Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2022 – 02:11 PM EDT

PDB ID	:	6NA5
Title	:	Crystal Structure of ECR in complex with NADP+
Authors	:	DeMirci, H.
Deposited on	:	2018-12-05
Resolution	:	1.75 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:

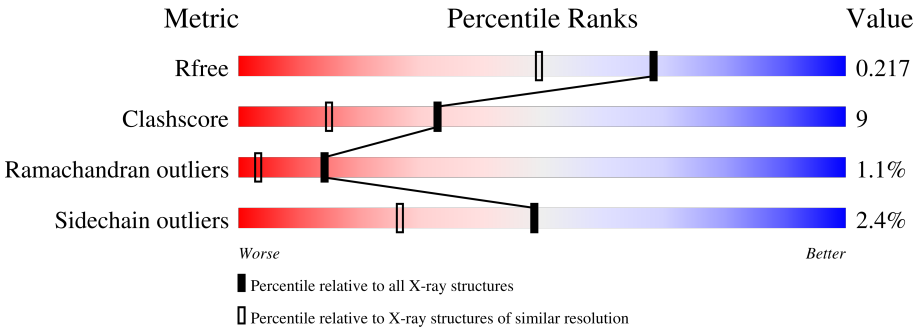
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	445	89% 10% ·
1	B	445	88% 10% ·
1	C	445	81% 17% ·
1	D	445	85% 13% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDP	A	501	X	-	-	-
2	NDP	B	501	X	-	-	-
2	NDP	C	501	X	-	-	-
2	NDP	D	501	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15737 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.

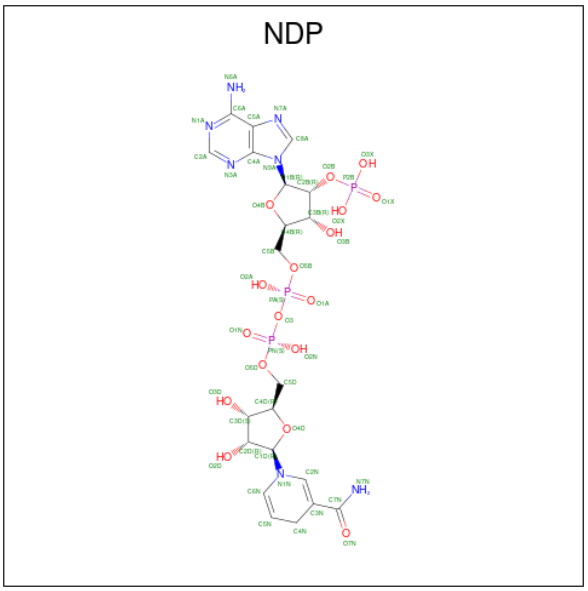
- Molecule 1 is a protein called Putative crotonyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total 3449	C 2169	N 621	O 646	S 13	0	2	0
1	B	445	Total 3449	C 2169	N 621	O 646	S 13	6	2	0
1	C	445	Total 3449	C 2169	N 621	O 646	S 13	6	2	0
1	D	445	Total 3449	C 2169	N 621	O 646	S 13	6	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP E4N096
A	0	HIS	-	expression tag	UNP E4N096
B	-1	ARG	-	expression tag	UNP E4N096
B	0	HIS	-	expression tag	UNP E4N096
C	-1	ARG	-	expression tag	UNP E4N096
C	0	HIS	-	expression tag	UNP E4N096
D	-1	ARG	-	expression tag	UNP E4N096
D	0	HIS	-	expression tag	UNP E4N096

- 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 water.

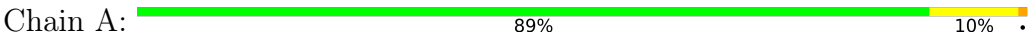
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	426	Total	O	0	0
			426	426		
3	B	408	Total	O	0	0
			408	408		
3	C	431	Total	O	0	0
			431	431		
3	D	484	Total	O	0	0
			484	484		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

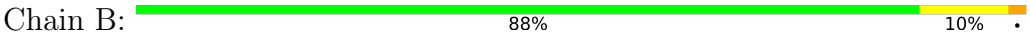
• Molecule 1: Putative crotonyl-CoA reductase

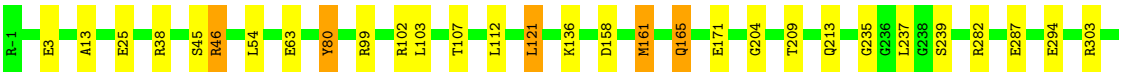
Chain A:

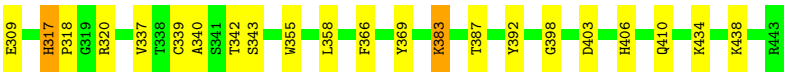


• Molecule 1: Putative crotonyl-CoA reductase

Chain B:

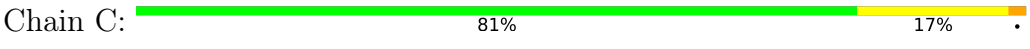


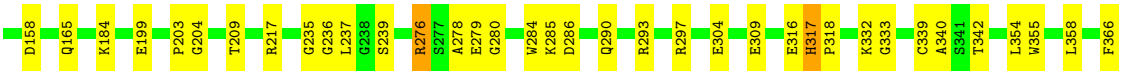




• Molecule 1: Putative crotonyl-CoA reductase

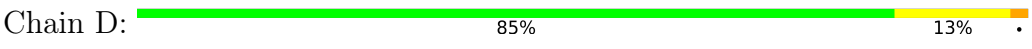
Chain C:

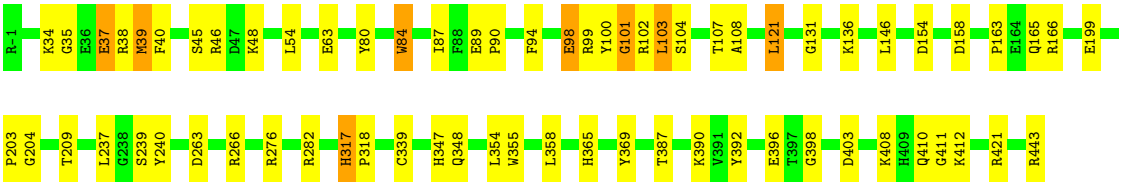




• Molecule 1: Putative crotonyl-CoA reductase

Chain D:




R-1
K34
G35
E36
E37
R38
M39
F40
S45
R46
D47
K48
L54
E63
Y80
W84
I87
F88
E89
P90
F94
E98
R99
Y100
G101
R102
L103
S104
T107
A108
L121
G131
K136
L146
D154
D158
P163
E164
Q165
R166
E199
P203
G204
T209
L237
G238
S239
Y240
D263
R266
R276
R282
H317
P318
C339
H347
Q348
L354
W355
L358
H365
Y369
T387
K390
V391
Y392
E396
T397
G398
D403
K408
H409
Q410
G411
K412
R421
R443

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.00Å 146.70Å 200.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 1.75 49.36 – 1.36	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.36-1.75) 80.9 (49.36-1.36)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.72 (at 1.36Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.217 0.195 , 0.217	Depositor DCC
R_{free} test set	2000 reflections (0.51%)	wwPDB-VP
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15737	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 25.49 % 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 3.1384e-03. 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

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	0.36	0/3531	0.57	2/4787 (0.0%)
1	B	0.37	0/3531	0.57	3/4787 (0.1%)
1	C	0.39	0/3531	0.62	2/4787 (0.0%)
1	D	0.41	0/3531	0.63	2/4787 (0.0%)
All	All	0.38	0/14124	0.60	9/19148 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	121	LEU	CA-CB-CG	7.69	132.98	115.30
1	D	121	LEU	CA-CB-CG	7.11	131.66	115.30
1	B	161	MET	CG-SD-CE	-6.61	89.63	100.20
1	B	121	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	358	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	121	LEU	CA-CB-CG	5.88	128.82	115.30
1	C	358	LEU	CA-CB-CG	5.37	127.66	115.30
1	D	358	LEU	CA-CB-CG	5.25	127.36	115.30
1	B	358	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	411	GLY	Peptide

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	3449	0	3379	46	0
1	B	3449	0	3379	51	0
1	C	3449	0	3379	79	0
1	D	3449	0	3379	58	0
2	A	48	0	25	7	0
2	B	48	0	25	10	0
2	C	48	0	25	7	0
2	D	48	0	25	9	0
3	A	426	0	0	25	1
3	B	408	0	0	23	2
3	C	431	0	0	48	3
3	D	484	0	0	28	4
All	All	15737	0	13616	239	5

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 (239) 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:280:GLY:C	3:C:601:HOH:O	1.84	1.13
1:C:377:ARG:NH2	3:C:603:HOH:O	1.82	1.12
1:C:278:ALA:HB2	3:C:610:HOH:O	1.50	1.10
2:D:501:NDP:O4D	2:D:501:NDP:C1D	1.63	1.08
1:A:282:ARG:NH1	3:A:601:HOH:O	1.85	1.07
1:A:34:LYS:NZ	1:A:37:GLU:OE1	1.86	1.07
1:C:217:ARG:CD	3:C:606:HOH:O	1.99	1.07
1:B:161:MET:SD	3:B:920:HOH:O	2.09	1.06
1:C:217:ARG:NE	3:C:606:HOH:O	1.88	1.02
1:D:37:GLU:HB3	3:D:624:HOH:O	1.58	1.01
1:D:99:ARG:NH2	3:D:603:HOH:O	1.95	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:NDP:P2B	3:A:610:HOH:O	2.21	0.98
1:B:366:PHE:H	2:B:501:NDP:H72N	1.11	0.98
1:C:309:GLU:OE1	3:C:602:HOH:O	1.82	0.98
1:A:-1:ARG:NH2	3:A:605:HOH:O	1.95	0.97
1:D:263:ASP:OD1	3:D:601:HOH:O	1.86	0.94
1:B:309:GLU:OE1	3:B:601:HOH:O	1.86	0.93
1:C:280:GLY:O	3:C:601:HOH:O	1.80	0.91
1:A:282:ARG:CZ	3:A:601:HOH:O	2.15	0.91
1:A:260:ARG:HD2	3:A:604:HOH:O	1.71	0.90
1:C:98:GLU:O	3:C:605:HOH:O	1.88	0.90
1:B:112:LEU:O	3:B:602:HOH:O	1.90	0.90
1:A:-1:ARG:NH2	3:A:606:HOH:O	1.98	0.90
1:D:136:LYS:HE3	3:D:941:HOH:O	1.72	0.89
1:C:297:ARG:NH2	3:C:601:HOH:O	1.83	0.88
1:C:407:ASN:ND2	3:C:611:HOH:O	2.07	0.88
1:C:278:ALA:N	3:C:610:HOH:O	2.07	0.87
1:B:171:GLU:OE2	3:B:604:HOH:O	1.91	0.87
1:D:34:LYS:O	1:D:37:GLU:HB2	1.76	0.86
1:A:261:LYS:NZ	3:A:610:HOH:O	2.10	0.85
1:A:165:GLN:OE1	3:A:603:HOH:O	1.93	0.84
1:B:410:GLN:NE2	3:B:608:HOH:O	2.11	0.84
1:B:343:SER:O	3:B:605:HOH:O	1.95	0.83
1:C:63:GLU:OE1	3:C:607:HOH:O	1.98	0.82
1:D:87:ILE:HG13	1:D:89:GLU:HB3	1.61	0.81
1:C:278:ALA:CA	3:C:610:HOH:O	2.28	0.81
1:D:282:ARG:NE	3:D:607:HOH:O	2.10	0.81
2:A:501:NDP:H2N	3:A:665:HOH:O	1.81	0.80
1:B:13:ALA:O	3:B:606:HOH:O	1.99	0.80
1:C:434:LYS:HE3	3:C:948:HOH:O	1.80	0.80
1:C:28:ARG:HD2	3:C:620:HOH:O	1.80	0.80
1:C:279:GLU:O	3:C:601:HOH:O	2.00	0.80
1:C:217:ARG:CZ	3:C:606:HOH:O	2.27	0.79
1:A:263:ASP:OD1	3:A:608:HOH:O	2.01	0.79
1:A:383:LYS:HD2	3:A:976:HOH:O	1.81	0.78
1:A:293:ARG:NH2	3:A:611:HOH:O	2.15	0.78
1:C:28:ARG:NH2	3:C:612:HOH:O	2.09	0.77
1:C:278:ALA:CB	3:C:610:HOH:O	2.15	0.76
1:A:-1:ARG:NH2	3:A:612:HOH:O	2.19	0.76
1:C:102:ARG:C	3:C:613:HOH:O	2.23	0.76
1:D:421:ARG:NE	3:D:604:HOH:O	1.95	0.74
1:D:131:GLY:O	3:D:605:HOH:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:NH2	3:A:604:HOH:O	1.94	0.73
1:C:40:PHE:HB3	1:C:48:LYS:HD3	1.68	0.73
1:C:47:ASP:O	3:C:609:HOH:O	2.06	0.73
1:B:366:PHE:N	2:B:501:NDP:H72N	1.86	0.70
1:B:3:GLU:OE1	3:B:607:HOH:O	2.09	0.69
1:D:98:GLU:O	3:D:606:HOH:O	2.09	0.69
1:C:28:ARG:NH1	3:C:620:HOH:O	2.22	0.69
1:C:28:ARG:NH1	3:C:622:HOH:O	2.24	0.69
1:C:102:ARG:O	3:C:613:HOH:O	2.10	0.69
1:C:239[B]:SER:HB2	1:C:387:THR:HG21	1.75	0.69
1:B:38:ARG:HB2	3:B:609:HOH:O	1.93	0.69
1:D:63:GLU:OE1	3:D:608:HOH:O	2.10	0.69
1:D:239[B]:SER:HB2	1:D:387:THR:HG21	1.76	0.68
1:C:28:ARG:CD	3:C:620:HOH:O	2.40	0.67
1:A:321:GLU:HG2	2:A:501:NDP:H62A	1.59	0.67
1:C:304:GLU:OE2	3:C:615:HOH:O	2.13	0.67
1:D:39:MET:N	3:D:614:HOH:O	2.27	0.67
1:A:166:ARG:NH1	3:A:609:HOH:O	2.08	0.66
1:D:392:TYR:HB3	1:D:396:GLU:HG3	1.77	0.66
1:C:63:GLU:CD	3:C:607:HOH:O	2.34	0.66
1:A:293:ARG:CZ	3:A:611:HOH:O	2.43	0.66
1:D:103:LEU:HG	1:D:104:SER:N	2.10	0.65
1:C:102:ARG:N	3:C:605:HOH:O	2.30	0.64
1:C:407:ASN:ND2	3:C:619:HOH:O	2.22	0.64
1:C:430:GLU:OE1	3:C:616:HOH:O	2.13	0.64
1:A:80:TYR:OH	2:A:501:NDP:O2A	2.12	0.63
1:C:103:LEU:HG	1:C:104:SER:N	2.14	0.63
2:B:501:NDP:H2N	3:B:611:HOH:O	1.98	0.63
1:D:45:SER:HA	1:D:48:LYS:HD2	1.80	0.63
1:A:260:ARG:CD	3:A:604:HOH:O	2.37	0.63
1:D:408:LYS:HA	1:D:408:LYS:HE3	1.81	0.63
1:A:293:ARG:CD	3:A:611:HOH:O	2.47	0.62
1:C:87:ILE:HG13	1:C:89:GLU:HB3	1.82	0.62
1:C:3:GLU:HG3	3:C:641:HOH:O	1.99	0.62
1:C:80:TYR:HB2	2:C:501:NDP:H52N	1.81	0.61
1:D:100:TYR:O	1:D:102:ARG:N	2.34	0.61
1:D:131:GLY:CA	3:D:605:HOH:O	2.48	0.61
1:D:421:ARG:NH1	3:D:604:HOH:O	2.34	0.60
1:C:131:GLY:HA3	3:C:636:HOH:O	2.02	0.60
1:C:49:ASP:OD2	1:C:51:ARG:HB2	2.01	0.60
1:B:340:ALA:HB2	2:B:501:NDP:H2D	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:PHE:HB3	1:D:48:LYS:HE2	1.84	0.58
1:B:239[B]:SER:HB2	1:B:387:THR:HG21	1.86	0.58
1:A:209:THR:HG21	2:A:501:NDP:H41N	1.86	0.58
1:B:209:THR:HG21	2:B:501:NDP:H41N	1.85	0.58
1:B:38:ARG:N	3:B:609:HOH:O	2.14	0.57
1:B:161:MET:HE1	1:C:332:LYS:C	2.25	0.57
1:D:38:ARG:NH2	3:D:618:HOH:O	2.37	0.57
1:A:237:LEU:HD21	1:A:339:CYS:SG	2.44	0.56
1:B:38:ARG:CB	3:B:609:HOH:O	2.53	0.56
1:B:63:GLU:HA	3:B:655:HOH:O	2.05	0.56
1:B:342:THR:HG22	2:B:501:NDP:O3D	2.05	0.56
2:B:501:NDP:O2D	3:B:611:HOH:O	2.18	0.56
1:A:383:LYS:NZ	3:A:607:HOH:O	1.99	0.56
1:C:438:LYS:NZ	3:C:629:HOH:O	2.39	0.55
1:A:34:LYS:O	1:A:34:LYS:HD3	2.07	0.55
1:C:99:ARG:O	3:C:618:HOH:O	2.18	0.55
1:C:217:ARG:HD3	3:C:606:HOH:O	1.83	0.55
1:A:25:GLU:HG3	3:A:636:HOH:O	2.06	0.55
2:D:501:NDP:H2D	3:D:909:HOH:O	2.07	0.54
1:A:289:HIS:HE1	3:D:894:HOH:O	1.90	0.54
1:D:390:LYS:NZ	3:D:621:HOH:O	2.40	0.54
1:D:131:GLY:HA3	3:D:605:HOH:O	2.07	0.54
1:B:392:TYR:OH	1:B:403:ASP:OD2	2.11	0.53
1:B:237:LEU:HD21	1:B:339:CYS:SG	2.48	0.53
1:C:237:LEU:HD21	1:C:339:CYS:SG	2.48	0.53
1:A:38:ARG:HD3	1:A:41:ASP:OD1	2.10	0.52
1:B:99:ARG:O	1:B:102:ARG:HG2	2.10	0.51
1:A:235:GLY:O	1:A:239[A]:SER:HB3	2.10	0.51
1:D:40:PHE:HB3	1:D:48:LYS:HG2	1.93	0.51
1:C:209:THR:HG21	2:C:501:NDP:H41N	1.92	0.51
1:C:340:ALA:HB2	2:C:501:NDP:H2D	1.91	0.51
1:B:136:LYS:CD	3:B:610:HOH:O	2.58	0.51
1:D:237:LEU:HD21	1:D:339:CYS:SG	2.51	0.50
1:D:54:LEU:HD12	1:D:398:GLY:HA2	1.93	0.50
1:C:3:GLU:HG2	1:C:21:LEU:HD22	1.93	0.50
1:C:184:LYS:HE3	3:C:860:HOH:O	2.11	0.50
1:B:112:LEU:N	3:B:602:HOH:O	2.43	0.50
1:C:98:GLU:HA	1:C:111:ASP:CG	2.32	0.50
1:A:340:ALA:HB2	2:A:501:NDP:H2D	1.94	0.49
1:B:161:MET:HE3	1:B:161:MET:HA	1.93	0.49
1:B:342:THR:HG21	3:B:735:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:ARG:NH2	3:D:602:HOH:O	1.92	0.49
1:D:209:THR:HG21	2:D:501:NDP:H41N	1.94	0.49
1:B:438:LYS:HD2	3:B:651:HOH:O	2.11	0.49
1:D:94:PHE:O	1:D:98:GLU:HB2	2.12	0.49
1:B:136:LYS:HD3	3:B:610:HOH:O	2.13	0.48
1:C:388:LEU:O	1:C:443:ARG:HD2	2.12	0.48
1:D:84:TRP:HZ3	2:D:501:NDP:O2D	1.95	0.48
1:C:403:ASP:HA	1:C:408:LYS:HE2	1.95	0.48
1:B:161:MET:HE1	1:C:333:GLY:N	2.29	0.47
1:C:146:LEU:HD11	1:C:165:GLN:HG2	1.95	0.47
1:A:266:ARG:HD3	3:A:784:HOH:O	2.14	0.47
1:B:38:ARG:CA	3:B:609:HOH:O	2.61	0.47
1:C:276:ARG:NH2	3:C:635:HOH:O	2.47	0.47
1:D:35:GLY:N	3:D:616:HOH:O	2.32	0.47
1:D:102:ARG:N	3:D:606:HOH:O	2.45	0.47
1:A:149:GLU:HG2	3:A:602:HOH:O	2.15	0.47
1:B:235:GLY:O	1:B:239[B]:SER:OG	2.24	0.47
1:B:282:ARG:O	1:B:294:GLU:HG3	2.14	0.47
1:B:287:GLU:O	1:B:320:ARG:NH2	2.47	0.47
1:D:63:GLU:CD	3:D:608:HOH:O	2.53	0.47
1:D:392:TYR:OH	1:D:403:ASP:OD2	2.27	0.47
1:C:80:TYR:CB	2:C:501:NDP:H52N	2.45	0.47
1:C:45:SER:HA	1:C:48:LYS:HE3	1.97	0.47
1:B:213:GLN:HG3	1:B:337:VAL:HG22	1.96	0.46
1:D:403:ASP:HA	1:D:408:LYS:HG2	1.97	0.46
1:B:165:GLN:CG	3:C:841:HOH:O	2.62	0.46
1:B:165:GLN:HG2	3:C:841:HOH:O	2.14	0.46
1:D:266:ARG:NE	3:D:601:HOH:O	2.11	0.46
1:C:438:LYS:HB2	1:C:438:LYS:HE2	1.67	0.46
1:A:94:PHE:O	1:A:98:GLU:HG3	2.16	0.46
1:D:100:TYR:HE2	1:D:107:THR:HG21	1.80	0.46
1:C:285:LYS:NZ	3:C:623:HOH:O	2.26	0.46
1:C:29:ALA:HB1	1:C:116:VAL:HG13	1.98	0.45
1:C:235:GLY:O	1:C:239[A]:SER:HB3	2.17	0.45
1:C:407:ASN:CG	3:C:619:HOH:O	2.54	0.45
1:B:103:LEU:HD23	1:B:107:THR:HG21	1.98	0.45
1:A:388:LEU:O	1:A:443:ARG:HD2	2.17	0.45
1:D:199:GLU:O	1:D:203:PRO:HD3	2.16	0.45
1:D:317:HIS:H	1:D:318:PRO:CD	2.28	0.45
1:C:102:ARG:HG3	3:C:605:HOH:O	2.17	0.45
1:B:25:GLU:HB2	3:B:650:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ARG:HD3	1:B:406:HIS:CE1	2.51	0.45
1:C:199:GLU:O	1:C:203:PRO:HD3	2.17	0.45
2:C:501:NDP:O5D	2:C:501:NDP:H1D	2.17	0.45
1:C:136:LYS:HE2	3:C:750:HOH:O	2.16	0.44
1:D:101:GLY:CA	1:D:108:ALA:HA	2.47	0.44
1:D:412:LYS:HG3	3:D:609:HOH:O	2.15	0.44
1:B:54:LEU:HD12	1:B:398:GLY:HA2	1.99	0.44
1:D:101:GLY:HA3	1:D:108:ALA:HA	1.99	0.44
1:D:101:GLY:O	1:D:108:ALA:HB2	2.18	0.44
1:A:136:LYS:NZ	3:A:633:HOH:O	2.50	0.44
1:A:342:THR:HG22	2:A:501:NDP:H3D	1.98	0.44
1:A:347:HIS:O	1:D:348:GLN:HA	2.18	0.44
1:C:-1:ARG:HG2	1:C:2:GLN:H	1.83	0.44
1:C:284:TRP:HA	1:C:290:GLN:HA	2.00	0.44
1:C:54:LEU:HD12	1:C:398:GLY:HA2	1.99	0.44
2:D:501:NDP:O4D	2:D:501:NDP:O2D	2.16	0.44
1:B:209:THR:OG1	2:B:501:NDP:H41N	2.18	0.44
1:C:46:ARG:HG3	1:C:406:HIS:CE1	2.53	0.43
1:B:317:HIS:H	1:B:318:PRO:CD	2.31	0.43
1:C:236:GLY:O	1:C:239[B]:SER:OG	2.35	0.43
1:C:318:PRO:HA	1:C:342:THR:OG1	2.18	0.43
1:A:199:GLU:O	1:A:203:PRO:HD3	2.18	0.43
1:A:317:HIS:H	1:A:318:PRO:CD	2.30	0.43
1:D:84:TRP:CH2	2:D:501:NDP:O3D	2.72	0.43
1:B:45:SER:HB2	3:B:871:HOH:O	2.19	0.43
1:C:317:HIS:H	1:C:318:PRO:CD	2.31	0.43
1:A:217:ARG:CZ	3:C:606:HOH:O	2.66	0.43
1:B:235:GLY:O	1:B:239[A]:SER:HB3	2.19	0.43
1:D:102:ARG:HG3	3:D:606:HOH:O	2.18	0.43
1:A:282:ARG:NH2	3:A:601:HOH:O	2.41	0.43
1:B:317:HIS:CG	1:B:318:PRO:HD3	2.54	0.43
1:D:146:LEU:HD11	1:D:165:GLN:HG2	2.00	0.43
1:B:303:ARG:NE	3:B:636:HOH:O	2.52	0.43
1:D:38:ARG:HD2	3:D:618:HOH:O	2.19	0.42
1:A:54:LEU:HD12	1:A:398:GLY:HA2	2.00	0.42
1:C:383:LYS:HA	1:C:383:LYS:HD3	1.94	0.42
2:D:501:NDP:O4D	2:D:501:NDP:C6N	2.67	0.42
1:D:40:PHE:CG	1:D:48:LYS:HG2	2.55	0.42
1:D:84:TRP:HH2	2:D:501:NDP:O3D	2.02	0.42
1:C:106:LEU:CD2	3:C:607:HOH:O	2.67	0.42
1:A:217:ARG:NE	3:C:606:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LYS:HG2	3:D:688:HOH:O	2.18	0.42
1:B:434:LYS:HB2	1:B:434:LYS:HE2	1.81	0.42
1:C:340:ALA:HB2	2:C:501:NDP:C2D	2.49	0.42
1:D:100:TYR:CE1	1:D:166:ARG:NH2	2.87	0.42
1:A:355:TRP:O	1:D:365:HIS:HB2	2.20	0.42
1:C:103:LEU:C	3:C:613:HOH:O	2.58	0.41
1:C:144:HIS:HB2	1:C:366:PHE:HZ	1.84	0.41
1:A:121:LEU:C	1:A:121:LEU:HD23	2.41	0.41
1:C:32:LEU:HD21	1:C:86:SER:HA	2.01	0.41
1:C:96:PHE:CD2	3:C:648:HOH:O	2.57	0.41
1:A:193:LYS:HE3	3:A:983:HOH:O	2.21	0.41
1:B:340:ALA:CB	2:B:501:NDP:H2D	2.49	0.41
1:C:342:THR:HG23	2:C:501:NDP:O3D	2.19	0.41
2:D:501:NDP:O4D	2:D:501:NDP:H6N	2.21	0.41
1:A:348:GLN:HA	1:D:347:HIS:O	2.21	0.41
1:B:80:TYR:HB2	2:B:501:NDP:C5D	2.51	0.41
1:B:165:GLN:O	1:B:165:GLN:HG3	2.20	0.41
1:D:46:ARG:HD2	3:D:838:HOH:O	2.21	0.41
1:D:317:HIS:CG	1:D:318:PRO:HD3	2.56	0.41
1:A:317:HIS:CG	1:A:318:PRO:HD3	2.56	0.40
1:D:154:ASP:HB2	1:D:163:PRO:HD3	2.03	0.40
1:C:101:GLY:CA	1:C:108:ALA:HA	2.51	0.40
1:D:240:TYR:OH	3:D:609:HOH:O	2.20	0.40

All (5) 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)
3:C:676:HOH:O	3:D:817:HOH:O[1_455]	1.67	0.53
3:B:683:HOH:O	3:D:951:HOH:O[3_554]	1.84	0.36
3:C:968:HOH:O	3:D:884:HOH:O[1_455]	1.85	0.35
3:B:972:HOH:O	3:D:866:HOH:O[4_555]	1.92	0.28
3:A:977:HOH:O	3:C:966:HOH:O[4_455]	2.06	0.14

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	445/445 (100%)	436 (98%)	6 (1%)	3 (1%)	22 8
1	B	445/445 (100%)	430 (97%)	12 (3%)	3 (1%)	22 8
1	C	445/445 (100%)	423 (95%)	17 (4%)	5 (1%)	14 3
1	D	445/445 (100%)	423 (95%)	14 (3%)	8 (2%)	8 1
All	All	1780/1780 (100%)	1712 (96%)	49 (3%)	19 (1%)	14 3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	317	HIS
1	B	158	ASP
1	B	317	HIS
1	C	158	ASP
1	C	317	HIS
1	D	37	GLU
1	D	101	GLY
1	D	158	ASP
1	D	317	HIS
1	A	204	GLY
1	B	204	GLY
1	C	101	GLY
1	C	103	LEU
1	D	103	LEU
1	C	204	GLY
1	D	39	MET
1	D	204	GLY
1	D	90	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	359/357 (101%)	352 (98%)	7 (2%)	57 37
1	B	359/357 (101%)	352 (98%)	7 (2%)	57 37
1	C	359/357 (101%)	347 (97%)	12 (3%)	38 15
1	D	359/357 (101%)	350 (98%)	9 (2%)	47 25
All	All	1436/1428 (101%)	1401 (98%)	35 (2%)	49 26

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	121	LEU
1	A	239[A]	SER
1	A	239[B]	SER
1	A	260	ARG
1	A	293	ARG
1	A	316	GLU
1	B	46	ARG
1	B	80	TYR
1	B	121	LEU
1	B	165	GLN
1	B	355	TRP
1	B	369	TYR
1	B	383	LYS
1	C	28	ARG
1	C	45	SER
1	C	80	TYR
1	C	121	LEU
1	C	276	ARG
1	C	286	ASP
1	C	293	ARG
1	C	316	GLU
1	C	354	LEU
1	C	355	TRP
1	C	369	TYR
1	C	438	LYS
1	D	80	TYR
1	D	84	TRP
1	D	98	GLU
1	D	121	LEU
1	D	276	ARG
1	D	354	LEU
1	D	355	TRP

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Mol	Chain	Res	Type
1	D	369	TYR
1	D	410	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	B	406	HIS
1	B	409	HIS

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 monosaccharides 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	501	-	45,52,52	3.94	17 (37%)	53,80,80	2.09	14 (26%)
2	NDP	C	501	-	45,52,52	4.02	18 (40%)	53,80,80	2.65	17 (32%)
2	NDP	A	501	-	45,52,52	4.01	21 (46%)	53,80,80	2.61	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NDP	B	501	-	45,52,52	3.98	19 (42%)	53,80,80	2.28	15 (28%)

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	501	-	3/3/14/17	8/30/77/77	0/5/5/5
2	NDP	C	501	-	3/3/14/17	11/30/77/77	0/5/5/5
2	NDP	A	501	-	3/3/14/17	11/30/77/77	0/5/5/5
2	NDP	B	501	-	3/3/14/17	10/30/77/77	0/5/5/5

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NDP	O4B-C1B	15.41	1.62	1.41
2	A	501	NDP	O4B-C1B	15.36	1.62	1.41
2	C	501	NDP	O4B-C1B	14.99	1.62	1.41
2	D	501	NDP	O4B-C1B	14.93	1.61	1.41
2	D	501	NDP	O4D-C1D	9.08	1.63	1.42
2	A	501	NDP	O4D-C1D	8.99	1.63	1.42
2	C	501	NDP	O4D-C1D	8.99	1.63	1.42
2	C	501	NDP	C2D-C1D	-8.78	1.25	1.53
2	C	501	NDP	O4B-C4B	-8.51	1.26	1.45
2	A	501	NDP	O4B-C4B	-8.41	1.26	1.45
2	B	501	NDP	O4D-C1D	8.28	1.61	1.42
2	B	501	NDP	O4B-C4B	-8.22	1.26	1.45
2	D	501	NDP	O4B-C4B	-8.00	1.27	1.45
2	B	501	NDP	C2D-C1D	-7.91	1.28	1.53
2	A	501	NDP	O4D-C4D	-7.84	1.27	1.45
2	D	501	NDP	C2D-C1D	-7.67	1.28	1.53
2	B	501	NDP	O4D-C4D	-7.59	1.28	1.45
2	D	501	NDP	O4D-C4D	-7.27	1.28	1.45
2	A	501	NDP	P2B-O2B	7.16	1.72	1.59
2	B	501	NDP	P2B-O2B	7.07	1.72	1.59
2	C	501	NDP	C4N-C3N	-6.60	1.36	1.49
2	C	501	NDP	P2B-O2B	6.57	1.71	1.59
2	A	501	NDP	C2D-C1D	-6.55	1.32	1.53
2	D	501	NDP	P2B-O2B	6.31	1.71	1.59
2	C	501	NDP	O4D-C4D	-6.29	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NDP	C4N-C3N	-6.00	1.38	1.49
2	B	501	NDP	C4N-C3N	-5.91	1.38	1.49
2	A	501	NDP	C4N-C3N	-5.73	1.38	1.49
2	D	501	NDP	O3D-C3D	-4.22	1.33	1.43
2	A	501	NDP	C7N-N7N	4.22	1.44	1.33
2	B	501	NDP	C4N-C5N	-3.92	1.38	1.48
2	C	501	NDP	C4N-C5N	-3.87	1.38	1.48
2	A	501	NDP	C4N-C5N	-3.83	1.38	1.48
2	C	501	NDP	O3D-C3D	-3.68	1.34	1.43
2	C	501	NDP	O2D-C2D	3.67	1.51	1.43
2	D	501	NDP	O2D-C2D	3.67	1.51	1.43
2	D	501	NDP	C7N-N7N	3.59	1.42	1.33
2	A	501	NDP	O2D-C2D	3.54	1.51	1.43
2	D	501	NDP	C4N-C5N	-3.54	1.39	1.48
2	C	501	NDP	C7N-N7N	3.54	1.42	1.33
2	B	501	NDP	O2D-C2D	3.52	1.51	1.43
2	B	501	NDP	C6A-N6A	3.52	1.46	1.34
2	D	501	NDP	C6A-N6A	3.50	1.46	1.34
2	A	501	NDP	C6A-N6A	3.50	1.46	1.34
2	A	501	NDP	C7N-C3N	3.47	1.56	1.48
2	D	501	NDP	C7N-C3N	3.44	1.56	1.48
2	C	501	NDP	C6A-N6A	3.41	1.46	1.34
2	B	501	NDP	O3D-C3D	-3.38	1.35	1.43
2	C	501	NDP	C6N-N1N	-3.30	1.29	1.37
2	A	501	NDP	PN-O5D	2.99	1.71	1.59
2	B	501	NDP	C6N-N1N	-2.96	1.29	1.37
2	B	501	NDP	C7N-C3N	2.96	1.55	1.48
2	A	501	NDP	O3D-C3D	-2.88	1.36	1.43
2	C	501	NDP	C7N-C3N	2.78	1.54	1.48
2	D	501	NDP	C6N-N1N	-2.68	1.30	1.37
2	B	501	NDP	PN-O5D	2.63	1.69	1.59
2	D	501	NDP	O7N-C7N	-2.61	1.18	1.24
2	D	501	NDP	C6N-C5N	2.56	1.37	1.33
2	B	501	NDP	C7N-N7N	2.56	1.40	1.33
2	C	501	NDP	O7N-C7N	-2.54	1.18	1.24
2	A	501	NDP	O2B-C2B	2.54	1.53	1.44
2	B	501	NDP	O2B-C2B	2.53	1.53	1.44
2	A	501	NDP	C6N-N1N	-2.45	1.31	1.37
2	C	501	NDP	C1D-N1N	-2.44	1.39	1.46
2	C	501	NDP	PN-O5D	2.33	1.68	1.59
2	A	501	NDP	C5D-C4D	2.30	1.58	1.51
2	A	501	NDP	C6N-C5N	2.28	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NDP	O2B-C2B	2.26	1.52	1.44
2	D	501	NDP	O2B-C2B	2.22	1.52	1.44
2	A	501	NDP	O7N-C7N	-2.21	1.19	1.24
2	B	501	NDP	C5D-C4D	2.16	1.58	1.51
2	B	501	NDP	O7N-C7N	-2.14	1.19	1.24
2	A	501	NDP	C3B-C4B	2.13	1.58	1.53
2	A	501	NDP	C3D-C4D	2.10	1.58	1.53
2	B	501	NDP	C1D-N1N	-2.02	1.40	1.46

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	NDP	O4D-C1D-N1N	10.31	128.20	108.06
2	A	501	NDP	O3X-P2B-O1X	-8.14	78.83	110.68
2	B	501	NDP	C4D-O4D-C1D	-7.85	92.14	109.47
2	A	501	NDP	O2B-P2B-O1X	-7.52	80.35	109.39
2	D	501	NDP	O4D-C1D-C2D	-7.23	90.88	106.64
2	A	501	NDP	O3X-P2B-O2X	-6.80	81.64	107.64
2	C	501	NDP	C4D-O4D-C1D	-6.25	95.69	109.47
2	C	501	NDP	C1D-N1N-C6N	-6.11	107.66	120.83
2	A	501	NDP	O2X-P2B-O1X	5.88	133.68	110.68
2	A	501	NDP	O2X-P2B-O2B	-5.63	80.78	105.99
2	C	501	NDP	C3N-C2N-N1N	-5.40	115.40	123.10
2	A	501	NDP	O3X-P2B-O2B	5.31	129.79	105.99
2	B	501	NDP	C3N-C2N-N1N	-4.97	116.00	123.10
2	C	501	NDP	N3A-C2A-N1A	-4.94	120.96	128.68
2	B	501	NDP	N3A-C2A-N1A	-4.90	121.02	128.68
2	C	501	NDP	C3D-C2D-C1D	-4.89	92.14	101.43
2	D	501	NDP	C3D-C2D-C1D	-4.85	92.21	101.43
2	D	501	NDP	N3A-C2A-N1A	-4.80	121.18	128.68
2	B	501	NDP	C1D-N1N-C6N	-4.74	110.62	120.83
2	B	501	NDP	O4D-C1D-C2D	-4.57	96.67	106.64
2	A	501	NDP	N3A-C2A-N1A	-4.54	121.59	128.68
2	D	501	NDP	O5D-C5D-C4D	-4.49	93.53	108.99
2	C	501	NDP	C5D-C4D-C3D	-4.33	98.97	115.18
2	B	501	NDP	O4D-C1D-N1N	4.10	116.08	108.06
2	B	501	NDP	C3N-C7N-N7N	-3.85	110.83	117.67
2	D	501	NDP	C4D-O4D-C1D	-3.76	101.19	109.47
2	C	501	NDP	O4D-C1D-C2D	-3.73	98.51	106.64
2	B	501	NDP	O7N-C7N-C3N	3.70	127.86	120.90
2	D	501	NDP	C1D-N1N-C6N	-3.68	112.89	120.83
2	A	501	NDP	C4D-O4D-C1D	-3.35	102.08	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	NDP	C3N-C2N-N1N	-3.33	118.34	123.10
2	B	501	NDP	C2D-C1D-N1N	3.06	120.96	113.30
2	D	501	NDP	C2D-C1D-N1N	3.05	120.95	113.30
2	C	501	NDP	C1D-N1N-C2N	2.99	126.09	121.11
2	A	501	NDP	PN-O3-PA	-2.90	122.87	132.83
2	C	501	NDP	C4A-C5A-N7A	-2.89	106.39	109.40
2	B	501	NDP	PN-O5D-C5D	-2.87	104.85	121.68
2	B	501	NDP	PN-O3-PA	-2.87	122.99	132.83
2	A	501	NDP	C3N-C2N-N1N	-2.78	119.12	123.10
2	A	501	NDP	C4A-C5A-N7A	-2.74	106.55	109.40
2	D	501	NDP	PN-O3-PA	-2.72	123.48	132.83
2	C	501	NDP	C3B-C2B-C1B	2.66	107.89	102.89
2	B	501	NDP	O3D-C3D-C4D	-2.66	103.37	111.05
2	B	501	NDP	C4A-C5A-N7A	-2.62	106.66	109.40
2	C	501	NDP	O2D-C2D-C1D	-2.59	101.37	110.02
2	D	501	NDP	C3B-C2B-C1B	2.57	107.73	102.89
2	C	501	NDP	PN-O3-PA	-2.53	124.14	132.83
2	D	501	NDP	O4D-C4D-C3D	-2.40	100.37	105.11
2	C	501	NDP	C3N-C7N-N7N	2.34	121.82	117.67
2	B	501	NDP	O5D-C5D-C4D	2.34	117.03	108.99
2	C	501	NDP	O7N-C7N-C3N	-2.31	116.54	120.90
2	C	501	NDP	C2D-C3D-C4D	-2.27	98.22	102.64
2	A	501	NDP	C1D-N1N-C6N	-2.20	116.09	120.83
2	A	501	NDP	C3N-C7N-N7N	2.19	121.55	117.67
2	D	501	NDP	C4A-C5A-N7A	-2.17	107.14	109.40
2	D	501	NDP	O4D-C1D-N1N	2.12	112.20	108.06
2	C	501	NDP	O2B-C2B-C3B	-2.11	104.05	111.68
2	D	501	NDP	C3N-C7N-N7N	2.08	121.37	117.67
2	B	501	NDP	O2D-C2D-C3D	-2.00	105.34	111.82

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	NDP	C4D
2	A	501	NDP	C3D
2	A	501	NDP	C2D
2	B	501	NDP	C4D
2	B	501	NDP	C3D
2	B	501	NDP	C2D
2	C	501	NDP	C4D
2	C	501	NDP	C3D
2	C	501	NDP	C2D

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Mol	Chain	Res	Type	Atom
2	D	501	NDP	C4D
2	D	501	NDP	C3D
2	D	501	NDP	C2D

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C2B-O2B-P2B-O1X
2	A	501	NDP	C5D-O5D-PN-O3
2	A	501	NDP	C5D-O5D-PN-O1N
2	A	501	NDP	C5D-O5D-PN-O2N
2	A	501	NDP	O4D-C4D-C5D-O5D
2	A	501	NDP	C3D-C4D-C5D-O5D
2	A	501	NDP	O4D-C1D-N1N-C2N
2	B	501	NDP	PN-O3-PA-O5B
2	B	501	NDP	O4D-C4D-C5D-O5D
2	C	501	NDP	C5D-O5D-PN-O3
2	C	501	NDP	C5D-O5D-PN-O1N
2	D	501	NDP	C3D-C4D-C5D-O5D
2	D	501	NDP	O4D-C1D-N1N-C2N
2	D	501	NDP	O4D-C4D-C5D-O5D
2	B	501	NDP	C3D-C4D-C5D-O5D
2	B	501	NDP	C2D-C1D-N1N-C2N
2	B	501	NDP	C2D-C1D-N1N-C6N
2	C	501	NDP	C2D-C1D-N1N-C2N
2	C	501	NDP	C2D-C1D-N1N-C6N
2	B	501	NDP	O4D-C1D-N1N-C2N
2	A	501	NDP	C2D-C1D-N1N-C6N
2	C	501	NDP	PN-O3-PA-O5B
2	D	501	NDP	C2B-O2B-P2B-O2X
2	D	501	NDP	C5D-O5D-PN-O3
2	B	501	NDP	O4D-C1D-N1N-C6N
2	C	501	NDP	O4D-C1D-N1N-C2N
2	C	501	NDP	O4D-C1D-N1N-C6N
2	A	501	NDP	C4D-C5D-O5D-PN
2	D	501	NDP	C2D-C1D-N1N-C6N
2	C	501	NDP	C3D-C4D-C5D-O5D
2	A	501	NDP	C2D-C1D-N1N-C2N
2	B	501	NDP	C2B-O2B-P2B-O3X
2	C	501	NDP	C2B-O2B-P2B-O3X
2	D	501	NDP	C2B-O2B-P2B-O3X
2	C	501	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	501	NDP	O4B-C4B-C5B-O5B
2	B	501	NDP	PA-O3-PN-O2N
2	C	501	NDP	C5D-O5D-PN-O2N
2	A	501	NDP	O4B-C4B-C5B-O5B
2	B	501	NDP	O4B-C4B-C5B-O5B

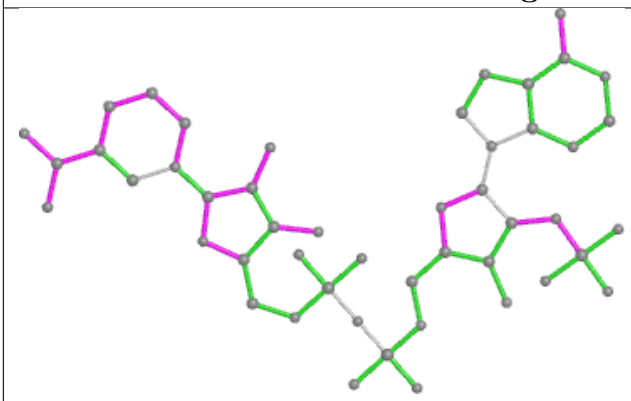
There are no ring outliers.

4 monomers are involved in 33 short contacts:

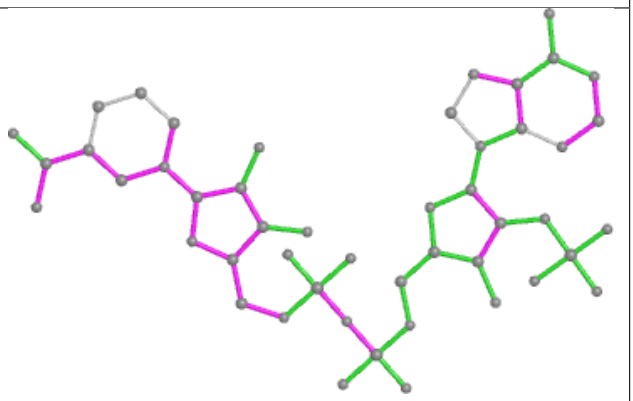
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	NDP	9	0
2	C	501	NDP	7	0
2	A	501	NDP	7	0
2	B	501	NDP	10	0

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.

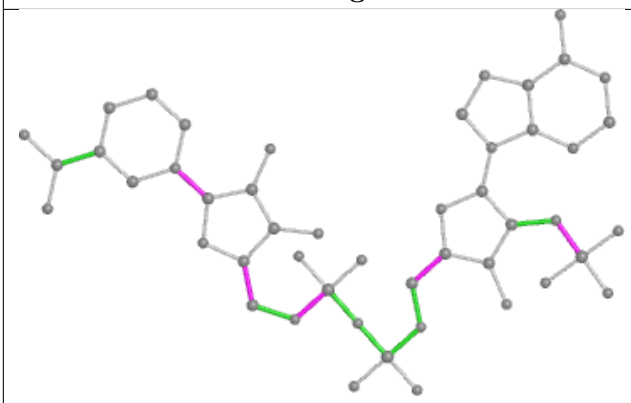
Ligand NDP D 501



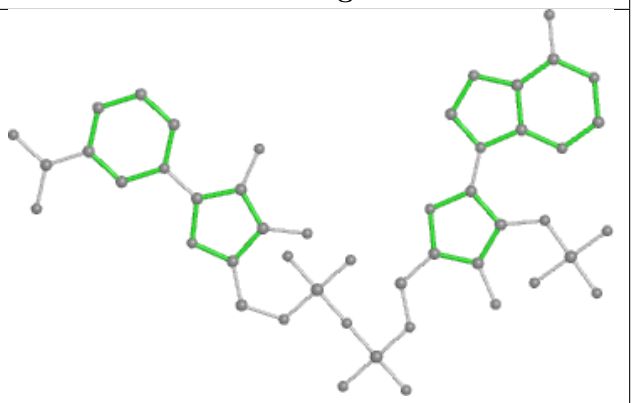
Bond lengths



Bond angles

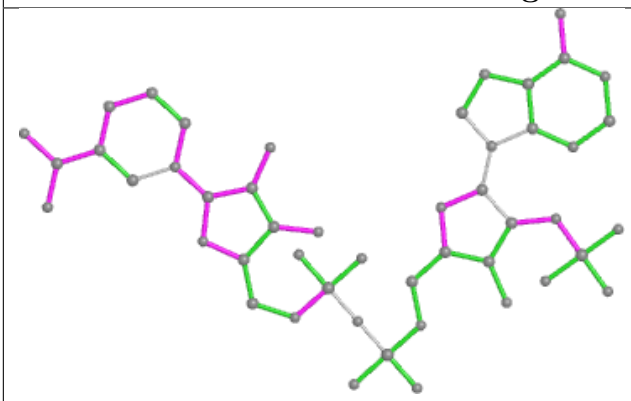


Torsions

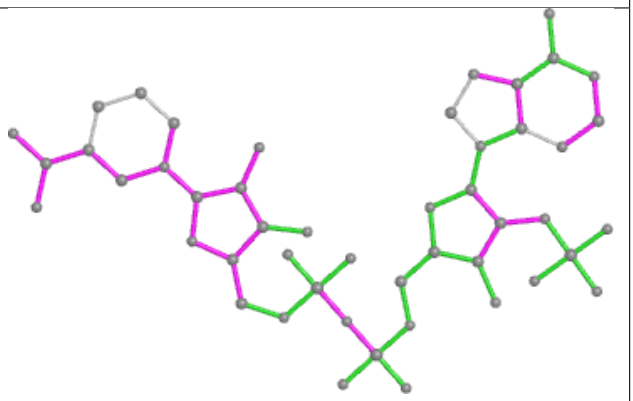


Rings

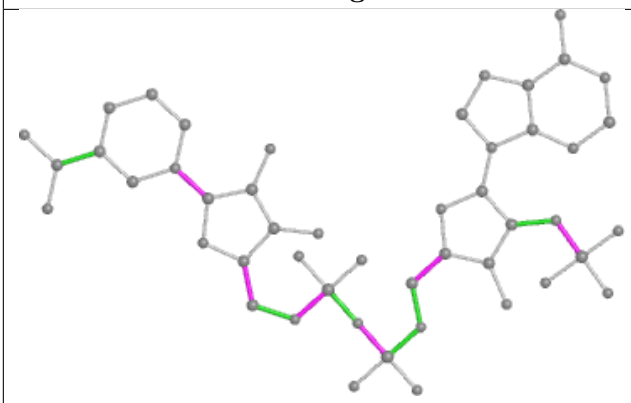
Ligand NDP C 501



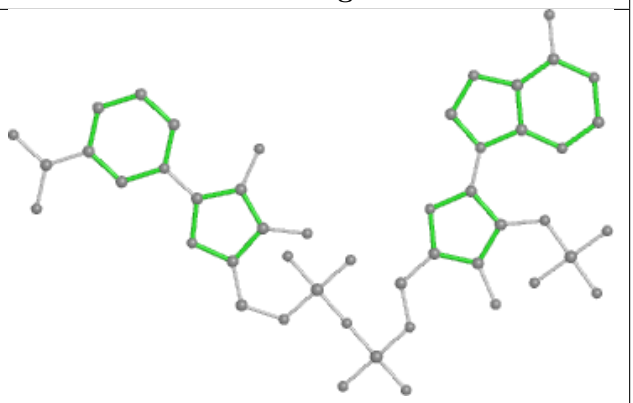
Bond lengths



Bond angles

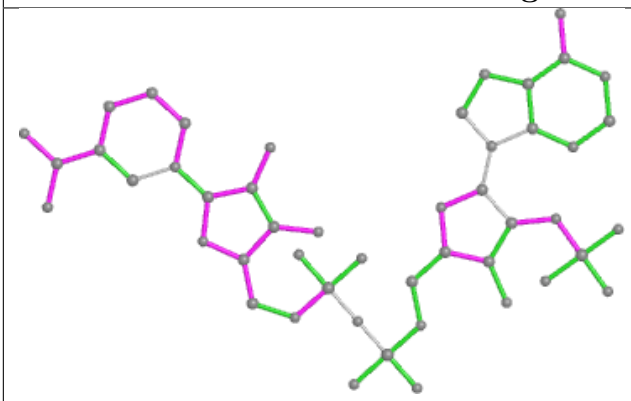


Torsions

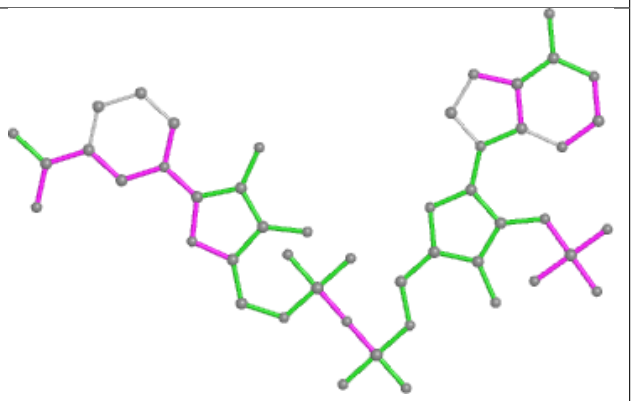


Rings

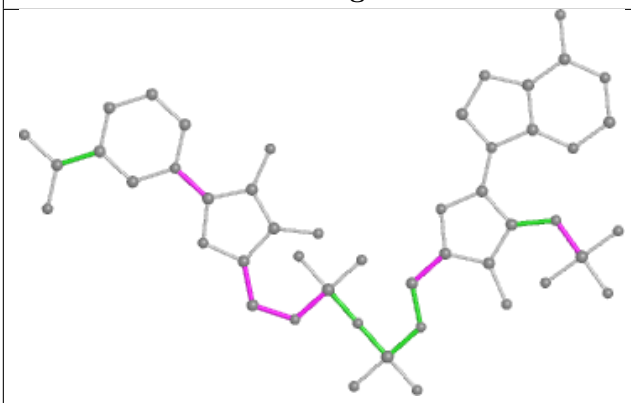
Ligand NDP A 501



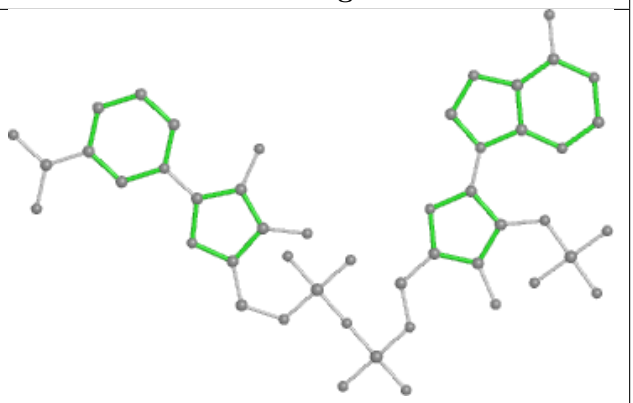
Bond lengths



Bond angles

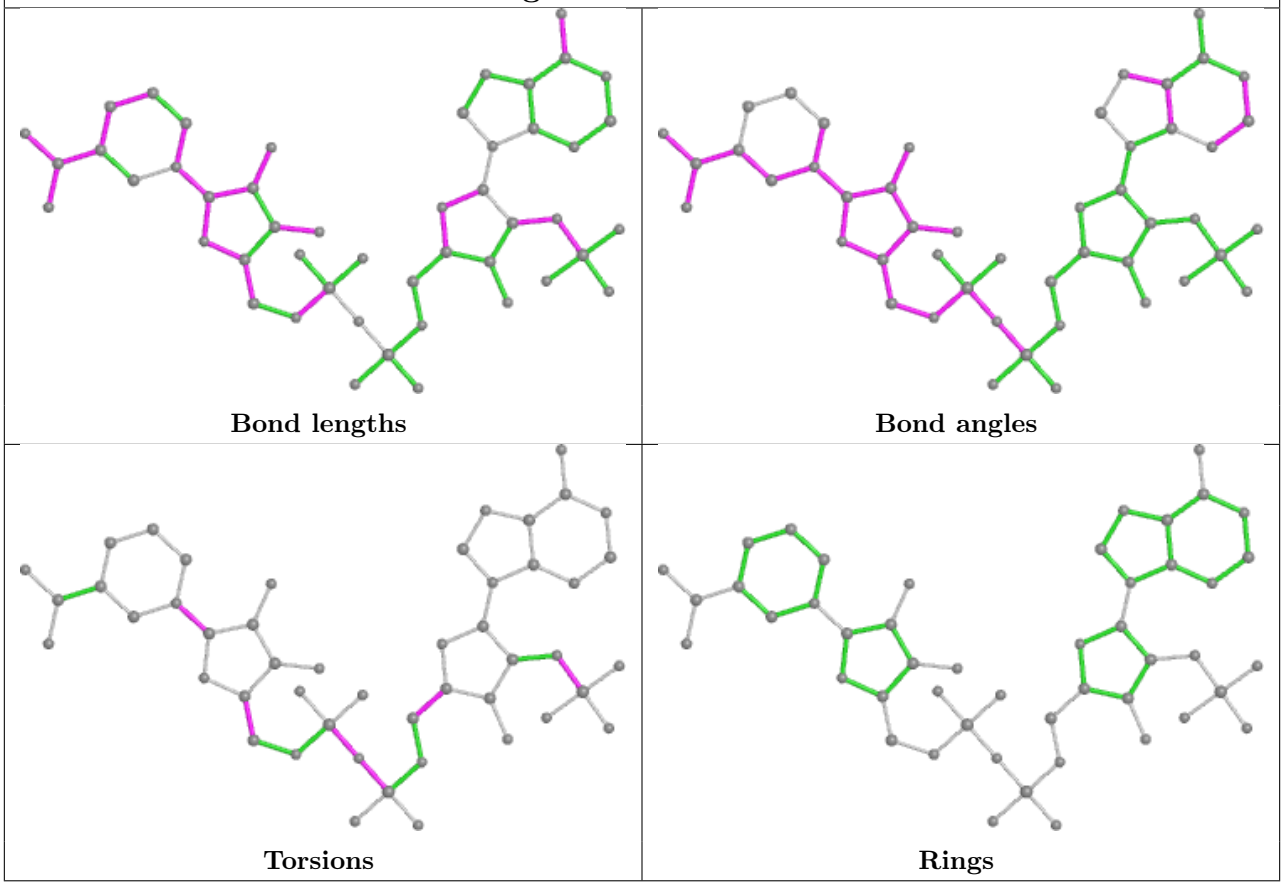


Torsions



Rings

Ligand NDP B 501



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

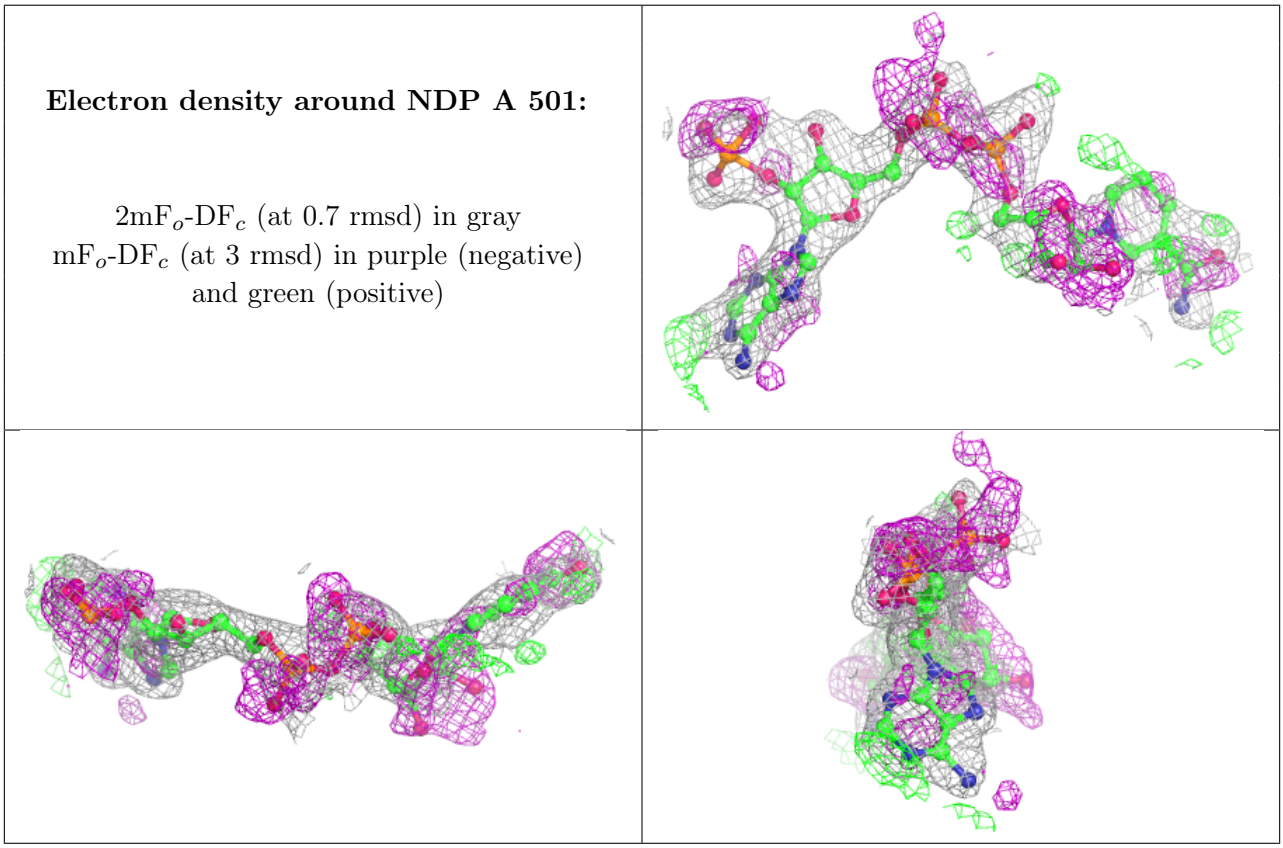
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

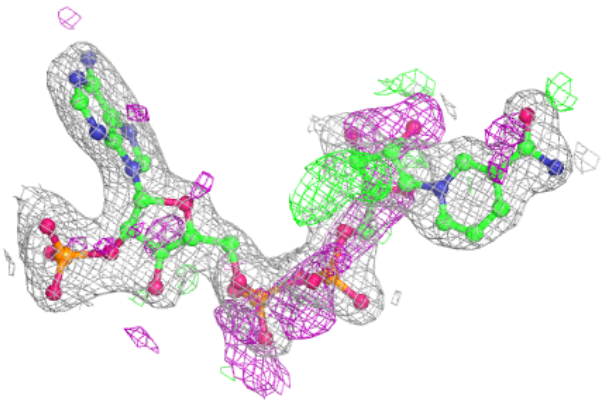
Electron density around NDP A 501:

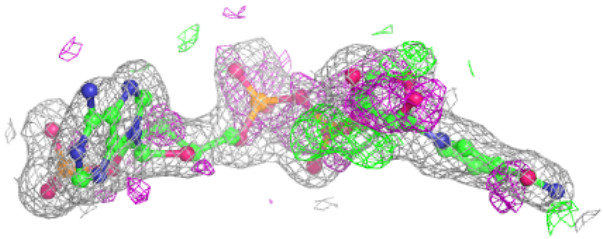
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

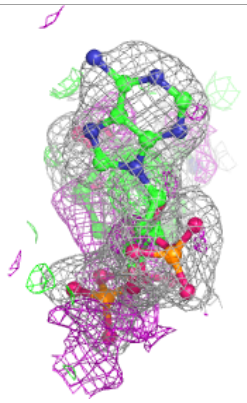


Electron density around NDP B 501:

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

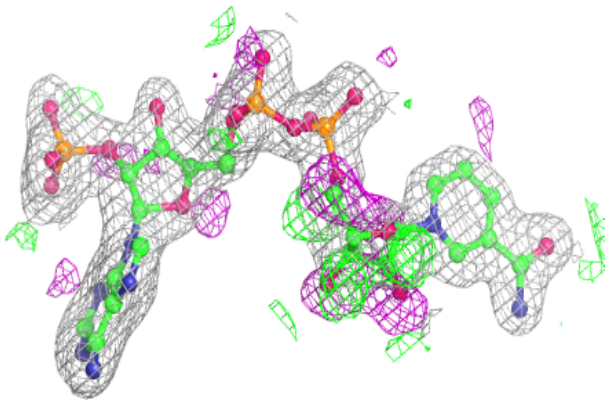


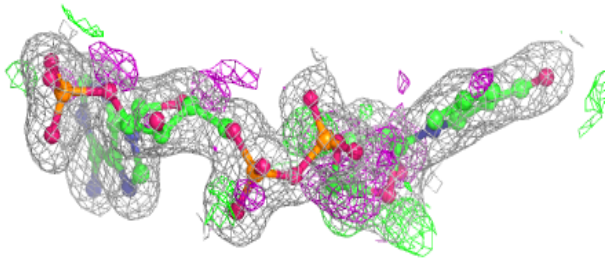


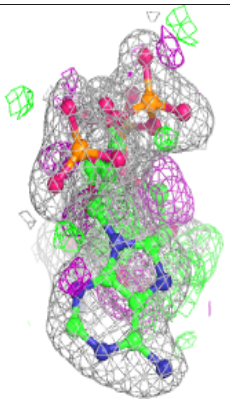


Electron density around NDP C 501:

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

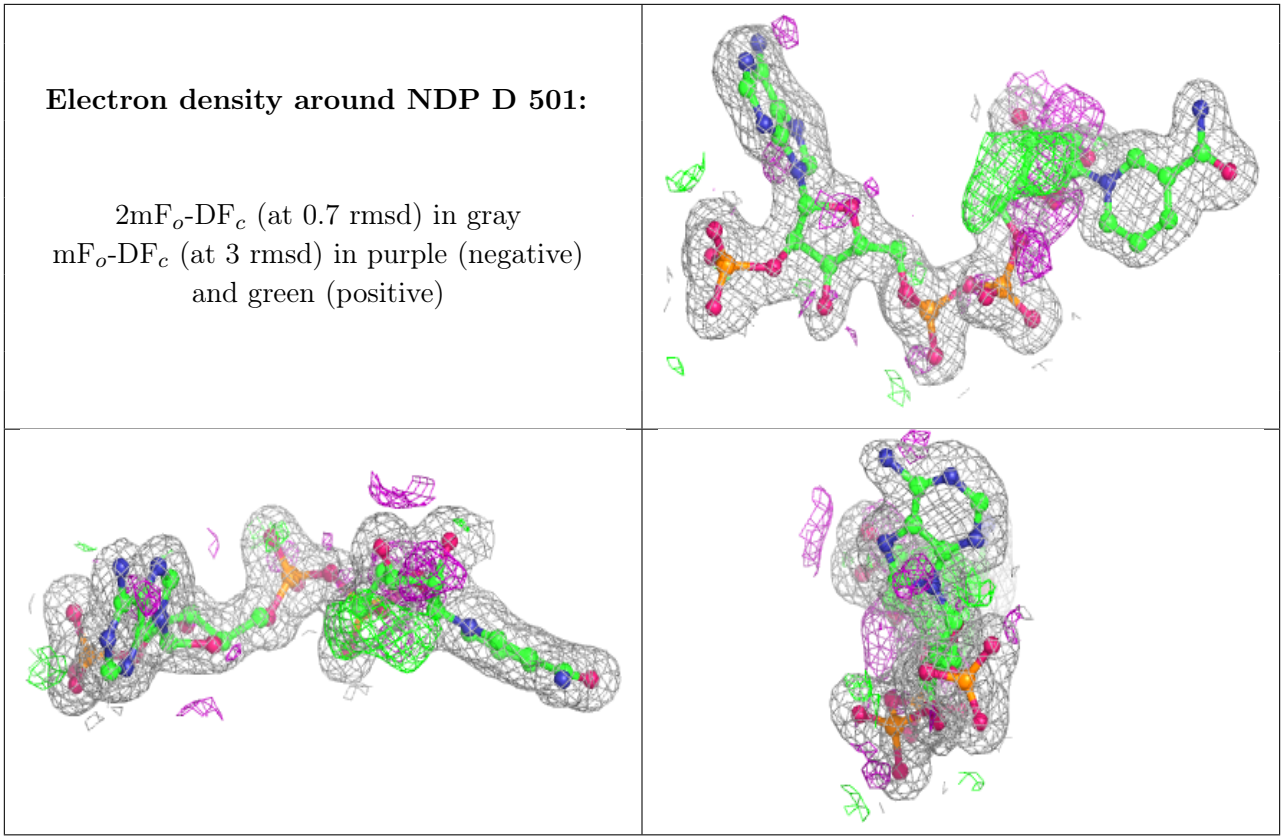






Electron density around NDP D 501:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.