



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:09 pm BST

PDB ID : 3F0R  
Title : Crystal Structure Analysis of Human HDAC8 complexed with trichostatin A in a new monoclinic crystal form  
Authors : Dowling, D.P.; Gantt, S.L.; Gattis, S.G.; Fierke, C.A.; Christianson, D.W.  
Deposited on : 2008-10-25  
Resolution : 2.54 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.

---

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 : 2.11  
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) : 2.11

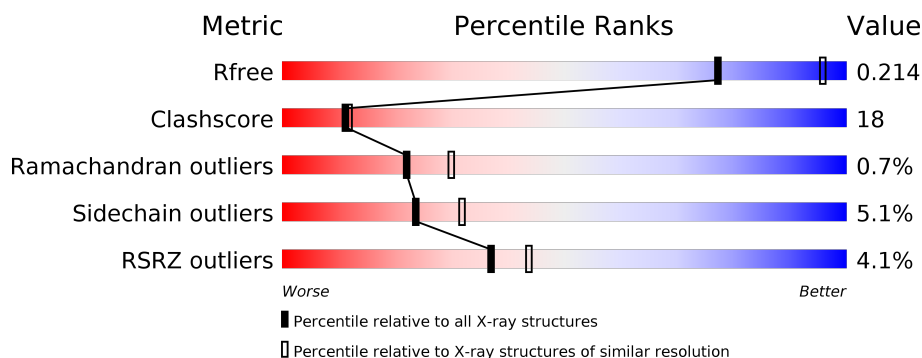
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 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	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 63%, yellow 27%, orange 2%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>63%</span> <span>27%</span> <span>• • 6%</span> </div> </div>
1	B	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 66%, yellow 26%, orange 2%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>66%</span> <span>26%</span> <span>• 6%</span> </div> </div>
1	C	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 7%, green 54%, yellow 35%, orange 2%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>7%</span> <span>54%</span> <span>35%</span> <span>• 9%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8703 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 Histone deacetylase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2839	1819	471	530	19			
1	B	366	Total	C	N	O	S	0	0	0
			2853	1828	474	532	19			
1	C	355	Total	C	N	O	S	0	0	0
			2769	1779	461	510	19			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	ILE	-	EXPRESSION TAG	UNP Q9BY41
A	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
A	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
A	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
A	382	SER	-	EXPRESSION TAG	UNP Q9BY41
A	383	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	388	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	378	ILE	-	EXPRESSION TAG	UNP Q9BY41
B	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
B	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
B	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
B	382	SER	-	EXPRESSION TAG	UNP Q9BY41
B	383	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	388	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	378	ILE	-	EXPRESSION TAG	UNP Q9BY41

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
C	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
C	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
C	382	SER	-	EXPRESSION TAG	UNP Q9BY41
C	383	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	388	HIS	-	EXPRESSION TAG	UNP Q9BY41

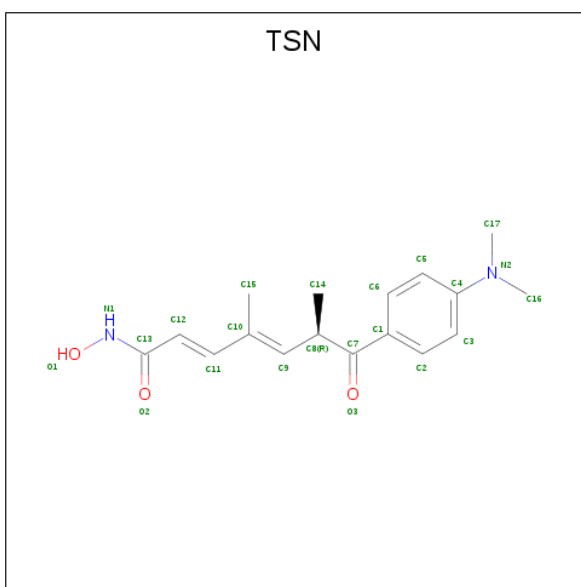
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0

- Molecule 4 is TRICHOSTATIN A (three-letter code: TSN) (formula: C<sub>17</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 22	C 17	N 2	O 3	0	0
4	A	1	Total 22	C 17	N 2	O 3	0	0
4	B	1	Total 22	C 17	N 2	O 3	0	0
4	B	1	Total 22	C 17	N 2	O 3	0	0
4	C	1	Total 22	C 17	N 2	O 3	0	0
4	C	1	Total 22	C 17	N 2	O 3	0	0

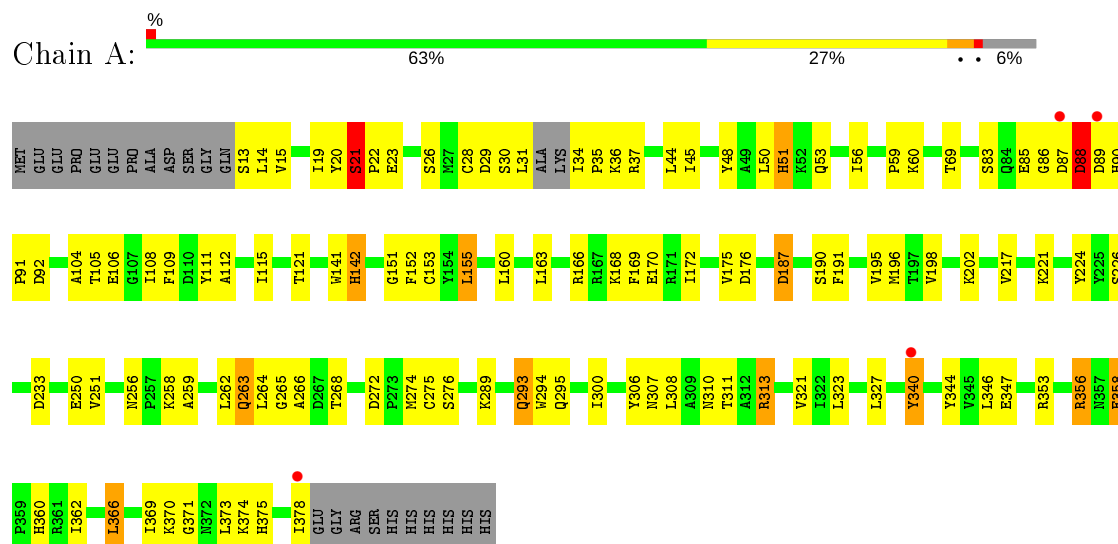
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	48	Total O 48 48	0	0
5	B	35	Total O 35 35	0	0
5	C	18	Total O 18 18	0	0

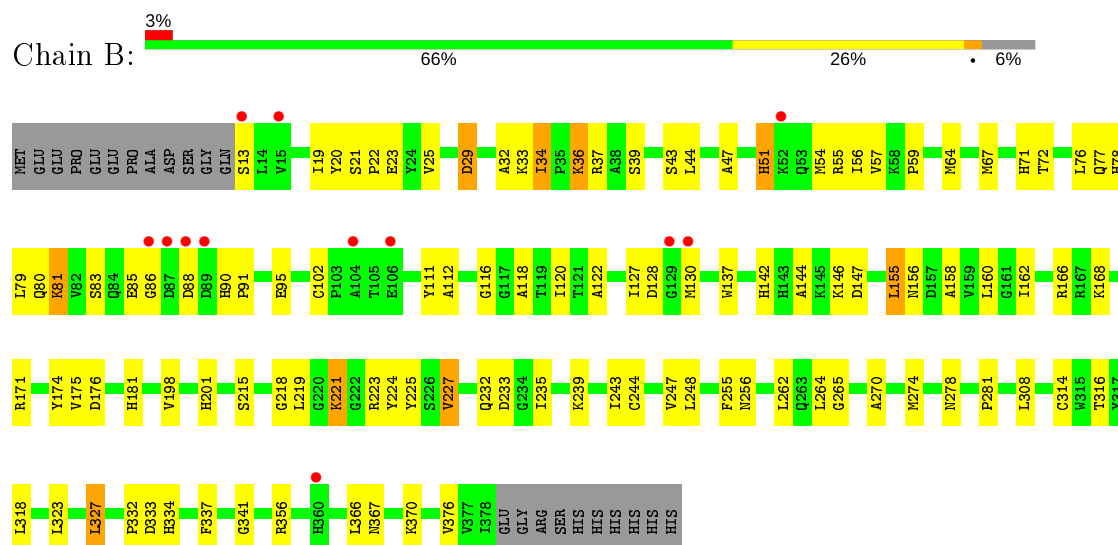
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Histone deacetylase 8

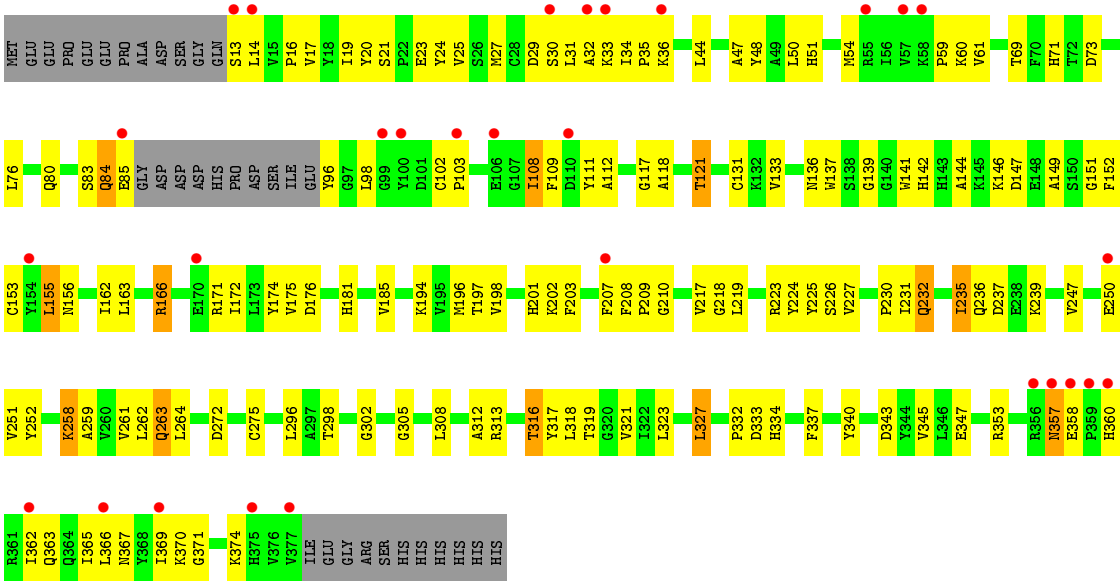


#### • Molecule 1: Histone deacetylase 8



#### • Molecule 1: Histone deacetylase 8





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.89Å 90.70Å 92.14Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	40.97 – 2.54 40.97 – 2.51	Depositor EDS
% Data completeness (in resolution range)	90.0 (40.97-2.54) 92.2 (40.97-2.51)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.210 , 0.258 0.211 , 0.214	Depositor DCC
$R_{free}$ test set	2311 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: TSN, ZN, K

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	0.38	0/2909	0.61	0/3947
1	B	0.36	0/2924	0.61	0/3968
1	C	0.33	0/2837	0.56	0/3847
All	All	0.36	0/8670	0.59	0/11762

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	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	TYR	Peptide
1	A	340	TYR	Peptide
1	C	305	GLY	Peptide

## 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	2839	0	2784	97	0
1	B	2853	0	2804	86	0
1	C	2769	0	2737	124	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	44	0	43	1	0
4	B	44	0	44	2	0
4	C	44	0	44	1	0
5	A	48	0	0	0	0
5	B	35	0	0	1	0
5	C	18	0	0	0	0
All	All	8703	0	8456	305	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 (305) 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:221:LYS:HE2	1:B:221:LYS:H	0.94	1.10
1:C:29:ASP:HB3	1:C:36:LYS:HD2	1.33	1.09
1:C:35:PRO:HB2	1:C:308:LEU:HD11	1.36	1.07
1:A:263:GLN:NE2	1:A:265:GLY:H	1.57	1.01
1:B:221:LYS:HE2	1:B:221:LYS:N	1.77	0.96
1:A:31:LEU:HB2	1:A:34:ILE:HG21	1.52	0.92
1:B:64:MET:HE2	1:B:76:LEU:HB3	1.52	0.91
1:B:221:LYS:CE	1:B:221:LYS:H	1.82	0.90
1:B:29:ASP:HB3	1:B:36:LYS:HA	1.57	0.87
1:B:232:GLN:HB3	1:B:356:ARG:HE	1.39	0.86
1:A:263:GLN:HE22	1:A:265:GLY:H	1.17	0.85
1:C:312:ALA:O	1:C:316:THR:HG23	1.78	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:HB2	1:C:34:ILE:HG12	1.64	0.80
1:B:19:ILE:HG22	1:B:59:PRO:HG3	1.62	0.80
1:A:233:ASP:HB2	1:A:356:ARG:HE	1.48	0.78
1:C:171:ARG:NH2	1:C:258:LYS:HE3	1.98	0.78
1:C:366:LEU:O	1:C:370:LYS:HG3	1.84	0.78
1:C:144:ALA:HB3	1:C:156:ASN:HB2	1.64	0.78
1:A:44:LEU:HD22	1:A:340:TYR:OH	1.84	0.77
1:A:69:THR:HG22	1:A:163:LEU:HD13	1.67	0.77
1:C:365:ILE:O	1:C:369:ILE:HG22	1.85	0.77
1:C:202:LYS:HA	1:C:231:ILE:O	1.85	0.76
1:A:34:ILE:N	1:A:35:PRO:HD3	2.00	0.76
1:C:357:ASN:HD22	1:C:362:ILE:HD11	1.51	0.75
1:C:232:GLN:CD	1:C:357:ASN:HB3	2.08	0.75
1:B:34:ILE:O	1:B:34:ILE:HG22	1.86	0.73
1:A:29:ASP:HB2	1:A:36:LYS:HA	1.69	0.73
1:C:198:VAL:HA	1:C:227:VAL:HG13	1.69	0.72
1:C:35:PRO:CB	1:C:308:LEU:HD11	2.15	0.72
1:B:22:PRO:HG2	1:B:23:GLU:OE2	1.90	0.72
1:C:239:LYS:HE2	1:C:362:ILE:CD1	2.20	0.71
1:A:105:THR:HG22	1:A:106:GLU:H	1.56	0.71
1:A:22:PRO:HG2	1:A:23:GLU:OE2	1.92	0.69
1:A:166:ARG:HH11	1:A:166:ARG:HG2	1.58	0.68
1:C:371:GLY:HA2	1:C:374:LYS:HE2	1.75	0.68
1:B:19:ILE:CG2	1:B:59:PRO:HG3	2.24	0.67
1:B:166:ARG:HG2	1:B:166:ARG:HH11	1.58	0.66
1:C:171:ARG:HH22	1:C:258:LYS:HE3	1.60	0.66
1:A:221:LYS:HG3	1:B:95:GLU:HG2	1.77	0.65
1:A:263:GLN:HE22	1:A:265:GLY:N	1.91	0.65
1:A:353:ARG:HH11	1:A:353:ARG:HB2	1.62	0.65
1:C:162:ILE:HG12	1:C:261:VAL:HG21	1.79	0.64
1:A:29:ASP:CB	1:A:36:LYS:HA	2.26	0.64
1:A:371:GLY:O	1:A:374:LYS:HB2	1.97	0.64
1:B:64:MET:HA	1:B:64:MET:HE3	1.80	0.64
1:A:13:SER:C	1:A:15:VAL:H	2.00	0.63
1:C:141:TRP:HB3	1:C:153:CYS:SG	2.39	0.63
1:C:19:ILE:HG22	1:C:59:PRO:HG3	1.80	0.63
1:B:32:ALA:O	1:B:33:LYS:HB2	1.99	0.63
1:A:20:TYR:CG	1:A:21:SER:N	2.67	0.62
1:B:44:LEU:HD23	1:B:316:THR:OG1	1.99	0.62
1:C:166:ARG:NH1	1:C:194:LYS:HB3	2.14	0.62
1:A:88:ASP:O	1:A:90:HIS:N	2.33	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:PRO:HB2	1:C:308:LEU:CD1	2.21	0.62
1:A:170:GLU:HG3	1:A:258:LYS:HZ2	1.65	0.62
1:A:13:SER:O	1:A:15:VAL:HG12	1.99	0.62
1:B:29:ASP:HB2	1:B:36:LYS:HE2	1.82	0.61
1:B:51:HIS:HB2	1:B:56:ILE:HD11	1.81	0.61
1:A:112:ALA:HB1	1:A:155:LEU:HB2	1.82	0.61
1:C:230:PRO:HG2	1:C:365:ILE:HD13	1.82	0.61
1:B:155:LEU:HD11	1:B:160:LEU:HD11	1.84	0.60
1:C:146:LYS:HG3	1:C:147:ASP:H	1.65	0.60
1:A:289:LYS:HE3	1:A:321:VAL:HG13	1.82	0.60
1:A:111:TYR:O	1:A:115:ILE:HG12	2.02	0.60
1:A:353:ARG:NH1	1:A:353:ARG:HB2	2.17	0.60
1:C:69:THR:HG22	1:C:163:LEU:HD13	1.83	0.59
1:C:171:ARG:HG3	1:C:171:ARG:HH11	1.67	0.59
1:C:313:ARG:NH1	1:C:345:VAL:O	2.36	0.59
1:B:37:ARG:HB2	1:B:308:LEU:HD22	1.85	0.58
1:C:239:LYS:HE2	1:C:362:ILE:HD12	1.84	0.58
1:C:76:LEU:O	1:C:80:GLN:HG3	2.02	0.58
1:C:44:LEU:HD23	1:C:316:THR:HG21	1.85	0.58
1:A:340:TYR:O	1:A:344:TYR:HA	2.02	0.58
1:A:262:LEU:HD11	1:A:264:LEU:HD21	1.84	0.58
1:B:367:ASN:HA	1:B:370:LYS:HE3	1.86	0.58
1:B:327:LEU:H	1:B:327:LEU:HD22	1.69	0.58
1:C:48:TYR:CE2	1:C:327:LEU:HB3	2.39	0.58
1:A:313:ARG:HG2	1:A:346:LEU:HD12	1.85	0.57
1:B:54:MET:HG2	1:B:323:LEU:HD21	1.85	0.57
1:A:263:GLN:NE2	1:A:265:GLY:N	2.41	0.57
1:A:87:ASP:HB3	1:A:104:ALA:HB3	1.86	0.57
1:C:146:LYS:HG3	1:C:147:ASP:N	2.19	0.57
1:C:31:LEU:HB2	1:C:34:ILE:CG1	2.33	0.57
1:A:362:ILE:O	1:A:366:LEU:HD22	2.05	0.56
1:A:45:ILE:HG23	1:A:50:LEU:HB2	1.86	0.56
1:B:264:LEU:HD13	1:B:318:LEU:HD13	1.87	0.56
1:B:29:ASP:CB	1:B:36:LYS:HA	2.33	0.56
1:B:367:ASN:O	1:B:370:LYS:HG2	2.06	0.56
1:B:174:TYR:CE1	1:B:176:ASP:HB2	2.39	0.56
1:B:232:GLN:HB3	1:B:356:ARG:NE	2.17	0.56
1:C:60:LYS:H	1:C:121:THR:HG21	1.70	0.56
1:C:235:ILE:CD1	1:C:239:LYS:HB3	2.36	0.55
1:A:170:GLU:H	1:A:258:LYS:HZ2	1.53	0.55
1:C:175:VAL:HG22	1:C:198:VAL:CG1	2.37	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASN:HB3	1:A:310:ASN:HB2	1.88	0.55
1:A:358:GLU:OE2	1:A:360:HIS:HB2	2.07	0.55
1:B:274:MET:HE1	4:B:804:TSN:H9	1.89	0.55
1:B:34:ILE:O	1:B:34:ILE:CG2	2.53	0.54
1:C:108:ILE:HG22	1:C:109:PHE:N	2.22	0.54
1:C:264:LEU:HD13	1:C:318:LEU:HD13	1.88	0.54
1:B:64:MET:HE2	1:B:76:LEU:CB	2.32	0.54
1:A:262:LEU:HD23	1:A:300:ILE:HD12	1.89	0.54
1:C:250:GLU:OE2	1:C:370:LYS:HG2	2.07	0.54
1:A:276:SER:O	1:A:353:ARG:NH2	2.40	0.54
1:C:236:GLN:O	1:C:237:ASP:C	2.46	0.54
1:C:319:THR:HG22	1:C:323:LEU:CD2	2.38	0.54
1:C:32:ALA:O	1:C:34:ILE:N	2.40	0.54
1:C:44:LEU:HD22	1:C:340:TYR:OH	2.07	0.54
1:A:34:ILE:N	1:A:35:PRO:CD	2.71	0.54
1:B:175:VAL:HB	1:B:262:LEU:HD13	1.90	0.54
1:C:98:LEU:HD12	1:C:103:PRO:O	2.08	0.53
1:A:175:VAL:HG22	1:A:198:VAL:CG1	2.38	0.53
1:C:333:ASP:HA	1:C:337:PHE:CD1	2.43	0.53
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.74	0.53
1:A:86:GLY:C	1:A:88:ASP:H	2.11	0.52
1:C:247:VAL:HG22	1:C:369:ILE:HD13	1.91	0.52
1:B:81:LYS:N	1:B:81:LYS:HE3	2.24	0.52
1:C:32:ALA:C	1:C:34:ILE:H	2.13	0.52
1:C:48:TYR:CB	1:C:50:LEU:HD13	2.39	0.52
1:C:44:LEU:HD23	1:C:316:THR:CG2	2.39	0.52
1:A:35:PRO:HB2	1:A:308:LEU:HD11	1.92	0.52
1:C:218:GLY:O	1:C:219:LEU:HD23	2.09	0.52
1:A:272:ASP:OD2	1:A:274:MET:HG2	2.10	0.52
1:A:51:HIS:HB2	1:A:56:ILE:HD11	1.92	0.52
1:C:83:SER:HB2	1:C:108:ILE:HG22	1.90	0.52
1:B:198:VAL:HG22	1:B:227:VAL:CG1	2.40	0.52
1:A:155:LEU:HD11	1:A:160:LEU:HD11	1.92	0.51
1:A:169:PHE:HB2	1:A:172:ILE:HD11	1.93	0.51
1:A:262:LEU:HD23	1:A:300:ILE:CD1	2.41	0.51
1:B:166:ARG:NH1	1:B:166:ARG:HG2	2.22	0.51
1:C:334:HIS:HE1	1:C:340:TYR:HE1	1.58	0.51
1:A:151:GLY:O	1:A:152:PHE:HB2	2.10	0.51
1:A:44:LEU:HD22	1:A:340:TYR:CZ	2.45	0.51
1:C:334:HIS:CE1	1:C:340:TYR:CE1	2.99	0.51
1:B:91:PRO:HA	5:B:421:HOH:O	2.09	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:C	1:A:15:VAL:N	2.65	0.50
1:A:294:TRP:O	1:A:295:GLN:HB2	2.11	0.50
1:C:175:VAL:HB	1:C:262:LEU:HD13	1.94	0.50
1:C:181:HIS:HB2	1:C:201:HIS:CD2	2.47	0.50
1:A:166:ARG:NH1	1:A:166:ARG:HG2	2.25	0.50
1:C:137:TRP:O	1:C:302:GLY:HA3	2.11	0.50
1:C:347:GLU:H	1:C:347:GLU:CD	2.14	0.50
1:A:217:VAL:C	1:A:226:SER:HB2	2.32	0.50
1:B:59:PRO:HB3	1:B:118:ALA:HA	1.92	0.50
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.75	0.50
1:C:363:GLN:HA	1:C:366:LEU:HD12	1.94	0.50
1:B:86:GLY:O	1:B:88:ASP:N	2.39	0.50
1:C:19:ILE:CG2	1:C:59:PRO:HG3	2.42	0.49
1:B:235:ILE:HD11	1:B:239:LYS:HB3	1.95	0.49
1:C:108:ILE:CG2	1:C:109:PHE:N	2.75	0.49
1:B:112:ALA:HB1	1:B:155:LEU:HB2	1.94	0.49
1:B:77:GLN:O	1:B:80:GLN:HB3	2.13	0.49
1:C:47:ALA:HB1	1:C:332:PRO:HG2	1.95	0.49
1:C:217:VAL:C	1:C:226:SER:HB2	2.32	0.49
1:C:252:TYR:HE1	1:C:296:LEU:HD11	1.78	0.49
1:C:17:VAL:HG23	1:C:131:CYS:HB3	1.95	0.49
1:C:235:ILE:HD13	1:C:239:LYS:HB3	1.95	0.49
1:A:175:VAL:HA	1:A:198:VAL:HG13	1.95	0.48
1:A:224:TYR:CD2	1:A:375:HIS:HB2	2.48	0.48
1:C:202:LYS:HB3	1:C:207:PHE:CE2	2.49	0.48
1:A:26:SER:O	1:A:30:SER:HB3	2.13	0.48
1:A:307:ASN:CG	1:A:310:ASN:HB2	2.34	0.48
1:A:83:SER:HB2	1:A:109:PHE:H	1.78	0.48
1:B:19:ILE:HG13	1:B:122:ALA:HB2	1.95	0.48
1:B:90:HIS:CG	1:B:91:PRO:HD2	2.49	0.48
1:C:366:LEU:O	1:C:369:ILE:HG23	2.12	0.48
1:C:24:TYR:CG	1:C:59:PRO:HG2	2.49	0.48
1:A:196:MET:SD	1:A:251:VAL:HG13	2.54	0.48
1:C:203:PHE:HE1	1:C:210:GLY:O	1.97	0.48
1:B:116:GLY:O	1:B:120:ILE:HG13	2.13	0.48
1:B:233:ASP:H	1:B:356:ARG:NE	2.11	0.47
1:C:232:GLN:CD	1:C:232:GLN:H	2.15	0.47
1:A:83:SER:O	1:A:106:GLU:HA	2.15	0.47
1:B:218:GLY:O	1:B:219:LEU:HD23	2.14	0.47
1:A:250:GLU:OE1	1:A:370:LYS:HG3	2.14	0.47
1:A:60:LYS:HE3	1:A:121:THR:OG1	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:CD1	1:A:21:SER:N	2.83	0.47
1:C:20:TYR:CG	1:C:21:SER:N	2.83	0.47
1:C:98:LEU:HD22	1:C:98:LEU:N	2.30	0.47
1:B:20:TYR:CG	1:B:21:SER:N	2.83	0.46
1:B:54:MET:CG	1:B:323:LEU:HD21	2.45	0.46
1:C:13:SER:O	1:C:14:LEU:HD23	2.15	0.46
1:A:172:ILE:HD12	1:A:259:ALA:HB3	1.97	0.46
1:A:187:ASP:HA	1:A:190:SER:OG	2.14	0.46
1:A:87:ASP:CB	1:A:104:ALA:HB3	2.45	0.46
1:A:191:PHE:CG	1:B:91:PRO:HB2	2.50	0.46
1:B:47:ALA:HB1	1:B:332:PRO:HB2	1.96	0.46
1:C:175:VAL:HA	1:C:198:VAL:HG13	1.97	0.46
1:A:170:GLU:HB2	1:A:258:LYS:HD3	1.98	0.46
1:C:227:VAL:HG21	1:C:369:ILE:HD12	1.97	0.46
1:C:32:ALA:O	1:C:33:LYS:HG2	2.16	0.46
1:C:172:ILE:HD13	1:C:259:ALA:HB3	1.97	0.46
1:C:208:PHE:CG	1:C:209:PRO:HA	2.51	0.46
1:B:79:LEU:O	1:B:83:SER:HB2	2.16	0.46
1:C:117:GLY:O	1:C:121:THR:HG22	2.16	0.46
1:A:358:GLU:CD	1:A:360:HIS:HB2	2.36	0.46
1:C:217:VAL:O	1:C:226:SER:HB2	2.16	0.46
1:C:247:VAL:O	1:C:251:VAL:HG23	2.16	0.46
1:A:28:CYS:O	1:A:111:TYR:HE1	1.99	0.45
1:A:307:ASN:CB	1:A:310:ASN:HB2	2.46	0.45
1:C:31:LEU:CB	1:C:34:ILE:HG12	2.41	0.45
1:A:293:GLN:O	1:A:295:GLN:HG2	2.16	0.45
1:B:223:ARG:HG2	1:B:223:ARG:NH1	2.32	0.45
1:B:225:TYR:CZ	1:B:376:VAL:HG13	2.52	0.45
1:C:171:ARG:NH1	1:C:171:ARG:HG3	2.30	0.45
1:C:59:PRO:HB3	1:C:118:ALA:HB2	1.99	0.45
1:A:19:ILE:CG2	1:A:59:PRO:HB3	2.47	0.45
1:A:13:SER:OG	1:A:14:LEU:N	2.49	0.45
1:B:128:ASP:O	1:B:130:MET:N	2.50	0.45
1:B:111:TYR:OH	4:B:805:TSN:H161	2.16	0.45
1:C:232:GLN:CD	1:C:232:GLN:N	2.70	0.45
1:A:37:ARG:HD2	1:A:311:THR:HG21	1.98	0.45
1:C:334:HIS:CE1	1:C:340:TYR:HE1	2.35	0.45
1:C:48:TYR:HB3	1:C:50:LEU:HD13	1.97	0.45
1:C:51:HIS:HA	1:C:54:MET:CE	2.47	0.45
1:C:174:TYR:CD1	1:C:185:VAL:HG11	2.52	0.45
1:B:255:PHE:O	1:B:256:ASN:C	2.54	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:SER:HB3	1:A:59:PRO:HD2	1.99	0.44
1:B:127:ILE:HG23	1:B:168:LYS:CD	2.47	0.44
1:A:172:ILE:HB	1:A:195:VAL:HG22	1.99	0.44
1:C:363:GLN:HA	1:C:366:LEU:HB2	1.98	0.44
1:A:202:LYS:HE3	1:A:233:ASP:OD2	2.18	0.44
1:B:181:HIS:HB2	1:B:201:HIS:CD2	2.52	0.44
1:B:20:TYR:CD2	1:B:20:TYR:C	2.90	0.44
1:C:16:PRO:HG2	1:C:54:MET:HG2	2.00	0.44
1:A:44:LEU:HD22	1:A:340:TYR:CE2	2.53	0.44
1:C:136:ASN:ND2	1:C:139:GLY:HA3	2.32	0.44
1:B:327:LEU:N	1:B:327:LEU:HD22	2.31	0.44
1:C:102:CYS:SG	1:C:149:ALA:HB1	2.58	0.44
1:A:256:ASN:HB3	1:A:378:ILE:HD13	1.98	0.44
1:A:48:TYR:CE2	1:A:327:LEU:HB3	2.51	0.44
1:B:25:VAL:O	1:B:29:ASP:OD1	2.36	0.44
1:B:43:SER:HB3	1:B:334:HIS:HD2	1.83	0.44
1:C:117:GLY:O	1:C:121:THR:CG2	2.66	0.44
1:A:347:GLU:H	1:A:347:GLU:CD	2.20	0.44
1:B:233:ASP:H	1:B:356:ARG:HE	1.66	0.44
1:B:44:LEU:HD23	1:B:316:THR:HG1	1.83	0.44
1:C:166:ARG:HH12	1:C:194:LYS:HB3	1.81	0.44
1:C:358:GLU:C	1:C:360:HIS:H	2.21	0.44
1:B:55:ARG:CD	1:B:130:MET:HE2	2.48	0.44
1:C:151:GLY:O	1:C:152:PHE:HB2	2.18	0.44
1:C:258:LYS:HD2	1:C:258:LYS:N	2.32	0.44
1:C:111:TYR:OH	4:C:803:TSN:H161	2.18	0.43
1:B:71:HIS:HA	1:B:146:LYS:O	2.18	0.43
1:C:44:LEU:CD2	1:C:316:THR:HG21	2.48	0.43
1:B:244:CYS:SG	1:B:248:LEU:HD12	2.58	0.43
1:B:55:ARG:HD3	1:B:130:MET:HE2	2.01	0.43
1:C:112:ALA:HB1	1:C:155:LEU:HB2	1.99	0.43
1:C:263:GLN:HB2	1:C:263:GLN:HE21	1.51	0.43
1:C:272:ASP:O	1:C:275:CYS:N	2.48	0.43
1:C:176:ASP:OD1	1:C:263:GLN:HG2	2.18	0.43
1:C:36:LYS:HB3	1:C:36:LYS:HE3	1.84	0.43
1:B:171:ARG:HG3	1:B:171:ARG:NH1	2.33	0.43
1:B:264:LEU:O	1:B:265:GLY:C	2.55	0.43
1:A:105:THR:HG22	1:A:106:GLU:N	2.26	0.43
1:A:170:GLU:HG3	1:A:258:LYS:NZ	2.32	0.43
1:A:50:LEU:HD22	1:A:323:LEU:HD12	2.00	0.43
1:C:44:LEU:CG	1:C:316:THR:HG21	2.49	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:HA	1:C:146:LYS:O	2.19	0.43
1:C:27:MET:HE3	1:C:30:SER:OG	2.18	0.43
1:B:72:THR:CG2	1:B:147:ASP:HB3	2.49	0.42
1:C:171:ARG:HA	1:C:194:LYS:O	2.18	0.42
1:B:144:ALA:HB3	1:B:156:ASN:HB2	2.00	0.42
1:A:141:TRP:HB3	1:A:153:CYS:SG	2.59	0.42
1:A:293:GLN:HE21	1:A:293:GLN:HB3	1.58	0.42
1:B:158:ALA:O	1:B:162:ILE:HG13	2.19	0.42
1:C:133:VAL:HA	1:C:298:THR:O	2.20	0.42
1:B:223:ARG:O	1:B:224:TYR:HB2	2.19	0.42
1:B:13:SER:HA	1:B:130:MET:O	2.20	0.42
1:B:57:VAL:CG2	1:B:130:MET:HE1	2.50	0.42
1:C:166:ARG:HH11	1:C:166:ARG:HG2	1.84	0.42
1:B:233:ASP:O	1:B:356:ARG:HG2	2.19	0.42
1:A:34:ILE:O	1:A:34:ILE:HG22	2.19	0.42
1:A:91:PRO:HG2	1:A:92:ASP:OD1	2.19	0.42
1:C:174:TYR:HB3	1:C:197:THR:HG22	2.02	0.41
1:C:60:LYS:O	1:C:61:VAL:C	2.59	0.41
1:A:258:LYS:HE2	1:A:258:LYS:HB3	1.91	0.41
1:A:369:ILE:O	1:A:373:LEU:HG	2.20	0.41
1:B:64:MET:HE1	1:B:67:MET:HE1	2.01	0.41
1:C:84:GLN:O	1:C:85:GLU:HB2	2.20	0.41
1:A:142:HIS:ND1	1:A:176:ASP:OD2	2.33	0.41
1:B:281:PRO:HB3	1:B:314:CYS:SG	2.60	0.41
1:C:232:GLN:OE1	1:C:357:ASN:HB3	2.20	0.41
1:B:64:MET:CE	1:B:76:LEU:HD13	2.50	0.41
1:C:20:TYR:HE1	1:C:25:VAL:HG21	1.85	0.41
1:A:263:GLN:HE21	1:A:263:GLN:C	2.24	0.41
1:C:317:TYR:O	1:C:321:VAL:HG23	2.21	0.41
1:A:266:ALA:C	1:A:268:THR:H	2.24	0.41
1:C:24:TYR:CD2	1:C:59:PRO:HG2	2.55	0.41
1:B:243:ILE:O	1:B:247:VAL:HG23	2.21	0.41
1:B:78:HIS:HE1	1:B:90:HIS:CD2	2.38	0.41
1:A:274:MET:O	1:A:275:CYS:C	2.58	0.41
1:B:333:ASP:HA	1:B:337:PHE:CD1	2.55	0.41
1:C:362:ILE:O	1:C:366:LEU:HG	2.21	0.41
1:C:31:LEU:HB2	1:C:34:ILE:CD1	2.50	0.41
1:C:34:ILE:HA	1:C:35:PRO:HD2	1.89	0.41
1:A:85:GLU:O	1:A:106:GLU:HG2	2.21	0.40
1:A:35:PRO:HD2	4:A:800:TSN:C2	2.51	0.40
1:B:270:ALA:HB2	1:B:278:ASN:OD1	2.20	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ILE:CG1	1:C:261:VAL:HG21	2.49	0.40
1:C:196:MET:HG3	1:C:225:TYR:O	2.21	0.40
1:A:166:ARG:C	1:A:168:LYS:H	2.23	0.40
1:B:314:CYS:O	1:B:318:LEU:HG	2.21	0.40
1:C:223:ARG:HG2	1:C:224:TYR:CD1	2.57	0.40
1:C:232:GLN:OE1	1:C:232:GLN:N	2.42	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	360/388 (93%)	329 (91%)	28 (8%)	3 (1%)	19	27
1	B	364/388 (94%)	334 (92%)	27 (7%)	3 (1%)	19	27
1	C	351/388 (90%)	317 (90%)	33 (9%)	1 (0%)	41	51
All	All	1075/1164 (92%)	980 (91%)	88 (8%)	7 (1%)	22	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	B	341	GLY
1	A	88	ASP
1	B	85	GLU
1	B	137	TRP
1	C	166	ARG
1	A	21	SER

### 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	306/326 (94%)	292 (95%)	14 (5%)	27	36
1	B	307/326 (94%)	293 (95%)	14 (5%)	27	36
1	C	297/326 (91%)	279 (94%)	18 (6%)	18	24
All	All	910/978 (93%)	864 (95%)	46 (5%)	24	32

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	51	HIS
1	A	53	GLN
1	A	88	ASP
1	A	108	ILE
1	A	142	HIS
1	A	155	LEU
1	A	187	ASP
1	A	263	GLN
1	A	293	GLN
1	A	313	ARG
1	A	356	ARG
1	A	358	GLU
1	A	366	LEU
1	B	29	ASP
1	B	34	ILE
1	B	36	LYS
1	B	39	SER
1	B	51	HIS
1	B	81	LYS
1	B	102	CYS
1	B	142	HIS
1	B	155	LEU
1	B	215	SER
1	B	221	LYS
1	B	227	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	327	LEU
1	B	366	LEU
1	C	23	GLU
1	C	73	ASP
1	C	84	GLN
1	C	96	TYR
1	C	108	ILE
1	C	121	THR
1	C	142	HIS
1	C	155	LEU
1	C	232	GLN
1	C	235	ILE
1	C	258	LYS
1	C	263	GLN
1	C	316	THR
1	C	327	LEU
1	C	343	ASP
1	C	353	ARG
1	C	357	ASN
1	C	367	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	77	GLN
1	A	232	GLN
1	A	263	GLN
1	A	293	GLN
1	B	51	HIS
1	B	78	HIS
1	B	90	HIS
1	B	136	ASN
1	B	236	GLN
1	B	253	GLN
1	B	372	ASN
1	C	80	GLN
1	C	124	GLN
1	C	136	ASN
1	C	228	ASN
1	C	236	GLN
1	C	293	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	295	GLN
1	C	372	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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$
4	TSN	C	803	-	22,22,22	2.27	5 (22%)	27,29,29	1.08	4 (14%)
4	TSN	A	800	-	22,22,22	2.28	5 (22%)	27,29,29	0.99	1 (3%)
4	TSN	B	805	-	22,22,22	2.62	9 (40%)	27,29,29	1.24	3 (11%)
4	TSN	A	801	2	22,22,22	2.36	7 (31%)	27,29,29	1.15	5 (18%)
4	TSN	B	804	2	22,22,22	2.31	6 (27%)	27,29,29	1.10	4 (14%)
4	TSN	C	802	2	22,22,22	2.38	8 (36%)	27,29,29	1.14	3 (11%)

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
4	TSN	C	803	-	-	0/23/23/23	0/1/1/1
4	TSN	A	800	-	-	0/23/23/23	0/1/1/1
4	TSN	B	805	-	-	1/23/23/23	0/1/1/1
4	TSN	A	801	2	-	0/23/23/23	0/1/1/1
4	TSN	B	804	2	-	0/23/23/23	0/1/1/1
4	TSN	C	802	2	-	1/23/23/23	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	805	TSN	C2-C1	5.22	1.48	1.39
4	A	800	TSN	C2-C1	5.05	1.47	1.39
4	C	803	TSN	C2-C1	4.75	1.47	1.39
4	A	801	TSN	C2-C1	4.72	1.47	1.39
4	B	805	TSN	C6-C1	4.69	1.47	1.39
4	A	800	TSN	C6-C1	4.58	1.47	1.39
4	C	802	TSN	C2-C1	4.53	1.47	1.39
4	B	805	TSN	C3-C4	4.46	1.48	1.39
4	B	804	TSN	C6-C1	4.36	1.46	1.39
4	C	803	TSN	C6-C1	4.35	1.46	1.39
4	B	804	TSN	C2-C1	4.30	1.46	1.39
4	C	802	TSN	C6-C1	4.26	1.46	1.39
4	A	801	TSN	C6-C1	4.22	1.46	1.39
4	A	800	TSN	C5-C4	4.10	1.47	1.39
4	B	804	TSN	C5-C4	4.06	1.47	1.39
4	C	803	TSN	C5-C4	4.02	1.47	1.39
4	A	801	TSN	C5-C4	4.00	1.47	1.39
4	C	802	TSN	C5-C4	3.92	1.47	1.39
4	C	803	TSN	C3-C4	3.92	1.47	1.39
4	C	802	TSN	C4-N2	3.91	1.46	1.37
4	A	800	TSN	C3-C4	3.90	1.47	1.39
4	B	805	TSN	C5-C4	3.88	1.46	1.39
4	A	801	TSN	C4-N2	3.83	1.46	1.37
4	A	801	TSN	C3-C4	3.78	1.46	1.39
4	B	805	TSN	C8-C7	3.76	1.57	1.53
4	B	804	TSN	C3-C4	3.72	1.46	1.39
4	C	802	TSN	C3-C4	3.71	1.46	1.39
4	B	804	TSN	C4-N2	3.67	1.46	1.37
4	B	805	TSN	C4-N2	3.64	1.46	1.37
4	C	803	TSN	C4-N2	3.52	1.45	1.37
4	A	800	TSN	C4-N2	3.07	1.44	1.37
4	B	805	TSN	C1-C7	2.76	1.53	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	802	TSN	C1-C7	2.34	1.52	1.49
4	C	802	TSN	C8-C7	2.25	1.55	1.53
4	A	801	TSN	C8-C9	2.17	1.54	1.51
4	B	805	TSN	C3-C2	2.16	1.42	1.38
4	B	804	TSN	C8-C9	2.14	1.54	1.51
4	C	802	TSN	C8-C9	2.03	1.54	1.51
4	B	805	TSN	C8-C9	2.02	1.54	1.51
4	A	801	TSN	C11-C10	2.01	1.50	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	805	TSN	C14-C8-C9	-3.94	107.06	110.75
4	C	802	TSN	C1-C7-C8	3.06	122.11	119.29
4	A	801	TSN	C1-C7-C8	2.86	121.94	119.29
4	B	804	TSN	C12-C13-N1	2.48	119.31	114.38
4	B	804	TSN	C1-C7-C8	2.44	121.55	119.29
4	C	803	TSN	C14-C8-C9	-2.42	108.48	110.75
4	C	803	TSN	C15-C10-C11	2.33	121.75	118.08
4	A	800	TSN	C15-C10-C11	2.29	121.69	118.08
4	A	801	TSN	C12-C13-N1	2.27	118.91	114.38
4	A	801	TSN	C14-C8-C9	-2.24	108.65	110.75
4	B	804	TSN	C15-C10-C11	2.23	121.59	118.08
4	B	805	TSN	C12-C13-N1	2.22	118.81	114.38
4	C	803	TSN	C1-C7-C8	2.15	121.28	119.29
4	B	805	TSN	C15-C10-C11	2.09	121.37	118.08
4	C	802	TSN	C12-C13-N1	2.07	118.51	114.38
4	A	801	TSN	C15-C10-C11	2.07	121.34	118.08
4	C	803	TSN	C12-C13-N1	2.05	118.47	114.38
4	C	802	TSN	C14-C8-C9	-2.05	108.83	110.75
4	A	801	TSN	O2-C13-N1	-2.03	119.13	122.89
4	B	804	TSN	C14-C8-C9	-2.01	108.86	110.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

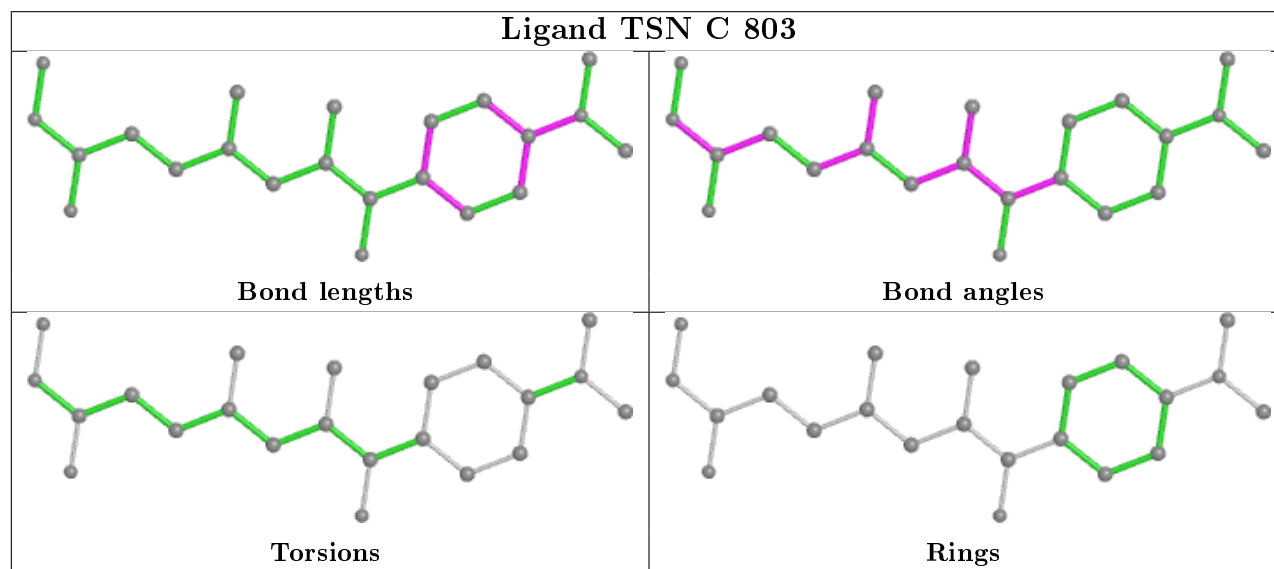
Mol	Chain	Res	Type	Atoms
4	B	805	TSN	O3-C7-C8-C9
4	C	802	TSN	C1-C7-C8-C14

There are no ring outliers.

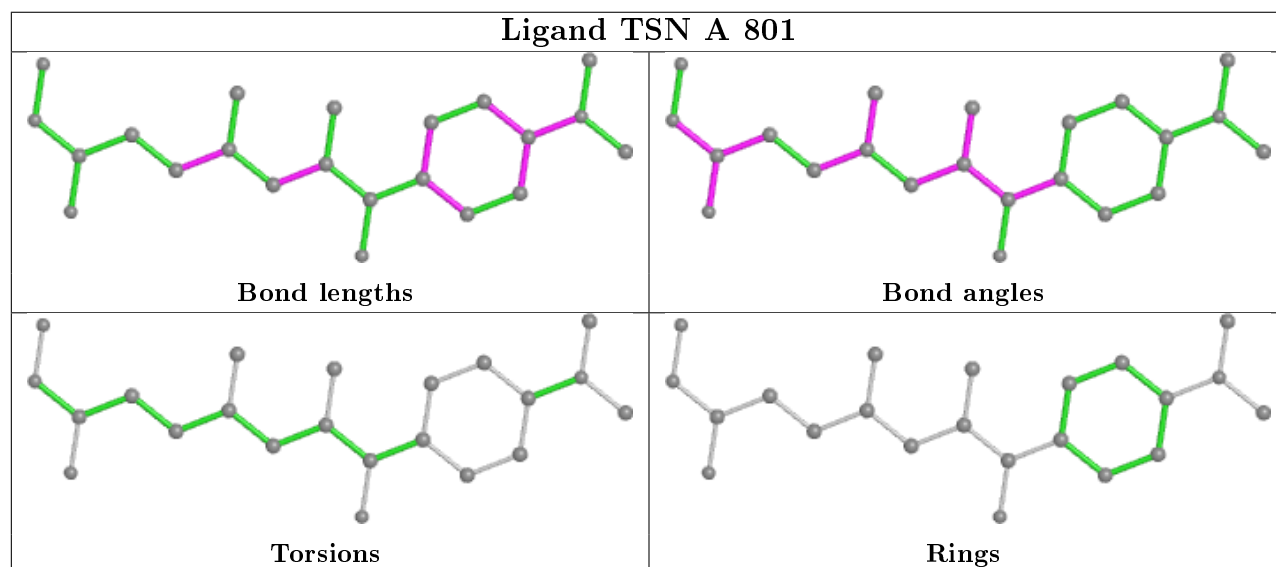
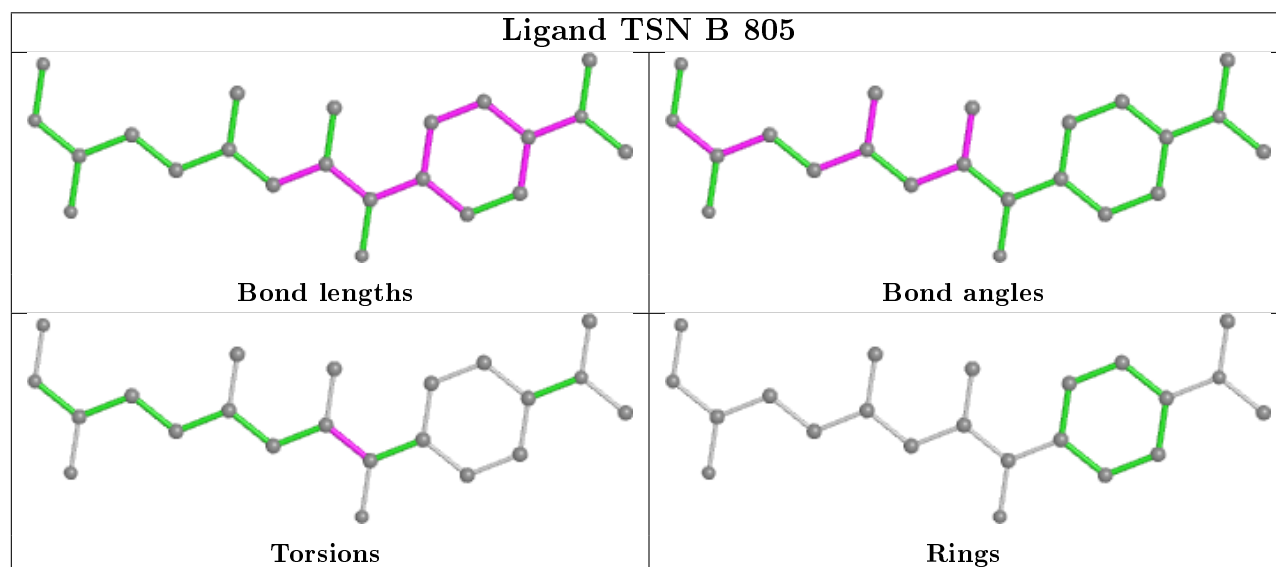
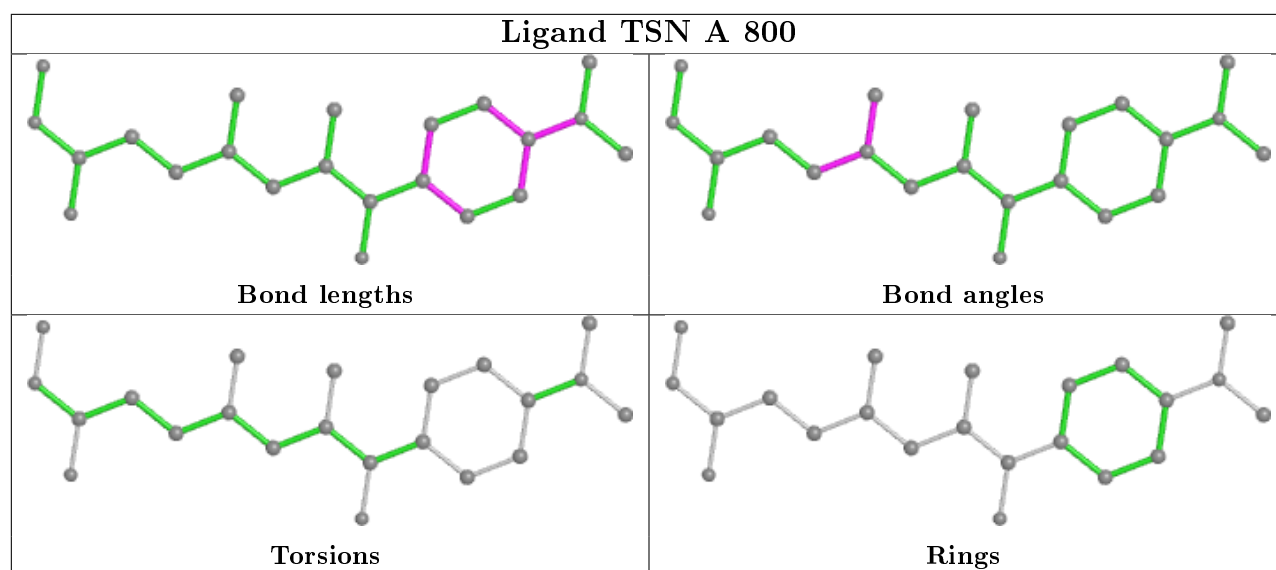
4 monomers are involved in 4 short contacts:

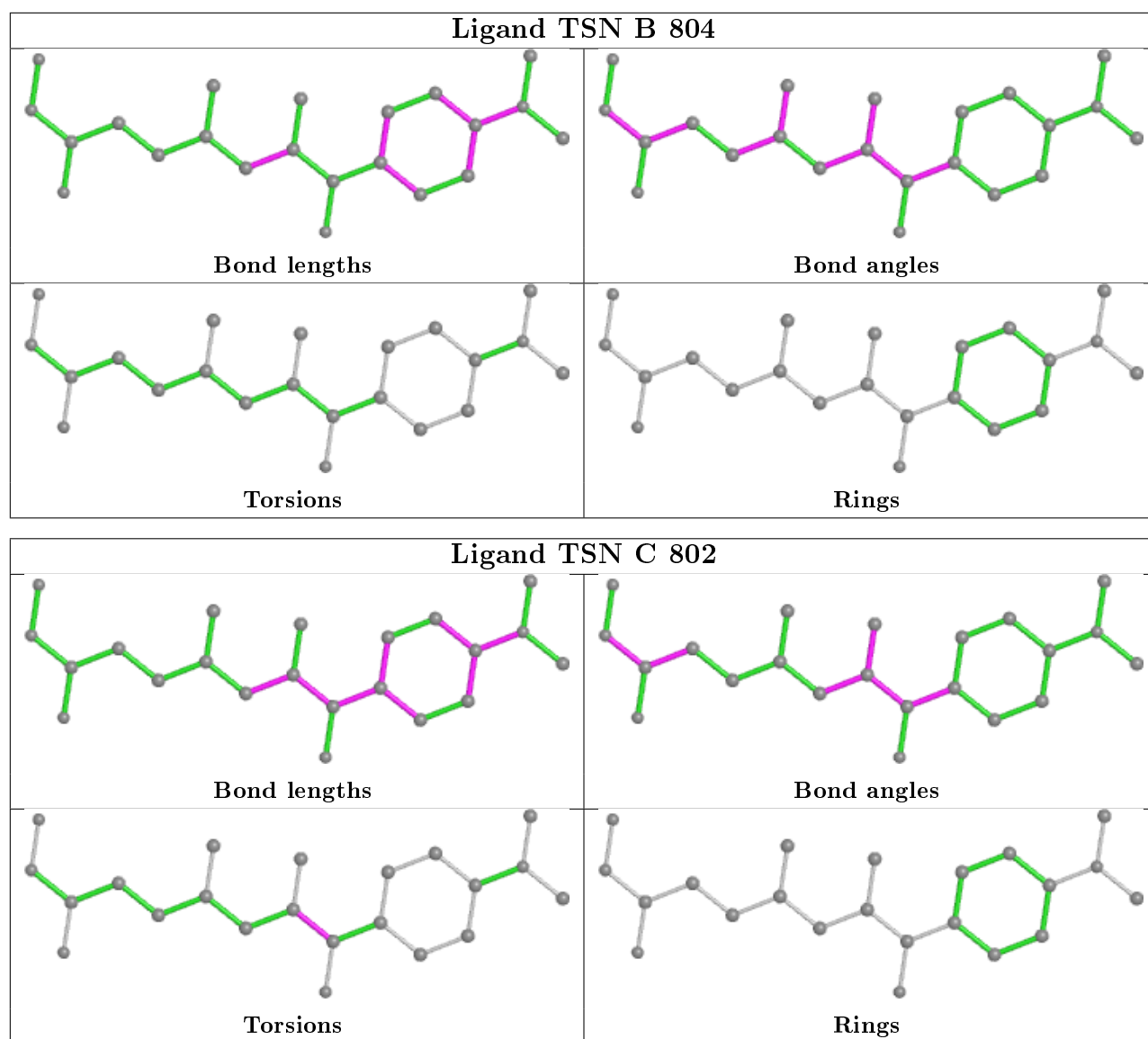
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	803	TSN	1	0
4	A	800	TSN	1	0
4	B	805	TSN	1	0
4	B	804	TSN	1	0

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	364/388 (93%)	0.01	4 (1%) 80 85	28, 45, 70, 96	0
1	B	366/388 (94%)	0.11	12 (3%) 46 53	31, 52, 76, 112	0
1	C	355/388 (91%)	0.47	29 (8%) 11 14	40, 68, 95, 106	0
All	All	1085/1164 (93%)	0.19	45 (4%) 37 44	28, 54, 86, 112	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	LYS	7.0
1	C	100	TYR	5.1
1	C	360	HIS	4.7
1	C	103	PRO	4.4
1	B	89	ASP	4.0
1	B	87	ASP	3.8
1	C	30	SER	3.8
1	C	362	ILE	3.4
1	C	32	ALA	3.4
1	A	89	ASP	3.3
1	B	130	MET	3.2
1	B	88	ASP	3.2
1	C	14	LEU	3.1
1	B	360	HIS	3.0
1	C	55	ARG	3.0
1	B	13	SER	3.0
1	B	86	GLY	2.9
1	C	13	SER	2.9
1	C	375	HIS	2.8
1	C	170	GLU	2.8
1	C	57	VAL	2.6
1	C	154	TYR	2.5
1	C	58	LYS	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	106	GLU	2.5
1	A	340	TYR	2.4
1	C	207	PHE	2.4
1	C	250	GLU	2.4
1	A	87	ASP	2.3
1	C	99	GLY	2.3
1	C	110	ASP	2.3
1	C	358	GLU	2.3
1	A	378	ILE	2.3
1	C	356	ARG	2.3
1	C	357	ASN	2.3
1	C	377	VAL	2.2
1	B	104	ALA	2.2
1	C	36	LYS	2.1
1	B	129	GLY	2.1
1	C	359	PRO	2.1
1	B	106	GLU	2.1
1	C	85	GLU	2.1
1	B	52	LYS	2.0
1	B	15	VAL	2.0
1	C	366	LEU	2.0
1	C	369	ILE	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 carbohydrates 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(Å <sup>2</sup> )	Q<0.9
4	TSN	A	800	22/22	0.76	0.32	91,93,95,98	0

*Continued on next page...*

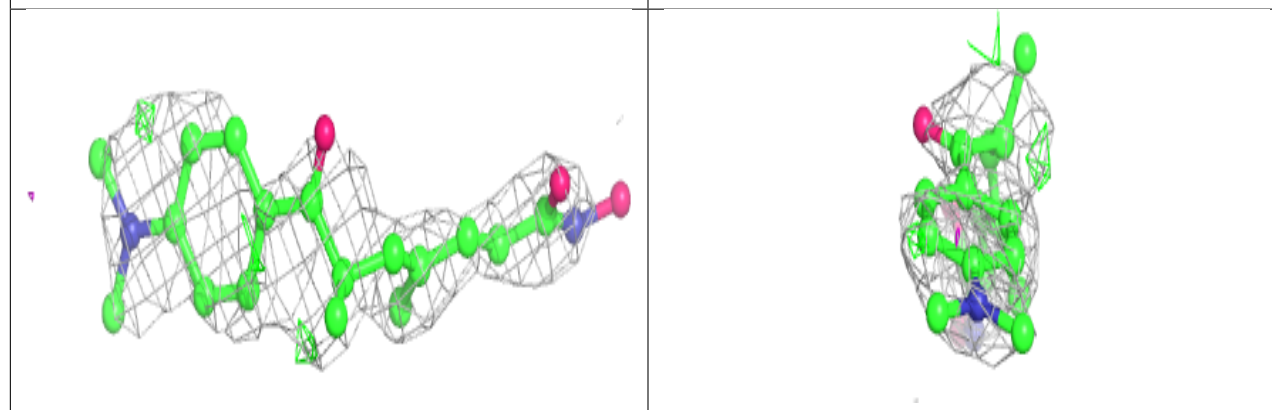
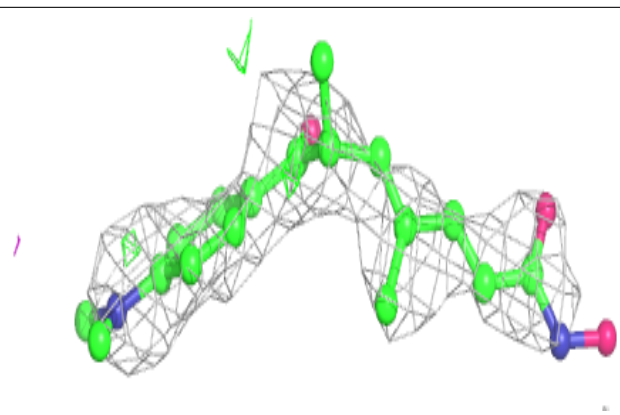
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TSN	B	805	22/22	0.81	0.28	75,77,78,79	0
4	TSN	C	803	22/22	0.81	0.31	97,98,102,102	0
4	TSN	C	802	22/22	0.88	0.34	86,97,101,102	0
4	TSN	B	804	22/22	0.90	0.27	54,63,70,72	0
3	K	C	407	1/1	0.93	0.10	63,63,63,63	0
4	TSN	A	801	22/22	0.95	0.24	76,78,80,81	0
3	K	C	408	1/1	0.97	0.10	57,57,57,57	0
2	ZN	A	400	1/1	0.99	0.14	42,42,42,42	0
3	K	B	404	1/1	0.99	0.14	46,46,46,46	0
3	K	B	405	1/1	0.99	0.13	34,34,34,34	0
3	K	A	402	1/1	0.99	0.14	36,36,36,36	0
2	ZN	B	403	1/1	0.99	0.16	35,35,35,35	0
2	ZN	C	406	1/1	0.99	0.14	47,47,47,47	0
3	K	A	401	1/1	0.99	0.10	37,37,37,37	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.

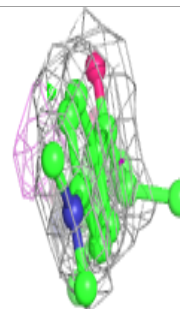
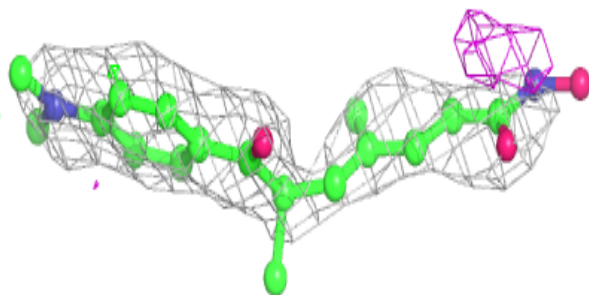
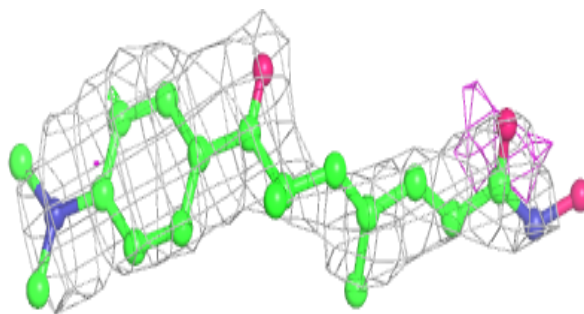
**Electron density around TSN A 800:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

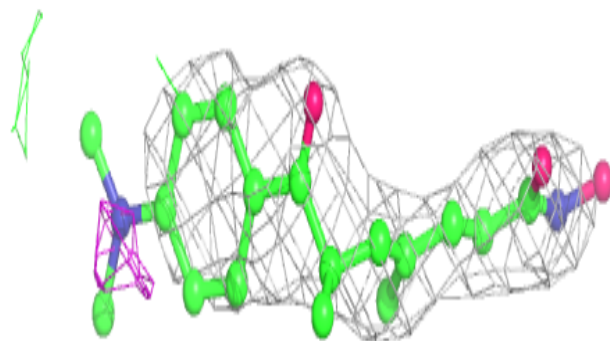
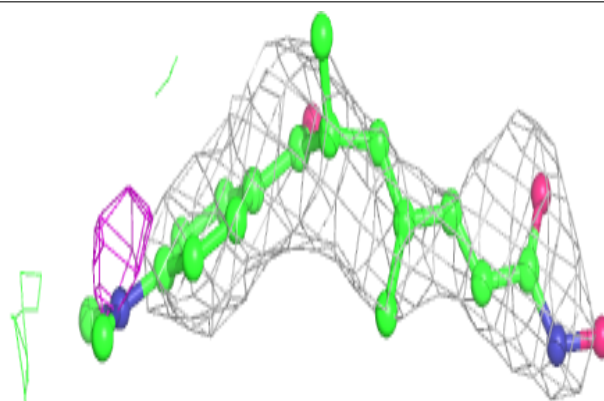


**Electron density around TSN B 805:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

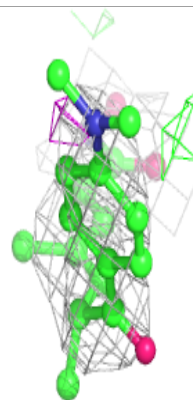
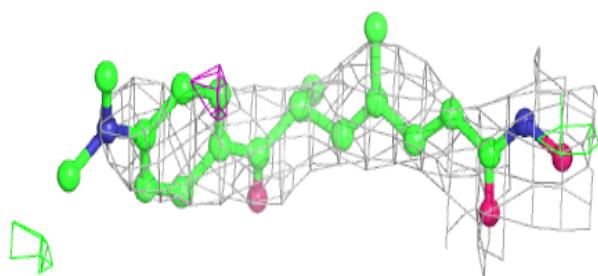
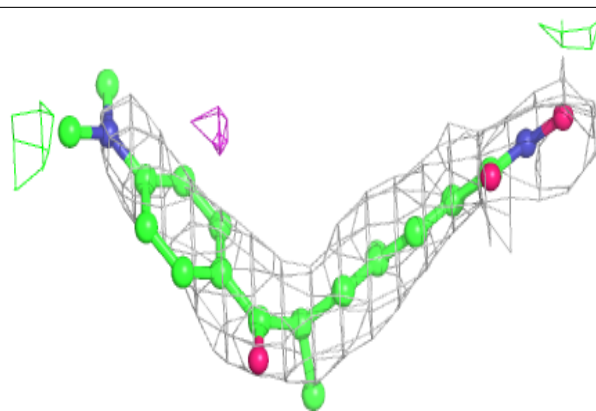
**Electron density around TSN C 803:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

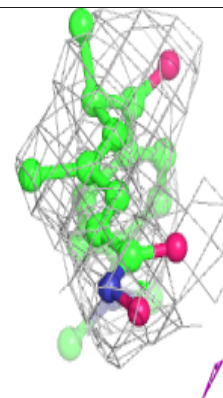
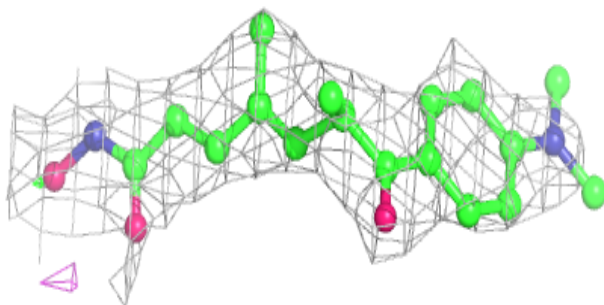
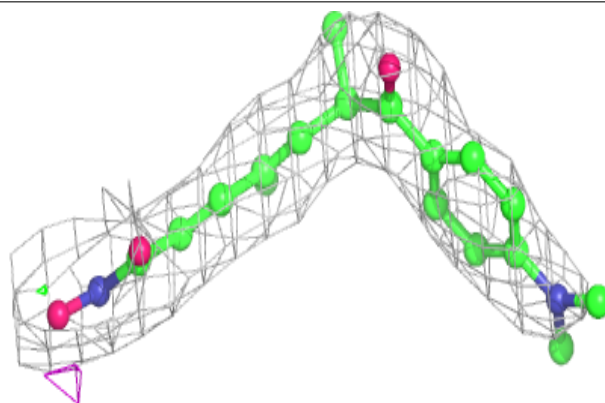


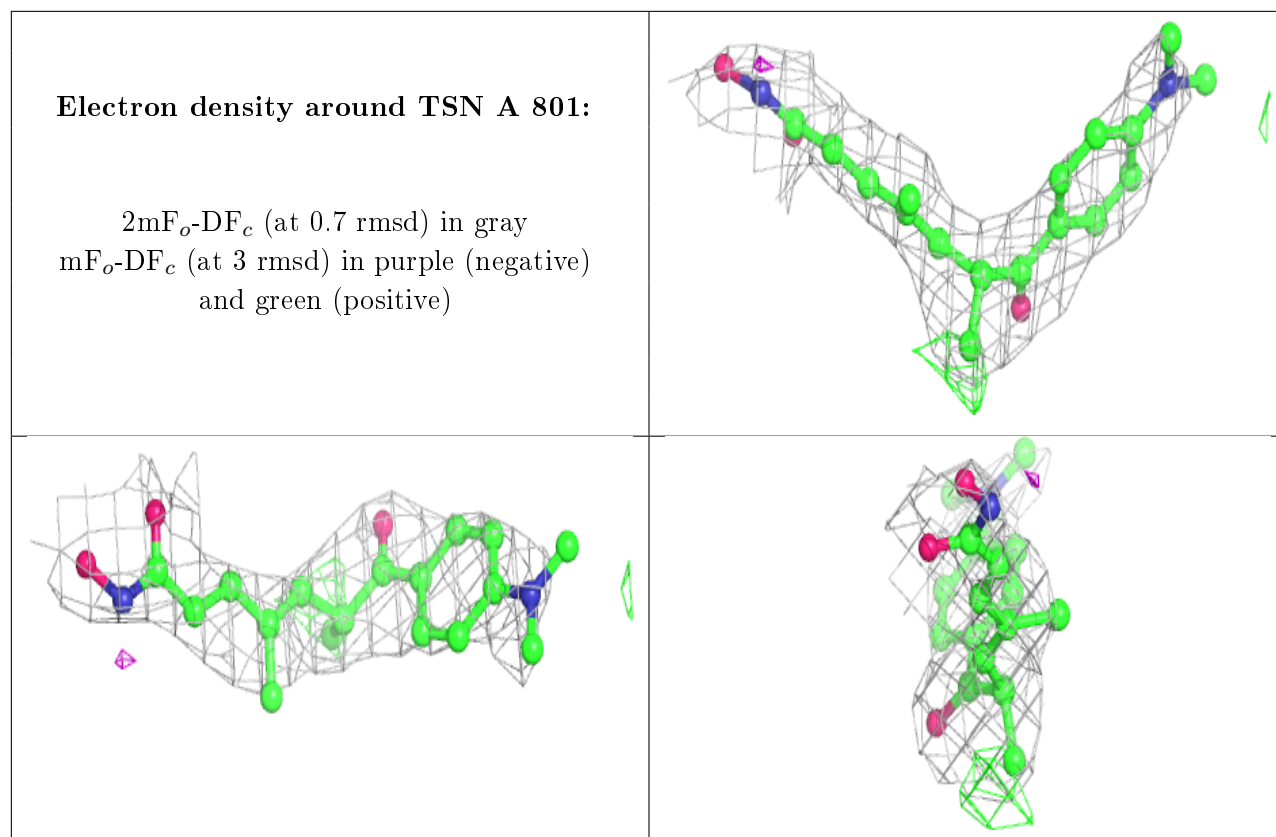
**Electron density around TSN C 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around TSN B 804:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.