



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:31 PM UTC

PDB ID : 9DRU / pdb_00009dru
Title : Crystal structure of 04709_4F04 Fab in complex with H1 HA from A/California/04/2009(H1N1)
Authors : Lin, T.H.; Wilson, I.A.
Deposited on : 2024-09-26
Resolution : 2.75 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

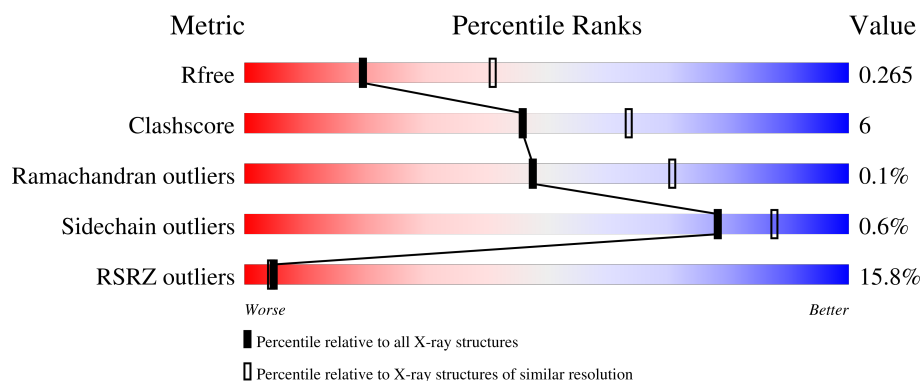
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	330	
2	B	175	
3	H	227	
4	L	209	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7415 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2575	1628	443	493	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	-	expression tag	UNP A0A6M3Z334
A	9	PRO	-	expression tag	UNP A0A6M3Z334
A	10	GLY	-	expression tag	UNP A0A6M3Z334
A	131	ASP	GLU	conflict	UNP A0A6M3Z334
A	194	LEU	ILE	conflict	UNP A0A6M3Z334
A	329	ILE	-	expression tag	UNP A0A6M3Z334

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A6J3XB93

- Molecule 3 is a protein called 04709_4F04, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	227	Total	C	N	O	S	0	0	0
			1692	1068	285	332	7			

- Molecule 4 is a protein called 04709_4F04, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	209	Total	C	N	O	S	0	0	0
			1594	1003	264	322	5			

- Molecule 5 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
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

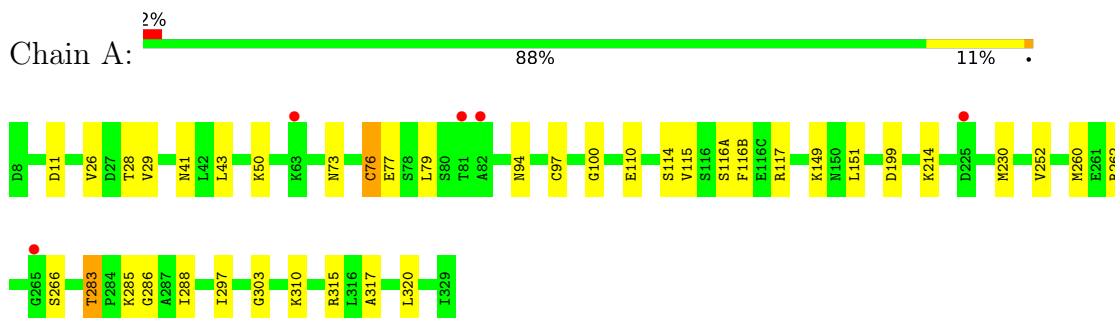
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total	O	0	0
			43	43		
6	B	38	Total	O	0	0
			38	38		
6	H	29	Total	O	0	0
			29	29		
6	L	10	Total	O	0	0
			10	10		

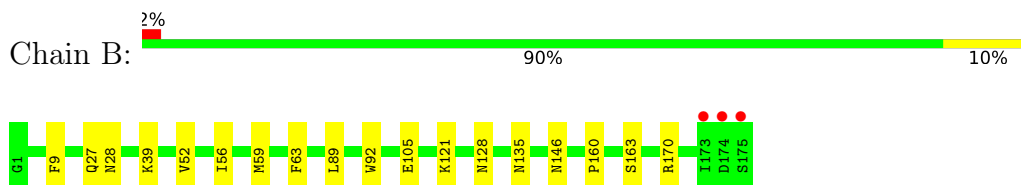
3 Residue-property plots

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.

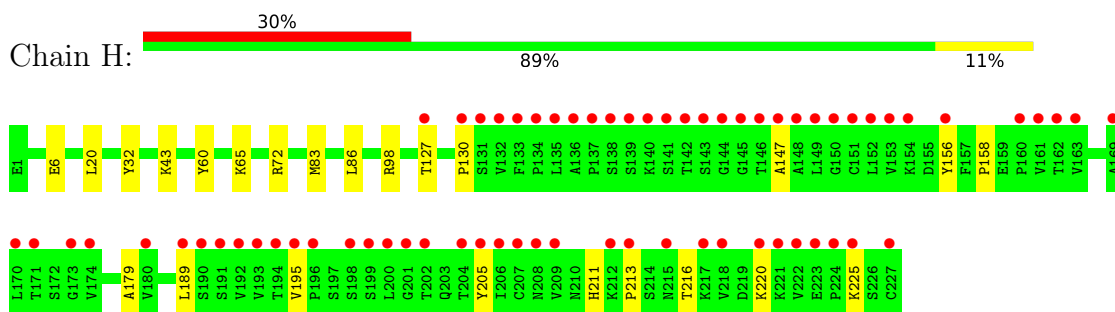
- Molecule 1: Hemagglutinin HA1 chain



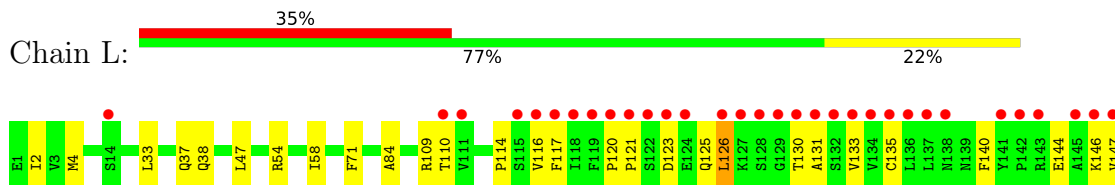
- Molecule 2: Hemagglutinin HA2 chain

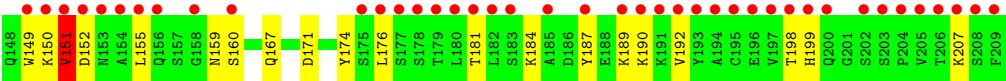


- Molecule 3: 04709_4F04, heavy chain



- Molecule 4: 04709_4F04, light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.40Å 115.40Å 206.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.98 – 2.75 29.98 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.98-2.75) 97.9 (29.98-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.76Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, R_{free}	0.212 , 0.265 0.212 , 0.265	Depositor DCC
R_{free} test set	2032 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7415	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.12	0/2640	0.32	0/3589
2	B	0.16	0/1434	0.32	0/1932
3	H	0.12	0/1734	0.30	0/2361
4	L	0.17	0/1630	0.44	0/2217
All	All	0.14	0/7438	0.34	0/10099

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	2575	0	2524	27	0
2	B	1406	0	1325	13	0
3	H	1692	0	1654	16	0
4	L	1594	0	1555	35	0
5	A	14	0	13	2	0
5	B	14	0	13	0	0
6	A	43	0	0	1	0
6	B	38	0	0	0	0
6	H	29	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	10	0	0	0	0
All	All	7415	0	7084	83	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 (83) 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:A:29:VAL:HG12	2:B:105:GLU:HG3	1.49	0.95
1:A:28:THR:HB	2:B:105:GLU:HG2	1.62	0.82
3:H:127:THR:HG22	3:H:158:PRO:HD3	1.69	0.73
4:L:121:PRO:HB3	4:L:131:ALA:HB1	1.70	0.72
4:L:189:LYS:O	4:L:190:LYS:HD2	1.90	0.71
1:A:97:CYS:HB3	5:A:401:NAG:H81	1.73	0.70
4:L:159:ASN:ND2	4:L:181:THR:O	2.22	0.70
1:A:115:VAL:HG11	1:A:116(B):PHE:HB2	1.72	0.70
1:A:199:ASP:OD1	1:A:214:LYS:NZ	2.25	0.69
4:L:123:ASP:HA	4:L:126:LEU:HG	1.74	0.68
1:A:11:ASP:HB3	2:B:27:GLN:O	1.97	0.64
1:A:283:THR:HG22	1:A:285:LYS:H	1.62	0.64
4:L:126:LEU:HA	4:L:184:LYS:HE3	1.80	0.63
3:H:225:LYS:HE3	4:L:120:PRO:HG3	1.81	0.62
1:A:94:ASN:HD22	5:A:401:NAG:H83	1.65	0.62
4:L:126:LEU:HD22	4:L:184:LYS:NZ	2.15	0.61
4:L:151:VAL:HG13	4:L:152:ASP:H	1.64	0.60
4:L:184:LYS:HZ3	4:L:187:TYR:HD2	1.50	0.60
4:L:140:PHE:HB2	4:L:199:HIS:CE1	2.39	0.58
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.87	0.57
4:L:144:GLU:HG2	4:L:146:LYS:HZ1	1.69	0.57
4:L:121:PRO:HG2	4:L:187:TYR:CE1	2.41	0.56
4:L:126:LEU:HD22	4:L:184:LYS:HZ1	1.72	0.55
4:L:54:ARG:HG2	4:L:58:ILE:HB	1.88	0.54
4:L:151:VAL:O	4:L:192:VAL:O	2.25	0.54
4:L:144:GLU:HG2	4:L:146:LYS:NZ	2.22	0.54
1:A:283:THR:HB	1:A:286:GLY:O	2.09	0.53
1:A:310:LYS:HG3	2:B:89:LEU:HD11	1.89	0.53
3:H:211:HIS:CD2	3:H:213:PRO:HD2	2.42	0.53
4:L:121:PRO:HG3	4:L:133:VAL:HG22	1.90	0.52
4:L:116:VAL:HG23	4:L:207:LYS:HD3	1.92	0.51
1:A:288:ILE:HG21	1:A:297:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6:GLU:N	3:H:6:GLU:OE1	2.43	0.51
1:A:100:GLY:HA3	1:A:230:MET:O	2.10	0.51
1:A:114:SER:HB2	1:A:266:SER:HB2	1.91	0.51
1:A:41:ASN:ND2	1:A:43:LEU:O	2.37	0.50
1:A:41:ASN:HB2	1:A:315:ARG:NH1	2.26	0.50
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.93	0.50
1:A:303:GLY:HA2	2:B:63:PHE:CE1	2.47	0.49
4:L:146:LYS:HB2	4:L:198:THR:HB	1.92	0.49
4:L:171:ASP:OD1	4:L:171:ASP:N	2.42	0.48
3:H:98:ARG:NH2	6:H:303:HOH:O	2.41	0.47
4:L:147:VAL:HG21	4:L:176:LEU:HD22	1.97	0.47
2:B:28:ASN:HD21	2:B:146:ASN:HD22	1.63	0.47
3:H:147:ALA:HA	4:L:117:PHE:HE2	1.79	0.47
3:H:130:PRO:HB3	3:H:156:TYR:HB3	1.96	0.47
4:L:109:ARG:NH2	4:L:110:THR:OG1	2.47	0.47
3:H:20:LEU:HG	3:H:83:MET:HE2	1.97	0.46
4:L:114:PRO:HD3	4:L:199:HIS:ND1	2.31	0.46
4:L:150:LYS:HD2	4:L:150:LYS:HA	1.73	0.46
3:H:60:TYR:HB2	3:H:65:LYS:HG3	1.98	0.45
1:A:73:ASN:HB3	1:A:76:CYS:SG	2.56	0.45
4:L:2:ILE:HG22	4:L:4:MET:HE3	1.97	0.45
1:A:260:MET:HE2	1:A:262:ARG:HG3	1.98	0.45
2:B:59:MET:HE1	2:B:92:TRP:CZ3	2.51	0.45
1:A:77:GLU:HG2	1:A:149:LYS:HD2	1.99	0.44
1:A:151:LEU:HB3	1:A:252:VAL:HG12	1.99	0.44
2:B:9:PHE:O	2:B:135:ASN:HA	2.16	0.44
1:A:117:ARG:HH12	1:A:149:LYS:NZ	2.16	0.44
4:L:135:CYS:HB2	4:L:149:TRP:CH2	2.52	0.44
4:L:159:ASN:OD1	4:L:160:SER:N	2.50	0.44
4:L:38:GLN:O	4:L:84:ALA:HB1	2.18	0.43
3:H:195:VAL:HG11	3:H:205:TYR:CE1	2.53	0.43
4:L:33:LEU:HD22	4:L:71:PHE:CG	2.53	0.43
1:A:116(A):SER:O	1:A:260:MET:HA	2.19	0.43
1:A:310:LYS:HD2	2:B:89:LEU:HD21	2.00	0.43
1:A:110:GLU:OE1	6:A:501:HOH:O	2.21	0.42
2:B:128:ASN:HB3	2:B:170:ARG:NH2	2.35	0.42
4:L:150:LYS:NZ	4:L:155:LEU:HD23	2.34	0.42
2:B:39:LYS:HE2	2:B:121:LYS:HZ1	1.84	0.42
2:B:160:PRO:HA	2:B:163:SER:HB3	2.02	0.42
4:L:184:LYS:NZ	4:L:187:TYR:CD2	2.87	0.42
1:A:76:CYS:HB3	1:A:79:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:43:LYS:HA	3:H:43:LYS:HD3	1.90	0.42
4:L:167:GLN:HG3	4:L:174:TYR:CE2	2.55	0.42
3:H:220:LYS:HD2	3:H:220:LYS:HA	1.91	0.41
3:H:130:PRO:HD2	3:H:216:THR:HG21	2.02	0.41
1:A:50:LYS:O	1:A:286:GLY:HA2	2.21	0.41
3:H:32:TYR:O	3:H:72:ARG:NH2	2.53	0.41
2:B:52:VAL:O	2:B:56:ILE:HG13	2.21	0.41
4:L:125:GLN:HG2	4:L:130:THR:O	2.22	0.40
1:A:26:VAL:HG21	1:A:317:ALA:HB2	2.04	0.40
3:H:179:ALA:HA	3:H:189:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	328/330 (99%)	321 (98%)	7 (2%)	0	100	100
2	B	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
3	H	225/227 (99%)	221 (98%)	4 (2%)	0	100	100
4	L	207/209 (99%)	184 (89%)	22 (11%)	1 (0%)	24	43
All	All	933/941 (99%)	897 (96%)	35 (4%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	151	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/290 (100%)	287 (99%)	3 (1%)	68	81
2	B	150/150 (100%)	150 (100%)	0	100	100
3	H	190/190 (100%)	190 (100%)	0	100	100
4	L	180/180 (100%)	178 (99%)	2 (1%)	65	79
All	All	810/810 (100%)	805 (99%)	5 (1%)	78	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	CYS
1	A	283	THR
1	A	320	LEU
4	L	126	LEU
4	L	151	VAL

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	150	ASN
1	A	275	HIS
2	B	62	GLN
2	B	146	ASN
3	H	30	ASN
3	H	39	GLN
3	H	77	ASN
4	L	37	GLN
4	L	38	GLN

5.3.3 RNA ⓘ

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	$\# Z > 2$
5	NAG	A	401	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
5	NAG	B	201	2	14,14,15	0.71	0	17,19,21	0.96	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
5	NAG	A	401	1	-	3/6/23/26	0/1/1/1
5	NAG	B	201	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	NAG	C1-O5-C5	2.23	115.18	112.19
5	B	201	NAG	C1-O5-C5	2.21	115.15	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

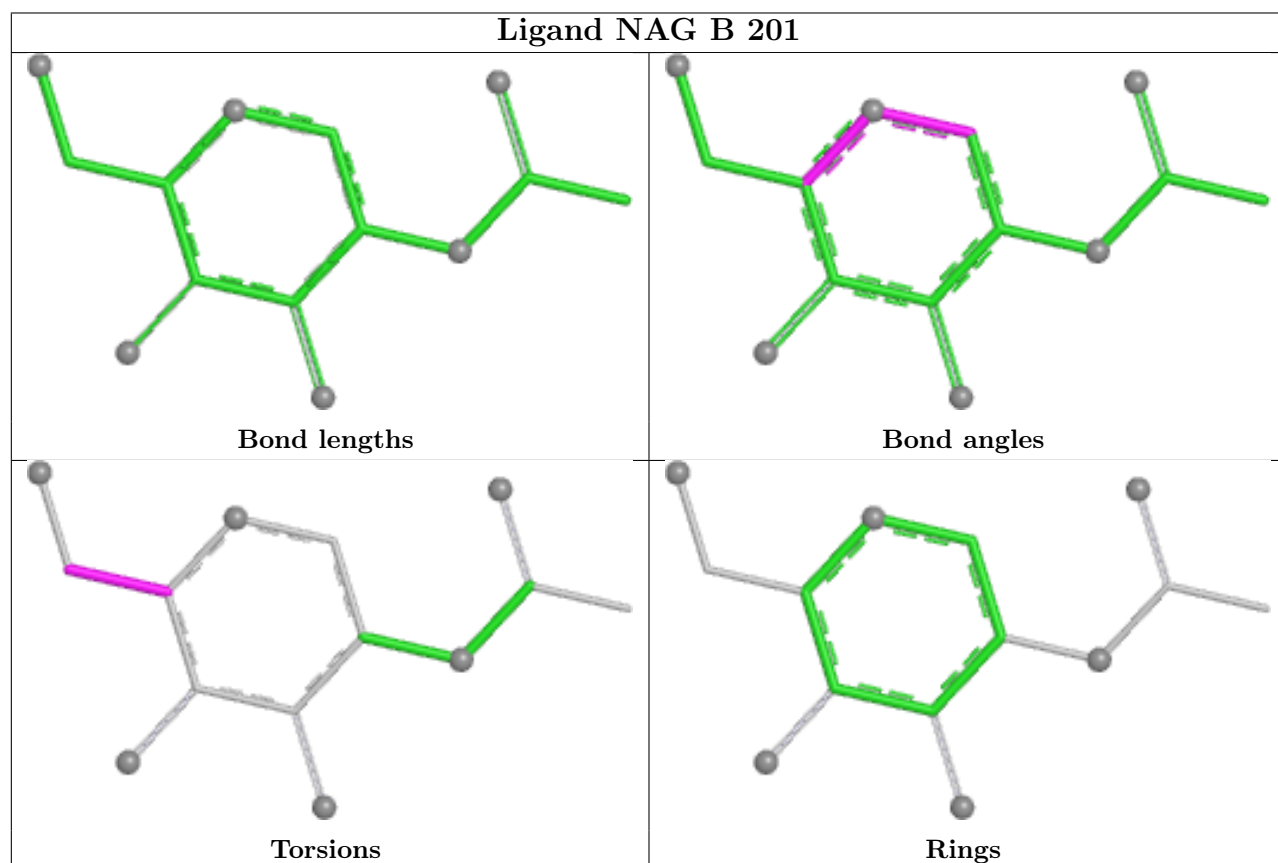
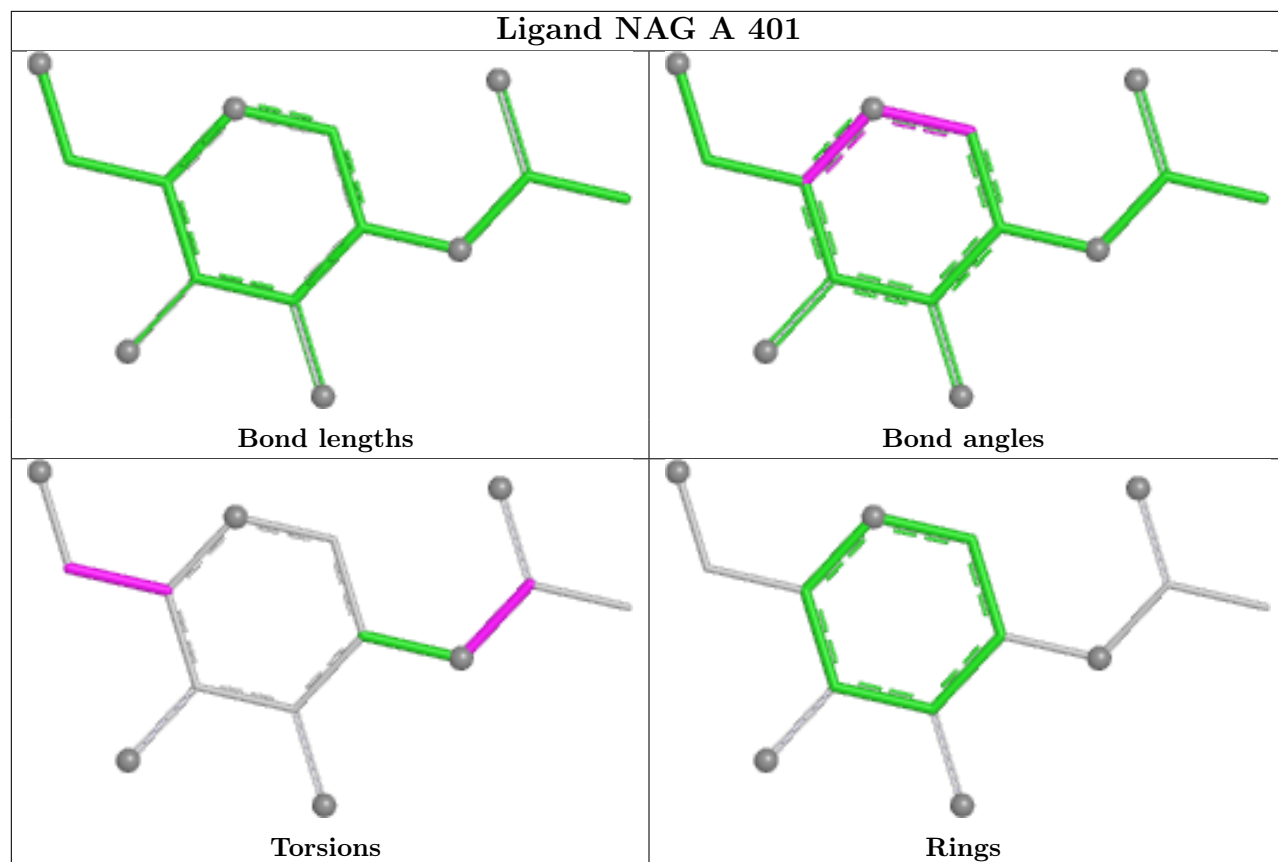
Mol	Chain	Res	Type	Atoms
5	A	401	NAG	C8-C7-N2-C2
5	A	401	NAG	O7-C7-N2-C2
5	A	401	NAG	O5-C5-C6-O6
5	B	201	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	NAG	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.



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	330/330 (100%)	-0.07	5 (1%) 72 71	24, 46, 69, 105	0
2	B	175/175 (100%)	-0.22	3 (1%) 69 67	21, 36, 69, 94	0
3	H	227/227 (100%)	1.21	68 (29%) 1 1	24, 55, 150, 175	0
4	L	209/209 (100%)	1.54	73 (34%) 1 0	27, 75, 125, 164	0
All	All	941/941 (100%)	0.57	149 (15%) 5 4	21, 48, 129, 175	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	136	ALA	7.2
3	H	135	LEU	7.0
4	L	209	PHE	7.0
4	L	133	VAL	7.0
4	L	205	VAL	6.6
3	H	142	THR	6.5
3	H	134	PRO	6.4
3	H	218	VAL	6.3
3	H	132	VAL	6.1
3	H	194	THR	6.0
3	H	138	SER	5.9
3	H	141	SER	5.4
4	L	195	CYS	5.3
4	L	194	ALA	5.3
3	H	143	SER	5.2
4	L	155	LEU	5.2
3	H	193	VAL	5.1
3	H	149	LEU	5.1
3	H	200	LEU	5.1
3	H	205	TYR	5.0
4	L	145	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
3	H	222	VAL	5.0
3	H	202	THR	4.9
4	L	185	ALA	4.8
4	L	152	ASP	4.7
4	L	134	VAL	4.7
3	H	148	ALA	4.7
4	L	118	ILE	4.7
4	L	187	TYR	4.7
3	H	161	VAL	4.6
3	H	133	PHE	4.6
3	H	137	PRO	4.5
4	L	197	VAL	4.4
3	H	196	PRO	4.4
3	H	151	CYS	4.4
4	L	192	VAL	4.3
4	L	119	PHE	4.3
3	H	195	VAL	4.2
4	L	204	PRO	4.2
4	L	151	VAL	4.2
3	H	170	LEU	4.1
4	L	202	SER	4.1
4	L	123	ASP	4.0
4	L	207	LYS	3.9
4	L	126	LEU	3.9
3	H	227	CYS	3.9
4	L	181	THR	3.9
3	H	190	SER	3.9
4	L	180	LEU	3.8
4	L	153	ASN	3.8
3	H	169	ALA	3.8
3	H	152	LEU	3.8
4	L	147	VAL	3.8
3	H	139	SER	3.6
4	L	132	SER	3.5
4	L	177	SER	3.5
4	L	179	THR	3.5
3	H	224	PRO	3.5
4	L	120	PRO	3.5
3	H	209	VAL	3.5
3	H	131	SER	3.4
1	A	81	THR	3.4
3	H	174	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
3	H	204	THR	3.4
3	H	206	ILE	3.3
3	H	150	GLY	3.3
3	H	192	VAL	3.3
2	B	173	ILE	3.3
4	L	156	GLN	3.2
3	H	153	VAL	3.2
3	H	198	SER	3.1
4	L	178	SER	3.1
3	H	212	LYS	3.1
4	L	160	SER	3.1
4	L	193	TYR	3.1
3	H	144	GLY	3.1
3	H	199	SER	3.0
4	L	121	PRO	3.0
4	L	14	SER	3.0
4	L	137	LEU	3.0
3	H	221	LYS	3.0
4	L	176	LEU	2.9
3	H	213	PRO	2.9
4	L	128	SER	2.9
4	L	203	SER	2.9
4	L	136	LEU	2.9
4	L	200	GLN	2.9
4	L	206	THR	2.9
1	A	63	LYS	2.9
3	H	189	LEU	2.9
4	L	199	HIS	2.9
1	A	265	GLY	2.9
4	L	130	THR	2.8
3	H	220	LYS	2.8
3	H	173	GLY	2.8
4	L	208	SER	2.8
4	L	124	GLU	2.8
4	L	149	TRP	2.8
4	L	196	GLU	2.8
3	H	201	GLY	2.7
4	L	122	SER	2.7
3	H	130	PRO	2.7
4	L	143	ARG	2.7
3	H	140	LYS	2.6
3	H	160	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
4	L	117	PHE	2.6
2	B	175	SER	2.6
4	L	190	LYS	2.6
3	H	215	ASN	2.6
4	L	138	ASN	2.6
1	A	82	ALA	2.5
4	L	141	TYR	2.5
3	H	146	THR	2.5
4	L	183	SER	2.5
3	H	162	THR	2.5
3	H	171	THR	2.5
4	L	146	LYS	2.5
3	H	223	GLU	2.5
4	L	154	ALA	2.5
3	H	145	GLY	2.4
4	L	129	GLY	2.4
2	B	174	ASP	2.4
4	L	131	ALA	2.4
4	L	116	VAL	2.4
4	L	182	LEU	2.3
3	H	154	LYS	2.3
4	L	115	SER	2.3
4	L	189	LYS	2.3
4	L	150	LYS	2.3
3	H	191	SER	2.3
4	L	127	LYS	2.3
3	H	180	VAL	2.3
4	L	191	LYS	2.2
3	H	156	TYR	2.2
4	L	175	SER	2.2
3	H	217	LYS	2.2
1	A	225	ASP	2.2
3	H	225	LYS	2.2
3	H	163	VAL	2.2
4	L	110	THR	2.2
3	H	207	CYS	2.2
3	H	208	ASN	2.1
4	L	111	VAL	2.1
4	L	142	PRO	2.1
4	L	135	CYS	2.1
3	H	147	ALA	2.1
3	H	127	THR	2.1

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Mol	Chain	Res	Type	RSRZ
4	L	198	THR	2.0
4	L	158	GLY	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](#)

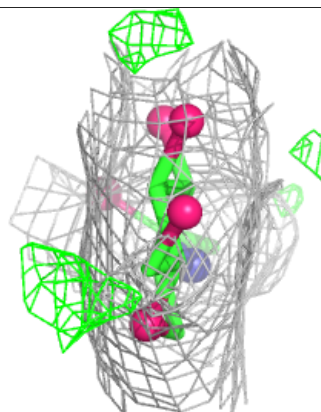
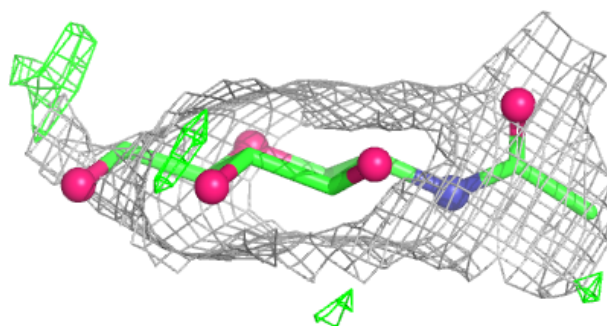
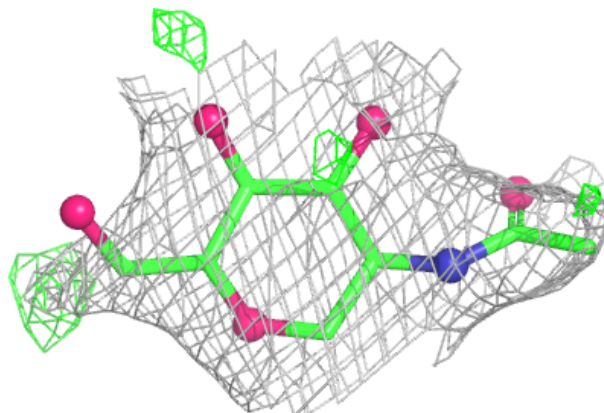
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	NAG	B	201	14/15	0.59	0.15	68,93,103,108	0
5	NAG	A	401	14/15	0.85	0.11	61,70,83,84	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.

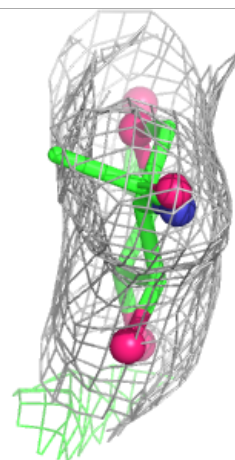
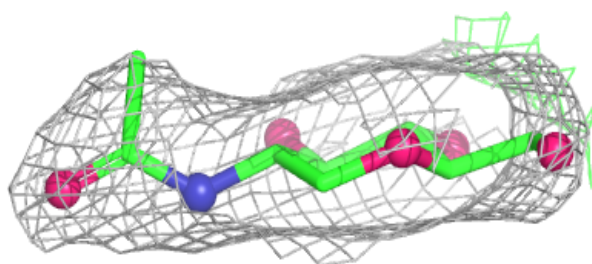
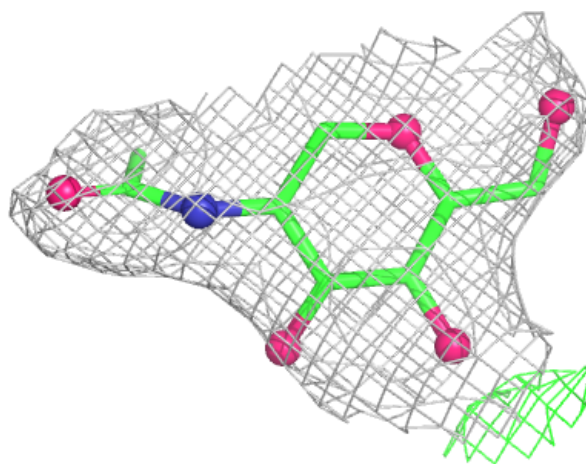
Electron density around NAG B 201:

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



Electron density around NAG A 401:

$2mF_o-DF_c$ (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.