Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2024 – 05:02 PM EST

PDB ID	:	5SVF
Title	:	IDH1 R132H in complex with IDH125
Authors	:	Xie, X.; Kulathila, R.
Deposited on	:	2016-08-05
Resolution	:	2.34 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

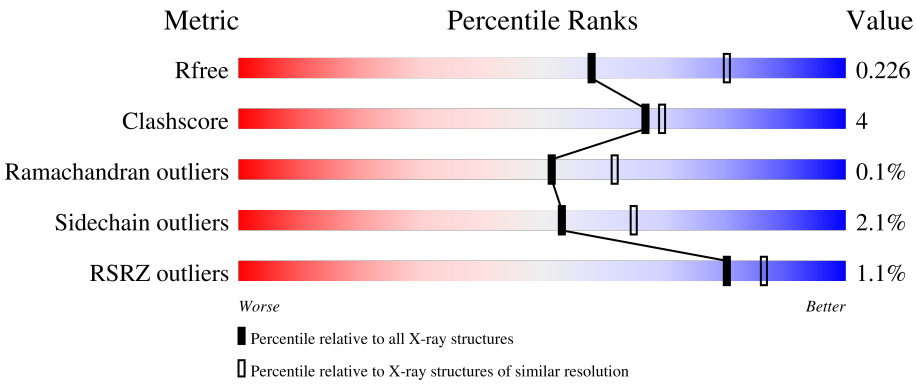
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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% 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	417	89% 6% 5%
1	B	417	87% 8% 5%
1	C	417	84% 11% • •
1	D	417	4% 79% 17% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13375 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.

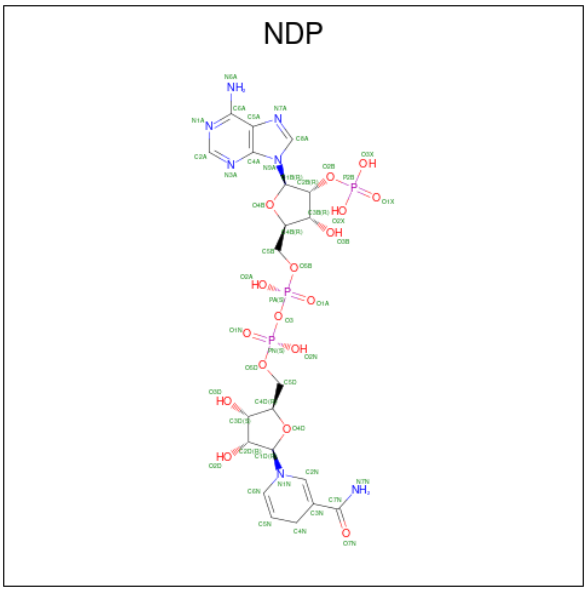
- Molecule 1 is a protein called Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	398	3156	2008	533	597	18	0	2	0
1	C	399	3155	2009	536	592	18	0	0	0
1	B	397	3158	2010	540	590	18	0	2	0
1	D	402	3194	2032	543	601	18	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

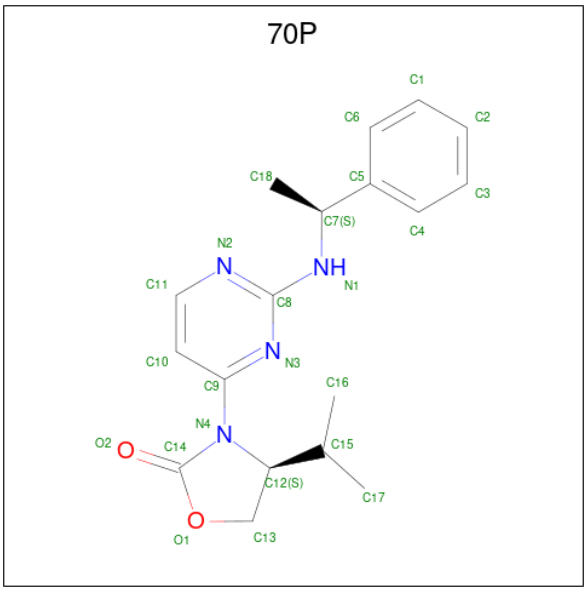
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O75874
A	-1	PRO	-	expression tag	UNP O75874
A	0	GLY	-	expression tag	UNP O75874
A	132	HIS	ARG	engineered mutation	UNP O75874
C	-2	GLY	-	expression tag	UNP O75874
C	-1	PRO	-	expression tag	UNP O75874
C	0	GLY	-	expression tag	UNP O75874
C	132	HIS	ARG	engineered mutation	UNP O75874
B	-2	GLY	-	expression tag	UNP O75874
B	-1	PRO	-	expression tag	UNP O75874
B	0	GLY	-	expression tag	UNP O75874
B	132	HIS	ARG	engineered mutation	UNP O75874
D	-2	GLY	-	expression tag	UNP O75874
D	-1	PRO	-	expression tag	UNP O75874
D	0	GLY	-	expression tag	UNP O75874
D	132	HIS	ARG	engineered mutation	UNP O75874

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



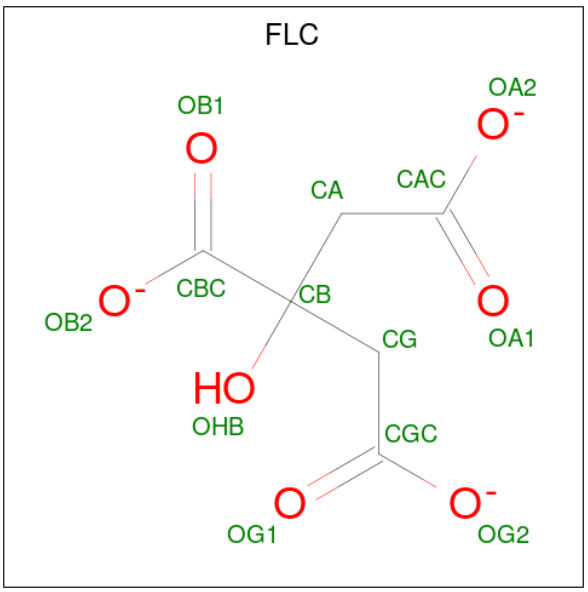
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	C	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	B	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	D	1	48	21	7	17	3	0	0

- Molecule 3 is (4S)-3-(2-{[(1S)-1-phenylethyl]amino}pyrimidin-4-yl)-4-(propan-2-yl)-1,3-oxazolidin-2-one (three-letter code: 70P) (formula: $C_{18}H_{22}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	24	18	4	2	0	0
3	C	1	24	18	4	2	0	0
3	B	1	24	18	4	2	0	0
3	D	1	24	18	4	2	0	0

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	13	6	7		0	0
4	C	1	13	6	7		0	0
4	B	1	13	6	7		0	0
4	D	1	13	6	7		0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O			
5	A	125	125	125		0	0
5	C	64	64	64		0	0

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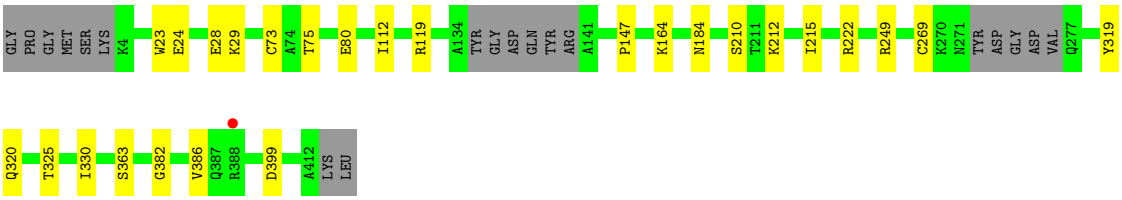
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	134	134	134	0	0
			Total	O		
5	D	49	49	49	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

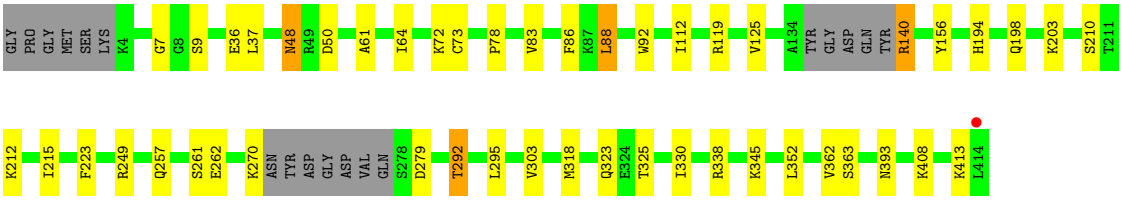
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain A:



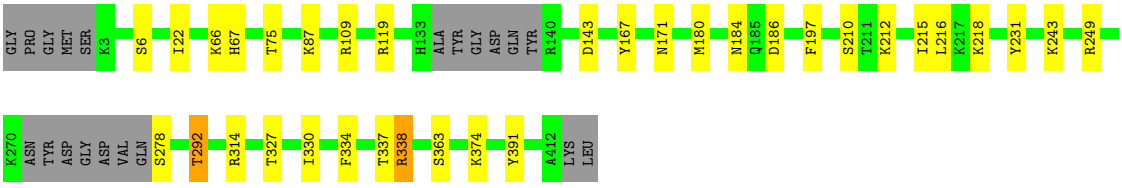
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain C:



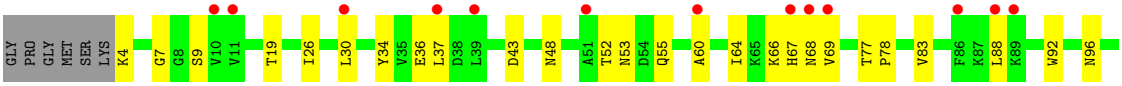
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

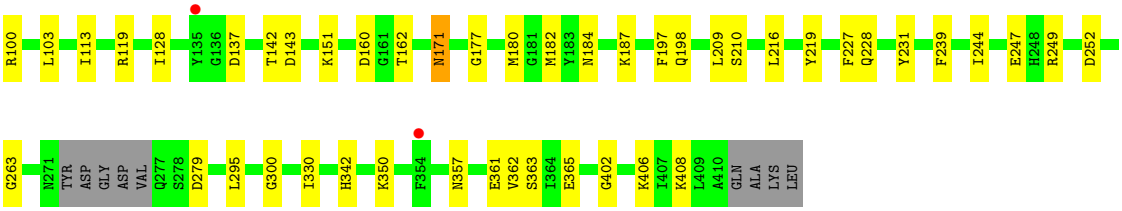
Chain B:



• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain D:




R100
L103
I113
R119
I128
Y135
G136
D137
T142
D143
K151
D160
G161
T162
N171
G177
M180
G181
M182
Y183
N184
K187
F197
Q198
L209
S210
L216
Y219
F227
Q228
Y231
F239
I244
E247
H248
R249
D252
G263
N271
TYR
ASP
GLY
ASP
VAL
Q277
S278
D279
L295
G300
I330
H342
K350
F354
N357
E361
V362
S363
I364
E365
G402
K406
I407
K408
L409
A410
GLN
ALA
LYS
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.98Å 154.99Å 162.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.75 – 2.34 112.32 – 2.34	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.75-2.34) 96.1 (112.32-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.223 0.183 , 0.226	Depositor DCC
R_{free} test set	4443 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13375	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, 70P, 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	0.49	1/3226 (0.0%)	0.59	0/4348
1	B	0.49	0/3228	0.56	0/4347
1	C	0.43	0/3219	0.55	1/4337 (0.0%)
1	D	0.46	0/3264	0.57	0/4400
All	All	0.47	1/12937 (0.0%)	0.57	1/17432 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	CYS	CB-SG	-7.09	1.70	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	88	LEU	CA-CB-CG	5.47	127.89	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3156	0	3131	12	1
1	B	3158	0	3152	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3155	0	3142	30	1
1	D	3194	0	3166	43	2
2	A	48	0	26	1	0
2	B	48	0	26	2	0
2	C	48	0	26	1	0
2	D	48	0	26	1	0
3	A	24	0	0	0	0
3	B	24	0	0	0	0
3	C	24	0	0	0	0
3	D	24	0	0	0	0
4	A	13	0	5	0	0
4	B	13	0	5	2	0
4	C	13	0	5	1	0
4	D	13	0	5	2	0
5	A	125	0	0	0	0
5	B	134	0	0	0	0
5	C	64	0	0	2	0
5	D	49	0	0	1	0
All	All	13375	0	12715	101	2

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 4.

All (101) 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)
2:B:501:NDP:H42N	4:B:503:FLC:HA2	1.60	0.84
1:B:180:MET:HE1	1:D:216:LEU:HD22	1.67	0.77
1:D:7:GLY:HA3	1:D:37:LEU:HD23	1.69	0.74
1:C:7:GLY:HA3	1:C:37:LEU:HD23	1.71	0.73
2:D:501:NDP:H42N	4:D:503:FLC:HA2	1.75	0.68
1:D:100:ARG:NH1	4:D:503:FLC:OA1	2.31	0.64
1:C:86:PHE:HB2	1:C:88:LEU:HD22	1.79	0.64
1:B:212:LYS:HG2	1:B:215:ILE:HD12	1.83	0.61
1:D:151:LYS:HE2	1:D:171:ASN:OD1	2.02	0.60
1:C:72:LYS:HG2	1:C:73:CYS:O	2.03	0.59
2:C:501:NDP:H42N	4:C:503:FLC:HA1	1.86	0.57
1:A:24:GLU:O	1:A:28[A]:GLU:HG2	2.04	0.57
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.87	0.56
1:D:113:ILE:HG23	1:D:119:ARG:HD3	1.86	0.56
1:A:319:TYR:HB2	1:A:325:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HE2	1:A:399:ASP:OD1	2.05	0.55
1:D:137:ASP:HA	1:D:182:MET:HG3	1.86	0.55
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.88	0.55
1:D:52:THR:O	1:D:55:GLN:HB2	2.07	0.55
1:C:125:VAL:HG22	1:C:262:GLU:HG2	1.89	0.53
1:D:160:ASP:OD1	1:D:160:ASP:N	2.26	0.52
1:C:325:THR:O	1:C:393:ASN:HB2	2.10	0.52
1:B:374:LYS:HD2	1:B:391:TYR:CZ	2.44	0.51
1:C:362:VAL:HG23	1:C:408:LYS:HD2	1.92	0.51
1:C:210:SER:HA	1:C:249:ARG:O	2.11	0.50
1:D:34:TYR:OH	1:D:406:LYS:HG2	2.12	0.49
1:D:361:GLU:O	1:D:365:GLU:HG3	2.13	0.49
1:D:210:SER:HA	1:D:249:ARG:O	2.12	0.49
1:D:357:ASN:O	1:D:361:GLU:HG3	2.12	0.49
1:D:96:ASN:O	1:D:100:ARG:HG3	2.13	0.49
1:D:330:ILE:HD12	1:D:363:SER:HB3	1.95	0.49
1:C:112:ILE:HD13	1:C:330:ILE:HG22	1.94	0.48
1:B:216:LEU:HD22	1:D:180:MET:HE1	1.94	0.48
1:B:243:LYS:N	1:B:243:LYS:HD3	2.28	0.47
1:D:128:ILE:HG12	1:D:263:GLY:HA2	1.96	0.47
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.96	0.47
1:B:22:ILE:HD11	1:B:327:THR:HB	1.96	0.47
1:D:53:ASN:HA	1:D:92:TRP:CH2	2.50	0.47
1:C:212:LYS:HG2	1:C:215:ILE:HD12	1.97	0.47
1:D:187:LYS:HA	1:D:187:LYS:HD2	1.82	0.46
1:C:61:ALA:HA	1:C:64:ILE:HD12	1.96	0.46
1:D:60:ALA:O	1:D:64:ILE:HG13	2.15	0.46
1:D:83:VAL:HA	1:D:88:LEU:HD12	1.98	0.46
1:B:75:THR:O	2:B:501:NDP:H2N	2.15	0.46
1:B:197:PHE:CZ	1:B:231:TYR:HB2	2.51	0.46
1:C:203:LYS:HB3	1:C:203:LYS:NZ	2.32	0.45
1:D:43:ASP:HB3	1:D:48:ASN:HD22	1.81	0.45
1:D:209:LEU:HD22	1:D:227:PHE:CG	2.52	0.45
1:C:194:HIS:O	1:C:198:GLN:HG2	2.17	0.45
1:D:197:PHE:CZ	1:D:231:TYR:HB2	2.51	0.45
1:D:198:GLN:HG3	1:D:300:GLY:HA2	1.99	0.45
1:C:295:LEU:O	1:C:303:VAL:HA	2.17	0.44
1:A:112:ILE:HD13	1:A:330:ILE:HG22	1.98	0.44
1:C:140:ARG:HH11	1:C:140:ARG:HG3	1.82	0.44
1:C:257:GLN:NE2	5:C:603:HOH:O	2.34	0.44
1:A:80:GLU:H	1:A:80:GLU:CD	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TRP:CD2	1:A:73:CYS:HB2	2.53	0.43
1:B:292:THR:HG21	1:B:338[A]:ARG:NH1	2.34	0.43
1:C:292:THR:HG21	1:C:338:ARG:HH11	1.84	0.43
1:B:210:SER:HA	1:B:249:ARG:O	2.18	0.43
1:B:334:PHE:HA	1:B:337:THR:OG1	2.19	0.43
1:B:143:ASP:HB2	1:D:219:TYR:HB2	2.00	0.43
1:D:26:ILE:HG23	1:D:30:LEU:HD12	2.01	0.43
1:D:279:ASP:OD1	1:D:279:ASP:N	2.45	0.43
1:D:402:GLY:O	1:D:406:LYS:HG3	2.19	0.43
4:B:503:FLC:OG1	4:B:503:FLC:OHB	2.33	0.43
1:D:113:ILE:CG2	1:D:119:ARG:HD3	2.49	0.43
1:B:216:LEU:HD22	1:D:180:MET:CE	2.49	0.43
1:A:75:THR:O	2:A:501:NDP:H2N	2.19	0.42
1:C:48:ASN:HD22	1:C:48:ASN:C	2.22	0.42
1:C:50:ASP:CG	1:C:88:LEU:HB2	2.39	0.42
1:C:318:MET:HB3	1:C:323:GLN:HB3	2.01	0.42
1:D:362:VAL:HG23	1:D:408:LYS:HD2	2.01	0.42
1:D:67:HIS:O	1:D:68:ASN:HB2	2.20	0.42
1:D:239:PHE:CD2	1:D:244:ILE:HG13	2.54	0.42
1:A:210:SER:HA	1:A:249:ARG:O	2.19	0.42
1:B:180:MET:HG2	1:D:219:TYR:CE2	2.54	0.42
1:B:167:TYR:HB3	1:D:142:THR:HG21	2.02	0.42
1:D:77:THR:HA	1:D:78:PRO:HD3	1.92	0.42
1:B:66:LYS:HE3	1:B:67:HIS:CE1	2.55	0.42
1:C:203:LYS:HB3	1:C:203:LYS:HZ2	1.84	0.41
1:C:257:GLN:HB2	5:C:638:HOH:O	2.19	0.41
1:C:261:SER:OG	1:C:262:GLU:N	2.53	0.41
1:D:69:VAL:HG22	1:D:342:HIS:HD2	1.85	0.41
1:B:186:ASP:OD1	1:D:177:GLY:HA2	2.20	0.41
1:C:83:VAL:HA	1:C:88:LEU:CD2	2.50	0.41
1:A:382:GLY:O	1:A:386:VAL:HG23	2.21	0.41
1:C:7:GLY:HA2	1:C:352:LEU:HD22	2.02	0.41
1:B:314:ARG:NH1	1:B:314:ARG:HG2	2.34	0.41
1:D:228:GLN:HG2	5:D:613:HOH:O	2.19	0.41
1:A:147:PRO:HD2	1:C:156:TYR:CE2	2.56	0.41
1:A:212:LYS:HE3	1:A:215:ILE:HD12	2.03	0.41
1:C:83:VAL:HA	1:C:88:LEU:HD23	2.01	0.41
1:B:314:ARG:CG	1:B:314:ARG:HH11	2.34	0.41
1:D:357:ASN:ND2	1:D:361:GLU:OE1	2.53	0.41
1:D:143:ASP:HB3	1:D:180:MET:HE3	2.03	0.41
1:D:103:LEU:HD12	1:D:295:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ARG:O	1:C:140:ARG:HG2	2.20	0.40
1:C:223:PHE:CE2	1:C:270:LYS:HG3	2.57	0.40
1:D:247:GLU:OE2	1:D:249:ARG:NH2	2.50	0.40
1:C:78:PRO:HD2	1:C:92:TRP:O	2.22	0.40

All (2) 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)
1:C:9:SER:OG	1:D:36:GLU:OE2[1_556]	2.13	0.07
1:A:320:GLN:O	1:D:350:LYS:NZ[2_555]	2.15	0.05

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	394/417 (94%)	385 (98%)	9 (2%)	0	100	100
1	B	393/417 (94%)	383 (98%)	10 (2%)	0	100	100
1	C	393/417 (94%)	381 (97%)	12 (3%)	0	100	100
1	D	399/417 (96%)	380 (95%)	18 (4%)	1 (0%)	41	47
All	All	1579/1668 (95%)	1529 (97%)	49 (3%)	1 (0%)	51	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	THR

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	338/351 (96%)	334 (99%)	4 (1%)	71	82
1	B	338/351 (96%)	327 (97%)	11 (3%)	38	46
1	C	337/351 (96%)	329 (98%)	8 (2%)	49	59
1	D	341/351 (97%)	334 (98%)	7 (2%)	53	65
All	All	1354/1404 (96%)	1324 (98%)	30 (2%)	53	63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ARG
1	A	164	LYS
1	A	184	ASN
1	A	222	ARG
1	C	36	GLU
1	C	48	ASN
1	C	119	ARG
1	C	140	ARG
1	C	279	ASP
1	C	292	THR
1	C	345	LYS
1	C	413	LYS
1	B	6	SER
1	B	87	LYS
1	B	109	ARG
1	B	119	ARG
1	B	171	ASN
1	B	184	ASN
1	B	218	LYS
1	B	278	SER
1	B	292	THR
1	B	338[A]	ARG
1	B	338[B]	ARG
1	D	4	LYS

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Mol	Chain	Res	Type
1	D	9	SER
1	D	19	THR
1	D	66	LYS
1	D	171	ASN
1	D	184	ASN
1	D	252	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	D	55	GLN
1	D	67	HIS
1	D	323	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	A	501	-	45,52,52	1.35	5 (11%)	53,80,80	1.19	4 (7%)
2	NDP	D	501	-	45,52,52	1.33	4 (8%)	53,80,80	1.21	4 (7%)
4	FLC	B	503	-	12,12,12	1.07	1 (8%)	17,17,17	1.27	2 (11%)
3	70P	D	502	-	26,26,26	1.31	2 (7%)	31,36,36	1.60	5 (16%)
3	70P	B	502	-	26,26,26	1.17	2 (7%)	31,36,36	1.33	4 (12%)
4	FLC	D	503	-	12,12,12	1.32	1 (8%)	17,17,17	1.73	2 (11%)
3	70P	A	502	-	26,26,26	1.15	1 (3%)	31,36,36	1.43	3 (9%)
3	70P	C	502	-	26,26,26	1.23	0	31,36,36	1.44	6 (19%)
2	NDP	B	501	-	45,52,52	1.44	5 (11%)	53,80,80	1.30	4 (7%)
4	FLC	C	503	-	12,12,12	0.95	0	17,17,17	1.44	2 (11%)
2	NDP	C	501	-	45,52,52	1.29	4 (8%)	53,80,80	1.24	4 (7%)
4	FLC	A	503	-	12,12,12	1.17	1 (8%)	17,17,17	1.43	4 (23%)

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	A	501	-	-	8/30/77/77	0/5/5/5
2	NDP	D	501	-	-	8/30/77/77	0/5/5/5
4	FLC	B	503	-	-	4/16/16/16	-
3	70P	D	502	-	-	0/16/29/29	0/3/3/3
3	70P	B	502	-	-	0/16/29/29	0/3/3/3
4	FLC	D	503	-	-	2/16/16/16	-
3	70P	A	502	-	-	0/16/29/29	0/3/3/3
3	70P	C	502	-	-	0/16/29/29	0/3/3/3
2	NDP	B	501	-	-	7/30/77/77	0/5/5/5
4	FLC	C	503	-	-	0/16/16/16	-
2	NDP	C	501	-	-	10/30/77/77	0/5/5/5
4	FLC	A	503	-	-	4/16/16/16	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NDP	C4N-C3N	-5.21	1.39	1.49
2	B	501	NDP	C4N-C3N	-5.05	1.40	1.49
2	D	501	NDP	C4N-C3N	-4.97	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NDP	C4N-C3N	-4.93	1.40	1.49
2	B	501	NDP	C6N-C5N	4.03	1.40	1.33
2	A	501	NDP	C6N-C5N	4.03	1.40	1.33
2	D	501	NDP	C6N-C5N	3.91	1.40	1.33
2	C	501	NDP	C6N-C5N	3.73	1.40	1.33
2	C	501	NDP	C4N-C5N	-3.52	1.39	1.48
2	D	501	NDP	C4N-C5N	-3.48	1.39	1.48
4	D	503	FLC	CB-CBC	-3.17	1.50	1.53
2	B	501	NDP	C4N-C5N	-3.17	1.40	1.48
2	B	501	NDP	P2B-O2B	3.11	1.65	1.59
2	A	501	NDP	C4N-C5N	-3.06	1.40	1.48
2	B	501	NDP	O4B-C1B	2.91	1.45	1.41
2	A	501	NDP	O4B-C1B	2.68	1.44	1.41
2	D	501	NDP	O4B-C1B	2.59	1.44	1.41
2	A	501	NDP	P2B-O2B	2.41	1.63	1.59
3	D	502	70P	C14-N4	2.41	1.40	1.36
3	D	502	70P	C8-N1	2.30	1.37	1.34
4	A	503	FLC	CB-CBC	-2.21	1.51	1.53
3	B	502	70P	C14-N4	2.16	1.39	1.36
3	A	502	70P	C8-N1	2.14	1.37	1.34
4	B	503	FLC	CB-CBC	-2.10	1.51	1.53
2	C	501	NDP	C2A-N3A	2.06	1.35	1.32
3	B	502	70P	C6-C5	2.03	1.42	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	NDP	N3A-C2A-N1A	-4.88	121.06	128.68
2	D	501	NDP	N3A-C2A-N1A	-4.75	121.26	128.68
2	B	501	NDP	N3A-C2A-N1A	-4.70	121.33	128.68
4	D	503	FLC	OB1-CBC-CB	-4.61	115.73	122.25
2	A	501	NDP	N3A-C2A-N1A	-4.37	121.84	128.68
4	C	503	FLC	OB2-CBC-CB	4.03	120.04	113.05
3	A	502	70P	C18-C7-N1	3.92	116.38	108.95
3	D	502	70P	C18-C7-N1	3.85	116.24	108.95
3	C	502	70P	C13-O1-C14	3.84	114.25	109.94
3	D	502	70P	C13-O1-C14	3.78	114.19	109.94
3	A	502	70P	C13-O1-C14	3.74	114.15	109.94
4	D	503	FLC	OB2-CBC-CB	3.44	119.03	113.05
3	D	502	70P	C10-C9-N3	-3.30	118.14	123.53
3	B	502	70P	C13-C12-C15	-3.18	110.23	115.04
2	B	501	NDP	C1D-N1N-C2N	-3.03	116.06	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NDP	O2B-P2B-O1X	-3.02	97.75	109.39
2	A	501	NDP	C1D-N1N-C2N	-2.99	116.14	121.11
3	B	502	70P	C13-O1-C14	2.94	113.25	109.94
4	A	503	FLC	OB1-CBC-CB	-2.90	118.15	122.25
3	B	502	70P	C10-C9-N3	-2.87	118.85	123.53
3	C	502	70P	O1-C13-C12	-2.83	102.40	105.66
3	A	502	70P	C10-C9-N3	-2.74	119.05	123.53
3	C	502	70P	C13-C12-C15	-2.73	110.91	115.04
3	C	502	70P	C18-C7-N1	2.70	114.07	108.95
2	A	501	NDP	C4A-C5A-N7A	-2.68	106.60	109.40
3	D	502	70P	C13-C12-C15	-2.68	110.99	115.04
4	A	503	FLC	OB2-CBC-CB	2.66	117.68	113.05
2	D	501	NDP	PN-O3-PA	-2.61	123.88	132.83
4	C	503	FLC	OB1-CBC-CB	-2.60	118.57	122.25
4	B	503	FLC	OB2-CBC-CB	2.56	117.50	113.05
2	C	501	NDP	C1D-N1N-C2N	-2.54	116.89	121.11
2	C	501	NDP	O4D-C1D-N1N	2.47	112.89	108.06
3	B	502	70P	C18-C7-N1	2.45	113.60	108.95
3	C	502	70P	O2-C14-N4	2.41	131.41	128.68
3	D	502	70P	O1-C13-C12	-2.41	102.90	105.66
3	C	502	70P	C10-C9-N3	-2.33	119.73	123.53
2	A	501	NDP	O2A-PA-O1A	2.29	123.57	112.24
2	D	501	NDP	O4D-C1D-N1N	2.29	112.52	108.06
4	A	503	FLC	CB-CA-CAC	-2.19	108.51	113.81
2	B	501	NDP	O7N-C7N-C3N	-2.17	116.80	120.90
2	D	501	NDP	O2B-C2B-C1B	-2.13	102.43	110.10
2	C	501	NDP	PN-O3-PA	-2.12	125.54	132.83
4	B	503	FLC	OG1-CGC-CG	-2.04	116.97	122.94
4	A	503	FLC	CA-CB-CBC	-2.03	105.74	110.11

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C2B-O2B-P2B-O2X
2	A	501	NDP	C5D-O5D-PN-O1N
2	A	501	NDP	C5D-O5D-PN-O2N
2	C	501	NDP	C2B-O2B-P2B-O1X
2	C	501	NDP	C5D-O5D-PN-O2N
2	B	501	NDP	C5D-O5D-PN-O2N
2	D	501	NDP	C5D-O5D-PN-O2N
4	B	503	FLC	CG-CB-CBC-OB1

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Mol	Chain	Res	Type	Atoms
4	B	503	FLC	CG-CB-CBC-OB2
4	B	503	FLC	OHB-CB-CBC-OB1
4	B	503	FLC	OHB-CB-CBC-OB2
2	C	501	NDP	O4B-C4B-C5B-O5B
2	D	501	NDP	O4B-C4B-C5B-O5B
2	C	501	NDP	C3B-C4B-C5B-O5B
4	D	503	FLC	CB-CG-CGC-OG1
2	A	501	NDP	O4B-C4B-C5B-O5B
4	D	503	FLC	CB-CG-CGC-OG2
2	C	501	NDP	C5D-O5D-PN-O3
2	B	501	NDP	C2B-O2B-P2B-O2X
2	B	501	NDP	C5D-O5D-PN-O3
2	D	501	NDP	C5D-O5D-PN-O3
2	D	501	NDP	C3B-C4B-C5B-O5B
2	B	501	NDP	O4D-C1D-N1N-C2N
2	B	501	NDP	C2D-C1D-N1N-C2N
2	C	501	NDP	C5D-O5D-PN-O1N
2	D	501	NDP	C5D-O5D-PN-O1N
2	A	501	NDP	C3B-C4B-C5B-O5B
4	A	503	FLC	CB-CG-CGC-OG2
2	A	501	NDP	O4D-C1D-N1N-C2N
4	A	503	FLC	CB-CG-CGC-OG1
2	C	501	NDP	O4D-C1D-N1N-C2N
2	D	501	NDP	O4D-C1D-N1N-C2N
2	A	501	NDP	C2D-C1D-N1N-C2N
2	C	501	NDP	C2D-C1D-N1N-C2N
2	D	501	NDP	C2D-C1D-N1N-C2N
2	C	501	NDP	O4D-C1D-N1N-C6N
2	B	501	NDP	O4D-C1D-N1N-C6N
2	A	501	NDP	C5D-O5D-PN-O3
2	C	501	NDP	C2B-O2B-P2B-O2X
4	A	503	FLC	CB-CA-CAC-OA1
2	B	501	NDP	C5D-O5D-PN-O1N
2	D	501	NDP	O4D-C1D-N1N-C6N
4	A	503	FLC	CB-CA-CAC-OA2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NDP	1	0
2	D	501	NDP	1	0

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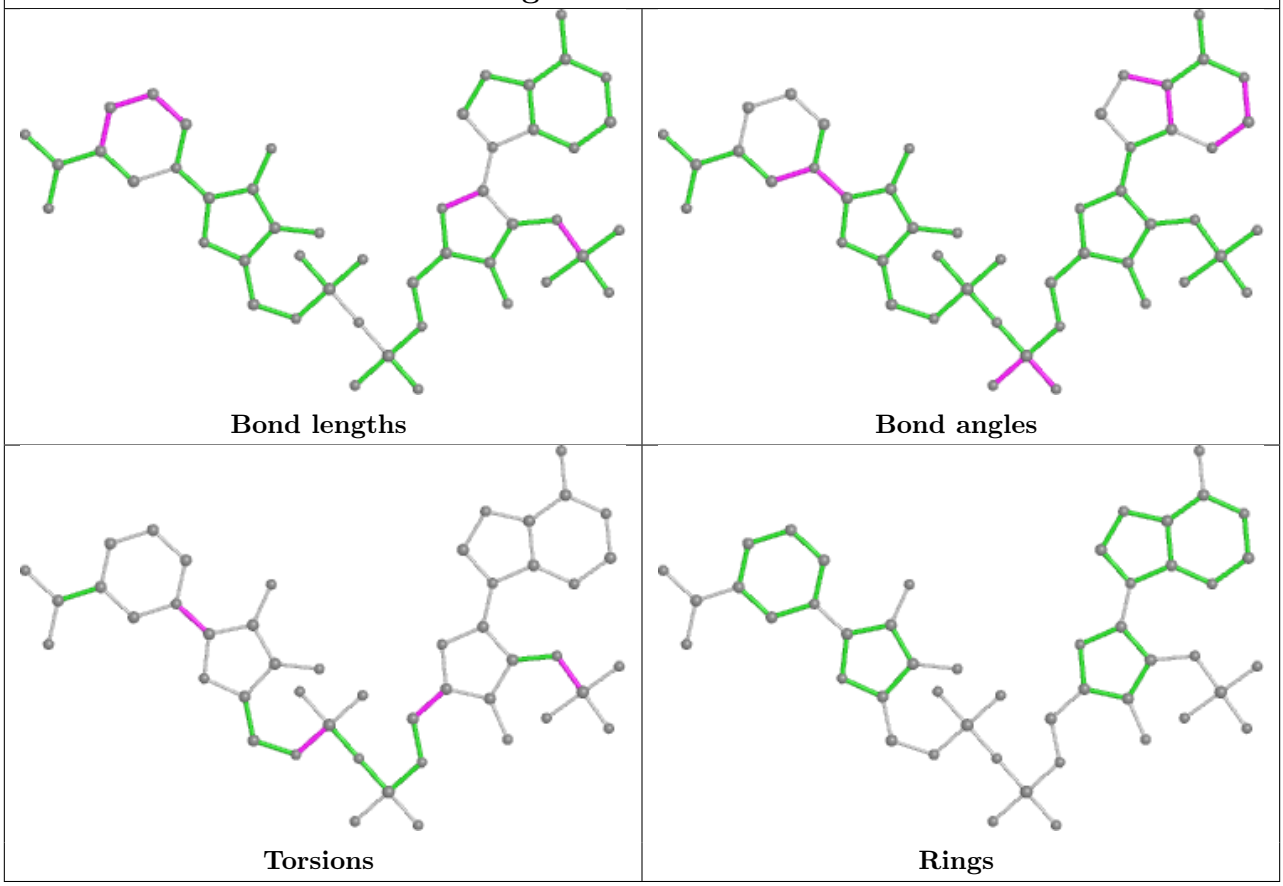
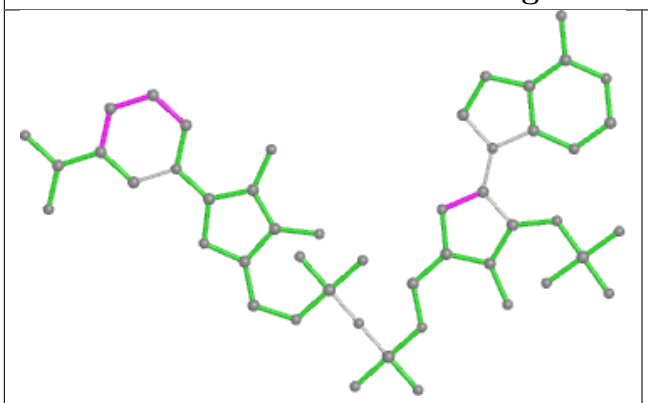
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	FLC	2	0
4	D	503	FLC	2	0
2	B	501	NDP	2	0
4	C	503	FLC	1	0
2	C	501	NDP	1	0

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.

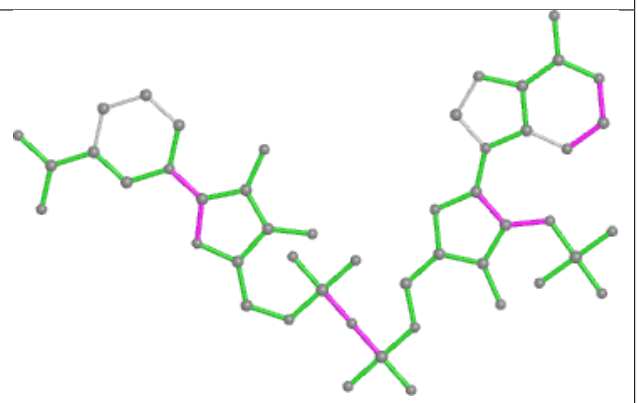
Ligand NDP A 501



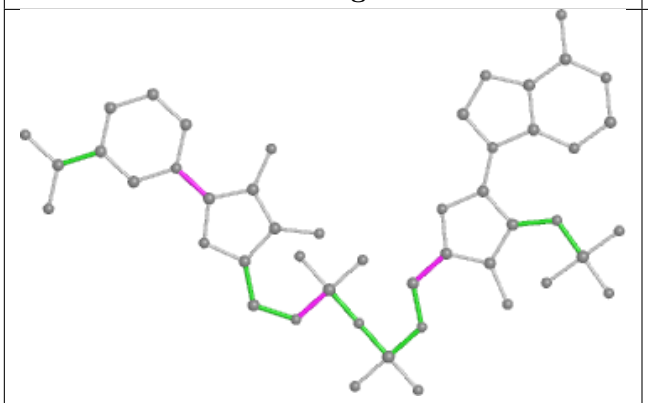
Ligand NDP D 501



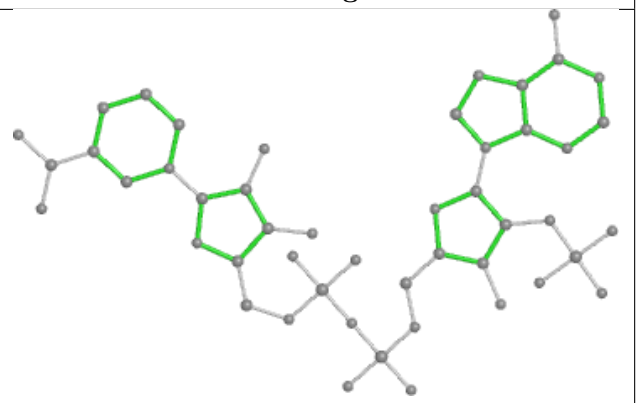
Bond lengths



Bond angles

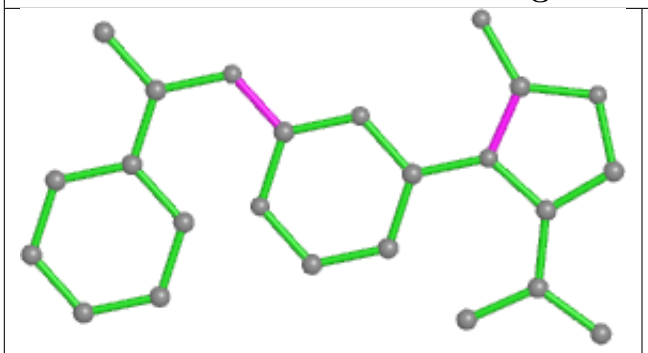


Torsions

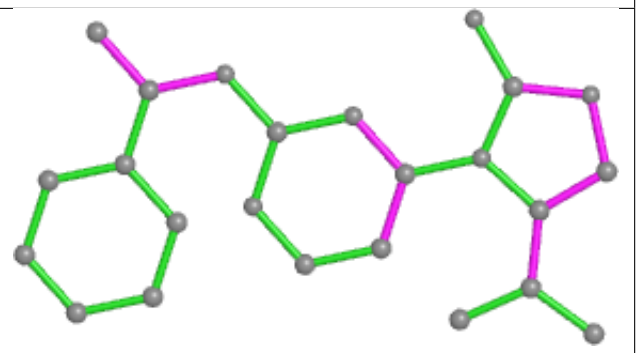


Rings

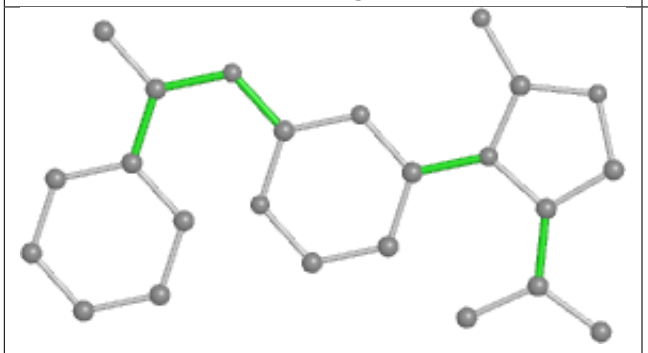
Ligand 70P D 502



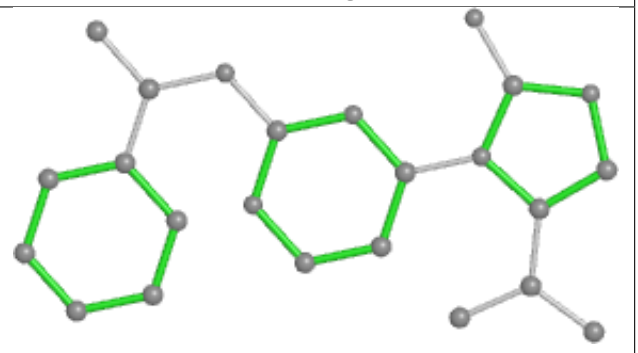
Bond lengths



Bond angles

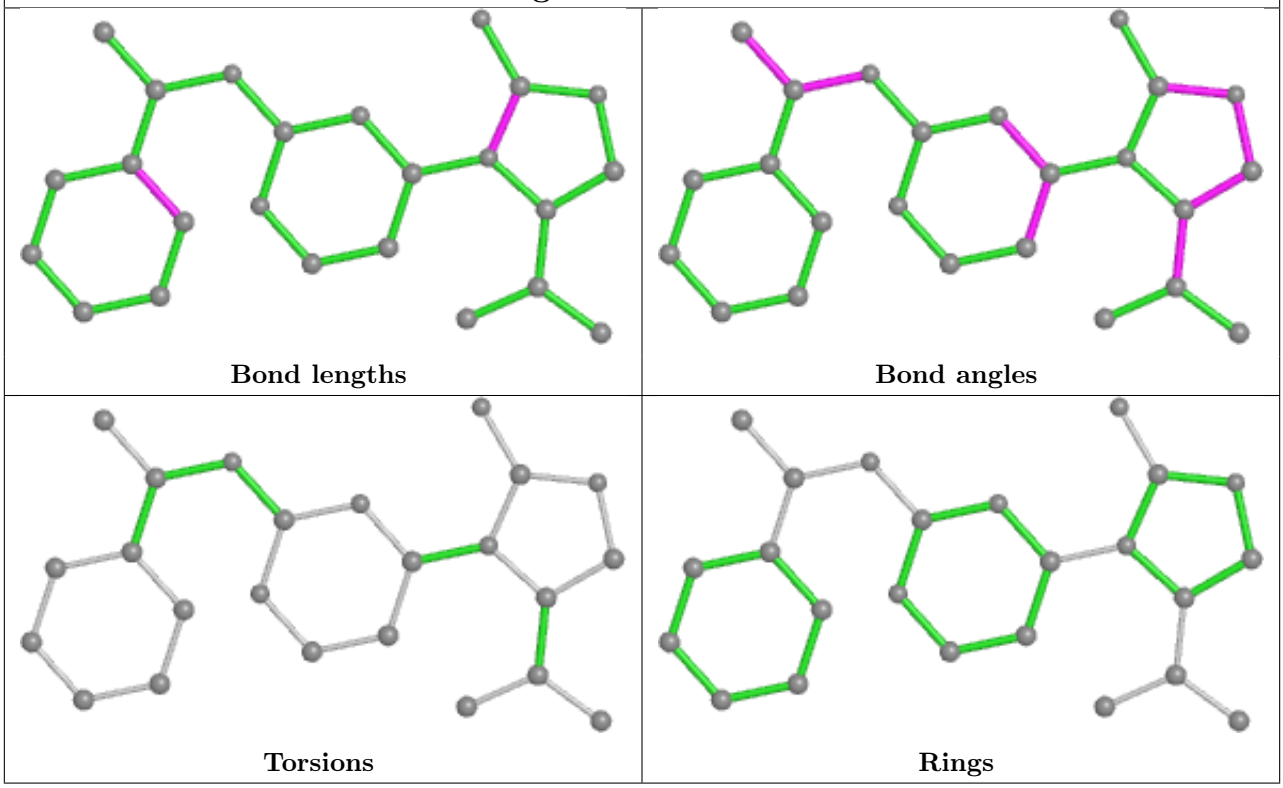


Torsions

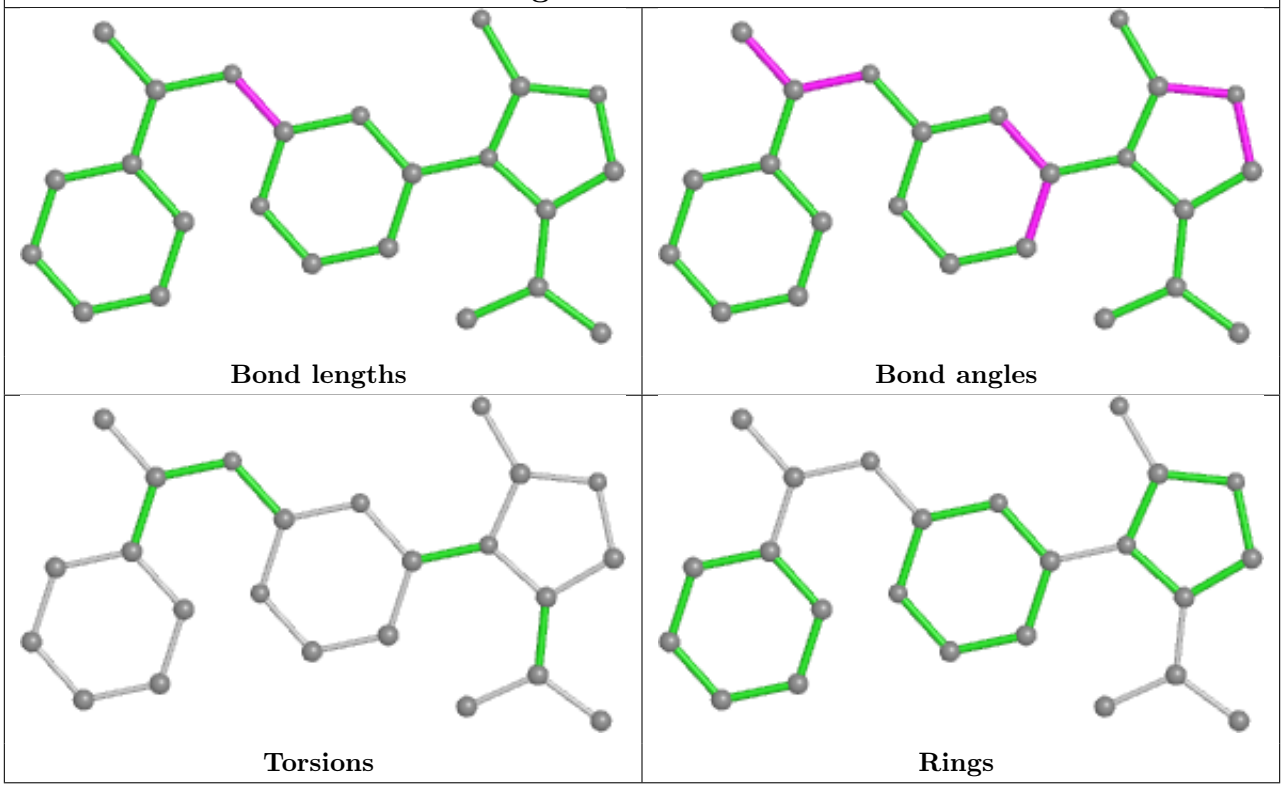


Rings

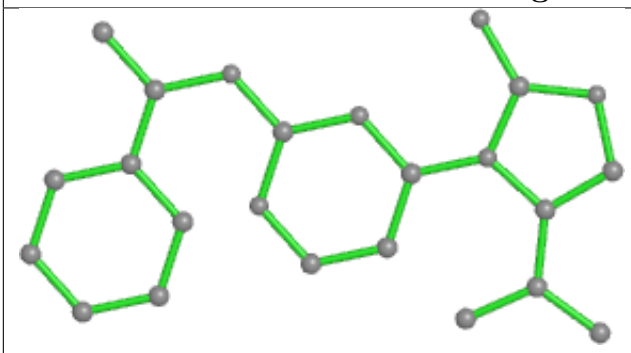
Ligand 70P B 502



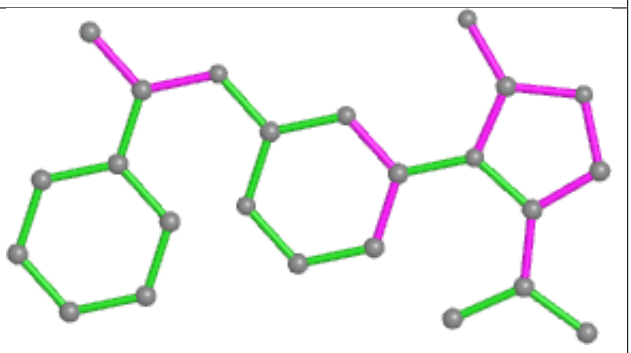
Ligand 70P A 502



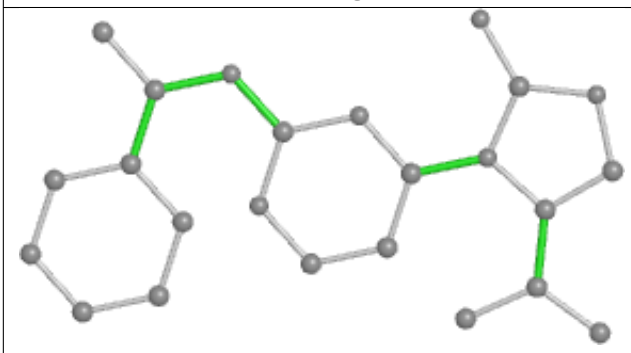
Ligand 70P C 502



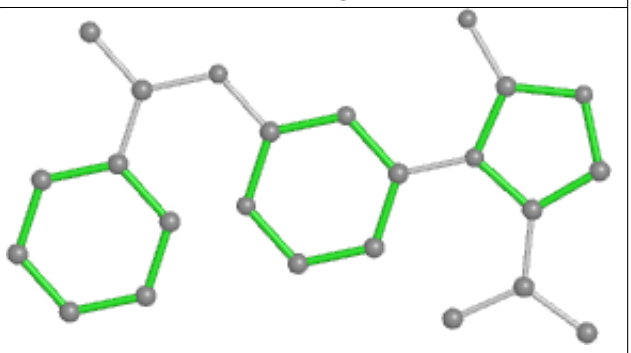
Bond lengths



Bond angles

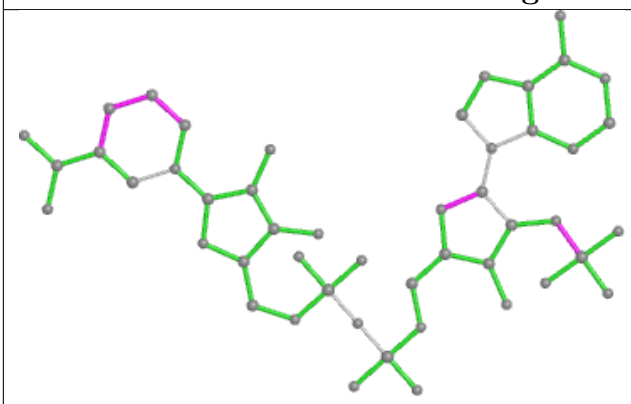


Torsions

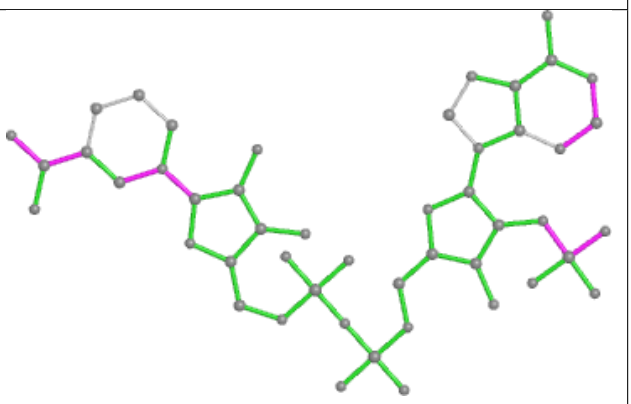


Rings

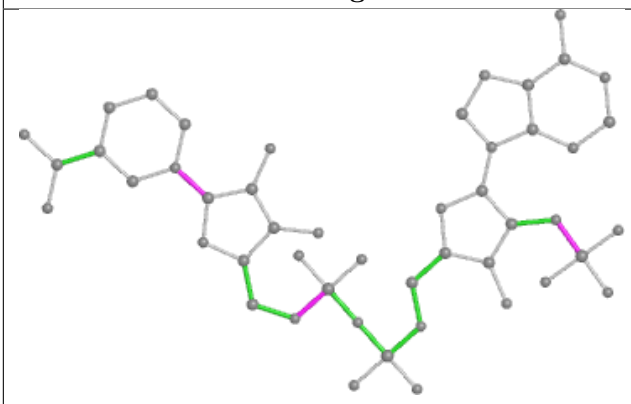
Ligand NDP B 501



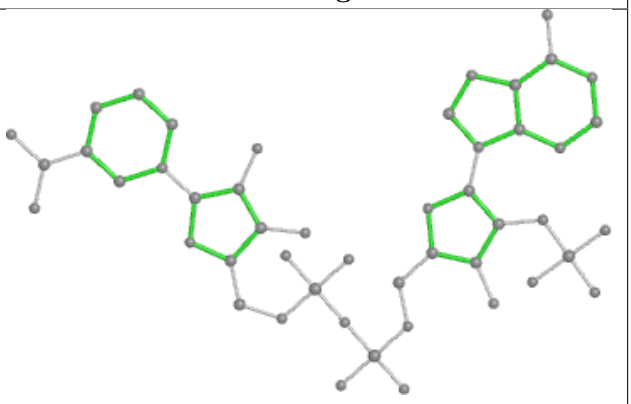
Bond lengths



Bond angles

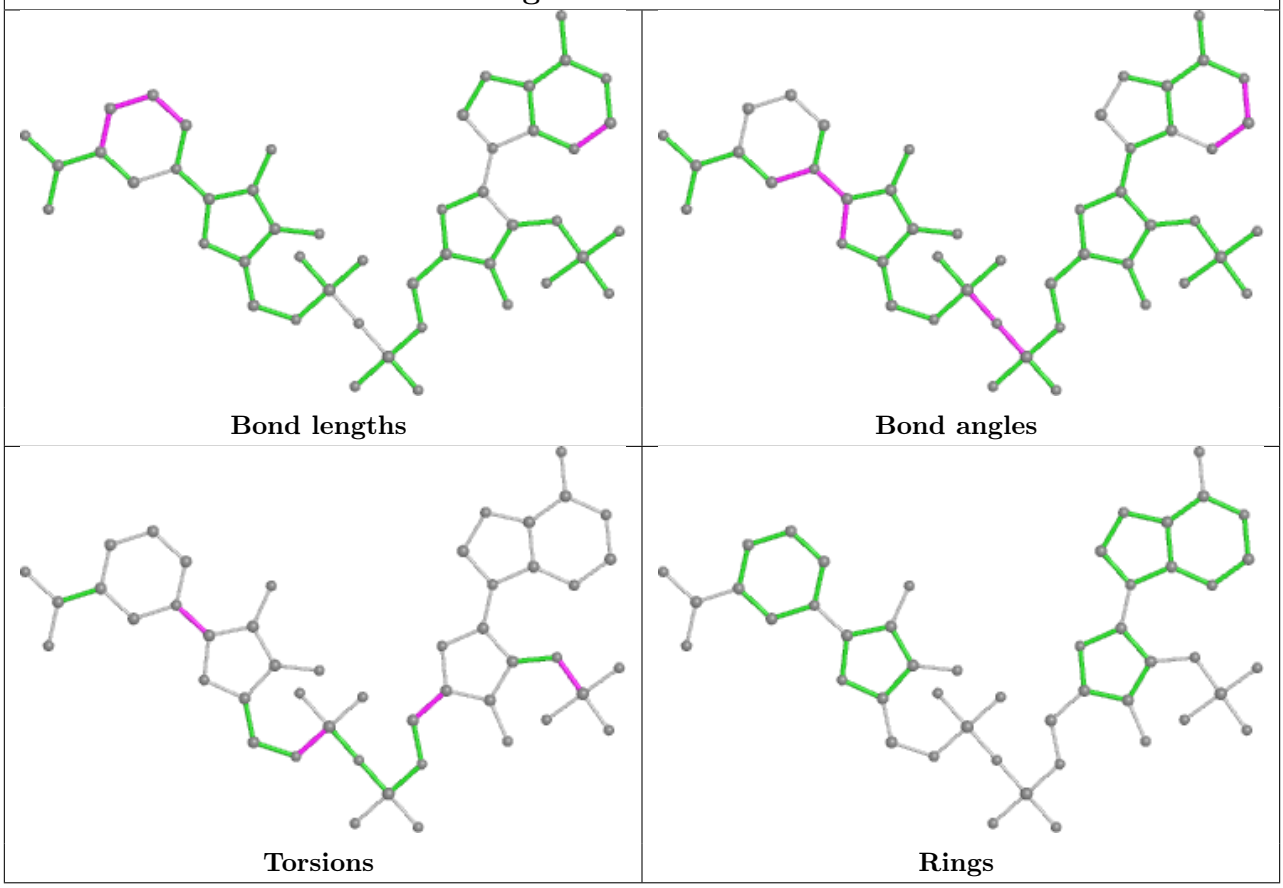


Torsions



Rings

Ligand NDP C 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 (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	398/417 (95%)	-0.12	1 (0%) 94 97	31, 41, 60, 83	0
1	B	397/417 (95%)	-0.14	0 100 100	31, 42, 55, 80	0
1	C	399/417 (95%)	0.04	1 (0%) 94 97	33, 51, 81, 101	0
1	D	402/417 (96%)	0.18	15 (3%) 41 52	35, 58, 81, 92	0
All	All	1596/1668 (95%)	-0.01	17 (1%) 80 86	31, 47, 75, 101	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	414	LEU	4.4
1	D	86	PHE	3.8
1	D	88	LEU	3.2
1	D	10	VAL	3.1
1	D	68	ASN	2.9
1	D	135	TYR	2.8
1	A	388	ARG	2.8
1	D	89	LYS	2.7
1	D	11	VAL	2.6
1	D	67	HIS	2.5
1	D	354	PHE	2.3
1	D	30	LEU	2.2
1	D	51	ALA	2.1
1	D	69	VAL	2.1
1	D	39	LEU	2.1
1	D	60	ALA	2.1
1	D	37	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

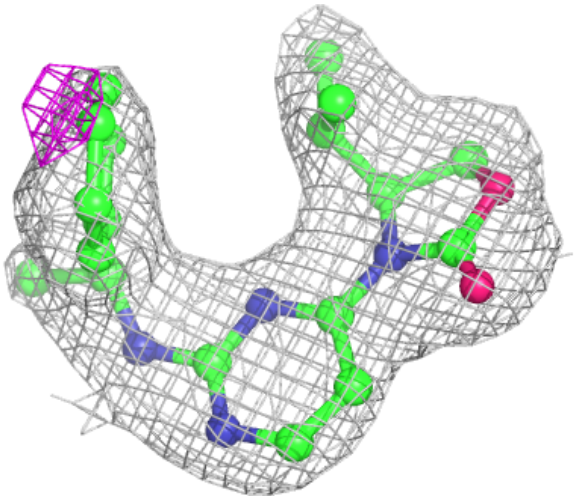
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

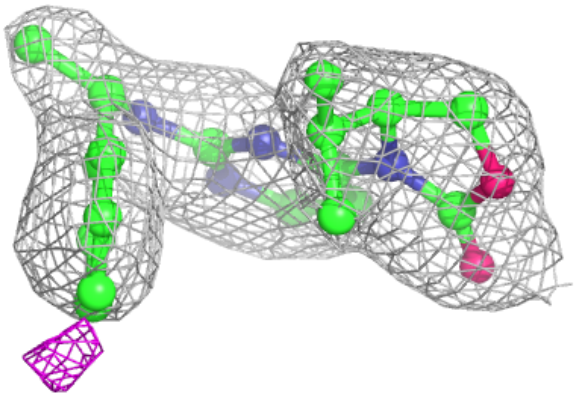
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FLC	D	503	13/13	0.88	0.16	70,77,81,84	0
4	FLC	B	503	13/13	0.90	0.25	54,62,71,82	0
4	FLC	C	503	13/13	0.90	0.22	79,83,85,86	0
4	FLC	A	503	13/13	0.91	0.17	55,66,76,81	0
3	70P	D	502	24/24	0.96	0.17	44,49,55,59	0
2	NDP	D	501	48/48	0.97	0.13	44,54,61,64	0
3	70P	C	502	24/24	0.97	0.15	40,47,53,58	0
3	70P	B	502	24/24	0.97	0.14	37,43,51,53	0
2	NDP	C	501	48/48	0.97	0.11	42,54,64,69	0
2	NDP	A	501	48/48	0.98	0.13	33,40,46,50	0
3	70P	A	502	24/24	0.98	0.14	31,40,46,50	0
2	NDP	B	501	48/48	0.98	0.13	31,37,44,62	0

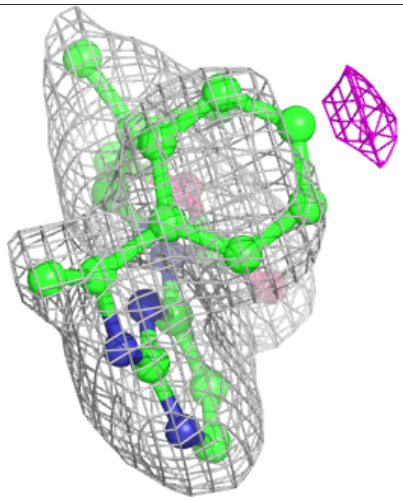
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 70P D 502:

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

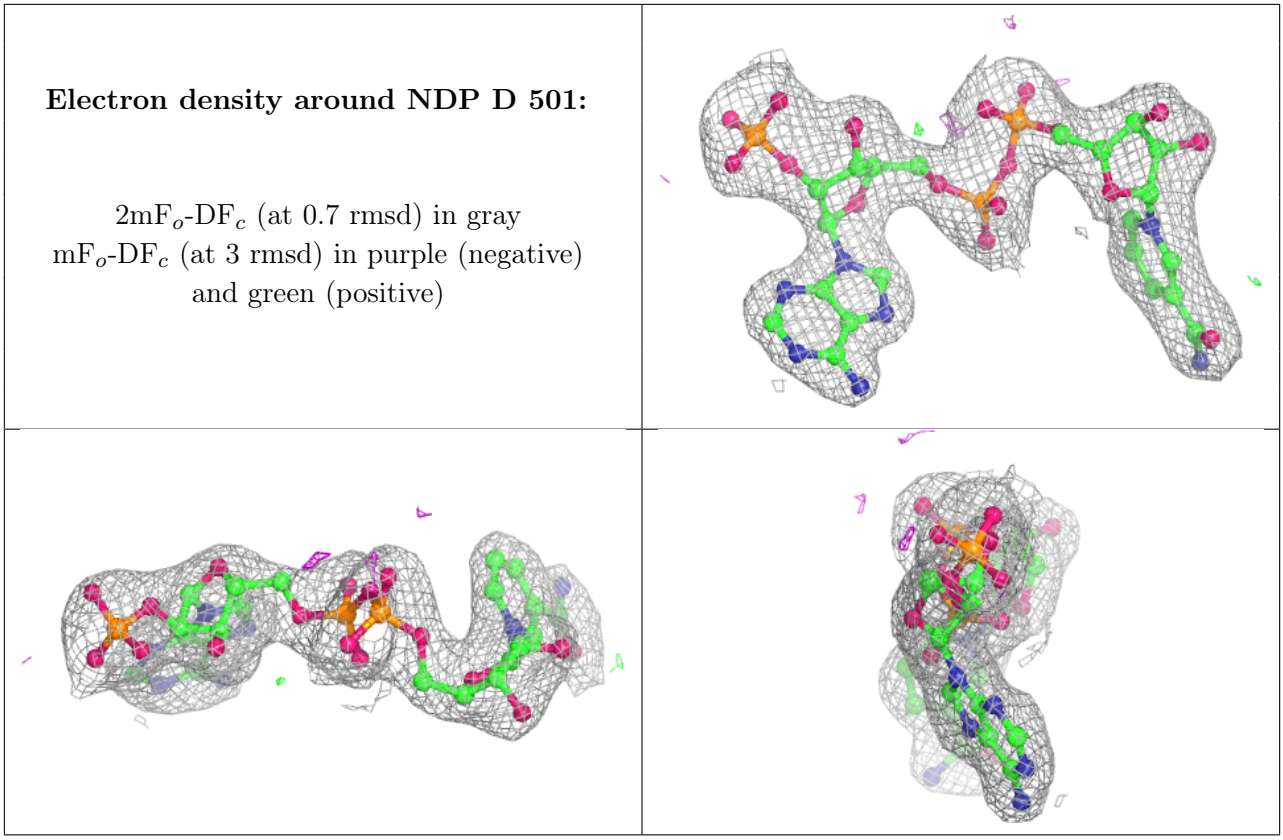






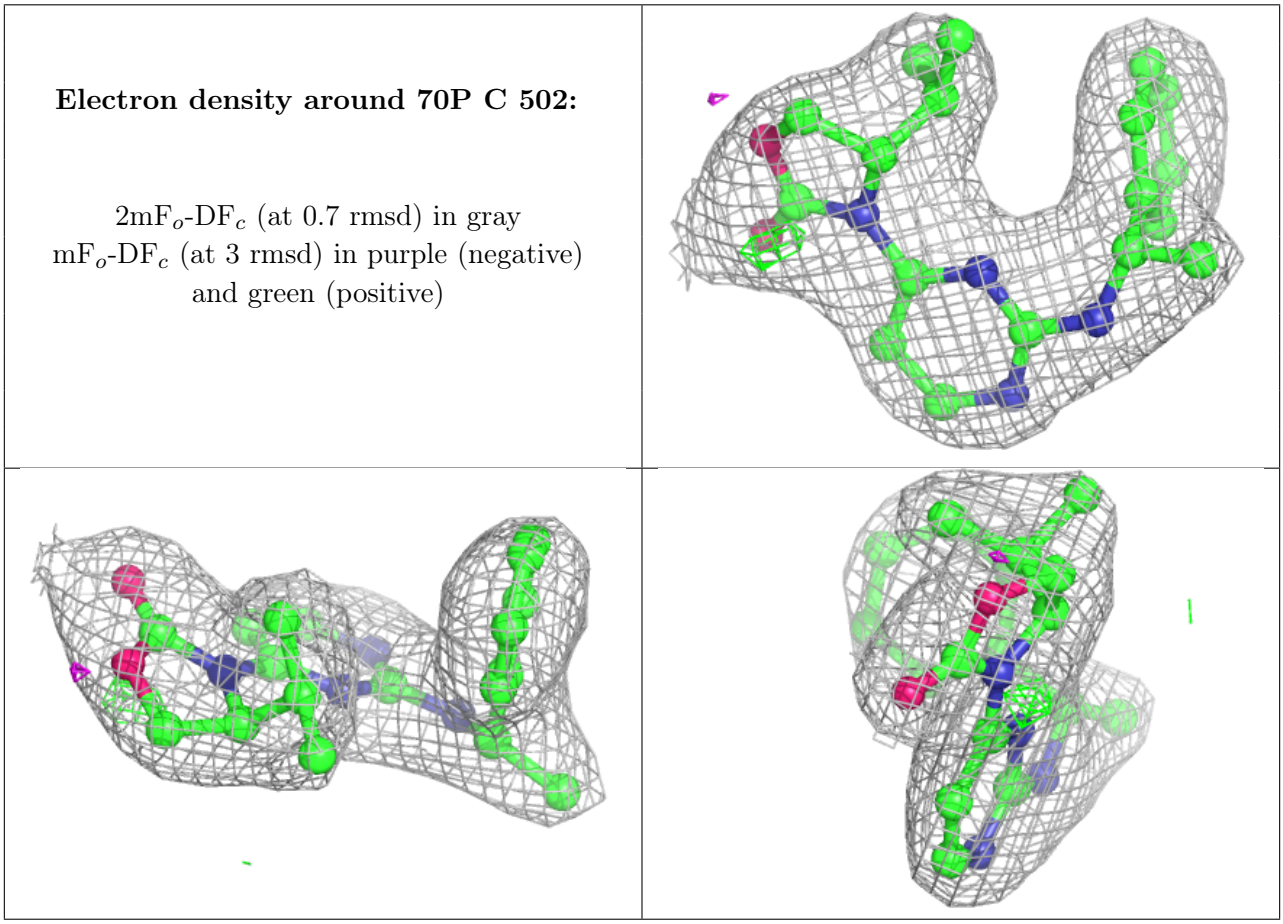
Electron density around NDP D 501:

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



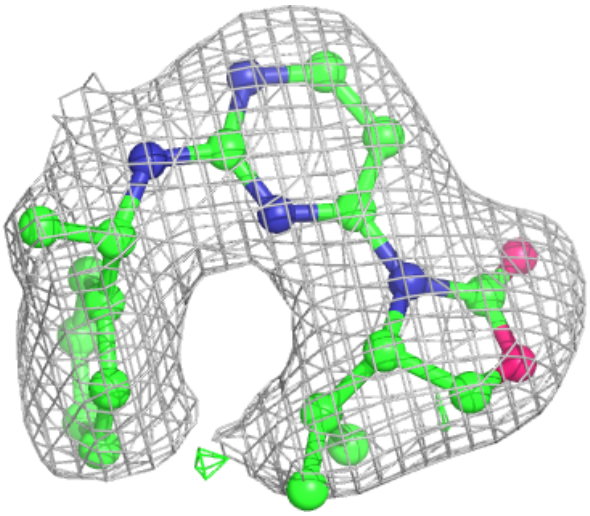
Electron density around 70P C 502:

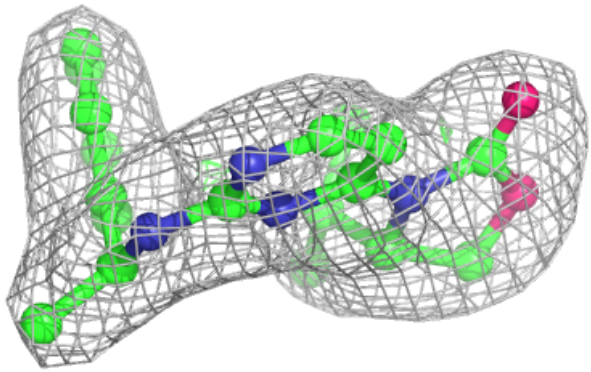
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

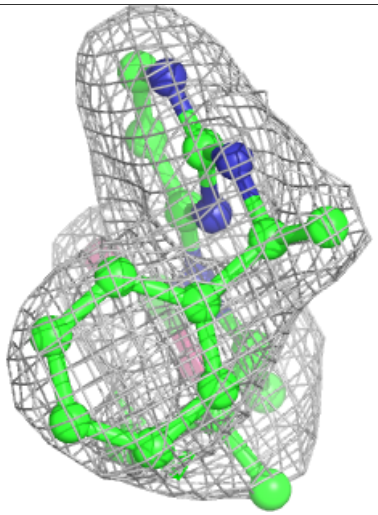


Electron density around 70P B 502:

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

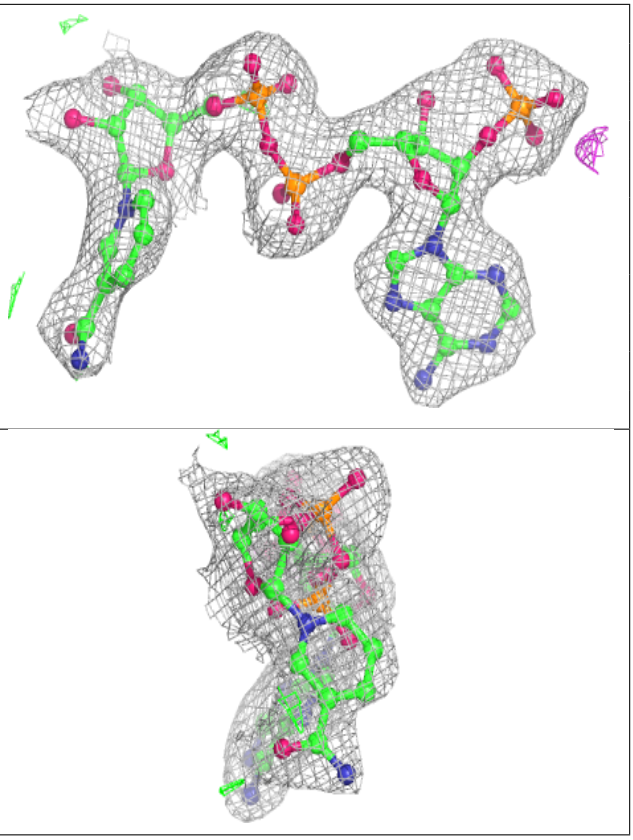






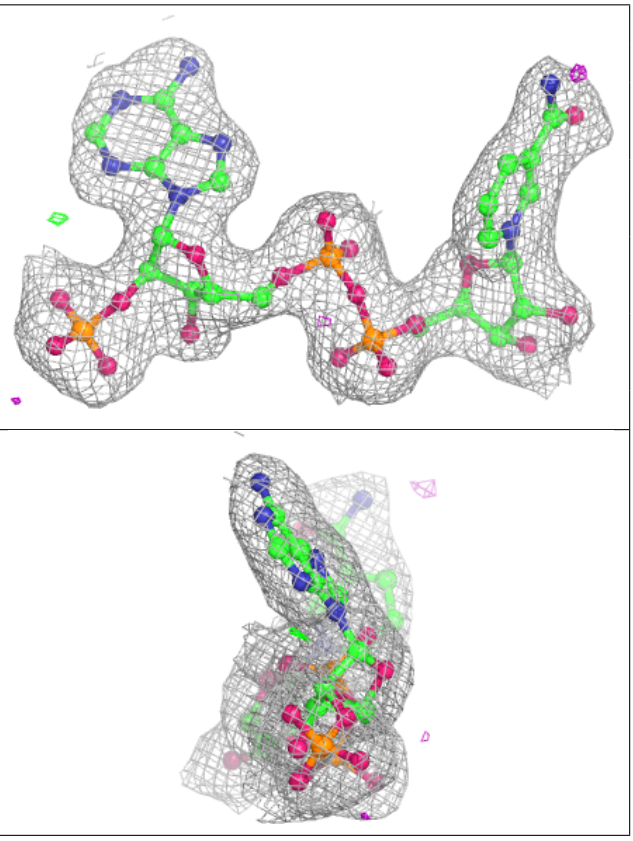
Electron density around NDP C 501:

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



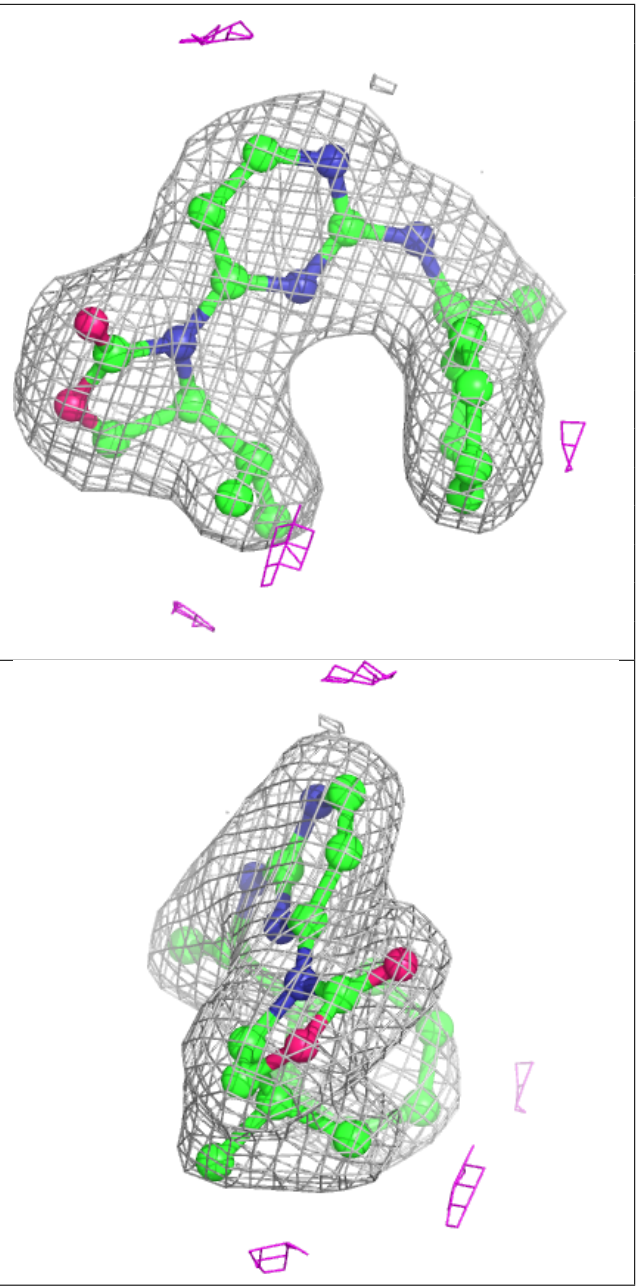
Electron density around NDP A 501:

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



Electron density around 70P A 502:

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:

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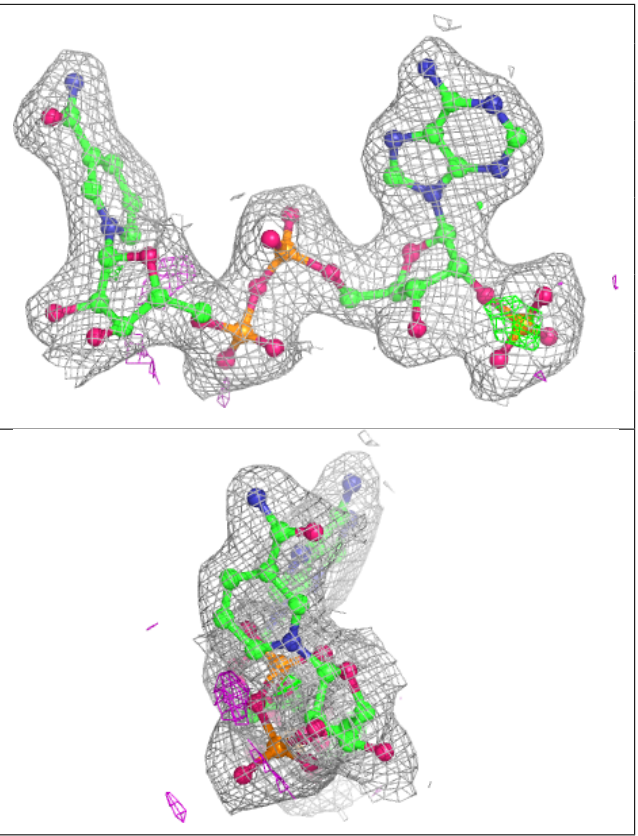
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.