



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:38 PM UTC

PDB ID : 7W5N / pdb_00007w5n
Title : The crystal structure of the reduced form of Gluconobacter oxydans WSH-004 SNDH
Authors : Li, D.; Hou, X.D.; Rao, Y.J.; Yin, D.J.; Zhou, J.W.; Chen, J.
Deposited on : 2021-11-30
Resolution : 2.99 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

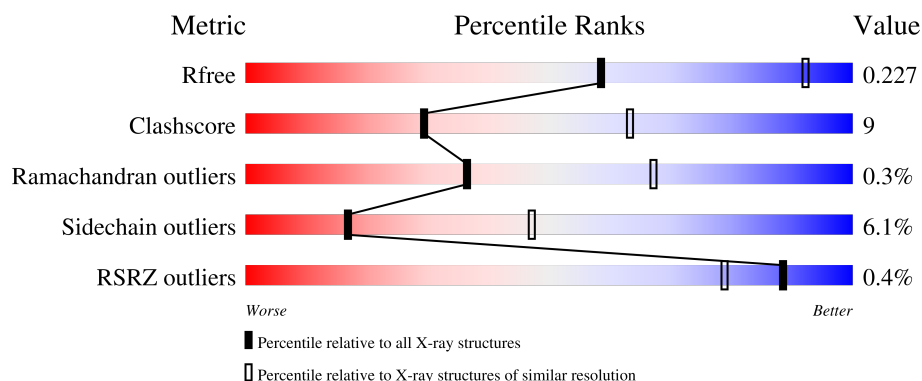
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

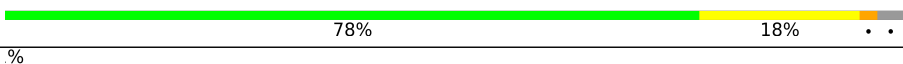
The reported resolution of this entry is 2.99 Å.

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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	504	
1	B	504	
1	C	504	
1	D	504	

2 Entry composition ⓘ

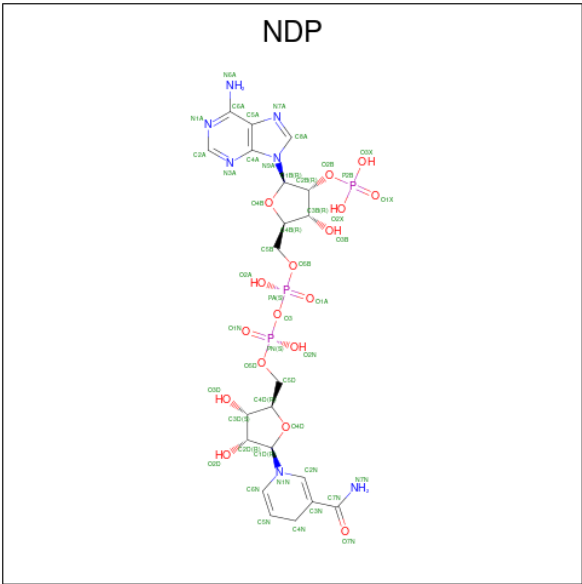
There are 3 unique types of molecules in this entry. The entry contains 15112 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-sorbose dehydrogenase, NAD(P) dependent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3722	2361	645	698	18			
1	B	491	Total	C	N	O	S	0	0	0
			3715	2357	644	696	18			
1	C	490	Total	C	N	O	S	0	0	0
			3708	2352	643	695	18			
1	D	491	Total	C	N	O	S	0	0	0
			3715	2357	644	696	18			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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

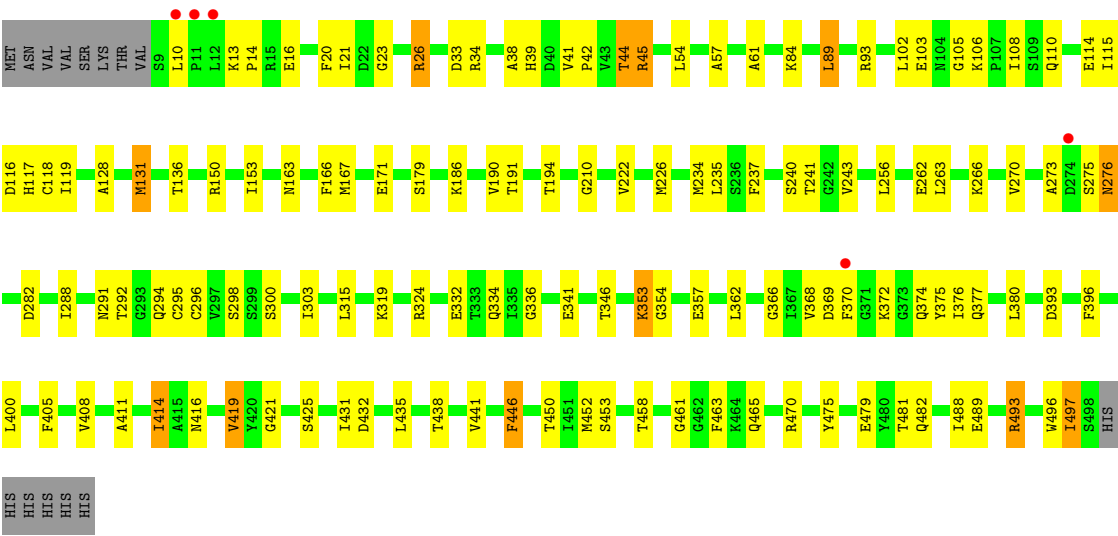
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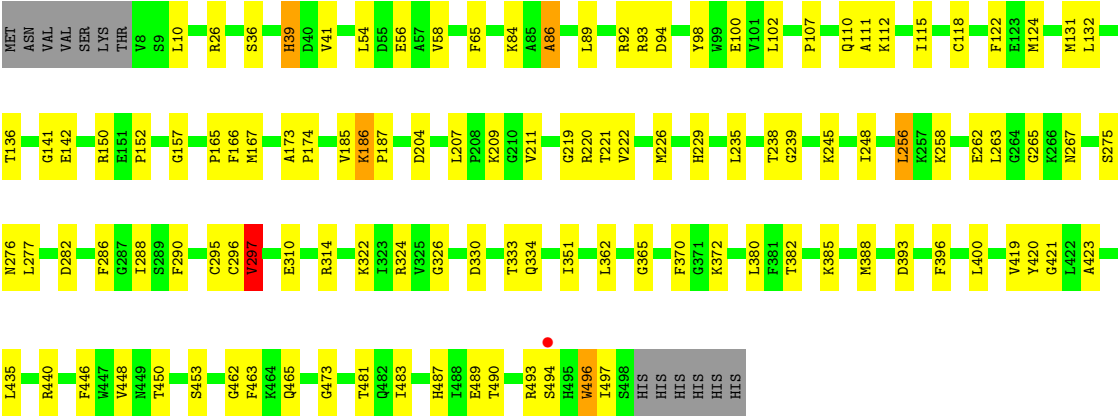
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	10	Total	O	0	0
			10	10		
3	C	16	Total	O	0	0
			16	16		
3	D	18	Total	O	0	0
			18	18		



● Molecule 1: L-sorbose dehydrogenase, NAD(P) dependent



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.24Å 118.82Å 109.02Å 90.00° 93.32° 90.00°	Depositor
Resolution (Å)	23.52 – 2.99 23.52 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.4 (23.52-2.99) 99.4 (23.52-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.31	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.99Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.171 , 0.219 0.181 , 0.227	Depositor DCC
R_{free} test set	3990 reflections (9.62%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15112	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP

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	1.03	0/3797	1.44	3/5142 (0.1%)
1	B	1.04	0/3790	1.44	5/5132 (0.1%)
1	C	1.04	0/3783	1.42	4/5122 (0.1%)
1	D	1.05	0/3790	1.44	12/5132 (0.2%)
All	All	1.04	0/15160	1.44	24/20528 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	SER	CA-C-O	-7.21	115.16	119.55
1	B	419	VAL	N-CA-C	-6.71	103.87	113.07
1	C	419	VAL	N-CA-C	-6.24	105.18	112.98
1	B	254	SER	O-C-N	6.15	125.38	120.83
1	D	141	GLY	CA-C-O	-5.95	118.16	122.45
1	B	254	SER	CA-C-O	-5.71	116.51	119.77
1	D	86	ALA	CA-C-N	5.49	126.03	120.00
1	D	86	ALA	C-N-CA	5.49	126.03	120.00
1	B	83	LEU	CA-C-O	-5.33	115.22	120.82
1	A	160	THR	CB-CA-C	5.33	116.84	108.63
1	A	254	SER	O-C-N	5.28	125.47	120.71
1	D	393	ASP	CA-CB-CG	5.27	117.87	112.60
1	D	107	PRO	CA-C-N	5.22	127.90	120.53
1	D	107	PRO	C-N-CA	5.22	127.90	120.53
1	D	39	HIS	N-CA-C	-5.22	107.56	114.04
1	D	157	GLY	CA-C-O	-5.17	116.57	120.76
1	D	496	TRP	N-CA-C	-5.17	106.83	113.23
1	D	462	GLY	CA-C-O	-5.16	116.47	121.11
1	D	276	ASN	CA-C-N	5.15	127.43	120.38
1	D	276	ASN	C-N-CA	5.15	127.43	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	ARG	CA-C-N	5.06	126.23	122.59
1	C	45	ARG	C-N-CA	5.06	126.23	122.59
1	C	26	ARG	CB-CA-C	5.04	118.60	109.37
1	B	28	GLY	CA-C-O	-5.03	117.86	122.24

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	3722	0	3711	73	0
1	B	3715	0	3704	61	0
1	C	3708	0	3695	89	0
1	D	3715	0	3704	59	0
2	A	48	0	26	7	0
2	B	48	0	26	3	0
2	C	48	0	26	2	0
2	D	48	0	26	3	0
3	A	16	0	0	0	0
3	B	10	0	0	0	0
3	C	16	0	0	1	0
3	D	18	0	0	0	0
All	All	15112	0	14918	259	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LYS:HB2	1:C:226:MET:HE1	1.33	1.05
1:B:396:PHE:HB2	2:B:601:NDP:H6N	1.34	1.03
1:C:396:PHE:HB2	2:C:601:NDP:H6N	1.41	1.02
1:A:186:LYS:HB2	1:A:226:MET:HE1	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PHE:HB2	2:A:601:NDP:H6N	1.54	0.89
1:C:34:ARG:HB3	1:C:44:THR:HG22	1.61	0.80
1:D:297:VAL:HG12	1:D:423:ALA:HB2	1.67	0.76
1:A:297:VAL:HG12	1:A:423:ALA:HB2	1.69	0.74
1:A:396:PHE:CB	2:A:601:NDP:H6N	2.18	0.74
1:B:234:MET:HG3	1:B:258:LYS:HB3	1.68	0.74
1:B:361:LEU:HD11	1:B:379:THR:HG23	1.70	0.73
1:C:39:HIS:HA	1:C:372:LYS:HD2	1.71	0.73
1:A:451:ILE:HG13	1:A:452:MET:HG3	1.71	0.72
1:C:16:GLU:HA	1:C:45:ARG:HB2	1.70	0.71
1:C:295:CYS:HB2	1:C:298:SER:HB3	1.72	0.71
1:B:361:LEU:HD21	1:B:365:GLY:HA3	1.75	0.69
1:D:186:LYS:HD2	1:D:222:VAL:HG23	1.76	0.68
1:A:474:LEU:HB2	1:C:131:MET:HE1	1.75	0.67
1:B:419:VAL:O	1:B:465:GLN:HB2	1.95	0.66
1:C:341:GLU:HG2	1:C:374:GLN:HE22	1.61	0.66
1:D:385:LYS:H	1:D:388:MET:HE3	1.62	0.64
1:B:396:PHE:CB	2:B:601:NDP:H6N	2.19	0.63
1:A:89:LEU:HD12	1:A:201:ILE:HD13	1.81	0.62
1:C:488:ILE:HG12	1:D:448:VAL:HB	1.81	0.62
1:A:111:ALA:O	1:A:115:ILE:HG12	1.99	0.62
1:C:366:GLY:O	1:C:377:GLN:HG2	2.00	0.62
1:B:470:ARG:O	1:B:479:GLU:HG3	2.00	0.61
1:C:497:ILE:HG22	1:D:322:LYS:HE3	1.83	0.61
1:D:94:ASP:OD1	1:D:112:LYS:NZ	2.29	0.61
1:C:419:VAL:O	1:C:465:GLN:HB2	2.01	0.61
1:B:361:LEU:HD11	1:B:379:THR:CG2	2.31	0.60
1:C:93:ARG:NH1	1:C:116:ASP:OD1	2.35	0.60
1:A:186:LYS:HB2	1:A:226:MET:CE	2.30	0.60
1:B:295:CYS:HB3	1:B:298:SER:HB3	1.84	0.59
1:B:351:ILE:HG22	1:B:355:LYS:HE2	1.84	0.59
1:C:241:THR:HA	1:C:263:LEU:HD13	1.83	0.59
1:D:219:GLY:HA3	2:D:601:NDP:C8A	2.32	0.59
1:D:207:LEU:HD11	1:D:211:VAL:HG11	1.85	0.59
1:A:32:PHE:HE1	1:A:217:GLY:HA2	1.68	0.58
1:B:390:ILE:HG22	1:B:395:ILE:HD11	1.84	0.58
1:D:93:ARG:HG3	1:D:115:ILE:HG21	1.85	0.58
1:D:89:LEU:HD11	1:D:166:PHE:CZ	2.39	0.58
1:B:164:PHE:HB2	1:B:168:ILE:HG13	1.85	0.57
1:A:118:CYS:SG	1:A:167:MET:HA	2.44	0.57
1:D:245:LYS:HA	1:D:248:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ALA:C	1:C:275:SER:H	2.12	0.57
1:A:266:LYS:HE2	1:A:300:SER:HB2	1.87	0.56
1:B:265:GLY:HA2	1:B:420:TYR:CG	2.41	0.56
1:D:100:GLU:OE2	1:D:165:PRO:HD2	2.05	0.56
1:D:26:ARG:NH2	1:D:56:GLU:OE1	2.38	0.56
1:B:241:THR:O	1:B:245:LYS:HG3	2.06	0.56
1:D:295:CYS:SG	1:D:297:VAL:HG23	2.46	0.56
1:A:459:PRO:HG3	1:A:475:TYR:CD2	2.39	0.56
1:B:382:THR:HG22	1:B:383:ASP:H	1.71	0.56
1:A:314:ARG:HA	1:A:317:VAL:HG22	1.88	0.55
1:C:362:LEU:HD12	1:C:380:LEU:HD12	1.87	0.55
1:A:396:PHE:HB2	2:A:601:NDP:C6N	2.30	0.55
1:A:489:GLU:OE2	1:B:450:THR:HG23	2.06	0.55
1:C:380:LEU:HD23	1:C:400:LEU:HD23	1.89	0.55
1:B:359:ALA:HB2	1:B:388:MET:HE1	1.88	0.55
1:C:39:HIS:O	1:C:41:VAL:HG13	2.07	0.55
1:C:222:VAL:HG12	1:C:226:MET:HE2	1.89	0.54
1:C:450:THR:HB	1:D:489:GLU:HB2	1.89	0.54
1:B:243:VAL:HG21	2:B:601:NDP:O2A	2.07	0.54
1:C:237:PHE:CZ	1:C:243:VAL:HB	2.42	0.54
1:D:92:ARG:NH2	1:D:204:ASP:OD2	2.37	0.54
1:B:274:ASP:OD1	1:B:274:ASP:C	2.50	0.54
1:C:186:LYS:CB	1:C:226:MET:HE1	2.24	0.54
1:A:70:TRP:CD1	1:A:180:GLY:HA2	2.43	0.54
1:B:297:VAL:HG23	1:B:452:MET:HE2	1.90	0.53
1:C:282:ASP:CG	1:D:496:TRP:H	2.16	0.53
1:A:436:ALA:O	1:A:440:ARG:HG3	2.09	0.53
1:B:48:ARG:NH1	1:B:189:GLU:OE2	2.42	0.52
1:C:222:VAL:HG12	1:C:226:MET:CE	2.38	0.52
1:D:58:VAL:HG11	1:D:229:HIS:CE1	2.44	0.52
1:C:396:PHE:CD1	2:C:601:NDP:H1D	2.45	0.52
1:D:124:MET:HE2	1:D:473:GLY:HA2	1.91	0.52
1:C:266:LYS:HE3	1:C:393:ASP:O	2.10	0.52
1:C:496:TRP:N	1:D:282:ASP:OD2	2.36	0.52
1:D:419:VAL:HB	1:D:465:GLN:OE1	2.10	0.52
1:A:131:MET:HE1	1:C:128:ALA:CA	2.40	0.51
1:B:270:VAL:HA	1:B:303:ILE:O	2.11	0.51
1:C:14:PRO:HG3	1:C:42:PRO:HB2	1.92	0.51
1:C:44:THR:HG21	1:C:103:GLU:OE2	2.11	0.51
1:D:185:VAL:HG12	1:D:187:PRO:HD3	1.92	0.51
1:A:30:ASP:HB2	1:A:48:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ARG:HH12	1:B:451:ILE:HG22	1.75	0.51
1:B:475:TYR:O	1:B:479:GLU:HG2	2.10	0.51
1:A:38:ALA:HB1	1:A:375:TYR:OH	2.11	0.51
1:C:163:ASN:HB2	1:C:294:GLN:O	2.11	0.51
1:D:267:ASN:ND2	1:D:296:CYS:O	2.40	0.51
1:C:489:GLU:OE1	1:D:450:THR:OG1	2.27	0.50
1:D:89:LEU:HD11	1:D:166:PHE:HZ	1.75	0.50
1:B:70:TRP:CH2	1:B:78:ARG:HA	2.47	0.50
1:A:34:ARG:HB3	1:A:44:THR:OG1	2.12	0.50
1:C:13:LYS:HG2	1:C:14:PRO:HD2	1.94	0.50
1:D:111:ALA:O	1:D:115:ILE:HG12	2.12	0.50
1:B:357:GLU:CB	1:B:388:MET:HE3	2.42	0.50
1:C:20:PHE:CZ	1:C:23:GLY:HA2	2.46	0.50
1:A:490:THR:HG23	1:C:432:ASP:HA	1.94	0.49
1:C:431:ILE:O	1:C:435:LEU:HB2	2.11	0.49
1:C:438:THR:HA	1:C:446:PHE:CZ	2.48	0.49
1:B:92:ARG:NH2	1:B:204:ASP:OD2	2.41	0.49
1:C:303:ILE:HD12	1:C:414:ILE:HB	1.94	0.49
1:A:49:CYS:HB2	1:A:216:THR:O	2.13	0.49
1:D:98:TYR:CZ	1:D:102:LEU:HD11	2.47	0.49
1:A:58:VAL:HG13	1:A:155:VAL:HG11	1.95	0.49
1:A:100:GLU:OE2	1:A:165:PRO:HD2	2.13	0.49
1:A:106:LYS:NZ	1:A:291:ASN:OD1	2.46	0.49
1:B:10:LEU:HD13	1:B:41:VAL:HG21	1.94	0.49
1:C:115:ILE:O	1:C:119:ILE:HG13	2.13	0.48
1:A:361:LEU:HD21	1:A:379:THR:HG23	1.94	0.48
1:C:458:THR:HG21	1:D:487:HIS:CE1	2.48	0.48
1:D:324:ARG:HG3	1:D:334:GLN:OE1	2.14	0.48
1:A:396:PHE:CG	2:A:601:NDP:H1D	2.48	0.48
1:A:496:TRP:CZ3	1:B:286:PHE:HA	2.49	0.48
1:D:150:ARG:NH1	1:D:481:THR:OG1	2.47	0.48
1:D:173:ALA:N	1:D:174:PRO:HD2	2.29	0.48
1:B:70:TRP:CZ3	1:B:78:ARG:HG2	2.48	0.47
1:B:135:ASP:O	1:C:136:THR:HG23	2.14	0.47
1:C:273:ALA:C	1:C:275:SER:N	2.71	0.47
1:C:461:GLY:HA3	1:C:470:ARG:HD3	1.96	0.47
1:C:470:ARG:O	1:C:479:GLU:HG3	2.14	0.47
1:C:262:GLU:OE1	1:C:461:GLY:HA2	2.14	0.47
1:B:309:ALA:HB1	1:B:404:HIS:NE2	2.30	0.47
1:A:104:ASN:OD1	1:A:106:LYS:HG3	2.15	0.47
1:A:54:LEU:O	1:A:58:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:GLY:HA2	1:D:370:PHE:CE2	2.50	0.47
1:B:357:GLU:HB3	1:B:388:MET:HE3	1.96	0.47
1:C:103:GLU:OE1	1:C:191:THR:HA	2.13	0.47
1:A:495:HIS:NE2	1:B:279:ASP:OD1	2.44	0.47
1:C:288:ILE:HD13	1:C:300:SER:HA	1.97	0.47
1:A:288:ILE:HG21	1:A:320:MET:HE3	1.97	0.47
1:B:309:ALA:HB1	1:B:404:HIS:CD2	2.50	0.47
1:C:496:TRP:CD2	1:D:286:PHE:HD1	2.33	0.46
1:D:419:VAL:O	1:D:465:GLN:HB2	2.15	0.46
2:D:601:NDP:H2D	2:D:601:NDP:H2N	1.61	0.46
1:C:319:LYS:NZ	1:D:497:ILE:O	2.49	0.46
1:D:310:GLU:HG2	1:D:314:ARG:NH2	2.31	0.46
1:D:265:GLY:HA2	1:D:420:TYR:CG	2.51	0.46
1:A:219:GLY:HA3	2:A:601:NDP:C8A	2.46	0.46
1:C:21:ILE:HB	1:C:26:ARG:HH21	1.81	0.46
2:D:601:NDP:O2A	2:D:601:NDP:H3D	2.16	0.46
1:C:105:GLY:O	1:C:336:GLY:HA3	2.17	0.45
1:C:296:CYS:HB2	3:C:707:HOH:O	2.16	0.45
1:C:416:ASN:HD21	1:C:441:VAL:HA	1.82	0.45
1:D:65:PHE:HE1	1:D:152:PRO:HB2	1.81	0.45
1:B:353:LYS:HE3	1:B:353:LYS:HB2	1.66	0.45
1:D:330:ASP:HB3	1:D:333:THR:HG23	1.96	0.45
1:A:64:ALA:HB3	1:A:182:THR:HG21	1.98	0.45
1:B:86:ALA:HB2	1:B:122:PHE:HB3	1.97	0.45
1:D:118:CYS:SG	1:D:167:MET:HA	2.55	0.45
1:A:70:TRP:O	1:A:78:ARG:HD3	2.16	0.45
1:A:288:ILE:HG12	1:A:400:LEU:HB2	1.98	0.45
1:C:475:TYR:CE1	1:D:483:ILE:HD12	2.51	0.45
1:A:131:MET:HE1	1:C:128:ALA:HA	1.99	0.45
1:C:190:VAL:HG23	1:C:191:THR:HG23	1.99	0.45
1:C:368:VAL:O	1:C:370:PHE:N	2.48	0.45
1:C:14:PRO:HG3	1:C:42:PRO:CB	2.47	0.45
1:A:361:LEU:HD21	1:A:379:THR:CG2	2.46	0.45
1:C:117:HIS:NE2	1:C:171:GLU:OE2	2.48	0.45
1:C:118:CYS:SG	1:C:167:MET:HA	2.57	0.45
1:A:22:ASP:C	1:A:24:GLU:H	2.25	0.44
1:C:324:ARG:NH2	1:C:332:GLU:O	2.46	0.44
1:D:86:ALA:HB2	1:D:122:PHE:HB3	1.98	0.44
1:C:270:VAL:HA	1:C:303:ILE:O	2.18	0.44
1:A:450:THR:HB	1:B:489:GLU:HB2	1.98	0.44
1:B:77:ASP:O	1:B:81:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ALA:N	1:B:174:PRO:HD2	2.33	0.44
1:A:124:MET:HE1	1:C:131:MET:HG2	1.98	0.44
1:A:361:LEU:HA	1:A:361:LEU:HD23	1.75	0.44
1:B:451:ILE:HG23	1:B:451:ILE:O	2.17	0.44
1:A:243:VAL:O	1:A:246:SER:HB2	2.18	0.44
1:C:61:ALA:HA	1:C:210:GLY:O	2.17	0.44
1:A:128:ALA:CB	1:A:477:VAL:HG21	2.48	0.44
1:C:276:ASN:C	1:C:276:ASN:HD22	2.24	0.44
1:B:244:GLY:O	1:B:248:ILE:HG13	2.17	0.44
1:D:238:THR:HG23	1:D:262:GLU:HB2	2.00	0.44
1:A:65:PHE:CZ	1:A:154:GLY:HA2	2.53	0.43
1:A:361:LEU:HD11	1:A:365:GLY:HA3	2.00	0.43
1:A:147:MET:HG3	1:D:136:THR:HG21	2.00	0.43
1:A:396:PHE:CD1	2:A:601:NDP:H1D	2.53	0.43
1:B:269:ILE:HG13	1:B:425:SER:HB3	1.99	0.43
1:C:353:LYS:O	1:C:357:GLU:HG3	2.19	0.43
1:C:493:ARG:O	1:C:493:ARG:HG3	2.18	0.43
1:D:385:LYS:N	1:D:388:MET:HE3	2.31	0.43
1:A:164:PHE:HB2	1:A:168:ILE:HG13	2.00	0.43
1:A:289:SER:O	1:A:292:THR:N	2.52	0.43
1:A:447:TRP:HB3	1:A:450:THR:HG23	2.01	0.43
1:C:89:LEU:HD22	1:C:115:ILE:HG23	2.01	0.43
1:A:89:LEU:CD1	1:A:201:ILE:HD13	2.47	0.43
1:B:58:VAL:HG11	1:B:229:HIS:CE1	2.53	0.43
1:B:362:LEU:HD13	1:B:382:THR:OG1	2.19	0.43
1:B:435:LEU:HD23	1:B:435:LEU:HA	1.90	0.43
1:B:349:ASP:O	1:B:352:ALA:HB3	2.19	0.43
1:C:110:GLN:O	1:C:114:GLU:HG3	2.19	0.43
1:A:224:GLN:O	1:A:228:GLU:HG2	2.19	0.43
1:B:8:VAL:HG11	1:B:329:PHE:CD1	2.54	0.42
1:D:275:SER:OG	1:D:277:LEU:HD23	2.19	0.42
1:D:351:ILE:HG21	1:D:365:GLY:O	2.19	0.42
1:C:332:GLU:OE1	1:C:332:GLU:HA	2.19	0.42
1:C:353:LYS:HG3	1:C:354:GLY:N	2.33	0.42
1:C:482:GLN:HG2	1:D:463:PHE:CG	2.54	0.42
1:A:266:LYS:NZ	1:A:390:ILE:O	2.50	0.42
1:A:435:LEU:HD12	1:A:435:LEU:HA	1.91	0.42
1:C:13:LYS:CG	1:C:14:PRO:HD2	2.49	0.42
1:C:21:ILE:HG23	1:C:57:ALA:HA	2.00	0.42
1:A:222:VAL:HG12	1:A:226:MET:HE3	2.02	0.42
1:B:89:LEU:HD21	1:B:166:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:CYS:O	1:B:121:CYS:HB2	2.20	0.42
1:B:361:LEU:HD12	1:B:361:LEU:HA	1.78	0.42
1:B:418:THR:HG23	1:B:420:TYR:O	2.18	0.42
1:C:131:MET:HE2	1:C:131:MET:HB3	1.62	0.42
1:C:291:ASN:O	1:C:294:GLN:HB2	2.19	0.42
1:D:435:LEU:HD23	1:D:435:LEU:HA	1.85	0.42
1:D:10:LEU:HD13	1:D:41:VAL:HG21	2.01	0.42
1:A:131:MET:HE1	1:C:128:ALA:N	2.35	0.42
2:A:601:NDP:H3D	2:A:601:NDP:O1A	2.19	0.42
1:B:353:LYS:HG3	1:B:357:GLU:HG3	2.01	0.42
1:A:258:LYS:HE2	1:A:258:LYS:HB3	1.78	0.42
1:B:240:SER:OG	1:B:243:VAL:HG23	2.20	0.42
1:A:274:ASP:OD1	1:A:274:ASP:C	2.63	0.41
1:C:38:ALA:HB1	1:C:375:TYR:OH	2.20	0.41
1:C:489:GLU:HB2	1:D:450:THR:HB	2.01	0.41
1:A:310:GLU:O	1:A:314:ARG:HG2	2.19	0.41
1:B:157:GLY:HA2	1:B:184:VAL:O	2.20	0.41
1:B:474:LEU:HD12	1:B:474:LEU:O	2.20	0.41
1:C:102:LEU:HD23	1:C:102:LEU:HA	1.84	0.41
1:D:131:MET:O	1:D:132:LEU:C	2.62	0.41
1:D:380:LEU:HD13	1:D:400:LEU:HD23	2.02	0.41
1:A:30:ASP:CG	1:A:48:ARG:HD2	2.46	0.41
1:A:62:ARG:O	1:A:66:GLU:HB2	2.21	0.41
1:A:317:VAL:CG1	1:A:380:LEU:HD23	2.50	0.41
1:C:166:PHE:CD1	1:C:194:THR:HB	2.55	0.41
1:D:36:SER:HB3	1:D:39:HIS:HB2	2.02	0.41
1:B:429:LYS:HA	1:B:429:LYS:HE2	2.01	0.41
1:C:324:ARG:HG3	1:C:334:GLN:OE1	2.20	0.41
1:A:33:ASP:OD1	1:A:45:ARG:HG3	2.21	0.41
1:A:302:LEU:HB3	1:A:402:SER:HA	2.02	0.41
1:C:153:ILE:HD13	1:C:234:MET:HB2	2.02	0.41
1:C:353:LYS:HE3	1:C:353:LYS:HB2	1.88	0.41
1:D:54:LEU:HD11	1:D:226:MET:HG2	2.03	0.41
1:D:362:LEU:HD13	1:D:382:THR:HG22	2.03	0.41
1:A:474:LEU:HD12	1:A:474:LEU:HA	1.92	0.41
1:C:341:GLU:CG	1:C:374:GLN:HE22	2.28	0.41
1:C:465:GLN:HG2	1:D:256:LEU:HB2	2.03	0.41
1:D:239:GLY:O	1:D:263:LEU:HA	2.21	0.41
1:A:30:ASP:OD2	1:A:30:ASP:N	2.50	0.40
1:B:157:GLY:O	1:B:235:LEU:HA	2.21	0.40
1:B:330:ASP:HB3	1:B:333:THR:OG1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:O	1:A:56:GLU:HG3	2.21	0.40
1:C:405:PHE:CD1	1:C:411:ALA:HB2	2.57	0.40
1:C:421:GLY:HA3	1:C:463:PHE:HB2	2.03	0.40
1:B:34:ARG:HB3	1:B:44:THR:OG1	2.21	0.40
1:B:237:PHE:CD1	1:B:237:PHE:C	2.99	0.40
1:A:148:VAL:HG13	1:A:483:ILE:HG23	2.03	0.40
1:A:291:ASN:O	1:A:294:GLN:HB2	2.20	0.40
1:C:150:ARG:NH1	1:C:481:THR:OG1	2.55	0.40
1:D:110:GLN:HG3	1:D:290:PHE:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	490/504 (97%)	473 (96%)	17 (4%)	0	100	100
1	B	489/504 (97%)	470 (96%)	17 (4%)	2 (0%)	30	62
1	C	488/504 (97%)	460 (94%)	27 (6%)	1 (0%)	43	73
1	D	489/504 (97%)	468 (96%)	19 (4%)	2 (0%)	30	62
All	All	1956/2016 (97%)	1871 (96%)	80 (4%)	5 (0%)	36	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	352	ALA
1	C	369	ASP
1	D	421	GLY
1	B	421	GLY
1	D	297	VAL

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	385/397 (97%)	357 (93%)	28 (7%)	13	40
1	B	384/397 (97%)	365 (95%)	19 (5%)	22	54
1	C	383/397 (96%)	356 (93%)	27 (7%)	14	42
1	D	384/397 (97%)	365 (95%)	19 (5%)	22	54
All	All	1536/1588 (97%)	1443 (94%)	93 (6%)	17	47

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	29	LYS
1	A	30	ASP
1	A	45	ARG
1	A	48	ARG
1	A	62	ARG
1	A	63	ARG
1	A	66	GLU
1	A	89	LEU
1	A	179	SER
1	A	186	LYS
1	A	209	LYS
1	A	221	THR
1	A	224	GLN
1	A	230	GLN
1	A	235	LEU
1	A	256	LEU
1	A	258	LYS
1	A	266	LYS
1	A	279	ASP
1	A	297	VAL
1	A	321	GLU
1	A	332	GLU
1	A	367	ILE

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Mol	Chain	Res	Type
1	A	382	THR
1	A	385	LYS
1	A	446	PHE
1	A	453	SER
1	B	8	VAL
1	B	9	SER
1	B	84	LYS
1	B	89	LEU
1	B	131	MET
1	B	163	ASN
1	B	256	LEU
1	B	332	GLU
1	B	353	LYS
1	B	362	LEU
1	B	380	LEU
1	B	382	THR
1	B	385	LYS
1	B	425	SER
1	B	442	ARG
1	B	446	PHE
1	B	450	THR
1	B	465	GLN
1	B	493	ARG
1	C	10	LEU
1	C	33	ASP
1	C	44	THR
1	C	54	LEU
1	C	84	LYS
1	C	89	LEU
1	C	106	LYS
1	C	108	ILE
1	C	131	MET
1	C	179	SER
1	C	235	LEU
1	C	240	SER
1	C	256	LEU
1	C	276	ASN
1	C	292	THR
1	C	315	LEU
1	C	346	THR
1	C	353	LYS
1	C	376	ILE

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Mol	Chain	Res	Type
1	C	408	VAL
1	C	414	ILE
1	C	425	SER
1	C	446	PHE
1	C	452	MET
1	C	453	SER
1	C	493	ARG
1	C	497	ILE
1	D	84	LYS
1	D	142	GLU
1	D	186	LYS
1	D	209	LYS
1	D	220	ARG
1	D	221	THR
1	D	235	LEU
1	D	256	LEU
1	D	258	LYS
1	D	288	ILE
1	D	297	VAL
1	D	372	LYS
1	D	396	PHE
1	D	440	ARG
1	D	446	PHE
1	D	453	SER
1	D	490	THR
1	D	493	ARG
1	D	494	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	224	GLN
1	B	224	GLN
1	B	276	ASN
1	B	343	GLN
1	C	276	ASN
1	C	374	GLN
1	C	482	GLN
1	D	343	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NDP	D	601	-	51,52,52	0.54	0	71,80,80	0.76	2 (2%)
2	NDP	C	601	-	51,52,52	0.50	0	71,80,80	0.89	3 (4%)
2	NDP	A	601	-	51,52,52	0.52	0	71,80,80	0.84	1 (1%)
2	NDP	B	601	-	51,52,52	0.50	0	71,80,80	0.83	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	D	601	-	-	18/34/77/77	0/5/5/5
2	NDP	C	601	-	-	15/34/77/77	0/5/5/5
2	NDP	A	601	-	-	18/34/77/77	0/5/5/5
2	NDP	B	601	-	-	15/34/77/77	0/5/5/5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	NDP	P2B-O2B-C2B	-5.00	110.08	123.43
2	A	601	NDP	P2B-O2B-C2B	-4.41	111.65	123.43
2	D	601	NDP	P2B-O2B-C2B	-4.31	111.92	123.43
2	B	601	NDP	P2B-O2B-C2B	-3.95	112.89	123.43
2	C	601	NDP	C3N-C2N-N1N	-2.84	119.04	123.20
2	B	601	NDP	O4D-C1D-C2D	-2.38	101.53	106.62
2	B	601	NDP	C3N-C2N-N1N	-2.37	119.72	123.20
2	D	601	NDP	C3D-C2D-C1D	2.22	105.66	101.46
2	C	601	NDP	C3D-C2D-C1D	2.02	105.28	101.46

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NDP	C5B-O5B-PA-O1A
2	A	601	NDP	C5B-O5B-PA-O2A
2	A	601	NDP	C5B-O5B-PA-O3
2	A	601	NDP	C5D-O5D-PN-O3
2	A	601	NDP	C5D-O5D-PN-O1N
2	A	601	NDP	C5D-O5D-PN-O2N
2	A	601	NDP	C2D-C1D-N1N-C2N
2	B	601	NDP	C5D-O5D-PN-O3
2	B	601	NDP	C5D-O5D-PN-O1N
2	B	601	NDP	C5D-O5D-PN-O2N
2	B	601	NDP	O4D-C4D-C5D-O5D
2	B	601	NDP	C2N-C3N-C7N-N7N
2	C	601	NDP	C5B-O5B-PA-O3
2	C	601	NDP	C5D-O5D-PN-O3
2	C	601	NDP	C5D-O5D-PN-O1N
2	C	601	NDP	C2D-C1D-N1N-C2N
2	C	601	NDP	C2N-C3N-C7N-N7N
2	D	601	NDP	C5B-O5B-PA-O3
2	D	601	NDP	C5D-O5D-PN-O3
2	D	601	NDP	C5D-O5D-PN-O1N
2	D	601	NDP	C5D-O5D-PN-O2N
2	D	601	NDP	C2D-C1D-N1N-C2N
2	D	601	NDP	C2N-C3N-C7N-N7N
2	A	601	NDP	C2D-C1D-N1N-C6N
2	C	601	NDP	C2D-C1D-N1N-C6N
2	D	601	NDP	C2D-C1D-N1N-C6N

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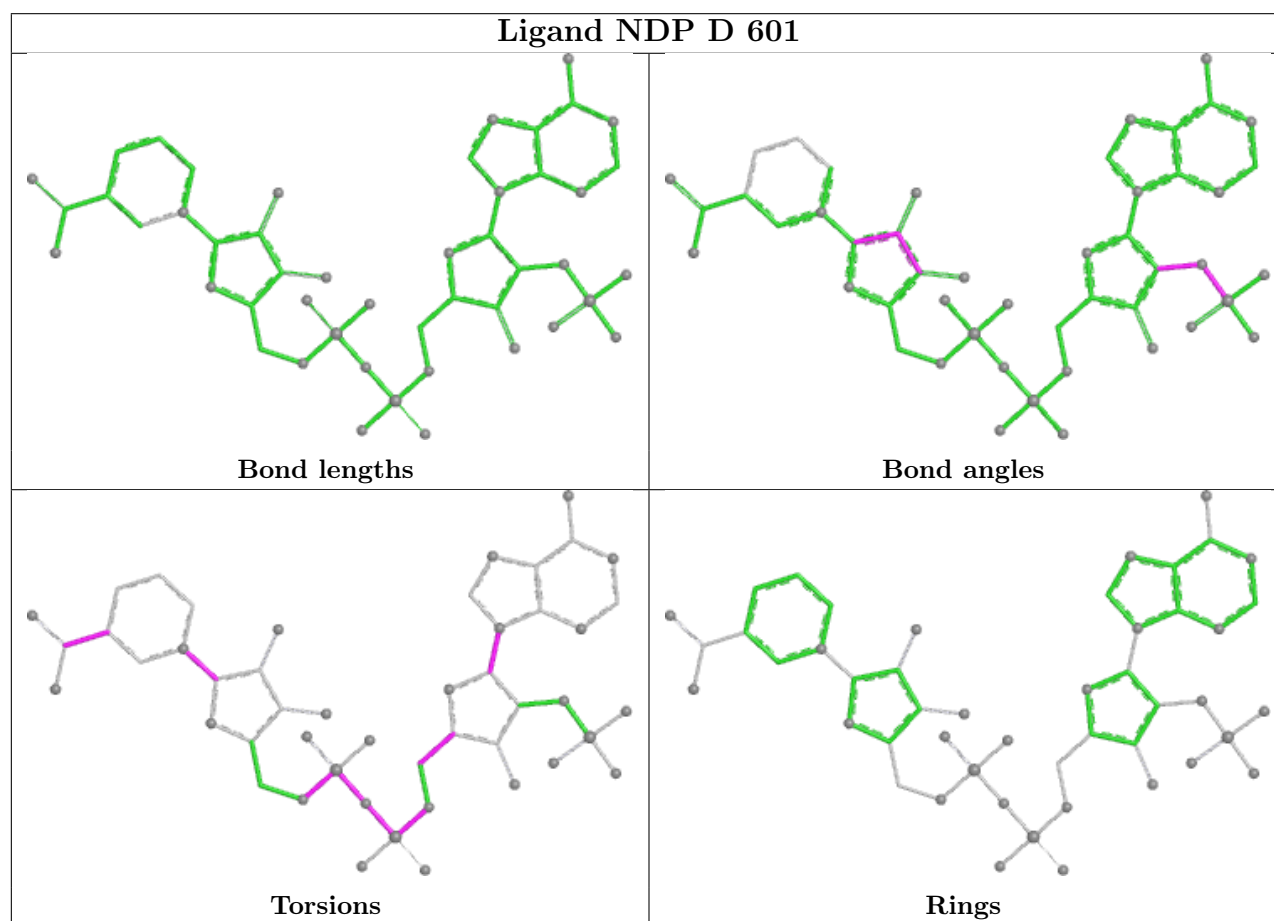
Mol	Chain	Res	Type	Atoms
2	A	601	NDP	O4B-C4B-C5B-O5B
2	B	601	NDP	C3D-C4D-C5D-O5D
2	B	601	NDP	C2D-C1D-N1N-C2N
2	B	601	NDP	C2D-C1D-N1N-C6N
2	D	601	NDP	C2B-C1B-N9A-C8A
2	A	601	NDP	C3B-C4B-C5B-O5B
2	A	601	NDP	C2B-C1B-N9A-C8A
2	D	601	NDP	C2B-C1B-N9A-C4A
2	B	601	NDP	C2B-C1B-N9A-C8A
2	A	601	NDP	C2N-C3N-C7N-N7N
2	A	601	NDP	PA-O3-PN-O5D
2	C	601	NDP	PA-O3-PN-O5D
2	C	601	NDP	C2B-C1B-N9A-C8A
2	A	601	NDP	PN-O3-PA-O1A
2	B	601	NDP	O4D-C1D-N1N-C2N
2	B	601	NDP	O4D-C1D-N1N-C6N
2	C	601	NDP	C2N-C3N-C7N-O7N
2	D	601	NDP	C2N-C3N-C7N-O7N
2	C	601	NDP	C5B-O5B-PA-O1A
2	D	601	NDP	C5B-O5B-PA-O1A
2	C	601	NDP	C4D-C5D-O5D-PN
2	C	601	NDP	O4B-C4B-C5B-O5B
2	A	601	NDP	C2B-C1B-N9A-C4A
2	B	601	NDP	C2B-C1B-N9A-C4A
2	A	601	NDP	O4D-C1D-N1N-C2N
2	D	601	NDP	O4D-C1D-N1N-C2N
2	C	601	NDP	C2B-C1B-N9A-C4A
2	C	601	NDP	O4B-C1B-N9A-C8A
2	C	601	NDP	O4D-C1D-N1N-C2N
2	D	601	NDP	PA-O3-PN-O5D
2	D	601	NDP	O4B-C4B-C5B-O5B
2	B	601	NDP	O4B-C1B-N9A-C8A
2	A	601	NDP	PN-O3-PA-O2A
2	B	601	NDP	PA-O3-PN-O2N
2	D	601	NDP	PN-O3-PA-O1A
2	A	601	NDP	O4B-C1B-N9A-C8A
2	D	601	NDP	O4B-C1B-N9A-C8A
2	B	601	NDP	C2B-O2B-P2B-O2X
2	D	601	NDP	PN-O3-PA-O2A
2	D	601	NDP	PA-O3-PN-O2N

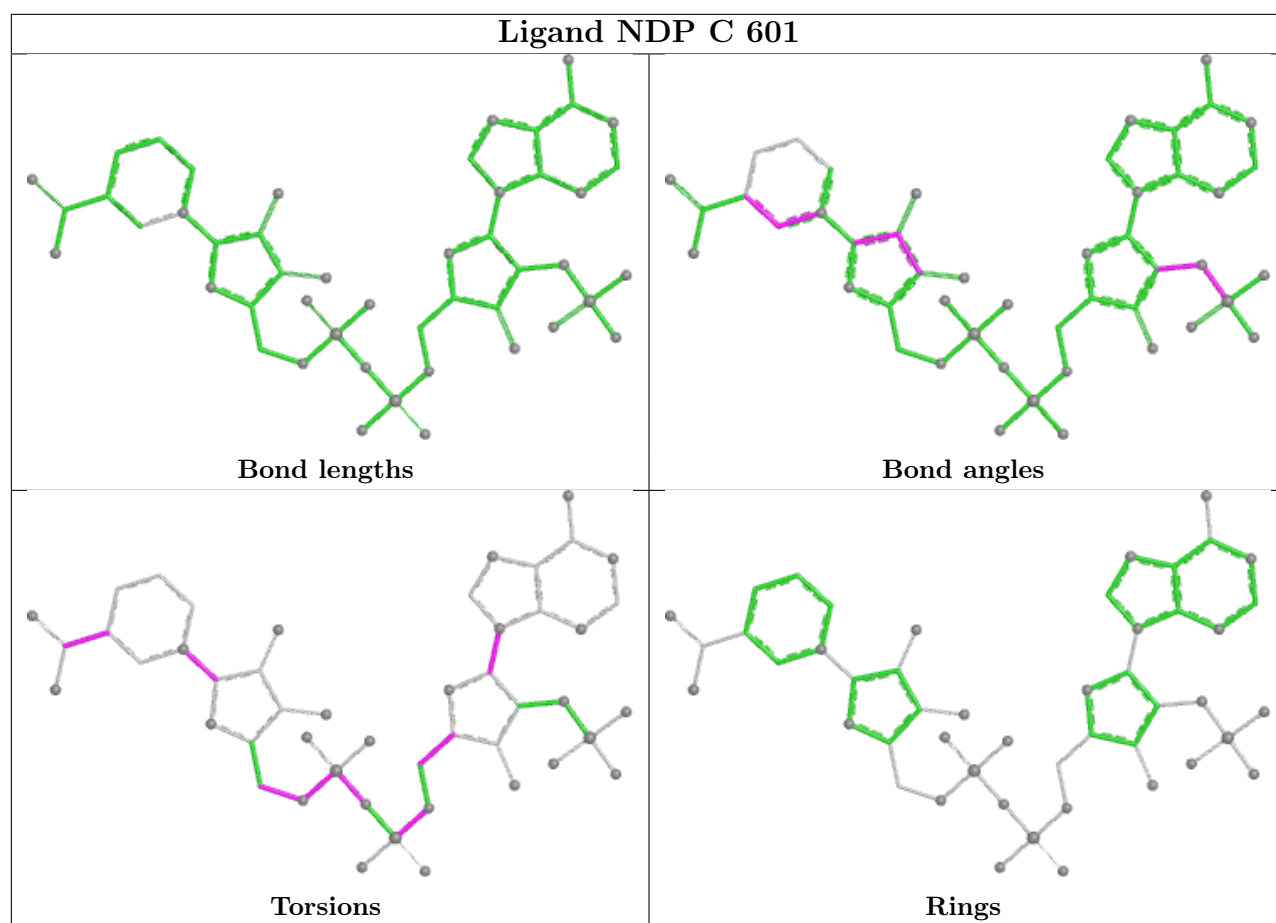
There are no ring outliers.

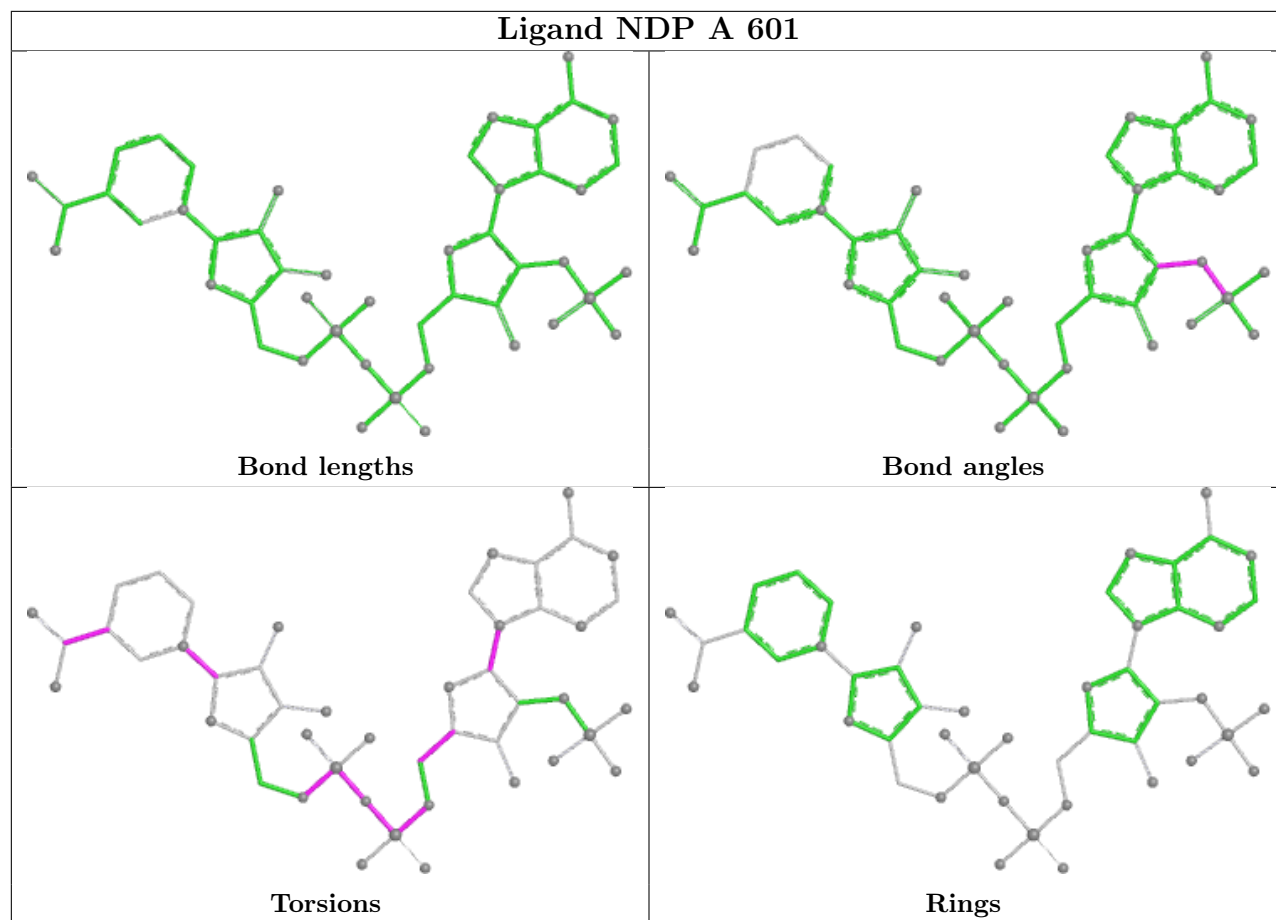
4 monomers are involved in 15 short contacts:

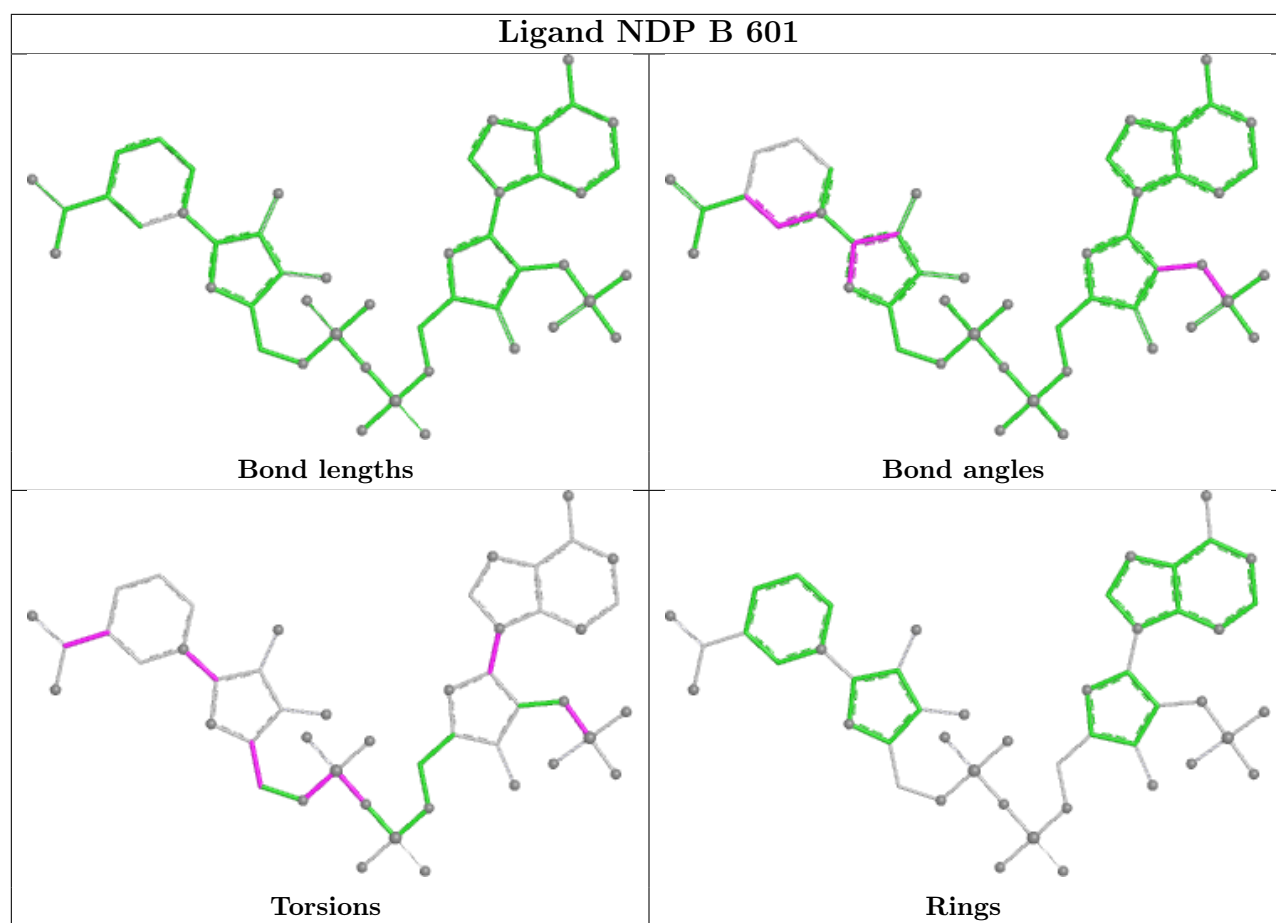
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	NDP	3	0
2	C	601	NDP	2	0
2	A	601	NDP	7	0
2	B	601	NDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	492/504 (97%)	-0.32	1 (0%) 91 85	6, 14, 33, 59	0
1	B	491/504 (97%)	-0.34	0 100 100	7, 15, 33, 56	0
1	C	490/504 (97%)	-0.16	5 (1%) 79 63	7, 22, 47, 79	0
1	D	491/504 (97%)	-0.34	1 (0%) 91 85	8, 14, 29, 57	0
All	All	1964/2016 (97%)	-0.29	7 (0%) 88 79	6, 16, 38, 79	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	10	LEU	4.5
1	C	370	PHE	2.9
1	C	12	LEU	2.9
1	A	30	ASP	2.8
1	D	494	SER	2.4
1	C	11	PRO	2.2
1	C	274	ASP	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](#)

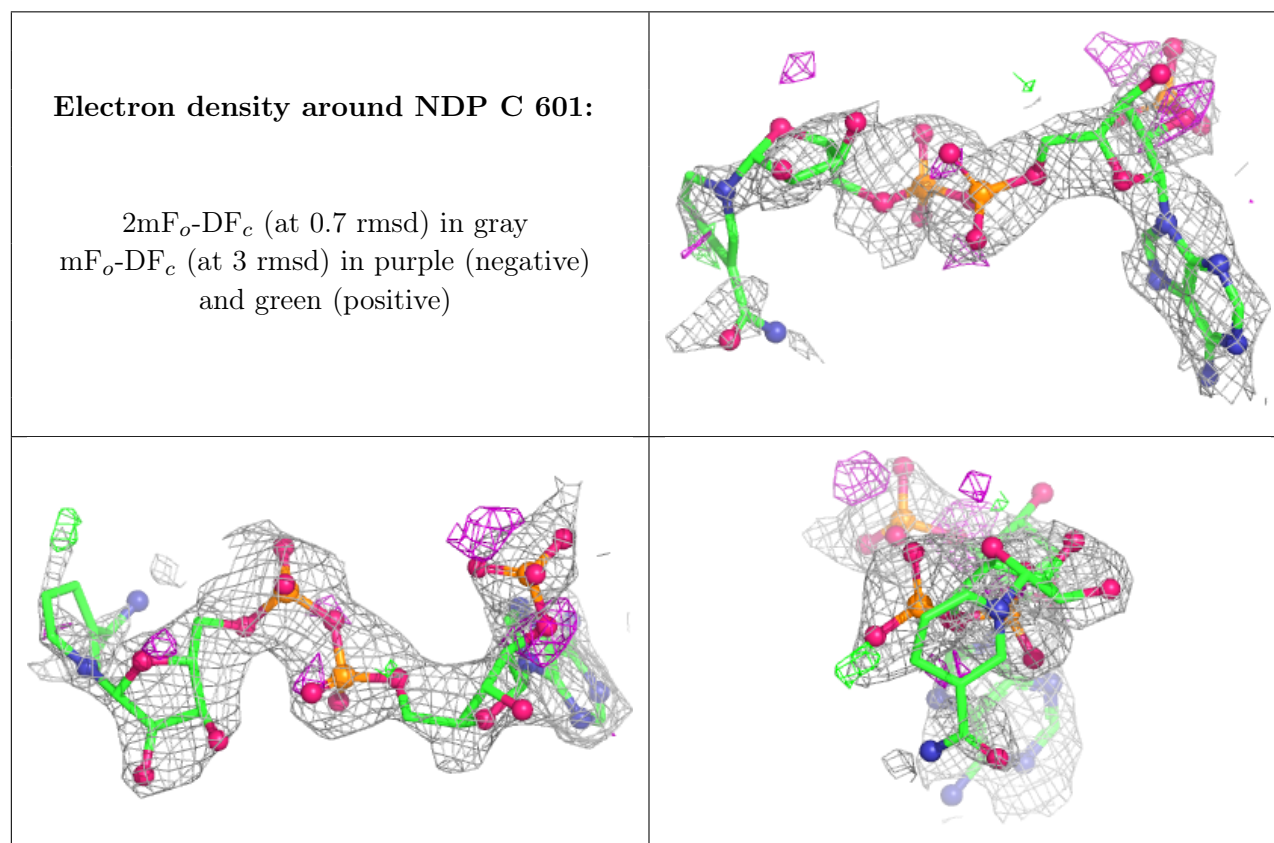
There are no oligosaccharides in this entry.

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.

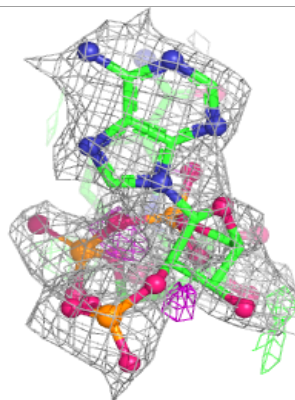
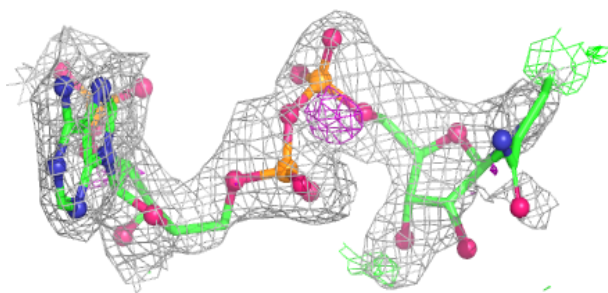
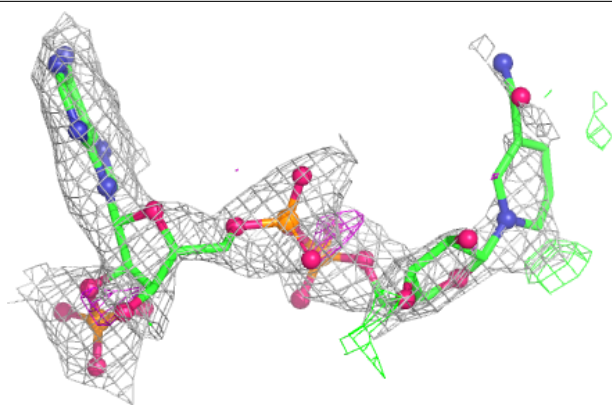
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	C	601	48/48	0.78	0.17	55,68,77,83	0
2	NDP	D	601	48/48	0.80	0.17	36,60,85,90	0
2	NDP	A	601	48/48	0.86	0.14	28,52,62,66	0
2	NDP	B	601	48/48	0.86	0.14	34,48,76,81	0

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.

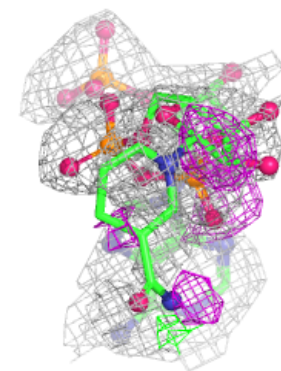
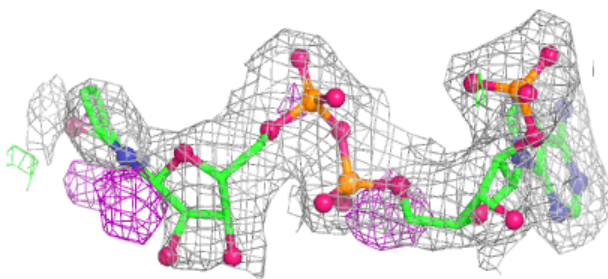
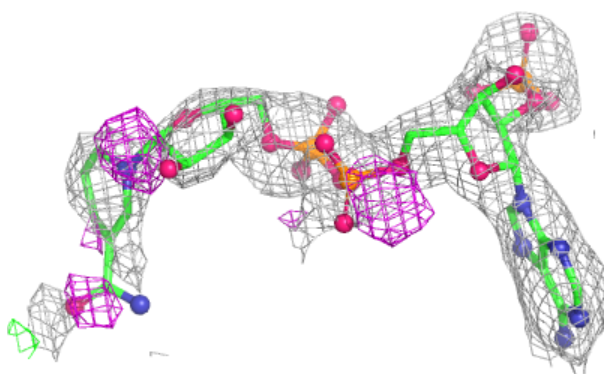


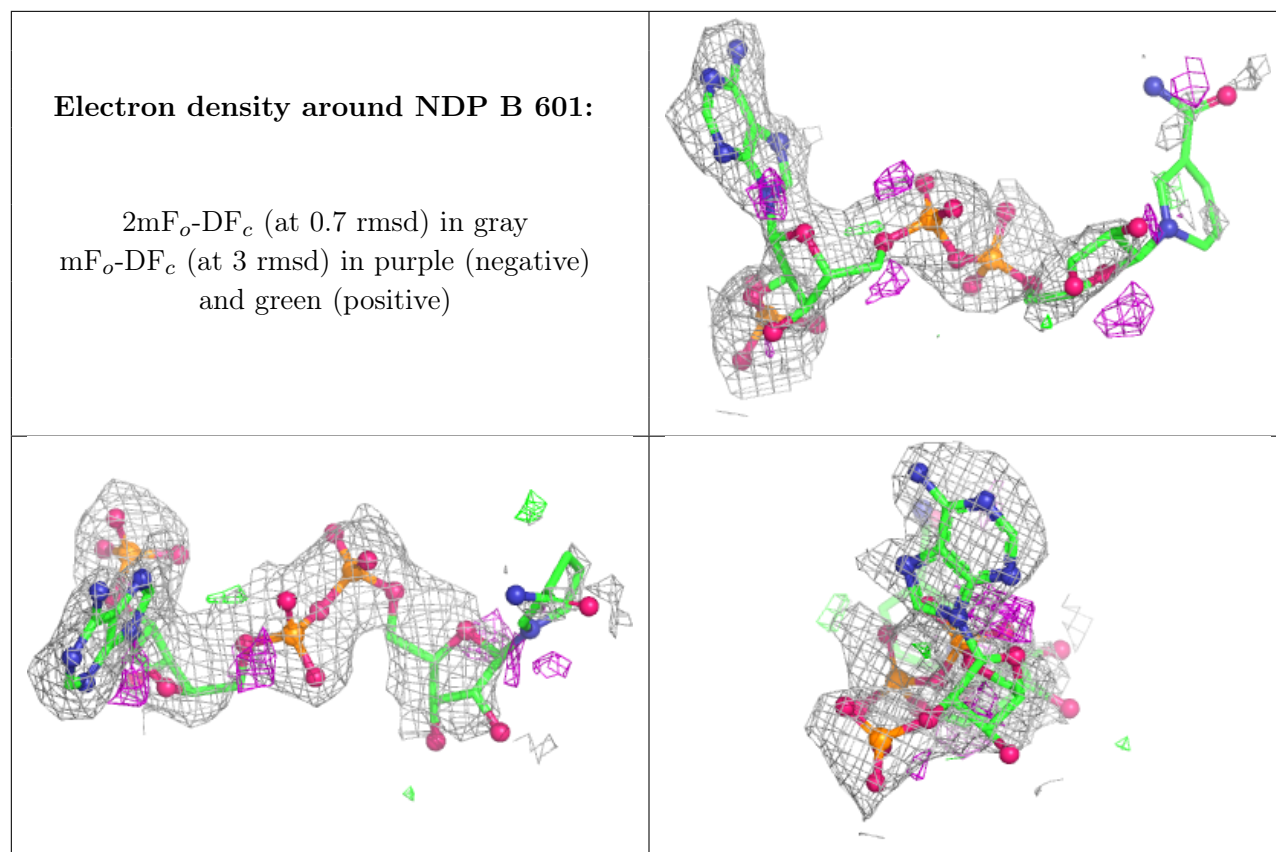
Electron density around NDP D 601:

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

**Electron density around NDP A 601:**

$2mF_o-DF_c$ (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.