



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 10:24 PM BST

PDB ID : 6OFC  
Title : Crystal structure of M. tuberculosis glutamine-dependent NAD<sup>+</sup> synthetase complexed with Sulfonamide derivative 1, pyrophosphate, and glutamine  
Authors : Chuenchor, W.; Doukov, T.I.; Gerratana, B.  
Deposited on : 2019-03-28  
Resolution : 3.14 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 : 2.13  
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) : 2.13

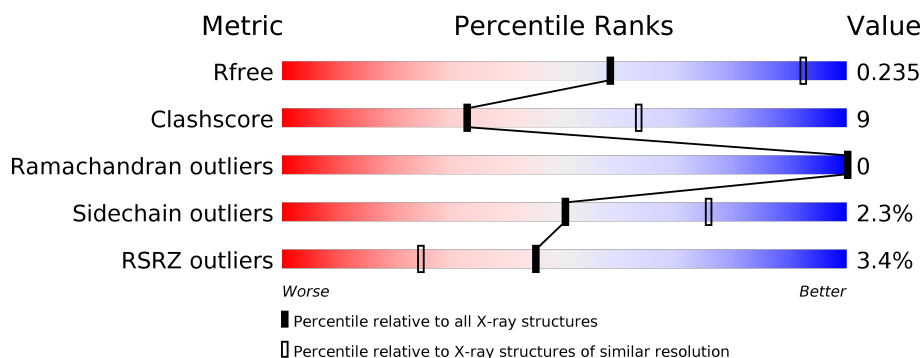
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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	679	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>•</div> </div> </div>
1	B	679	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>••</div> </div> </div>
1	C	679	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>•</div> </div> </div>
1	D	679	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>••</div> </div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SFH	A	702	-	-	-	X
2	SFH	A	703[A]	-	-	-	X
2	SFH	A	703[B]	-	-	-	X
2	SFH	B	702	-	-	-	X
3	CL	A	704	-	-	-	X
4	POP	B	705	-	-	-	X
5	GLN	B	706	-	-	-	X
5	GLN	C	702	-	-	-	X
5	GLN	D	703	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20893 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.

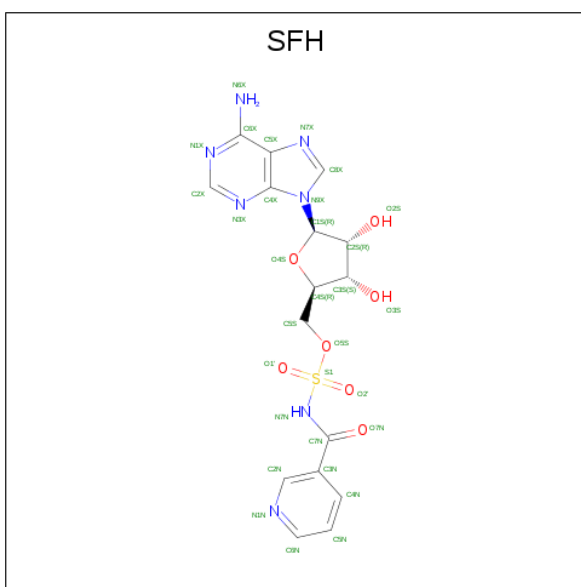
- Molecule 1 is a protein called Glutamine-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	0	0
			5081	3216	910	940	15			
1	B	669	Total	C	N	O	S	0	0	0
			5158	3265	925	953	15			
1	C	665	Total	C	N	O	S	0	0	0
			5153	3263	921	954	15			
1	D	661	Total	C	N	O	S	0	0	0
			5125	3247	916	947	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	ALA	CYS	engineered mutation	UNP P9WJJ2
B	176	ALA	CYS	engineered mutation	UNP P9WJJ2
C	176	ALA	CYS	engineered mutation	UNP P9WJJ2
D	176	ALA	CYS	engineered mutation	UNP P9WJJ2

- Molecule 2 is 5'-O-[(pyridine-3-carbonyl)sulfamoyl]adenosine (three-letter code: SFH) (formula: C<sub>16</sub>H<sub>17</sub>N<sub>7</sub>O<sub>7</sub>S) (labeled as "Ligand of Interest" by author).



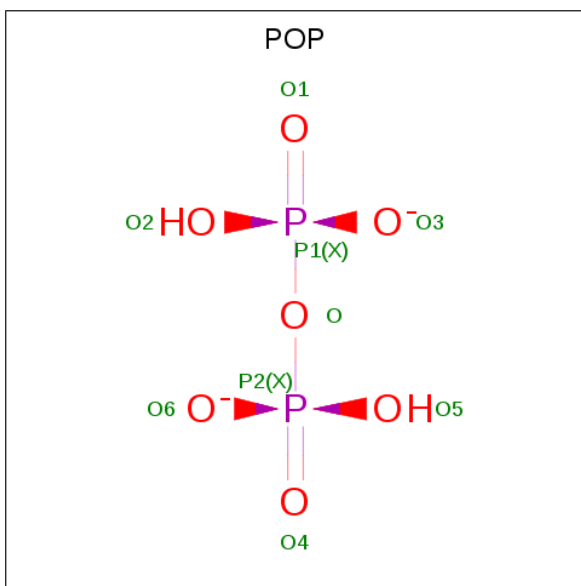
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	16	7	7	1		
2	A	1	Total	C	N	O	S	0	0
			31	16	7	7	1		
2	A	1	Total	C	N	O	S	0	1
			62	32	14	14	2		
2	B	1	Total	C	N	O	S	0	0
			31	16	7	7	1		
2	B	1	Total	C	N	O	S	0	0
			31	16	7	7	1		
2	B	1	Total	C	N	O	S	0	0
			31	16	7	7	1		
2	C	1	Total	C	N	O	S	0	0
			31	16	7	7	1		
2	D	1	Total	C	N	O	S	0	0
			31	16	7	7	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	2	Total	Cl	0	0
			2	2		
3	D	1	Total	Cl	0	0
			1	1		

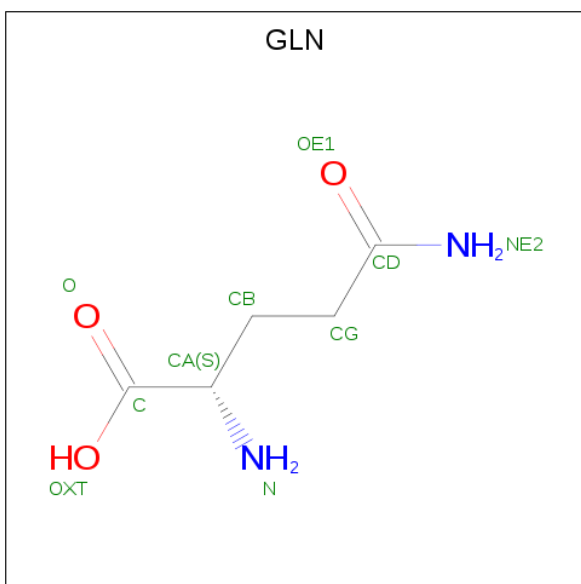
- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>) (labeled

as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			10	5	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			10	5	2	3		
5	D	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

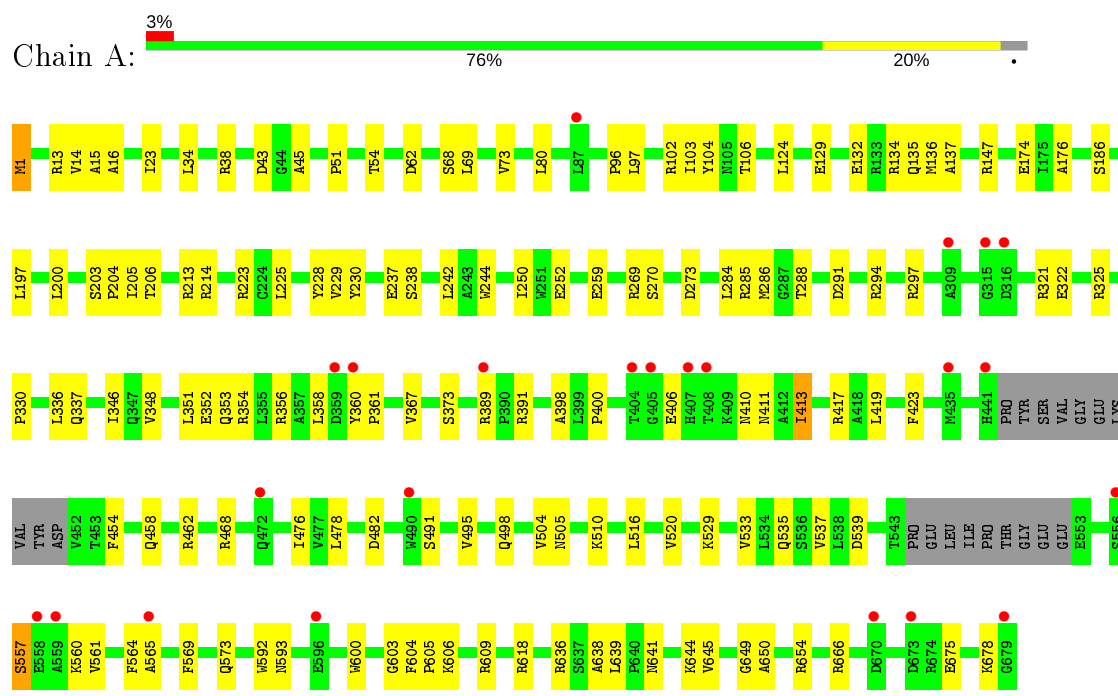
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	10	Total	O	0	0
			10	10		
7	B	8	Total	O	0	0
			8	8		
7	C	12	Total	O	0	0
			12	12		
7	D	12	Total	O	0	0
			12	12		

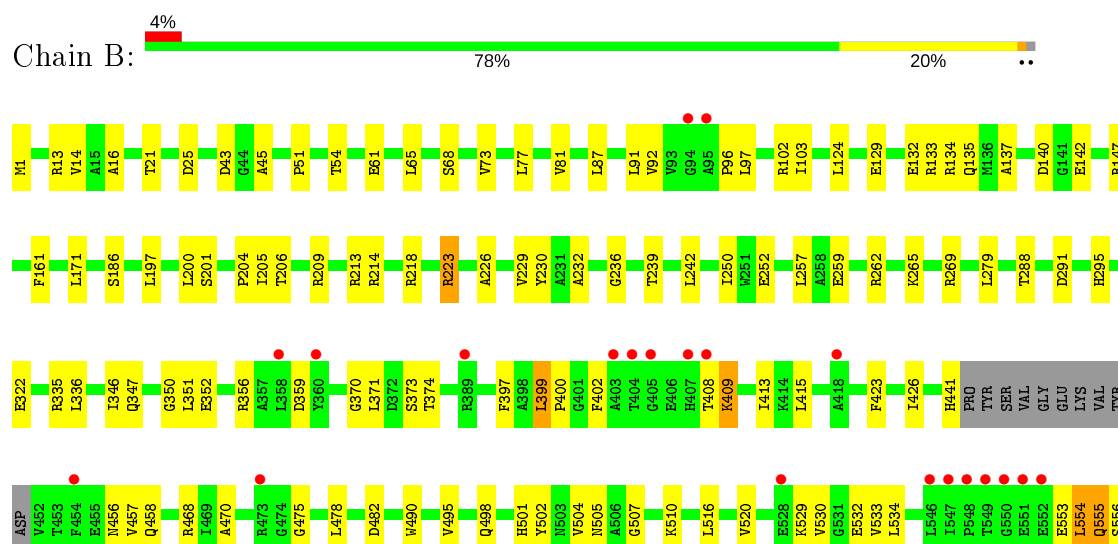
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

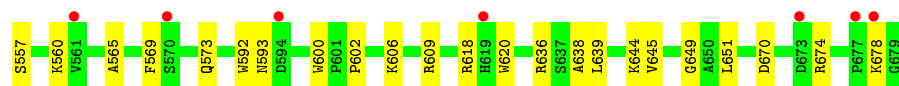
- Molecule 1: Glutamine-dependent NAD(+) synthetase



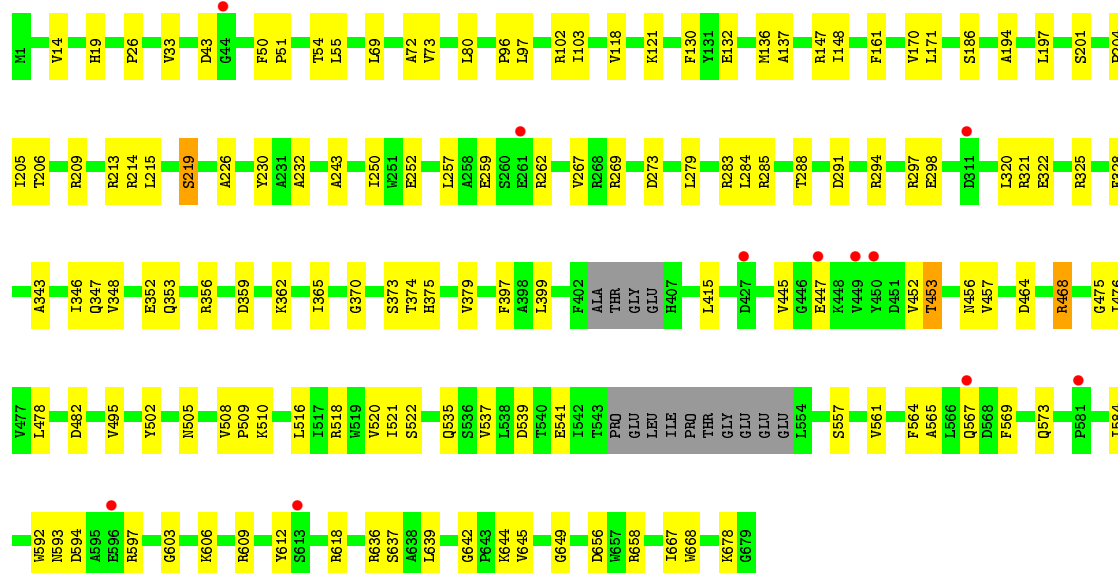
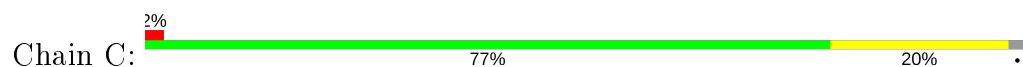
- Molecule 1: Glutamine-dependent NAD(+) synthetase



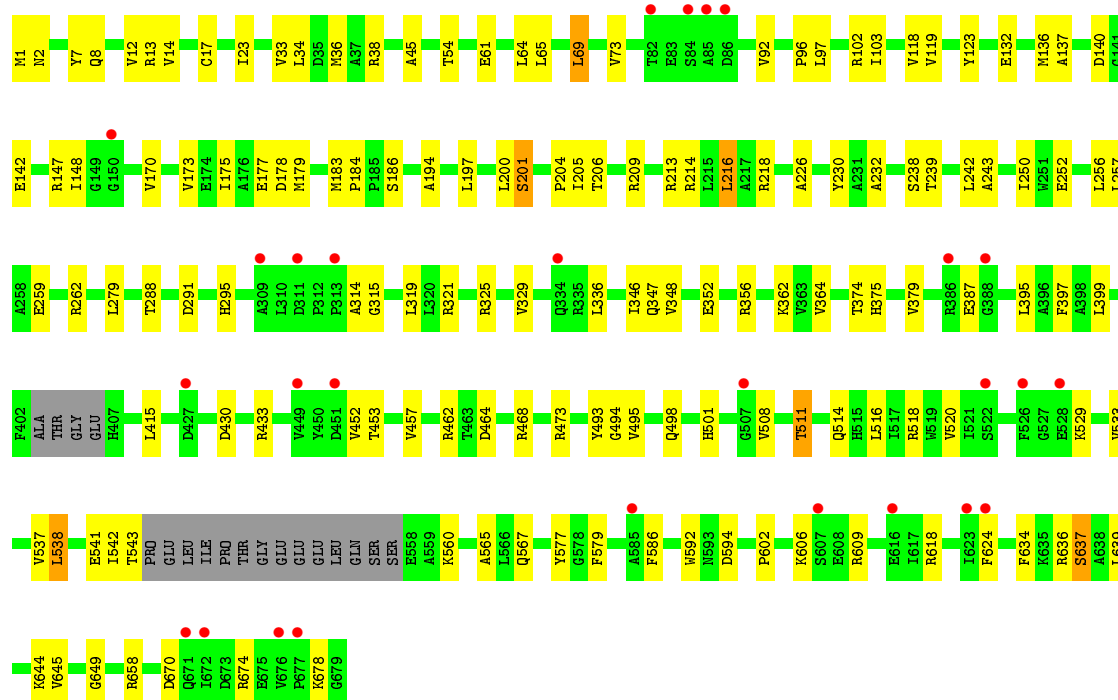
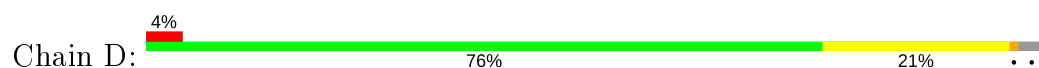




• Molecule 1: Glutamine-dependent NAD(+) synthetase



• Molecule 1: Glutamine-dependent NAD(+) synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.27Å 179.27Å 208.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.09 – 3.14 36.09 – 3.14	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.09-3.14) 98.8 (36.09-3.14)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.186 , 0.235 0.186 , 0.235	Depositor DCC
$R_{free}$ test set	2967 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	1.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2273e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, POP, SFH, CL

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	0.37	0/5199	0.55	0/7066
1	B	0.37	0/5279	0.56	0/7176
1	C	0.38	0/5274	0.57	0/7167
1	D	0.37	0/5245	0.55	0/7127
All	All	0.38	0/20997	0.56	0/28536

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	5081	0	4953	88	0
1	B	5158	0	5044	95	0
1	C	5153	0	5041	93	0
1	D	5125	0	5015	107	0
2	A	124	0	0	2	0
2	B	93	0	0	2	0
2	C	31	0	0	0	0
2	D	31	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	9	0	0	2	0
5	B	10	0	7	4	0
5	C	10	0	7	3	0
5	D	10	0	7	0	0
6	B	6	0	8	0	0
6	D	6	0	8	1	0
7	A	10	0	0	0	0
7	B	8	0	0	0	0
7	C	12	0	0	1	0
7	D	12	0	0	0	0
All	All	20893	0	20090	356	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 9.

All (356) 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)
5:C:702:GLN:NE2	7:C:801:HOH:O	2.04	0.89
1:B:606:LYS:HA	1:B:609:ARG:HD3	1.57	0.86
1:D:102:ARG:HD3	1:D:137:ALA:HB2	1.57	0.85
1:C:102:ARG:HD3	1:C:137:ALA:HB2	1.61	0.82
1:D:14:VAL:HG23	1:D:250:ILE:HD13	1.64	0.78
1:D:493:TYR:HA	1:D:498:GLN:HG2	1.64	0.78
5:B:706:GLN:HB2	1:D:218:ARG:HH11	1.50	0.77
1:D:542:ILE:HD12	1:D:543:THR:HG23	1.67	0.77
1:A:606:LYS:HA	1:A:609:ARG:HD3	1.67	0.76
1:C:606:LYS:HA	1:C:609:ARG:HD3	1.67	0.76
1:B:346:ILE:HD11	1:B:645:VAL:HG22	1.67	0.74
1:A:174:GLU:OE2	1:A:228:TYR:OH	2.06	0.74
1:C:285:ARG:NH2	1:D:65:LEU:O	2.22	0.72
1:A:102:ARG:HD3	1:A:137:ALA:HB2	1.73	0.71
1:C:365:ILE:HD12	1:C:478:LEU:HD23	1.72	0.70
1:A:618:ARG:HH12	1:A:678:LYS:HG2	1.55	0.70
1:B:129:GLU:OE2	1:B:209:ARG:NH2	2.23	0.70
1:D:325:ARG:NH2	1:D:594:ASP:O	2.24	0.69
1:A:252:GLU:OE1	1:A:321:ARG:NH2	2.24	0.69
1:A:498:GLN:NE2	1:A:638:ALA:O	2.26	0.69
1:D:362:LYS:NZ	1:D:473:ARG:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:ILE:HD11	1:D:645:VAL:HA	1.75	0.69
5:B:706:GLN:HB2	1:D:218:ARG:NH1	2.07	0.68
1:D:606:LYS:HA	1:D:609:ARG:HD3	1.76	0.68
1:A:529:LYS:O	1:A:533:VAL:HG23	1.94	0.68
1:A:14:VAL:HG23	1:A:250:ILE:HD13	1.73	0.68
1:D:73:VAL:HG11	1:D:96:PRO:HD2	1.75	0.67
1:C:43:ASP:OD2	1:C:269:ARG:NH2	2.28	0.66
1:C:204:PRO:O	1:C:209:ARG:NH1	2.29	0.66
1:A:495:VAL:O	1:D:468:ARG:NH2	2.29	0.65
1:B:373:SER:OG	4:B:705:POP:O4	2.11	0.65
1:D:514:GLN:HE21	1:D:518:ARG:HH12	1.44	0.65
1:B:482:ASP:OD2	1:B:510:LYS:NZ	2.31	0.64
1:B:13:ARG:HB3	1:B:45:ALA:HA	1.80	0.64
1:B:644:LYS:HE3	1:B:649:GLY:HA2	1.78	0.64
1:D:514:GLN:NE2	1:D:518:ARG:HH12	1.96	0.64
1:B:102:ARG:HD3	1:B:137:ALA:HB2	1.80	0.63
1:D:226:ALA:HA	1:D:279:LEU:HD13	1.80	0.63
1:B:553:GLU:HG3	1:B:555:GLN:HG2	1.80	0.62
1:D:397:PHE:HB3	1:D:399:LEU:HD21	1.81	0.62
1:B:350:GLY:HA2	1:D:239:THR:HG21	1.82	0.61
1:C:325:ARG:NH2	1:C:594:ASP:O	2.33	0.61
1:A:297:ARG:NH2	1:B:142:GLU:OE2	2.33	0.61
1:C:518:ARG:HH11	1:C:603:GLY:HA3	1.66	0.61
1:A:618:ARG:NH1	1:A:678:LYS:HG2	2.16	0.60
1:C:537:VAL:O	1:C:541:GLU:HG2	2.01	0.60
1:C:561:VAL:O	1:C:567:GLN:NE2	2.31	0.60
1:A:353:GLN:OE1	1:A:356:ARG:NH2	2.35	0.60
1:A:346:ILE:HD11	1:A:645:VAL:HA	1.83	0.60
1:A:13:ARG:HB3	1:A:45:ALA:HA	1.84	0.59
1:B:204:PRO:HG2	1:B:209:ARG:HH12	1.67	0.59
1:A:468:ARG:NH2	1:D:495:VAL:O	2.36	0.59
1:B:495:VAL:O	1:C:468:ARG:NH2	2.36	0.59
1:D:252:GLU:OE1	1:D:321:ARG:NH2	2.30	0.59
1:A:411:ASN:HB3	1:A:537:VAL:HG22	1.85	0.58
1:B:218:ARG:NH1	5:B:706:GLN:HG2	2.18	0.58
1:D:618:ARG:NH1	1:D:678:LYS:HG2	2.18	0.58
1:D:186:SER:HB2	1:D:197:LEU:HD13	1.84	0.58
1:C:51:PRO:O	1:C:54:THR:OG1	2.22	0.58
1:A:346:ILE:HD11	1:A:645:VAL:HG22	1.85	0.58
1:C:186:SER:HB2	1:C:197:LEU:HD13	1.86	0.58
1:D:214:ARG:HH22	1:D:256:LEU:HD22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:LYS:HE3	1:A:649:GLY:HA2	1.86	0.57
1:C:252:GLU:OE1	1:C:321:ARG:NH2	2.30	0.57
1:D:494:GLY:H	1:D:498:GLN:HE21	1.52	0.57
1:A:510:LYS:HD2	1:A:564:PHE:HE2	1.70	0.57
1:B:456:ASN:OD1	1:C:468:ARG:NH1	2.37	0.57
1:A:62:ASP:OD1	1:A:135:GLN:NE2	2.36	0.57
1:C:284:LEU:HD11	1:D:103:ILE:HG23	1.86	0.57
1:B:457:VAL:HA	1:C:468:ARG:HD2	1.86	0.56
1:B:346:ILE:HD11	1:B:645:VAL:HA	1.85	0.56
1:B:295:HIS:CD2	1:D:140:ASP:HB2	2.40	0.56
1:B:186:SER:HB2	1:B:197:LEU:HD13	1.87	0.56
1:C:452:VAL:HG12	1:C:456:ASN:OD1	2.06	0.56
1:A:322:GLU:CD	1:A:322:GLU:H	2.09	0.56
1:C:353:GLN:OE1	1:C:356:ARG:NH2	2.38	0.56
1:C:510:LYS:HG2	1:C:564:PHE:HD2	1.71	0.56
1:D:537:VAL:O	1:D:541:GLU:HG2	2.06	0.56
1:B:14:VAL:HG23	1:B:250:ILE:HD13	1.87	0.56
1:D:430:ASP:OD1	1:D:433:ARG:NH1	2.39	0.56
1:B:140:ASP:HB2	1:D:295:HIS:CD2	2.41	0.55
1:C:97:LEU:O	1:C:103:ILE:HA	2.07	0.55
1:A:510:LYS:HD2	1:A:564:PHE:CE2	2.42	0.55
1:A:352:GLU:O	1:A:356:ARG:HG3	2.07	0.55
1:B:201:SER:O	1:B:232:ALA:HA	2.07	0.55
1:B:288:THR:HA	1:B:291:ASP:HB2	1.89	0.55
1:A:482:ASP:HA	1:A:505:ASN:O	2.07	0.55
1:C:257:LEU:HD21	1:C:321:ARG:HH12	1.72	0.55
1:A:351:LEU:HD22	1:A:504:VAL:HG11	1.87	0.55
1:B:400:PRO:HG3	1:B:409:LYS:HE3	1.88	0.55
1:B:618:ARG:HH11	1:B:678:LYS:HA	1.72	0.55
1:A:654:ARG:O	1:D:658:ARG:NH2	2.37	0.55
1:A:124:LEU:HB3	1:A:132:GLU:HB3	1.89	0.55
1:A:15:ALA:HA	1:A:270:SER:O	2.06	0.55
1:B:213:ARG:HD3	1:B:230:TYR:OH	2.06	0.54
1:C:518:ARG:NH1	1:C:603:GLY:HA3	2.22	0.54
1:C:535:GLN:NE2	1:C:539:ASP:OD1	2.40	0.54
1:A:213:ARG:HD3	1:A:230:TYR:CZ	2.43	0.54
1:B:226:ALA:HA	1:B:279:LEU:HD13	1.90	0.54
1:A:565:ALA:HB1	1:A:592:TRP:CH2	2.42	0.54
1:B:97:LEU:O	1:B:103:ILE:HA	2.08	0.54
1:D:346:ILE:CD1	1:D:645:VAL:HA	2.37	0.54
1:A:51:PRO:O	1:A:54:THR:OG1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ARG:HB3	1:D:45:ALA:HA	1.89	0.53
1:D:670:ASP:CG	1:D:674:ARG:HH12	2.11	0.53
1:A:294:ARG:NH2	1:B:140:ASP:OD1	2.42	0.53
1:C:19:HIS:HA	1:C:267:VAL:HG12	1.91	0.53
1:C:618:ARG:HH12	1:C:678:LYS:HG2	1.74	0.53
1:C:565:ALA:HB1	1:C:592:TRP:CZ2	2.43	0.53
1:B:204:PRO:HG2	1:B:209:ARG:NH1	2.23	0.52
1:D:518:ARG:HG2	1:D:538:LEU:HD21	1.91	0.52
1:A:73:VAL:HG11	1:A:96:PRO:HD2	1.89	0.52
1:A:285:ARG:NH2	1:B:65:LEU:O	2.42	0.52
1:C:636:ARG:HA	1:C:639:LEU:HD13	1.91	0.52
1:D:670:ASP:OD1	1:D:674:ARG:NH2	2.39	0.52
1:B:397:PHE:HB3	1:B:399:LEU:HD21	1.91	0.52
1:D:132:GLU:HG2	1:D:136:MET:HE3	1.91	0.52
1:D:97:LEU:O	1:D:103:ILE:HA	2.10	0.52
1:D:201:SER:O	1:D:232:ALA:HA	2.10	0.51
1:C:362:LYS:O	1:C:476:ILE:HG12	2.10	0.51
1:B:498:GLN:NE2	1:B:638:ALA:O	2.43	0.51
1:C:644:LYS:HE3	1:C:649:GLY:HA2	1.91	0.51
1:D:364:VAL:HG22	1:D:395:LEU:HD12	1.93	0.51
1:A:348:VAL:O	1:A:352:GLU:HG3	2.10	0.51
1:C:226:ALA:HA	1:C:279:LEU:HD13	1.93	0.51
1:D:464:ASP:O	1:D:468:ARG:HG2	2.10	0.51
1:D:514:GLN:HG2	1:D:518:ARG:NH1	2.26	0.51
1:B:490:TRP:NE1	1:B:557:SER:HB3	2.26	0.51
1:C:453:THR:O	1:C:457:VAL:HG23	2.11	0.51
1:D:618:ARG:HH12	1:D:678:LYS:HG2	1.75	0.51
1:B:351:LEU:HD22	1:B:504:VAL:HG21	1.93	0.51
1:C:464:ASP:O	1:C:468:ARG:HG2	2.11	0.51
1:C:482:ASP:HA	1:C:505:ASN:O	2.11	0.51
1:B:16:ALA:HB2	1:B:229:VAL:HG13	1.94	0.50
1:B:218:ARG:HH11	5:B:706:GLN:HG2	1.75	0.50
1:C:375:HIS:O	1:C:379:VAL:HG23	2.10	0.50
6:D:704:GOL:O3	6:D:704:GOL:O1	2.25	0.50
1:A:186:SER:HB2	1:A:197:LEU:HD13	1.94	0.50
1:D:204:PRO:O	1:D:209:ARG:NH1	2.44	0.50
1:A:1:MET:HG2	1:A:675:GLU:OE1	2.11	0.50
1:B:529:LYS:O	1:B:532:GLU:HG2	2.11	0.50
1:C:132:GLU:HG2	1:C:136:MET:HE3	1.93	0.50
1:C:346:ILE:HD11	1:C:645:VAL:HA	1.92	0.50
1:D:213:ARG:HD3	1:D:230:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ILE:N	1:D:178:ASP:OD2	2.40	0.50
1:D:374:THR:HG23	1:D:415:LEU:HD22	1.94	0.50
1:B:346:ILE:CD1	1:B:645:VAL:HA	2.42	0.49
1:D:34:LEU:HD11	1:D:38:ARG:HH21	1.77	0.49
1:D:336:LEU:HD23	1:D:602:PRO:HD2	1.94	0.49
1:C:273:ASP:O	1:C:321:ARG:NH1	2.45	0.49
1:C:298:GLU:CD	1:C:298:GLU:H	2.15	0.49
1:A:398:ALA:O	1:A:400:PRO:HD3	2.12	0.49
1:A:213:ARG:HD3	1:A:230:TYR:OH	2.12	0.49
1:A:214:ARG:NH1	1:A:259:GLU:OE1	2.46	0.49
1:C:516:LEU:O	1:C:520:VAL:HG23	2.12	0.49
1:D:529:LYS:O	1:D:533:VAL:HG23	2.13	0.49
1:C:328:PHE:CG	1:C:509:PRO:HG2	2.47	0.49
1:C:618:ARG:HH11	1:C:678:LYS:HA	1.78	0.49
1:D:636:ARG:O	1:D:639:LEU:HB2	2.13	0.49
1:B:213:ARG:HD3	1:B:230:TYR:CZ	2.47	0.49
1:B:468:ARG:HD2	1:C:457:VAL:HA	1.93	0.49
1:A:104:TYR:O	1:A:106:THR:HG23	2.13	0.49
1:A:129:GLU:HB2	1:A:242:LEU:HD21	1.95	0.49
1:D:644:LYS:HE3	1:D:649:GLY:HA2	1.95	0.49
1:B:322:GLU:CD	1:B:322:GLU:H	2.17	0.48
1:C:521:ILE:HG13	1:C:522:SER:N	2.29	0.48
1:C:374:THR:HG23	1:C:415:LEU:HD22	1.95	0.48
1:D:516:LEU:O	1:D:520:VAL:HG23	2.14	0.48
1:A:516:LEU:O	1:A:520:VAL:HG23	2.13	0.48
1:A:618:ARG:HH11	1:A:678:LYS:HA	1.78	0.48
1:B:636:ARG:O	1:B:639:LEU:HB2	2.14	0.48
1:C:205:ILE:HD12	1:C:206:THR:H	1.78	0.48
1:C:26:PRO:HG2	1:C:72:ALA:HB3	1.96	0.48
1:A:391:ARG:NH1	1:A:419:LEU:O	2.46	0.48
1:A:43:ASP:OD2	1:A:269:ARG:NH2	2.47	0.48
1:C:213:ARG:HD3	1:C:230:TYR:CZ	2.49	0.48
1:B:124:LEU:HB3	1:B:132:GLU:HB3	1.94	0.48
1:A:273:ASP:O	1:A:321:ARG:NH1	2.47	0.48
1:B:565:ALA:HB1	1:B:592:TRP:CH2	2.48	0.48
1:D:288:THR:HA	1:D:291:ASP:HB2	1.95	0.48
1:D:636:ARG:HA	1:D:639:LEU:HD13	1.96	0.48
1:A:284:LEU:HD12	1:B:102:ARG:HA	1.96	0.48
1:A:406:GLU:O	1:A:410:ASN:N	2.47	0.47
1:D:399:LEU:HB2	1:D:462:ARG:HG2	1.94	0.47
1:D:352:GLU:O	1:D:356:ARG:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ALA:HB2	1:A:229:VAL:HG13	1.97	0.47
1:B:600:TRP:CD2	1:B:609:ARG:HG2	2.49	0.47
1:B:670:ASP:OD2	1:B:674:ARG:NH2	2.45	0.47
1:C:346:ILE:CD1	1:C:645:VAL:HA	2.44	0.47
1:B:288:THR:HG21	1:D:177:GLU:HG2	1.96	0.47
1:C:285:ARG:HG2	1:D:65:LEU:HD13	1.95	0.47
1:A:603:GLY:O	1:A:605:PRO:HD3	2.14	0.47
1:A:23:ILE:HD13	1:A:238:SER:HB2	1.97	0.47
1:B:600:TRP:CE3	1:B:609:ARG:HG2	2.50	0.47
1:C:618:ARG:NH1	1:C:678:LYS:HG2	2.29	0.47
1:D:514:GLN:HE21	1:D:518:ARG:HH22	1.61	0.47
1:D:64:LEU:HA	1:D:69:LEU:HD22	1.96	0.47
1:C:322:GLU:H	1:C:322:GLU:CD	2.19	0.47
1:B:288:THR:HG22	1:D:123:TYR:HB3	1.96	0.46
1:B:73:VAL:HG11	1:B:96:PRO:HD2	1.97	0.46
1:C:343:ALA:HB3	1:C:516:LEU:HD21	1.98	0.46
1:D:119:VAL:HG11	1:D:173:VAL:O	2.16	0.46
1:B:529:LYS:O	1:B:533:VAL:HG13	2.16	0.46
1:C:205:ILE:HD11	1:C:262:ARG:NH2	2.31	0.46
1:C:215:LEU:O	1:C:219:SER:HB3	2.15	0.46
1:D:514:GLN:HE21	1:D:518:ARG:NH1	2.13	0.46
1:B:336:LEU:HD23	1:B:602:PRO:HD2	1.98	0.46
1:C:118:VAL:HG21	1:C:148:ILE:HD12	1.97	0.46
1:B:370:GLY:HA3	4:B:705:POP:P2	2.56	0.46
1:B:161:PHE:HB2	1:B:171:LEU:HB3	1.98	0.45
1:B:346:ILE:HG13	1:B:347:GLN:N	2.30	0.45
1:B:371:LEU:HD12	1:B:554:LEU:HD12	1.99	0.45
1:B:77:LEU:O	1:B:81:VAL:HG23	2.14	0.45
1:C:297:ARG:NH2	1:D:142:GLU:OE2	2.46	0.45
1:D:205:ILE:HD11	1:D:262:ARG:NH2	2.31	0.45
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.79	0.45
1:B:61:GLU:OE1	1:B:135:GLN:NE2	2.47	0.45
1:C:205:ILE:HD11	1:C:262:ARG:HH21	1.81	0.45
1:D:375:HIS:O	1:D:379:VAL:HG23	2.17	0.45
1:D:453:THR:O	1:D:457:VAL:HG23	2.16	0.45
1:A:458:GLN:O	1:A:462:ARG:HG3	2.17	0.45
1:B:21:THR:O	1:B:236:GLY:HA3	2.17	0.45
1:B:409:LYS:O	1:B:413:ILE:HG13	2.17	0.45
1:D:179:MET:HA	1:D:184:PRO:HB3	1.99	0.45
1:D:204:PRO:HB3	1:D:242:LEU:HD13	1.97	0.45
1:B:43:ASP:OD2	1:B:269:ARG:NH2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:SER:OG	1:A:498:GLN:HB2	2.17	0.45
1:D:634:PHE:HA	1:D:637:SER:HB2	1.97	0.45
1:B:470:ALA:HB1	1:B:475:GLY:O	2.17	0.45
2:B:702:SFH:O2S	1:C:475:GLY:O	2.35	0.45
1:D:183:MET:HB3	1:D:183:MET:HE2	1.79	0.45
1:A:225:LEU:HD11	1:A:286:MET:SD	2.58	0.44
1:C:370:GLY:O	1:C:374:THR:OG1	2.26	0.44
1:D:132:GLU:HG2	1:D:136:MET:CE	2.46	0.44
1:D:565:ALA:HB1	1:D:592:TRP:CZ2	2.52	0.44
1:A:417:ARG:HD3	1:A:417:ARG:HA	1.65	0.44
1:C:201:SER:O	1:C:232:ALA:HA	2.16	0.44
1:A:417:ARG:NH2	1:A:423:PHE:H	2.15	0.44
1:A:69:LEU:O	1:A:73:VAL:HG23	2.17	0.44
1:B:507:GLY:HA3	1:B:645:VAL:HG23	1.99	0.44
1:B:501:HIS:NE2	2:B:703:SFH:O4S	2.51	0.44
1:C:482:ASP:HB2	1:C:508:VAL:O	2.17	0.44
1:B:636:ARG:HD2	1:B:651:LEU:HB3	1.99	0.44
1:C:73:VAL:HG11	1:C:96:PRO:HD2	2.00	0.44
1:A:535:GLN:NE2	1:A:539:ASP:OD1	2.47	0.44
1:A:600:TRP:CD2	1:A:609:ARG:HG2	2.52	0.44
1:B:129:GLU:OE1	1:D:644:LYS:NZ	2.50	0.44
1:B:478:LEU:HD12	1:B:502:TYR:O	2.17	0.44
1:C:294:ARG:NH2	1:D:140:ASP:OD1	2.50	0.44
1:D:252:GLU:HB3	1:D:257:LEU:HD13	1.99	0.44
1:D:325:ARG:HB3	1:D:592:TRP:CZ2	2.52	0.44
1:B:374:THR:HG23	1:B:415:LEU:HD22	1.99	0.44
1:A:367:VAL:HA	1:A:373:SER:HB2	2.00	0.44
1:A:97:LEU:O	1:A:103:ILE:HA	2.17	0.44
1:B:413:ILE:HG12	1:B:423:PHE:CZ	2.52	0.44
1:A:354:ARG:NH2	1:A:641:ASN:OD1	2.37	0.43
1:B:87:LEU:HD12	1:B:91:LEU:HD11	2.00	0.43
1:D:348:VAL:O	1:D:352:GLU:HG3	2.17	0.43
1:A:34:LEU:HD21	1:A:38:ARG:HH21	1.82	0.43
1:C:14:VAL:HG23	1:C:250:ILE:HD13	2.00	0.43
1:C:593:ASN:HA	1:C:612:TYR:O	2.19	0.43
1:A:468:ARG:HD2	1:D:457:VAL:HA	2.00	0.43
1:A:636:ARG:O	1:A:639:LEU:HB2	2.18	0.43
1:B:569:PHE:O	1:B:573:GLN:HG2	2.18	0.43
1:C:288:THR:HA	1:C:291:ASP:HB2	2.00	0.43
1:A:288:THR:HA	1:A:291:ASP:HB2	2.00	0.43
1:A:557:SER:O	1:A:561:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ALA:HB1	1:A:592:TRP:CZ2	2.54	0.43
1:B:468:ARG:NH2	1:C:495:VAL:O	2.50	0.43
1:B:482:ASP:HA	1:B:505:ASN:O	2.18	0.43
2:A:702:SFH:O4S	1:D:501:HIS:NE2	2.52	0.43
1:C:33:VAL:HG21	1:C:54:THR:HG21	1.99	0.43
1:D:205:ILE:HD12	1:D:206:THR:H	1.83	0.43
1:D:17:CYS:HB3	1:D:36:MET:CE	2.49	0.43
1:C:226:ALA:HB2	1:C:283:ARG:NH2	2.34	0.43
1:D:7:TYR:CE1	1:D:12:VAL:HA	2.54	0.43
1:A:176:ALA:N	1:A:200:LEU:O	2.46	0.43
1:A:666:ARG:NH2	1:B:25:ASP:OD1	2.48	0.43
1:C:397:PHE:HB3	1:C:399:LEU:HD21	2.01	0.43
1:B:399:LEU:HA	1:B:426:ILE:O	2.19	0.43
1:C:130:PHE:CZ	5:C:702:GLN:HG3	2.54	0.43
1:C:121:LYS:NZ	5:C:702:GLN:OE1	2.34	0.43
1:B:205:ILE:HD12	1:B:206:THR:H	1.84	0.42
1:B:415:LEU:HA	1:B:533:VAL:HG21	2.02	0.42
1:A:237:GLU:HB2	1:A:244:TRP:CD1	2.53	0.42
1:B:530:VAL:O	1:B:534:LEU:HG	2.19	0.42
1:C:170:VAL:HG12	1:C:194:ALA:HA	2.01	0.42
1:C:347:GLN:OE1	1:C:508:VAL:HG21	2.18	0.42
1:D:118:VAL:HG21	1:D:148:ILE:HD12	2.01	0.42
1:B:214:ARG:NH1	1:B:259:GLU:OE1	2.48	0.42
1:D:567:GLN:OE1	1:D:624:PHE:HB2	2.19	0.42
1:B:92:VAL:HG12	1:B:200:LEU:HD11	2.01	0.42
1:B:402:PHE:CD1	1:B:458:GLN:NE2	2.88	0.42
1:C:214:ARG:NH1	1:C:259:GLU:OE1	2.46	0.42
1:D:560:LYS:HD2	1:D:560:LYS:HA	1.74	0.42
1:B:205:ILE:HD11	1:B:262:ARG:NH2	2.34	0.42
1:D:374:THR:HG23	1:D:415:LEU:CD2	2.50	0.42
1:D:670:ASP:OD2	1:D:674:ARG:NH1	2.43	0.42
1:A:482:ASP:OD1	1:A:510:LYS:HE2	2.20	0.42
1:C:348:VAL:O	1:C:352:GLU:HG3	2.19	0.42
1:B:346:ILE:HB	1:D:243:ALA:HB3	2.02	0.42
1:D:347:GLN:OE1	1:D:508:VAL:HG21	2.20	0.42
1:D:92:VAL:CG1	1:D:200:LEU:HD11	2.49	0.42
1:A:325:ARG:HB3	1:A:592:TRP:CZ2	2.55	0.42
1:C:569:PHE:O	1:C:573:GLN:HG2	2.20	0.42
1:B:239:THR:HA	1:B:242:LEU:O	2.20	0.41
1:C:510:LYS:HG2	1:C:564:PHE:CD2	2.52	0.41
1:D:8:GLN:NE2	1:D:314:ALA:HB1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:GLU:O	1:B:356:ARG:HG3	2.19	0.41
1:B:618:ARG:HH12	1:B:678:LYS:HG2	1.85	0.41
1:D:23:ILE:HD13	1:D:238:SER:HB2	2.02	0.41
1:D:319:LEU:HD22	1:D:586:PHE:HE2	1.85	0.41
1:D:257:LEU:HD21	1:D:321:ARG:HH12	1.85	0.41
1:D:2:ASN:ND2	1:D:315:GLY:HA2	2.34	0.41
1:B:51:PRO:O	1:B:54:THR:OG1	2.37	0.41
1:B:516:LEU:O	1:B:520:VAL:HG23	2.20	0.41
1:D:214:ARG:NH1	1:D:259:GLU:OE1	2.49	0.41
1:D:577:TYR:HB3	1:D:579:PHE:CE1	2.55	0.41
1:A:482:ASP:CG	1:A:510:LYS:HG3	2.41	0.41
1:C:226:ALA:HB2	1:C:283:ARG:HH21	1.85	0.41
1:C:33:VAL:HG22	1:C:50:PHE:CD1	2.56	0.41
1:C:502:TYR:CZ	1:C:642:GLY:HA2	2.56	0.41
1:A:413:ILE:HD12	1:A:423:PHE:CE2	2.56	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.86	0.41
1:C:636:ARG:O	1:C:639:LEU:HB2	2.20	0.41
1:A:604:PHE:O	1:A:609:ARG:HD2	2.21	0.41
1:C:97:LEU:HA	1:C:97:LEU:HD23	1.89	0.41
1:A:204:PRO:HB3	1:A:242:LEU:HD13	2.02	0.41
1:D:170:VAL:HG12	1:D:194:ALA:HA	2.02	0.41
1:B:124:LEU:HD12	1:B:133:ARG:HD2	2.03	0.41
1:C:573:GLN:CB	1:C:584:ILE:HG12	2.51	0.41
1:C:658:ARG:HE	1:D:61:GLU:CD	2.24	0.41
1:D:213:ARG:HD3	1:D:230:TYR:OH	2.21	0.41
1:A:203:SER:OG	1:A:213:ARG:NE	2.53	0.41
1:A:476:ILE:HG22	2:A:703[A]:SFH:O2S	2.21	0.41
1:C:161:PHE:HB2	1:C:171:LEU:HB3	2.03	0.41
1:B:265:LYS:NZ	1:D:387:GLU:OE2	2.54	0.41
1:A:205:ILE:HD12	1:A:206:THR:H	1.85	0.41
1:A:330:PRO:HG2	1:A:336:LEU:HA	2.02	0.41
1:A:358:LEU:HB2	1:A:361:PRO:HD3	2.02	0.41
1:A:644:LYS:HG3	1:A:650:ALA:HB2	2.04	0.41
1:B:252:GLU:HB3	1:B:257:LEU:HD13	2.02	0.41
1:C:325:ARG:NH2	1:C:597:ARG:O	2.54	0.41
1:A:132:GLU:HG2	1:A:136:MET:CE	2.52	0.40
1:C:205:ILE:HG22	1:C:243:ALA:O	2.20	0.40
1:D:33:VAL:HG21	1:D:54:THR:HG21	2.04	0.40
1:D:567:GLN:OE1	1:D:567:GLN:HA	2.21	0.40
1:D:97:LEU:HD23	1:D:97:LEU:HA	1.87	0.40
1:A:360:TYR:HB3	1:A:389:ARG:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:HG3	1:D:216:LEU:HD21	2.02	0.40
1:B:620:TRP:CE3	1:B:620:TRP:HA	2.56	0.40
1:A:569:PHE:O	1:A:573:GLN:HG2	2.21	0.40
1:C:667:ILE:HG13	1:C:668:TRP:CE3	2.56	0.40
1:D:329:VAL:HG23	1:D:511:THR:HG23	2.03	0.40
1:C:26:PRO:HA	1:C:55:LEU:O	2.21	0.40
1:C:273:ASP:OD2	1:C:320:LEU:N	2.45	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	654/679 (96%)	622 (95%)	32 (5%)	0	100	100
1	B	665/679 (98%)	630 (95%)	35 (5%)	0	100	100
1	C	659/679 (97%)	627 (95%)	32 (5%)	0	100	100
1	D	655/679 (96%)	623 (95%)	32 (5%)	0	100	100
All	All	2633/2716 (97%)	2502 (95%)	131 (5%)	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	518/547 (95%)	506 (98%)	12 (2%)	50	75
1	B	528/547 (96%)	512 (97%)	16 (3%)	41	70
1	C	531/547 (97%)	519 (98%)	12 (2%)	50	75
1	D	527/547 (96%)	518 (98%)	9 (2%)	60	82
All	All	2104/2188 (96%)	2055 (98%)	49 (2%)	50	75

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	68	SER
1	A	134	ARG
1	A	147	ARG
1	A	223	ARG
1	A	337	GLN
1	A	413	ILE
1	A	454	PHE
1	A	478	LEU
1	A	557	SER
1	A	560	LYS
1	A	593	ASN
1	B	1	MET
1	B	68	SER
1	B	134	ARG
1	B	147	ARG
1	B	223	ARG
1	B	335	ARG
1	B	359	ASP
1	B	399	LEU
1	B	408	THR
1	B	409	LYS
1	B	441	HIS
1	B	554	LEU
1	B	555	GLN
1	B	556	SER
1	B	560	LYS
1	B	593	ASN
1	C	69	LEU
1	C	147	ARG
1	C	219	SER
1	C	359	ASP
1	C	373	SER

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Mol	Chain	Res	Type
1	C	445	VAL
1	C	447	GLU
1	C	453	THR
1	C	468	ARG
1	C	557	SER
1	C	637	SER
1	C	656	ASP
1	D	1	MET
1	D	69	LEU
1	D	147	ARG
1	D	201	SER
1	D	216	LEU
1	D	452	VAL
1	D	511	THR
1	D	538	LEU
1	D	637	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	A	458	GLN
1	A	515	HIS
1	B	295	HIS
1	B	296	HIS
1	B	345	ASN
1	B	458	GLN
1	B	555	GLN
1	C	345	ASN
1	C	456	ASN
1	C	535	GLN
1	D	111	HIS
1	D	295	HIS
1	D	345	ASN
1	D	456	ASN
1	D	498	GLN
1	D	514	GLN
1	D	535	GLN
1	D	590	HIS

### 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 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	GLN	B	706	-	5,9,9	0.36	0	5,11,11	0.20	0
5	GLN	C	702	-	5,9,9	0.22	0	5,11,11	0.26	0
5	GLN	D	703	-	5,9,9	0.54	0	5,11,11	0.51	0
6	GOL	D	704	-	5,5,5	0.93	0	5,5,5	0.86	0
2	SFH	B	703	-	31,34,34	8.50	14 (45%)	35,50,50	2.52	11 (31%)
2	SFH	C	701	-	31,34,34	8.43	13 (41%)	35,50,50	2.09	10 (28%)
2	SFH	A	701	-	31,34,34	8.26	14 (45%)	35,50,50	2.18	10 (28%)
2	SFH	A	703[A]	-	31,34,34	8.20	13 (41%)	35,50,50	2.53	12 (34%)
2	SFH	A	702	-	31,34,34	8.25	15 (48%)	35,50,50	2.88	11 (31%)
2	SFH	B	702	-	31,34,34	8.01	14 (45%)	35,50,50	3.10	12 (34%)
2	SFH	D	701	-	31,34,34	8.66	14 (45%)	35,50,50	2.23	13 (37%)
2	SFH	A	703[B]	-	31,34,34	8.08	15 (48%)	35,50,50	3.17	12 (34%)
2	SFH	B	701	-	31,34,34	8.28	14 (45%)	35,50,50	2.17	12 (34%)
4	POP	B	705	-	6,8,8	0.75	0	13,13,13	1.18	1 (7%)
6	GOL	B	707	-	5,5,5	0.77	0	5,5,5	1.00	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	GLN	B	706	-	-	0/5/9/9	-
5	GLN	C	702	-	-	0/5/9/9	-
5	GLN	D	703	-	-	1/5/9/9	-
6	GOL	D	704	-	-	4/4/4/4	-
2	SFH	B	703	-	-	6/14/35/35	0/4/4/4
2	SFH	C	701	-	-	5/14/35/35	0/4/4/4
2	SFH	A	701	-	-	5/14/35/35	0/4/4/4
2	SFH	A	703[A]	-	-	3/14/35/35	0/4/4/4
2	SFH	A	702	-	-	4/14/35/35	0/4/4/4
2	SFH	B	702	-	-	6/14/35/35	0/4/4/4
2	SFH	D	701	-	-	4/14/35/35	0/4/4/4
2	SFH	A	703[B]	-	-	6/14/35/35	0/4/4/4
2	SFH	B	701	-	-	7/14/35/35	0/4/4/4
4	POP	B	705	-	-	1/6/6/6	-
6	GOL	B	707	-	-	2/4/4/4	-

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	SFH	O1'-S1	30.70	1.68	1.42
2	C	701	SFH	O1'-S1	29.98	1.67	1.42
2	A	701	SFH	O1'-S1	28.90	1.66	1.42
2	B	703	SFH	O2'-S1	28.74	1.66	1.42
2	B	703	SFH	O1'-S1	28.73	1.66	1.42
2	A	703[A]	SFH	O1'-S1	28.52	1.66	1.42
2	B	701	SFH	O1'-S1	28.26	1.66	1.42
2	A	702	SFH	O2'-S1	27.65	1.65	1.42
2	D	701	SFH	O2'-S1	27.30	1.65	1.42
2	A	702	SFH	O1'-S1	27.24	1.65	1.42
2	A	703[B]	SFH	O1'-S1	27.02	1.65	1.42
2	B	702	SFH	O1'-S1	26.96	1.65	1.42
2	B	701	SFH	O2'-S1	26.67	1.65	1.42
2	A	703[A]	SFH	O2'-S1	26.29	1.64	1.42
2	A	703[B]	SFH	O2'-S1	26.26	1.64	1.42
2	A	701	SFH	O2'-S1	25.98	1.64	1.42
2	C	701	SFH	O2'-S1	25.66	1.64	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	SFH	O2'-S1	25.58	1.64	1.42
2	A	701	SFH	O4S-C1S	16.05	1.63	1.41
2	D	701	SFH	O4S-C1S	15.74	1.63	1.41
2	B	701	SFH	O4S-C1S	15.73	1.63	1.41
2	C	701	SFH	O4S-C1S	15.54	1.62	1.41
2	A	703[A]	SFH	O4S-C1S	14.20	1.60	1.41
2	A	702	SFH	C2S-C1S	-13.83	1.32	1.53
2	C	701	SFH	C2S-C1S	-13.82	1.32	1.53
2	A	703[B]	SFH	C2S-C1S	-13.73	1.32	1.53
2	A	702	SFH	O4S-C1S	13.66	1.60	1.41
2	B	702	SFH	O4S-C1S	13.64	1.60	1.41
2	B	702	SFH	C2S-C1S	-13.64	1.33	1.53
2	A	703[B]	SFH	O4S-C1S	13.58	1.60	1.41
2	B	703	SFH	C2S-C1S	-13.57	1.33	1.53
2	A	703[A]	SFH	C2S-C1S	-13.52	1.33	1.53
2	D	701	SFH	C2S-C1S	-13.42	1.33	1.53
2	A	701	SFH	C2S-C1S	-13.32	1.33	1.53
2	B	701	SFH	C2S-C1S	-13.08	1.33	1.53
2	B	703	SFH	O4S-C1S	13.03	1.59	1.41
2	A	703[B]	SFH	C7N-N7N	7.98	1.48	1.39
2	B	702	SFH	C7N-N7N	7.90	1.48	1.39
2	C	701	SFH	C7N-N7N	7.86	1.48	1.39
2	B	703	SFH	C7N-N7N	7.85	1.48	1.39
2	A	702	SFH	C7N-N7N	7.78	1.48	1.39
2	D	701	SFH	C7N-N7N	7.68	1.48	1.39
2	B	701	SFH	C7N-N7N	7.10	1.47	1.39
2	C	701	SFH	C3S-C4S	-6.86	1.35	1.53
2	A	703[B]	SFH	C3S-C4S	-6.81	1.35	1.53
2	B	701	SFH	C3S-C4S	-6.76	1.35	1.53
2	D	701	SFH	C3S-C4S	-6.74	1.35	1.53
2	A	701	SFH	C3S-C4S	-6.71	1.35	1.53
2	B	703	SFH	C3S-C4S	-6.65	1.36	1.53
2	B	702	SFH	C3S-C4S	-6.60	1.36	1.53
2	A	702	SFH	C3S-C4S	-6.56	1.36	1.53
2	A	703[A]	SFH	C7N-N7N	6.41	1.46	1.39
2	A	703[A]	SFH	C3S-C4S	-6.40	1.36	1.53
2	A	701	SFH	C7N-N7N	5.93	1.46	1.39
2	B	703	SFH	S1-N7N	5.90	1.70	1.59
2	A	702	SFH	S1-N7N	5.87	1.70	1.59
2	A	703[B]	SFH	S1-N7N	5.84	1.70	1.59
2	B	702	SFH	S1-N7N	5.57	1.69	1.59
2	D	701	SFH	S1-N7N	5.30	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	SFH	S1-N7N	5.16	1.69	1.59
2	B	701	SFH	S1-N7N	5.02	1.68	1.59
2	A	703[A]	SFH	S1-N7N	4.94	1.68	1.59
2	C	701	SFH	C3N-C7N	4.77	1.60	1.50
2	D	701	SFH	C3N-C7N	4.64	1.59	1.50
2	A	703[A]	SFH	O5S-S1	4.43	1.69	1.59
2	A	703[B]	SFH	C3N-C7N	4.36	1.59	1.50
2	B	702	SFH	C4X-N3X	4.29	1.41	1.35
2	B	703	SFH	C3N-C7N	4.28	1.59	1.50
2	A	701	SFH	S1-N7N	4.19	1.67	1.59
2	B	702	SFH	C3N-C7N	4.15	1.58	1.50
2	A	702	SFH	C3N-C7N	4.09	1.58	1.50
2	B	702	SFH	C3S-C2S	4.05	1.64	1.53
2	B	703	SFH	C3S-C2S	3.98	1.64	1.53
2	B	701	SFH	O4S-C4S	3.90	1.53	1.45
2	A	703[A]	SFH	C3S-C2S	3.88	1.64	1.53
2	A	702	SFH	C3S-C2S	3.83	1.63	1.53
2	B	701	SFH	C3N-C7N	3.81	1.58	1.50
2	A	703[A]	SFH	O4S-C4S	3.81	1.53	1.45
2	B	703	SFH	C4X-N3X	3.72	1.40	1.35
2	D	701	SFH	O4S-C4S	3.64	1.53	1.45
2	A	703[B]	SFH	C3S-C2S	3.62	1.63	1.53
2	B	701	SFH	C3S-C2S	3.62	1.63	1.53
2	A	701	SFH	O4S-C4S	3.62	1.53	1.45
2	A	701	SFH	C3S-C2S	3.62	1.63	1.53
2	A	702	SFH	C4X-N3X	3.61	1.40	1.35
2	A	701	SFH	C3N-C7N	3.54	1.57	1.50
2	A	703[A]	SFH	C3N-C7N	3.53	1.57	1.50
2	A	703[B]	SFH	O4S-C4S	3.51	1.52	1.45
2	A	702	SFH	O4S-C4S	3.50	1.52	1.45
2	A	703[B]	SFH	C4X-N3X	3.47	1.40	1.35
2	B	702	SFH	O4S-C4S	3.44	1.52	1.45
2	B	702	SFH	O5S-S1	3.43	1.66	1.59
2	B	703	SFH	O4S-C4S	3.41	1.52	1.45
2	B	703	SFH	O5S-S1	3.36	1.66	1.59
2	A	703[A]	SFH	C4X-N3X	3.32	1.40	1.35
2	A	702	SFH	O5S-S1	3.29	1.66	1.59
2	C	701	SFH	O4S-C4S	3.29	1.52	1.45
2	A	703[B]	SFH	O5S-S1	3.18	1.66	1.59
2	C	701	SFH	C3S-C2S	3.16	1.62	1.53
2	D	701	SFH	C3S-C2S	3.13	1.61	1.53
2	A	701	SFH	O5S-S1	3.01	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	SFH	O5S-S1	2.96	1.65	1.59
2	B	701	SFH	C4X-N3X	2.60	1.39	1.35
2	C	701	SFH	O5S-S1	2.58	1.65	1.59
2	A	701	SFH	C4X-N3X	2.57	1.39	1.35
2	B	702	SFH	C4N-C3N	2.50	1.43	1.39
2	D	701	SFH	C4X-N3X	2.43	1.39	1.35
2	D	701	SFH	O5S-S1	2.41	1.64	1.59
2	B	702	SFH	O5S-C5S	-2.34	1.37	1.46
2	A	703[B]	SFH	O5S-C5S	-2.33	1.37	1.46
2	D	701	SFH	C6X-N6X	2.33	1.42	1.34
2	A	702	SFH	C4N-C3N	2.33	1.43	1.39
2	A	702	SFH	O5S-C5S	-2.33	1.37	1.46
2	A	703[B]	SFH	C4N-C3N	2.33	1.43	1.39
2	B	703	SFH	O5S-C5S	-2.31	1.37	1.46
2	C	701	SFH	C6X-N6X	2.26	1.42	1.34
2	A	701	SFH	C6X-N6X	2.23	1.42	1.34
2	B	701	SFH	C6X-N6X	2.18	1.42	1.34
2	C	701	SFH	C4X-N3X	2.16	1.38	1.35
2	B	703	SFH	C4N-C3N	2.14	1.43	1.39
2	B	701	SFH	O5S-C5S	-2.09	1.38	1.46
2	D	701	SFH	O5S-C5S	-2.07	1.38	1.46
2	A	702	SFH	C6X-N6X	2.06	1.41	1.34
2	A	703[A]	SFH	C6X-N6X	2.06	1.41	1.34
2	A	703[B]	SFH	C6X-N6X	2.04	1.41	1.34
2	A	701	SFH	O5S-C5S	-2.01	1.38	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703[B]	SFH	C3N-C7N-N7N	10.11	128.32	116.09
2	B	702	SFH	C3N-C7N-N7N	10.06	128.26	116.09
2	A	703[B]	SFH	O2'-S1-O1'	-8.43	107.62	120.76
2	A	702	SFH	C3N-C7N-N7N	8.38	126.23	116.09
2	A	701	SFH	O2'-S1-O1'	-8.33	107.78	120.76
2	B	702	SFH	O2'-S1-O1'	-7.95	108.37	120.76
2	A	703[A]	SFH	C3N-C7N-N7N	7.80	125.53	116.09
2	A	702	SFH	O2'-S1-O1'	-7.77	108.65	120.76
2	B	703	SFH	C3N-C7N-N7N	6.42	123.86	116.09
2	D	701	SFH	C7N-N7N-S1	6.12	131.09	123.38
2	A	702	SFH	C3S-C2S-C1S	6.12	110.19	100.98
2	B	702	SFH	O7N-C7N-C3N	-6.06	110.14	120.94
2	B	703	SFH	C3S-C2S-C1S	5.90	109.86	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703[A]	SFH	C3S-C2S-C1S	5.81	109.72	100.98
2	B	701	SFH	O2'-S1-O1'	-5.77	111.78	120.76
2	B	703	SFH	O2'-S1-O1'	-5.67	111.92	120.76
2	A	703[B]	SFH	O7N-C7N-C3N	-5.55	111.04	120.94
2	B	702	SFH	O5S-C5S-C4S	-5.31	97.72	107.62
2	A	703[B]	SFH	C3S-C2S-C1S	5.21	108.81	100.98
2	C	701	SFH	O2'-S1-O1'	-5.19	112.67	120.76
2	A	703[A]	SFH	O2'-S1-O1'	-5.17	112.70	120.76
2	A	702	SFH	O7N-C7N-C3N	-5.11	111.83	120.94
2	A	703[B]	SFH	O5S-C5S-C4S	-4.99	98.31	107.62
2	B	701	SFH	C3N-C7N-N7N	4.96	122.09	116.09
2	A	701	SFH	N3X-C2X-N1X	-4.67	121.38	128.68
2	B	701	SFH	N3X-C2X-N1X	-4.64	121.43	128.68
2	B	703	SFH	N3X-C2X-N1X	-4.59	121.50	128.68
2	C	701	SFH	C5S-O5S-S1	-4.55	107.98	117.37
2	D	701	SFH	O2'-S1-O1'	-4.47	113.80	120.76
2	C	701	SFH	N3X-C2X-N1X	-4.46	121.71	128.68
2	A	703[A]	SFH	C2S-C3S-C4S	4.45	111.30	102.64
2	D	701	SFH	N3X-C2X-N1X	-4.44	121.74	128.68
2	B	702	SFH	N3X-C2X-N1X	-4.26	122.01	128.68
2	B	702	SFH	C3S-C2S-C1S	4.14	107.21	100.98
2	D	701	SFH	C3N-C7N-N7N	4.04	120.97	116.09
2	A	703[A]	SFH	O7N-C7N-C3N	-4.04	113.74	120.94
2	B	703	SFH	O7N-C7N-C3N	-3.95	113.89	120.94
2	A	703[B]	SFH	C6N-N1N-C2N	3.84	123.48	116.85
2	A	702	SFH	O5S-C5S-C4S	-3.83	100.47	107.62
2	A	702	SFH	N3X-C2X-N1X	-3.74	122.83	128.68
2	A	703[B]	SFH	O5S-S1-O1'	3.73	117.00	105.59
2	B	702	SFH	O5S-S1-O1'	3.63	116.67	105.59
2	A	703[A]	SFH	N3X-C2X-N1X	-3.60	123.05	128.68
2	C	701	SFH	C3N-C7N-N7N	3.57	120.41	116.09
2	B	702	SFH	C6N-N1N-C2N	3.57	123.03	116.85
2	B	703	SFH	O5S-C5S-C4S	-3.57	100.96	107.62
2	C	701	SFH	C7N-N7N-S1	3.56	127.87	123.38
2	A	702	SFH	C2S-C3S-C4S	3.51	109.47	102.64
2	B	703	SFH	C2S-C3S-C4S	3.47	109.38	102.64
2	B	703	SFH	O5S-S1-O1'	3.42	116.05	105.59
2	A	702	SFH	O5S-S1-O1'	3.40	115.98	105.59
2	A	702	SFH	C6N-N1N-C2N	3.37	122.68	116.85
2	A	703[B]	SFH	N3X-C2X-N1X	-3.36	123.43	128.68
2	D	701	SFH	C5S-O5S-S1	-3.28	110.61	117.37
2	A	703[B]	SFH	O4S-C1S-C2S	-3.26	102.17	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703[B]	SFH	C4X-C5X-N7X	-3.23	106.04	109.40
2	B	701	SFH	O7N-C7N-C3N	-3.21	115.20	120.94
2	B	701	SFH	C5S-O5S-S1	-3.21	110.74	117.37
2	A	703[A]	SFH	C6N-N1N-C2N	3.11	122.22	116.85
2	A	703[A]	SFH	O5S-S1-O1'	3.11	115.08	105.59
2	A	701	SFH	C5S-O5S-S1	-3.09	110.99	117.37
2	A	701	SFH	O5S-S1-O1'	3.02	114.81	105.59
2	A	703[A]	SFH	C4X-C5X-N7X	-3.02	106.26	109.40
2	B	701	SFH	C3S-C2S-C1S	3.01	105.50	100.98
2	D	701	SFH	C3S-C2S-C1S	2.92	105.38	100.98
2	B	701	SFH	C6N-N1N-C2N	2.84	121.77	116.85
2	B	702	SFH	O4S-C1S-C2S	-2.75	102.91	106.93
2	D	701	SFH	O5S-S1-O2'	2.66	113.72	105.59
2	D	701	SFH	C2S-C3S-C4S	2.65	107.79	102.64
2	A	701	SFH	C4X-C5X-N7X	-2.62	106.67	109.40
2	B	702	SFH	C5X-C6X-N6X	-2.61	116.39	120.35
2	B	702	SFH	C4X-C5X-N7X	-2.55	106.74	109.40
2	B	703	SFH	C6N-N1N-C2N	2.54	121.25	116.85
2	C	701	SFH	O5S-C5S-C4S	-2.53	102.91	107.62
2	A	701	SFH	C6N-N1N-C2N	2.50	121.17	116.85
2	B	701	SFH	O5S-S1-O2'	2.49	113.21	105.59
2	B	703	SFH	C5X-C6X-N6X	-2.48	116.58	120.35
2	D	701	SFH	O7N-C7N-C3N	-2.47	116.53	120.94
2	D	701	SFH	C4X-C5X-N7X	-2.46	106.83	109.40
2	C	701	SFH	O7N-C7N-C3N	-2.45	116.56	120.94
2	A	703[B]	SFH	C5S-O5S-S1	-2.43	112.36	117.37
2	B	701	SFH	C4X-C5X-N7X	-2.42	106.88	109.40
2	C	701	SFH	C6N-N1N-C2N	2.40	121.01	116.85
2	D	701	SFH	C5S-C4S-C3S	-2.37	106.28	115.18
2	A	701	SFH	O2S-C2S-C1S	-2.32	102.28	110.85
2	A	701	SFH	C3S-C2S-C1S	2.30	104.44	100.98
2	A	703[B]	SFH	C5S-C4S-C3S	-2.29	106.61	115.18
2	C	701	SFH	O2S-C2S-C1S	-2.28	102.42	110.85
2	A	701	SFH	O5S-S1-O2'	2.27	112.52	105.59
2	A	702	SFH	C4X-C5X-N7X	-2.26	107.04	109.40
2	D	701	SFH	O3S-C3S-C2S	-2.23	104.62	111.82
2	D	701	SFH	C6N-N1N-C2N	2.20	120.65	116.85
2	B	701	SFH	O5S-C5S-C4S	-2.20	103.52	107.62
4	B	705	POP	O5-P2-O	2.18	111.95	104.64
2	B	702	SFH	C5S-O5S-S1	-2.15	112.93	117.37
2	C	701	SFH	C5S-C4S-C3S	-2.14	107.18	115.18
2	A	703[A]	SFH	C5S-O5S-S1	-2.11	113.01	117.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	703	SFH	C4X-C5X-N7X	-2.10	107.21	109.40
2	B	701	SFH	O5S-S1-N7N	-2.07	99.83	105.60
2	B	701	SFH	C5S-C4S-C3S	-2.07	107.44	115.18
2	A	703[A]	SFH	O2S-C2S-C3S	-2.07	105.14	111.82
2	A	701	SFH	C3N-C7N-N7N	2.05	118.56	116.09
2	A	703[A]	SFH	C3N-C2N-N1N	-2.04	120.48	123.49
2	A	702	SFH	C5S-C4S-C3S	-2.03	107.56	115.18

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	703	SFH	C3S-C4S-C5S-O5S
2	B	703	SFH	C7N-N7N-S1-O1'
2	B	703	SFH	C7N-N7N-S1-O2'
2	C	701	SFH	C3S-C4S-C5S-O5S
2	C	701	SFH	O4S-C4S-C5S-O5S
2	C	701	SFH	C5S-O5S-S1-N7N
2	C	701	SFH	C5S-O5S-S1-O2'
2	A	701	SFH	C3S-C4S-C5S-O5S
2	A	701	SFH	O4S-C4S-C5S-O5S
2	A	701	SFH	C5S-O5S-S1-O2'
2	A	702	SFH	C7N-N7N-S1-O1'
2	A	702	SFH	C7N-N7N-S1-O2'
2	B	702	SFH	C3S-C4S-C5S-O5S
2	B	702	SFH	C7N-N7N-S1-O1'
2	B	702	SFH	C7N-N7N-S1-O2'
2	D	701	SFH	C3S-C4S-C5S-O5S
2	D	701	SFH	O4S-C4S-C5S-O5S
2	D	701	SFH	C5S-O5S-S1-N7N
2	D	701	SFH	C5S-O5S-S1-O2'
2	A	703[B]	SFH	C3S-C4S-C5S-O5S
2	A	703[B]	SFH	C7N-N7N-S1-O1'
2	A	703[B]	SFH	C7N-N7N-S1-O2'
2	B	701	SFH	C3S-C4S-C5S-O5S
2	B	701	SFH	O4S-C4S-C5S-O5S
2	B	701	SFH	C7N-N7N-S1-O1'
2	B	701	SFH	C7N-N7N-S1-O2'
2	B	701	SFH	C5S-O5S-S1-O2'
4	B	705	POP	P2-O-P1-O3
6	B	707	GOL	C1-C2-C3-O3
6	B	707	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	D	704	GOL	O1-C1-C2-C3
6	D	704	GOL	C1-C2-C3-O3
2	C	701	SFH	C5S-O5S-S1-O1'
2	A	701	SFH	C5S-O5S-S1-O1'
2	A	703[A]	SFH	C5S-O5S-S1-O2'
2	A	702	SFH	C5S-O5S-S1-O2'
2	B	702	SFH	C5S-O5S-S1-O2'
6	D	704	GOL	O2-C2-C3-O3
5	D	703	GLN	CA-CB-CG-CD
2	B	703	SFH	C5S-O5S-S1-O1'
2	B	703	SFH	C5S-O5S-S1-O2'
2	A	702	SFH	C5S-O5S-S1-O1'
2	B	702	SFH	C5S-O5S-S1-O1'
2	A	703[B]	SFH	C5S-O5S-S1-O1'
2	A	703[B]	SFH	C5S-O5S-S1-O2'
2	B	701	SFH	C5S-O5S-S1-O1'
2	A	701	SFH	C5S-O5S-S1-N7N
2	A	703[A]	SFH	C5S-O5S-S1-N7N
2	B	702	SFH	C5S-O5S-S1-N7N
2	B	701	SFH	C5S-O5S-S1-N7N
6	D	704	GOL	O1-C1-C2-O2
2	B	703	SFH	O4S-C4S-C5S-O5S
2	A	703[B]	SFH	O4S-C4S-C5S-O5S
2	A	703[A]	SFH	C5S-O5S-S1-O1'

There are no ring outliers.

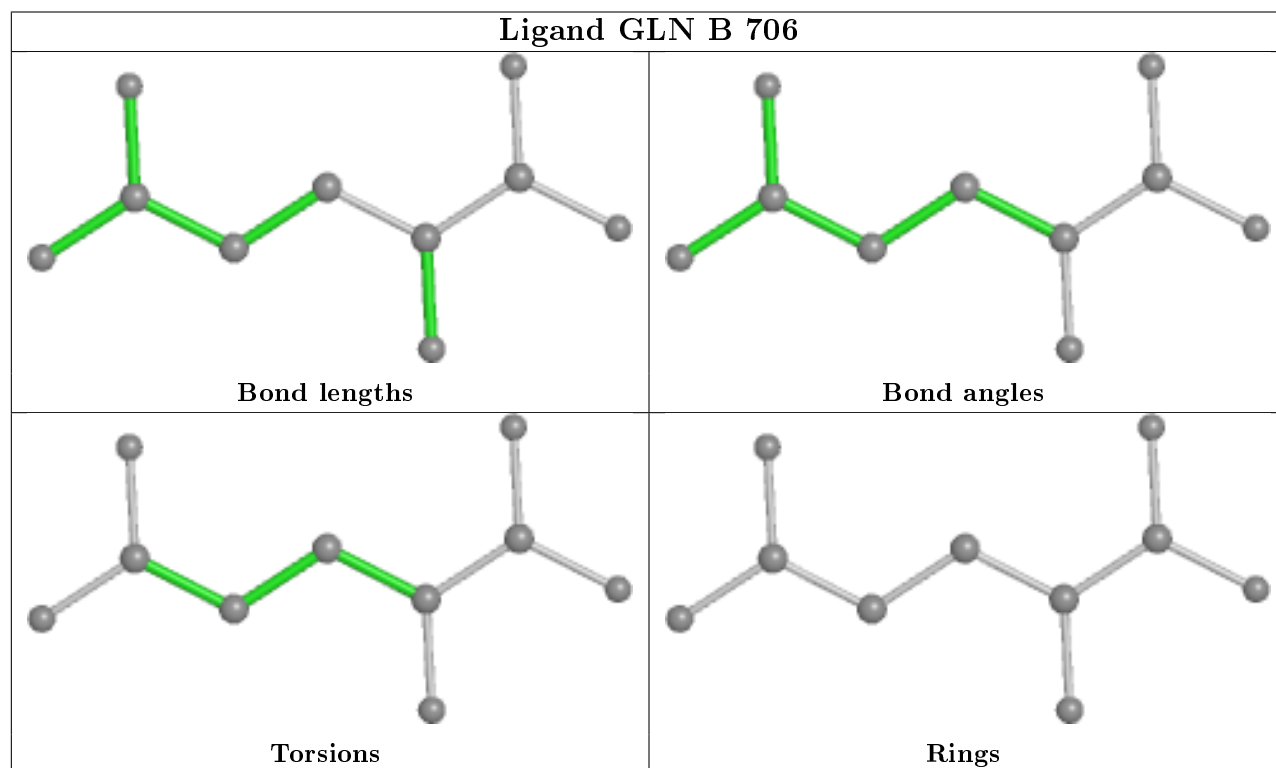
8 monomers are involved in 14 short contacts:

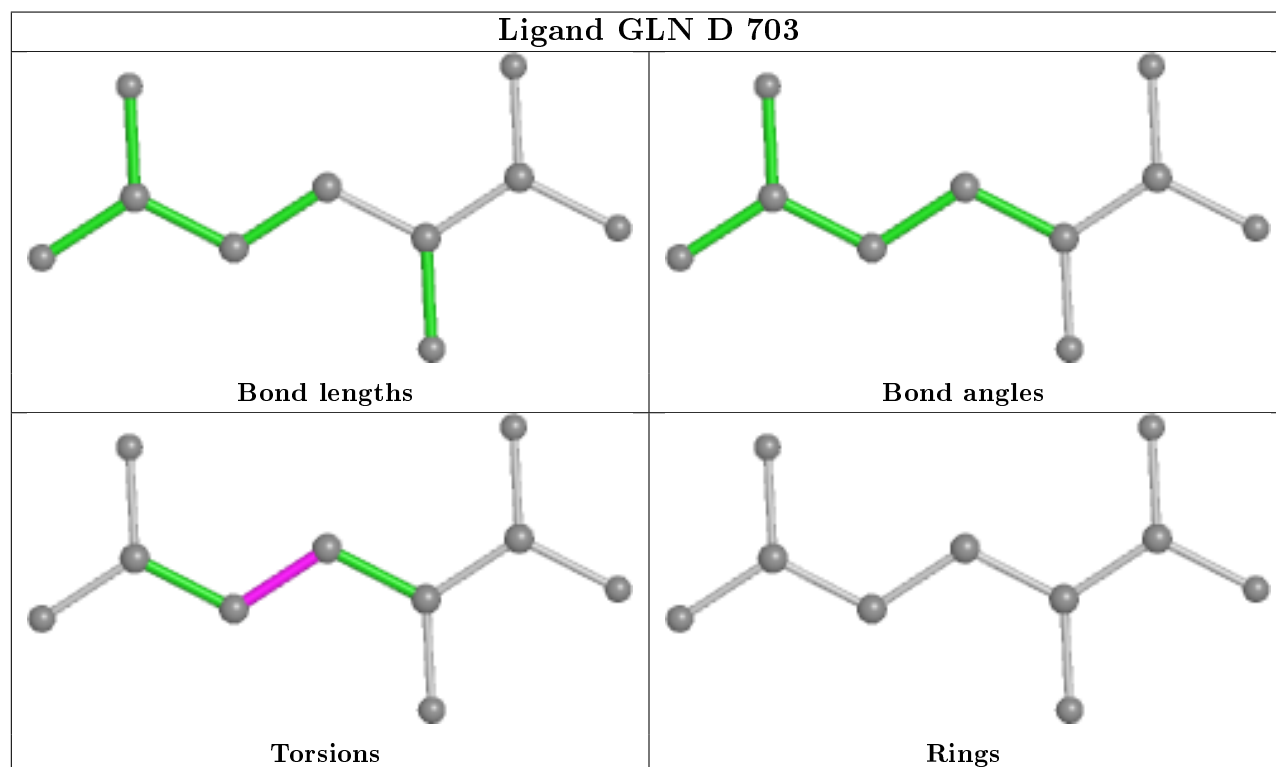
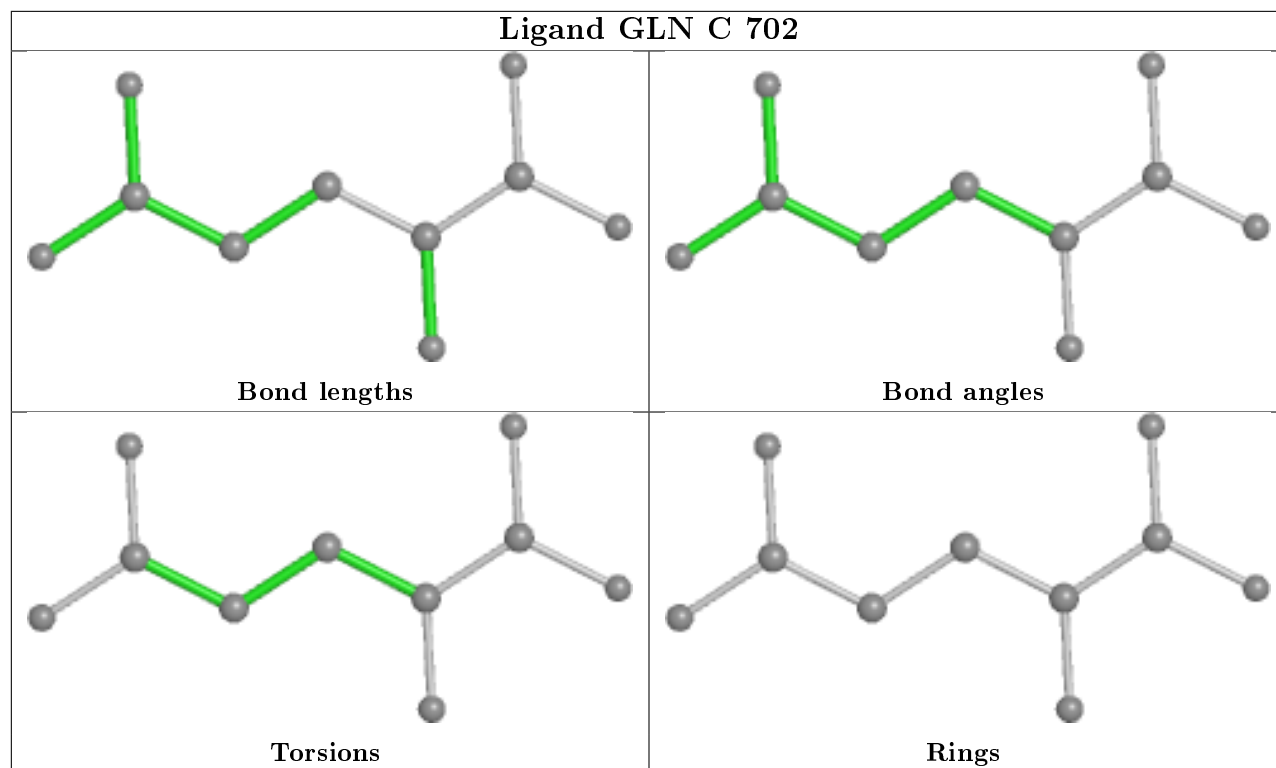
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	706	GLN	4	0
5	C	702	GLN	3	0
6	D	704	GOL	1	0
2	B	703	SFH	1	0
2	A	703[A]	SFH	1	0
2	A	702	SFH	1	0
2	B	702	SFH	1	0
4	B	705	POP	2	0

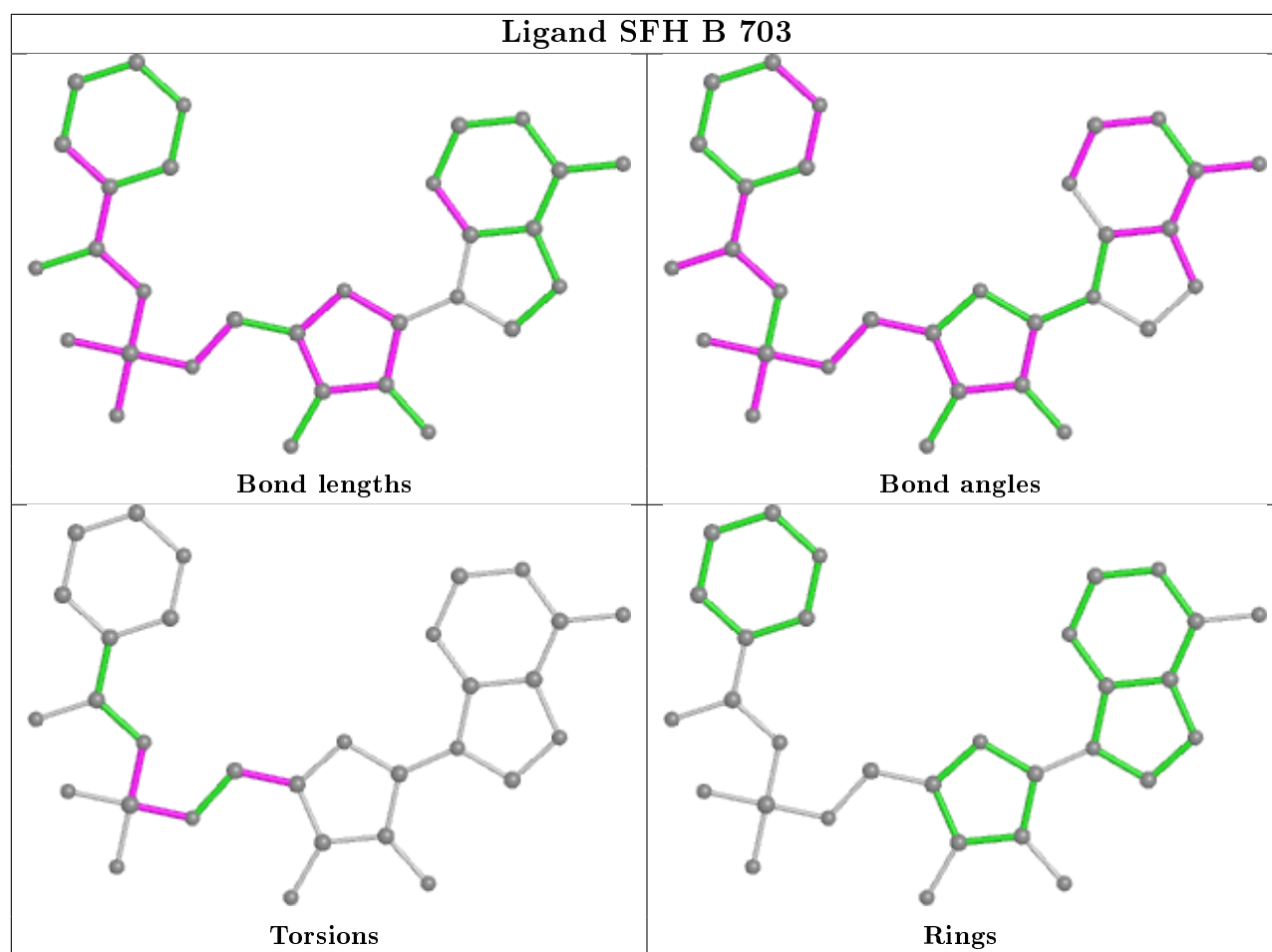
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is



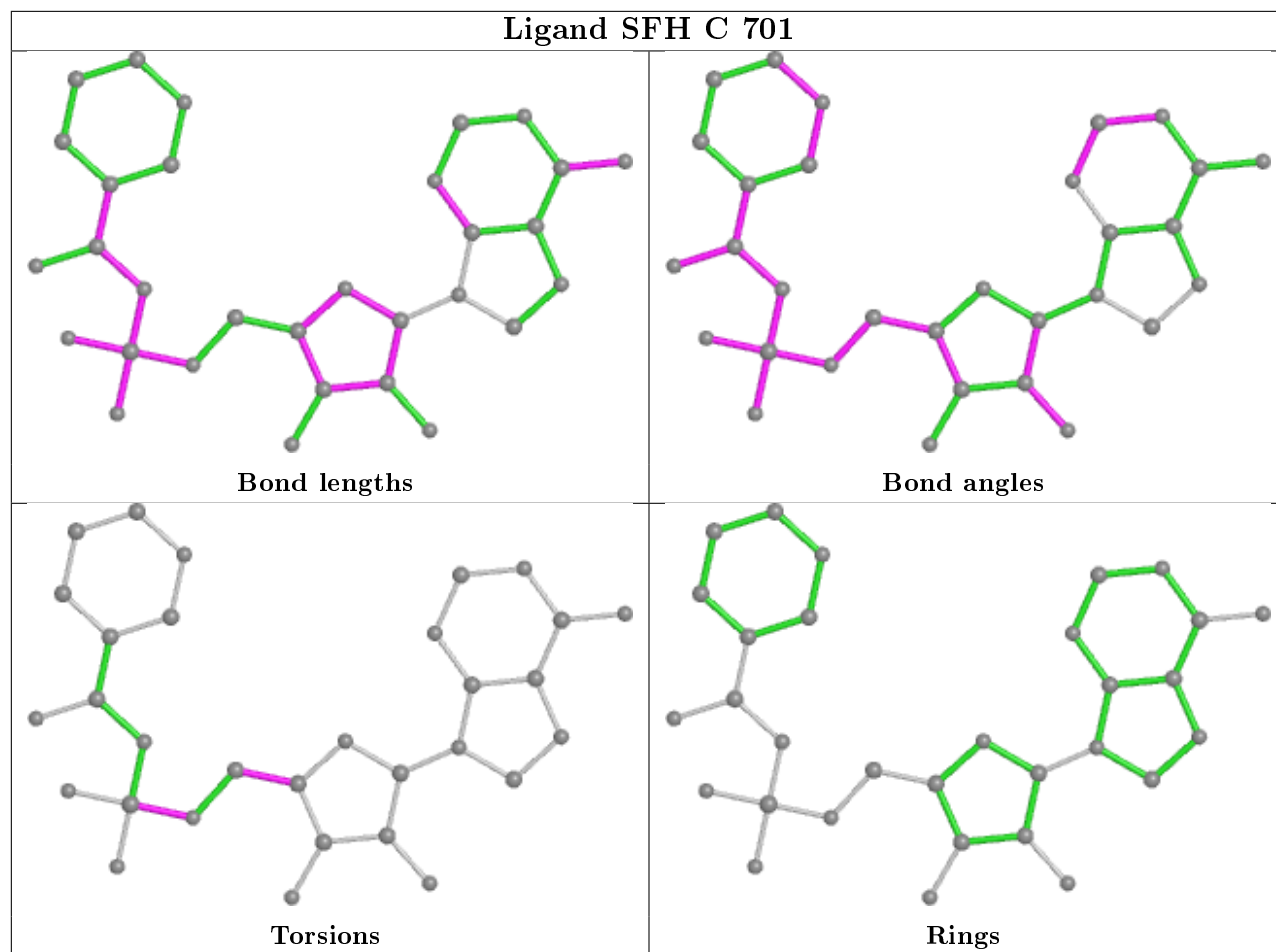
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

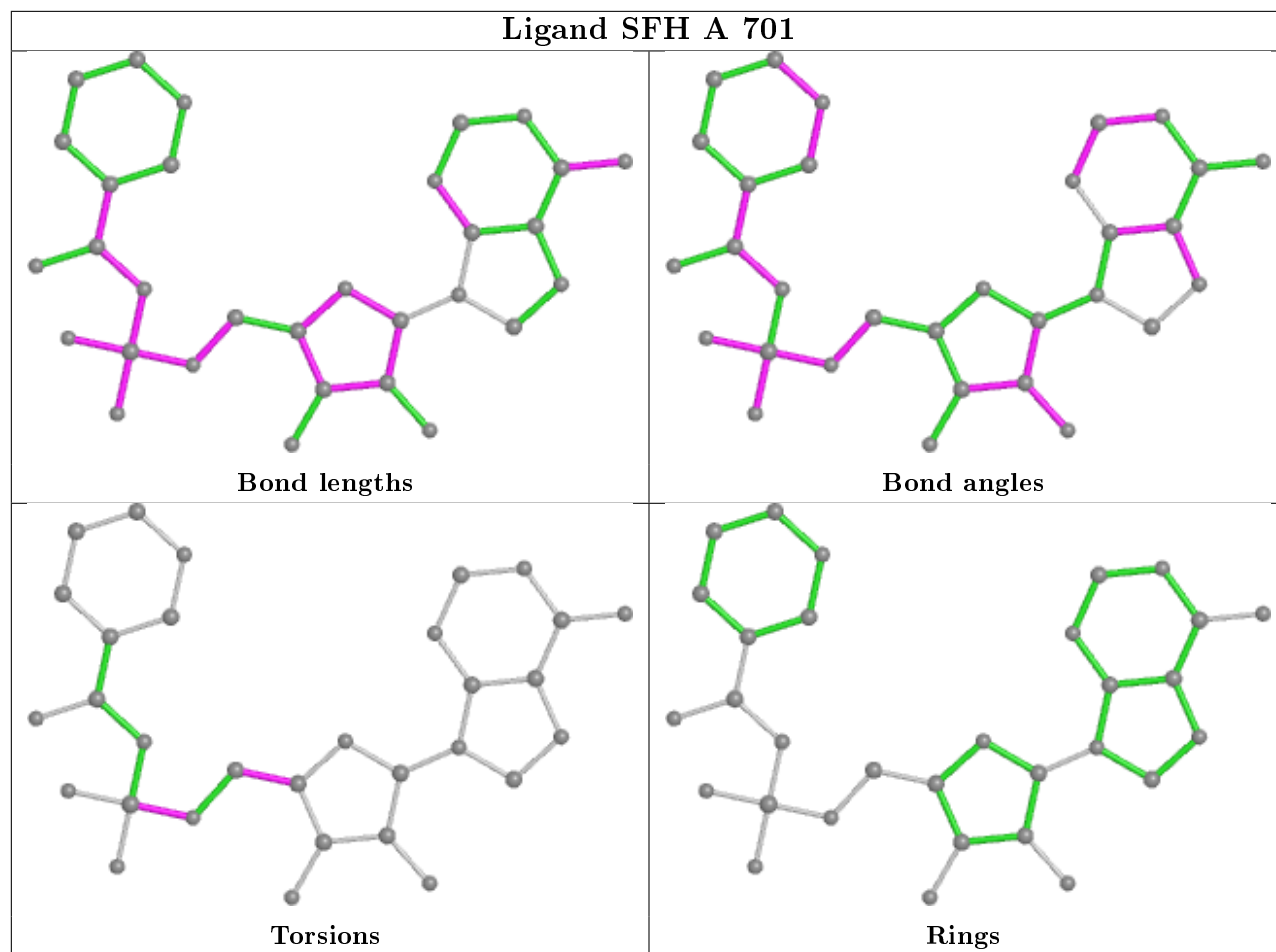


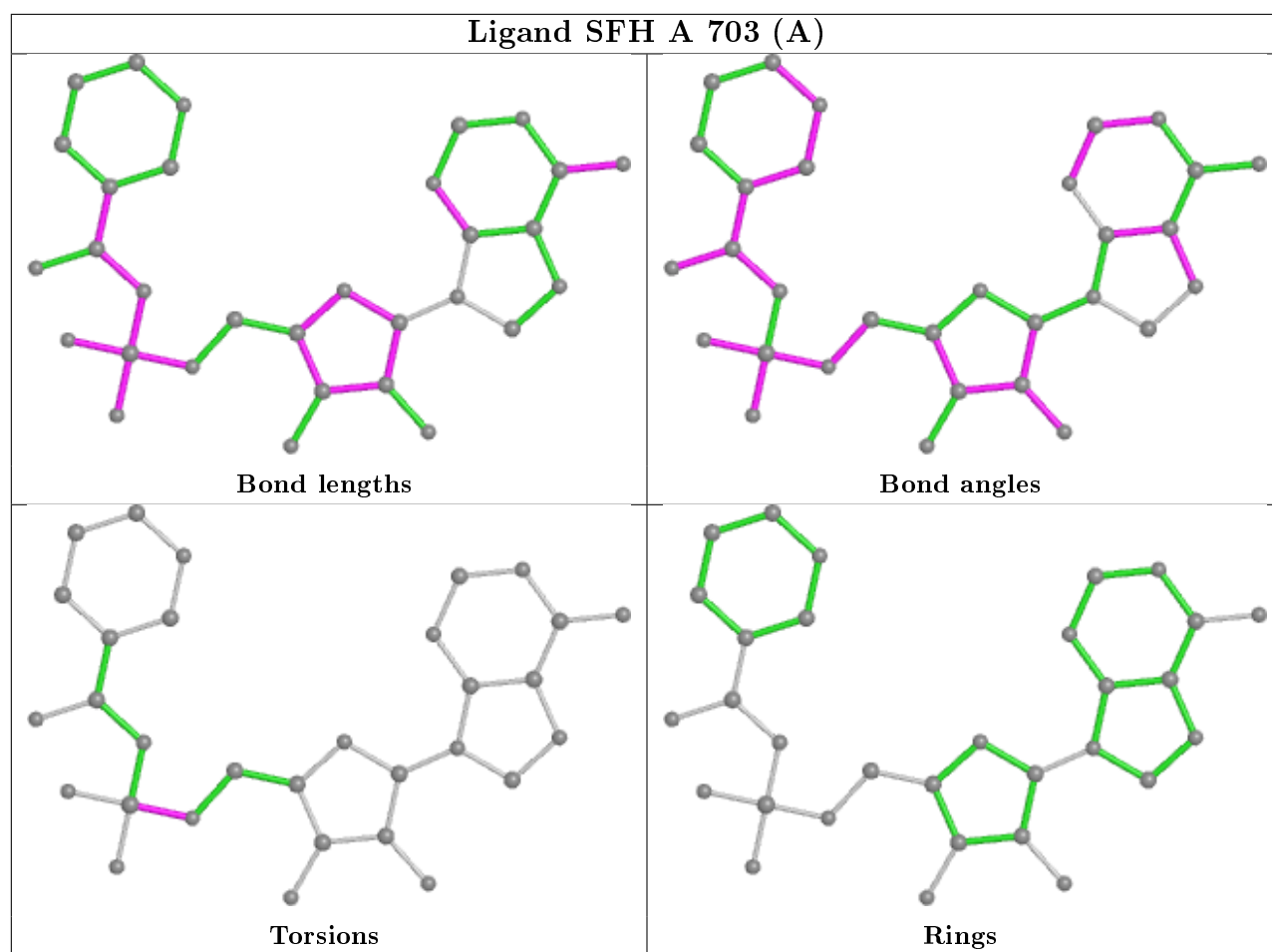




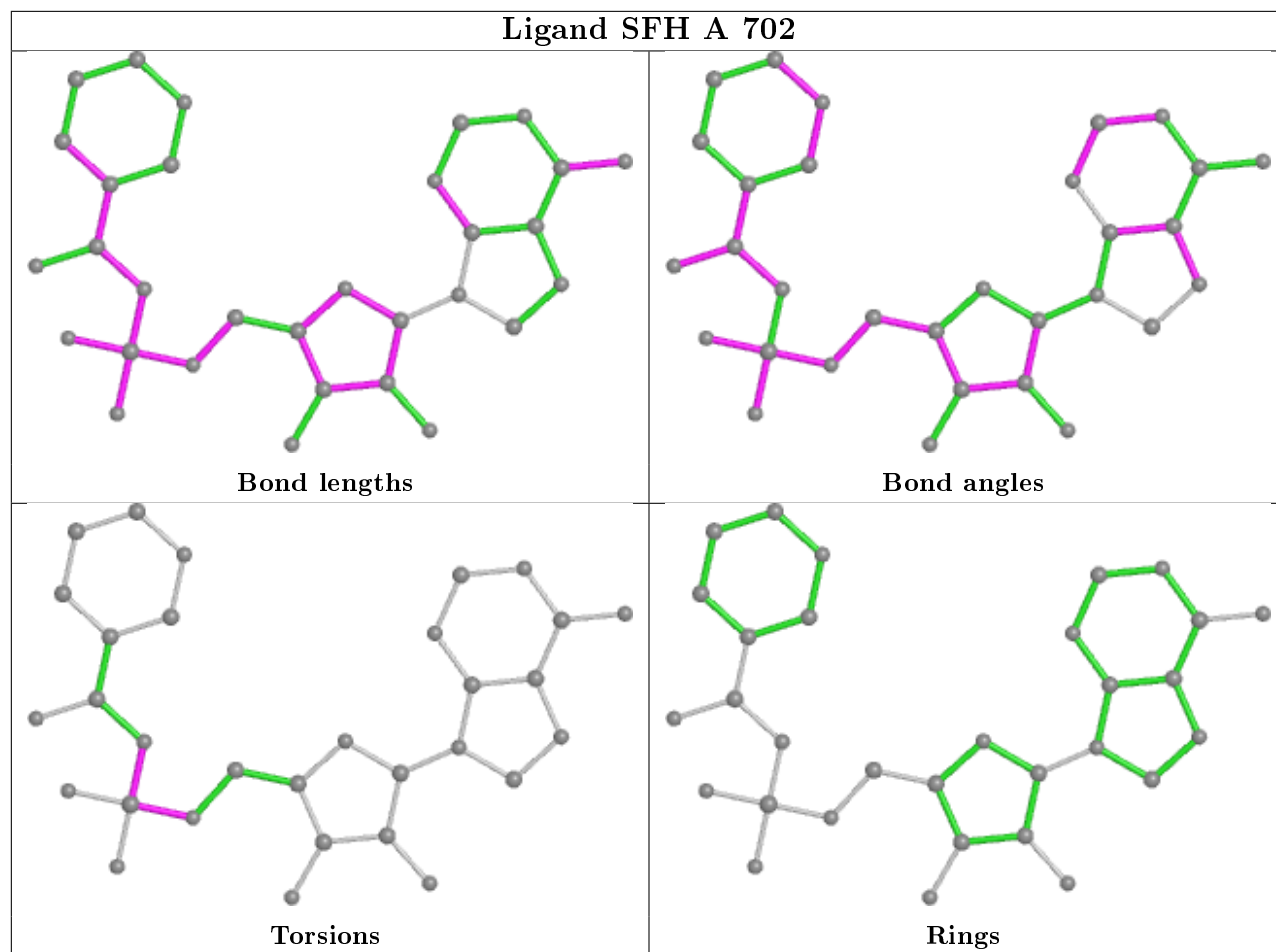
## Ligand SFH C 701

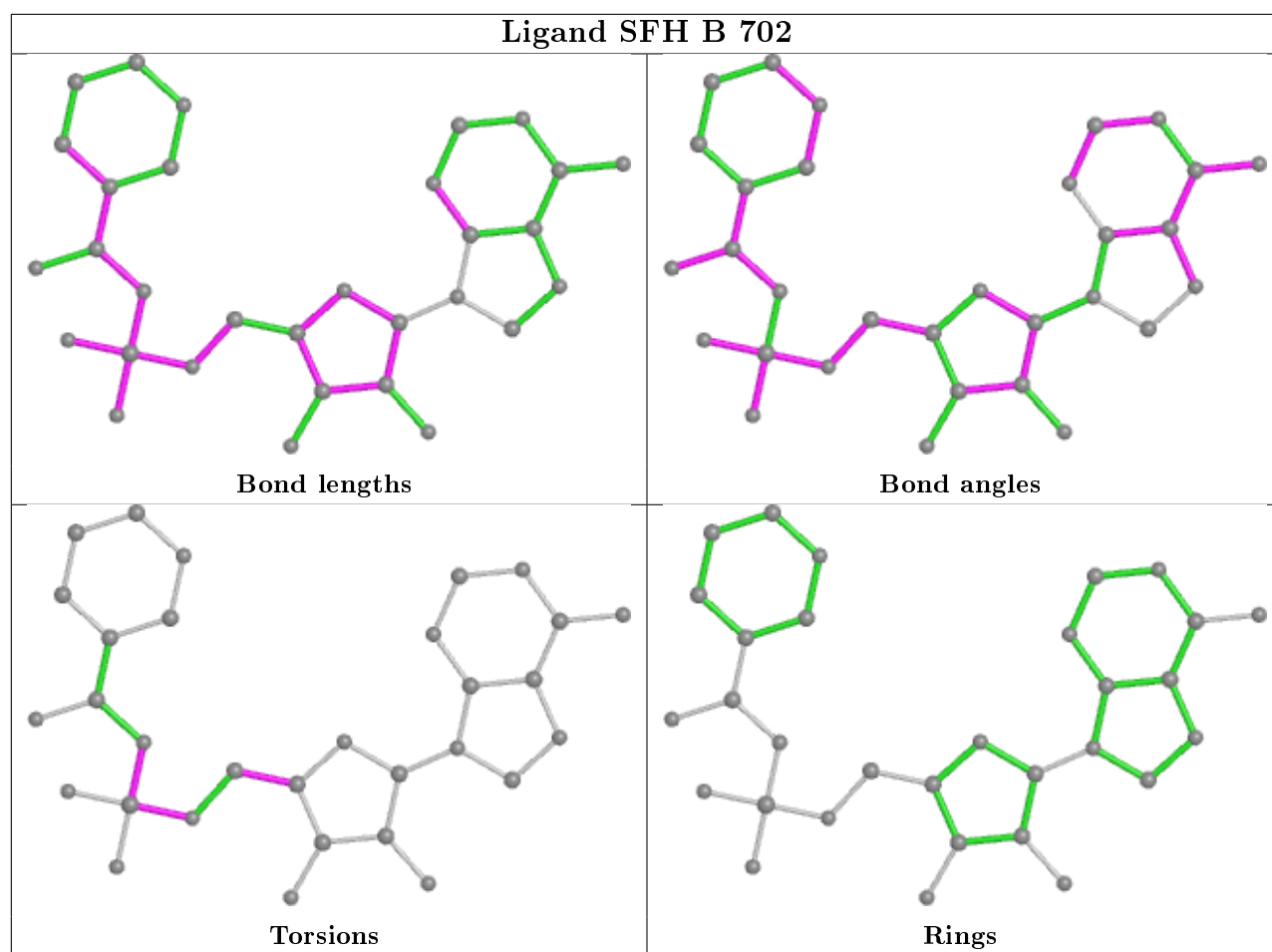






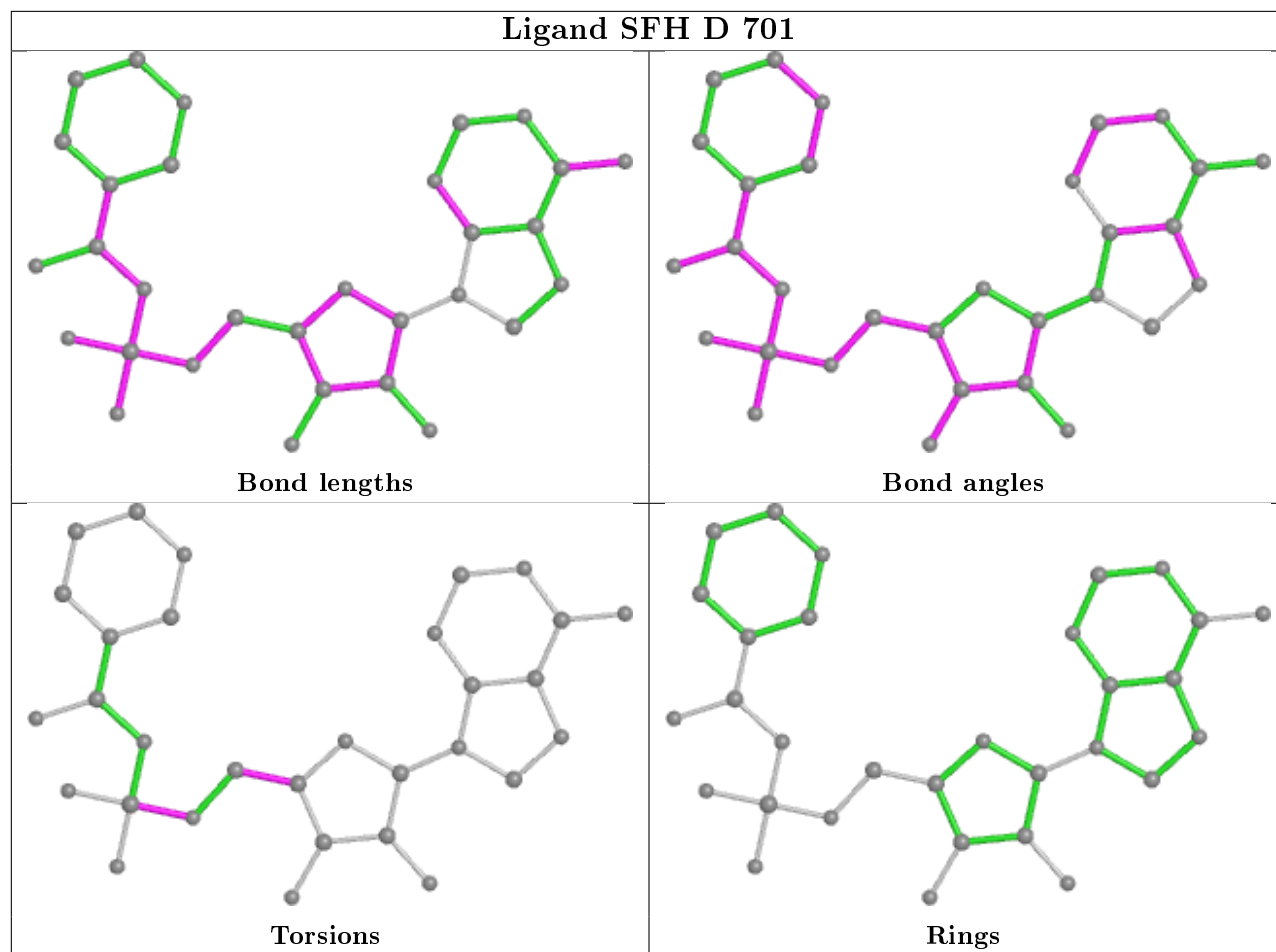
## Ligand SFH A 702

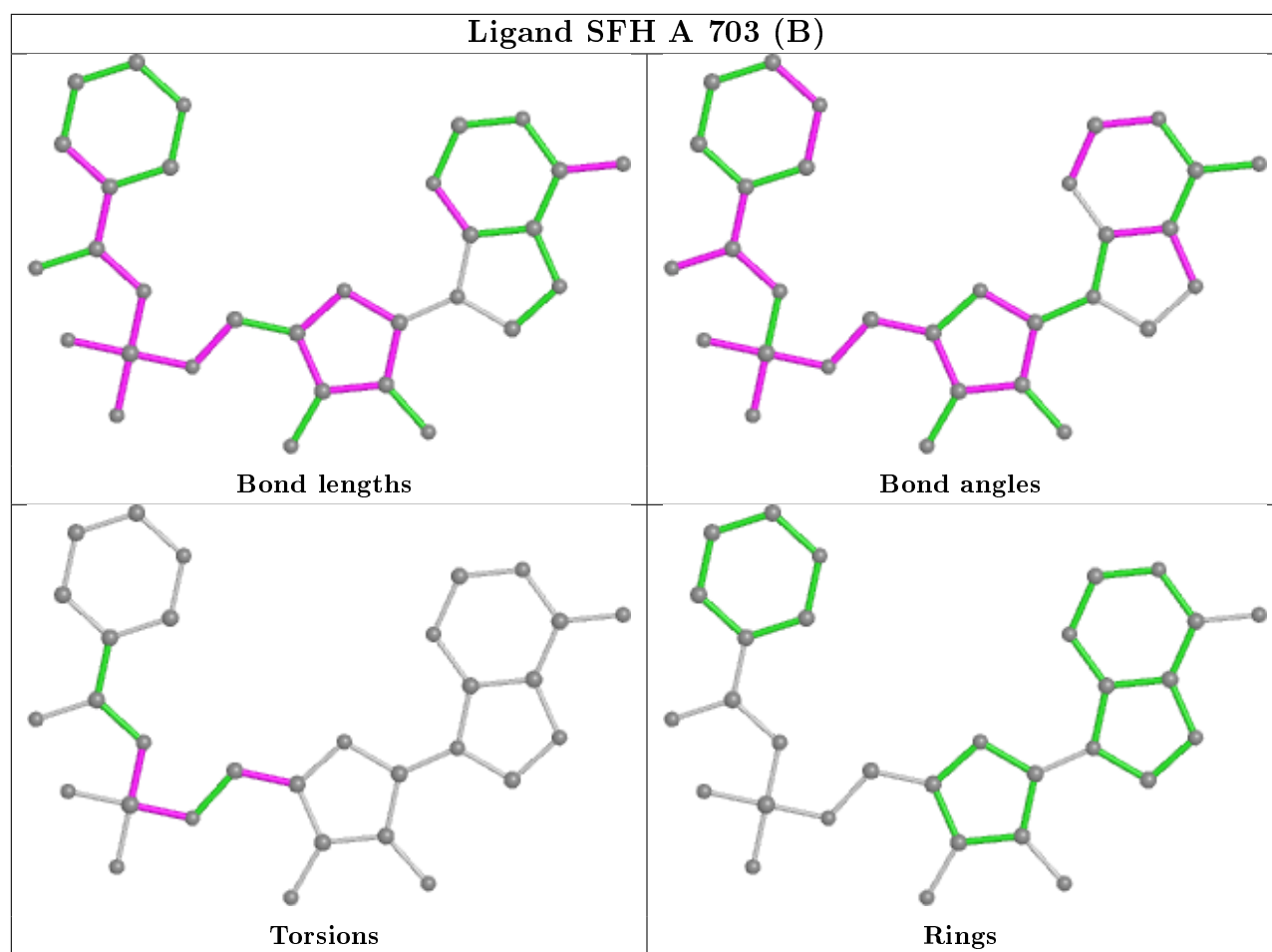




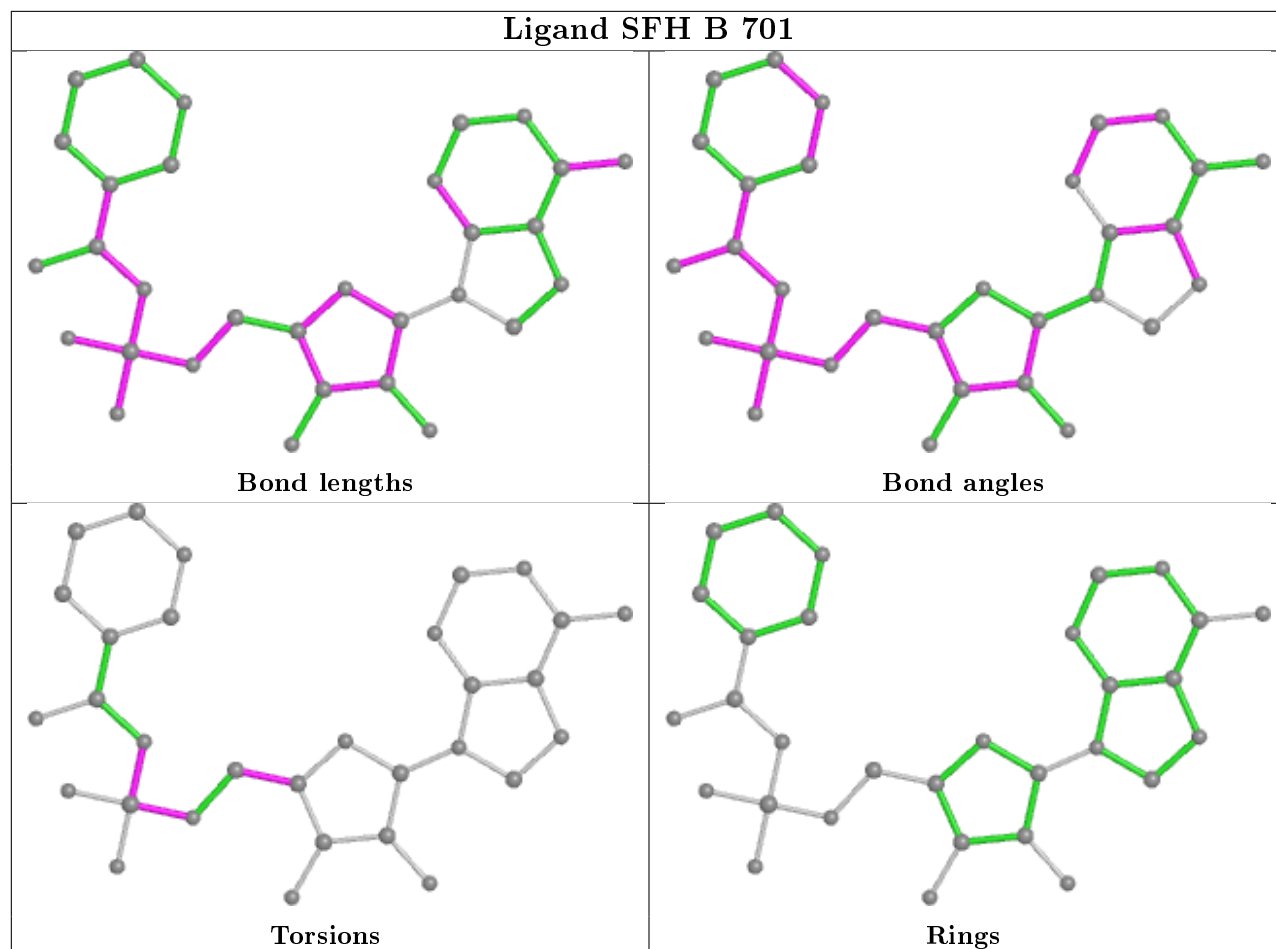


## Ligand SFH D 701

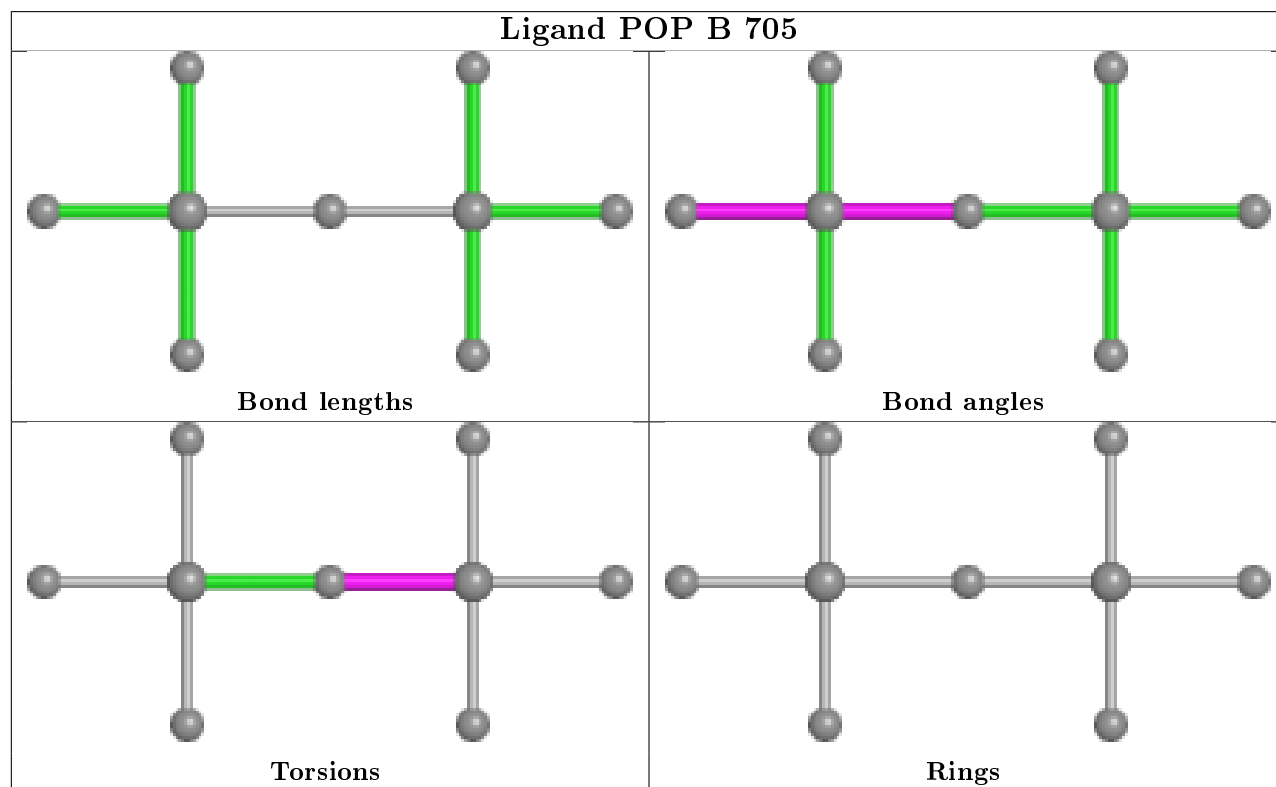




## Ligand SFH B 701



## Ligand POP B 705



## 5.7 Other polymers

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<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	660/679 (97%)	0.30	23 (3%)	44 23	35, 53, 75, 121	0
1	B	669/679 (98%)	0.33	28 (4%)	36 18	35, 49, 74, 107	0
1	C	665/679 (97%)	0.18	11 (1%)	70 51	32, 46, 66, 88	0
1	D	661/679 (97%)	0.35	27 (4%)	37 19	32, 50, 72, 106	0
All	All	2655/2716 (97%)	0.29	89 (3%)	45 24	32, 50, 72, 121	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	550	GLY	5.6
1	B	404	THR	4.7
1	D	676	VAL	4.6
1	B	548	PRO	4.3
1	D	449	VAL	3.9
1	D	84	SER	3.9
1	D	334	GLN	3.6
1	B	405	GLY	3.6
1	A	405	GLY	3.4
1	B	94	GLY	3.4
1	D	672	ILE	3.4
1	B	561	VAL	3.3
1	D	677	PRO	3.3
1	D	309	ALA	3.1
1	B	546	LEU	3.0
1	A	596	GLU	3.0
1	A	441	HIS	2.9
1	B	619	HIS	2.9
1	D	616	GLU	2.9
1	C	427	ASP	2.9
1	B	389	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	671	GLN	2.7
1	C	447	GLU	2.7
1	B	473	ARG	2.7
1	B	360	TYR	2.7
1	B	552	GLU	2.7
1	B	570	SER	2.7
1	D	522	SER	2.6
1	C	581	PRO	2.6
1	A	389	ARG	2.6
1	D	386	ARG	2.6
1	D	427	ASP	2.6
1	B	549	THR	2.6
1	B	403	ALA	2.6
1	A	315	GLY	2.6
1	A	673	ASP	2.5
1	B	408	THR	2.5
1	D	623	ILE	2.5
1	C	613	SER	2.5
1	C	450	TYR	2.5
1	C	311	ASP	2.5
1	B	358	LEU	2.5
1	B	454	PHE	2.4
1	C	567	GLN	2.4
1	C	449	VAL	2.4
1	A	490	TRP	2.4
1	A	435	MET	2.4
1	B	678	LYS	2.4
1	D	528	GLU	2.4
1	A	316	ASP	2.3
1	A	404	THR	2.3
1	A	670	ASP	2.3
1	A	565	ALA	2.3
1	C	44	GLY	2.2
1	A	408	THR	2.2
1	A	556	SER	2.2
1	D	86	ASP	2.2
1	D	313	PRO	2.2
1	D	150	GLY	2.2
1	B	418	ALA	2.2
1	B	673	ASP	2.2
1	D	607	SER	2.2
1	B	551	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	360	TYR	2.2
1	B	594	ASP	2.2
1	D	526	PHE	2.2
1	A	679	GLY	2.2
1	A	359	ASP	2.1
1	A	87	LEU	2.1
1	D	451	ASP	2.1
1	D	85	ALA	2.1
1	A	472	GLN	2.1
1	A	407	HIS	2.1
1	B	407	HIS	2.1
1	D	82	THR	2.1
1	B	677	PRO	2.1
1	D	388	GLY	2.1
1	A	559	ALA	2.1
1	B	95	ALA	2.1
1	D	507	GLY	2.1
1	B	528	GLU	2.1
1	D	311	ASP	2.0
1	C	261	GLU	2.0
1	C	596	GLU	2.0
1	B	547	ILE	2.0
1	D	585	ALA	2.0
1	D	624	PHE	2.0
1	A	558	GLU	2.0
1	A	309	ALA	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.

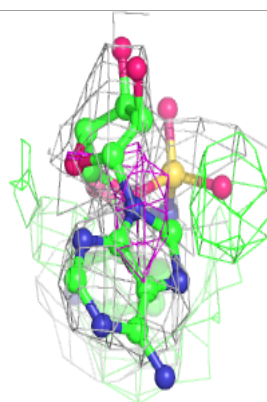
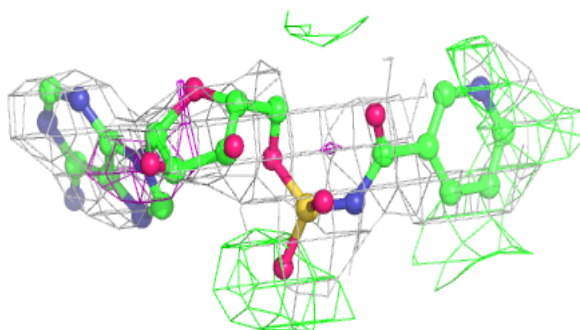
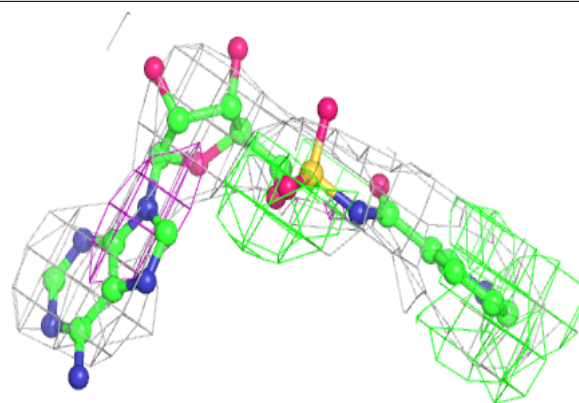
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SFH	A	703[A]	31/31	0.53	0.50	64,74,87,89	31
2	SFH	A	703[B]	31/31	0.53	0.50	64,74,84,87	31
5	GLN	D	703	10/10	0.62	0.53	63,74,82,95	0
4	POP	B	705	9/9	0.68	0.45	55,62,69,72	9
5	GLN	B	706	10/10	0.75	0.58	51,55,62,69	0
3	CL	A	704	1/1	0.75	0.89	80,80,80,80	0
2	SFH	A	702	31/31	0.76	0.47	58,76,93,96	0
2	SFH	B	702	31/31	0.79	0.45	49,72,89,90	0
6	GOL	B	707	6/6	0.79	0.31	46,48,53,55	0
5	GLN	C	702	10/10	0.80	0.41	50,56,70,83	0
2	SFH	B	703	31/31	0.80	0.32	53,68,96,103	0
2	SFH	A	701	31/31	0.80	0.33	60,67,73,87	0
2	SFH	D	701	31/31	0.82	0.30	51,61,88,91	0
6	GOL	D	704	6/6	0.82	0.29	42,45,50,50	0
3	CL	A	705	1/1	0.86	0.31	60,60,60,60	0
3	CL	B	704	1/1	0.87	0.78	64,64,64,64	0
2	SFH	B	701	31/31	0.88	0.25	54,57,67,72	0
2	SFH	C	701	31/31	0.89	0.26	41,51,74,76	0
3	CL	D	702	1/1	0.93	0.56	63,63,63,63	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.

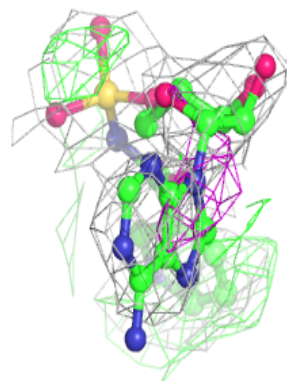
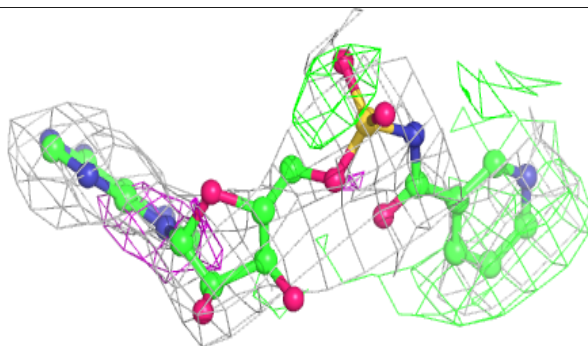
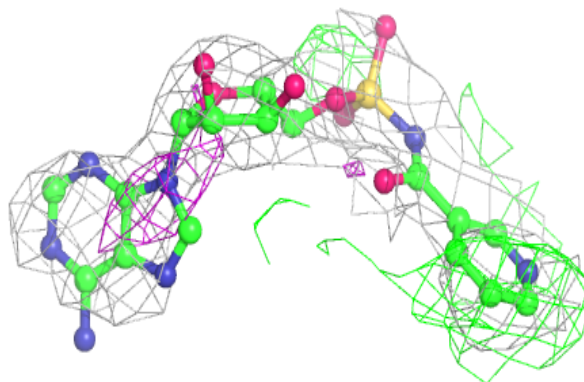


**Electron density around SFH A 703 (A):**

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

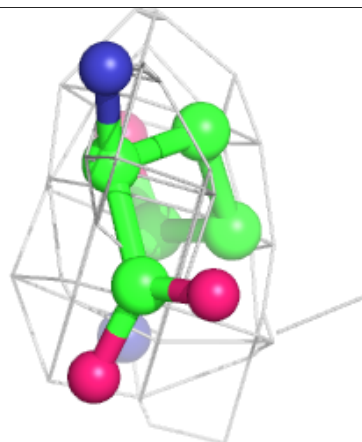
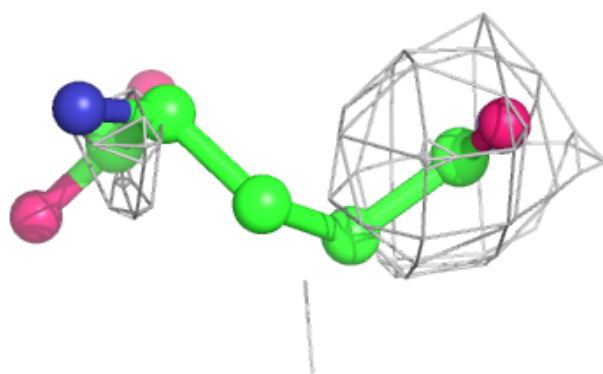
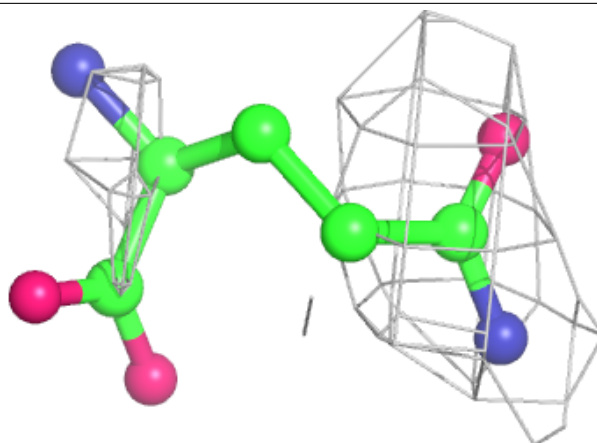
**Electron density around SFH A 703 (B):**

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

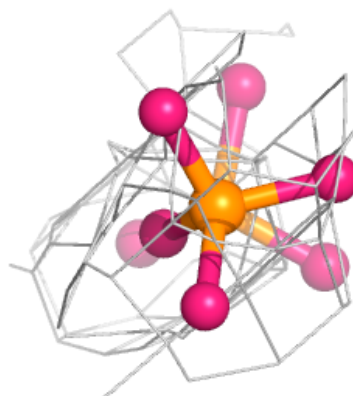
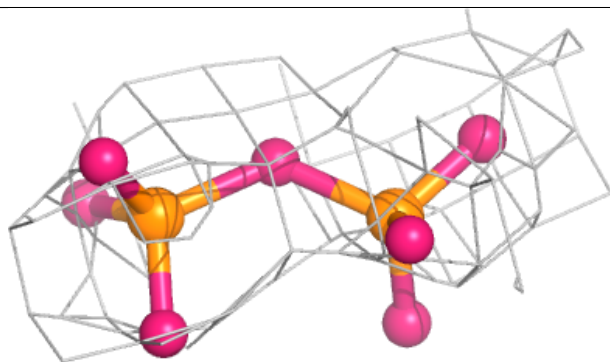
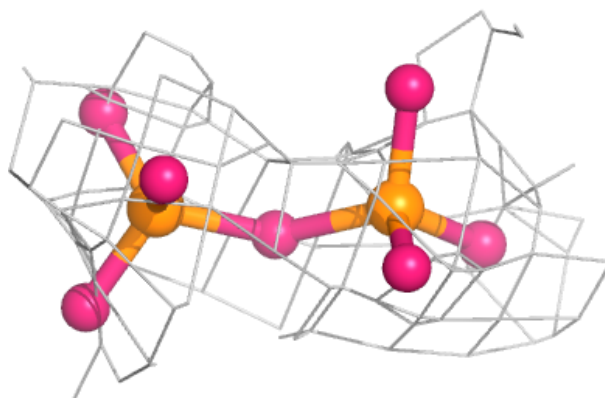


**Electron density around GLN D 703:**

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

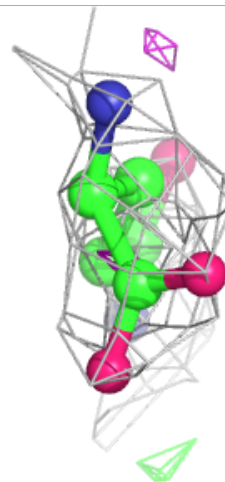
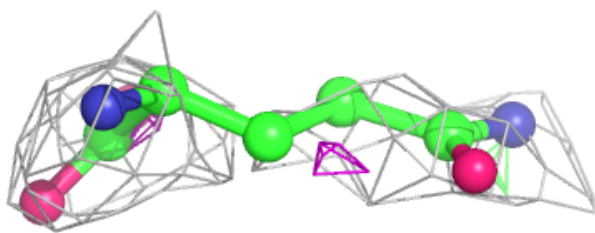
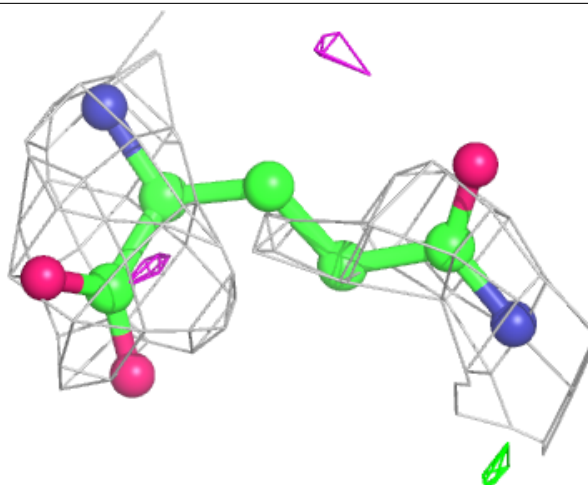
**Electron density around POP B 705:**

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



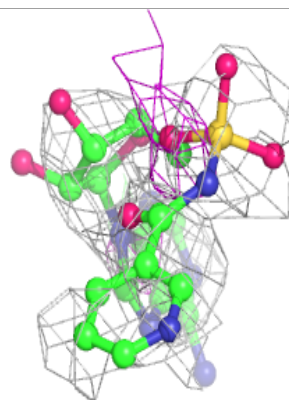
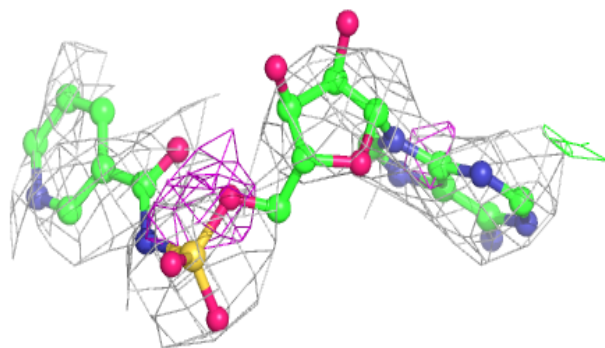
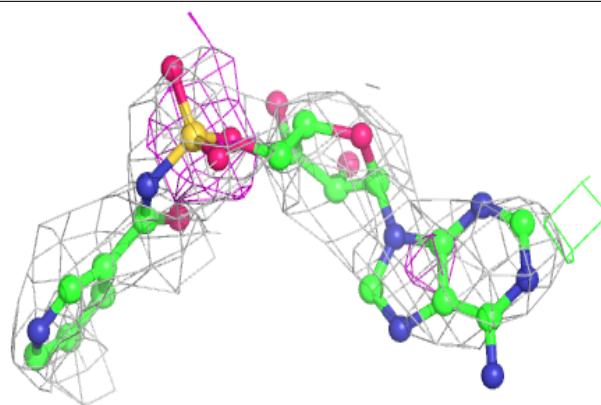
**Electron density around GLN B 706:**

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

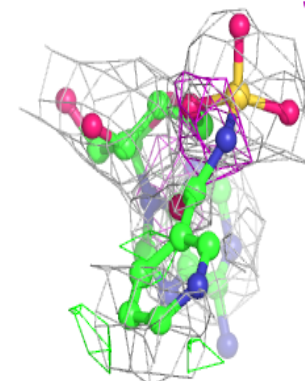
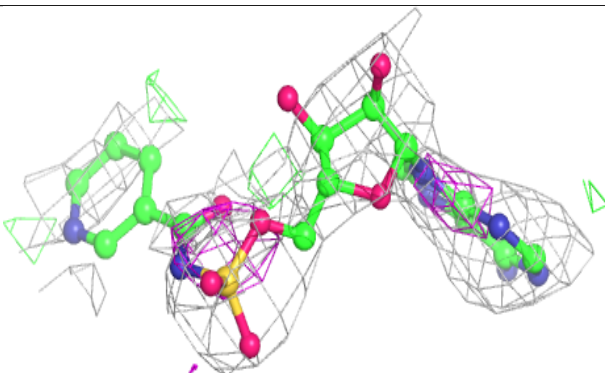
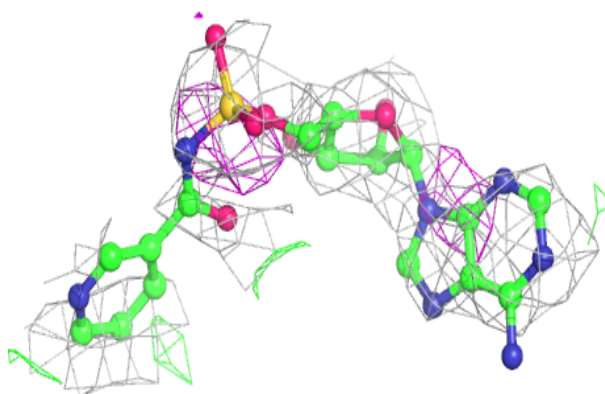


**Electron density around SFH A 702:**

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

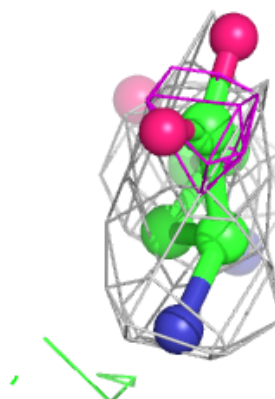
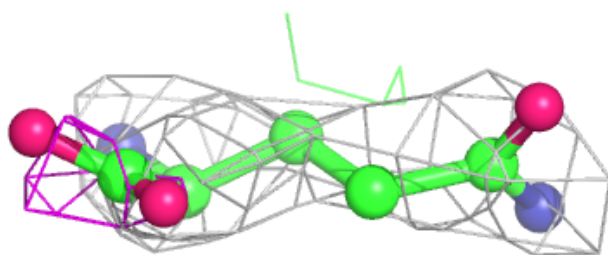
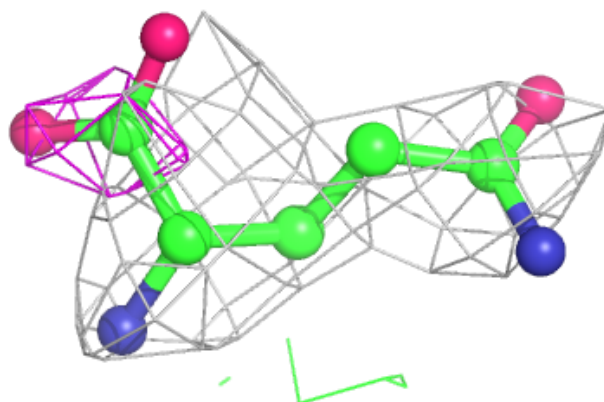
**Electron density around SFH B 702:**

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

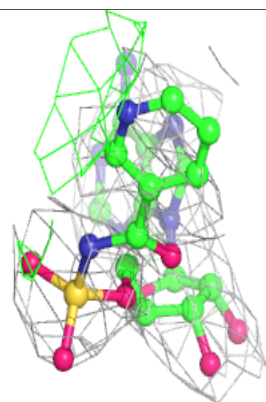
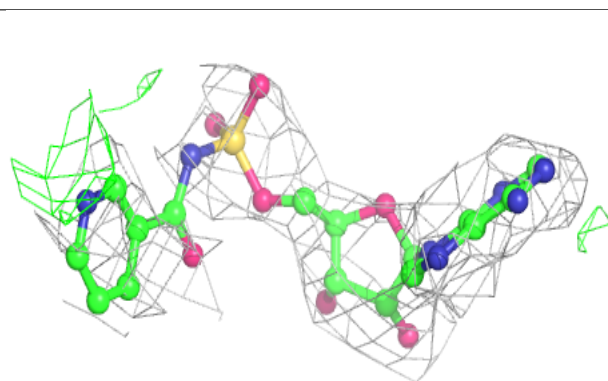
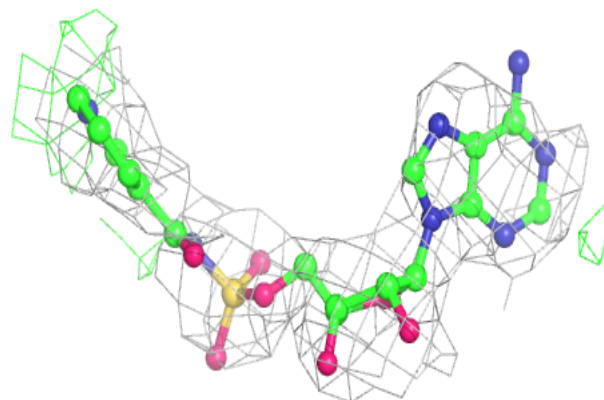


**Electron density around GLN C 702:**

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

**Electron density around SFH B 703:**

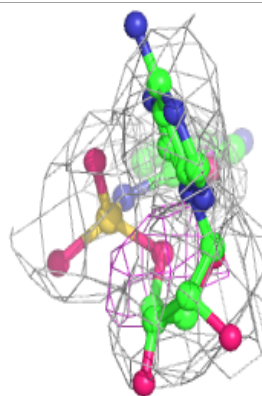
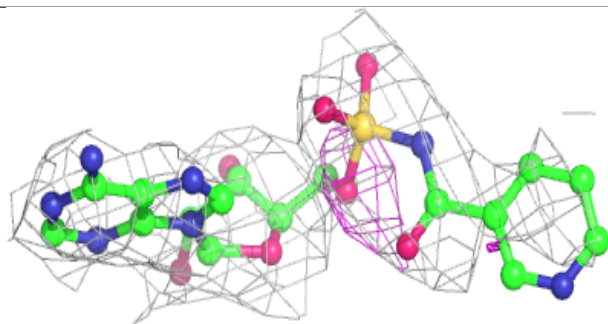
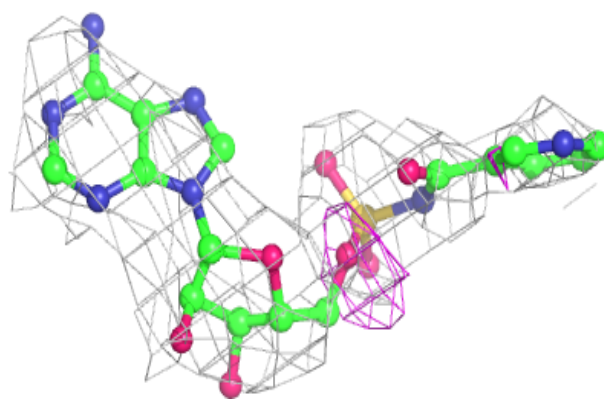
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



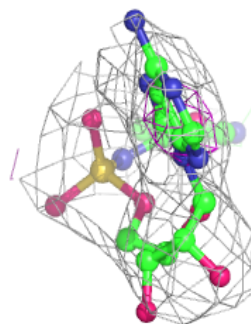
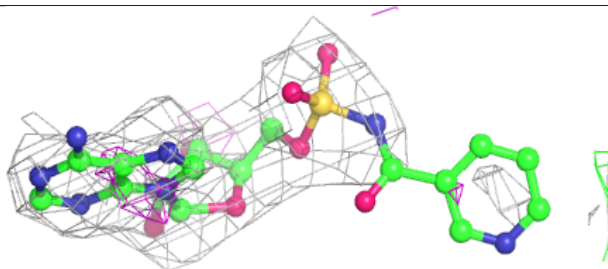
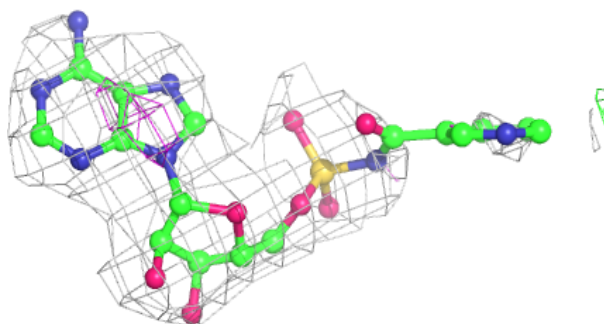


**Electron density around SFH A 701:**

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

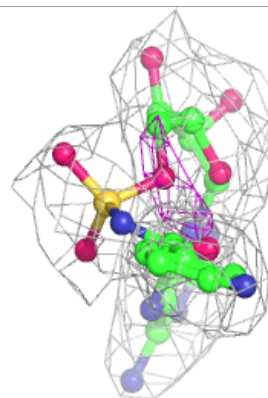
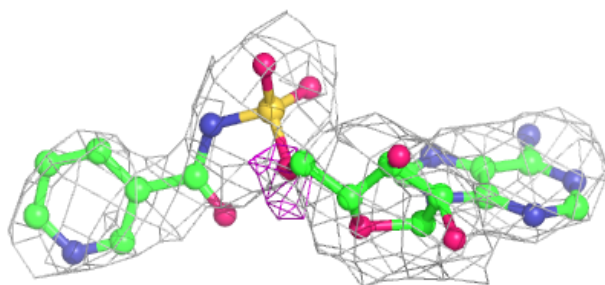
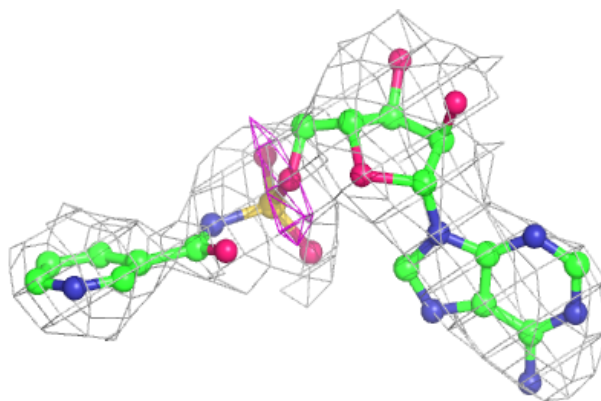
**Electron density around SFH D 701:**

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

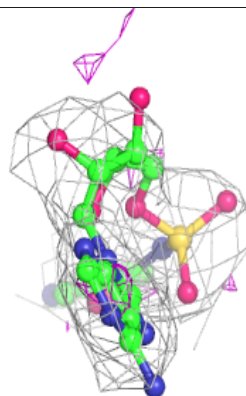
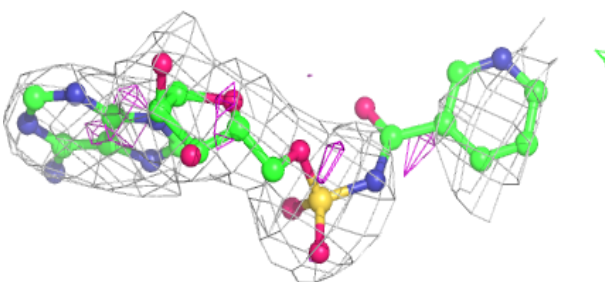
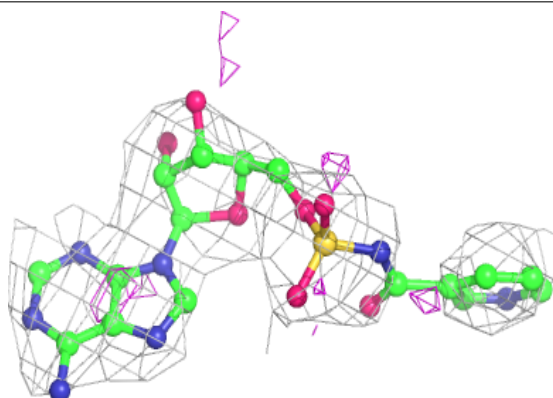


**Electron density around SFH B 701:**

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

**Electron density around SFH C 701:**

$2mF_o - DF_c$  (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.