



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2019 – 07:06 PM EDT

PDB ID : 6NTT  
Title : X-ray Crystal Structure of Soybean Trypsin Inhibitor (Kunitz) Complexed with 1,5-Disulfonyl Naphthalene  
Authors : McPherson, A.  
Deposited on : 2019-01-30  
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](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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

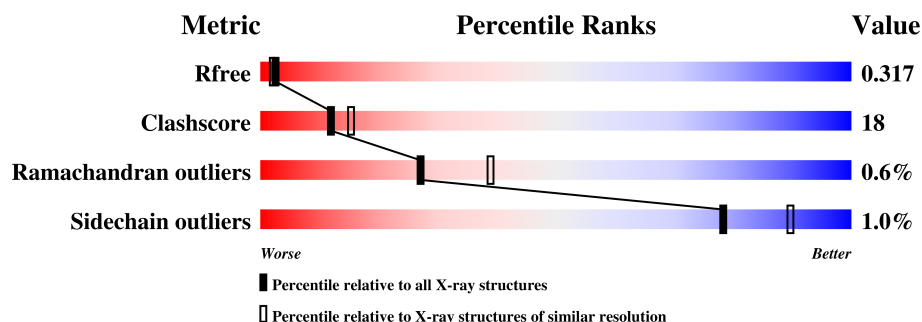
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	216	<div> <div style="width: 64%; background-color: green;"></div> <div style="width: 16%; background-color: yellow;"></div> <div style="width: 19%; background-color: grey;"></div> <div style="width: 1%; background-color: red;"></div> </div> <div>64% 16% . 19%</div>
1	B	216	<div> <div style="width: 63%; background-color: green;"></div> <div style="width: 19%; background-color: yellow;"></div> <div style="width: 19%; background-color: grey;"></div> </div> <div>63% 19% 19%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	21D	A	201[A]	-	-	X	-
2	21D	A	201[B]	-	-	X	-
2	21D	B	201[A]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MES	A	202[A]	-	-	X	-

## 2 Entry composition [i](#)

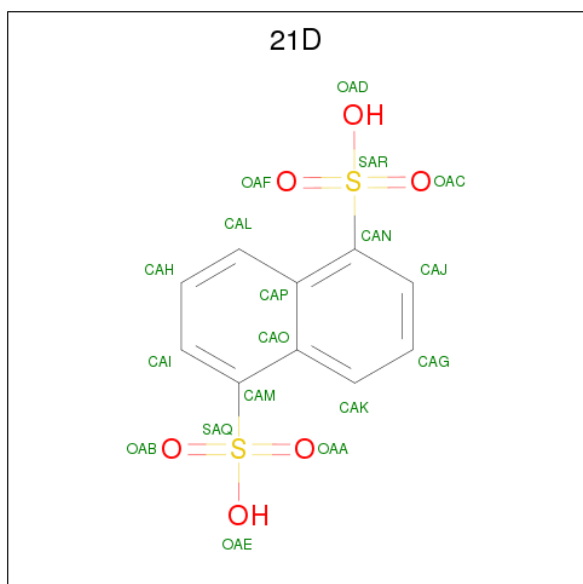
There are 4 unique types of molecules in this entry. The entry contains 3130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Trypsin inhibitor A.

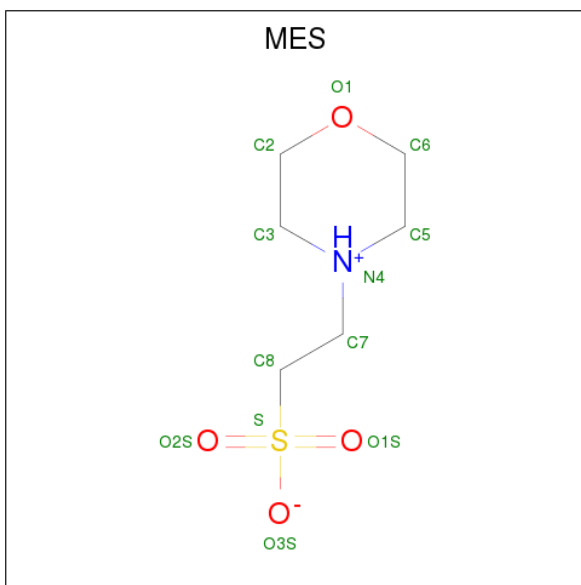
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	2	0
			1376	871	232	267	6			
1	B	176	Total	C	N	O	S	0	0	0
			1373	868	232	267	6			

- Molecule 2 is naphthalene-1,5-disulfonic acid (three-letter code: 21D) (formula:  $C_{10}H_8O_6S_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	1
			36	20	12	4		
2	B	1	Total	C	O	S	0	1
			36	20	12	4		
2	B	1	Total	C	O	S	0	1
			36	20	12	4		

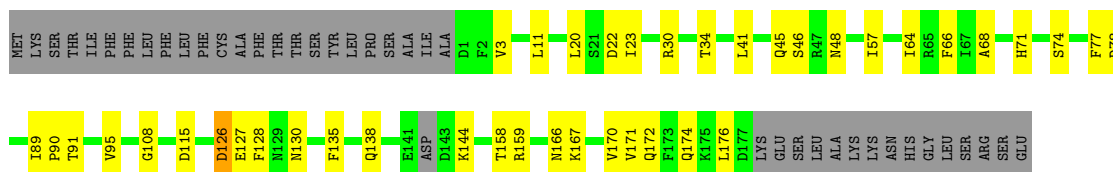
- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	102	Total	O	0	0
			102	102		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.88Å 64.68Å 69.08Å 90.00° 97.52° 90.00°	Depositor
Resolution (Å)	32.61 – 2.40 32.61 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (32.61-2.40) 88.4 (32.61-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.209 , 0.306 0.215 , 0.317	Depositor DCC
$R_{free}$ test set	1153 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3130	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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: 21D, MES

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	0.65	0/1408	0.76	0/1905
1	B	0.65	0/1400	0.76	0/1896
All	All	0.65	0/2808	0.76	0/3801

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	GLY	Peptide

### 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	1376	0	1348	37	0
1	B	1373	0	1340	46	0
2	A	36	0	12	21	0
2	B	72	0	27	17	0
3	A	24	0	26	9	0
3	B	24	0	26	2	0
4	A	123	0	0	7	0
4	B	102	0	0	8	0
All	All	3130	0	2779	105	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 18.

All (105) 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)
1:B:22:ASP:CB	1:B:172:GLN:HE22	1.62	1.12
2:A:201[A]:21D:H4	4:A:308:HOH:O	1.49	1.11
1:A:159:ARG:HH22	3:A:202[A]:MES:C2	1.72	1.01
1:B:30:ARG:CZ	2:B:201[A]:21D:OAD	2.09	1.01
2:A:201[B]:21D:OAF	4:A:305:HOH:O	1.80	1.00
2:A:201[B]:21D:OAD	2:B:201[B]:21D:CAK	2.10	0.99
2:A:201[B]:21D:OAA	4:A:303:HOH:O	1.73	0.99
2:A:201[B]:21D:OAD	4:A:306:HOH:O	1.83	0.97
1:B:22:ASP:HB2	1:B:172:GLN:HE22	1.36	0.89
1:B:45:GLN:NE2	1:B:159:ARG:HH11	1.71	0.88
1:B:45:GLN:HE21	1:B:159:ARG:HH11	1.14	0.87
2:A:201[B]:21D:OAD	2:B:201[B]:21D:CAG	2.24	0.86
1:A:94:SER:OG	1:A:110[B]:ASN:ND2	2.09	0.85
1:A:110[B]:ASN:HD22	1:A:113:ALA:HB2	1.41	0.84
1:A:159:ARG:HH22	3:A:202[A]:MES:H21	1.41	0.83
1:A:108:GLY:O	1:A:110[B]:ASN:OD1	1.97	0.82
2:A:201[A]:21D:OAE	4:A:308:HOH:O	1.99	0.80
1:A:48:ASN:HD22	2:A:201[A]:21D:H2	1.47	0.80
1:A:159:ARG:HH22	3:A:202[A]:MES:H22	1.43	0.80
1:A:142:ASP:CG	1:A:143:ASP:H	1.86	0.80
2:B:201[A]:21D:OAA	2:B:201[A]:21D:H4	1.82	0.79
1:B:45:GLN:NE2	1:B:159:ARG:NH1	2.31	0.79
1:B:22:ASP:HB3	1:B:172:GLN:HE22	1.47	0.79
1:B:22:ASP:CB	1:B:172:GLN:NE2	2.45	0.77
2:A:201[A]:21D:OAF	2:A:201[A]:21D:H3	1.86	0.75
1:A:62:TYR:O	1:A:63:ARG:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201[A]:21D:H4	2:A:201[A]:21D:OAE	1.88	0.73
1:B:45:GLN:HE21	1:B:159:ARG:NH1	1.88	0.72
1:A:30:ARG:CZ	2:A:201[A]:21D:OAA	2.38	0.71
1:B:23:ILE:HD12	1:B:128:PHE:CE2	2.27	0.70
1:A:159:ARG:NH2	3:A:202[A]:MES:H22	2.07	0.67
1:A:30:ARG:NH2	2:A:201[A]:21D:OAA	2.27	0.67
2:B:201[B]:21D:H4	2:B:201[B]:21D:OAA	1.95	0.67
1:B:89:ILE:HD11	2:B:202[B]:21D:H2	1.76	0.67
1:B:23:ILE:HG22	1:B:23:ILE:O	1.95	0.67
1:B:30:ARG:NH1	2:B:201[A]:21D:OAD	2.28	0.65
1:B:144:LYS:HA	4:B:352:HOH:O	1.96	0.65
2:A:201[B]:21D:H4	2:A:201[B]:21D:OAB	1.94	0.65
1:B:22:ASP:HB3	1:B:172:GLN:NE2	2.09	0.65
1:A:142:ASP:CG	1:A:143:ASP:N	2.50	0.64
1:B:23:ILE:HD12	1:B:128:PHE:CZ	2.34	0.63
1:A:115:ASP:HB3	1:A:138:GLN:CD	2.22	0.59
1:A:159:ARG:NH2	3:A:202[A]:MES:C2	2.55	0.56
1:B:90:PRO:HG2	1:B:108:GLY:HA2	1.87	0.56
1:A:48:ASN:CB	2:A:201[A]:21D:H2	2.36	0.56
1:B:48:ASN:HD22	2:B:201[A]:21D:H5	1.71	0.55
1:B:176:LEU:HD12	4:B:369:HOH:O	2.06	0.55
3:B:203:MES:H52	4:B:368:HOH:O	2.07	0.55
1:A:176:LEU:O	1:A:177:ASP:HB2	2.06	0.55
1:A:48:ASN:HB3	2:A:201[A]:21D:H2	1.89	0.54
1:A:48:ASN:ND2	2:A:201[A]:21D:H2	2.20	0.54
1:B:30:ARG:HG3	1:B:30:ARG:NH1	2.22	0.54
1:B:176:LEU:CD1	4:B:369:HOH:O	2.56	0.54
1:B:22:ASP:HB2	1:B:172:GLN:NE2	2.17	0.53
1:B:115:ASP:OD2	1:B:138:GLN:HB2	2.08	0.53
2:A:201[A]:21D:OAB	2:B:201[A]:21D:CAP	2.57	0.52
1:B:127:GLU:O	1:B:127:GLU:CG	2.58	0.52
1:A:23:ILE:HD13	3:A:202[A]:MES:H61	1.92	0.52
1:B:144:LYS:NZ	4:B:306:HOH:O	2.31	0.52
1:B:3:VAL:HG12	1:B:11:LEU:HD13	1.91	0.52
1:B:30:ARG:NH2	2:B:201[A]:21D:OAD	2.44	0.51
1:A:119:ARG:NH2	4:A:315:HOH:O	2.43	0.51
1:B:46:SER:OG	2:B:201[B]:21D:OAE	2.29	0.50
1:A:77:PHE:HB2	1:A:91:THR:HB	1.92	0.50
1:A:58:ILE:HG23	1:A:75:LEU:CD2	2.42	0.50
2:B:201[B]:21D:H3	4:B:304:HOH:O	2.12	0.49
1:B:30:ARG:HG3	1:B:30:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:HD11	2:B:202[A]:21D:CAP	2.44	0.48
1:B:22:ASP:CA	1:B:172:GLN:HE22	2.24	0.47
2:B:201[A]:21D:CAK	2:B:201[A]:21D:OAA	2.58	0.47
1:B:68:ALA:HB3	1:B:71:HIS:CD2	2.49	0.47
1:B:77:PHE:HB2	1:B:91:THR:HB	1.96	0.47
1:B:89:ILE:HG12	2:B:202[B]:21D:H3	1.96	0.47
1:A:58:ILE:HG12	1:A:75:LEU:HD22	1.97	0.47
1:A:111:LYS:HE2	4:A:382:HOH:O	2.14	0.47
1:B:130:ASN:HB2	1:B:170:VAL:CG1	2.46	0.46
1:B:64:ILE:HD12	1:B:66:PHE:O	2.15	0.46
1:B:159:ARG:HG3	4:B:324:HOH:O	2.15	0.46
1:B:95:VAL:HG21	1:B:135:PHE:CG	2.51	0.46
1:B:127:GLU:O	1:B:127:GLU:HG2	2.16	0.46
1:A:18:TYR:CE2	1:A:176:LEU:HD13	2.50	0.46
1:A:11:LEU:HD22	1:A:17:TYR:CE2	2.51	0.45
1:A:11:LEU:HB2	1:A:67:ILE:HB	1.99	0.44
1:A:23:ILE:HD12	3:A:202[B]:MES:O3S	2.18	0.44
2:B:202[B]:21D:H3	2:B:202[B]:21D:OAF	2.19	0.43
1:A:71:HIS:HB3	1:A:72:PRO:HD2	1.98	0.43
3:A:202[B]:MES:H52	3:A:202[B]:MES:H82	1.70	0.43
1:B:20:LEU:HD11	1:B:174:GLN:NE2	2.34	0.43
1:B:89:ILE:CD1	2:B:202[B]:21D:H2	2.47	0.43
1:B:57:ILE:HD11	1:B:78:ASP:HB3	2.01	0.43
2:A:201[A]:21D:OAF	2:A:201[A]:21D:CAL	2.60	0.42
1:B:126:ASP:OD2	1:B:170:VAL:HG11	2.19	0.42
1:B:34:THR:HG22	1:B:158:THR:HG21	2.02	0.42
3:B:203:MES:C5	4:B:368:HOH:O	2.67	0.42
1:A:176:LEU:O	1:A:177:ASP:CB	2.68	0.41
2:A:201[B]:21D:OAB	2:A:201[B]:21D:CAK	2.66	0.41
1:A:2:PHE:HB3	1:A:10:PRO:HB3	2.02	0.41
1:A:48:ASN:HB3	2:A:201[A]:21D:CAH	2.49	0.41
1:B:130:ASN:HB3	1:B:171:VAL:O	2.21	0.41
1:A:99:LEU:HA	1:A:99:LEU:HD23	1.96	0.41
2:A:201[A]:21D:OAE	2:A:201[A]:21D:CAK	2.62	0.40
1:A:159:ARG:NH2	3:A:202[A]:MES:H21	2.21	0.40
1:A:39:CYS:HB3	1:A:40:PRO:HD2	2.03	0.40
1:B:166:ASN:O	1:B:167:LYS:C	2.59	0.40
1:A:89:ILE:HG13	1:A:89:ILE:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	171/216 (79%)	157 (92%)	13 (8%)	1 (1%)	27	39
1	B	172/216 (80%)	158 (92%)	13 (8%)	1 (1%)	27	39
All	All	343/432 (79%)	315 (92%)	26 (8%)	2 (1%)	27	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	126	ASP
1	A	13	ASN

### 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	153/187 (82%)	150 (98%)	3 (2%)	58	77
1	B	152/187 (81%)	151 (99%)	1 (1%)	85	93
All	All	305/374 (82%)	301 (99%)	4 (1%)	78	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110[A]	ASN
1	A	110[B]	ASN
1	A	142	ASP
1	B	74	SER

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

Mol	Chain	Res	Type
1	B	45	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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	$\# Z  > 2$
2	21D	A	201[A]	-	19,19,19	0.40	0	30,30,30	0.25	0
2	21D	A	201[B]	-	19,19,19	0.49	0	30,30,30	0.32	0
3	MES	A	202[A]	-	12,12,12	0.70	0	14,16,16	0.42	0
3	MES	A	202[B]	-	12,12,12	0.76	0	14,16,16	0.44	0
2	21D	B	201[A]	-	19,19,19	0.31	0	30,30,30	0.18	0
2	21D	B	201[B]	-	19,19,19	0.44	0	30,30,30	0.21	0
2	21D	B	202[A]	-	19,19,19	0.38	0	30,30,30	0.22	0
2	21D	B	202[B]	-	19,19,19	0.35	0	30,30,30	0.45	1 (3%)
3	MES	B	203	-	12,12,12	0.74	0	14,16,16	0.39	0
3	MES	B	204	-	12,12,12	0.75	0	14,16,16	0.36	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
2	21D	A	201[A]	-	-	0/12/12/12	0/2/2/2
2	21D	A	201[B]	-	-	0/12/12/12	0/2/2/2
3	MES	A	202[A]	-	-	0/6/14/14	0/1/1/1
3	MES	A	202[B]	-	-	0/6/14/14	0/1/1/1
2	21D	B	201[A]	-	-	0/12/12/12	0/2/2/2
2	21D	B	201[B]	-	-	0/12/12/12	0/2/2/2
2	21D	B	202[A]	-	-	0/12/12/12	0/2/2/2
2	21D	B	202[B]	-	-	0/12/12/12	0/2/2/2
3	MES	B	203	-	-	0/6/14/14	0/1/1/1
3	MES	B	204	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	202[B]	21D	OAF-SAR-CAN	2.31	108.71	106.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201[A]	21D	14	0
2	A	201[B]	21D	7	0
3	A	202[A]	MES	7	0
3	A	202[B]	MES	2	0
2	B	201[A]	21D	7	0
2	B	201[B]	21D	5	0
2	B	202[A]	21D	1	0
2	B	202[B]	21D	4	0
3	B	203	MES	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	138:GLN	C	139:GLN	N	13.79

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.