Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 09:16 AM EDT

PDB ID	:	1XU9
Title	:	Crystal Structure of the Interface Closed Conformation of 11b-hydroxysteroid dehydrogenase isozyme 1
Authors	:	Hosfield, D.J.; Wu, Y.; Skene, R.J.; Hilger, M.; Jennings, A.; Snell, G.P.; Aertgeerts, K.
Deposited on	:	2004-10-25
Resolution	:	1.55 Å(reported)

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

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

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

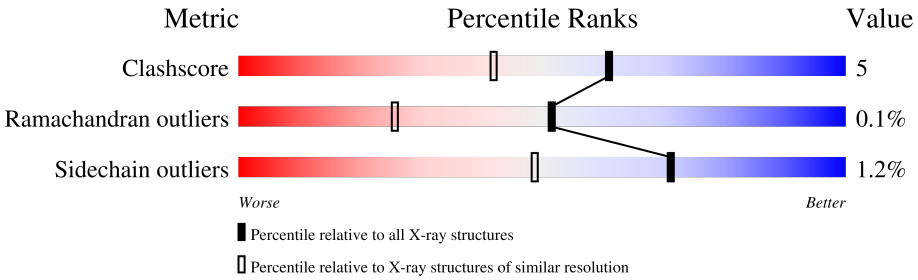
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.55 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	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)

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	A	286	86% 8% 6%
1	B	286	86% 7% • 6%
1	C	286	85% 5% 10%
1	D	286	85% 6% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9889 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 Corticosteroid 11-beta-dehydrogenase, isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	11	0
			2109	1346	355	392	16			
1	B	270	Total	C	N	O	S	0	12	0
			2121	1355	357	392	17			
1	C	258	Total	C	N	O	S	0	10	0
			2012	1282	341	375	14			
1	D	258	Total	C	N	O	S	0	12	0
			2016	1283	339	377	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP P28845
A	8	LYS	-	cloning artifact	UNP P28845
A	9	HIS	-	cloning artifact	UNP P28845
A	10	GLN	-	cloning artifact	UNP P28845
A	11	HIS	-	cloning artifact	UNP P28845
A	12	GLN	-	cloning artifact	UNP P28845
A	13	HIS	-	cloning artifact	UNP P28845
A	14	GLN	-	cloning artifact	UNP P28845
A	15	HIS	-	cloning artifact	UNP P28845
A	16	GLN	-	cloning artifact	UNP P28845
A	17	HIS	-	cloning artifact	UNP P28845
A	18	GLN	-	cloning artifact	UNP P28845
A	19	HIS	-	cloning artifact	UNP P28845
A	20	GLN	-	cloning artifact	UNP P28845
A	21	GLN	-	cloning artifact	UNP P28845
A	22	PRO	-	cloning artifact	UNP P28845
A	23	LEU	-	cloning artifact	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	7	MET	-	initiating methionine	UNP P28845
B	8	LYS	-	cloning artifact	UNP P28845
B	9	HIS	-	cloning artifact	UNP P28845

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	cloning artifact	UNP P28845
B	11	HIS	-	cloning artifact	UNP P28845
B	12	GLN	-	cloning artifact	UNP P28845
B	13	HIS	-	cloning artifact	UNP P28845
B	14	GLN	-	cloning artifact	UNP P28845
B	15	HIS	-	cloning artifact	UNP P28845
B	16	GLN	-	cloning artifact	UNP P28845
B	17	HIS	-	cloning artifact	UNP P28845
B	18	GLN	-	cloning artifact	UNP P28845
B	19	HIS	-	cloning artifact	UNP P28845
B	20	GLN	-	cloning artifact	UNP P28845
B	21	GLN	-	cloning artifact	UNP P28845
B	22	PRO	-	cloning artifact	UNP P28845
B	23	LEU	-	cloning artifact	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
C	7	MET	-	initiating methionine	UNP P28845
C	8	LYS	-	cloning artifact	UNP P28845
C	9	HIS	-	cloning artifact	UNP P28845
C	10	GLN	-	cloning artifact	UNP P28845
C	11	HIS	-	cloning artifact	UNP P28845
C	12	GLN	-	cloning artifact	UNP P28845
C	13	HIS	-	cloning artifact	UNP P28845
C	14	GLN	-	cloning artifact	UNP P28845
C	15	HIS	-	cloning artifact	UNP P28845
C	16	GLN	-	cloning artifact	UNP P28845
C	17	HIS	-	cloning artifact	UNP P28845
C	18	GLN	-	cloning artifact	UNP P28845
C	19	HIS	-	cloning artifact	UNP P28845
C	20	GLN	-	cloning artifact	UNP P28845
C	21	GLN	-	cloning artifact	UNP P28845
C	22	PRO	-	cloning artifact	UNP P28845
C	23	LEU	-	cloning artifact	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
D	7	MET	-	initiating methionine	UNP P28845
D	8	LYS	-	cloning artifact	UNP P28845
D	9	HIS	-	cloning artifact	UNP P28845
D	10	GLN	-	cloning artifact	UNP P28845
D	11	HIS	-	cloning artifact	UNP P28845
D	12	GLN	-	cloning artifact	UNP P28845
D	13	HIS	-	cloning artifact	UNP P28845
D	14	GLN	-	cloning artifact	UNP P28845
D	15	HIS	-	cloning artifact	UNP P28845

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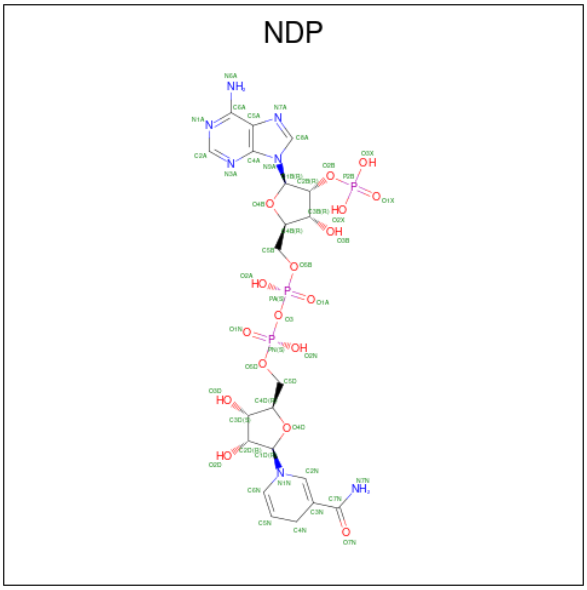
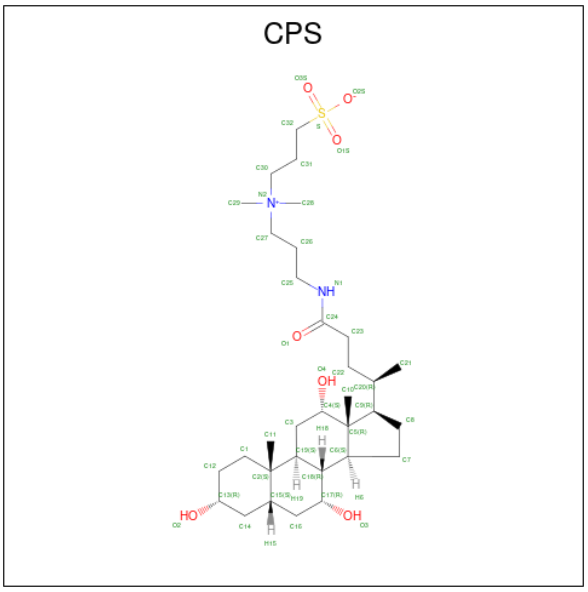
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	cloning artifact	UNP P28845
D	17	HIS	-	cloning artifact	UNP P28845
D	18	GLN	-	cloning artifact	UNP P28845
D	19	HIS	-	cloning artifact	UNP P28845
D	20	GLN	-	cloning artifact	UNP P28845
D	21	GLN	-	cloning artifact	UNP P28845
D	22	PRO	-	cloning artifact	UNP P28845
D	23	LEU	-	cloning artifact	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

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



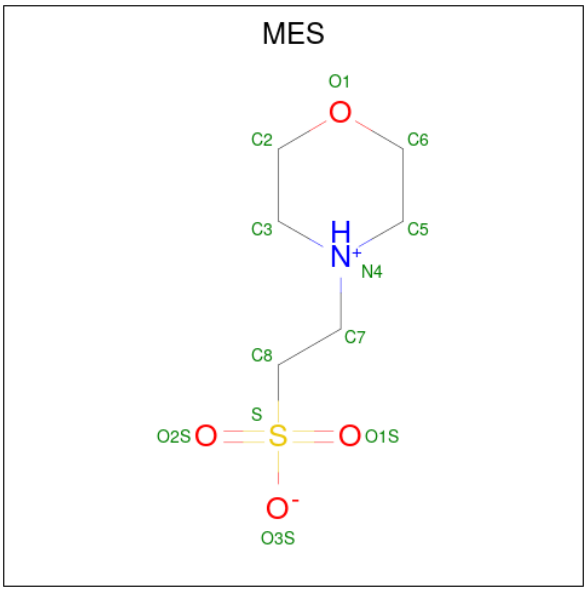
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
3	B	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
3	C	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
3	D	1	Total	C	N	O	S	0	0
			42	32	2	7	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	350	Total	O	0	0
			350	350		
5	B	293	Total	O	0	0
			293	293		
5	C	339	Total	O	0	0
			339	339		
5	D	277	Total	O	0	0
			277	277		

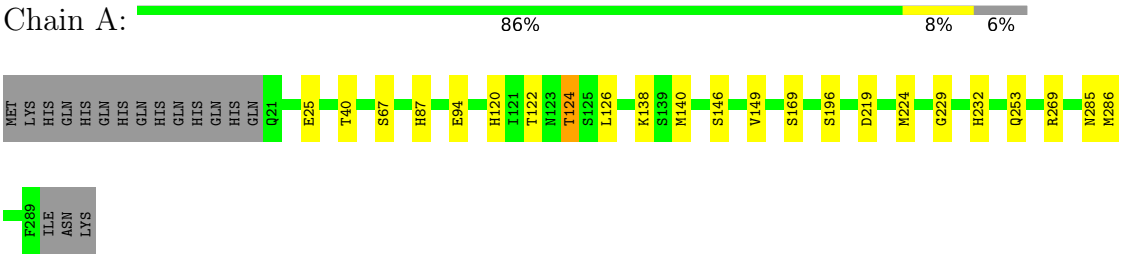
3 Residue-property plots (i)

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.

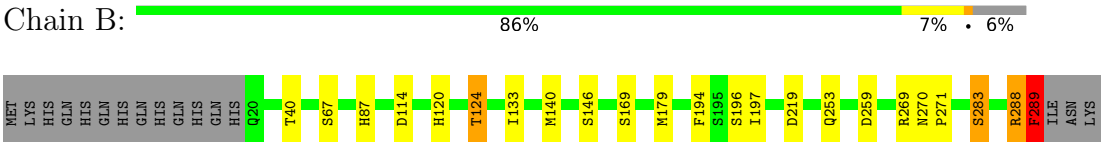
• Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain A:



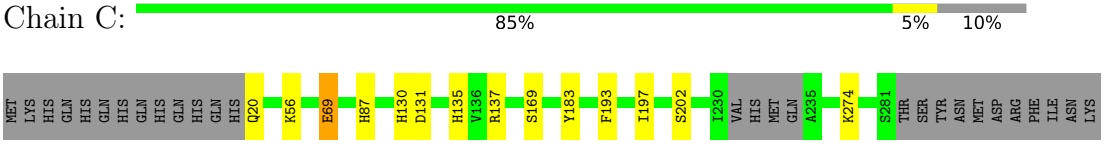
• Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain B:



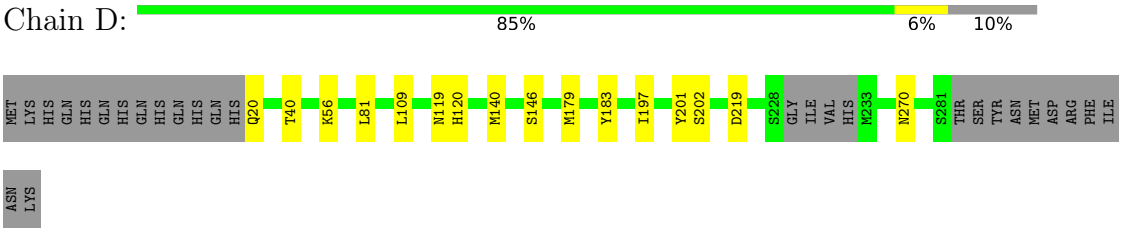
• Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain C:



• Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain D:



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	57.43Å 152.67Å 73.92Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55	Depositor
% Data completeness (in resolution range)	92.1 (20.00-1.55)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.157 , 0.181	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9889	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

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: CPS, MES, 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	0.45	0/2192	0.67	1/2960 (0.0%)
1	B	0.78	4/2205 (0.2%)	1.14	7/2977 (0.2%)
1	C	0.43	0/2087	0.65	0/2817
1	D	0.41	0/2101	0.63	1/2833 (0.0%)
All	All	0.54	4/8585 (0.0%)	0.80	9/11587 (0.1%)

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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	PHE	CD1-CE1	19.26	1.77	1.39
1	B	289	PHE	CB-CG	-15.72	1.24	1.51
1	B	289	PHE	CG-CD2	13.16	1.58	1.38
1	B	289	PHE	C-O	8.09	1.38	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	289	PHE	CB-CG-CD1	-35.98	95.61	120.80
1	B	289	PHE	CB-CG-CD2	32.85	143.80	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	289	PHE	CA-CB-CG	9.35	136.34	113.90
1	A	219	ASP	CB-CG-OD2	7.26	124.83	118.30
1	D	219	ASP	CB-CG-OD2	6.33	123.99	118.30
1	B	289	PHE	CG-CD1-CE1	6.09	127.50	120.80
1	B	219	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	114	ASP	CB-CG-OD2	5.63	123.36	118.30
1	B	259	ASP	CB-CG-OD2	5.34	123.11	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	SER	Peptide
1	B	169	SER	Peptide
1	C	169	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2109	0	2145	29	0
1	B	2121	0	2161	29	0
1	C	2012	0	2054	12	0
1	D	2016	0	2056	11	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
2	C	48	0	26	0	0
2	D	48	0	26	1	0
3	A	42	0	58	0	0
3	B	42	0	58	1	0
3	C	42	0	58	3	0
3	D	42	0	58	3	0
4	A	12	0	12	0	0
5	A	350	0	0	19	0
5	B	293	0	0	7	0
5	C	339	0	0	11	0
5	D	277	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9889	0	8764	79	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 5.

All (79) 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:B:289:PHE:CD1	1:B:289:PHE:CE1	1.77	1.67
1:A:126:LEU:HB2	1:B:289:PHE:CE1	1.42	1.52
1:A:126:LEU:CB	1:B:289:PHE:CE1	2.02	1.30
5:A:2739:HOH:O	1:B:289:PHE:CE1	1.98	1.16
5:A:2739:HOH:O	1:B:289:PHE:CD2	2.06	1.09
1:A:196[B]:SER:OG	5:A:1946:HOH:O	1.83	0.95
1:A:67[B]:SER:OG	5:A:1974:HOH:O	2.00	0.79
1:B:67[B]:SER:OG	5:B:1892:HOH:O	2.00	0.78
1:A:126:LEU:N	1:B:289:PHE:CE1	2.56	0.70
1:A:224:MET:O	1:A:232:HIS:HE1	1.75	0.69
1:B:253:GLN:OE1	5:B:2819:HOH:O	2.10	0.69
1:B:196[B]:SER:OG	5:B:1712:HOH:O	1.95	0.69
1:B:288:ARG:CG	1:B:289:PHE:H	2.05	0.69
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.79	0.66
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.79	0.66
1:A:126:LEU:O	1:B:289:PHE:CD1	2.50	0.64
1:A:124[B]:THR:CG2	5:A:2365:HOH:O	2.44	0.63
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.82	0.61
1:A:124[B]:THR:HG21	5:A:1548:HOH:O	2.02	0.60
1:A:94:GLU:CD	5:A:1820:HOH:O	2.40	0.59
1:A:124[B]:THR:HG21	5:A:2365:HOH:O	2.02	0.59
1:C:202[A]:SER:OG	5:C:532:HOH:O	2.16	0.58
1:D:197:ILE:C	5:D:533:HOH:O	2.41	0.58
1:B:124:THR:O	5:B:2529:HOH:O	2.17	0.58
1:B:288:ARG:CG	1:B:289:PHE:N	2.67	0.57
1:C:56:LYS:NZ	5:C:404:HOH:O	2.37	0.56
1:A:126:LEU:HB3	1:B:289:PHE:CE1	2.26	0.56
1:A:269:ARG:NE	5:A:2252:HOH:O	2.38	0.55
1:A:224:MET:O	1:A:232:HIS:CE1	2.58	0.55
5:A:2739:HOH:O	1:B:289:PHE:CD1	2.58	0.55
1:B:288:ARG:HG2	1:B:289:PHE:N	2.21	0.55
1:B:283:SER:HB2	5:B:2162:HOH:O	2.07	0.54
1:B:288:ARG:HG2	1:B:289:PHE:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLY:O	1:A:232:HIS:HD2	1.90	0.54
1:A:124[B]:THR:CG2	5:A:1548:HOH:O	2.57	0.53
1:D:120:HIS:HE1	1:D:146:SER:OG	1.91	0.53
1:A:140:MET:HB3	5:A:1708:HOH:O	2.09	0.52
1:A:120:HIS:HE1	1:A:146:SER:OG	1.93	0.52
1:B:120:HIS:HE1	1:B:146:SER:OG	1.93	0.52
1:B:87:HIS:HD2	5:B:1603:HOH:O	1.92	0.51
1:B:269:ARG:HG3	1:B:271:PRO:HD3	1.92	0.51
1:C:87:HIS:HD2	5:C:306:HOH:O	1.93	0.51
3:B:6:CPS:H4	3:B:6:CPS:H21A	1.93	0.51
1:A:286:MET:SD	1:B:179[B]:MET:HE3	2.51	0.50
3:C:293:CPS:H32	5:C:376:HOH:O	2.12	0.49
3:C:293:CPS:H4	3:C:293:CPS:H21A	1.96	0.47
1:C:135:HIS:HD2	5:C:372:HOH:O	1.96	0.47
1:D:140[A]:MET:HG2	5:D:314:HOH:O	2.14	0.46
1:A:124[B]:THR:HG23	5:A:2365:HOH:O	2.10	0.46
3:D:293:CPS:H21A	3:D:293:CPS:H4	1.98	0.46
1:C:69[A]:GLU:HG3	5:C:334:HOH:O	2.16	0.45
1:A:253:GLN:NE2	5:A:2092:HOH:O	2.50	0.45
1:B:140:MET:HE3	1:B:140:MET:HA	1.97	0.45
1:D:183:TYR:CZ	3:D:293:CPS:H16	2.51	0.45
1:C:137:ARG:NH1	5:C:373:HOH:O	2.48	0.45
1:C:274:LYS:HD2	5:C:440:HOH:O	2.17	0.44
1:A:122:THR:O	1:A:124[B]:THR:HG23	2.17	0.44
3:D:293:CPS:H29A	3:D:293:CPS:H31	1.82	0.44
1:D:179[B]:MET:HE3	5:D:535:HOH:O	2.18	0.44
1:A:138:LYS:NZ	5:A:2815:HOH:O	2.41	0.44
1:A:286:MET:SD	1:B:179[B]:MET:CE	3.06	0.43
1:D:56:LYS:HE2	1:D:81:LEU:HD22	2.00	0.43
1:B:194:PHE:HA	1:B:197[A]:ILE:HG12	2.01	0.43
1:A:87:HIS:HE1	5:A:2028:HOH:O	2.01	0.43
1:C:20:GLN:HA	5:C:532:HOH:O	2.17	0.42
1:D:201:TYR:CE2	5:D:533:HOH:O	2.71	0.42
1:C:130:HIS:N	5:C:370:HOH:O	2.53	0.42
1:C:183:TYR:CZ	3:C:293:CPS:H16	2.55	0.42
1:D:20:GLN:HA	5:D:434:HOH:O	2.20	0.42
1:D:202[A]:SER:OG	5:D:434:HOH:O	2.22	0.41
1:B:288:ARG:CD	1:B:289:PHE:H	2.32	0.41
1:C:193:PHE:CZ	1:C:197[B]:ILE:HD13	2.55	0.41
1:A:253:GLN:NE2	5:A:2822:HOH:O	2.51	0.41
1:D:119:ASN:ND2	2:D:4:NDP:H4D	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:HD2	5:A:1625:HOH:O	2.04	0.41
1:A:149:VAL:HG22	1:B:133:ILE:HD13	2.02	0.40
1:C:274:LYS:HE2	5:C:469:HOH:O	2.21	0.40
1:B:140:MET:HB3	5:B:2368:HOH:O	2.20	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	278/286 (97%)	268 (96%)	10 (4%)	0	100 100
1	B	280/286 (98%)	269 (96%)	10 (4%)	1 (0%)	34 14
1	C	264/286 (92%)	257 (97%)	7 (3%)	0	100 100
1	D	266/286 (93%)	257 (97%)	9 (3%)	0	100 100
All	All	1088/1144 (95%)	1051 (97%)	36 (3%)	1 (0%)	51 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	ARG

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	237/243 (98%)	233 (98%)	4 (2%)	60	32
1	B	239/243 (98%)	235 (98%)	4 (2%)	60	32
1	C	225/243 (93%)	222 (99%)	3 (1%)	69	44
1	D	228/243 (94%)	226 (99%)	2 (1%)	78	61
All	All	929/972 (96%)	916 (99%)	13 (1%)	71	41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	124[A]	THR
1	A	124[B]	THR
1	A	285	ASN
1	B	124	THR
1	B	270	ASN
1	B	283	SER
1	B	289	PHE
1	C	69[A]	GLU
1	C	69[B]	GLU
1	C	131	ASP
1	D	109	LEU
1	D	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	87	HIS
1	A	105	GLN
1	A	119	ASN
1	A	120	HIS
1	A	232	HIS
1	A	234	GLN
1	A	253	GLN
1	A	270	ASN
1	A	285	ASN
1	B	87	HIS
1	B	119	ASN
1	B	120	HIS
1	B	234	GLN

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Mol	Chain	Res	Type
1	B	270	ASN
1	C	87	HIS
1	C	119	ASN
1	C	135	HIS
1	C	270	ASN
1	D	119	ASN
1	D	120	HIS
1	D	135	HIS
1	D	270	ASN

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)

9 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	$\#\|Z\| > 2$
3	CPS	A	5	-	45,45,45	1.42	2 (4%)	69,70,70	1.13	5 (7%)
2	NDP	B	2	-	45,52,52	1.56	5 (11%)	53,80,80	1.63	12 (22%)
4	MES	A	293	-	12,12,12	1.76	1 (8%)	14,16,16	1.36	1 (7%)
2	NDP	C	3	-	45,52,52	1.54	5 (11%)	53,80,80	1.67	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CPS	C	293	-	45,45,45	1.37	1 (2%)	69,70,70	1.21	4 (5%)
3	CPS	D	293	-	45,45,45	1.12	1 (2%)	69,70,70	1.16	3 (4%)
2	NDP	A	1	-	45,52,52	1.56	4 (8%)	53,80,80	1.71	13 (24%)
3	CPS	B	6	-	45,45,45	1.32	2 (4%)	69,70,70	1.23	6 (8%)
2	NDP	D	4	-	45,52,52	1.61	4 (8%)	53,80,80	1.73	15 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CPS	A	5	-	-	0/25/90/90	0/4/4/4
2	NDP	B	2	-	-	6/30/77/77	0/5/5/5
4	MES	A	293	-	-	0/6/14/14	0/1/1/1
2	NDP	C	3	-	-	6/30/77/77	0/5/5/5
3	CPS	C	293	-	-	1/25/90/90	0/4/4/4
3	CPS	D	293	-	-	6/25/90/90	0/4/4/4
2	NDP	A	1	-	-	5/30/77/77	0/5/5/5
3	CPS	B	6	-	-	6/25/90/90	0/4/4/4
2	NDP	D	4	-	-	8/30/77/77	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5	CPS	C32-S	-8.04	1.66	1.77
3	C	293	CPS	C32-S	-7.95	1.66	1.77
3	B	6	CPS	C32-S	-7.55	1.66	1.77
3	D	293	CPS	C32-S	-6.45	1.68	1.77
2	D	4	NDP	C4A-N3A	5.89	1.43	1.35
2	A	1	NDP	C4N-C3N	-5.78	1.38	1.49
4	A	293	MES	C8-S	-5.75	1.69	1.77
2	B	2	NDP	C4N-C3N	-5.22	1.39	1.49
2	C	3	NDP	C4N-C3N	-5.06	1.40	1.49
2	D	4	NDP	C4N-C3N	-5.05	1.40	1.49
2	B	2	NDP	C4A-N3A	5.00	1.42	1.35
2	C	3	NDP	C4A-N3A	4.98	1.42	1.35
2	A	1	NDP	C4A-N3A	4.90	1.42	1.35
2	B	2	NDP	C4N-C5N	-3.99	1.38	1.48
2	A	1	NDP	C4N-C5N	-3.83	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	NDP	C4N-C5N	-3.83	1.38	1.48
2	C	3	NDP	C4N-C5N	-3.64	1.39	1.48
2	C	3	NDP	C6N-C5N	3.10	1.38	1.33
2	A	1	NDP	C6N-C5N	3.07	1.38	1.33
2	D	4	NDP	C6N-C5N	2.90	1.38	1.33
2	B	2	NDP	C6N-C5N	2.75	1.38	1.33
2	B	2	NDP	C2A-N3A	2.55	1.36	1.32
2	C	3	NDP	C3B-C2B	-2.22	1.48	1.52
3	B	6	CPS	C30-N2	-2.03	1.48	1.52
3	A	5	CPS	C30-N2	-2.01	1.48	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	293	CPS	O1S-S-C32	5.72	113.80	106.92
3	D	293	CPS	O3S-S-C32	5.24	113.22	106.92
2	A	1	NDP	O4D-C1D-N1N	4.39	116.64	108.06
2	D	4	NDP	N3A-C2A-N1A	-4.28	121.98	128.68
2	B	2	NDP	O4D-C1D-N1N	4.00	115.88	108.06
2	A	1	NDP	N3A-C2A-N1A	-3.75	122.81	128.68
4	A	293	MES	C5-N4-C3	3.74	117.26	108.83
2	C	3	NDP	C4A-C5A-N7A	-3.71	105.53	109.40
2	B	2	NDP	C4A-C5A-N7A	-3.70	105.54	109.40
2	C	3	NDP	O4D-C1D-N1N	3.69	115.27	108.06
2	D	4	NDP	O4D-C1D-N1N	3.55	115.00	108.06
2	D	4	NDP	C4A-C5A-N7A	-3.48	105.78	109.40
2	A	1	NDP	C3N-C2N-N1N	-3.40	118.24	123.10
2	C	3	NDP	C3N-C2N-N1N	-3.30	118.39	123.10
2	C	3	NDP	N3A-C2A-N1A	-3.29	123.54	128.68
2	D	4	NDP	O3B-C3B-C2B	-3.25	101.93	111.17
2	A	1	NDP	O3B-C3B-C2B	-3.21	102.06	111.17
3	A	5	CPS	C31-C32-S	-3.15	108.42	113.25
3	B	6	CPS	O3S-S-C32	3.11	110.66	106.92
3	B	6	CPS	O1S-S-C32	3.07	110.61	106.92
2	A	1	NDP	O3D-C3D-C2D	-3.06	101.92	111.82
3	A	5	CPS	C19-C18-C17	-3.01	108.28	111.88
2	B	2	NDP	O2B-C2B-C1B	2.98	120.82	110.10
2	C	3	NDP	O2B-C2B-C1B	2.93	120.64	110.10
2	D	4	NDP	O2D-C2D-C1D	2.92	119.77	110.02
3	B	6	CPS	C19-C18-C17	-2.87	108.45	111.88
3	B	6	CPS	C5-C9-C20	-2.83	116.12	119.50
2	C	3	NDP	O3B-C3B-C2B	-2.80	103.20	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	NDP	O2B-P2B-O1X	-2.80	98.60	109.39
2	B	2	NDP	C3N-C2N-N1N	-2.80	119.11	123.10
2	A	1	NDP	O2B-C2B-C1B	2.78	120.12	110.10
2	B	2	NDP	N3A-C2A-N1A	-2.78	124.33	128.68
2	C	3	NDP	O2D-C2D-C1D	2.72	119.11	110.02
2	D	4	NDP	C2A-N1A-C6A	2.71	123.39	118.75
2	A	1	NDP	O2D-C2D-C1D	2.70	119.04	110.02
3	A	5	CPS	O2S-S-C32	2.66	110.07	105.77
2	A	1	NDP	C2A-N1A-C6A	2.64	123.27	118.75
2	B	2	NDP	O3B-C3B-C4B	-2.63	103.46	111.05
2	B	2	NDP	O3B-C3B-C2B	-2.62	103.73	111.17
2	D	4	NDP	O2B-P2B-O1X	-2.60	99.37	109.39
2	B	2	NDP	O3D-C3D-C2D	-2.59	103.44	111.82
3	D	293	CPS	C19-C18-C17	-2.57	108.80	111.88
2	A	1	NDP	C4A-C5A-N7A	-2.54	106.75	109.40
2	D	4	NDP	C2B-C3B-C4B	2.50	107.43	101.99
2	B	2	NDP	O2D-C2D-C1D	2.49	118.35	110.02
3	B	6	CPS	C31-C32-S	-2.43	109.53	113.25
2	B	2	NDP	C2A-N1A-C6A	2.42	122.89	118.75
2	C	3	NDP	O3D-C3D-C2D	-2.36	104.20	111.82
2	D	4	NDP	O3D-C3D-C2D	-2.34	104.24	111.82
3	B	6	CPS	C29-N2-C30	-2.32	103.56	109.46
2	D	4	NDP	O3X-P2B-O2X	2.31	116.48	107.64
2	C	3	NDP	C2A-N1A-C6A	2.30	122.69	118.75
3	A	5	CPS	C19-C18-C6	2.28	112.85	109.71
2	A	1	NDP	O3D-C3D-C4D	-2.26	104.52	111.05
3	D	293	CPS	O1S-S-C32	2.23	109.60	106.92
3	C	293	CPS	C19-C18-C17	-2.22	109.22	111.88
3	A	5	CPS	O3S-S-C32	2.22	109.59	106.92
2	D	4	NDP	O3B-C3B-C4B	-2.21	104.65	111.05
2	C	3	NDP	C1D-N1N-C6N	-2.19	116.11	120.83
2	A	1	NDP	O3B-C3B-C4B	-2.18	104.75	111.05
2	D	4	NDP	C5B-C4B-C3B	-2.15	107.14	115.18
3	C	293	CPS	C19-C18-C6	2.11	112.61	109.71
2	A	1	NDP	C5B-C4B-C3B	-2.09	107.33	115.18
2	A	1	NDP	C2D-C3D-C4D	2.09	106.71	102.64
2	B	2	NDP	N6A-C6A-N1A	2.09	122.91	118.57
2	D	4	NDP	O2B-C2B-C1B	2.08	117.60	110.10
2	C	3	NDP	C2B-C3B-C4B	2.07	106.49	101.99
3	C	293	CPS	O2S-S-C32	2.05	109.08	105.77
2	D	4	NDP	C3N-C7N-N7N	2.03	121.27	117.67
2	D	4	NDP	O2N-PN-O1N	2.03	122.26	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NDP	O2N-PN-O1N	2.01	122.15	112.24

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NDP	O4D-C1D-N1N-C6N
2	B	2	NDP	O4D-C1D-N1N-C6N
2	C	3	NDP	O4D-C1D-N1N-C6N
2	D	4	NDP	O4D-C1D-N1N-C6N
3	C	293	CPS	C30-C31-C32-S
3	D	293	CPS	N2-C30-C31-C32
3	D	293	CPS	C30-C31-C32-S
3	D	293	CPS	C31-C30-N2-C28
3	D	293	CPS	C31-C30-N2-C29
3	B	6	CPS	C26-C27-N2-C30
3	D	293	CPS	C31-C30-N2-C27
2	A	1	NDP	C1B-C2B-O2B-P2B
2	B	2	NDP	C1B-C2B-O2B-P2B
3	B	6	CPS	C26-C27-N2-C29
3	B	6	CPS	C31-C32-S-O1S
3	B	6	CPS	C26-C27-N2-C28
2	B	2	NDP	C2B-O2B-P2B-O2X
2	D	4	NDP	C2B-O2B-P2B-O2X
2	A	1	NDP	PN-O3-PA-O1A
2	B	2	NDP	PN-O3-PA-O1A
2	C	3	NDP	C5D-O5D-PN-O1N
2	D	4	NDP	C5D-O5D-PN-O1N
2	D	4	NDP	O4B-C4B-C5B-O5B
3	D	293	CPS	C26-C25-N1-C24
2	B	2	NDP	O4B-C4B-C5B-O5B
2	C	3	NDP	C1B-C2B-O2B-P2B
2	C	3	NDP	O4B-C4B-C5B-O5B
3	B	6	CPS	C31-C32-S-O3S
2	C	3	NDP	C5D-O5D-PN-O3
2	D	4	NDP	C5D-O5D-PN-O3
2	D	4	NDP	PN-O3-PA-O1A
2	D	4	NDP	PN-O3-PA-O2A
2	A	1	NDP	C2N-C3N-C7N-N7N
2	B	2	NDP	C2N-C3N-C7N-N7N
2	C	3	NDP	C2N-C3N-C7N-N7N
2	D	4	NDP	C2N-C3N-C7N-N7N

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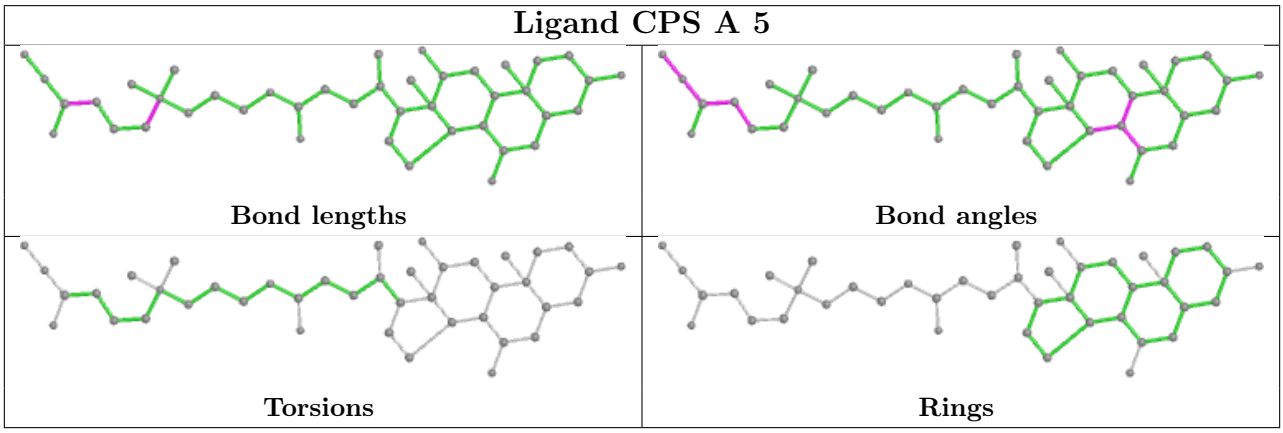
Mol	Chain	Res	Type	Atoms
2	A	1	NDP	O4B-C4B-C5B-O5B
3	B	6	CPS	C31-C32-S-O2S

There are no ring outliers.

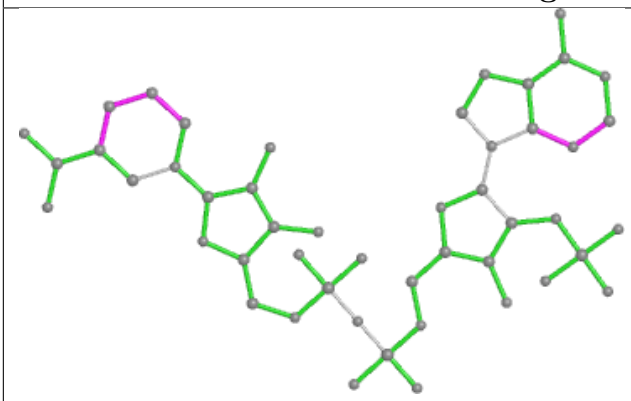
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	293	CPS	3	0
3	D	293	CPS	3	0
3	B	6	CPS	1	0
2	D	4	NDP	1	0

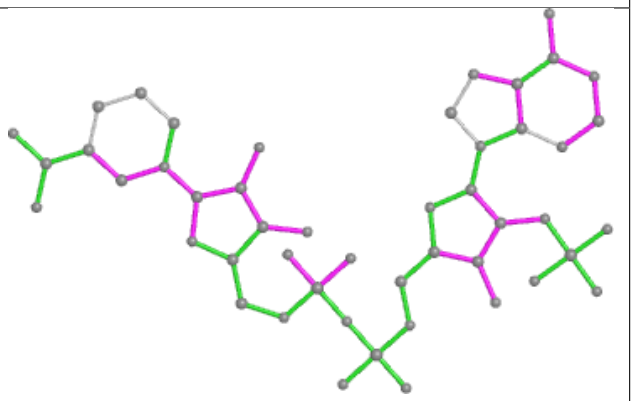
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



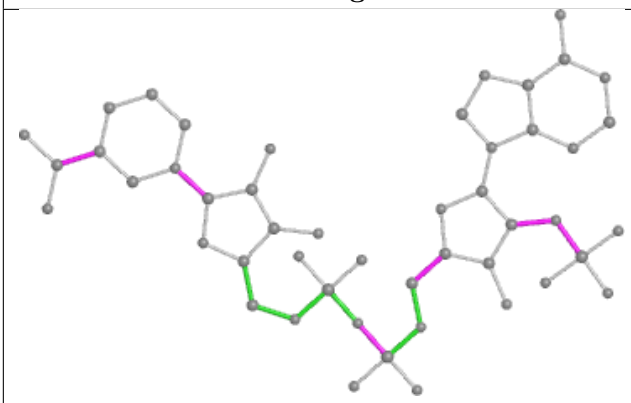
Ligand NDP B 2



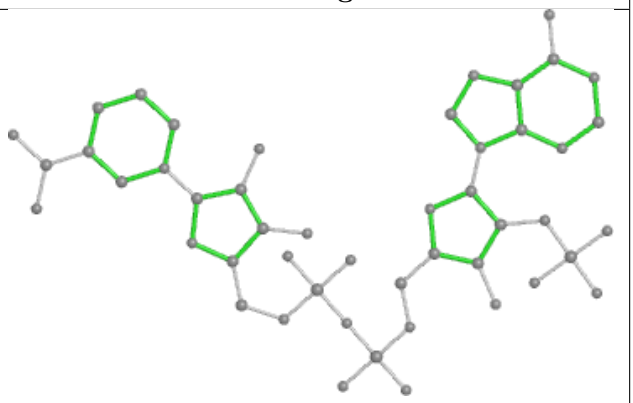
Bond lengths



Bond angles

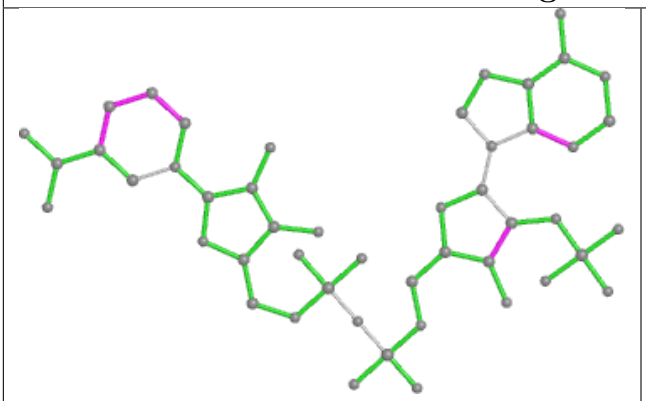


Torsions

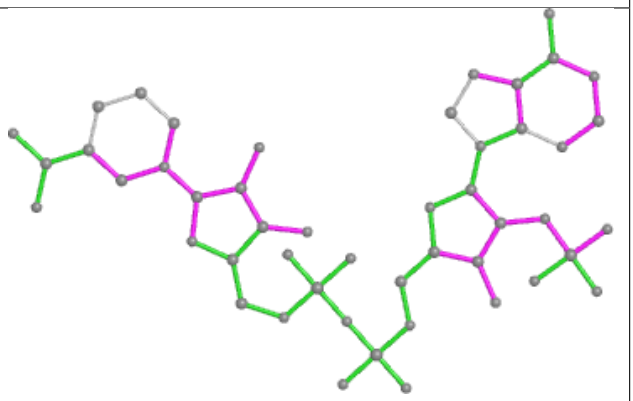


Rings

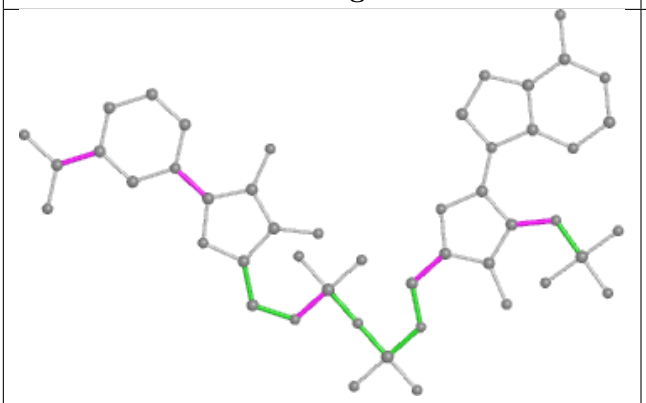
Ligand NDP C 3



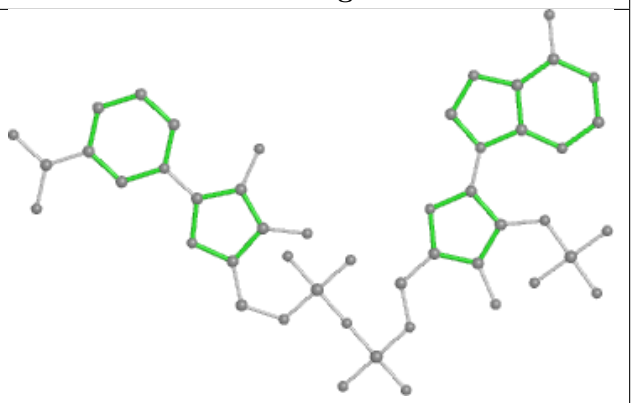
Bond lengths



Bond angles

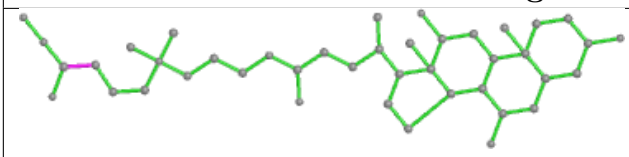


Torsions

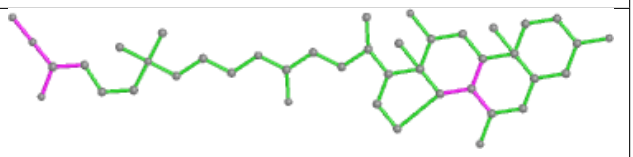


Rings

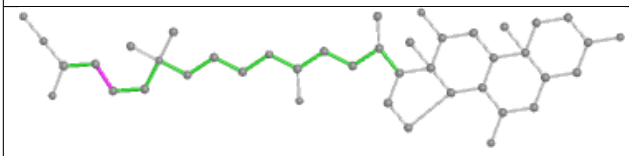
Ligand CPS C 293



Bond lengths



Bond angles



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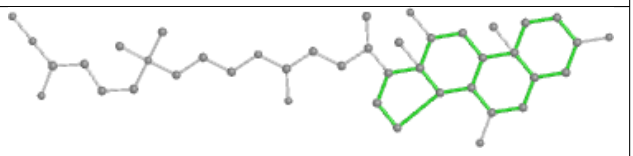
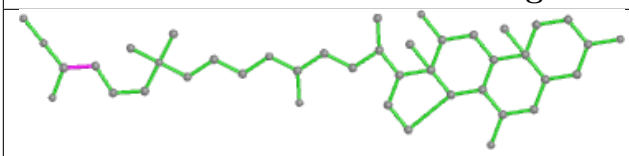


Rings

Ligand CPS D 293



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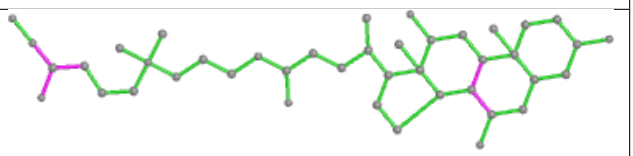
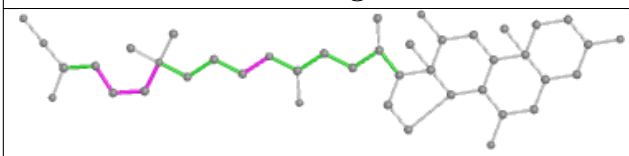
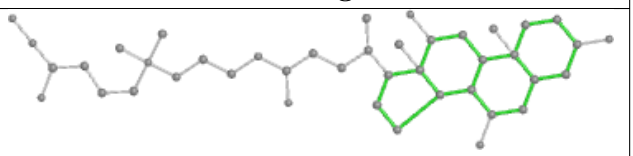


Bond angles

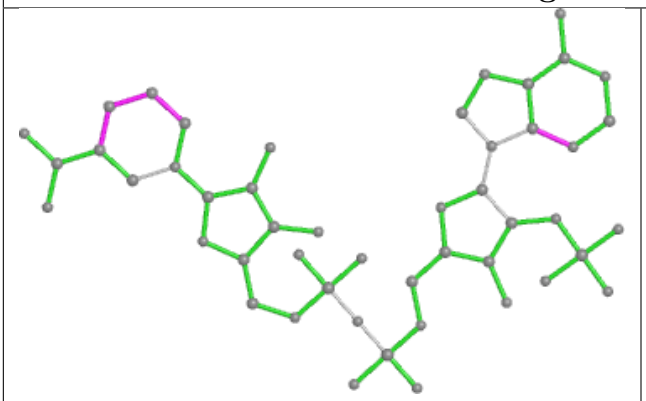


Torsions

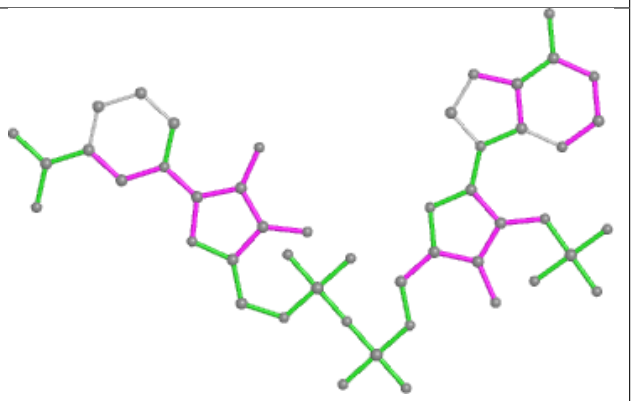


Rings

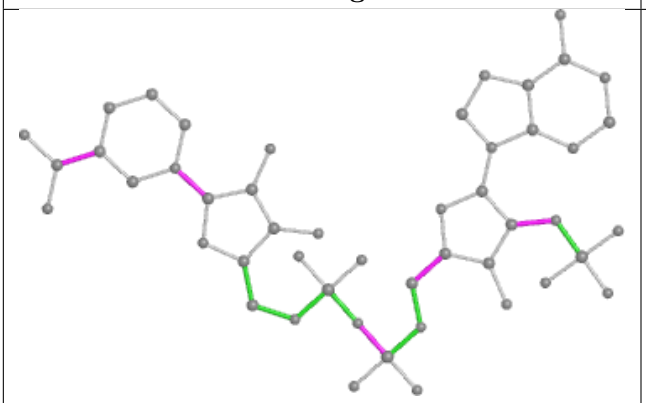
Ligand NDP A 1



Bond lengths



Bond angles



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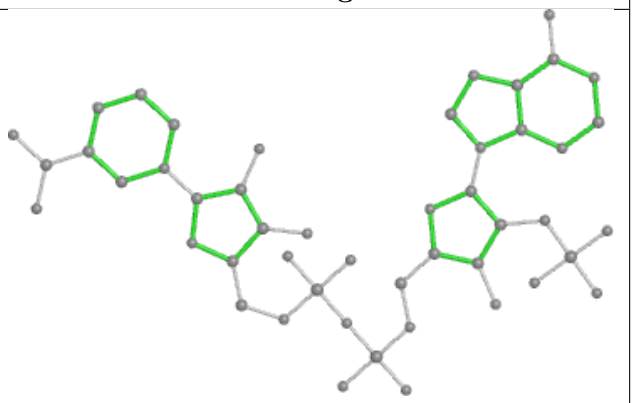
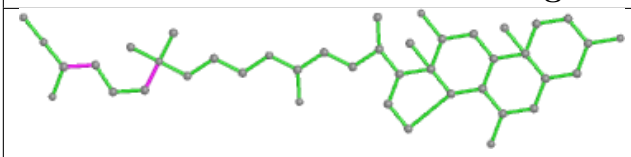


Rings

Ligand CPS B 6



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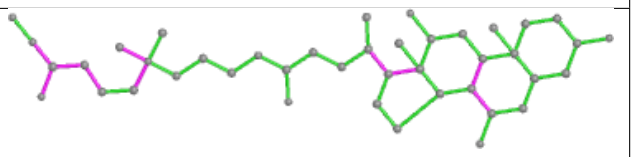
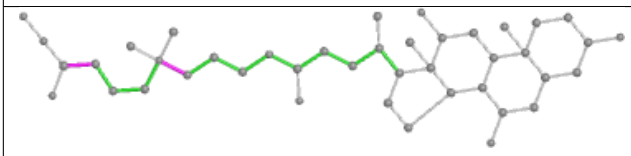
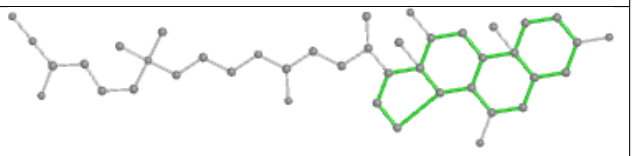


Bond angles

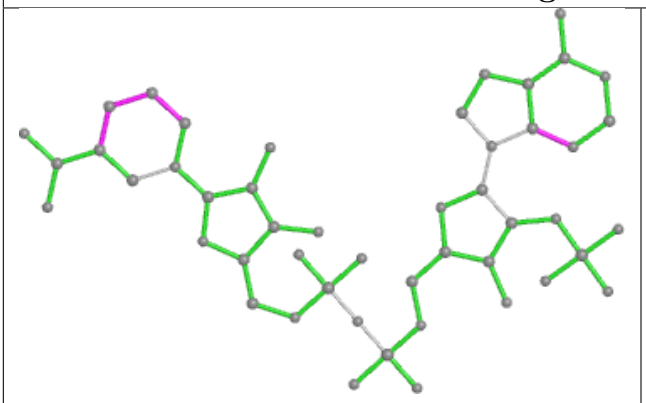


Torsions

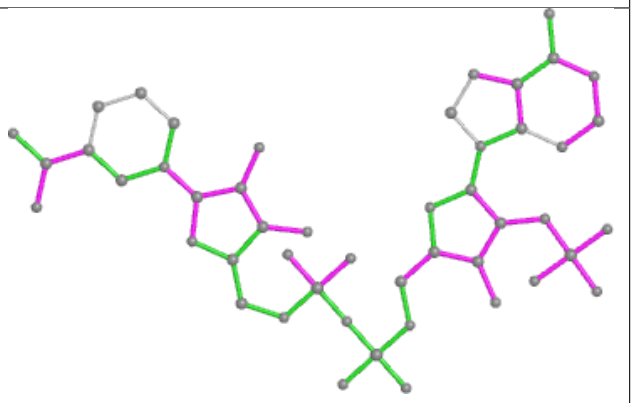


Rings

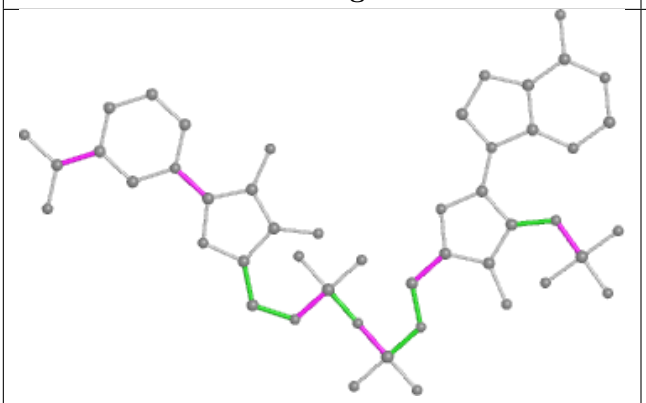
Ligand NDP D 4



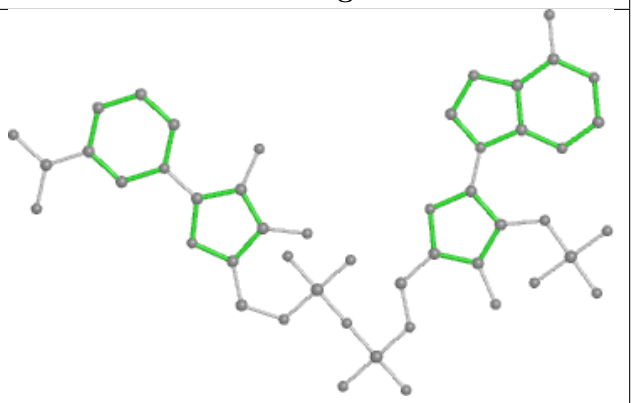
Bond lengths



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

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.