



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:41 AM UTC

PDB ID : 7KN4 / pdb_00007kn4
Title : Crystal structure of SARS-CoV-2 spike protein receptor-binding domain complexed with a pre-pandemic antibody S-E6 Fab
Authors : Liu, H.; Wilson, I.A.
Deposited on : 2020-11-04
Resolution : 2.70 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

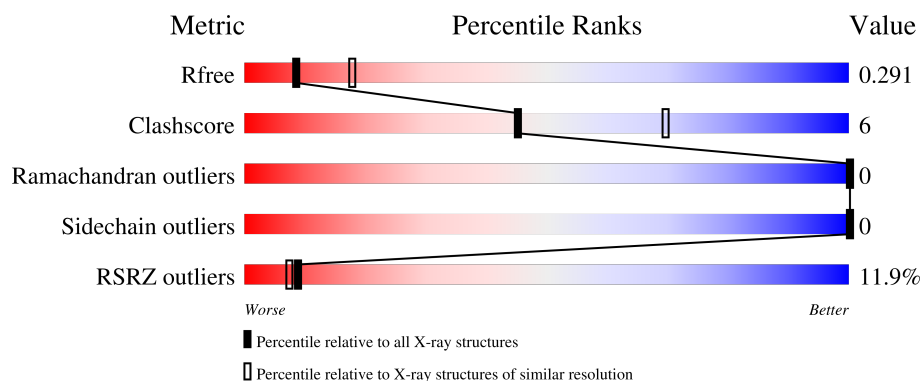
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	231	
1	B	231	
2	H	223	
2	M	223	
3	L	216	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	N	216	 A horizontal bar chart showing the quality of chain N. The bar is divided into three segments: a red segment at the beginning labeled '9%', a green segment in the middle labeled '84%', and a yellow segment at the end labeled '13%'. A small grey dot is located at the far right end of the bar.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8955 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1469	941	242	278	8			
1	B	182	Total	C	N	O	S	0	0	0
			1287	828	209	242	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
B	542	SER	-	expression tag	UNP P0DTC2
B	543	GLY	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
B	548	HIS	-	expression tag	UNP P0DTC2
B	549	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called S-E6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1556	994	253	303	6			
2	M	216	Total	C	N	O	S	0	0	0
			1564	1000	253	305	6			

- Molecule 3 is a protein called S-E6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1538	967	256	311	4			
3	N	211	Total	C	N	O	S	0	0	0
			1513	952	248	309	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

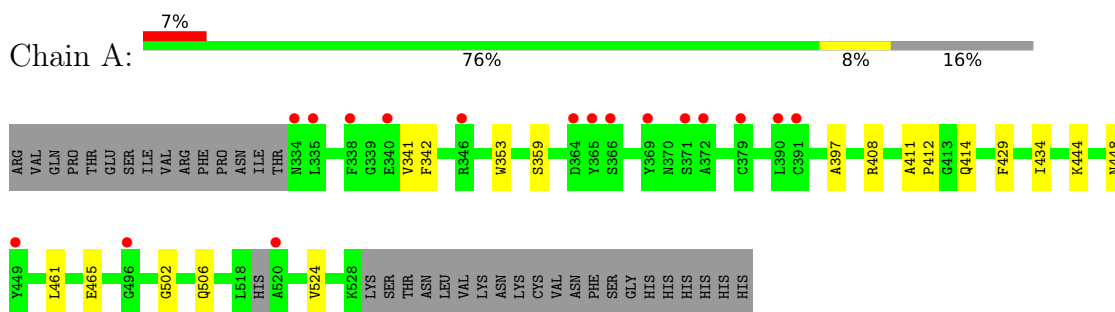


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

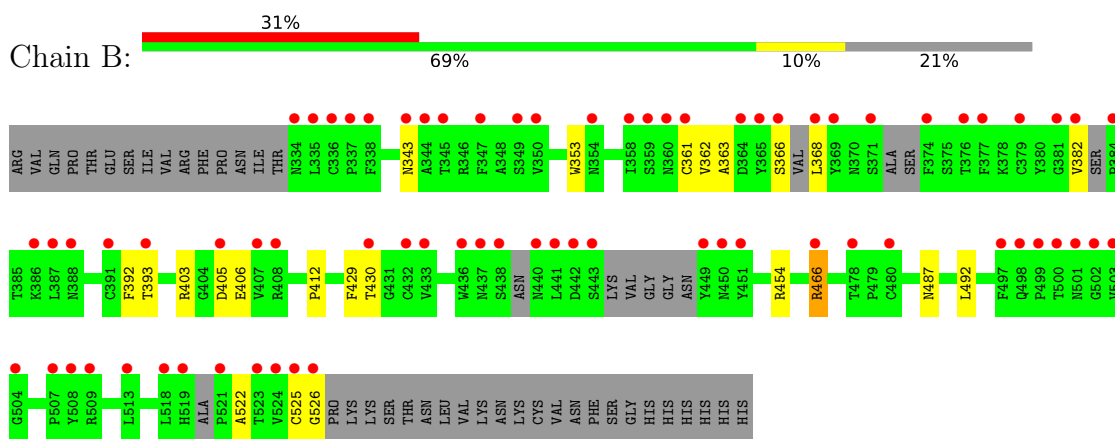
3 Residue-property plots [i](#)

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.

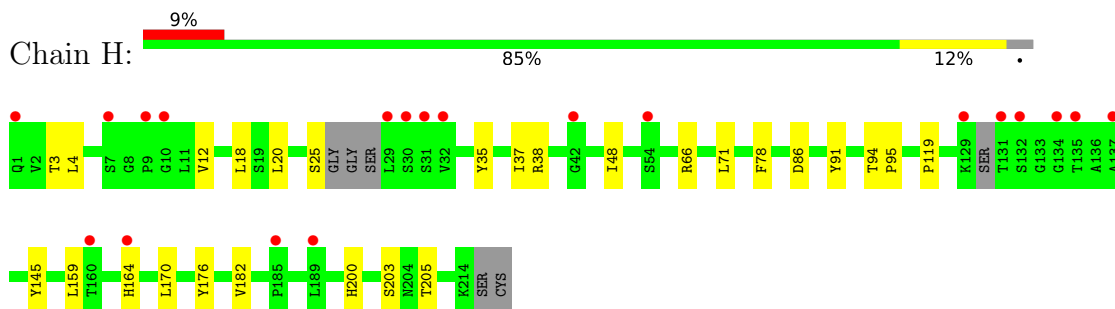
- Molecule 1: Spike protein S1



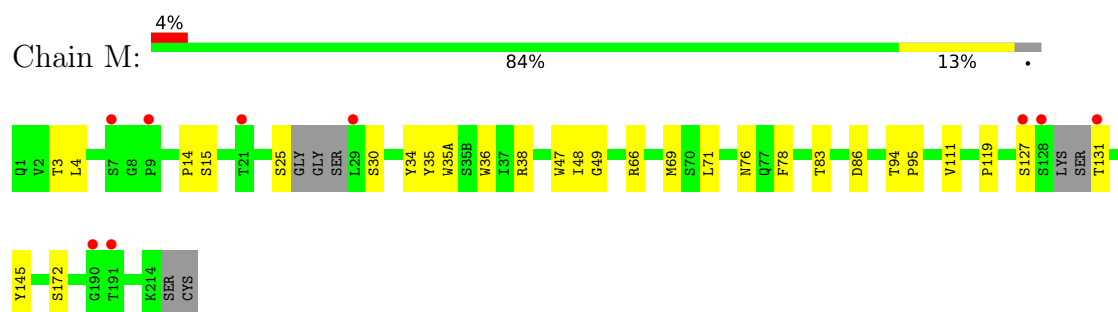
- Molecule 1: Spike protein S1



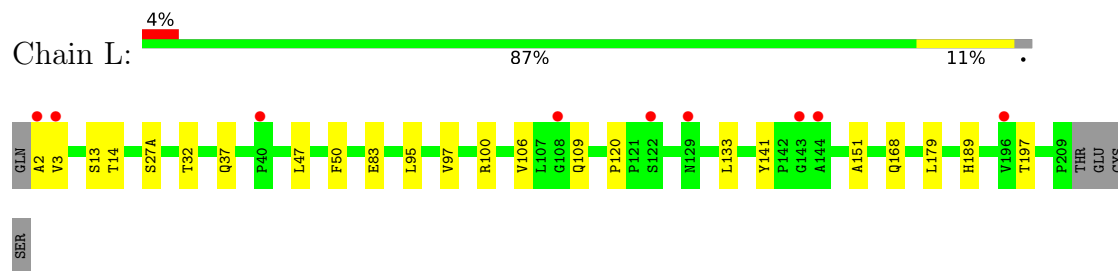
- Molecule 2: S-E6 Fab heavy chain



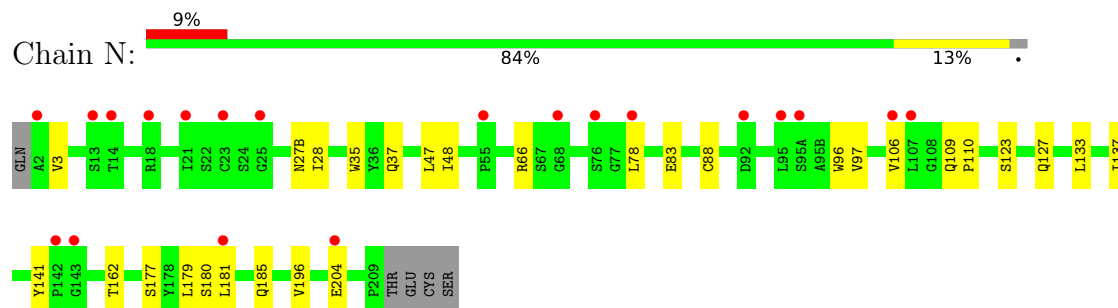
- Molecule 2: S-E6 Fab heavy chain



- Molecule 3: S-E6 Fab light chain



- Molecule 3: S-E6 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	242.11Å 70.23Å 91.89Å 90.00° 108.47° 90.00°	Depositor
Resolution (Å)	49.38 – 2.70 49.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	87.1 (49.38-2.70) 87.3 (49.38-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.241 , 0.291 0.241 , 0.291	Depositor DCC
R_{free} test set	1791 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8955	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.11	0/1510	0.33	0/2060
1	B	0.34	0/1320	0.57	4/1800 (0.2%)
2	H	0.14	0/1596	0.35	0/2191
2	M	0.12	0/1604	0.34	0/2200
3	L	0.15	0/1578	0.37	1/2166 (0.0%)
3	N	0.26	1/1553 (0.1%)	0.44	1/2137 (0.0%)
All	All	0.20	1/9161 (0.0%)	0.40	6/12554 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	27(B)	ASN	CA-C	-6.29	1.48	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	204	GLU	N-CA-CB	6.89	121.78	110.69
1	B	466	ARG	CG-CD-NE	-6.53	97.63	112.00
1	B	466	ARG	CB-CG-CD	-5.83	97.89	111.30
1	B	466	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	B	466	ARG	NH1-CZ-NH2	5.74	126.77	119.30
3	L	197	THR	OG1-CB-CG2	5.31	119.92	109.30

There are no chirality outliers.

There are no planarity outliers.

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	1469	0	1317	12	0
1	B	1287	0	1013	22	0
2	H	1556	0	1454	16	0
2	M	1564	0	1490	18	0
3	L	1538	0	1439	16	0
3	N	1513	0	1389	23	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
All	All	8955	0	8128	101	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 6.

All (101) 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:403:ARG:NH2	1:B:405:ASP:OD2	2.04	0.89
3:N:179:LEU:HG	3:N:181:LEU:HD12	1.61	0.83
2:M:36:TRP:HD1	2:M:69:MET:HE3	1.43	0.80
3:N:3:VAL:HG22	3:N:97:VAL:HG21	1.63	0.79
1:B:403:ARG:HG3	1:B:406:GLU:HG3	1.66	0.78
2:H:66:ARG:HG2	2:M:172:SER:HB2	1.68	0.76
2:M:3:THR:HB	2:M:25:SER:HB2	1.68	0.75
2:H:12:VAL:HG21	2:H:18:LEU:HD23	1.68	0.74
3:N:179:LEU:HD11	3:N:181:LEU:HD11	1.72	0.71
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.72	0.70
3:L:3:VAL:HG22	3:L:97:VAL:HG11	1.74	0.69
3:L:133:LEU:HD12	3:L:179:LEU:HD23	1.73	0.69
1:B:366:SER:O	1:B:368:LEU:N	2.25	0.68
1:B:363:ALA:O	1:B:526:GLY:HA2	1.93	0.68
3:N:109:GLN:HG3	3:N:110:PRO:HD2	1.77	0.66
3:N:179:LEU:HG	3:N:181:LEU:CD1	2.26	0.65
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.79	0.64
1:B:353:TRP:CE3	1:B:466:ARG:NH1	2.66	0.63
3:L:83:GLU:HG2	3:L:106:VAL:HG23	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:28:ILE:O	3:N:66:ARG:NH2	2.34	0.60
2:H:164:HIS:NE2	3:L:168:GLN:HG2	2.17	0.59
1:A:408:ARG:HH21	1:A:408:ARG:HG3	1.67	0.58
3:L:32:THR:HG21	3:L:50:PHE:HD1	1.69	0.58
3:N:181:LEU:HB3	3:N:185:GLN:OE1	2.03	0.58
2:M:30:SER:HB2	2:M:76:ASN:OD1	2.03	0.57
3:L:109:GLN:HB2	3:L:141:TYR:CZ	2.40	0.56
2:M:38:ARG:HB3	2:M:48:ILE:HD11	1.86	0.56
1:B:353:TRP:CZ3	1:B:466:ARG:NH1	2.74	0.55
3:N:180:SER:O	3:N:181:LEU:HG	2.06	0.55
1:A:461:LEU:HD22	1:A:465:GLU:HB3	1.89	0.54
3:N:35:TRP:HB2	3:N:48:ILE:HB	1.90	0.54
1:B:403:ARG:HH21	1:B:405:ASP:CG	2.15	0.53
3:N:78:LEU:HD21	3:N:106:VAL:HG22	1.90	0.53
3:N:123:SER:O	3:N:127:GLN:HG2	2.09	0.53
1:A:359:SER:HA	1:A:524:VAL:HG22	1.91	0.53
2:M:4:LEU:HD21	2:M:35(A):TRP:HZ3	1.74	0.53
1:B:403:ARG:NE	1:B:405:ASP:OD1	2.42	0.53
1:A:444:LYS:HB3	1:A:448:ASN:HB2	1.91	0.52
3:L:27(A):SER:OG	2:M:15:SER:HB2	2.09	0.52
3:N:162:THR:HG23	3:N:177:SER:HB2	1.92	0.52
2:M:71:LEU:HD23	2:M:78:PHE:HB3	1.92	0.51
1:A:342:PHE:HZ	1:A:434:ILE:HD13	1.75	0.51
2:M:119:PRO:HB3	2:M:145:TYR:HB3	1.92	0.51
3:N:179:LEU:CD1	3:N:181:LEU:HD11	2.39	0.50
3:N:179:LEU:CG	3:N:181:LEU:CD1	2.89	0.50
3:N:133:LEU:HD12	3:N:179:LEU:HD23	1.92	0.50
2:H:203:SER:OG	2:H:205:THR:OG1	2.27	0.50
3:L:32:THR:CG2	3:L:50:PHE:HA	2.43	0.49
1:B:353:TRP:NE1	1:B:466:ARG:HB2	2.28	0.49
2:M:127:SER:HB3	2:M:131:THR:N	2.28	0.48
2:M:35:TYR:O	2:M:95:PRO:HD2	2.13	0.48
2:M:4:LEU:HD11	2:M:94:THR:HG22	1.96	0.47
3:L:32:THR:HG21	3:L:50:PHE:HA	1.97	0.47
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.95	0.47
1:B:403:ARG:HG3	1:B:406:GLU:CG	2.40	0.47
1:B:403:ARG:NH2	1:B:405:ASP:CG	2.70	0.47
3:N:109:GLN:HB3	3:N:141:TYR:CE1	2.50	0.47
2:M:47:TRP:CZ2	2:M:49:GLY:HA2	2.50	0.46
3:L:120:PRO:HA	3:L:133:LEU:HD23	1.98	0.46
1:B:392:PHE:N	1:B:522:ALA:HB1	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:PRO:HG3	1:B:429:PHE:HB3	1.96	0.46
3:L:151:ALA:HB1	3:L:189:HIS:CD2	2.51	0.46
2:M:47:TRP:CD2	3:N:96:TRP:HB3	2.51	0.46
2:H:71:LEU:HD23	2:H:78:PHE:HB3	1.97	0.45
1:A:408:ARG:HG3	1:A:408:ARG:NH2	2.30	0.45
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.98	0.45
2:H:66:ARG:HH22	2:H:86:ASP:CG	2.25	0.44
1:B:487:ASN:ND2	2:M:34:TYR:OH	2.51	0.44
2:M:66:ARG:NH2	2:M:86:ASP:OD1	2.51	0.44
1:A:502:GLY:O	1:A:506:GLN:HG3	2.18	0.44
3:N:83:GLU:HG2	3:N:106:VAL:HG23	1.99	0.43
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.99	0.43
3:L:100:ARG:O	3:L:100:ARG:HD3	2.18	0.43
2:H:35:TYR:O	2:H:95:PRO:HD2	2.18	0.42
3:N:47:LEU:O	3:N:48:ILE:HD13	2.19	0.42
1:B:343:ASN:HD22	4:B:1501:NAG:H83	1.84	0.42
1:B:454:ARG:HA	1:B:492:LEU:HD23	2.00	0.42
3:L:95:LEU:HD21	2:M:14:PRO:HG2	2.00	0.42
2:H:4:LEU:HD11	2:H:94:THR:HG22	2.01	0.42
2:M:83:THR:C	2:M:111:VAL:HG11	2.44	0.42
1:B:353:TRP:CD2	1:B:466:ARG:NH1	2.87	0.42
2:H:200:HIS:ND1	2:H:203:SER:HB3	2.35	0.42
1:A:411:ALA:HB3	1:A:414:GLN:HG3	2.01	0.42
3:N:137:ILE:HG12	3:N:196:VAL:HG21	2.01	0.42
1:B:361:CYS:SG	1:B:362:VAL:N	2.91	0.41
1:A:341:VAL:HG11	1:A:397:ALA:HB1	2.02	0.41
2:H:18:LEU:HD11	2:H:20:LEU:HD11	2.01	0.41
3:L:2:ALA:N	3:L:97:VAL:HG13	2.36	0.41
1:B:393:THR:HA	1:B:522:ALA:HA	2.02	0.41
1:B:382:VAL:HG22	1:B:430:THR:OG1	2.21	0.41
2:H:3:THR:HB	2:H:25:SER:HB2	2.02	0.41
2:H:170:LEU:HD13	2:H:176:TYR:CZ	2.56	0.41
1:A:353:TRP:CD1	1:A:353:TRP:H	2.39	0.41
1:A:359:SER:HA	1:A:524:VAL:CG2	2.51	0.41
1:B:362:VAL:HA	1:B:525:CYS:O	2.21	0.40
2:H:38:ARG:HB3	2:H:48:ILE:HD11	2.03	0.40
2:H:37:ILE:O	2:H:91:TYR:N	2.38	0.40
1:B:430:THR:HG23	1:B:430:THR:O	2.21	0.40
3:L:13:SER:OG	3:L:14:THR:N	2.54	0.40
3:N:35:TRP:CH2	3:N:88:CYS:HB3	2.56	0.40
3:N:179:LEU:CG	3:N:181:LEU:HD11	2.51	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	190/231 (82%)	179 (94%)	11 (6%)	0	100	100
1	B	168/231 (73%)	158 (94%)	10 (6%)	0	100	100
2	H	211/223 (95%)	200 (95%)	11 (5%)	0	100	100
2	M	210/223 (94%)	199 (95%)	11 (5%)	0	100	100
3	L	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
3	N	209/216 (97%)	205 (98%)	4 (2%)	0	100	100
All	All	1197/1340 (89%)	1145 (96%)	52 (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	148/203 (73%)	148 (100%)	0	100	100
1	B	105/203 (52%)	105 (100%)	0	100	100
2	H	162/190 (85%)	162 (100%)	0	100	100
2	M	168/190 (88%)	168 (100%)	0	100	100
3	L	163/181 (90%)	163 (100%)	0	100	100
3	N	158/181 (87%)	158 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	904/1148 (79%)	904 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	501	ASN
1	B	394	ASN
1	B	414	GLN
2	H	58	ASN
3	L	79	GLN
2	M	164	HIS
3	N	31	ASN
3	N	127	GLN
3	N	171	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1501	1	14,14,15	1.24	1 (7%)	17,19,21	2.85	3 (17%)
4	NAG	B	1501	1	14,14,15	1.28	1 (7%)	17,19,21	2.57	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1501	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1501	1	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1501	NAG	O5-C1	4.58	1.51	1.43
4	A	1501	NAG	O5-C1	4.47	1.51	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1501	NAG	C1-O5-C5	10.18	125.83	112.19
4	A	1501	NAG	C1-O5-C5	9.84	125.37	112.19
4	A	1501	NAG	C2-N2-C7	4.90	129.46	122.90
4	A	1501	NAG	C1-C2-N2	2.60	114.53	110.43

There are no chirality outliers.

All (9) torsion outliers are listed below:

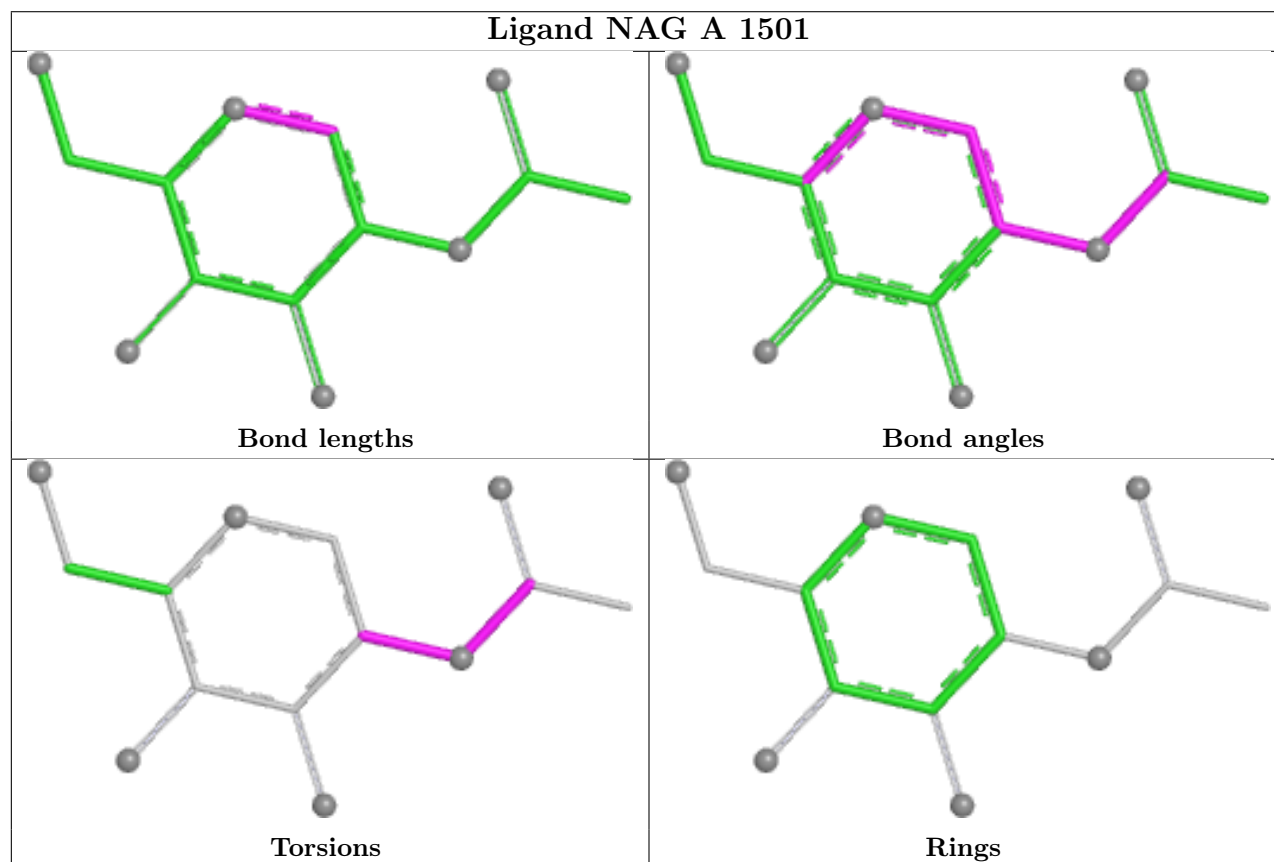
Mol	Chain	Res	Type	Atoms
4	B	1501	NAG	O5-C5-C6-O6
4	A	1501	NAG	C8-C7-N2-C2
4	A	1501	NAG	O7-C7-N2-C2
4	B	1501	NAG	C8-C7-N2-C2
4	B	1501	NAG	O7-C7-N2-C2
4	A	1501	NAG	C1-C2-N2-C7
4	B	1501	NAG	C4-C5-C6-O6
4	A	1501	NAG	C3-C2-N2-C7
4	B	1501	NAG	C1-C2-N2-C7

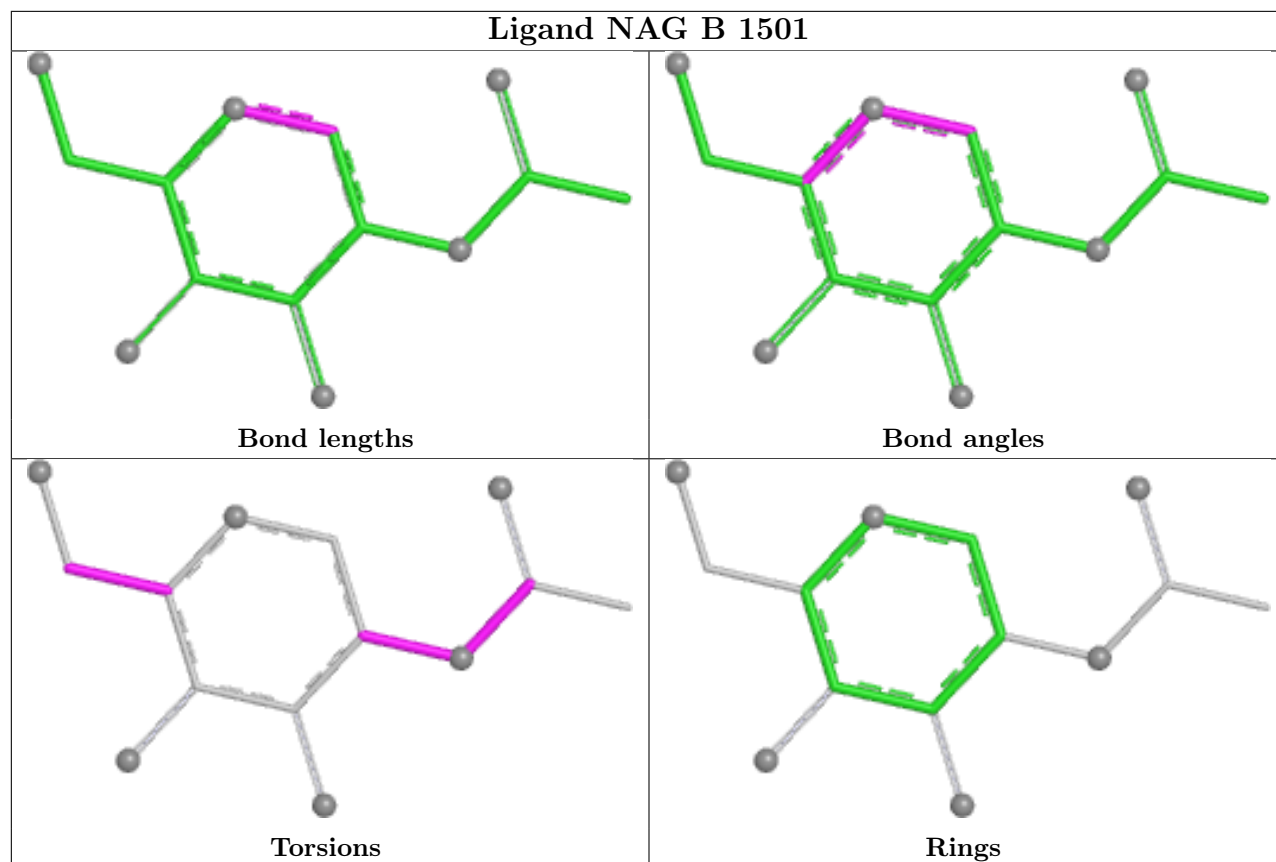
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1501	NAG	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, 95th 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	194/231 (83%)	0.63	17 (8%) 15 13	24, 37, 79, 100	0
1	B	182/231 (78%)	1.82	72 (39%) 1 0	38, 74, 115, 145	0
2	H	217/223 (97%)	0.60	20 (9%) 14 12	21, 37, 73, 85	0
2	M	216/223 (96%)	0.55	9 (4%) 40 37	22, 42, 74, 96	0
3	L	211/216 (97%)	0.39	9 (4%) 40 36	19, 38, 61, 87	0
3	N	211/216 (97%)	0.86	20 (9%) 14 11	22, 54, 80, 97	0
All	All	1231/1340 (91%)	0.79	147 (11%) 9 7	19, 45, 87, 145	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	HIS	6.2
1	B	360	ASN	6.0
1	A	520	ALA	5.5
1	B	384	PRO	5.2
1	B	366	SER	5.2
1	B	359	SER	5.2
1	B	526	GLY	5.2
2	M	131	THR	5.1
3	L	108	GLY	5.1
1	B	440	ASN	4.9
2	H	132	SER	4.6
3	N	181	LEU	4.6
1	B	442	ASP	4.5
2	H	29	LEU	4.3
1	B	334	ASN	4.3
1	B	438	SER	4.2
1	B	500	THR	4.1
1	B	501	ASN	4.1
3	N	13	SER	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	382	VAL	4.0
2	H	189	LEU	3.9
2	H	31	SER	3.9
1	B	432	CYS	3.9
3	N	2	ALA	3.8
1	A	391	CYS	3.7
1	B	523	THR	3.7
1	B	407	VAL	3.6
1	B	507	PRO	3.6
1	B	525	CYS	3.5
1	B	502	GLY	3.5
3	N	107	LEU	3.4
2	H	135	THR	3.4
3	L	2	ALA	3.3
3	L	143	GLY	3.3
2	H	131	THR	3.3
1	B	513	LEU	3.3
2	M	9	PRO	3.3
1	B	433	VAL	3.3
3	L	40	PRO	3.2
1	B	336	CYS	3.2
1	B	509	ARG	3.2
1	B	443	SER	3.2
1	B	335	LEU	3.1
2	M	29	LEU	3.1
1	B	361	CYS	3.1
3	N	23	CYS	3.1
1	B	365	TYR	3.1
1	B	338	PHE	3.1
1	B	369	TYR	3.1
1	B	451	TYR	3.1
2	M	7	SER	3.1
1	B	450	ASN	3.1
1	A	366	SER	3.1
1	B	345	THR	3.0
2	M	191	THR	3.0
1	B	344	ALA	3.0
2	H	42	GLY	2.9
1	B	347	PHE	2.9
2	H	129	LYS	2.9
1	B	358	ILE	2.8
3	N	25	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	391	CYS	2.7
1	B	436	TRP	2.7
1	B	405	ASP	2.7
1	B	498	GLN	2.7
1	A	334	ASN	2.7
3	N	68	GLY	2.7
1	B	350	VAL	2.7
1	B	376	THR	2.7
2	H	134	GLY	2.7
1	B	388	ASN	2.7
1	B	408	ARG	2.7
1	B	393	THR	2.7
3	N	204	GLU	2.6
1	B	437	ASN	2.6
1	B	521	PRO	2.6
1	A	379	CYS	2.6
1	A	449	TYR	2.6
1	A	496	GLY	2.6
2	H	160	THR	2.5
3	L	129	ASN	2.5
1	A	335	LEU	2.5
1	B	497	PHE	2.5
1	B	466	ARG	2.5
1	B	381	GLY	2.5
1	B	349	SER	2.5
2	H	30	SER	2.5
2	M	128	SER	2.5
3	N	21	ILE	2.5
1	B	449	TYR	2.4
3	N	106	VAL	2.4
1	A	371	SER	2.4
1	B	337	PRO	2.4
3	N	143	GLY	2.4
1	B	441	LEU	2.4
3	N	14	THR	2.4
3	N	142	PRO	2.4
1	B	503	VAL	2.4
2	H	32	VAL	2.4
1	B	368	LEU	2.4
1	B	371	SER	2.4
2	M	127	SER	2.4
1	B	364	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	18	ARG	2.4
1	B	387	LEU	2.3
1	B	508	TYR	2.3
1	A	338	PHE	2.3
1	B	524	VAL	2.3
1	A	365	TYR	2.3
1	A	346	ARG	2.3
2	H	54	SER	2.3
1	A	372	ALA	2.2
1	B	478	THR	2.2
1	B	343	ASN	2.2
3	N	76	SER	2.2
1	B	377	PHE	2.2
2	H	1	GLN	2.2
1	A	364	ASP	2.2
2	M	190	GLY	2.2
2	H	7	SER	2.2
3	L	3	VAL	2.2
3	N	55	PRO	2.2
1	B	386	LYS	2.2
2	H	10	GLY	2.2
2	H	137	ALA	2.1
3	N	95	LEU	2.1
3	N	92	ASP	2.1
3	L	122	SER	2.1
2	H	9	PRO	2.1
1	A	369	TYR	2.1
3	L	144	ALA	2.1
2	H	185	PRO	2.1
3	N	78	LEU	2.1
1	B	354	ASN	2.1
1	B	504	GLY	2.1
3	N	95(A)	SER	2.1
2	M	21	THR	2.1
1	A	340	GLU	2.0
1	B	499	PRO	2.0
1	A	390	LEU	2.0
1	B	518	LEU	2.0
1	B	379	CYS	2.0
1	B	480	CYS	2.0
3	L	196	VAL	2.0
1	B	374	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	430	THR	2.0
2	H	164	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

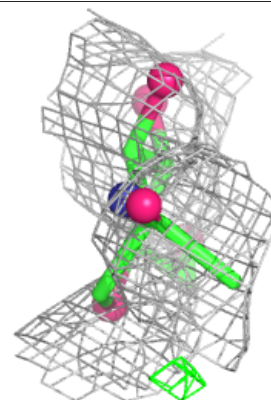
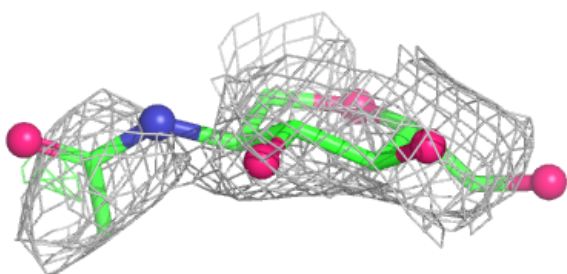
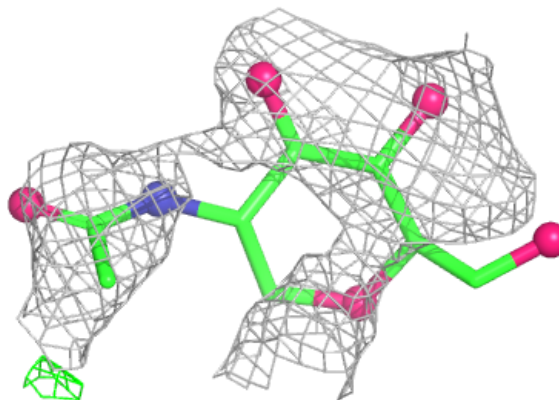
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	NAG	B	1501	14/15	0.48	0.23	125,129,131,131	0
4	NAG	A	1501	14/15	0.64	0.20	75,79,82,82	0

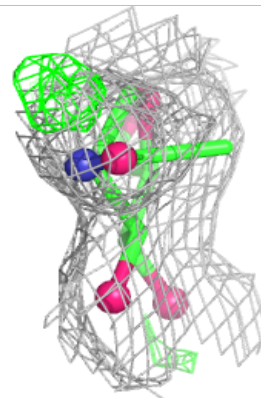
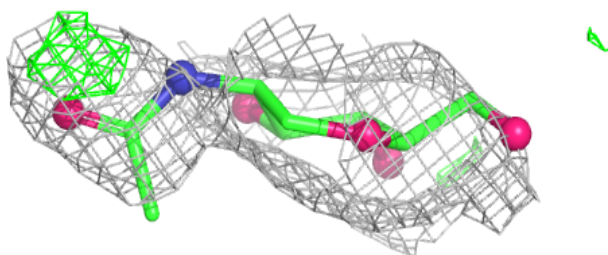
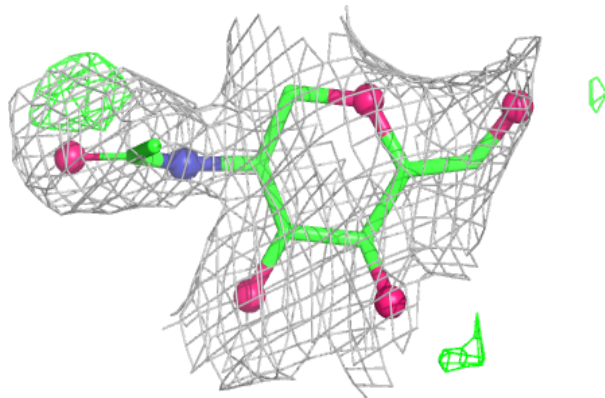
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG B 1501:

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

**Electron density around NAG A 1501:**

$2mF_o-DF_c$ (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.