



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:42 PM UTC

PDB ID : 7QBF / pdb_00007qbf
Title : TC:CD320 in complex with nanobody TC-Nb34
Authors : Bloch, J.S.; Locher, K.P.
Deposited on : 2021-11-19
Resolution : 1.85 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

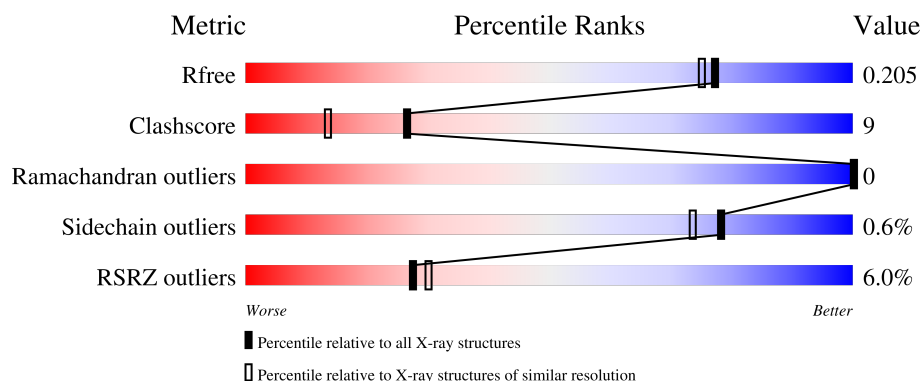
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	5% 89% 10%
2	C	147	3% 50% 47%
3	B	137	9% 82% 9% 9%

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	IOD	A	508	-	-	X	-
5	EDO	A	517	-	-	X	-
5	EDO	A	520	-	-	X	-
5	EDO	A	529	-	-	X	-
6	CNC	A	536[A]	X	-	-	-
6	CNC	A	536[B]	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10278 atoms, of which 4733 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	409	Total	C	H	N	O	S	0	9	0
			6481	2079	3207	576	600	19			

- Molecule 2 is a protein called CD320 antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	78	Total	C	H	N	O	S	0	0	0
			1085	345	500	103	125	12			

- Molecule 3 is a protein called Anti-transcobalamin-2 nanobody TC-Nb34.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	B	125	Total	C	H	N	O	S	0	3	0
			1831	599	864	170	192	6			

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	I	0	0
			12	12		
4	C	4	Total	I	0	0
			4	4		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



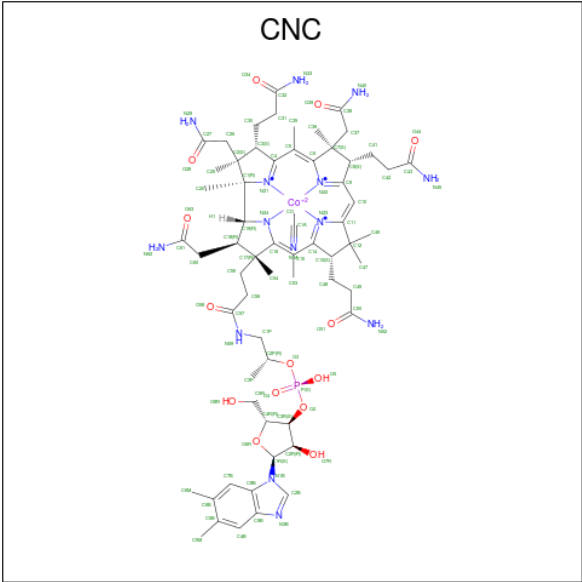
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is CYANOCOBALAMIN (CCD ID: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	Co	N	O	P	0	1
			186	126	2	28	28	2		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	2	Total	Ca	0	0
			2	2		

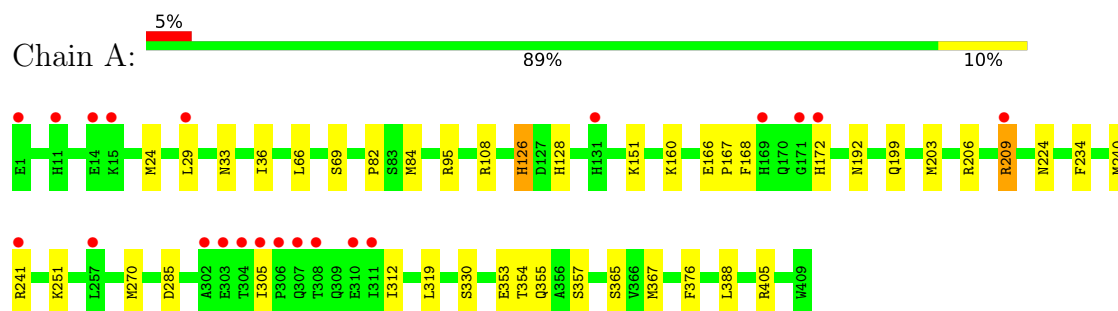
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	297	Total	O	0	0
			297	297		
8	C	49	Total	O	0	0
			49	49		
8	B	61	Total	O	0	0
			61	61		

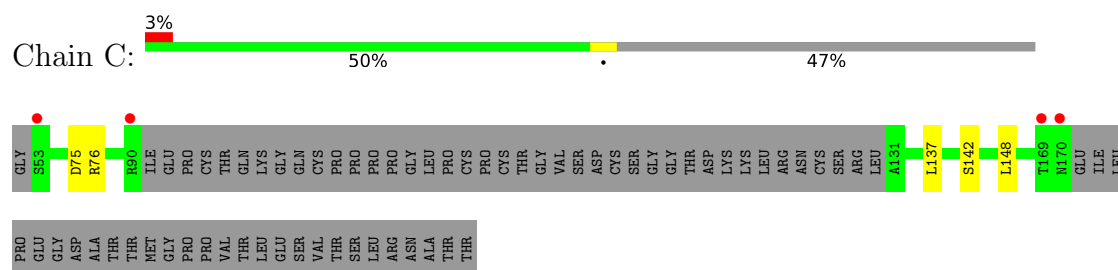
3 Residue-property plots [i](#)

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.

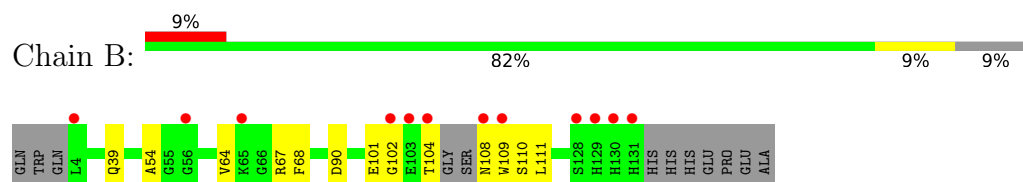
• Molecule 1: Transcobalamin-2



• Molecule 2: CD320 antigen



• Molecule 3: Anti-transcobalamin-2 nanobody TC-Nb34



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.82Å 104.82Å 167.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 1.85 49.27 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.27-1.85) 99.7 (49.27-1.85)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.174 , 0.205 0.175 , 0.205	Depositor DCC
R_{free} test set	3973 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.0	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	0.96	EDS
Total number of atoms	10278	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: CA, CNC, IOD, EDO

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	0.54	1/3363 (0.0%)	0.69	3/4553 (0.1%)
2	C	0.47	0/595	0.66	0/807
3	B	0.41	0/995	0.64	0/1347
All	All	0.51	1/4953 (0.0%)	0.68	3/6707 (0.0%)

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
3	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	MET	SD-CE	-5.12	1.66	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	MET	CG-SD-CE	-8.89	81.34	100.90
1	A	126	HIS	CA-C-N	5.19	127.75	120.28
1	A	126	HIS	C-N-CA	5.19	127.75	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	39[B]	GLN	Mainchain

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	3274	3207	3255	53	0
2	C	585	500	516	3	0
3	B	967	864	893	10	0
4	A	12	0	0	4	0
4	C	4	0	0	1	0
5	A	92	138	138	30	0
5	B	12	18	18	1	0
5	C	4	6	6	0	0
6	A	186	0	174	27	0
7	C	2	0	0	0	0
8	A	297	0	0	9	0
8	B	61	0	0	2	0
8	C	49	0	0	1	0
All	All	5545	4733	5000	95	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 9.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:HD2	1:A:209:ARG:HH22	1.34	0.90
2:C:142:SER:OG	8:C:301:HOH:O	1.72	0.90
6:A:536[A]:CNC:C4	6:A:536[A]:CNC:H4B	2.18	0.74
5:A:525:EDO:O2	8:A:601:HOH:O	2.08	0.71
1:A:209:ARG:HH21	1:A:209:ARG:CB	2.04	0.71
6:A:536[A]:CNC:H2B	6:A:536[A]:CNC:C14	2.21	0.70
6:A:536[B]:CNC:H552	6:A:536[B]:CNC:H531	1.74	0.69
3:B:109[B]:TRP:HE3	3:B:110[B]:SER:H	1.39	0.68
1:A:192:ASN:OD1	8:A:602:HOH:O	2.11	0.68
6:A:536[B]:CNC:O51	6:A:536[B]:CNC:O8R	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:101:GLU:HB2	8:B:323:HOH:O	1.96	0.66
1:A:388:LEU:HD21	5:A:517:EDO:H22	1.78	0.65
1:A:95:ARG:HH22	5:A:513:EDO:H11	1.62	0.65
1:A:241:ARG:NE	1:A:241:ARG:HA	2.14	0.63
1:A:224:ASN:HD22	5:A:517:EDO:H11	1.66	0.61
6:A:536[B]:CNC:H203	6:A:536[B]:CNC:H301	1.83	0.60
1:A:305:ILE:O	1:A:305:ILE:HG22	2.00	0.60
8:A:781:HOH:O	4:C:206:IOD:I	2.86	0.59
1:A:354:THR:H	5:A:529:EDO:C1	2.15	0.59
1:A:270:MET:HA	1:A:270:MET:HE2	1.84	0.57
1:A:69:SER:HB2	5:A:535:EDO:H22	1.86	0.57
1:A:126:HIS:HB2	5:A:516:EDO:H22	1.88	0.56
6:A:536[B]:CNC:H531	6:A:536[B]:CNC:C55	2.35	0.56
3:B:67:ARG:NH2	3:B:90:ASP:OD2	2.28	0.55
1:A:209:ARG:NH2	1:A:240:MET:HG3	2.21	0.55
1:A:84:MET:HB2	5:A:526:EDO:H12	1.88	0.55
3:B:64:VAL:HG13	3:B:68:PHE:CG	2.43	0.54
1:A:354:THR:H	5:A:529:EDO:H11	1.73	0.54
5:A:520:EDO:H12	8:A:674:HOH:O	2.06	0.54
1:A:319:LEU:HB2	5:A:520:EDO:H21	1.89	0.54
1:A:151:LYS:NZ	8:A:606:HOH:O	2.40	0.54
1:A:209:ARG:HH21	1:A:209:ARG:CG	2.20	0.54
6:A:536[B]:CNC:C4	6:A:536[B]:CNC:C1A	2.87	0.53
1:A:95:ARG:HH22	5:A:513:EDO:C1	2.22	0.53
1:A:319:LEU:HB2	5:A:520:EDO:H12	1.91	0.52
1:A:388:LEU:O	6:A:536[A]:CNC:H311	2.10	0.52
2:C:75:ASP:O	2:C:76:ARG:HB2	2.09	0.52
1:A:209:ARG:HH21	1:A:209:ARG:HB2	1.76	0.51
6:A:536[A]:CNC:N23	6:A:536[A]:CNC:C2B	2.73	0.51
1:A:209:ARG:NH2	1:A:209:ARG:CG	2.73	0.50
1:A:69:SER:HB2	5:A:535:EDO:C2	2.41	0.50
1:A:33:ASN:HB3	1:A:36:ILE:HD12	1.94	0.50
1:A:285:ASP:HB3	4:A:512:IOD:I	2.82	0.49
1:A:355:GLN:HG3	5:A:514:EDO:H22	1.94	0.49
6:A:536[A]:CNC:N21	6:A:536[A]:CNC:N3B	2.61	0.49
6:A:536[B]:CNC:H422	6:A:536[B]:CNC:H361	1.95	0.49
1:A:203:MET:HE1	3:B:111:LEU:HD11	1.95	0.48
1:A:224:ASN:HA	5:A:534:EDO:H21	1.95	0.48
6:A:536[B]:CNC:C35	6:A:536[B]:CNC:H302	2.43	0.48
3:B:54:ALA:HB3	8:B:319:HOH:O	2.14	0.48
1:A:357:SER:HB3	5:A:514:EDO:H21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:HB3	5:A:517:EDO:H21	1.97	0.46
6:A:536[B]:CNC:H302	6:A:536[B]:CNC:H353	1.98	0.46
3:B:108:ASN:HD22	3:B:108:ASN:N	2.13	0.46
5:A:513:EDO:H12	8:A:655:HOH:O	2.15	0.45
1:A:209:ARG:HG2	1:A:234:PHE:CE2	2.51	0.45
1:A:160:LYS:NZ	5:A:533:EDO:H11	2.32	0.45
1:A:365:SER:OG	4:A:508:IOD:I	3.03	0.45
6:A:536[A]:CNC:H491	6:A:536[A]:CNC:C46	2.47	0.45
6:A:536[B]:CNC:O28	6:A:536[B]:CNC:H3	2.17	0.45
3:B:102:GLY:HA3	3:B:109[A]:TRP:CE3	2.52	0.44
1:A:224:ASN:HA	5:A:534:EDO:C2	2.48	0.44
1:A:353:GLU:HG3	4:A:508:IOD:I	2.87	0.44
6:A:536[A]:CNC:H531	6:A:536[A]:CNC:H543	2.00	0.44
3:B:64:VAL:CG1	3:B:68:PHE:HB2	2.48	0.44
1:A:224:ASN:HD22	5:A:517:EDO:C1	2.29	0.44
1:A:405:ARG:HG3	5:A:520:EDO:H11	2.00	0.43
5:A:524:EDO:H22	6:A:536[A]:CNC:N1A	2.34	0.43
6:A:536[A]:CNC:N40	6:A:536[A]:CNC:H362	2.16	0.43
1:A:166:GLU:HB3	1:A:167:PRO:CD	2.49	0.43
1:A:354:THR:N	5:A:529:EDO:H11	2.34	0.43
1:A:376:PHE:CG	6:A:536[B]:CNC:H462	2.53	0.43
1:A:126:HIS:N	5:A:516:EDO:H21	2.33	0.43
6:A:536[A]:CNC:H552	6:A:536[A]:CNC:C53	2.49	0.43
1:A:367:MET:HE3	4:A:507:IOD:I	2.89	0.42
3:B:104:THR:C	3:B:109[A]:TRP:CH2	2.97	0.42
1:A:354:THR:OG1	5:A:529:EDO:H12	2.18	0.42
6:A:536[A]:CNC:N23	6:A:536[A]:CNC:N3B	2.68	0.42
6:A:536[A]:CNC:H491	6:A:536[A]:CNC:H461	2.01	0.42
6:A:536[A]:CNC:H2B	6:A:536[A]:CNC:N23	2.35	0.42
1:A:29:LEU:HD11	8:A:808:HOH:O	2.19	0.42
1:A:312:ILE:O	1:A:330:SER:HA	2.20	0.42
6:A:536[B]:CNC:H351	6:A:536[B]:CNC:C36	2.50	0.41
1:A:126:HIS:N	5:A:516:EDO:C2	2.83	0.41
1:A:199:GLN:O	1:A:203:MET:HG3	2.21	0.41
1:A:319:LEU:HB2	5:A:520:EDO:C2	2.51	0.41
6:A:536[A]:CNC:H531	6:A:536[A]:CNC:H552	2.03	0.41
2:C:137:LEU:HB2	2:C:148:LEU:HD12	2.01	0.41
1:A:108:ARG:NE	8:A:609:HOH:O	2.42	0.41
6:A:536[B]:CNC:C46	6:A:536[B]:CNC:H491	2.51	0.41
6:A:536[B]:CNC:H541	6:A:536[B]:CNC:H602	1.83	0.40
5:A:526:EDO:H21	8:A:668:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:HIS:CE1	1:A:160:LYS:HD3	2.57	0.40
1:A:168:PHE:CD2	5:B:203:EDO:H12	2.57	0.40
1:A:66:LEU:HD11	1:A:82:PRO:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	416/409 (102%)	412 (99%)	4 (1%)	0	100	100
2	C	74/147 (50%)	72 (97%)	2 (3%)	0	100	100
3	B	124/137 (90%)	119 (96%)	5 (4%)	0	100	100
All	All	614/693 (89%)	603 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	357/348 (103%)	354 (99%)	3 (1%)	73	67
2	C	70/129 (54%)	70 (100%)	0	100	100
3	B	101/108 (94%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	528/585 (90%)	525 (99%)	3 (1%)	78	73

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	HIS
1	A	209	ARG
1	A	251	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	138	GLN
1	A	378	GLN
3	B	13	GLN
3	B	108	ASN

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](#)

Of 47 ligands modelled in this entry, 18 are monoatomic - leaving 29 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	EDO	A	527	-	3,3,3	0.49	0	2,2,2	0.54	0
5	EDO	B	201	-	3,3,3	0.39	0	2,2,2	0.42	0
5	EDO	A	514	-	3,3,3	0.40	0	2,2,2	0.56	0
5	EDO	A	525	-	3,3,3	0.28	0	2,2,2	0.24	0
5	EDO	A	528	-	3,3,3	0.42	0	2,2,2	0.41	0
5	EDO	A	531	-	3,3,3	0.42	0	2,2,2	0.11	0
5	EDO	A	521	-	3,3,3	0.56	0	2,2,2	0.34	0
5	EDO	A	517	-	3,3,3	0.74	0	2,2,2	0.85	0
5	EDO	A	533	-	3,3,3	0.62	0	2,2,2	0.31	0
5	EDO	A	535	-	3,3,3	0.67	0	2,2,2	0.36	0
5	EDO	A	518	-	3,3,3	0.98	0	2,2,2	0.28	0
5	EDO	A	523	-	3,3,3	0.51	0	2,2,2	0.26	0
5	EDO	A	515	-	3,3,3	0.55	0	2,2,2	0.73	0
5	EDO	A	522	-	3,3,3	0.48	0	2,2,2	0.35	0
5	EDO	A	524	-	3,3,3	0.46	0	2,2,2	0.36	0
6	CNC	A	536[B]	-	93,103,103	3.06	38 (40%)	149,171,171	3.96	64 (42%)
5	EDO	A	520	-	3,3,3	0.40	0	2,2,2	0.34	0
5	EDO	A	519	-	3,3,3	0.52	0	2,2,2	0.39	0
5	EDO	C	207	-	3,3,3	0.48	0	2,2,2	0.07	0
5	EDO	A	534	-	3,3,3	0.42	0	2,2,2	0.69	0
5	EDO	A	529	-	3,3,3	0.55	0	2,2,2	0.89	0
5	EDO	A	530	-	3,3,3	0.52	0	2,2,2	0.62	0
5	EDO	A	526	-	3,3,3	0.26	0	2,2,2	0.77	0
5	EDO	A	532	-	3,3,3	0.55	0	2,2,2	0.33	0
5	EDO	A	516	-	3,3,3	0.66	0	2,2,2	0.99	0
5	EDO	B	202	-	3,3,3	0.49	0	2,2,2	0.54	0
5	EDO	B	203	-	3,3,3	0.79	0	2,2,2	0.17	0
6	CNC	A	536[A]	-	93,103,103	3.17	37 (39%)	149,171,171	4.12	55 (36%)
5	EDO	A	513	-	3,3,3	0.40	0	2,2,2	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	527	-	-	0/1/1/1	-
5	EDO	B	201	-	-	1/1/1/1	-
5	EDO	A	514	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	525	-	-	0/1/1/1	-
5	EDO	A	528	-	-	1/1/1/1	-
5	EDO	A	531	-	-	1/1/1/1	-
5	EDO	A	521	-	-	1/1/1/1	-
5	EDO	A	517	-	-	0/1/1/1	-
5	EDO	A	533	-	-	0/1/1/1	-
5	EDO	A	535	-	-	0/1/1/1	-
5	EDO	A	518	-	-	0/1/1/1	-
5	EDO	A	523	-	-	1/1/1/1	-
5	EDO	A	515	-	-	0/1/1/1	-
5	EDO	A	522	-	-	1/1/1/1	-
5	EDO	A	524	-	-	0/1/1/1	-
6	CNC	A	536[B]	-	1/1/36/38	2/56/235/235	0/3/11/11
5	EDO	A	520	-	-	1/1/1/1	-
5	EDO	A	519	-	-	0/1/1/1	-
5	EDO	C	207	-	-	1/1/1/1	-
5	EDO	A	534	-	-	1/1/1/1	-
5	EDO	A	529	-	-	0/1/1/1	-
5	EDO	A	530	-	-	1/1/1/1	-
5	EDO	A	526	-	-	0/1/1/1	-
5	EDO	A	532	-	-	1/1/1/1	-
5	EDO	A	516	-	-	0/1/1/1	-
5	EDO	B	202	-	-	1/1/1/1	-
5	EDO	B	203	-	-	1/1/1/1	-
6	CNC	A	536[A]	-	1/1/36/38	5/56/235/235	0/3/11/11
5	EDO	A	513	-	-	1/1/1/1	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	536[B]	CNC	C10-C11	9.73	1.64	1.37
6	A	536[A]	CNC	C10-C11	9.47	1.63	1.37
6	A	536[A]	CNC	C10-C9	9.30	1.65	1.39
6	A	536[B]	CNC	C10-C9	8.96	1.64	1.39
6	A	536[A]	CNC	C3R-C4R	-8.26	1.31	1.52
6	A	536[B]	CNC	C3R-C4R	-7.91	1.32	1.52
6	A	536[A]	CNC	C6-C5	6.98	1.55	1.36
6	A	536[B]	CNC	C6-C5	6.84	1.55	1.36
6	A	536[A]	CNC	C1-C19	6.48	1.72	1.54
6	A	536[A]	CNC	C57-N59	6.36	1.48	1.33
6	A	536[A]	CNC	C4-C5	6.31	1.69	1.43
6	A	536[B]	CNC	C4-C5	6.23	1.68	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	536[B]	CNC	C57-N59	6.22	1.48	1.33
6	A	536[A]	CNC	O6R-C4R	5.76	1.57	1.45
6	A	536[B]	CNC	C1-C19	5.70	1.70	1.54
6	A	536[A]	CNC	C19-N24	-5.67	1.37	1.49
6	A	536[A]	CNC	C2R-C1R	-5.33	1.36	1.53
6	A	536[A]	CNC	C54-C17	-5.27	1.46	1.54
6	A	536[B]	CNC	C2R-C1R	-5.12	1.37	1.53
6	A	536[B]	CNC	O6R-C4R	5.10	1.56	1.45
6	A	536[B]	CNC	C36-C7	-5.05	1.46	1.54
6	A	536[A]	CNC	C1-C2	-4.96	1.47	1.58
6	A	536[A]	CNC	C50-N52	4.72	1.48	1.32
6	A	536[A]	CNC	C38-N40	4.62	1.47	1.32
6	A	536[B]	CNC	C50-N52	4.62	1.47	1.32
6	A	536[B]	CNC	C54-C17	-4.62	1.47	1.54
6	A	536[B]	CNC	C1-C2	-4.54	1.48	1.58
6	A	536[B]	CNC	C38-N40	4.50	1.47	1.32
6	A	536[B]	CNC	C61-N62	4.43	1.47	1.32
6	A	536[A]	CNC	C2R-C3R	4.25	1.62	1.53
6	A	536[B]	CNC	C27-N29	4.23	1.46	1.32
6	A	536[A]	CNC	C61-N62	4.22	1.46	1.32
6	A	536[A]	CNC	C27-N29	4.20	1.46	1.32
6	A	536[A]	CNC	C43-N45	4.19	1.46	1.32
6	A	536[A]	CNC	C36-C7	-4.19	1.47	1.54
6	A	536[B]	CNC	C32-N33	4.18	1.46	1.32
6	A	536[A]	CNC	C32-N33	4.15	1.46	1.32
6	A	536[A]	CNC	C14-C15	4.15	1.60	1.43
6	A	536[B]	CNC	C43-N45	4.11	1.46	1.32
6	A	536[B]	CNC	C19-N24	-3.93	1.41	1.49
6	A	536[B]	CNC	C14-C15	3.79	1.58	1.43
6	A	536[A]	CNC	O6R-C1R	3.76	1.50	1.42
6	A	536[B]	CNC	C2R-C3R	3.74	1.61	1.53
6	A	536[A]	CNC	C7-C6	3.57	1.62	1.54
6	A	536[A]	CNC	C3-C4	-3.35	1.43	1.51
6	A	536[A]	CNC	C56-C57	3.35	1.58	1.51
6	A	536[A]	CNC	C16-C15	3.28	1.57	1.42
6	A	536[B]	CNC	O6R-C1R	3.13	1.49	1.42
6	A	536[B]	CNC	P-O2	3.12	1.68	1.59
6	A	536[B]	CNC	C16-C15	3.08	1.56	1.42
6	A	536[B]	CNC	C26-C2	3.03	1.62	1.55
6	A	536[B]	CNC	C3-C4	-3.01	1.44	1.51
6	A	536[B]	CNC	C55-C56	3.00	1.59	1.53
6	A	536[A]	CNC	P-O2	3.00	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	536[B]	CNC	C56-C57	2.93	1.57	1.51
6	A	536[B]	CNC	C26-C27	2.92	1.61	1.51
6	A	536[A]	CNC	C55-C56	2.89	1.59	1.53
6	A	536[B]	CNC	C5M-C5B	2.77	1.56	1.51
6	A	536[A]	CNC	C9B-N3B	-2.76	1.34	1.39
6	A	536[B]	CNC	C7-C6	2.76	1.61	1.54
6	A	536[A]	CNC	P-O3	2.71	1.67	1.59
6	A	536[B]	CNC	C8B-N1B	-2.63	1.34	1.39
6	A	536[B]	CNC	C37-C38	2.57	1.60	1.51
6	A	536[A]	CNC	C35-C5	2.54	1.56	1.50
6	A	536[B]	CNC	C35-C5	2.52	1.55	1.50
6	A	536[B]	CNC	C12-C11	2.47	1.59	1.51
6	A	536[B]	CNC	C9B-N3B	-2.47	1.35	1.39
6	A	536[B]	CNC	C8B-C9B	-2.41	1.36	1.40
6	A	536[B]	CNC	P-O3	2.40	1.66	1.59
6	A	536[A]	CNC	C26-C2	2.39	1.61	1.55
6	A	536[A]	CNC	C26-C27	2.38	1.59	1.51
6	A	536[A]	CNC	C8B-N1B	-2.27	1.34	1.39
6	A	536[A]	CNC	C12-C11	2.25	1.58	1.51
6	A	536[A]	CNC	C6M-C6B	2.04	1.54	1.51
6	A	536[A]	CNC	C55-C17	2.03	1.59	1.54

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	536[A]	CNC	C3-C4-C5	-20.32	89.82	123.82
6	A	536[B]	CNC	C9-C10-C11	-14.82	104.05	125.84
6	A	536[A]	CNC	C36-C7-C37	-14.76	85.65	110.74
6	A	536[B]	CNC	C3-C4-C5	-14.20	100.06	123.82
6	A	536[A]	CNC	C9-C10-C11	-13.26	106.33	125.84
6	A	536[B]	CNC	C36-C7-C37	-13.21	88.28	110.74
6	A	536[A]	CNC	C25-C2-C26	-11.98	85.93	109.74
6	A	536[A]	CNC	C8-C9-C10	-11.44	98.99	123.33
6	A	536[B]	CNC	C25-C2-C26	-11.19	87.50	109.74
6	A	536[B]	CNC	C26-C2-C3	-9.88	90.19	107.42
6	A	536[A]	CNC	C16-C15-C14	-9.67	108.16	121.29
6	A	536[A]	CNC	C26-C2-C1	-9.54	95.27	110.00
6	A	536[B]	CNC	C8-C9-C10	-9.45	103.21	123.33
6	A	536[B]	CNC	C6-C5-C4	-9.26	105.06	121.55
6	A	536[A]	CNC	C13-C14-C15	-9.18	108.46	123.82
6	A	536[A]	CNC	C1-C19-C18	-9.16	107.99	121.75
6	A	536[B]	CNC	C36-C7-C8	8.80	128.30	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	536[B]	CNC	C19-C1-N21	-8.80	90.59	101.69
6	A	536[B]	CNC	C16-C15-C14	-8.64	109.56	121.29
6	A	536[A]	CNC	C26-C2-C3	-8.40	92.77	107.42
6	A	536[B]	CNC	C37-C7-C8	-8.32	86.41	108.37
6	A	536[A]	CNC	C7-C6-C5	-8.32	115.07	128.07
6	A	536[A]	CNC	C37-C7-C6	-8.29	81.43	107.11
6	A	536[A]	CNC	C25-C2-C1	7.77	125.37	113.75
6	A	536[B]	CNC	C30-C3-C2	-7.73	101.94	119.00
6	A	536[B]	CNC	C1-C19-C18	-7.73	110.15	121.75
6	A	536[B]	CNC	C13-C14-C15	-7.60	111.10	123.82
6	A	536[A]	CNC	C30-C3-C2	-7.24	103.03	119.00
6	A	536[B]	CNC	C19-N24-C16	-7.15	100.53	111.96
6	A	536[A]	CNC	C6-C5-C4	-7.13	108.85	121.55
6	A	536[B]	CNC	C18-C19-N24	7.00	113.06	101.92
6	A	536[A]	CNC	C12-C11-C10	-6.78	117.45	123.54
6	A	536[A]	CNC	C12-C11-N23	-6.75	104.29	111.49
6	A	536[B]	CNC	C25-C2-C3	6.70	129.94	112.91
6	A	536[A]	CNC	C5-C6-N22	-6.31	114.33	123.88
6	A	536[B]	CNC	C25-C2-C1	6.25	123.10	113.75
6	A	536[A]	CNC	C10-C9-N22	-6.06	118.83	125.74
6	A	536[B]	CNC	C37-C7-C6	-6.02	88.46	107.11
6	A	536[B]	CNC	C35-C5-C6	-5.93	112.86	122.41
6	A	536[A]	CNC	C25-C2-C3	5.72	127.43	112.91
6	A	536[A]	CNC	C8-C7-C6	5.67	110.54	100.92
6	A	536[B]	CNC	N1B-C2B-N3B	-5.37	106.32	113.94
6	A	536[A]	CNC	C18-C19-N24	5.36	110.45	101.92
6	A	536[B]	CNC	C26-C2-C1	-5.18	102.00	110.00
6	A	536[A]	CNC	C37-C7-C8	-5.04	95.07	108.37
6	A	536[A]	CNC	C36-C7-C8	5.03	121.34	112.05
6	A	536[A]	CNC	C5M-C5B-C4B	-5.01	110.75	119.57
6	A	536[A]	CNC	C8-C9-N22	4.96	120.56	110.77
6	A	536[B]	CNC	C8B-N1B-C1R	-4.95	117.04	125.41
6	A	536[A]	CNC	C7-C8-C9	-4.78	94.84	100.89
6	A	536[B]	CNC	C9B-C8B-N1B	4.75	107.41	105.30
6	A	536[B]	CNC	C8-C7-C6	4.53	108.61	100.92
6	A	536[B]	CNC	C10-C9-N22	-4.46	120.65	125.74
6	A	536[A]	CNC	C1-C2-C3	4.38	107.10	101.60
6	A	536[B]	CNC	C8-C9-N22	4.29	119.24	110.77
6	A	536[B]	CNC	C17-C18-C19	-4.25	97.53	102.70
6	A	536[B]	CNC	C5M-C5B-C4B	-4.19	112.18	119.57
6	A	536[B]	CNC	O28-C27-N29	-4.19	111.36	122.53
6	A	536[B]	CNC	C9B-N3B-C2B	4.11	109.45	104.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	536[A]	CNC	C1-C19-N24	-4.11	99.73	106.29
6	A	536[A]	CNC	C15-C14-N23	-4.03	118.77	126.67
6	A	536[B]	CNC	C12-C11-N23	-4.01	107.22	111.49
6	A	536[B]	CNC	C8B-N1B-C2B	3.84	109.74	106.26
6	A	536[B]	CNC	C3-C4-N21	3.79	116.70	111.98
6	A	536[A]	CNC	C5M-C5B-C6B	3.72	128.35	120.76
6	A	536[B]	CNC	C1-C2-C3	3.72	106.28	101.60
6	A	536[B]	CNC	C53-C15-C14	3.71	124.30	116.79
6	A	536[B]	CNC	C7-C8-C9	-3.64	96.28	100.89
6	A	536[A]	CNC	C7-C6-N22	-3.56	101.46	107.94
6	A	536[B]	CNC	C17-C16-C15	-3.54	121.38	126.70
6	A	536[B]	CNC	C5-C4-N21	-3.53	118.52	124.19
6	A	536[A]	CNC	N1B-C2B-N3B	-3.49	108.99	113.94
6	A	536[A]	CNC	C9B-C8B-N1B	3.46	106.84	105.30
6	A	536[A]	CNC	C19-N24-C16	-3.45	106.44	111.96
6	A	536[B]	CNC	C10-C11-N23	-3.40	119.41	124.92
6	A	536[B]	CNC	C56-C55-C17	-3.38	109.07	115.58
6	A	536[B]	CNC	C5M-C5B-C6B	3.37	127.65	120.76
6	A	536[B]	CNC	C15-C14-N23	-3.35	120.10	126.67
6	A	536[A]	CNC	C5-C4-N21	-3.23	119.00	124.19
6	A	536[B]	CNC	C3R-C2R-C1R	3.06	106.61	99.89
6	A	536[A]	CNC	O28-C27-N29	-3.05	114.39	122.53
6	A	536[A]	CNC	C35-C5-C4	2.98	122.82	116.79
6	A	536[B]	CNC	C2-C1-C19	2.97	123.89	118.77
6	A	536[B]	CNC	O7R-C2R-C3R	-2.95	102.94	111.19
6	A	536[B]	CNC	C2-C1-N21	2.93	105.86	101.78
6	A	536[A]	CNC	C36-C7-C6	2.89	127.36	112.41
6	A	536[A]	CNC	C10-C11-N23	-2.82	120.35	124.92
6	A	536[A]	CNC	C2-C26-C27	2.75	122.83	115.19
6	A	536[B]	CNC	C2-C3-C4	-2.71	98.59	101.64
6	A	536[B]	CNC	C8B-C9B-N3B	-2.71	107.07	110.00
6	A	536[B]	CNC	C1R-N1B-C2B	2.68	133.05	127.09
6	A	536[B]	CNC	C12-C13-C14	-2.67	98.38	101.86
6	A	536[B]	CNC	C2R-C1R-N1B	-2.62	106.79	113.30
6	A	536[A]	CNC	C41-C8-C9	-2.57	106.69	111.19
6	A	536[B]	CNC	C60-C18-C17	-2.56	108.81	115.82
6	A	536[B]	CNC	C7-C6-C5	-2.55	124.08	128.07
6	A	536[A]	CNC	C60-C18-C17	-2.53	108.89	115.82
6	A	536[A]	CNC	C3R-C2R-C1R	2.48	105.35	99.89
6	A	536[B]	CNC	C1-C19-N24	-2.44	102.39	106.29
6	A	536[A]	CNC	O58-C57-N59	-2.43	118.27	123.03
6	A	536[B]	CNC	O6R-C1R-N1B	-2.35	103.57	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	536[B]	CNC	O39-C38-N40	-2.29	116.42	122.53
6	A	536[A]	CNC	C8B-N1B-C1R	-2.26	121.59	125.41
6	A	536[A]	CNC	C8B-N1B-C2B	2.24	108.30	106.26
6	A	536[B]	CNC	C2-C26-C27	2.22	121.36	115.19
6	A	536[A]	CNC	C9B-N3B-C2B	2.22	107.12	104.40
6	A	536[B]	CNC	C7-C37-C38	2.22	120.83	114.28
6	A	536[B]	CNC	O6R-C1R-C2R	-2.19	101.93	106.62
6	A	536[A]	CNC	C2R-C1R-N1B	-2.17	107.92	113.30
6	A	536[B]	CNC	C35-C5-C4	2.16	121.17	116.79
6	A	536[B]	CNC	C41-C8-C7	-2.14	108.28	114.19
6	A	536[A]	CNC	C55-C56-C57	-2.14	106.48	111.25
6	A	536[B]	CNC	C55-C17-C16	-2.13	111.52	116.17
6	A	536[A]	CNC	C20-C1-C2	-2.08	109.84	113.28
6	A	536[B]	CNC	C1P-N59-C57	-2.07	118.26	122.69
6	A	536[A]	CNC	C2-C1-N21	2.06	104.65	101.78
6	A	536[A]	CNC	C54-C17-C55	-2.06	105.84	109.27
6	A	536[A]	CNC	C17-C16-C15	-2.05	123.61	126.70
6	A	536[A]	CNC	C35-C5-C6	-2.02	119.16	122.41

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	536[A]	CNC	N24
6	A	536[B]	CNC	N24

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	536[A]	CNC	C2R-C3R-O2-P
6	A	536[A]	CNC	C4R-C3R-O2-P
5	A	532	EDO	O1-C1-C2-O2
5	A	513	EDO	O1-C1-C2-O2
5	A	520	EDO	O1-C1-C2-O2
5	A	523	EDO	O1-C1-C2-O2
5	B	202	EDO	O1-C1-C2-O2
6	A	536[A]	CNC	N59-C1P-C2P-C3P
5	A	521	EDO	O1-C1-C2-O2
5	A	531	EDO	O1-C1-C2-O2
6	A	536[A]	CNC	N59-C1P-C2P-O3
6	A	536[B]	CNC	C13-C48-C49-C50
5	A	522	EDO	O1-C1-C2-O2
5	A	514	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	528	EDO	O1-C1-C2-O2
5	B	203	EDO	O1-C1-C2-O2
5	C	207	EDO	O1-C1-C2-O2
5	B	201	EDO	O1-C1-C2-O2
6	A	536[B]	CNC	O6R-C1R-N1B-C8B
6	A	536[A]	CNC	C13-C48-C49-C50
5	A	530	EDO	O1-C1-C2-O2
5	A	534	EDO	O1-C1-C2-O2

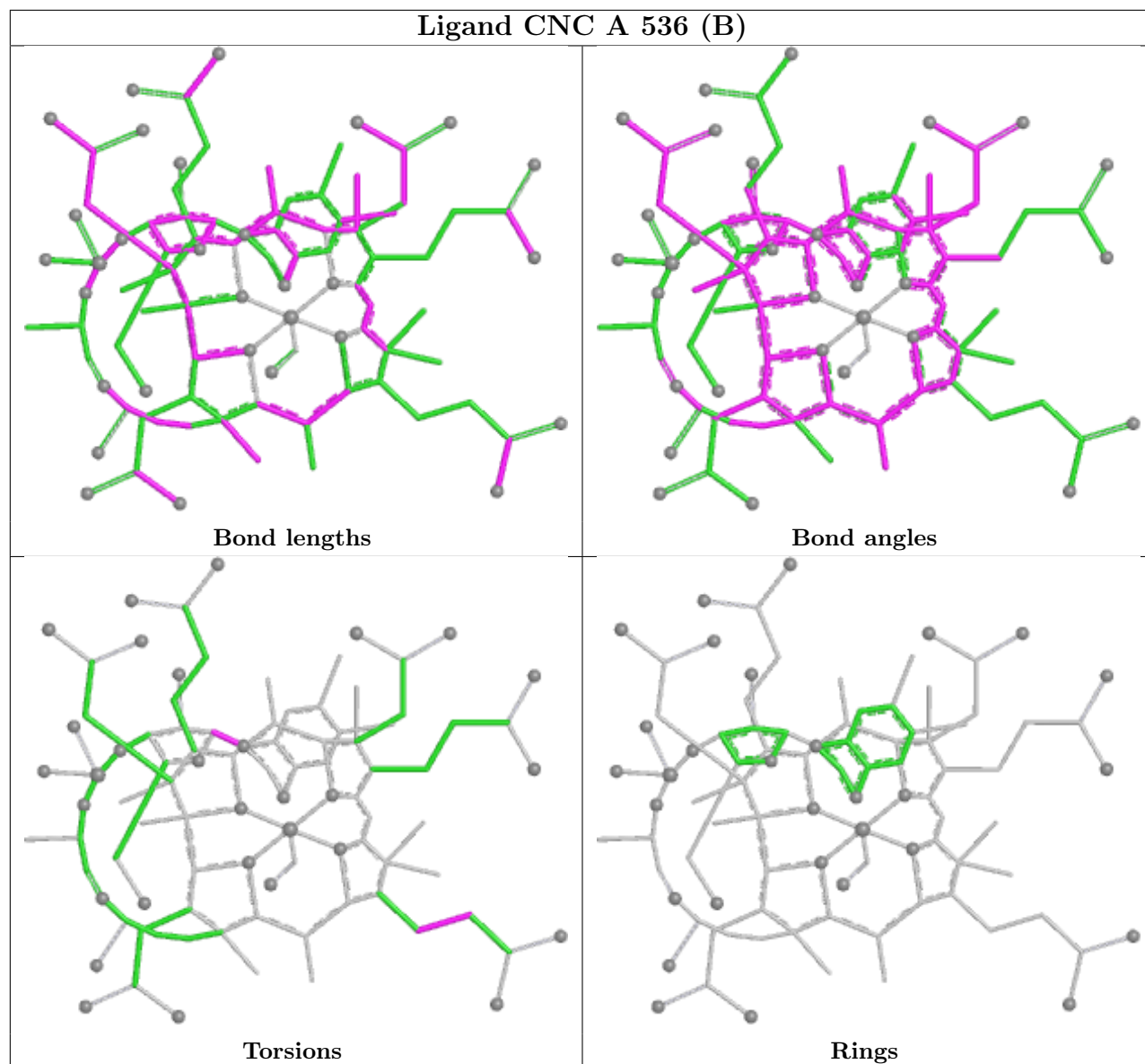
There are no ring outliers.

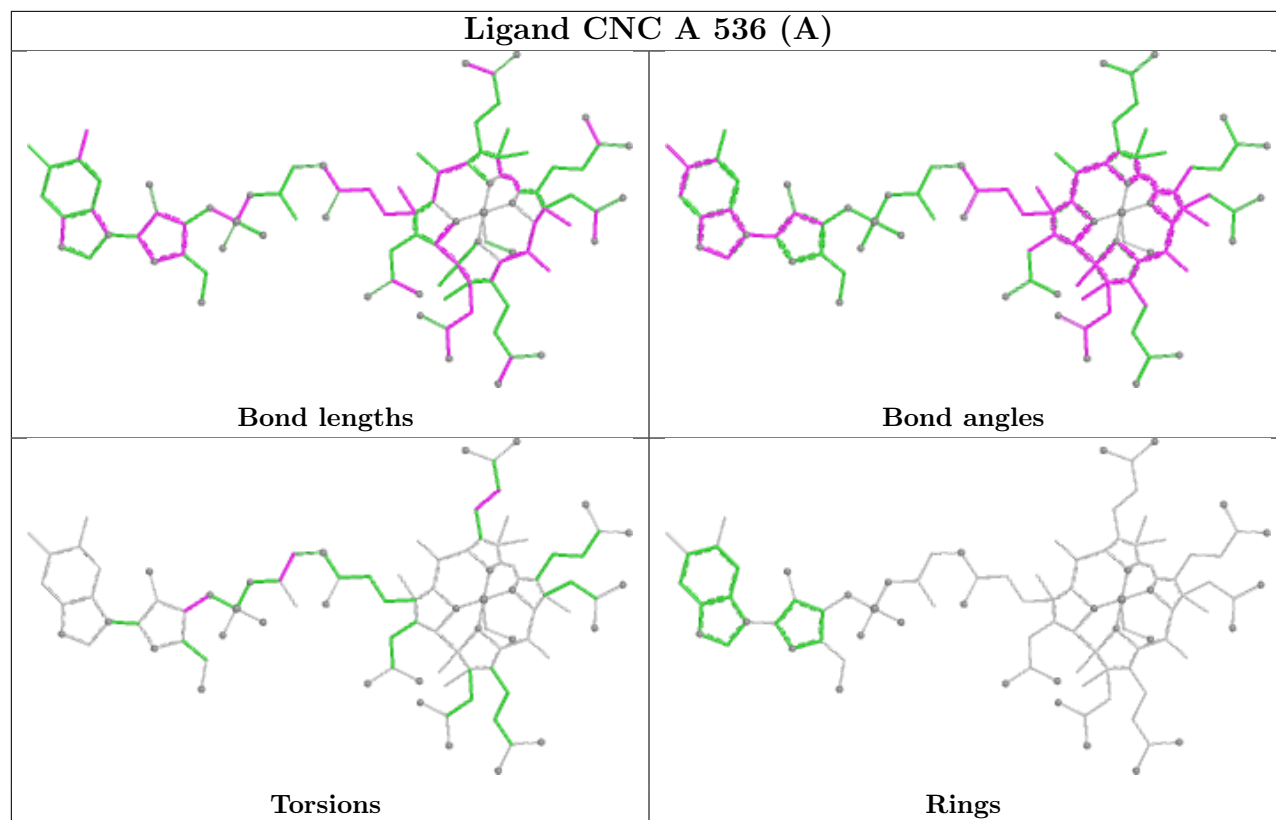
15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	514	EDO	2	0
5	A	525	EDO	1	0
5	A	517	EDO	4	0
5	A	533	EDO	1	0
5	A	535	EDO	2	0
5	A	524	EDO	1	0
6	A	536[B]	CNC	13	0
5	A	520	EDO	5	0
5	A	534	EDO	2	0
5	A	529	EDO	4	0
5	A	526	EDO	2	0
5	A	516	EDO	3	0
5	B	203	EDO	1	0
6	A	536[A]	CNC	14	0
5	A	513	EDO	3	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.

Ligand CNC A 536 (B)





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	409/409 (100%)	-0.04	21 (5%)	33 36	17, 36, 65, 134	7 (1%)
2	C	78/147 (53%)	0.36	4 (5%)	33 36	27, 41, 75, 100	0
3	B	125/137 (91%)	0.82	12 (9%)	13 13	27, 49, 82, 102	2 (1%)
All	All	612/693 (88%)	0.18	37 (6%)	27 30	17, 39, 72, 134	9 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	109[A]	TRP	10.2
3	B	4	LEU	6.4
1	A	169[A]	HIS	6.2
1	A	305	ILE	6.2
1	A	11[A]	HIS	5.6
3	B	131	HIS	5.2
3	B	104	THR	5.0
3	B	129	HIS	4.5
2	C	170	ASN	4.5
1	A	308	THR	4.4
1	A	172	HIS	4.2
1	A	304	THR	3.8
2	C	90	ARG	3.5
1	A	15[A]	LYS	3.3
3	B	102	GLY	3.2
1	A	302	ALA	3.1
1	A	241	ARG	3.0
3	B	108	ASN	2.9
1	A	306	PRO	2.8
2	C	169	THR	2.8
3	B	103	GLU	2.6
3	B	128	SER	2.6
2	C	53	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	B	130	HIS	2.5
1	A	307	GLN	2.5
1	A	311	ILE	2.4
1	A	1	GLU	2.4
1	A	171	GLY	2.4
1	A	257	LEU	2.3
1	A	14[A]	GLU	2.3
1	A	209	ARG	2.2
1	A	303	GLU	2.2
3	B	56	GLY	2.2
1	A	29	LEU	2.2
3	B	65	LYS	2.1
1	A	131	HIS	2.1
1	A	310	GLU	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	IOD	A	507	1/1	0.70	0.16	208,208,208,208	0
5	EDO	A	523	4/4	0.72	0.17	46,66,84,88	0
5	EDO	A	522	4/4	0.80	0.17	60,72,82,82	0
5	EDO	A	529	4/4	0.80	0.15	43,52,67,67	0
5	EDO	B	203	4/4	0.80	0.22	51,61,69,69	0
5	EDO	A	517	4/4	0.81	0.24	32,51,61,63	0
5	EDO	A	535	4/4	0.82	0.26	44,55,57,66	0
5	EDO	A	521	4/4	0.85	0.15	41,50,72,86	0
5	EDO	A	532	4/4	0.85	0.14	45,54,60,72	0

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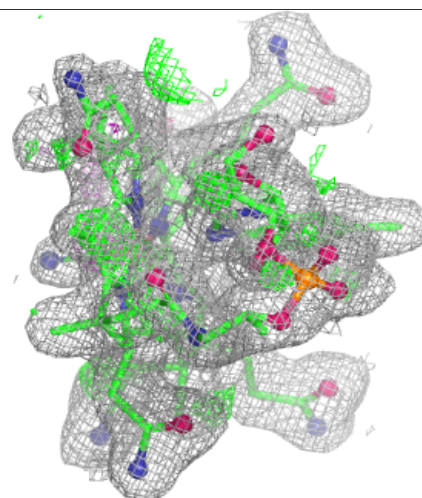
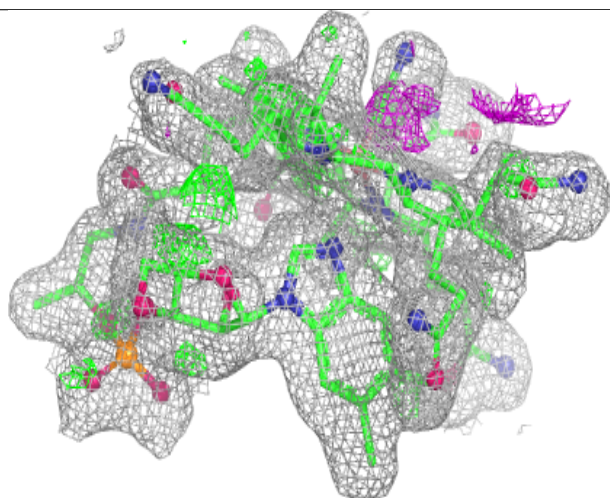
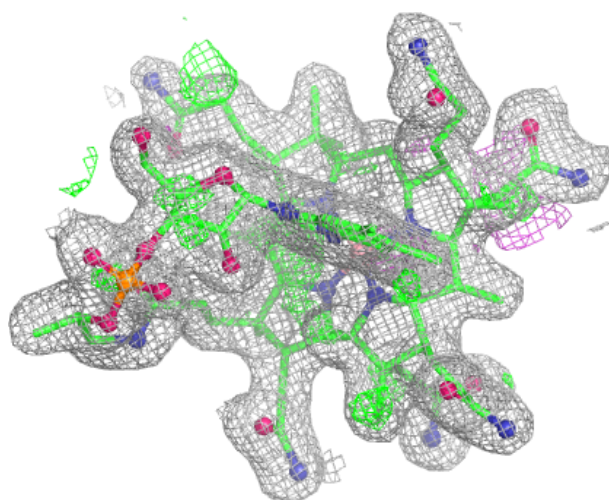
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	530	4/4	0.87	0.13	36,43,50,57	0
5	EDO	A	520	4/4	0.87	0.41	42,51,62,62	0
4	IOD	A	511	1/1	0.88	0.42	122,122,122,122	0
5	EDO	A	524	4/4	0.88	0.17	43,57,68,69	0
5	EDO	A	526	4/4	0.88	0.32	36,44,58,70	0
5	EDO	A	513	4/4	0.88	0.14	29,38,65,78	0
5	EDO	B	201	4/4	0.89	0.16	54,65,74,89	0
5	EDO	A	518	4/4	0.89	0.20	30,46,55,55	0
4	IOD	A	510	1/1	0.90	0.28	118,118,118,118	0
4	IOD	A	509	1/1	0.90	0.38	153,153,153,153	0
4	IOD	A	512	1/1	0.90	0.42	130,130,130,130	0
5	EDO	A	516	4/4	0.91	0.16	31,42,57,57	0
5	EDO	A	528	4/4	0.91	0.20	43,52,60,68	0
5	EDO	A	525	4/4	0.92	0.12	32,46,60,63	0
4	IOD	A	502	1/1	0.93	0.33	126,126,126,126	0
5	EDO	A	531	4/4	0.93	0.10	46,55,58,60	0
5	EDO	A	514	4/4	0.93	0.12	37,46,61,61	0
5	EDO	A	534	4/4	0.94	0.15	29,45,66,66	0
5	EDO	A	527	4/4	0.94	0.11	39,47,52,62	0
5	EDO	C	207	4/4	0.94	0.13	31,50,77,77	0
5	EDO	A	515	4/4	0.94	0.11	34,44,53,53	0
5	EDO	A	533	4/4	0.94	0.12	35,51,66,75	0
4	IOD	A	504	1/1	0.95	0.10	74,74,74,74	1
5	EDO	B	202	4/4	0.96	0.09	30,39,41,47	0
4	IOD	A	508	1/1	0.97	0.07	52,52,52,52	1
6	CNC	A	536[A]	93/93	0.97	0.08	20,23,27,34	93
6	CNC	A	536[B]	93/93	0.97	0.08	19,23,29,38	93
4	IOD	A	501	1/1	0.98	0.04	37,37,37,37	1
5	EDO	A	519	4/4	0.98	0.10	28,39,46,46	0
4	IOD	A	505	1/1	0.98	0.05	45,45,45,45	1
4	IOD	A	506	1/1	0.98	0.05	43,43,43,43	1
4	IOD	C	203	1/1	0.98	0.07	53,53,53,53	1
4	IOD	C	206	1/1	0.98	0.05	45,45,45,45	1
4	IOD	C	204	1/1	0.99	0.04	48,48,48,48	1
4	IOD	C	205	1/1	0.99	0.05	35,35,35,35	1
7	CA	C	201	1/1	0.99	0.02	25,25,25,25	0
4	IOD	A	503	1/1	1.00	0.02	37,37,37,37	1
7	CA	C	202	1/1	1.00	0.02	30,30,30,30	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.

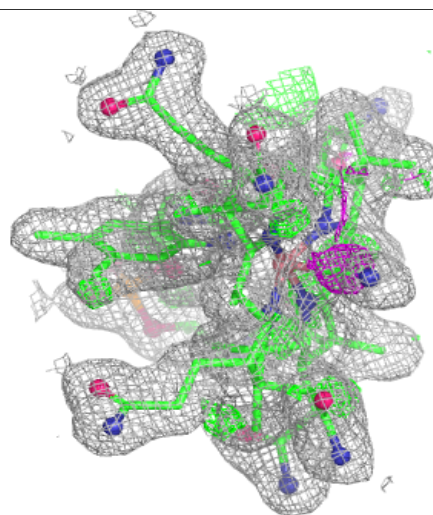
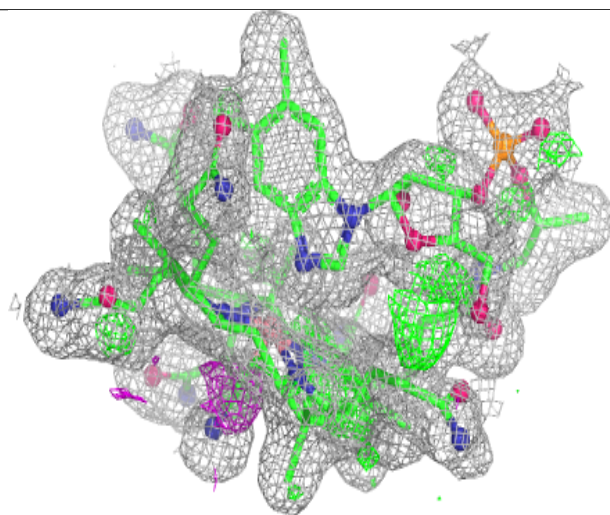
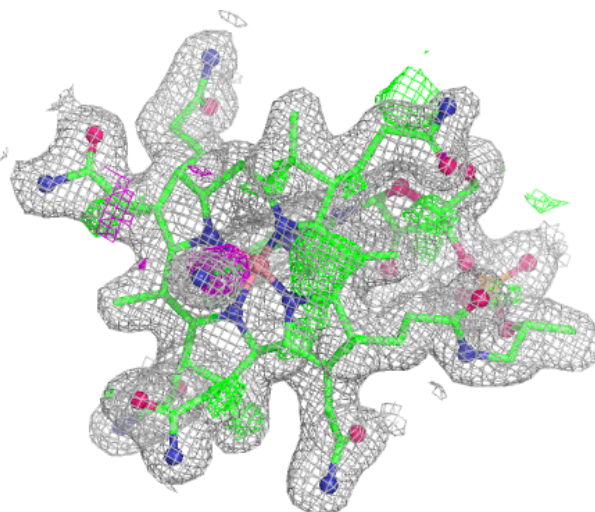
Electron density around CNC A 536 (A):

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



Electron density around CNC A 536 (B):

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



6.5 Other polymers ⓘ

There are no such residues in this entry.