



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:05 PM UTC

PDB ID : 8HB9 / pdb_00008hb9
Title : Crystal Structure of Human IDH1 R132H Mutant in Complex with NADPH and Compound IHMT-IDH1-053
Authors : Guo, G.; Wang, B.; Liu, J.; Liu, Q.
Deposited on : 2022-10-27
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

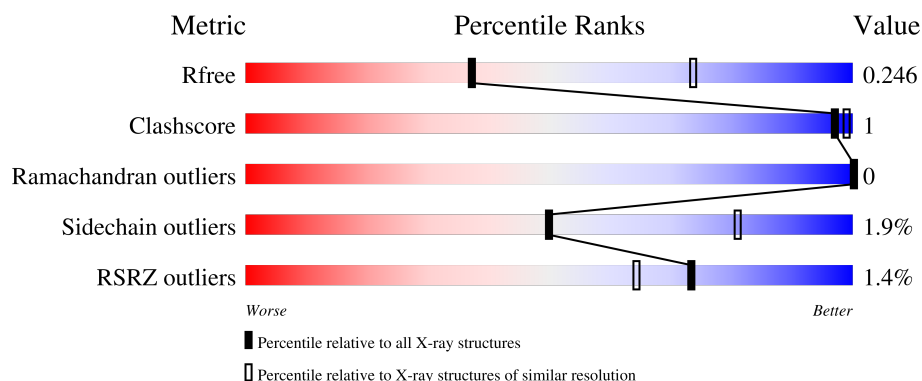
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

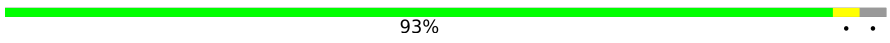
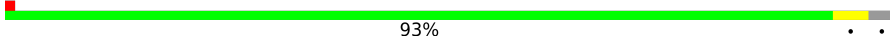
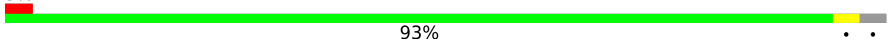
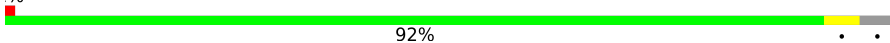
The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	414	 93%
1	BBB	414	 93%
1	CCC	414	 93%
1	DDD	414	 92%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13391 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.

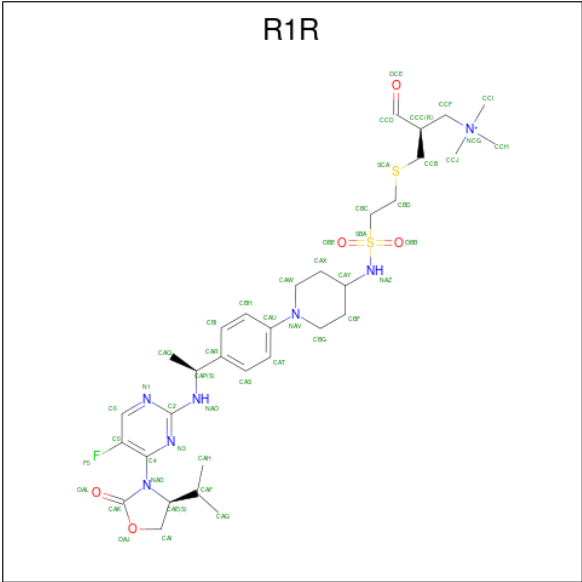
- Molecule 1 is a protein called Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	400	Total	C	N	O	S	0	6	0
			3183	2027	543	595	18			
1	BBB	402	Total	C	N	O	S	0	5	0
			3199	2036	541	604	18			
1	CCC	400	Total	C	N	O	S	0	1	0
			3160	2012	536	594	18			
1	DDD	399	Total	C	N	O	S	0	5	0
			3180	2026	539	595	20			

There are 4 discrepancies between the modelled and reference sequences:

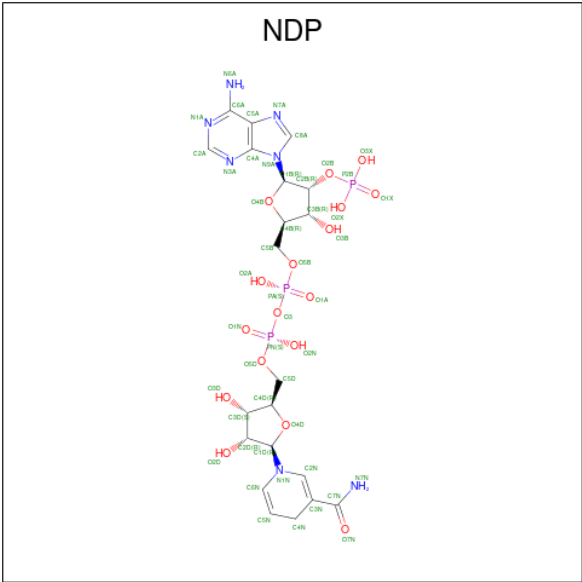
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	132	HIS	ARG	engineered mutation	UNP O75874
BBB	132	HIS	ARG	engineered mutation	UNP O75874
CCC	132	HIS	ARG	engineered mutation	UNP O75874
DDD	132	HIS	ARG	engineered mutation	UNP O75874

- Molecule 2 is [2-[2-[[1-[4-[(1S)-1-[[5-fluoranyl-4-[(4S)-2-oxidanylidene-4-propan-2-yl-1,3-oxazolidin-3-yl]pyrimidin-2-yl]amino]ethyl]phenyl]piperidin-4-yl]sulfamoyl]ethylsulfanylmethyl]-3-oxidanylidene-propyl]-trimethyl-azanium (CCD ID: R1R) (formula: C₃₂H₄₉FN₇O₅S₂) (labeled as "Ligand of Interest" by depositor).



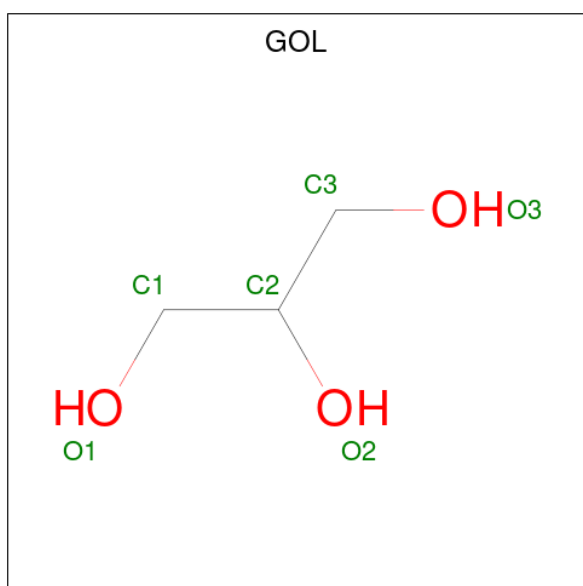
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total 37	C 25	F 1	N 6	O 4	S 1	0	0
2	BBB	1	Total 37	C 25	F 1	N 6	O 4	S 1	0	0
2	CCC	1	Total 37	C 25	F 1	N 6	O 4	S 1	0	0
2	DDD	1	Total 37	C 25	F 1	N 6	O 4	S 1	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



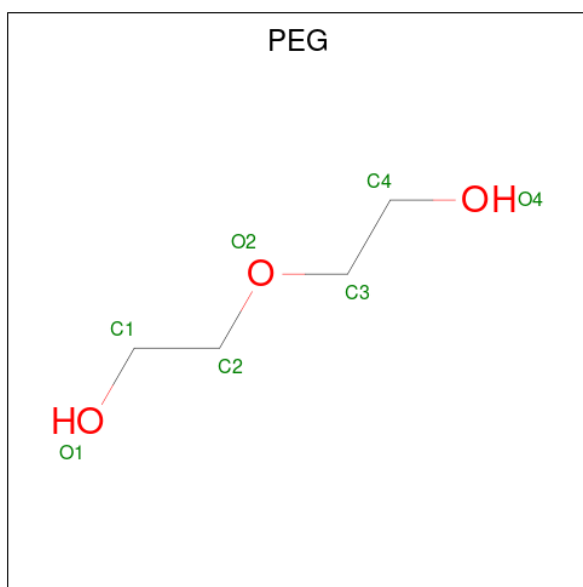
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	BBB	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	CCC	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	DDD	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	BBB	1	Total	C	O	0	0
			6	3	3		
4	CCC	1	Total	C	O	0	0
			6	3	3		
4	DDD	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			7	4	3		
5	AAA	1	Total	C	O	0	0
			7	4	3		
5	AAA	1	Total	C	O	0	0
			7	4	3		
5	AAA	1	Total	C	O	0	0
			7	4	3		
5	DDD	1	Total	C	O	0	0
			7	4	3		

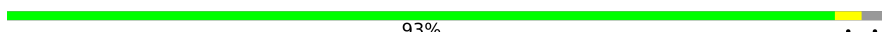
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	87	Total	O	0	0
			87	87		
6	BBB	91	Total	O	0	0
			91	91		
6	CCC	38	Total	O	0	0
			38	38		
6	DDD	36	Total	O	0	0
			36	36		

3 Residue-property plots [i](#)

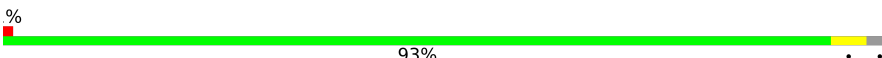
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 AAA:  93%

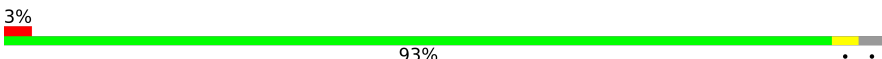


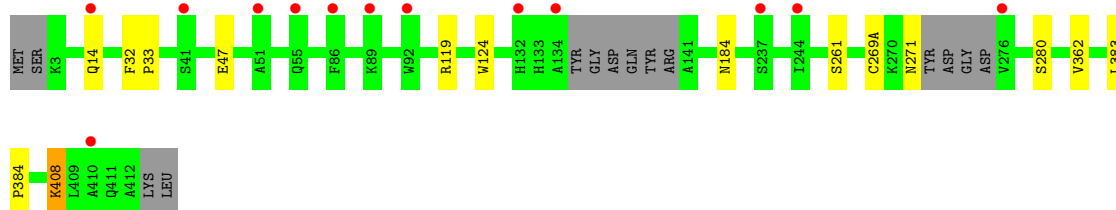
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain BBB:  93%

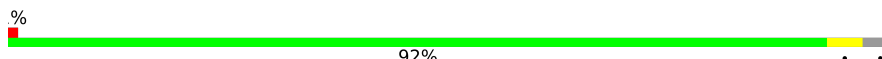


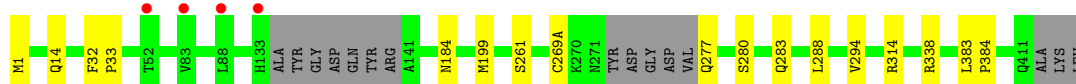
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain CCC:  93%



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain DDD:  92%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.76Å 76.43Å 171.97Å 90.00° 98.27° 90.00°	Depositor
Resolution (Å)	13.08 – 2.80 13.08 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (13.08-2.80) 98.9 (13.08-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.216 , 0.243 0.220 , 0.246	Depositor DCC
R_{free} test set	2624 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13391	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, GOL, PEG, R1R

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	AAA	1.01	0/3266	1.50	0/4402
1	BBB	1.00	0/3278	1.50	0/4418
1	CCC	1.00	0/3227	1.50	0/4349
1	DDD	1.01	0/3259	1.50	0/4388
All	All	1.01	0/13030	1.50	0/17557

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 [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	AAA	3183	0	3165	5	0
1	BBB	3199	0	3178	7	0
1	CCC	3160	0	3137	6	0
1	DDD	3180	0	3181	6	0
2	AAA	37	0	0	0	0
2	BBB	37	0	0	0	0
2	CCC	37	0	0	0	0
2	DDD	37	0	0	0	0
3	AAA	48	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	48	0	26	0	0
3	CCC	48	0	26	0	0
3	DDD	48	0	26	1	0
4	AAA	24	0	32	0	0
4	BBB	6	0	8	0	0
4	CCC	6	0	8	0	0
4	DDD	6	0	8	0	0
5	AAA	28	0	40	0	0
5	DDD	7	0	10	0	0
6	AAA	87	0	0	0	0
6	BBB	91	0	0	1	0
6	CCC	38	0	0	2	0
6	DDD	36	0	0	0	0
All	All	13391	0	12871	24	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 1.

All (24) 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:BBB:276:VAL:N	6:BBB:601:HOH:O	2.36	0.58
1:DDD:14[B]:GLN:HA	1:DDD:14[B]:GLN:OE1	2.06	0.55
1:CCC:14:GLN:NE2	6:CCC:601:HOH:O	2.43	0.51
1:BBB:14[B]:GLN:HA	1:BBB:14[B]:GLN:OE1	2.09	0.51
1:AAA:119:ARG:HD2	1:AAA:124:TRP:O	2.13	0.49
1:CCC:119:ARG:HD2	1:CCC:124:TRP:O	2.14	0.47
1:AAA:362:VAL:HG23	1:AAA:408:LYS:HD2	1.96	0.47
1:CCC:362:VAL:HG23	1:CCC:408:LYS:HD2	1.96	0.47
1:BBB:14[B]:GLN:NE2	1:BBB:24:GLU:OE1	2.50	0.45
1:DDD:383:LEU:N	1:DDD:384:PRO:CD	2.82	0.43
1:DDD:283:GLN:HG2	1:DDD:288:LEU:HD11	2.01	0.43
1:BBB:212:LYS:HE2	1:BBB:215:ILE:HD12	2.01	0.42
1:BBB:383:LEU:N	1:BBB:384:PRO:CD	2.82	0.42
1:AAA:32:PHE:N	1:AAA:33:PRO:CD	2.83	0.42
1:AAA:383:LEU:N	1:AAA:384:PRO:CD	2.83	0.42
1:BBB:119:ARG:HD2	1:BBB:124:TRP:O	2.18	0.42
1:DDD:199:MET:HE1	1:DDD:294:VAL:HG21	2.02	0.42
1:BBB:32:PHE:N	1:BBB:33:PRO:CD	2.82	0.42
1:DDD:314:ARG:NH2	3:DDD:502:NDP:O3X	2.50	0.42
1:CCC:32:PHE:N	1:CCC:33:PRO:CD	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:383:LEU:N	1:CCC:384:PRO:CD	2.82	0.41
1:DDD:32:PHE:N	1:DDD:33:PRO:CD	2.83	0.41
1:CCC:271:ASN:ND2	6:CCC:604:HOH:O	2.53	0.41

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	AAA	400/414 (97%)	394 (98%)	6 (2%)	0	100	100
1	BBB	401/414 (97%)	394 (98%)	7 (2%)	0	100	100
1	CCC	395/414 (95%)	389 (98%)	6 (2%)	0	100	100
1	DDD	398/414 (96%)	391 (98%)	7 (2%)	0	100	100
All	All	1594/1656 (96%)	1568 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	340/350 (97%)	335 (98%)	5 (2%)	57	84
1	BBB	343/350 (98%)	336 (98%)	7 (2%)	48	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CCC	337/350 (96%)	331 (98%)	6 (2%)	51 82
1	DDD	343/350 (98%)	336 (98%)	7 (2%)	48 80
All	All	1363/1400 (97%)	1338 (98%)	25 (2%)	50 82

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	184	ASN
1	AAA	261	SER
1	AAA	269(A)	CYS
1	AAA	280	SER
1	AAA	408	LYS
1	BBB	184	ASN
1	BBB	261	SER
1	BBB	269(A)	CYS
1	BBB	276	VAL
1	BBB	280	SER
1	BBB	348	ASN
1	BBB	387	GLN
1	CCC	47	GLU
1	CCC	184	ASN
1	CCC	261	SER
1	CCC	269(A)	CYS
1	CCC	280	SER
1	CCC	408	LYS
1	DDD	1	MET
1	DDD	184	ASN
1	DDD	261	SER
1	DDD	269(A)	CYS
1	DDD	277	GLN
1	DDD	280	SER
1	DDD	338	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	PEG	AAA	510	-	6,6,6	0.17	0	5,5,5	0.10	0
4	GOL	BBB	503	-	5,5,5	0.11	0	5,5,5	0.32	0
3	NDP	CCC	502	-	51,52,52	0.52	0	71,80,80	0.65	1 (1%)
4	GOL	CCC	503	-	5,5,5	0.11	0	5,5,5	0.31	0
5	PEG	AAA	509	-	6,6,6	0.16	0	5,5,5	0.07	0
2	R1R	CCC	501	1	40,40,50	2.56	7 (17%)	53,58,72	2.32	19 (35%)
4	GOL	AAA	508	-	5,5,5	0.09	0	5,5,5	0.30	0
3	NDP	BBB	502	-	51,52,52	0.52	0	71,80,80	0.69	1 (1%)
2	R1R	AAA	501	1	40,40,50	2.44	8 (20%)	53,58,72	2.15	18 (33%)
4	GOL	AAA	504	-	5,5,5	0.10	0	5,5,5	0.26	0
2	R1R	DDD	501	1	40,40,50	2.63	8 (20%)	53,58,72	2.24	17 (32%)
4	GOL	AAA	503	-	5,5,5	0.09	0	5,5,5	0.34	0
3	NDP	AAA	502	-	51,52,52	0.51	0	71,80,80	0.66	1 (1%)
5	PEG	AAA	505	-	6,6,6	0.16	0	5,5,5	0.06	0
4	GOL	DDD	503	-	5,5,5	0.11	0	5,5,5	0.28	0
4	GOL	AAA	507	-	5,5,5	0.09	0	5,5,5	0.26	0
5	PEG	AAA	506	-	6,6,6	0.15	0	5,5,5	0.08	0
3	NDP	DDD	502	-	51,52,52	0.50	0	71,80,80	0.66	1 (1%)
5	PEG	DDD	504	-	6,6,6	0.18	0	5,5,5	0.11	0
2	R1R	BBB	501	1	40,40,50	2.74	10 (25%)	53,58,72	2.65	19 (35%)

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	PEG	AAA	510	-	-	2/4/4/4	-
4	GOL	BBB	503	-	-	0/4/4/4	-
3	NDP	CCC	502	-	-	10/34/77/77	0/5/5/5
4	GOL	CCC	503	-	-	4/4/4/4	-
5	PEG	AAA	509	-	-	1/4/4/4	-
2	R1R	CCC	501	1	-	3/26/51/63	0/4/4/4
4	GOL	AAA	508	-	-	4/4/4/4	-
3	NDP	BBB	502	-	-	5/34/77/77	0/5/5/5
2	R1R	AAA	501	1	-	3/26/51/63	0/4/4/4
4	GOL	AAA	504	-	-	2/4/4/4	-
2	R1R	DDD	501	1	-	4/26/51/63	0/4/4/4
4	GOL	AAA	503	-	-	0/4/4/4	-
3	NDP	AAA	502	-	-	6/34/77/77	0/5/5/5
5	PEG	AAA	505	-	-	2/4/4/4	-
4	GOL	DDD	503	-	-	2/4/4/4	-
4	GOL	AAA	507	-	-	0/4/4/4	-
5	PEG	AAA	506	-	-	3/4/4/4	-
3	NDP	DDD	502	-	-	5/34/77/77	0/5/5/5
5	PEG	DDD	504	-	-	1/4/4/4	-
2	R1R	BBB	501	1	-	2/26/51/63	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	501	R1R	SBA-NAZ	8.90	1.75	1.61
2	DDD	501	R1R	SBA-NAZ	8.06	1.74	1.61
2	AAA	501	R1R	OBE-SBA	7.99	1.54	1.43
2	DDD	501	R1R	OBE-SBA	7.77	1.54	1.43
2	CCC	501	R1R	SBA-NAZ	7.75	1.73	1.61
2	CCC	501	R1R	OBE-SBA	7.59	1.53	1.43
2	BBB	501	R1R	CBC-SBA	7.41	1.84	1.76
2	CCC	501	R1R	OBB-SBA	7.14	1.53	1.43
2	DDD	501	R1R	OBB-SBA	7.02	1.53	1.43
2	AAA	501	R1R	SBA-NAZ	6.97	1.72	1.61
2	BBB	501	R1R	OBB-SBA	6.74	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	501	R1R	OBB-SBA	6.37	1.52	1.43
2	CCC	501	R1R	CBC-SBA	5.93	1.82	1.76
2	DDD	501	R1R	CBC-SBA	5.88	1.82	1.76
2	BBB	501	R1R	OBE-SBA	5.79	1.51	1.43
2	DDD	501	R1R	CAR-CAP	-4.25	1.41	1.52
2	CCC	501	R1R	CAR-CAP	-4.23	1.41	1.52
2	AAA	501	R1R	CAR-CAP	-4.20	1.41	1.52
2	BBB	501	R1R	OAJ-CAI	-4.17	1.37	1.45
2	BBB	501	R1R	CAR-CAP	-4.07	1.41	1.52
2	AAA	501	R1R	CBC-SBA	3.67	1.80	1.76
2	AAA	501	R1R	OAJ-CAI	-3.42	1.39	1.45
2	AAA	501	R1R	C6-N1	2.92	1.40	1.34
2	CCC	501	R1R	C6-N1	2.72	1.40	1.34
2	AAA	501	R1R	F5-C5	-2.69	1.28	1.35
2	BBB	501	R1R	C6-N1	2.56	1.39	1.34
2	DDD	501	R1R	C6-N1	2.36	1.39	1.34
2	CCC	501	R1R	F5-C5	-2.28	1.29	1.35
2	BBB	501	R1R	F5-C5	-2.28	1.29	1.35
2	DDD	501	R1R	F5-C5	-2.26	1.29	1.35
2	BBB	501	R1R	CBG-NAV	2.24	1.50	1.46
2	BBB	501	R1R	C4-NAD	-2.09	1.34	1.39
2	DDD	501	R1R	C4-NAD	-2.07	1.34	1.39

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	501	R1R	OBE-SBA-OBB	-8.52	107.43	119.34
2	CCC	501	R1R	OBE-SBA-OBB	-7.43	108.95	119.34
2	BBB	501	R1R	CBG-CBF-CAY	-6.97	99.66	110.67
2	DDD	501	R1R	OBE-SBA-OBB	-6.40	110.39	119.34
2	AAA	501	R1R	N1-C2-N3	-5.99	120.63	126.42
2	AAA	501	R1R	OBE-SBA-OBB	-5.96	111.00	119.34
2	CCC	501	R1R	N1-C2-N3	-5.74	120.88	126.42
2	BBB	501	R1R	OBB-SBA-NAZ	5.69	115.21	107.11
2	BBB	501	R1R	N1-C2-N3	-5.47	121.13	126.42
2	CCC	501	R1R	OAJ-CAI-CAE	-5.47	99.45	105.63
2	DDD	501	R1R	OAJ-CAI-CAE	-5.32	99.62	105.63
2	DDD	501	R1R	N1-C2-N3	-5.19	121.40	126.42
2	BBB	501	R1R	OBE-SBA-NAZ	-5.17	99.76	107.11
2	AAA	501	R1R	OAJ-CAI-CAE	-4.43	100.63	105.63
2	DDD	501	R1R	C5-C6-N1	-4.35	119.00	122.68
2	CCC	501	R1R	C5-C6-N1	-4.12	119.21	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	501	R1R	OAJ-CAI-CAE	-3.94	101.18	105.63
2	BBB	501	R1R	C5-C6-N1	-3.93	119.36	122.68
2	AAA	501	R1R	CAX-CAW-NAV	-3.78	102.35	110.92
2	DDD	501	R1R	CAX-CAW-NAV	-3.77	102.38	110.92
2	AAA	501	R1R	C5-C6-N1	-3.73	119.53	122.68
2	DDD	501	R1R	OAL-CAK-NAD	-3.70	124.00	128.52
2	CCC	501	R1R	OAL-CAK-NAD	-3.66	124.05	128.52
2	BBB	501	R1R	OAL-CAK-NAD	-3.64	124.07	128.52
2	AAA	501	R1R	C4-NAD-CAK	3.64	130.57	124.91
2	CCC	501	R1R	CAX-CAW-NAV	-3.62	102.72	110.92
2	CCC	501	R1R	CBD-CBC-SBA	-3.57	107.08	112.55
2	CCC	501	R1R	C4-NAD-CAK	3.57	130.46	124.91
2	DDD	501	R1R	CAI-CAE-NAD	3.53	103.15	100.11
2	CCC	501	R1R	CAX-CAY-CBF	3.48	116.81	110.80
2	BBB	501	R1R	CBD-CBC-SBA	-3.47	107.23	112.55
2	DDD	501	R1R	CAX-CAY-CBF	3.42	116.72	110.80
2	AAA	501	R1R	OAL-CAK-NAD	-3.42	124.35	128.52
2	BBB	501	R1R	CAI-CAE-NAD	3.38	103.03	100.11
2	BBB	501	R1R	C4-NAD-CAK	3.38	130.16	124.91
2	DDD	501	R1R	CBD-CBC-SBA	-3.37	107.38	112.55
2	DDD	501	R1R	C4-NAD-CAK	3.34	130.11	124.91
2	AAA	501	R1R	CAX-CAY-CBF	3.23	116.38	110.80
3	DDD	502	NDP	P2B-O2B-C2B	-3.21	114.85	123.43
2	AAA	501	R1R	OBE-SBA-NAZ	3.14	111.59	107.11
2	BBB	501	R1R	CBG-NAV-CAU	3.11	126.58	118.11
2	BBB	501	R1R	CBF-CAY-NAZ	3.07	115.98	110.47
2	BBB	501	R1R	CAE-NAD-CAK	-3.00	105.27	111.42
2	DDD	501	R1R	CAE-NAD-CAK	-2.99	105.28	111.42
2	DDD	501	R1R	CBG-NAV-CAW	2.94	118.19	111.57
3	AAA	502	NDP	P2B-O2B-C2B	-2.91	115.67	123.43
3	BBB	502	NDP	P2B-O2B-C2B	-2.89	115.71	123.43
2	CCC	501	R1R	CAE-NAD-CAK	-2.83	105.61	111.42
2	AAA	501	R1R	CAE-NAD-CAK	-2.83	105.61	111.42
2	BBB	501	R1R	C2-N3-C4	2.81	123.02	113.99
2	AAA	501	R1R	F5-C5-C4	2.81	122.54	119.87
2	DDD	501	R1R	OBE-SBA-NAZ	2.78	111.07	107.11
2	CCC	501	R1R	OBE-SBA-NAZ	2.77	111.05	107.11
2	BBB	501	R1R	CAI-CAE-CAF	-2.76	110.97	115.02
2	DDD	501	R1R	C2-N3-C4	2.76	122.85	113.99
2	CCC	501	R1R	F5-C5-C4	2.76	122.49	119.87
2	CCC	501	R1R	CBG-NAV-CAW	2.75	117.75	111.57
2	AAA	501	R1R	C2-N3-C4	2.74	122.77	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	501	R1R	C2-N3-C4	2.70	122.66	113.99
2	CCC	501	R1R	CAI-OAJ-CAK	-2.67	107.02	109.94
2	CCC	501	R1R	C6-N1-C2	2.67	119.47	115.81
2	AAA	501	R1R	C6-N1-C2	2.65	119.45	115.81
3	CCC	502	NDP	P2B-O2B-C2B	-2.61	116.47	123.43
2	AAA	501	R1R	CAI-CAE-NAD	2.54	102.30	100.11
2	DDD	501	R1R	C6-N1-C2	2.45	119.18	115.81
2	AAA	501	R1R	CBG-NAV-CAW	2.45	117.07	111.57
2	BBB	501	R1R	C6-N1-C2	2.44	119.16	115.81
2	CCC	501	R1R	CAI-CAE-NAD	2.41	102.19	100.11
2	AAA	501	R1R	NAO-C2-N3	2.13	120.44	117.09
2	DDD	501	R1R	CAI-OAJ-CAK	-2.10	107.65	109.94
2	CCC	501	R1R	N3-C4-NAD	2.09	118.27	116.10
2	DDD	501	R1R	C4-NAD-CAE	2.08	124.61	122.12
2	CCC	501	R1R	NAO-C2-N3	2.08	120.35	117.09
2	AAA	501	R1R	OBE-SBA-CBC	-2.06	105.67	108.70
2	BBB	501	R1R	N3-C4-NAD	2.05	118.23	116.10
2	AAA	501	R1R	N3-C4-NAD	2.04	118.21	116.10
2	BBB	501	R1R	C4-NAD-CAE	2.03	124.55	122.12

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	501	R1R	CAY-NAZ-SBA-OBE
2	CCC	501	R1R	CAY-NAZ-SBA-OBE
2	DDD	501	R1R	CAY-NAZ-SBA-OBE
3	AAA	502	NDP	C5D-O5D-PN-O3
3	AAA	502	NDP	C5D-O5D-PN-O1N
3	AAA	502	NDP	C5D-O5D-PN-O2N
3	BBB	502	NDP	C5D-O5D-PN-O3
3	BBB	502	NDP	C5D-O5D-PN-O1N
3	BBB	502	NDP	C5D-O5D-PN-O2N
3	CCC	502	NDP	C5D-O5D-PN-O3
3	CCC	502	NDP	C5D-O5D-PN-O1N
3	CCC	502	NDP	C5D-O5D-PN-O2N
3	CCC	502	NDP	C2N-C3N-C7N-O7N
3	DDD	502	NDP	O4B-C4B-C5B-O5B
4	CCC	503	GOL	C1-C2-C3-O3
4	CCC	503	GOL	O2-C2-C3-O3
4	DDD	503	GOL	C1-C2-C3-O3
3	DDD	502	NDP	C3B-C4B-C5B-O5B

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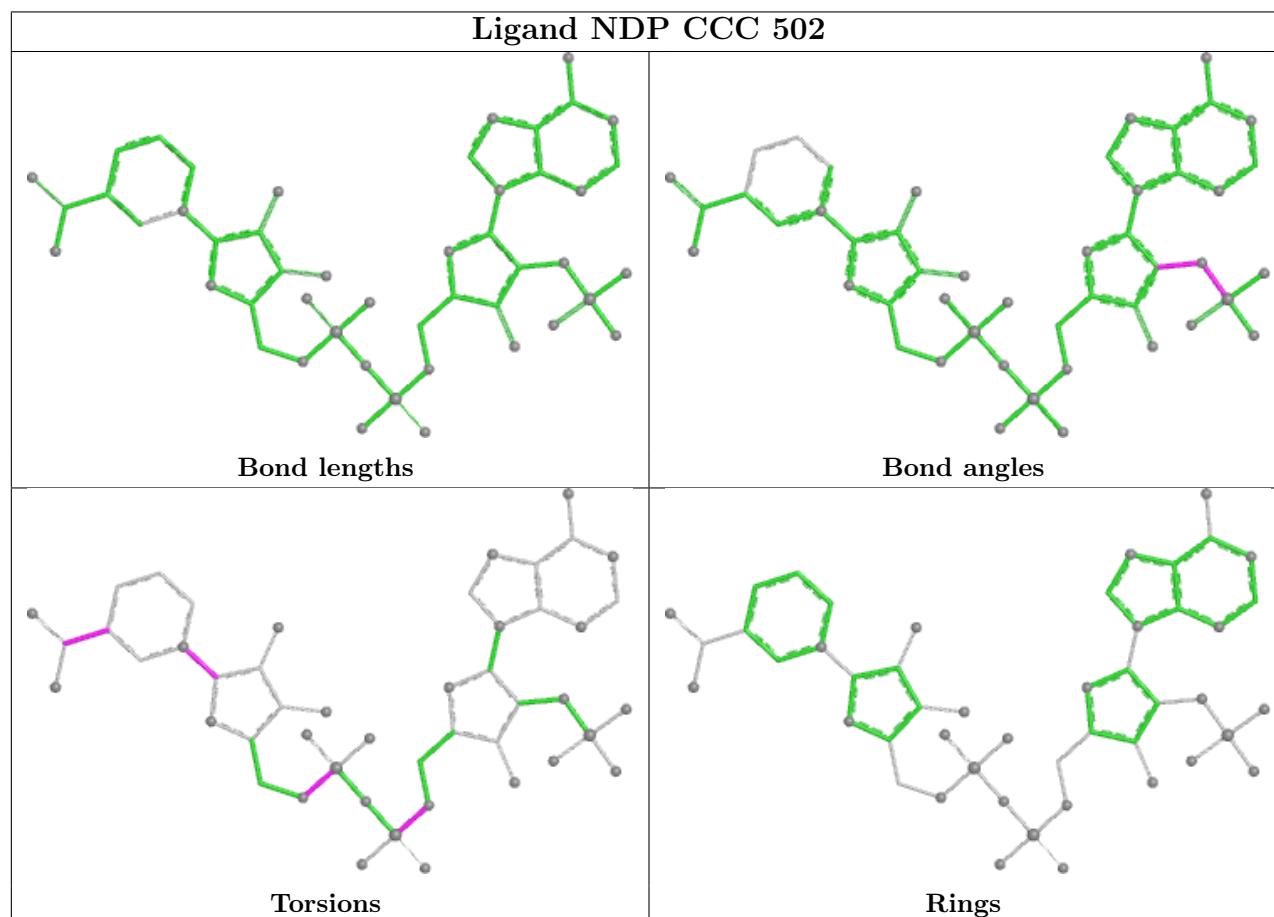
Mol	Chain	Res	Type	Atoms
5	AAA	505	PEG	O1-C1-C2-O2
5	AAA	510	PEG	O2-C3-C4-O4
5	DDD	504	PEG	O2-C3-C4-O4
4	AAA	504	GOL	C1-C2-C3-O3
4	AAA	508	GOL	O1-C1-C2-C3
4	AAA	508	GOL	C1-C2-C3-O3
4	CCC	503	GOL	O1-C1-C2-C3
5	AAA	506	PEG	O2-C3-C4-O4
4	AAA	504	GOL	O2-C2-C3-O3
5	AAA	509	PEG	O1-C1-C2-O2
2	AAA	501	R1R	CAY-NAZ-SBA-OBB
2	CCC	501	R1R	CAY-NAZ-SBA-OBB
2	DDD	501	R1R	CAY-NAZ-SBA-OBB
3	CCC	502	NDP	C2D-C1D-N1N-C2N
5	AAA	510	PEG	O1-C1-C2-O2
3	CCC	502	NDP	C2D-C1D-N1N-C6N
4	AAA	508	GOL	O2-C2-C3-O3
4	CCC	503	GOL	O1-C1-C2-O2
3	AAA	502	NDP	O4D-C1D-N1N-C2N
3	CCC	502	NDP	C2N-C3N-C7N-N7N
2	BBB	501	R1R	CAX-CAY-NAZ-SBA
3	DDD	502	NDP	PN-O3-PA-O5B
4	DDD	503	GOL	O2-C2-C3-O3
2	AAA	501	R1R	CAY-NAZ-SBA-CBC
2	CCC	501	R1R	CAY-NAZ-SBA-CBC
2	DDD	501	R1R	CAY-NAZ-SBA-CBC
5	AAA	506	PEG	O1-C1-C2-O2
3	BBB	502	NDP	O4D-C1D-N1N-C2N
3	CCC	502	NDP	O4D-C1D-N1N-C2N
3	DDD	502	NDP	O4D-C1D-N1N-C2N
3	AAA	502	NDP	C5B-O5B-PA-O1A
3	CCC	502	NDP	C5B-O5B-PA-O1A
3	CCC	502	NDP	O4D-C1D-N1N-C6N
5	AAA	505	PEG	O2-C3-C4-O4
5	AAA	506	PEG	C1-C2-O2-C3
3	AAA	502	NDP	C2B-O2B-P2B-O2X
3	DDD	502	NDP	C2B-O2B-P2B-O3X
3	BBB	502	NDP	C2N-C3N-C7N-N7N
2	BBB	501	R1R	CBF-CAY-NAZ-SBA
4	AAA	508	GOL	O1-C1-C2-O2
2	DDD	501	R1R	NAO-CAP-CAR-CAS

There are no ring outliers.

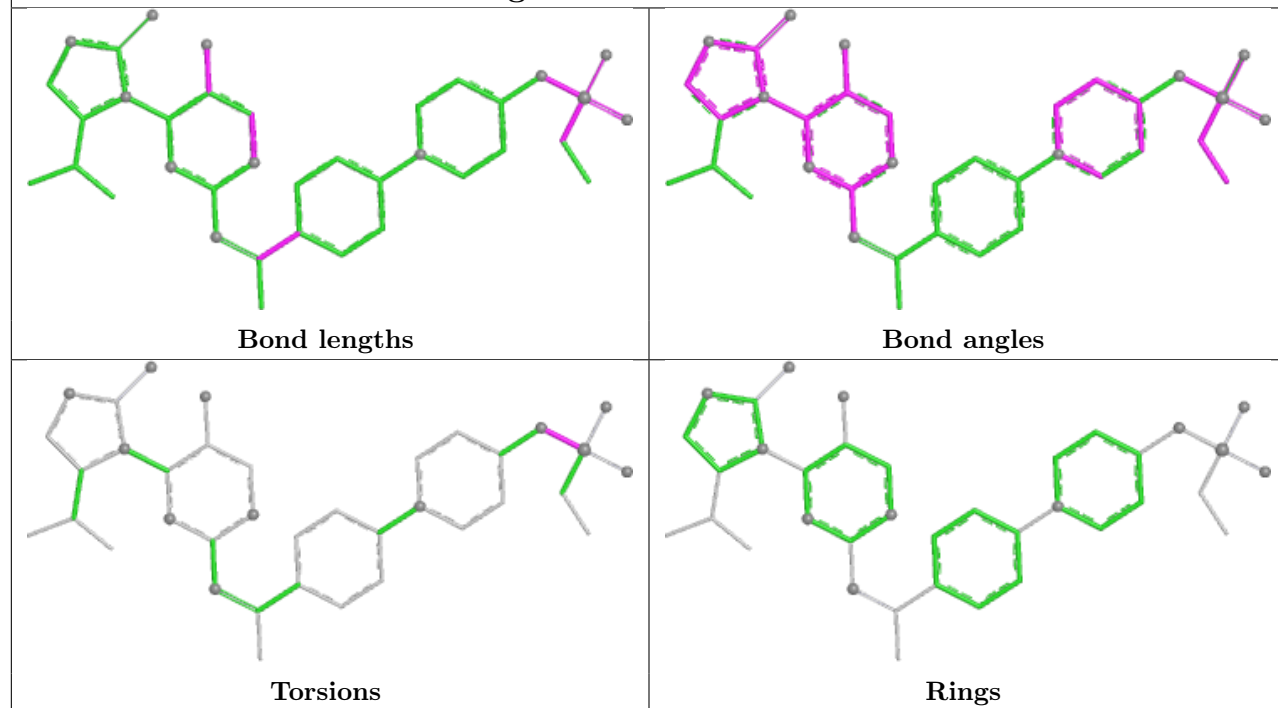
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DDD	502	NDP	1	0

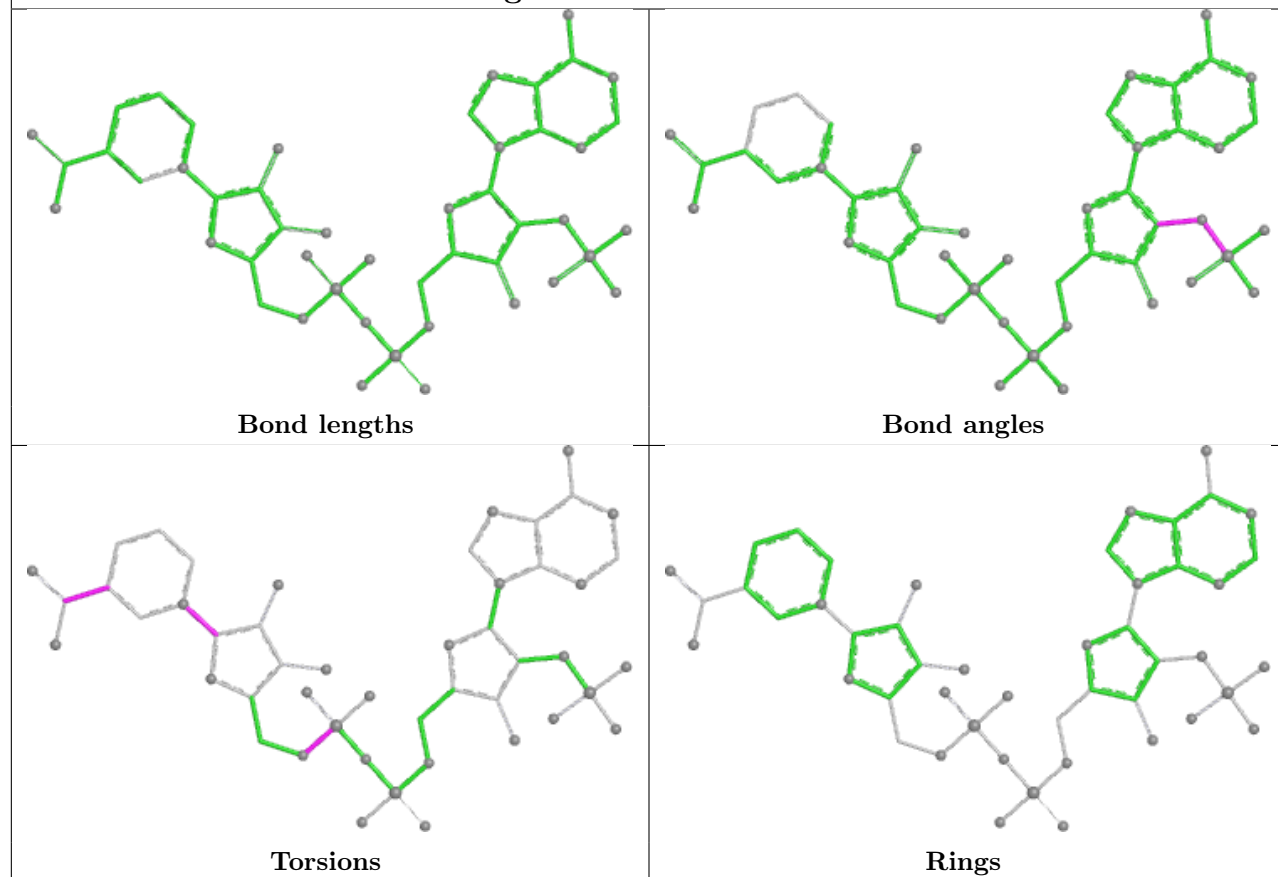
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



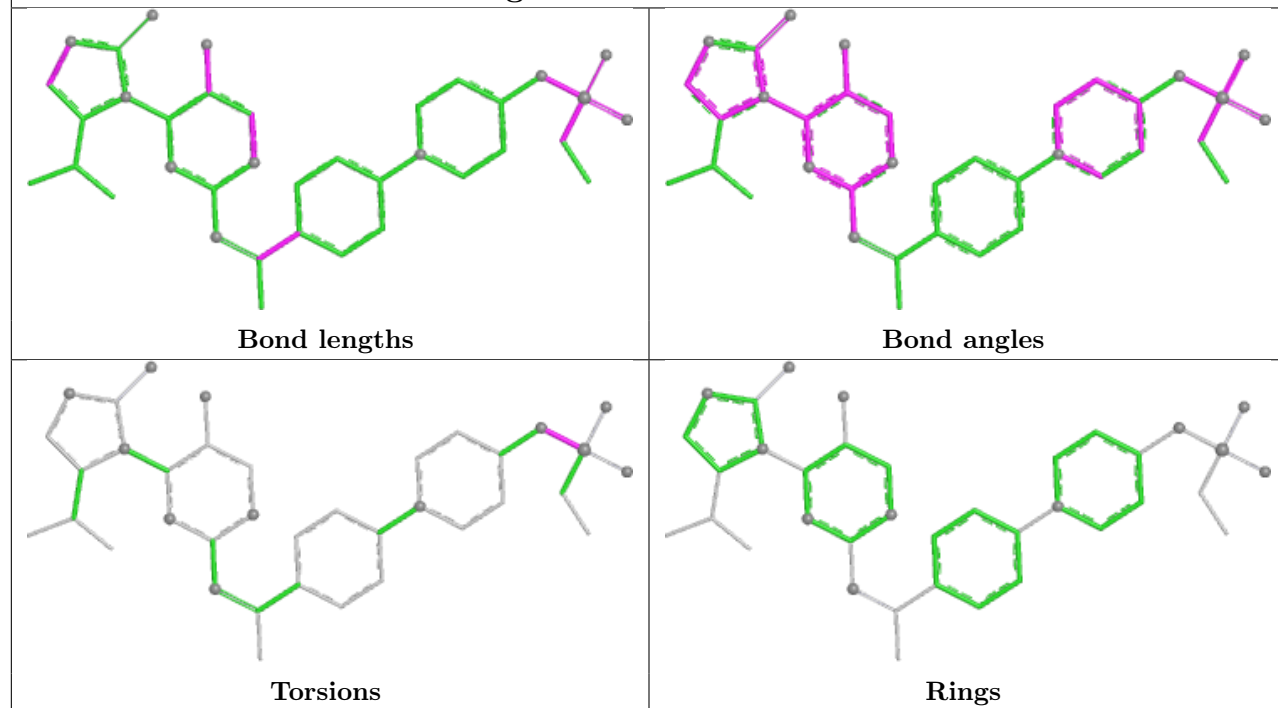
Ligand R1R CCC 501



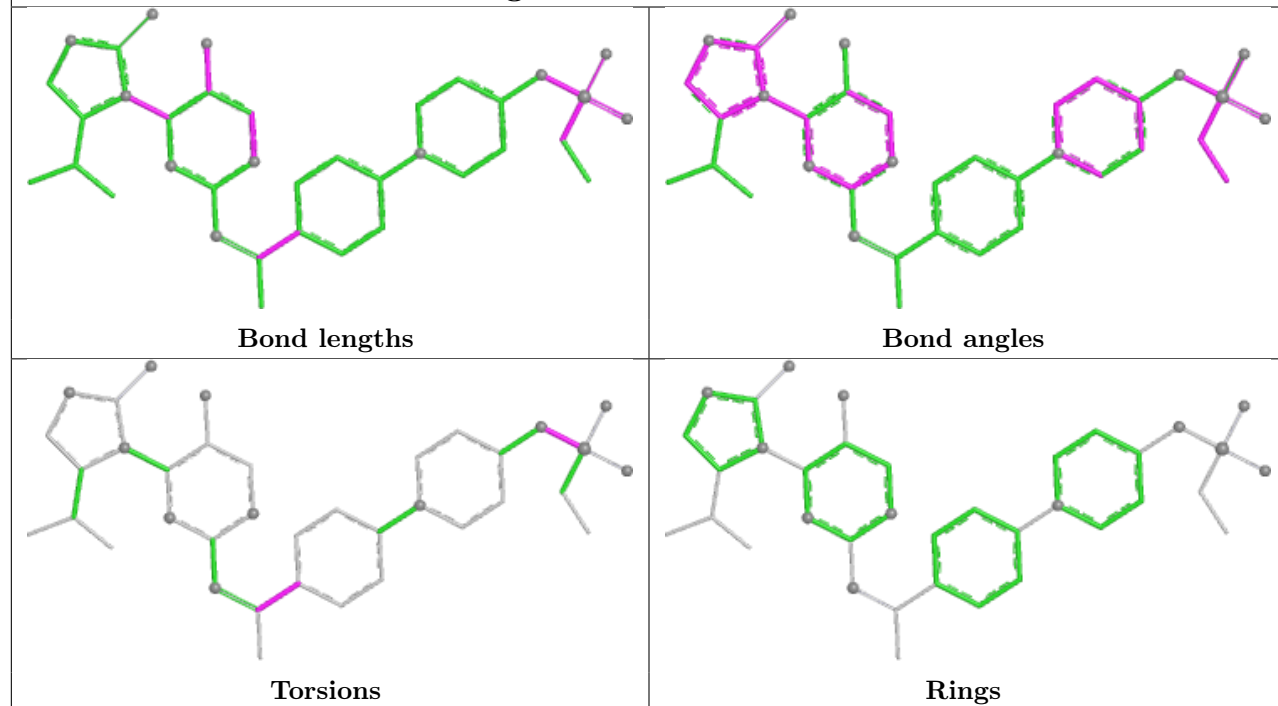
Ligand NDP BBB 502



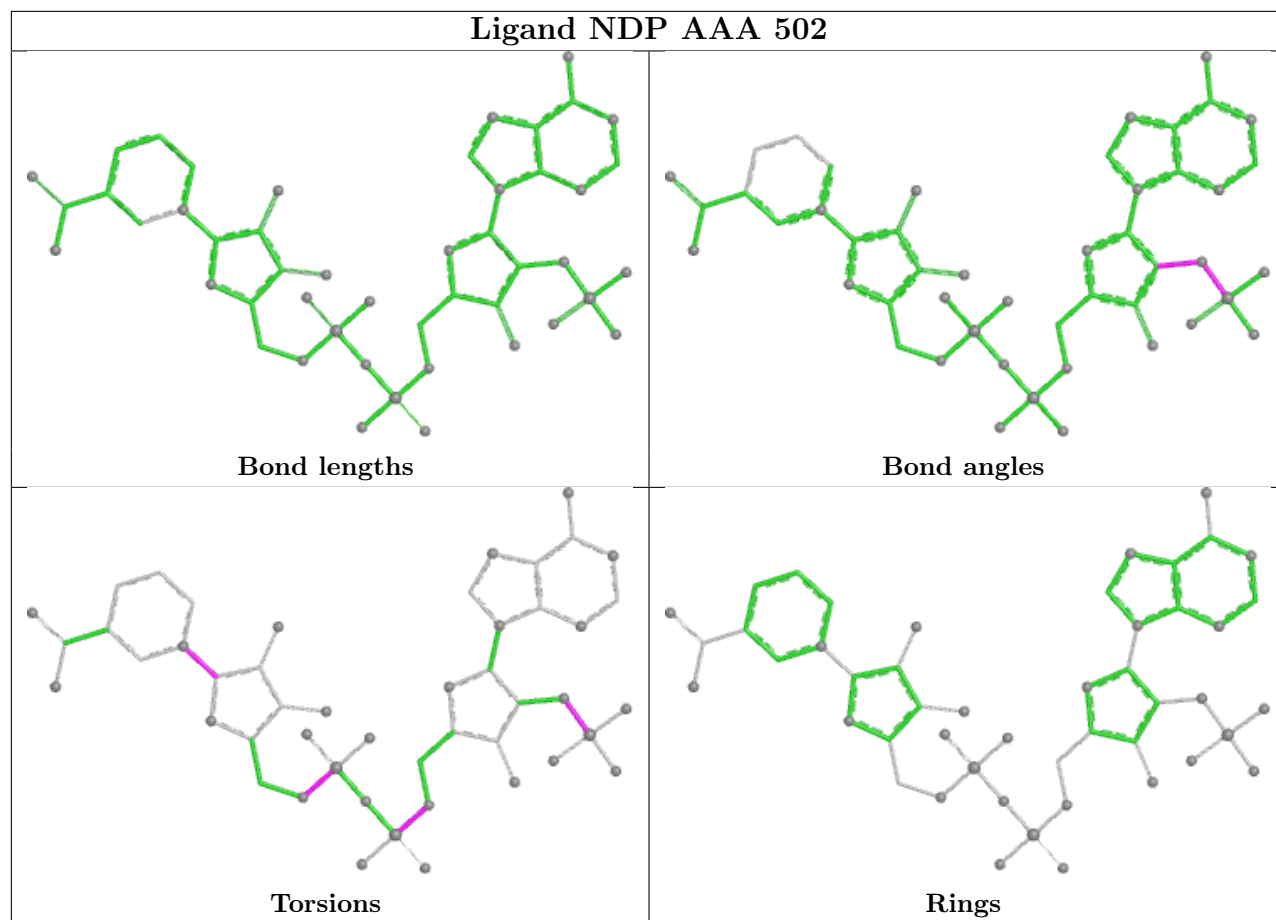
Ligand R1R AAA 501



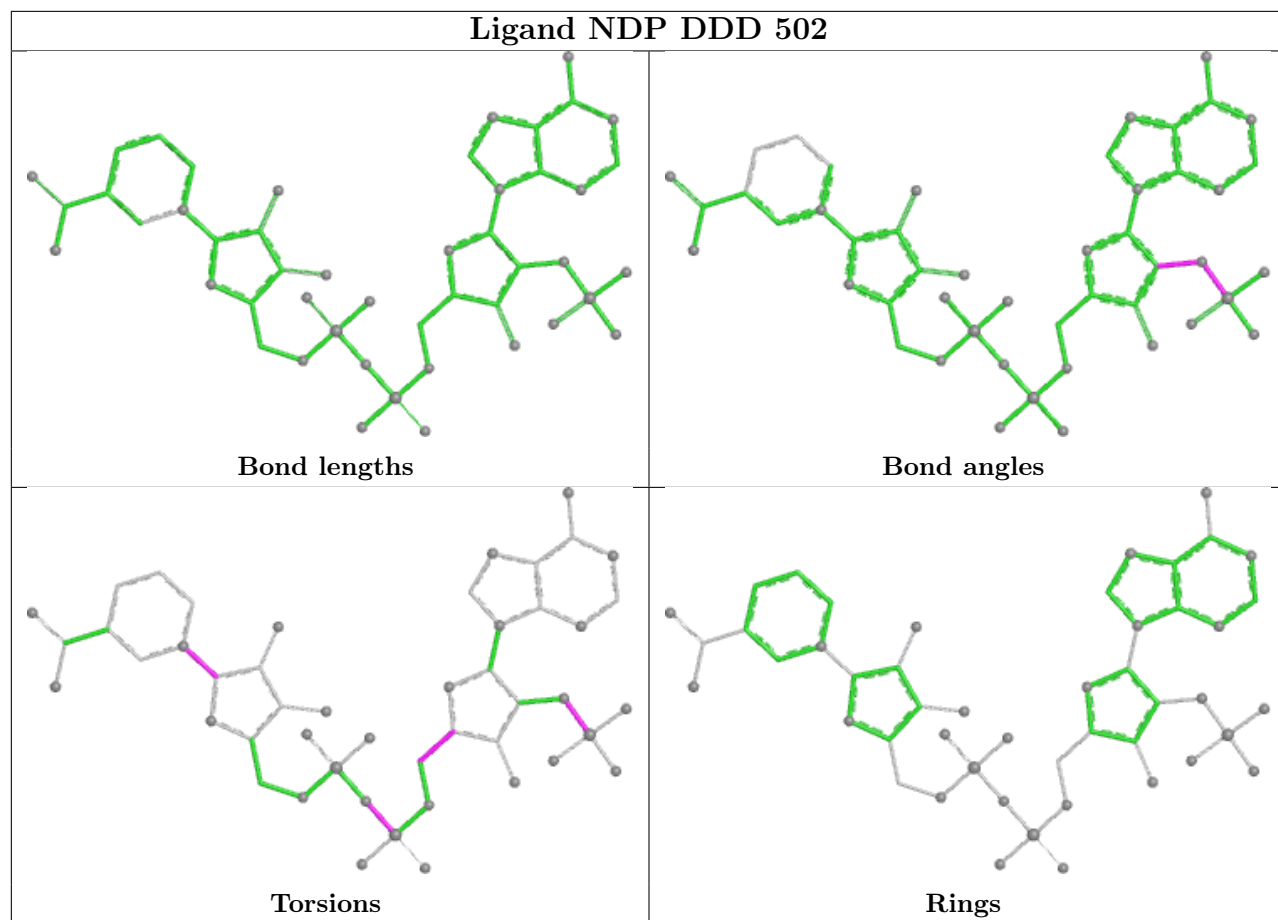
Ligand R1R DDD 501



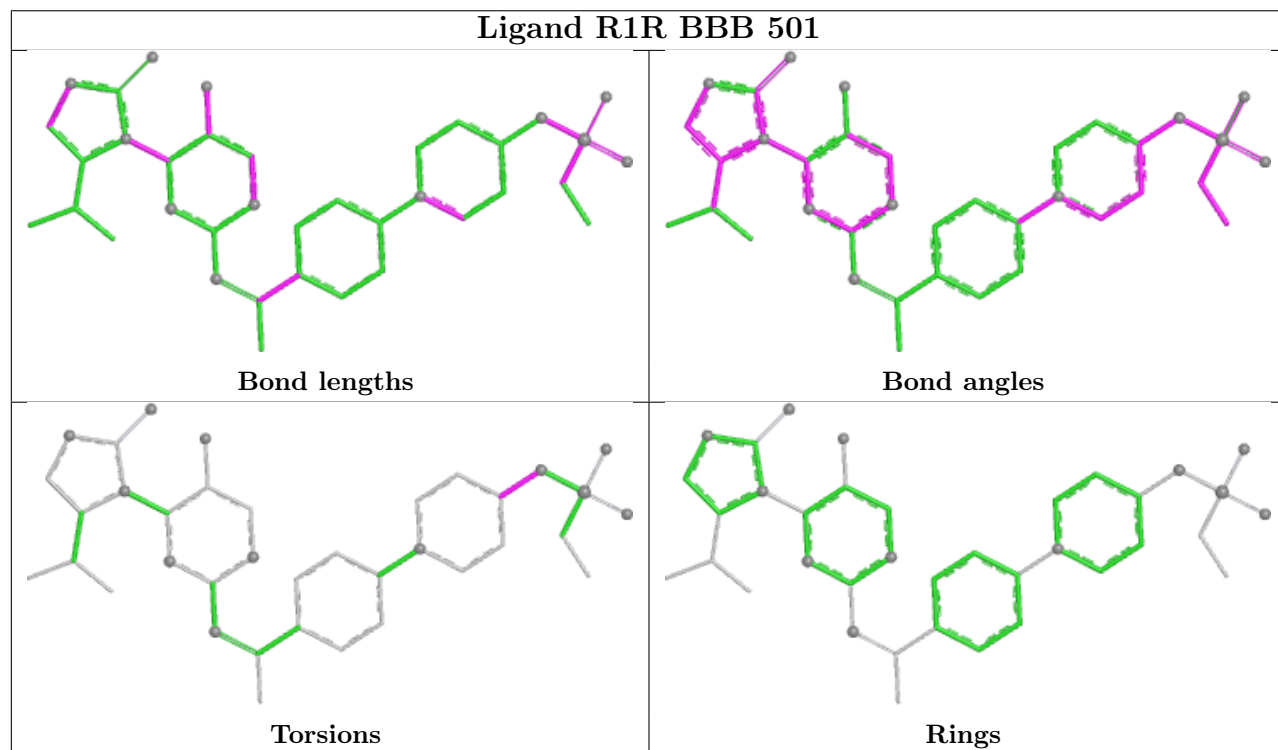
Ligand NDP AAA 502



Ligand NDP DDD 502



Ligand R1R BBB 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

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	AAA	400/414 (96%)	-0.26	1 (0%) 90 86	19, 33, 55, 69	6 (1%)
1	BBB	402/414 (97%)	-0.29	4 (0%) 79 72	15, 32, 52, 75	5 (1%)
1	CCC	400/414 (96%)	0.30	13 (3%) 49 39	30, 52, 92, 109	1 (0%)
1	DDD	399/414 (96%)	0.13	4 (1%) 79 72	20, 49, 88, 102	5 (1%)
All	All	1601/1656 (96%)	-0.03	22 (1%) 73 64	15, 41, 78, 109	17 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	276	VAL	3.4
1	DDD	52	THR	3.3
1	CCC	134	ALA	3.2
1	DDD	88	LEU	3.2
1	BBB	134	ALA	3.0
1	CCC	237	SER	2.8
1	DDD	83	VAL	2.7
1	BBB	271	ASN	2.7
1	CCC	14	GLN	2.6
1	CCC	55	GLN	2.6
1	CCC	41	SER	2.6
1	BBB	132	HIS	2.5
1	DDD	133	HIS	2.5
1	CCC	132	HIS	2.5
1	CCC	92	TRP	2.3
1	AAA	132[A]	HIS	2.3
1	CCC	86	PHE	2.2
1	CCC	410	ALA	2.2
1	CCC	244	ILE	2.1
1	CCC	89	LYS	2.0
1	CCC	51	ALA	2.0
1	CCC	276	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

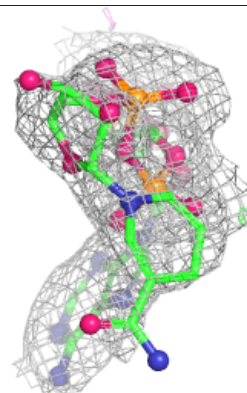
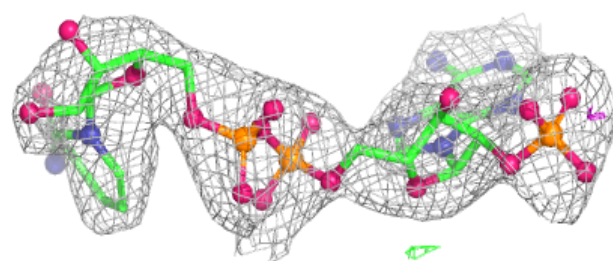
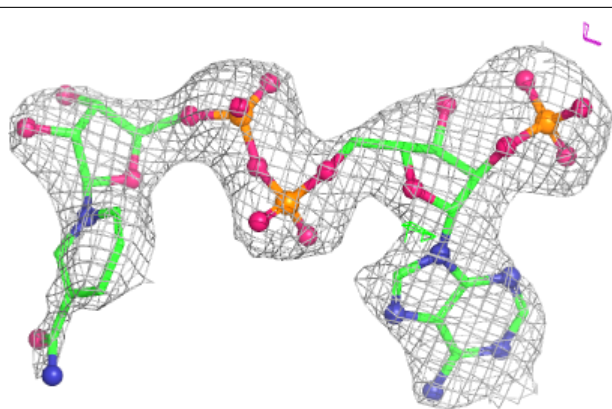
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	AAA	509	7/7	0.58	0.15	71,73,74,75	0
4	GOL	CCC	503	6/6	0.64	0.15	60,63,63,63	0
5	PEG	AAA	510	7/7	0.65	0.14	72,73,73,74	0
4	GOL	AAA	508	6/6	0.73	0.13	59,61,63,63	0
5	PEG	DDD	504	7/7	0.74	0.10	59,60,61,61	0
4	GOL	DDD	503	6/6	0.76	0.13	32,33,33,33	0
5	PEG	AAA	505	7/7	0.81	0.11	59,60,61,62	0
4	GOL	BBB	503	6/6	0.81	0.14	44,45,45,45	0
4	GOL	AAA	503	6/6	0.86	0.14	68,69,69,72	0
4	GOL	AAA	504	6/6	0.89	0.14	65,66,68,68	0
4	GOL	AAA	507	6/6	0.90	0.10	53,56,56,57	0
3	NDP	DDD	502	48/48	0.90	0.10	53,62,75,77	0
5	PEG	AAA	506	7/7	0.90	0.11	54,56,60,60	0
2	R1R	CCC	501	37/47	0.91	0.08	30,35,48,50	0
2	R1R	AAA	501	37/47	0.92	0.08	34,39,49,50	0
2	R1R	DDD	501	37/47	0.92	0.08	33,37,52,53	0
2	R1R	BBB	501	37/47	0.92	0.08	28,31,42,43	0
3	NDP	CCC	502	48/48	0.93	0.09	36,42,59,65	0
3	NDP	BBB	502	48/48	0.97	0.06	24,26,32,35	0
3	NDP	AAA	502	48/48	0.98	0.05	18,19,23,24	0

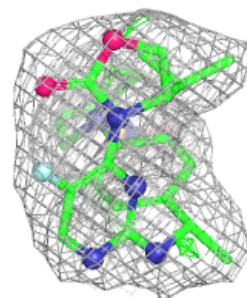
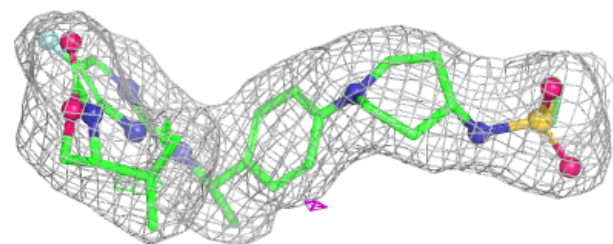
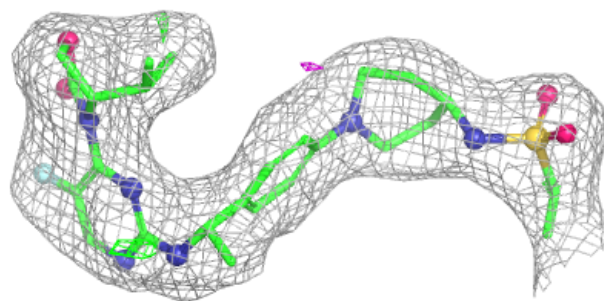
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP DDD 502:

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

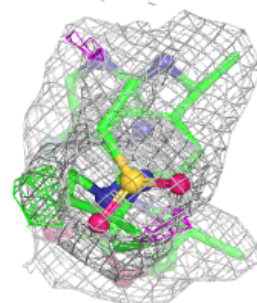
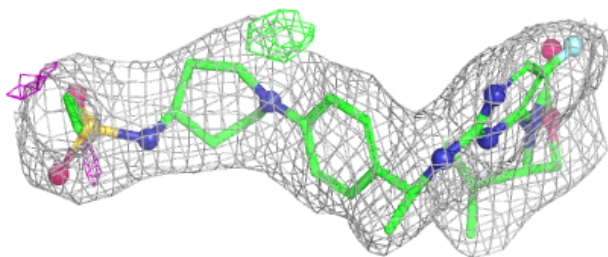
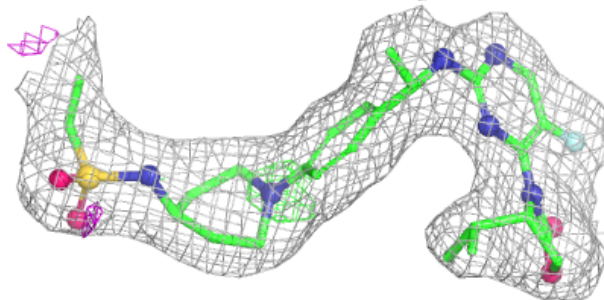
**Electron density around R1R CCC 501:**

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

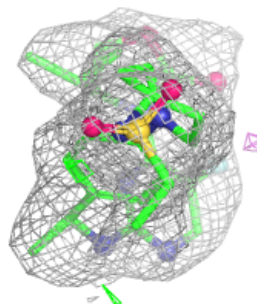
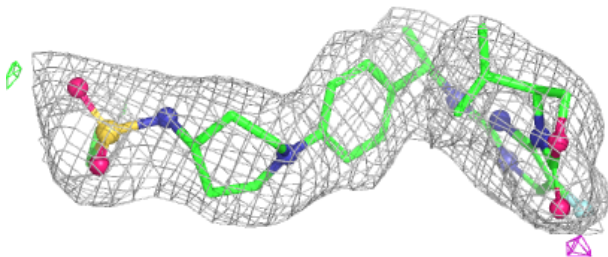
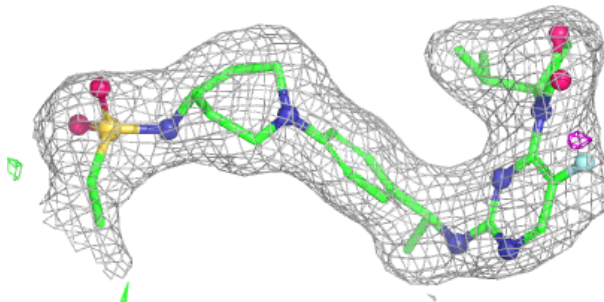


Electron density around R1R AAA 501:

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

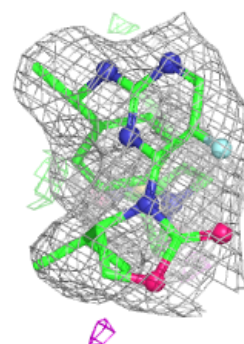
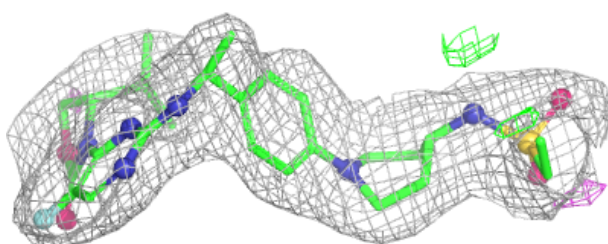
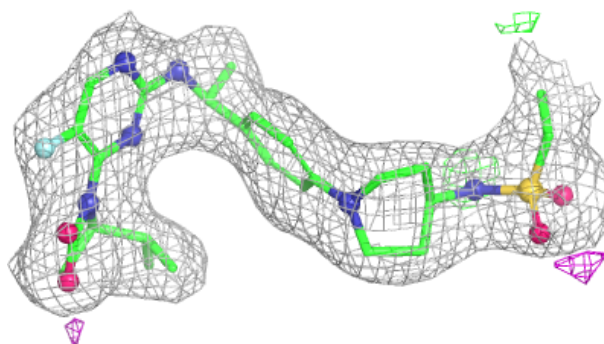
**Electron density around R1R DDD 501:**

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

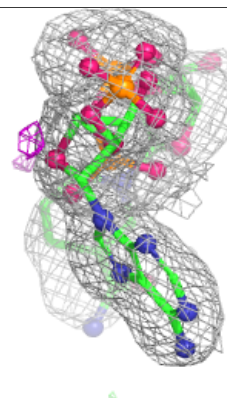
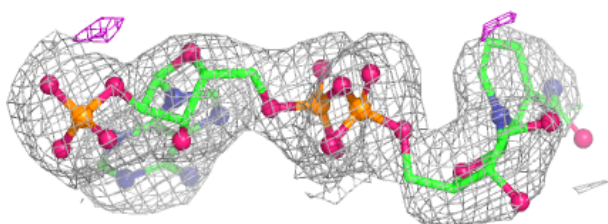
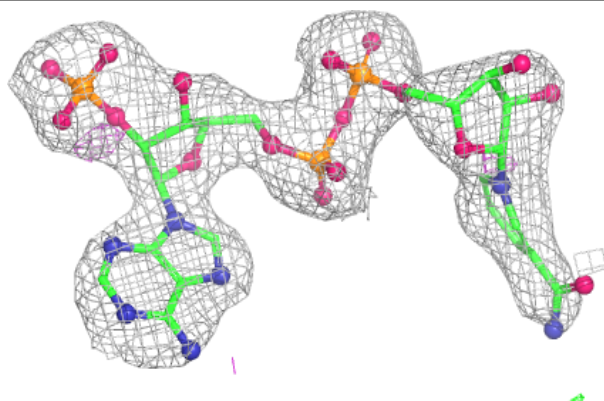


Electron density around R1R BBB 501:

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

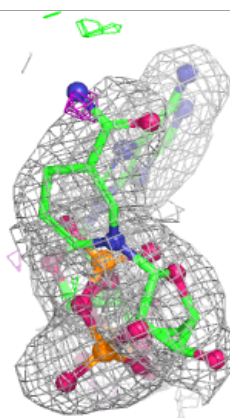
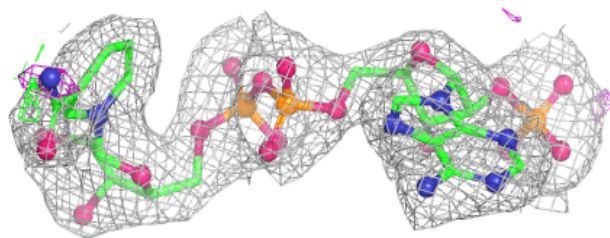
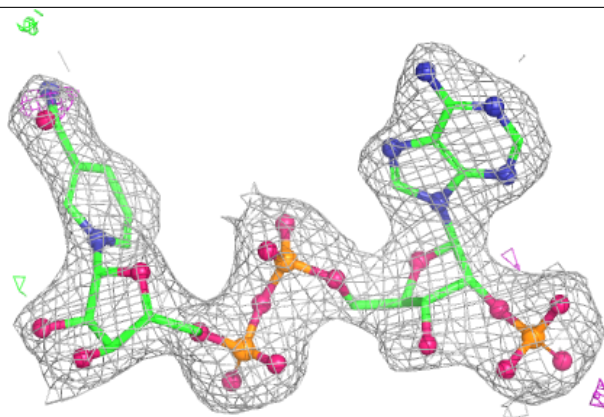
**Electron density around NDP CCC 502:**

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

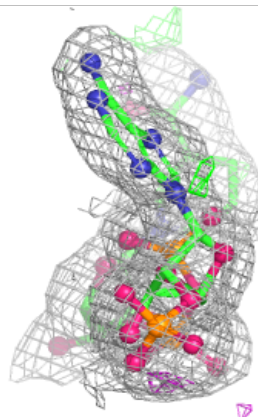
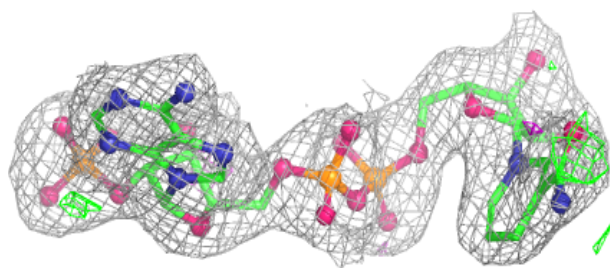
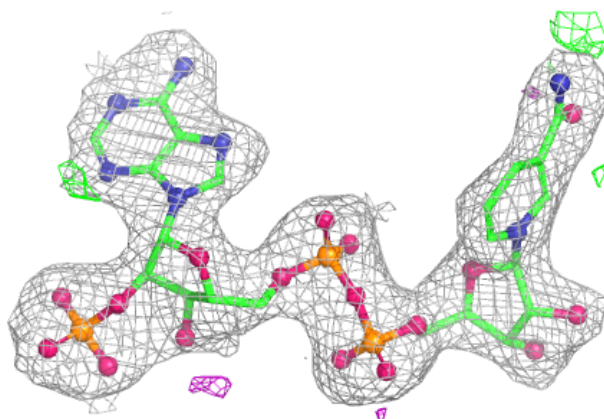


Electron density around NDP BBB 502:

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

**Electron density around NDP AAA 502:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.