



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2021 – 05:04 pm BST

PDB ID : 7B92  
Title : Structure of a minimal SF3B core in complex with sudemycin D6 (form II)  
Authors : Cretu, C.; Pena, V.  
Deposited on : 2020-12-14  
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](mailto: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.

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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

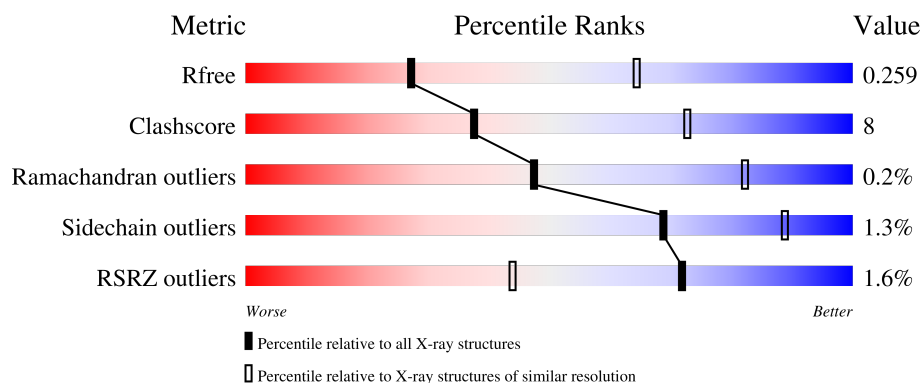
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

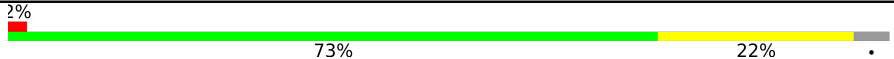



The reported resolution of this entry is 3.00 Å.

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  $\geq 3$ , 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 14792 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	862	Total	C	N	O	S	0	0	0
			6812	4332	1162	1287	31			

There are 44 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	1199	PHE	-	expression tag	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

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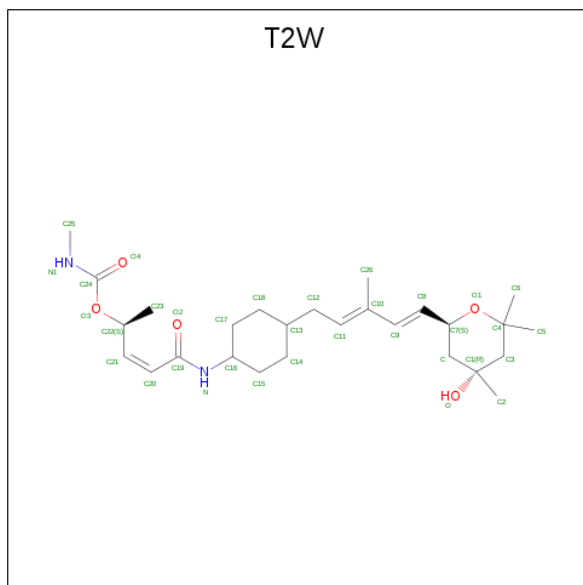
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q7RTV0
D	-5	SER	-	expression tag	UNP Q7RTV0
D	-4	PRO	-	expression tag	UNP Q7RTV0
D	-3	GLY	-	expression tag	UNP Q7RTV0
D	-2	SER	-	expression tag	UNP Q7RTV0
D	-1	ARG	-	expression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

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

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

- 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	0	0
			34	27	2	5		

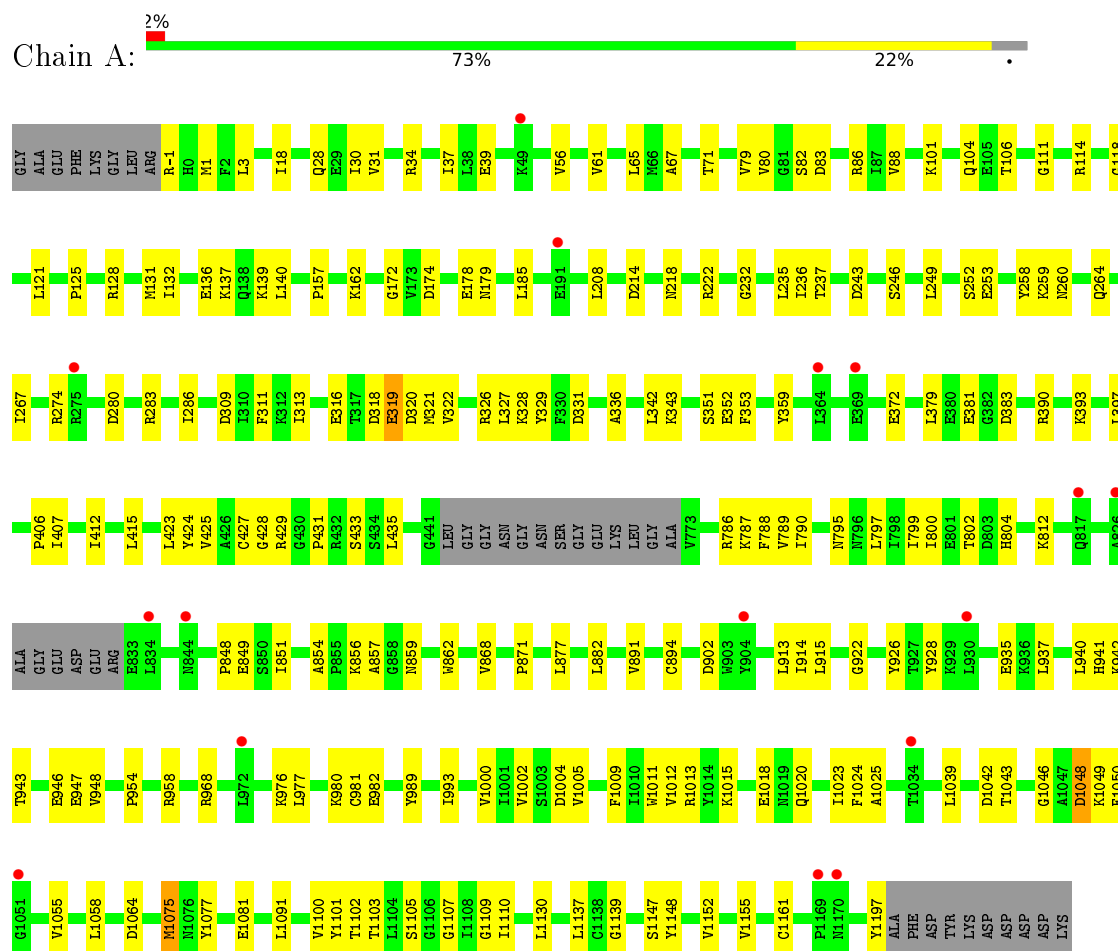
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	O	0	0
			1	1		

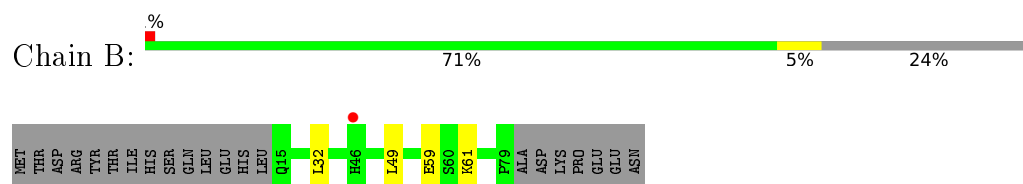
### 3 Residue-property plots [i](#)

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.

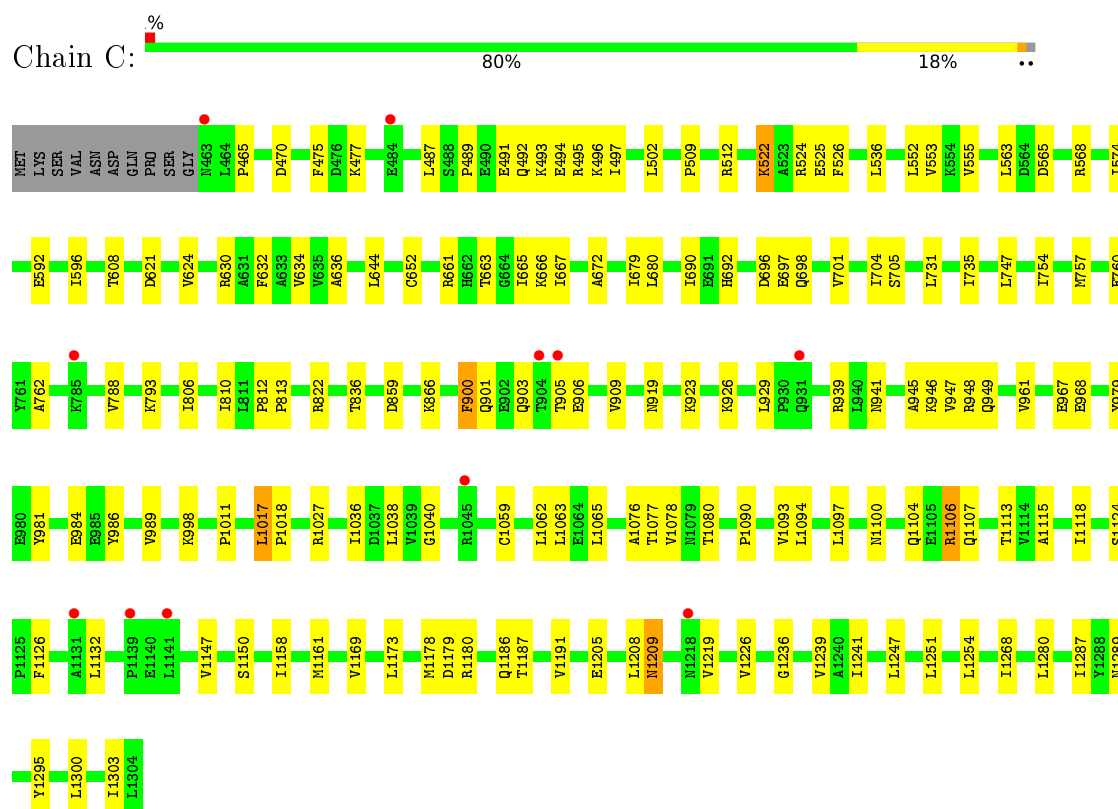
#### • Molecule 1: Splicing factor 3B subunit 3



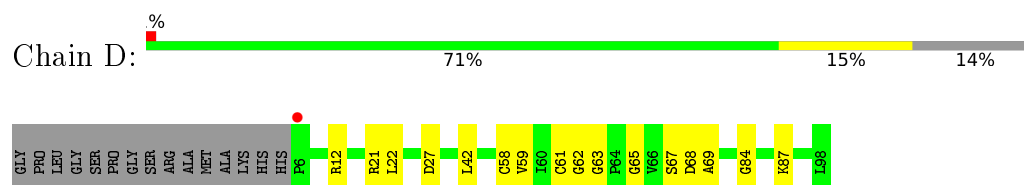
#### • Molecule 2: Splicing factor 3B subunit 5



#### • 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 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.43Å 107.43Å 361.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.52 – 3.00 49.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.52-3.00) 98.9 (49.06-3.00)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.223 , 0.258 0.224 , 0.259	Depositor DCC
$R_{free}$ test set	2427 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	107.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.26	0/6960	0.45	0/9438
2	B	0.26	0/551	0.39	0/744
3	C	0.25	0/6835	0.41	0/9256
4	D	0.25	0/709	0.42	0/952
All	All	0.25	0/15055	0.43	0/20390

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	6812	0	6731	123	0
2	B	535	0	504	5	0
3	C	6707	0	6915	99	0
4	D	700	0	682	8	0
5	D	3	0	0	0	0
6	D	34	0	0	0	0
7	D	1	0	0	0	0
All	All	14792	0	14832	228	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 8.

All (228) 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:1186:GLN:HB2	3:C:1226:VAL:HG12	1.62	0.81
3:C:665:ILE:HG23	3:C:690:ILE:HD11	1.64	0.80
3:C:1219:VAL:HG21	3:C:1268:ILE:HD11	1.65	0.79
1:A:926:TYR:HE1	1:A:942:LYS:HE3	1.48	0.79
3:C:1036:ILE:HD11	3:C:1065:LEU:HD13	1.66	0.77
3:C:522:LYS:NZ	3:C:525:GLU:OE1	2.17	0.76
3:C:1289:ASN:HB3	3:C:1295:TYR:H	1.52	0.75
1:A:316:GLU:OE2	1:A:326:ARG:NH2	2.21	0.72
1:A:428:GLY:HA3	1:A:433:SER:HA	1.71	0.72
1:A:379:LEU:HD13	1:A:381:GLU:H	1.52	0.71
1:A:1011:TRP:HB2	1:A:1025:ALA:HB3	1.71	0.71
3:C:553:VAL:HG21	3:C:592:GLU:HB3	1.73	0.70
3:C:945:ALA:HB1	3:C:989:VAL:HG21	1.74	0.70
2:B:32:LEU:HD11	3:C:1287:ILE:HG21	1.72	0.70
3:C:906:GLU:OE1	3:C:906:GLU:N	2.25	0.70
4:D:61:CYS:SG	4:D:62:GLY:N	2.66	0.69
3:C:900:PHE:O	3:C:939:ARG:NH2	2.27	0.66
1:A:246:SER:O	1:A:260:ASN:ND2	2.29	0.65
3:C:524:ARG:HD2	3:C:563:LEU:HD23	1.79	0.65
1:A:412:ILE:HG12	1:A:423:LEU:HG	1.77	0.65
1:A:797:LEU:HD13	1:A:871:PRO:HG3	1.79	0.65
3:C:866:LYS:HG3	3:C:909:VAL:HG11	1.79	0.65
1:A:280:ASP:HB2	1:A:857:ALA:HB1	1.80	0.64
3:C:757:MET:HE3	3:C:762:ALA:HA	1.81	0.63
1:A:882:LEU:HD22	1:A:926:TYR:HE2	1.64	0.62
1:A:260:ASN:HB3	1:A:264:GLN:HG2	1.82	0.62
1:A:34:ARG:HB2	1:A:37:ILE:HB	1.83	0.61
3:C:754:ILE:HG12	3:C:757:MET:HE1	1.82	0.61
3:C:497:ILE:HD11	3:C:526:PHE:CG	2.36	0.60
1:A:1100:VAL:HG22	1:A:1110:ILE:HG22	1.83	0.60
4:D:21:ARG:HG3	4:D:65:GLY:HA3	1.83	0.60
3:C:1040:GLY:HA3	3:C:1080:THR:HG22	1.82	0.60
1:A:877:LEU:HD23	1:A:935:GLU:HG2	1.84	0.60
3:C:661:ARG:NH1	3:C:696:ASP:OD2	2.36	0.59
3:C:731:LEU:O	3:C:735:ILE:HG12	2.03	0.58
3:C:496:LYS:HE2	3:C:526:PHE:HZ	1.70	0.57
3:C:1113:THR:HG23	3:C:1150:SER:HA	1.86	0.57
1:A:1077:TYR:HB2	1:A:1155:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:PHE:HZ	1:A:1046:GLY:HA3	1.68	0.57
1:A:981:CYS:SG	1:A:1020:GLN:HA	2.45	0.56
3:C:493:LYS:HE2	3:C:526:PHE:HA	1.86	0.56
1:A:868:VAL:O	1:A:877:LEU:N	2.37	0.56
3:C:665:ILE:HD13	3:C:705:SER:HB3	1.87	0.56
1:A:267:ILE:HD13	1:A:322:VAL:HG13	1.88	0.55
1:A:101:LYS:HD3	1:A:104:GLN:HB2	1.89	0.55
3:C:465:PRO:HD2	3:C:502:LEU:HD12	1.88	0.55
1:A:114:ARG:NE	1:A:136:GLU:OE1	2.32	0.55
1:A:1064:ASP:OD1	1:A:1064:ASP:N	2.40	0.55
1:A:318:ASP:HB3	1:A:321:MET:O	2.07	0.55
1:A:431:PRO:HG3	1:A:854:ALA:HB2	1.88	0.55
1:A:1000:VAL:HG13	1:A:1012:VAL:HB	1.88	0.55
1:A:913:LEU:HD22	1:A:915:LEU:HD12	1.89	0.54
1:A:319:GLU:HG2	1:A:320:ASP:N	2.23	0.54
3:C:1158:ILE:HB	3:C:1161:MET:HB3	1.89	0.54
1:A:86:ARG:NH1	1:A:1139:GLY:O	2.41	0.54
1:A:941:HIS:HD2	1:A:976:LYS:HA	1.72	0.54
1:A:30:ILE:HD11	1:A:342:LEU:HD11	1.90	0.54
1:A:854:ALA:HB3	1:A:856:LYS:HE3	1.90	0.53
1:A:140:LEU:HD22	1:A:157:PRO:HB2	1.90	0.53
1:A:319:GLU:HG2	1:A:320:ASP:H	1.74	0.53
3:C:553:VAL:HG13	3:C:596:ILE:HG23	1.90	0.53
3:C:672:ALA:HA	3:C:679:ILE:CD1	2.39	0.53
1:A:253:GLU:HA	1:A:286:ILE:HG22	1.91	0.53
1:A:283:ARG:NH2	2:B:59:GLU:OE1	2.42	0.53
3:C:735:ILE:HD12	3:C:747:LEU:HD12	1.91	0.52
4:D:12:ARG:HA	4:D:84:GLY:HA3	1.90	0.52
1:A:862:TRP:HZ2	1:A:915:LEU:HD11	1.74	0.52
1:A:232:GLY:HA2	1:A:252:SER:HA	1.92	0.52
3:C:522:LYS:CE	3:C:525:GLU:OE1	2.58	0.52
1:A:1:MET:HG2	1:A:3:LEU:HD21	1.91	0.52
1:A:328:LYS:HB3	1:A:372:GLU:HG3	1.92	0.52
1:A:1130:LEU:HD12	1:A:1161:CYS:HA	1.90	0.52
3:C:701:VAL:HA	3:C:704:ILE:HG22	1.91	0.52
1:A:788:PHE:HB3	1:A:799:ILE:HG23	1.91	0.52
1:A:1103:THR:HG22	1:A:1105:SER:H	1.75	0.52
3:C:919:ASN:HA	3:C:961:VAL:HG21	1.90	0.52
3:C:1132:LEU:HD13	3:C:1147:VAL:HG13	1.92	0.51
3:C:536:LEU:HD11	3:C:574:ILE:HD13	1.92	0.51
3:C:984:GLU:HG2	3:C:989:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:HA	1:A:427:CYS:HB3	1.92	0.51
1:A:940:LEU:HB3	1:A:941:HIS:ND1	2.25	0.51
3:C:565:ASP:HB2	3:C:568:ARG:HE	1.75	0.51
4:D:27:ASP:OD1	4:D:67:SER:OG	2.23	0.51
1:A:1015:LYS:HD3	1:A:1018:GLU:HG3	1.93	0.51
3:C:1251:LEU:HD23	3:C:1254:LEU:HD12	1.92	0.51
3:C:621:ASP:HB3	3:C:624:VAL:HG22	1.92	0.51
3:C:636:ALA:HB2	3:C:644:LEU:HD22	1.92	0.51
3:C:941:ASN:OD1	3:C:981:TYR:OH	2.29	0.50
1:A:131:MET:HE3	1:A:139:LYS:HD2	1.93	0.50
1:A:968:ARG:HG2	1:A:982:GLU:HB2	1.94	0.50
1:A:179:ASN:ND2	1:A:214:ASP:HA	2.27	0.50
1:A:34:ARG:NE	1:A:39:GLU:OE1	2.38	0.50
3:C:522:LYS:HE3	3:C:525:GLU:OE1	2.12	0.50
1:A:1147:SER:OG	1:A:1152:VAL:HG23	2.13	0.49
1:A:80:VAL:HB	1:A:88:VAL:HG23	1.93	0.49
1:A:208:LEU:HD23	1:A:259:LYS:HD2	1.94	0.49
1:A:848:PRO:HB2	1:A:851:ILE:HG22	1.95	0.49
3:C:812:PRO:HB2	3:C:813:PRO:HD3	1.95	0.49
1:A:214:ASP:O	1:A:218:ASN:N	2.46	0.48
1:A:236:ILE:HB	1:A:249:LEU:HB2	1.94	0.48
1:A:336:ALA:HA	1:A:351:SER:HA	1.95	0.48
3:C:1062:LEU:HG	3:C:1077:THR:HG23	1.95	0.48
1:A:28:GLN:HE22	1:A:343:LYS:HD3	1.78	0.48
3:C:806:ILE:HG12	3:C:810:ILE:HD12	1.96	0.48
1:A:353:PHE:HB3	1:A:406:PRO:HD3	1.96	0.48
1:A:429:ARG:NH1	2:B:59:GLU:O	2.38	0.48
4:D:58:CYS:HB3	4:D:63:GLY:H	1.79	0.48
3:C:946:LYS:HA	3:C:949:GLN:HG2	1.94	0.48
1:A:1012:VAL:HG22	1:A:1023:ILE:HG12	1.95	0.48
1:A:274:ARG:NH1	1:A:309:ASP:OD1	2.35	0.47
1:A:18:ILE:HD12	1:A:67:ALA:HB2	1.94	0.47
1:A:1101:TYR:CZ	1:A:1109:GLY:HA3	2.49	0.47
3:C:509:PRO:HG3	3:C:512:ARG:HH21	1.79	0.47
3:C:901:GLN:HA	3:C:939:ARG:HH21	1.77	0.47
3:C:968:GLU:OE1	3:C:968:GLU:N	2.39	0.47
3:C:475:PHE:CG	3:C:502:LEU:HD23	2.50	0.47
3:C:1090:PRO:O	3:C:1094:LEU:HB2	2.15	0.47
1:A:812:LYS:NZ	1:A:849:GLU:OE2	2.27	0.47
1:A:993:ILE:HG22	1:A:1002:VAL:HA	1.95	0.47
3:C:1187:THR:O	3:C:1191:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LYS:HG2	1:A:222:ARG:NH2	2.30	0.47
1:A:407:ILE:HG23	1:A:425:VAL:HG13	1.96	0.47
1:A:407:ILE:HG21	1:A:1102:THR:OG1	2.15	0.47
3:C:1076:ALA:O	3:C:1080:THR:HG23	2.14	0.47
1:A:947:GLU:HG2	1:A:948:VAL:H	1.79	0.47
3:C:903:GLN:HB3	3:C:905:THR:O	2.14	0.47
1:A:1055:VAL:HB	1:A:1075:MET:HB3	1.96	0.47
1:A:352:GLU:OE2	1:A:429:ARG:NH2	2.48	0.46
1:A:383:ASP:N	1:A:383:ASP:OD1	2.49	0.46
3:C:592:GLU:O	3:C:596:ILE:HG12	2.15	0.46
1:A:61:VAL:HB	1:A:83:ASP:HB3	1.98	0.46
1:A:1048:ASP:HB3	1:A:1050:PHE:H	1.81	0.46
1:A:1103:THR:HG22	1:A:1105:SER:N	2.31	0.46
3:C:698:GLN:HB3	3:C:701:VAL:HG12	1.98	0.46
3:C:1036:ILE:O	3:C:1080:THR:HG21	2.16	0.46
1:A:894:CYS:HB3	1:A:954:PRO:HG3	1.97	0.45
1:A:981:CYS:SG	1:A:982:GLU:N	2.89	0.45
3:C:1078:VAL:HG22	3:C:1118:ILE:HD11	1.97	0.45
1:A:1081:GLU:HB3	1:A:1103:THR:HG23	1.99	0.45
4:D:59:VAL:HG13	4:D:87:LYS:HA	1.97	0.45
3:C:565:ASP:OD2	3:C:565:ASP:N	2.47	0.45
1:A:79:VAL:HG12	1:A:121:LEU:HD21	1.99	0.45
1:A:1103:THR:HB	1:A:1107:GLY:H	1.80	0.45
1:A:243:ASP:OD1	1:A:243:ASP:N	2.48	0.45
1:A:316:GLU:OE1	1:A:316:GLU:HA	2.16	0.45
1:A:989:TYR:HE2	3:C:1303:ILE:HG13	1.82	0.45
3:C:1106:ARG:HG3	3:C:1107:GLN:N	2.31	0.45
3:C:497:ILE:HD11	3:C:526:PHE:CD2	2.50	0.45
3:C:979:TYR:CD1	3:C:1011:PRO:HG3	2.52	0.44
1:A:786:ARG:NH1	1:A:802:THR:O	2.50	0.44
3:C:747:LEU:HD23	3:C:788:VAL:HG12	1.99	0.44
3:C:998:LYS:HA	3:C:1038:LEU:HD13	2.00	0.44
4:D:42:LEU:HD11	4:D:68:ASP:HB3	1.99	0.44
1:A:812:LYS:HB2	1:A:812:LYS:HE3	1.71	0.44
1:A:311:PHE:CD1	1:A:329:TYR:HA	2.53	0.44
1:A:862:TRP:HZ2	1:A:915:LEU:CD1	2.30	0.44
3:C:470:ASP:OD1	3:C:470:ASP:N	2.51	0.44
1:A:902:ASP:N	1:A:902:ASP:OD1	2.48	0.44
1:A:390:ARG:NH1	1:A:393:LYS:HB2	2.33	0.43
1:A:415:LEU:HD21	1:A:790:ILE:HD13	2.01	0.43
1:A:83:ASP:O	1:A:111:GLY:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:HIS:CD2	1:A:976:LYS:HA	2.52	0.43
3:C:630:ARG:O	3:C:634:VAL:HG23	2.18	0.43
3:C:1178:MET:O	3:C:1180:ARG:N	2.44	0.43
3:C:1247:LEU:HD22	3:C:1280:LEU:HD22	1.99	0.43
1:A:1049:LYS:NZ	3:C:1300:LEU:O	2.48	0.43
4:D:22:LEU:HG	4:D:69:ALA:HB2	2.00	0.43
1:A:1004:ASP:OD1	1:A:1005:VAL:N	2.52	0.43
3:C:946:LYS:HG3	3:C:949:GLN:NE2	2.34	0.43
3:C:1205:GLU:O	3:C:1209:ASN:HB2	2.18	0.43
3:C:1208:LEU:HB2	3:C:1241:ILE:HD11	1.99	0.43
1:A:313:ILE:HG12	1:A:327:LEU:HG	2.00	0.43
3:C:652:CYS:O	3:C:692:HIS:NE2	2.44	0.43
3:C:984:GLU:HG3	3:C:986:TYR:H	1.84	0.43
3:C:948:ARG:NH1	3:C:984:GLU:OE2	2.44	0.43
3:C:1124:SER:HB3	3:C:1126:PHE:CE1	2.54	0.43
3:C:929:LEU:HD12	3:C:967:GLU:HG3	2.01	0.42
1:A:56:VAL:HG11	1:A:1137:LEU:HD22	2.01	0.42
2:B:49:LEU:HD12	2:B:49:LEU:HA	1.92	0.42
3:C:477:LYS:O	3:C:495:ARG:NH2	2.51	0.42
1:A:958:ARG:NH1	1:A:980:LYS:HD2	2.34	0.42
1:A:82:SER:OG	1:A:83:ASP:N	2.52	0.42
3:C:696:ASP:OD1	3:C:697:GLU:N	2.52	0.42
1:A:359:TYR:HD1	1:A:397:LEU:HA	1.85	0.42
3:C:1100:ASN:O	3:C:1104:GLN:HG2	2.19	0.42
1:A:1091:LEU:HD12	1:A:1197:TYR:HD2	1.84	0.42
3:C:493:LYS:HB2	3:C:493:LYS:HE3	1.93	0.42
1:A:928:TYR:HD2	1:A:937:LEU:HB3	1.85	0.42
1:A:1011:TRP:HB3	1:A:1024:PHE:CZ	2.54	0.42
3:C:489:PRO:O	3:C:491:GLU:N	2.50	0.42
3:C:552:LEU:HA	3:C:555:VAL:HG12	2.02	0.42
1:A:125:PRO:HG2	1:A:174:ASP:HA	2.00	0.42
3:C:1093:VAL:O	3:C:1097:LEU:HD23	2.19	0.42
3:C:1169:VAL:HG12	3:C:1173:LEU:HD13	2.02	0.41
1:A:31:VAL:HG12	1:A:65:LEU:HD21	2.02	0.41
1:A:128:ARG:NH1	1:A:178:GLU:O	2.50	0.41
1:A:1039:LEU:HB2	1:A:1043:THR:OG1	2.20	0.41
3:C:760:GLU:CD	3:C:760:GLU:H	2.24	0.41
3:C:906:GLU:CG	3:C:947:VAL:HG22	2.50	0.41
3:C:939:ARG:HA	3:C:939:ARG:HD3	1.83	0.41
1:A:352:GLU:HB2	2:B:61:LYS:HE3	2.01	0.41
1:A:415:LEU:HD12	1:A:795:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:568:ARG:HD3	3:C:608:THR:OG1	2.20	0.41
3:C:1017:LEU:HB3	3:C:1018:PRO:HD3	2.02	0.41
3:C:1236:GLY:O	3:C:1239:VAL:HG22	2.21	0.41
3:C:665:ILE:HG21	3:C:704:ILE:HG23	2.02	0.41
1:A:172:GLY:O	1:A:237:THR:OG1	2.23	0.41
3:C:663:THR:O	3:C:667:ILE:HG13	2.21	0.41
3:C:1097:LEU:HD11	3:C:1115:ALA:HB3	2.01	0.41
1:A:787:LYS:O	1:A:800:ILE:HG12	2.21	0.41
1:A:71:THR:HG22	3:C:680:LEU:HD23	2.01	0.41
1:A:185:LEU:HD21	1:A:235:LEU:HD21	2.02	0.41
1:A:318:ASP:O	1:A:320:ASP:N	2.52	0.41
1:A:424:TYR:CE2	1:A:871:PRO:HB3	2.56	0.41
1:A:1042:ASP:HA	1:A:1058:LEU:HD12	2.02	0.41
1:A:86:ARG:HG2	1:A:106:THR:HG23	2.02	0.41
1:A:922:GLY:HA2	1:A:946:GLU:O	2.21	0.41
3:C:672:ALA:HA	3:C:679:ILE:HD11	2.02	0.41
1:A:118:GLY:HA2	1:A:132:ILE:HD11	2.03	0.40
1:A:162:LYS:HG2	1:A:222:ARG:HH22	1.85	0.40
3:C:487:LEU:HD12	3:C:487:LEU:HA	1.82	0.40
3:C:793:LYS:HB2	3:C:836:THR:HG23	2.03	0.40
3:C:926:LYS:HE3	3:C:926:LYS:HB3	1.86	0.40
1:A:943:THR:HG21	1:A:977:LEU:HB2	2.02	0.40
1:A:246:SER:O	1:A:258:TYR:OH	2.39	0.40
1:A:789:VAL:HG13	1:A:891:VAL:HG13	2.03	0.40
1:A:804:HIS:NE2	1:A:859:ASN:O	2.55	0.40
3:C:666:LYS:HD2	3:C:704:ILE:HD11	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	856/899 (95%)	801 (94%)	52 (6%)	3 (0%)	34	72
2	B	63/86 (73%)	62 (98%)	1 (2%)	0	100	100
3	C	840/852 (99%)	813 (97%)	26 (3%)	1 (0%)	51	85
4	D	91/108 (84%)	77 (85%)	14 (15%)	0	100	100
All	All	1850/1945 (95%)	1753 (95%)	93 (5%)	4 (0%)	47	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	A	137	LYS
1	A	914	ILE
3	C	1179	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	749/774 (97%)	742 (99%)	7 (1%)	78	92
2	B	57/77 (74%)	57 (100%)	0	100	100
3	C	728/737 (99%)	714 (98%)	14 (2%)	57	84
4	D	80/90 (89%)	80 (100%)	0	100	100
All	All	1614/1678 (96%)	1593 (99%)	21 (1%)	69	89

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ARG
1	A	331	ASP
1	A	435	LEU
1	A	1013	ARG
1	A	1048	ASP
1	A	1075	MET
1	A	1148	TYR

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Mol	Chain	Res	Type
3	C	492	GLN
3	C	494	GLU
3	C	522	LYS
3	C	632	PHE
3	C	822	ARG
3	C	859	ASP
3	C	900	PHE
3	C	923	LYS
3	C	1017	LEU
3	C	1027	ARG
3	C	1059	CYS
3	C	1063	LEU
3	C	1106	ARG
3	C	1209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	518	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	0.30	0	37,49,49	0.63	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
6	T2W	D	104	4	-	4/25/51/51	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	2.90	129.96	122.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

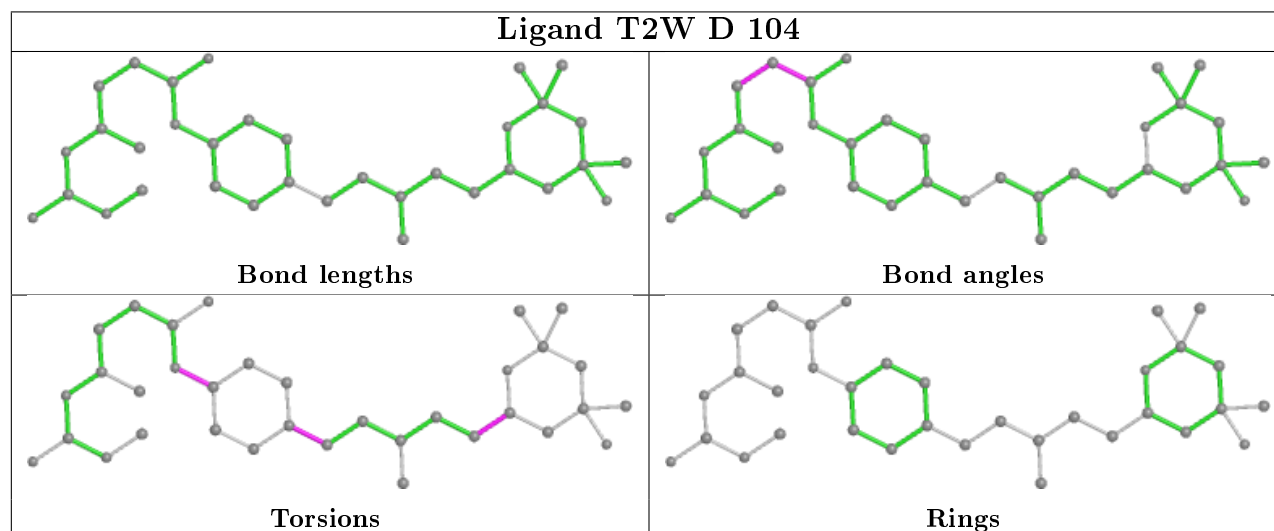
Mol	Chain	Res	Type	Atoms
6	D	104	T2W	C15-C16-N-C19
6	D	104	T2W	C11-C12-C13-C18
6	D	104	T2W	O1-C7-C8-C9
6	D	104	T2W	C11-C12-C13-C14

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	862/899 (95%)	0.11	16 (1%) 66 37	63, 102, 140, 162	0
2	B	65/86 (75%)	0.38	1 (1%) 73 46	74, 88, 109, 125	0
3	C	842/852 (98%)	-0.03	11 (1%) 77 51	64, 102, 132, 162	0
4	D	93/108 (86%)	-0.19	1 (1%) 80 56	62, 82, 122, 151	0
All	All	1862/1945 (95%)	0.04	29 (1%) 72 44	62, 101, 137, 162	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	6	PRO	4.9
3	C	463	ASN	3.1
1	A	49	LYS	3.1
1	A	844	ASN	3.0
3	C	905	THR	3.0
1	A	191	GLU	3.0
1	A	972	LEU	2.9
1	A	1051	GLY	2.8
3	C	484	GLU	2.6
3	C	1139	PRO	2.5
3	C	1045	ARG	2.4
3	C	1141	LEU	2.4
1	A	1169	PRO	2.4
1	A	1170	ASN	2.3
1	A	364	LEU	2.3
1	A	834	LEU	2.3
1	A	930	LEU	2.3
1	A	369	GLU	2.2
1	A	275	ARG	2.2
3	C	931	GLN	2.2
3	C	1218	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1034	THR	2.1
3	C	1131	ALA	2.1
1	A	817	GLN	2.1
2	B	46	HIS	2.1
1	A	904	TYR	2.1
1	A	826	ALA	2.1
3	C	904	THR	2.1
3	C	785	LYS	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	T2W	D	104	34/34	0.88	0.37	94,105,121,124	0
5	ZN	D	103	1/1	0.97	0.20	97,97,97,97	0
5	ZN	D	102	1/1	0.97	0.18	69,69,69,69	0
5	ZN	D	101	1/1	1.00	0.19	78,78,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.