



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:04 PM UTC

PDB ID : 7QIV / pdb_00007qiv
Title : Structure of human C3b in complex with the EWE nanobody
Authors : Pedersen, H.; Andersen, G.R.
Deposited on : 2021-12-16
Resolution : 2.80 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

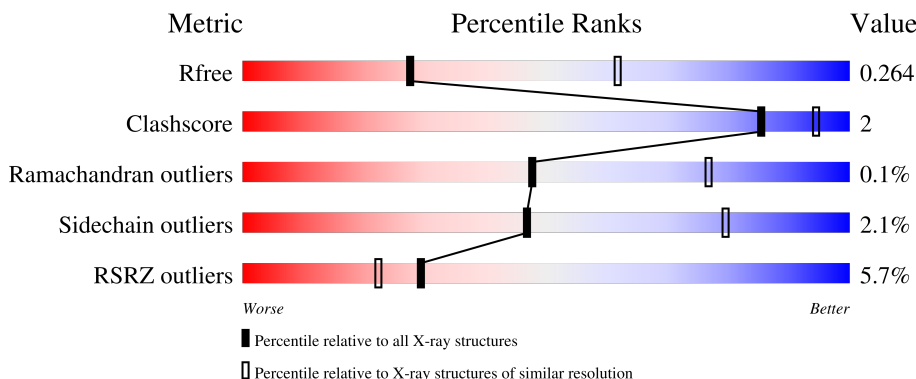
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	645	 2% 93% 6% •
2	B	915	 9% 90% 8% ••
3	C	133	 3% 84% 8% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13155 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4969	3164	843	947	15			

- Molecule 2 is a protein called Complement C3b alpha' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	903	Total	C	N	O	S	4	0	0
			7208	4569	1212	1389	38			

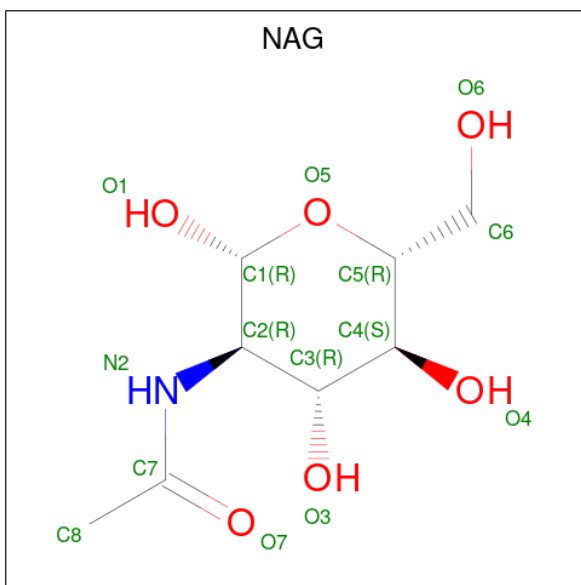
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	conflict	UNP P01024

- Molecule 3 is a protein called Nanobody EWE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	124	Total	C	N	O	S	1	0	0
			950	591	170	184	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

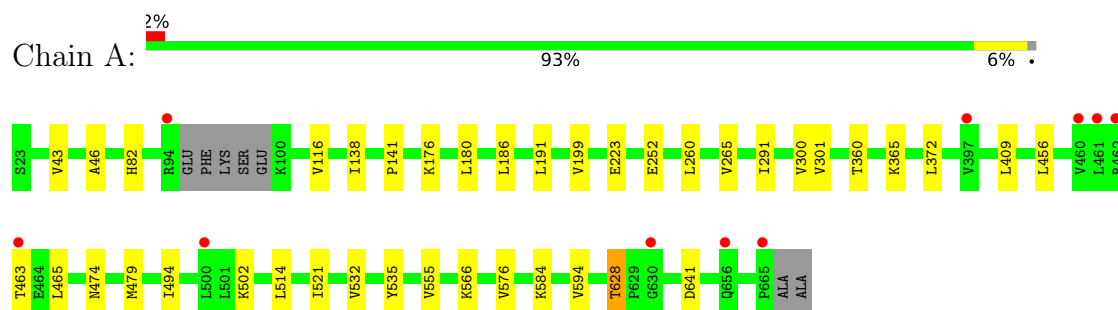


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	14	0
			14	8	1	5		
4	B	1	Total	C	N	O	14	0
			14	8	1	5		

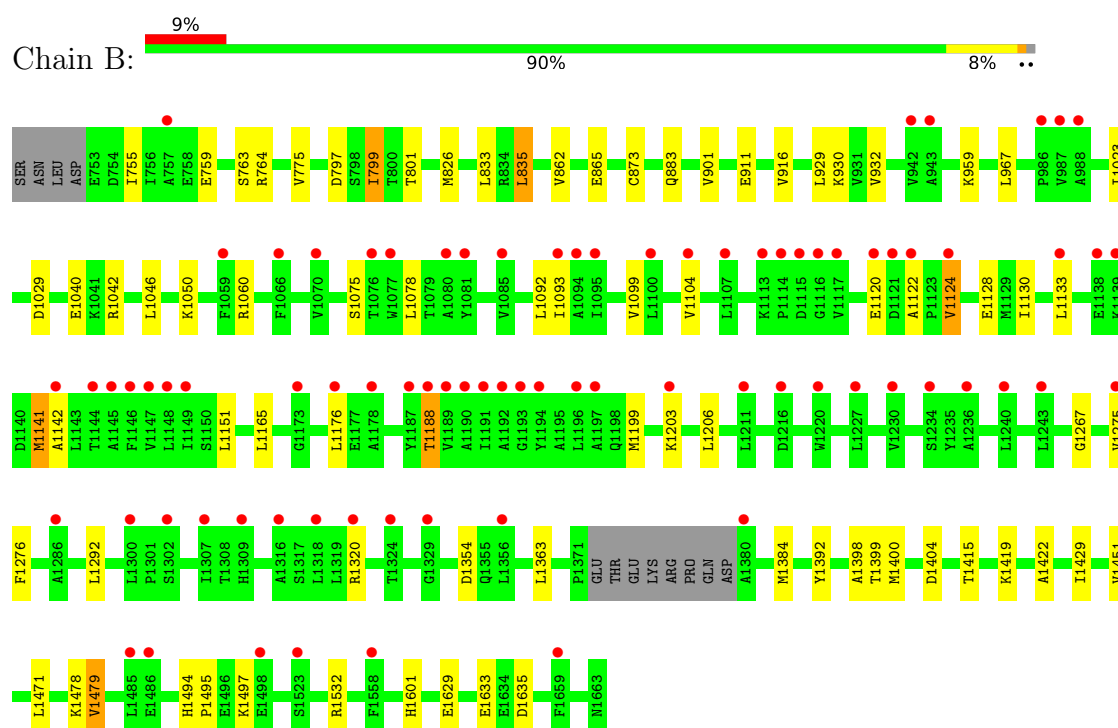
3 Residue-property plots

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.

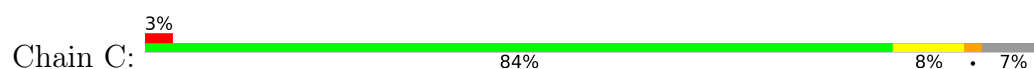
• Molecule 1: Complement C3 beta chain



• Molecule 2: Complement C3b alpha' chain



• Molecule 3: Nanobody EWE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	255.31Å 64.88Å 144.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.31 – 2.80 48.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.31-2.80) 98.6 (48.31-2.80)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.235 , 0.275 0.232 , 0.264	Depositor DCC
R_{free} test set	1607 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	83.2	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13155	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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	0.19	0/5069	0.41	0/6889
2	B	0.20	0/7352	0.44	0/9954
3	C	0.17	0/971	0.42	0/1313
All	All	0.19	0/13392	0.43	0/18156

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	4969	0	5031	18	0
2	B	7208	0	7135	38	1
3	C	950	0	901	6	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
All	All	13155	0	13093	58	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 2.

All (58) 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)
2:B:835:LEU:HG	2:B:929:LEU:HD23	1.83	0.61
2:B:1046:LEU:HG	2:B:1093:ILE:HD11	1.83	0.61
1:A:141:PRO:O	2:B:930:LYS:NZ	2.37	0.58
2:B:833:LEU:HG	2:B:835:LEU:HD13	1.87	0.57
3:C:102:ALA:HB3	3:C:116:TYR:HB2	1.87	0.57
2:B:1050:LYS:HG3	2:B:1093:ILE:HD13	1.87	0.57
2:B:1399:THR:OG1	2:B:1400:MET:N	2.38	0.56
1:A:594:VAL:HG12	2:B:775:VAL:HG22	1.89	0.56
1:A:474:ASN:HB3	1:A:514:LEU:HD11	1.88	0.54
2:B:862:VAL:HG22	2:B:916:VAL:HG12	1.90	0.53
2:B:1128:GLU:HB3	2:B:1267:GLY:HA2	1.90	0.53
2:B:1151:LEU:HB3	2:B:1165:LEU:HD11	1.91	0.53
2:B:1141:MET:HE2	2:B:1176:LEU:HD23	1.93	0.51
2:B:1203:LYS:HB2	2:B:1206:LEU:HG	1.91	0.51
1:A:372:LEU:HB2	1:A:409:LEU:HB2	1.94	0.50
2:B:1494:HIS:HD1	2:B:1497:LYS:HB2	1.76	0.49
2:B:1354:ASP:OD1	2:B:1354:ASP:N	2.41	0.49
1:A:494:ILE:HD12	1:A:502:LYS:HB3	1.95	0.48
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.95	0.48
1:A:260:LEU:O	2:B:801:THR:OG1	2.29	0.47
1:A:360:THR:HG21	1:A:372:LEU:HD23	1.96	0.47
1:A:291:ILE:HD13	1:A:300:VAL:HB	1.96	0.47
2:B:1029:ASP:OD2	2:B:1042:ARG:NH2	2.44	0.47
3:C:36:ASN:HA	3:C:57:ARG:HB2	1.96	0.47
1:A:628:THR:HB	1:A:641:ASP:HB3	1.96	0.47
2:B:1075:SER:HB3	2:B:1078:LEU:HB3	1.97	0.47
2:B:1060:ARG:NH1	2:B:1099:VAL:HG22	2.31	0.46
2:B:1363:LEU:HD22	2:B:1479:VAL:HG23	1.97	0.46
1:A:46:ALA:HB3	1:A:82:HIS:HB3	1.97	0.46
2:B:1532:ARG:NH2	2:B:1629:GLU:OE2	2.40	0.46
1:A:176:LYS:HA	2:B:1320:ARG:HH12	1.81	0.46
1:A:456:LEU:HB2	1:A:535:TYR:HE2	1.81	0.46
3:C:32:ILE:HD11	3:C:38:MET:HG3	1.98	0.46
1:A:566:LYS:HE3	1:A:584:LYS:HD2	1.98	0.45
3:C:95:THR:HG23	3:C:124:THR:HA	1.98	0.45
2:B:799:ILE:HG23	2:B:826:MET:HA	1.97	0.45
2:B:1601:HIS:ND1	2:B:1633:GLU:OE2	2.49	0.45
1:A:465:LEU:HD21	1:A:521:ILE:HG13	2.00	0.44
3:C:54:THR:HG21	3:C:108:PRO:HB2	2.00	0.44
2:B:873:CYS:HB3	2:B:901:VAL:HB	2.00	0.44
2:B:1124:VAL:HG11	2:B:1130:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:HG2	1:A:301:VAL:HG22	1.99	0.44
2:B:763:SER:OG	2:B:911:GLU:OE2	2.34	0.43
2:B:1384:MET:HE1	2:B:1495:PRO:HB3	1.99	0.43
2:B:1415:THR:HG22	2:B:1419:LYS:HE2	2.01	0.43
2:B:1120:GLU:HG3	2:B:1122:ALA:H	1.82	0.43
2:B:1104:VAL:HG13	2:B:1151:LEU:HD22	2.01	0.42
2:B:1392:TYR:CG	2:B:1398:ALA:HB2	2.55	0.42
3:C:56:ASN:HB2	3:C:61:ARG:H	1.84	0.42
1:A:138:ILE:HG13	1:A:223:GLU:HB3	2.00	0.42
1:A:479:MET:HE3	1:A:479:MET:HB2	1.90	0.42
2:B:1142:ALA:HB2	2:B:1188:THR:HG23	2.01	0.41
1:A:180:LEU:HD11	1:A:191:LEU:HD21	2.01	0.41
2:B:1203:LYS:H	2:B:1206:LEU:HD12	1.85	0.41
2:B:1023:ILE:HG13	2:B:1276:PHE:HB2	2.03	0.41
2:B:1422:ALA:HB2	2:B:1429:ILE:HB	2.03	0.41
2:B:1404:ASP:HB3	2:B:1478:LYS:HB3	2.03	0.41
2:B:865:GLU:HB2	2:B:883:GLN:HG2	2.03	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)
2:B:959:LYS:NZ	2:B:1635:ASP:OD2[3_455]	2.00	0.20

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	634/645 (98%)	616 (97%)	18 (3%)	0	100	100
2	B	899/915 (98%)	866 (96%)	32 (4%)	1 (0%)	48	77
3	C	122/133 (92%)	117 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1655/1693 (98%)	1599 (97%)	55 (3%)	1 (0%)	48 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1199	MET

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	562/567 (99%)	551 (98%)	11 (2%)	48 80
2	B	798/810 (98%)	781 (98%)	17 (2%)	47 79
3	C	98/107 (92%)	96 (98%)	2 (2%)	48 80
All	All	1458/1484 (98%)	1428 (98%)	30 (2%)	47 79

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	116	VAL
1	A	186	LEU
1	A	199	VAL
1	A	265	VAL
1	A	365	LYS
1	A	463	THR
1	A	532	VAL
1	A	555	VAL
1	A	576	VAL
1	A	628	THR
2	B	755	ILE
2	B	759	GLU
2	B	799	ILE
2	B	835	LEU

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Mol	Chain	Res	Type
2	B	932	VAL
2	B	967	LEU
2	B	1040	GLU
2	B	1092	LEU
2	B	1124	VAL
2	B	1133	LEU
2	B	1141	MET
2	B	1188	THR
2	B	1275	VAL
2	B	1292	LEU
2	B	1451	VAL
2	B	1471	LEU
2	B	1479	VAL
3	C	32	ILE
3	C	54	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	392	GLN
1	A	417	GLN
1	A	453	ASN
1	A	506	GLN
1	A	580	GLN
1	A	661	GLN
2	B	827	GLN
2	B	989	GLN
2	B	1061	GLN
2	B	1259	GLN
2	B	1299	GLN
2	B	1349	HIS
2	B	1503	ASN
2	B	1617	ASN
2	B	1642	ASN
3	C	122	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	$\# Z > 2$
4	NAG	A	2000	1	14,14,15	0.36	0	17,19,21	0.35	0
4	NAG	B	1701	2	14,14,15	0.33	0	17,19,21	0.46	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
4	NAG	A	2000	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1701	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2000	NAG	C4-C5-C6-O6
4	A	2000	NAG	O5-C5-C6-O6

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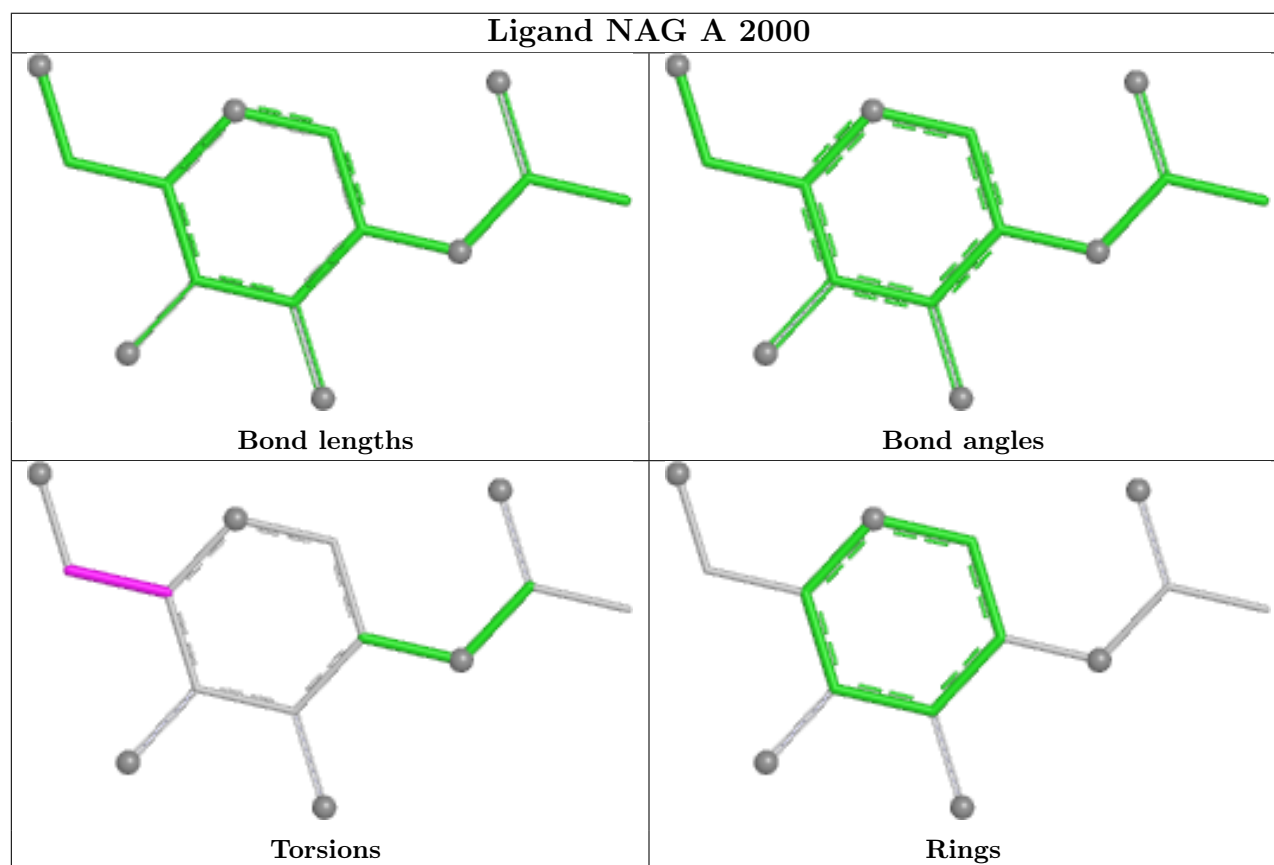
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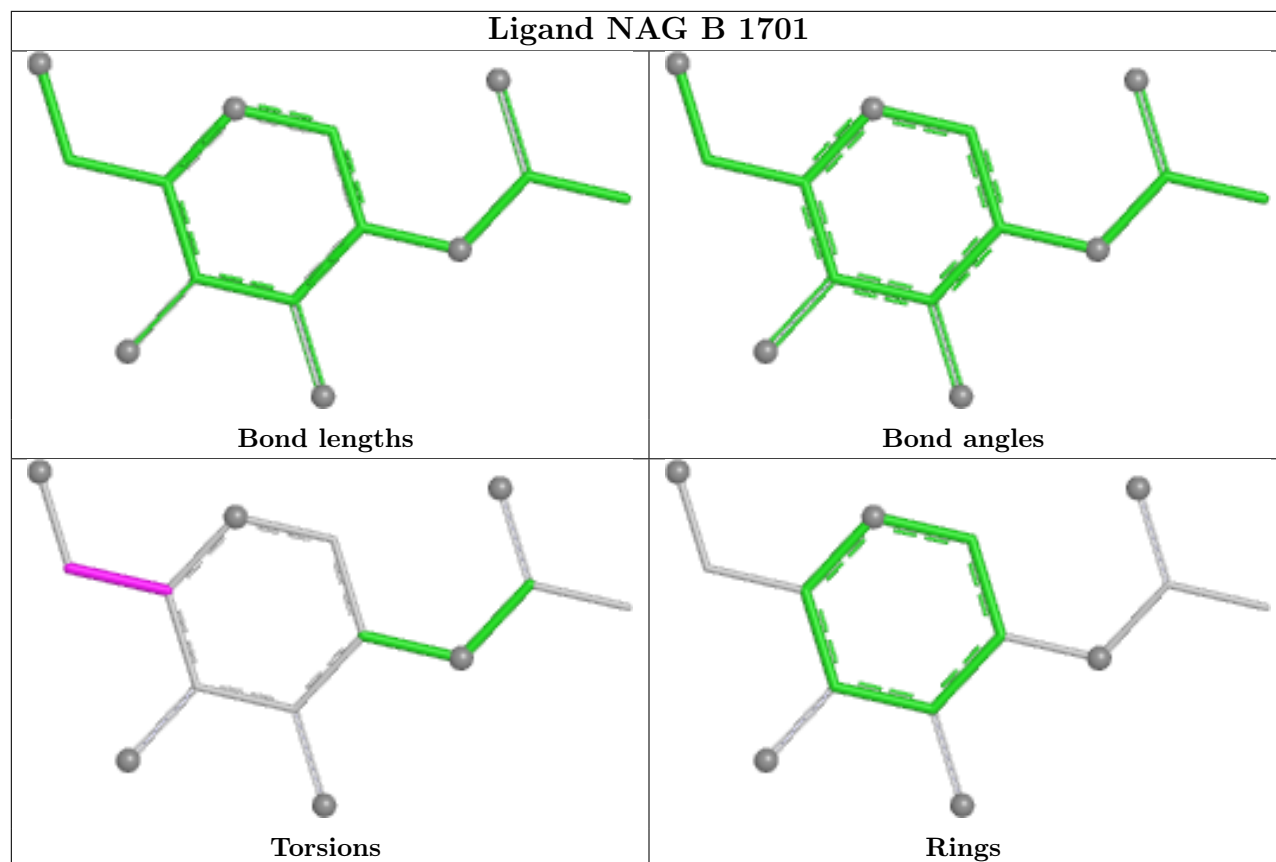
Mol	Chain	Res	Type	Atoms
4	B	1701	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	638/645 (98%)	0.03	10 (1%)	70 61	50, 85, 135, 191	0
2	B	903/915 (98%)	0.60	81 (8%)	15 11	49, 115, 202, 271	1 (0%)
3	C	124/133 (93%)	0.49	4 (3%)	50 40	86, 130, 180, 223	0
All	All	1665/1693 (98%)	0.38	95 (5%)	29 22	49, 102, 189, 271	1 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1196	LEU	6.3
1	A	462	ARG	4.9
1	A	461	LEU	4.9
2	B	1133	LEU	4.4
2	B	1142	ALA	4.3
2	B	1193	GLY	4.2
2	B	1122	ALA	4.1
2	B	1146	PHE	4.0
2	B	1104	VAL	3.7
2	B	1145	ALA	3.7
2	B	1380	ALA	3.6
2	B	1115	ASP	3.5
3	C	112	ASN	3.5
2	B	1148	LEU	3.5
2	B	1318	LEU	3.4
1	A	397	VAL	3.4
2	B	1197	ALA	3.4
2	B	1300	LEU	3.3
2	B	1203	LYS	3.2
3	C	128	HIS	3.2
2	B	987	VAL	3.2
2	B	1190	ALA	3.1
2	B	1194	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	986	PRO	3.1
2	B	1139	LYS	3.0
2	B	1076	THR	3.0
1	A	94	ARG	2.9
2	B	1189	VAL	2.9
2	B	1558	PHE	2.9
2	B	1095	ILE	2.9
2	B	1356	LEU	2.9
2	B	1093	ILE	2.8
2	B	1485	LEU	2.8
2	B	1192	ALA	2.8
2	B	1211	LEU	2.8
2	B	1216	ASP	2.8
3	C	110	THR	2.8
2	B	1187	TYR	2.8
2	B	1117	VAL	2.7
2	B	1120	GLU	2.7
2	B	1080	ALA	2.7
2	B	1094	ALA	2.7
2	B	942	VAL	2.7
2	B	1070	VAL	2.6
2	B	1275	VAL	2.6
2	B	1220	TRP	2.6
2	B	1081	TYR	2.6
2	B	1144	THR	2.6
2	B	1059	PHE	2.6
2	B	1178	ALA	2.6
2	B	1234	SER	2.6
2	B	1236	ALA	2.5
2	B	1121	ASP	2.5
2	B	1100	LEU	2.5
2	B	1173	GLY	2.5
1	A	463	THR	2.5
2	B	1320	ARG	2.4
2	B	757	ALA	2.4
2	B	1149	ILE	2.4
2	B	1147	VAL	2.4
1	A	665	PRO	2.4
2	B	1138	GLU	2.4
1	A	500	LEU	2.4
2	B	1107	LEU	2.4
2	B	1114	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	988	ALA	2.3
2	B	1240	LEU	2.3
2	B	1523	SER	2.3
1	A	460	VAL	2.3
2	B	1329	GLY	2.3
2	B	1113	LYS	2.3
2	B	1227	LEU	2.3
2	B	1243	LEU	2.2
2	B	1302	SER	2.2
2	B	943	ALA	2.2
2	B	1176	LEU	2.2
2	B	1191	ILE	2.2
2	B	1188	THR	2.2
1	A	656	GLN	2.2
2	B	1309	HIS	2.2
2	B	1498	GLU	2.2
2	B	1124	VAL	2.1
2	B	1659	PHE	2.1
2	B	1324	THR	2.1
2	B	1066	PHE	2.1
2	B	1316	ALA	2.1
3	C	6	VAL	2.1
2	B	1077	TRP	2.1
2	B	1085	VAL	2.1
1	A	630	GLY	2.1
2	B	1116	GLY	2.1
2	B	1486	GLU	2.1
2	B	1307	ILE	2.0
2	B	1286	ALA	2.0
2	B	1230	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

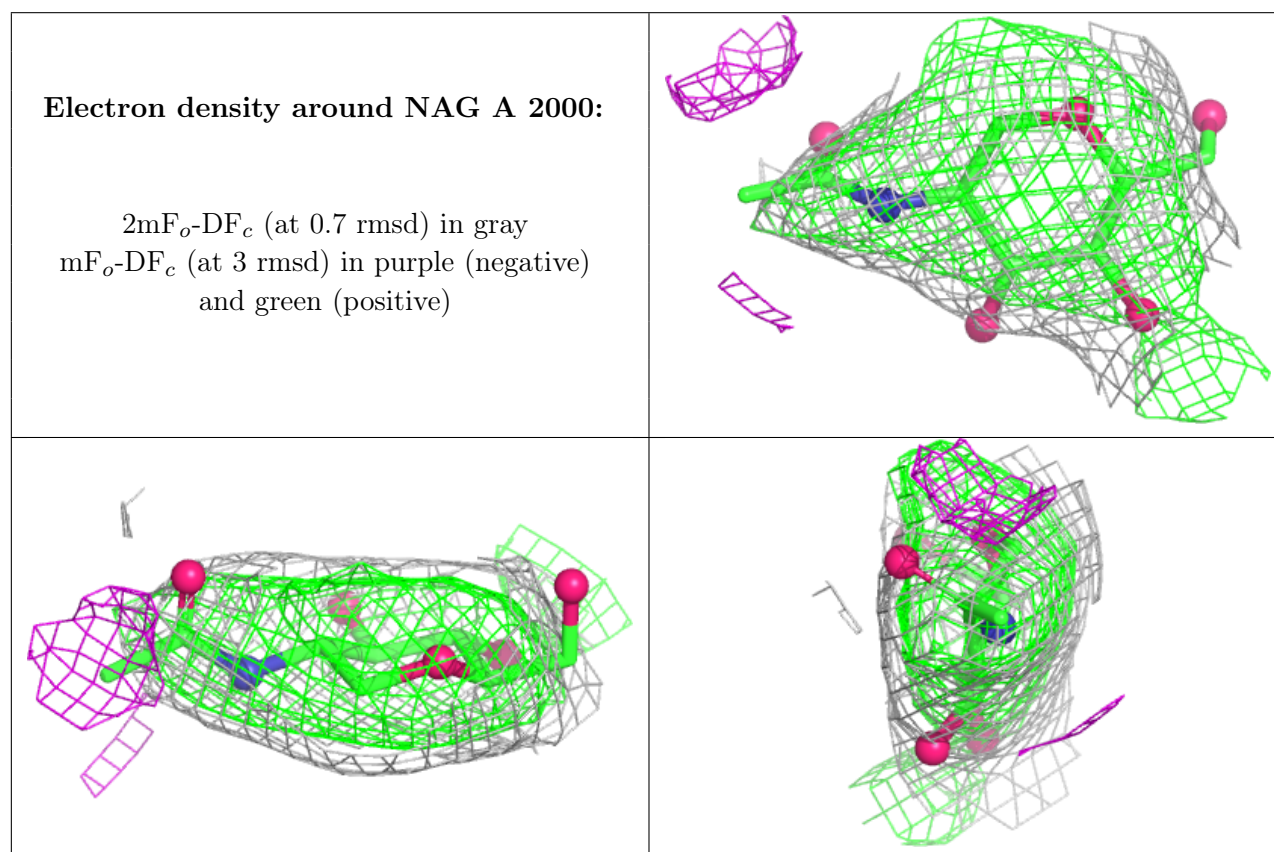
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

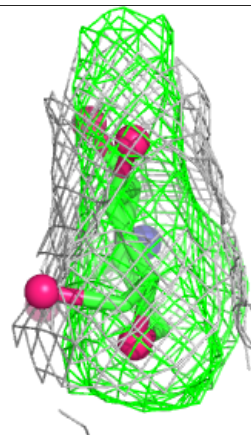
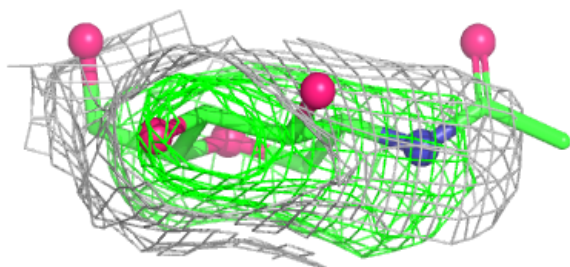
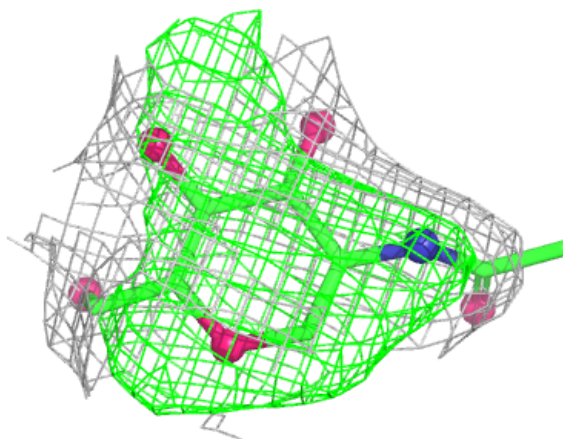
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	2000	14/15	-	-	92,112,118,134	14
4	NAG	B	1701	14/15	-	-	118,120,123,126	14

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 1701:

$2mF_o-DF_c$ (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.