



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:58 AM UTC

PDB ID : 8ZAZ / pdb_00008zaz
Title : Crystal structure of Chitinase 3-like protein 1
Authors : Zhao, H.L.; Huang, M.D.; Jiang, L.G.
Deposited on : 2024-04-25
Resolution : 2.31 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

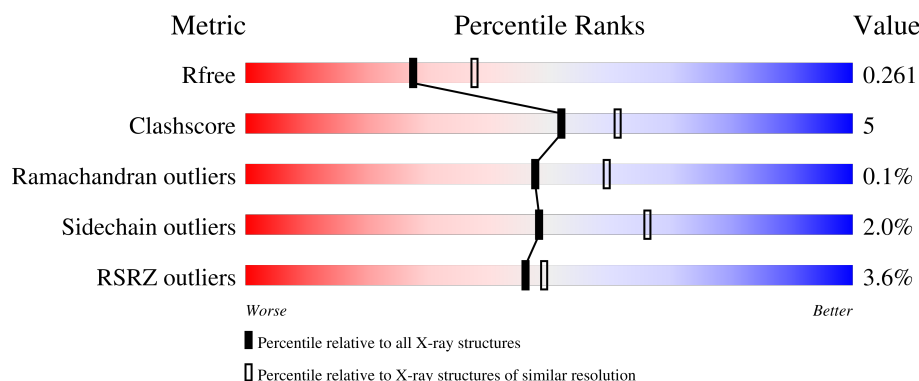
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	362	
1	B	362	
1	C	362	
1	D	362	

2 Entry composition [i](#)

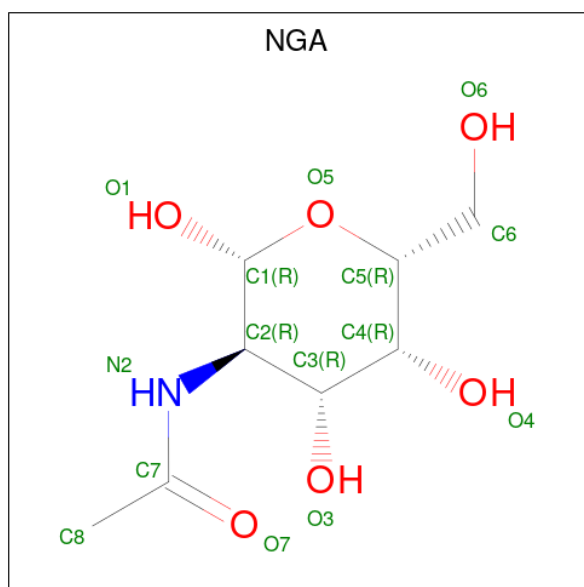
There are 3 unique types of molecules in this entry. The entry contains 11724 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chitinase-3-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2853	1823	492	527	11			
1	B	361	Total	C	N	O	S	0	0	0
			2853	1823	492	527	11			
1	C	361	Total	C	N	O	S	0	0	0
			2853	1823	492	527	11			
1	D	361	Total	C	N	O	S	0	0	0
			2853	1823	492	527	11			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		

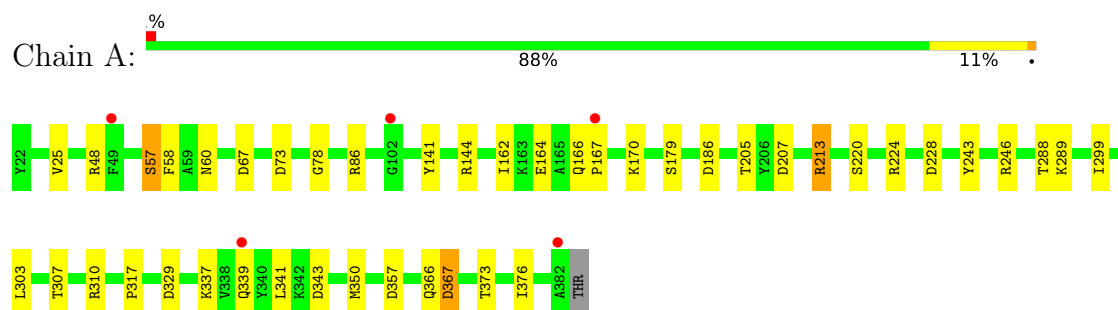
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	81	Total	O	0	0
			81	81		
3	C	57	Total	O	0	0
			57	57		
3	D	37	Total	O	0	0
			37	37		

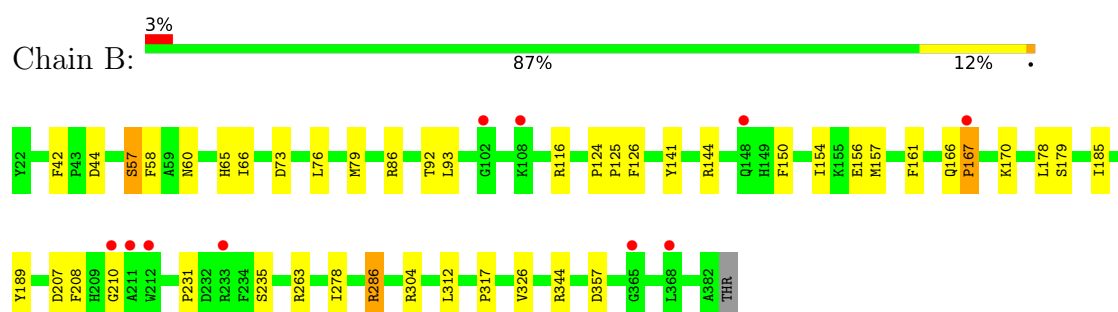
3 Residue-property plots [i](#)

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.

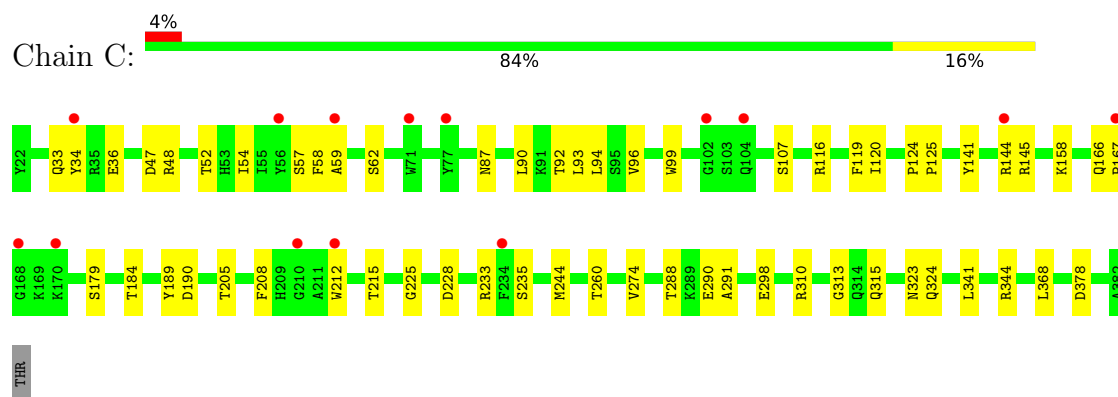
• Molecule 1: Chitinase-3-like protein 1



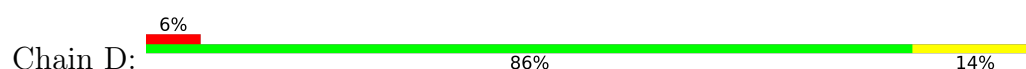
• Molecule 1: Chitinase-3-like protein 1

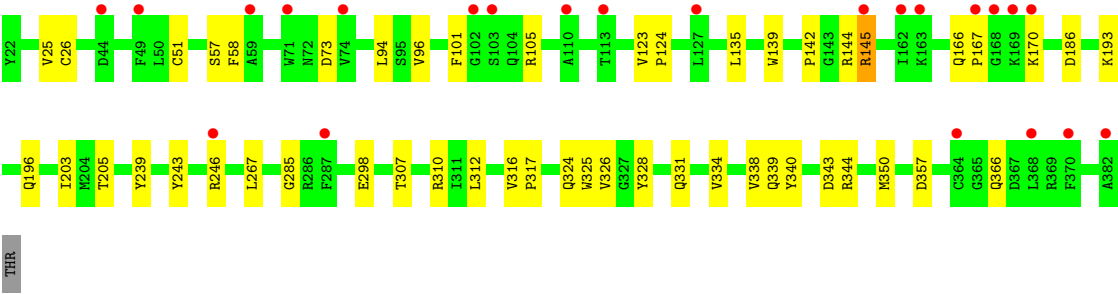


• Molecule 1: Chitinase-3-like protein 1



• Molecule 1: Chitinase-3-like protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.48Å 122.39Å 137.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 2.31 49.97 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.97-2.31) 100.0 (49.97-2.31)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.201 , 0.257 0.207 , 0.261	Depositor DCC
R_{free} test set	3966 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11724	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.79% 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: NGA

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	0.68	0/2929	1.19	11/3968 (0.3%)
1	B	0.71	1/2929 (0.0%)	1.20	6/3968 (0.2%)
1	C	0.61	0/2929	1.15	7/3968 (0.2%)
1	D	0.59	0/2929	1.14	7/3968 (0.2%)
All	All	0.65	1/11716 (0.0%)	1.17	31/15872 (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
1	A	0	3
1	B	0	3
1	C	0	4
1	D	0	1
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	326	VAL	C-N	5.54	1.36	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	THR	CA-CB-OG1	-7.02	99.07	109.60
1	D	73	ASP	CA-CB-CG	6.97	119.57	112.60
1	C	36	GLU	CB-CA-C	-6.89	98.61	109.70
1	A	67	ASP	CA-CB-CG	6.82	119.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	357	ASP	CA-CB-CG	6.42	119.02	112.60
1	B	207	ASP	CB-CA-C	-6.17	102.79	111.80
1	C	52	THR	CA-CB-OG1	-6.16	100.36	109.60
1	A	307	THR	CA-CB-OG1	-5.94	100.69	109.60
1	C	228	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	207	ASP	CB-CA-C	-5.88	103.38	111.73
1	A	373	THR	CA-CB-OG1	-5.82	100.88	109.60
1	D	343	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	357	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	65	HIS	CA-CB-CG	5.65	119.45	113.80
1	A	343	ASP	CA-CB-CG	5.64	118.24	112.60
1	D	239	TYR	N-CA-CB	5.64	118.18	110.01
1	A	339	GLN	N-CA-CB	5.55	118.06	110.01
1	A	228	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	167	PRO	N-CA-C	5.51	120.20	112.26
1	B	60	ASN	CB-CG-ND2	5.40	124.50	116.40
1	D	339	GLN	N-CA-CB	5.39	118.53	110.22
1	B	73	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	310	ARG	N-CA-CB	5.30	118.91	110.16
1	D	316	VAL	N-CA-CB	5.30	117.31	111.64
1	C	378	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	329	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	164	GLU	CB-CG-CD	5.23	121.48	112.60
1	D	357	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	73	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	190	ASP	CB-CA-C	5.00	119.91	111.41

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	246	ARG	Sidechain
1	A	310	ARG	Sidechain
1	B	263	ARG	Sidechain
1	B	286	ARG	Sidechain
1	B	344	ARG	Sidechain
1	C	116	ARG	Sidechain
1	C	233	ARG	Sidechain
1	C	310	ARG	Sidechain
1	C	344	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	246	ARG	Sidechain

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	2853	0	2778	18	0
1	B	2853	0	2778	33	1
1	C	2853	0	2776	34	0
1	D	2853	0	2778	26	1
2	A	15	0	14	1	0
2	B	15	0	14	0	0
2	C	15	0	14	0	0
2	D	15	0	14	0	0
3	A	77	0	0	5	0
3	B	81	0	0	11	0
3	C	57	0	0	10	0
3	D	37	0	0	9	0
All	All	11724	0	11166	109	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 5.

All (109) 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:D:326:VAL:HG22	3:D:524:HOH:O	1.54	1.08
1:D:324:GLN:C	3:D:501:HOH:O	2.03	1.01
1:D:144:ARG:HA	3:D:523:HOH:O	1.65	0.96
1:D:26:CYS:HG	1:D:51:CYS:HG	0.99	0.92
1:B:157:MET:SD	3:B:550:HOH:O	2.26	0.92
1:B:166:GLN:HG2	1:B:167:PRO:HD3	1.56	0.88
1:B:231:PRO:HD2	3:B:515:HOH:O	1.79	0.82
1:B:210:GLY:O	1:B:231:PRO:HD2	1.81	0.81
1:C:323:ASN:N	3:C:501:HOH:O	2.13	0.81
1:D:344:ARG:HG3	3:D:530:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:HG2	3:C:526:HOH:O	1.83	0.78
1:D:340:TYR:CE2	3:D:530:HOH:O	2.38	0.77
1:A:162:ILE:O	3:A:501:HOH:O	2.06	0.72
1:B:66:ILE:HG23	3:B:504:HOH:O	1.90	0.71
1:D:328:TYR:HB3	3:D:524:HOH:O	1.91	0.70
1:C:274:VAL:HA	3:C:511:HOH:O	1.91	0.70
1:A:166:GLN:HG2	1:A:167:PRO:HD3	1.72	0.69
1:B:189:TYR:CG	3:B:581:HOH:O	2.45	0.69
1:B:66:ILE:C	3:B:504:HOH:O	2.36	0.69
1:B:161:PHE:CE1	3:B:550:HOH:O	2.46	0.69
1:B:312:LEU:O	1:C:315:GLN:NE2	2.26	0.68
1:B:178:LEU:HD13	3:B:581:HOH:O	1.94	0.67
1:C:189:TYR:CE2	3:C:536:HOH:O	2.47	0.67
1:B:189:TYR:CD2	3:B:581:HOH:O	2.49	0.66
1:C:158:LYS:HA	3:C:541:HOH:O	1.96	0.64
1:C:57:SER:HB2	1:C:58:PHE:CD1	2.33	0.64
1:C:225:GLY:HA2	1:C:313:GLY:HA3	1.80	0.63
1:D:340:TYR:CD2	3:D:530:HOH:O	2.52	0.63
1:B:210:GLY:O	1:B:231:PRO:CD	2.46	0.63
1:C:324:GLN:N	3:C:501:HOH:O	2.31	0.62
1:B:141:TYR:CE1	1:B:179:SER:HB2	2.34	0.61
1:C:166:GLN:HG2	1:C:167:PRO:HD3	1.82	0.60
1:C:225:GLY:CA	1:C:313:GLY:HA3	2.32	0.60
1:C:184:THR:HG22	3:C:536:HOH:O	2.02	0.59
1:D:96:VAL:HG12	1:D:135:LEU:HD11	1.84	0.59
1:B:126:PHE:CE2	3:B:504:HOH:O	2.56	0.58
1:C:368:LEU:HD12	3:C:535:HOH:O	2.06	0.56
1:D:331:GLN:HE22	1:D:366:GLN:HE22	1.53	0.56
1:D:193:LYS:O	1:D:196:GLN:HG2	2.06	0.56
1:C:166:GLN:HG2	1:C:167:PRO:CD	2.36	0.56
1:A:350:MET:HG2	3:A:503:HOH:O	2.07	0.54
1:B:178:LEU:HD22	1:B:189:TYR:CE1	2.44	0.53
1:B:178:LEU:HD22	1:B:189:TYR:CZ	2.44	0.53
1:C:48:ARG:O	1:C:87:ASN:ND2	2.41	0.52
1:A:141:TYR:CE1	1:A:179:SER:HB2	2.46	0.51
1:A:186:ASP:OD1	1:A:243:TYR:OH	2.26	0.50
1:C:288:THR:HG23	1:C:298:GLU:OE1	2.12	0.50
1:D:285:GLY:HA3	1:D:298:GLU:OE2	2.13	0.49
1:C:144:ARG:HH11	1:C:144:ARG:HG2	1.78	0.49
1:B:92:THR:C	1:B:93:LEU:HD12	2.38	0.48
1:A:48:ARG:CD	1:A:86:ARG:HB3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:TRP:O	1:C:215:THR:OG1	2.26	0.47
1:A:25:VAL:C	3:A:503:HOH:O	2.58	0.47
1:D:101:PHE:O	1:D:105:ARG:NH1	2.47	0.47
1:B:166:GLN:CG	1:B:167:PRO:HD3	2.37	0.47
1:D:325:TRP:HB2	3:D:501:HOH:O	2.14	0.47
1:A:213:ARG:HG3	1:A:213:ARG:HH11	1.81	0.46
1:C:166:GLN:N	1:C:167:PRO:HD2	2.31	0.46
1:D:186:ASP:OD1	1:D:243:TYR:OH	2.24	0.46
1:B:126:PHE:CD2	3:B:504:HOH:O	2.56	0.45
1:B:44:ASP:CG	1:B:79:MET:CE	2.90	0.45
1:C:107:SER:OG	1:C:145:ARG:NH1	2.48	0.45
1:A:299:ILE:O	1:A:303:LEU:HG	2.16	0.45
1:B:150:PHE:CZ	1:B:154:ILE:HD11	2.51	0.45
1:C:33:GLN:HG3	1:C:34:TYR:CD1	2.51	0.45
1:B:44:ASP:CG	1:B:79:MET:HE3	2.41	0.45
1:C:290:GLU:O	1:C:291:ALA:C	2.59	0.45
1:D:94:LEU:O	1:D:135:LEU:HD12	2.17	0.45
1:C:54:ILE:HG13	1:C:90:LEU:HD11	1.99	0.45
1:C:124:PRO:N	1:C:125:PRO:HD2	2.32	0.45
1:D:267:LEU:HG	3:D:501:HOH:O	2.16	0.44
1:B:208:PHE:HB3	1:B:235:SER:HB3	1.98	0.44
1:D:96:VAL:CG1	1:D:135:LEU:HD11	2.46	0.44
1:D:139:TRP:O	1:D:142:PRO:HD3	2.17	0.44
1:A:57:SER:HA	1:A:58:PHE:HA	1.78	0.44
1:C:99:TRP:NE1	3:C:508:HOH:O	2.47	0.44
1:C:57:SER:HA	1:C:58:PHE:HA	1.81	0.44
1:D:123:VAL:HB	1:D:124:PRO:HD3	2.00	0.44
1:A:288:THR:O	1:A:289:LYS:C	2.61	0.44
1:D:144:ARG:O	1:D:145:ARG:CB	2.66	0.43
1:D:57:SER:HA	1:D:58:PHE:HA	1.70	0.43
1:A:78:GLY:HA3	1:B:167:PRO:HB2	2.01	0.43
1:C:92:THR:C	1:C:93:LEU:HD12	2.43	0.43
1:A:366:GLN:O	1:A:367:ASP:C	2.61	0.43
1:B:116:ARG:NE	1:B:156:GLU:OE1	2.49	0.43
1:A:220:SER:OG	1:A:337:LYS:NZ	2.52	0.42
1:B:124:PRO:N	1:B:125:PRO:CD	2.82	0.42
1:B:42:PHE:HB3	1:B:79:MET:HE1	2.01	0.42
1:C:57:SER:HB2	1:C:58:PHE:CE1	2.54	0.42
1:B:44:ASP:H	1:B:79:MET:HE2	1.85	0.42
1:C:141:TYR:CE1	1:C:179:SER:HB2	2.55	0.42
1:C:208:PHE:HB3	1:C:235:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG12	3:A:503:HOH:O	2.20	0.41
1:B:185:ILE:HA	1:B:189:TYR:CD2	2.55	0.41
1:A:376:ILE:HA	3:A:523:HOH:O	2.20	0.41
1:B:166:GLN:N	1:B:167:PRO:CD	2.84	0.41
1:D:334:VAL:O	1:D:338:VAL:HG23	2.19	0.41
1:A:166:GLN:N	1:A:167:PRO:CD	2.84	0.41
1:C:288:THR:HA	3:C:504:HOH:O	2.20	0.41
1:A:60:ASN:ND2	2:A:401:NGA:N2	2.67	0.41
1:B:304:ARG:HD3	3:B:576:HOH:O	2.20	0.41
1:C:119:PHE:O	1:C:120:ILE:C	2.64	0.41
1:B:57:SER:HA	1:B:58:PHE:HA	1.88	0.41
1:B:86:ARG:HH11	1:B:86:ARG:HG2	1.86	0.41
1:C:225:GLY:HA3	1:C:313:GLY:HA3	2.03	0.40
1:D:25:VAL:O	1:D:350:MET:HA	2.21	0.40
1:D:144:ARG:O	1:D:145:ARG:HG2	2.21	0.40
1:C:59:ALA:HB2	1:C:94:LEU:HD11	2.03	0.40
1:D:166:GLN:HB3	1:D:167:PRO:HD3	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)
1:B:278:ILE:O	1:D:145:ARG:NH2[3_545]	2.07	0.13

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	359/362 (99%)	353 (98%)	5 (1%)	1 (0%)	36	45
1	B	359/362 (99%)	350 (98%)	9 (2%)	0	100	100
1	C	359/362 (99%)	346 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	359/362 (99%)	344 (96%)	14 (4%)	1 (0%)	36	45
All	All	1436/1448 (99%)	1393 (97%)	41 (3%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	145	ARG
1	A	367	ASP

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	301/302 (100%)	294 (98%)	7 (2%)	44	62
1	B	301/302 (100%)	295 (98%)	6 (2%)	48	66
1	C	301/302 (100%)	296 (98%)	5 (2%)	53	70
1	D	301/302 (100%)	295 (98%)	6 (2%)	48	66
All	All	1204/1208 (100%)	1180 (98%)	24 (2%)	48	66

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	144	ARG
1	A	170	LYS
1	A	205	THR
1	A	213	ARG
1	A	317	PRO
1	A	341	LEU
1	B	57	SER
1	B	76	LEU
1	B	144	ARG
1	B	170	LYS
1	B	286	ARG

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Mol	Chain	Res	Type
1	B	317	PRO
1	C	62	SER
1	C	96	VAL
1	C	205	THR
1	C	244	MET
1	C	341	LEU
1	D	170	LYS
1	D	203	ILE
1	D	205	THR
1	D	307	THR
1	D	312	LEU
1	D	317	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	89	ASN
1	A	314	GLN
1	B	85	ASN
1	B	171	GLN
1	B	309	HIS
1	B	374	ASN
1	C	85	ASN
1	C	89	ASN
1	C	149	HIS
1	D	85	ASN
1	D	89	ASN
1	D	309	HIS
1	D	314	GLN
1	D	366	GLN
1	D	374	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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$
2	NGA	A	401	-	15,15,15	0.54	0	21,21,21	2.55	7 (33%)
2	NGA	D	401	-	15,15,15	0.48	0	21,21,21	1.23	2 (9%)
2	NGA	B	401	-	15,15,15	0.56	0	21,21,21	2.14	7 (33%)
2	NGA	C	401	-	15,15,15	0.34	0	21,21,21	1.64	5 (23%)

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
2	NGA	A	401	-	-	3/6/26/26	0/1/1/1
2	NGA	D	401	-	-	2/6/26/26	0/1/1/1
2	NGA	B	401	-	-	4/6/26/26	0/1/1/1
2	NGA	C	401	-	-	4/6/26/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NGA	O5-C1-C2	-7.14	102.34	109.52
2	A	401	NGA	O1-C1-O5	6.01	128.26	110.41
2	B	401	NGA	C4-C3-C2	4.49	116.94	110.40
2	C	401	NGA	O5-C1-C2	-4.46	105.04	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NGA	O1-C1-O5	4.02	122.36	110.41
2	D	401	NGA	O1-C1-O5	3.59	121.06	110.41
2	B	401	NGA	O1-C1-C2	-3.40	102.16	109.22
2	A	401	NGA	O5-C5-C4	3.26	115.57	109.70
2	B	401	NGA	O3-C3-C2	-3.13	103.35	109.58
2	A	401	NGA	C4-C3-C2	3.00	114.77	110.40
2	A	401	NGA	O1-C1-C2	-2.91	103.18	109.22
2	B	401	NGA	C2-N2-C7	2.81	129.68	123.11
2	B	401	NGA	O4-C4-C3	2.65	116.61	110.38
2	C	401	NGA	O1-C1-O5	2.53	117.93	110.41
2	A	401	NGA	C1-C2-N2	-2.50	107.84	110.73
2	C	401	NGA	C2-N2-C7	2.47	128.89	123.11
2	C	401	NGA	C1-C2-C3	-2.28	107.44	110.54
2	C	401	NGA	O5-C5-C4	2.10	113.49	109.70
2	B	401	NGA	O5-C5-C6	2.07	111.58	106.44
2	A	401	NGA	O5-C5-C6	2.04	111.49	106.44
2	D	401	NGA	C2-N2-C7	2.01	127.82	123.11

There are no chirality outliers.

All (13) torsion outliers are listed below:

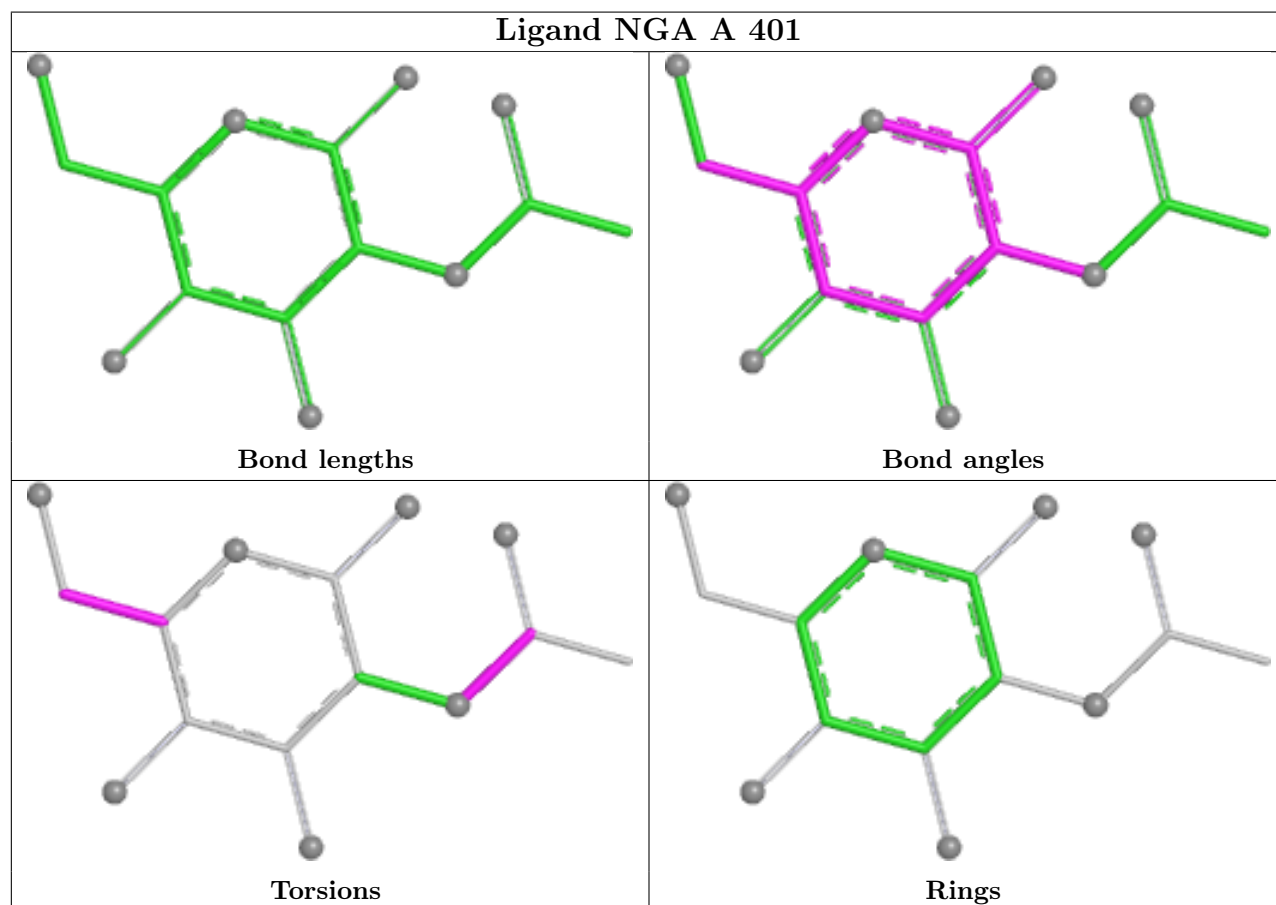
Mol	Chain	Res	Type	Atoms
2	A	401	NGA	C8-C7-N2-C2
2	A	401	NGA	O7-C7-N2-C2
2	C	401	NGA	C8-C7-N2-C2
2	C	401	NGA	O7-C7-N2-C2
2	B	401	NGA	C8-C7-N2-C2
2	B	401	NGA	O7-C7-N2-C2
2	D	401	NGA	C4-C5-C6-O6
2	D	401	NGA	O5-C5-C6-O6
2	C	401	NGA	O5-C5-C6-O6
2	B	401	NGA	C4-C5-C6-O6
2	A	401	NGA	O5-C5-C6-O6
2	B	401	NGA	O5-C5-C6-O6
2	C	401	NGA	C4-C5-C6-O6

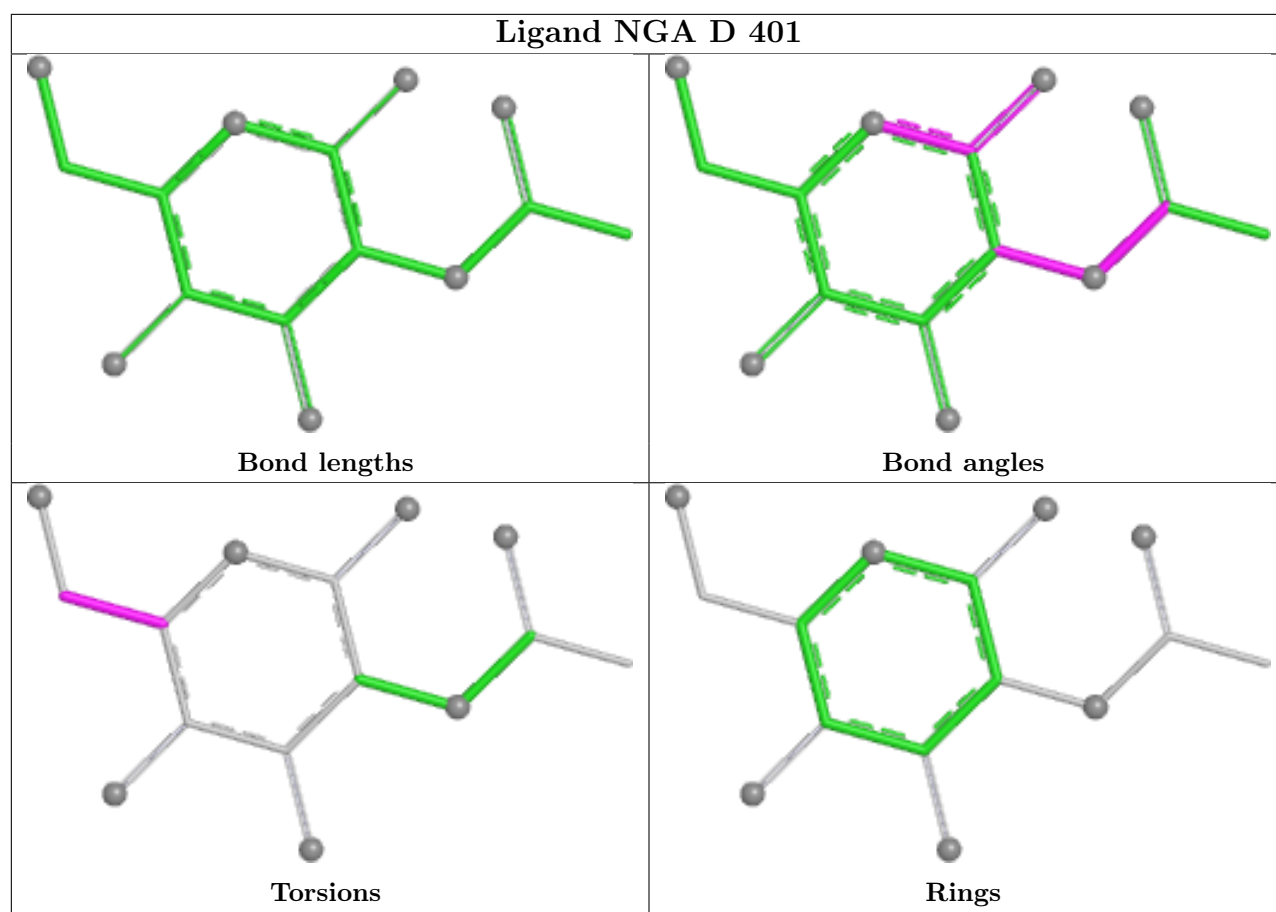
There are no ring outliers.

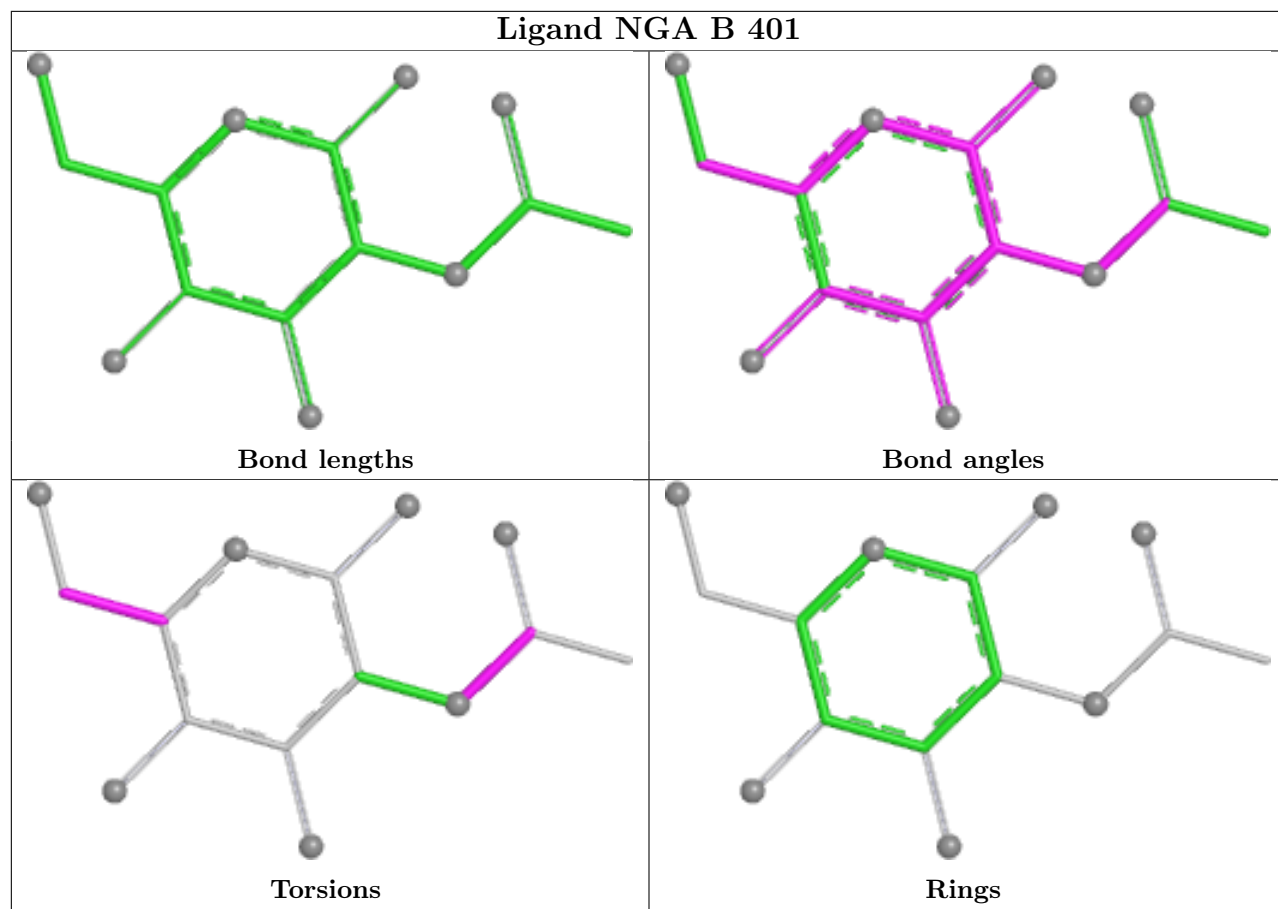
1 monomer is involved in 1 short contact:

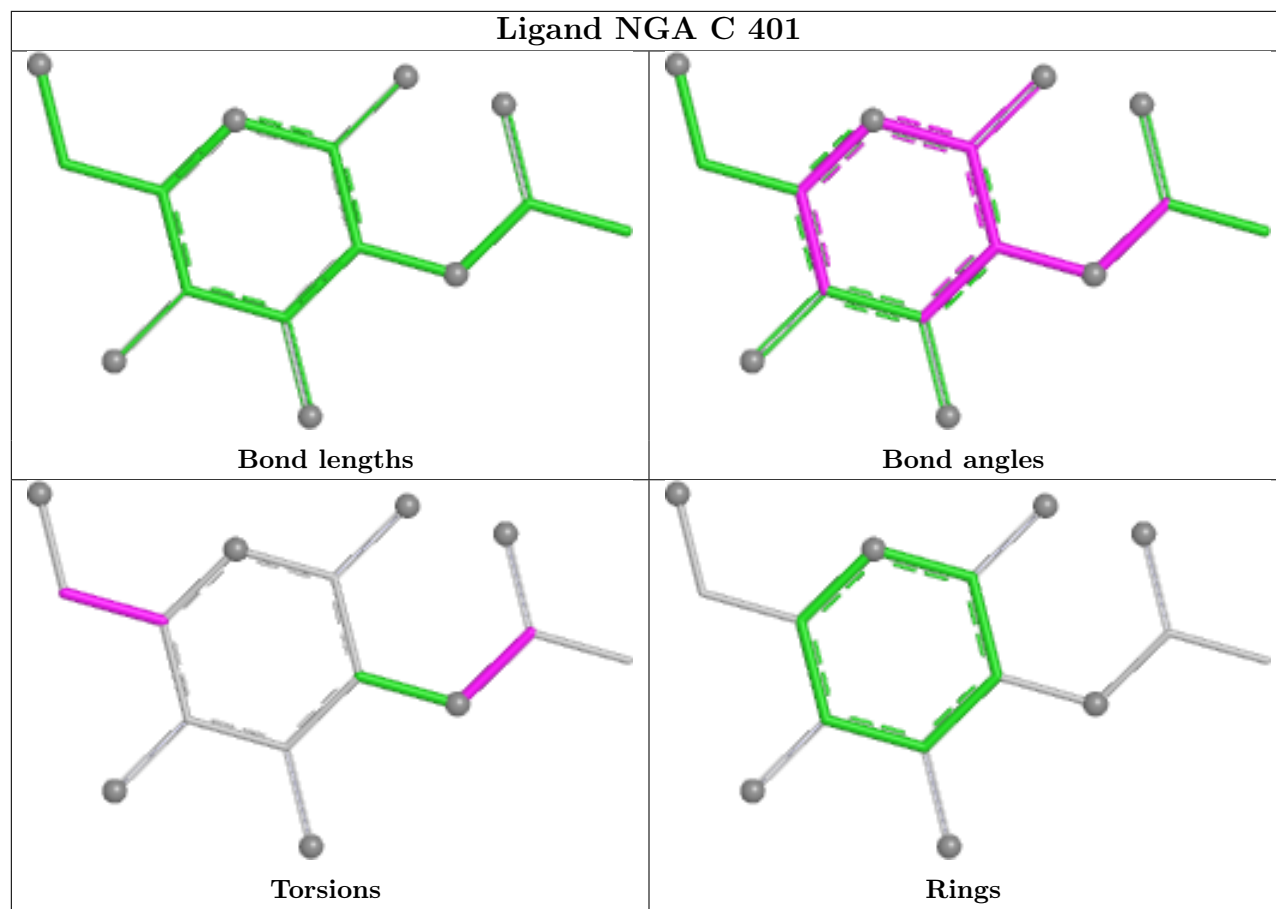
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NGA	1	0

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	361/362 (99%)	-0.10	5 (1%) 73 75	27, 41, 75, 102	0
1	B	361/362 (99%)	-0.05	10 (2%) 55 57	23, 38, 75, 101	0
1	C	361/362 (99%)	0.41	14 (3%) 43 46	30, 52, 88, 136	0
1	D	361/362 (99%)	0.68	23 (6%) 25 28	30, 62, 103, 148	0
All	All	1444/1448 (99%)	0.23	52 (3%) 46 49	23, 47, 90, 148	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	PHE	4.5
1	B	211	ALA	4.2
1	D	167	PRO	4.1
1	C	167	PRO	3.6
1	C	170	LYS	3.5
1	B	102	GLY	3.3
1	C	71	TRP	3.0
1	C	212	TRP	3.0
1	D	145	ARG	3.0
1	D	163	LYS	2.9
1	D	287	PHE	2.9
1	D	246	ARG	2.8
1	B	212	TRP	2.8
1	B	365	GLY	2.8
1	A	102	GLY	2.8
1	B	167	PRO	2.7
1	D	162	ILE	2.7
1	D	168	GLY	2.7
1	D	49	PHE	2.7
1	D	110	ALA	2.6
1	C	210	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	169	LYS	2.5
1	C	104	GLN	2.5
1	D	127	LEU	2.5
1	A	382	ALA	2.5
1	A	49	PHE	2.5
1	D	74	VAL	2.5
1	D	44	ASP	2.5
1	D	368	LEU	2.4
1	B	108	LYS	2.4
1	A	167	PRO	2.4
1	D	382	ALA	2.4
1	D	102	GLY	2.4
1	C	102	GLY	2.3
1	D	370	PHE	2.3
1	D	71	TRP	2.3
1	B	210	GLY	2.3
1	C	77	TYR	2.3
1	A	339	GLN	2.2
1	C	56	TYR	2.2
1	B	368	LEU	2.2
1	B	148	GLN	2.2
1	B	233	ARG	2.2
1	D	170	LYS	2.2
1	C	144	ARG	2.1
1	D	103	SER	2.1
1	C	168	GLY	2.1
1	D	113	THR	2.0
1	D	59	ALA	2.0
1	C	34	TYR	2.0
1	C	59	ALA	2.0
1	D	364	CYS	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](#)

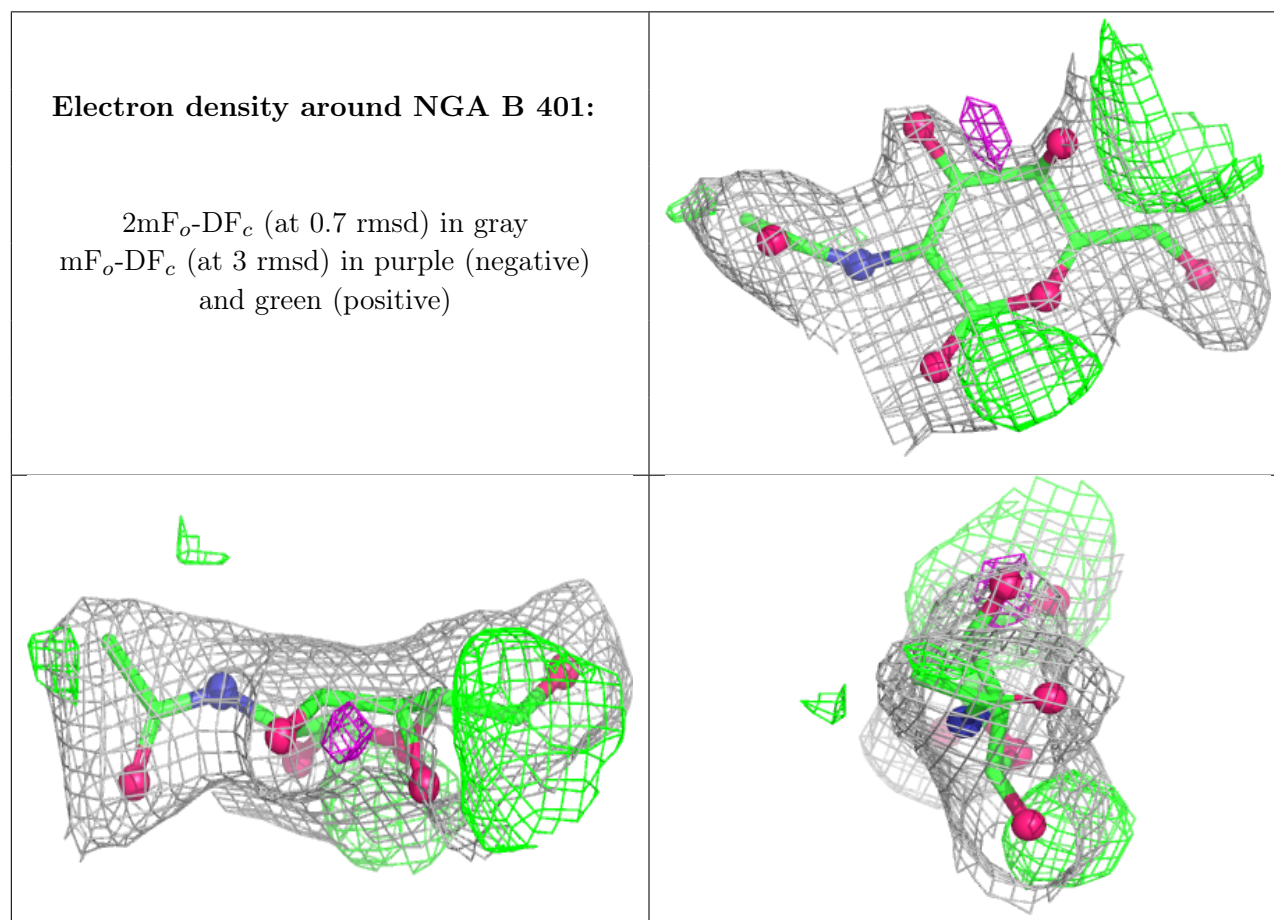
There are no oligosaccharides in this entry.

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.

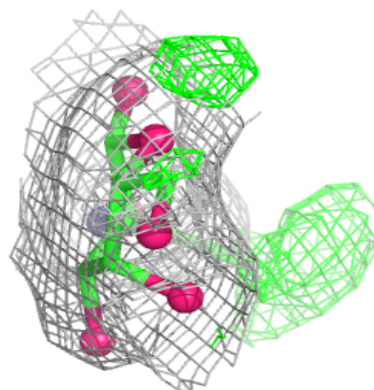
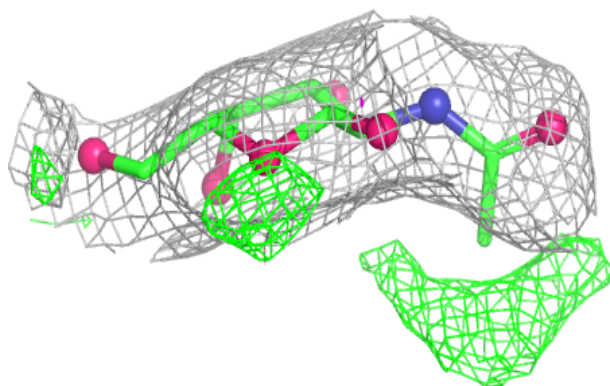
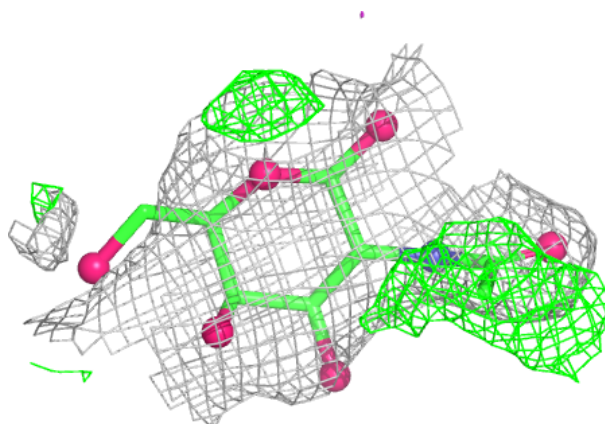
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NGA	B	401	15/15	0.71	0.16	46,59,75,79	0
2	NGA	C	401	15/15	0.72	0.16	73,86,100,102	0
2	NGA	D	401	15/15	0.72	0.16	73,89,103,115	0
2	NGA	A	401	15/15	0.85	0.15	54,67,93,93	0

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.



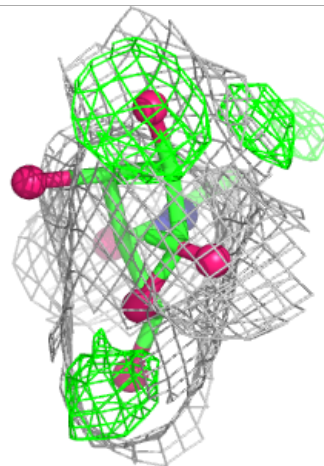
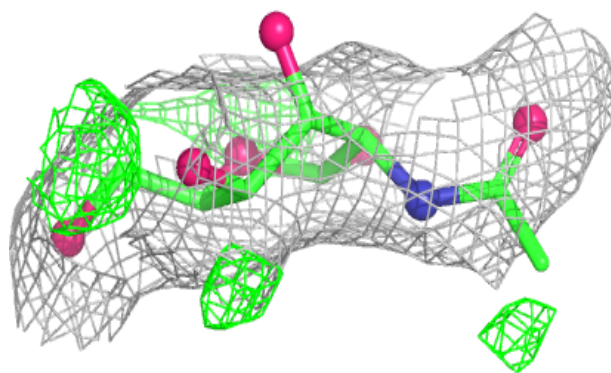
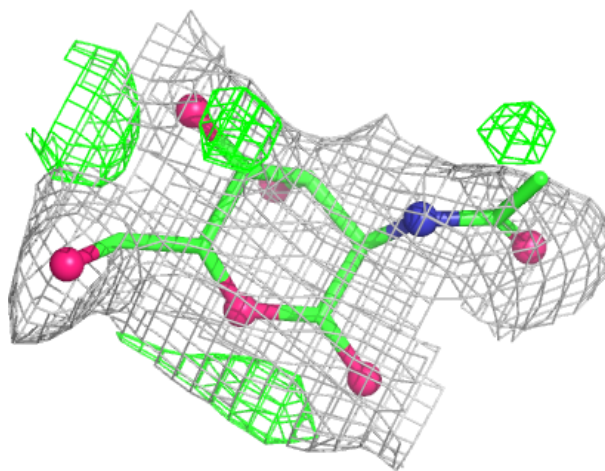
Electron density around NGA C 401:

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



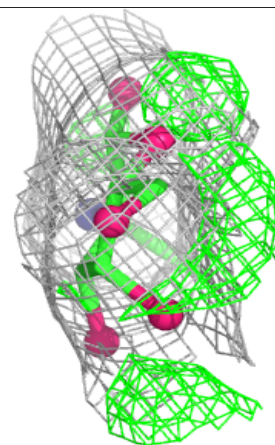
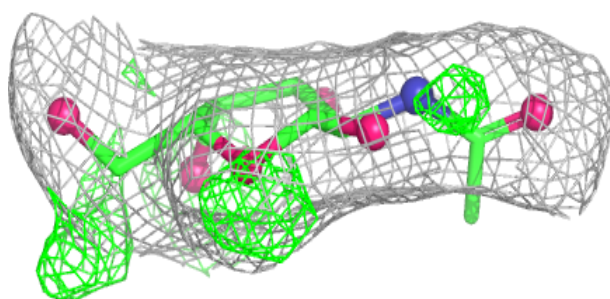
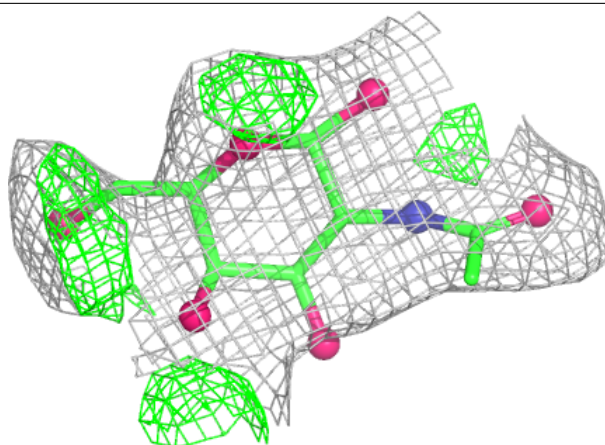
Electron density around NGA D 401:

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



Electron density around NGA 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.