



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:21 AM UTC

PDB ID : 2WOX / pdb_00002wox
Title : Betaine aldehyde dehydrogenase from Pseudomonas aeruginosa with NAD(P)
H-catalytic thiol adduct.
Authors : Gonzalez-Segura, L.; Rudino-Pinera, E.; Diaz-Sanchez, A.G.; Munoz-Clares,
R.A.
Deposited on : 2009-07-30
Resolution : 2.30 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

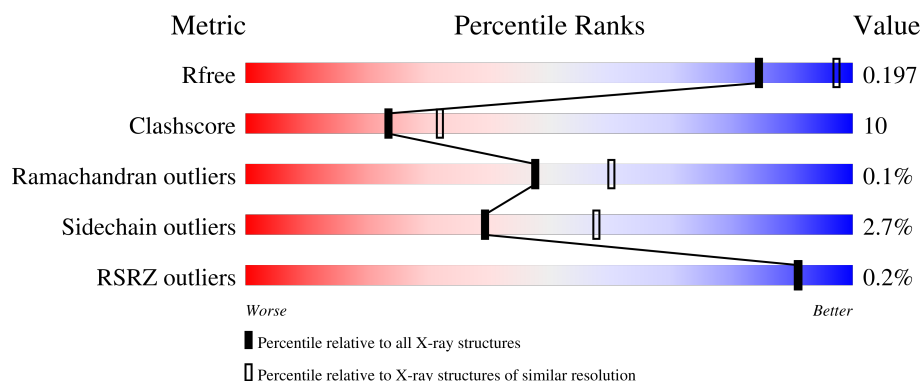
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	489	 83% 16% .
1	B	489	 83% 15% .
1	C	489	 86% 13% .
1	D	489	 85% 15% .

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
2	NDP	B	1491	X	-	-	-
2	NDP	D	1491	X	-	-	-
4	GOL	A	1494	-	-	X	-
4	GOL	B	1496	-	-	X	-
4	GOL	C	1497	-	-	X	-
4	GOL	C	1499	-	-	X	-
4	GOL	D	1496	-	X	-	-
5	7PE	A	1496	-	-	X	-
5	7PE	C	1501	-	-	X	-
6	BME	C	1600	-	-	X	-

2 Entry composition ⓘ

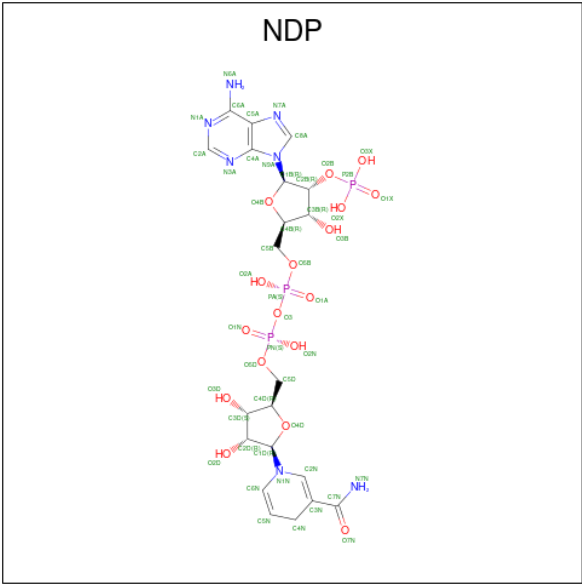
There are 7 unique types of molecules in this entry. The entry contains 16607 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETAINES ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	7	0
			3797	2382	667	733	15			
1	B	489	Total	C	N	O	S	0	5	0
			3787	2376	666	730	15			
1	C	489	Total	C	N	O	S	0	4	0
			3778	2371	664	728	15			
1	D	489	Total	C	N	O	S	0	3	0
			3770	2365	663	727	15			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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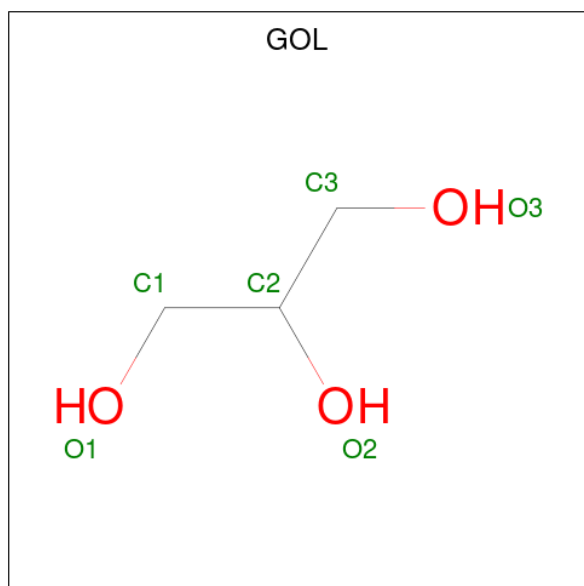
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	1
			60	26	7	23	4		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		
3	B	2	Total	K	0	0
			2	2		
3	C	2	Total	K	0	0
			2	2		
3	D	2	Total	K	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



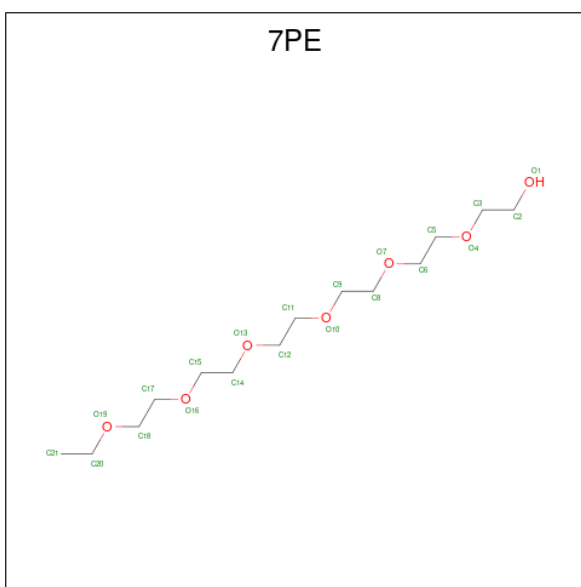
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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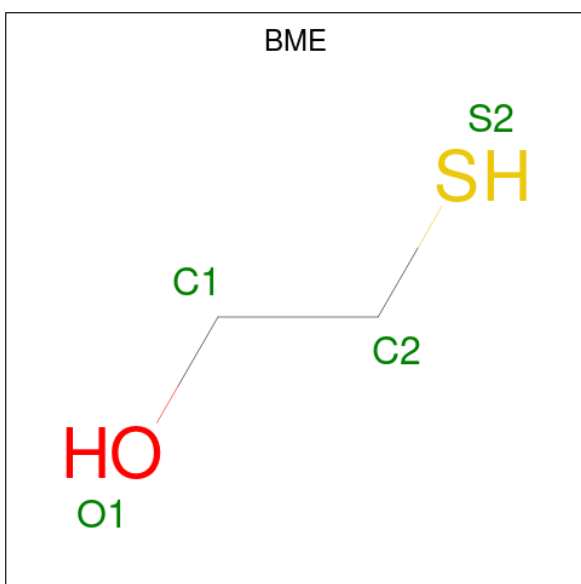
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-(2-(2-(2-(2-ETHOXYETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHANOL (CCD ID: 7PE) (formula: C₁₄H₃₀O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 21	C 14	O 7	0	0
5	A	1	Total 11	C 7	O 4	0	0
5	B	1	Total 16	C 10	O 6	0	0
5	B	1	Total 8	C 5	O 3	0	0
5	C	1	Total 15	C 10	O 5	0	0

- Molecule 6 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: $\text{C}_2\text{H}_6\text{OS}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	C	1	Total	C	O	S	0	0
			4	2	1	1		

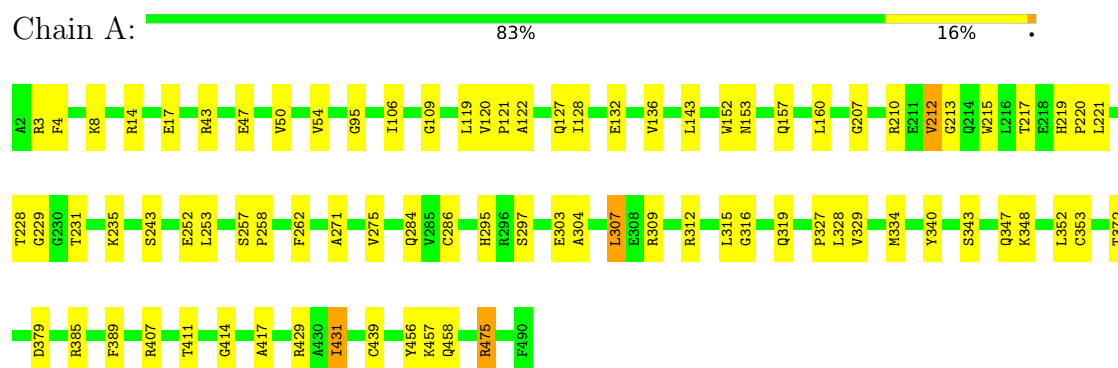
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	225	Total	O	0	0
			225	225		
7	B	265	Total	O	0	0
			265	265		
7	C	363	Total	O	0	0
			363	363		
7	D	235	Total	O	0	0
			235	235		

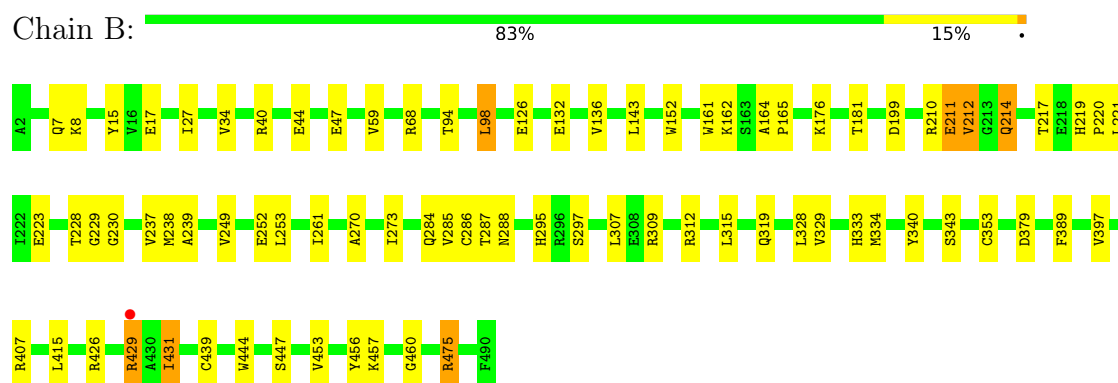
3 Residue-property plots [i](#)

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.

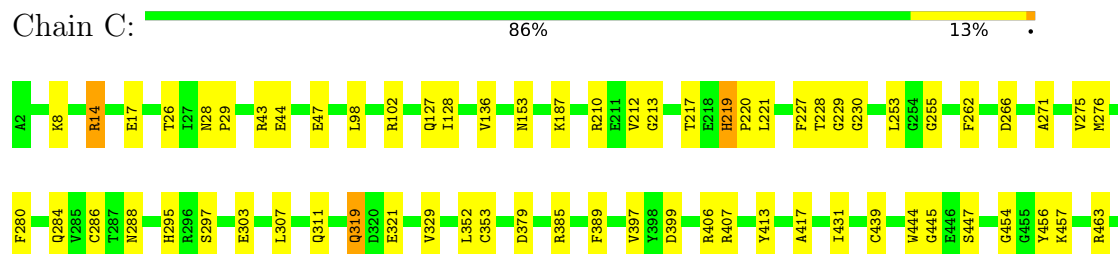
• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE



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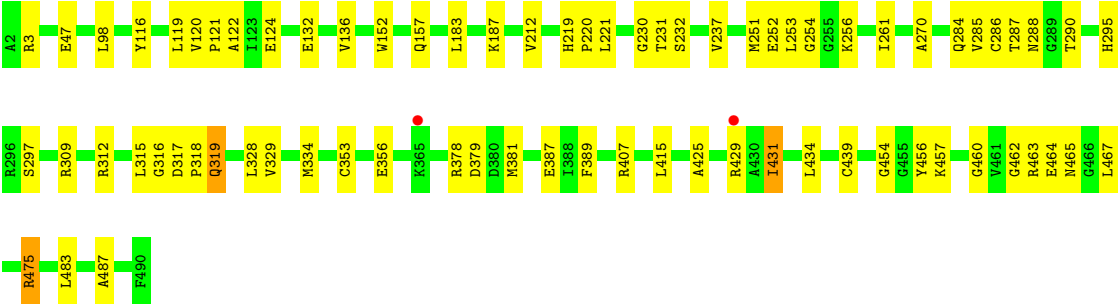
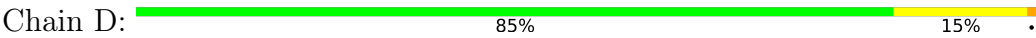


• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE





● Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.75Å 151.75Å 242.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.41 – 2.30 63.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (63.41-2.30) 98.7 (63.41-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.159 , 0.198 0.131 , 0.197	Depositor DCC
R_{free} test set	7081 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16607	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BME, K, NDP, GOL, 7PE

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	0.43	0/3865	0.78	3/5237 (0.1%)
1	B	0.47	0/3855	0.79	2/5223 (0.0%)
1	C	0.54	1/3846 (0.0%)	0.81	5/5211 (0.1%)
1	D	0.50	0/3838	0.76	3/5200 (0.1%)
All	All	0.49	1/15404 (0.0%)	0.79	13/20871 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	ARG	C-O	-5.13	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	HIS	CA-C-N	6.78	126.41	119.56
1	C	219	HIS	C-N-CA	6.78	126.41	119.56
1	A	262	PHE	CA-C-N	6.12	125.81	119.82
1	A	262	PHE	C-N-CA	6.12	125.81	119.82
1	A	457	LYS	CB-CA-C	-6.07	109.59	116.63
1	B	457	LYS	CB-CA-C	-5.87	109.80	116.54
1	D	457	LYS	CB-CA-C	-5.78	109.37	117.23
1	D	460	GLY	N-CA-C	5.72	118.92	110.63
1	C	457	LYS	CB-CA-C	-5.64	108.44	116.34
1	D	183	LEU	N-CA-C	5.43	117.00	111.14
1	B	460	GLY	N-CA-C	5.34	118.38	110.63
1	C	262	PHE	CA-C-N	5.14	124.81	119.56
1	C	262	PHE	C-N-CA	5.14	124.81	119.56

There are no chirality outliers.

There are no planarity outliers.

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	3797	0	3761	82	0
1	B	3787	0	3752	78	0
1	C	3778	0	3744	69	0
1	D	3770	0	3736	66	0
2	A	48	0	25	17	0
2	B	48	0	24	18	0
2	C	60	0	14	9	0
2	D	48	0	24	15	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	6	0	8	8	0
4	B	30	0	40	15	0
4	C	36	0	48	10	0
4	D	24	0	32	2	0
5	A	32	0	41	16	0
5	B	24	0	24	9	0
5	C	15	0	21	12	0
6	A	4	0	5	2	0
6	C	4	0	5	5	0
7	A	225	0	0	3	0
7	B	265	0	0	7	0
7	C	363	0	0	7	0
7	D	235	0	0	5	0
All	All	16607	0	15304	314	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 10.

All (314) 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)
5:A:1496:7PE:H111	7:A:2224:HOH:O	1.28	1.24
1:C:307[B]:LEU:HD21	1:C:352:LEU:CG	1.67	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:NH2	4:B:1496:GOL:H12	1.54	1.20
1:B:68:ARG:HH22	4:B:1496:GOL:C1	1.55	1.19
1:A:307[B]:LEU:HD21	1:A:352:LEU:CD2	1.85	1.07
1:A:157:GLN:HE22	5:A:1496:7PE:H121	1.12	1.06
1:C:307[B]:LEU:CD2	1:C:352:LEU:HG	1.85	1.05
1:B:252:GLU:HB3	2:B:1491:NDP:O7N	1.54	1.03
4:A:1494:GOL:H11	5:A:1496:7PE:O19	1.59	1.01
1:C:389:PHE:CE1	2:C:1491[A]:NDP:H2D	1.95	1.00
1:B:286[A]:CYS:SG	2:B:1491:NDP:C5N	2.50	0.98
1:A:157:GLN:HE22	5:A:1496:7PE:C12	1.78	0.97
1:C:447:SER:H	4:C:1499:GOL:H2	1.29	0.96
1:D:252:GLU:HB3	2:D:1491:NDP:O7N	1.64	0.95
1:A:228:THR:HG23	2:A:1491:NDP:C5N	1.96	0.95
4:A:1494:GOL:H12	5:A:1496:7PE:H172	1.52	0.92
1:B:68:ARG:HH22	4:B:1496:GOL:H12	0.75	0.92
1:C:307[B]:LEU:HD21	1:C:352:LEU:HG	0.91	0.88
1:B:284:GLN:HE22	1:B:329:VAL:H	1.22	0.88
1:D:378:ARG:HG3	1:D:381:MET:HE3	1.54	0.88
1:D:286[A]:CYS:SG	2:D:1491:NDP:C5N	2.57	0.87
1:C:219:HIS:HD2	1:C:221:LEU:H	1.23	0.87
1:C:307[B]:LEU:HD23	1:C:353:CYS:SG	2.14	0.86
1:D:284:GLN:HE22	1:D:329:VAL:H	1.19	0.86
1:A:307[B]:LEU:HD21	1:A:352:LEU:HG	1.59	0.85
1:C:210:ARG:HG3	2:C:1491[B]:NDP:H1D	1.57	0.85
1:A:307[B]:LEU:HD21	1:A:352:LEU:CG	2.06	0.85
1:B:143:LEU:HD23	1:B:475:ARG:HG2	1.58	0.84
1:D:389:PHE:CE1	2:D:1491:NDP:H2D	2.11	0.84
1:B:286[A]:CYS:HB3	2:B:1491:NDP:H71N	1.42	0.84
1:B:219:HIS:HD2	1:B:221:LEU:H	1.24	0.83
1:C:286[B]:CYS:SG	7:C:2356:HOH:O	2.35	0.83
4:A:1494:GOL:C1	5:A:1496:7PE:O19	2.28	0.82
4:A:1494:GOL:H11	5:A:1496:7PE:C18	2.10	0.82
1:B:199:ASP:HB2	5:B:1499:7PE:H122	1.61	0.82
1:C:307[B]:LEU:HD21	1:C:352:LEU:CD2	2.09	0.82
4:B:1496:GOL:H2	7:B:2265:HOH:O	1.79	0.81
1:C:456:TYR:CZ	1:D:475:ARG:HD3	2.14	0.81
1:B:389:PHE:CE1	2:B:1491:NDP:H2D	2.15	0.81
1:C:187:LYS:HZ3	4:C:1495:GOL:H12	1.44	0.80
1:D:219:HIS:HD2	1:D:221:LEU:H	1.29	0.80
1:B:447:SER:H	5:B:1500:7PE:C12	1.95	0.79
1:A:303:GLU:O	1:A:307[B]:LEU:HG	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLN:HE22	1:C:329:VAL:H	1.27	0.79
1:D:286[A]:CYS:HB3	2:D:1491:NDP:H71N	1.48	0.78
1:A:157:GLN:NE2	5:A:1496:7PE:H121	1.97	0.78
1:A:307[B]:LEU:CD2	1:A:352:LEU:CD2	2.62	0.77
1:B:230:GLY:HA2	2:B:1491:NDP:O3D	1.84	0.77
1:B:295:HIS:CD2	1:B:297:SER:H	2.02	0.77
1:B:199:ASP:N	5:B:1499:7PE:H121	2.00	0.76
1:B:353:CYS:SG	7:B:2126:HOH:O	2.44	0.76
1:A:252:GLU:O	2:A:1491:NDP:H5N	1.84	0.76
1:A:307[B]:LEU:CD2	1:A:352:LEU:HD23	2.15	0.76
1:D:230:GLY:HA2	2:D:1491:NDP:O3D	1.86	0.76
4:A:1494:GOL:H32	5:A:1496:7PE:H151	1.68	0.75
1:B:199:ASP:H	5:B:1499:7PE:H121	1.49	0.74
1:A:228:THR:CG2	2:A:1491:NDP:H42N	2.18	0.74
1:A:284:GLN:HE22	1:A:329:VAL:H	1.35	0.74
1:A:295:HIS:HD2	1:A:297:SER:OG	1.71	0.73
2:B:1491:NDP:H42N	7:B:2195:HOH:O	1.89	0.73
1:A:153:ASN:ND2	2:A:1491:NDP:N7N	2.36	0.72
1:C:307[A]:LEU:HD13	6:C:1600:BME:S2	2.30	0.72
1:D:353:CYS:SG	7:D:2091:HOH:O	2.47	0.72
1:C:444:TRP:CD1	5:C:1501:7PE:H82	2.25	0.71
1:C:445:GLY:HA3	5:C:1501:7PE:H112	1.72	0.71
1:A:475:ARG:HD3	1:B:456:TYR:CZ	2.26	0.71
1:B:219:HIS:CD2	1:B:221:LEU:H	2.07	0.70
1:A:228:THR:HG23	2:A:1491:NDP:C4N	2.23	0.69
1:C:187:LYS:NZ	4:C:1495:GOL:H12	2.07	0.69
1:A:219:HIS:HD2	1:A:221:LEU:H	1.42	0.68
2:D:1491:NDP:H42N	7:D:2235:HOH:O	1.93	0.67
1:A:307[B]:LEU:HD21	1:A:352:LEU:HD23	1.67	0.67
4:B:1496:GOL:O3	7:B:2264:HOH:O	2.12	0.67
1:C:219:HIS:CD2	1:C:221:LEU:H	2.10	0.67
1:C:307[B]:LEU:CD2	1:C:353:CYS:SG	2.82	0.67
1:A:228:THR:HG23	2:A:1491:NDP:H5N	1.77	0.67
5:C:1501:7PE:H172	7:C:2363:HOH:O	1.95	0.66
1:A:429[A]:ARG:HG3	1:D:483:LEU:HD13	1.76	0.66
1:A:219:HIS:CD2	1:A:221:LEU:H	2.14	0.66
1:C:288:ASN:OD1	5:C:1501:7PE:H81	1.96	0.65
1:D:219:HIS:CD2	1:D:221:LEU:H	2.13	0.65
6:C:1600:BME:H12	7:C:2119:HOH:O	1.96	0.65
5:A:1496:7PE:C11	7:A:2224:HOH:O	2.07	0.65
1:D:379:ASP:OD2	1:D:407:ARG:HD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:ARG:HD3	1:D:456:TYR:CZ	2.32	0.64
1:A:143:LEU:HD23	1:A:475:ARG:HG2	1.80	0.64
1:B:47:GLU:OE1	1:B:219:HIS:HE1	1.81	0.64
1:C:445:GLY:HA2	5:C:1501:7PE:H91	1.79	0.64
1:C:307[B]:LEU:CD2	1:C:352:LEU:CD2	2.76	0.64
1:D:116:TYR:OH	1:D:465:ASN:HA	1.98	0.63
1:D:47:GLU:OE1	1:D:219:HIS:HE1	1.80	0.63
1:A:353[B]:CYS:SG	6:A:1600:BME:S2	2.95	0.63
4:A:1494:GOL:C1	5:A:1496:7PE:C18	2.77	0.62
1:C:47:GLU:OE1	1:C:219:HIS:HE1	1.82	0.62
1:D:295:HIS:HD2	1:D:297:SER:OG	1.82	0.62
1:A:307[A]:LEU:HD11	6:A:1600:BME:H12	1.80	0.61
1:C:303:GLU:O	1:C:307[B]:LEU:HG	2.00	0.61
1:C:307[A]:LEU:CD1	6:C:1600:BME:S2	2.88	0.61
1:D:387:GLU:OE2	7:D:2186:HOH:O	2.16	0.61
1:A:456:TYR:CZ	1:B:475:ARG:HD3	2.36	0.61
1:B:199:ASP:H	5:B:1499:7PE:C12	2.13	0.61
1:A:157:GLN:NE2	5:A:1496:7PE:C12	2.59	0.60
1:A:389:PHE:CE1	2:A:1491:NDP:H2D	2.36	0.60
1:D:286[A]:CYS:SG	2:D:1491:NDP:C2D	2.89	0.60
1:D:231:THR:HA	1:D:253:LEU:HD13	1.82	0.60
1:A:307[B]:LEU:HD21	1:A:352:LEU:HD21	1.81	0.60
1:B:261[B]:ILE:HD13	1:B:270:ALA:HB1	1.84	0.60
1:B:295:HIS:HD2	1:B:297:SER:H	1.46	0.60
1:B:8:LYS:HE2	1:B:17:GLU:OE2	2.02	0.59
5:C:1501:7PE:H211	1:D:487:ALA:O	2.02	0.59
1:B:210:ARG:C	1:B:211:GLU:HG3	2.28	0.59
4:B:1490:GOL:H2	2:B:1491:NDP:N7A	2.18	0.59
1:B:379:ASP:OD2	1:B:407:ARG:HD2	2.03	0.59
4:A:1494:GOL:C3	5:A:1496:7PE:H151	2.33	0.59
1:C:445:GLY:CA	5:C:1501:7PE:H91	2.33	0.59
1:A:228:THR:CG2	2:A:1491:NDP:C5N	2.78	0.58
1:C:379:ASP:OD2	1:C:407:ARG:HD2	2.04	0.58
1:D:253:LEU:O	2:D:1491:NDP:N7N	2.36	0.58
1:B:252:GLU:CB	2:B:1491:NDP:O7N	2.42	0.58
1:D:286[A]:CYS:CB	2:D:1491:NDP:H71N	2.14	0.57
1:C:295:HIS:CD2	1:C:297:SER:H	2.23	0.57
4:B:1490:GOL:H2	2:B:1491:NDP:H61A	1.70	0.57
1:C:219:HIS:CD2	1:C:220:PRO:HD2	2.39	0.57
1:A:119:LEU:HD21	1:D:122:ALA:HB2	1.87	0.56
1:B:229:GLY:O	1:B:253:LEU:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:GLN:HE22	1:D:329:VAL:N	1.96	0.56
1:D:295:HIS:CD2	1:D:297:SER:H	2.23	0.56
1:C:230:GLY:HA2	2:C:1491[A]:NDP:O3D	2.06	0.56
1:A:43:ARG:HG3	1:A:215:TRP:CE2	2.40	0.56
4:A:1494:GOL:H12	5:A:1496:7PE:C17	2.31	0.56
1:C:447:SER:H	4:C:1499:GOL:C2	2.09	0.56
1:A:50:VAL:O	1:A:54:VAL:HG23	2.05	0.56
1:B:286[A]:CYS:CB	2:B:1491:NDP:H71N	2.14	0.56
1:C:389:PHE:CZ	2:C:1491[A]:NDP:H2D	2.37	0.55
1:B:286[A]:CYS:HB3	2:B:1491:NDP:N7N	2.17	0.55
4:C:1497:GOL:H32	7:C:2338:HOH:O	2.07	0.55
1:D:315:LEU:C	1:D:315:LEU:HD23	2.32	0.55
1:D:237:VAL:HG12	1:D:251:MET:HE1	1.88	0.54
1:D:285:VAL:HB	1:D:288:ASN:OD1	2.07	0.54
1:A:379:ASP:OD2	1:A:407:ARG:HD2	2.07	0.54
1:A:295:HIS:CD2	1:A:297:SER:H	2.26	0.54
1:D:464:GLU:O	1:D:465:ASN:HB2	2.07	0.54
1:B:397:VAL:O	1:B:407:ARG:NH2	2.41	0.54
1:D:328:LEU:HD12	1:D:334:MET:HA	1.89	0.54
1:C:280:PHE:CD2	5:C:1501:7PE:H141	2.43	0.53
1:D:462:GLY:C	1:D:463:ARG:HG2	2.33	0.53
1:D:120:VAL:HB	1:D:121:PRO:HD3	1.91	0.53
1:D:286[B]:CYS:SG	1:D:287:THR:HG23	2.49	0.53
1:C:444:TRP:HD1	5:C:1501:7PE:H82	1.70	0.53
1:A:228:THR:HG23	2:A:1491:NDP:H42N	1.84	0.52
1:A:315:LEU:C	1:A:315:LEU:HD23	2.34	0.52
1:B:285:VAL:HB	1:B:288:ASN:OD1	2.10	0.51
1:D:116:TYR:OH	1:D:465:ASN:CA	2.58	0.51
1:C:284:GLN:HE22	1:C:329:VAL:N	2.03	0.51
1:B:211:GLU:O	1:B:212:VAL:C	2.52	0.51
1:C:276:MET:HE3	5:C:1501:7PE:H122	1.91	0.51
1:A:229:GLY:O	2:A:1491:NDP:H6N	2.11	0.51
1:B:162:LYS:O	1:B:165:PRO:HD2	2.10	0.50
1:D:261:ILE:HD12	1:D:270:ALA:HB1	1.92	0.50
1:A:153:ASN:HD21	2:A:1491:NDP:H72N	1.53	0.50
1:A:379:ASP:OD2	1:A:407:ARG:CD	2.59	0.50
1:D:415:LEU:HD21	2:D:1491:NDP:H72N	1.76	0.50
1:B:59:VAL:HG11	5:B:1499:7PE:H92	1.94	0.50
1:B:152:TRP:CE3	1:B:329:VAL:HG11	2.47	0.50
1:C:454:GLY:HA3	1:C:463:ARG:HD3	1.93	0.50
1:D:415:LEU:HD21	2:D:1491:NDP:N7N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:TYR:OH	1:D:465:ASN:C	2.55	0.49
1:A:295:HIS:CD2	1:A:297:SER:OG	2.58	0.49
1:A:152:TRP:CE3	1:A:329:VAL:HG11	2.48	0.49
1:A:243:SER:HB3	1:B:239:ALA:HB2	1.95	0.49
1:D:152:TRP:CE3	1:D:329:VAL:HG11	2.48	0.49
1:B:238:MET:HG3	1:B:249:VAL:HG21	1.93	0.49
1:C:307[B]:LEU:HG	1:C:352:LEU:HD21	1.93	0.49
1:A:353[A]:CYS:O	1:A:372:THR:HA	2.13	0.49
1:B:453:VAL:HG21	4:B:1495:GOL:H31	1.94	0.49
1:C:311:GLN:HG3	6:C:1600:BME:H21	1.96	0.48
1:C:102:ARG:NH2	1:C:321:GLU:HG2	2.28	0.48
6:C:1600:BME:C1	7:C:2119:HOH:O	2.57	0.48
1:A:120:VAL:HB	1:A:121:PRO:HD3	1.95	0.48
1:A:328:LEU:HD12	1:A:334:MET:HA	1.95	0.48
1:D:284:GLN:NE2	1:D:329:VAL:H	2.00	0.48
1:A:417:ALA:O	1:A:439:CYS:HA	2.14	0.48
1:C:397:VAL:O	1:C:407:ARG:NH2	2.47	0.48
1:D:254:GLY:HA2	2:D:1491:NDP:O2D	2.14	0.48
1:A:304:ALA:HA	1:A:307[B]:LEU:HD12	1.95	0.48
4:B:1497:GOL:H12	7:B:2002:HOH:O	2.14	0.48
1:D:232:SER:HB3	7:D:2150:HOH:O	2.14	0.47
1:A:307[A]:LEU:HD13	1:A:353[A]:CYS:SG	2.54	0.47
1:D:462:GLY:O	1:D:463:ARG:HG2	2.13	0.47
1:A:122:ALA:HB2	1:D:119:LEU:HD21	1.96	0.47
1:A:228:THR:HG21	2:A:1491:NDP:H42N	1.94	0.47
1:A:229:GLY:O	1:A:253:LEU:HA	2.14	0.47
1:C:447:SER:HB3	4:C:1499:GOL:H31	1.96	0.47
1:C:406[A]:ARG:NH1	7:C:2300:HOH:O	2.44	0.47
1:A:231:THR:HA	1:A:253:LEU:HD13	1.97	0.47
1:C:8:LYS:HE2	1:C:17:GLU:OE2	2.15	0.47
1:B:161:TRP:HZ3	4:B:1495:GOL:H12	1.80	0.46
1:C:230:GLY:HA2	2:C:1491[A]:NDP:HO3N	1.79	0.46
1:C:276:MET:HE3	5:C:1501:7PE:C12	2.44	0.46
1:B:328:LEU:HD12	1:B:334:MET:HA	1.97	0.46
1:D:219:HIS:CD2	1:D:220:PRO:HD2	2.50	0.46
1:A:271:ALA:O	1:A:275[A]:VAL:HG22	2.15	0.46
1:A:347:GLN:O	1:A:348:LYS:HB2	2.16	0.46
1:B:286[A]:CYS:CB	2:B:1491:NDP:N7N	2.77	0.46
1:B:431:ILE:HG13	1:B:439:CYS:HB3	1.98	0.46
1:D:295:HIS:CD2	1:D:297:SER:OG	2.68	0.46
1:D:286[A]:CYS:SG	2:D:1491:NDP:O2D	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1495:7PE:H121	5:A:1495:7PE:H152	1.66	0.46
1:A:229:GLY:HA2	2:A:1491:NDP:O4D	2.15	0.45
4:B:1496:GOL:H32	7:B:2262:HOH:O	2.16	0.45
1:A:431:ILE:HG13	1:A:439:CYS:HB3	1.98	0.45
1:D:315:LEU:HD23	1:D:316:GLY:N	2.31	0.45
1:A:229:GLY:C	2:A:1491:NDP:H1D	2.41	0.45
1:D:187:LYS:HZ3	4:D:1497:GOL:H11	1.82	0.45
1:D:219:HIS:HA	1:D:220:PRO:HD3	1.81	0.45
1:C:286[A]:CYS:SG	2:C:1491[A]:NDP:C2D	3.03	0.45
5:A:1495:7PE:H51	1:D:467:LEU:HD22	1.99	0.45
1:C:389:PHE:CD1	2:C:1491[A]:NDP:H2D	2.49	0.45
1:D:431:ILE:HD12	1:D:434:LEU:HD12	1.98	0.45
1:A:95:GLY:O	1:A:327:PRO:HD2	2.17	0.45
1:B:27:ILE:CD1	1:B:34:VAL:HG22	2.47	0.45
1:B:176:LYS:HD2	1:B:212:VAL:HG22	1.98	0.44
1:A:8:LYS:HE2	1:A:17:GLU:OE2	2.18	0.44
1:A:307[B]:LEU:HD23	1:A:352:LEU:HD23	1.95	0.44
1:B:44:GLU:HG2	7:B:2061:HOH:O	2.16	0.44
1:A:431:ILE:CG1	1:A:439:CYS:HB3	2.47	0.44
1:A:127:GLN:C	1:A:128:ILE:HG13	2.41	0.44
1:C:210:ARG:HG3	2:C:1491[B]:NDP:C1D	2.38	0.44
1:D:256:LYS:HE3	1:D:290:THR:OG1	2.17	0.44
4:B:1490:GOL:C2	2:B:1491:NDP:H61A	2.30	0.44
1:D:152:TRP:CZ3	1:D:329:VAL:HG11	2.53	0.44
1:B:286[B]:CYS:SG	1:B:287:THR:HG23	2.57	0.44
1:B:211:GLU:O	1:B:214[A]:GLN:N	2.49	0.44
1:B:199:ASP:CB	5:B:1499:7PE:H122	2.41	0.43
1:C:213:GLY:O	1:C:217:THR:HG23	2.18	0.43
1:C:286[A]:CYS:SG	2:C:1491[A]:NDP:O2D	2.71	0.43
1:B:284:GLN:HE22	1:B:329:VAL:N	2.02	0.43
1:C:219:HIS:HA	1:C:220:PRO:HD3	1.74	0.43
1:A:286:CYS:SG	2:A:1491:NDP:C2D	3.03	0.43
1:B:253:LEU:O	2:B:1491:NDP:N7N	2.51	0.43
1:C:266:ASP:HB3	7:C:2215:HOH:O	2.17	0.43
1:D:317:ASP:OD1	1:D:318:PRO:HD2	2.19	0.43
1:B:286[B]:CYS:SG	1:B:415:LEU:HD21	2.59	0.43
1:C:319:GLN:HE21	1:C:319:GLN:HA	1.83	0.43
1:A:284:GLN:HE22	1:A:329:VAL:N	2.11	0.43
1:B:98:LEU:HD12	1:B:98:LEU:HA	1.89	0.43
1:C:271:ALA:O	1:C:275:VAL:HG22	2.18	0.43
1:A:257:SER:HA	1:A:258:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:GLY:HA3	1:D:463:ARG:HD3	2.00	0.42
1:A:219:HIS:CD2	1:A:220:PRO:HD2	2.54	0.42
1:A:271:ALA:O	1:A:275[B]:VAL:HG23	2.19	0.42
1:C:229:GLY:O	1:C:253:LEU:HA	2.18	0.42
1:B:199:ASP:N	5:B:1499:7PE:C12	2.77	0.42
1:B:199:ASP:O	5:B:1499:7PE:H142	2.20	0.42
1:A:47:GLU:OE1	1:A:219:HIS:HE1	2.03	0.42
1:A:153:ASN:OD1	2:A:1491:NDP:N7N	2.52	0.42
1:A:315:LEU:HD23	1:A:316:GLY:N	2.34	0.42
1:B:161:TRP:CZ3	4:B:1495:GOL:H12	2.54	0.42
1:B:475:ARG:H	1:B:475:ARG:HG3	1.62	0.42
1:B:286[A]:CYS:HB2	2:B:1491:NDP:H42N	2.01	0.42
1:A:340:TYR:O	1:A:343:SER:HB3	2.19	0.42
1:A:475:ARG:H	1:A:475:ARG:HG3	1.67	0.42
1:B:415:LEU:HD21	2:B:1491:NDP:N7N	2.34	0.42
1:D:425:ALA:O	1:D:429[B]:ARG:HB3	2.19	0.42
1:C:447:SER:N	4:C:1499:GOL:H2	2.13	0.42
1:A:153:ASN:CG	2:A:1491:NDP:N7N	2.78	0.42
1:B:228:THR:HG23	2:B:1491:NDP:C3N	2.50	0.42
1:D:286[A]:CYS:HB2	2:D:1491:NDP:H42N	2.02	0.41
1:D:454:GLY:CA	1:D:463:ARG:HD3	2.50	0.41
1:B:309:ARG:O	1:B:312:ARG:HG2	2.20	0.41
1:D:157:GLN:OE1	4:D:1495:GOL:H11	2.19	0.41
1:D:431:ILE:HG13	1:D:439:CYS:HB3	2.02	0.41
1:B:152:TRP:CD2	1:B:329:VAL:HG11	2.55	0.41
1:A:3:ARG:HD3	1:A:4:PHE:CZ	2.55	0.41
1:A:385:ARG:NH1	7:A:2165:HOH:O	2.54	0.41
1:B:126:GLU:OE2	1:D:124:GLU:OE1	2.39	0.41
1:C:417:ALA:O	1:C:439:CYS:HA	2.21	0.41
1:C:28:ASN:HA	1:C:29:PRO:HD3	1.96	0.41
1:B:143:LEU:O	1:B:223:GLU:HG3	2.21	0.41
1:B:219:HIS:HA	1:B:220:PRO:HD3	1.89	0.41
1:B:286[A]:CYS:SG	2:B:1491:NDP:C2D	3.08	0.41
1:D:309:ARG:O	1:D:312:ARG:HG2	2.21	0.41
1:A:235:LYS:HE3	1:A:458:GLN:OE1	2.20	0.41
1:B:15:TYR:CD1	4:B:1498:GOL:H31	2.55	0.41
1:B:315:LEU:C	1:B:315:LEU:HD23	2.46	0.41
1:C:280:PHE:CE2	5:C:1501:7PE:H141	2.55	0.41
1:A:207:GLY:HA3	1:A:212:VAL:HG11	2.02	0.41
1:B:94:THR:HG22	1:B:181:THR:HG21	2.03	0.41
1:B:217:THR:HG21	1:B:237:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLN:HE21	1:B:333:HIS:CD2	2.39	0.41
1:B:285:VAL:HB	1:B:288:ASN:CG	2.46	0.41
1:B:340:TYR:O	1:B:343:SER:HB3	2.21	0.41
1:C:127:GLN:C	1:C:128:ILE:HG13	2.45	0.41
1:C:295:HIS:HE1	1:C:399:ASP:O	2.02	0.41
1:A:106:ILE:HD12	1:A:106:ILE:N	2.36	0.40
1:B:426:ARG:HB2	1:B:429[B]:ARG:NH1	2.36	0.40
1:A:109:GLY:C	1:A:160:LEU:HD13	2.46	0.40
1:C:255:GLY:HA2	1:C:413:TYR:CD1	2.56	0.40
1:C:307[B]:LEU:CG	1:C:352:LEU:HD21	2.52	0.40
1:D:319:GLN:HE21	1:D:319:GLN:HA	1.85	0.40
1:D:463:ARG:HG2	1:D:463:ARG:HH11	1.86	0.40
1:A:213:GLY:O	1:A:217:THR:HG23	2.22	0.40
1:A:309:ARG:O	1:A:312:ARG:HG2	2.22	0.40
1:B:164:ALA:HB3	1:B:165:PRO:HD3	2.02	0.40
1:B:273:ILE:HG23	1:B:444:TRP:HB2	2.04	0.40
2:D:1491:NDP:C4N	7:D:2235:HOH:O	2.62	0.40
1:B:7:GLN:OE1	4:B:1497:GOL:H11	2.21	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	494/489 (101%)	482 (98%)	11 (2%)	1 (0%)	43	55
1	B	492/489 (101%)	477 (97%)	15 (3%)	0	100	100
1	C	491/489 (100%)	476 (97%)	15 (3%)	0	100	100
1	D	490/489 (100%)	478 (98%)	12 (2%)	0	100	100
All	All	1967/1956 (101%)	1913 (97%)	53 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	GLY

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	397/390 (102%)	386 (97%)	11 (3%)	38	56
1	B	395/390 (101%)	381 (96%)	14 (4%)	32	48
1	C	394/390 (101%)	382 (97%)	12 (3%)	36	53
1	D	393/390 (101%)	384 (98%)	9 (2%)	44	63
All	All	1579/1560 (101%)	1533 (97%)	46 (3%)	39	55

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	132	GLU
1	A	136	VAL
1	A	210	ARG
1	A	212	VAL
1	A	307[A]	LEU
1	A	307[B]	LEU
1	A	319	GLN
1	A	411	THR
1	A	431	ILE
1	A	475	ARG
1	B	40	ARG
1	B	98	LEU
1	B	132	GLU
1	B	136	VAL
1	B	211	GLU
1	B	212	VAL
1	B	214[A]	GLN
1	B	214[B]	GLN
1	B	307	LEU
1	B	319	GLN

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Mol	Chain	Res	Type
1	B	429[A]	ARG
1	B	429[B]	ARG
1	B	431	ILE
1	B	475	ARG
1	C	14	ARG
1	C	26	THR
1	C	43	ARG
1	C	44[A]	GLU
1	C	44[B]	GLU
1	C	98	LEU
1	C	136	VAL
1	C	212	VAL
1	C	319	GLN
1	C	385	ARG
1	C	431	ILE
1	C	475	ARG
1	D	3	ARG
1	D	98	LEU
1	D	132	GLU
1	D	136	VAL
1	D	212	VAL
1	D	319	GLN
1	D	356	GLU
1	D	431	ILE
1	D	475	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	127	GLN
1	A	157	GLN
1	A	219	HIS
1	A	284	GLN
1	A	295	HIS
1	A	319	GLN
1	B	127	GLN
1	B	219	HIS
1	B	284	GLN
1	B	295	HIS
1	B	319	GLN
1	C	127	GLN

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Mol	Chain	Res	Type
1	C	219	HIS
1	C	284	GLN
1	C	295	HIS
1	C	319	GLN
1	D	219	HIS
1	D	284	GLN
1	D	295	HIS
1	D	319	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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	7PE	A	1495	-	20,20,20	1.55	4 (20%)	19,19,19	1.56	5 (26%)
6	BME	A	1600	-	3,3,3	0.35	0	2,2,2	0.25	0
2	NDP	B	1491	-	51,52,52	2.85	16 (31%)	71,80,80	2.42	20 (28%)
4	GOL	C	1500	-	5,5,5	0.64	0	5,5,5	1.31	1 (20%)
4	GOL	B	1498	-	5,5,5	0.35	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	7PE	B	1500	-	7,7,20	0.32	0	6,6,19	0.32	0
4	GOL	A	1494	-	5,5,5	0.37	0	5,5,5	0.40	0
2	NDP	C	1491[A]	-	51,52,52	1.65	11 (21%)	71,80,80	2.00	12 (16%)
4	GOL	D	1494	-	5,5,5	0.31	0	5,5,5	0.28	0
5	7PE	A	1496	-	10,10,20	0.31	0	9,9,19	0.34	0
4	GOL	D	1496	-	5,5,5	1.33	0	5,5,5	2.47	4 (80%)
4	GOL	C	1496	-	5,5,5	0.35	0	5,5,5	0.29	0
4	GOL	B	1490	-	5,5,5	0.63	0	5,5,5	0.71	0
5	7PE	B	1499	-	15,15,20	1.94	2 (13%)	14,14,19	4.91	2 (14%)
6	BME	C	1600	1	3,3,3	0.33	0	2,2,2	0.21	0
4	GOL	C	1497	-	5,5,5	0.47	0	5,5,5	0.32	0
4	GOL	B	1495	-	5,5,5	0.28	0	5,5,5	0.61	0
4	GOL	C	1495	-	5,5,5	0.25	0	5,5,5	0.51	0
4	GOL	D	1497	-	5,5,5	0.39	0	5,5,5	0.69	0
2	NDP	D	1491	-	51,52,52	2.85	18 (35%)	71,80,80	2.42	20 (28%)
4	GOL	D	1495	-	5,5,5	0.33	0	5,5,5	0.31	0
4	GOL	C	1498	-	5,5,5	0.29	0	5,5,5	0.15	0
4	GOL	C	1499	-	5,5,5	0.46	0	5,5,5	1.40	1 (20%)
4	GOL	B	1497	-	5,5,5	0.50	0	5,5,5	0.62	0
4	GOL	B	1496	-	5,5,5	0.29	0	5,5,5	0.50	0
2	NDP	A	1491	-	51,52,52	1.50	6 (11%)	71,80,80	2.62	15 (21%)
5	7PE	C	1501	-	14,14,20	0.41	0	13,13,19	0.58	0
2	NDP	C	1491[B]	-	51,52,52	68.20	11 (21%)	71,80,80	4.09	18 (25%)

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	7PE	A	1495	-	-	11/18/18/18	-
6	BME	A	1600	-	-	1/1/1/1	-
2	NDP	B	1491	-	1/1/14/17	7/34/77/77	0/5/5/5
4	GOL	C	1500	-	-	2/4/4/4	-
4	GOL	B	1498	-	-	4/4/4/4	-
5	7PE	B	1500	-	-	4/5/5/18	-
4	GOL	A	1494	-	-	2/4/4/4	-
2	NDP	C	1491[A]	-	-	7/34/77/77	0/5/5/5
4	GOL	D	1494	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7PE	A	1496	-	-	2/8/8/18	-
4	GOL	D	1496	-	-	4/4/4/4	-
4	GOL	C	1496	-	-	0/4/4/4	-
4	GOL	B	1490	-	-	1/4/4/4	-
5	7PE	B	1499	-	-	6/13/13/18	-
6	BME	C	1600	1	-	0/1/1/1	-
4	GOL	C	1497	-	-	3/4/4/4	-
4	GOL	B	1495	-	-	4/4/4/4	-
4	GOL	C	1495	-	-	0/4/4/4	-
4	GOL	D	1497	-	-	2/4/4/4	-
2	NDP	D	1491	-	1/1/14/17	7/34/77/77	0/5/5/5
4	GOL	D	1495	-	-	2/4/4/4	-
4	GOL	C	1498	-	-	4/4/4/4	-
4	GOL	C	1499	-	-	2/4/4/4	-
4	GOL	B	1497	-	-	4/4/4/4	-
4	GOL	B	1496	-	-	3/4/4/4	-
2	NDP	A	1491	-	-	12/34/77/77	0/5/5/5
5	7PE	C	1501	-	-	6/12/12/18	-
2	NDP	C	1491[B]	-	-	16/34/77/77	0/5/5/5

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1491[B]	NDP	C1D-N1N	465.01	14.25	1.46
2	C	1491[B]	NDP	PN-O3	144.39	3.15	1.59
2	D	1491	NDP	PN-O3	-14.37	1.44	1.59
2	B	1491	NDP	PN-O3	-14.36	1.44	1.59
2	C	1491[A]	NDP	C2N-C3N	6.68	1.53	1.35
2	C	1491[B]	NDP	C2N-C3N	6.68	1.53	1.35
2	D	1491	NDP	C2N-C3N	6.64	1.53	1.35
2	B	1491	NDP	C2N-C3N	6.63	1.53	1.35
2	A	1491	NDP	C2N-C3N	6.62	1.53	1.35
5	B	1499	7PE	C6-C5	-5.67	1.19	1.49
2	C	1491[A]	NDP	C4N-C5N	-4.38	1.37	1.49
2	C	1491[B]	NDP	C4N-C5N	-4.38	1.37	1.49
5	B	1499	7PE	O7-C6	-4.18	1.24	1.42
2	B	1491	NDP	C5A-N7A	-3.86	1.32	1.39
2	D	1491	NDP	C5A-N7A	-3.85	1.32	1.39
2	B	1491	NDP	PN-O5D	-3.65	1.45	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1491	NDP	PN-O5D	-3.64	1.45	1.59
2	C	1491[A]	NDP	C4N-C3N	3.49	1.56	1.50
2	C	1491[B]	NDP	C4N-C3N	3.49	1.56	1.50
2	D	1491	NDP	C8A-N9A	-3.48	1.31	1.37
2	B	1491	NDP	C8A-N9A	-3.48	1.31	1.37
2	D	1491	NDP	C4A-N9A	-3.39	1.30	1.37
2	B	1491	NDP	C4A-N9A	-3.39	1.30	1.37
5	A	1495	7PE	C11-C12	-3.18	1.33	1.49
5	A	1495	7PE	C8-C9	-3.07	1.33	1.49
5	A	1495	7PE	C5-C6	-3.06	1.33	1.49
2	A	1491	NDP	C1D-N1N	-2.96	1.38	1.46
2	B	1491	NDP	P2B-O2B	-2.95	1.54	1.59
2	B	1491	NDP	O5D-C5D	2.94	1.55	1.44
2	D	1491	NDP	P2B-O2B	-2.94	1.54	1.59
2	D	1491	NDP	O5D-C5D	2.92	1.55	1.44
5	A	1495	7PE	C3-C2	-2.91	1.34	1.49
2	C	1491[A]	NDP	C3D-C4D	2.72	1.59	1.53
2	B	1491	NDP	C3D-C4D	2.71	1.59	1.53
2	A	1491	NDP	C3D-C4D	2.70	1.59	1.53
2	D	1491	NDP	C3D-C4D	2.69	1.59	1.53
2	B	1491	NDP	P2B-O3X	-2.66	1.44	1.54
2	D	1491	NDP	P2B-O3X	-2.66	1.44	1.54
2	D	1491	NDP	P2B-O2X	-2.64	1.45	1.54
2	B	1491	NDP	P2B-O2X	-2.63	1.45	1.54
2	D	1491	NDP	C4N-C3N	2.63	1.55	1.50
2	B	1491	NDP	C4N-C3N	2.60	1.54	1.50
2	A	1491	NDP	C4N-C3N	2.57	1.54	1.50
2	D	1491	NDP	PN-O2N	-2.47	1.43	1.55
2	B	1491	NDP	PN-O2N	-2.46	1.43	1.55
2	B	1491	NDP	P2B-O1X	-2.45	1.42	1.50
2	D	1491	NDP	P2B-O1X	-2.45	1.42	1.50
2	C	1491[A]	NDP	C8A-N7A	2.34	1.36	1.31
2	C	1491[B]	NDP	C8A-N7A	2.34	1.36	1.31
2	C	1491[A]	NDP	PA-O3	2.30	1.62	1.59
2	C	1491[B]	NDP	PA-O3	2.30	1.62	1.59
2	A	1491	NDP	C5A-N7A	-2.24	1.35	1.39
2	D	1491	NDP	PA-O3	-2.23	1.57	1.59
2	C	1491[A]	NDP	C1D-N1N	2.22	1.52	1.46
2	B	1491	NDP	PA-O3	-2.22	1.57	1.59
2	C	1491[A]	NDP	C5A-N7A	-2.21	1.35	1.39
2	C	1491[B]	NDP	C5A-N7A	-2.21	1.35	1.39
2	D	1491	NDP	C5A-C4A	-2.21	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1491	NDP	C5A-C4A	-2.18	1.35	1.39
2	A	1491	NDP	C8A-N7A	2.13	1.35	1.31
2	C	1491[B]	NDP	O4D-C4D	-2.06	1.40	1.45
2	C	1491[A]	NDP	C7N-C3N	2.05	1.53	1.48
2	C	1491[B]	NDP	C7N-C3N	2.05	1.53	1.48
2	C	1491[A]	NDP	C4A-N9A	-2.03	1.33	1.37
2	C	1491[B]	NDP	C4A-N9A	-2.03	1.33	1.37
2	C	1491[A]	NDP	PN-O3	2.02	1.61	1.59
2	D	1491	NDP	C4N-C5N	2.00	1.54	1.49
2	D	1491	NDP	C7N-C3N	2.00	1.53	1.48

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1491[B]	NDP	C2D-C1D-N1N	-23.11	56.47	113.31
5	B	1499	7PE	O7-C6-C5	14.79	175.30	110.11
2	A	1491	NDP	O4D-C1D-N1N	13.75	134.30	108.08
2	C	1491[B]	NDP	O4D-C1D-N1N	-13.54	82.26	108.08
2	C	1491[B]	NDP	O2N-PN-O3	-10.99	77.56	107.27
5	B	1499	7PE	O4-C5-C6	10.70	174.82	111.82
2	C	1491[A]	NDP	C2D-C1D-N1N	9.70	137.15	113.31
2	D	1491	NDP	C3N-C2N-N1N	-8.73	110.39	123.20
2	B	1491	NDP	C3N-C2N-N1N	-8.70	110.43	123.20
2	A	1491	NDP	C3N-C2N-N1N	-8.66	110.49	123.20
2	C	1491[B]	NDP	C1D-N1N-C6N	-8.64	102.51	120.77
2	C	1491[B]	NDP	O3-PN-O1N	-8.29	85.78	110.70
2	B	1491	NDP	C2D-C1D-N1N	7.64	132.10	113.31
2	D	1491	NDP	C2D-C1D-N1N	7.63	132.07	113.31
2	D	1491	NDP	O4D-C1D-N1N	7.05	121.53	108.08
2	B	1491	NDP	O4D-C1D-N1N	7.05	121.52	108.08
2	B	1491	NDP	C5A-C4A-N3A	-5.59	119.02	126.72
2	D	1491	NDP	C5A-C4A-N3A	-5.59	119.02	126.72
2	A	1491	NDP	C5A-C4A-N3A	-5.54	119.09	126.72
2	B	1491	NDP	O5D-C5D-C4D	-5.13	91.54	108.99
2	D	1491	NDP	O5D-C5D-C4D	-5.12	91.57	108.99
2	A	1491	NDP	N3A-C2A-N1A	-5.08	120.90	128.58
2	C	1491[A]	NDP	N3A-C2A-N1A	-5.07	120.91	128.58
2	C	1491[B]	NDP	N3A-C2A-N1A	-5.07	120.91	128.58
2	A	1491	NDP	C1D-N1N-C6N	-4.82	110.57	120.77
2	C	1491[A]	NDP	C5A-C4A-N3A	-4.80	120.11	126.72
2	C	1491[B]	NDP	C5A-C4A-N3A	-4.80	120.11	126.72
2	C	1491[B]	NDP	C1D-N1N-C2N	4.43	128.44	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1491	NDP	O4D-C4D-C5D	4.37	123.33	109.33
2	B	1491	NDP	N3A-C2A-N1A	-4.18	122.26	128.58
2	D	1491	NDP	N3A-C2A-N1A	-4.15	122.30	128.58
2	D	1491	NDP	C1D-N1N-C6N	-4.04	112.22	120.77
2	B	1491	NDP	C1D-N1N-C6N	-4.03	112.24	120.77
2	A	1491	NDP	N3A-C4A-N9A	3.78	133.59	127.17
2	C	1491[A]	NDP	N9A-C8A-N7A	-3.73	108.64	113.94
2	C	1491[B]	NDP	N9A-C8A-N7A	-3.73	108.64	113.94
2	C	1491[A]	NDP	O4D-C1D-N1N	3.68	115.10	108.08
2	A	1491	NDP	C2A-N3A-C4A	3.65	120.74	111.83
2	D	1491	NDP	N9A-C8A-N7A	-3.58	108.85	113.94
2	B	1491	NDP	N9A-C8A-N7A	-3.57	108.86	113.94
2	D	1491	NDP	C2A-N3A-C4A	3.55	120.50	111.83
4	D	1496	GOL	O1-C1-C2	3.55	126.34	110.38
2	B	1491	NDP	C2A-N3A-C4A	3.55	120.49	111.83
2	A	1491	NDP	N9A-C8A-N7A	-3.49	108.98	113.94
2	C	1491[A]	NDP	C2A-N3A-C4A	3.38	120.08	111.83
2	C	1491[B]	NDP	C2A-N3A-C4A	3.38	120.08	111.83
2	C	1491[B]	NDP	O4D-C4D-C5D	3.23	119.68	109.33
2	B	1491	NDP	C4A-C5A-N7A	-3.12	107.01	110.58
2	D	1491	NDP	N3A-C4A-N9A	3.10	132.44	127.17
2	D	1491	NDP	C4A-C5A-N7A	-3.09	107.05	110.58
2	B	1491	NDP	N3A-C4A-N9A	3.09	132.42	127.17
2	C	1491[A]	NDP	N3A-C4A-N9A	3.03	132.33	127.17
2	C	1491[B]	NDP	N3A-C4A-N9A	3.03	132.33	127.17
2	A	1491	NDP	C2D-C1D-N1N	-3.01	105.90	113.31
2	C	1491[A]	NDP	C6N-N1N-C2N	-2.98	116.13	119.32
2	C	1491[B]	NDP	C6N-N1N-C2N	-2.98	116.13	119.32
2	C	1491[A]	NDP	C4A-N9A-C8A	2.81	108.69	105.74
2	C	1491[B]	NDP	C4A-N9A-C8A	2.81	108.69	105.74
2	A	1491	NDP	C6N-N1N-C2N	-2.77	116.36	119.32
2	B	1491	NDP	C6N-N1N-C2N	-2.72	116.40	119.32
2	B	1491	NDP	C5A-N7A-C8A	2.68	107.67	103.45
2	D	1491	NDP	C5A-N7A-C8A	2.67	107.64	103.45
2	D	1491	NDP	C6N-N1N-C2N	-2.66	116.47	119.32
5	A	1495	7PE	O13-C12-C11	2.65	122.45	110.35
4	D	1496	GOL	O2-C2-C1	2.64	120.10	109.18
5	A	1495	7PE	O4-C5-C6	2.62	122.31	110.35
2	D	1491	NDP	O3X-P2B-O2X	2.62	117.63	107.80
2	A	1491	NDP	C4A-N9A-C8A	2.62	108.49	105.74
2	B	1491	NDP	O3X-P2B-O2X	2.61	117.59	107.80
2	D	1491	NDP	O3X-P2B-O2B	-2.58	95.81	105.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1491	NDP	O3X-P2B-O2B	-2.58	95.81	105.85
2	B	1491	NDP	C5A-C4A-N9A	2.52	108.56	105.81
2	A	1491	NDP	C5A-N7A-C8A	2.51	107.39	103.45
2	D	1491	NDP	C5A-C4A-N9A	2.50	108.53	105.81
2	C	1491[A]	NDP	C5A-N7A-C8A	2.48	107.34	103.45
2	C	1491[B]	NDP	C5A-N7A-C8A	2.48	107.34	103.45
2	C	1491[A]	NDP	C4A-C5A-N7A	-2.46	107.77	110.58
2	C	1491[B]	NDP	C4A-C5A-N7A	-2.46	107.77	110.58
2	A	1491	NDP	C4A-C5A-N7A	-2.41	107.82	110.58
5	A	1495	7PE	O4-C3-C2	2.40	120.68	110.11
4	D	1496	GOL	O3-C3-C2	2.35	120.95	110.38
2	D	1491	NDP	PN-O5D-C5D	2.33	134.72	121.35
2	B	1491	NDP	PN-O5D-C5D	2.33	134.72	121.35
4	C	1499	GOL	O1-C1-C2	2.32	120.82	110.38
4	C	1500	GOL	O2-C2-C3	-2.26	99.81	109.18
5	A	1495	7PE	O10-C9-C8	2.24	120.57	110.35
2	C	1491[B]	NDP	O2N-PN-O1N	2.24	122.86	112.44
4	D	1496	GOL	O2-C2-C3	-2.23	99.94	109.18
2	A	1491	NDP	C5D-C4D-C3D	2.20	123.12	115.21
5	A	1495	7PE	O7-C8-C9	2.18	120.27	110.35
2	C	1491[A]	NDP	C3N-C2N-N1N	-2.16	120.03	123.20
2	C	1491[B]	NDP	C3N-C2N-N1N	-2.16	120.03	123.20
2	D	1491	NDP	C4A-N9A-C8A	2.08	107.92	105.74
2	B	1491	NDP	C4A-N9A-C8A	2.05	107.89	105.74
2	B	1491	NDP	O4B-C1B-C2B	-2.03	103.09	106.59
2	B	1491	NDP	O4D-C4D-C5D	2.02	115.81	109.33
2	D	1491	NDP	O4B-C1B-C2B	-2.02	103.11	106.59
2	D	1491	NDP	O4D-C4D-C5D	2.02	115.80	109.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1491	NDP	C1D
2	D	1491	NDP	C1D

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1491	NDP	C5B-O5B-PA-O1A
2	A	1491	NDP	C5B-O5B-PA-O3
2	B	1491	NDP	C5D-O5D-PN-O3
2	B	1491	NDP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	B	1491	NDP	C5D-O5D-PN-O2N
2	B	1491	NDP	O4D-C1D-N1N-C2N
2	C	1491[A]	NDP	C5D-O5D-PN-O3
2	C	1491[A]	NDP	C5D-O5D-PN-O2N
2	C	1491[A]	NDP	O4D-C1D-N1N-C2N
2	C	1491[A]	NDP	C2N-C3N-C7N-N7N
2	C	1491[B]	NDP	PA-O3-PN-O5D
2	C	1491[B]	NDP	C5D-O5D-PN-O3
2	C	1491[B]	NDP	C5D-O5D-PN-O1N
2	C	1491[B]	NDP	C2N-C3N-C7N-N7N
2	D	1491	NDP	C5D-O5D-PN-O3
2	D	1491	NDP	C5D-O5D-PN-O1N
2	D	1491	NDP	C5D-O5D-PN-O2N
2	D	1491	NDP	O4D-C1D-N1N-C2N
4	A	1494	GOL	C1-C2-C3-O3
4	B	1497	GOL	C1-C2-C3-O3
4	B	1498	GOL	C1-C2-C3-O3
4	C	1499	GOL	C1-C2-C3-O3
4	C	1500	GOL	O1-C1-C2-C3
4	D	1496	GOL	O1-C1-C2-C3
4	D	1497	GOL	C1-C2-C3-O3
2	A	1491	NDP	C3D-C4D-C5D-O5D
2	C	1491[B]	NDP	O4D-C1D-N1N-C2N
5	A	1495	7PE	C15-C14-O13-C12
2	C	1491[B]	NDP	C2D-C1D-N1N-C6N
4	B	1497	GOL	O1-C1-C2-O2
4	D	1496	GOL	O1-C1-C2-O2
5	A	1495	7PE	O1-C2-C3-O4
5	B	1500	7PE	O16-C17-C18-O19
4	B	1490	GOL	C1-C2-C3-O3
4	B	1495	GOL	O1-C1-C2-C3
4	B	1495	GOL	C1-C2-C3-O3
4	B	1496	GOL	C1-C2-C3-O3
4	B	1497	GOL	O1-C1-C2-C3
4	B	1498	GOL	O1-C1-C2-C3
4	C	1497	GOL	O1-C1-C2-C3
4	C	1497	GOL	C1-C2-C3-O3
4	C	1498	GOL	O1-C1-C2-C3
4	C	1498	GOL	C1-C2-C3-O3
4	D	1496	GOL	C1-C2-C3-O3
2	C	1491[B]	NDP	C2D-C1D-N1N-C2N
4	A	1494	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	1495	GOL	O2-C2-C3-O3
4	C	1498	GOL	O1-C1-C2-O2
4	C	1499	GOL	O2-C2-C3-O3
4	C	1500	GOL	O1-C1-C2-O2
4	D	1496	GOL	O2-C2-C3-O3
5	B	1499	7PE	O16-C17-C18-O19
4	B	1497	GOL	O2-C2-C3-O3
4	B	1498	GOL	O2-C2-C3-O3
4	D	1497	GOL	O2-C2-C3-O3
5	C	1501	7PE	O13-C14-C15-O16
5	A	1496	7PE	C18-C17-O16-C15
4	B	1495	GOL	O1-C1-C2-O2
5	B	1499	7PE	O7-C8-C9-O10
2	B	1491	NDP	C4D-C5D-O5D-PN
2	D	1491	NDP	C4D-C5D-O5D-PN
4	D	1495	GOL	O1-C1-C2-O2
5	C	1501	7PE	C18-C17-O16-C15
5	A	1495	7PE	C14-C15-O16-C17
2	C	1491[B]	NDP	C3D-C4D-C5D-O5D
5	B	1500	7PE	C18-C17-O16-C15
5	C	1501	7PE	C17-C18-O19-C20
5	A	1496	7PE	C15-C14-O13-C12
2	A	1491	NDP	C2D-C1D-N1N-C6N
5	A	1495	7PE	C2-C3-O4-C5
5	B	1499	7PE	C15-C14-O13-C12
2	A	1491	NDP	C4D-C5D-O5D-PN
2	A	1491	NDP	C2B-C1B-N9A-C8A
2	B	1491	NDP	C2B-C1B-N9A-C8A
2	C	1491[A]	NDP	C2B-C1B-N9A-C8A
2	C	1491[B]	NDP	C2B-C1B-N9A-C8A
2	D	1491	NDP	C2B-C1B-N9A-C8A
2	C	1491[B]	NDP	PN-O3-PA-O1A
5	A	1495	7PE	O16-C17-C18-O19
2	A	1491	NDP	C4N-C3N-C7N-O7N
2	C	1491[B]	NDP	C5D-O5D-PN-O2N
2	C	1491[A]	NDP	C4D-C5D-O5D-PN
5	C	1501	7PE	O7-C8-C9-O10
2	A	1491	NDP	O4D-C1D-N1N-C6N
5	A	1495	7PE	C12-C11-O10-C9
5	B	1499	7PE	O13-C14-C15-O16
2	C	1491[B]	NDP	PN-O3-PA-O2A
2	B	1491	NDP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	D	1491	NDP	C2D-C1D-N1N-C2N
5	B	1499	7PE	C12-C11-O10-C9
5	B	1500	7PE	C15-C14-O13-C12
5	B	1499	7PE	C14-C15-O16-C17
4	B	1496	GOL	O1-C1-C2-C3
4	D	1495	GOL	O1-C1-C2-C3
2	C	1491[B]	NDP	O4D-C4D-C5D-O5D
5	A	1495	7PE	C18-C17-O16-C15
5	C	1501	7PE	C12-C11-O10-C9
4	C	1497	GOL	O2-C2-C3-O3
4	C	1498	GOL	O2-C2-C3-O3
2	A	1491	NDP	C2N-C3N-C7N-N7N
2	C	1491[B]	NDP	O4D-C1D-N1N-C6N
5	A	1495	7PE	C11-C12-O13-C14
4	B	1496	GOL	O2-C2-C3-O3
5	C	1501	7PE	C11-C12-O13-C14
6	A	1600	BME	O1-C1-C2-S2
2	C	1491[A]	NDP	O4B-C1B-N9A-C8A
2	C	1491[B]	NDP	O4B-C1B-N9A-C8A
5	A	1495	7PE	O7-C8-C9-O10
5	A	1495	7PE	O4-C5-C6-O7
5	A	1495	7PE	O10-C11-C12-O13
2	A	1491	NDP	O4B-C1B-N9A-C8A
2	A	1491	NDP	C2B-O2B-P2B-O1X
4	B	1498	GOL	O1-C1-C2-O2
5	B	1500	7PE	O13-C14-C15-O16
2	A	1491	NDP	PN-O3-PA-O2A
2	C	1491[B]	NDP	PA-O3-PN-O2N

There are no ring outliers.

23 monomers are involved in 127 short contacts:

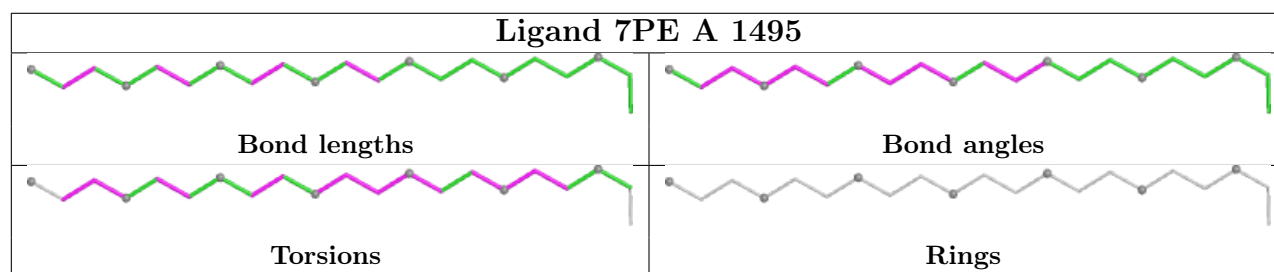
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1495	7PE	2	0
6	A	1600	BME	2	0
2	B	1491	NDP	18	0
4	B	1498	GOL	1	0
5	B	1500	7PE	1	0
4	A	1494	GOL	8	0
2	C	1491[A]	NDP	7	0
5	A	1496	7PE	14	0
4	B	1490	GOL	3	0

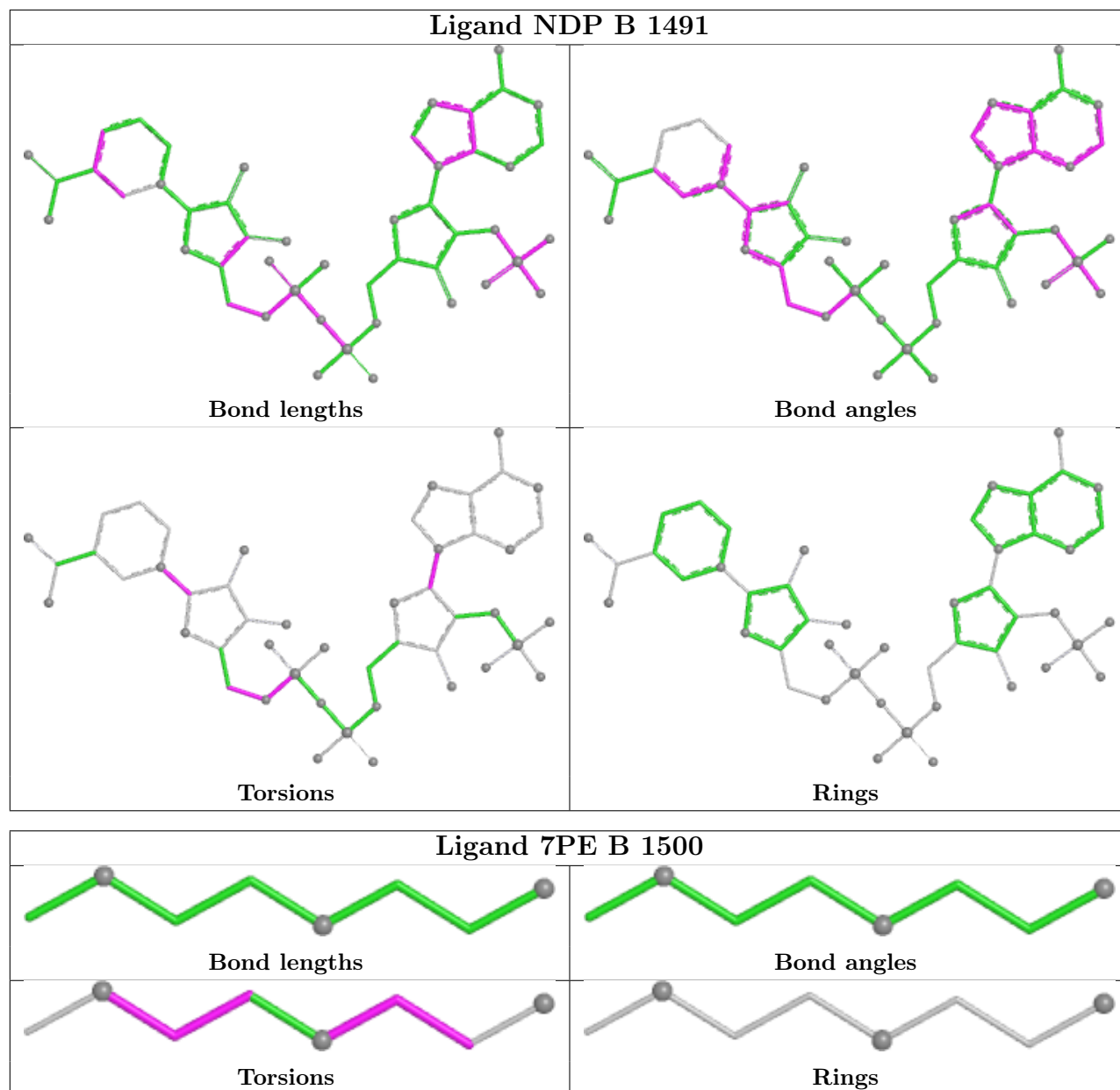
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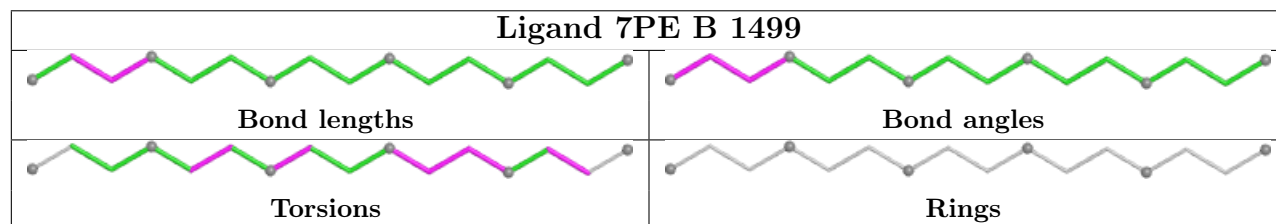
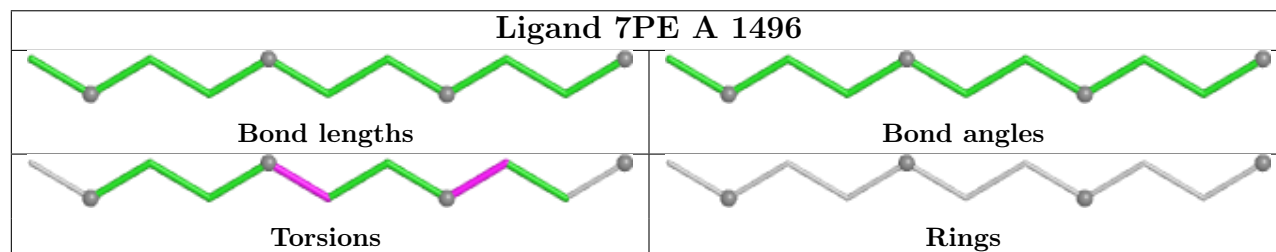
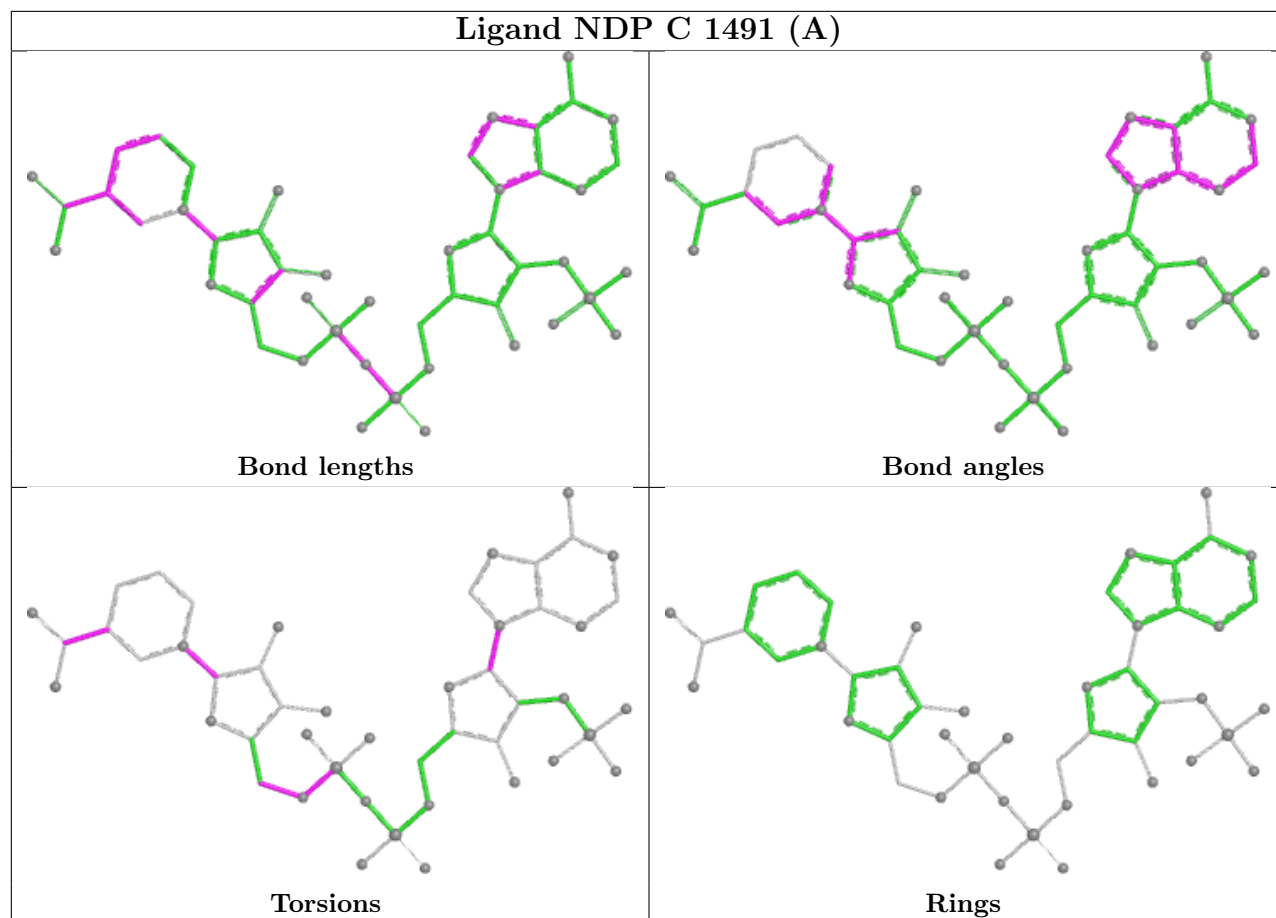
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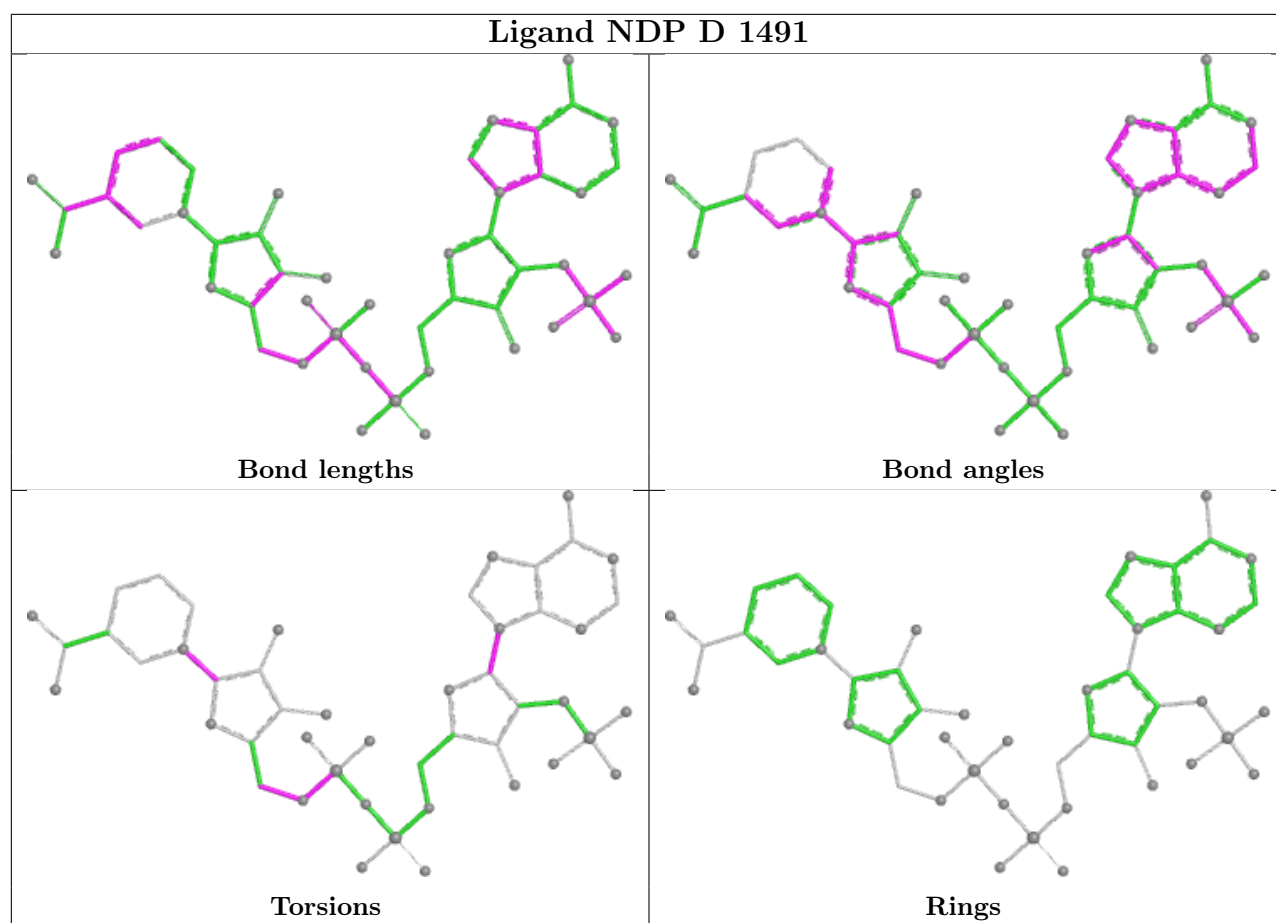
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1499	7PE	8	0
6	C	1600	BME	5	0
4	C	1497	GOL	4	0
4	B	1495	GOL	3	0
4	C	1495	GOL	2	0
4	D	1497	GOL	1	0
2	D	1491	NDP	15	0
4	D	1495	GOL	1	0
4	C	1499	GOL	4	0
4	B	1497	GOL	2	0
4	B	1496	GOL	6	0
2	A	1491	NDP	17	0
5	C	1501	7PE	12	0
2	C	1491[B]	NDP	2	0

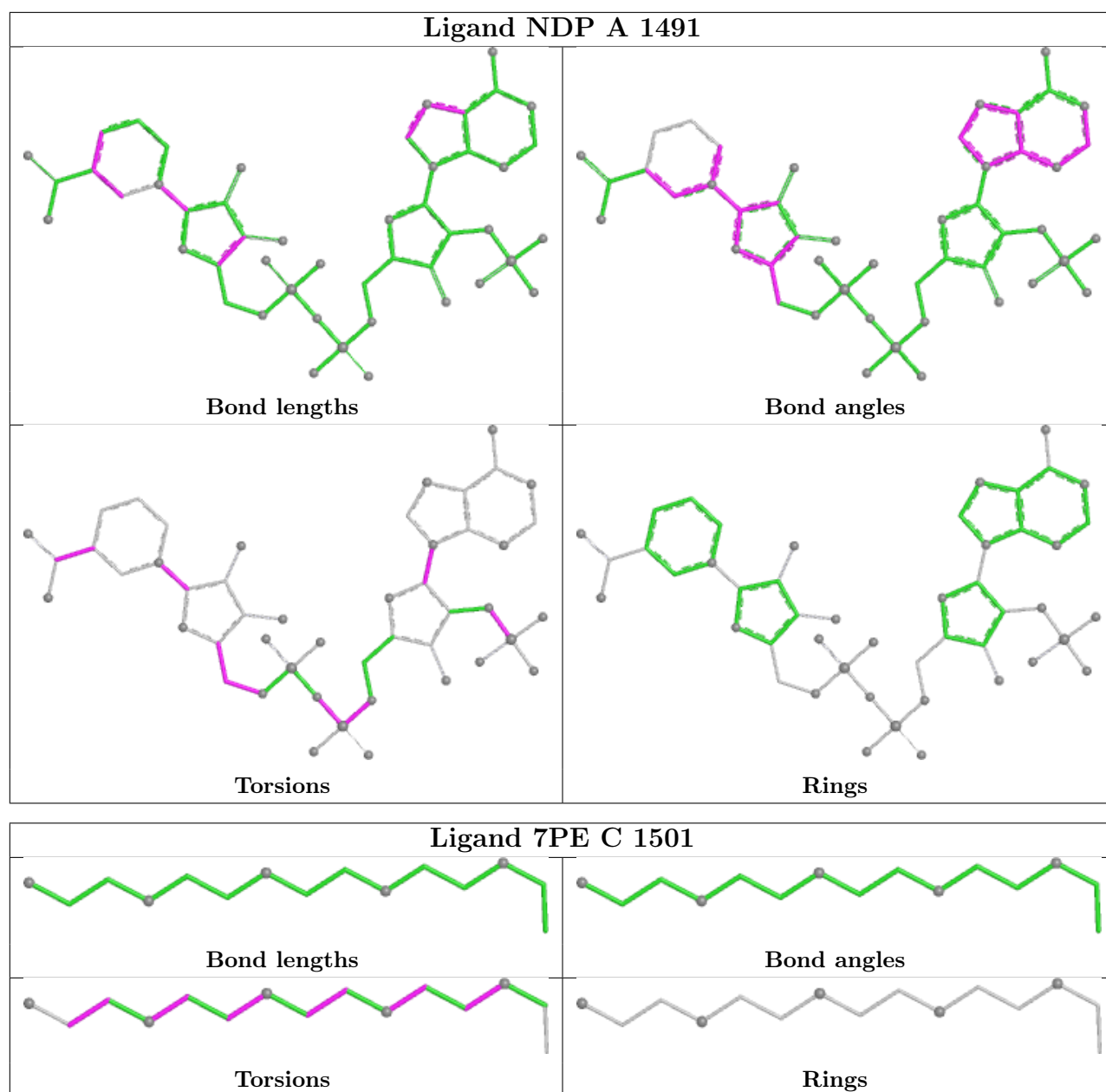
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

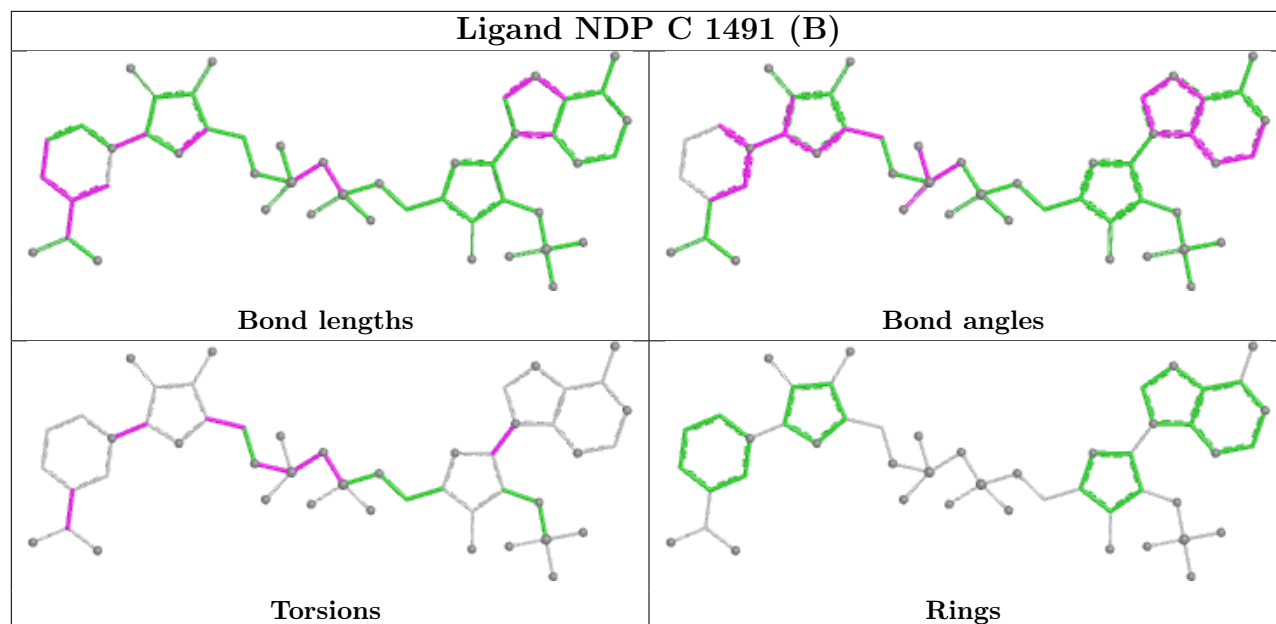












5.7 Other polymers [i](#)

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 [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	489/489 (100%)	-0.88	0 100 100	11, 45, 75, 102	7 (1%)
1	B	489/489 (100%)	-0.92	1 (0%) 91 91	17, 40, 72, 91	5 (1%)
1	C	489/489 (100%)	-1.13	0 100 100	16, 31, 51, 82	4 (0%)
1	D	489/489 (100%)	-0.88	2 (0%) 88 89	22, 42, 73, 93	3 (0%)
All	All	1956/1956 (100%)	-0.95	3 (0%) 91 91	11, 40, 71, 102	19 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	429[A]	ARG	7.5
1	B	429[A]	ARG	6.7
1	D	365	LYS	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](#)

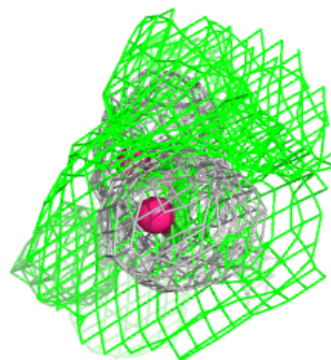
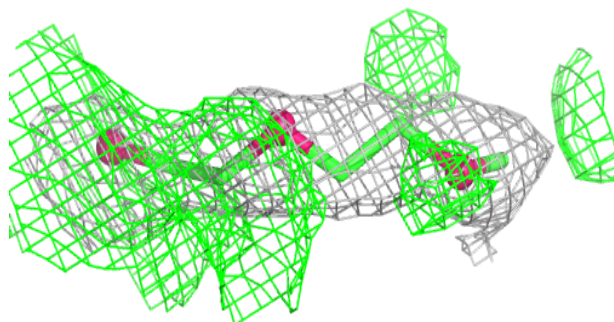
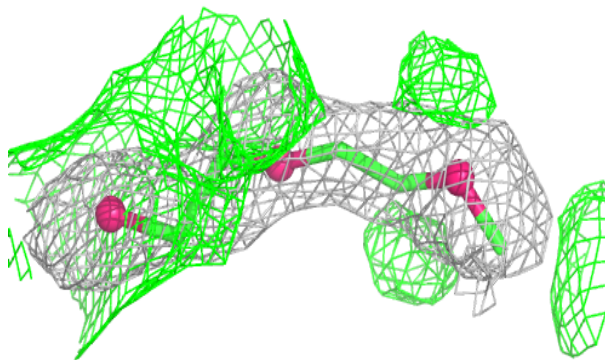
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
6	BME	A	1600	4/4	0.84	0.22	113,135,136,139	4
4	GOL	C	1498	6/6	0.85	0.19	56,83,100,102	0
6	BME	C	1600	4/4	0.85	0.26	107,107,108,116	4
4	GOL	B	1495	6/6	0.86	0.22	68,85,90,91	0
5	7PE	B	1500	8/21	0.86	0.25	35,57,60,77	8
5	7PE	A	1495	21/21	0.87	0.24	48,80,122,160	0
4	GOL	B	1490	6/6	0.88	0.16	74,90,102,105	0
4	GOL	D	1496	6/6	0.88	0.21	86,91,97,102	0
5	7PE	B	1499	16/21	0.89	0.22	31,77,144,213	0
4	GOL	C	1499	6/6	0.89	0.26	20,70,158,248	0
4	GOL	B	1496	6/6	0.90	0.21	61,82,117,166	0
4	GOL	C	1495	6/6	0.91	0.14	53,59,63,78	0
3	K	A	1493	1/1	0.92	0.13	75,75,75,75	0
4	GOL	B	1498	6/6	0.92	0.14	52,76,84,107	0
5	7PE	A	1496	11/21	0.92	0.17	48,67,126,167	0
4	GOL	A	1494	6/6	0.92	0.20	88,89,94,96	0
2	NDP	A	1491	48/48	0.92	0.16	28,78,160,189	48
2	NDP	D	1491	48/48	0.92	0.17	29,71,151,205	48
4	GOL	C	1500	6/6	0.92	0.15	60,69,82,88	0
4	GOL	C	1497	6/6	0.93	0.16	60,68,77,80	0
4	GOL	D	1497	6/6	0.93	0.11	49,63,78,85	0
3	K	B	1493	1/1	0.93	0.09	53,53,53,53	1
4	GOL	D	1495	6/6	0.93	0.14	51,84,102,116	0
2	NDP	C	1491[A]	48/48	0.94	0.18	20,55,145,171	48
5	7PE	C	1501	15/21	0.94	0.18	33,84,146,170	0
3	K	D	1493	1/1	0.94	0.07	56,56,56,56	1
2	NDP	C	1491[B]	48/48	0.94	0.18	20,50,138,169	48
4	GOL	C	1496	6/6	0.95	0.11	43,58,78,93	0
3	K	C	1493	1/1	0.96	0.08	53,53,53,53	0
4	GOL	D	1494	6/6	0.96	0.12	54,67,116,128	0
4	GOL	B	1497	6/6	0.96	0.09	41,43,65,72	0
3	K	A	1492	1/1	0.97	0.06	67,67,67,67	0
3	K	B	1501	1/1	0.97	0.08	60,60,60,60	0
2	NDP	B	1491	48/48	0.97	0.10	12,39,128,150	48
3	K	D	1492	1/1	0.97	0.06	59,59,59,59	0
3	K	C	1492	1/1	0.99	0.04	41,41,41,41	0

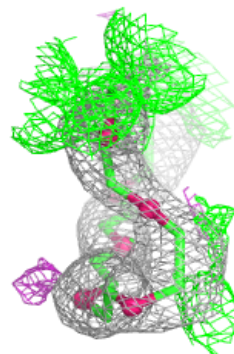
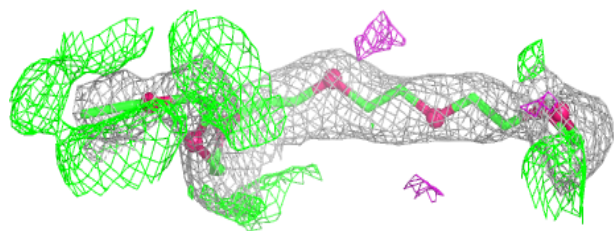
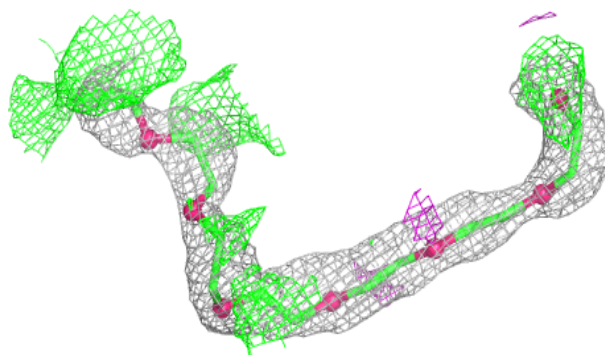
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 7PE B 1500:

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

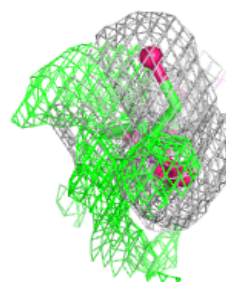
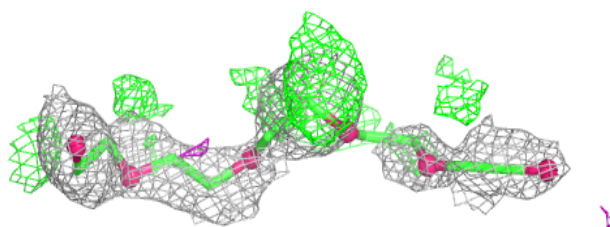
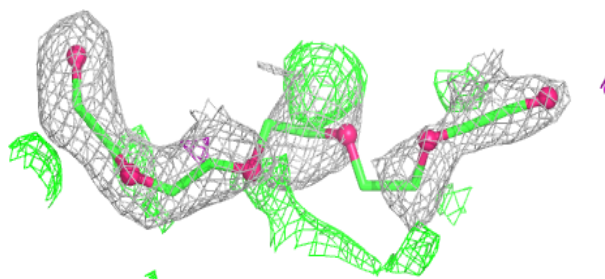
**Electron density around 7PE A 1495:**

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

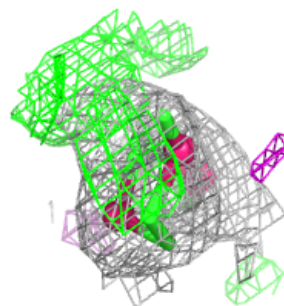
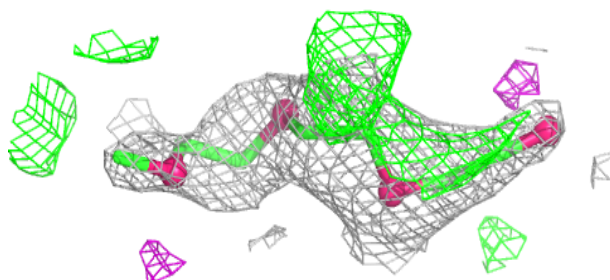
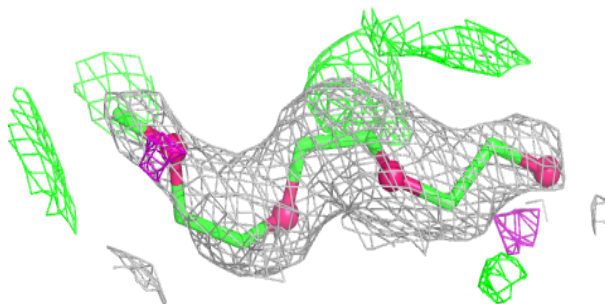


Electron density around 7PE B 1499:

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

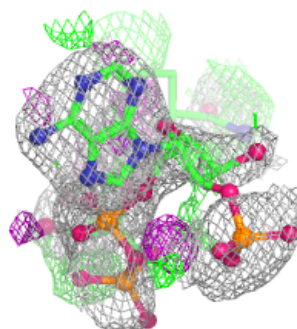
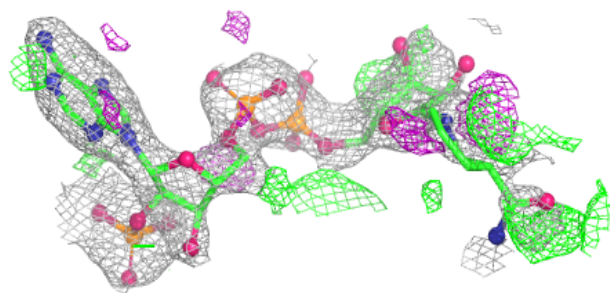
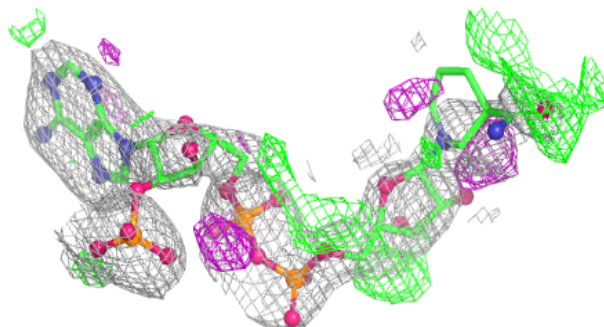
**Electron density around 7PE A 1496:**

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

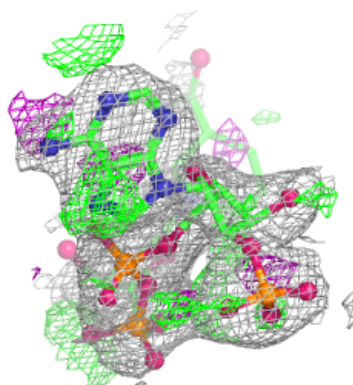
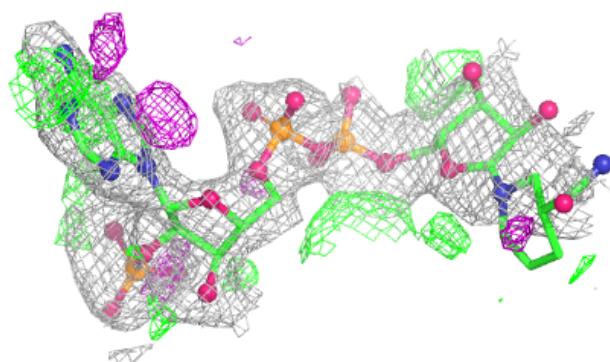
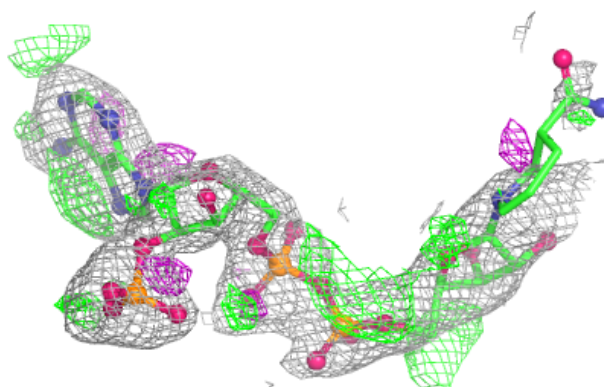


Electron density around NDP A 1491:

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

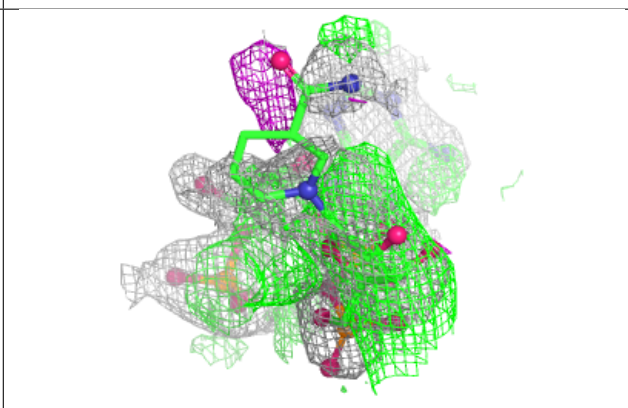
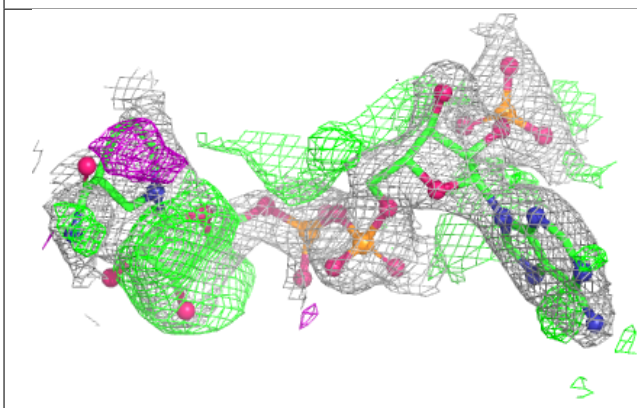
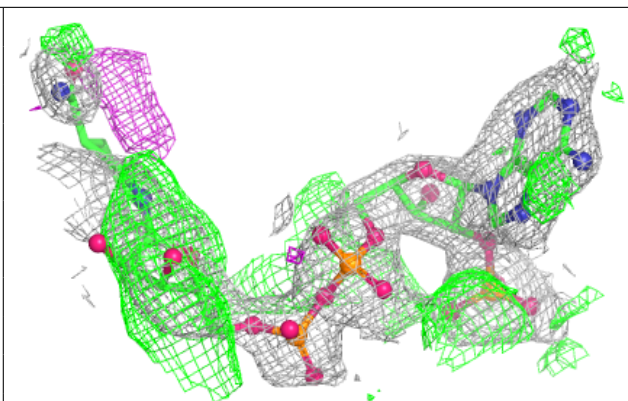
**Electron density around NDP D 1491:**

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

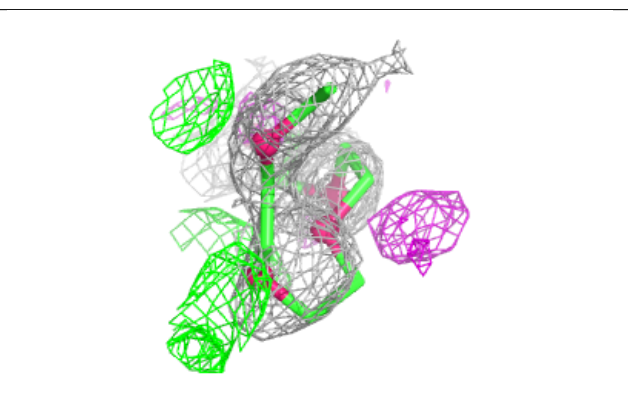
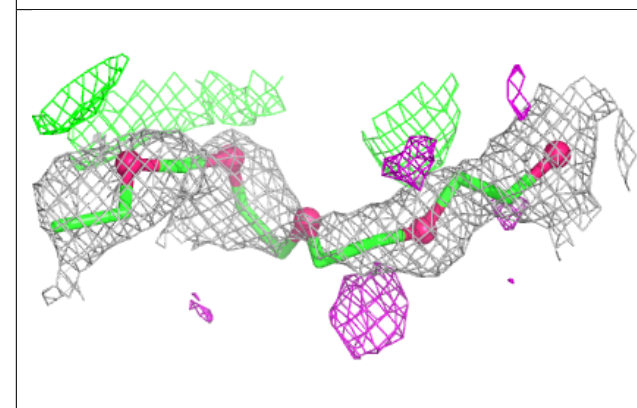
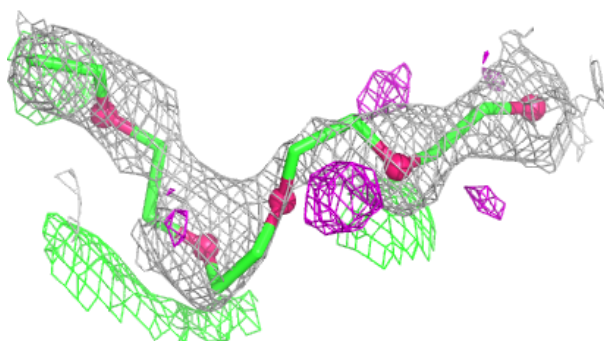


Electron density around NDP C 1491 (A):

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

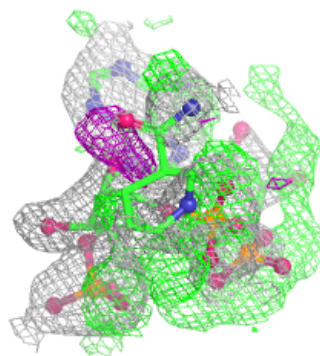
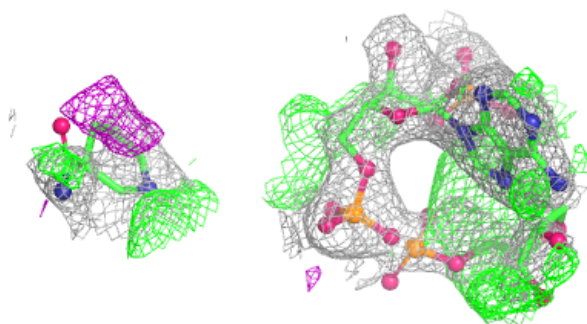
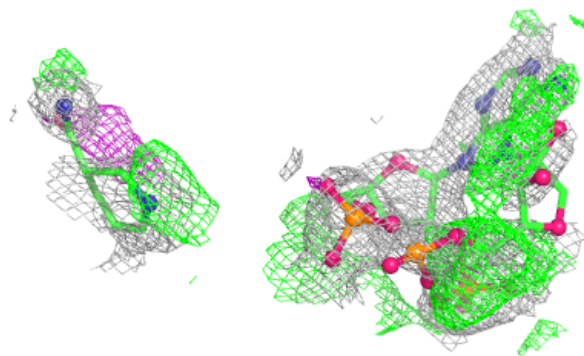
**Electron density around 7PE C 1501:**

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



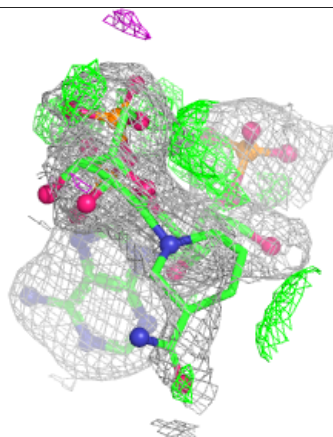
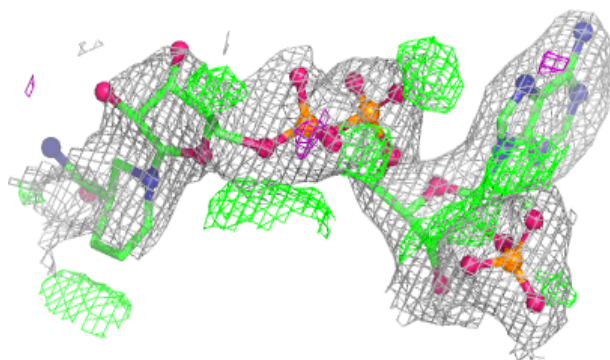
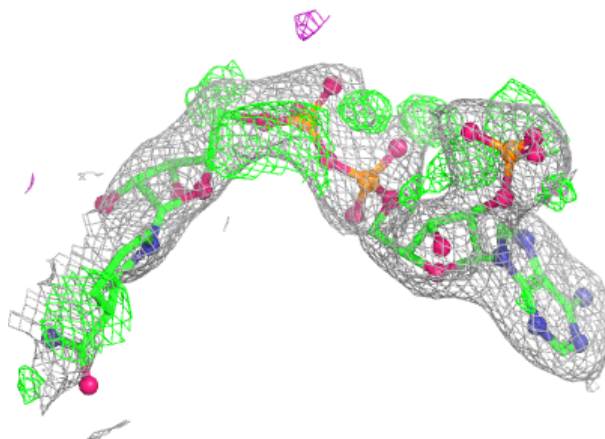
Electron density around NDP C 1491 (B):

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



Electron density around NDP B 1491:

$2mF_o - DF_c$ (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.