Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 03:41 pm BST

PDB ID	:	2XGT
Title	:	Asparaginyl-tRNA synthetase from Brugia malayi complexed with the sulphamoyl analogue of asparaginyl-adenylate
Authors	:	Crepin, T.; Haertlein, M.; Kron, M.; Cusack, S.
Deposited on	:	2010-06-07
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*
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.

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

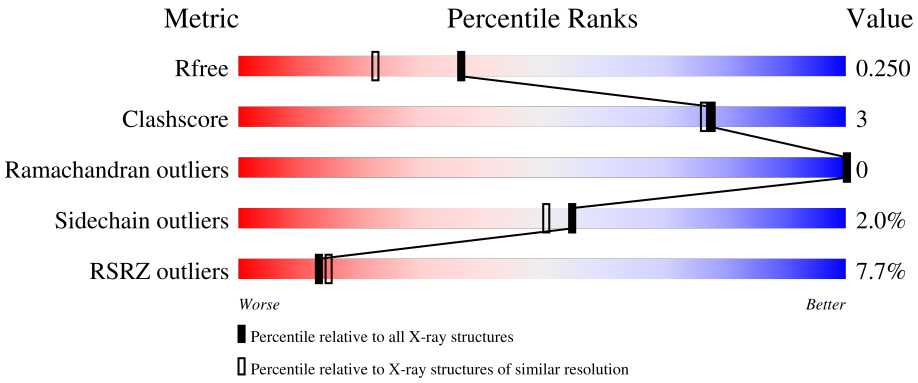
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	435	6% 90% 8% .
1	B	435	10% 92% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7526 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.

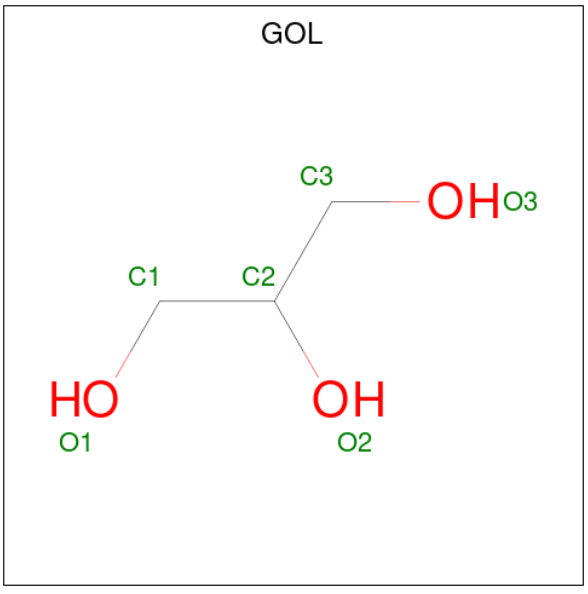
- Molecule 1 is a protein called ASPARAGINYL-TRNA SYNTHETASE, CYTOPLASMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3456	2202	597	635	22			
1	B	433	Total	C	N	O	S	0	0	0
			3504	2230	603	649	22			

There are 4 discrepancies between the modelled and reference sequences:

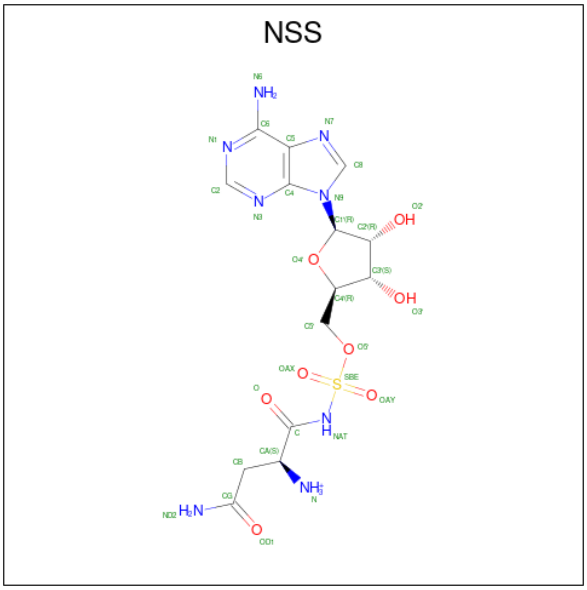
Chain	Residue	Modelled	Actual	Comment	Reference
A	265	VAL	LEU	conflict	UNP A8PWE4
A	454	GLN	LYS	conflict	UNP A8PWE4
B	265	VAL	LEU	conflict	UNP A8PWE4
B	454	GLN	LYS	conflict	UNP A8PWE4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0

- Molecule 3 is 5'-O-[N-(L-ASPARAGINYL)SULFAMOYL]ADENOSINE (three-letter code: NSS) (formula: $C_{14}H_{21}N_8O_8S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 31 14 8 8 1	0	0
3	B	1	Total C N O S 31 14 8 8 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is water.

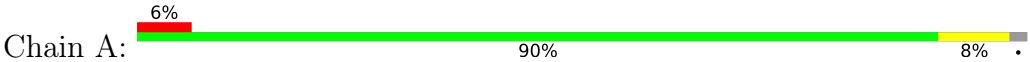
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	288	Total O 288 288	0	0
5	B	208	Total O 208 208	0	0

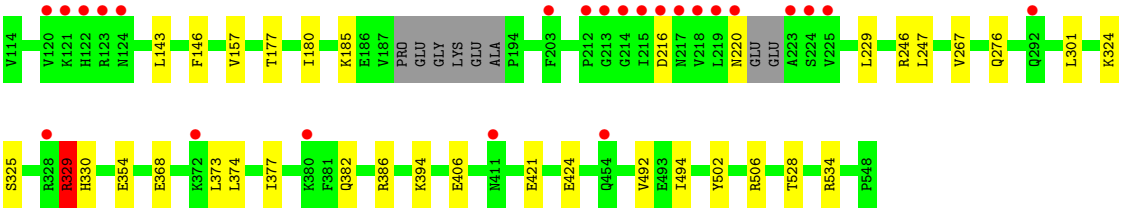
3 Residue-property plots (i)

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

• Molecule 1: ASPARAGINYL-TRNA SYNTHETASE, CYTOPLASMIC

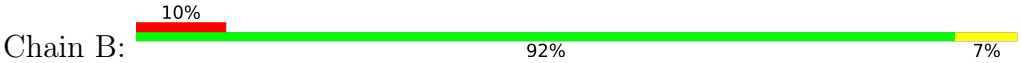
Chain A:

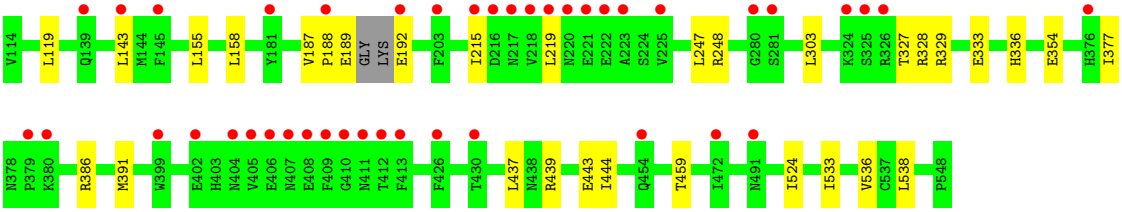




• Molecule 1: ASPARAGINYL-TRNA SYNTHETASE, CYTOPLASMIC

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.51Å 125.70Å 144.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.92 – 1.90 29.40 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.9 (94.92-1.90) 88.9 (29.40-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.202 , 0.250 0.203 , 0.250	Depositor DCC
R_{free} test set	2136 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7526	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NSS, GOL

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	0.60	0/3533	0.71	1/4778 (0.0%)
1	B	0.57	0/3583	0.66	0/4849
All	All	0.59	0/7116	0.69	1/9627 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	329	ARG	NE-CZ-NH1	8.74	124.67	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3456	0	3409	21	0
1	B	3504	0	3445	21	0
2	A	6	0	8	0	0
3	A	31	0	21	0	0
3	B	31	0	21	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	288	0	0	3	0
5	B	208	0	0	1	0
All	All	7526	0	6904	41	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 3.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:HD11	1:B:158:LEU:HD11	1.36	1.02
1:A:424:GLU:OE2	5:A:2218:HOH:O	2.06	0.72
1:A:247:LEU:HD21	1:A:374:LEU:HD13	1.74	0.69
1:A:247:LEU:HD23	1:A:528:THR:HG22	1.79	0.65
1:B:215:ILE:CG2	1:B:219:LEU:HD12	2.30	0.61
1:B:354:GLU:OE1	1:B:386:ARG:HD2	2.01	0.61
1:B:143:LEU:CD1	1:B:158:LEU:HD11	2.23	0.60
1:B:327:THR:HG22	1:B:329:ARG:H	1.67	0.60
1:A:354:GLU:OE1	1:A:386:ARG:HD2	2.05	0.57
1:A:329:ARG:HH11	1:A:329:ARG:HG3	1.70	0.56
1:A:329:ARG:HH11	1:A:329:ARG:CG	2.18	0.56
1:A:157:VAL:HG11	1:A:180:ILE:HD13	1.87	0.56
1:B:247:LEU:HD22	1:B:377:ILE:HD12	1.87	0.55
1:A:267:VAL:HG13	1:B:538:LEU:HD22	1.89	0.55
1:B:443:GLU:HG2	1:B:444:ILE:HG23	1.89	0.54
1:A:247:LEU:HD23	1:A:528:THR:CG2	2.38	0.53
1:B:336:HIS:HE2	3:B:1550:NSS:H5'1	1.74	0.51
1:B:215:ILE:HG22	1:B:219:LEU:HD12	1.92	0.51
1:B:328:ARG:NH1	5:B:2120:HOH:O	2.41	0.50
1:B:391:MET:O	1:B:437:LEU:HD12	2.12	0.49
1:A:246:ARG:HB3	1:A:373:LEU:HD21	1.94	0.49
1:B:119:LEU:CD1	1:B:155:LEU:HD22	2.42	0.49
1:B:354:GLU:OE1	1:B:386:ARG:CD	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HD21	1:A:534:ARG:HD2	1.96	0.48
1:A:247:LEU:HD22	1:A:377:ILE:HD12	1.96	0.47
1:B:248:ARG:HG3	1:B:524:ILE:HD11	1.97	0.47
1:A:386:ARG:NH2	5:A:2180:HOH:O	2.48	0.46
1:A:330:HIS:HE1	1:A:421:GLU:OE2	1.98	0.46
1:B:533:ILE:O	1:B:536:VAL:HG22	2.17	0.44
1:A:394:LYS:HB3	5:A:2201:HOH:O	2.18	0.44
1:A:506:ARG:N	1:A:506:ARG:HD2	2.33	0.43
1:A:301:LEU:HD22	1:A:502:TYR:CZ	2.55	0.42
1:A:492:VAL:HG23	1:A:494:ILE:HG13	2.00	0.42
1:A:301:LEU:HD22	1:A:502:TYR:CE2	2.55	0.42
1:B:327:THR:HG22	1:B:328:ARG:N	2.35	0.42
1:A:329:ARG:CG	1:A:329:ARG:NH1	2.83	0.41
1:B:391:MET:O	1:B:437:LEU:HA	2.20	0.41
1:B:439:ARG:HA	1:B:459:THR:O	2.21	0.41
1:A:146:PHE:HB2	1:A:157:VAL:HB	2.03	0.41
1:B:187:VAL:O	1:B:189:GLU:N	2.54	0.41
1:B:248:ARG:HG3	1:B:524:ILE:CD1	2.52	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	421/435 (97%)	409 (97%)	12 (3%)	0	100	100
1	B	429/435 (99%)	417 (97%)	12 (3%)	0	100	100
All	All	850/870 (98%)	826 (97%)	24 (3%)	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	372/378 (98%)	360 (97%)	12 (3%)	39 30
1	B	377/378 (100%)	374 (99%)	3 (1%)	81 82
All	All	749/756 (99%)	734 (98%)	15 (2%)	55 51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	177	THR
1	A	185	LYS
1	A	216	ASP
1	A	220	ASN
1	A	276	GLN
1	A	324	LYS
1	A	325	SER
1	A	329	ARG
1	A	368	GLU
1	A	382	GLN
1	A	406	GLU
1	B	192	GLU
1	B	303	LEU
1	B	333	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	165	GLN
1	A	276	GLN
1	A	330	HIS
1	A	454	GLN
1	A	531	ASN
1	A	532	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	122	HIS
1	B	209	ASN
1	B	261	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	NSS	B	1550	4	29,33,33	1.11	3 (10%)	32,49,49	1.69	3 (9%)
3	NSS	A	1550	4	29,33,33	1.24	4 (13%)	32,49,49	1.48	6 (18%)
2	GOL	A	1549	-	5,5,5	0.34	0	5,5,5	0.13	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
3	NSS	B	1550	4	-	0/18/39/39	0/3/3/3
3	NSS	A	1550	4	-	0/18/39/39	0/3/3/3
2	GOL	A	1549	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1550	NSS	OAX-SBE	2.59	1.44	1.42
3	B	1550	NSS	C-NAT	-2.42	1.32	1.37
3	B	1550	NSS	C5-C4	2.24	1.46	1.40
3	A	1550	NSS	C5-C4	2.24	1.46	1.40
3	A	1550	NSS	C-NAT	-2.22	1.33	1.37
3	A	1550	NSS	C2-N3	2.04	1.35	1.32
3	B	1550	NSS	OAX-SBE	2.02	1.44	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1550	NSS	OAY-SBE-OAX	-6.80	110.17	120.76
3	A	1550	NSS	N3-C2-N1	-4.31	121.95	128.68
3	B	1550	NSS	N3-C2-N1	-3.59	123.07	128.68
3	A	1550	NSS	OAY-SBE-OAX	-3.36	115.53	120.76
3	A	1550	NSS	C-NAT-SBE	-2.59	120.42	124.61
3	A	1550	NSS	C1'-N9-C4	-2.45	122.34	126.64
3	B	1550	NSS	C1'-N9-C4	-2.37	122.48	126.64
3	A	1550	NSS	C4-C5-N7	-2.24	107.06	109.40
3	A	1550	NSS	CB-CA-C	-2.13	104.12	109.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1549	GOL	C1-C2-C3-O3
2	A	1549	GOL	O2-C2-C3-O3

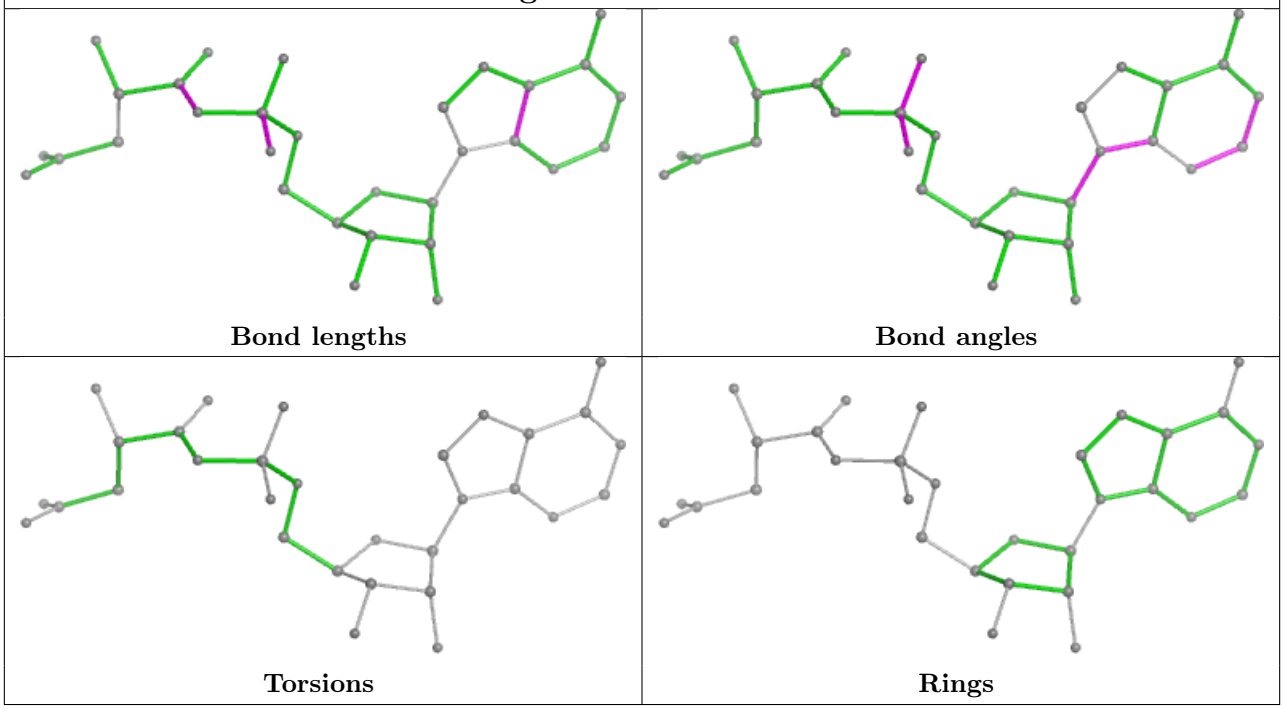
There are no ring outliers.

1 monomer is involved in 1 short contact:

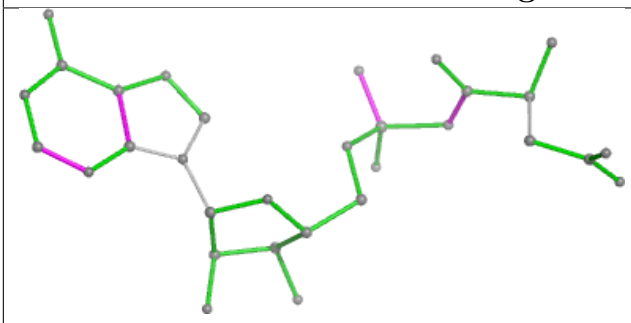
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1550	NSS	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

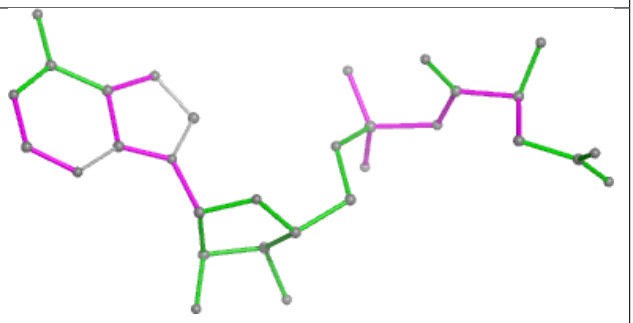
Ligand NSS B 1550



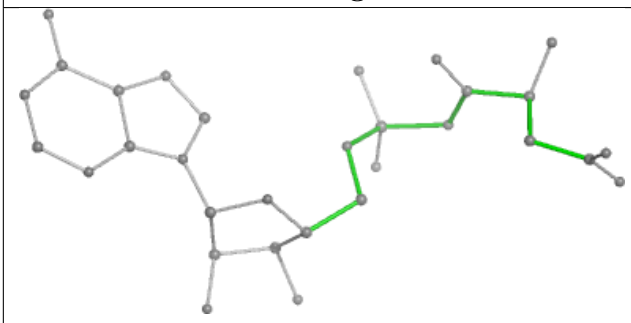
Ligand NSS A 1550



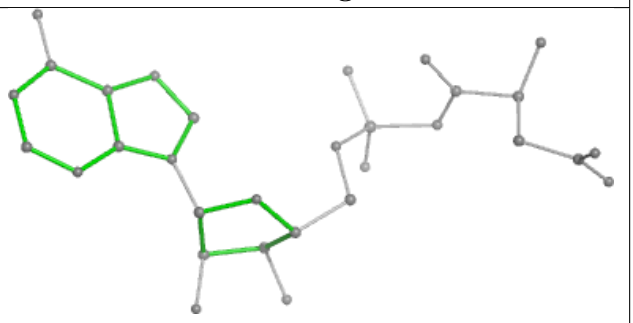
Bond lengths



Bond angles



Torsions



Rings

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	427/435 (98%)	0.37	24 (5%) 24 27	7, 17, 34, 58	0
1	B	433/435 (99%)	0.54	42 (9%) 7 9	9, 21, 41, 53	0
All	All	860/870 (98%)	0.46	66 (7%) 13 15	7, 19, 37, 58	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	VAL	6.0
1	B	217	ASN	5.9
1	B	222	GLU	5.9
1	A	216	ASP	5.6
1	B	221	GLU	5.5
1	B	223	ALA	5.2
1	A	217	ASN	5.2
1	B	220	ASN	5.0
1	B	409	PHE	5.0
1	A	220	ASN	4.9
1	B	216	ASP	4.9
1	A	223	ALA	4.6
1	B	411	ASN	4.6
1	A	120	VAL	4.3
1	B	412	THR	4.2
1	B	426	PHE	4.2
1	A	123	ARG	4.0
1	B	410	GLY	3.9
1	B	218	VAL	3.9
1	B	143	LEU	3.7
1	B	405	VAL	3.7
1	B	181	TYR	3.6
1	B	188	PRO	3.5
1	B	215	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	404	ASN	3.3
1	A	122	HIS	3.3
1	B	203	PHE	3.2
1	A	121	LYS	3.2
1	B	380	LYS	3.2
1	B	407	ASN	3.2
1	A	380	LYS	3.1
1	B	324	LYS	3.1
1	A	225	VAL	3.0
1	A	219	LEU	2.9
1	B	491	ASN	2.9
1	A	328	ARG	2.9
1	B	219	LEU	2.9
1	A	292	GLN	2.8
1	A	124	ASN	2.8
1	A	203	PHE	2.7
1	A	224	SER	2.6
1	B	145	PHE	2.6
1	B	192	GLU	2.6
1	B	408	GLU	2.5
1	A	372	LYS	2.5
1	A	454	GLN	2.5
1	B	376	HIS	2.4
1	B	472	ILE	2.4
1	B	225	VAL	2.4
1	A	212	PRO	2.4
1	B	399	TRP	2.4
1	B	379	PRO	2.4
1	B	280	GLY	2.3
1	A	213	GLY	2.3
1	B	413	PHE	2.3
1	B	139	GLN	2.2
1	B	326	ARG	2.1
1	B	454	GLN	2.1
1	A	215	ILE	2.1
1	B	402	GLU	2.1
1	B	325	SER	2.1
1	A	411	ASN	2.1
1	B	430	THR	2.1
1	B	406	GLU	2.1
1	A	214	GLY	2.0
1	B	281	SER	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)

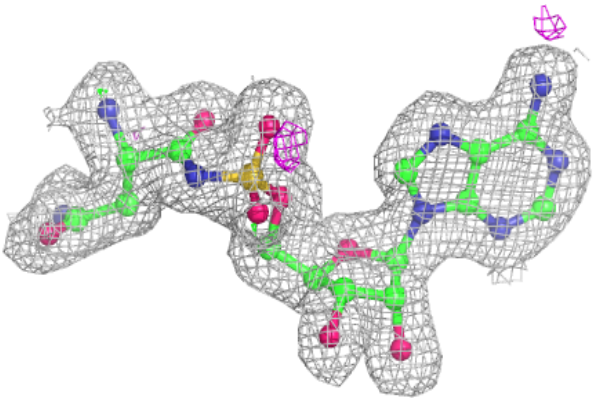
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

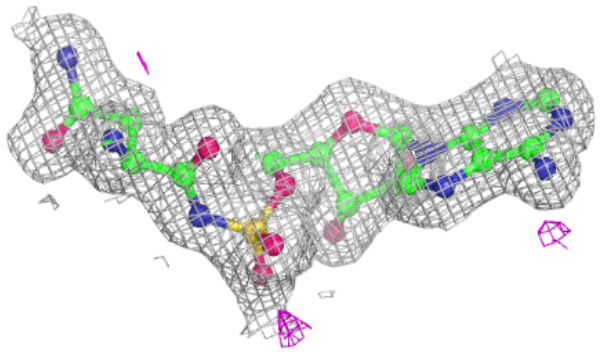
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	1549	6/6	0.87	0.18	39,40,41,41	0
4	MG	B	1551	1/1	0.96	0.09	26,26,26,26	0
3	NSS	B	1550	31/31	0.97	0.12	10,14,17,18	0
3	NSS	A	1550	31/31	0.97	0.10	7,10,12,14	0
4	MG	A	1551	1/1	1.00	0.06	15,15,15,15	0

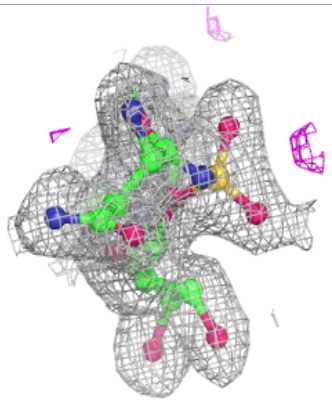
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NSS B 1550:

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

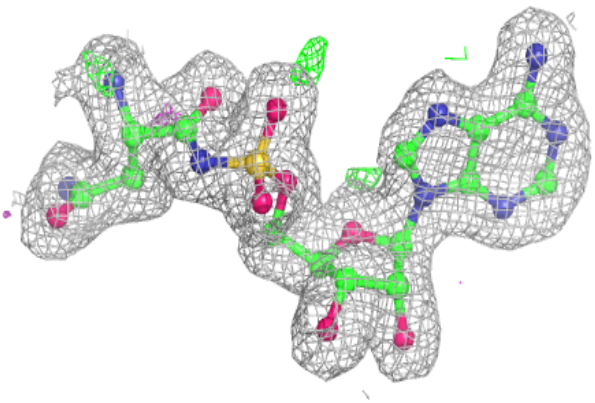


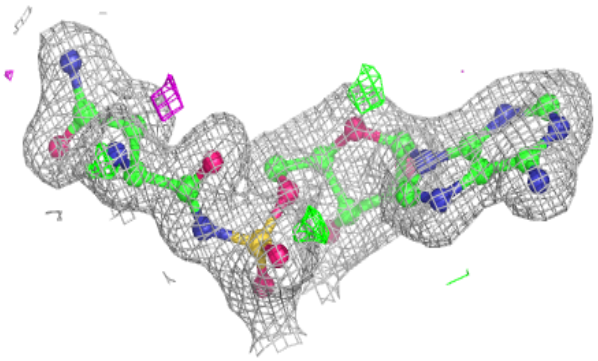


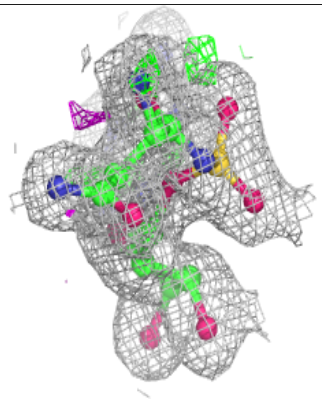


Electron density around NSS A 1550:

$2mF_o$-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.