



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2024 – 02:25 PM EST

PDB ID : 8TC8  
Title : Human asparaginyl-tRNA synthetase bound to adenosine 5'-sulfamate  
Authors : Dogovski, C.; Metcalfe, R.D.; Xie, S.C.; Morton, C.J.; Tilley, L.; Griffin, M.D.W.  
Deposited on : 2023-06-30  
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

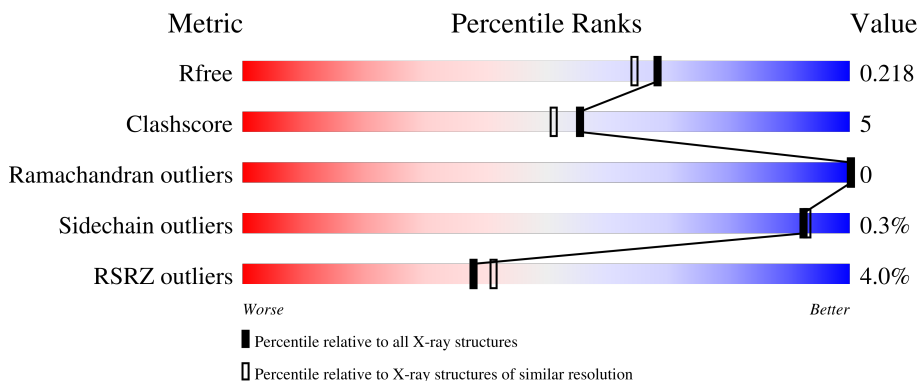
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	 2% 70% 9% 21%
1	B	548	 2% 70% 9% 21%
1	C	548	 5% 72% 7% 21%
1	D	548	 4% 72% 8% 21%

## 2 Entry composition [i](#)

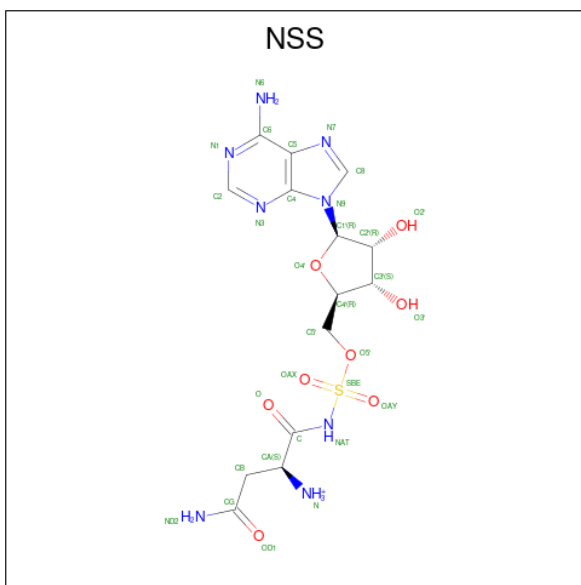
There are 5 unique types of molecules in this entry. The entry contains 15900 atoms, of which 80 are hydrogens and 0 are deuteriums.

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 Asparagine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	435	Total 3508	C 2230	N 604	O 648	S 26	0	0	0
1	B	433	Total 3491	C 2221	N 601	O 643	S 26	0	0	0
1	C	434	Total 3504	C 2228	N 603	O 647	S 26	0	0	0
1	D	434	Total 3504	C 2228	N 603	O 647	S 26	0	0	0

- Molecule 2 is 5'-O-[N-(L-ASPARAGINYL)SULFAMOYL]ADENOSINE (three-letter code: NSS) (formula: C<sub>14</sub>H<sub>21</sub>N<sub>8</sub>O<sub>8</sub>S) (labeled as "Ligand of Interest" by depositor).



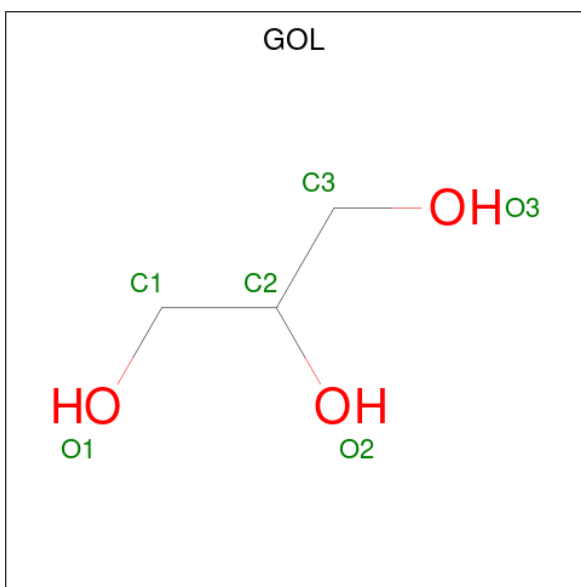
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
2	A	1	Total 51	C 14	H 20	N 8	O 8	S 1	0	0
2	B	1	Total 51	C 14	H 20	N 8	O 8	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	C	1	Total	C	H	N	O	S	0	0
			51	14	20	8	8	1		
2	D	1	Total	C	H	N	O	S	0	0
			51	14	20	8	8	1		

- Molecule 3 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
3	A	1	Total	C O	0	0
			6	3 3		
3	A	1	Total	C O	0	0
			6	3 3		
3	A	1	Total	C O	0	0
			6	3 3		
3	A	1	Total	C O	0	0
			6	3 3		
3	A	1	Total	C O	0	0
			6	3 3		
3	A	1	Total	C O	0	0
			6	3 3		
3	B	1	Total	C O	0	0
			6	3 3		
3	B	1	Total	C O	0	0
			6	3 3		
3	B	1	Total	C O	0	0
			6	3 3		

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	423	Total O 423 423	0	0
5	B	459	Total O 459 459	0	0
5	C	330	Total O 330 330	0	0
5	D	377	Total O 377 377	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.85Å 126.28Å 160.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 1.90 49.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-1.90) 99.7 (49.29-1.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.181 , 0.217 0.182 , 0.218	Depositor DCC
$R_{free}$ test set	9326 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtrriage
Anisotropy	0.496	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.57 % 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 9.7419e-05. 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, NSS, NA

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	0.42	0/3593	0.62	0/4861
1	B	0.42	0/3576	0.61	0/4839
1	C	0.39	0/3589	0.59	0/4857
1	D	0.39	0/3589	0.60	0/4857
All	All	0.40	0/14347	0.61	0/19414

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	3508	0	3433	38	0
1	B	3491	0	3420	42	0
1	C	3504	0	3429	34	0
1	D	3504	0	3429	36	0
2	A	31	20	20	0	0
2	B	31	20	20	1	0
2	C	31	20	20	0	0
2	D	31	20	20	0	0
3	A	36	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	36	0	46	4	0
3	C	12	0	16	0	0
3	D	12	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	423	0	0	13	1
5	B	459	0	0	10	0
5	C	330	0	0	9	1
5	D	377	0	0	9	0
All	All	15820	80	13915	143	1

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 5.

All (143) 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:C:189:PRO:HG2	1:C:192:LYS:HD2	1.57	0.86
1:B:292:GLU:OE1	5:B:701:HOH:O	1.93	0.86
1:A:534:ARG:NH1	5:A:703:HOH:O	2.12	0.83
1:B:451:ARG:NE	5:B:704:HOH:O	2.12	0.82
3:A:606:GOL:O2	5:A:701:HOH:O	1.98	0.82
1:A:129:LYS:NZ	5:A:705:HOH:O	2.14	0.80
1:B:109:LEU:HB3	1:B:110:PRO:HD2	1.65	0.77
1:D:535:ASP:OD2	5:D:701:HOH:O	2.02	0.77
1:C:535:ASP:OD2	5:C:701:HOH:O	2.01	0.77
1:A:408:GLU:OE1	5:A:702:HOH:O	2.03	0.76
1:D:167:CYS:SG	5:D:1025:HOH:O	2.45	0.74
1:B:534:ARG:NH1	5:B:706:HOH:O	2.16	0.72
1:B:324:GLU:OE2	5:B:702:HOH:O	2.07	0.70
1:A:163:GLU:HG3	5:A:707:HOH:O	1.91	0.70
1:D:143:ASN:OD1	1:D:166:GLN:NE2	2.24	0.70
1:C:534:ARG:NH1	5:C:703:HOH:O	2.21	0.70
1:B:288:ASP:OD1	5:B:703:HOH:O	2.10	0.70
1:C:188:THR:HB	1:C:192:LYS:HD3	1.75	0.69
1:B:213:ALA:H	3:B:602:GOL:H12	1.56	0.69
1:C:414:GLU:O	1:C:417:GLU:HG2	1.93	0.68
1:D:414:GLU:O	1:D:417:GLU:HG2	1.94	0.67
1:C:189:PRO:HG2	1:C:192:LYS:CD	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:GLU:OE2	5:B:705:HOH:O	2.13	0.66
1:D:406:LYS:HD2	1:D:410:GLY:O	1.96	0.66
1:A:535:ASP:OD2	5:A:704:HOH:O	2.14	0.65
1:A:382:GLN:HB2	5:A:930:HOH:O	1.96	0.65
1:C:109:LEU:HB3	1:C:110:PRO:HD2	1.77	0.65
1:A:324:GLU:OE2	5:A:706:HOH:O	2.15	0.65
1:A:143:ASN:OD1	1:A:166:GLN:NE2	2.31	0.64
1:C:324:GLU:OE2	5:C:702:HOH:O	2.14	0.64
1:D:224:SER:HB2	5:D:817:HOH:O	1.98	0.63
1:B:521:GLU:O	1:B:525:THR:HG23	1.98	0.62
1:A:433:GLU:HG2	5:A:726:HOH:O	2.00	0.61
1:B:433:GLU:HG2	5:B:736:HOH:O	2.00	0.61
1:A:414:GLU:O	1:A:417:GLU:HG2	2.00	0.61
1:D:521:GLU:O	1:D:525:THR:HG23	2.01	0.60
1:D:111:GLU:O	1:D:111:GLU:HG2	2.03	0.59
1:D:471:GLU:OE1	3:D:603:GOL:H12	2.02	0.59
1:B:414:GLU:O	1:B:417:GLU:HG2	2.03	0.59
1:B:421:GLU:O	1:B:425:ARG:HG3	2.02	0.59
1:A:253:THR:HB	5:A:868:HOH:O	2.03	0.58
1:B:472:ILE:HG13	1:B:473:VAL:HG23	1.84	0.58
1:B:481:ASP:OD1	5:B:707:HOH:O	2.17	0.58
1:C:109:LEU:HB3	1:C:110:PRO:CD	2.33	0.58
1:D:534:ARG:NH1	5:D:704:HOH:O	2.30	0.58
1:C:189:PRO:CG	1:C:192:LYS:HD2	2.31	0.56
1:A:521:GLU:O	1:A:525:THR:HG23	2.05	0.56
1:B:275:GLN:HE22	1:B:292:GLU:CD	2.09	0.56
1:D:433:GLU:HG2	5:D:714:HOH:O	2.06	0.56
1:B:390:ARG:NE	5:B:708:HOH:O	2.20	0.55
1:D:539:TYR:CD1	1:D:548:PRO:HG2	2.42	0.55
1:A:547:THR:HG23	1:D:275:GLN:OE1	2.08	0.54
1:C:109:LEU:N	5:C:706:HOH:O	2.39	0.54
1:C:433:GLU:HG2	5:C:734:HOH:O	2.06	0.54
1:C:375:HIS:HE1	5:C:769:HOH:O	1.91	0.54
1:B:275:GLN:OE1	1:C:547:THR:HG23	2.09	0.53
1:D:109:LEU:HB3	1:D:110:PRO:HD2	1.90	0.52
1:C:414:GLU:N	1:C:417:GLU:OE2	2.35	0.52
1:D:472:ILE:HG13	1:D:473:VAL:HG23	1.91	0.52
1:B:409:ASP:OD1	1:B:411:THR:HG23	2.10	0.52
1:D:375:HIS:HD2	5:D:755:HOH:O	1.92	0.52
1:B:225:ASP:OD2	1:B:227:ASP:HB2	2.09	0.51
1:B:337:HIS:HE2	2:B:601:NSS:H5'1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASP:OD1	1:A:226:VAL:N	2.43	0.51
1:C:539:TYR:CD1	1:C:548:PRO:HG2	2.45	0.51
1:C:222:GLU:HG3	1:C:223:GLU:HG3	1.92	0.51
1:A:166:GLN:OE1	5:A:707:HOH:O	2.19	0.51
1:C:547:THR:HA	1:C:548:PRO:C	2.29	0.51
1:D:138:ARG:HD3	5:D:936:HOH:O	2.09	0.51
1:B:469:VAL:HG11	1:B:526:TRP:HB2	1.93	0.51
1:C:469:VAL:HG11	1:C:526:TRP:HB2	1.92	0.51
1:B:547:THR:HG23	1:C:275:GLN:OE1	2.11	0.50
1:D:138:ARG:NH2	5:D:705:HOH:O	2.38	0.50
1:B:452:CYS:HB3	1:B:454:GLU:OE2	2.11	0.50
1:D:109:LEU:HB3	1:D:110:PRO:CD	2.42	0.50
1:B:358:VAL:HG11	1:B:466:MET:CE	2.42	0.49
1:D:547:THR:HA	1:D:548:PRO:C	2.32	0.49
1:A:548:PRO:HB3	1:D:501:TRP:CD1	2.48	0.49
1:A:138:ARG:NH2	1:A:140:GLN:OE1	2.46	0.48
1:C:138:ARG:NH2	1:C:140:GLN:OE1	2.46	0.48
1:C:532:HIS:ND1	1:C:534:ARG:HG2	2.29	0.48
1:A:408:GLU:HB3	5:A:702:HOH:O	2.14	0.48
1:B:213:ALA:N	3:B:602:GOL:H12	2.24	0.48
1:C:472:ILE:HG13	1:C:473:VAL:HG23	1.95	0.48
1:A:172:LEU:O	3:A:603:GOL:H11	2.13	0.48
1:A:110:PRO:O	1:A:127:ARG:NH1	2.46	0.47
1:B:439:ARG:HA	1:B:459:THR:O	2.14	0.47
1:A:421:GLU:O	1:A:425:ARG:HG3	2.14	0.47
1:A:439:ARG:HA	1:A:459:THR:O	2.14	0.47
1:D:439:ARG:HA	1:D:459:THR:O	2.15	0.47
1:A:220:ILE:HG22	1:A:220:ILE:O	2.14	0.47
1:C:439:ARG:HA	1:C:459:THR:O	2.14	0.47
1:B:253:THR:HG21	5:C:893:HOH:O	2.15	0.47
1:A:415:PHE:CG	3:A:602:GOL:H32	2.50	0.46
1:C:371:GLY:O	1:C:375:HIS:ND1	2.49	0.46
1:B:213:ALA:HB2	3:B:602:GOL:H2	1.98	0.46
1:B:547:THR:HG22	5:C:908:HOH:O	2.15	0.45
1:B:547:THR:HA	1:B:548:PRO:C	2.36	0.45
1:C:355:GLU:OE2	1:C:387:PRO:HA	2.17	0.45
1:C:189:PRO:HD2	1:C:192:LYS:CD	2.46	0.45
1:D:525:THR:HG21	1:D:533:ILE:HA	1.98	0.45
1:A:547:THR:HA	1:A:548:PRO:C	2.37	0.44
1:D:137:LEU:C	1:D:137:LEU:HD23	2.37	0.44
1:D:414:GLU:N	1:D:417:GLU:OE2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:PRO:HD2	1:D:444:ILE:HD11	1.98	0.44
1:C:137:LEU:C	1:C:137:LEU:HD23	2.38	0.44
1:B:168:TYR:CZ	1:B:172:LEU:HD11	2.53	0.44
1:B:190:LYS:H	1:B:190:LYS:HG2	1.41	0.44
1:B:109:LEU:HB3	1:B:110:PRO:CD	2.42	0.44
1:A:115:VAL:HG12	1:A:116:LYS:O	2.18	0.43
1:B:452:CYS:HB3	1:B:454:GLU:CD	2.38	0.43
1:B:548:PRO:HB3	1:C:501:TRP:CD1	2.54	0.43
1:A:124:ARG:NH2	1:A:196:GLY:O	2.50	0.43
1:A:375:HIS:HB2	5:A:1030:HOH:O	2.18	0.43
1:D:110:PRO:O	1:D:127:ARG:NH1	2.47	0.43
1:D:355:GLU:OE2	1:D:387:PRO:HA	2.19	0.43
1:C:443:GLU:HB2	5:C:950:HOH:O	2.19	0.43
1:D:532:HIS:ND1	1:D:534:ARG:HG2	2.34	0.43
1:B:138:ARG:NH2	1:B:140:GLN:OE1	2.51	0.42
1:A:472:ILE:HG13	1:A:473:VAL:HG23	2.02	0.42
1:A:525:THR:HG21	1:A:533:ILE:HA	2.01	0.42
1:C:406:LYS:HD2	1:C:410:GLY:O	2.19	0.42
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.89	0.42
1:B:503:THR:HG22	1:B:507:LYS:HE3	2.02	0.42
1:A:308:LEU:HB2	1:A:309:PRO:HD3	2.02	0.42
1:A:275:GLN:OE1	1:D:547:THR:HG23	2.20	0.41
1:B:303:TYR:OH	1:C:548:PRO:O	2.31	0.41
1:D:497:THR:HB	1:D:498:PRO:HD3	2.01	0.41
1:B:241:ASN:O	1:B:244:LYS:HG2	2.20	0.41
1:D:443:GLU:OE1	1:D:443:GLU:N	2.52	0.41
1:A:383:PRO:HA	1:A:384:PRO:HD3	1.92	0.41
1:B:383:PRO:HA	1:B:384:PRO:HD3	1.90	0.41
3:B:605:GOL:H32	5:B:1067:HOH:O	2.20	0.41
1:D:525:THR:CG2	1:D:533:ILE:HA	2.50	0.41
1:A:451:ARG:NH1	1:A:456:SER:O	2.47	0.40
1:A:480:PHE:HB2	1:A:510:THR:OG1	2.20	0.40
1:A:275:GLN:HE22	1:A:292:GLU:CD	2.25	0.40
1:B:137:LEU:C	1:B:137:LEU:HD23	2.41	0.40
1:B:501:TRP:CD1	1:C:548:PRO:HB3	2.56	0.40
1:C:441:PRO:HD2	1:C:444:ILE:HD11	2.04	0.40
1:D:469:VAL:HG11	1:D:526:TRP:HB2	2.03	0.40
1:A:501:TRP:CD1	1:D:548:PRO:HB3	2.57	0.40
1:D:375:HIS:CD2	5:D:755:HOH:O	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:963:HOH:O	5:C:929:HOH:O[4_455]	2.14	0.06

### 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	431/548 (79%)	415 (96%)	16 (4%)	0	100	100
1	B	429/548 (78%)	413 (96%)	16 (4%)	0	100	100
1	C	430/548 (78%)	415 (96%)	15 (4%)	0	100	100
1	D	430/548 (78%)	412 (96%)	18 (4%)	0	100	100
All	All	1720/2192 (78%)	1655 (96%)	65 (4%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/485 (79%)	382 (100%)	1 (0%)	92	93
1	B	381/485 (79%)	380 (100%)	1 (0%)	92	93
1	C	383/485 (79%)	382 (100%)	1 (0%)	92	93
1	D	383/485 (79%)	382 (100%)	1 (0%)	92	93
All	All	1530/1940 (79%)	1526 (100%)	4 (0%)	92	93

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

Mol	Chain	Res	Type
1	A	198	HIS
1	B	190	LYS
1	C	198	HIS
1	D	182	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	$\# Z  > 2$
2	NSS	D	601	4	29,33,33	4.18	14 (48%)	32,49,49	2.32	8 (25%)
3	GOL	A	604	4	5,5,5	1.17	0	5,5,5	1.06	0
3	GOL	B	603	-	5,5,5	0.89	0	5,5,5	1.11	0
3	GOL	B	602	-	5,5,5	0.98	0	5,5,5	1.34	1 (20%)
3	GOL	D	602	-	5,5,5	1.01	0	5,5,5	0.94	0
3	GOL	A	603	-	5,5,5	0.95	0	5,5,5	1.32	0
3	GOL	C	603	4	5,5,5	1.10	0	5,5,5	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	604	-	5,5,5	1.09	0	5,5,5	1.02	0
3	GOL	B	605	4	5,5,5	1.19	0	5,5,5	1.19	1 (20%)
2	NSS	B	601	4	29,33,33	3.89	13 (44%)	32,49,49	2.57	11 (34%)
3	GOL	A	607	-	5,5,5	0.86	0	5,5,5	0.89	0
2	NSS	C	601	4	29,33,33	4.28	14 (48%)	32,49,49	2.07	7 (21%)
3	GOL	A	605	-	5,5,5	0.63	0	5,5,5	1.28	1 (20%)
3	GOL	A	602	-	5,5,5	1.40	1 (20%)	5,5,5	1.05	0
3	GOL	C	602	-	5,5,5	0.83	0	5,5,5	1.07	0
3	GOL	D	603	4	5,5,5	0.95	0	5,5,5	1.32	0
2	NSS	A	601	4	29,33,33	3.97	13 (44%)	32,49,49	2.48	11 (34%)
3	GOL	B	606	-	5,5,5	1.10	0	5,5,5	0.78	0
3	GOL	A	606	-	5,5,5	1.01	0	5,5,5	0.87	0
3	GOL	B	607	-	5,5,5	0.76	0	5,5,5	1.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NSS	D	601	4	-	0/18/39/39	0/3/3/3
3	GOL	A	604	4	-	0/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	D	602	-	-	4/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	C	603	4	-	0/4/4/4	-
3	GOL	B	604	-	-	0/4/4/4	-
3	GOL	B	605	4	-	2/4/4/4	-
2	NSS	B	601	4	-	0/18/39/39	0/3/3/3
3	GOL	A	607	-	-	4/4/4/4	-
2	NSS	C	601	4	-	0/18/39/39	0/3/3/3
3	GOL	A	605	-	-	1/4/4/4	-
3	GOL	A	602	-	-	4/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
3	GOL	D	603	4	-	4/4/4/4	-
2	NSS	A	601	4	-	0/18/39/39	0/3/3/3
3	GOL	B	606	-	-	2/4/4/4	-
3	GOL	A	606	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	607	-	-	2/4/4/4	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NSS	OAY-SBE	9.71	1.50	1.42
2	C	601	NSS	OAX-SBE	9.57	1.50	1.42
2	C	601	NSS	OAY-SBE	9.55	1.50	1.42
2	D	601	NSS	OAY-SBE	9.39	1.50	1.42
2	D	601	NSS	OAX-SBE	9.31	1.50	1.42
2	C	601	NSS	C2'-C1'	9.22	1.67	1.53
2	D	601	NSS	C2'-C1'	9.16	1.67	1.53
2	A	601	NSS	C2'-C3'	-9.07	1.28	1.53
2	C	601	NSS	C2'-C3'	-9.06	1.28	1.53
2	A	601	NSS	C2'-C1'	8.98	1.67	1.53
2	D	601	NSS	C2'-C3'	-8.96	1.28	1.53
2	B	601	NSS	C2'-C3'	-8.95	1.28	1.53
2	B	601	NSS	OAX-SBE	8.84	1.49	1.42
2	B	601	NSS	C2'-C1'	8.64	1.66	1.53
2	A	601	NSS	OAX-SBE	8.42	1.49	1.42
2	B	601	NSS	OAY-SBE	8.28	1.49	1.42
2	C	601	NSS	O4'-C1'	-6.80	1.31	1.41
2	D	601	NSS	O4'-C1'	-6.48	1.32	1.41
2	C	601	NSS	SBE-NAT	5.14	1.69	1.59
2	B	601	NSS	O4'-C1'	-5.03	1.34	1.41
2	D	601	NSS	O4'-C4'	4.74	1.55	1.45
2	C	601	NSS	O4'-C4'	4.62	1.55	1.45
2	A	601	NSS	O4'-C1'	-4.45	1.34	1.41
2	B	601	NSS	SBE-NAT	4.31	1.67	1.59
2	D	601	NSS	SBE-NAT	4.18	1.67	1.59
2	A	601	NSS	SBE-NAT	4.13	1.67	1.59
2	D	601	NSS	C5'-C4'	-4.11	1.38	1.51
2	B	601	NSS	O4'-C4'	3.97	1.53	1.45
2	A	601	NSS	C5'-C4'	-3.90	1.39	1.51
2	C	601	NSS	C5'-C4'	-3.85	1.39	1.51
2	B	601	NSS	C5'-C4'	-3.84	1.39	1.51
2	A	601	NSS	CG-ND2	3.77	1.45	1.32
2	A	601	NSS	O4'-C4'	3.73	1.53	1.45
2	C	601	NSS	C-NAT	3.59	1.44	1.37
2	D	601	NSS	O5'-SBE	3.49	1.67	1.59
2	B	601	NSS	CG-ND2	3.49	1.44	1.32
2	C	601	NSS	CG-ND2	3.45	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NSS	CG-ND2	3.42	1.43	1.32
2	B	601	NSS	C-NAT	3.41	1.43	1.37
2	A	601	NSS	C-NAT	3.40	1.43	1.37
2	C	601	NSS	O5'-SBE	3.32	1.66	1.59
3	A	602	GOL	O2-C2	-2.95	1.34	1.43
2	D	601	NSS	C-NAT	2.90	1.43	1.37
2	B	601	NSS	C6-N6	2.88	1.44	1.34
2	A	601	NSS	C6-N6	2.86	1.44	1.34
2	D	601	NSS	C6-N6	2.81	1.44	1.34
2	C	601	NSS	C6-N6	2.79	1.44	1.34
2	C	601	NSS	O3'-C3'	2.74	1.49	1.43
2	B	601	NSS	O5'-SBE	2.70	1.65	1.59
2	A	601	NSS	O5'-SBE	2.57	1.65	1.59
2	B	601	NSS	O3'-C3'	2.31	1.48	1.43
2	A	601	NSS	O3'-C3'	2.29	1.48	1.43
2	D	601	NSS	O-C	-2.20	1.19	1.23
2	D	601	NSS	O3'-C3'	2.19	1.48	1.43
2	C	601	NSS	C3'-C4'	2.10	1.58	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NSS	OAY-SBE-OAX	-10.02	105.15	120.76
2	A	601	NSS	OAY-SBE-OAX	-9.55	105.88	120.76
2	D	601	NSS	OAY-SBE-OAX	-8.99	106.76	120.76
2	C	601	NSS	OAY-SBE-OAX	-7.36	109.29	120.76
2	B	601	NSS	N3-C2-N1	-4.98	120.89	128.68
2	C	601	NSS	N3-C2-N1	-4.80	121.17	128.68
2	A	601	NSS	N3-C2-N1	-4.73	121.28	128.68
2	D	601	NSS	N3-C2-N1	-4.51	121.63	128.68
2	A	601	NSS	CA-CB-CG	3.98	120.16	112.24
2	B	601	NSS	CA-CB-CG	3.62	119.43	112.24
2	D	601	NSS	C3'-C2'-C1'	3.60	106.40	100.98
2	B	601	NSS	C2'-C3'-C4'	3.40	109.25	102.64
2	C	601	NSS	C-NAT-SBE	-3.30	119.27	124.61
2	C	601	NSS	C3'-C2'-C1'	3.20	105.80	100.98
2	D	601	NSS	CB-CA-C	-3.04	102.01	109.09
2	B	601	NSS	C-NAT-SBE	-3.01	119.73	124.61
2	A	601	NSS	C-NAT-SBE	-2.91	119.89	124.61
2	D	601	NSS	C-NAT-SBE	-2.86	119.98	124.61
2	A	601	NSS	CB-CA-C	-2.85	102.44	109.09
2	B	601	NSS	O4'-C4'-C3'	-2.71	99.75	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NSS	O5'-SBE-OAY	2.69	113.81	105.59
2	A	601	NSS	C2'-C3'-C4'	2.68	107.84	102.64
2	A	601	NSS	O2'-C2'-C1'	-2.63	101.13	110.85
2	B	601	NSS	CB-CA-C	-2.58	103.07	109.09
2	C	601	NSS	CB-CA-C	-2.47	103.33	109.09
2	B	601	NSS	O2'-C2'-C1'	-2.46	101.77	110.85
2	D	601	NSS	O2'-C2'-C1'	-2.43	101.87	110.85
2	B	601	NSS	O2'-C2'-C3'	2.36	119.45	111.82
2	B	601	NSS	O-C-CA	2.27	124.98	120.18
3	A	605	GOL	C3-C2-C1	-2.22	103.08	111.70
2	A	601	NSS	O2'-C2'-C3'	2.18	118.88	111.82
2	B	601	NSS	O5'-SBE-OAY	2.17	112.21	105.59
2	C	601	NSS	O5'-C5'-C4'	2.14	111.62	107.62
2	D	601	NSS	O5'-SBE-OAY	2.07	111.90	105.59
3	B	602	GOL	C3-C2-C1	-2.05	103.73	111.70
2	A	601	NSS	C4-C5-N7	-2.05	107.26	109.40
3	B	605	GOL	C3-C2-C1	-2.05	103.74	111.70
2	C	601	NSS	C2'-C3'-C4'	2.04	106.60	102.64
2	D	601	NSS	C2'-C3'-C4'	2.01	106.56	102.64
2	A	601	NSS	C3'-C2'-C1'	2.01	104.01	100.98

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	C1-C2-C3-O3
3	A	603	GOL	C1-C2-C3-O3
3	A	606	GOL	O1-C1-C2-C3
3	A	607	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-C3
3	B	603	GOL	C1-C2-C3-O3
3	B	607	GOL	C1-C2-C3-O3
3	C	602	GOL	C1-C2-C3-O3
3	D	603	GOL	C1-C2-C3-O3
3	D	603	GOL	O2-C2-C3-O3
3	D	603	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-C3
3	A	607	GOL	C1-C2-C3-O3
3	B	605	GOL	C1-C2-C3-O3
3	B	606	GOL	C1-C2-C3-O3
3	D	602	GOL	O1-C1-C2-C3

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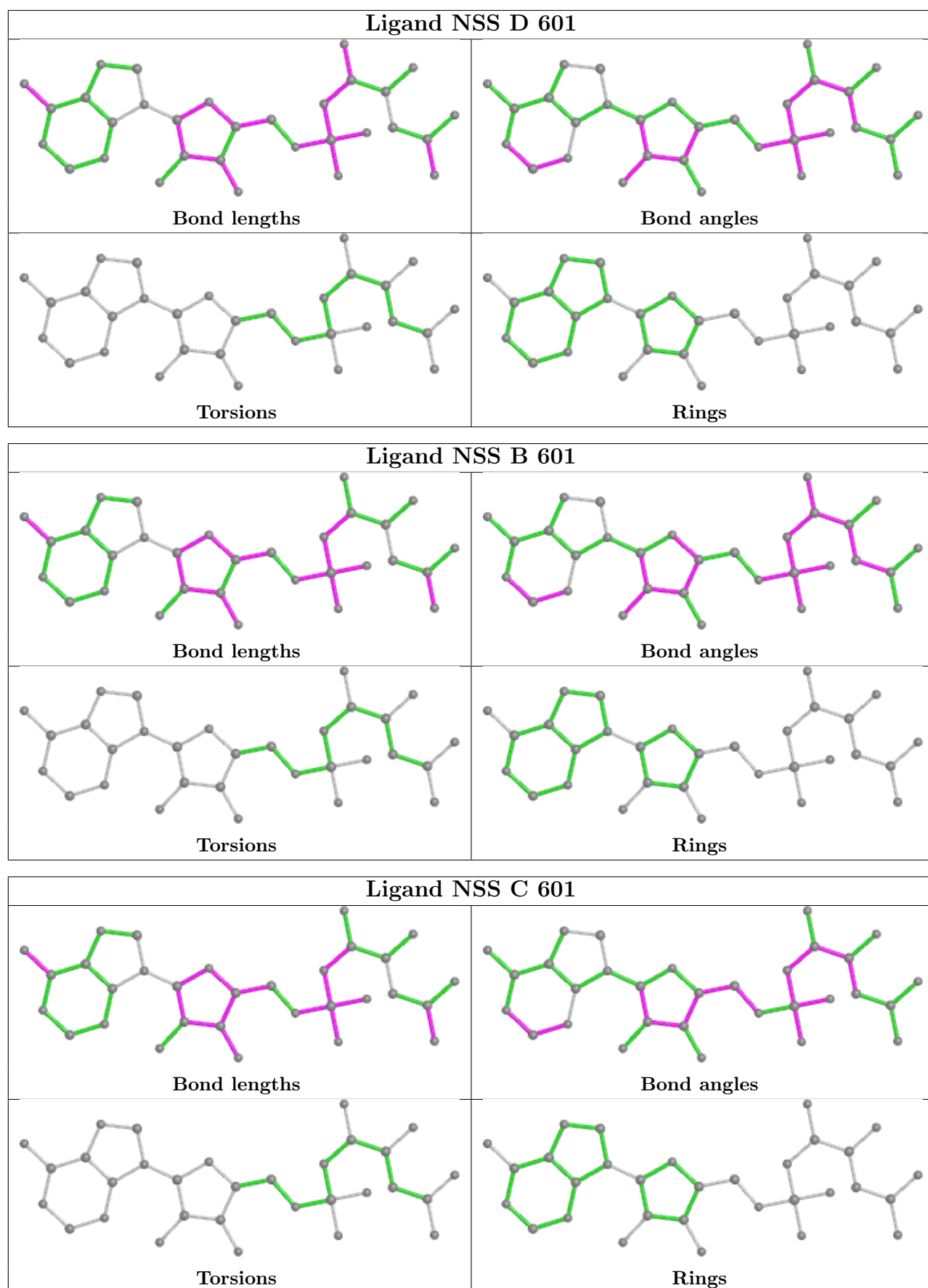
Mol	Chain	Res	Type	Atoms
3	D	602	GOL	C1-C2-C3-O3
3	D	603	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-O2
3	A	607	GOL	O1-C1-C2-O2
3	B	607	GOL	O2-C2-C3-O3
3	D	602	GOL	O1-C1-C2-O2
3	A	602	GOL	O2-C2-C3-O3
3	A	603	GOL	O2-C2-C3-O3
3	A	607	GOL	O2-C2-C3-O3
3	C	602	GOL	O2-C2-C3-O3
3	D	602	GOL	O2-C2-C3-O3
3	A	605	GOL	C1-C2-C3-O3
3	B	603	GOL	O2-C2-C3-O3
3	B	606	GOL	O2-C2-C3-O3
3	B	605	GOL	O2-C2-C3-O3
3	A	606	GOL	O1-C1-C2-O2

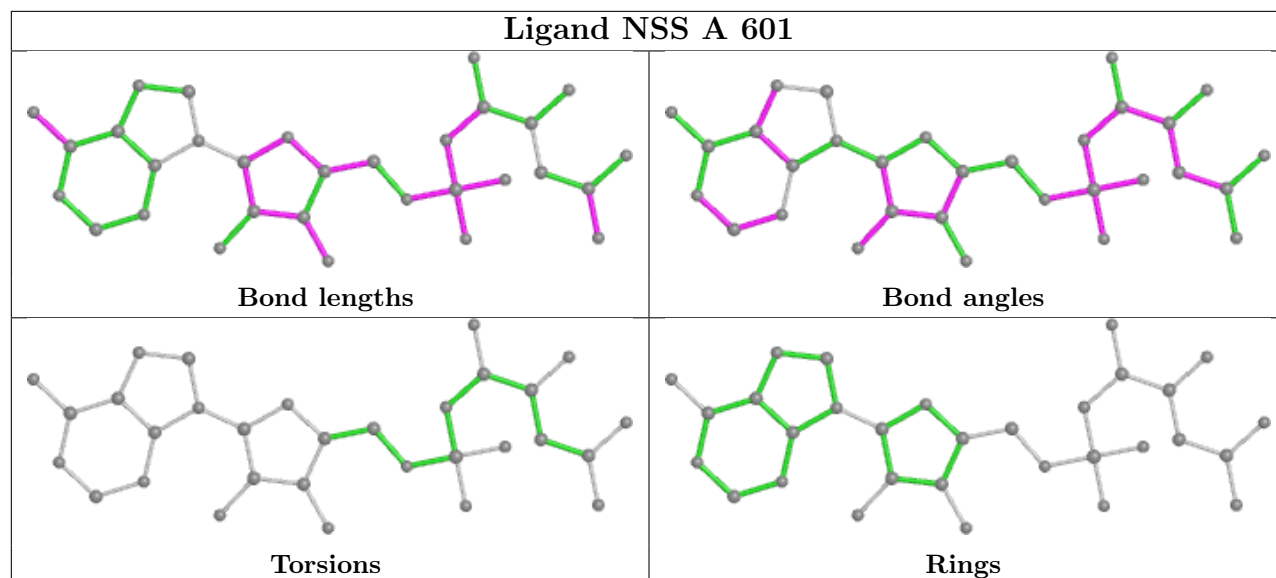
There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GOL	3	0
3	A	603	GOL	1	0
3	B	605	GOL	1	0
2	B	601	NSS	1	0
3	A	602	GOL	1	0
3	D	603	GOL	1	0
3	A	606	GOL	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	435/548 (79%)	-0.06	11 (2%) 57 60	20, 31, 52, 111	0
1	B	433/548 (79%)	-0.15	9 (2%) 63 66	18, 31, 53, 101	0
1	C	434/548 (79%)	0.17	26 (5%) 21 24	21, 36, 74, 115	0
1	D	434/548 (79%)	0.03	23 (5%) 26 29	20, 33, 69, 135	0
All	All	1736/2192 (79%)	-0.00	69 (3%) 38 41	18, 33, 61, 135	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	LEU	6.2
1	C	222	GLU	5.8
1	B	110	PRO	5.7
1	C	412	PHE	5.7
1	C	191	GLY	5.6
1	C	190	LYS	5.5
1	A	220	ILE	5.4
1	C	109	LEU	5.4
1	D	408	GLU	5.2
1	D	412	PHE	5.2
1	D	190	LYS	5.1
1	C	408	GLU	5.1
1	C	411	THR	5.1
1	C	410	GLY	4.7
1	C	223	GLU	4.7
1	C	110	PRO	4.6
1	C	189	PRO	4.5
1	D	191	GLY	4.5
1	C	192	LYS	4.4
1	D	193	GLN	4.2
1	A	110	PRO	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	111	GLU	4.0
1	C	193	GLN	4.0
1	C	407	LYS	3.9
1	D	192	LYS	3.8
1	C	214	GLY	3.5
1	C	111	GLU	3.4
1	D	409	ASP	3.3
1	D	111	GLU	3.3
1	D	109	LEU	3.3
1	D	223	GLU	3.2
1	D	268	VAL	3.2
1	A	221	ASN	3.0
1	A	111	GLU	3.0
1	A	222	GLU	3.0
1	A	223	GLU	3.0
1	D	222	GLU	3.0
1	D	317	ILE	3.0
1	C	221	ASN	2.9
1	D	189	PRO	2.9
1	D	411	THR	2.8
1	C	409	ASP	2.8
1	A	317	ILE	2.8
1	B	317	ILE	2.8
1	D	338	VAL	2.8
1	A	338	VAL	2.7
1	D	269	THR	2.7
1	C	143	ASN	2.6
1	C	405	VAL	2.6
1	C	144	LEU	2.5
1	D	221	ASN	2.4
1	C	268	VAL	2.4
1	D	318	ALA	2.4
1	C	317	ILE	2.4
1	B	193	GLN	2.3
1	C	318	ALA	2.3
1	D	327	ARG	2.3
1	B	338	VAL	2.3
1	B	385	LYS	2.3
1	C	269	THR	2.3
1	C	413	TYR	2.2
1	D	188	THR	2.2
1	B	214	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	318	ALA	2.2
1	D	407	LYS	2.2
1	A	269	THR	2.1
1	A	316	CYS	2.1
1	A	270	PRO	2.0
1	D	110	PRO	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.

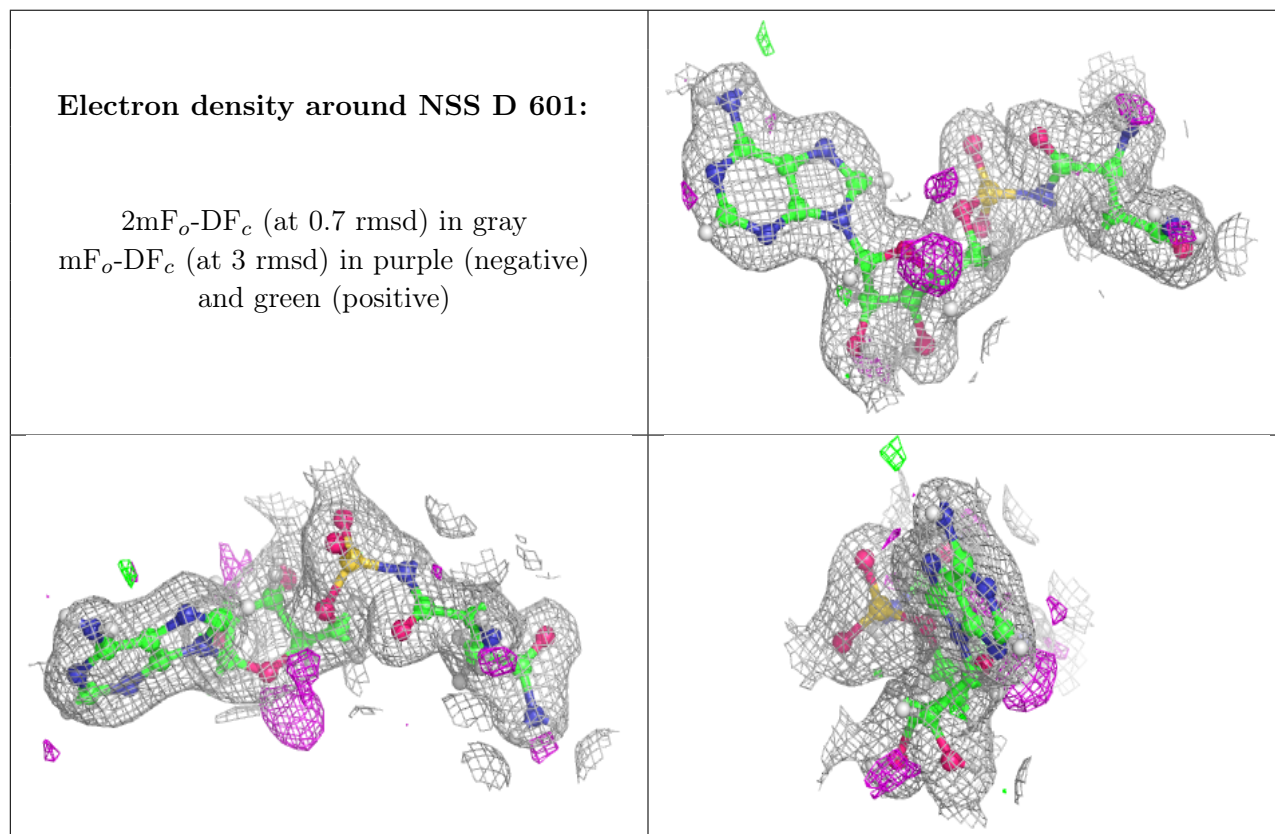
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	606	6/6	0.86	0.16	42,46,52,59	0
3	GOL	B	606	6/6	0.87	0.19	48,54,60,68	0
3	GOL	A	607	6/6	0.88	0.20	44,47,57,63	0
3	GOL	B	607	6/6	0.88	0.28	40,51,59,63	0
3	GOL	B	602	6/6	0.89	0.23	37,49,52,52	0
3	GOL	C	602	6/6	0.89	0.14	39,52,55,57	0
3	GOL	D	603	6/6	0.89	0.12	35,46,51,55	0
3	GOL	A	603	6/6	0.90	0.22	36,45,51,57	0
3	GOL	B	605	6/6	0.90	0.14	40,45,58,60	0
3	GOL	A	604	6/6	0.91	0.14	31,42,48,58	0
3	GOL	B	603	6/6	0.92	0.11	38,48,56,58	0
3	GOL	D	602	6/6	0.93	0.13	39,48,61,62	0
3	GOL	A	605	6/6	0.94	0.12	35,48,58,77	0
3	GOL	C	603	6/6	0.94	0.09	36,43,45,56	0
3	GOL	A	602	6/6	0.95	0.13	34,37,43,47	0
3	GOL	B	604	6/6	0.96	0.14	28,36,40,44	0
4	NA	C	604	1/1	0.96	0.07	38,38,38,38	0

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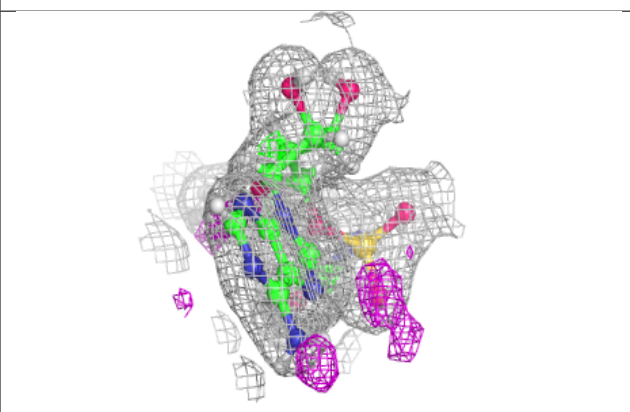
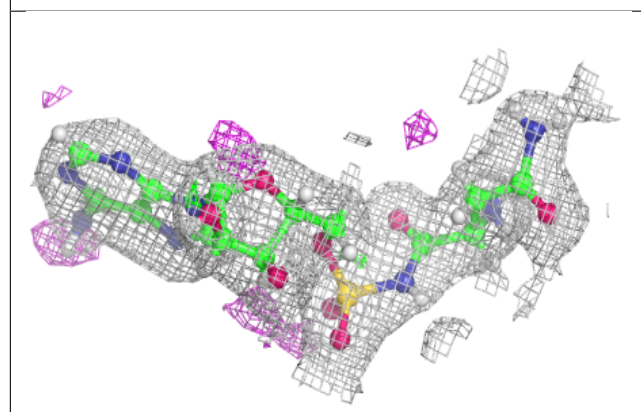
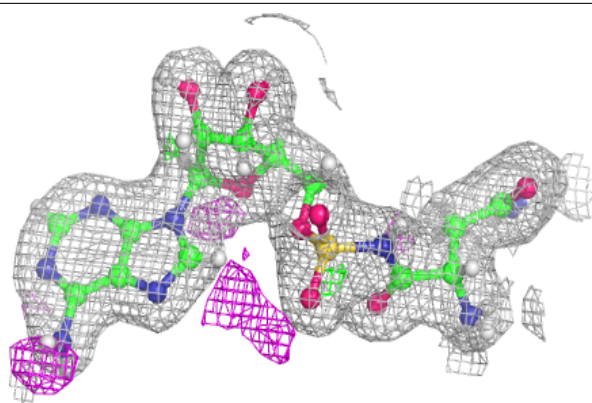
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NSS	D	601	31/31	0.97	0.10	19,26,34,43	0
2	NSS	A	601	31/31	0.98	0.10	19,25,31,35	0
2	NSS	B	601	31/31	0.98	0.10	20,24,32,33	0
2	NSS	C	601	31/31	0.98	0.10	19,29,34,41	0
4	NA	D	604	1/1	0.98	0.03	30,30,30,30	0
4	NA	A	608	1/1	0.99	0.05	31,31,31,31	0
4	NA	B	608	1/1	0.99	0.04	30,30,30,30	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.

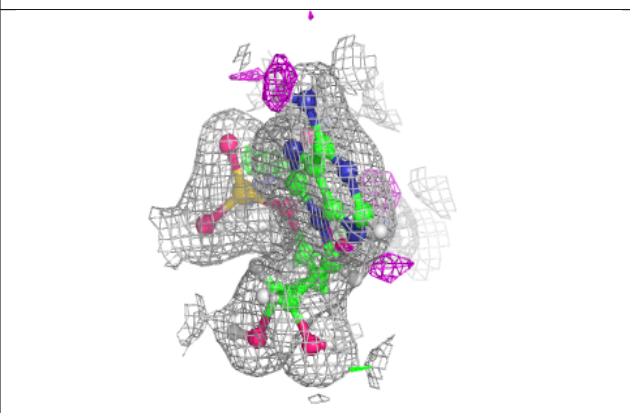
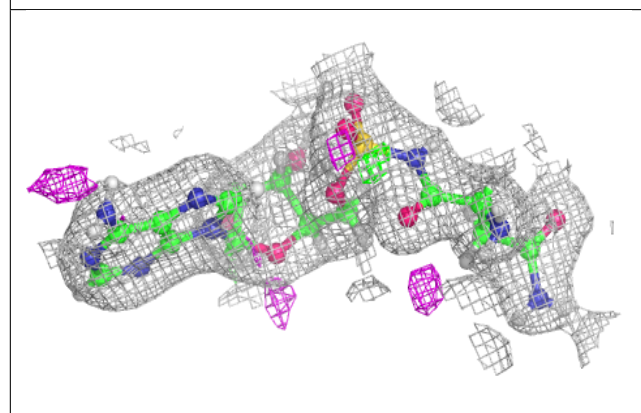
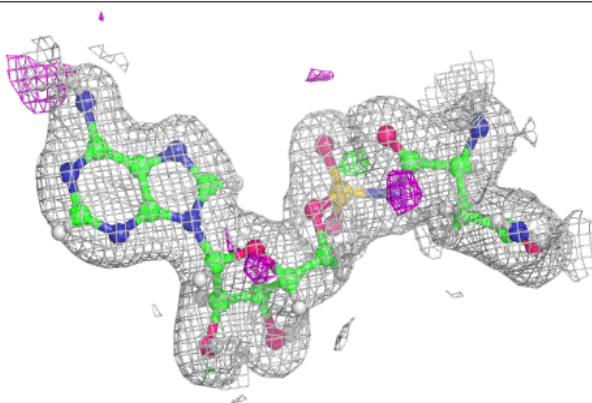


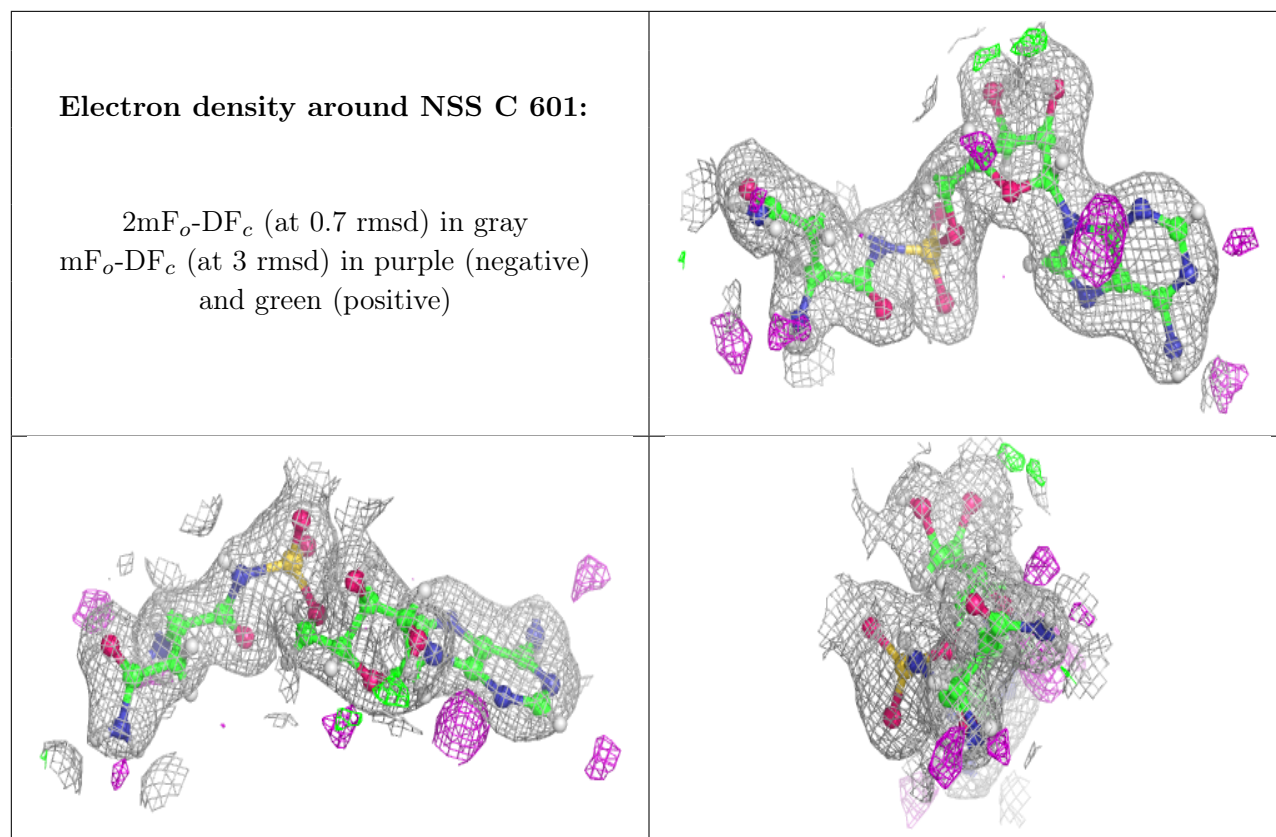
**Electron density around NSS A 601:**

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

**Electron density around NSS B 601:**

$2mF_o-DF_c$  (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.