Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2021 – 05:05 pm BST

PDB ID	:	7B91
Title	:	Structure of a minimal SF3B core in complex with pladienolide D (form I)
Authors	:	Cretu, C.; Pena, V.
Deposited on	:	2020-12-13
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

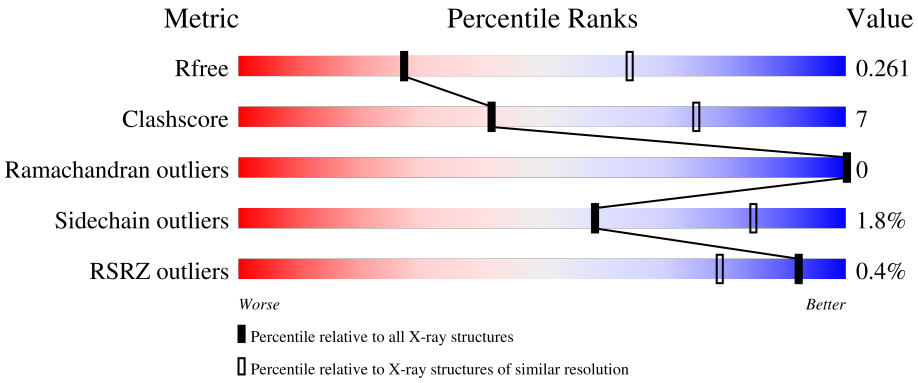
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 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 <=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	% 78% 18% .
2	B	86	65% 12% 23%
3	C	852	78% 20% .
4	D	108	80% 5% 16%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14776 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	861	Total	C	N	O	S	0	0	0
			6801	4326	1158	1286	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	66	Total	C	N	O	S	0	0	0
			540	343	94	98	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	91	Total	C	N	O	S	0	0	0
			685	418	121	133	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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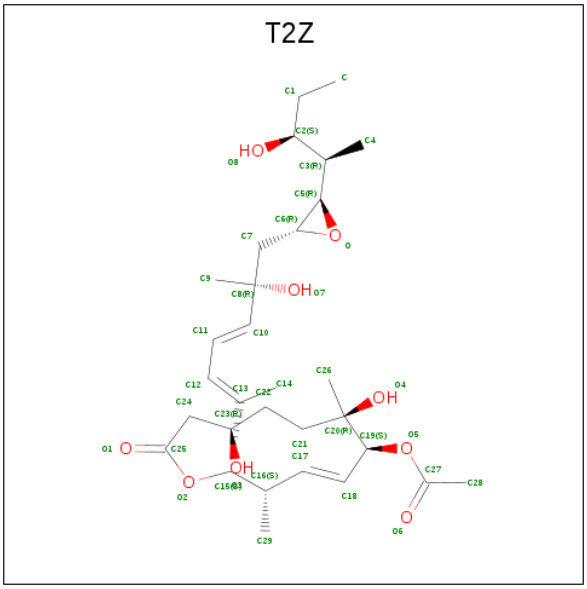
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q7RTV0
D	-5	SER	-	expression tag	UNP Q7RTV0
D	-4	PRO	-	expression tag	UNP Q7RTV0
D	-3	GLY	-	expression tag	UNP Q7RTV0
D	-2	SER	-	expression tag	UNP Q7RTV0
D	-1	ARG	-	expression tag	UNP Q7RTV0
D	0	ALA	-	expression tag	UNP Q7RTV0

- Molecule 5 is [(2 {S},3 {S},4 {E},6 {S},7 {R},10 {R})-3,7-dimethyl-2-[(2 {E},4 {E},6 {R})-6-methyl-6-oxidanyl-7-[(2 {R},3 {R})-3-[(2 {R},3 {S})-3-oxidanylpentan-2-yl]oxiran-2-yl]hepta-2,4-dien-2-yl]-7,10-bis(oxidanyl)-12-oxidanylidene-1-oxacyclododec-4-en-6-yl] ethanoate (three-letter code: T2Z) (formula: $C_{30}H_{48}O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 39 30 9	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

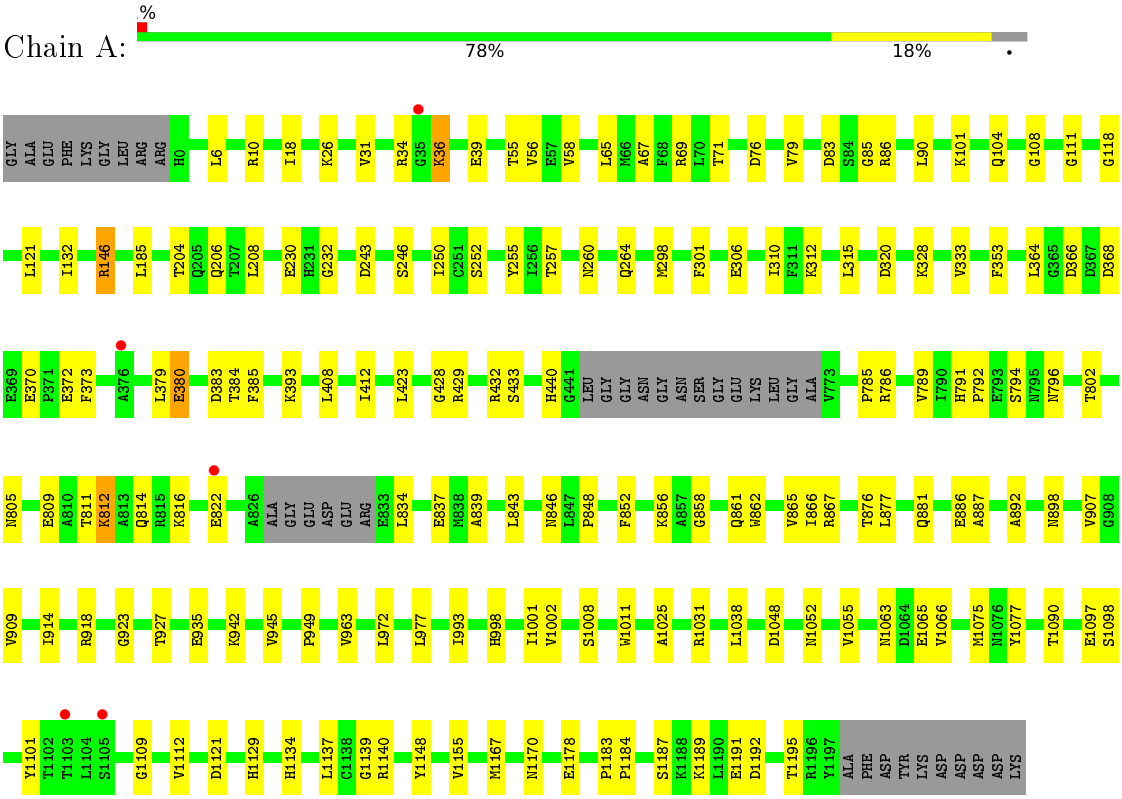
- Molecule 7 is water.

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

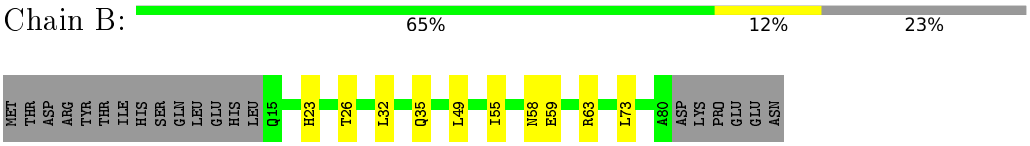
3 Residue-property plots (i)

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.

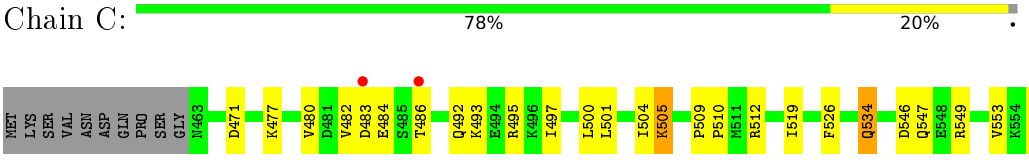
- Molecule 1: Splicing factor 3B subunit 3

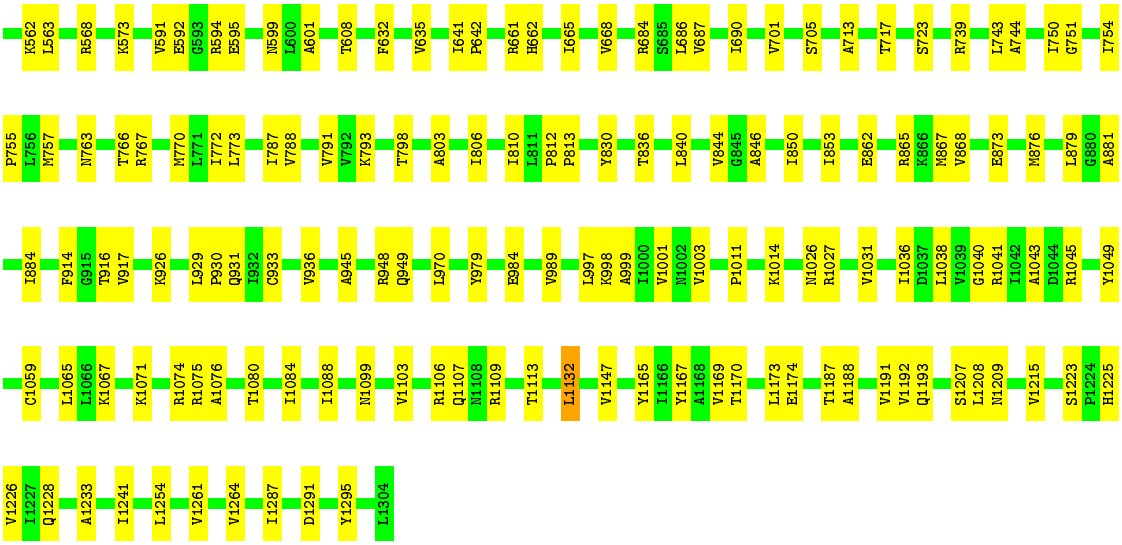


- Molecule 2: Splicing factor 3B subunit 5



- Molecule 3: Splicing factor 3B subunit 1





• 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	106.08Å 109.80Å 251.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.33 – 3.00 50.33 – 2.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.33-3.00) 99.8 (50.33-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.210 , 0.255 0.216 , 0.261	Depositor DCC
R_{free} test set	3563 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	100.3	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14776	wwPDB-VP
Average B, all atoms (Å^2)	96.0	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.*

[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: ZN, T2Z

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	0/6949	0.46	0/9424
2	B	0.26	0/556	0.41	0/751
3	C	0.25	0/6835	0.42	0/9256
4	D	0.26	0/693	0.44	0/930
All	All	0.26	0/15033	0.44	0/20361

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	6801	0	6718	98	0
2	B	540	0	509	12	0
3	C	6707	0	6915	105	0
4	D	685	0	663	3	0
5	D	39	0	0	0	0
6	D	3	0	0	0	0
7	D	1	0	0	0	0
All	All	14776	0	14805	208	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 7.

All (208) 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:668:VAL:HG11	3:C:690:ILE:HG21	1.58	0.84
1:A:1011:TRP:HB2	1:A:1025:ALA:HB3	1.63	0.78
1:A:34:ARG:NH2	1:A:39:GLU:OE1	2.19	0.75
1:A:185:LEU:HB3	1:A:206:GLN:HE21	1.51	0.73
3:C:1036:ILE:HD11	3:C:1065:LEU:HD13	1.69	0.73
1:A:246:SER:O	1:A:260:ASN:ND2	2.23	0.71
1:A:90:LEU:HD23	1:A:101:LYS:HA	1.72	0.70
1:A:310:ILE:HD11	1:A:333:VAL:HG22	1.75	0.69
3:C:949:GLN:HB2	3:C:989:VAL:HG12	1.76	0.67
3:C:793:LYS:HB2	3:C:836:THR:HG23	1.76	0.66
2:B:32:LEU:HD11	3:C:1287:ILE:HG21	1.78	0.65
1:A:858:GLY:HA3	1:A:861:GLN:HG2	1.79	0.64
3:C:788:VAL:HA	3:C:791:VAL:HG12	1.79	0.63
3:C:754:ILE:HG12	3:C:757:MET:HE2	1.80	0.63
1:A:83:ASP:OD2	1:A:1140:ARG:NH1	2.32	0.62
3:C:933:CYS:HA	3:C:936:VAL:HG12	1.81	0.62
1:A:428:GLY:HA3	1:A:433:SER:HA	1.82	0.61
3:C:471:ASP:OD1	3:C:505:LYS:NZ	2.33	0.60
3:C:1076:ALA:O	3:C:1080:THR:HG23	2.00	0.60
1:A:83:ASP:O	1:A:111:GLY:N	2.33	0.60
1:A:786:ARG:NH1	1:A:802:THR:O	2.35	0.60
3:C:595:GLU:O	3:C:599:ASN:ND2	2.33	0.60
3:C:1040:GLY:HA3	3:C:1080:THR:HG22	1.83	0.60
1:A:1055:VAL:HB	1:A:1075:MET:HB3	1.84	0.59
1:A:328:LYS:HE2	1:A:372:GLU:HB3	1.84	0.59
1:A:1001:ILE:HG13	1:A:1038:LEU:HD21	1.85	0.59
1:A:232:GLY:HA2	1:A:252:SER:HA	1.85	0.58
3:C:744:ALA:HB1	3:C:787:ILE:HD12	1.84	0.58
1:A:412:ILE:HG12	1:A:423:LEU:HG	1.84	0.58
1:A:816:LYS:NZ	1:A:846:ASN:OD1	2.36	0.58
3:C:662:HIS:HB2	3:C:701:VAL:HG12	1.86	0.58
1:A:353:PHE:O	1:A:432:ARG:NH1	2.34	0.57
1:A:18:ILE:HD12	1:A:67:ALA:HB2	1.87	0.57
3:C:1223:SER:HB2	3:C:1226:VAL:HG22	1.86	0.57
1:A:208:LEU:HD22	1:A:250:ILE:HD11	1.87	0.56
1:A:1063:ASN:HB3	1:A:1066:VAL:HG12	1.87	0.56
3:C:945:ALA:HB1	3:C:989:VAL:HG11	1.88	0.55
1:A:79:VAL:HG22	1:A:121:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:TYR:CZ	1:A:1109:GLY:HA3	2.43	0.54
1:A:1191:GLU:O	1:A:1195:THR:HG23	2.08	0.54
3:C:484:GLU:OE1	3:C:486:THR:N	2.34	0.53
1:A:230:GLU:OE1	1:A:255:TYR:HB2	2.08	0.53
3:C:1084:ILE:O	3:C:1088:ILE:HG13	2.08	0.53
1:A:320:ASP:OD1	1:A:320:ASP:N	2.36	0.53
1:A:789:VAL:HG11	1:A:892:ALA:HA	1.89	0.53
1:A:1077:TYR:HB2	1:A:1155:VAL:HG21	1.91	0.53
1:A:71:THR:O	1:A:146:ARG:NH2	2.41	0.53
1:A:429:ARG:NH1	2:B:59:GLU:O	2.38	0.53
3:C:1192:VAL:HG21	3:C:1215:VAL:HG21	1.91	0.52
1:A:1090:THR:HG22	1:A:1097:GLU:HA	1.91	0.52
3:C:979:TYR:CG	3:C:1011:PRO:HG2	2.44	0.52
1:A:328:LYS:NZ	1:A:370:GLU:O	2.43	0.52
3:C:501:LEU:HD12	3:C:534:GLN:HG2	1.91	0.52
3:C:865:ARG:HA	3:C:868:VAL:HG12	1.92	0.51
3:C:1132:LEU:HD22	3:C:1147:VAL:HG13	1.91	0.51
3:C:632:PHE:HA	3:C:635:VAL:HG12	1.92	0.51
3:C:850:ILE:HA	3:C:853:ILE:HD11	1.93	0.51
1:A:10:ARG:HD3	1:A:55:THR:HG21	1.92	0.51
3:C:546:ASP:OD1	3:C:549:ARG:NH2	2.44	0.50
3:C:830:TYR:HA	3:C:867:MET:HE2	1.93	0.50
3:C:1099:ASN:O	3:C:1103:VAL:HG22	2.12	0.50
1:A:118:GLY:HA2	1:A:132:ILE:HD11	1.93	0.50
3:C:665:ILE:HD12	3:C:705:SER:HB3	1.93	0.50
3:C:553:VAL:HG21	3:C:592:GLU:HB3	1.94	0.50
3:C:998:LYS:HA	3:C:1038:LEU:HD13	1.92	0.50
3:C:483:ASP:OD1	3:C:483:ASP:N	2.40	0.50
1:A:86:ARG:NH1	1:A:1139:GLY:O	2.44	0.50
1:A:1098:SER:HB3	1:A:1112:VAL:HG12	1.94	0.50
3:C:1080:THR:O	3:C:1084:ILE:HG23	2.11	0.49
3:C:754:ILE:HD13	3:C:766:THR:HG22	1.93	0.49
1:A:243:ASP:OD1	1:A:243:ASP:N	2.38	0.49
3:C:1041:ARG:HH22	3:C:1045:ARG:HE	1.60	0.49
1:A:1129:HIS:NE2	1:A:1178:GLU:HG2	2.28	0.49
3:C:668:VAL:HG23	3:C:686:LEU:HD22	1.95	0.49
3:C:1026:ASN:HD22	3:C:1031:VAL:HG11	1.78	0.49
3:C:1059:CYS:SG	3:C:1084:ILE:HD11	2.53	0.49
1:A:230:GLU:OE2	1:A:257:THR:OG1	2.30	0.49
3:C:755:PRO:HA	3:C:798:THR:HG21	1.94	0.48
3:C:1291:ASP:OD1	3:C:1291:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASN:HB3	1:A:264:GLN:HG2	1.94	0.48
3:C:751:GLY:CA	3:C:791:VAL:HG23	2.43	0.48
3:C:948:ARG:NH2	3:C:984:GLU:OE1	2.46	0.48
3:C:601:ALA:HB1	3:C:635:VAL:HG23	1.95	0.48
1:A:366:ASP:OD1	1:A:366:ASP:N	2.46	0.48
1:A:886:GLU:HB3	1:A:909:VAL:HG11	1.95	0.48
1:A:301:PHE:HE2	1:A:315:LEU:HD11	1.78	0.48
1:A:993:ILE:HG22	1:A:1002:VAL:HG22	1.94	0.48
1:A:185:LEU:HB3	1:A:206:GLN:NE2	2.26	0.48
1:A:306:GLU:OE2	2:B:63:ARG:NE	2.46	0.48
1:A:373:PHE:HB3	1:A:385:PHE:CD2	2.49	0.48
1:A:791:HIS:HD2	1:A:792:PRO:HD2	1.79	0.48
4:D:7:ASP:OD2	4:D:7:ASP:N	2.47	0.48
3:C:1193:GLN:HB2	3:C:1233:ALA:HA	1.96	0.47
1:A:898:ASN:ND2	1:A:972:LEU:O	2.47	0.47
3:C:493:LYS:O	3:C:497:ILE:HG12	2.14	0.47
1:A:805:ASN:N	1:A:861:GLN:O	2.48	0.47
3:C:687:VAL:HG21	3:C:723:SER:O	2.15	0.47
3:C:493:LYS:HG2	3:C:526:PHE:HD1	1.79	0.47
3:C:881:ALA:HA	3:C:884:ILE:HD13	1.96	0.47
1:A:945:VAL:HG21	1:A:963:VAL:HG21	1.95	0.47
1:A:429:ARG:HH12	2:B:59:GLU:C	2.16	0.47
1:A:1008:SER:HB2	1:A:1031:ARG:HG3	1.97	0.47
1:A:927:THR:OG1	1:A:977:LEU:HD11	2.14	0.47
3:C:873:GLU:HG2	3:C:916:THR:OG1	2.15	0.47
3:C:1071:LYS:HE3	3:C:1075:ARG:HH22	1.80	0.46
1:A:877:LEU:HD13	1:A:935:GLU:HG2	1.96	0.46
3:C:846:ALA:HB2	3:C:879:LEU:HD12	1.97	0.46
1:A:433:SER:HB3	1:A:785:PRO:HD3	1.98	0.46
3:C:806:ILE:HG23	3:C:810:ILE:HD12	1.97	0.46
1:A:373:PHE:HB3	1:A:385:PHE:HD2	1.81	0.46
1:A:206:GLN:OE1	1:A:232:GLY:N	2.44	0.46
1:A:380:GLU:OE1	1:A:380:GLU:N	2.48	0.46
3:C:1170:THR:O	3:C:1174:GLU:HG3	2.16	0.46
1:A:1129:HIS:CE1	1:A:1178:GLU:HG2	2.51	0.46
1:A:848:PRO:HD2	1:A:852:PHE:HE2	1.81	0.46
3:C:504:ILE:HG21	3:C:555:VAL:HG11	1.98	0.46
1:A:809:GLU:O	1:A:812:LYS:HG3	2.16	0.46
1:A:862:TRP:HB3	1:A:887:ALA:HB2	1.98	0.46
1:A:945:VAL:HG22	1:A:963:VAL:HG11	1.98	0.46
1:A:1189:LYS:HA	1:A:1192:ASP:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:770:MET:SD	3:C:773:LEU:HD11	2.56	0.45
3:C:763:ASN:OD1	3:C:767:ARG:NH1	2.41	0.45
3:C:1173:LEU:HD13	3:C:1192:VAL:HG12	1.99	0.45
3:C:568:ARG:HD3	3:C:608:THR:OG1	2.17	0.45
2:B:32:LEU:HD13	3:C:1295:TYR:CG	2.52	0.45
3:C:754:ILE:HA	3:C:757:MET:HE2	1.98	0.45
1:A:385:PHE:CD1	1:A:385:PHE:N	2.85	0.45
3:C:547:GLN:HB3	4:D:95:LYS:NZ	2.32	0.44
3:C:812:PRO:HB2	3:C:813:PRO:HD3	1.99	0.44
1:A:791:HIS:ND1	1:A:794:SER:HB3	2.32	0.44
1:A:312:LYS:HE3	1:A:364:LEU:O	2.18	0.44
2:B:23:HIS:H	2:B:26:THR:HG1	1.64	0.44
1:A:839:ALA:O	1:A:843:LEU:HD12	2.17	0.44
1:A:1134:HIS:ND1	1:A:1167:MET:HG2	2.33	0.44
3:C:999:ALA:O	3:C:1003:VAL:HG22	2.18	0.44
3:C:1026:ASN:OD1	3:C:1027:ARG:N	2.50	0.44
4:D:22:LEU:HG	4:D:69:ALA:HB2	1.99	0.44
3:C:757:MET:HB2	3:C:757:MET:HE3	1.93	0.44
1:A:69:ARG:HB2	1:A:76:ASP:OD1	2.17	0.44
3:C:500:LEU:HD13	3:C:519:ILE:HB	2.00	0.44
3:C:665:ILE:HA	3:C:668:VAL:HG12	1.99	0.44
3:C:948:ARG:H	3:C:948:ARG:HG2	1.53	0.44
1:A:56:VAL:HG11	1:A:1137:LEU:HD22	1.99	0.44
1:A:848:PRO:HD2	1:A:852:PHE:CE2	2.52	0.44
3:C:926:LYS:HA	3:C:929:LEU:HD12	1.99	0.44
1:A:914:ILE:O	1:A:918:ARG:HA	2.17	0.43
3:C:739:ARG:HA	3:C:743:LEU:HB2	1.99	0.43
1:A:865:VAL:HG23	1:A:881:GLN:HA	1.99	0.43
3:C:772:ILE:HD12	3:C:772:ILE:H	1.83	0.43
3:C:1067:LYS:HB2	3:C:1067:LYS:HE3	1.83	0.43
3:C:573:LYS:HB2	3:C:573:LYS:HE2	1.81	0.43
1:A:923:GLY:HA3	1:A:949:PRO:HD3	1.99	0.43
3:C:788:VAL:O	3:C:791:VAL:HG12	2.19	0.43
3:C:1208:LEU:HB2	3:C:1241:ILE:HD11	2.00	0.43
1:A:36:LYS:O	1:A:58:VAL:HG22	2.18	0.43
2:B:32:LEU:HA	2:B:35:GLN:HG2	2.00	0.43
3:C:477:LYS:O	3:C:495:ARG:NH2	2.49	0.43
1:A:31:VAL:HG23	1:A:65:LEU:HD21	2.01	0.43
1:A:1183:PRO:N	1:A:1184:PRO:HD2	2.34	0.43
1:A:408:LEU:HD11	2:B:55:ILE:HD13	2.00	0.42
1:A:867:ARG:NH1	1:A:876:THR:HG21	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:ASP:HB2	1:A:1052:ASN:HB2	2.01	0.42
3:C:803:ALA:HB1	3:C:844:VAL:HA	2.01	0.42
3:C:557:ASP:HB2	3:C:599:ASN:CG	2.39	0.42
3:C:713:ALA:O	3:C:717:THR:HG23	2.19	0.42
3:C:1225:HIS:O	3:C:1228:GLN:HG2	2.19	0.42
3:C:836:THR:O	3:C:840:LEU:HG	2.19	0.42
1:A:383:ASP:OD1	1:A:384:THR:N	2.53	0.42
1:A:886:GLU:OE2	1:A:942:LYS:NZ	2.51	0.42
1:A:1187:SER:O	1:A:1191:GLU:HG2	2.20	0.42
3:C:497:ILE:HD11	3:C:526:PHE:CD2	2.53	0.42
3:C:1167:TYR:CE1	3:C:1207:SER:HB3	2.55	0.42
2:B:49:LEU:HD12	2:B:49:LEU:HA	1.88	0.42
3:C:665:ILE:O	3:C:668:VAL:HG12	2.20	0.42
1:A:866:ILE:HD13	1:A:907:VAL:HG21	2.02	0.42
1:A:101:LYS:HD3	1:A:104:GLN:HB2	2.01	0.41
3:C:509:PRO:N	3:C:510:PRO:HD2	2.35	0.41
3:C:933:CYS:HB3	3:C:970:LEU:HD21	2.01	0.41
3:C:1165:TYR:O	3:C:1169:VAL:HG23	2.20	0.41
1:A:1065:GLU:N	1:A:1065:GLU:OE1	2.53	0.41
3:C:1187:THR:O	3:C:1191:VAL:HG23	2.21	0.41
1:A:834:LEU:HD12	1:A:837:GLU:HB2	2.01	0.41
3:C:997:LEU:O	3:C:1001:VAL:HG23	2.20	0.41
1:A:811:THR:O	1:A:814:GLN:HG3	2.20	0.41
3:C:929:LEU:N	3:C:930:PRO:HD2	2.36	0.41
1:A:805:ASN:ND2	2:B:58:ASN:HB3	2.34	0.41
1:A:794:SER:OG	1:A:796:ASN:ND2	2.54	0.41
3:C:661:ARG:H	3:C:661:ARG:HG2	1.65	0.41
3:C:862:GLU:HG3	3:C:865:ARG:NH1	2.36	0.41
3:C:1014:LYS:HG2	3:C:1049:TYR:O	2.20	0.41
3:C:1043:ALA:CB	3:C:1084:ILE:HG22	2.50	0.41
3:C:1188:ALA:O	3:C:1192:VAL:HG13	2.21	0.41
1:A:379:LEU:HG	1:A:380:GLU:H	1.86	0.41
1:A:384:THR:OG1	1:A:385:PHE:N	2.54	0.41
1:A:805:ASN:HD21	2:B:58:ASN:HB3	1.85	0.41
3:C:641:ILE:N	3:C:642:PRO:HD2	2.36	0.41
3:C:1254:LEU:HD23	3:C:1254:LEU:HA	1.84	0.41
3:C:1261:VAL:HA	3:C:1264:VAL:HG22	2.03	0.41
3:C:559:ILE:O	3:C:563:LEU:HG	2.21	0.40
3:C:591:VAL:HG12	3:C:594:ARG:NH2	2.37	0.40
3:C:1109:ARG:O	3:C:1113:THR:HG23	2.21	0.40
1:A:6:LEU:HD23	1:A:6:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:THR:CG2	2:B:73:LEU:HD21	2.51	0.40
3:C:480:VAL:HG12	3:C:482:VAL:HG12	2.03	0.40
3:C:555:VAL:O	3:C:559:ILE:HG12	2.21	0.40
3:C:876:MET:SD	3:C:917:VAL:HG23	2.61	0.40
3:C:750:ILE:O	3:C:754:ILE:HG13	2.22	0.40
1:A:85:GLY:HA3	1:A:108:GLY:O	2.22	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	855/899 (95%)	808 (94%)	47 (6%)	0	100	100
2	B	64/86 (74%)	64 (100%)	0	0	100	100
3	C	840/852 (99%)	813 (97%)	27 (3%)	0	100	100
4	D	89/108 (82%)	85 (96%)	4 (4%)	0	100	100
All	All	1848/1945 (95%)	1770 (96%)	78 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	748/774 (97%)	733 (98%)	15 (2%)	55 83
2	B	57/77 (74%)	57 (100%)	0	100 100
3	C	728/737 (99%)	715 (98%)	13 (2%)	59 85
4	D	78/90 (87%)	77 (99%)	1 (1%)	69 89
All	All	1611/1678 (96%)	1582 (98%)	29 (2%)	59 85

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	36	LYS
1	A	146	ARG
1	A	298	MET
1	A	368	ASP
1	A	380	GLU
1	A	393	LYS
1	A	440	HIS
1	A	812	LYS
1	A	822	GLU
1	A	856	LYS
1	A	998	HIS
1	A	1121	ASP
1	A	1148	TYR
1	A	1170	ASN
3	C	492	GLN
3	C	505	LYS
3	C	512	ARG
3	C	534	GLN
3	C	562	LYS
3	C	684	ARG
3	C	914	PHE
3	C	931	GLN
3	C	1074	ARG
3	C	1106	ARG
3	C	1107	GLN
3	C	1132	LEU
3	C	1209	ASN
4	D	55	GLN

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

Mol	Chain	Res	Type
1	A	805	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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
5	T2Z	D	1401	-	38,40,40	0.15	0	45,58,58	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	T2Z	D	1401	-	-	3/59/64/64	0/1/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

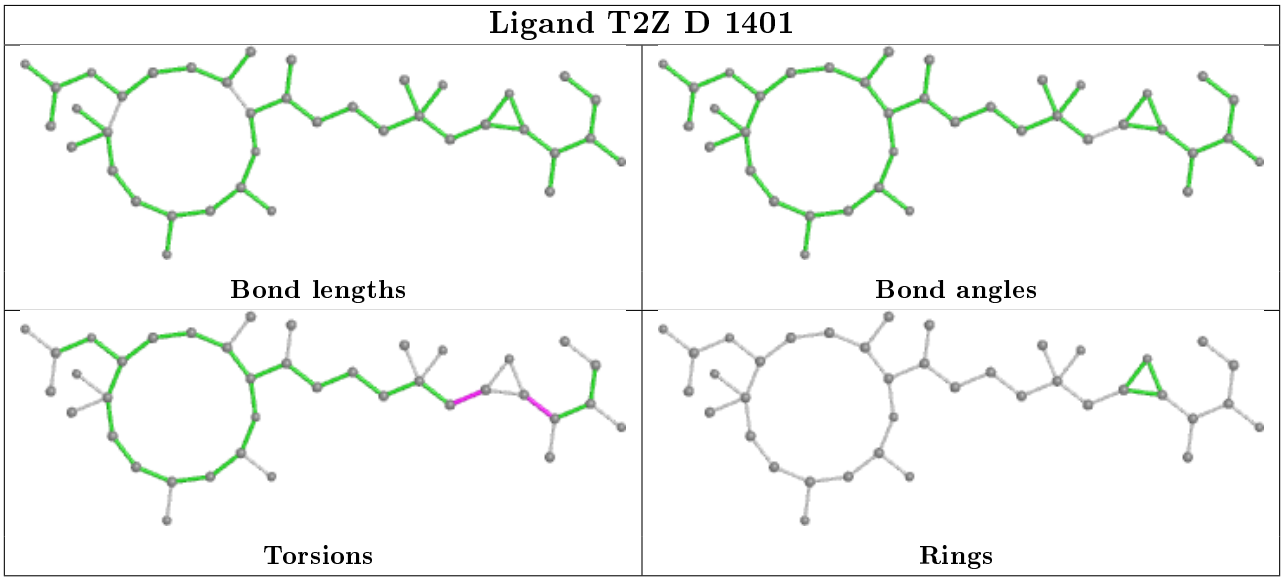
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1401	T2Z	C4-C3-C5-O
5	D	1401	T2Z	C4-C3-C5-C6
5	D	1401	T2Z	C5-C6-C7-C8

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.



5.7 Other polymers (i)

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	861/899 (95%)	-0.07	5 (0%) 89 72	58, 94, 127, 154	0
2	B	66/86 (76%)	0.14	0 100 100	70, 83, 101, 127	0
3	C	842/852 (98%)	-0.24	2 (0%) 95 87	61, 99, 124, 171	0
4	D	91/108 (84%)	-0.29	0 100 100	64, 80, 114, 124	0
All	All	1860/1945 (95%)	-0.15	7 (0%) 92 79	58, 95, 125, 171	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	822	GLU	2.7
3	C	483	ASP	2.7
1	A	376	ALA	2.6
1	A	35	GLY	2.4
1	A	1105	SER	2.2
1	A	1103	THR	2.1
3	C	486	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
5	T2Z	D	1401	39/39	0.91	0.31	64,80,90,93	0
6	ZN	D	1402	1/1	0.99	0.19	94,94,94,94	0
6	ZN	D	1403	1/1	0.99	0.20	85,85,85,85	0
6	ZN	D	1404	1/1	0.99	0.19	70,70,70,70	0

6.5 Other polymers

There are no such residues in this entry.