Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2020 – 02:59 am BST

PDB ID	:	3KBO
Title	:	2.14 Angstrom Crystal Structure of Putative Oxidoreductase (ycdW) from Salmonella typhimurium in Complex with NADP
Authors	:	Minasov, G.; Wawrzak, Z.; Skarina, T.; Onopriyenko, O.; Papazisi, L.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2009-10-20
Resolution	:	2.14 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

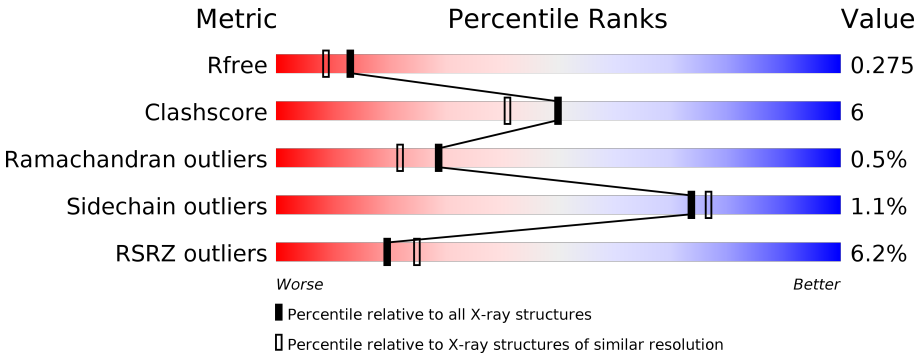
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 <=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	315	3% 83% 16%
1	B	315	7% 86% 12%
1	C	315	3% 89% 10%
1	D	315	10% 83% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10785 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.

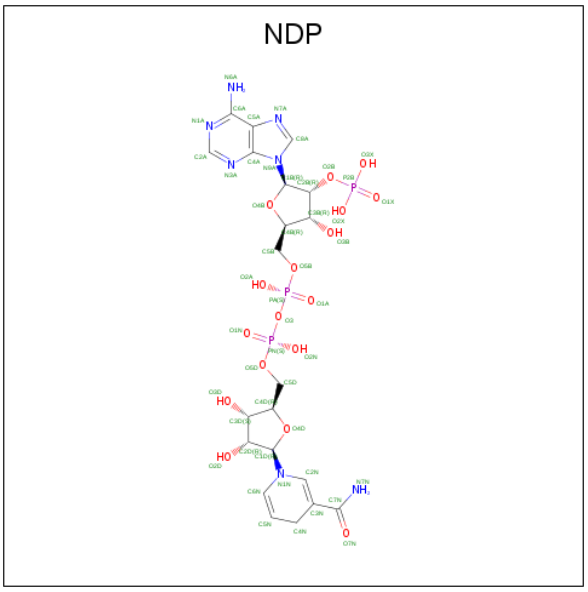
- Molecule 1 is a protein called Glyoxylate/hydroxypyruvate reductase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	Se	0	4	0
			2510	1606	442	453	1	8			
1	B	312	Total	C	N	O	S	Se	0	2	0
			2490	1595	439	447	1	8			
1	C	312	Total	C	N	O	S	Se	0	1	0
			2484	1592	438	445	1	8			
1	D	312	Total	C	N	O	S	Se	0	2	0
			2490	1595	439	447	1	8			

There are 12 discrepancies between the modelled and reference sequences:

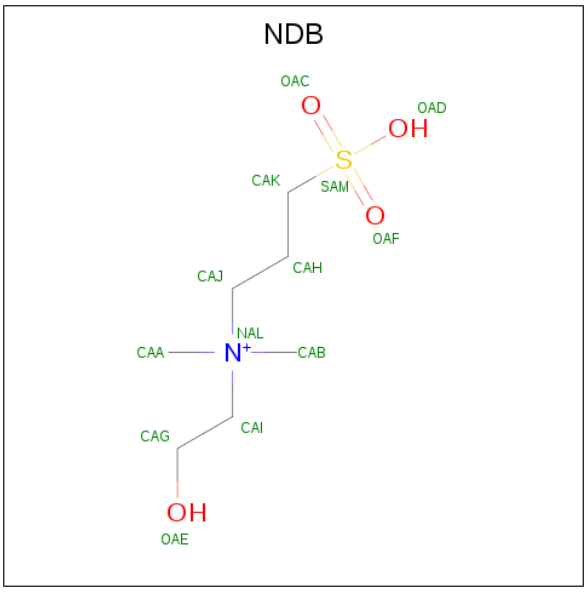
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8ZQ30
A	-1	ASN	-	EXPRESSION TAG	UNP Q8ZQ30
A	0	ALA	-	EXPRESSION TAG	UNP Q8ZQ30
B	-2	SER	-	EXPRESSION TAG	UNP Q8ZQ30
B	-1	ASN	-	EXPRESSION TAG	UNP Q8ZQ30
B	0	ALA	-	EXPRESSION TAG	UNP Q8ZQ30
C	-2	SER	-	EXPRESSION TAG	UNP Q8ZQ30
C	-1	ASN	-	EXPRESSION TAG	UNP Q8ZQ30
C	0	ALA	-	EXPRESSION TAG	UNP Q8ZQ30
D	-2	SER	-	EXPRESSION TAG	UNP Q8ZQ30
D	-1	ASN	-	EXPRESSION TAG	UNP Q8ZQ30
D	0	ALA	-	EXPRESSION TAG	UNP Q8ZQ30

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
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 N-(2-hydroxyethyl)-N,N-dimethyl-3-sulfopropan-1-aminium (three-letter code: NDB) (formula: $C_7H_{18}NO_4S$).

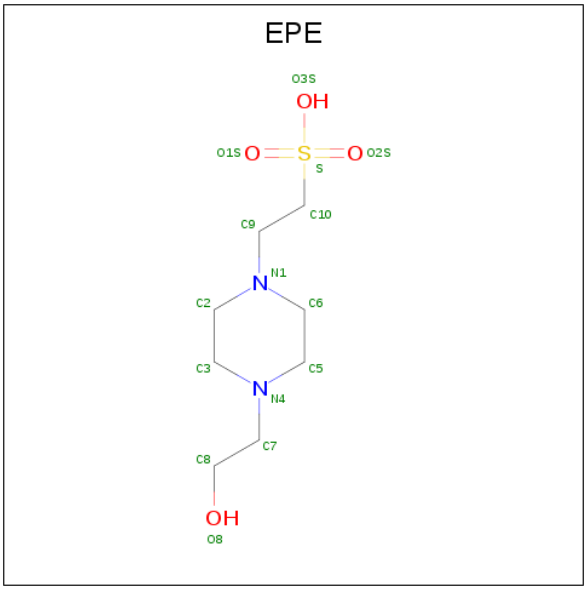


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 13 7 1 4 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Cl 2 2	0	0
4	A	2	Total Cl 2 2	0	0
4	D	2	Total Cl 2 2	0	0
4	C	2	Total Cl 2 2	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O S 15 8 2 4 1	0	0
5	D	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 6 is water.

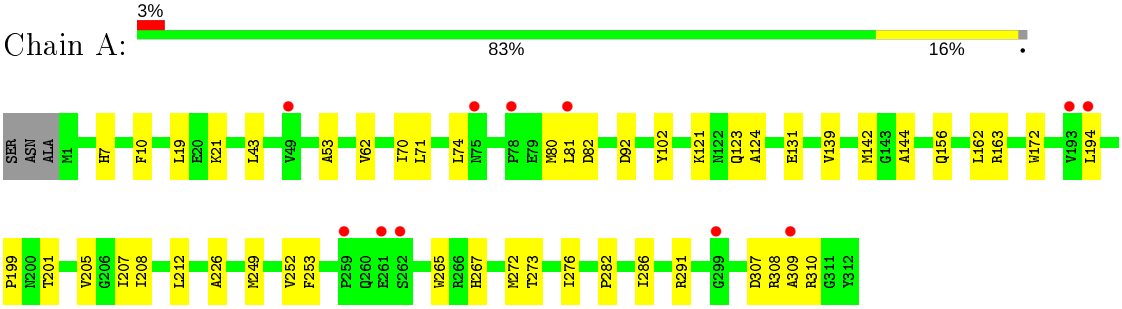
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	147	Total O 152 152	0	6
6	B	125	Total O 127 127	0	2
6	C	179	Total O 184 184	0	5
6	D	104	Total O 105 105	0	1

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.

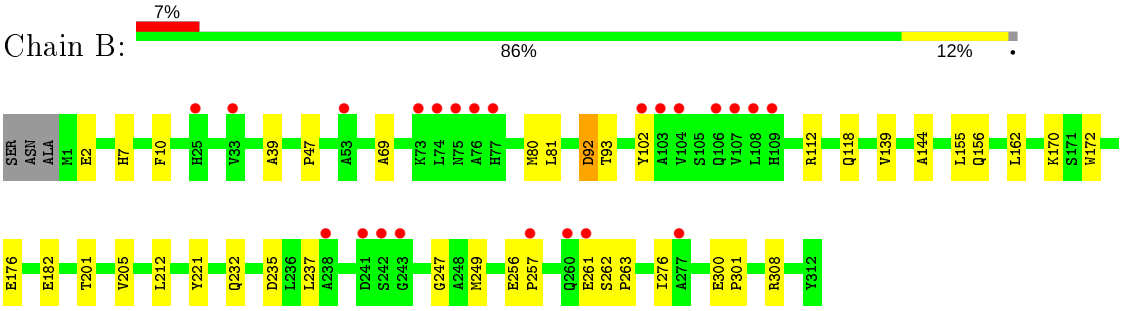
- Molecule 1: Glyoxylate/hydroxypyruvate reductase A

Chain A:



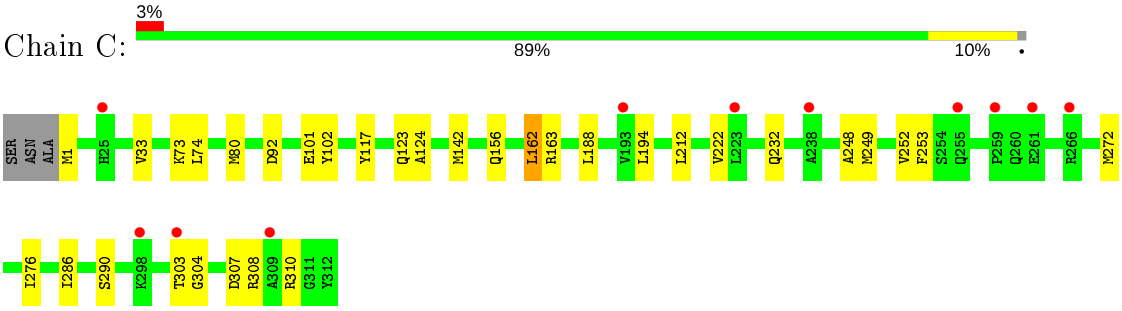
- Molecule 1: Glyoxylate/hydroxypyruvate reductase A

Chain B:



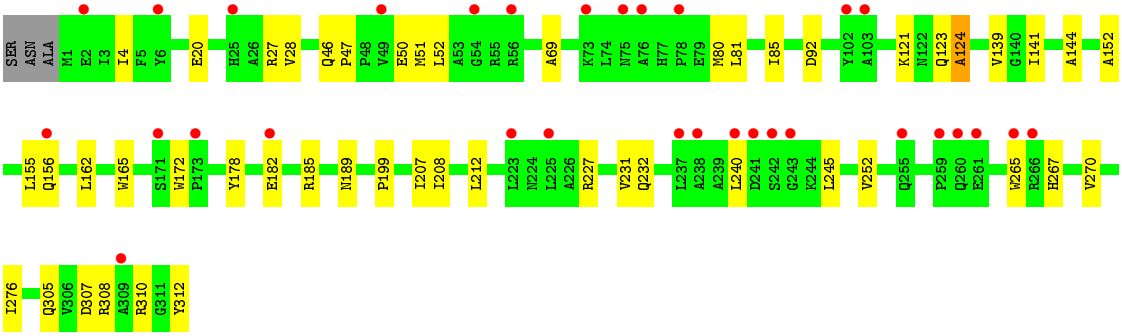
- Molecule 1: Glyoxylate/hydroxypyruvate reductase A

Chain C:



- Molecule 1: Glyoxylate/hydroxypyruvate reductase A

Chain D:


SER ASN ALA M1 E2 I3 I4 F5 Y6 E20 H25 A26 R27 V28 Q46 P47 P48 V49 E50 M51 L52 A53 G54 R55 R56 A69 K73 L74 N75 A76 H77 P78 E79 M80 L81 I85 D92 Y102 A103 K121 N122 Q123 A124 V139 G140 I141 A144 A152
L155 Q156 L162 W165 S171 W172 P173 Y178 E182 R185 N189 P199 I207 I208 L212 L223 M224 L225 A226 R227 V231 Q232 L237 A238 A239 L240 D241 S242 G243 K244 L245 V252 Q255 P259 Q260 E261 W265 R266 H267 V270
I276 Q305 V306 D307 R308 A309 R310 G311 Y312

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	279.62Å 45.59Å 112.33Å 90.00° 101.58° 90.00°	Depositor
Resolution (Å)	29.93 – 2.14 29.83 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.93-2.14) 98.0 (29.83-2.14)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.48 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.211 , 0.269 0.219 , 0.275	Depositor DCC
R_{free} test set	3806 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.831	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10785	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 85.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2269e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, NDB, EPE, CL

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	0.66	0/2568	0.71	0/3485
1	B	0.59	0/2548	0.68	0/3457
1	C	0.70	0/2542	0.72	0/3449
1	D	0.54	0/2548	0.67	0/3457
All	All	0.63	0/10206	0.69	0/13848

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

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	2510	0	2490	34	0
1	B	2490	0	2478	29	0
1	C	2484	0	2474	22	0
1	D	2490	0	2478	41	0
2	A	48	0	25	2	0
2	B	48	0	26	1	0
2	C	48	0	26	0	0
2	D	48	0	26	1	0
3	A	13	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	B	15	0	17	0	0
5	D	15	0	17	0	0
6	A	152	0	0	2	0
6	B	127	0	0	3	0
6	C	184	0	0	1	0
6	D	105	0	0	3	0
All	All	10785	0	10075	118	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 6.

All (118) 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:D:232[B]:GLN:N	1:D:232[B]:GLN:HE21	1.64	0.96
1:A:121:LYS:NZ	1:D:267:HIS:O	2.23	0.70
1:A:121:LYS:NZ	1:D:270:VAL:O	2.22	0.69
1:C:156:GLN:HB2	1:C:162:LEU:HD13	1.79	0.65
1:A:307:ASP:HB3	1:A:310:ARG:HG2	1.79	0.64
1:A:139:VAL:HB	1:A:162:LEU:HD22	1.81	0.63
1:A:131:GLU:HA	6:A:403:HOH:O	1.98	0.63
1:D:232[B]:GLN:H	1:D:232[B]:GLN:HE21	1.44	0.63
1:D:123:GLN:O	1:D:124:ALA:HB3	1.99	0.63
1:D:47:PRO:HG2	1:D:80:MSE:HE1	1.81	0.62
1:B:276:ILE:HD13	1:C:117:TYR:CE2	2.35	0.62
1:B:201:THR:O	1:B:205:VAL:HG23	1.99	0.62
1:D:52:LEU:HD12	1:D:80:MSE:HE2	1.81	0.62
1:D:208:ILE:HB	1:D:231:VAL:HG22	1.82	0.61
1:C:303:THR:HB	1:C:304:GLY:HA2	1.87	0.57
1:C:307:ASP:HB3	1:C:310:ARG:HG2	1.86	0.57
1:A:273:THR:HB	1:A:276:ILE:HD11	1.87	0.57
1:A:139:VAL:HB	1:A:162:LEU:CD2	2.35	0.56
1:D:144:ALA:HB1	1:D:172:TRP:CH2	2.41	0.56
1:A:212:LEU:HD23	1:A:212:LEU:C	2.27	0.55
1:B:182:GLU:CD	1:B:182:GLU:H	2.10	0.55
1:C:252:VAL:C	1:C:253:PHE:CD2	2.80	0.55
1:B:300:GLU:HB3	1:B:301:PRO:CD	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MSE:HG3	1:A:194:LEU:HD11	1.90	0.54
1:D:310:ARG:HD2	1:D:312:TYR:CZ	2.42	0.54
1:A:308:ARG:HB3	6:A:426:HOH:O	2.08	0.53
1:C:276:ILE:C	1:C:276:ILE:HD12	2.28	0.53
1:A:253:PHE:CZ	1:A:272:MSE:HE3	2.43	0.53
1:A:144:ALA:HB1	1:A:172:TRP:CH2	2.44	0.53
1:A:70:ILE:HG22	1:A:71:LEU:N	2.22	0.53
1:C:74:LEU:HD21	1:C:308:ARG:NH2	2.23	0.52
1:D:141:ILE:HD12	1:D:152:ALA:HB2	1.91	0.52
1:A:53:ALA:HA	1:A:80:MSE:HA	1.92	0.52
1:D:69:ALA:HB3	6:D:373:HOH:O	2.08	0.52
1:A:282:PRO:O	1:A:286:ILE:HG12	2.09	0.51
1:B:139:VAL:HB	1:B:162:LEU:HD23	1.91	0.51
1:D:20:GLU:HG2	1:D:28:VAL:HG23	1.92	0.51
1:A:201:THR:O	1:A:205:VAL:HG23	2.11	0.51
1:D:139:VAL:HG11	1:D:155:LEU:HD13	1.93	0.51
1:A:124:ALA:HA	1:D:265:TRP:CE3	2.46	0.51
1:A:265:TRP:CE3	1:D:124:ALA:HA	2.46	0.51
1:B:262:SER:HA	6:B:379[A]:HOH:O	2.11	0.51
1:B:47:PRO:HG2	1:B:80:MSE:HE1	1.93	0.50
1:D:232[B]:GLN:HE21	1:D:232[B]:GLN:CA	2.24	0.50
1:B:300:GLU:HB3	1:B:301:PRO:HD2	1.93	0.50
1:D:240:LEU:HD23	1:D:245:LEU:HB2	1.93	0.50
1:A:207:ILE:HG23	1:A:208:ILE:HG13	1.93	0.49
1:D:305:GLN:HB2	6:D:320:HOH:O	2.13	0.49
1:D:165:TRP:HA	1:D:178:TYR:O	2.13	0.49
1:D:139:VAL:HB	1:D:162:LEU:HD23	1.95	0.48
1:B:276:ILE:HD13	1:C:117:TYR:CZ	2.49	0.48
1:D:123:GLN:O	1:D:124:ALA:CB	2.61	0.48
1:D:46:GLN:N	1:D:47:PRO:CD	2.77	0.48
1:D:85:ILE:O	1:D:308:ARG:NH1	2.48	0.47
1:C:73:LYS:HG2	1:C:80:MSE:CE	2.43	0.47
1:D:81:LEU:HD11	1:D:85:ILE:HG21	1.96	0.47
1:B:176:GLU:HG2	6:B:384:HOH:O	2.13	0.47
1:B:102:TYR:OH	1:B:249:MSE:HE2	2.15	0.47
1:D:182:GLU:CD	1:D:182:GLU:H	2.17	0.47
1:D:199:PRO:HD3	2:D:313:NDP:H52A	1.97	0.47
1:A:62:VAL:CG2	1:A:70:ILE:HD12	2.45	0.47
1:C:253:PHE:CD2	1:C:253:PHE:N	2.82	0.47
1:D:212:LEU:C	1:D:212:LEU:HD23	2.36	0.46
1:B:170:LYS:NZ	2:B:313:NDP:O3X	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ILE:C	1:D:276:ILE:HD12	2.35	0.46
1:C:102:TYR:OH	1:C:249:MSE:HE2	2.15	0.46
1:B:2:GLU:HB3	1:B:39:ALA:HA	1.98	0.46
1:D:47:PRO:HG2	1:D:80:MSE:CE	2.45	0.46
1:A:19:LEU:HD22	1:A:43:LEU:HD22	1.98	0.45
1:A:252:VAL:C	1:A:253:PHE:CD2	2.89	0.45
1:A:253:PHE:CE1	1:A:272:MSE:HE3	2.51	0.45
1:B:144:ALA:HB1	1:B:172:TRP:CH2	2.51	0.45
1:B:276:ILE:CD1	1:C:117:TYR:CE2	2.99	0.45
1:A:7:HIS:CD2	1:A:10:PHE:CD2	3.04	0.45
1:C:142:MSE:HG3	1:C:194:LEU:HD11	1.97	0.45
1:C:212:LEU:C	1:C:212:LEU:HD23	2.36	0.45
1:D:232[B]:GLN:N	1:D:232[B]:GLN:NE2	2.48	0.45
1:A:81:LEU:O	1:A:82:ASP:C	2.55	0.45
1:A:123:GLN:O	1:A:124:ALA:C	2.55	0.45
1:B:7:HIS:CD2	1:B:10:PHE:CD2	3.05	0.45
1:B:221:TYR:HA	1:B:247:GLY:O	2.17	0.44
1:B:237:LEU:HD11	1:B:263:PRO:HG2	1.98	0.44
1:B:69:ALA:HB3	6:B:453:HOH:O	2.16	0.44
1:D:156:GLN:HB2	1:D:162:LEU:CD1	2.47	0.44
1:D:227:ARG:CA	1:D:252:VAL:HG21	2.48	0.43
1:B:92:ASP:O	1:B:93:THR:OG1	2.33	0.43
1:B:102:TYR:CZ	1:B:249:MSE:HE2	2.54	0.43
1:C:33:VAL:O	1:C:33:VAL:HG23	2.17	0.43
1:C:1:MSE:N	6:C:424:HOH:O	2.52	0.43
1:C:286:ILE:O	1:C:290:SER:CB	2.67	0.43
1:A:226:ALA:HA	2:A:313:NDP:H1D	2.00	0.42
1:A:267:HIS:O	1:D:121:LYS:NZ	2.53	0.42
1:B:81:LEU:HD23	1:B:308:ARG:NH2	2.34	0.42
1:B:261:GLU:O	1:B:262:SER:C	2.58	0.42
1:D:207:ILE:O	1:D:212:LEU:HD13	2.19	0.42
1:C:123:GLN:O	1:C:124:ALA:HB3	2.20	0.42
1:B:212:LEU:C	1:B:212:LEU:HD23	2.39	0.42
1:D:307:ASP:HB3	1:D:310:ARG:HG2	2.01	0.42
1:D:310:ARG:HD2	1:D:312:TYR:CE2	2.55	0.42
1:C:188:LEU:HD11	1:C:212:LEU:HG	2.02	0.42
1:A:307:ASP:OD2	1:A:309:ALA:HB3	2.20	0.41
3:A:314:NDB:HAG	3:A:314:NDB:HAH	2.00	0.41
1:B:139:VAL:HG11	1:B:155:LEU:HD13	2.02	0.41
1:C:222:VAL:O	1:C:248:ALA:HA	2.20	0.41
1:D:46:GLN:N	1:D:47:PRO:HD3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:PRO:HD3	2:A:313:NDP:H52A	2.01	0.41
1:A:71:LEU:HA	1:A:74:LEU:HG	2.01	0.41
1:B:256:GLU:HA	1:B:257:PRO:C	2.40	0.41
1:D:156:GLN:N	1:D:162:LEU:HD11	2.35	0.41
1:D:185:ARG:HB3	6:D:376:HOH:O	2.20	0.41
1:B:112:ARG:HD3	1:C:101:GLU:OE1	2.20	0.41
1:B:156:GLN:N	1:B:162:LEU:HD11	2.36	0.41
1:B:232[B]:GLN:HB3	1:B:235:ASP:HB2	2.02	0.41
1:C:276:ILE:C	1:C:276:ILE:CD1	2.88	0.41
1:D:4:ILE:HD12	1:D:51:MSE:HE3	2.02	0.41
1:A:102:TYR:OH	1:A:249:MSE:HE2	2.22	0.40
1:A:19:LEU:HD22	1:A:43:LEU:CD2	2.51	0.40
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.90	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	314/315 (100%)	302 (96%)	11 (4%)	1 (0%)	41	36
1	B	312/315 (99%)	296 (95%)	15 (5%)	1 (0%)	41	36
1	C	311/315 (99%)	301 (97%)	9 (3%)	1 (0%)	41	36
1	D	312/315 (99%)	291 (93%)	18 (6%)	3 (1%)	15	8
All	All	1249/1260 (99%)	1190 (95%)	53 (4%)	6 (0%)	29	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	92	ASP
1	D	124	ALA

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Mol	Chain	Res	Type
1	D	189	ASN
1	A	92	ASP
1	B	92	ASP
1	D	92	ASP

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	261/251 (104%)	257 (98%)	4 (2%)	65	68
1	B	259/251 (103%)	258 (100%)	1 (0%)	91	93
1	C	258/251 (103%)	254 (98%)	4 (2%)	62	65
1	D	259/251 (103%)	257 (99%)	2 (1%)	81	85
All	All	1037/1004 (103%)	1026 (99%)	11 (1%)	73	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	156	GLN
1	A	163	ARG
1	A	291	ARG
1	B	118	GLN
1	C	162	LEU
1	C	163	ARG
1	C	232	GLN
1	C	272	MSE
1	D	27	ARG
1	D	50	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	17	ASN

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 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
2	NDP	D	313	-	45,52,52	1.96	9 (20%)	53,80,80	1.33	5 (9%)
5	EPE	D	314	-	15,15,15	0.69	1 (6%)	18,20,20	1.41	2 (11%)
5	EPE	B	314	-	15,15,15	0.85	1 (6%)	18,20,20	1.48	3 (16%)
3	NDB	A	314	-	12,12,12	1.78	2 (16%)	16,17,17	1.56	3 (18%)
2	NDP	C	313	-	45,52,52	2.03	10 (22%)	53,80,80	1.28	6 (11%)
2	NDP	A	313	-	45,52,52	1.97	9 (20%)	53,80,80	1.39	5 (9%)
2	NDP	B	313	-	45,52,52	2.00	8 (17%)	53,80,80	1.40	7 (13%)

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	313	-	-	5/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	D	314	-	-	3/9/19/19	0/1/1/1
5	EPE	B	314	-	-	2/9/19/19	0/1/1/1
3	NDB	A	314	-	-	4/12/12/12	-
2	NDP	C	313	-	-	6/30/77/77	0/5/5/5
2	NDP	A	313	-	-	5/30/77/77	0/5/5/5
2	NDP	B	313	-	-	10/30/77/77	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	313	NDP	O7N-C7N	7.31	1.41	1.24
2	D	313	NDP	O7N-C7N	6.93	1.40	1.24
2	A	313	NDP	O7N-C7N	6.60	1.40	1.24
2	C	313	NDP	C4N-C3N	-6.45	1.37	1.49
2	C	313	NDP	O7N-C7N	6.37	1.39	1.24
2	A	313	NDP	C4N-C3N	-5.92	1.38	1.49
2	D	313	NDP	C4N-C3N	-5.70	1.38	1.49
2	B	313	NDP	C4N-C3N	-5.37	1.39	1.49
2	B	313	NDP	C2A-N3A	4.80	1.39	1.32
2	D	313	NDP	C2A-N3A	4.47	1.39	1.32
2	A	313	NDP	C2A-N3A	4.40	1.39	1.32
2	C	313	NDP	C2A-N3A	4.20	1.38	1.32
3	A	314	NDB	CAK-SAM	4.10	1.83	1.77
2	C	313	NDP	C2A-N1A	3.56	1.40	1.33
2	D	313	NDP	C2A-N1A	3.51	1.40	1.33
2	B	313	NDP	C2A-N1A	3.35	1.40	1.33
2	A	313	NDP	C4N-C5N	-3.07	1.40	1.48
2	D	313	NDP	C4N-C5N	-3.04	1.40	1.48
2	B	313	NDP	C4N-C5N	-2.99	1.41	1.48
2	C	313	NDP	C4N-C5N	-2.96	1.41	1.48
2	A	313	NDP	C2A-N1A	2.83	1.39	1.33
5	B	314	EPE	C10-S	2.80	1.81	1.77
2	A	313	NDP	O2D-C2D	-2.76	1.36	1.43
2	C	313	NDP	P2B-O2B	2.67	1.64	1.59
3	A	314	NDB	CAI-NAL	-2.67	1.46	1.52
2	A	313	NDP	C6N-C5N	2.56	1.37	1.33
2	D	313	NDP	C6N-C5N	2.52	1.37	1.33
2	B	313	NDP	C6N-C5N	2.51	1.37	1.33
2	B	313	NDP	O4D-C4D	-2.50	1.39	1.45
2	C	313	NDP	PN-O2N	-2.46	1.43	1.55
2	C	313	NDP	O4D-C4D	-2.37	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	313	NDP	O4D-C4D	-2.36	1.39	1.45
2	C	313	NDP	O2D-C2D	-2.34	1.37	1.43
5	D	314	EPE	C10-S	2.26	1.80	1.77
2	C	313	NDP	C6N-C5N	2.25	1.37	1.33
2	A	313	NDP	O4D-C1D	2.23	1.47	1.42
2	A	313	NDP	PN-O2N	-2.12	1.45	1.55
2	B	313	NDP	P2B-O2B	2.11	1.63	1.59
2	D	313	NDP	C7N-C3N	2.10	1.53	1.48
2	D	313	NDP	PN-O2N	-2.05	1.45	1.55

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	313	NDP	N3A-C2A-N1A	-6.40	118.67	128.68
2	D	313	NDP	N3A-C2A-N1A	-5.90	119.46	128.68
2	A	313	NDP	N3A-C2A-N1A	-5.80	119.62	128.68
5	D	314	EPE	O2S-S-C10	4.84	112.75	106.92
2	C	313	NDP	N3A-C2A-N1A	-4.83	121.13	128.68
3	A	314	NDB	OAD-SAM-CAK	3.71	111.77	105.77
5	B	314	EPE	O2S-S-C10	3.33	110.93	106.92
2	B	313	NDP	C1B-N9A-C4A	-3.05	121.28	126.64
2	D	313	NDP	O2N-PN-O1N	3.01	127.12	112.24
2	C	313	NDP	C1B-N9A-C4A	-2.78	121.77	126.64
2	A	313	NDP	O2N-PN-O1N	2.72	125.69	112.24
2	A	313	NDP	C3N-C2N-N1N	-2.69	119.26	123.10
2	B	313	NDP	O2N-PN-O1N	2.63	125.24	112.24
2	A	313	NDP	C1B-N9A-C4A	-2.58	122.11	126.64
3	A	314	NDB	OAC-SAM-CAK	2.47	109.89	106.92
3	A	314	NDB	CAH-CAJ-NAL	-2.37	110.35	115.38
5	B	314	EPE	C6-N1-C2	2.36	114.14	108.83
2	D	313	NDP	O3X-P2B-O2B	2.33	116.45	105.99
2	C	313	NDP	C3D-C2D-C1D	2.27	105.75	101.43
2	C	313	NDP	C3N-C2N-N1N	-2.23	119.92	123.10
2	C	313	NDP	O3X-P2B-O2X	2.19	116.01	107.64
5	B	314	EPE	O3S-S-C10	2.19	109.31	105.77
2	A	313	NDP	O3X-P2B-O2X	2.16	115.90	107.64
2	B	313	NDP	O5B-PA-O1A	2.15	117.47	109.07
2	B	313	NDP	C4A-C5A-N7A	-2.13	107.18	109.40
2	B	313	NDP	C2D-C1D-N1N	2.10	118.58	113.30
2	B	313	NDP	O3X-P2B-O2B	2.10	115.40	105.99
2	D	313	NDP	C1B-N9A-C4A	-2.09	122.97	126.64
5	D	314	EPE	C2-C3-N4	2.08	114.90	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	313	NDP	O2N-PN-O1N	2.06	122.42	112.24
2	D	313	NDP	O3X-P2B-O1X	-2.04	102.69	110.68

There are no chirality outliers.

All (35) torsion outliers are listed below:

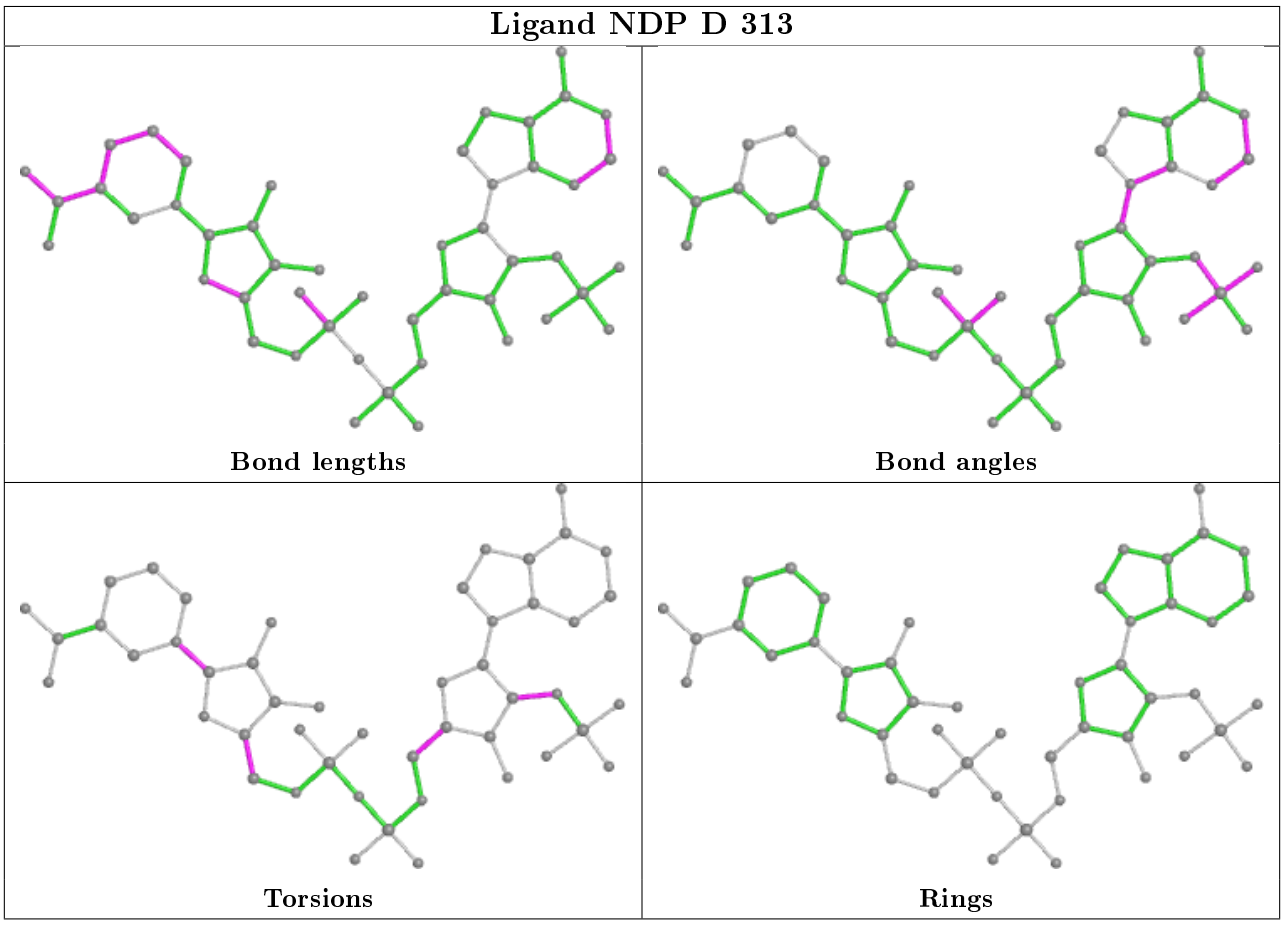
Mol	Chain	Res	Type	Atoms
2	B	313	NDP	C5B-O5B-PA-O1A
2	B	313	NDP	C5B-O5B-PA-O2A
3	A	314	NDB	CAH-CAJ-NAL-CAA
3	A	314	NDB	CAH-CAJ-NAL-CAB
2	B	313	NDP	O4B-C4B-C5B-O5B
2	B	313	NDP	C3B-C4B-C5B-O5B
2	D	313	NDP	C3B-C2B-O2B-P2B
2	C	313	NDP	C3B-C2B-O2B-P2B
2	A	313	NDP	C3B-C2B-O2B-P2B
2	B	313	NDP	C3B-C2B-O2B-P2B
3	A	314	NDB	CAH-CAJ-NAL-CAI
2	C	313	NDP	C1B-C2B-O2B-P2B
2	C	313	NDP	C3D-C4D-C5D-O5D
2	B	313	NDP	C3D-C4D-C5D-O5D
2	A	313	NDP	C1B-C2B-O2B-P2B
2	C	313	NDP	O4D-C4D-C5D-O5D
2	B	313	NDP	O4D-C4D-C5D-O5D
2	A	313	NDP	O4D-C1D-N1N-C2N
2	D	313	NDP	C1B-C2B-O2B-P2B
2	D	313	NDP	O4D-C1D-N1N-C2N
3	A	314	NDB	CAJ-CAH-CAK-SAM
5	D	314	EPE	S-C10-C9-N1
5	B	314	EPE	C10-C9-N1-C2
2	B	313	NDP	O4D-C1D-N1N-C2N
2	C	313	NDP	O4D-C1D-N1N-C2N
5	B	314	EPE	C10-C9-N1-C6
2	D	313	NDP	C3D-C4D-C5D-O5D
2	B	313	NDP	C1B-C2B-O2B-P2B
2	A	313	NDP	O4B-C4B-C5B-O5B
2	C	313	NDP	O4B-C4B-C5B-O5B
2	B	313	NDP	C5B-O5B-PA-O3
2	D	313	NDP	O4B-C4B-C5B-O5B
5	D	314	EPE	C8-C7-N4-C5
2	A	313	NDP	C5B-O5B-PA-O1A
5	D	314	EPE	C8-C7-N4-C3

There are no ring outliers.

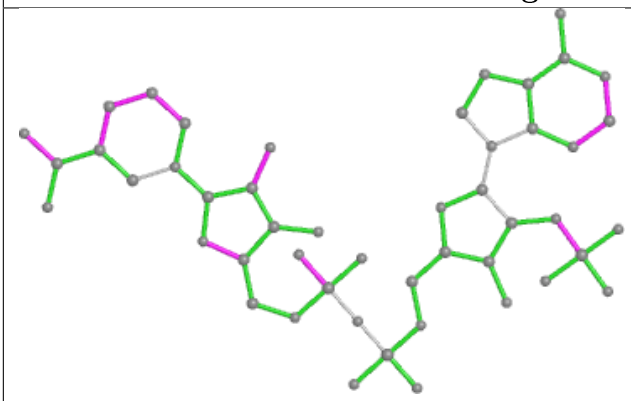
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	313	NDP	1	0
3	A	314	NDB	1	0
2	A	313	NDP	2	0
2	B	313	NDP	1	0

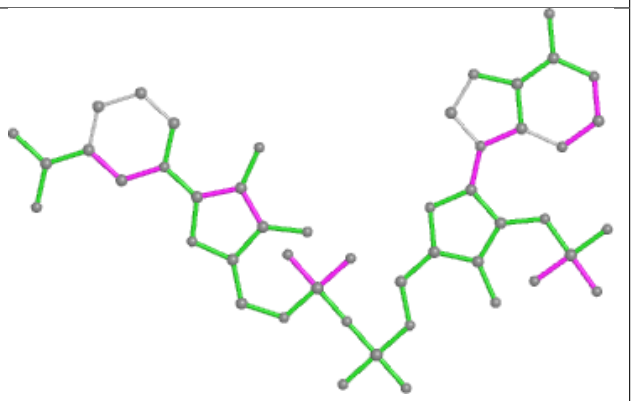
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



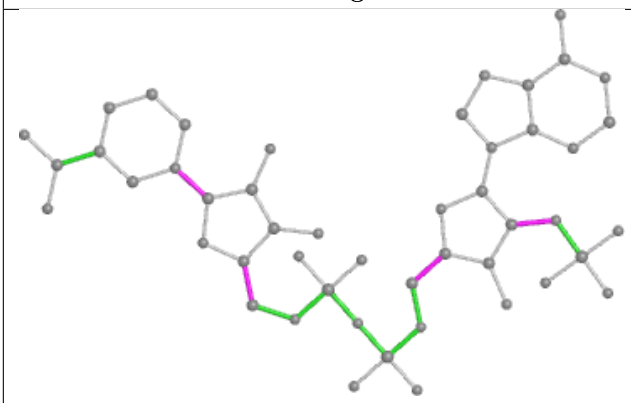
Ligand NDP C 313



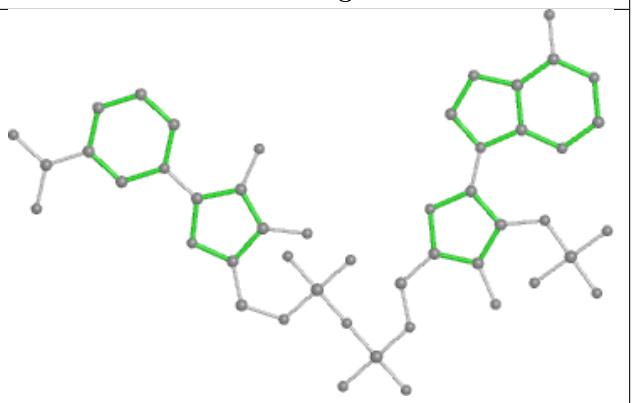
Bond lengths



Bond angles

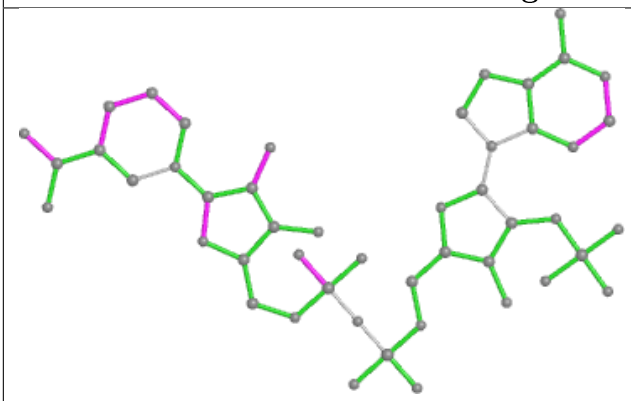


Torsions

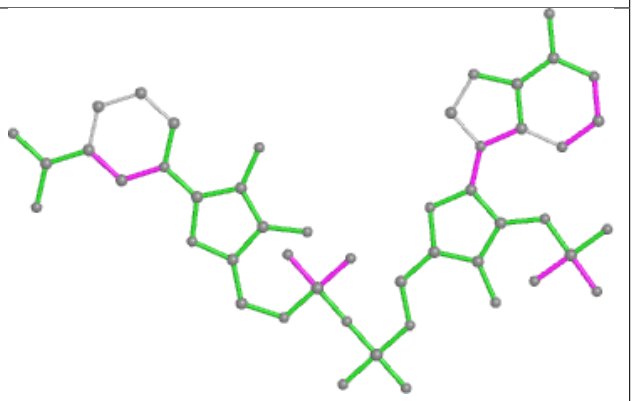


Rings

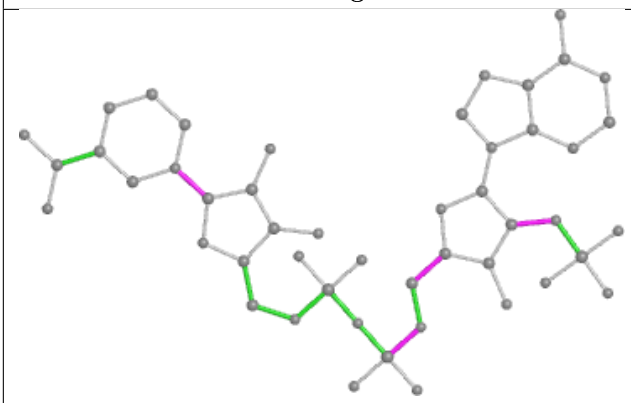
Ligand NDP A 313



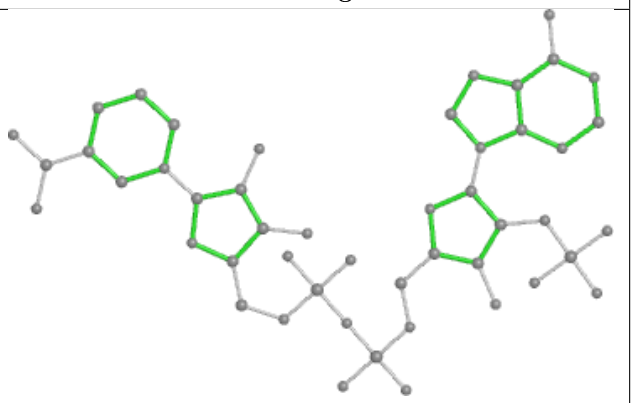
Bond lengths



Bond angles

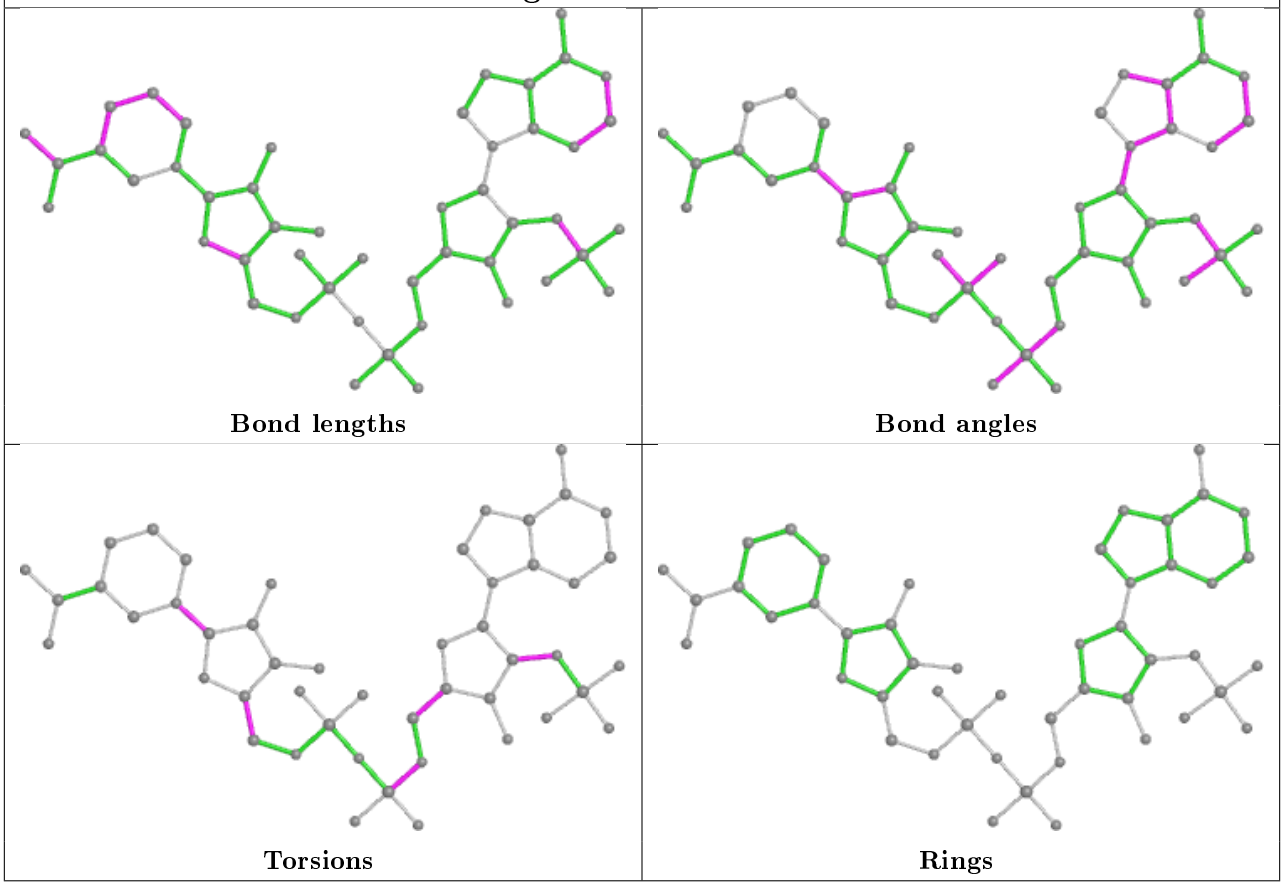


Torsions



Rings

Ligand NDP B 313



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	304/315 (96%)	0.33	11 (3%) 42 50	9, 29, 49, 58	0
1	B	304/315 (96%)	0.44	23 (7%) 13 17	17, 34, 53, 68	0
1	C	304/315 (96%)	0.22	11 (3%) 42 50	14, 28, 41, 51	0
1	D	304/315 (96%)	0.63	31 (10%) 6 8	16, 39, 54, 67	0
All	All	1216/1260 (96%)	0.41	76 (6%) 20 25	9, 31, 52, 68	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	LYS	5.3
1	D	75	ASN	4.9
1	C	261	GLU	4.9
1	B	75	ASN	4.8
1	A	299	GLY	4.2
1	B	25	HIS	4.2
1	B	76	ALA	4.2
1	A	261	GLU	4.1
1	B	33	VAL	3.9
1	D	76	ALA	3.9
1	B	260	GLN	3.7
1	D	241	ASP	3.6
1	C	303	THR	3.5
1	A	81	LEU	3.5
1	D	238	ALA	3.4
1	A	262	SER	3.3
1	B	103	ALA	3.1
1	D	56	ARG	3.0
1	D	171	SER	2.9
1	B	74	LEU	2.8
1	B	241	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	309	ALA	2.7
1	A	259	PRO	2.7
1	D	49	VAL	2.7
1	C	25	HIS	2.7
1	A	309	ALA	2.7
1	D	182	GLU	2.6
1	C	255	GLN	2.6
1	B	102	TYR	2.6
1	D	173	PRO	2.6
1	D	240	LEU	2.5
1	D	261	GLU	2.5
1	B	108	LEU	2.5
1	D	266	ARG	2.5
1	A	78	PRO	2.5
1	D	242	SER	2.5
1	D	156	GLN	2.5
1	C	238	ALA	2.5
1	D	243	GLY	2.5
1	C	223	LEU	2.4
1	D	237	LEU	2.4
1	A	49	VAL	2.4
1	D	2	GLU	2.4
1	D	54	GLY	2.4
1	C	193	VAL	2.4
1	A	75	ASN	2.4
1	D	309	ALA	2.4
1	D	25	HIS	2.3
1	A	193	VAL	2.3
1	D	103	ALA	2.3
1	B	106	GLN	2.3
1	B	261	GLU	2.3
1	B	238	ALA	2.2
1	D	223	LEU	2.2
1	D	255	GLN	2.2
1	D	265	TRP	2.2
1	A	194	LEU	2.2
1	B	53	ALA	2.2
1	B	242	SER	2.2
1	C	259	PRO	2.1
1	D	78	PRO	2.1
1	D	102	TYR	2.1
1	D	259	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	77	HIS	2.1
1	B	109	HIS	2.1
1	D	73	LYS	2.1
1	B	243	GLY	2.1
1	B	257	PRO	2.1
1	D	225	LEU	2.0
1	B	107	VAL	2.0
1	B	277	ALA	2.0
1	D	260	GLN	2.0
1	B	104	VAL	2.0
1	C	266	ARG	2.0
1	C	298	LYS	2.0
1	D	6	TYR	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 carbohydrates 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EPE	D	314	15/15	0.76	0.20	48,57,61,62	0
5	EPE	B	314	15/15	0.81	0.17	41,56,64,64	0
4	CL	B	316	1/1	0.90	0.06	61,61,61,61	0
4	CL	B	315	1/1	0.90	0.17	54,54,54,54	0
3	NDB	A	314	13/13	0.92	0.20	31,33,40,45	0
4	CL	D	316	1/1	0.93	0.11	62,62,62,62	0
4	CL	C	315	1/1	0.93	0.04	63,63,63,63	0
4	CL	A	315	1/1	0.93	0.14	52,52,52,52	0
4	CL	D	315	1/1	0.94	0.23	55,55,55,55	0
4	CL	C	314	1/1	0.94	0.08	44,44,44,44	0

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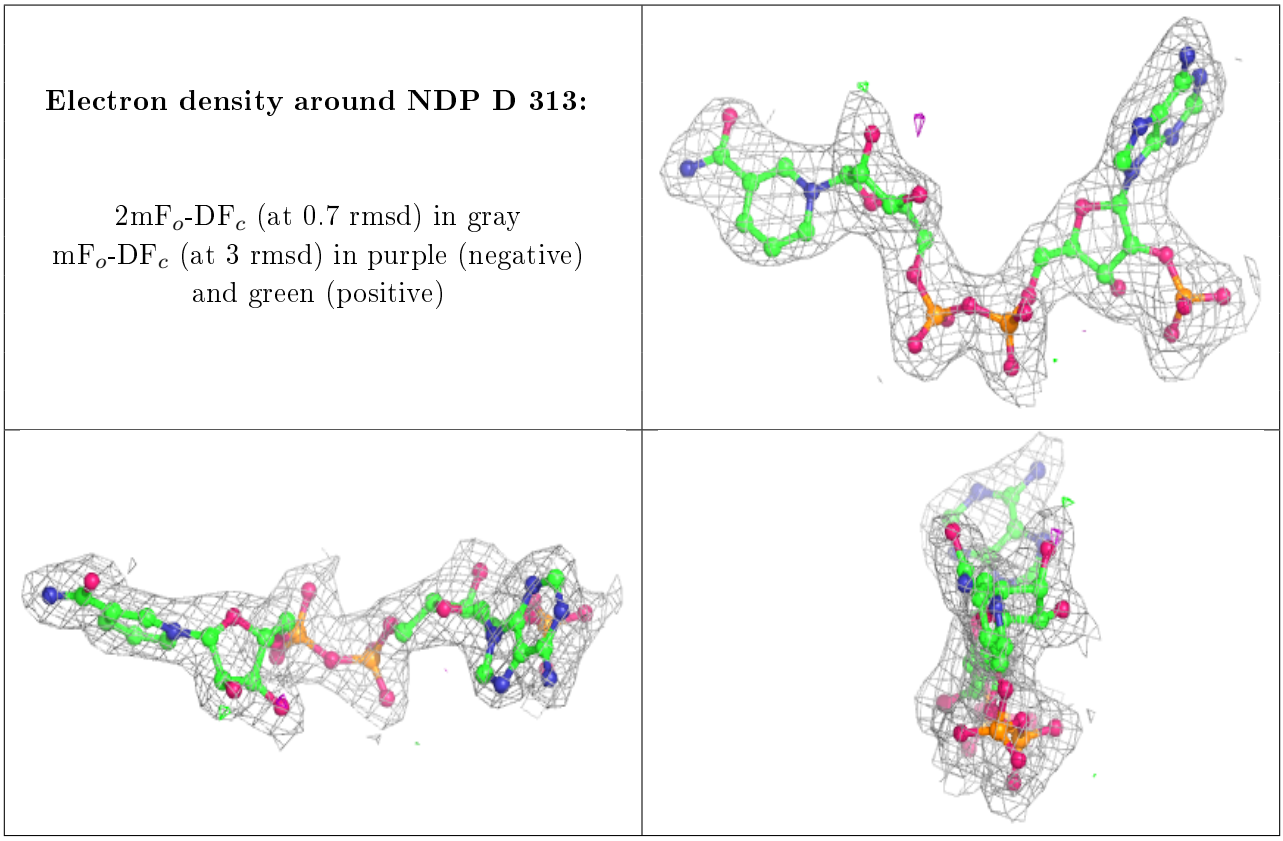
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NDP	D	313	48/48	0.95	0.11	20,28,35,37	0
2	NDP	B	313	48/48	0.96	0.10	15,25,29,34	0
2	NDP	C	313	48/48	0.97	0.09	13,19,24,27	0
4	CL	A	316	1/1	0.97	0.04	62,62,62,62	0
2	NDP	A	313	48/48	0.97	0.10	11,19,25,27	0

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.

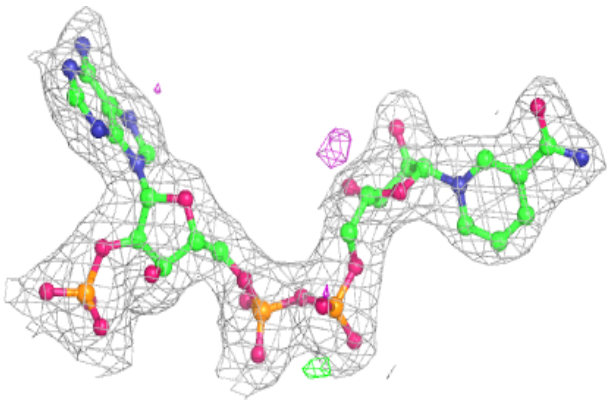
Electron density around NDP D 313:

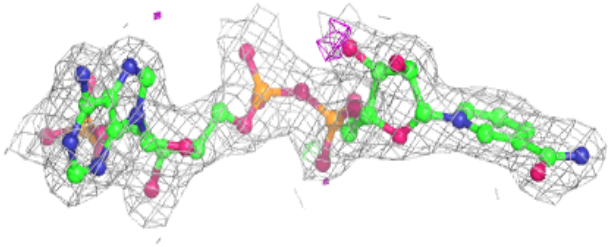
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

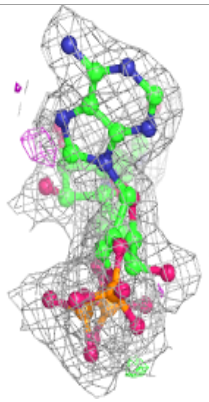


Electron density around NDP B 313:

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

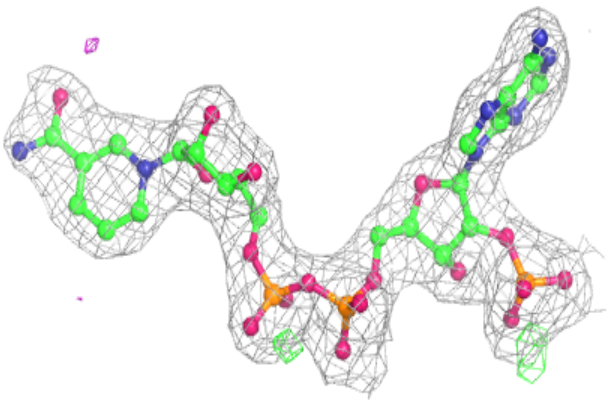


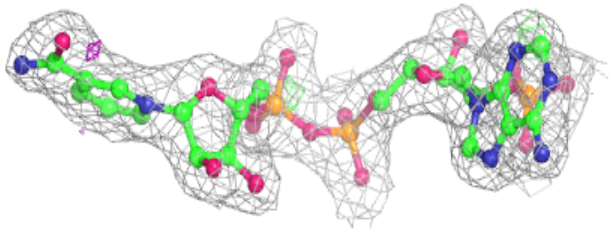


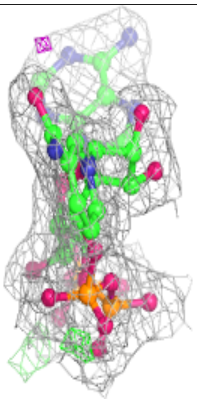


Electron density around NDP C 313:

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

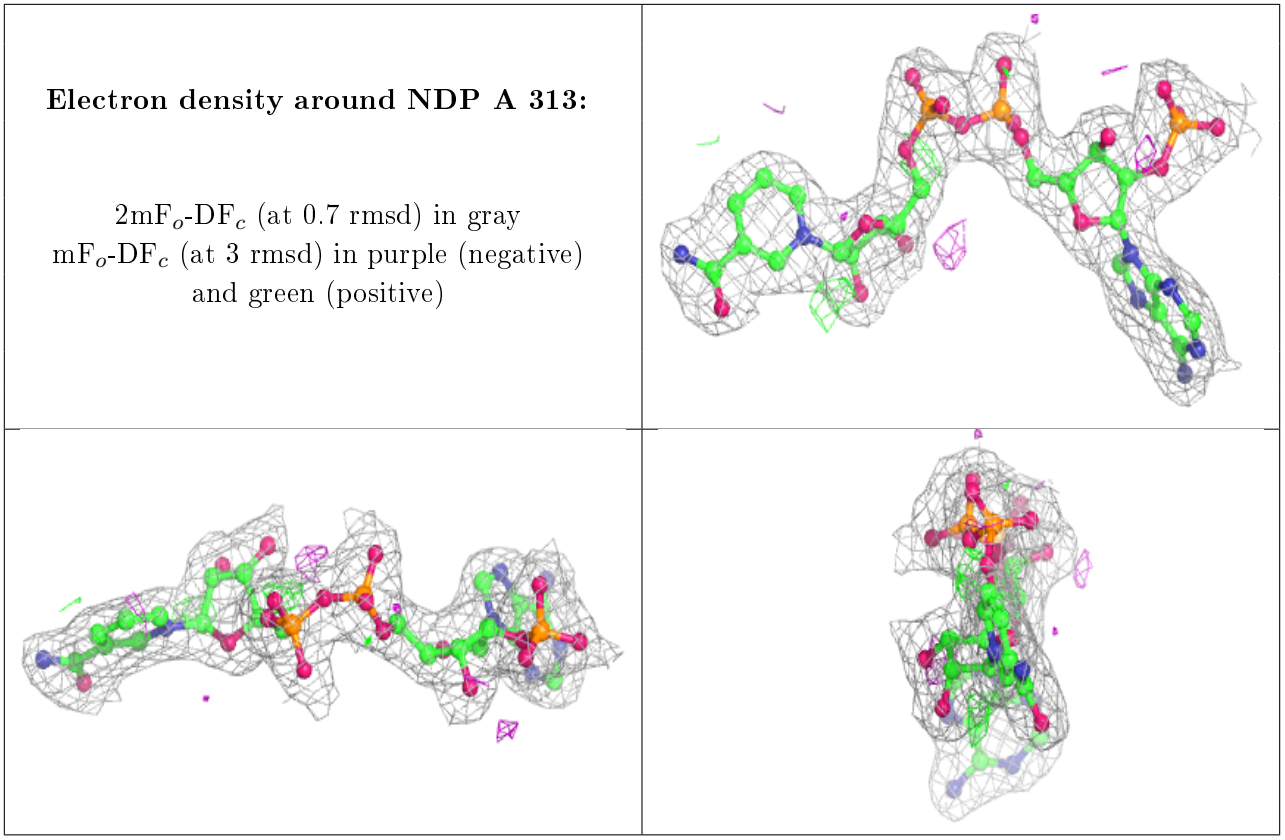






Electron density around NDP A 313:

$2mF_o$-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.