



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:35 PM UTC

PDB ID : 7QBG / pdb_00007qbg
Title : TC:CD320 in complex with nanobody TC-Nb4
Authors : Bloch, J.S.; Locher, K.P.
Deposited on : 2021-11-19
Resolution : 2.69 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:

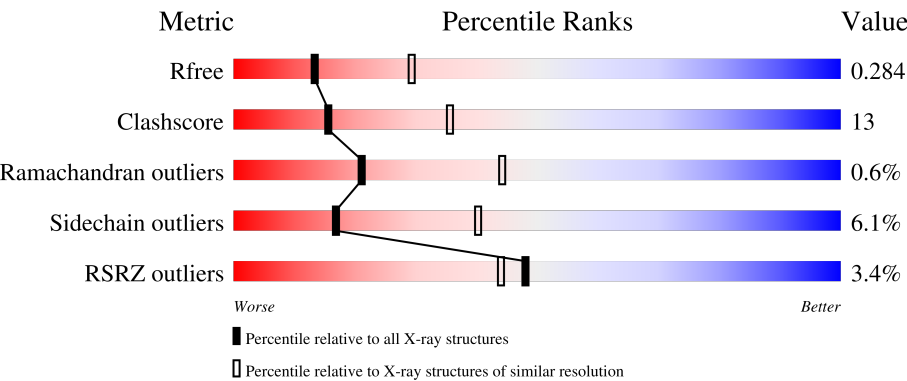
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	409	2% 68% 22% • 7%
1	C	409	3% 69% 24% • 5%
2	B	147	3% 37% 18% • 42%
2	D	147	3% 41% 13% • 45%
3	E	135	3% 60% 28% • • 7%

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Mol	Chain	Length	Quality of chain
3	G	135	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CNC	A	501	X	-	-	-
4	CNC	C	501	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9349 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 Transcobalamin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2972	1899	517	538	18			
1	C	388	Total	C	N	O	S	0	0	0
			3020	1932	525	545	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLN	ARG	conflict	UNP P20062
C	209	GLN	ARG	conflict	UNP P20062

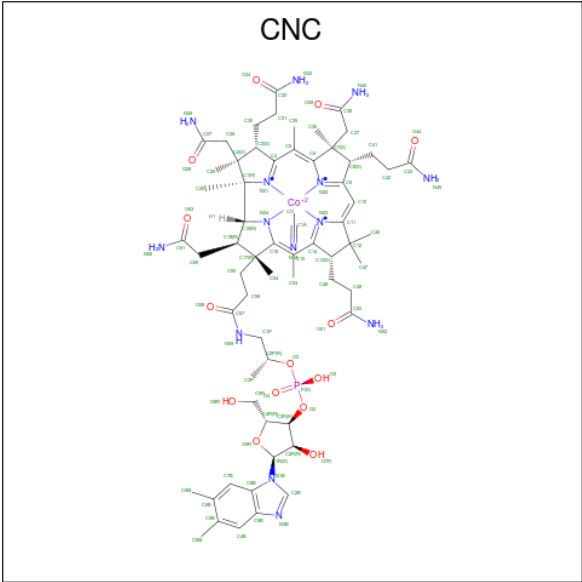
- Molecule 2 is a protein called CD320 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	85	Total	C	N	O	S	0	0	0
			628	371	110	135	12			
2	D	81	Total	C	N	O	S	0	0	0
			604	359	103	130	12			

- Molecule 3 is a protein called Anti-TC:CD320 nanobody TC-Nb4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	125	Total	C	N	O	S	0	0	0
			944	590	164	185	5			
3	G	121	Total	C	N	O	S	0	0	0
			924	579	161	179	5			

- Molecule 4 is CYANOCOBALAMIN (CCD ID: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Co	N	O	P	2	0
			93	63	1	14	14	1		
4	C	1	Total	C	Co	N	O	P	1	0
			93	63	1	14	14	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Ca	0	0
			2	2		
6	D	2	Total	Ca	0	0
			2	2		
6	E	1	Total	Ca	0	0
			1	1		
6	G	1	Total	Ca	0	0
			1	1		

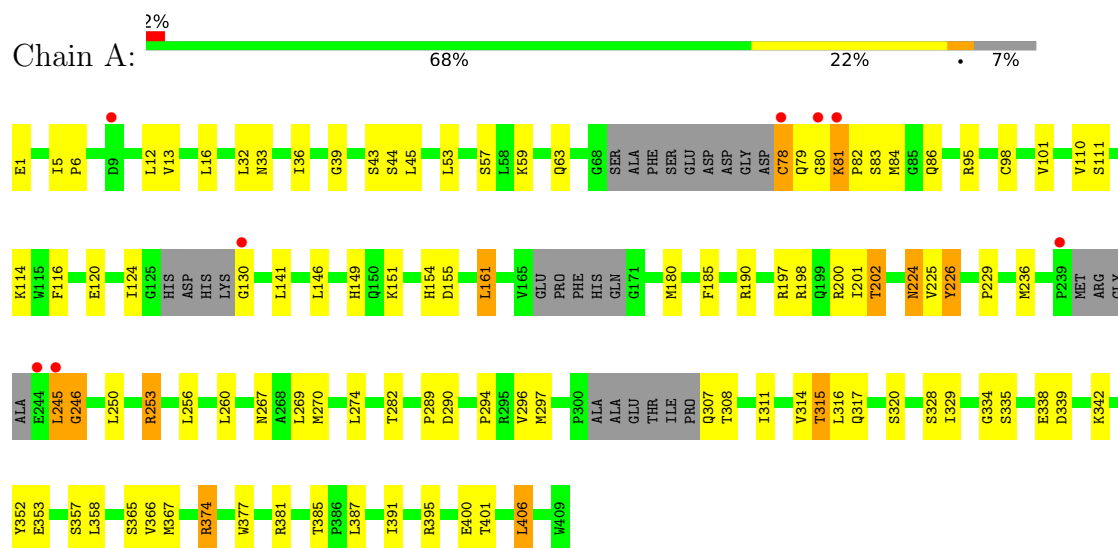
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	21	Total	O	0	0
			21	21		
7	B	2	Total	O	0	0
			2	2		
7	C	16	Total	O	0	0
			16	16		
7	D	1	Total	O	0	0
			1	1		
7	E	5	Total	O	0	0
			5	5		
7	G	2	Total	O	0	0
			2	2		

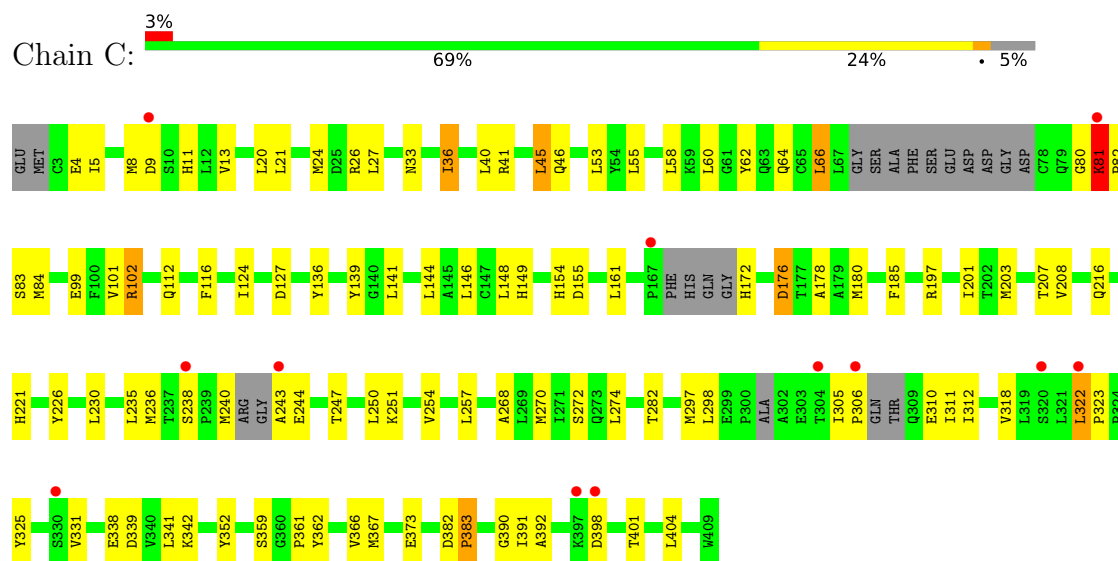
3 Residue-property plots [i](#)

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.

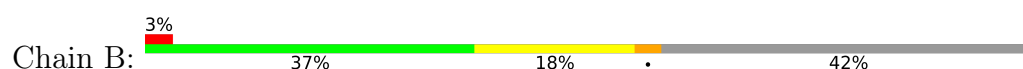
• Molecule 1: Transcobalamin-2



• Molecule 1: Transcobalamin-2

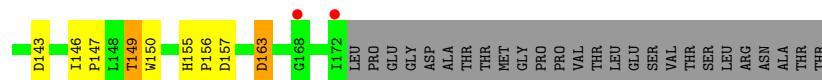


• Molecule 2: CD320 antigen





Chain D:



Chain E: 3% 60% 28% 7%



Chain G: 6% 59% 28% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.34Å 116.42Å 125.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.69 48.92 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.92-2.69) 97.3 (48.92-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.227 , 0.285 0.227 , 0.284	Depositor DCC
R_{free} test set	2128 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9349	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: CNC, GOL, CA

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	0.53	0/3031	0.80	4/4101 (0.1%)
1	C	0.47	0/3082	0.70	2/4174 (0.0%)
2	B	0.71	0/638	1.16	5/866 (0.6%)
2	D	0.43	0/614	0.68	0/834
3	E	0.63	0/966	1.12	10/1311 (0.8%)
3	G	0.52	0/944	0.82	2/1279 (0.2%)
All	All	0.53	0/9275	0.83	23/12565 (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	C	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	97	LYS	N-CA-C	7.94	120.01	111.36
2	B	72	TRP	N-CA-C	-7.78	103.36	112.92
3	E	124	SER	N-CA-C	7.59	120.70	109.24
2	B	70	LEU	CA-C-O	-7.50	113.60	121.55
3	E	123	PRO	N-CA-C	7.16	123.48	113.53
3	E	123	PRO	CA-C-N	-7.13	110.66	122.21
3	E	123	PRO	C-N-CA	-7.13	110.66	122.21
1	A	224	ASN	CB-CA-C	6.48	121.31	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	PRO	N-CA-CB	6.41	110.06	103.00
3	E	126	GLY	N-CA-C	6.23	120.53	112.68
2	B	70	LEU	N-CA-C	-6.15	101.99	110.35
1	A	226	TYR	CB-CA-C	6.07	121.16	110.85
3	E	97	LYS	CA-C-O	-6.06	114.00	120.42
1	C	80	GLY	CA-C-O	-5.93	114.64	120.75
1	C	81	LYS	CB-CA-C	5.91	121.80	110.17
2	B	153	ASP	CA-CB-CG	5.72	118.32	112.60
3	E	77	SER	N-CA-C	-5.63	105.03	112.24
3	E	122	GLN	N-CA-C	-5.50	97.61	109.01
1	A	246	GLY	CA-C-O	-5.32	115.27	120.75
3	G	97	LYS	CA-C-O	-5.26	114.85	120.42
3	E	125	ASN	CB-CA-C	5.24	120.85	110.42
1	A	224	ASN	CA-CB-CG	5.22	117.82	112.60
3	E	97	LYS	N-CA-C	5.02	116.83	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	168	GLY	Peptide
1	C	102	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	A	2972	0	3004	70	0
1	C	3020	0	3044	71	0
2	B	628	0	545	18	0
2	D	604	0	533	17	0
3	E	944	0	901	35	0
3	G	924	0	891	27	0
4	A	93	0	87	13	0
4	C	93	0	87	11	0
5	A	12	0	16	5	0
5	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
6	D	2	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
7	A	21	0	0	4	0
7	B	2	0	0	0	0
7	C	16	0	0	1	0
7	D	1	0	0	0	0
7	E	5	0	0	0	0
7	G	2	0	0	0	0
All	All	9349	0	9116	247	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 13.

All (247) 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)
4:A:501:CNC:C19	4:A:501:CNC:C1	1.75	1.55
3:E:82:ALA:O	3:E:83:ASP:OD1	1.65	1.14
2:B:137:LEU:HD23	2:B:148:LEU:HD23	1.42	1.01
4:A:501:CNC:C19	4:A:501:CNC:H262	1.91	0.98
1:C:84:MET:HE2	3:E:123:PRO:HG2	1.46	0.96
4:A:501:CNC:C19	4:A:501:CNC:C26	2.52	0.88
3:E:82:ALA:O	3:E:83:ASP:CG	2.17	0.86
3:G:112:THR:HG23	3:G:143:THR:HA	1.59	0.85
4:C:501:CNC:C14	4:C:501:CNC:H2B	2.11	0.80
2:B:129:ARG:HD2	2:B:143:ASP:OD2	1.81	0.80
2:B:167:CYS:C	2:B:169:THR:HG23	2.09	0.78
1:A:185:PHE:HB3	1:A:201:ILE:HG23	1.65	0.77
1:C:84:MET:CE	3:E:123:PRO:HG2	2.16	0.74
4:A:501:CNC:C1	4:A:501:CNC:C18	2.67	0.73
1:A:154:HIS:CG	2:D:149:THR:HG21	2.24	0.72
1:C:244:GLU:O	1:C:247:THR:OG1	2.07	0.71
3:E:104:MET:HB3	3:E:107:LEU:HD21	1.72	0.70
1:C:322:LEU:HD23	1:C:323:PRO:HA	1.74	0.70
2:D:146:ILE:HD13	2:D:150:TRP:HB2	1.74	0.69
2:B:137:LEU:HD23	2:B:148:LEU:CD2	2.18	0.69
1:A:236:MET:HE2	1:A:282:THR:HG22	1.75	0.69
1:A:366:VAL:HG12	1:A:367:MET:HG3	1.75	0.68
1:C:33:ASN:HB3	1:C:36:ILE:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:CYS:SG	2:D:90:ARG:N	2.66	0.68
3:E:33:VAL:HG11	3:E:107:LEU:HD12	1.76	0.67
2:B:131:ALA:HA	2:B:138:ARG:HH22	1.61	0.66
1:A:6:PRO:HD2	1:A:253:ARG:HD2	1.78	0.65
3:E:109:PRO:HA	3:E:144:VAL:HG13	1.77	0.65
1:A:84:MET:HG3	1:A:116:PHE:HB2	1.79	0.65
1:A:197:ARG:HD2	1:A:200:ARG:HD3	1.78	0.65
1:C:341:LEU:HD23	1:C:352:TYR:CD2	2.32	0.64
1:C:312:ILE:HD11	1:C:398:ASP:HB2	1.78	0.64
1:A:289:PRO:HA	5:A:502:GOL:H11	1.80	0.63
1:C:362:TYR:OH	7:C:601:HOH:O	2.14	0.63
1:C:66:LEU:HA	3:E:124:SER:HB3	1.80	0.63
4:A:501:CNC:C20	4:A:501:CNC:H18	2.28	0.63
2:B:167:CYS:O	2:B:169:THR:HG23	1.99	0.63
3:E:89:PHE:O	3:E:90:ILE:HD13	1.99	0.63
1:A:130:GLY:N	7:A:603:HOH:O	2.30	0.62
1:C:339:ASP:HA	1:C:342:LYS:HG3	1.81	0.62
1:A:226:TYR:HA	1:A:270:MET:HE2	1.81	0.62
2:B:129:ARG:HD2	2:B:143:ASP:CG	2.23	0.61
1:C:155:ASP:HB3	1:C:197:ARG:HE	1.66	0.61
1:C:270:MET:HA	1:C:270:MET:HE2	1.82	0.61
3:G:89:PHE:O	3:G:90:ILE:HD13	2.00	0.61
1:C:305:ILE:HD12	1:C:306:PRO:HD2	1.83	0.60
2:D:138:ARG:NH2	2:D:143:ASP:OD2	2.34	0.60
1:A:81:LYS:HB3	1:A:82:PRO:HA	1.82	0.60
4:A:501:CNC:C19	4:A:501:CNC:C20	2.75	0.60
3:G:88:ARG:NH1	3:G:111:ASP:OD2	2.34	0.60
2:D:146:ILE:HD12	2:D:147:PRO:O	2.01	0.59
3:E:121:TYR:CZ	3:E:123:PRO:HG3	2.37	0.59
3:G:130:ARG:HH12	3:G:132:GLU:CD	2.11	0.58
1:C:8:MET:HE1	1:C:257:LEU:HD23	1.85	0.57
1:C:139:TYR:HD2	1:C:161:LEU:HD13	1.69	0.57
1:C:310:GLU:CD	1:C:310:GLU:H	2.13	0.56
2:B:149:THR:HB	1:C:154:HIS:CD2	2.39	0.56
3:E:82:ALA:C	3:E:83:ASP:OD1	2.47	0.56
3:G:49:THR:HB	3:G:52:ILE:HD11	1.87	0.56
2:D:85:ASP:N	2:D:85:ASP:OD1	2.39	0.56
3:G:97:LYS:HB3	3:G:99:THR:HG23	1.86	0.56
4:A:501:CNC:H4B	4:A:501:CNC:C4	2.36	0.56
3:E:44:ALA:HA	3:E:99:THR:HG22	1.87	0.56
3:E:97:LYS:HB3	3:E:99:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:O	1:A:250:LEU:HG	2.06	0.55
1:A:13:VAL:HG12	1:A:45:LEU:HD21	1.89	0.55
1:C:84:MET:HG3	1:C:116:PHE:HB2	1.90	0.54
1:C:9:ASP:OD2	1:C:11:HIS:N	2.37	0.54
4:C:501:CNC:N23	4:C:501:CNC:C2B	2.70	0.54
3:G:119:ALA:HB3	3:G:135:TYR:HB2	1.89	0.54
1:C:318:VAL:HG22	1:C:404:LEU:HB2	1.89	0.54
1:C:155:ASP:HB3	1:C:197:ARG:NE	2.23	0.54
3:E:83:ASP:HA	3:E:86:LYS:HB2	1.89	0.54
1:A:353:GLU:HB2	1:A:365:SER:HB3	1.88	0.53
1:A:357:SER:HB2	4:A:501:CNC:H2R	1.88	0.53
1:C:236:MET:HE2	1:C:282:THR:HG22	1.90	0.53
1:C:247:THR:O	1:C:251:LYS:HG3	2.07	0.53
3:G:94:ASP:HB3	3:G:97:LYS:HB2	1.89	0.53
1:A:294:PRO:HB2	2:B:171:GLU:HB2	1.91	0.53
3:E:65:GLU:HG2	3:E:66:ARG:N	2.24	0.53
3:G:44:ALA:HA	3:G:99:THR:HG22	1.90	0.53
1:C:21:LEU:O	1:C:24:MET:HB2	2.09	0.53
1:A:1:GLU:HB2	1:A:245:LEU:HB3	1.90	0.52
3:G:79:THR:HB	3:G:91:ILE:HD11	1.90	0.52
1:C:382:ASP:OD2	1:C:383:PRO:HA	2.09	0.52
3:E:108:GLU:O	3:E:144:VAL:HG11	2.09	0.52
1:A:197:ARG:O	1:A:200:ARG:N	2.42	0.52
1:C:197:ARG:O	1:C:201:ILE:HG13	2.09	0.52
1:C:81:LYS:HE3	3:E:123:PRO:HD2	1.90	0.52
1:C:226:TYR:HB3	1:C:270:MET:SD	2.50	0.52
1:C:250:LEU:O	1:C:254:VAL:HG23	2.10	0.52
2:B:141:LEU:HD12	2:B:160:ASP:OD2	2.10	0.51
4:C:501:CNC:H8	4:C:501:CNC:O39	2.10	0.51
2:D:157:ASP:N	2:D:163:ASP:OD1	2.39	0.51
2:B:58:LYS:HD3	2:B:67:CYS:HB3	1.91	0.51
3:G:43:CYS:HB2	3:G:57:TRP:CZ2	2.45	0.51
1:C:325:TYR:CD2	1:C:367:MET:HE1	2.46	0.51
3:E:89:PHE:C	3:E:90:ILE:HD13	2.36	0.51
1:A:98:CYS:SG	1:A:289:PRO:HB2	2.50	0.51
2:B:59:PHE:HE2	2:B:73:ARG:HH11	1.57	0.50
2:D:163:ASP:OD2	2:D:163:ASP:N	2.42	0.50
1:A:154:HIS:ND1	2:D:149:THR:HG21	2.25	0.50
4:A:501:CNC:O39	4:A:501:CNC:H8	2.11	0.50
1:C:101:VAL:HG12	1:C:149:HIS:ND1	2.27	0.50
1:A:338:GLU:N	1:A:391:ILE:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ASP:HB2	1:C:401:THR:HB	1.93	0.50
3:E:33:VAL:HG22	3:E:37:GLY:HA3	1.93	0.50
3:G:27:GLU:CD	3:G:139:GLY:H	2.20	0.50
1:C:141:LEU:HA	1:C:180:MET:HE2	1.94	0.49
3:E:121:TYR:CE2	3:E:123:PRO:HG3	2.48	0.49
1:C:62:TYR:HA	1:C:82:PRO:HG2	1.94	0.49
1:C:99:GLU:HG2	1:C:102:ARG:NH2	2.28	0.49
2:D:130:LEU:HG	3:G:95:ASN:O	2.13	0.49
1:A:101:VAL:HG12	1:A:149:HIS:ND1	2.28	0.49
4:C:501:CNC:C6	4:C:501:CNC:C1A	2.80	0.49
1:C:84:MET:HE1	1:C:112:GLN:HB3	1.95	0.49
1:C:390:GLY:HA3	4:C:501:CNC:HM53	1.94	0.49
1:C:178:ALA:HB1	1:C:208:VAL:HG13	1.94	0.48
3:G:58:PHE:CD2	3:G:68:GLY:HA2	2.47	0.48
4:A:501:CNC:C18	4:A:501:CNC:C20	2.92	0.48
1:A:198:ARG:O	1:A:202:THR:HG23	2.13	0.48
3:G:64:LYS:HG2	3:G:65:GLU:N	2.27	0.48
1:A:342:LYS:HD3	1:A:352:TYR:OH	2.14	0.48
1:C:366:VAL:HG12	1:C:367:MET:HG2	1.96	0.48
1:A:59:LYS:O	1:A:63:GLN:HB2	2.13	0.48
3:E:88:ARG:NH2	3:E:111:ASP:OD2	2.47	0.48
1:A:151:LYS:HE2	2:D:155:HIS:CD2	2.49	0.47
4:A:501:CNC:H2B	4:A:501:CNC:C14	2.43	0.47
1:A:197:ARG:NH2	7:A:605:HOH:O	2.46	0.47
3:E:84:SER:O	3:E:88:ARG:NH1	2.48	0.47
2:B:130:LEU:HD21	3:E:98:ASN:HB2	1.97	0.47
1:A:226:TYR:O	1:A:229:PRO:HD2	2.14	0.47
2:B:135:GLY:O	2:B:148:LEU:HG	2.14	0.47
1:A:33:ASN:HB3	1:A:36:ILE:HD12	1.96	0.47
1:C:216:GLN:HA	1:C:221:HIS:O	2.15	0.47
4:C:501:CNC:N21	4:C:501:CNC:N3B	2.62	0.47
4:C:501:CNC:N23	4:C:501:CNC:N3B	2.63	0.47
1:A:315:THR:HG22	7:A:604:HOH:O	2.15	0.46
1:A:374:ARG:HD2	1:A:374:ARG:HA	1.45	0.46
1:A:381:ARG:HB3	1:A:387:LEU:HD21	1.96	0.46
1:C:146:LEU:HA	1:C:146:LEU:HD23	1.58	0.46
1:A:250:LEU:HA	1:A:253:ARG:HG2	1.97	0.46
1:A:366:VAL:HG12	1:A:367:MET:CG	2.46	0.46
2:B:129:ARG:HD2	2:B:143:ASP:OD1	2.15	0.46
1:A:120:GLU:O	1:A:124:ILE:HG13	2.16	0.46
1:C:36:ILE:HD11	1:C:268:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:GLU:HB3	1:C:247:THR:HG23	1.97	0.46
2:D:58:LYS:HG3	2:D:69:PRO:HA	1.98	0.46
1:A:32:LEU:HD11	1:A:57:SER:HB3	1.98	0.46
1:A:63:GLN:HE22	5:A:503:GOL:C3	2.29	0.46
4:C:501:CNC:C14	4:C:501:CNC:C2B	2.89	0.46
1:A:44:SER:O	1:A:296:VAL:HG12	2.16	0.45
1:C:33:ASN:CB	1:C:36:ILE:HG13	2.45	0.45
1:A:307:GLN:HG2	1:A:308:THR:H	1.82	0.45
1:A:316:LEU:HD12	1:A:317:GLN:H	1.81	0.45
1:C:124:ILE:HD13	1:C:136:TYR:OH	2.17	0.45
3:E:65:GLU:HG2	3:E:66:ARG:H	1.80	0.45
1:A:256:LEU:O	1:A:260:LEU:HD12	2.16	0.45
1:C:27:LEU:HD11	1:C:53:LEU:HD21	1.98	0.45
3:E:61:ALA:HB3	3:E:64:LYS:HB3	1.98	0.45
1:A:154:HIS:CD2	1:A:155:ASP:H	2.35	0.45
4:C:501:CNC:H422	4:C:501:CNC:H361	1.99	0.45
3:G:86:LYS:O	3:G:86:LYS:HG3	2.16	0.45
1:C:312:ILE:HG22	1:C:331:VAL:O	2.17	0.45
4:C:501:CNC:H552	4:C:501:CNC:H531	1.99	0.45
1:C:40:LEU:HD12	1:C:40:LEU:HA	1.74	0.44
1:C:240:MET:HG3	1:C:243:ALA:N	2.33	0.44
1:A:290:ASP:H	5:A:502:GOL:C1	2.30	0.44
1:A:197:ARG:O	1:A:198:ARG:C	2.60	0.44
1:C:13:VAL:HG12	1:C:45:LEU:HD21	1.99	0.44
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.88	0.44
2:B:137:LEU:HB3	2:B:148:LEU:HD21	2.00	0.44
1:C:203:MET:O	1:C:207:THR:HG23	2.17	0.44
2:D:71:THR:HG22	2:D:72:TRP:HD1	1.83	0.44
3:E:40:ARG:HG3	3:E:103:GLN:OE1	2.18	0.44
1:A:16:LEU:HD21	1:A:274:LEU:HD23	1.99	0.44
1:A:95:ARG:HD2	1:A:95:ARG:HA	1.70	0.43
4:A:501:CNC:H541	4:A:501:CNC:H602	1.54	0.43
1:A:5:ILE:HD13	1:A:253:ARG:HB3	1.99	0.43
1:A:80:GLY:O	1:A:81:LYS:HB2	2.18	0.43
1:C:55:LEU:O	1:C:58:LEU:HB2	2.18	0.43
3:E:59:ARG:HB3	3:E:115:TYR:CE2	2.53	0.43
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.84	0.43
2:B:78:LEU:HD12	2:B:86:GLU:HG3	2.01	0.43
3:G:88:ARG:HH12	3:G:111:ASP:CG	2.27	0.43
1:A:110:VAL:HG13	1:A:146:LEU:CD2	2.49	0.43
1:C:161:LEU:HD23	1:C:185:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:89:PHE:CD2	3:E:89:PHE:N	2.86	0.43
1:A:39:GLY:O	1:A:43:SER:HB3	2.18	0.43
1:A:328:SER:C	1:A:329:ILE:HD12	2.44	0.43
3:G:27:GLU:N	3:G:27:GLU:OE1	2.52	0.43
1:C:60:LEU:O	1:C:64:GLN:HB2	2.18	0.42
1:C:141:LEU:HA	1:C:180:MET:CE	2.50	0.42
1:C:141:LEU:HD13	1:C:180:MET:HE2	2.00	0.42
3:G:69:VAL:HG13	3:G:85:VAL:HG21	2.01	0.42
1:A:290:ASP:H	5:A:502:GOL:H2	1.83	0.42
3:E:89:PHE:HA	3:E:103:GLN:O	2.18	0.42
1:A:1:GLU:HB2	1:A:245:LEU:CB	2.49	0.42
1:A:81:LYS:O	3:G:124:SER:OG	2.37	0.42
1:A:154:HIS:HD2	7:A:618:HOH:O	2.01	0.42
1:A:297:MET:HE2	1:A:297:MET:HB2	1.94	0.42
1:A:307:GLN:HG2	1:A:308:THR:N	2.35	0.42
1:C:230:LEU:HA	1:C:230:LEU:HD12	1.81	0.42
1:A:267:ASN:HB3	1:A:270:MET:HB2	2.00	0.42
1:C:62:TYR:O	1:C:66:LEU:HB2	2.20	0.42
1:C:361:PRO:HG2	1:C:392:ALA:HB2	2.01	0.42
1:A:377:TRP:CZ3	1:A:406:LEU:HB2	2.55	0.42
4:A:501:CNC:H18	4:A:501:CNC:H201	1.98	0.42
3:E:91:ILE:H	3:E:91:ILE:HG13	1.67	0.42
1:A:63:GLN:HE22	5:A:503:GOL:H31	1.85	0.42
3:G:89:PHE:C	3:G:90:ILE:HD13	2.45	0.42
1:A:141:LEU:HD13	1:A:180:MET:HE3	2.02	0.41
1:A:334:GLY:O	1:A:395:ARG:HD3	2.19	0.41
3:E:85:VAL:HA	3:E:88:ARG:HH11	1.84	0.41
1:C:20:LEU:HD22	1:C:36:ILE:HD13	2.02	0.41
3:G:107:LEU:HD12	3:G:144:VAL:HG21	2.02	0.41
1:C:45:LEU:HG	1:C:298:LEU:HD21	2.01	0.41
1:A:111:SER:HA	1:A:114:LYS:HD3	2.02	0.41
3:G:57:TRP:CD1	3:G:102:LEU:HB2	2.55	0.41
1:C:4:GLU:O	1:C:5:ILE:HD13	2.20	0.41
2:D:59:PHE:HE2	2:D:85:ASP:HA	1.86	0.41
3:G:74:SER:HB3	3:G:75:ARG:HG3	2.03	0.41
1:A:78:CYS:HB3	1:A:79:GLN:H	1.75	0.41
1:C:81:LYS:HD2	3:E:124:SER:O	2.21	0.41
3:E:85:VAL:HA	3:E:88:ARG:NH1	2.35	0.41
1:A:86:GLN:HG2	1:A:358:LEU:HD11	2.01	0.41
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.90	0.41
1:A:335:SER:HB3	1:A:339:ASP:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:TYR:HD2	1:C:161:LEU:CD1	2.32	0.41
1:C:176:ASP:OD1	1:C:176:ASP:N	2.50	0.41
1:C:338:GLU:N	1:C:391:ILE:O	2.50	0.41
2:D:137:LEU:HD12	2:D:138:ARG:H	1.86	0.41
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.95	0.41
1:C:41:ARG:HA	1:C:41:ARG:HD2	1.80	0.40
3:E:34:GLN:O	3:E:37:GLY:N	2.53	0.40
1:C:46:GLN:NE2	1:C:297:MET:HG2	2.36	0.40
1:C:84:MET:CE	1:C:112:GLN:HB3	2.52	0.40
2:D:155:HIS:CD2	2:D:156:PRO:HD2	2.56	0.40
3:E:130:ARG:HD2	3:E:132:GLU:OE2	2.21	0.40
4:C:501:CNC:H562	4:C:501:CNC:H18	1.95	0.40
3:G:54:ASP:OD1	3:G:74:SER:HB2	2.21	0.40
1:A:314:VAL:HG13	1:A:400:GLU:O	2.22	0.40
1:C:4:GLU:C	1:C:5:ILE:HD13	2.46	0.40
2:D:137:LEU:HD12	2:D:138:ARG:N	2.36	0.40
3:G:102:LEU:HD12	3:G:102:LEU:HA	1.85	0.40
2:B:147:PRO:HD2	2:B:150:TRP:CD2	2.57	0.40
3:G:25:LEU:HD23	3:G:25:LEU:H	1.87	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	369/409 (90%)	357 (97%)	11 (3%)	1 (0%)	36	60
1	C	376/409 (92%)	360 (96%)	14 (4%)	2 (0%)	24	48
2	B	81/147 (55%)	77 (95%)	3 (4%)	1 (1%)	10	27
2	D	77/147 (52%)	70 (91%)	7 (9%)	0	100	100
3	E	123/135 (91%)	111 (90%)	10 (8%)	2 (2%)	7	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	117/135 (87%)	111 (95%)	5 (4%)	1 (1%)	14	35
All	All	1143/1382 (83%)	1086 (95%)	50 (4%)	7 (1%)	21	44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	83	ASP
2	B	71	THR
1	C	81	LYS
3	E	50	PRO
3	G	46	SER
1	A	81	LYS
1	C	383	PRO

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	322/348 (92%)	303 (94%)	19 (6%)	18	42
1	C	326/348 (94%)	308 (94%)	18 (6%)	19	45
2	B	73/129 (57%)	66 (90%)	7 (10%)	8	20
2	D	72/129 (56%)	69 (96%)	3 (4%)	26	55
3	E	102/112 (91%)	94 (92%)	8 (8%)	11	29
3	G	100/112 (89%)	94 (94%)	6 (6%)	17	41
All	All	995/1178 (84%)	934 (94%)	61 (6%)	17	40

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	53	LEU
1	A	78	CYS
1	A	83	SER

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Mol	Chain	Res	Type
1	A	161	LEU
1	A	190	ARG
1	A	202	THR
1	A	224	ASN
1	A	225	VAL
1	A	245	LEU
1	A	253	ARG
1	A	269	LEU
1	A	311	ILE
1	A	315	THR
1	A	320	SER
1	A	374	ARG
1	A	385	THR
1	A	401	THR
1	A	406	LEU
2	B	71	THR
2	B	73	ARG
2	B	84	SER
2	B	128	SER
2	B	143	ASP
2	B	170	ASN
2	B	171	GLU
1	C	26	ARG
1	C	36	ILE
1	C	45	LEU
1	C	66	LEU
1	C	81	LYS
1	C	83	SER
1	C	127	ASP
1	C	144	LEU
1	C	172	HIS
1	C	176	ASP
1	C	235	LEU
1	C	238	SER
1	C	272	SER
1	C	274	LEU
1	C	311	ILE
1	C	322	LEU
1	C	359	SER
1	C	373	GLU
2	D	54	CYS
2	D	149	THR

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Mol	Chain	Res	Type
2	D	163	ASP
3	E	26	VAL
3	E	73	SER
3	E	75	ARG
3	E	89	PHE
3	E	91	ILE
3	E	97	LYS
3	E	124	SER
3	E	134	SER
3	G	24	GLN
3	G	25	LEU
3	G	89	PHE
3	G	91	ILE
3	G	96	VAL
3	G	106	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	63	GLN
1	A	154	HIS
1	A	261	GLN
2	B	155	HIS
2	B	170	ASN
1	C	19	HIS
1	C	64	GLN
1	C	192	ASN
1	C	317	GLN
1	C	389	GLN
2	D	155	HIS
3	E	34	GLN
3	E	125	ASN
3	G	60	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](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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	GOL	A	503	-	5,5,5	0.95	0	5,5,5	1.22	1 (20%)
4	CNC	A	501	-	93,103,103	3.34	42 (45%)	149,171,171	4.87	68 (45%)
5	GOL	A	502	-	5,5,5	1.36	1 (20%)	5,5,5	1.06	0
5	GOL	C	502	-	5,5,5	1.37	1 (20%)	5,5,5	1.31	1 (20%)
4	CNC	C	501	-	93,103,103	3.33	41 (44%)	149,171,171	4.40	62 (41%)

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	GOL	A	503	-	-	2/4/4/4	-
4	CNC	A	501	-	1/1/36/38	7/56/235/235	0/3/11/11
5	GOL	A	502	-	-	2/4/4/4	-
5	GOL	C	502	-	-	2/4/4/4	-
4	CNC	C	501	-	1/1/36/38	1/56/235/235	0/3/11/11

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	CNC	C10-C9	9.91	1.67	1.39
4	C	501	CNC	C10-C11	9.72	1.64	1.37
4	A	501	CNC	C3R-C4R	-9.71	1.27	1.52
4	A	501	CNC	C10-C9	9.63	1.66	1.39
4	A	501	CNC	C10-C11	9.28	1.63	1.37
4	C	501	CNC	C3R-C4R	-8.52	1.30	1.52
4	A	501	CNC	C1-C19	7.86	1.75	1.54
4	C	501	CNC	C1-C19	7.18	1.74	1.54
4	C	501	CNC	C6-C5	7.07	1.56	1.36
4	A	501	CNC	C57-N59	7.02	1.50	1.33
4	A	501	CNC	C4-C5	6.85	1.71	1.43
4	C	501	CNC	C4-C5	6.71	1.70	1.43
4	A	501	CNC	C6-C5	6.70	1.55	1.36
4	C	501	CNC	C57-N59	6.52	1.48	1.33
4	A	501	CNC	C2R-C1R	-6.38	1.33	1.53
4	C	501	CNC	C2R-C1R	-6.33	1.33	1.53
4	C	501	CNC	O6R-C4R	5.92	1.58	1.45
4	C	501	CNC	C1-C2	-5.81	1.45	1.58
4	A	501	CNC	C19-N24	-5.57	1.37	1.49
4	A	501	CNC	O6R-C4R	5.48	1.57	1.45
4	A	501	CNC	C9B-N3B	-5.32	1.29	1.39
4	C	501	CNC	C19-N24	-5.30	1.38	1.49
4	A	501	CNC	C3-C4	-5.29	1.38	1.51
4	A	501	CNC	C54-C17	-5.13	1.46	1.54
4	C	501	CNC	C54-C17	-4.70	1.46	1.54
4	C	501	CNC	C50-N52	4.70	1.48	1.32
4	C	501	CNC	C38-N40	4.65	1.47	1.32
4	C	501	CNC	C36-C7	-4.65	1.47	1.54
4	C	501	CNC	O6R-C1R	4.59	1.52	1.42
4	C	501	CNC	C61-N62	4.46	1.47	1.32
4	C	501	CNC	C3-C4	-4.37	1.41	1.51
4	A	501	CNC	C7-C6	4.34	1.64	1.54
4	C	501	CNC	C43-N45	4.33	1.46	1.32
4	C	501	CNC	C27-N29	4.23	1.46	1.32
4	A	501	CNC	C38-N40	4.21	1.46	1.32
4	A	501	CNC	C2R-C3R	4.15	1.62	1.53
4	A	501	CNC	O6R-C1R	4.15	1.51	1.42
4	A	501	CNC	C14-C15	4.15	1.60	1.43
4	C	501	CNC	C32-N33	4.11	1.46	1.32
4	C	501	CNC	C14-C15	4.08	1.59	1.43
4	A	501	CNC	C50-N52	4.04	1.45	1.32
4	A	501	CNC	C43-N45	4.02	1.45	1.32
4	A	501	CNC	C27-N29	3.99	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	CNC	C61-N62	3.97	1.45	1.32
4	A	501	CNC	C32-N33	3.79	1.45	1.32
4	C	501	CNC	C2R-C3R	3.74	1.61	1.53
4	A	501	CNC	C2B-N1B	-3.58	1.31	1.37
4	C	501	CNC	C16-C15	3.57	1.58	1.42
4	C	501	CNC	C7-C6	3.55	1.62	1.54
4	A	501	CNC	C4B-C5B	-3.52	1.34	1.39
4	A	501	CNC	C16-C15	3.28	1.57	1.42
4	C	501	CNC	C17-C16	3.25	1.61	1.54
4	C	501	CNC	C56-C57	3.21	1.57	1.51
4	C	501	CNC	C35-C5	3.19	1.57	1.50
4	A	501	CNC	C2-C3	3.15	1.66	1.57
4	A	501	CNC	C8B-C9B	-3.13	1.35	1.40
4	C	501	CNC	C12-C11	2.99	1.61	1.51
4	A	501	CNC	C26-C2	2.98	1.62	1.55
4	A	501	CNC	C1-C2	-2.92	1.52	1.58
4	C	501	CNC	C9B-N3B	-2.92	1.34	1.39
4	A	501	CNC	C56-C57	2.91	1.57	1.51
4	C	501	CNC	P-O2	2.89	1.68	1.59
5	C	502	GOL	C3-C2	2.89	1.62	1.51
4	A	501	CNC	C35-C5	2.86	1.56	1.50
4	C	501	CNC	C2B-N1B	-2.81	1.32	1.37
4	C	501	CNC	C8B-N1B	-2.78	1.33	1.39
4	A	501	CNC	O3-C2P	-2.74	1.38	1.45
4	A	501	CNC	C55-C56	2.65	1.59	1.53
4	A	501	CNC	C8B-N1B	-2.55	1.34	1.39
4	C	501	CNC	C55-C56	2.52	1.58	1.53
4	A	501	CNC	P-O2	2.48	1.66	1.59
4	C	501	CNC	C8B-C9B	-2.42	1.36	1.40
4	A	501	CNC	O63-C61	-2.38	1.16	1.23
4	A	501	CNC	C26-C27	2.38	1.59	1.51
4	A	501	CNC	O58-C57	-2.37	1.18	1.23
4	A	501	CNC	C12-C11	2.32	1.59	1.51
4	C	501	CNC	P-O3	2.26	1.66	1.59
4	A	501	CNC	C36-C7	-2.25	1.50	1.54
5	A	502	GOL	C3-C2	2.24	1.60	1.51
4	C	501	CNC	C25-C2	-2.20	1.50	1.54
4	C	501	CNC	C26-C2	2.18	1.60	1.55
4	C	501	CNC	O28-C27	-2.15	1.17	1.23
4	C	501	CNC	C37-C38	2.15	1.58	1.51
4	C	501	CNC	C6M-C6B	2.13	1.55	1.51
4	A	501	CNC	C37-C38	2.08	1.58	1.51

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	CNC	C3-C4-C5	-24.37	83.04	123.82
4	A	501	CNC	C36-C7-C37	-19.82	77.04	110.74
4	A	501	CNC	C25-C2-C26	-19.64	70.71	109.74
4	A	501	CNC	C3-C4-C5	-19.60	91.02	123.82
4	C	501	CNC	C36-C7-C37	-15.75	83.96	110.74
4	A	501	CNC	C26-C2-C3	-15.56	80.27	107.42
4	A	501	CNC	C26-C2-C1	-14.47	87.65	110.00
4	C	501	CNC	C8-C9-C10	-13.63	94.32	123.33
4	C	501	CNC	C25-C2-C26	-13.46	83.00	109.74
4	A	501	CNC	C8-C9-C10	-12.98	95.70	123.33
4	A	501	CNC	C7-C6-C5	-12.92	107.87	128.07
4	C	501	CNC	C26-C2-C1	-11.53	92.20	110.00
4	A	501	CNC	C13-C14-C15	-11.40	104.74	123.82
4	C	501	CNC	C1-C19-C18	-11.16	104.99	121.75
4	A	501	CNC	C12-C11-N23	-10.87	99.88	111.49
4	A	501	CNC	C37-C7-C8	-10.34	81.08	108.37
4	A	501	CNC	C37-C7-C6	-10.33	75.12	107.11
4	C	501	CNC	C26-C2-C3	-9.90	90.15	107.42
4	C	501	CNC	C13-C14-C15	-9.79	107.44	123.82
4	C	501	CNC	C12-C11-N23	-9.53	101.32	111.49
4	A	501	CNC	C17-C16-C15	-9.05	113.09	126.70
4	C	501	CNC	C7-C6-C5	-9.03	113.96	128.07
4	A	501	CNC	C1-C19-C18	-8.76	108.60	121.75
4	C	501	CNC	C25-C2-C1	8.45	126.38	113.75
4	A	501	CNC	C35-C5-C4	7.58	132.15	116.79
4	C	501	CNC	C18-C19-N24	7.56	113.95	101.92
4	A	501	CNC	C9-C10-C11	-7.41	114.94	125.84
4	C	501	CNC	C30-C3-C2	-7.37	102.75	119.00
4	C	501	CNC	C37-C7-C8	-7.24	89.26	108.37
4	C	501	CNC	C37-C7-C6	-7.14	85.01	107.11
4	C	501	CNC	C9-C10-C11	-6.96	115.61	125.84
4	A	501	CNC	C5M-C5B-C4B	-6.53	108.07	119.57
4	C	501	CNC	C5-C4-N21	-6.51	113.72	124.19
4	A	501	CNC	C6-C5-C4	-6.46	110.04	121.55
4	A	501	CNC	C12-C11-C10	-6.41	117.78	123.54
4	A	501	CNC	C2-C26-C27	6.20	132.43	115.19
4	A	501	CNC	C18-C19-N24	6.12	111.66	101.92
4	A	501	CNC	C30-C3-C2	-5.71	106.40	119.00
4	C	501	CNC	C36-C7-C8	5.68	122.54	112.05
4	A	501	CNC	C36-C7-C8	5.62	122.42	112.05
4	C	501	CNC	C12-C11-C10	-5.54	118.56	123.54
4	C	501	CNC	C35-C5-C4	5.52	127.98	116.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CNC	C7-C6-N22	-5.50	97.91	107.94
4	C	501	CNC	C6-C5-C4	-5.26	112.18	121.55
4	C	501	CNC	C25-C2-C3	5.24	126.22	112.91
4	C	501	CNC	C7-C6-N22	-5.19	98.49	107.94
4	A	501	CNC	C5M-C5B-C6B	5.08	131.14	120.76
4	A	501	CNC	C25-C2-C3	4.94	125.47	112.91
4	C	501	CNC	C8-C7-C6	4.90	109.24	100.92
4	A	501	CNC	C16-C15-C14	-4.84	114.72	121.29
4	A	501	CNC	C7-C37-C38	4.79	128.45	114.28
4	A	501	CNC	C5-C4-N21	-4.77	116.52	124.19
4	C	501	CNC	C19-N24-C16	-4.72	104.42	111.96
4	A	501	CNC	C41-C8-C9	4.69	119.38	111.19
4	C	501	CNC	C16-C15-C14	-4.63	115.00	121.29
4	C	501	CNC	C17-C16-C15	-4.49	119.94	126.70
4	A	501	CNC	C5-C6-N22	-4.48	117.10	123.88
4	A	501	CNC	C19-C1-N21	-4.46	96.06	101.69
4	C	501	CNC	C5M-C5B-C4B	-4.37	111.88	119.57
4	C	501	CNC	C1-C2-C3	4.35	107.08	101.60
4	A	501	CNC	C20-C1-C2	-4.32	106.15	113.28
4	A	501	CNC	C13-C12-C11	-4.14	95.31	100.86
4	C	501	CNC	N1B-C2B-N3B	-4.06	108.17	113.94
4	A	501	CNC	N1B-C2B-N3B	-4.01	108.25	113.94
4	C	501	CNC	C35-C5-C6	-3.87	116.18	122.41
4	C	501	CNC	C41-C8-C9	3.74	117.70	111.19
4	A	501	CNC	O28-C27-N29	-3.69	112.68	122.53
4	C	501	CNC	C8B-N1B-C2B	3.63	109.55	106.26
4	A	501	CNC	C25-C2-C1	3.60	119.14	113.75
4	C	501	CNC	O28-C27-N29	-3.54	113.09	122.53
4	A	501	CNC	C15-C14-N23	-3.51	119.80	126.67
4	C	501	CNC	C55-C17-C18	-3.43	104.56	111.12
4	C	501	CNC	C30-C31-C32	-3.41	100.98	112.55
4	A	501	CNC	C7B-C8B-C9B	-3.41	118.39	122.47
4	A	501	CNC	C9B-N3B-C2B	3.38	108.55	104.40
4	A	501	CNC	C17-C16-N24	-3.30	105.37	110.91
4	A	501	CNC	C18-C17-C16	3.29	105.55	100.34
4	C	501	CNC	C5M-C5B-C6B	3.25	127.39	120.76
4	A	501	CNC	C60-C18-C17	-3.21	107.04	115.82
4	C	501	CNC	C8B-N1B-C1R	-3.21	119.98	125.41
4	C	501	CNC	C60-C18-C17	-3.18	107.12	115.82
4	C	501	CNC	C5-C6-N22	-3.16	119.11	123.88
4	C	501	CNC	C26-C27-N29	2.98	125.71	116.49
4	C	501	CNC	C55-C17-C16	2.96	122.61	116.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CNC	C35-C5-C6	-2.93	117.69	122.41
4	C	501	CNC	C9B-N3B-C2B	2.88	107.93	104.40
4	C	501	CNC	C3R-C2R-C1R	2.86	106.19	99.89
4	A	501	CNC	C19-N24-C16	-2.84	107.41	111.96
4	A	501	CNC	C6M-C6B-C5B	-2.78	115.08	120.76
4	C	501	CNC	P-O3-C2P	-2.78	111.61	121.10
4	C	501	CNC	C36-C7-C6	2.76	126.71	112.41
4	A	501	CNC	C8B-N1B-C2B	2.74	108.75	106.26
4	C	501	CNC	O2-C3R-C2R	-2.74	101.86	111.68
4	A	501	CNC	C4B-C9B-C8B	2.73	122.67	120.16
4	C	501	CNC	C2-C1-C19	-2.71	114.11	118.77
4	A	501	CNC	C2-C1-C19	2.70	123.42	118.77
4	C	501	CNC	C10-C11-N23	-2.65	120.62	124.92
4	C	501	CNC	C13-C14-N23	2.64	115.00	109.39
4	A	501	CNC	C5R-C4R-C3R	-2.63	106.54	114.84
4	A	501	CNC	C20-C1-N21	2.57	114.50	110.26
4	A	501	CNC	C41-C8-C7	-2.57	107.12	114.19
4	C	501	CNC	C2R-C1R-N1B	-2.53	107.02	113.30
4	A	501	CNC	C7B-C8B-N1B	2.47	136.28	131.39
4	A	501	CNC	C3R-C2R-C1R	2.40	105.17	99.89
4	C	501	CNC	C53-C15-C16	2.40	125.56	120.42
4	A	501	CNC	O39-C38-N40	-2.38	116.17	122.53
4	A	501	CNC	C53-C15-C14	2.37	121.58	116.79
4	A	501	CNC	P-O3-C2P	-2.36	113.04	121.10
4	A	501	CNC	C2P-C1P-N59	2.36	116.39	112.92
4	C	501	CNC	C18-C60-C61	2.35	120.01	114.04
4	C	501	CNC	C13-C12-C11	-2.31	97.76	100.86
4	A	501	CNC	C6M-C6B-C7B	2.24	123.51	119.57
4	A	501	CNC	C8-C7-C6	2.23	104.71	100.92
5	C	502	GOL	O2-C2-C3	2.23	118.42	109.18
4	A	501	CNC	C60-C61-N62	2.22	121.51	116.19
4	A	501	CNC	O63-C61-N62	-2.20	116.65	122.53
4	A	501	CNC	C47-C12-C46	-2.19	105.77	109.41
4	C	501	CNC	C2-C26-C27	2.17	121.23	115.19
4	A	501	CNC	C2R-C3R-C4R	2.15	107.00	103.24
4	A	501	CNC	O7R-C2R-C1R	2.15	117.49	110.10
4	C	501	CNC	O58-C57-N59	-2.14	118.82	123.03
4	A	501	CNC	C10-C11-N23	-2.13	121.46	124.92
4	A	501	CNC	C15-C16-N24	-2.12	120.25	122.38
5	A	503	GOL	C3-C2-C1	-2.08	104.15	111.80
4	C	501	CNC	C20-C1-C19	2.07	114.34	110.23
4	C	501	CNC	C12-C13-C14	-2.05	99.18	101.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CNC	C1-C2-C3	2.04	104.17	101.60
4	C	501	CNC	O7R-C2R-C3R	-2.04	105.48	111.19
4	C	501	CNC	C42-C41-C8	-2.02	108.92	114.65
4	C	501	CNC	O3-C2P-C1P	2.02	110.94	106.94
4	A	501	CNC	C3P-C2P-C1P	-2.00	107.56	111.42
4	C	501	CNC	C41-C8-C7	-2.00	108.68	114.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	501	CNC	N24
4	C	501	CNC	N24

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	CNC	C2P-O3-P-O2
5	A	503	GOL	O1-C1-C2-C3
4	A	501	CNC	C18-C17-C55-C56
4	A	501	CNC	C16-C17-C55-C56
4	A	501	CNC	C3R-C4R-C5R-O8R
5	A	502	GOL	C1-C2-C3-O3
5	C	502	GOL	C1-C2-C3-O3
5	A	502	GOL	O2-C2-C3-O3
5	A	503	GOL	O1-C1-C2-O2
4	C	501	CNC	C13-C48-C49-C50
4	A	501	CNC	O6R-C4R-C5R-O8R
4	A	501	CNC	C2R-C3R-O2-P
5	C	502	GOL	O2-C2-C3-O3
4	A	501	CNC	C4R-C3R-O2-P

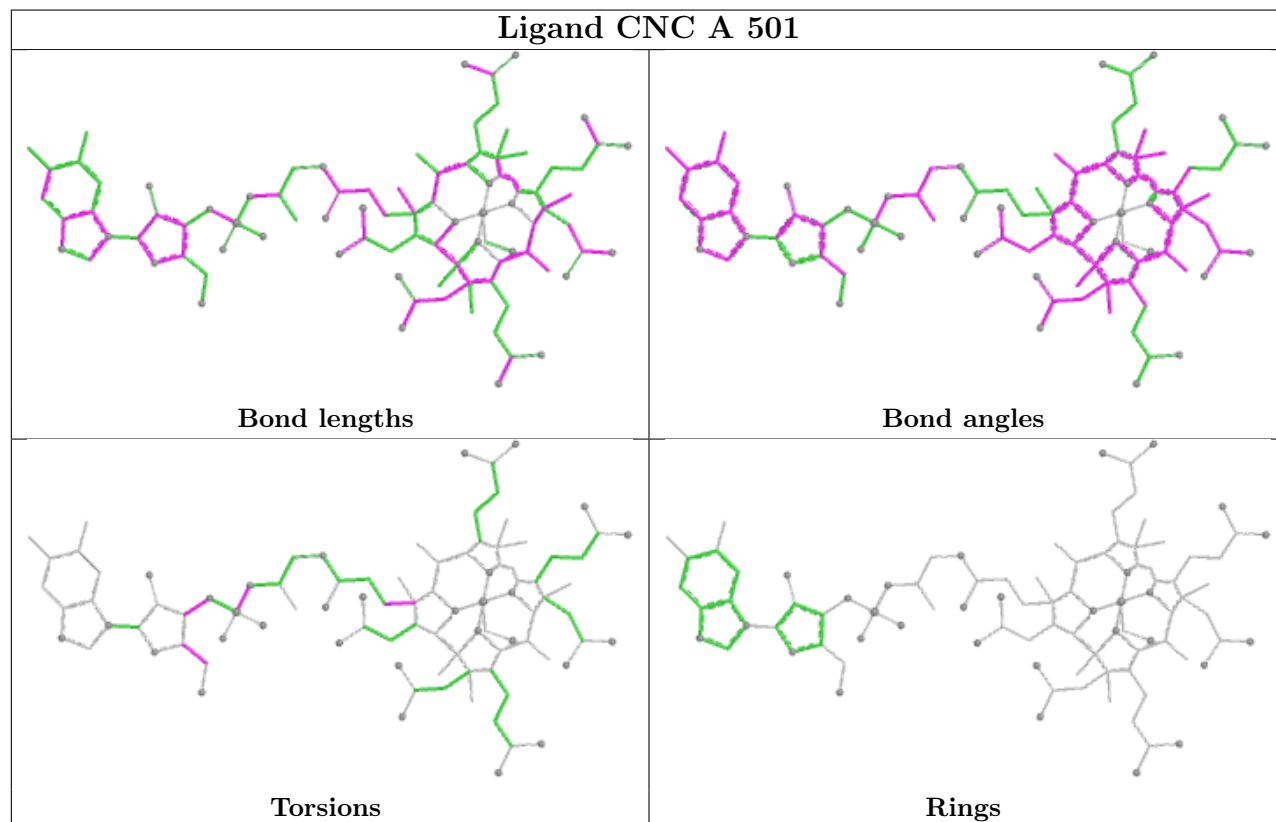
There are no ring outliers.

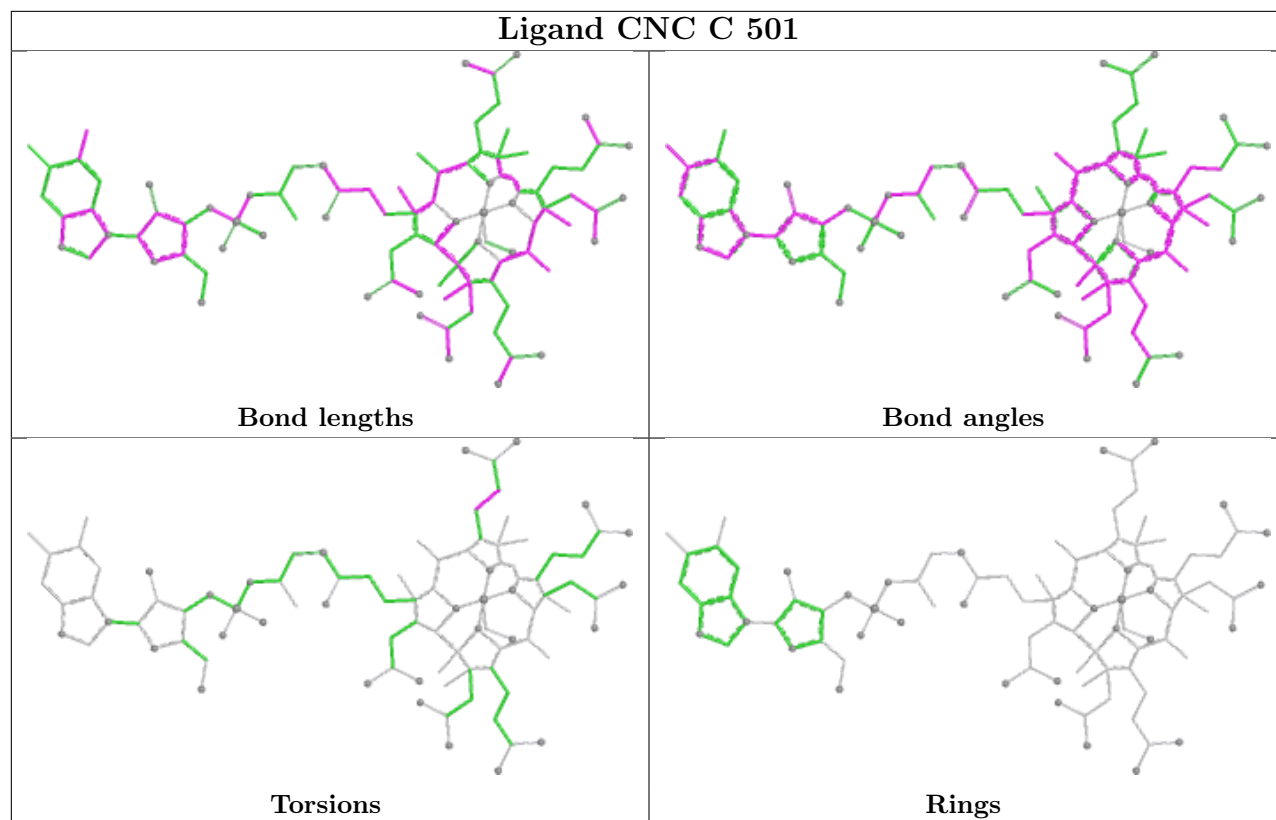
4 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	GOL	2	0
4	A	501	CNC	13	0
5	A	502	GOL	3	0
4	C	501	CNC	11	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	381/409 (93%)	-0.02	8 (2%) 63 61	32, 49, 76, 105	0
1	C	388/409 (94%)	0.19	12 (3%) 51 48	36, 58, 92, 122	0
2	B	85/147 (57%)	0.58	4 (4%) 36 33	44, 75, 96, 107	0
2	D	81/147 (55%)	0.51	4 (4%) 35 31	45, 76, 99, 112	0
3	E	125/135 (92%)	0.50	4 (3%) 50 46	49, 69, 96, 106	0
3	G	121/135 (89%)	0.94	8 (6%) 24 21	52, 90, 117, 213	0
All	All	1181/1382 (85%)	0.28	40 (3%) 48 44	32, 61, 100, 213	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	78	SER	5.5
1	A	80	GLY	5.2
2	B	168	GLY	3.8
3	E	124	SER	3.2
2	D	168	GLY	3.2
1	C	243	ALA	3.1
1	A	81	LYS	3.1
1	C	167	PRO	3.1
3	G	79	THR	3.1
3	G	145	SER	3.0
1	C	398	ASP	3.0
1	A	239	PRO	2.9
3	E	147	HIS	2.9
1	C	322	LEU	2.9
2	D	130	LEU	2.8
1	C	238	SER	2.8
3	G	80	ASN	2.8
1	A	244	GLU	2.7
2	B	171	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	G	96	VAL	2.7
3	G	23	ARG	2.6
2	B	169	THR	2.5
1	C	397	LYS	2.5
1	A	78	CYS	2.5
1	C	320	SER	2.5
2	D	172	ILE	2.5
1	A	245	LEU	2.4
3	E	125	ASN	2.4
1	C	330	SER	2.3
2	B	93	PRO	2.3
1	C	304	THR	2.3
1	A	130	GLY	2.3
2	D	139	CYS	2.3
1	C	81	LYS	2.2
1	C	9	ASP	2.2
3	G	34	GLN	2.1
3	E	91	ILE	2.1
1	C	306	PRO	2.1
1	A	9	ASP	2.0
3	G	50	PRO	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	GOL	A	502	6/6	0.83	0.30	53,56,60,66	0
5	GOL	C	502	6/6	0.89	0.16	59,63,67,70	0

Continued on next page...

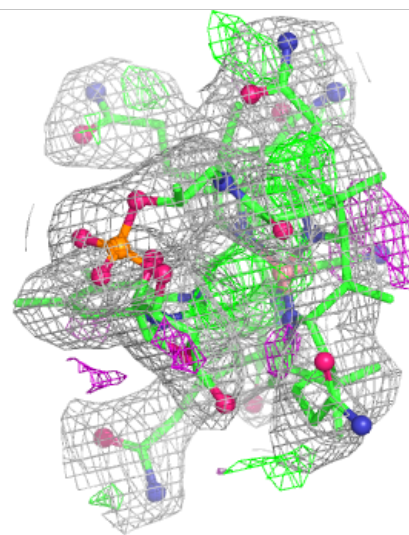
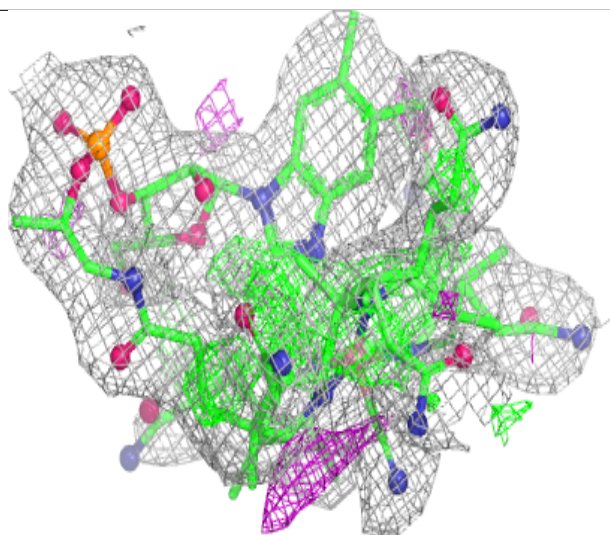
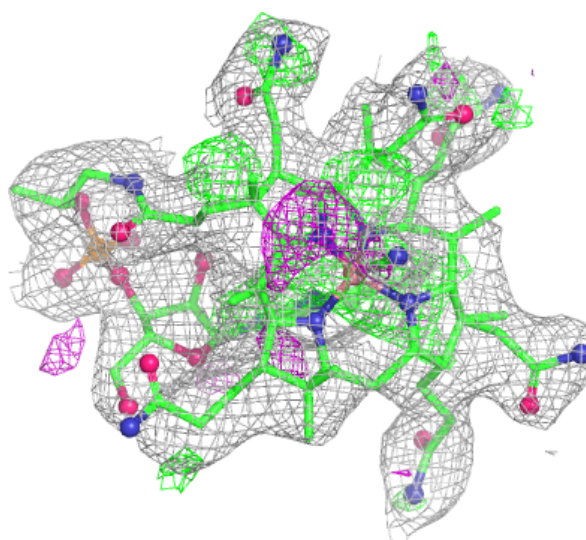
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	E	201	1/1	0.92	0.11	59,59,59,59	0
4	CNC	A	501	93/93	0.94	0.13	27,40,48,57	7
5	GOL	A	503	6/6	0.94	0.09	58,66,67,70	0
4	CNC	C	501	93/93	0.95	0.10	35,46,53,66	11
6	CA	G	201	1/1	0.98	0.03	56,56,56,56	0
6	CA	D	202	1/1	0.99	0.03	75,75,75,75	0
6	CA	B	201	1/1	0.99	0.05	70,70,70,70	0
6	CA	B	202	1/1	0.99	0.02	50,50,50,50	0
6	CA	D	201	1/1	1.00	0.06	47,47,47,47	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.

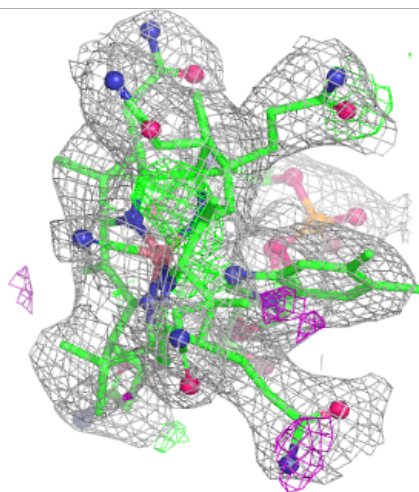
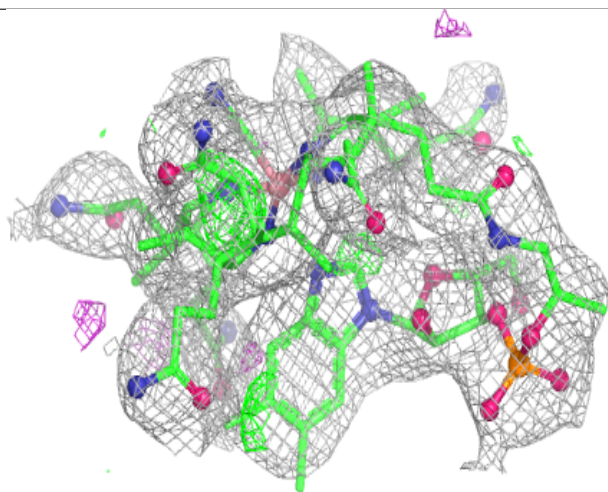
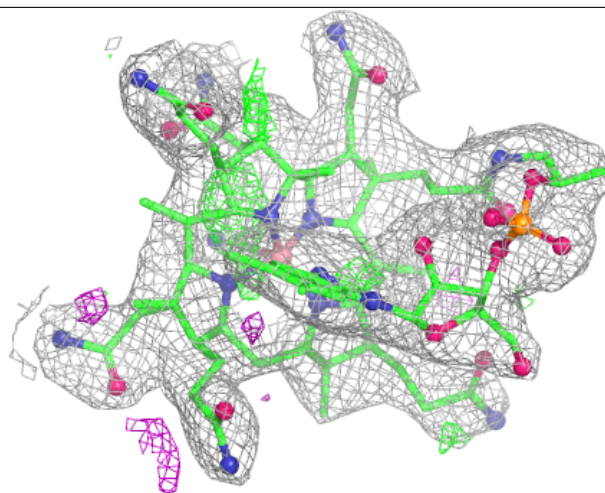
Electron density around CNC A 501:

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 CNC C 501:

$2mF_o-DF_c$ (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.