



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:29 PM UTC

PDB ID : 8COE / pdb_00008coe
Title : complement C5 in complex with the LCP0195 nanobody
Authors : Andersen, G.R.; Pedersen, D.V.
Deposited on : 2023-02-28
Resolution : 4.20 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

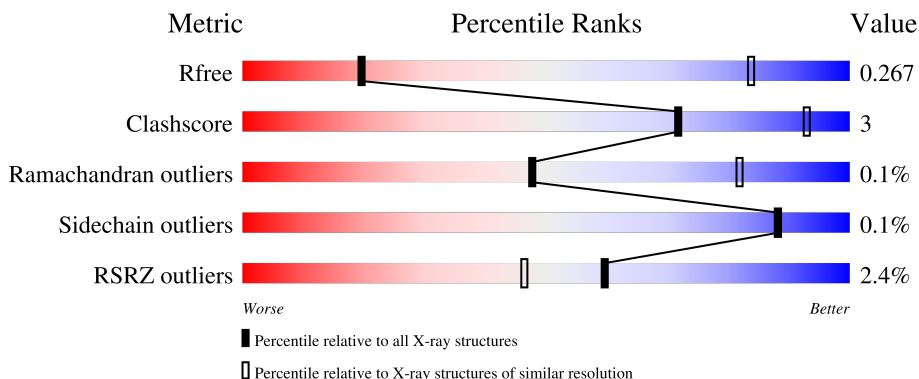
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	C	655	 2% 90% 9%
2	A	999	 3% 86% 9%
3	B	132	 3% 80% 12% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13741 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 C5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	650	5132	3290	824	1005	13	0	0	0

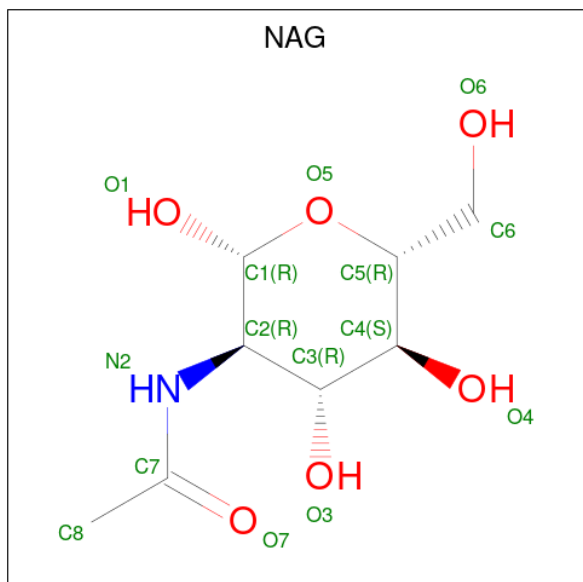
- Molecule 2 is a protein called Complement C5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	961	7631	4884	1271	1437	39	0	0	0

- Molecule 3 is a protein called LCP0195.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	124	964	597	171	191	5	0	1	0

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

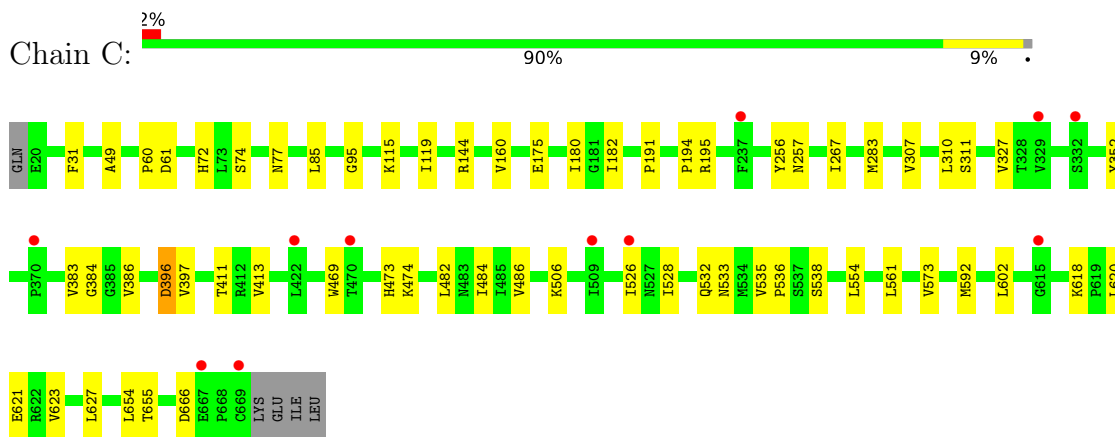


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

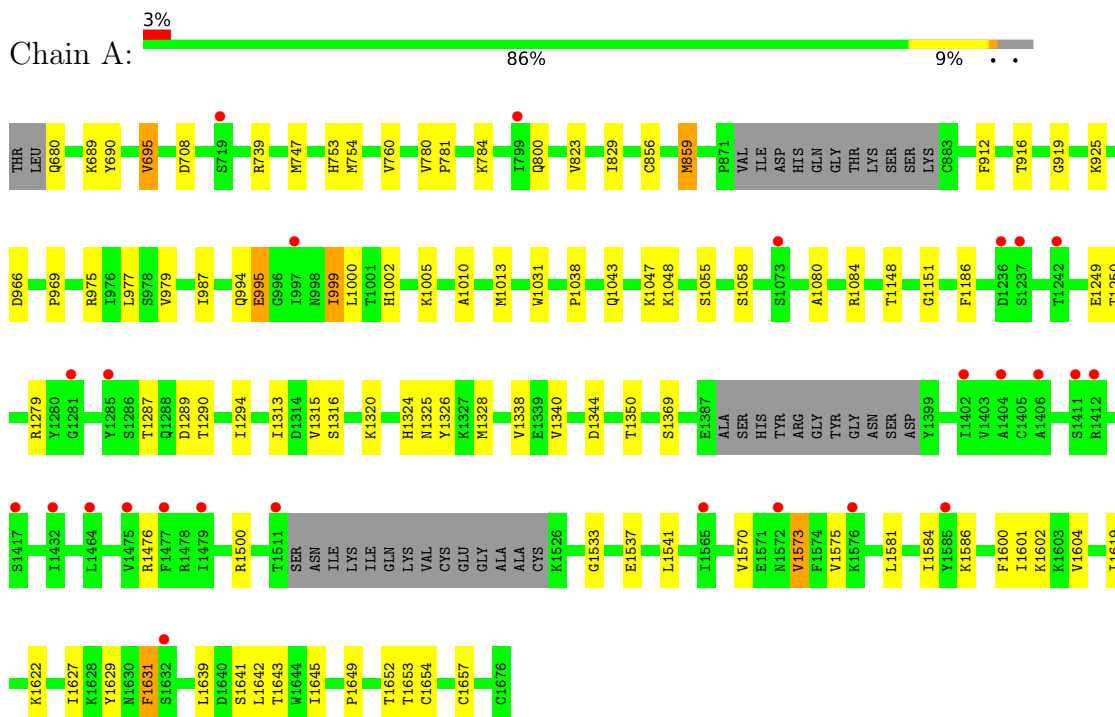
3 Residue-property plots [i](#)

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: Complement C5 beta chain



- Molecule 2: Complement C5 alpha chain



- Molecule 3: LCP0195

Chain B:  3% 80% 12% •• 6%



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	194.83Å 194.83Å 207.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 4.20 48.71 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.71-4.20) 99.9 (48.71-4.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 4.00Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.248 , 0.269 0.248 , 0.267	Depositor DCC
R_{free} test set	2022 reflections (6.20%)	wwPDB-VP
Wilson B-factor (Å ²)	196.7	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 183.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.077 for -h,k,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13741	wwPDB-VP
Average B, all atoms (Å ²)	242.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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	C	0.31	0/5252	0.81	11/7145 (0.2%)
2	A	0.36	0/7788	0.86	15/10546 (0.1%)
3	B	0.43	1/984 (0.1%)	1.00	6/1330 (0.5%)
All	All	0.34	1/14024 (0.0%)	0.86	32/19021 (0.2%)

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
2	A	0	5
3	B	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	28	ARG	CB-CG	-5.03	1.37	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	695	VAL	N-CA-CB	-7.90	98.80	112.08
3	B	34	ALA	N-CA-C	7.75	121.58	109.96
3	B	28	ARG	CG-CD-NE	7.07	127.55	112.00
2	A	1627	ILE	CA-C-N	6.68	131.52	122.84
2	A	1627	ILE	C-N-CA	6.68	131.52	122.84
3	B	28	ARG	CB-CA-C	-6.38	96.04	110.07
2	A	1500	ARG	CB-CA-C	6.35	120.61	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	PRO	CB-CA-C	6.07	121.65	112.55
3	B	100	ARG	CB-CA-C	6.05	120.43	109.37
3	B	3	VAL	CB-CA-C	-6.03	101.52	110.33
2	A	1326	TYR	CB-CA-C	-5.94	96.38	109.56
1	C	257	ASN	N-CA-C	5.81	118.40	111.71
1	C	95	GLY	N-CA-C	-5.75	103.81	112.89
1	C	61	ASP	N-CA-CB	5.72	120.09	110.77
2	A	781	PRO	CA-C-N	5.54	132.12	121.54
2	A	781	PRO	C-N-CA	5.54	132.12	121.54
2	A	1586	LYS	CB-CG-CD	5.43	123.78	111.30
1	C	396	ASP	N-CA-CB	-5.41	101.80	110.51
3	B	59	THR	N-CA-C	5.37	116.80	107.93
2	A	994	GLN	CA-C-N	5.34	131.75	121.54
2	A	994	GLN	C-N-CA	5.34	131.75	121.54
1	C	666	ASP	CA-C-N	-5.29	109.83	122.74
1	C	666	ASP	C-N-CA	-5.29	109.83	122.74
1	C	533	ASN	CA-C-N	5.28	131.26	122.54
1	C	533	ASN	C-N-CA	5.28	131.26	122.54
2	A	1629	TYR	CA-C-N	5.15	132.47	123.91
2	A	1629	TYR	C-N-CA	5.15	132.47	123.91
2	A	859	MET	CG-SD-CE	-5.12	89.63	100.90
2	A	1631	PHE	CA-CB-CG	-5.09	108.71	113.80
1	C	61	ASP	CA-C-N	-5.09	113.80	122.56
1	C	61	ASP	C-N-CA	-5.09	113.80	122.56
2	A	760	VAL	N-CA-C	-5.08	102.08	109.29

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1316	SER	Mainchain
2	A	1631	PHE	Sidechain
2	A	919	GLY	Mainchain
2	A	995	GLU	Mainchain
2	A	999	ILE	Mainchain
3	B	28	ARG	Sidechain

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	C	5132	0	5040	31	0
2	A	7631	0	7656	52	1
3	B	964	0	898	10	0
4	A	14	0	13	0	0
All	All	13741	0	13607	90	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 3.

All (90) 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:A:1320:LYS:HB2	2:A:1344:ASP:OD2	1.89	0.71
2:A:1600:PHE:HB3	2:A:1639:LEU:HD11	1.70	0.71
2:A:969:PRO:HG3	2:A:1601:ILE:HD12	1.74	0.69
2:A:987:ILE:HD11	2:A:1294:ILE:HD12	1.77	0.65
3:B:23:CYS:HB3	3:B:80:LEU:HB3	1.79	0.64
3:B:52:ILE:O	3:B:73:ARG:NH2	2.30	0.64
2:A:1537:GLU:HB2	2:A:1541:LEU:HD11	1.83	0.61
2:A:975:ARG:HG3	2:A:1340:VAL:HB	1.84	0.58
1:C:191:PRO:HB3	2:A:1055:SER:HA	1.86	0.58
1:C:623:VAL:O	1:C:627:LEU:HD13	2.05	0.57
2:A:999:ILE:HG13	2:A:1000:LEU:HG	1.86	0.56
1:C:180:ILE:HG13	1:C:182:ILE:H	1.70	0.56
1:C:307:VAL:O	1:C:311:SER:N	2.36	0.56
2:A:1084:ARG:HB2	2:A:1151:GLY:HA2	1.89	0.54
3:B:32:ASP:HB2	3:B:103:GLN:HG2	1.90	0.54
3:B:3:VAL:HG22	3:B:28:ARG:HD2	1.90	0.54
1:C:386:VAL:H	1:C:411:THR:HB	1.72	0.53
1:C:554:LEU:HD11	1:C:655:THR:HG21	1.89	0.53
2:A:1043:GLN:HG3	2:A:1047:LYS:HE3	1.90	0.53
1:C:620:LEU:HG	2:A:800:GLN:HG2	1.91	0.52
2:A:708:ASP:OD2	2:A:1476:ARG:HD3	2.09	0.52
2:A:780:VAL:HG22	2:A:784:LYS:HB3	1.92	0.51
3:B:84:MET:HE2	3:B:87:LEU:HD21	1.92	0.51
1:C:195:ARG:HG3	2:A:1058:SER:HA	1.92	0.51
1:C:384:GLY:HA3	1:C:413:VAL:HG23	1.93	0.51
1:C:160:VAL:HG22	1:C:175:GLU:HB3	1.93	0.50
2:A:975:ARG:NH2	2:A:1344:ASP:O	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4:GLN:HB2	3:B:26:SER:HB3	1.94	0.50
2:A:995:GLU:O	2:A:1048:LYS:NZ	2.46	0.49
3:B:52:ILE:HG13	3:B:71:ASN:HD22	1.77	0.49
1:C:144:ARG:NH2	1:C:602:LEU:O	2.43	0.49
2:A:966:ASP:OD2	2:A:1369:SER:HB2	2.13	0.48
1:C:618:LYS:HB3	1:C:621:GLU:HG2	1.97	0.47
2:A:1602:LYS:HE3	2:A:1639:LEU:HD13	1.96	0.47
1:C:115:LYS:HB2	1:C:654:LEU:HD21	1.96	0.47
2:A:739:ARG:HG2	2:A:747:MET:HG2	1.97	0.47
2:A:1622:LYS:HD2	2:A:1642:LEU:HB3	1.96	0.47
2:A:859:MET:HE2	2:A:912:PHE:HE1	1.79	0.47
2:A:1639:LEU:HD23	2:A:1643:THR:HG21	1.97	0.47
2:A:979:VAL:HG12	2:A:1328:MET:HE1	1.97	0.46
1:C:74:SER:H	1:C:77:ASN:HB2	1.81	0.46
2:A:1570:VAL:HG22	2:A:1575:VAL:HG22	1.98	0.46
2:A:1320:LYS:HE2	2:A:1344:ASP:OD2	2.16	0.46
2:A:1324:HIS:CE1	2:A:1338:VAL:HG21	2.50	0.46
1:C:506:LYS:HD3	1:C:536:PRO:HG2	1.97	0.46
3:B:32:ASP:HB3	3:B:54:TRP:CD1	2.50	0.46
1:C:620:LEU:HD13	1:C:620:LEU:HA	1.80	0.45
2:A:1324:HIS:HE1	2:A:1338:VAL:HG21	1.80	0.45
2:A:1533:GLY:HA2	2:A:1641:SER:HA	1.98	0.45
2:A:1313:ILE:HA	2:A:1350:THR:HG22	1.98	0.45
1:C:573:VAL:HG12	1:C:592:MET:HG2	1.98	0.45
2:A:754:MET:HE2	2:A:754:MET:HB3	1.87	0.45
1:C:191:PRO:HD2	1:C:194:PRO:HB3	2.00	0.44
2:A:1619:ILE:HG12	2:A:1645:ILE:HG23	1.98	0.44
2:A:680:GLN:HG3	2:A:753:HIS:HB2	1.98	0.44
1:C:267:ILE:HG23	1:C:327:VAL:HG22	2.00	0.44
2:A:999:ILE:HD11	2:A:1290:THR:HG21	1.98	0.44
2:A:977:LEU:HD21	2:A:1315:VAL:HG11	1.99	0.44
3:B:52:ILE:HG23	3:B:58:ASP:O	2.18	0.44
2:A:823:VAL:HG11	2:A:916:THR:HG21	2.00	0.44
2:A:1573:VAL:HG13	2:A:1604:VAL:HG12	2.00	0.44
2:A:689:LYS:HB3	2:A:689:LYS:HE3	1.88	0.43
1:C:538:SER:HB3	1:C:561:LEU:HB2	2.00	0.43
1:C:283:MET:HA	1:C:310:LEU:HD22	2.01	0.43
2:A:1005:LYS:HD2	2:A:1010:ALA:HB1	2.01	0.43
1:C:473:HIS:CD2	1:C:474:LYS:HE2	2.54	0.43
1:C:31:PHE:HB2	1:C:119:ILE:HG22	2.01	0.42
1:C:49:ALA:HB1	1:C:72:HIS:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1249:GLU:HB2	2:A:1289:ASP:HB3	2.00	0.42
1:C:396:ASP:OD1	1:C:397:VAL:N	2.48	0.42
1:C:469:TRP:HB2	1:C:484:ILE:HG12	2.01	0.42
3:B:3:VAL:CG2	3:B:28:ARG:HD2	2.50	0.42
2:A:1186:PHE:HA	2:A:1250:THR:HG22	2.01	0.42
1:C:352:TYR:HE1	1:C:383:VAL:HG11	1.85	0.41
2:A:859:MET:HE2	2:A:912:PHE:CE1	2.55	0.41
2:A:1002:HIS:CE1	2:A:1279:ARG:HH12	2.38	0.41
2:A:690:TYR:CE1	2:A:695:VAL:HG11	2.55	0.41
2:A:1080:ALA:HB2	2:A:1148:THR:HG22	2.02	0.41
2:A:1649:PRO:HB2	2:A:1652:THR:HG22	2.01	0.41
2:A:1581:LEU:HD11	2:A:1584:ILE:HG12	2.02	0.41
2:A:829:ILE:HG13	2:A:925:LYS:HG2	2.03	0.41
1:C:532:GLN:HA	1:C:535:VAL:HG23	2.02	0.41
2:A:1031:TRP:HB3	2:A:1038:PRO:HB3	2.01	0.41
1:C:85:LEU:HD23	1:C:85:LEU:HA	1.90	0.41
2:A:1013:MET:HE3	2:A:1287:THR:HB	2.02	0.41
2:A:987:ILE:CD1	2:A:1294:ILE:HD12	2.49	0.41
2:A:1654:CYS:H	2:A:1657:CYS:HB2	1.86	0.40
1:C:482:LEU:HB3	1:C:528:ILE:HB	2.04	0.40
2:A:977:LEU:HB3	2:A:1338:VAL:HG13	2.02	0.40
1:C:486:VAL:HG21	1:C:526:ILE:HD12	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:A:1325:ASN:O	2:A:1653:THR:OG1[7_554]	2.18	0.02

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	C	648/655 (99%)	622 (96%)	25 (4%)	1 (0%)	43	77
2	A	953/999 (95%)	903 (95%)	49 (5%)	1 (0%)	48	82
3	B	123/132 (93%)	116 (94%)	7 (6%)	0	100	100
All	All	1724/1786 (96%)	1641 (95%)	81 (5%)	2 (0%)	48	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1573	VAL
1	C	256	TYR

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	C	575/580 (99%)	575 (100%)	0	100	100
2	A	855/886 (96%)	854 (100%)	1 (0%)	88	88
3	B	98/105 (93%)	98 (100%)	0	100	100
All	All	1528/1571 (97%)	1527 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	856	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	70	HIS
1	C	72	HIS
1	C	139	GLN
1	C	355	ASN
1	C	374	GLN

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Mol	Chain	Res	Type
1	C	434	ASN
1	C	447	GLN
1	C	472	ASN
1	C	481	HIS
1	C	574	HIS
1	C	591	ASN
1	C	642	ASN
2	A	909	ASN
2	A	1183	GLN
2	A	1319	HIS
2	A	1448	GLN
3	B	71	ASN
3	B	103	GLN

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](#)

1 ligand is 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	2	14,14,15	1.55	1 (7%)	17,19,21	1.45	3 (17%)

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	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2000	NAG	O5-C1	-5.34	1.34	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2000	NAG	C4-C3-C2	4.20	117.17	111.02
4	A	2000	NAG	C3-C4-C5	2.97	115.62	110.23
4	A	2000	NAG	C1-O5-C5	-2.27	109.14	112.19

There are no chirality outliers.

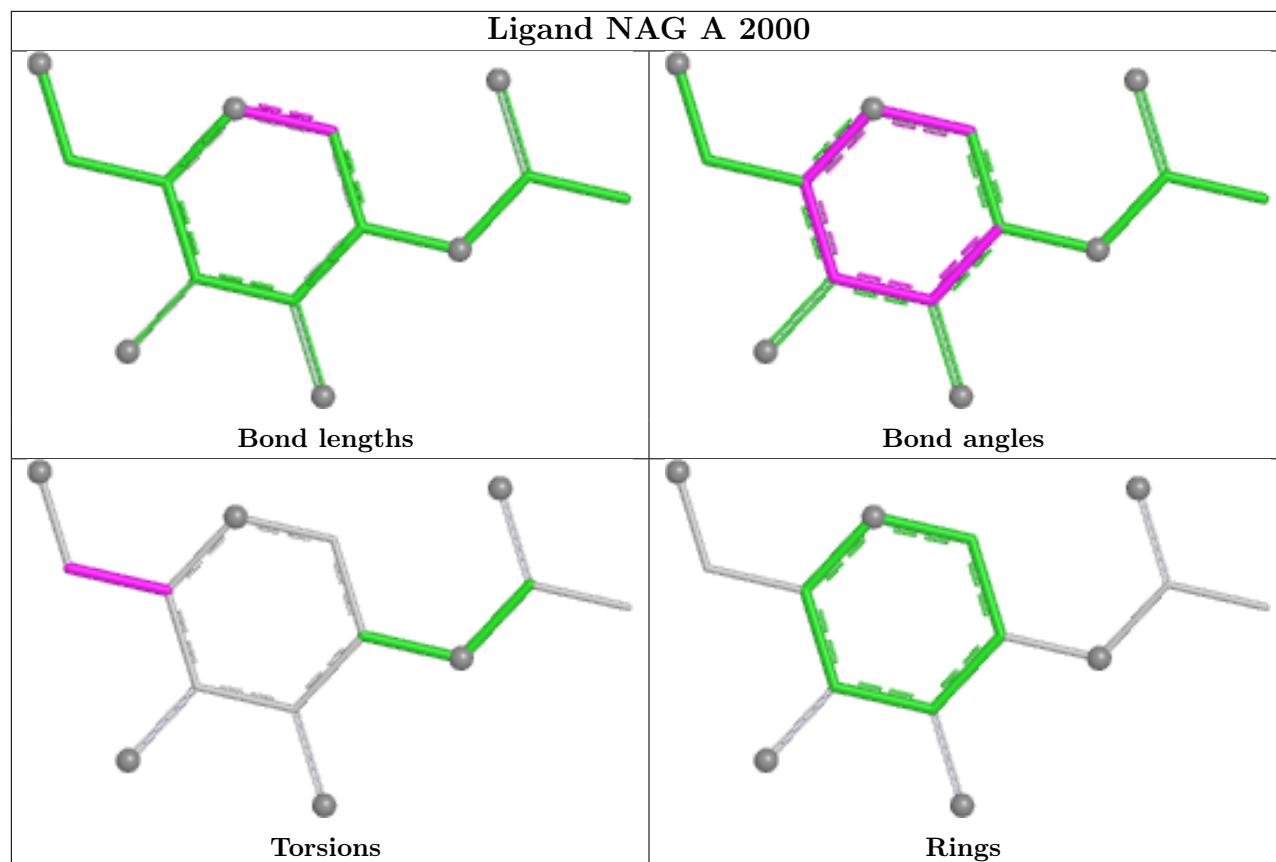
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2000	NAG	O5-C5-C6-O6
4	A	2000	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	C	650/655 (99%)	0.10	11 (1%) 69 54	167, 222, 271, 300	0
2	A	961/999 (96%)	0.13	26 (2%) 56 43	168, 240, 379, 451	0
3	B	124/132 (93%)	0.29	4 (3%) 50 39	110, 218, 260, 275	1 (0%)
All	All	1735/1786 (97%)	0.13	41 (2%) 59 46	110, 232, 360, 451	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	422	LEU	5.0
1	C	669	CYS	3.8
2	A	1402	ILE	3.4
2	A	1281	GLY	3.3
2	A	1242	THR	3.3
1	C	615	GLY	3.2
2	A	1576	LYS	3.1
2	A	1572	ASN	3.0
1	C	509	ILE	2.9
2	A	1285	TYR	2.6
1	C	667	GLU	2.6
3	B	106	TYR	2.6
2	A	1565	ILE	2.6
1	C	237	PHE	2.5
2	A	1475	VAL	2.5
2	A	1411	SER	2.5
2	A	1511	THR	2.4
2	A	1479	ILE	2.4
1	C	370	PRO	2.3
2	A	1406	ALA	2.3
1	C	332	SER	2.3
2	A	1073	SER	2.3
2	A	1477	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
3	B	35	MET	2.3
2	A	1237	SER	2.3
2	A	1464	LEU	2.3
2	A	1585	TYR	2.2
2	A	1432	ILE	2.2
1	C	470	THR	2.2
1	C	526	ILE	2.2
3	B	73	ARG	2.2
2	A	1417	SER	2.2
2	A	1404	ALA	2.1
3	B	58	ASP	2.1
1	C	329	VAL	2.1
2	A	719	SER	2.1
2	A	799	ILE	2.1
2	A	997	ILE	2.1
2	A	1236	ASP	2.1
2	A	1412	ARG	2.1
2	A	1632	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](#)

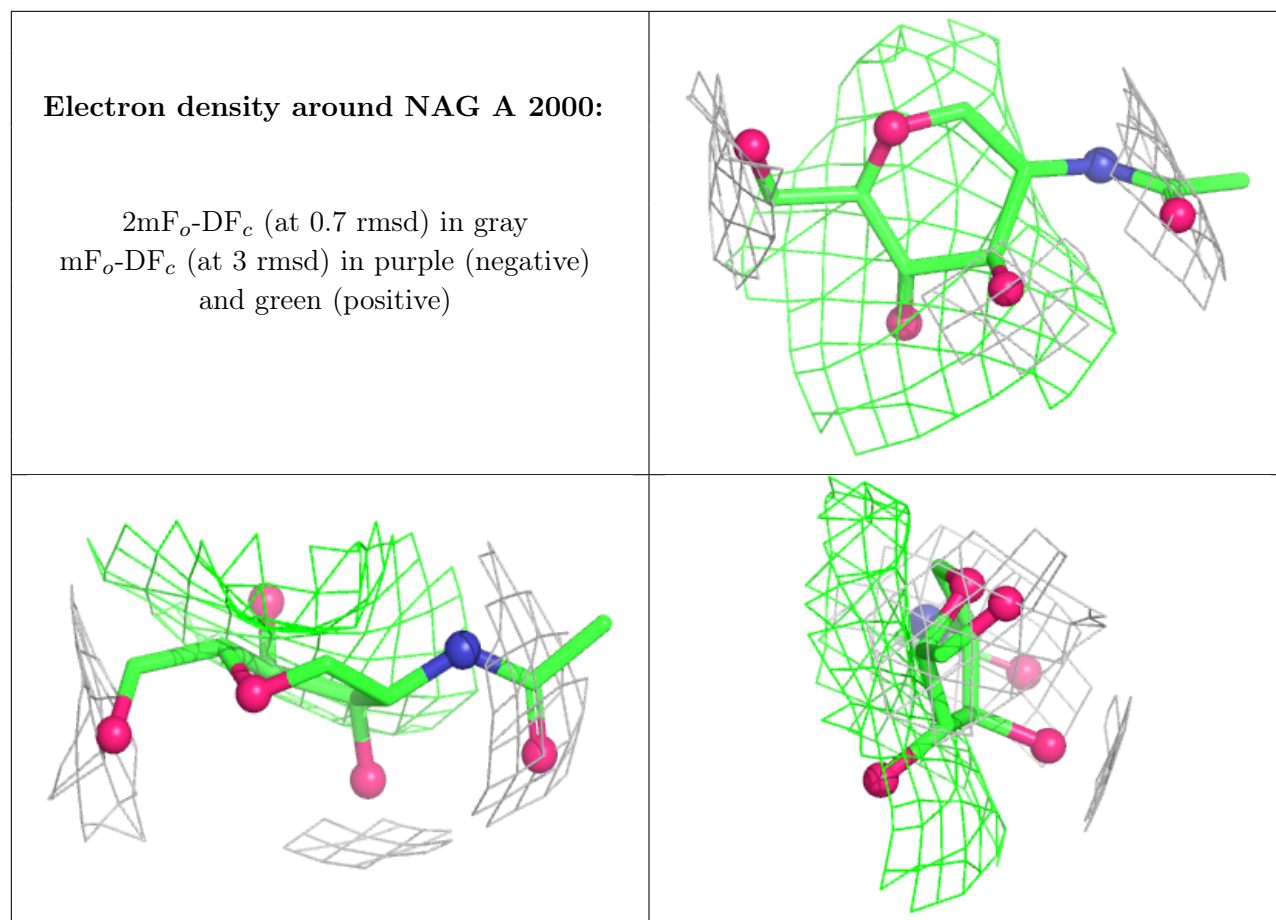
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
4	NAG	A	2000	14/15	0.71	0.19	248,258,271,281	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.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.