ASN:HA	3:C:961:VAL:HG21	1.89	0.55
3:C:1076:ALA:O	3:C:1080:THR:HG23	2.06	0.55
1:A:1103:THR:HB	1:A:1107:GLY:H	1.72	0.54
1:A:882:LEU:HD22	1:A:926:TYR:HE2	1.72	0.53
3:C:533:ASN:O	3:C:537:PRO:HD2	2.08	0.53
1:A:28:GLN:HE22	1:A:343:LYS:HD3	1.72	0.53
3:C:906:GLU:HG2	3:C:946:LYS:HB3	1.91	0.53
3:C:493:LYS:O	3:C:497:ILE:HG12	2.09	0.53
3:C:500:LEU:HD11	3:C:518:GLN:HB3	1.91	0.53
3:C:652:CYS:O	3:C:692:HIS:NE2	2.36	0.53
4:D:42:LEU:HD11	4:D:68:ASP:HB3	1.90	0.53
3:C:984:GLU:HG2	3:C:989:VAL:HB	1.91	0.53
3:C:1169:VAL:HG12	3:C:1173:LEU:HD13	1.90	0.53
3:C:884:ILE:HG23	3:C:888:LEU:HB3	1.90	0.53
1:A:392:LEU:HD13	1:A:395:LEU:O	2.09	0.52
4:D:12:ARG:HA	4:D:84:GLY:HA3	1.91	0.52
1:A:243:ASP:OD1	1:A:243:ASP:N	2.41	0.52
1:A:1013:ARG:HG3	1:A:1064:ASP:HB3	1.92	0.52
1:A:365:GLY:O	1:A:367:ASP:N	2.41	0.52
1:A:1100:VAL:HG22	1:A:1110:ILE:HG22	1.91	0.52
1:A:431:PRO:HG3	1:A:854:ALA:HB2	1.92	0.52
3:C:735:ILE:HD12	3:C:747:LEU:HD12	1.92	0.52
3:C:900:PHE:HA	3:C:903:GLN:HE21	1.74	0.51
1:A:118:GLY:HA2	1:A:132:ILE:HD11	1.92	0.51
3:C:1017:LEU:HD23	3:C:1050:VAL:HG11	1.91	0.51
3:C:1114:VAL:O	3:C:1118:ILE:HG13	2.11	0.51
1:A:1103:THR:HG22	1:A:1105:SER:N	2.24	0.51
1:A:83:ASP:O	1:A:111:GLY:N	2.40	0.51
3:C:539:LEU:HD21	3:C:581:LEU:HD11	1.92	0.50
1:A:253:GLU:HA	1:A:286:ILE:HG22	1.94	0.50
2:B:38:ASP:HB3	3:C:1281:ILE:HD11	1.93	0.50
1:A:847:LEU:HB3	1:A:852:PHE:HD2	1.77	0.50
3:C:573:LYS:O	3:C:576:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:ILE:HD12	1:A:1011:TRP:CD1	2.48	0.49
3:C:754:ILE:HG12	3:C:757:MET:HE1	1.95	0.49
3:C:757:MET:HE3	3:C:762:ALA:HA	1.93	0.49
1:A:214:ASP:O	1:A:218:ASN:N	2.45	0.49
3:C:553:VAL:HG13	3:C:596:ILE:HG23	1.94	0.49
3:C:1040:GLY:HA3	3:C:1080:THR:HG22	1.94	0.49
3:C:1054:GLU:O	3:C:1058:ILE:HG12	2.12	0.49
1:A:1189:LYS:O	1:A:1193:ILE:HG12	2.11	0.49
3:C:1017:LEU:HD23	3:C:1050:VAL:HG21	1.94	0.49
1:A:902:ASP:N	1:A:902:ASP:OD1	2.46	0.48
3:C:735:ILE:HG22	3:C:772:ILE:HG13	1.95	0.48
3:C:1237:LEU:HB3	3:C:1246:MET:HE1	1.95	0.48
1:A:1096:SER:HB2	1:A:1198:ALA:HB1	1.94	0.48
1:A:929:LYS:HB3	1:A:938:GLU:HB3	1.95	0.48
3:C:1006:MET:SD	3:C:1013:ILE:HD11	2.53	0.48
1:A:162:LYS:HG2	1:A:222:ARG:NH1	2.28	0.48
1:A:415:LEU:HD21	1:A:790:ILE:HD13	1.94	0.48
1:A:1101:TYR:CZ	1:A:1109:GLY:HA3	2.49	0.48
1:A:1147:SER:OG	1:A:1152:VAL:HG23	2.14	0.48
3:C:1132:LEU:HD22	3:C:1147:VAL:HG13	1.96	0.48
3:C:552:LEU:O	3:C:555:VAL:HG12	2.14	0.48
3:C:1182:LEU:HB3	3:C:1226:VAL:HG11	1.95	0.48
3:C:631:ALA:O	3:C:635:VAL:HG13	2.13	0.47
3:C:475:PHE:HD1	3:C:498:MET:HG2	1.79	0.47
1:A:415:LEU:HD12	1:A:795:ASN:HB3	1.95	0.47
3:C:1036:ILE:O	3:C:1080:THR:HG21	2.14	0.47
1:A:1181:ARG:NH1	1:A:1189:LYS:HD2	2.30	0.47
1:A:185:LEU:HD22	1:A:206:GLN:HE21	1.79	0.46
3:C:652:CYS:HB3	3:C:692:HIS:HE1	1.80	0.46
1:A:311:PHE:CD1	1:A:329:TYR:HA	2.50	0.46
3:C:1158:ILE:HB	3:C:1161:MET:HB3	1.98	0.46
4:D:21:ARG:HD3	4:D:67:SER:O	2.16	0.46
1:A:-1:ARG:HD3	1:A:-1:ARG:HA	1.78	0.46
1:A:236:ILE:HB	1:A:249:LEU:HB2	1.98	0.46
1:A:274:ARG:NH2	1:A:309:ASP:OD1	2.41	0.46
1:A:995:THR:HG22	1:A:1000:VAL:HG23	1.97	0.45
3:C:946:LYS:HG3	3:C:949:GLN:HE21	1.81	0.45
1:A:894:CYS:HB3	1:A:954:PRO:HG3	1.98	0.45
3:C:765:TYR:O	3:C:769:VAL:HG23	2.16	0.45
3:C:811:LEU:HD11	3:C:844:VAL:HG21	1.97	0.45
3:C:1071:LYS:HB2	4:D:27:ASP:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:21:ARG:HG3	4:D:65:GLY:HA3	1.98	0.45
1:A:185:LEU:HB3	1:A:206:GLN:HE21	1.82	0.45
4:D:8:LEU:HD23	4:D:88:ILE:HG21	1.97	0.45
3:C:734:GLY:HA3	3:C:746:PHE:CE2	2.52	0.45
1:A:961:ILE:HD12	1:A:970:TYR:CD2	2.51	0.45
3:C:717:THR:HA	3:C:718:PRO:HA	1.82	0.45
1:A:922:GLY:HA2	1:A:946:GLU:O	2.18	0.44
4:D:42:LEU:HD13	4:D:70:TYR:CZ	2.52	0.44
1:A:804:HIS:NE2	1:A:859:ASN:O	2.50	0.44
1:A:913:LEU:HD22	1:A:915:LEU:HD12	1.98	0.44
1:A:304:GLN:HE21	1:A:308:GLY:HA2	1.83	0.44
3:C:1247:LEU:O	3:C:1251:LEU:HG	2.17	0.44
4:D:31:VAL:HG11	4:D:86:PRO:HB2	2.00	0.44
1:A:877:LEU:HD23	1:A:935:GLU:HG2	1.99	0.43
1:A:1123:PHE:HE1	1:A:1190:LEU:HD23	1.82	0.43
3:C:665:ILE:HG12	3:C:690:ILE:HG13	1.99	0.43
3:C:1254:LEU:HD23	3:C:1254:LEU:HA	1.80	0.43
3:C:676:GLY:O	3:C:679:ILE:HG13	2.18	0.43
1:A:999:ARG:NH1	1:A:1042:ASP:OD1	2.49	0.43
1:A:1181:ARG:HH12	1:A:1189:LYS:HD2	1.83	0.43
1:A:185:LEU:HB3	1:A:206:GLN:NE2	2.34	0.43
3:C:1081:PHE:HA	3:C:1084:ILE:HG12	2.00	0.43
1:A:914:ILE:O	1:A:918:ARG:HA	2.19	0.43
1:A:212:GLU:OE1	1:A:223:LYS:HD2	2.19	0.43
1:A:353:PHE:O	1:A:432:ARG:NH1	2.46	0.43
1:A:429:ARG:HH22	2:B:59:GLU:C	2.21	0.43
1:A:69:ARG:HB2	1:A:76:ASP:OD1	2.19	0.43
3:C:696:ASP:OD2	3:C:701:VAL:HG11	2.19	0.43
3:C:701:VAL:HA	3:C:704:ILE:HG22	2.01	0.42
3:C:929:LEU:HD23	3:C:929:LEU:HA	1.91	0.42
3:C:988:GLU:HA	3:C:1030:LYS:HD3	2.01	0.42
1:A:30:ILE:HD11	1:A:342:LEU:HD11	2.01	0.42
3:C:614:ARG:N	3:C:615:PRO:HD2	2.33	0.42
1:A:360:GLN:HB3	1:A:396:VAL:HG23	2.00	0.42
1:A:1012:VAL:HG22	1:A:1023:ILE:HG12	2.01	0.42
1:A:405:SER:HA	1:A:406:PRO:HA	1.83	0.42
1:A:847:LEU:HD22	1:A:852:PHE:CE2	2.55	0.42
3:C:1026:ASN:HD22	3:C:1031:VAL:HG11	1.84	0.42
3:C:794:GLN:O	3:C:798:THR:HG23	2.20	0.42
3:C:827:ARG:HD3	3:C:827:ARG:HA	1.78	0.42
1:A:113:ARG:HB2	1:A:116:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ILE:HG12	1:A:306:GLU:OE2	2.20	0.42
1:A:217:LEU:HD23	1:A:219:HIS:HE1	1.85	0.42
2:B:43:TYR:CG	2:B:53:PHE:HE2	2.38	0.42
1:A:828:GLY:O	1:A:831:GLU:HG2	2.19	0.41
3:C:666:LYS:HD2	3:C:704:ILE:HD11	2.02	0.41
3:C:812:PRO:HB2	3:C:813:PRO:HD3	2.02	0.41
1:A:911:LYS:HD3	1:A:924:PHE:HE2	1.86	0.41
1:A:1183:PRO:HB2	1:A:1184:PRO:HD3	2.02	0.41
3:C:1132:LEU:HD11	3:C:1150:SER:HB3	2.02	0.41
1:A:1110:ILE:HD12	1:A:1112:VAL:HG23	2.02	0.41
1:A:1123:PHE:CZ	1:A:1193:ILE:HG13	2.56	0.41
2:B:33:VAL:HG23	2:B:75:PRO:HD2	2.03	0.41
3:C:926:LYS:HE3	3:C:926:LYS:HB3	1.91	0.41
1:A:965:LYS:HB3	1:A:988:ASN:O	2.21	0.41
1:A:812:LYS:HE3	1:A:812:LYS:HB2	1.71	0.41
1:A:125:PRO:HG2	1:A:174:ASP:HA	2.01	0.41
1:A:208:LEU:HD22	1:A:250:ILE:HD11	2.02	0.41
1:A:28:GLN:NE2	1:A:343:LYS:HD3	2.36	0.41
1:A:317:THR:HA	1:A:322:VAL:HA	2.03	0.41
1:A:940:LEU:HD22	1:A:941:HIS:ND1	2.36	0.41
2:B:32:LEU:HD21	3:C:1287:ILE:HB	2.03	0.41
3:C:939:ARG:HA	3:C:939:ARG:HD3	1.70	0.41
3:C:1000:ILE:O	3:C:1004:ILE:HG22	2.21	0.41
1:A:828:GLY:O	1:A:832:ARG:HG3	2.20	0.40
1:A:1081:GLU:HB3	1:A:1103:THR:HG23	2.03	0.40
3:C:1179:ASP:O	3:C:1181:ASP:N	2.46	0.40
3:C:1165:TYR:O	3:C:1169:VAL:HG23	2.21	0.40
1:A:847:LEU:HB3	1:A:852:PHE:CD2	2.55	0.40
3:C:1129:LEU:HD23	3:C:1129:LEU:HA	1.90	0.40
1:A:892:ALA:HB3	1:A:952:ILE:HG22	2.04	0.40
1:A:968:ARG:HG2	1:A:982:GLU:HB2	2.03	0.40
1:A:1000:VAL:HG13	1:A:1012:VAL:HB	2.03	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	865/899 (96%)	817 (94%)	47 (5%)	1 (0%)	51	85
2	B	63/86 (73%)	60 (95%)	2 (3%)	1 (2%)	9	40
3	C	840/852 (99%)	819 (98%)	21 (2%)	0	100	100
4	D	91/108 (84%)	88 (97%)	3 (3%)	0	100	100
All	All	1859/1945 (96%)	1784 (96%)	73 (4%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	900	GLY
2	B	56	ALA

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	754/774 (97%)	746 (99%)	8 (1%)	73	90
2	B	57/77 (74%)	56 (98%)	1 (2%)	59	85
3	C	728/737 (99%)	719 (99%)	9 (1%)	71	90
4	D	80/90 (89%)	80 (100%)	0	100	100
All	All	1619/1678 (96%)	1601 (99%)	18 (1%)	73	90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	MET
1	A	368	ASP
1	A	390	ARG
1	A	440	HIS

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Mol	Chain	Res	Type
1	A	1013	ARG
1	A	1048	ASP
1	A	1075	MET
1	A	1148	TYR
2	B	58	ASN
3	C	467	LEU
3	C	532	PHE
3	C	602	LYS
3	C	939	ARG
3	C	1009	MET
3	C	1027	ARG
3	C	1053	ARG
3	C	1054	GLU
3	C	1184	HIS

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	206	GLN
3	C	949	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	T2W	D	104	4	34,35,35	0.32	0	37,49,49	0.52	1 (2%)
7	SCN	D	105	5	1,2,2	0.88	0	0,1,1	0.00	-

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	T2W	D	104	4	-	2/25/51/51	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(°)
6	D	104	T2W	C21-C20-C19	2.29	128.43	122.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

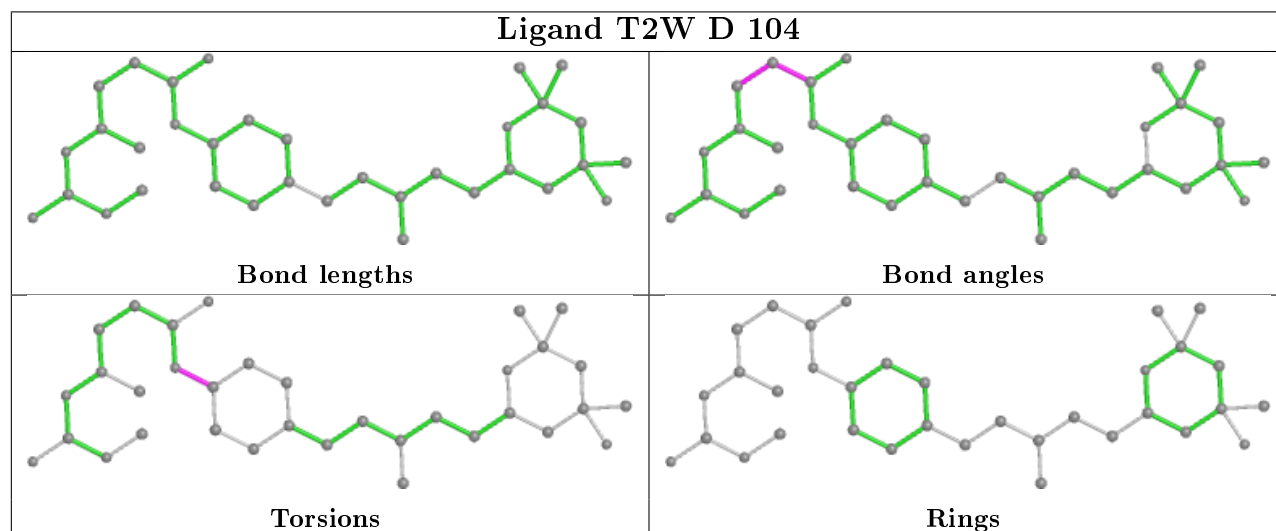
Mol	Chain	Res	Type	Atoms
6	D	104	T2W	C17-C16-N-C19
6	D	104	T2W	C15-C16-N-C19

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 [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	869/899 (96%)	-0.01	11 (1%) 77 51	70, 109, 147, 169	0
2	B	65/86 (75%)	0.30	2 (3%) 49 21	82, 100, 117, 133	0
3	C	842/852 (98%)	-0.21	1 (0%) 95 89	77, 116, 143, 166	0
4	D	93/108 (86%)	-0.15	0 100 100	78, 94, 133, 148	0
All	All	1869/1945 (96%)	-0.10	14 (0%) 87 69	70, 112, 144, 169	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	THR	3.9
2	B	15	GLN	3.3
1	A	0	HIS	2.6
3	C	578	ILE	2.5
1	A	383	ASP	2.4
1	A	385	PHE	2.3
2	B	60	SER	2.3
1	A	1102	THR	2.2
1	A	326	ARG	2.2
1	A	1048	ASP	2.1
1	A	1034	THR	2.1
1	A	379	LEU	2.1
1	A	381	GLU	2.1
1	A	1103	THR	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](#)

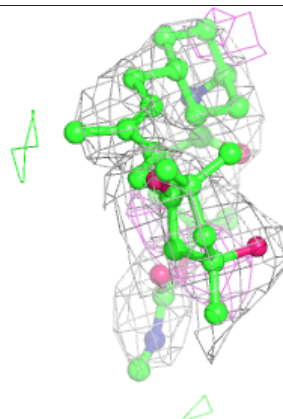
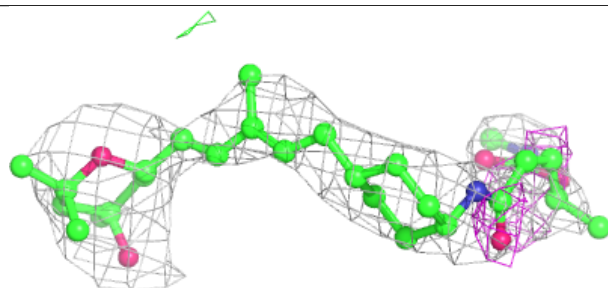
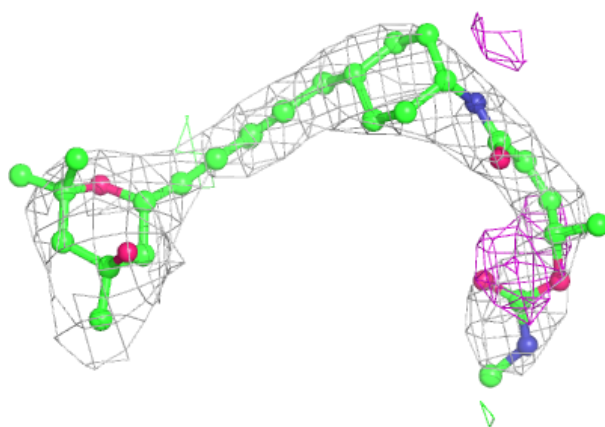
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	T2W	D	104	34/34	0.89	0.42	91,107,117,125	0
5	ZN	D	101	1/1	0.97	0.13	105,105,105,105	0
7	SCN	D	105	3/3	0.98	0.16	115,115,119,123	0
5	ZN	D	102	1/1	0.99	0.22	99,99,99,99	0
5	ZN	D	103	1/1	0.99	0.20	80,80,80,80	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 T2W D 104:

$2mF_o-DF_c$ (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.