Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 10:50 PM EST

PDB ID	:	1YVE
Title	:	ACETOHYDROXY ACID ISOMEROREDUCTASE COMPLEXED WITH NADPH, MAGNESIUM AND INHIBITOR IPOHA (N-HYDROXY-N-ISOPROPYLOXAMATE)
Authors	:	Biou, V.; Dumas, R.; Cohen-Addad, C.; Douce, R.; Job, D.; Pebay-Peyroula, E.
Deposited on	:	1996-10-11
Resolution	:	1.65 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:

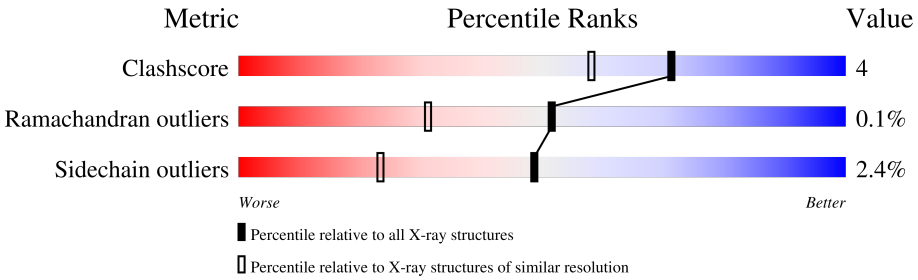
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.65 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))
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	524	91% 6% ·
1	J	524	89% 8% ·
1	K	524	88% 9% · ·
1	L	524	89% 8% · ·

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17729 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 ACETOHYDROXY ACID ISOMEROREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	513	Total	C	N	O	S	0	0	0
			3934	2491	670	755	18			
1	J	510	Total	C	N	O	S	0	0	0
			3915	2480	667	750	18			
1	K	510	Total	C	N	O	S	0	0	0
			3915	2480	667	750	18			
1	L	513	Total	C	N	O	S	0	0	0
			3933	2491	670	754	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	79	ASP	ASN	conflict	UNP Q01292
J	79	ASP	ASN	conflict	UNP Q01292
K	79	ASP	ASN	conflict	UNP Q01292
L	79	ASP	ASN	conflict	UNP Q01292

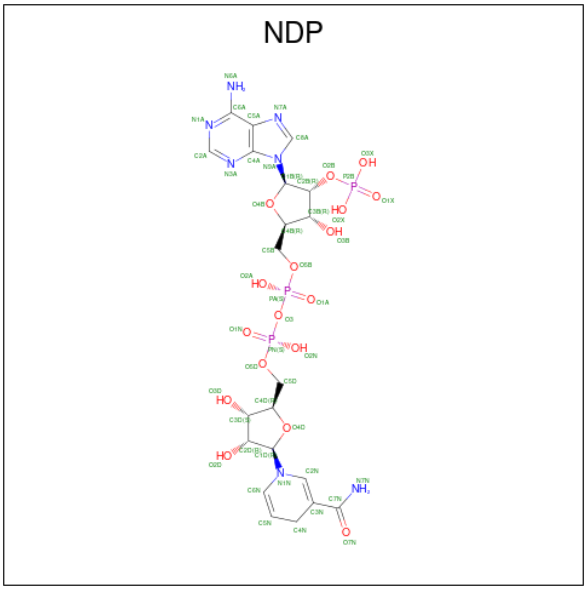
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	2	Total	Mg	0	0
			2	2		
2	J	2	Total	Mg	0	0
			2	2		
2	K	2	Total	Mg	0	0
			2	2		
2	L	2	Total	Mg	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

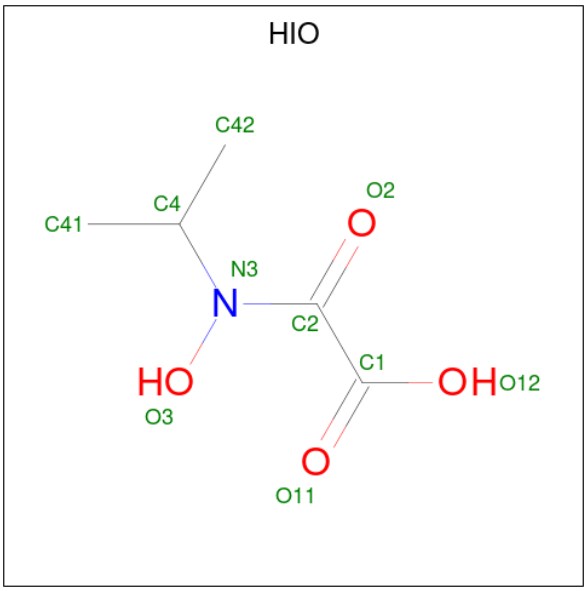
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0

- Molecule 4 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
4	I	1	Total C N O P 48 21 7 17 3	0	0
4	K	1	Total C N O P 48 21 7 17 3	0	0
4	K	1	Total C N O P 48 21 7 17 3	0	0
4	L	1	Total C N O P 48 21 7 17 3	0	0

- Molecule 5 is N-HYDROXY-N-ISOPROPYLOXAMIC ACID (three-letter code: HIO) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C N O 10 5 1 4	0	0
5	J	1	Total C N O 10 5 1 4	0	0
5	K	1	Total C N O 10 5 1 4	0	0
5	L	1	Total C N O 10 5 1 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	567	Total O 567 567	0	0
6	J	419	Total O 419 419	0	0
6	K	416	Total O 416 416	0	0
6	L	387	Total O 387 387	0	0

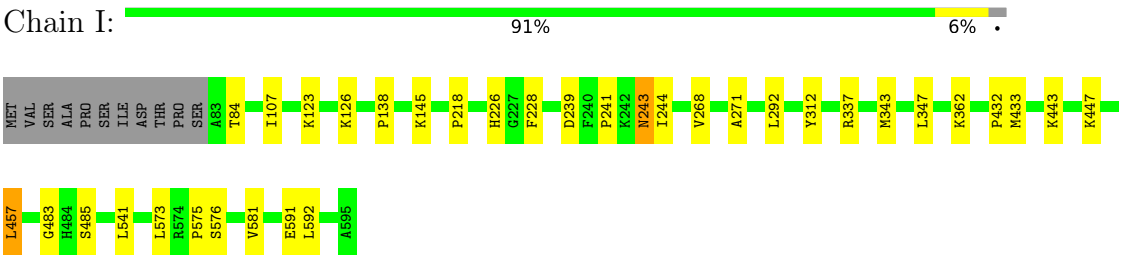
3 Residue-property plots (i)

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. 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.

Note EDS was not executed.

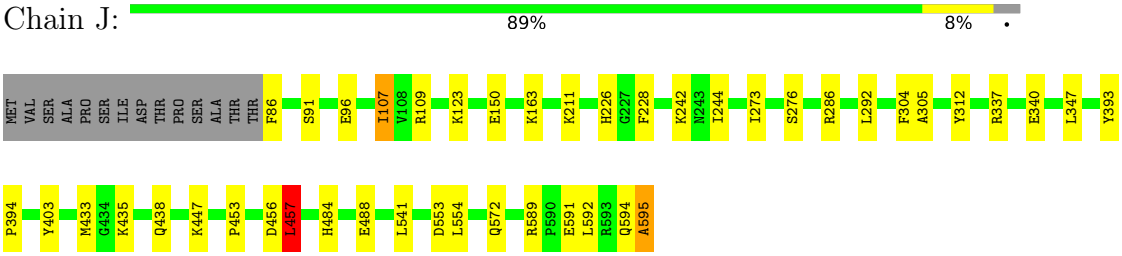
• Molecule 1: ACETOHYDROXY ACID ISOMEROREDUCTASE

Chain I:



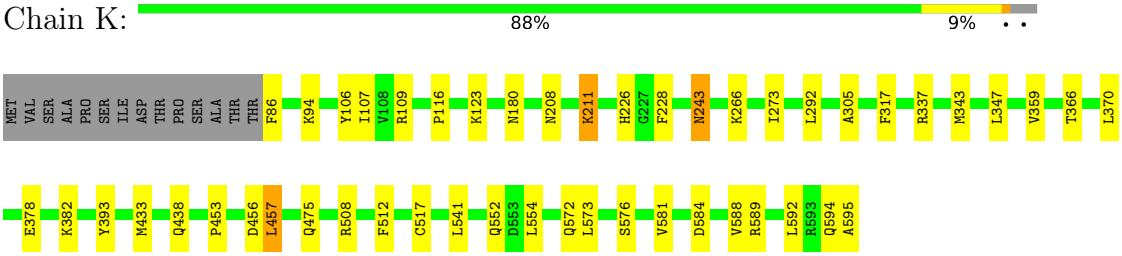
• Molecule 1: ACETOHYDROXY ACID ISOMEROREDUCTASE

Chain J:



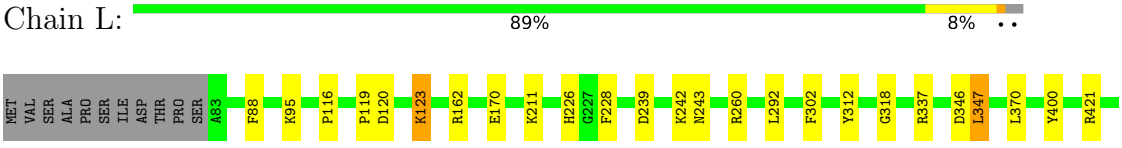
• Molecule 1: ACETOHYDROXY ACID ISOMEROREDUCTASE

Chain K:



• Molecule 1: ACETOHYDROXY ACID ISOMEROREDUCTASE

Chain L:




M433
G434
K435
Q438
K443
R452
G458
R480
E492
R508
L541
L554
D561
P575
S580
F587
V588
R589
L592
R593
Q594
A595

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.43Å 61.94Å 162.54Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	10.00 – 1.65	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.65)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.197 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17729	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NDP, CL, HIO

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	I	0.54	0/4013	0.69	2/5426 (0.0%)
1	J	0.53	0/3994	0.68	2/5399 (0.0%)
1	K	0.52	0/3994	0.68	1/5399 (0.0%)
1	L	0.46	0/4012	0.63	1/5426 (0.0%)
All	All	0.51	0/16013	0.67	6/21650 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	421	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	I	581	VAL	CB-CA-C	-6.17	99.68	111.40
1	J	595	ALA	N-CA-C	-5.41	96.38	111.00
1	J	457	LEU	CA-CB-CG	5.04	126.89	115.30
1	I	483	GLY	N-CA-C	5.03	125.69	113.10
1	K	581	VAL	CB-CA-C	-5.03	101.84	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	138	PRO	Mainchain
1	I	241	PRO	Mainchain
1	I	573	LEU	Mainchain

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	I	3934	0	3896	21	0
1	J	3915	0	3877	28	0
1	K	3915	0	3877	34	0
1	L	3933	0	3896	26	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
4	I	48	0	26	1	0
4	K	96	0	52	2	0
4	L	48	0	26	0	0
5	I	10	0	7	0	0
5	J	10	0	7	0	0
5	K	10	0	7	2	0
5	L	10	0	7	0	0
6	I	567	0	0	18	0
6	J	419	0	0	10	0
6	K	416	0	0	16	0
6	L	387	0	0	11	0
All	All	17729	0	15678	112	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 4.

All (112) 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:K:211:LYS:HE3	1:K:211:LYS:H	1.38	0.88
6:K:791:HOH:O	1:L:438:GLN:HG3	1.80	0.81
1:J:457:LEU:HB3	6:J:744:HOH:O	1.82	0.80
1:J:403:TYR:OH	1:J:484:HIS:HE1	1.73	0.71
6:K:985:HOH:O	1:L:162:ARG:HB2	1.91	0.70
1:I:575:PRO:HG2	6:I:945:HOH:O	1.93	0.68
1:L:593:ARG:O	1:L:594:GLN:HB2	1.94	0.67
1:K:438:GLN:HG3	6:L:834:HOH:O	1.95	0.67
1:K:123:LYS:HD3	6:K:662:HOH:O	1.96	0.65
1:K:337:ARG:HD2	1:K:541:LEU:HD13	1.77	0.65
1:K:94:LYS:HE2	6:K:668:HOH:O	1.97	0.64
1:I:457:LEU:HA	6:I:1161:HOH:O	1.97	0.63
1:I:362:LYS:HG3	6:I:986:HOH:O	1.96	0.63
1:J:123:LYS:HG3	1:J:286:ARG:HG2	1.81	0.62
1:I:271:ALA:HB1	6:I:946:HOH:O	2.00	0.62
1:K:211:LYS:HE3	1:K:211:LYS:N	2.11	0.61
1:I:443:LYS:HE3	6:I:1039:HOH:O	2.00	0.61
1:J:273:ILE:HD13	6:J:755:HOH:O	2.00	0.60
1:I:432:PRO:HB3	6:I:906:HOH:O	2.01	0.59
6:K:791:HOH:O	1:L:435:LYS:HD2	2.01	0.59
1:I:84:THR:O	1:I:485:SER:HB3	2.02	0.59
4:I:600:NDP:H8A	6:I:763:HOH:O	2.03	0.58
1:L:370:LEU:HB2	6:L:693:HOH:O	2.04	0.57
1:K:86:PHE:CD2	1:K:305:ALA:HB1	2.39	0.57
1:L:575:PRO:HB3	6:L:974:HOH:O	2.04	0.56
1:J:484:HIS:HD2	1:J:488:GLU:OE1	1.90	0.55
1:L:226:HIS:CD2	1:L:228:PHE:HB2	2.42	0.55
1:J:572:GLN:HA	6:J:767:HOH:O	2.06	0.54
1:L:116:PRO:O	1:L:119:PRO:HD2	2.08	0.53
1:K:584:ASP:HA	1:K:594:GLN:HB3	1.89	0.53
6:I:1054:HOH:O	1:J:438:GLN:HG3	2.06	0.53
1:K:378:GLU:O	1:K:382:LYS:HG3	2.09	0.52
4:K:605:NDP:P2B	1:L:162:ARG:HH21	2.33	0.52
1:L:452:ARG:CZ	6:L:942:HOH:O	2.57	0.52
1:J:337:ARG:HD2	1:J:541:LEU:HD13	1.92	0.51
1:J:591:GLU:H	1:J:591:GLU:CD	2.13	0.51
1:J:594:GLN:HG2	1:J:595:ALA:H	1.75	0.51
1:L:260:ARG:HD3	1:L:587:PHE:CE2	2.45	0.51
1:J:453:PRO:HG2	1:J:456:ASP:HB2	1.93	0.51
1:K:576:SER:HA	6:K:946:HOH:O	2.10	0.51
1:I:362:LYS:HD3	6:I:982:HOH:O	2.11	0.50
1:K:359:VAL:HB	1:K:457:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:226:HIS:CD2	1:K:228:PHE:HB2	2.46	0.50
1:L:589:ARG:HA	6:L:664:HOH:O	2.12	0.50
1:L:443:LYS:HE3	6:L:832:HOH:O	2.12	0.50
1:K:393:TYR:HB3	6:K:926:HOH:O	2.11	0.50
4:K:605:NDP:H8A	6:L:658:HOH:O	2.11	0.50
1:K:366:THR:HB	6:K:965:HOH:O	2.12	0.49
1:K:508:ARG:NH1	1:K:594:GLN:HB2	2.28	0.49
1:K:109:ARG:CZ	1:K:573:LEU:HD23	2.43	0.49
1:J:433:MET:HG2	6:J:637:HOH:O	2.13	0.48
1:J:96:GLU:OE1	1:J:109:ARG:HD2	2.13	0.48
1:J:226:HIS:CD2	1:J:228:PHE:HB2	2.47	0.48
1:K:594:GLN:HG2	1:K:595:ALA:N	2.28	0.48
6:I:1054:HOH:O	1:J:435:LYS:HD2	2.13	0.48
5:K:603:HIO:O11	5:K:603:HIO:H4	2.14	0.47
1:K:208:ASN:HA	1:K:211:LYS:NZ	2.28	0.47
1:L:337:ARG:HD2	1:L:541:LEU:HD13	1.96	0.47
1:L:480:ARG:NH2	1:L:561:ASP:OD1	2.44	0.47
1:I:447:LYS:HG2	6:I:1128:HOH:O	2.15	0.47
1:I:447:LYS:HE3	6:I:1129:HOH:O	2.14	0.47
1:K:243:ASN:H	1:K:243:ASN:HD22	1.63	0.46
1:I:126:LYS:HA	1:I:126:LYS:HD2	1.63	0.46
1:I:226:HIS:CD2	1:I:228:PHE:HB2	2.51	0.46
1:K:343:MET:HG2	1:K:347:LEU:HB3	1.97	0.46
1:L:88:PHE:O	1:L:95:LYS:HE2	2.16	0.46
1:J:86:PHE:CD2	1:J:305:ALA:HB1	2.51	0.45
1:L:443:LYS:HD3	1:L:443:LYS:HA	1.84	0.45
1:J:123:LYS:HG3	1:J:286:ARG:CG	2.46	0.45
1:J:457:LEU:HA	6:J:743:HOH:O	2.16	0.45
1:J:457:LEU:HD12	6:J:964:HOH:O	2.17	0.45
1:K:106:TYR:O	1:K:107:ILE:HD12	2.17	0.45
1:K:208:ASN:HA	1:K:211:LYS:HZ2	1.82	0.45
1:K:347:LEU:HD21	6:K:1008:HOH:O	2.16	0.44
1:J:107:ILE:HD11	1:J:304:PHE:HB3	1.99	0.44
1:K:589:ARG:HD2	6:K:877:HOH:O	2.17	0.44
1:L:580:SER:HA	6:L:886:HOH:O	2.16	0.44
1:K:273:ILE:HD13	6:K:958:HOH:O	2.16	0.44
1:L:508:ARG:HD2	1:L:595:ALA:CB	2.48	0.44
1:K:433:MET:HG2	6:K:764:HOH:O	2.18	0.43
1:J:242:LYS:HA	1:J:242:LYS:HD3	1.84	0.43
1:K:266:LYS:HE2	6:K:678:HOH:O	2.18	0.43
1:J:447:LYS:HD2	6:J:944:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:572:GLN:HB2	6:J:1007:HOH:O	2.17	0.43
1:I:145:LYS:HD3	6:I:741:HOH:O	2.19	0.43
1:K:453:PRO:HG2	1:K:456:ASP:HB2	2.00	0.43
1:I:337:ARG:HD2	1:I:541:LEU:HD13	2.01	0.42
1:J:337:ARG:HA	6:J:657:HOH:O	2.18	0.42
1:I:343:MET:HG2	1:I:347:LEU:HB3	2.02	0.42
1:L:120:ASP:O	1:L:123:LYS:HD3	2.20	0.42
1:J:276:SER:HB3	1:J:304:PHE:CZ	2.54	0.42
1:J:393:TYR:HB3	6:J:711:HOH:O	2.20	0.42
1:I:591:GLU:HG2	1:I:592:LEU:HD13	2.03	0.41
6:K:776:HOH:O	1:L:433:MET:HG2	2.21	0.41
1:I:243:ASN:HD22	1:I:243:ASN:H	1.68	0.41
1:K:317:PHE:CZ	1:K:475:GLN:HG3	2.55	0.41
1:K:572:GLN:HB2	6:K:941:HOH:O	2.20	0.41
1:L:170:GLU:HB3	6:L:891:HOH:O	2.18	0.41
1:K:370:LEU:HD23	1:K:370:LEU:HA	1.89	0.41
1:I:123:LYS:HE3	6:I:844:HOH:O	2.20	0.41
1:J:589:ARG:HB2	1:J:592:LEU:HD13	2.02	0.41
1:L:242:LYS:HD3	6:L:605:HOH:O	2.19	0.41
1:I:433:MET:HG2	6:I:683:HOH:O	2.20	0.41
6:I:1100:HOH:O	1:J:340:GLU:HG2	2.20	0.41
1:L:458:GLY:HA2	6:L:944:HOH:O	2.21	0.41
1:I:575:PRO:HG3	6:I:946:HOH:O	2.20	0.41
1:K:517:CYS:SG	5:K:603:HIO:H421	2.61	0.41
1:I:218:PRO:HD2	6:I:884:HOH:O	2.21	0.40
1:L:318:GLY:HA3	1:L:492:GLU:OE2	2.21	0.40
1:K:552:GLN:HG2	6:K:979:HOH:O	2.21	0.40
1:L:347:LEU:HD12	1:L:347:LEU:HA	1.93	0.40
1:K:512:PHE:CZ	1:K:588:VAL:HG11	2.57	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	I	511/524 (98%)	498 (98%)	12 (2%)	1 (0%)	47 28
1	J	508/524 (97%)	496 (98%)	11 (2%)	1 (0%)	47 28
1	K	508/524 (97%)	496 (98%)	12 (2%)	0	100 100
1	L	511/524 (98%)	493 (96%)	17 (3%)	1 (0%)	47 28
All	All	2038/2096 (97%)	1983 (97%)	52 (3%)	3 (0%)	51 31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	163	LYS
1	L	594	GLN
1	I	268	VAL

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	I	423/433 (98%)	415 (98%)	8 (2%)	57 34
1	J	421/433 (97%)	409 (97%)	12 (3%)	42 16
1	K	421/433 (97%)	413 (98%)	8 (2%)	57 34
1	L	423/433 (98%)	411 (97%)	12 (3%)	43 18
All	All	1688/1732 (98%)	1648 (98%)	40 (2%)	49 23

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	107	ILE
1	I	239	ASP
1	I	243	ASN
1	I	244	ILE
1	I	292	LEU
1	I	312	TYR
1	I	457	LEU
1	I	576	SER

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Mol	Chain	Res	Type
1	J	91	SER
1	J	107	ILE
1	J	150	GLU
1	J	211	LYS
1	J	244	ILE
1	J	292	LEU
1	J	312	TYR
1	J	347	LEU
1	J	394	PRO
1	J	457	LEU
1	J	553	ASP
1	J	554	LEU
1	K	116	PRO
1	K	180	ASN
1	K	211	LYS
1	K	243	ASN
1	K	292	LEU
1	K	457	LEU
1	K	554	LEU
1	K	592	LEU
1	L	123	LYS
1	L	211	LYS
1	L	239	ASP
1	L	243	ASN
1	L	292	LEU
1	L	302	PHE
1	L	312	TYR
1	L	346	ASP
1	L	347	LEU
1	L	400	TYR
1	L	554	LEU
1	L	592	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	238	GLN
1	I	243	ASN
1	J	238	GLN
1	J	310	GLN
1	J	484	HIS
1	J	572	GLN

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Mol	Chain	Res	Type
1	K	166	ASN
1	K	238	GLN
1	K	243	ASN
1	K	310	GLN
1	K	572	GLN
1	L	238	GLN
1	L	243	ASN
1	L	552	GLN
1	L	572	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)

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	HIO	I	603	2	8,9,9	1.01	0	8,12,12	2.70	5 (62%)
4	NDP	I	600	-	45,52,52	1.75	8 (17%)	53,80,80	1.20	3 (5%)
5	HIO	J	603	2	8,9,9	2.16	1 (12%)	8,12,12	2.42	4 (50%)
4	NDP	L	600	-	45,52,52	1.71	10 (22%)	53,80,80	1.27	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NDP	K	605	-	45,52,52	1.72	10 (22%)	53,80,80	1.37	5 (9%)
4	NDP	K	600	2	45,52,52	1.64	10 (22%)	53,80,80	1.27	4 (7%)
5	HIO	K	603	2	8,9,9	2.53	1 (12%)	8,12,12	3.89	4 (50%)
5	HIO	L	603	2	8,9,9	2.45	3 (37%)	8,12,12	3.23	4 (50%)

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	HIO	I	603	2	-	3/8/12/12	-
4	NDP	I	600	-	-	12/30/77/77	0/5/5/5
5	HIO	J	603	2	-	3/8/12/12	-
4	NDP	L	600	-	-	10/30/77/77	0/5/5/5
4	NDP	K	605	-	-	10/30/77/77	0/5/5/5
4	NDP	K	600	2	-	9/30/77/77	0/5/5/5
5	HIO	K	603	2	-	4/8/12/12	-
5	HIO	L	603	2	-	4/8/12/12	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	603	HIO	C2-N3	6.90	1.41	1.34
5	L	603	HIO	C2-N3	5.69	1.40	1.34
5	J	603	HIO	C2-N3	5.59	1.40	1.34
4	K	605	NDP	P2B-O2B	-5.49	1.48	1.59
4	I	600	NDP	P2B-O2B	-5.30	1.49	1.59
4	L	600	NDP	P2B-O2B	-5.10	1.49	1.59
4	I	600	NDP	C4N-C3N	-4.32	1.41	1.49
4	K	605	NDP	C4N-C3N	-4.28	1.41	1.49
4	K	600	NDP	C4N-C3N	-4.13	1.41	1.49
4	K	600	NDP	C6N-C5N	4.11	1.40	1.33
4	L	600	NDP	C4N-C3N	-3.97	1.42	1.49
4	K	600	NDP	P2B-O2B	-3.87	1.52	1.59
4	I	600	NDP	P2B-O1X	-3.85	1.38	1.50
4	L	600	NDP	P2B-O1X	-3.81	1.38	1.50
4	L	600	NDP	P2B-O2X	-3.72	1.40	1.54
4	K	605	NDP	P2B-O3X	-3.49	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	600	NDP	P2B-O3X	-3.46	1.41	1.54
4	I	600	NDP	C4N-C5N	-3.44	1.39	1.48
4	I	600	NDP	P2B-O3X	-3.43	1.41	1.54
4	I	600	NDP	C6N-C5N	3.42	1.39	1.33
4	K	600	NDP	P2B-O3X	-3.37	1.41	1.54
4	K	605	NDP	C7N-C3N	3.36	1.55	1.48
4	K	600	NDP	P2B-O1X	-3.25	1.40	1.50
4	K	605	NDP	C6N-C5N	3.14	1.38	1.33
4	I	600	NDP	P2B-O2X	-3.09	1.42	1.54
4	K	605	NDP	P2B-O2X	-3.07	1.43	1.54
4	L	600	NDP	C4N-C5N	-2.98	1.41	1.48
4	K	600	NDP	C4N-C5N	-2.97	1.41	1.48
4	K	605	NDP	C4N-C5N	-2.87	1.41	1.48
4	K	605	NDP	P2B-O1X	-2.82	1.41	1.50
4	L	600	NDP	C6N-C5N	2.78	1.38	1.33
4	K	600	NDP	C7N-C3N	2.74	1.54	1.48
4	K	600	NDP	P2B-O2X	-2.58	1.44	1.54
5	L	603	HIO	O12-C1	2.57	1.38	1.30
5	L	603	HIO	O2-C2	2.46	1.28	1.23
4	K	600	NDP	C6N-N1N	2.31	1.43	1.37
4	K	605	NDP	O4B-C1B	2.22	1.44	1.41
4	L	600	NDP	O4B-C1B	2.22	1.44	1.41
4	K	605	NDP	C5A-N7A	-2.19	1.31	1.39
4	I	600	NDP	O4B-C1B	2.18	1.44	1.41
4	L	600	NDP	C7N-C3N	2.16	1.53	1.48
4	K	600	NDP	C5A-N7A	-2.04	1.32	1.39
4	L	600	NDP	C5A-N7A	-2.02	1.32	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	603	HIO	C41-C4-N3	6.99	117.36	109.90
5	K	603	HIO	C41-C4-N3	6.83	117.19	109.90
5	K	603	HIO	O11-C1-C2	5.59	130.63	123.07
4	K	605	NDP	N3A-C2A-N1A	-5.59	119.94	128.68
5	K	603	HIO	C42-C4-N3	5.47	115.73	109.90
4	K	600	NDP	N3A-C2A-N1A	-5.20	120.55	128.68
5	I	603	HIO	O11-C1-C2	5.13	130.01	123.07
4	I	600	NDP	N3A-C2A-N1A	-4.93	120.98	128.68
4	L	600	NDP	N3A-C2A-N1A	-4.72	121.31	128.68
5	J	603	HIO	O11-C1-C2	4.42	129.04	123.07
5	L	603	HIO	C42-C4-N3	-4.33	105.28	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	603	HIO	C41-C4-N3	3.46	113.59	109.90
5	I	603	HIO	O2-C2-N3	-3.39	116.41	120.62
4	K	605	NDP	C2A-N1A-C6A	3.12	124.08	118.75
4	L	600	NDP	C2A-N1A-C6A	3.07	124.01	118.75
4	K	600	NDP	C3N-C2N-N1N	-2.98	118.84	123.10
5	L	603	HIO	O12-C1-O11	-2.93	116.90	123.61
4	K	605	NDP	C5A-C6A-N6A	2.86	124.69	120.35
5	K	603	HIO	O12-C1-O11	-2.83	117.13	123.61
4	L	600	NDP	N6A-C6A-N1A	2.79	124.36	118.57
4	K	600	NDP	C3B-C2B-C1B	-2.71	97.80	102.89
4	K	605	NDP	C4A-C5A-N7A	-2.67	106.62	109.40
5	I	603	HIO	C41-C4-N3	2.66	112.74	109.90
5	I	603	HIO	C42-C4-N3	-2.59	107.13	109.90
4	L	600	NDP	C5A-C6A-N1A	-2.59	114.48	120.35
4	I	600	NDP	C3N-C2N-N1N	-2.58	119.42	123.10
4	K	600	NDP	O3D-C3D-C4D	-2.53	103.73	111.05
5	J	603	HIO	O12-C1-O11	-2.46	117.99	123.61
4	I	600	NDP	C2A-N1A-C6A	2.42	122.89	118.75
4	K	605	NDP	C3N-C2N-N1N	-2.36	119.72	123.10
4	L	600	NDP	C4A-C5A-N7A	-2.32	106.99	109.40
5	J	603	HIO	O2-C2-C1	-2.31	115.20	118.32
4	L	600	NDP	C3N-C2N-N1N	-2.06	120.15	123.10
5	L	603	HIO	O11-C1-C2	2.04	125.83	123.07
5	I	603	HIO	O12-C1-C2	-2.04	109.11	113.84

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	600	NDP	C5B-O5B-PA-O2A
4	K	600	NDP	C5B-O5B-PA-O2A
4	K	600	NDP	C2B-O2B-P2B-O3X
4	K	605	NDP	C5B-O5B-PA-O2A
4	K	605	NDP	C2B-O2B-P2B-O3X
4	L	600	NDP	C5B-O5B-PA-O2A
5	I	603	HIO	O11-C1-C2-N3
5	I	603	HIO	O2-C2-N3-O3
5	I	603	HIO	C41-C4-N3-O3
5	J	603	HIO	O11-C1-C2-N3
5	J	603	HIO	O2-C2-N3-O3
5	J	603	HIO	C41-C4-N3-O3
5	K	603	HIO	O11-C1-C2-N3

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Mol	Chain	Res	Type	Atoms
5	K	603	HIO	O2-C2-N3-O3
5	K	603	HIO	C41-C4-N3-O3
5	L	603	HIO	O11-C1-C2-N3
5	L	603	HIO	O2-C2-N3-O3
5	L	603	HIO	C41-C4-N3-O3
4	I	600	NDP	C1B-C2B-O2B-P2B
4	K	600	NDP	C1B-C2B-O2B-P2B
4	K	605	NDP	C1B-C2B-O2B-P2B
4	L	600	NDP	C1B-C2B-O2B-P2B
4	I	600	NDP	C3B-C2B-O2B-P2B
4	K	600	NDP	C3B-C2B-O2B-P2B
4	K	605	NDP	C3B-C2B-O2B-P2B
4	L	600	NDP	C3B-C2B-O2B-P2B
4	I	600	NDP	PA-O3-PN-O1N
4	K	600	NDP	PA-O3-PN-O1N
4	I	600	NDP	C5B-O5B-PA-O3
4	I	600	NDP	C2B-O2B-P2B-O3X
4	K	600	NDP	C5B-O5B-PA-O3
4	K	605	NDP	C5B-O5B-PA-O3
4	L	600	NDP	C5B-O5B-PA-O3
4	L	600	NDP	C2B-O2B-P2B-O3X
4	K	605	NDP	PA-O3-PN-O2N
4	L	600	NDP	PA-O3-PN-O2N
4	L	600	NDP	C5B-O5B-PA-O1A
5	K	603	HIO	C42-C4-N3-O3
5	L	603	HIO	C42-C4-N3-O3
4	I	600	NDP	O4D-C1D-N1N-C6N
4	I	600	NDP	C2D-C1D-N1N-C6N
4	K	600	NDP	O4D-C1D-N1N-C6N
4	K	605	NDP	O4D-C1D-N1N-C6N
4	L	600	NDP	O4D-C1D-N1N-C6N
4	I	600	NDP	PA-O3-PN-O2N
4	K	600	NDP	C2D-C1D-N1N-C6N
4	K	605	NDP	C2D-C1D-N1N-C6N
4	L	600	NDP	C2D-C1D-N1N-C6N
4	I	600	NDP	C2D-C1D-N1N-C2N
4	K	600	NDP	PA-O3-PN-O2N
4	K	605	NDP	PA-O3-PN-O1N
4	L	600	NDP	PA-O3-PN-O1N
4	I	600	NDP	O4D-C1D-N1N-C2N
4	I	600	NDP	C5B-O5B-PA-O1A
4	K	605	NDP	C5B-O5B-PA-O1A

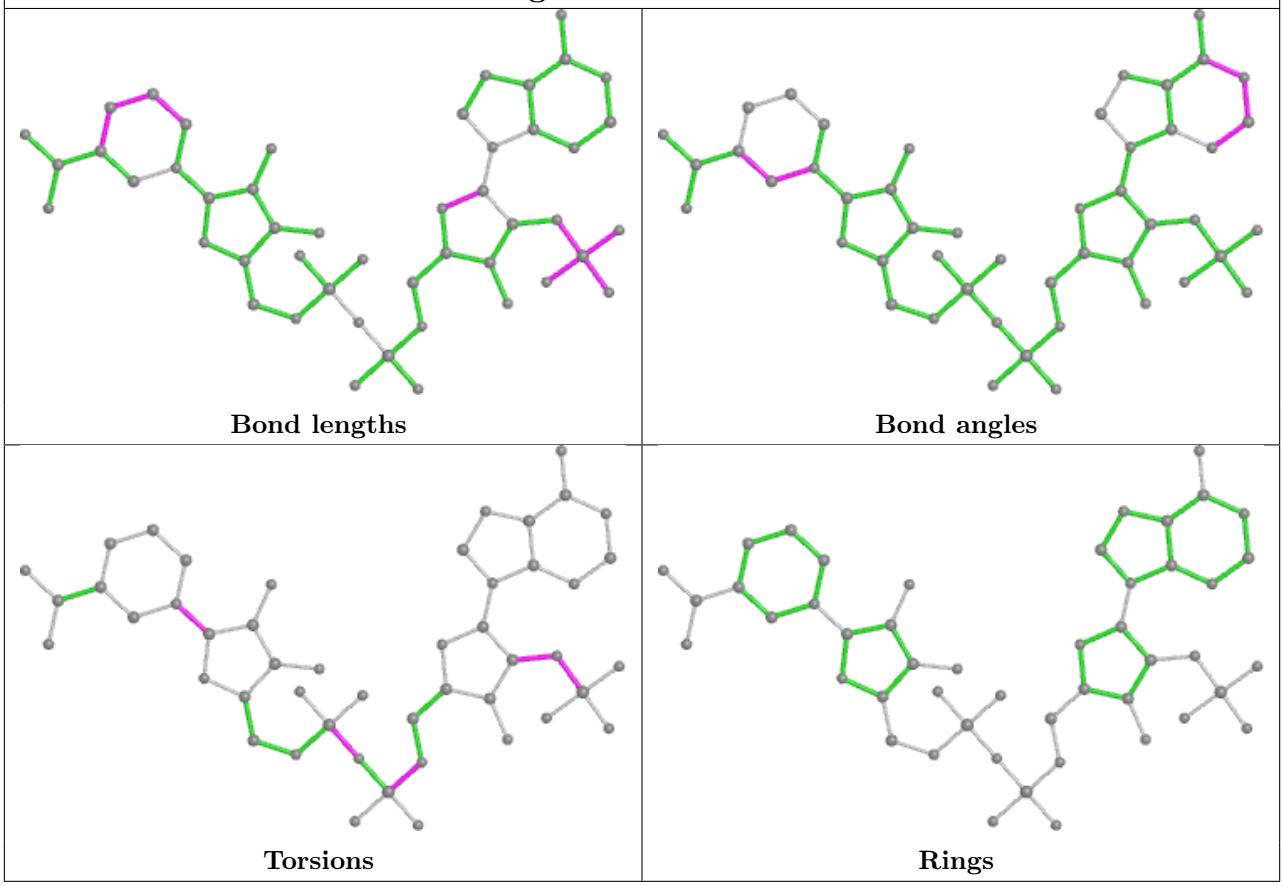
There are no ring outliers.

3 monomers are involved in 5 short contacts:

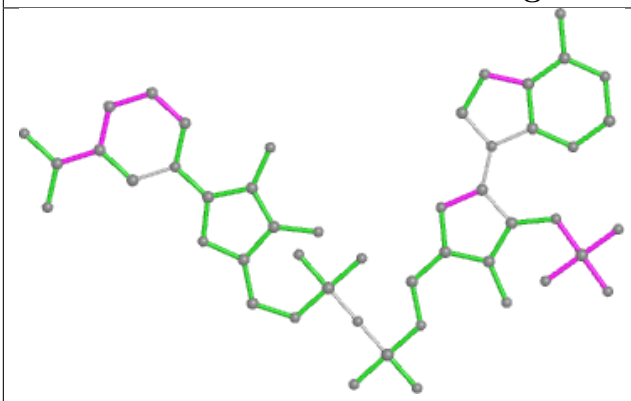
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	600	NDP	1	0
4	K	605	NDP	2	0
5	K	603	HIO	2	0

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.

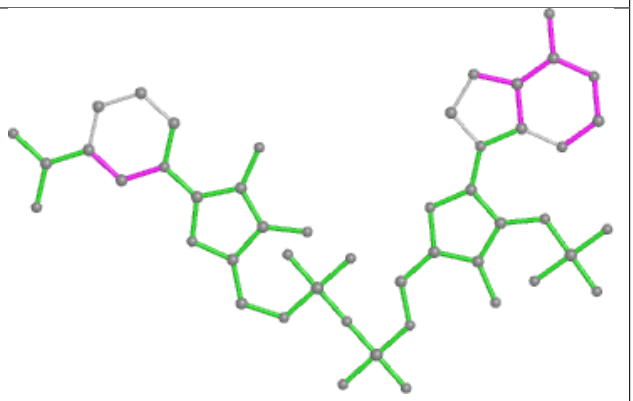
Ligand NDP I 600



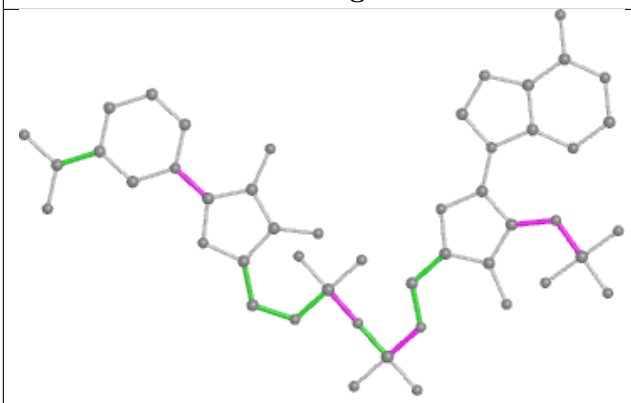
Ligand NDP L 600



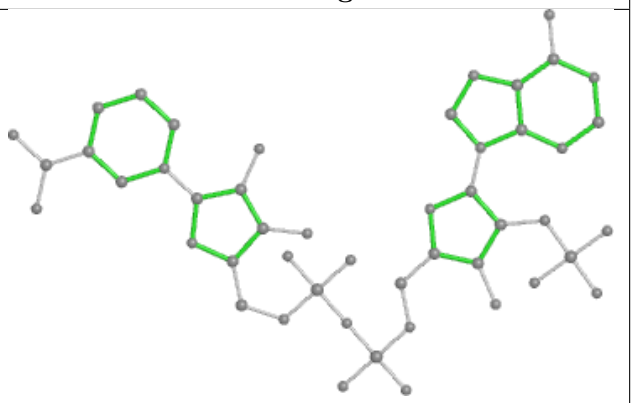
Bond lengths



Bond angles

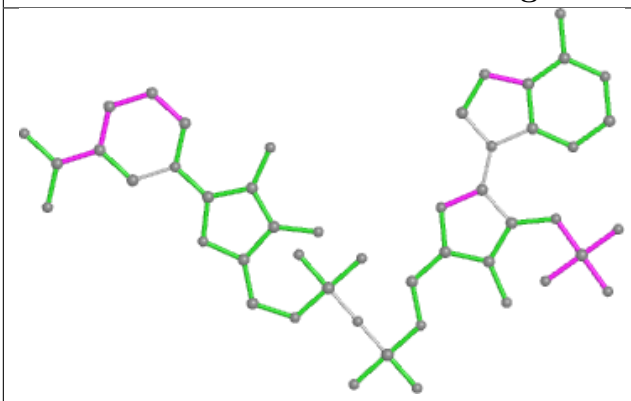


Torsions

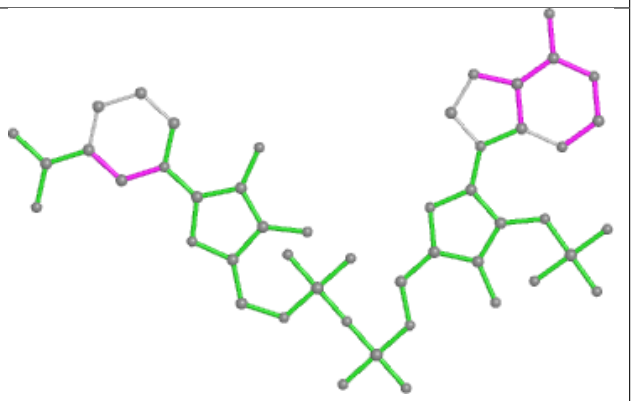


Rings

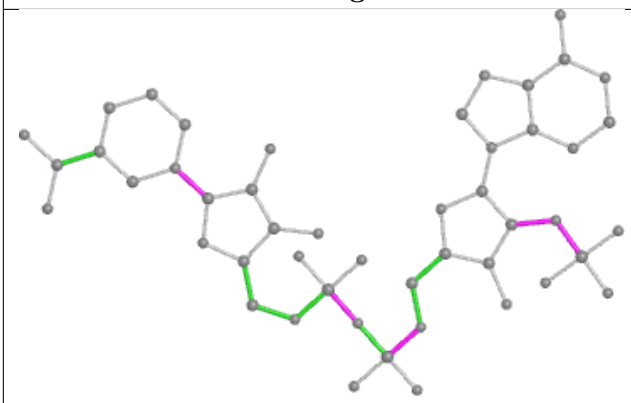
Ligand NDP K 605



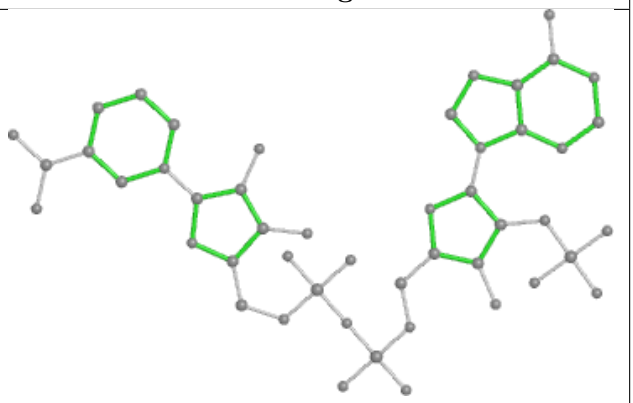
Bond lengths



Bond angles

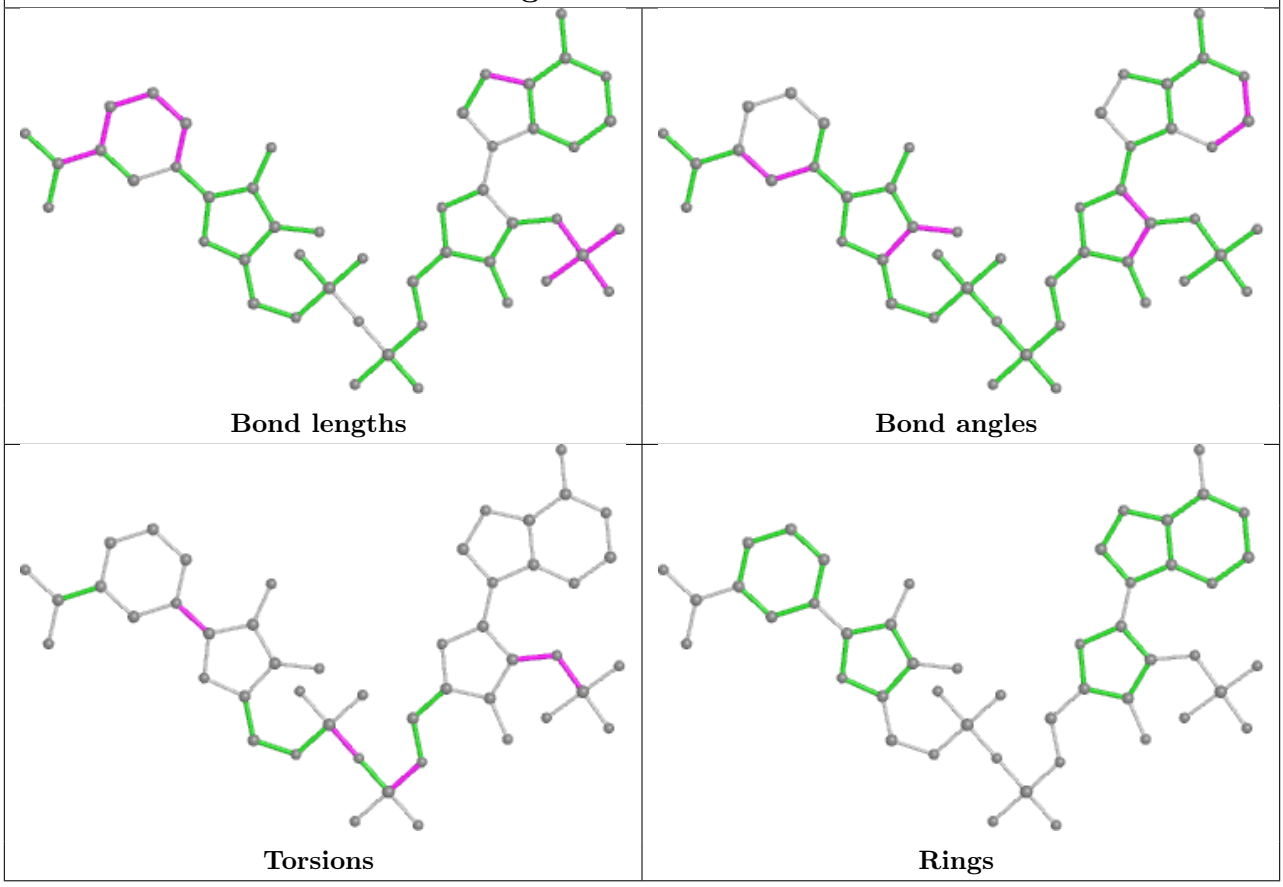


Torsions



Rings

Ligand NDP K 600



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.