



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:41 am BST

PDB ID : 3ZQA
Title : CRYSTALLOGRAPHIC STRUCTURE OF BETAIN ALDEHYDE DEHYDROGENASE MUTANT C286A FROM PSEUDOMONAS AERUGINOSA IN COMPLEX WITH NADPH
Authors : Diaz-Sanchez, A.G.; Gonzalez-Segura, L.; Rudino-Pinera, E.; Lira-Rocha, A.; Torres-Larios, A.; Munoz-Clares, R.A.
Deposited on : 2011-06-08
Resolution : 2.45 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

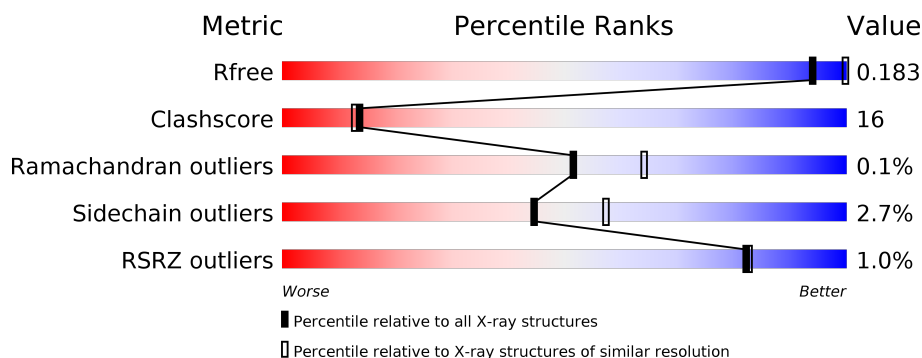
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 on 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	490	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>•</div> </div> </div>
1	B	490	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>•</div> </div> </div>
1	C	490	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>•</div> </div> </div>
1	D	490	<div> <div></div> <div> <div>80%</div> <div>19%</div> <div>•</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1491	-	-	X	X
2	GOL	A	1493	-	-	X	-
2	GOL	A	1499	-	-	X	-
2	GOL	B	1496	-	-	X	-
2	GOL	C	1492	-	-	X	-
2	GOL	D	1495	-	-	X	-
3	PG4	A	1495	-	-	X	-
4	EDO	A	1498	-	-	X	-
4	EDO	C	1497	-	-	X	X
6	K	B	1499	-	-	-	X
7	TOE	C	1496	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17530 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	8	0
			3801	2386	670	732	13			
1	B	489	Total	C	N	O	S	0	2	0
			3760	2361	661	725	13			
1	C	489	Total	C	N	O	S	0	2	0
			3751	2358	657	723	13			
1	D	489	Total	C	N	O	S	0	3	0
			3765	2364	664	724	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	CYS	engineered mutation	UNP Q9HTJ1
B	286	ALA	CYS	engineered mutation	UNP Q9HTJ1
C	286	ALA	CYS	engineered mutation	UNP Q9HTJ1
D	286	ALA	CYS	engineered mutation	UNP Q9HTJ1

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



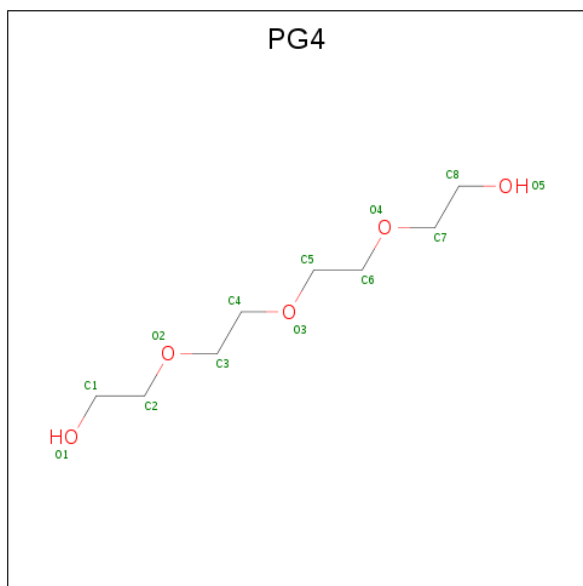
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total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

Continued on next page...

Continued from previous page...

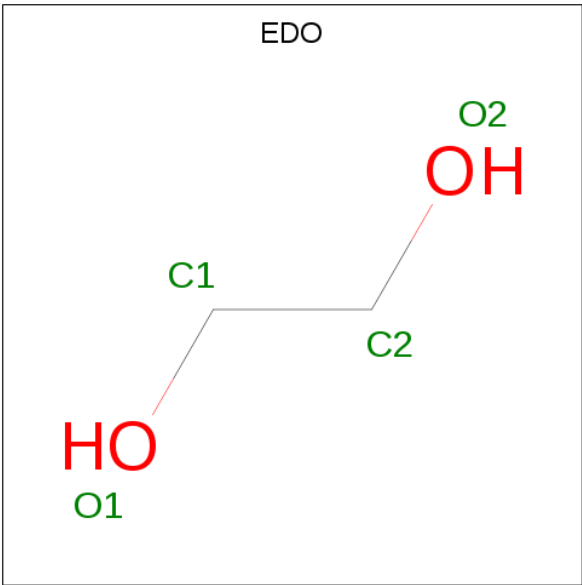
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



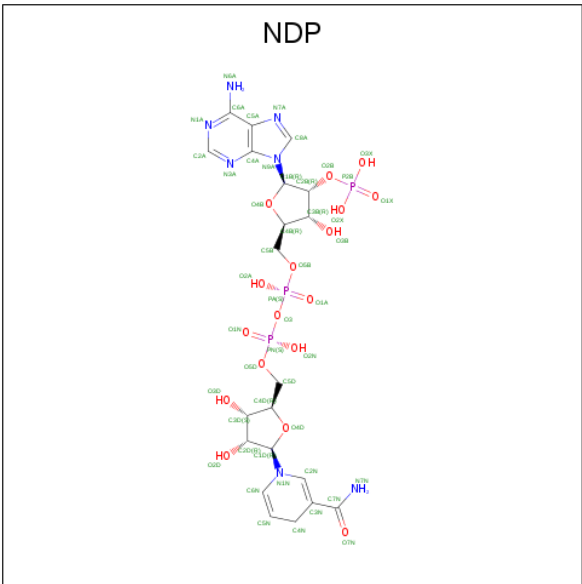
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			96	42	14	34	6		

Continued on next page...

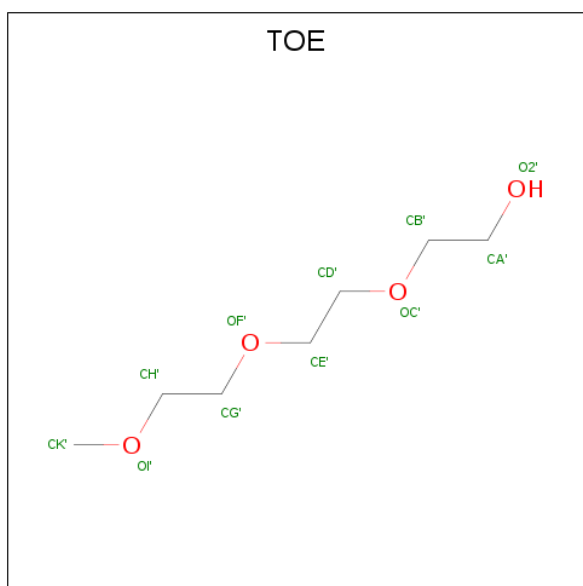
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	1
			96	42	14	34	6		
5	C	1	Total	C	N	O	P	0	1
			96	42	14	34	6		
5	D	1	Total	C	N	O	P	0	1
			96	42	14	34	6		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 7 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (three-letter code: TOE) (formula: C₇H₁₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	7	4		

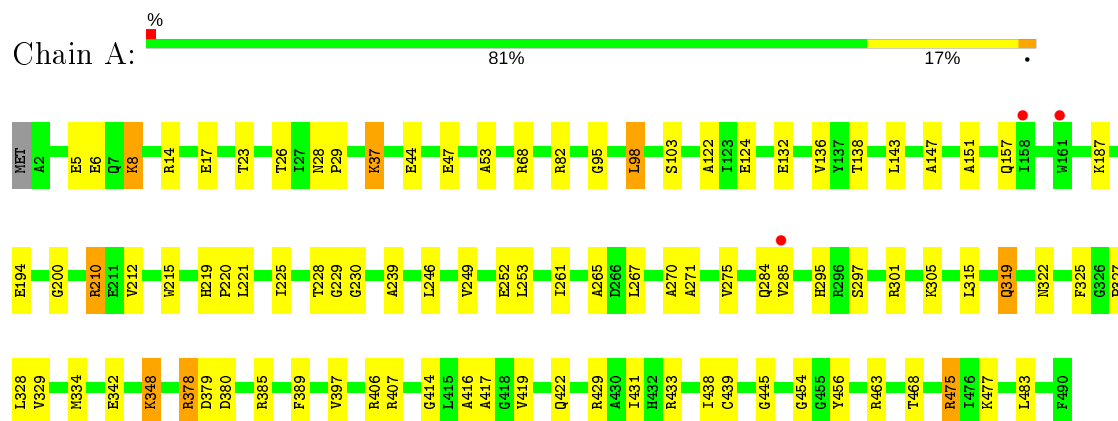
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	649	Total 649	O 649	0	0
8	B	421	Total 421	O 421	0	0
8	C	410	Total 410	O 410	0	0
8	D	411	Total 411	O 411	0	0

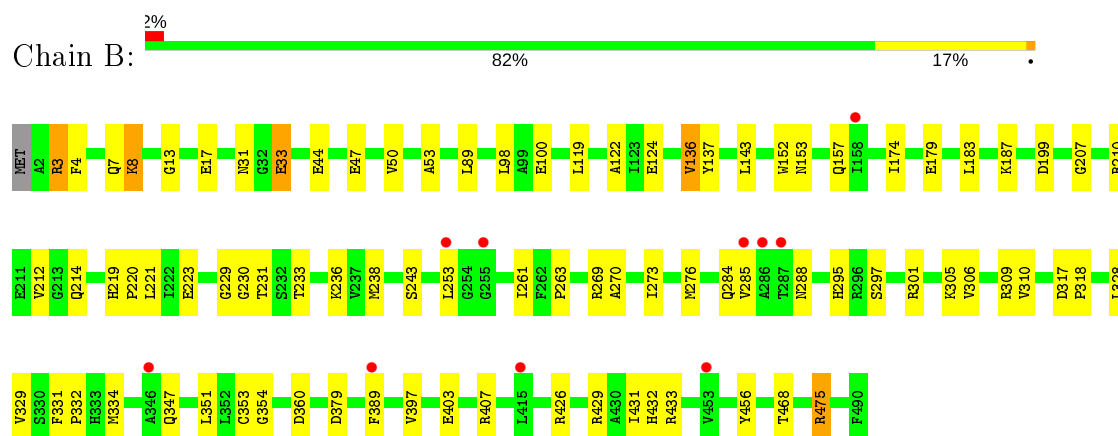
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

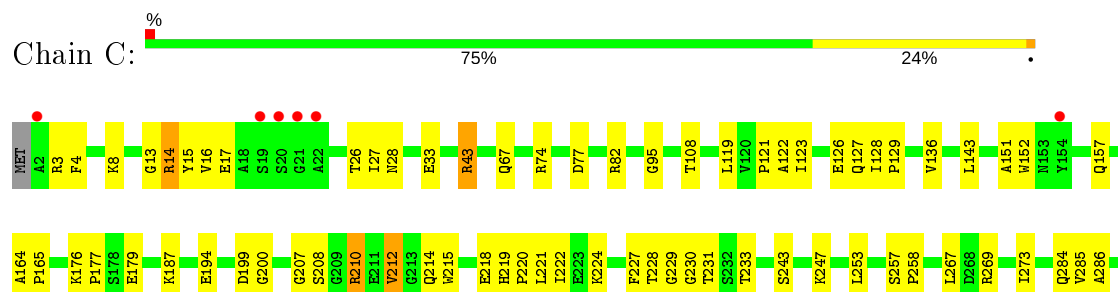
• Molecule 1: BETAINES ALDEHYDE DEHYDROGENASE

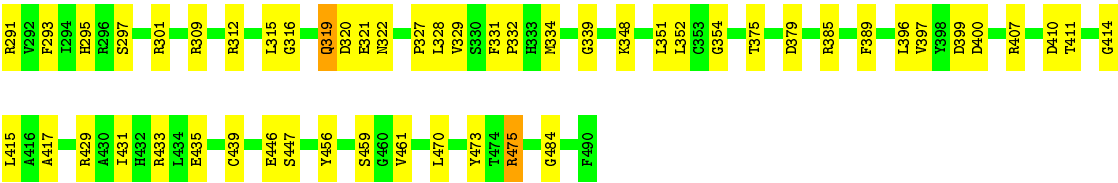


• Molecule 1: BETAINES ALDEHYDE DEHYDROGENASE

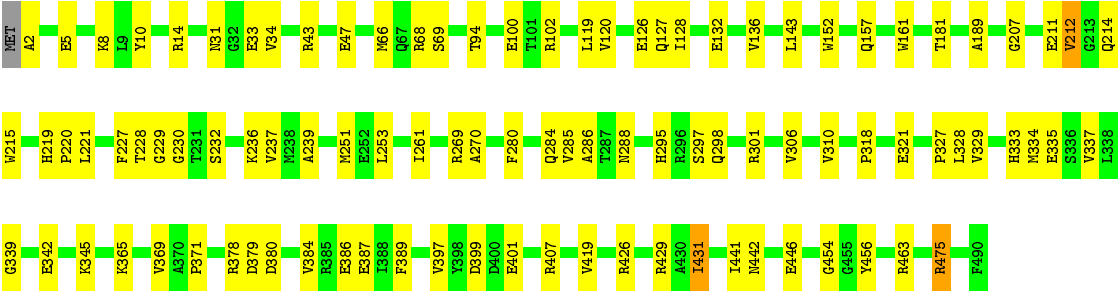
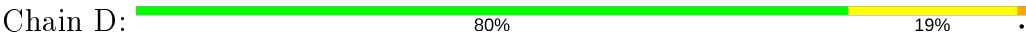


• Molecule 1: BETAINES ALDEHYDE DEHYDROGENASE





• 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	151.44Å 151.44Å 241.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.52 – 2.45 38.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.52-2.45) 99.9 (38.52-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.155 , 0.191 0.145 , 0.183	Depositor DCC
R_{free} test set	7150 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17530	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: GOL, K, EDO, PG4, NDP, TOE

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	0.52	0/3878	0.59	0/5253
1	B	0.40	0/3831	0.53	0/5191
1	C	0.41	0/3825	0.55	0/5184
1	D	0.42	0/3839	0.55	0/5201
All	All	0.44	0/15373	0.55	0/20829

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3801	0	3781	87	0
1	B	3760	0	3733	86	0
1	C	3751	0	3732	129	0
1	D	3765	0	3746	95	0
2	A	42	0	56	23	0
2	B	42	0	56	22	0
2	C	24	0	32	10	0
2	D	30	0	40	13	0
3	A	13	0	18	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	6	16	0
4	C	4	0	6	9	0
5	A	96	0	52	23	0
5	B	96	0	52	16	0
5	C	96	0	52	19	0
5	D	96	0	52	15	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	C	11	0	16	23	0
8	A	649	0	0	57	1
8	B	421	0	0	40	0
8	C	410	0	0	56	0
8	D	411	0	0	37	0
All	All	17530	0	15430	494	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (494) 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)
3:A:1495:PG4:H31	4:A:1498:EDO:C1	1.44	1.44
2:B:1494:GOL:H11	8:B:2012:HOH:O	1.32	1.29
3:A:1495:PG4:H41	4:A:1498:EDO:O2	1.18	1.28
1:C:322:ASN:HB3	8:C:2280:HOH:O	1.23	1.27
3:A:1495:PG4:C3	4:A:1498:EDO:H12	1.64	1.26
1:D:5:GLU:HB3	8:D:2010:HOH:O	1.36	1.22
3:A:1495:PG4:H82	8:A:2646:HOH:O	1.37	1.22
2:A:1491:GOL:H11	5:A:1500[A]:NDP:O2D	1.35	1.21
2:A:1491:GOL:C1	5:A:1500[A]:NDP:O2D	1.88	1.19
2:D:1493:GOL:O2	8:D:2290:HOH:O	1.65	1.15
5:A:1500[A]:NDP:H51N	8:A:2648:HOH:O	1.45	1.15
3:A:1495:PG4:H11	8:A:2346:HOH:O	1.47	1.14
3:A:1495:PG4:H12	2:A:1499:GOL:C3	1.79	1.13
1:B:301:ARG:HG3	8:B:2333:HOH:O	1.49	1.13
3:A:1495:PG4:C4	4:A:1498:EDO:O2	1.96	1.13
3:A:1495:PG4:H12	2:A:1499:GOL:H32	1.18	1.10
2:D:1495:GOL:O1	5:D:1496[A]:NDP:N6A	1.82	1.09
5:A:1500[A]:NDP:H3D	8:A:2496:HOH:O	1.52	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33[A]:GLU:OE1	8:B:2082:HOH:O	1.71	1.06
7:C:1496:TOE:H5	4:C:1497:EDO:H12	1.07	1.04
1:C:157:GLN:OE1	7:C:1496:TOE:CA'	2.07	1.01
2:A:1491:GOL:C1	5:A:1500[A]:NDP:HO2N	1.68	1.00
1:A:348:LYS:HE3	8:A:2510:HOH:O	1.61	0.99
7:C:1496:TOE:CB'	4:C:1497:EDO:H12	1.92	0.99
7:C:1496:TOE:H5	4:C:1497:EDO:C1	1.94	0.98
1:A:429[B]:ARG:HD2	8:A:2587:HOH:O	1.63	0.96
3:A:1495:PG4:H31	4:A:1498:EDO:C2	1.96	0.95
1:A:468:THR:HG23	8:A:2625:HOH:O	1.67	0.95
7:C:1496:TOE:H15	8:C:2410:HOH:O	1.67	0.94
2:D:1491:GOL:H31	8:D:2256:HOH:O	1.67	0.94
5:D:1496[B]:NDP:N7N	8:D:2290:HOH:O	2.00	0.94
1:C:157:GLN:OE1	7:C:1496:TOE:H3	1.66	0.93
1:C:187:LYS:HE2	8:C:2016:HOH:O	1.70	0.91
3:A:1495:PG4:H51	8:A:2343:HOH:O	1.69	0.91
1:C:352:LEU:HB2	8:C:2309:HOH:O	1.69	0.91
1:C:301:ARG:HG3	8:C:2271:HOH:O	1.72	0.89
5:A:1500[A]:NDP:H5N	8:A:2341:HOH:O	1.73	0.88
1:D:236:LYS:HD3	8:D:2168:HOH:O	1.73	0.86
1:A:445:GLY:HA3	2:A:1492:GOL:H11	1.57	0.86
7:C:1496:TOE:CK'	8:C:2410:HOH:O	2.19	0.86
4:A:1498:EDO:H21	2:A:1499:GOL:H31	1.57	0.85
1:C:301:ARG:CG	8:C:2271:HOH:O	2.24	0.85
1:C:219:HIS:HD2	1:C:221:LEU:H	1.21	0.85
3:A:1495:PG4:C3	4:A:1498:EDO:C1	2.34	0.85
1:D:301:ARG:NH1	8:D:2309:HOH:O	2.10	0.85
1:A:228:THR:CG2	5:A:1500[B]:NDP:H41N	2.07	0.84
8:A:2413:HOH:O	1:B:238:MET:CE	2.24	0.84
1:A:261:ILE:HD12	1:A:270:ALA:HB1	1.59	0.84
1:B:89:LEU:HD22	8:B:2080:HOH:O	1.76	0.84
5:B:1498[B]:NDP:N7N	8:B:2309:HOH:O	1.58	0.84
2:D:1494:GOL:C1	8:D:2256:HOH:O	2.26	0.83
1:D:219:HIS:HD2	1:D:221:LEU:H	1.24	0.83
1:A:468:THR:CG2	8:A:2625:HOH:O	2.23	0.83
3:A:1495:PG4:H31	4:A:1498:EDO:H12	0.83	0.83
1:A:301:ARG:NH1	8:A:2452:HOH:O	2.11	0.82
2:C:1492:GOL:O1	7:C:1496:TOE:H4	1.79	0.82
1:C:431:ILE:HD12	1:C:439:CYS:HB3	1.61	0.81
1:D:236:LYS:CD	8:D:2168:HOH:O	2.26	0.81
1:C:151:ALA:HA	8:C:2176:HOH:O	1.78	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2324:HOH:O	1:B:432:HIS:ND1	2.13	0.81
1:B:219:HIS:HD2	1:B:221:LEU:H	1.29	0.80
1:B:89:LEU:CD2	8:B:2080:HOH:O	2.31	0.79
5:C:1495[B]:NDP:N7N	8:C:2237:HOH:O	1.82	0.79
1:A:219:HIS:HD2	1:A:221:LEU:H	1.29	0.79
1:C:352:LEU:HD13	8:C:2309:HOH:O	1.83	0.79
1:C:74:ARG:NH1	8:C:2099:HOH:O	2.08	0.78
1:A:284:GLN:HE22	1:A:329:VAL:H	1.28	0.78
2:B:1495:GOL:O2	8:B:2309:HOH:O	2.03	0.77
2:B:1494:GOL:C1	8:B:2012:HOH:O	2.03	0.77
1:A:82:ARG:NH2	8:A:2218:HOH:O	2.16	0.77
1:C:219:HIS:CD2	1:C:221:LEU:H	2.01	0.77
1:B:7:GLN:NE2	8:B:2018:HOH:O	2.06	0.76
1:D:426:ARG:NH2	8:D:2377:HOH:O	2.18	0.76
1:A:215:TRP:CD1	8:A:2384:HOH:O	2.38	0.76
1:C:210:ARG:CG	8:C:2208:HOH:O	2.33	0.76
2:B:1496:GOL:H2	5:B:1498[B]:NDP:N7A	2.01	0.76
1:C:143:LEU:HD23	1:C:475:ARG:HG2	1.67	0.76
2:B:1496:GOL:H2	5:B:1498[A]:NDP:N7A	2.01	0.76
5:A:1500[A]:NDP:C5D	8:A:2648:HOH:O	2.12	0.75
1:A:249:VAL:O	8:A:2397:HOH:O	2.03	0.75
1:A:322[A]:ASN:ND2	8:A:2487:HOH:O	2.19	0.75
2:A:1499:GOL:H2	5:A:1500[B]:NDP:O7N	1.86	0.75
1:A:228:THR:HG21	5:A:1500[B]:NDP:H41N	1.68	0.75
2:C:1492:GOL:C1	8:C:2373:HOH:O	2.33	0.75
5:A:1500[A]:NDP:O2N	8:A:2650:HOH:O	2.05	0.74
1:A:348:LYS:CE	8:A:2510:HOH:O	2.25	0.74
8:A:2636:HOH:O	2:B:1491:GOL:H11	1.87	0.74
1:C:285:VAL:HG13	4:C:1497:EDO:H11	1.67	0.74
2:D:1495:GOL:O1	5:D:1496[B]:NDP:N6A	1.84	0.74
5:B:1498[A]:NDP:O3D	8:B:2364:HOH:O	2.02	0.73
8:A:2413:HOH:O	1:B:238:MET:HE3	1.83	0.73
1:C:461:VAL:HA	8:C:2378:HOH:O	1.88	0.73
1:D:298:GLN:OE1	8:D:2296:HOH:O	2.06	0.73
1:B:347:GLN:OE1	8:B:2349:HOH:O	2.05	0.73
1:B:157:GLN:OE1	2:B:1492:GOL:H12	1.89	0.73
1:C:233:THR:OG1	8:C:2228:HOH:O	2.06	0.73
2:A:1491:GOL:H12	5:A:1500[A]:NDP:O2D	1.89	0.73
1:A:378:ARG:NH2	8:A:2512:HOH:O	2.22	0.73
1:C:295:HIS:HD2	1:C:297:SER:OG	1.72	0.73
1:D:284:GLN:HE22	1:D:329:VAL:H	1.36	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ASP:OD2	1:D:407:ARG:HD2	1.89	0.72
1:A:14:ARG:HD2	8:A:2037:HOH:O	1.90	0.71
1:D:68:ARG:NH1	8:D:2136:HOH:O	2.19	0.71
3:A:1495:PG4:C3	4:A:1498:EDO:O2	2.38	0.71
1:C:475:ARG:HD3	1:D:456:TYR:CZ	2.26	0.71
3:A:1495:PG4:H41	4:A:1498:EDO:HO2	1.56	0.70
8:A:2322:HOH:O	1:C:129:PRO:HB3	1.90	0.70
1:C:352:LEU:CB	8:C:2309:HOH:O	2.34	0.70
1:B:379:ASP:OD2	1:B:407:ARG:HD2	1.91	0.70
2:C:1492:GOL:H12	8:C:2373:HOH:O	1.90	0.70
1:C:27:ILE:HG22	1:C:28:ASN:N	2.06	0.70
1:D:161:TRP:CE3	8:D:2245:HOH:O	2.44	0.70
1:B:179:GLU:OE1	8:B:2262:HOH:O	2.10	0.69
1:C:415:LEU:HB2	1:C:459[B]:SER:OG	1.92	0.69
1:C:228:THR:CG2	5:C:1495[B]:NDP:H41N	2.23	0.69
3:A:1495:PG4:H21	4:A:1498:EDO:H12	1.75	0.69
5:C:1495[A]:NDP:O3D	8:C:2329:HOH:O	2.10	0.69
1:D:228:THR:CG2	5:D:1496[B]:NDP:H41N	2.22	0.69
1:D:236:LYS:HE2	2:D:1495:GOL:H11	1.75	0.69
1:C:157:GLN:OE1	7:C:1496:TOE:H2	1.89	0.68
4:A:1498:EDO:C2	2:A:1499:GOL:H31	2.24	0.68
5:A:1500[A]:NDP:C5N	8:A:2341:HOH:O	2.34	0.68
2:A:1493:GOL:O1	8:A:2013:HOH:O	2.11	0.68
1:A:215:TRP:NE1	8:A:2384:HOH:O	2.27	0.68
2:C:1492:GOL:HO1	7:C:1496:TOE:H4	1.58	0.68
5:A:1500[A]:NDP:C5D	8:A:2496:HOH:O	2.42	0.67
5:A:1500[A]:NDP:H52N	8:A:2496:HOH:O	1.95	0.67
1:C:400:ASP:HB3	8:C:2334:HOH:O	1.93	0.67
1:C:219:HIS:CD2	1:C:221:LEU:HB2	2.30	0.67
1:C:352:LEU:CD1	8:C:2309:HOH:O	2.40	0.67
1:D:378:ARG:NH1	1:D:380:ASP:OD1	2.26	0.67
1:A:157:GLN:HE22	3:A:1495:PG4:H61	1.60	0.66
1:A:422:GLN:HG2	2:A:1496:GOL:H12	1.77	0.66
1:C:187:LYS:NZ	2:C:1491:GOL:H12	2.10	0.66
1:C:15:TYR:OH	8:C:2015:HOH:O	2.09	0.65
1:D:345:LYS:HD2	8:D:2338:HOH:O	1.96	0.65
1:D:31:ASN:OD1	1:D:33:GLU:HB2	1.97	0.65
1:C:187:LYS:HZ3	2:C:1491:GOL:H12	1.61	0.65
1:B:219:HIS:CD2	1:B:221:LEU:H	2.14	0.65
1:A:265:ALA:O	8:A:2428:HOH:O	2.15	0.65
1:D:219:HIS:CD2	1:D:221:LEU:H	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLU:OE2	8:B:2192:HOH:O	2.13	0.65
1:C:229:GLY:O	5:C:1495[B]:NDP:H1D	1.96	0.64
1:B:263:PRO:HD2	8:B:2316:HOH:O	1.96	0.64
1:D:47:GLU:OE1	1:D:219:HIS:HE1	1.78	0.64
2:B:1496:GOL:H2	5:B:1498[B]:NDP:C8A	2.28	0.64
1:D:215:TRP:HD1	8:D:2105:HOH:O	1.78	0.64
2:D:1494:GOL:H12	8:D:2256:HOH:O	1.95	0.63
1:B:47:GLU:OE1	1:B:219:HIS:HE1	1.81	0.63
1:A:103[B]:SER:OG	8:A:2254:HOH:O	2.15	0.63
1:D:232:SER:HB3	8:D:2279:HOH:O	1.98	0.62
1:D:43:ARG:NH2	8:D:2105:HOH:O	2.31	0.62
3:A:1495:PG4:C1	8:A:2346:HOH:O	2.23	0.62
1:C:322:ASN:CB	8:C:2280:HOH:O	2.03	0.62
1:C:3:ARG:HB2	1:C:33:GLU:OE2	1.98	0.62
1:B:284:GLN:HE22	1:B:329:VAL:H	1.47	0.62
1:B:230:GLY:N	5:B:1498[B]:NDP:H4D	2.15	0.62
1:C:210:ARG:HG3	8:C:2208:HOH:O	1.98	0.62
1:C:295:HIS:CD2	1:C:297:SER:H	2.17	0.62
5:D:1496[B]:NDP:H41N	8:D:2407:HOH:O	2.00	0.61
1:A:151:ALA:HB1	8:A:2341:HOH:O	1.99	0.61
2:C:1492:GOL:H11	8:C:2373:HOH:O	1.97	0.61
2:B:1496:GOL:H2	5:B:1498[A]:NDP:C8A	2.28	0.61
1:C:33:GLU:OE1	8:C:2003:HOH:O	2.16	0.61
1:A:295:HIS:CD2	1:A:297:SER:H	2.19	0.61
1:A:284:GLN:HE22	1:A:329:VAL:N	1.98	0.61
1:D:295:HIS:CD2	1:D:297:SER:H	2.19	0.61
1:A:187:LYS:HZ1	2:A:1493:GOL:H32	1.66	0.60
2:D:1491:GOL:C3	8:D:2256:HOH:O	2.37	0.60
1:A:397:VAL:O	1:A:407:ARG:NH2	2.34	0.60
1:D:284:GLN:HE22	1:D:329:VAL:N	1.98	0.60
5:A:1500[A]:NDP:C4N	8:A:2341:HOH:O	2.49	0.60
5:B:1498[A]:NDP:O2N	8:B:2261:HOH:O	2.16	0.60
1:C:4:PHE:HA	8:C:2010:HOH:O	2.00	0.60
1:A:285:VAL:HG13	4:A:1498:EDO:H11	1.83	0.60
1:C:210:ARG:HG2	8:C:2208:HOH:O	1.97	0.60
1:C:446:GLU:OE1	8:C:2368:HOH:O	2.17	0.59
1:B:389:PHE:CE1	5:B:1498[B]:NDP:H2D	2.37	0.59
1:C:319:GLN:HE21	1:C:319:GLN:HA	1.66	0.59
1:C:375:THR:HG22	8:C:2309:HOH:O	2.02	0.59
3:A:1495:PG4:C2	8:A:2346:HOH:O	2.49	0.59
1:B:468:THR:HA	8:B:2406:HOH:O	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLN:HE22	1:C:329:VAL:H	1.49	0.59
5:C:1495[B]:NDP:O2N	8:C:2176:HOH:O	2.16	0.58
1:D:386:GLU:HG2	8:D:2224:HOH:O	2.01	0.58
1:C:389:PHE:CE1	5:C:1495[B]:NDP:H2D	2.38	0.58
1:B:119:LEU:HD21	1:C:122:ALA:HB2	1.84	0.58
2:B:1495:GOL:H11	8:B:2254:HOH:O	2.03	0.58
3:A:1495:PG4:H31	4:A:1498:EDO:O2	2.02	0.58
1:C:301:ARG:NH2	8:C:2269:HOH:O	2.36	0.58
3:A:1495:PG4:C1	2:A:1499:GOL:C3	2.70	0.58
1:D:207:GLY:HA3	1:D:212:VAL:CG1	2.33	0.58
1:A:157:GLN:NE2	3:A:1495:PG4:H61	2.18	0.58
1:B:214:GLN:OE1	8:B:2279:HOH:O	2.16	0.58
1:B:295:HIS:CD2	1:B:297:SER:H	2.21	0.58
1:D:269:ARG:NH1	1:D:442:ASN:O	2.37	0.58
1:B:231:THR:HA	1:B:253:LEU:HD13	1.85	0.58
1:A:47:GLU:OE1	1:A:219:HIS:HE1	1.87	0.58
1:A:379:ASP:OD2	1:A:407:ARG:HD2	2.04	0.58
1:A:475:ARG:HD3	1:B:456:TYR:CZ	2.39	0.58
1:B:276:MET:CE	2:B:1491:GOL:H12	2.34	0.57
5:D:1496[B]:NDP:C4N	8:D:2407:HOH:O	2.53	0.57
1:A:98:LEU:HD22	1:A:319:GLN:HA	1.86	0.57
1:C:208:SER:O	1:C:212:VAL:HG13	2.04	0.57
1:D:328:LEU:HD12	1:D:334:MET:HA	1.86	0.57
1:D:236:LYS:HD2	8:D:2168:HOH:O	1.99	0.57
1:B:236:LYS:HD2	8:B:2299:HOH:O	2.05	0.57
1:D:295:HIS:HD2	1:D:297:SER:OG	1.88	0.57
1:C:27:ILE:HG22	1:C:28:ASN:H	1.70	0.56
1:C:295:HIS:CD2	1:C:297:SER:OG	2.56	0.56
1:C:301:ARG:HG2	8:C:2271:HOH:O	2.00	0.56
1:D:102:ARG:HH22	1:D:321:GLU:HG2	1.69	0.56
1:D:228:THR:HG21	5:D:1496[B]:NDP:H41N	1.87	0.56
8:B:2232:HOH:O	1:C:433:ARG:HD2	2.05	0.56
1:D:306:VAL:O	1:D:310:VAL:HG23	2.06	0.56
5:A:1500[A]:NDP:C4D	8:A:2648:HOH:O	2.50	0.56
1:A:228:THR:CG2	5:A:1500[B]:NDP:C4N	2.83	0.56
1:B:7:GLN:OE1	2:B:1493:GOL:H11	2.05	0.56
1:B:236:LYS:HE3	8:B:2295:HOH:O	2.04	0.56
1:D:232:SER:CB	8:D:2279:HOH:O	2.53	0.56
1:D:397:VAL:O	1:D:407:ARG:NH2	2.39	0.56
1:A:433:ARG:NH1	8:A:2595:HOH:O	2.31	0.56
1:B:429[B]:ARG:HD2	8:B:2386:HOH:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1496:TOE:CB'	4:C:1497:EDO:C1	2.69	0.56
1:C:95:GLY:HA2	8:C:2045:HOH:O	2.06	0.56
1:A:194:GLU:OE1	8:A:2217:HOH:O	2.18	0.55
1:B:276:MET:HE3	2:B:1491:GOL:H12	1.88	0.55
1:C:3:ARG:NH2	8:C:2002:HOH:O	2.39	0.55
3:A:1495:PG4:C3	4:A:1498:EDO:C2	2.79	0.55
7:C:1496:TOE:H8	8:C:2184:HOH:O	2.06	0.55
1:C:320:ASP:OD1	1:C:321:GLU:N	2.40	0.55
7:C:1496:TOE:CE'	8:C:2184:HOH:O	2.55	0.55
3:A:1495:PG4:C5	8:A:2343:HOH:O	2.42	0.55
5:C:1495[B]:NDP:H8A	8:C:2408:HOH:O	2.06	0.55
1:D:230:GLY:N	5:D:1496[B]:NDP:H4D	2.21	0.55
1:C:379:ASP:OD2	1:C:407:ARG:HD2	2.07	0.54
1:D:389:PHE:CE1	5:D:1496[B]:NDP:H2D	2.42	0.54
1:B:229:GLY:O	5:B:1498[B]:NDP:H1D	2.08	0.54
1:A:483:LEU:HD13	1:D:429[A]:ARG:HG2	1.88	0.54
1:B:44:GLU:HG3	8:B:2037:HOH:O	2.07	0.54
1:C:410:ASP:OD2	8:C:2323:HOH:O	2.18	0.53
1:B:153:ASN:OD1	5:B:1498[B]:NDP:H5N	2.08	0.53
1:C:484:GLY:O	1:D:269:ARG:NH2	2.39	0.53
1:D:14[A]:ARG:CZ	8:D:2035:HOH:O	2.55	0.53
1:B:210:ARG:HB2	8:B:2277:HOH:O	2.07	0.53
1:D:253:LEU:O	5:D:1496[B]:NDP:H2N	2.08	0.53
1:C:200:GLY:O	8:C:2194:HOH:O	2.19	0.53
1:D:261:ILE:HD12	1:D:270:ALA:HB1	1.89	0.53
2:B:1493:GOL:H12	8:B:2009:HOH:O	2.08	0.53
1:B:3:ARG:NH2	8:B:2005:HOH:O	2.23	0.53
1:D:219:HIS:CD2	1:D:220:PRO:HD2	2.43	0.53
1:C:219:HIS:HD2	1:C:221:LEU:N	1.99	0.53
1:C:77:ASP:OD2	8:C:2105:HOH:O	2.19	0.53
1:D:269:ARG:NH1	1:D:442:ASN:HB3	2.24	0.52
3:A:1495:PG4:O1	2:A:1499:GOL:H2	2.10	0.52
1:C:456:TYR:CZ	1:D:475:ARG:HD3	2.44	0.52
7:C:1496:TOE:CB'	4:C:1497:EDO:C2	2.88	0.52
1:C:228:THR:HG21	5:C:1495[B]:NDP:H41N	1.92	0.52
1:A:239:ALA:HB2	1:B:243:SER:HB3	1.92	0.52
1:B:4:PHE:CD1	2:B:1493:GOL:H2	2.45	0.52
2:D:1493:GOL:H32	8:D:2406:HOH:O	2.10	0.52
1:D:152:TRP:CE3	1:D:329:VAL:HG11	2.44	0.52
1:A:433:ARG:CD	8:A:2595:HOH:O	2.58	0.52
1:B:89:LEU:HD11	1:B:183:LEU:HD13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ILE:CG2	1:C:28:ASN:N	2.72	0.52
1:C:315:LEU:C	1:C:315:LEU:HD23	2.30	0.52
1:B:3:ARG:HD3	8:B:2006:HOH:O	2.09	0.52
1:A:433:ARG:HD2	8:A:2595:HOH:O	2.10	0.51
1:B:305:LYS:HG2	1:B:309:ARG:HH12	1.75	0.51
1:D:333:HIS:O	1:D:337:VAL:HG23	2.11	0.51
1:A:252:GLU:OE1	2:A:1499:GOL:H12	2.09	0.51
1:B:261:ILE:HD13	1:B:270:ALA:HB1	1.91	0.51
1:B:301:ARG:HD3	8:B:2331:HOH:O	2.10	0.51
1:A:406[B]:ARG:HG2	1:A:406[B]:ARG:HH11	1.74	0.51
1:A:419:VAL:HG22	1:A:431:ILE:HD13	1.92	0.51
1:A:271:ALA:O	1:A:275[A]:VAL:HG22	2.11	0.51
1:B:44:GLU:CG	8:B:2037:HOH:O	2.59	0.51
1:B:433:ARG:NH2	8:B:2370:HOH:O	2.40	0.51
1:B:429[B]:ARG:CG	8:B:2386:HOH:O	2.59	0.50
1:A:8:LYS:HE2	1:A:17:GLU:OE2	2.11	0.50
1:A:295:HIS:HD2	1:A:297:SER:OG	1.93	0.50
1:D:143:LEU:HD23	1:D:475:ARG:CG	2.41	0.50
1:A:147:ALA:HB3	1:A:225:ILE:CD1	2.41	0.50
1:B:285:VAL:HB	1:B:288:ASN:OD1	2.12	0.50
1:C:291:ARG:HD3	8:C:2264:HOH:O	2.11	0.50
1:A:132:GLU:O	8:A:2308:HOH:O	2.19	0.50
1:C:214:GLN:O	1:C:218:GLU:HG3	2.11	0.50
1:D:157:GLN:OE1	2:D:1492:GOL:H12	2.11	0.50
1:A:143:LEU:HD23	1:A:475:ARG:HG2	1.93	0.50
1:D:345:LYS:CD	8:D:2338:HOH:O	2.58	0.50
1:B:403:GLU:O	1:B:407:ARG:HG3	2.12	0.50
8:B:2401:HOH:O	1:C:121:PRO:HA	2.11	0.50
1:A:456:TYR:CZ	1:B:475:ARG:HD3	2.47	0.49
1:C:284:GLN:HE22	1:C:329:VAL:N	2.09	0.49
1:C:309:ARG:O	1:C:312:ARG:HG2	2.12	0.49
1:A:230:GLY:N	5:A:1500[B]:NDP:H4D	2.27	0.49
1:A:379:ASP:OD2	1:A:407:ARG:CD	2.60	0.49
1:D:318:PRO:HG3	1:D:327:PRO:HD2	1.94	0.49
5:A:1500[A]:NDP:C3D	8:A:2496:HOH:O	2.29	0.49
1:C:28:ASN:OD1	1:C:28:ASN:C	2.50	0.49
1:C:328:LEU:HD12	1:C:334:MET:HA	1.94	0.49
1:D:401:GLU:HB2	8:D:2363:HOH:O	2.12	0.49
1:D:69[B]:SER:OG	1:D:120:VAL:HB	2.12	0.49
1:B:233:THR:OG1	8:B:2296:HOH:O	2.20	0.49
1:C:108:THR:HG21	7:C:1496:TOE:H12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1495[A]:NDP:H8A	8:C:2408:HOH:O	2.12	0.49
1:B:284:GLN:HE22	1:B:329:VAL:N	2.09	0.49
7:C:1496:TOE:CB'	4:C:1497:EDO:O2	2.61	0.49
2:D:1493:GOL:C3	8:D:2406:HOH:O	2.60	0.49
5:D:1496[B]:NDP:O2A	5:D:1496[B]:NDP:O1N	2.30	0.49
1:D:295:HIS:HE1	1:D:399:ASP:O	1.96	0.49
1:C:429:ARG:HD3	8:C:2357:HOH:O	2.11	0.49
1:A:219:HIS:CD2	1:A:221:LEU:H	2.18	0.48
1:D:365:LYS:HE3	8:D:2087:HOH:O	2.13	0.48
1:C:315:LEU:O	2:C:1493:GOL:H32	2.14	0.48
1:B:429[B]:ARG:HG3	8:B:2386:HOH:O	2.12	0.48
1:D:236:LYS:HE2	2:D:1495:GOL:C1	2.41	0.48
1:D:345:LYS:NZ	8:D:2338:HOH:O	2.21	0.48
1:B:152:TRP:CE3	1:B:329:VAL:HG11	2.48	0.48
3:A:1495:PG4:H22	8:A:2346:HOH:O	2.13	0.48
3:A:1495:PG4:H12	2:A:1499:GOL:C2	2.43	0.48
5:C:1495[A]:NDP:H2B	5:C:1495[A]:NDP:H8A	1.67	0.48
1:C:322:ASN:ND2	8:C:2280:HOH:O	2.47	0.48
1:A:380:ASP:OD2	8:A:2546:HOH:O	2.20	0.47
1:A:380:ASP:OD1	8:A:2544:HOH:O	2.20	0.47
1:B:157:GLN:OE1	2:B:1492:GOL:C1	2.61	0.47
1:B:210:ARG:HG3	2:B:1496:GOL:H32	1.96	0.47
5:C:1495[B]:NDP:H42N	4:C:1497:EDO:O1	2.14	0.47
1:C:43:ARG:HG3	1:C:215:TRP:CE2	2.50	0.47
1:C:43:ARG:NH2	8:C:2061:HOH:O	2.35	0.47
1:C:267:LEU:HD23	1:C:267:LEU:HA	1.56	0.47
1:D:229:GLY:O	5:D:1496[B]:NDP:H1D	2.14	0.47
1:C:179:GLU:HG3	1:C:207:GLY:O	2.14	0.47
1:A:122:ALA:HB2	1:D:119:LEU:HD21	1.95	0.47
1:D:454:GLY:HA3	1:D:463:ARG:HD3	1.95	0.47
1:D:475:ARG:NH1	8:D:2394:HOH:O	2.46	0.47
1:C:447:SER:H	7:C:1496:TOE:H16	1.78	0.47
8:C:2390:HOH:O	1:D:446:GLU:HB3	2.15	0.47
1:B:269:ARG:HG2	1:B:273:ILE:HD12	1.97	0.47
1:A:389:PHE:CE1	5:A:1500[B]:NDP:H2D	2.49	0.47
1:C:351:LEU:HD21	1:C:354:GLY:O	2.15	0.47
1:D:387:GLU:OE2	8:D:2359:HOH:O	2.20	0.47
1:C:219:HIS:NE2	1:C:221:LEU:HB2	2.30	0.47
1:D:284:GLN:NE2	1:D:329:VAL:H	2.09	0.47
1:B:143:LEU:HD23	1:B:475:ARG:HG2	1.97	0.46
1:B:351:LEU:HD21	1:B:354:GLY:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1496:TOE:H8	8:C:2366:HOH:O	2.14	0.46
1:C:379:ASP:OD2	1:C:407:ARG:CD	2.62	0.46
1:A:284:GLN:NE2	1:A:329:VAL:H	2.06	0.46
1:C:224:LYS:HE3	1:C:473:TYR:CE1	2.51	0.46
2:B:1496:GOL:O2	5:B:1498[B]:NDP:H8A	2.15	0.46
1:A:219:HIS:CD2	1:A:220:PRO:HD2	2.50	0.46
1:B:187:LYS:NZ	8:B:2265:HOH:O	2.45	0.46
1:B:301:ARG:CD	8:B:2331:HOH:O	2.62	0.46
1:D:143:LEU:HD23	1:D:475:ARG:HG3	1.98	0.46
2:B:1496:GOL:O2	5:B:1498[A]:NDP:H8A	2.16	0.46
1:D:229:GLY:O	1:D:253:LEU:HA	2.15	0.46
5:C:1495[B]:NDP:H52A	8:C:2176:HOH:O	2.16	0.46
1:C:152:TRP:CE3	1:C:329:VAL:HG11	2.51	0.46
1:A:23:THR:HG21	1:A:37[B]:LYS:HE3	1.97	0.45
1:B:475:ARG:H	1:B:475:ARG:HG3	1.62	0.45
1:C:227:PHE:CZ	5:C:1495[A]:NDP:H51A	2.51	0.45
1:C:67:GLN:HG2	8:C:2091:HOH:O	2.15	0.45
1:B:122:ALA:HB2	1:C:119:LEU:HD21	1.97	0.45
1:C:269:ARG:O	1:C:273:ILE:HG13	2.16	0.45
1:D:295:HIS:CE1	1:D:399:ASP:O	2.69	0.45
1:D:339:GLY:O	1:D:342:GLU:HB2	2.16	0.45
2:A:1491:GOL:H12	5:A:1500[A]:NDP:HO2N	1.64	0.45
1:B:317:ASP:OD1	1:B:318:PRO:HD2	2.17	0.45
1:A:267:LEU:HB3	1:A:305:LYS:HD2	1.98	0.45
1:B:210:ARG:HG3	2:B:1496:GOL:C3	2.47	0.45
1:B:219:HIS:HA	1:B:220:PRO:HD3	1.76	0.45
1:C:230:GLY:N	5:C:1495[B]:NDP:H4D	2.31	0.45
1:C:227:PHE:HE2	5:C:1495[A]:NDP:O4B	1.99	0.45
1:C:8:LYS:HB3	1:C:16:VAL:O	2.17	0.45
1:B:426:ARG:NH1	8:B:2316:HOH:O	2.49	0.45
2:A:1492:GOL:H32	8:A:2604:HOH:O	2.16	0.45
1:B:223:GLU:HB3	8:B:2288:HOH:O	2.17	0.45
1:C:257:SER:HA	1:C:258:PRO:HD3	1.68	0.45
1:D:127:GLN:C	1:D:128:ILE:HG13	2.37	0.45
1:A:147:ALA:HB3	1:A:225:ILE:HD13	1.98	0.45
1:A:5:GLU:HG2	8:A:2013:HOH:O	2.17	0.45
1:A:6:GLU:O	2:A:1494:GOL:H32	2.17	0.45
5:C:1495[B]:NDP:H2B	5:C:1495[B]:NDP:H8A	1.75	0.45
1:C:231:THR:HA	1:C:253:LEU:HD13	1.99	0.45
1:D:286:ALA:HB2	5:D:1496[B]:NDP:C2N	2.46	0.45
1:D:419:VAL:HG22	1:D:431:ILE:HD13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:NH2	8:A:2376:HOH:O	2.51	0.44
1:C:339:GLY:HA3	2:C:1494:GOL:H12	1.99	0.44
2:D:1494:GOL:H11	8:D:2256:HOH:O	2.05	0.44
1:A:53:ALA:HA	1:A:200:GLY:O	2.17	0.44
5:C:1495[B]:NDP:O2A	5:C:1495[B]:NDP:O1N	2.36	0.44
1:C:397:VAL:O	1:C:407:ARG:NH2	2.51	0.44
1:A:95:GLY:O	1:A:327:PRO:HD2	2.17	0.44
1:C:4:PHE:CA	8:C:2010:HOH:O	2.63	0.44
1:D:334:MET:HG3	1:D:369:VAL:CG2	2.47	0.44
1:C:187:LYS:HD3	1:C:187:LYS:HA	1.85	0.44
1:C:219:HIS:CD2	1:C:220:PRO:HD2	2.52	0.44
1:A:295:HIS:HD2	1:A:297:SER:H	1.65	0.44
1:A:406[B]:ARG:NH1	1:A:406[B]:ARG:HG2	2.33	0.44
1:C:123:ILE:HD11	1:C:470:LEU:HD11	2.00	0.44
1:C:375:THR:CG2	8:C:2309:HOH:O	2.62	0.44
1:C:417:ALA:O	1:C:439:CYS:HA	2.18	0.44
1:B:431:ILE:HD12	1:B:431:ILE:HA	1.88	0.43
1:C:95:GLY:O	1:C:327:PRO:HD2	2.18	0.43
1:C:447:SER:H	7:C:1496:TOE:CK'	2.30	0.43
1:B:328:LEU:HD12	1:B:334:MET:HA	2.00	0.43
1:C:27:ILE:CG2	1:C:28:ASN:H	2.30	0.43
1:C:315:LEU:HD23	1:C:316:GLY:N	2.33	0.43
2:C:1492:GOL:H31	2:C:1492:GOL:HO1	1.63	0.43
8:A:2588:HOH:O	1:D:132:GLU:HG2	2.18	0.43
1:D:295:HIS:HD2	1:D:297:SER:CB	2.31	0.43
1:A:187:LYS:HE2	8:A:2019:HOH:O	2.19	0.43
1:B:50:VAL:HA	1:B:174:ILE:HD11	2.01	0.43
1:C:253:LEU:O	5:C:1495[B]:NDP:H2N	2.19	0.43
1:C:435:GLU:HG2	8:D:2394:HOH:O	2.17	0.43
1:D:236:LYS:HE3	1:D:236:LYS:HB3	1.82	0.43
1:A:219:HIS:HA	1:A:220:PRO:HD3	1.81	0.43
1:A:454:GLY:HA3	1:A:463:ARG:HD3	1.99	0.43
7:C:1496:TOE:CH'	8:C:2371:HOH:O	2.67	0.43
7:C:1496:TOE:H14	8:C:2410:HOH:O	2.04	0.43
1:D:219:HIS:HA	1:D:220:PRO:HD3	1.86	0.43
1:C:286:ALA:HB2	5:C:1495[B]:NDP:C2N	2.48	0.43
1:C:82:ARG:NH2	1:C:194:GLU:OE1	2.51	0.43
1:C:331:PHE:N	1:C:332:PRO:CD	2.82	0.43
8:A:2262:HOH:O	1:D:66:MET:HE3	2.18	0.43
1:A:187:LYS:NZ	2:A:1493:GOL:H11	2.33	0.42
1:A:229:GLY:O	1:A:253:LEU:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:VAL:O	1:B:310:VAL:HG23	2.19	0.42
1:A:44[B]:GLU:OE1	8:A:2056:HOH:O	2.22	0.42
1:C:176:LYS:NZ	1:C:177:PRO:O	2.51	0.42
1:C:218:GLU:OE1	8:C:2061:HOH:O	2.21	0.42
1:D:143:LEU:HD23	1:D:475:ARG:HG2	2.01	0.42
1:B:124:GLU:OE1	1:D:126:GLU:OE1	2.38	0.42
1:B:331:PHE:N	1:B:332:PRO:CD	2.82	0.42
1:C:219:HIS:HA	1:C:220:PRO:HD3	1.76	0.42
1:B:8:LYS:HD3	1:B:17:GLU:OE2	2.19	0.42
7:C:1496:TOE:H13	8:C:2371:HOH:O	2.19	0.42
1:D:68:ARG:NH2	8:D:2136:HOH:O	2.53	0.42
2:A:1499:GOL:O3	8:A:2610:HOH:O	2.13	0.42
5:A:1500[A]:NDP:H8A	5:A:1500[A]:NDP:H2B	1.71	0.42
1:B:44:GLU:H	1:B:44:GLU:CD	2.23	0.42
1:C:293:PHE:HA	1:C:396:LEU:O	2.19	0.42
1:B:53:ALA:HB2	8:B:2259:HOH:O	2.18	0.42
1:D:220:PRO:HG2	8:D:2046:HOH:O	2.19	0.42
1:A:417:ALA:O	1:A:439:CYS:HA	2.19	0.42
1:C:8:LYS:HE2	1:C:17:GLU:OE2	2.20	0.42
1:C:152:TRP:HD1	8:C:2180:HOH:O	2.03	0.42
1:C:3:ARG:HD3	1:C:4:PHE:CZ	2.55	0.42
1:D:229:GLY:C	5:D:1496[B]:NDP:H1D	2.40	0.42
1:D:2:ALA:HA	1:D:34:VAL:O	2.20	0.42
1:B:136:VAL:HG23	1:B:137:TYR:N	2.35	0.42
1:B:31:ASN:OD1	1:B:33[A]:GLU:HB2	2.19	0.42
1:C:221:LEU:HD23	1:C:221:LEU:HA	1.85	0.42
1:A:246:LEU:HD13	1:B:253:LEU:HD12	2.02	0.41
1:B:389:PHE:HA	8:B:2366:HOH:O	2.20	0.41
1:D:335:GLU:HA	1:D:335:GLU:OE1	2.20	0.41
1:A:28:ASN:HA	1:A:29:PRO:HD3	1.91	0.41
1:A:68:ARG:NH1	8:A:2165:HOH:O	2.33	0.41
7:C:1496:TOE:CB'	4:C:1497:EDO:HO2	2.32	0.41
1:C:164:ALA:HB3	1:C:165:PRO:CD	2.51	0.41
1:D:10:TYR:CD1	1:D:189:ALA:HB1	2.54	0.41
1:D:207:GLY:HA3	1:D:212:VAL:HG13	2.02	0.41
1:A:187:LYS:HZ3	2:A:1493:GOL:H11	1.85	0.41
3:A:1495:PG4:C2	4:A:1498:EDO:H12	2.47	0.41
2:B:1496:GOL:C2	5:B:1498[B]:NDP:C8A	2.96	0.41
1:C:14:ARG:HB3	1:C:14:ARG:HE	1.64	0.41
1:B:229:GLY:HA2	5:B:1498[B]:NDP:O4D	2.20	0.41
1:D:100:GLU:HG2	1:D:280:PHE:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1496[B]:NDP:O7N	8:D:2407:HOH:O	2.22	0.41
1:D:94:THR:HG22	1:D:181:THR:HG21	2.02	0.41
1:D:310:VAL:HG13	1:D:371:PRO:HB2	2.03	0.41
1:C:295:HIS:HE1	1:C:399:ASP:O	2.04	0.41
1:A:124:GLU:OE1	1:C:126:GLU:OE1	2.39	0.41
2:B:1496:GOL:C2	5:B:1498[A]:NDP:C8A	2.96	0.41
1:D:227:PHE:CE2	1:D:237:VAL:HG21	2.56	0.41
1:B:13:GLY:HA3	1:B:199:ASP:OD1	2.21	0.41
1:A:315:LEU:HA	1:A:325:PHE:O	2.21	0.41
1:B:179:GLU:HG3	1:B:207:GLY:O	2.21	0.41
1:D:102:ARG:NH2	1:D:321:GLU:HG2	2.34	0.41
1:D:441:ILE:O	1:D:442:ASN:HB2	2.21	0.41
1:A:44[A]:GLU:OE1	8:A:2056:HOH:O	2.21	0.41
1:D:285:VAL:HB	1:D:288:ASN:OD1	2.21	0.41
1:D:379:ASP:HA	1:D:384:VAL:HG11	2.03	0.41
1:C:243:SER:HB3	1:D:239:ALA:HB2	2.02	0.40
1:A:416:ALA:HA	1:A:438:ILE:O	2.21	0.40
1:B:229:GLY:O	1:B:253:LEU:HA	2.21	0.40
1:C:127:GLN:C	1:C:128:ILE:HG13	2.42	0.40
1:C:222:ILE:O	1:C:247:LYS:HE3	2.21	0.40
1:A:138:THR:HA	1:A:477:LYS:O	2.21	0.40
1:B:295:HIS:HD2	1:B:297:SER:CB	2.34	0.40
1:C:13:GLY:HA3	1:C:199:ASP:OD1	2.22	0.40
1:A:328:LEU:HD12	1:A:334:MET:HA	2.04	0.40
1:C:295:HIS:HD2	1:C:297:SER:H	1.67	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2509:HOH:O	8:A:2544:HOH:O[6_554]	2.15	0.05

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	495/490 (101%)	479 (97%)	15 (3%)	1 (0%)	47	57
1	B	489/490 (100%)	474 (97%)	15 (3%)	0	100	100
1	C	489/490 (100%)	470 (96%)	18 (4%)	1 (0%)	47	57
1	D	490/490 (100%)	473 (96%)	17 (4%)	0	100	100
All	All	1963/1960 (100%)	1896 (97%)	65 (3%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	GLY
1	C	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%)	383 (96%)	14 (4%)	36	47
1	B	391/390 (100%)	380 (97%)	11 (3%)	43	56
1	C	391/390 (100%)	380 (97%)	11 (3%)	43	56
1	D	392/390 (100%)	384 (98%)	8 (2%)	55	67
All	All	1571/1560 (101%)	1527 (97%)	44 (3%)	44	56

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	26	THR
1	A	37[A]	LYS
1	A	37[B]	LYS
1	A	98	LEU
1	A	136	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	210	ARG
1	A	212	VAL
1	A	319	GLN
1	A	342	GLU
1	A	348	LYS
1	A	378	ARG
1	A	385	ARG
1	A	475	ARG
1	B	3	ARG
1	B	8	LYS
1	B	33[A]	GLU
1	B	33[B]	GLU
1	B	98	LEU
1	B	136	VAL
1	B	212	VAL
1	B	353	CYS
1	B	360	ASP
1	B	397	VAL
1	B	475	ARG
1	C	14	ARG
1	C	26	THR
1	C	43	ARG
1	C	136	VAL
1	C	210	ARG
1	C	212	VAL
1	C	319	GLN
1	C	348	LYS
1	C	385	ARG
1	C	411	THR
1	C	475	ARG
1	D	8	LYS
1	D	136	VAL
1	D	211	GLU
1	D	212	VAL
1	D	214	GLN
1	D	251	MET
1	D	431	ILE
1	D	475	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	83	ASN
1	A	157	GLN
1	A	219	HIS
1	A	284	GLN
1	A	295	HIS
1	B	219	HIS
1	B	284	GLN
1	B	295	HIS
1	B	319	GLN
1	C	7	GLN
1	C	83	ASN
1	C	219	HIS
1	C	284	GLN
1	C	295	HIS
1	C	319	GLN
1	D	7	GLN
1	D	83	ASN
1	D	214	GLN
1	D	219	HIS
1	D	284	GLN
1	D	295	HIS
1	D	319	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 43 ligands modelled in this entry, 8 are monoatomic - leaving 35 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	NDP	C	1495[A]	-	45,52,52	1.52	4 (8%)	53,80,80	1.11	4 (7%)
2	GOL	A	1496	-	5,5,5	0.33	0	5,5,5	1.24	0
2	GOL	B	1496	-	5,5,5	0.13	0	5,5,5	0.34	0
5	NDP	C	1495[B]	-	45,52,52	2.36	9 (20%)	53,80,80	2.64	19 (35%)
4	EDO	C	1497	-	3,3,3	0.48	0	2,2,2	0.40	0
2	GOL	C	1494	-	5,5,5	0.45	0	5,5,5	0.18	0
2	GOL	B	1493	-	5,5,5	0.41	0	5,5,5	0.30	0
2	GOL	A	1491	-	5,5,5	0.30	0	5,5,5	0.36	0
2	GOL	B	1497	-	5,5,5	0.43	0	5,5,5	0.52	0
2	GOL	B	1492	-	5,5,5	0.60	0	5,5,5	0.47	0
2	GOL	D	1495	-	5,5,5	0.32	0	5,5,5	0.90	0
5	NDP	A	1500[A]	-	45,52,52	1.51	3 (6%)	53,80,80	1.04	3 (5%)
2	GOL	B	1491	-	5,5,5	0.27	0	5,5,5	0.89	0
2	GOL	C	1493	-	5,5,5	0.36	0	5,5,5	0.35	0
2	GOL	A	1493	-	5,5,5	0.36	0	5,5,5	0.31	0
2	GOL	B	1495	-	5,5,5	0.61	0	5,5,5	0.55	0
2	GOL	A	1497	-	5,5,5	0.34	0	5,5,5	1.06	0
2	GOL	C	1491	-	5,5,5	0.30	0	5,5,5	0.33	0
2	GOL	A	1492	-	5,5,5	0.41	0	5,5,5	0.31	0
2	GOL	D	1492	-	5,5,5	0.42	0	5,5,5	0.23	0
7	TOE	C	1496	-	10,10,10	0.41	0	9,9,9	0.81	0
2	GOL	A	1494	-	5,5,5	0.42	0	5,5,5	0.66	0
5	NDP	D	1496[A]	-	45,52,52	1.72	10 (22%)	53,80,80	1.34	11 (20%)
2	GOL	A	1499	-	5,5,5	0.27	0	5,5,5	0.52	0
5	NDP	B	1498[A]	-	45,52,52	1.47	4 (8%)	53,80,80	1.39	8 (15%)
5	NDP	D	1496[B]	-	45,52,52	2.27	11 (24%)	53,80,80	3.20	18 (33%)
2	GOL	D	1491	-	5,5,5	0.35	0	5,5,5	0.20	0
3	PG4	A	1495	-	12,12,12	0.29	0	11,11,11	0.98	0
5	NDP	B	1498[B]	-	45,52,52	1.52	5 (11%)	53,80,80	1.91	13 (24%)
2	GOL	D	1494	-	5,5,5	0.23	0	5,5,5	0.45	0
4	EDO	A	1498	-	3,3,3	0.47	0	2,2,2	0.40	0
5	NDP	A	1500[B]	-	45,52,52	1.80	12 (26%)	53,80,80	1.61	12 (22%)
2	GOL	B	1494	-	5,5,5	0.34	0	5,5,5	0.50	0
2	GOL	D	1493	-	5,5,5	0.26	0	5,5,5	0.99	0
2	GOL	C	1492	-	5,5,5	0.36	0	5,5,5	1.18	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	NDP	C	1495[A]	-	-	13/30/77/77	0/5/5/5
2	GOL	A	1496	-	-	4/4/4/4	-
2	GOL	B	1496	-	-	3/4/4/4	-
5	NDP	C	1495[B]	-	-	10/30/77/77	0/5/5/5
4	EDO	C	1497	-	-	0/1/1/1	-
2	GOL	C	1494	-	-	2/4/4/4	-
2	GOL	B	1493	-	-	2/4/4/4	-
2	GOL	A	1491	-	-	4/4/4/4	-
2	GOL	B	1497	-	-	4/4/4/4	-
2	GOL	B	1492	-	-	2/4/4/4	-
2	GOL	D	1495	-	-	4/4/4/4	-
5	NDP	A	1500[A]	-	-	16/30/77/77	0/5/5/5
2	GOL	B	1491	-	-	4/4/4/4	-
2	GOL	C	1493	-	-	2/4/4/4	-
2	GOL	A	1493	-	-	2/4/4/4	-
2	GOL	B	1495	-	-	4/4/4/4	-
2	GOL	A	1497	-	-	4/4/4/4	-
2	GOL	C	1491	-	-	0/4/4/4	-
2	GOL	A	1492	-	-	0/4/4/4	-
2	GOL	D	1492	-	-	3/4/4/4	-
7	TOE	C	1496	-	-	3/8/8/8	-
2	GOL	A	1494	-	-	4/4/4/4	-
5	NDP	D	1496[A]	-	-	10/30/77/77	0/5/5/5
2	GOL	A	1499	-	-	2/4/4/4	-
5	NDP	B	1498[A]	-	-	6/30/77/77	0/5/5/5
5	NDP	D	1496[B]	-	-	10/30/77/77	0/5/5/5
2	GOL	D	1491	-	-	2/4/4/4	-
3	PG4	A	1495	-	-	5/10/10/10	-
5	NDP	B	1498[B]	-	-	8/30/77/77	0/5/5/5
2	GOL	D	1494	-	-	0/4/4/4	-
4	EDO	A	1498	-	-	0/1/1/1	-
5	NDP	A	1500[B]	-	-	5/30/77/77	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1494	-	-	4/4/4/4	-
2	GOL	D	1493	-	-	4/4/4/4	-
2	GOL	C	1492	-	-	4/4/4/4	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1495[B]	NDP	C1D-N1N	-11.54	1.13	1.46
5	D	1496[B]	NDP	C1D-N1N	-9.60	1.19	1.46
5	A	1500[A]	NDP	C8A-N7A	7.28	1.47	1.34
5	C	1495[A]	NDP	C8A-N7A	7.28	1.47	1.34
5	C	1495[B]	NDP	C8A-N7A	6.06	1.45	1.34
5	B	1498[A]	NDP	C8A-N7A	5.94	1.45	1.34
5	B	1498[B]	NDP	C8A-N7A	5.90	1.45	1.34
5	A	1500[B]	NDP	C8A-N7A	5.76	1.45	1.34
5	D	1496[B]	NDP	C8A-N7A	4.72	1.43	1.34
5	D	1496[A]	NDP	C8A-N7A	4.71	1.43	1.34
5	A	1500[A]	NDP	C6N-C5N	3.67	1.39	1.33
5	C	1495[A]	NDP	C6N-C5N	3.55	1.39	1.33
5	D	1496[B]	NDP	C6N-N1N	-3.32	1.29	1.37
5	A	1500[B]	NDP	P2B-O3X	-3.27	1.42	1.54
5	D	1496[B]	NDP	P2B-O2X	-3.25	1.42	1.54
5	C	1495[A]	NDP	C5A-C4A	3.20	1.49	1.40
5	A	1500[B]	NDP	C6N-N1N	-3.17	1.29	1.37
5	D	1496[A]	NDP	P2B-O2X	-3.15	1.42	1.54
5	D	1496[B]	NDP	P2B-O1X	-3.09	1.40	1.50
5	D	1496[A]	NDP	PA-O2A	-3.08	1.40	1.55
5	C	1495[B]	NDP	C6N-N1N	-3.04	1.29	1.37
5	A	1500[A]	NDP	C5A-C4A	3.04	1.49	1.40
5	D	1496[A]	NDP	P2B-O1X	-2.99	1.40	1.50
5	A	1500[B]	NDP	P2B-O2X	-2.96	1.43	1.54
5	B	1498[B]	NDP	C6N-N1N	-2.92	1.30	1.37
5	D	1496[A]	NDP	P2B-O3X	-2.92	1.43	1.54
5	D	1496[B]	NDP	P2B-O3X	-2.91	1.43	1.54
5	D	1496[B]	NDP	C4A-N3A	-2.90	1.31	1.35
5	D	1496[A]	NDP	C4A-N3A	-2.73	1.31	1.35
5	A	1500[B]	NDP	P2B-O1X	-2.73	1.41	1.50
5	D	1496[A]	NDP	O4B-C4B	-2.68	1.39	1.45
5	A	1500[B]	NDP	PA-O2A	-2.68	1.42	1.55
5	B	1498[A]	NDP	PA-O2A	-2.63	1.43	1.55
5	D	1496[B]	NDP	PA-O1A	-2.59	1.41	1.50
5	A	1500[B]	NDP	PA-O1A	-2.59	1.41	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1496[B]	NDP	O4B-C4B	-2.58	1.39	1.45
5	D	1496[A]	NDP	PA-O1A	-2.57	1.41	1.50
5	D	1496[B]	NDP	P2B-O2B	-2.44	1.54	1.59
5	A	1500[B]	NDP	O7N-C7N	-2.40	1.18	1.24
5	D	1496[A]	NDP	O7N-C7N	-2.35	1.18	1.24
5	D	1496[A]	NDP	P2B-O2B	-2.35	1.54	1.59
5	C	1495[B]	NDP	PA-O1A	-2.34	1.42	1.50
5	B	1498[B]	NDP	C6N-C5N	2.32	1.37	1.33
5	C	1495[B]	NDP	P2B-O2X	-2.32	1.45	1.54
5	A	1500[B]	NDP	O4B-C4B	-2.26	1.39	1.45
5	D	1496[B]	NDP	C4N-C5N	-2.24	1.43	1.48
5	A	1500[B]	NDP	C5A-C4A	2.22	1.46	1.40
5	B	1498[A]	NDP	C5A-C4A	2.22	1.46	1.40
5	C	1495[B]	NDP	C4N-C5N	-2.22	1.43	1.48
5	A	1500[B]	NDP	C6N-C5N	2.21	1.37	1.33
5	C	1495[B]	NDP	O7N-C7N	-2.21	1.19	1.24
5	B	1498[B]	NDP	C5A-C4A	2.18	1.46	1.40
5	B	1498[A]	NDP	P2B-O2X	-2.16	1.46	1.54
5	C	1495[B]	NDP	C5A-C4A	2.16	1.46	1.40
5	B	1498[B]	NDP	P2B-O2X	-2.15	1.46	1.54
5	A	1500[B]	NDP	C4N-C5N	-2.12	1.43	1.48
5	C	1495[B]	NDP	P2B-O3X	-2.06	1.46	1.54
5	C	1495[A]	NDP	O4B-C1B	2.04	1.43	1.41

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1496[B]	NDP	C1D-N1N-C6N	-10.00	99.29	120.83
5	D	1496[B]	NDP	O4D-C1D-N1N	8.64	124.94	108.06
5	C	1495[B]	NDP	C1D-N1N-C6N	-8.37	102.79	120.83
5	D	1496[B]	NDP	C1D-N1N-C2N	7.99	134.41	121.11
5	D	1496[B]	NDP	O5D-C5D-C4D	-7.76	82.29	108.99
5	D	1496[B]	NDP	C2D-C1D-N1N	-7.68	94.06	113.30
5	C	1495[B]	NDP	C2D-C1D-N1N	-6.59	96.79	113.30
5	C	1495[B]	NDP	O4D-C1D-N1N	6.36	120.49	108.06
5	C	1495[B]	NDP	C1D-N1N-C2N	6.31	131.61	121.11
5	D	1496[B]	NDP	O4D-C4D-C5D	5.92	128.85	109.37
5	C	1495[B]	NDP	O4D-C1D-C2D	-5.10	95.52	106.64
5	C	1495[B]	NDP	O5D-C5D-C4D	-5.06	91.59	108.99
5	B	1498[B]	NDP	O4D-C1D-C2D	-5.04	95.65	106.64
5	A	1500[B]	NDP	O4D-C1D-C2D	-5.03	95.67	106.64
5	B	1498[B]	NDP	C2D-C1D-N1N	-5.02	100.73	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1498[B]	NDP	O4D-C4D-C5D	4.93	125.58	109.37
5	D	1496[B]	NDP	O4D-C1D-C2D	-4.93	95.91	106.64
5	B	1498[B]	NDP	O5D-C5D-C4D	-4.31	94.15	108.99
5	D	1496[B]	NDP	C5D-C4D-C3D	-4.22	99.35	115.18
5	D	1496[B]	NDP	C3N-C7N-N7N	4.21	125.14	117.67
5	A	1500[B]	NDP	C5D-C4D-C3D	-4.05	100.02	115.18
5	D	1496[A]	NDP	N3A-C2A-N1A	-3.76	122.81	128.68
5	D	1496[B]	NDP	N3A-C2A-N1A	-3.72	122.87	128.68
5	C	1495[B]	NDP	N3A-C2A-N1A	-3.68	122.93	128.68
5	C	1495[B]	NDP	O2B-P2B-O1X	-3.66	95.27	109.39
5	B	1498[A]	NDP	N3A-C2A-N1A	-3.53	123.16	128.68
5	B	1498[B]	NDP	N3A-C2A-N1A	-3.51	123.19	128.68
5	C	1495[A]	NDP	N3A-C2A-N1A	-3.47	123.25	128.68
5	A	1500[A]	NDP	N3A-C2A-N1A	-3.41	123.36	128.68
5	A	1500[B]	NDP	O5D-C5D-C4D	-3.32	97.58	108.99
5	B	1498[B]	NDP	O7N-C7N-C3N	-3.30	114.69	120.90
5	A	1500[B]	NDP	N3A-C2A-N1A	-3.19	123.69	128.68
5	B	1498[B]	NDP	C5D-C4D-C3D	-3.18	103.25	115.18
5	A	1500[B]	NDP	C3N-C7N-N7N	3.09	123.15	117.67
5	B	1498[B]	NDP	C3N-C7N-N7N	2.95	122.91	117.67
5	D	1496[B]	NDP	O7N-C7N-C3N	-2.84	115.55	120.90
5	A	1500[B]	NDP	O7N-C7N-C3N	-2.80	115.63	120.90
5	C	1495[B]	NDP	C2A-N1A-C6A	2.77	123.50	118.75
5	C	1495[B]	NDP	O4D-C4D-C5D	2.75	118.42	109.37
5	C	1495[B]	NDP	C3N-C7N-N7N	2.64	122.36	117.67
5	A	1500[B]	NDP	C2A-N1A-C6A	2.63	123.26	118.75
5	D	1496[B]	NDP	O4B-C1B-C2B	-2.60	102.07	106.59
5	C	1495[B]	NDP	O4B-C1B-C2B	-2.55	102.16	106.59
5	B	1498[A]	NDP	C3N-C2N-N1N	-2.52	119.50	123.10
5	B	1498[A]	NDP	C3D-C2D-C1D	2.51	106.20	101.43
5	D	1496[B]	NDP	O2B-P2B-O1X	-2.45	99.92	109.39
5	A	1500[A]	NDP	C2A-N1A-C6A	2.43	122.91	118.75
5	D	1496[A]	NDP	C3D-C2D-C1D	2.41	106.01	101.43
5	D	1496[A]	NDP	O2B-P2B-O1X	-2.40	100.12	109.39
5	C	1495[A]	NDP	C2A-N1A-C6A	2.40	122.86	118.75
5	D	1496[B]	NDP	PN-O3-PA	-2.38	124.66	132.83
5	B	1498[B]	NDP	O2B-P2B-O1X	-2.37	100.25	109.39
5	B	1498[A]	NDP	O2B-P2B-O1X	-2.35	100.33	109.39
5	D	1496[A]	NDP	C1D-N1N-C6N	-2.32	115.82	120.83
5	D	1496[A]	NDP	C2A-N1A-C6A	2.32	122.72	118.75
5	A	1500[A]	NDP	PN-O3-PA	-2.32	124.87	132.83
5	C	1495[B]	NDP	O3X-P2B-O2X	2.30	116.41	107.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1495[B]	NDP	O2A-PA-O5B	2.28	118.35	107.75
5	C	1495[A]	NDP	PN-O3-PA	-2.28	125.01	132.83
5	D	1496[B]	NDP	C2A-N1A-C6A	2.27	122.63	118.75
5	C	1495[B]	NDP	O5B-PA-O1A	-2.25	100.27	109.07
5	B	1498[A]	NDP	O7N-C7N-C3N	2.25	125.13	120.90
5	D	1496[A]	NDP	O3B-C3B-C4B	-2.24	104.57	111.05
5	D	1496[A]	NDP	O3X-P2B-O2X	2.23	116.15	107.64
5	A	1500[B]	NDP	C3B-C2B-C1B	-2.21	98.73	102.89
5	C	1495[B]	NDP	O7N-C7N-C3N	-2.21	116.74	120.90
5	A	1500[B]	NDP	O4B-C1B-C2B	-2.20	102.78	106.59
5	D	1496[B]	NDP	O3X-P2B-O2X	2.17	115.93	107.64
5	B	1498[B]	NDP	O2D-C2D-C1D	2.17	117.27	110.02
5	A	1500[B]	NDP	O2D-C2D-C1D	2.16	117.24	110.02
5	C	1495[B]	NDP	O3B-C3B-C2B	-2.15	105.06	111.17
5	D	1496[B]	NDP	O2D-C2D-C1D	2.14	117.18	110.02
5	C	1495[A]	NDP	O4D-C1D-N1N	2.14	112.23	108.06
5	D	1496[A]	NDP	C3N-C2N-N1N	-2.14	120.05	123.10
5	D	1496[A]	NDP	O7N-C7N-N7N	-2.13	117.89	122.88
5	C	1495[B]	NDP	O2D-C2D-C1D	2.12	117.11	110.02
5	D	1496[A]	NDP	O4B-C1B-C2B	-2.11	102.93	106.59
5	B	1498[B]	NDP	O2N-PN-O1N	2.11	122.65	112.24
5	D	1496[A]	NDP	C3B-C2B-C1B	-2.09	98.95	102.89
5	D	1496[B]	NDP	C3B-C2B-C1B	-2.07	99.00	102.89
5	C	1495[B]	NDP	O2N-PN-O1N	2.05	122.38	112.24
5	B	1498[A]	NDP	O3D-C3D-C2D	-2.05	105.19	111.82
5	B	1498[A]	NDP	C2A-N1A-C6A	2.04	122.24	118.75
5	B	1498[B]	NDP	C2A-N1A-C6A	2.04	122.24	118.75
5	A	1500[B]	NDP	O2B-P2B-O1X	-2.04	101.54	109.39
5	A	1500[B]	NDP	O4D-C4D-C5D	2.03	116.07	109.37
5	B	1498[B]	NDP	O4B-C1B-C2B	-2.01	103.10	106.59
5	B	1498[A]	NDP	O3B-C3B-C4B	-2.01	105.23	111.05

There are no chirality outliers.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1495[A]	NDP	C5B-O5B-PA-O2A
5	C	1495[A]	NDP	C5B-O5B-PA-O3
5	C	1495[A]	NDP	C2B-O2B-P2B-O2X
5	C	1495[A]	NDP	C5D-O5D-PN-O3
5	C	1495[A]	NDP	C5D-O5D-PN-O2N
2	A	1496	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1496	GOL	C1-C2-C3-O3
2	B	1496	GOL	O1-C1-C2-C3
5	C	1495[B]	NDP	C5B-O5B-PA-O2A
5	C	1495[B]	NDP	C5B-O5B-PA-O3
5	C	1495[B]	NDP	C2B-O2B-P2B-O1X
5	C	1495[B]	NDP	O4D-C4D-C5D-O5D
5	C	1495[B]	NDP	C3D-C4D-C5D-O5D
5	C	1495[B]	NDP	O4D-C1D-N1N-C2N
2	A	1491	GOL	O1-C1-C2-O2
2	A	1491	GOL	O1-C1-C2-C3
2	B	1497	GOL	O1-C1-C2-C3
2	D	1495	GOL	O1-C1-C2-O2
2	D	1495	GOL	O1-C1-C2-C3
5	A	1500[A]	NDP	C5B-O5B-PA-O1A
5	A	1500[A]	NDP	C5B-O5B-PA-O2A
5	A	1500[A]	NDP	C2B-O2B-P2B-O1X
5	A	1500[A]	NDP	C5D-O5D-PN-O1N
5	A	1500[A]	NDP	C5D-O5D-PN-O2N
2	B	1491	GOL	O1-C1-C2-C3
2	C	1493	GOL	C1-C2-C3-O3
2	A	1497	GOL	C1-C2-C3-O3
2	A	1494	GOL	C1-C2-C3-O3
5	D	1496[A]	NDP	C5B-O5B-PA-O1A
5	D	1496[A]	NDP	C2B-O2B-P2B-O1X
5	B	1498[A]	NDP	C5D-O5D-PN-O1N
5	B	1498[A]	NDP	O4D-C1D-N1N-C2N
5	D	1496[B]	NDP	C5B-O5B-PA-O1A
5	D	1496[B]	NDP	C5B-O5B-PA-O2A
5	D	1496[B]	NDP	C5B-O5B-PA-O3
5	D	1496[B]	NDP	C2B-O2B-P2B-O1X
5	D	1496[B]	NDP	O4D-C4D-C5D-O5D
5	D	1496[B]	NDP	C3D-C4D-C5D-O5D
5	D	1496[B]	NDP	O4D-C1D-N1N-C2N
2	D	1491	GOL	O1-C1-C2-C3
5	B	1498[B]	NDP	C5B-O5B-PA-O1A
5	B	1498[B]	NDP	C5B-O5B-PA-O3
5	B	1498[B]	NDP	O4D-C4D-C5D-O5D
5	B	1498[B]	NDP	C3D-C4D-C5D-O5D
5	B	1498[B]	NDP	O4D-C1D-N1N-C2N
5	A	1500[B]	NDP	O4D-C4D-C5D-O5D
5	A	1500[B]	NDP	C3D-C4D-C5D-O5D
5	A	1500[B]	NDP	O4D-C1D-N1N-C2N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1494	GOL	O1-C1-C2-C3
2	D	1493	GOL	O1-C1-C2-C3
2	D	1493	GOL	C1-C2-C3-O3
2	C	1492	GOL	O2-C2-C3-O3
5	C	1495[A]	NDP	C3B-C4B-C5B-O5B
5	D	1496[A]	NDP	O4D-C1D-N1N-C2N
7	C	1496	TOE	OC'-CD'-CE'-OF'
2	A	1496	GOL	O2-C2-C3-O3
2	B	1497	GOL	O1-C1-C2-O2
2	D	1495	GOL	O2-C2-C3-O3
2	A	1497	GOL	O2-C2-C3-O3
2	D	1492	GOL	O2-C2-C3-O3
2	A	1494	GOL	O2-C2-C3-O3
5	C	1495[A]	NDP	O4B-C4B-C5B-O5B
7	C	1496	TOE	OF'-CG'-CH'-OI'
2	C	1494	GOL	O1-C1-C2-C3
2	B	1493	GOL	O1-C1-C2-C3
2	A	1491	GOL	C1-C2-C3-O3
2	B	1497	GOL	C1-C2-C3-O3
2	B	1492	GOL	O1-C1-C2-C3
2	D	1495	GOL	C1-C2-C3-O3
2	A	1493	GOL	O1-C1-C2-C3
2	B	1495	GOL	O1-C1-C2-C3
2	B	1495	GOL	C1-C2-C3-O3
2	A	1497	GOL	O1-C1-C2-C3
2	D	1492	GOL	O1-C1-C2-C3
2	D	1492	GOL	C1-C2-C3-O3
2	A	1494	GOL	O1-C1-C2-C3
2	A	1499	GOL	O1-C1-C2-C3
2	B	1494	GOL	C1-C2-C3-O3
2	C	1492	GOL	O1-C1-C2-C3
2	C	1492	GOL	C1-C2-C3-O3
2	A	1496	GOL	O1-C1-C2-O2
2	B	1496	GOL	O1-C1-C2-O2
2	A	1491	GOL	O2-C2-C3-O3
2	B	1492	GOL	O1-C1-C2-O2
2	B	1491	GOL	O1-C1-C2-O2
2	B	1491	GOL	O2-C2-C3-O3
2	C	1493	GOL	O2-C2-C3-O3
2	A	1493	GOL	O1-C1-C2-O2
2	B	1494	GOL	O1-C1-C2-O2
2	D	1493	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1493	GOL	O2-C2-C3-O3
3	A	1495	PG4	O1-C1-C2-O2
5	A	1500[A]	NDP	O4B-C4B-C5B-O5B
3	A	1495	PG4	O2-C3-C4-O3
3	A	1495	PG4	O3-C5-C6-O4
2	A	1497	GOL	O1-C1-C2-O2
5	A	1500[A]	NDP	O4D-C1D-N1N-C2N
5	A	1500[A]	NDP	C3B-C4B-C5B-O5B
5	C	1495[A]	NDP	O4D-C1D-N1N-C2N
2	B	1493	GOL	O1-C1-C2-O2
2	B	1495	GOL	O1-C1-C2-O2
5	C	1495[A]	NDP	O4D-C4D-C5D-O5D
3	A	1495	PG4	C3-C4-O3-C5
3	A	1495	PG4	C1-C2-O2-C3
5	D	1496[A]	NDP	C5B-O5B-PA-O3
5	B	1498[A]	NDP	C5D-O5D-PN-O3
5	C	1495[A]	NDP	PA-O3-PN-O1N
5	D	1496[A]	NDP	PN-O3-PA-O2A
5	B	1498[A]	NDP	PN-O3-PA-O2A
2	B	1491	GOL	C1-C2-C3-O3
5	C	1495[B]	NDP	C5B-O5B-PA-O1A
5	D	1496[A]	NDP	C5B-O5B-PA-O2A
5	B	1498[A]	NDP	C5D-O5D-PN-O2N
5	B	1498[B]	NDP	C5B-O5B-PA-O2A
2	B	1495	GOL	O2-C2-C3-O3
2	D	1491	GOL	O1-C1-C2-O2
2	C	1492	GOL	O1-C1-C2-O2
5	A	1500[A]	NDP	O4D-C4D-C5D-O5D
5	A	1500[A]	NDP	PA-O3-PN-O1N
5	A	1500[B]	NDP	C4D-C5D-O5D-PN
2	C	1494	GOL	O1-C1-C2-O2
2	B	1497	GOL	O2-C2-C3-O3
5	D	1496[B]	NDP	C4D-C5D-O5D-PN
5	B	1498[B]	NDP	C4D-C5D-O5D-PN
5	C	1495[A]	NDP	C3D-C4D-C5D-O5D
5	C	1495[B]	NDP	PN-O3-PA-O1A
5	D	1496[B]	NDP	PN-O3-PA-O1A
2	A	1499	GOL	O1-C1-C2-O2
2	B	1494	GOL	O2-C2-C3-O3
5	A	1500[A]	NDP	C3D-C4D-C5D-O5D
7	C	1496	TOE	O2'-CA'-CB'-OC'
5	A	1500[A]	NDP	C5B-O5B-PA-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1500[A]	NDP	C2B-O2B-P2B-O3X
5	A	1500[A]	NDP	C5D-O5D-PN-O3
2	A	1494	GOL	O1-C1-C2-O2
5	D	1496[A]	NDP	C2B-O2B-P2B-O2X
5	D	1496[A]	NDP	C5D-O5D-PN-O3
5	C	1495[A]	NDP	PA-O3-PN-O2N
5	C	1495[B]	NDP	PN-O3-PA-O2A
5	A	1500[A]	NDP	PN-O3-PA-O2A
5	D	1496[A]	NDP	PN-O3-PA-O1A
2	B	1496	GOL	C1-C2-C3-O3
5	C	1495[A]	NDP	C2N-C3N-C7N-N7N
5	C	1495[B]	NDP	C2N-C3N-C7N-N7N
5	A	1500[A]	NDP	C2N-C3N-C7N-N7N
5	D	1496[A]	NDP	C2N-C3N-C7N-N7N
5	B	1498[A]	NDP	C2N-C3N-C7N-N7N
5	D	1496[B]	NDP	C2N-C3N-C7N-N7N
5	B	1498[B]	NDP	C2N-C3N-C7N-N7N
5	A	1500[B]	NDP	C2N-C3N-C7N-N7N

There are no ring outliers.

33 monomers are involved in 170 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1495[A]	NDP	5	0
2	A	1496	GOL	1	0
2	B	1496	GOL	10	0
5	C	1495[B]	NDP	14	0
4	C	1497	EDO	9	0
2	C	1494	GOL	1	0
2	B	1493	GOL	3	0
2	A	1491	GOL	5	0
2	B	1492	GOL	2	0
2	D	1495	GOL	4	0
5	A	1500[A]	NDP	17	0
2	B	1491	GOL	3	0
2	C	1493	GOL	1	0
2	A	1493	GOL	4	0
2	B	1495	GOL	2	0
2	C	1491	GOL	2	0
2	A	1492	GOL	2	0
2	D	1492	GOL	1	0
7	C	1496	TOE	23	0

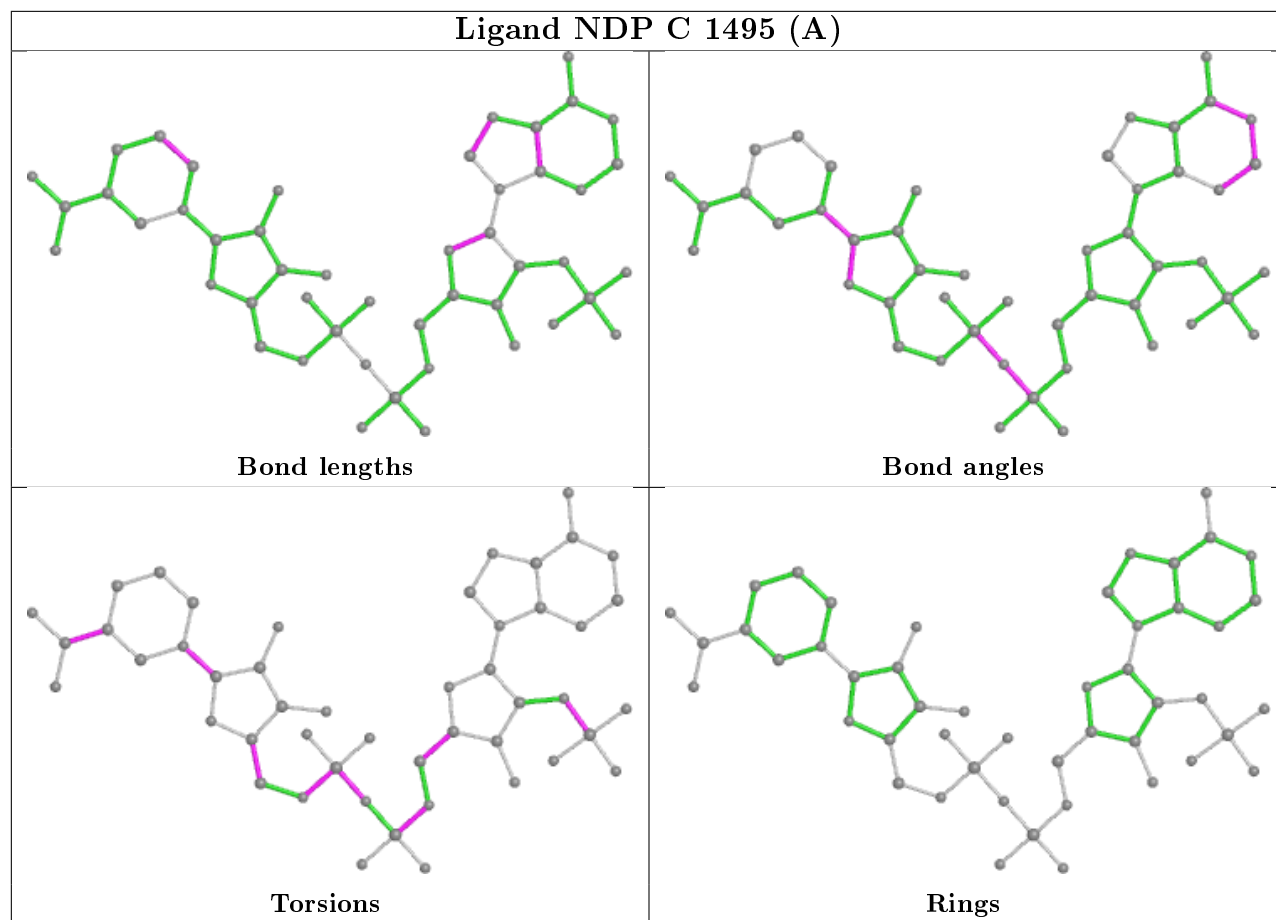
Continued on next page...

Continued from previous page...

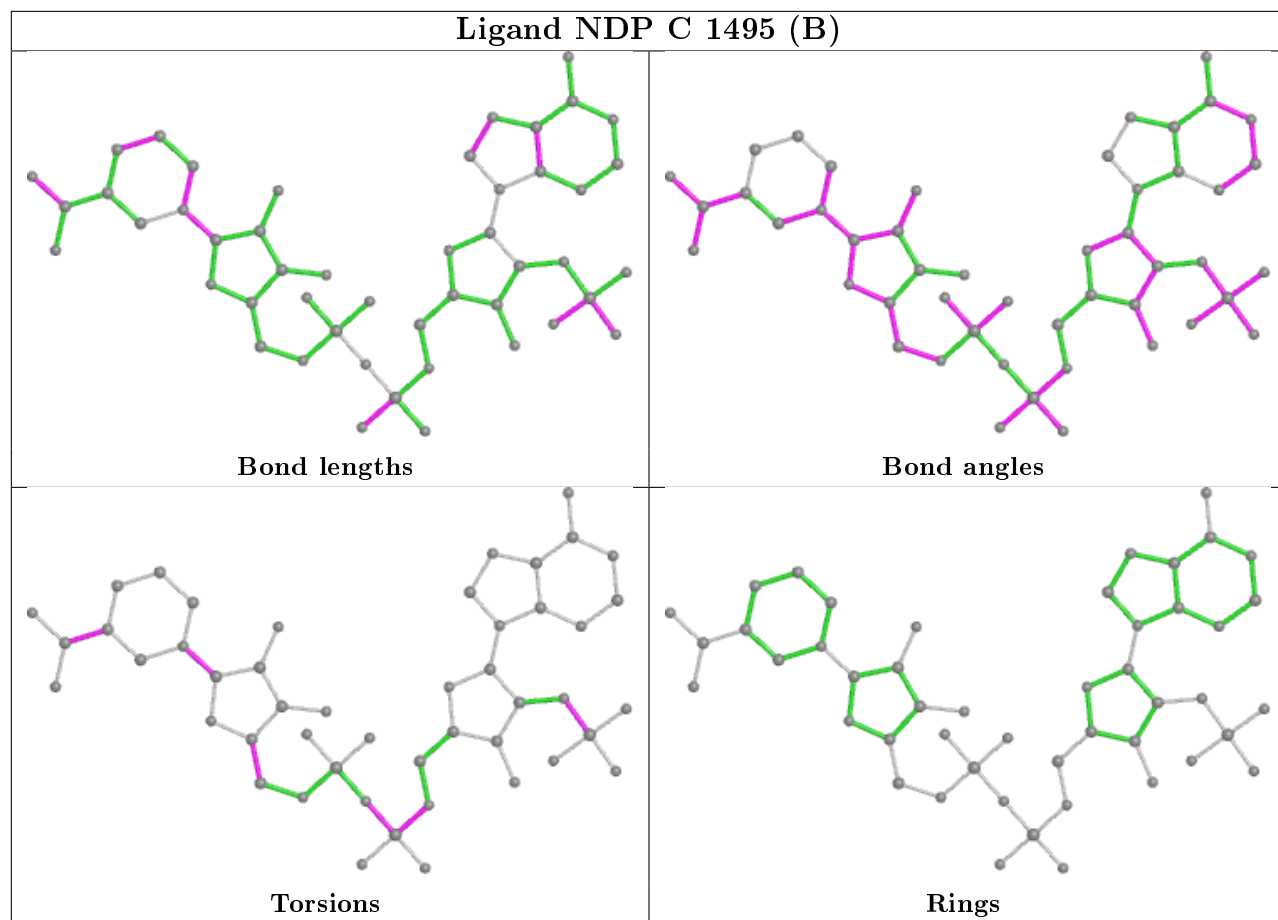
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1494	GOL	1	0
5	D	1496[A]	NDP	1	0
2	A	1499	GOL	10	0
5	B	1498[A]	NDP	6	0
5	D	1496[B]	NDP	14	0
2	D	1491	GOL	2	0
3	A	1495	PG4	27	0
5	B	1498[B]	NDP	10	0
2	D	1494	GOL	3	0
4	A	1498	EDO	16	0
5	A	1500[B]	NDP	6	0
2	B	1494	GOL	2	0
2	D	1493	GOL	3	0
2	C	1492	GOL	6	0

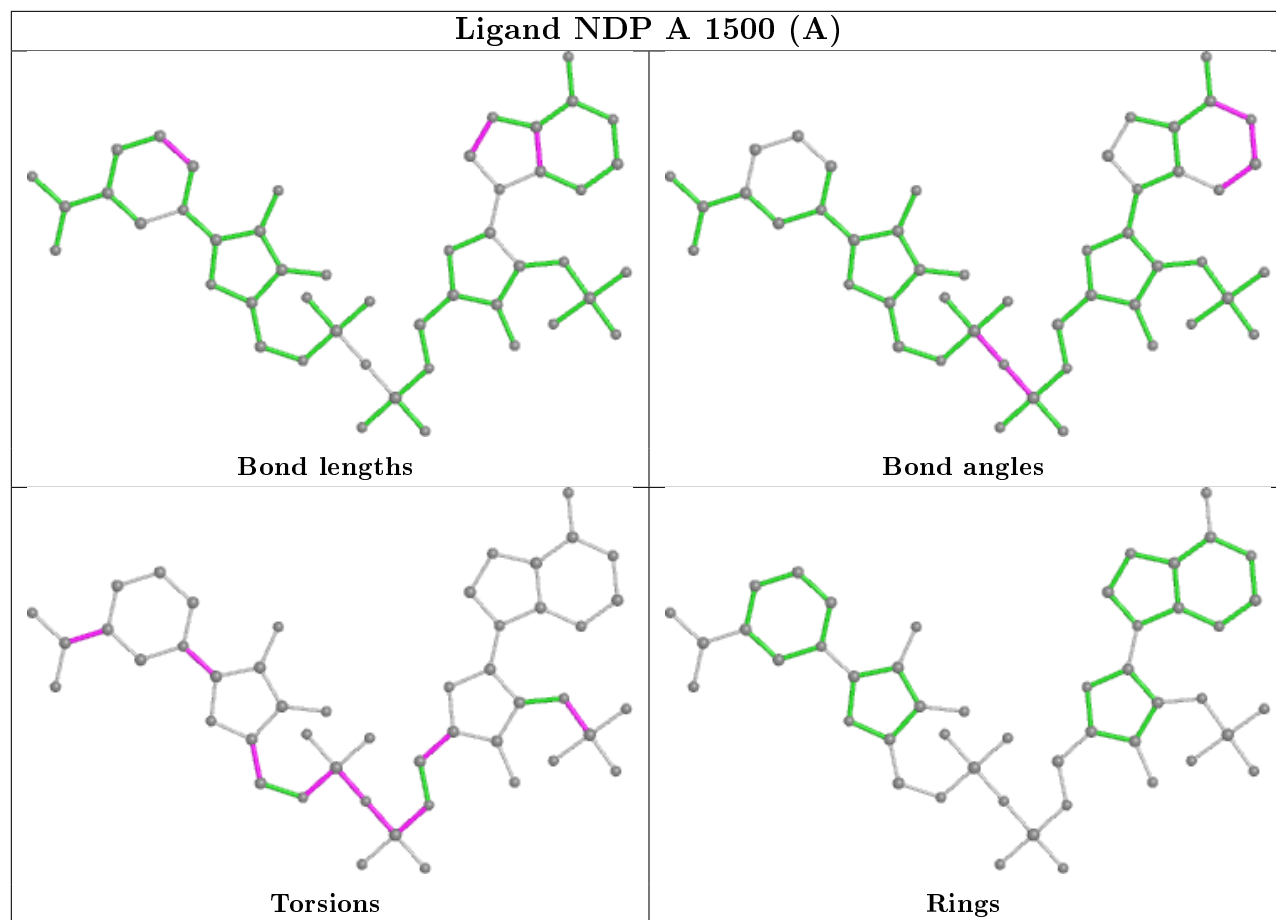
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 NDP C 1495 (A)

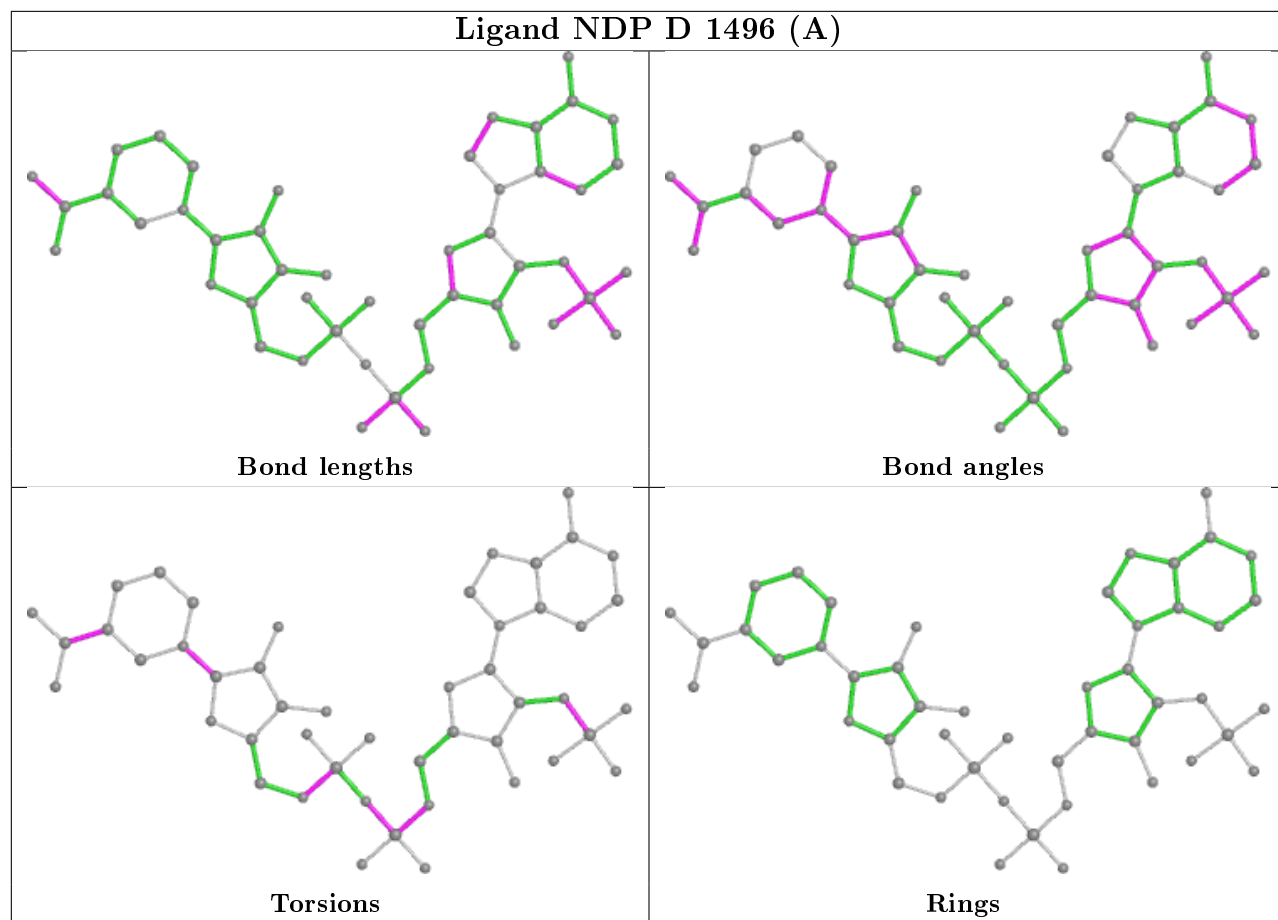


Ligand NDP C 1495 (B)

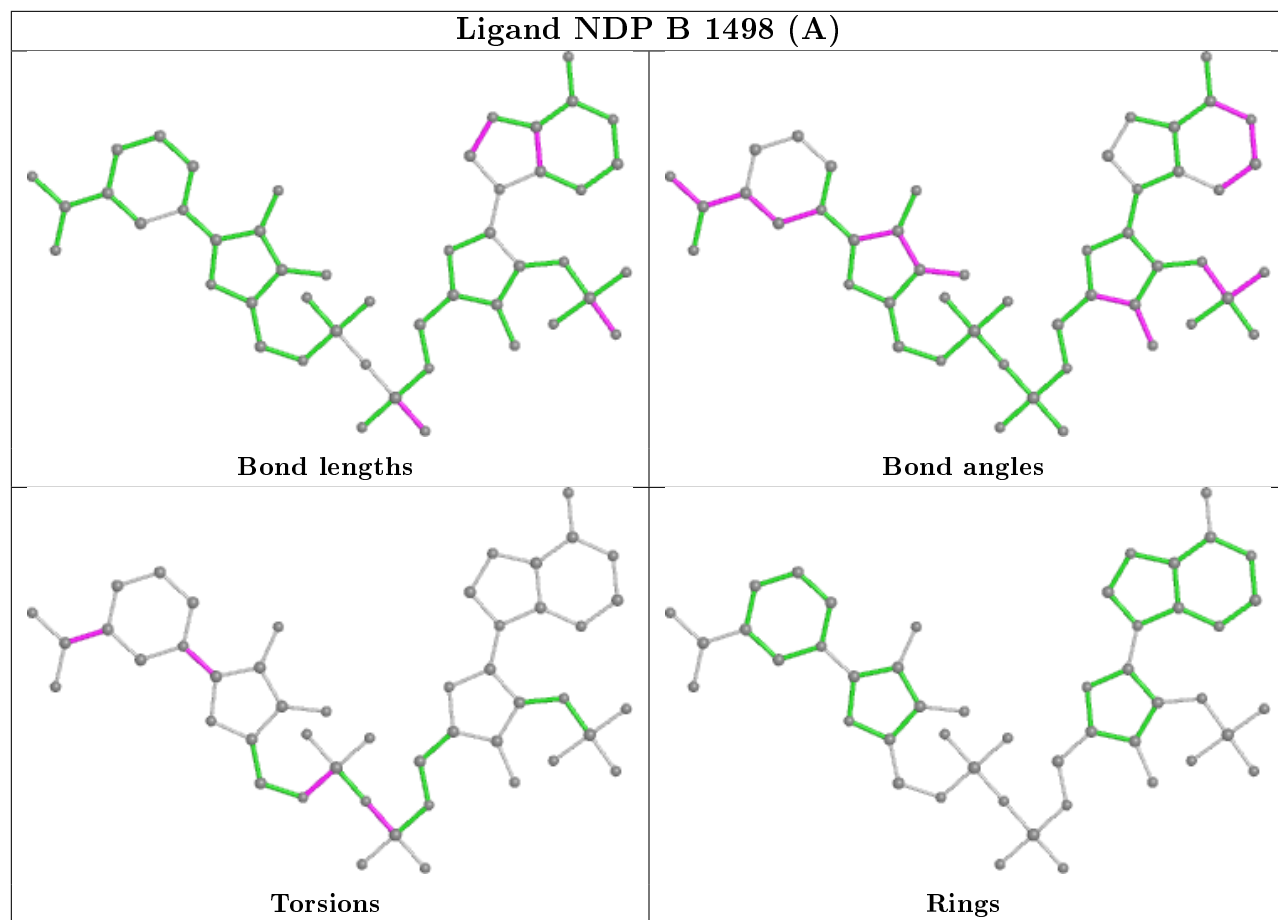




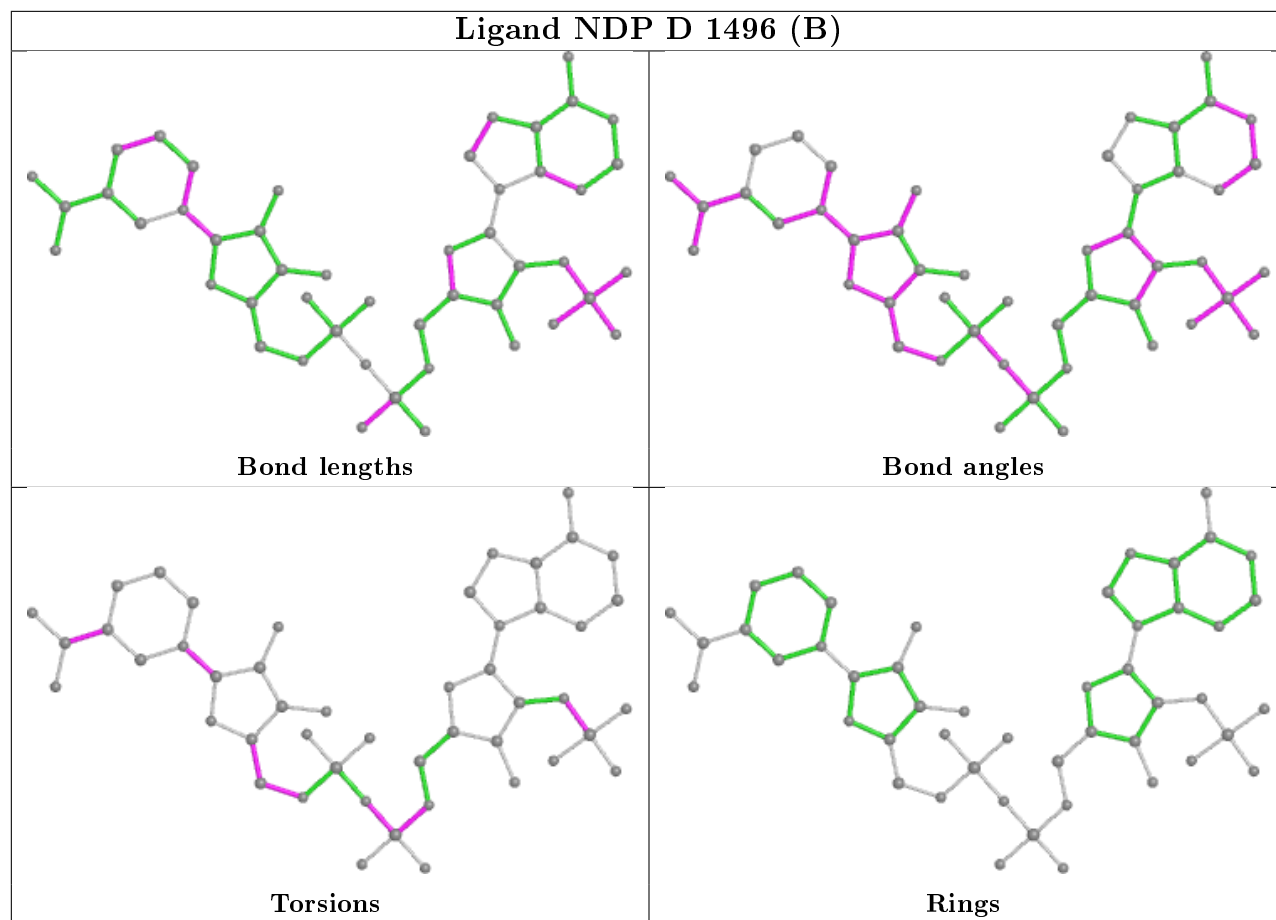
Ligand NDP D 1496 (A)



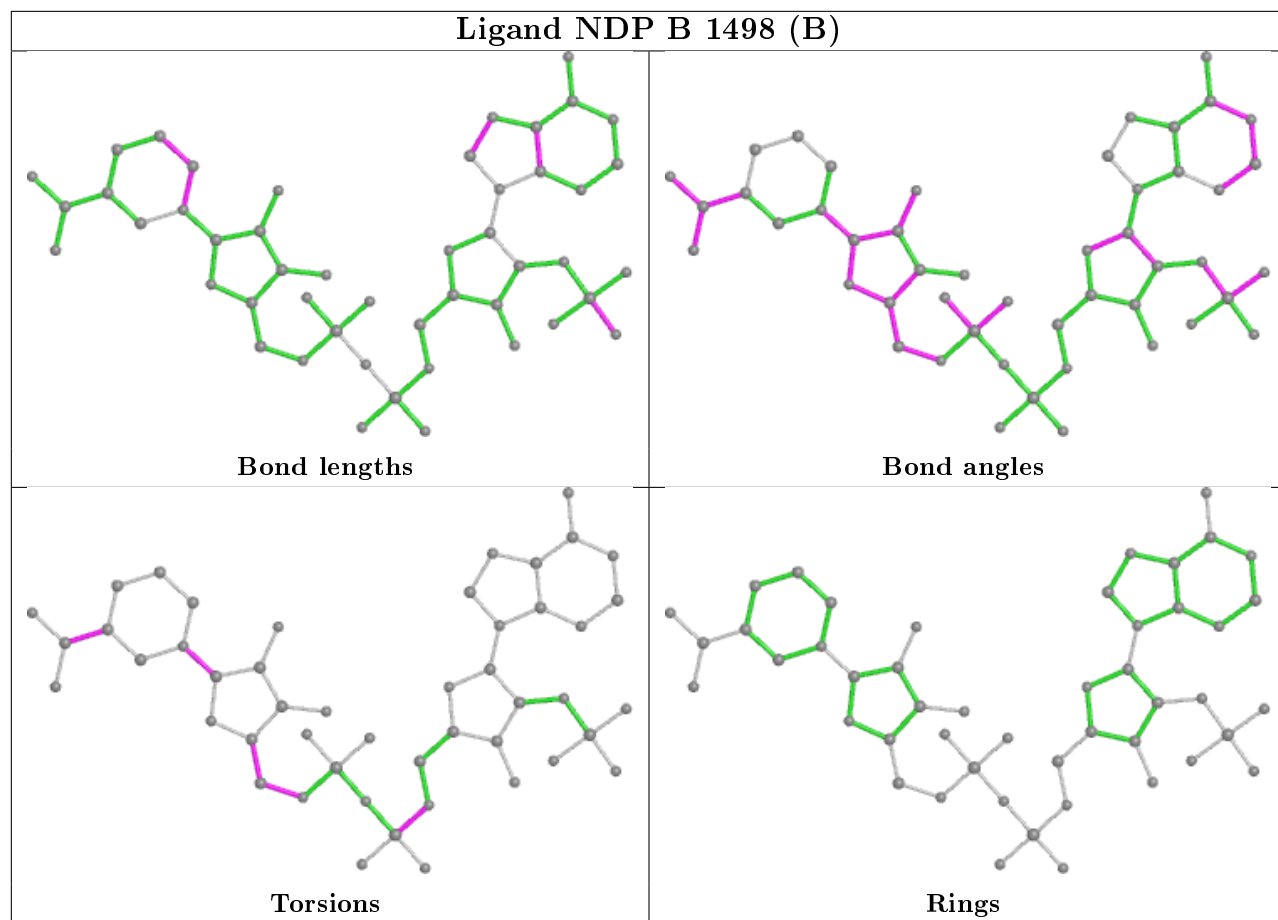
Ligand NDP B 1498 (A)

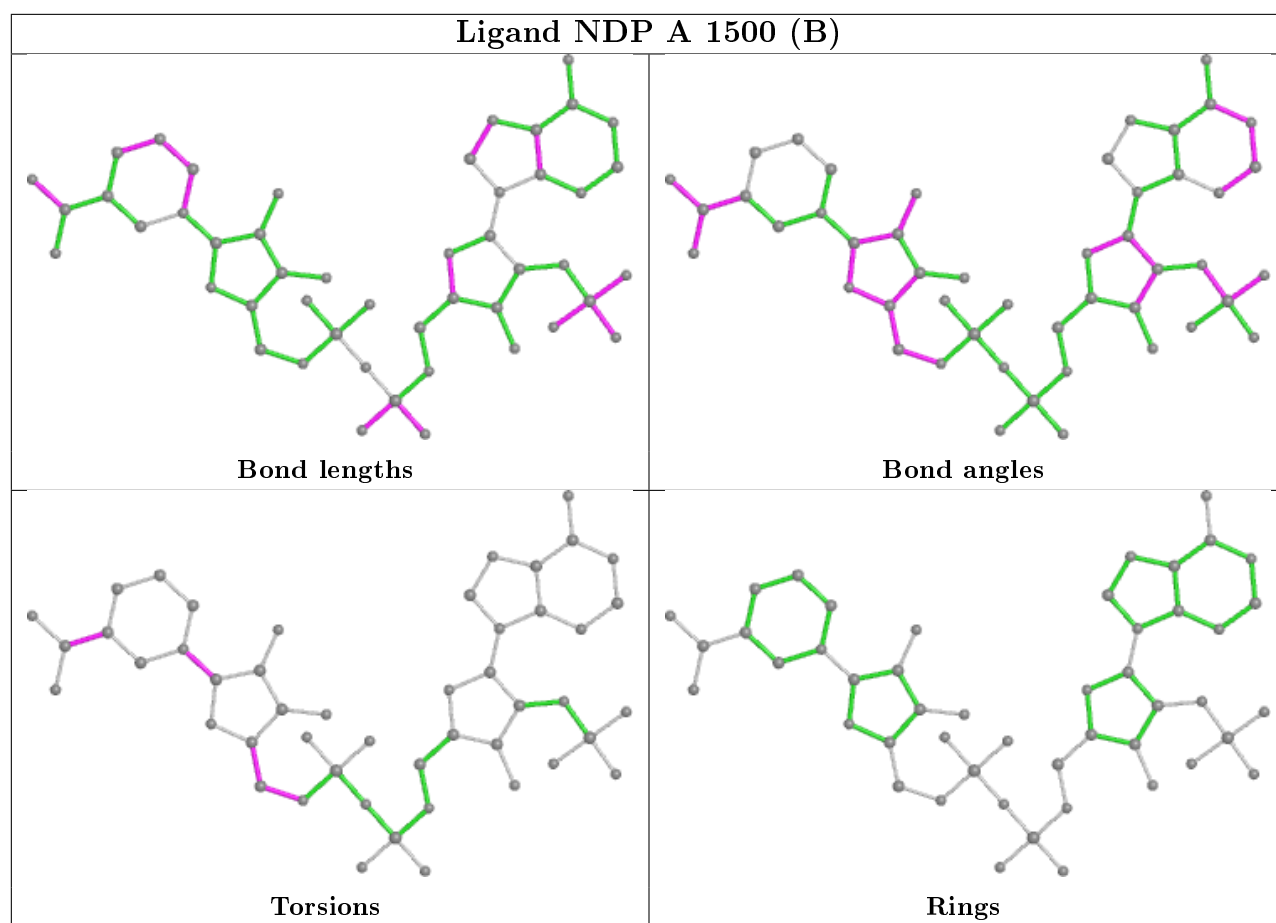


Ligand NDP D 1496 (B)



Ligand NDP B 1498 (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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	489/490 (99%)	-0.59	3 (0%) 89 89	19, 29, 47, 73	0
1	B	489/490 (99%)	-0.35	10 (2%) 65 62	18, 41, 65, 89	0
1	C	489/490 (99%)	-0.56	6 (1%) 79 77	23, 40, 64, 96	0
1	D	489/490 (99%)	-0.66	0 100 100	21, 36, 61, 82	0
All	All	1956/1960 (99%)	-0.54	19 (0%) 82 83	18, 36, 62, 96	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	ALA	4.1
1	B	285	VAL	3.5
1	B	287	THR	3.0
1	B	415	LEU	2.9
1	C	21	GLY	2.7
1	A	285	VAL	2.5
1	B	255	GLY	2.5
1	B	346	ALA	2.5
1	C	19	SER	2.4
1	C	2	ALA	2.4
1	B	253	LEU	2.4
1	C	20	SER	2.2
1	B	453	VAL	2.2
1	B	158	ILE	2.2
1	C	154	TYR	2.1
1	C	22	ALA	2.1
1	A	158	ILE	2.1
1	A	161	TRP	2.1
1	B	389	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
2	GOL	B	1496	6/6	0.47	0.30	70,79,87,87	0
6	K	D	1498	1/1	0.72	0.14	92,92,92,92	0
2	GOL	C	1493	6/6	0.74	0.37	79,93,97,97	0
4	EDO	C	1497	4/4	0.75	0.68	53,63,64,74	0
2	GOL	A	1497	6/6	0.77	0.18	57,65,70,79	0
6	K	A	1501	1/1	0.77	0.13	56,56,56,56	0
2	GOL	B	1491	6/6	0.78	0.35	77,83,86,87	0
2	GOL	D	1495	6/6	0.79	0.22	71,75,84,90	0
6	K	B	1499	1/1	0.79	0.41	106,106,106,106	0
6	K	D	1497	1/1	0.80	0.14	59,59,59,59	0
2	GOL	A	1491	6/6	0.80	0.44	14,33,38,39	6
5	NDP	B	1498[A]	48/48	0.81	0.28	38,54,80,85	48
2	GOL	A	1492	6/6	0.81	0.42	58,71,73,73	0
5	NDP	B	1498[B]	48/48	0.81	0.28	23,58,80,85	48
2	GOL	C	1494	6/6	0.82	0.26	70,79,84,87	0
5	NDP	C	1495[B]	48/48	0.85	0.23	24,53,68,71	48
6	K	C	1499	1/1	0.85	0.14	99,99,99,99	0
5	NDP	C	1495[A]	48/48	0.85	0.23	41,54,68,72	48
2	GOL	D	1491	6/6	0.86	0.32	41,69,82,88	0
3	PG4	A	1495	13/13	0.86	0.43	54,57,70,73	0
7	TOE	C	1496	11/11	0.86	0.40	45,56,66,67	0
2	GOL	D	1493	6/6	0.86	0.44	51,61,65,69	0
2	GOL	B	1495	6/6	0.87	0.57	42,53,59,65	0
2	GOL	A	1496	6/6	0.88	0.16	33,61,73,82	0
6	K	A	1502	1/1	0.89	0.10	71,71,71,71	0
2	GOL	B	1493	6/6	0.90	0.15	59,63,64,70	0
2	GOL	B	1494	6/6	0.90	0.14	63,74,81,84	0

Continued on next page...

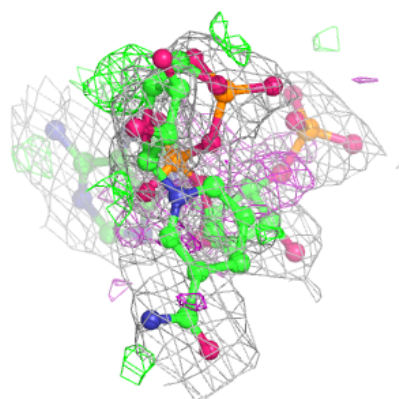
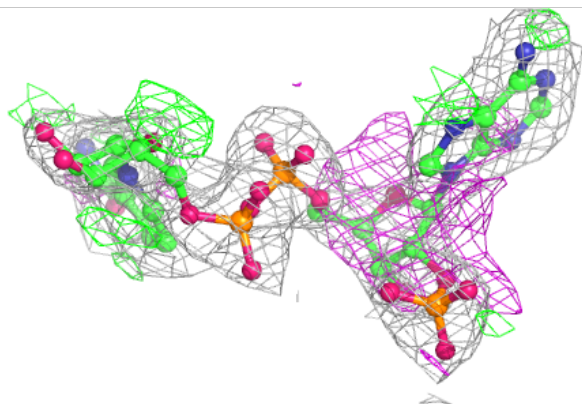
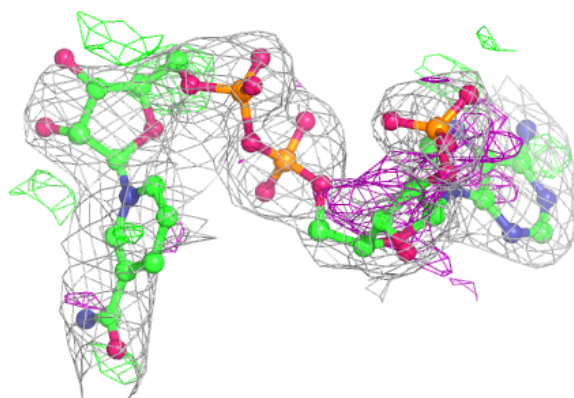
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	B	1497	6/6	0.90	0.13	93,97,97,98	0
2	GOL	D	1494	6/6	0.91	0.18	42,47,64,64	0
2	GOL	B	1492	6/6	0.91	0.60	51,68,75,79	0
2	GOL	A	1494	6/6	0.91	0.23	50,72,85,88	0
2	GOL	C	1491	6/6	0.92	0.16	69,72,76,76	0
2	GOL	A	1493	6/6	0.92	0.12	54,57,67,74	0
5	NDP	A	1500[B]	48/48	0.92	0.19	23,40,46,54	48
6	K	C	1498	1/1	0.92	0.13	79,79,79,79	0
5	NDP	A	1500[A]	48/48	0.92	0.19	20,41,48,53	48
2	GOL	D	1492	6/6	0.93	0.51	45,46,51,55	0
6	K	B	1500	1/1	0.93	0.07	70,70,70,70	0
5	NDP	D	1496[B]	48/48	0.94	0.16	18,35,48,50	48
4	EDO	A	1498	4/4	0.94	0.53	44,48,52,67	0
5	NDP	D	1496[A]	48/48	0.94	0.16	27,35,46,50	48
2	GOL	A	1499	6/6	0.95	0.42	42,55,57,60	0
2	GOL	C	1492	6/6	0.95	0.29	51,56,58,60	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.

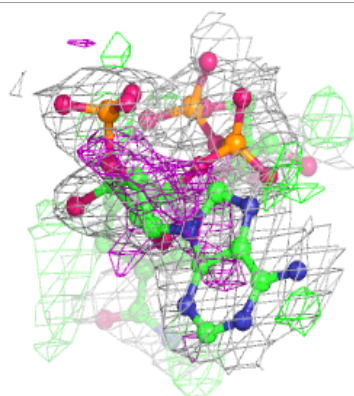
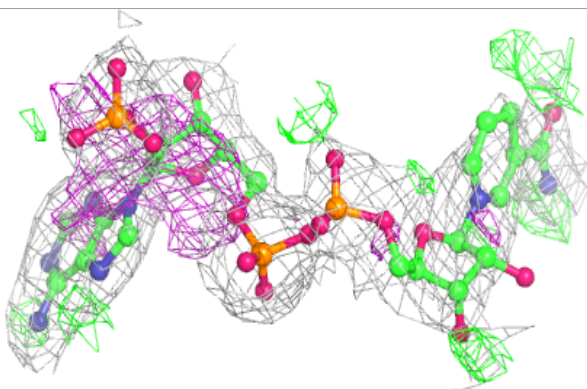
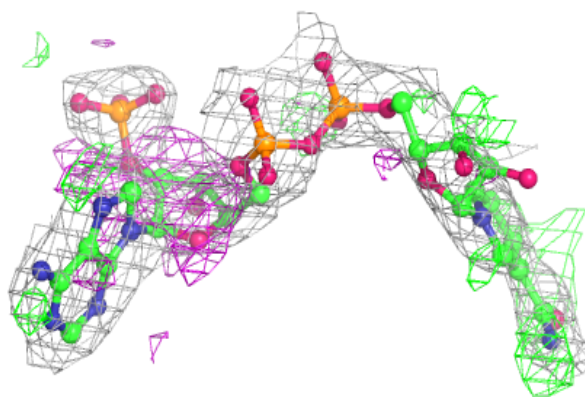
Electron density around NDP B 1498 (A):

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

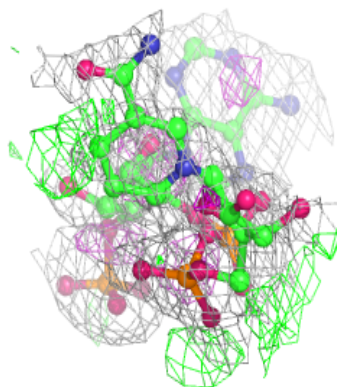
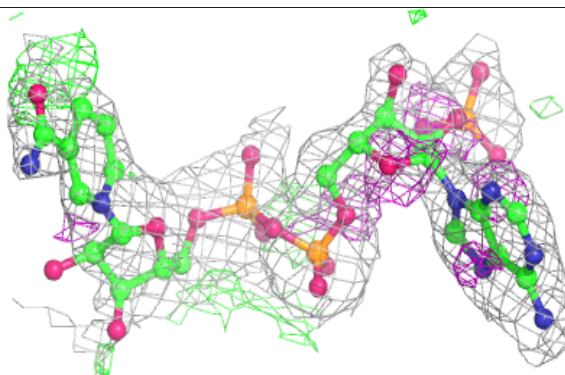
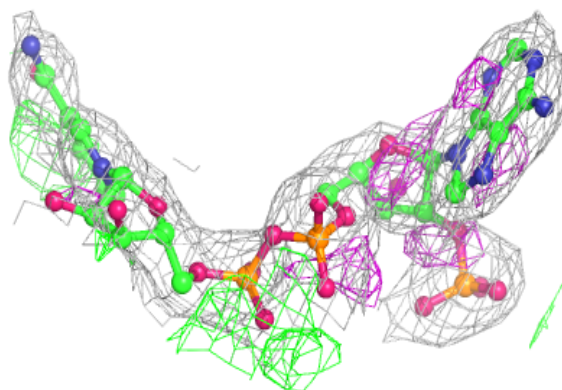


Electron density around NDP B 1498 (B):

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

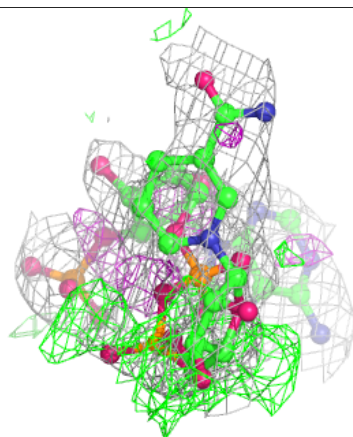
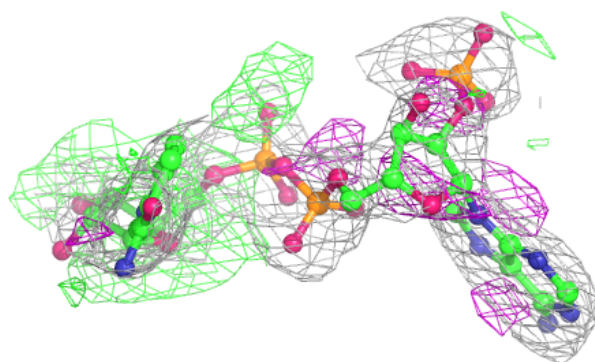
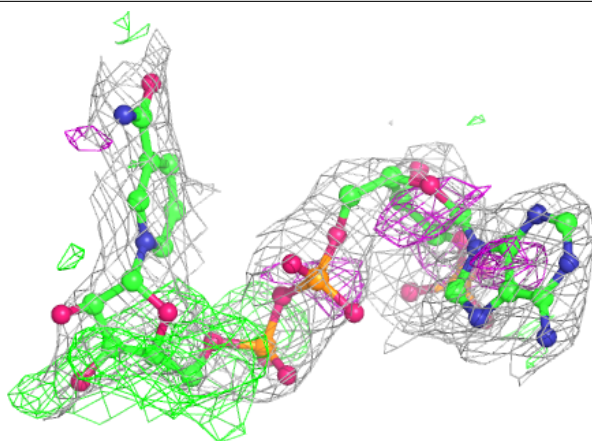
**Electron density around NDP C 1495 (B):**

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

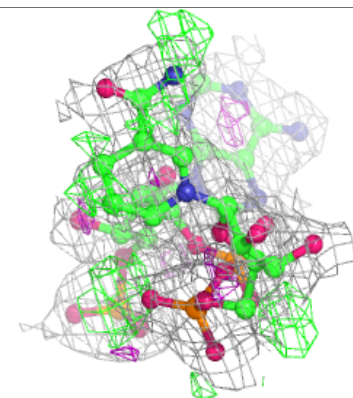
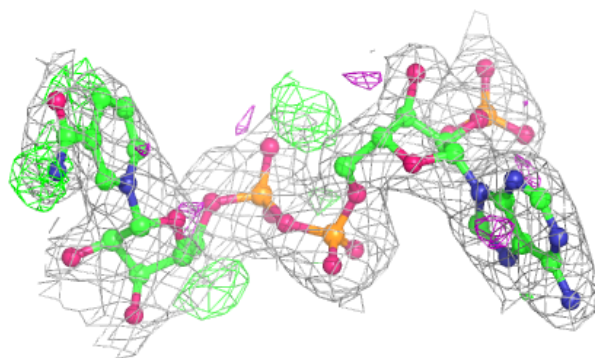
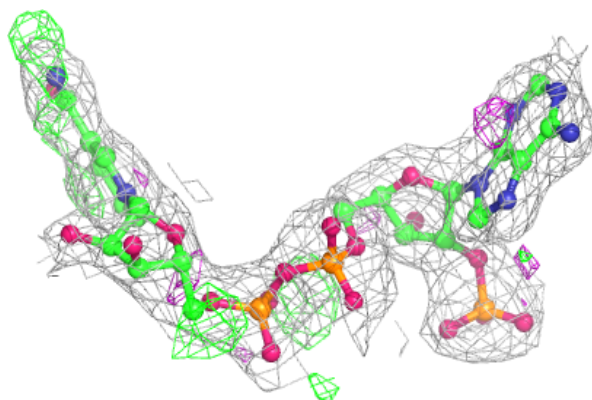


Electron density around NDP C 1495 (A):

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

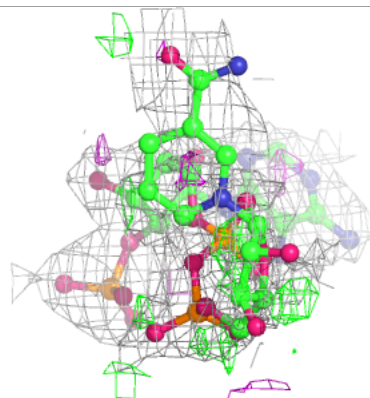
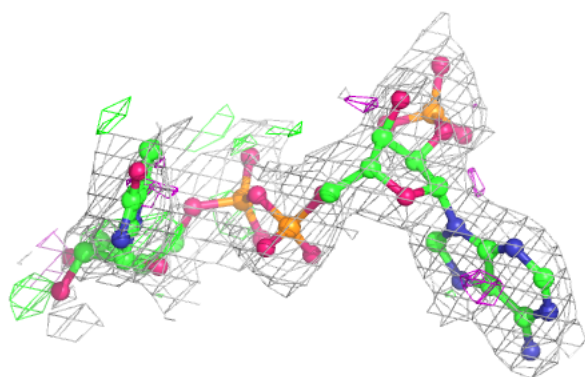
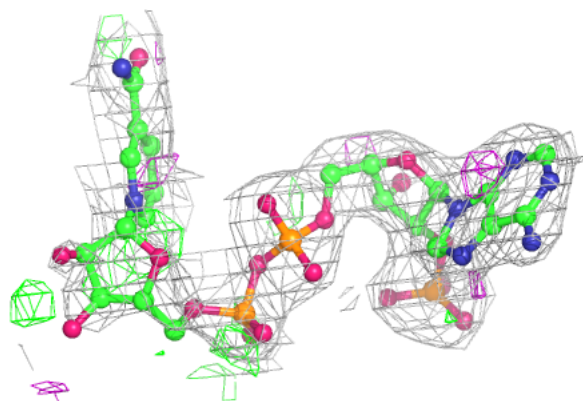
**Electron density around NDP A 1500 (B):**

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

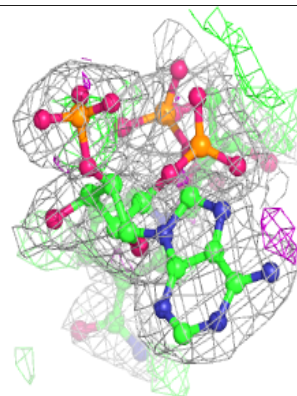
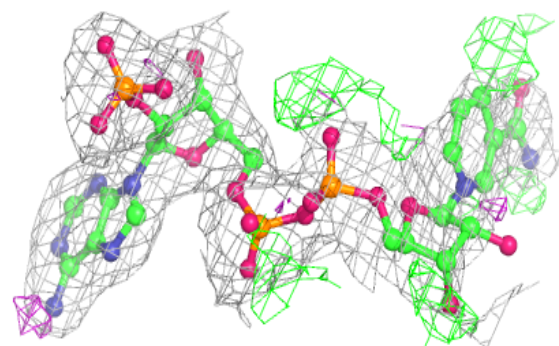
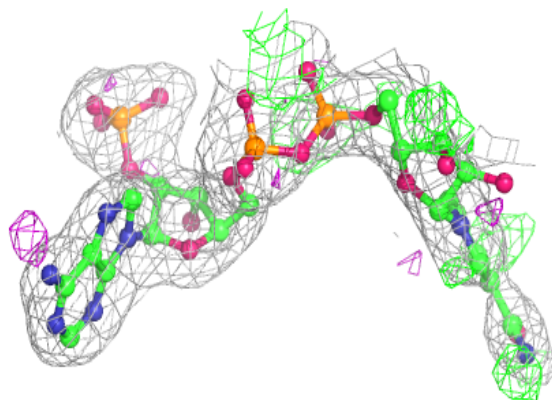


Electron density around NDP A 1500 (A):

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

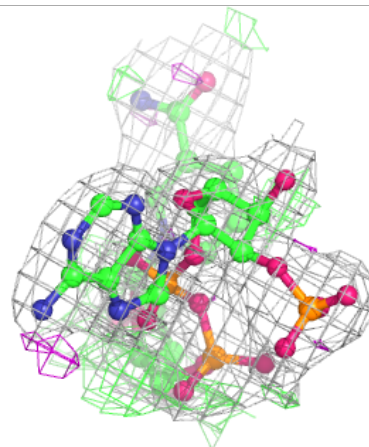
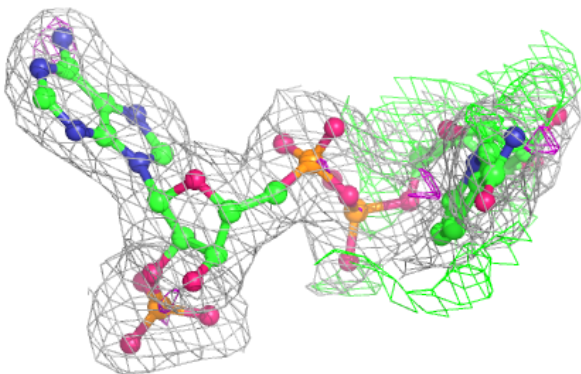
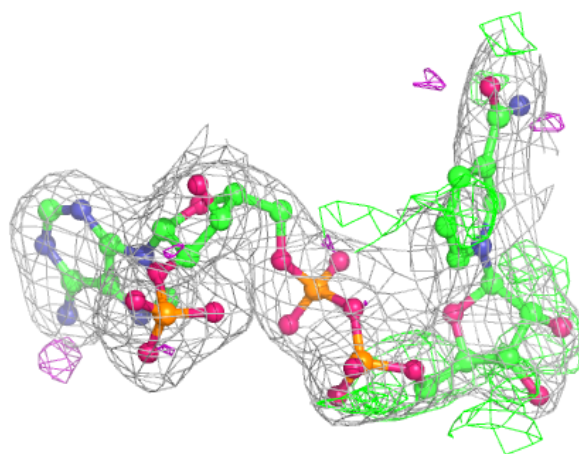
**Electron density around NDP D 1496 (B):**

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



Electron density around NDP D 1496 (A):

$2mF_o-DF_c$ (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.