Full wwPDB X-ray Structure Validation Report (i)

Jul 7, 2022 – 01:34 am BST

PDB ID	:	7PJN
Title	:	Crystal Structure of Ivosidenib-resistant IDH1 variant R132C S280F in complex with NADPH and inhibitor DS-1001B
Authors	:	Reinbold, R.; Rabe, P.; Abboud, M.I.; Schofield, C.J.; Clifton, I.J.
Deposited on	:	2021-08-24
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

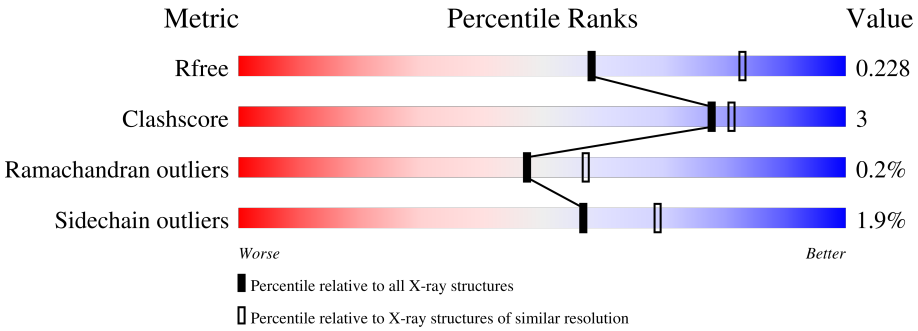
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)

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	422	91% 5% ·
1	C	422	86% 9% · ·
1	D	422	88% 9% ·
2	B	422	88% 8% ·

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 24994 atoms, of which 12019 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
1	A	406	Total	C	H	N	O	S	0	5	0
			6160	2004	3018	526	591	21			
1	C	404	Total	C	H	N	O	S	0	8	1
			5975	1968	2898	507	583	19			
1	D	408	Total	C	H	N	O	S	0	0	0
			5959	1970	2885	503	582	19			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	CYS	ARG	engineered mutation	UNP O75874
A	280	PHE	SER	engineered mutation	UNP O75874
A	415	LEU	-	expression tag	UNP O75874
A	416	GLU	-	expression tag	UNP O75874
A	417	HIS	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
C	132	CYS	ARG	engineered mutation	UNP O75874
C	280	PHE	SER	engineered mutation	UNP O75874
C	415	LEU	-	expression tag	UNP O75874
C	416	GLU	-	expression tag	UNP O75874
C	417	HIS	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874
D	132	CYS	ARG	engineered mutation	UNP O75874
D	280	PHE	SER	engineered mutation	UNP O75874
D	415	LEU	-	expression tag	UNP O75874

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	416	GLU	-	expression tag	UNP O75874
D	417	HIS	-	expression tag	UNP O75874
D	418	HIS	-	expression tag	UNP O75874
D	419	HIS	-	expression tag	UNP O75874
D	420	HIS	-	expression tag	UNP O75874
D	421	HIS	-	expression tag	UNP O75874
D	422	HIS	-	expression tag	UNP O75874

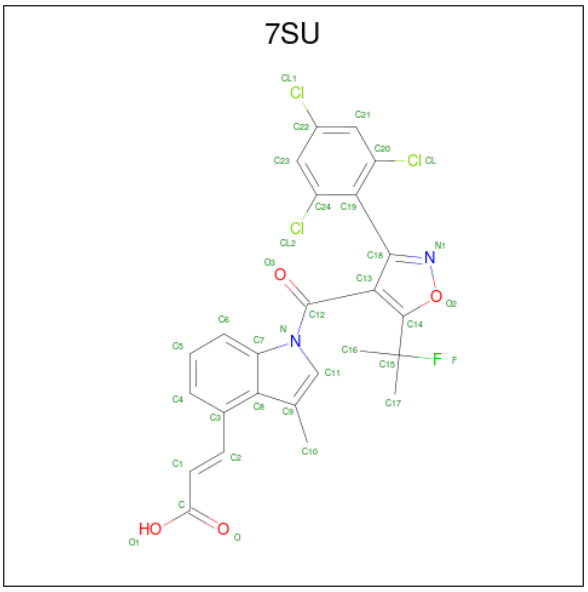
- Molecule 2 is a protein called Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	405	Total	C	H	N	O	S	0	4	0
			6123	2004	2983	519	597	20			

There are 10 discrepancies between the modelled and reference sequences:

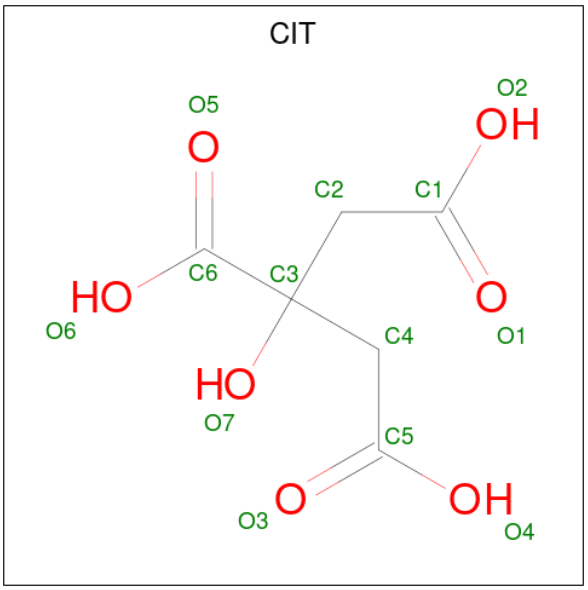
Chain	Residue	Modelled	Actual	Comment	Reference
B	132	CYS	ARG	engineered mutation	UNP O75874
B	280	PHE	SER	engineered mutation	UNP O75874
B	415	LEU	-	expression tag	UNP O75874
B	416	GLU	-	expression tag	UNP O75874
B	417	HIS	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874

- Molecule 3 is (E)-3-(1-(5-(2-fluoropropan-2-yl)-3-(2,4,6-trichlorophenyl)isoxazole-4-carbonyl)-3-methyl-1H-indol-4-yl)acrylic acid (three-letter code: 7SU) (formula: $C_{25}H_{18}Cl_3FN_2O_4$) (labeled as "Ligand of Interest" by depositor).



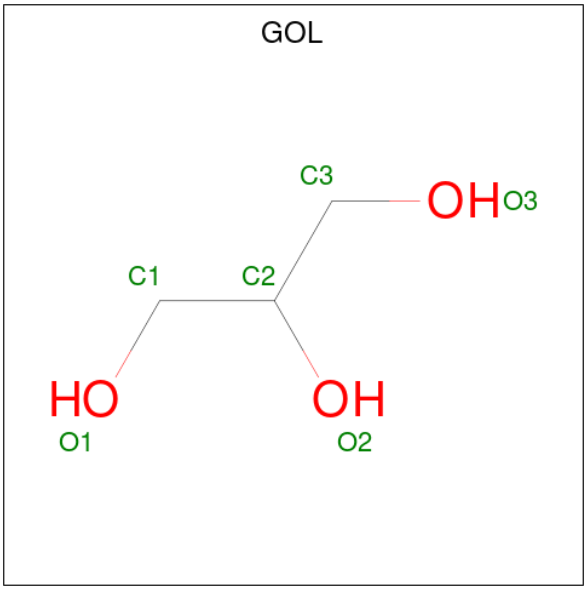
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	H	N	O	0	0
			53	25	3	1	18	2	4		
3	B	1	Total	C	Cl	F	H	N	O	0	0
			53	25	3	1	18	2	4		
3	C	1	Total	C	Cl	F	H	N	O	0	0
			53	25	3	1	18	2	4		
3	D	1	Total	C	Cl	F	H	N	O	0	0
			53	25	3	1	18	2	4		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 18 6 5 7	0	0
4	A	1	Total C H O 18 6 5 7	0	0
4	B	1	Total C H O 18 6 5 7	0	0
4	C	1	Total C H O 18 6 5 7	0	0
4	D	1	Total C H O 18 6 5 7	0	0

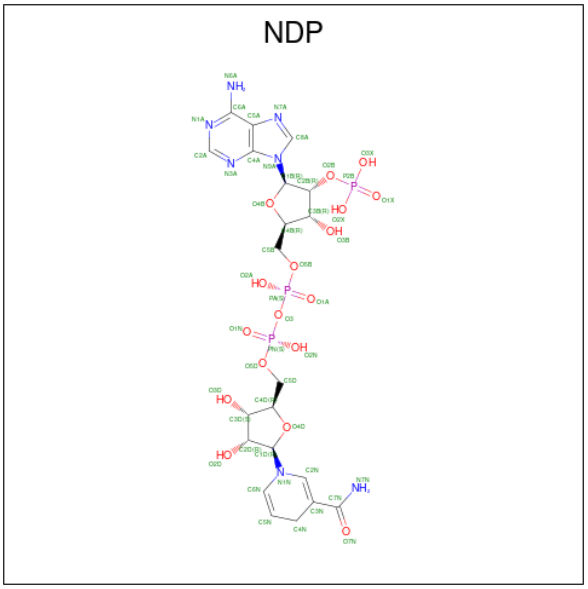
- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 9 3 3 3	0	0
5	B	1	Total C H O 9 3 3 3	0	0
5	B	1	Total C H O 9 3 3 3	0	0
5	C	1	Total C H O 9 3 3 3	0	0
5	C	1	Total C H O 9 3 3 3	0	0
5	D	1	Total C H O 9 3 3 3	0	0

- Molecule 6 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	P	0	0
			78	21	30	7	17	3		
6	B	1	Total	C	H	N	O	P	0	0
			78	21	30	7	17	3		
6	C	1	Total	C	H	N	O	P	0	0
			78	21	30	7	17	3		
6	D	1	Total	C	H	N	O	P	0	0
			78	21	30	7	17	3		

- Molecule 7 is water.

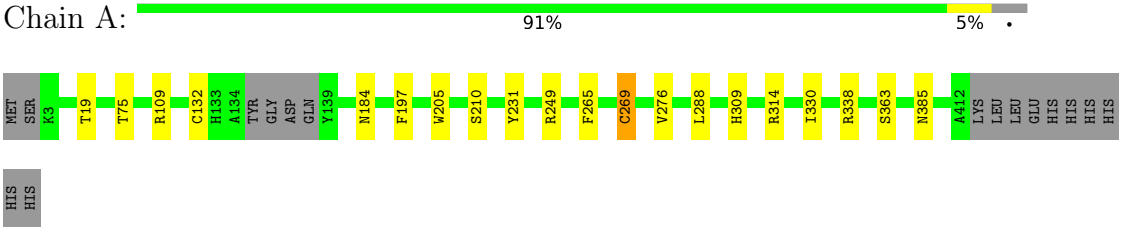
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	39	Total	O	0	0
			39	39		
7	B	43	Total	O	0	1
			44	44		
7	C	19	Total	O	0	0
			19	19		
7	D	7	Total	O	0	0
			7	7		

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.

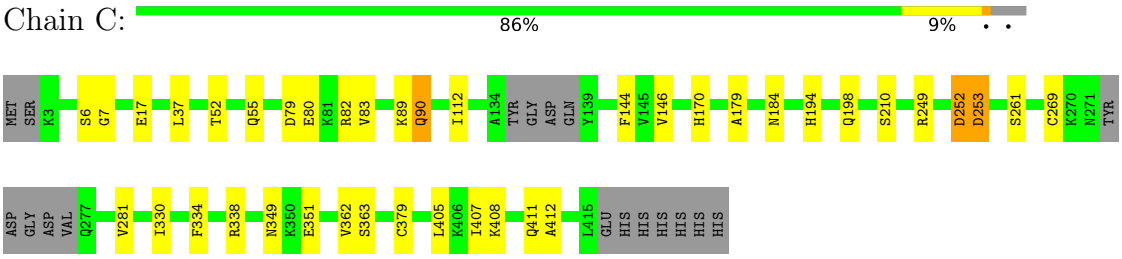
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain A:



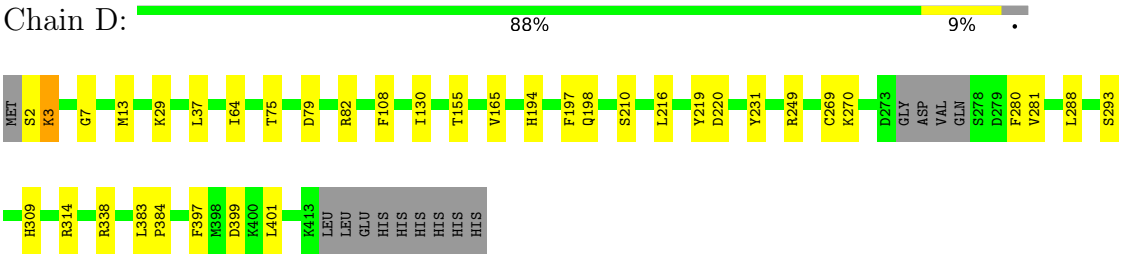
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain C:



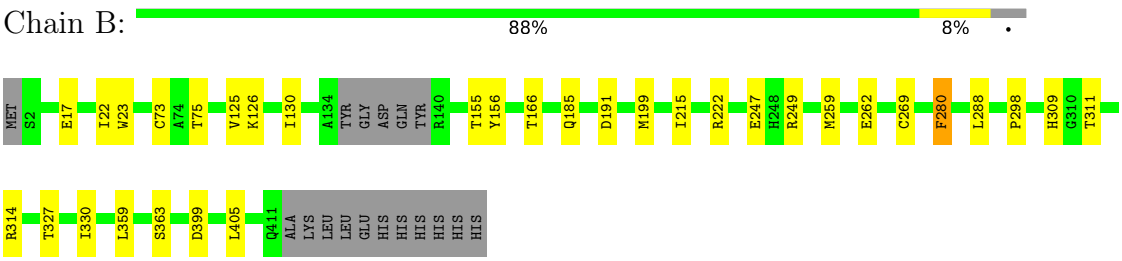
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain D:



- Molecule 2: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.18Å 153.05Å 164.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.36 – 2.45 55.36 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.36-2.45) 99.9 (55.36-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.186 , 0.228 0.186 , 0.228	Depositor DCC
R_{free} test set	3675 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24994	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, 7SU, CIT, GOL, 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	0.32	0/3221	0.49	0/4360
1	C	0.32	0/3169	0.49	0/4294
1	D	0.29	0/3139	0.46	0/4258
2	B	0.32	0/3213	0.50	0/4351
All	All	0.31	0/12742	0.48	0/17263

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	3142	3018	3000	8	0
1	C	3077	2898	2870	24	0
1	D	3074	2885	2885	20	0
2	B	3140	2983	2965	21	0
3	A	35	18	0	1	0
3	B	35	18	0	2	0
3	C	35	18	0	0	0
3	D	35	18	0	2	0
4	A	26	10	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	13	5	5	1	0
4	C	13	5	5	0	0
4	D	13	5	5	0	0
5	A	6	3	8	0	0
5	B	12	6	16	0	0
5	C	12	6	16	0	0
5	D	6	3	8	0	0
6	A	48	30	26	5	0
6	B	48	30	26	2	0
6	C	48	30	26	0	0
6	D	48	30	26	2	0
7	A	39	0	0	0	0
7	B	44	0	0	0	0
7	C	19	0	0	0	0
7	D	7	0	0	0	0
All	All	12975	12019	11897	73	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 3.

All (73) 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)
6:A:604:NDP:O3B	6:A:604:NDP:O2X	2.07	0.72
1:C:17:GLU:OE2	1:C:82:ARG:NH1	2.31	0.64
1:D:397:PHE:CE2	1:D:401:LEU:HD11	2.37	0.60
1:A:288:LEU:HG	1:A:309:HIS:HB3	1.84	0.58
1:D:75:THR:O	6:D:604:NDP:H2N	2.05	0.56
1:C:89:LYS:O	1:C:90:GLN:CB	2.54	0.55
1:C:7:GLY:HA3	1:C:37:LEU:HD23	1.91	0.53
2:B:280:PHE:CZ	1:C:252:ASP:HB3	2.44	0.52
1:C:52:THR:HG22	1:C:55:GLN:HB3	1.91	0.52
2:B:125:VAL:HG23	2:B:126:LYS:HG3	1.92	0.52
1:D:29:LYS:NZ	1:D:399:ASP:OD1	2.42	0.51
1:C:252:ASP:OD1	1:C:252:ASP:N	2.35	0.51
2:B:280:PHE:CE1	1:C:252:ASP:HB3	2.46	0.51
2:B:288:LEU:HG	2:B:309:HIS:HB3	1.93	0.50
2:B:247:GLU:OE1	2:B:249:ARG:NH1	2.41	0.50
2:B:359:LEU:HD13	2:B:405:LEU:HD22	1.93	0.50
2:B:314:ARG:NH2	6:B:604:NDP:O3X	2.44	0.49
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:VAL:HG11	1:C:405:LEU:HA	1.94	0.49
3:A:601:7SU:C17	3:A:601:7SU:C12	2.91	0.48
1:D:3:LYS:HG2	1:D:3:LYS:O	2.12	0.48
1:C:351:GLU:OE1	1:D:2:SER:N	2.46	0.48
1:D:314:ARG:NE	6:D:604:NDP:O2X	2.47	0.47
1:A:205:TRP:HB3	1:A:265:PHE:HA	1.96	0.47
1:D:194:HIS:O	1:D:198:GLN:HG2	2.13	0.47
1:C:362:VAL:HG13	1:C:408:LYS:HD2	1.97	0.46
2:B:75:THR:O	6:B:604:NDP:H2N	2.16	0.46
1:D:220:ASP:OD1	1:D:270:LYS:HE2	2.16	0.46
2:B:259:MET:HE3	1:C:281:VAL:HA	1.97	0.46
1:A:210:SER:HA	1:A:249:ARG:O	2.16	0.45
1:D:13:MET:CE	1:D:64:ILE:HD11	2.47	0.45
1:C:194:HIS:O	1:C:198:GLN:HG2	2.16	0.45
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.99	0.45
6:A:604:NDP:HO3A	6:A:604:NDP:P2B	2.38	0.45
4:B:603:CIT:C6	4:B:603:CIT:O1	2.65	0.45
2:B:185:GLN:OE1	1:C:170:HIS:NE2	2.46	0.44
1:C:144:PHE:CZ	1:C:179:ALA:HB3	2.52	0.44
1:A:132:CYS:HA	1:A:269:CYS:O	2.18	0.44
1:D:130:ILE:HD11	3:D:601:7SU:C9	2.48	0.44
2:B:156:TYR:CE1	1:C:146:VAL:HG13	2.53	0.44
2:B:155:THR:HG22	2:B:166:THR:HG23	1.99	0.43
1:C:407:ILE:O	1:C:411:GLN:HG2	2.17	0.43
2:B:280:PHE:CD1	2:B:280:PHE:N	2.83	0.43
1:D:288:LEU:HB3	1:D:309:HIS:HB3	1.99	0.43
1:D:197:PHE:CZ	1:D:231:TYR:HB2	2.53	0.43
1:C:80:GLU:O	1:C:83:VAL:HG22	2.18	0.43
2:B:23:TRP:CD2	2:B:73:CYS:HB2	2.54	0.43
1:D:216:LEU:HB3	1:D:219:TYR:HB3	2.00	0.43
1:D:383:LEU:N	1:D:384:PRO:HD2	2.34	0.43
6:A:604:NDP:C8A	6:A:604:NDP:H52A	2.49	0.42
1:D:7:GLY:HA3	1:D:37:LEU:HD23	2.01	0.42
3:B:601:7SU:C12	3:B:601:7SU:C16	2.98	0.42
1:C:79:ASP:O	1:C:83:VAL:HG13	2.19	0.42
1:D:130:ILE:HD11	3:D:601:7SU:C11	2.49	0.42
2:B:17:GLU:OE1	2:B:311:THR:OG1	2.31	0.42
1:C:252:ASP:O	1:C:253:ASP:CB	2.68	0.42
1:D:108:PHE:O	1:D:293:SER:HA	2.20	0.42
1:C:112:ILE:HD11	1:C:334:PHE:CG	2.55	0.41
2:B:191:ASP:HB3	2:B:298:PRO:HG3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ARG:NE	6:A:604:NDP:O2X	2.51	0.41
2:B:125:VAL:HG22	2:B:262:GLU:HB2	2.03	0.41
1:A:197:PHE:CZ	1:A:231:TYR:HB2	2.56	0.41
1:D:155:THR:HA	1:D:165:VAL:O	2.21	0.41
2:B:22:ILE:HD11	2:B:327:THR:HB	2.03	0.41
2:B:130:ILE:HD11	3:B:601:7SU:C9	2.50	0.41
1:D:210:SER:HA	1:D:249:ARG:O	2.21	0.41
1:C:210:SER:HA	1:C:249:ARG:O	2.21	0.40
1:D:79:ASP:H	1:D:82:ARG:HB2	1.86	0.40
1:A:75:THR:O	6:A:604:NDP:H2N	2.21	0.40
2:B:330:ILE:HD12	2:B:363:SER:HB3	2.03	0.40
1:C:6:SER:O	1:C:349:ASN:ND2	2.54	0.40
1:C:52:THR:HG22	1:C:52:THR:O	2.22	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	407/422 (96%)	394 (97%)	13 (3%)	0	100 100
1	C	406/422 (96%)	387 (95%)	16 (4%)	3 (1%)	22 25
1	D	404/422 (96%)	387 (96%)	17 (4%)	0	100 100
2	B	404/422 (96%)	388 (96%)	16 (4%)	0	100 100
All	All	1621/1688 (96%)	1556 (96%)	62 (4%)	3 (0%)	47 57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	90	GLN
1	C	253	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	412	ALA

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	320/358 (89%)	313 (98%)	7 (2%)	52	64
1	C	300/358 (84%)	294 (98%)	6 (2%)	55	67
1	D	298/358 (83%)	293 (98%)	5 (2%)	60	73
2	B	315/357 (88%)	310 (98%)	5 (2%)	62	74
All	All	1233/1431 (86%)	1210 (98%)	23 (2%)	57	69

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	109	ARG
1	A	184	ASN
1	A	269	CYS
1	A	276	VAL
1	A	338	ARG
1	A	385	ASN
2	B	199	MET
2	B	222	ARG
2	B	269	CYS
2	B	280	PHE
2	B	399	ASP
1	C	184	ASN
1	C	252	ASP
1	C	261	SER
1	C	269	CYS
1	C	338	ARG
1	C	379	CYS
1	D	3	LYS
1	D	269	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	280	PHE
1	D	281	VAL
1	D	338	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CSD	B	379	2	3,7,8	0.89	0	1,8,10	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSD	B	379	2	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	379	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

19 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	$\#\|Z\| > 2$
5	GOL	B	605	-	5,5,5	1.01	0	5,5,5	0.91	0
3	7SU	B	601	-	31,38,38	1.05	1 (3%)	32,58,58	0.72	0
5	GOL	C	602	-	5,5,5	0.82	0	5,5,5	0.94	0
4	CIT	A	602	-	12,12,12	0.99	0	17,17,17	1.72	1 (5%)
4	CIT	D	603	-	12,12,12	0.99	0	17,17,17	1.54	2 (11%)
5	GOL	B	602	-	5,5,5	0.84	0	5,5,5	1.01	0
3	7SU	C	601	-	31,38,38	0.82	2 (6%)	32,58,58	1.48	4 (12%)
4	CIT	C	603	-	12,12,12	1.06	0	17,17,17	1.59	2 (11%)
4	CIT	B	603	-	12,12,12	1.08	0	17,17,17	1.81	6 (35%)
5	GOL	C	604	-	5,5,5	0.91	0	5,5,5	1.03	0
6	NDP	D	604	-	45,52,52	0.50	0	53,80,80	0.71	1 (1%)
6	NDP	C	605	-	45,52,52	0.52	0	53,80,80	0.62	1 (1%)
5	GOL	A	603	-	5,5,5	0.87	0	5,5,5	1.01	0
3	7SU	A	601	-	31,38,38	1.17	1 (3%)	32,58,58	1.73	4 (12%)
6	NDP	A	604	-	45,52,52	0.54	0	53,80,80	0.81	1 (1%)
6	NDP	B	604	-	45,52,52	0.53	0	53,80,80	0.65	1 (1%)
3	7SU	D	601	-	31,38,38	0.84	2 (6%)	32,58,58	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CIT	A	605	-	12,12,12	1.00	0	17,17,17	1.60	2 (11%)
5	GOL	D	602	-	5,5,5	0.98	0	5,5,5	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	605	-	-	2/4/4/4	-
3	7SU	B	601	-	-	0/7/23/23	0/4/4/4
5	GOL	C	602	-	-	2/4/4/4	-
4	CIT	A	602	-	-	14/16/16/16	-
4	CIT	D	603	-	-	11/16/16/16	-
5	GOL	B	602	-	-	3/4/4/4	-
3	7SU	C	601	-	-	3/7/23/23	0/4/4/4
4	CIT	C	603	-	-	10/16/16/16	-
4	CIT	B	603	-	-	2/16/16/16	-
5	GOL	C	604	-	-	1/4/4/4	-
6	NDP	D	604	-	-	11/30/77/77	0/5/5/5
6	NDP	C	605	-	-	16/30/77/77	0/5/5/5
5	GOL	A	603	-	-	2/4/4/4	-
3	7SU	A	601	-	-	3/7/23/23	0/4/4/4
6	NDP	A	604	-	-	12/30/77/77	0/5/5/5
6	NDP	B	604	-	-	11/30/77/77	0/5/5/5
3	7SU	D	601	-	-	0/7/23/23	0/4/4/4
4	CIT	A	605	-	-	9/16/16/16	-
5	GOL	D	602	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	7SU	C13-C12	-5.41	1.44	1.51
3	B	601	7SU	C13-C12	-4.13	1.45	1.51
3	D	601	7SU	C13-C12	-2.40	1.48	1.51
3	D	601	7SU	F-C15	-2.15	1.38	1.41
3	C	601	7SU	F-C15	-2.11	1.38	1.41
3	C	601	7SU	C13-C12	-2.05	1.48	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	602	CIT	O6-C6-C3	5.01	121.75	113.05
3	A	601	7SU	C3-C2-C1	5.00	134.75	126.93
4	B	603	CIT	O6-C6-C3	4.70	121.21	113.05
3	A	601	7SU	C8-C3-C2	4.47	126.43	121.96
3	C	601	7SU	C3-C2-C1	4.36	133.74	126.93
4	A	605	CIT	O6-C6-C3	4.26	120.45	113.05
3	A	601	7SU	C4-C3-C2	-4.25	114.16	120.64
3	C	601	7SU	C8-C3-C2	4.18	126.14	121.96
4	C	603	CIT	O6-C6-C3	4.10	120.17	113.05
4	D	603	CIT	O6-C6-C3	4.01	120.02	113.05
3	C	601	7SU	C4-C3-C2	-3.92	114.65	120.64
3	A	601	7SU	C13-C12-N	3.28	121.79	118.10
4	B	603	CIT	O5-C6-C3	-2.49	118.73	122.25
6	B	604	NDP	C5A-C6A-N6A	2.35	123.93	120.35
6	A	604	NDP	C5A-C6A-N6A	2.33	123.90	120.35
4	C	603	CIT	C3-C4-C5	-2.33	108.17	113.81
6	C	605	NDP	C5A-C6A-N6A	2.27	123.80	120.35
6	D	604	NDP	C5A-C6A-N6A	2.19	123.68	120.35
4	B	603	CIT	O4-C5-C4	2.17	121.30	114.35
4	B	603	CIT	O2-C1-O1	-2.15	117.94	123.30
4	D	603	CIT	O4-C5-C4	2.15	121.25	114.35
3	C	601	7SU	C13-C12-N	2.11	120.48	118.10
4	B	603	CIT	O4-C5-O3	-2.08	118.12	123.30
4	B	603	CIT	C3-C4-C5	-2.06	108.82	113.81
4	A	605	CIT	O4-C5-C4	2.05	120.92	114.35

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	7SU	C1-C2-C3-C4
3	A	601	7SU	C1-C2-C3-C8
3	C	601	7SU	C1-C2-C3-C4
3	C	601	7SU	C1-C2-C3-C8
4	A	602	CIT	C1-C2-C3-O7
4	A	602	CIT	C1-C2-C3-C4
4	A	602	CIT	C1-C2-C3-C6
4	A	602	CIT	C2-C3-C6-O5
4	A	602	CIT	C2-C3-C6-O6
4	A	602	CIT	O7-C3-C6-O5
4	A	602	CIT	O7-C3-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	605	CIT	C1-C2-C3-O7
4	A	605	CIT	C1-C2-C3-C4
4	A	605	CIT	C1-C2-C3-C6
4	C	603	CIT	O7-C3-C6-O5
4	C	603	CIT	O7-C3-C6-O6
4	D	603	CIT	C2-C3-C6-O5
4	D	603	CIT	C2-C3-C6-O6
4	D	603	CIT	O7-C3-C6-O5
4	D	603	CIT	O7-C3-C6-O6
5	B	602	GOL	C1-C2-C3-O3
5	B	605	GOL	O1-C1-C2-C3
5	C	602	GOL	O1-C1-C2-C3
5	D	602	GOL	C1-C2-C3-O3
5	D	602	GOL	O2-C2-C3-O3
6	A	604	NDP	C5B-O5B-PA-O1A
6	A	604	NDP	C5B-O5B-PA-O3
6	A	604	NDP	PN-O3-PA-O5B
6	B	604	NDP	C5B-O5B-PA-O1A
6	B	604	NDP	C2B-O2B-P2B-O3X
6	B	604	NDP	C5D-O5D-PN-O1N
6	C	605	NDP	C5B-O5B-PA-O3
6	C	605	NDP	PA-O3-PN-O5D
6	C	605	NDP	C5D-O5D-PN-O1N
6	C	605	NDP	C5D-O5D-PN-O2N
6	D	604	NDP	PN-O3-PA-O5B
6	D	604	NDP	O4B-C4B-C5B-O5B
6	D	604	NDP	C2B-O2B-P2B-O1X
6	D	604	NDP	C5D-O5D-PN-O2N
6	D	604	NDP	C3B-C4B-C5B-O5B
4	D	603	CIT	C2-C3-C4-C5
4	D	603	CIT	C6-C3-C4-C5
6	A	604	NDP	C3B-C2B-O2B-P2B
4	A	602	CIT	C2-C3-C4-C5
4	A	602	CIT	C6-C3-C4-C5
4	C	603	CIT	C1-C2-C3-C6
5	A	603	GOL	C1-C2-C3-O3
6	A	604	NDP	C1B-C2B-O2B-P2B
4	C	603	CIT	C4-C3-C6-O5
5	A	603	GOL	O2-C2-C3-O3
5	B	602	GOL	O2-C2-C3-O3
5	B	605	GOL	O1-C1-C2-O2
4	A	602	CIT	O2-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	601	7SU	C-C1-C2-C3
4	A	602	CIT	O1-C1-C2-C3
4	C	603	CIT	C1-C2-C3-O7
6	A	604	NDP	PA-O3-PN-O1N
6	C	605	NDP	PN-O3-PA-O1A
6	D	604	NDP	PA-O3-PN-O1N
3	C	601	7SU	C-C1-C2-C3
4	A	605	CIT	O7-C3-C6-O5
4	A	605	CIT	O7-C3-C6-O6
4	A	605	CIT	C4-C3-C6-O5
4	A	605	CIT	C4-C3-C6-O6
4	C	603	CIT	C4-C3-C6-O6
4	D	603	CIT	O7-C3-C4-C5
5	C	602	GOL	O1-C1-C2-O2
6	B	604	NDP	C5B-O5B-PA-O3
6	C	605	NDP	C2B-O2B-P2B-O3X
6	D	604	NDP	C2B-O2B-P2B-O2X
6	A	604	NDP	PA-O3-PN-O2N
6	B	604	NDP	C5D-O5D-PN-O2N
6	C	605	NDP	C5B-O5B-PA-O1A
6	C	605	NDP	C5B-O5B-PA-O2A
6	C	605	NDP	C2D-C1D-N1N-C2N
4	A	605	CIT	C2-C3-C6-O6
6	A	604	NDP	O4D-C1D-N1N-C2N
6	B	604	NDP	O4D-C1D-N1N-C2N
6	C	605	NDP	O4D-C1D-N1N-C2N
6	A	604	NDP	C2D-C1D-N1N-C2N
6	D	604	NDP	O4D-C1D-N1N-C2N
6	C	605	NDP	PN-O3-PA-O2A
6	B	604	NDP	C2D-C1D-N1N-C2N
4	C	603	CIT	C1-C2-C3-C4
4	B	603	CIT	C3-C4-C5-O4
6	D	604	NDP	C2D-C1D-N1N-C2N
4	C	603	CIT	C2-C3-C6-O6
4	C	603	CIT	C3-C4-C5-O4
6	C	605	NDP	C1B-C2B-O2B-P2B
4	B	603	CIT	C3-C4-C5-O3
4	C	603	CIT	C3-C4-C5-O3
6	C	605	NDP	C2D-C1D-N1N-C6N
4	D	603	CIT	O2-C1-C2-C3
6	C	605	NDP	O4D-C1D-N1N-C6N
4	D	603	CIT	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	603	CIT	C3-C4-C5-O4
4	A	605	CIT	C2-C3-C6-O5
4	D	603	CIT	C3-C4-C5-O3
5	B	602	GOL	O1-C1-C2-O2
6	B	604	NDP	C5D-O5D-PN-O3
6	C	605	NDP	C5D-O5D-PN-O3
4	A	602	CIT	C3-C4-C5-O3
6	D	604	NDP	PA-O3-PN-O2N
5	C	604	GOL	O1-C1-C2-C3
4	A	602	CIT	O7-C3-C4-C5
6	C	605	NDP	C3B-C2B-O2B-P2B
6	A	604	NDP	C5D-O5D-PN-O1N
6	B	604	NDP	C5B-O5B-PA-O2A
6	D	604	NDP	C5D-O5D-PN-O1N
6	A	604	NDP	O4D-C1D-N1N-C6N
6	B	604	NDP	O4D-C1D-N1N-C6N
6	A	604	NDP	C2D-C1D-N1N-C6N
6	B	604	NDP	C2D-C1D-N1N-C6N
4	A	602	CIT	C3-C4-C5-O4

There are no ring outliers.

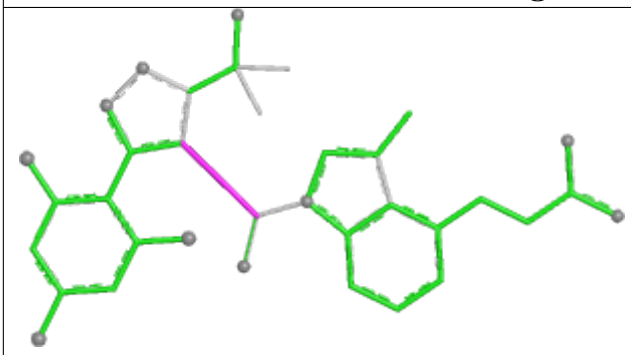
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	7SU	2	0
4	B	603	CIT	1	0
6	D	604	NDP	2	0
3	A	601	7SU	1	0
6	A	604	NDP	5	0
6	B	604	NDP	2	0
3	D	601	7SU	2	0

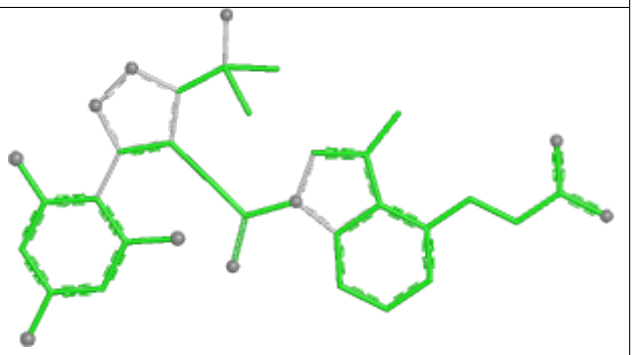
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

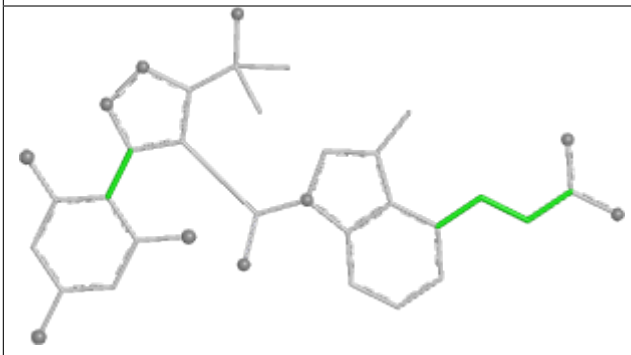
Ligand 7SU B 601



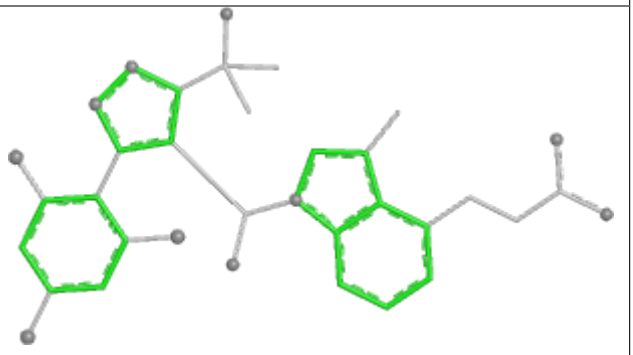
Bond lengths



Bond angles

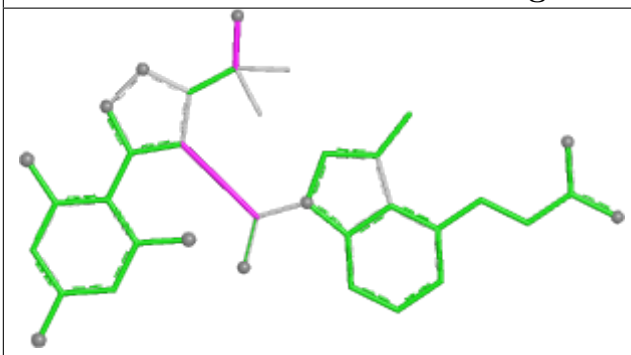


Torsions

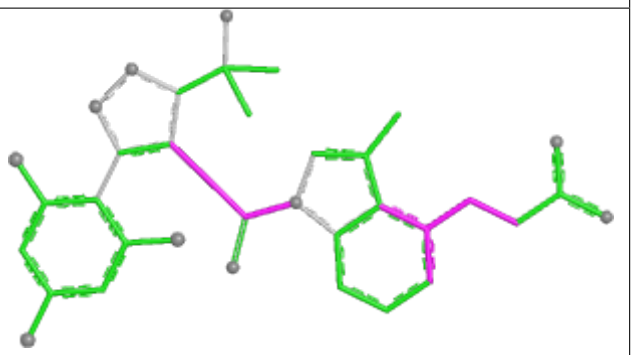


Rings

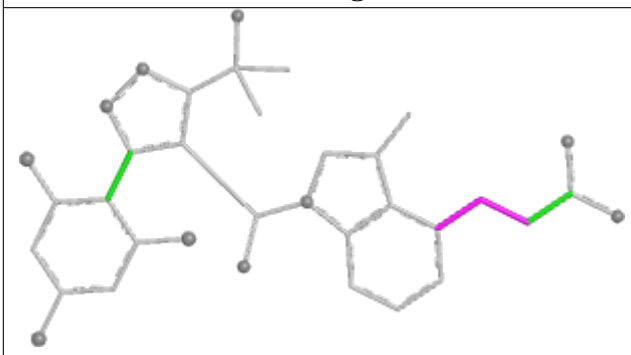
Ligand 7SU C 601



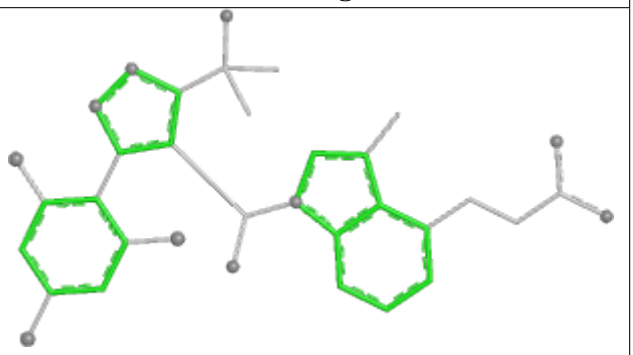
Bond lengths



Bond angles

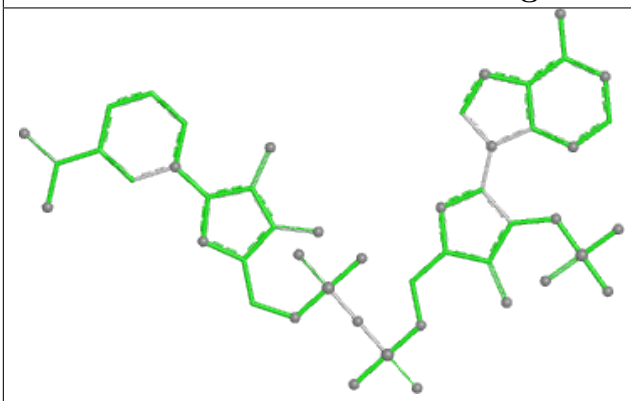


Torsions

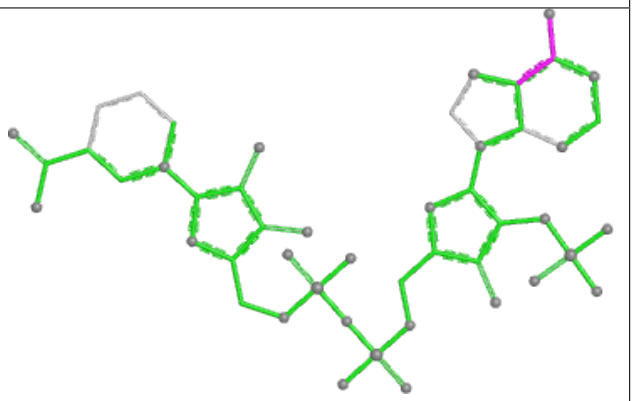


Rings

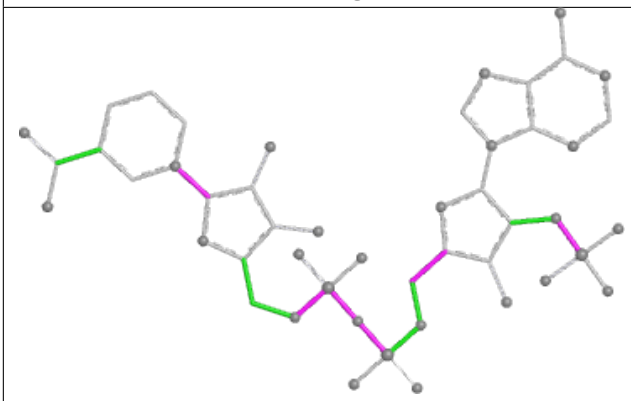
Ligand NDP D 604



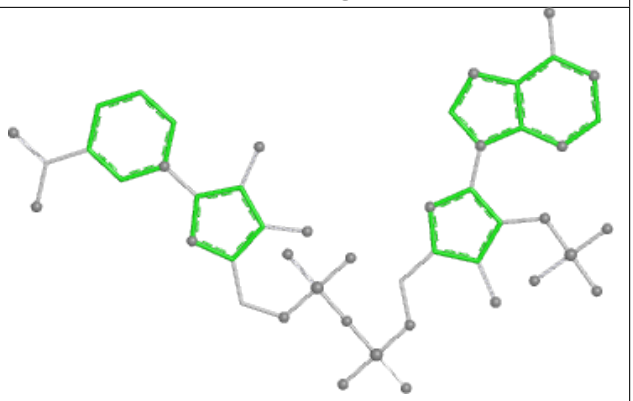
Bond lengths



Bond angles

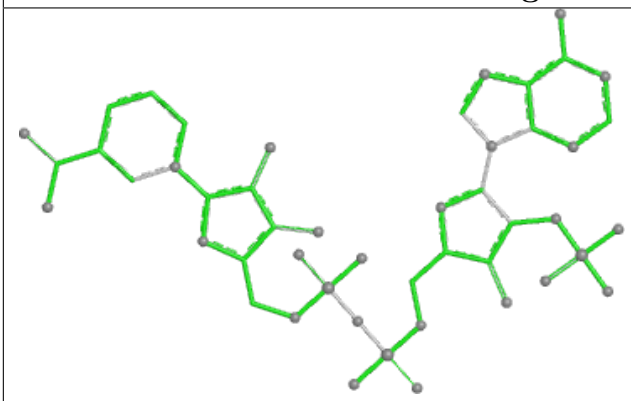


Torsions

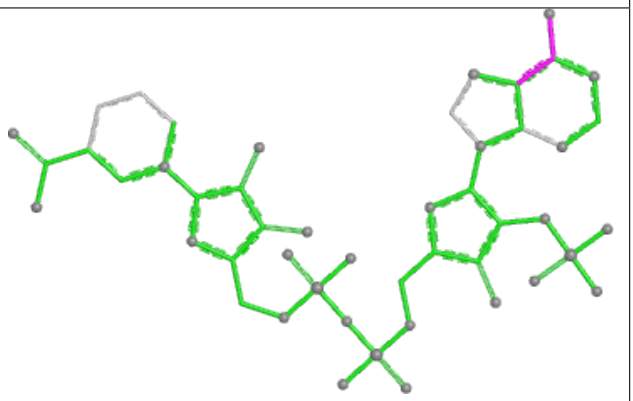


Rings

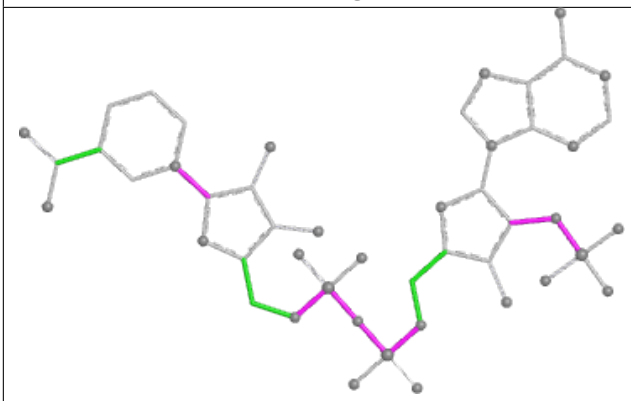
Ligand NDP C 605



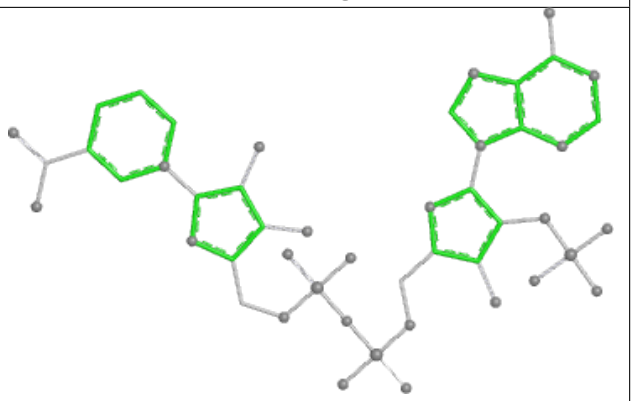
Bond lengths



Bond angles

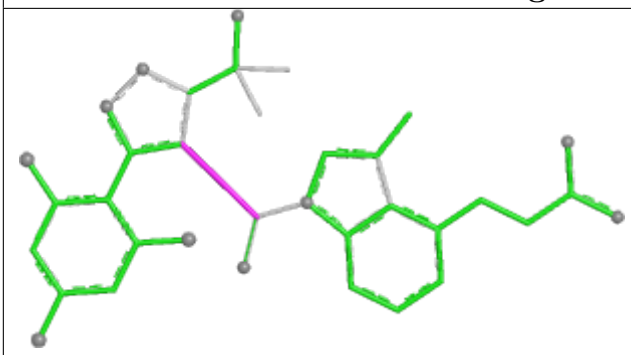


Torsions

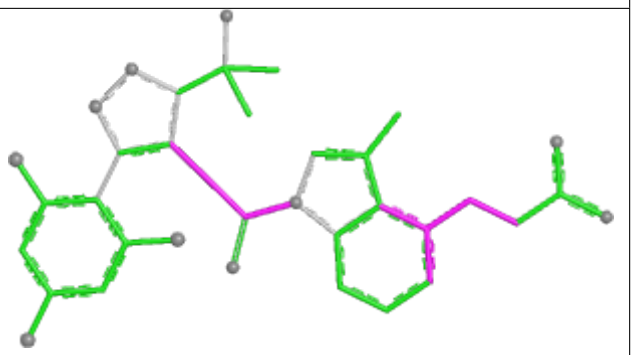


Rings

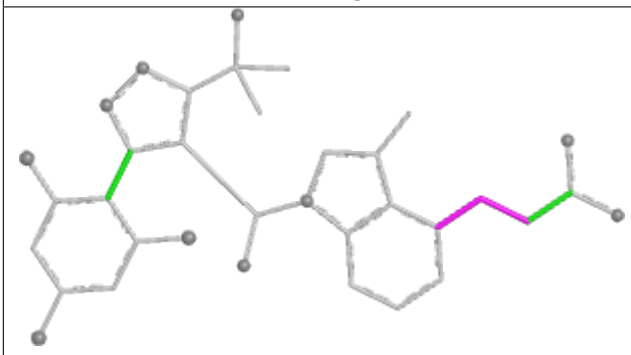
Ligand 7SU A 601



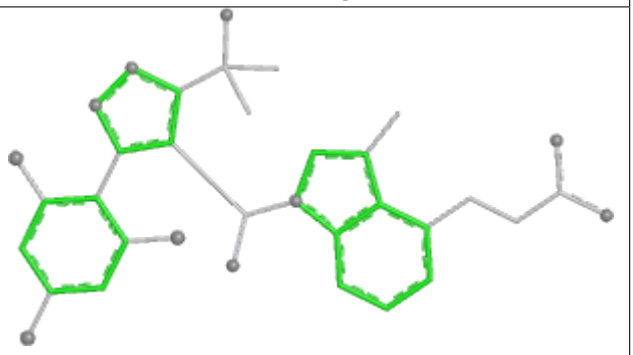
Bond lengths



Bond angles

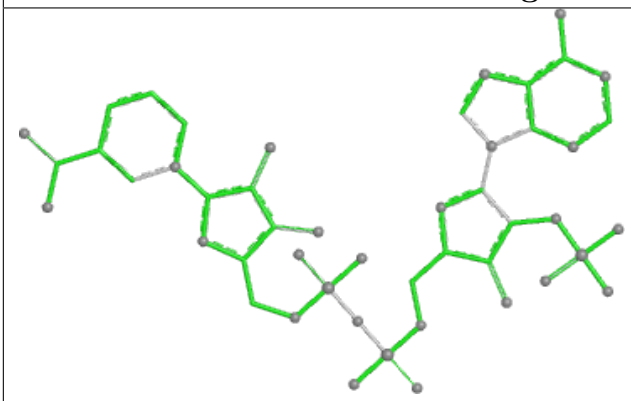


Torsions

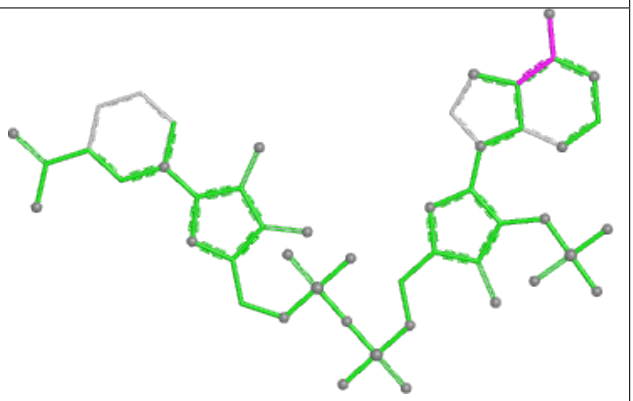


Rings

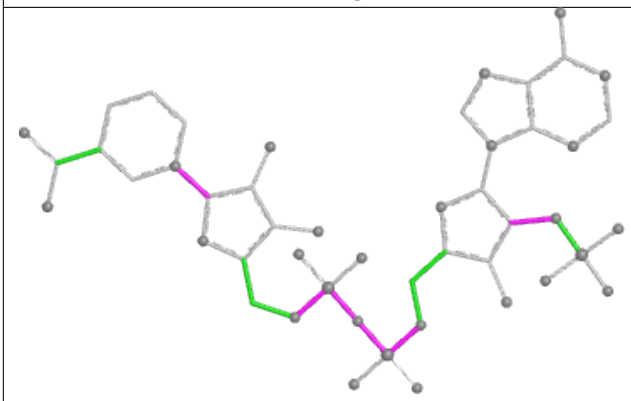
Ligand NDP A 604



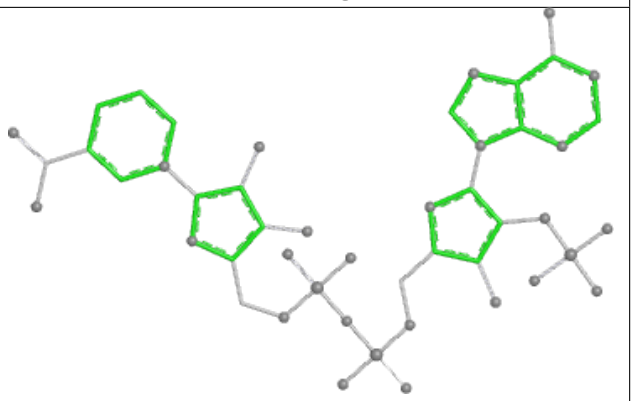
Bond lengths



Bond angles

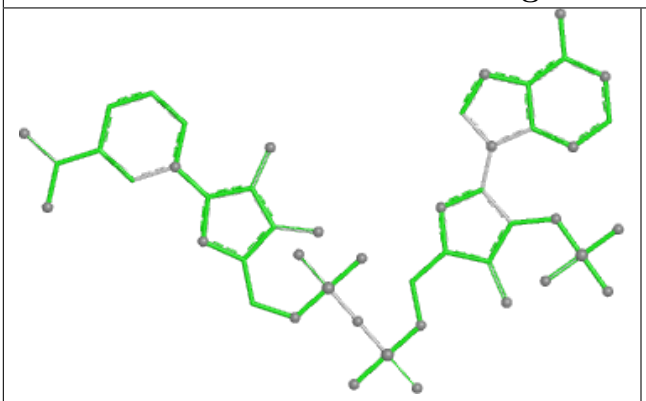


Torsions

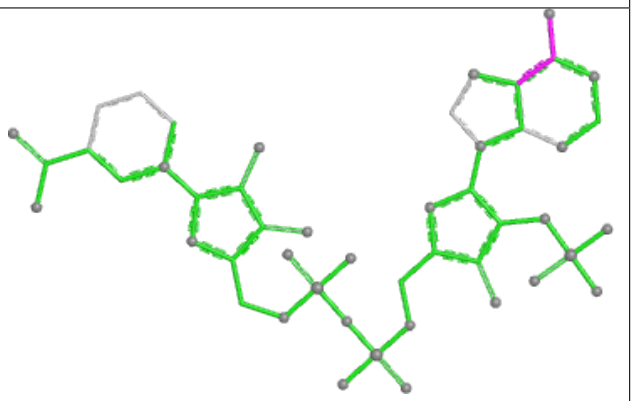


Rings

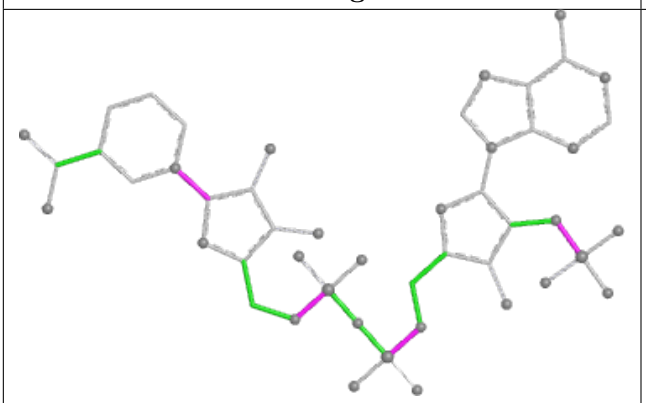
Ligand NDP B 604



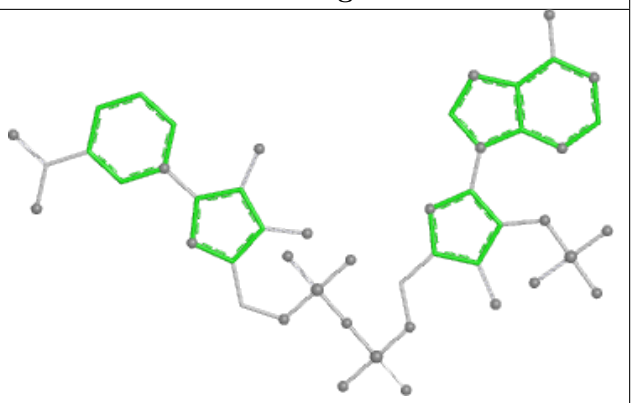
Bond lengths



Bond angles

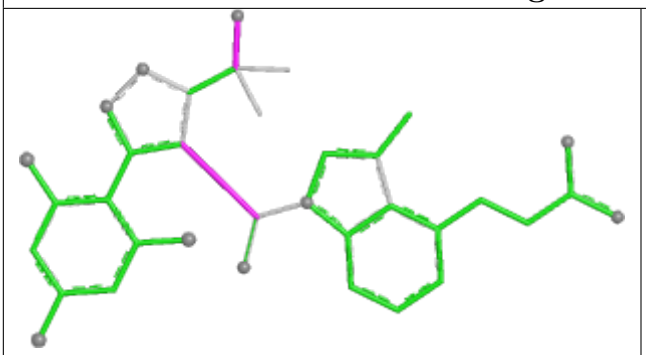


Torsions

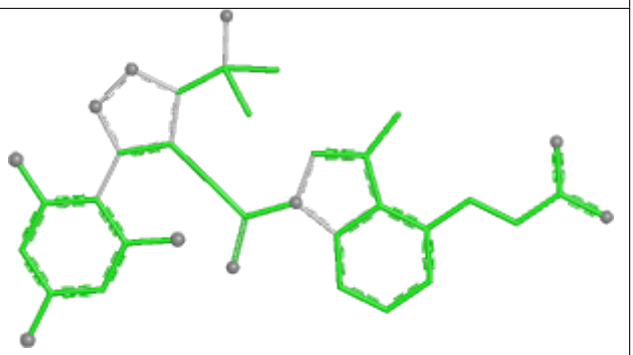


Rings

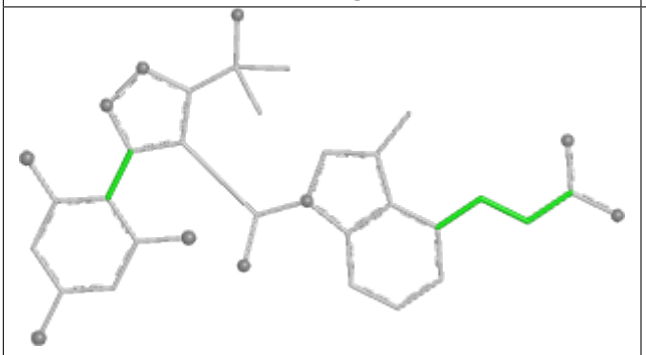
Ligand 7SU D 601



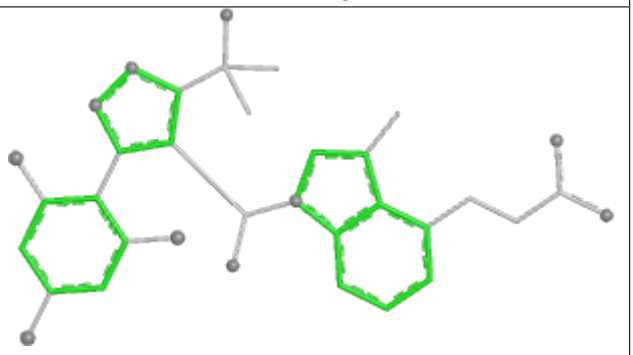
Bond lengths



Bond angles



Torsions



Rings

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.

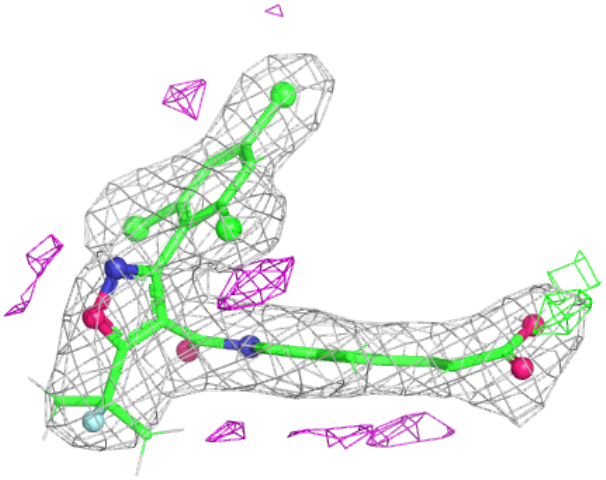
6.4 Ligands

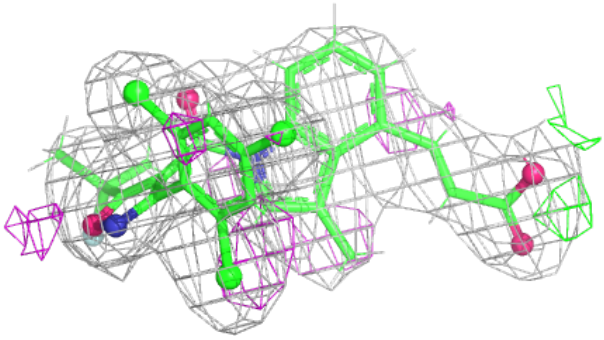
Unable to reproduce the depositors R factor - this section is therefore empty.

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 7SU A 601:

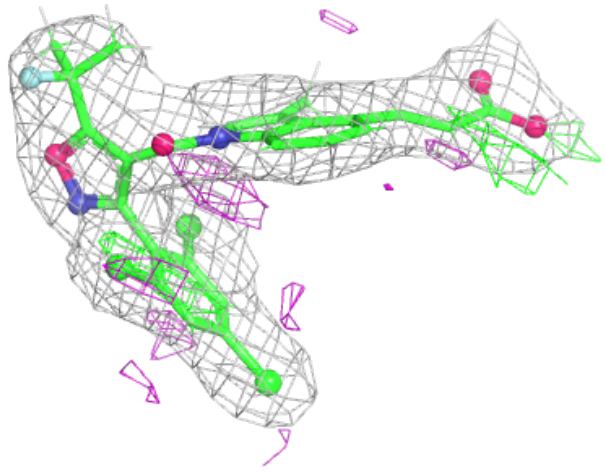
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

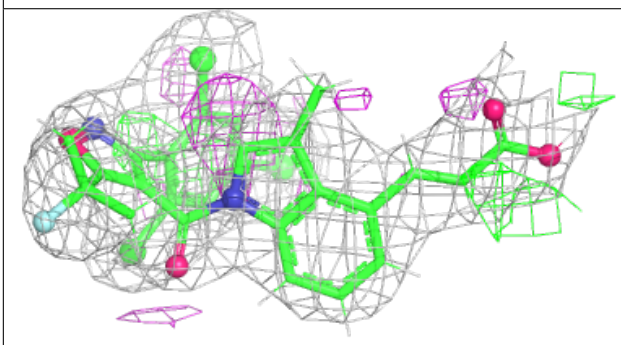


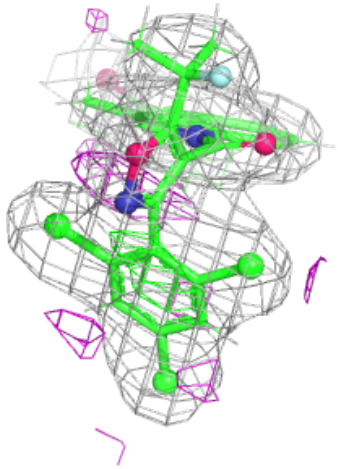


Electron density around 7SU B 601:

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

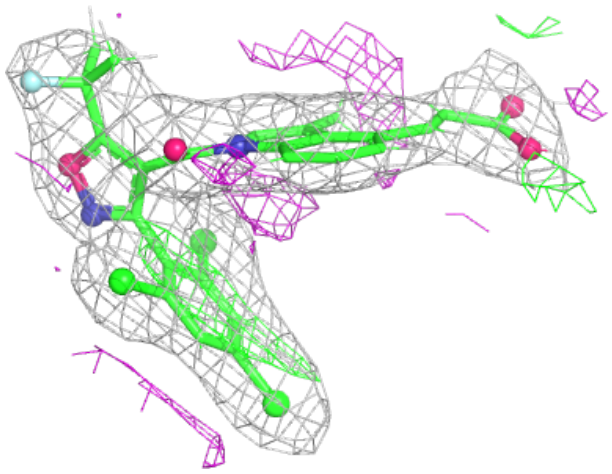


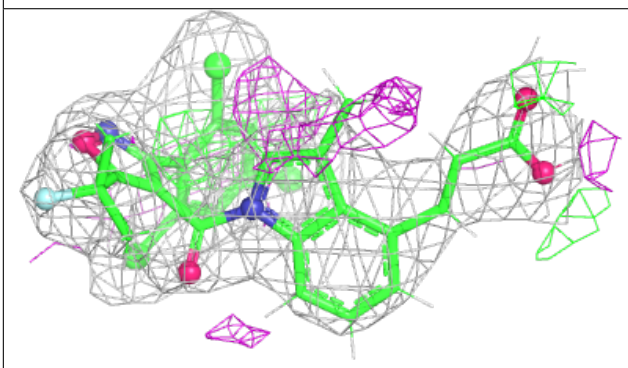




Electron density around 7SU C 601:

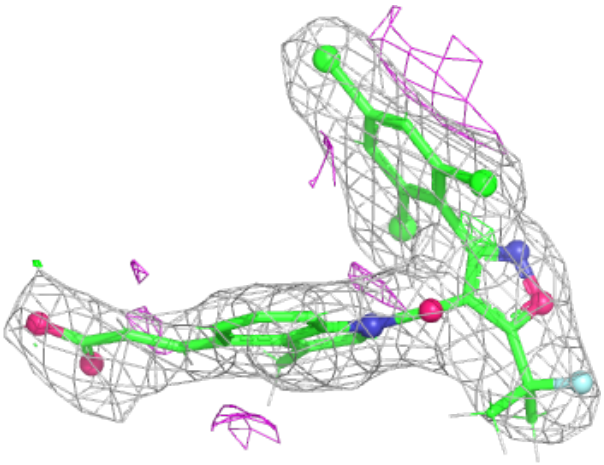
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

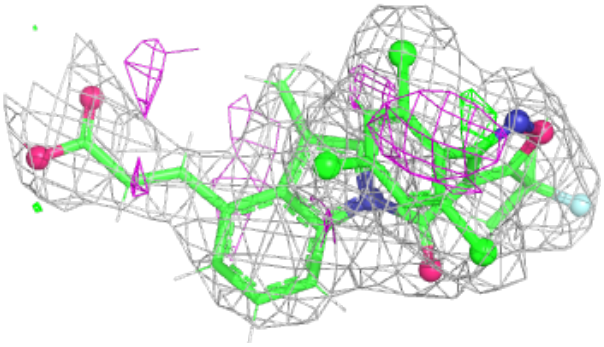


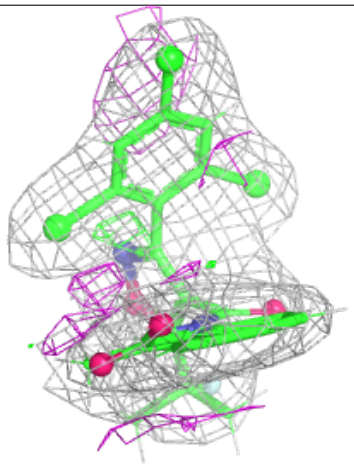


Electron density around 7SU D 601:

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

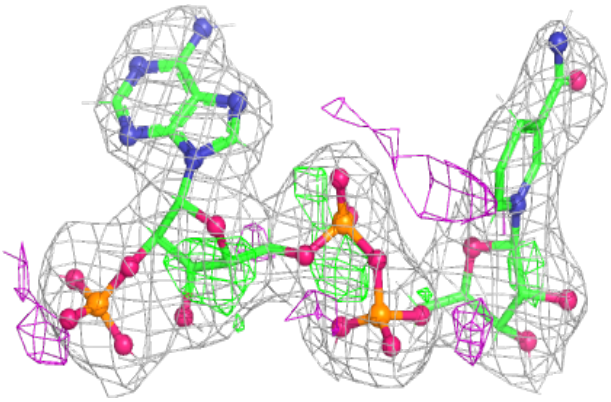


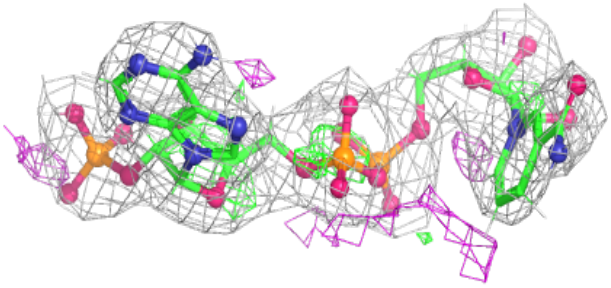


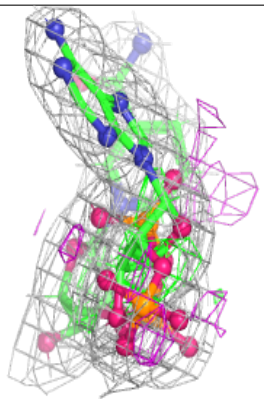


Electron density around NDP A 604:

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

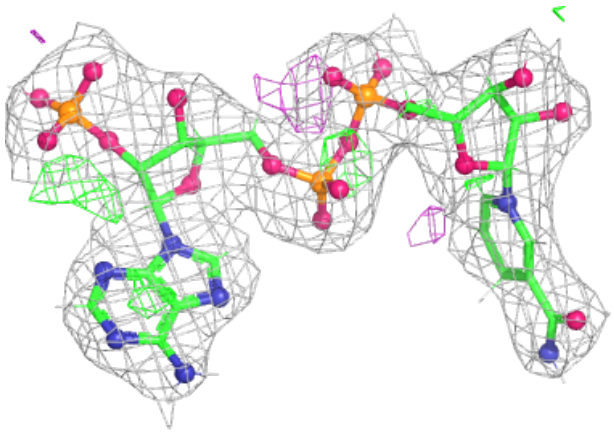


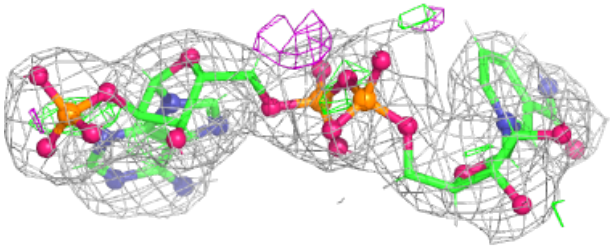


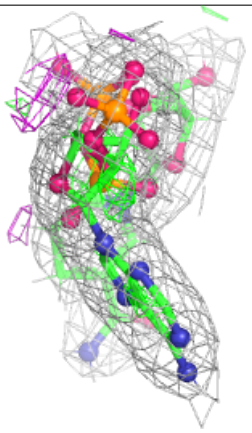


Electron density around NDP B 604:

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

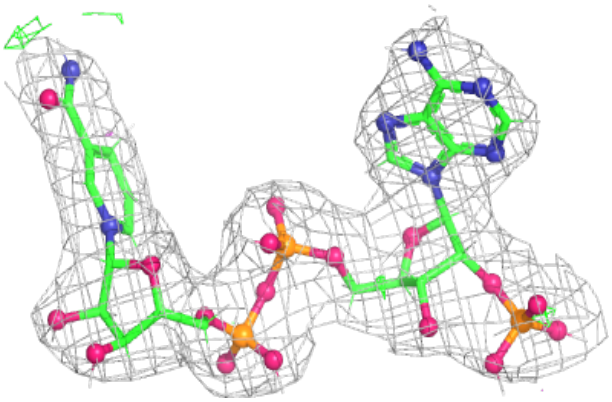


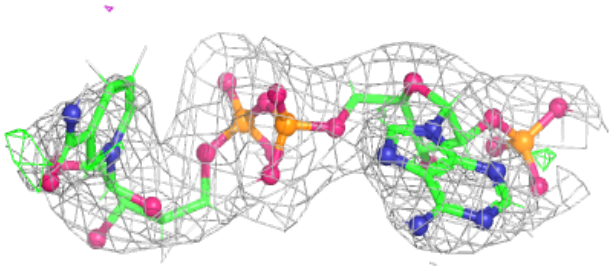


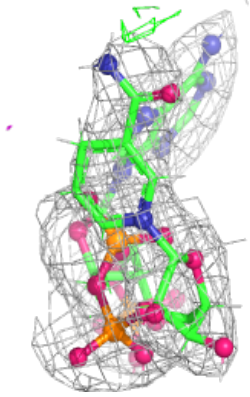


Electron density around NDP C 605:

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

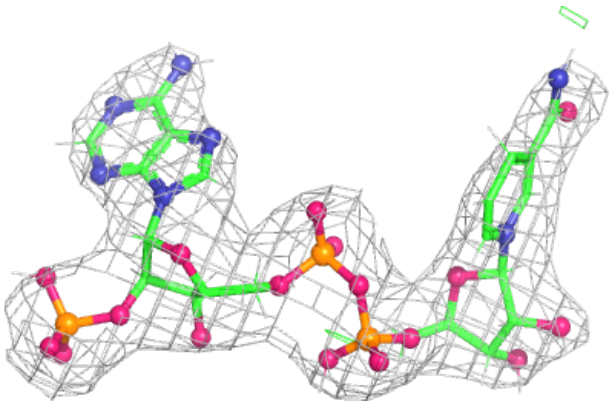


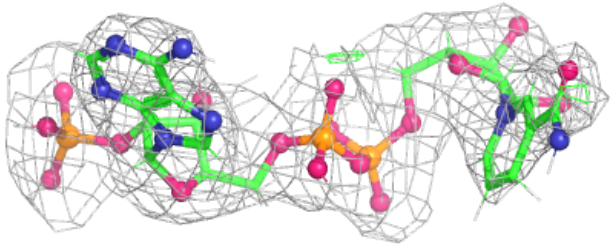


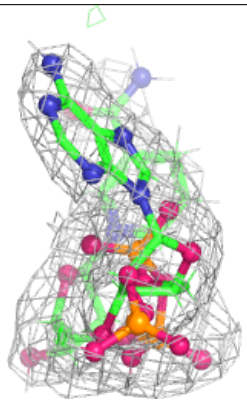


Electron density around NDP D 604:

$2mF_o$-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.