



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:22 PM UTC

PDB ID : 1XU7 / pdb_00001xu7
Title : Crystal Structure of the Interface Open Conformation of Tetrameric 11b-HSD1
Authors : Hosfield, D.J.; Wu, Y.; Skene, R.J.; Hilger, M.; Jennings, A.; Snell, G.P.; Aertgeerts, K.
Deposited on : 2004-10-25
Resolution : 1.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

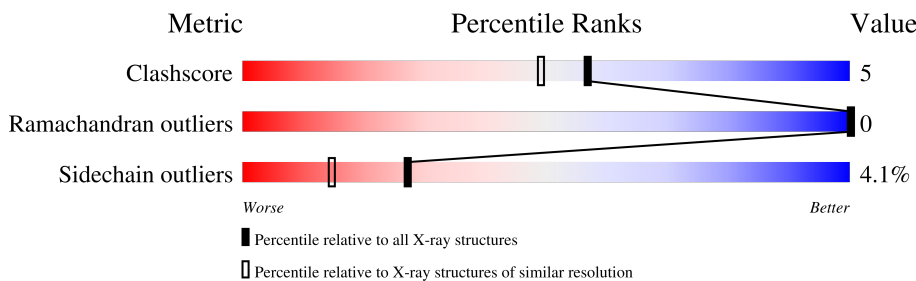
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	286	84% 8% 8%
1	B	286	81% 10% 8%
1	C	286	80% 11% 8%
1	D	286	80% 11% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8921 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	263	Total	C	N	O	S	0	10	0
			2014	1284	341	374	15			
1	B	262	Total	C	N	O	S	0	10	0
			2008	1281	340	372	15			
1	C	262	Total	C	N	O	S	0	9	0
			2008	1281	340	372	15			
1	D	261	Total	C	N	O	S	0	10	0
			2001	1277	339	370	15			

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

Continued on next page...

Continued from previous page...

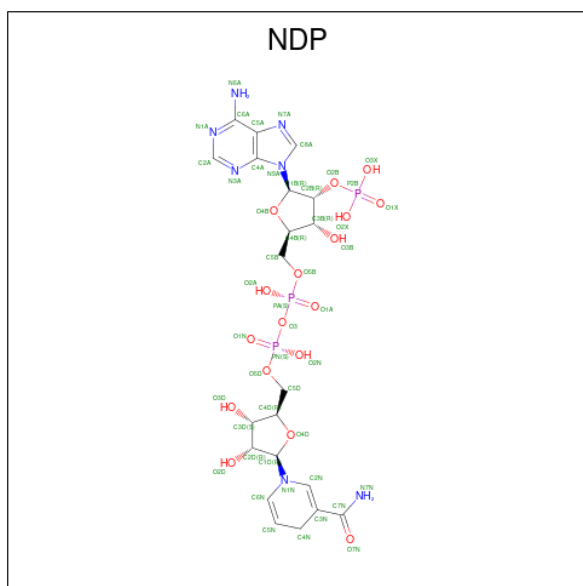
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	cloning artifact	UNP P28845
B	11	HIS	-	cloning artifact	UNP P28845
B	12	GLN	-	cloning artifact	UNP P28845
B	13	HIS	-	cloning artifact	UNP P28845
B	14	GLN	-	cloning artifact	UNP P28845
B	15	HIS	-	cloning artifact	UNP P28845
B	16	GLN	-	cloning 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

Continued on next page...

Continued from previous page...

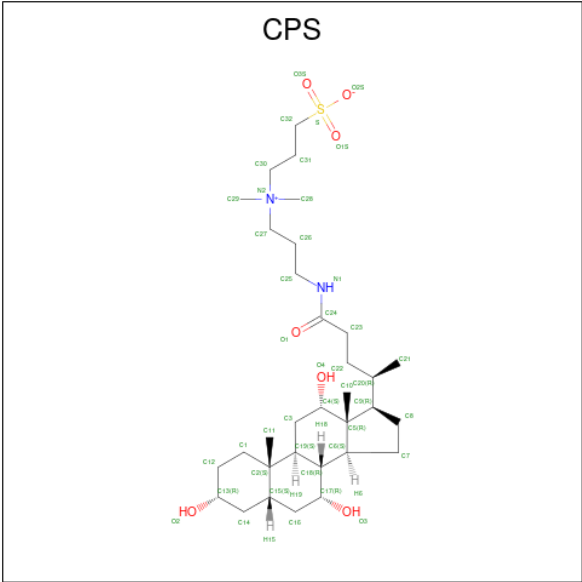
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	cloning artifact	UNP P28845
D	17	HIS	-	cloning artifact	UNP P28845
D	18	GLN	-	cloning artifact	UNP P28845
D	19	HIS	-	cloning artifact	UNP P28845
D	20	GLN	-	cloning artifact	UNP P28845
D	21	GLN	-	cloning artifact	UNP P28845
D	22	PRO	-	cloning 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 (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (CCD ID: 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	A	1	Total	C	O				0	0
			22	19	3					
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	C	1	Total	C	O				0	0
			22	19	3					
3	D	1	Total	C	N	O	S	0	0	
			42	32	2	7	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	113	Total	O	0	0
			113	113		
4	C	140	Total	O	0	0
			140	140		
4	D	104	Total	O	0	0
			104	104		

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.

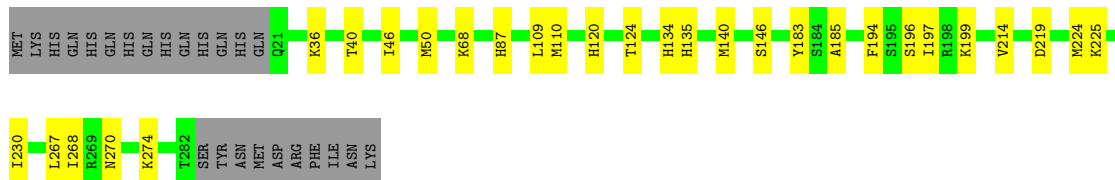
- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain A: 



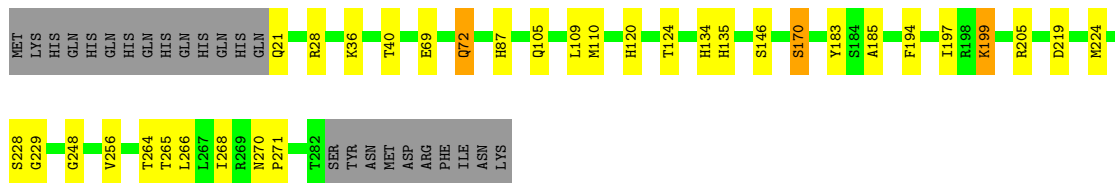
- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain B: 



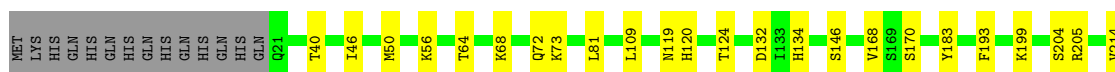
- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain C: 



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

Chain D: 





4 Data and refinement statistics

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	56.43Å 159.62Å 73.54Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.1 (20.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.197 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8921	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: NDP, CPS

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	0.37	0/2048	0.75	0/2766
1	B	0.38	0/2042	0.77	0/2758
1	C	0.38	0/2042	0.76	0/2758
1	D	0.37	0/2035	0.76	0/2748
All	All	0.37	0/8167	0.76	0/11030

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	A	2014	0	2041	15	0
1	B	2008	0	2036	15	0
1	C	2008	0	2038	20	0
1	D	2001	0	2029	14	0
2	A	48	0	26	0	0
2	B	48	0	26	1	0
2	C	48	0	24	4	0
2	D	48	0	24	5	0
3	A	64	0	88	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	58	3	0
3	C	64	0	88	5	0
3	D	42	0	58	3	0
4	A	129	0	0	2	0
4	B	113	0	0	3	0
4	C	140	0	0	4	0
4	D	104	0	0	1	0
All	All	8921	0	8536	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)
2:D:528:NDP:N3A	2:D:528:NDP:C4A	1.73	1.50
2:D:528:NDP:O5B	2:D:528:NDP:C5B	1.64	1.46
2:C:526:NDP:O3B	2:C:526:NDP:C3B	1.64	1.43
1:A:196[A]:SER:HB2	4:B:973:HOH:O	1.80	0.81
1:C:69:GLU:O	1:C:72:GLN:HG3	1.82	0.79
4:A:961:HOH:O	1:B:196[A]:SER:HB2	1.84	0.78
2:D:528:NDP:C4A	2:D:528:NDP:C2A	2.62	0.77
2:D:528:NDP:C5B	2:D:528:NDP:PA	2.73	0.76
2:C:526:NDP:O3B	2:C:526:NDP:C2B	2.34	0.75
1:A:224:MET:O	1:A:232:HIS:HE1	1.70	0.74
1:D:219:ASP:HA	1:D:224:MET:HE3	1.71	0.71
2:C:526:NDP:O3B	2:C:526:NDP:C4B	2.40	0.65
1:C:105:GLN:HG3	4:C:836:HOH:O	1.97	0.63
1:D:132:ASP:HB2	4:D:863:HOH:O	1.98	0.63
1:C:219:ASP:HA	1:C:224:MET:HE3	1.84	0.58
1:C:40:THR:OG1	1:C:120:HIS:HD2	1.85	0.58
2:C:526:NDP:C3B	2:C:526:NDP:HO3A	2.08	0.57
1:B:219:ASP:HA	1:B:224:MET:HE3	1.91	0.53
1:D:257:TYR:CE2	1:D:268:ILE:HD11	2.43	0.53
1:C:271:PRO:HB2	3:C:2:CPS:H7	1.91	0.53
1:A:219:ASP:HA	1:A:224:MET:HE3	1.90	0.52
1:D:120:HIS:HE1	1:D:146:SER:OG	1.92	0.52
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.91	0.52
3:B:525:CPS:H4	3:B:525:CPS:H21A	1.91	0.52
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.91	0.51
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PHE:HA	1:B:197:ILE:HG12	1.91	0.50
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.94	0.50
1:A:46:ILE:HG22	1:A:50:MET:HE2	1.94	0.49
1:B:120:HIS:HE1	1:B:146:SER:OG	1.96	0.49
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.96	0.48
1:C:265:THR:HA	1:C:268:ILE:HD12	1.94	0.48
1:C:185:ALA:HB2	1:D:193:PHE:HB2	1.96	0.48
1:C:228:SER:HA	1:C:229:GLY:HA2	1.62	0.47
1:C:248:GLY:HA3	1:C:256:VAL:CG2	2.44	0.47
1:C:120:HIS:HE1	1:C:146:SER:OG	1.96	0.47
1:A:266:LEU:HD23	3:C:2:CPS:H10	1.96	0.47
1:A:120:HIS:HE1	1:A:146:SER:OG	1.97	0.46
1:D:46:ILE:HG22	1:D:50:MET:HE2	1.96	0.46
1:C:134:HIS:CG	1:C:135:HIS:N	2.83	0.46
1:C:199:LYS:HE2	4:C:800:HOH:O	2.16	0.46
1:A:94:GLU:OE1	1:A:138:LYS:NZ	2.46	0.46
1:A:224:MET:O	1:A:232:HIS:CE1	2.61	0.46
2:D:528:NDP:N3A	2:D:528:NDP:H1B	2.32	0.45
1:B:274:LYS:HA	1:B:274:LYS:HD2	1.81	0.44
3:C:527:CPS:H29B	3:C:527:CPS:H261	1.84	0.44
3:C:527:CPS:H21A	3:C:527:CPS:H4	1.99	0.44
1:A:194:PHE:HA	1:A:197:ILE:HG12	1.99	0.44
1:A:229:GLY:O	1:A:232:HIS:HD2	2.01	0.44
1:D:214:VAL:HG11	1:D:268:ILE:HD13	2.00	0.44
3:B:525:CPS:H29A	3:B:525:CPS:H261	1.65	0.43
1:D:264:THR:O	1:D:268:ILE:HG23	2.18	0.43
1:D:40:THR:HA	1:D:64:THR:HG22	2.01	0.43
1:C:170:SER:HB3	4:C:801:HOH:O	2.18	0.43
1:D:183:TYR:CZ	3:D:529:CPS:H16	2.53	0.43
1:B:214:VAL:HG11	1:B:268:ILE:HG12	2.00	0.43
1:A:140:MET:HE2	1:B:140:MET:HE2	2.01	0.43
1:B:134:HIS:CG	1:B:135:HIS:N	2.87	0.43
1:C:270:ASN:C	1:C:270:ASN:HD22	2.27	0.42
1:C:36:LYS:HG2	1:C:110:MET:HB3	2.00	0.42
1:B:46:ILE:HG22	1:B:50:MET:HE2	2.01	0.42
2:B:524:NDP:H8A	4:B:642:HOH:O	2.19	0.42
1:A:170:SER:HB3	4:A:546:HOH:O	2.19	0.42
1:A:140:MET:HE3	1:A:140:MET:HA	2.00	0.42
1:B:36:LYS:HG2	1:B:110:MET:HB3	2.02	0.42
1:D:119:ASN:HD22	1:D:168:VAL:HG21	1.85	0.41
1:D:56:LYS:HE2	1:D:81:LEU:HD22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:523:CPS:H272	3:A:523:CPS:H31	1.78	0.41
1:B:183:TYR:CZ	3:B:525:CPS:H16	2.55	0.41
1:B:270:ASN:C	1:B:270:ASN:HD22	2.28	0.41
1:D:274:LYS:HA	1:D:274:LYS:HD2	1.86	0.41
3:D:529:CPS:H31A	3:D:529:CPS:H271	1.83	0.41
1:C:194:PHE:HA	1:C:197:ILE:HG12	2.02	0.41
1:C:264:THR:O	1:C:268:ILE:HG13	2.20	0.41
3:A:523:CPS:H4	3:A:523:CPS:H21A	2.02	0.41
1:B:87:HIS:HD2	4:B:808:HOH:O	2.04	0.41
1:C:183:TYR:CZ	3:C:527:CPS:H16	2.56	0.40
3:D:529:CPS:H4	3:D:529:CPS:H21A	2.02	0.40
1:C:87:HIS:HD2	4:C:818:HOH:O	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	261/286 (91%)	252 (97%)	9 (3%)	0	100	100
1	B	260/286 (91%)	249 (96%)	11 (4%)	0	100	100
1	C	260/286 (91%)	250 (96%)	10 (4%)	0	100	100
1	D	259/286 (91%)	249 (96%)	10 (4%)	0	100	100
All	All	1040/1144 (91%)	1000 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	220/243 (90%)	214 (97%)	6 (3%)	39	27
1	B	219/243 (90%)	212 (97%)	7 (3%)	34	22
1	C	219/243 (90%)	210 (96%)	9 (4%)	27	15
1	D	218/243 (90%)	204 (94%)	14 (6%)	16	6
All	All	876/972 (90%)	840 (96%)	36 (4%)	27	15

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	26	GLU
1	A	204[A]	SER
1	A	266	LEU
1	A	268	ILE
1	A	269	ARG
1	B	68	LYS
1	B	109	LEU
1	B	124[A]	THR
1	B	199	LYS
1	B	225	LYS
1	B	230	ILE
1	B	267	LEU
1	C	21	GLN
1	C	28	ARG
1	C	72	GLN
1	C	109	LEU
1	C	124[A]	THR
1	C	170	SER
1	C	199	LYS
1	C	205	ARG
1	C	266	LEU
1	D	68	LYS
1	D	72	GLN
1	D	73	LYS
1	D	109	LEU
1	D	124[A]	THR
1	D	134	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	170	SER
1	D	199	LYS
1	D	204[A]	SER
1	D	205	ARG
1	D	262	LEU
1	D	268	ILE
1	D	276	LEU
1	D	281	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) 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	270	ASN
1	B	77	HIS
1	B	119	ASN
1	B	120	HIS
1	B	270	ASN
1	C	24	ASN
1	C	77	HIS
1	C	105	GLN
1	C	119	ASN
1	C	120	HIS
1	C	270	ASN
1	D	21	GLN
1	D	87	HIS
1	D	105	GLN
1	D	119	ASN
1	D	120	HIS
1	D	160	GLN
1	D	270	ASN

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](#)

10 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	C	527	-	45,45,45	2.03	11 (24%)	70,70,70	1.06	4 (5%)
3	CPS	A	1	-	25,25,45	0.57	0	39,41,70	1.45	9 (23%)
3	CPS	C	2	-	25,25,45	0.57	0	39,41,70	1.09	2 (5%)
3	CPS	B	525	-	45,45,45	1.89	11 (24%)	70,70,70	1.18	6 (8%)
2	NDP	C	526	-	51,52,52	4.58	26 (50%)	71,80,80	2.29	19 (26%)
2	NDP	A	522	-	51,52,52	3.95	24 (47%)	71,80,80	2.34	18 (25%)
2	NDP	B	524	-	51,52,52	4.16	28 (54%)	71,80,80	2.40	19 (26%)
2	NDP	D	528	-	51,52,52	5.41	35 (68%)	71,80,80	2.33	18 (25%)
3	CPS	A	523	-	45,45,45	1.96	10 (22%)	70,70,70	1.01	4 (5%)
3	CPS	D	529	-	45,45,45	1.90	11 (24%)	70,70,70	1.03	4 (5%)

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	C	527	-	-	2/25/90/90	0/4/4/4
3	CPS	A	1	-	-	-	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CPS	C	2	-	-	-	0/4/4/4
3	CPS	B	525	-	-	5/25/90/90	0/4/4/4
2	NDP	C	526	-	-	3/34/77/77	0/5/5/5
2	NDP	A	522	-	-	5/34/77/77	0/5/5/5
2	NDP	B	524	-	-	6/34/77/77	0/5/5/5
2	NDP	D	528	-	-	7/34/77/77	0/5/5/5
3	CPS	A	523	-	-	4/25/90/90	0/4/4/4
3	CPS	D	529	-	-	4/25/90/90	0/4/4/4

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	528	NDP	C4A-N3A	21.10	1.73	1.34
2	C	526	NDP	C4A-N3A	15.27	1.63	1.34
2	D	528	NDP	C3B-C2B	-12.67	1.25	1.53
2	C	526	NDP	C2A-N1A	12.56	1.56	1.33
2	B	524	NDP	C4A-N3A	11.20	1.55	1.34
2	D	528	NDP	C4A-N9A	-10.67	1.15	1.37
2	B	524	NDP	C3B-C2B	-10.36	1.30	1.53
2	B	524	NDP	C5A-C4A	-10.13	1.21	1.39
2	A	522	NDP	C3B-C2B	-9.76	1.31	1.53
2	C	526	NDP	C3B-C2B	-9.55	1.32	1.53
2	D	528	NDP	C5A-N7A	-9.38	1.22	1.39
2	A	522	NDP	C2A-N3A	9.21	1.50	1.33
2	C	526	NDP	C4A-N9A	-8.97	1.19	1.37
2	D	528	NDP	C5A-C4A	-8.78	1.23	1.39
2	B	524	NDP	C4A-N9A	-8.70	1.19	1.37
2	C	526	NDP	O3B-C3B	8.63	1.64	1.43
2	C	526	NDP	C5A-N7A	-8.46	1.23	1.39
2	C	526	NDP	C4N-C5N	-8.30	1.27	1.49
2	A	522	NDP	C5A-N7A	-8.30	1.23	1.39
2	A	522	NDP	C4A-N3A	7.85	1.49	1.34
2	D	528	NDP	P2B-O2X	-7.72	1.26	1.54
2	A	522	NDP	PN-O3	7.70	1.67	1.59
2	A	522	NDP	C5A-C4A	-7.57	1.25	1.39
3	C	527	CPS	C32-S	-7.53	1.67	1.77
2	A	522	NDP	C5A-C6A	7.36	1.61	1.41
2	D	528	NDP	C4N-C5N	-7.25	1.30	1.49
3	D	529	CPS	C32-S	-7.23	1.67	1.77
2	B	524	NDP	C5A-C6A	7.16	1.60	1.41
2	D	528	NDP	C2A-N1A	7.14	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	522	NDP	C4A-N9A	-6.87	1.23	1.37
2	B	524	NDP	C5A-N7A	-6.82	1.26	1.39
3	A	523	CPS	C32-S	-6.50	1.68	1.77
2	B	524	NDP	C6N-N1N	6.49	1.53	1.37
3	B	525	CPS	C32-S	-6.38	1.68	1.77
2	C	526	NDP	C5A-C4A	-6.29	1.27	1.39
2	D	528	NDP	O3B-C3B	6.29	1.58	1.43
2	D	528	NDP	C5A-C6A	6.22	1.58	1.41
2	A	522	NDP	O3B-C3B	6.03	1.57	1.43
2	A	522	NDP	C8A-N7A	5.99	1.43	1.31
2	C	526	NDP	C5A-C6A	5.77	1.57	1.41
2	D	528	NDP	C1D-N1N	-5.56	1.31	1.46
2	B	524	NDP	C4N-C5N	-5.53	1.34	1.49
2	D	528	NDP	PA-O3	5.41	1.65	1.59
2	D	528	NDP	O5B-C5B	5.17	1.64	1.44
2	B	524	NDP	C2A-N3A	5.12	1.43	1.33
2	A	522	NDP	C4N-C5N	-4.94	1.36	1.49
2	B	524	NDP	P2B-O2B	4.87	1.68	1.59
2	B	524	NDP	C1D-N1N	-4.86	1.33	1.46
3	C	527	CPS	C3-C19	4.85	1.61	1.53
2	D	528	NDP	O4D-C4D	4.85	1.55	1.45
2	A	522	NDP	C2D-C3D	-4.81	1.40	1.53
2	B	524	NDP	C2D-C3D	-4.74	1.40	1.53
2	C	526	NDP	C2A-N3A	-4.74	1.25	1.33
2	B	524	NDP	PA-O2A	-4.71	1.33	1.55
2	D	528	NDP	C2D-C3D	-4.66	1.40	1.53
2	C	526	NDP	P2B-O2X	-4.63	1.37	1.54
2	D	528	NDP	P2B-O2B	4.58	1.67	1.59
2	D	528	NDP	C6A-N6A	4.53	1.45	1.34
2	B	524	NDP	PN-O3	-4.48	1.54	1.59
2	B	524	NDP	O3B-C3B	4.41	1.53	1.43
3	A	523	CPS	C3-C19	4.36	1.60	1.53
2	D	528	NDP	C6A-N1A	4.33	1.47	1.35
2	D	528	NDP	C6N-C5N	4.30	1.46	1.33
2	C	526	NDP	P2B-O1X	-4.27	1.37	1.50
2	A	522	NDP	O3D-C3D	4.25	1.53	1.43
2	A	522	NDP	PA-O3	-4.24	1.54	1.59
2	B	524	NDP	O3D-C3D	4.14	1.53	1.43
3	B	525	CPS	C3-C19	4.04	1.60	1.53
2	C	526	NDP	O4D-C4D	3.96	1.53	1.45
2	D	528	NDP	C2B-C1B	3.95	1.62	1.53
2	D	528	NDP	C2N-C3N	3.92	1.46	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	524	NDP	C2B-C1B	3.91	1.62	1.53
2	C	526	NDP	C8A-N7A	3.86	1.39	1.31
2	A	522	NDP	O4B-C4B	3.79	1.53	1.45
3	C	527	CPS	C20-C9	3.74	1.60	1.54
3	D	529	CPS	C20-C9	3.67	1.60	1.54
3	B	525	CPS	C20-C9	3.62	1.60	1.54
3	A	523	CPS	C20-C9	3.54	1.60	1.54
2	B	524	NDP	C3D-C4D	-3.46	1.44	1.53
2	C	526	NDP	C6N-C5N	3.44	1.43	1.33
2	A	522	NDP	C3D-C4D	-3.44	1.44	1.53
3	C	527	CPS	C10-C5	3.42	1.59	1.54
2	D	528	NDP	PA-O2A	-3.35	1.39	1.55
2	D	528	NDP	PN-O2N	-3.34	1.39	1.55
3	B	525	CPS	C18-C19	3.33	1.60	1.53
2	A	522	NDP	C2B-C1B	3.28	1.61	1.53
3	D	529	CPS	C2-C15	3.27	1.60	1.55
2	D	528	NDP	C2D-C1D	3.25	1.63	1.53
3	C	527	CPS	C18-C19	3.21	1.60	1.53
3	A	523	CPS	C5-C4	3.20	1.59	1.54
2	D	528	NDP	C8A-N7A	3.18	1.37	1.31
2	B	524	NDP	PA-O3	3.18	1.62	1.59
3	D	529	CPS	C3-C19	3.18	1.58	1.53
2	B	524	NDP	C8A-N7A	3.17	1.37	1.31
3	A	523	CPS	C18-C19	3.16	1.59	1.53
3	C	527	CPS	C2-C15	3.11	1.60	1.55
3	D	529	CPS	C16-C15	3.08	1.58	1.53
2	C	526	NDP	PA-O1A	-3.08	1.40	1.50
3	A	523	CPS	C16-C15	3.06	1.58	1.53
3	C	527	CPS	C16-C17	3.04	1.58	1.52
2	D	528	NDP	O3D-C3D	3.03	1.50	1.43
2	C	526	NDP	PA-O5B	-3.01	1.47	1.59
2	C	526	NDP	C3B-C4B	-2.95	1.45	1.53
2	D	528	NDP	P2B-O1X	-2.94	1.41	1.50
2	D	528	NDP	PA-O5B	-2.94	1.47	1.59
3	A	523	CPS	C2-C15	2.93	1.60	1.55
2	C	526	NDP	C5B-C4B	2.92	1.60	1.51
2	C	526	NDP	O3D-C3D	2.88	1.50	1.43
2	B	524	NDP	P2B-O2X	-2.86	1.44	1.54
2	A	522	NDP	C7N-C3N	-2.80	1.42	1.48
3	B	525	CPS	C8-C9	2.79	1.60	1.54
2	D	528	NDP	O4D-C1D	2.78	1.48	1.42
3	A	523	CPS	C16-C17	2.77	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	525	CPS	C5-C6	-2.73	1.50	1.55
2	D	528	NDP	C2A-N3A	-2.73	1.29	1.33
2	B	524	NDP	C5B-C4B	2.71	1.59	1.51
3	B	525	CPS	C5-C4	2.70	1.58	1.54
2	C	526	NDP	C6N-N1N	2.70	1.43	1.37
3	C	527	CPS	C5-C4	2.68	1.58	1.54
3	A	523	CPS	C8-C9	2.64	1.59	1.54
3	A	523	CPS	C14-C15	2.63	1.58	1.53
2	C	526	NDP	C2D-C3D	-2.63	1.46	1.53
3	B	525	CPS	C16-C17	2.60	1.57	1.52
3	C	527	CPS	C14-C15	2.59	1.57	1.53
3	D	529	CPS	C10-C5	2.55	1.58	1.54
2	A	522	NDP	C1B-N9A	-2.55	1.39	1.46
2	C	526	NDP	C2N-C3N	2.51	1.42	1.35
2	B	524	NDP	O4D-C4D	2.50	1.50	1.45
3	D	529	CPS	C16-C17	2.48	1.57	1.52
3	D	529	CPS	C18-C19	2.45	1.58	1.53
3	D	529	CPS	C5-C6	-2.42	1.51	1.55
2	C	526	NDP	PA-O2A	-2.39	1.44	1.55
3	B	525	CPS	C16-C15	2.38	1.57	1.53
3	B	525	CPS	C14-C15	2.38	1.57	1.53
3	D	529	CPS	C8-C9	2.37	1.59	1.54
3	B	525	CPS	C2-C15	2.37	1.59	1.55
3	D	529	CPS	C3-C4	2.35	1.57	1.53
2	C	526	NDP	C2B-C1B	2.32	1.58	1.53
2	A	522	NDP	PN-O2N	-2.31	1.44	1.55
2	D	528	NDP	C3D-C4D	-2.30	1.47	1.53
2	B	524	NDP	C6A-N6A	2.29	1.40	1.34
2	B	524	NDP	C6N-C5N	2.28	1.40	1.33
2	B	524	NDP	C2N-C3N	2.24	1.41	1.35
3	C	527	CPS	C16-C15	2.20	1.57	1.53
2	A	522	NDP	C6N-C5N	2.20	1.39	1.33
2	D	528	NDP	O4B-C1B	-2.16	1.37	1.42
2	D	528	NDP	PN-O3	2.16	1.61	1.59
3	C	527	CPS	C8-C9	2.13	1.58	1.54
2	B	524	NDP	C2D-C1D	2.12	1.60	1.53
2	A	522	NDP	C2D-C1D	-2.10	1.46	1.53
2	C	526	NDP	O5D-C5D	2.09	1.52	1.44
2	D	528	NDP	P2B-O3X	-2.09	1.47	1.54
2	A	522	NDP	O5B-C5B	2.07	1.52	1.44
2	D	528	NDP	C7N-C3N	-2.07	1.44	1.48
2	B	524	NDP	PN-O2N	-2.07	1.45	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	522	NDP	P2B-O2X	-2.02	1.47	1.54

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	528	NDP	C5A-C4A-N9A	9.23	115.87	105.81
2	B	524	NDP	C5A-C4A-N9A	9.06	115.69	105.81
2	A	522	NDP	C5A-C4A-N9A	8.75	115.35	105.81
2	C	526	NDP	C5A-C4A-N9A	8.54	115.12	105.81
2	D	528	NDP	N9A-C8A-N7A	-6.72	104.40	113.94
2	A	522	NDP	N9A-C8A-N7A	-6.58	104.59	113.94
2	B	524	NDP	N9A-C8A-N7A	-6.42	104.82	113.94
2	B	524	NDP	N3A-C2A-N1A	-6.40	118.89	128.58
2	C	526	NDP	N9A-C8A-N7A	-6.02	105.39	113.94
2	A	522	NDP	N3A-C2A-N1A	-6.02	119.47	128.58
2	C	526	NDP	N3A-C2A-N1A	-6.01	119.48	128.58
2	B	524	NDP	O4D-C1D-N1N	5.91	119.36	108.08
2	A	522	NDP	O4B-C1B-N9A	5.60	118.84	108.09
2	D	528	NDP	N3A-C2A-N1A	-5.51	120.25	128.58
2	B	524	NDP	O4B-C1B-N9A	5.47	118.59	108.09
2	C	526	NDP	O4B-C1B-N9A	5.25	118.18	108.09
2	D	528	NDP	O4D-C1D-N1N	5.24	118.09	108.08
2	C	526	NDP	O4D-C1D-N1N	4.98	117.58	108.08
2	D	528	NDP	O4B-C1B-N9A	4.56	116.84	108.09
2	A	522	NDP	O4D-C1D-N1N	4.47	116.61	108.08
2	D	528	NDP	C2D-C3D-C4D	4.06	110.46	102.61
2	A	522	NDP	C2B-C3B-C4B	3.90	110.38	101.99
2	C	526	NDP	C2B-C3B-C4B	3.88	110.34	101.99
2	A	522	NDP	O3B-C3B-C4B	-3.80	100.17	111.08
2	B	524	NDP	O3D-C3D-C4D	-3.79	100.19	111.08
2	A	522	NDP	C3N-C2N-N1N	-3.61	117.90	123.20
2	B	524	NDP	O3B-C3B-C4B	-3.58	100.80	111.08
2	D	528	NDP	C2B-C3B-C4B	3.52	109.57	101.99
3	D	529	CPS	C9-C5-C4	-3.50	114.52	117.67
2	B	524	NDP	C2D-C3D-C4D	3.48	109.33	102.61
3	B	525	CPS	C9-C5-C4	-3.45	114.56	117.67
2	B	524	NDP	C2B-C3B-C4B	3.44	109.40	101.99
2	D	528	NDP	O3D-C3D-C4D	-3.44	101.21	111.08
2	A	522	NDP	C5A-C4A-N3A	-3.43	121.99	126.72
2	C	526	NDP	C2A-N3A-C4A	3.42	120.19	111.83
2	A	522	NDP	C2D-C3D-C4D	3.41	109.20	102.61
2	C	526	NDP	O3D-C3D-C4D	-3.40	101.30	111.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	522	NDP	O3D-C3D-C4D	-3.37	101.40	111.08
2	D	528	NDP	C3D-C2D-C1D	3.36	107.82	101.46
3	C	527	CPS	C9-C5-C4	-3.34	114.66	117.67
2	C	526	NDP	O3B-C3B-C4B	-3.26	101.72	111.08
2	D	528	NDP	C5A-C4A-N3A	-3.25	122.24	126.72
2	C	526	NDP	C5A-C4A-N3A	-3.22	122.28	126.72
2	D	528	NDP	C3N-C2N-N1N	-3.19	118.53	123.20
2	D	528	NDP	C2A-N3A-C4A	3.18	119.60	111.83
2	B	524	NDP	C2A-N3A-C4A	3.18	119.60	111.83
2	B	524	NDP	C3N-C2N-N1N	-3.17	118.56	123.20
2	B	524	NDP	N3A-C4A-N9A	-3.15	121.81	127.17
2	A	522	NDP	C3B-C2B-C1B	3.15	108.84	102.81
2	D	528	NDP	O3B-C3B-C4B	-3.13	102.10	111.08
2	A	522	NDP	C2A-N3A-C4A	3.12	119.46	111.83
2	D	528	NDP	N3A-C4A-N9A	-3.10	121.89	127.17
2	D	528	NDP	C3B-C2B-C1B	3.08	108.71	102.81
2	B	524	NDP	C5A-C4A-N3A	-3.06	122.51	126.72
2	C	526	NDP	C2D-C3D-C4D	3.01	108.43	102.61
2	C	526	NDP	C3N-C2N-N1N	-2.98	118.83	123.20
3	A	1	CPS	C16-C15-C14	-2.93	107.88	111.23
2	A	522	NDP	C3D-C2D-C1D	2.88	106.91	101.46
2	A	522	NDP	O3D-C3D-C2D	-2.85	102.68	111.82
3	B	525	CPS	C25-N1-C24	2.83	128.09	122.82
2	A	522	NDP	O3B-C3B-C2B	-2.82	103.28	111.19
2	C	526	NDP	O3D-C3D-C2D	-2.81	102.79	111.82
3	C	527	CPS	C3-C19-C18	2.78	115.01	110.89
3	B	525	CPS	C7-C6-C5	2.77	106.23	103.54
2	B	524	NDP	O3D-C3D-C2D	-2.74	103.04	111.82
2	D	528	NDP	O3D-C3D-C2D	-2.71	103.13	111.82
2	C	526	NDP	N3A-C4A-N9A	-2.69	122.59	127.17
2	A	522	NDP	N3A-C4A-N9A	-2.66	122.65	127.17
2	B	524	NDP	C3D-C2D-C1D	2.65	106.47	101.46
2	C	526	NDP	C3B-C2B-C1B	2.63	107.85	102.81
3	B	525	CPS	C3-C19-C18	2.61	114.76	110.89
2	C	526	NDP	C3D-C2D-C1D	2.61	106.39	101.46
3	A	1	CPS	C1-C2-C15	2.57	111.43	107.75
2	B	524	NDP	O3B-C3B-C2B	-2.51	104.15	111.19
2	C	526	NDP	O2B-P2B-O1X	-2.46	100.55	109.33
3	A	1	CPS	C14-C15-C2	2.45	115.27	112.66
2	C	526	NDP	O3B-C3B-C2B	-2.45	104.33	111.19
2	C	526	NDP	C6N-N1N-C2N	2.44	121.93	119.32
3	A	1	CPS	C16-C15-C2	2.38	115.19	112.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	CPS	C3-C19-C18	2.38	114.42	110.89
3	A	1	CPS	C3-C19-C18	2.37	114.41	110.89
3	A	523	CPS	C7-C6-C5	2.36	105.83	103.54
2	B	524	NDP	C1D-N1N-C6N	-2.35	115.80	120.77
2	B	524	NDP	C3B-C2B-C1B	2.35	107.31	102.81
3	D	529	CPS	C7-C6-C5	2.35	105.82	103.54
3	A	1	CPS	C11-C2-C15	-2.34	106.52	110.44
3	C	2	CPS	C10-C5-C6	2.34	115.91	111.68
3	A	523	CPS	C9-C5-C4	-2.33	115.57	117.67
3	C	527	CPS	C7-C6-C5	2.28	105.75	103.54
3	D	529	CPS	C3-C19-C18	2.27	114.25	110.89
3	A	1	CPS	C10-C5-C6	2.26	115.78	111.68
3	C	527	CPS	C31-C32-S	-2.25	109.80	113.25
3	A	523	CPS	O1S-S-C32	2.24	110.12	106.73
3	A	1	CPS	C19-C18-C17	-2.24	109.04	111.86
2	D	528	NDP	C1D-N1N-C6N	-2.20	116.11	120.77
3	D	529	CPS	O2S-S-C32	2.20	110.31	106.00
3	A	523	CPS	C3-C19-C18	2.17	114.11	110.89
3	A	1	CPS	C11-C2-C1	-2.16	104.87	108.31
2	B	524	NDP	O2N-PN-O1N	2.14	122.41	112.44
3	B	525	CPS	O2S-S-C32	2.01	109.93	106.00
2	D	528	NDP	P2B-O2B-C2B	-2.00	118.08	123.43
2	A	522	NDP	O2N-PN-O1N	2.00	121.77	112.44
3	B	525	CPS	C5-C9-C20	-2.00	117.06	119.48

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	528	NDP	O4D-C1D-N1N-C6N
3	A	523	CPS	N2-C30-C31-C32
3	D	529	CPS	C26-C27-N2-C30
3	B	525	CPS	C26-C25-N1-C24
3	B	525	CPS	C26-C27-N2-C28
3	D	529	CPS	C26-C27-N2-C29
3	B	525	CPS	C26-C27-N2-C29
3	D	529	CPS	C26-C27-N2-C28
2	A	522	NDP	O4D-C1D-N1N-C6N
2	B	524	NDP	O4D-C1D-N1N-C6N
2	C	526	NDP	O4D-C1D-N1N-C6N
3	D	529	CPS	N1-C25-C26-C27
3	B	525	CPS	C26-C27-N2-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	525	CPS	C25-C26-C27-N2
2	A	522	NDP	C1B-C2B-O2B-P2B
3	A	523	CPS	C31-C32-S-O3S
3	A	523	CPS	C26-C25-N1-C24
3	C	527	CPS	N1-C25-C26-C27
2	A	522	NDP	PN-O3-PA-O1A
2	B	524	NDP	PN-O3-PA-O1A
3	A	523	CPS	N1-C25-C26-C27
3	C	527	CPS	C26-C25-N1-C24
2	B	524	NDP	C2B-O2B-P2B-O2X
2	D	528	NDP	C2B-O2B-P2B-O2X
2	A	522	NDP	C2N-C3N-C7N-N7N
2	B	524	NDP	C2N-C3N-C7N-N7N
2	C	526	NDP	C2N-C3N-C7N-N7N
2	D	528	NDP	C2N-C3N-C7N-N7N
2	D	528	NDP	PN-O3-PA-O1A
2	D	528	NDP	PN-O3-PA-O2A
2	C	526	NDP	O4B-C4B-C5B-O5B
2	A	522	NDP	C2B-O2B-P2B-O2X
2	D	528	NDP	C2B-O2B-P2B-O3X
2	D	528	NDP	C2B-O2B-P2B-O1X
2	B	524	NDP	C1B-C2B-O2B-P2B
2	B	524	NDP	PN-O3-PA-O2A

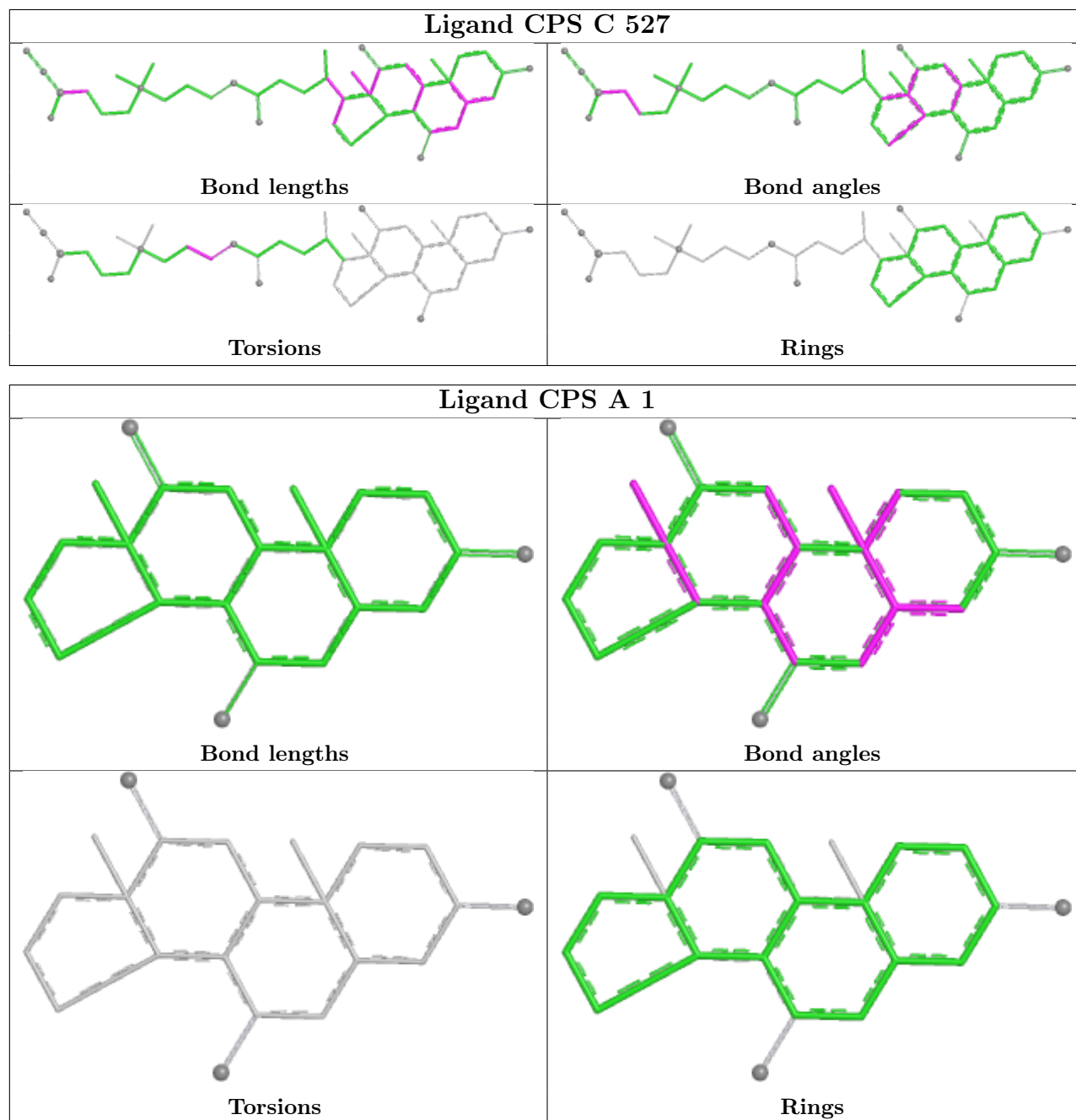
There are no ring outliers.

8 monomers are involved in 23 short contacts:

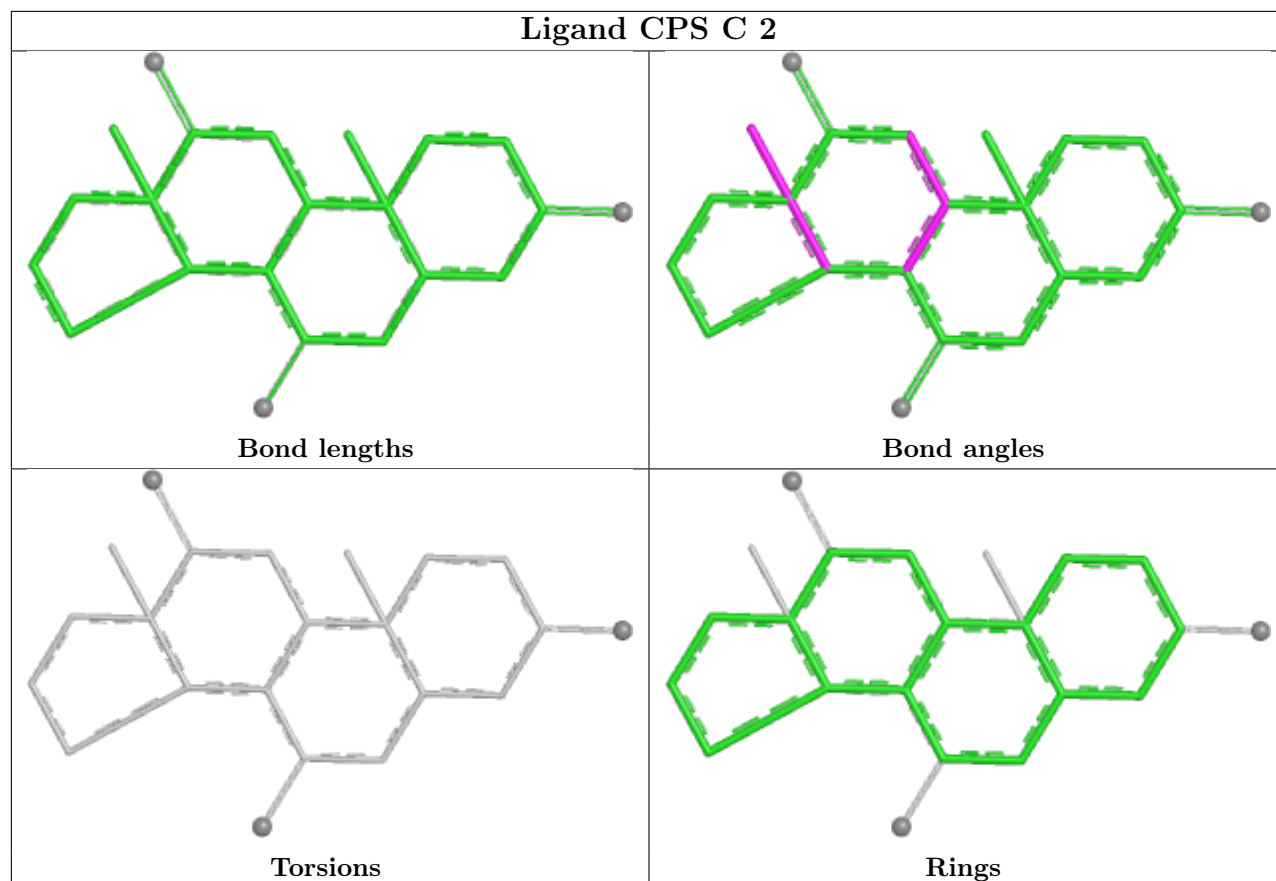
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	527	CPS	3	0
3	C	2	CPS	2	0
3	B	525	CPS	3	0
2	C	526	NDP	4	0
2	B	524	NDP	1	0
2	D	528	NDP	5	0
3	A	523	CPS	2	0
3	D	529	CPS	3	0

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.

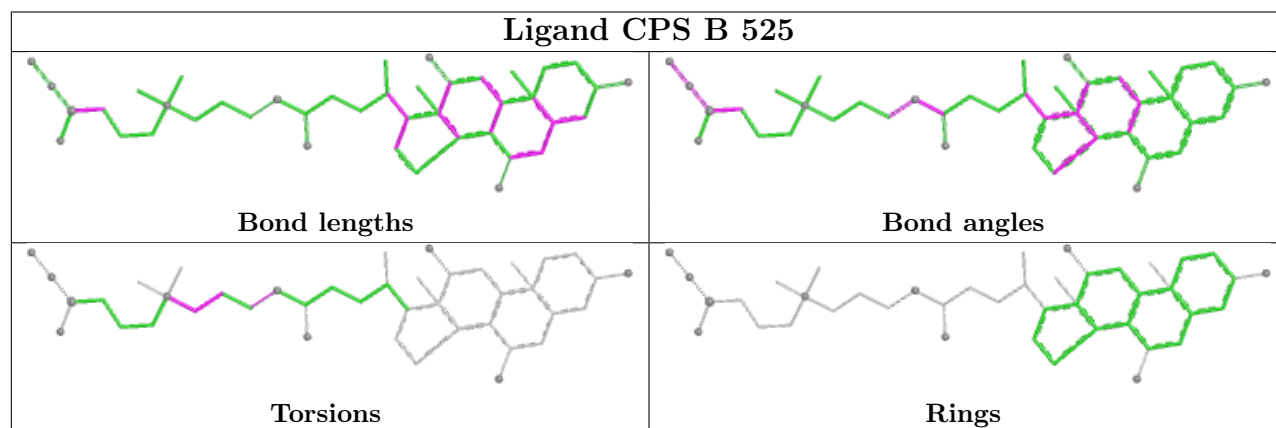
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

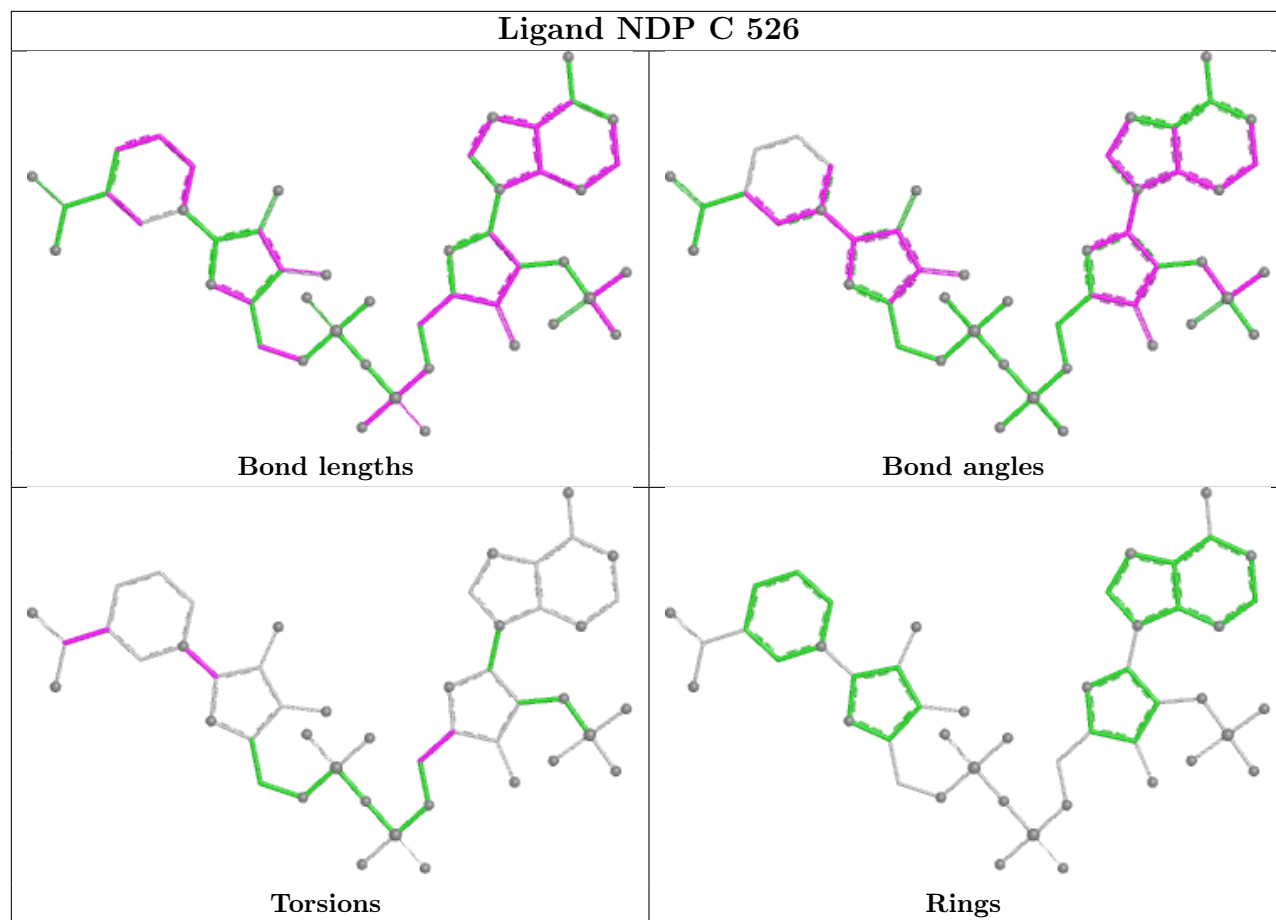


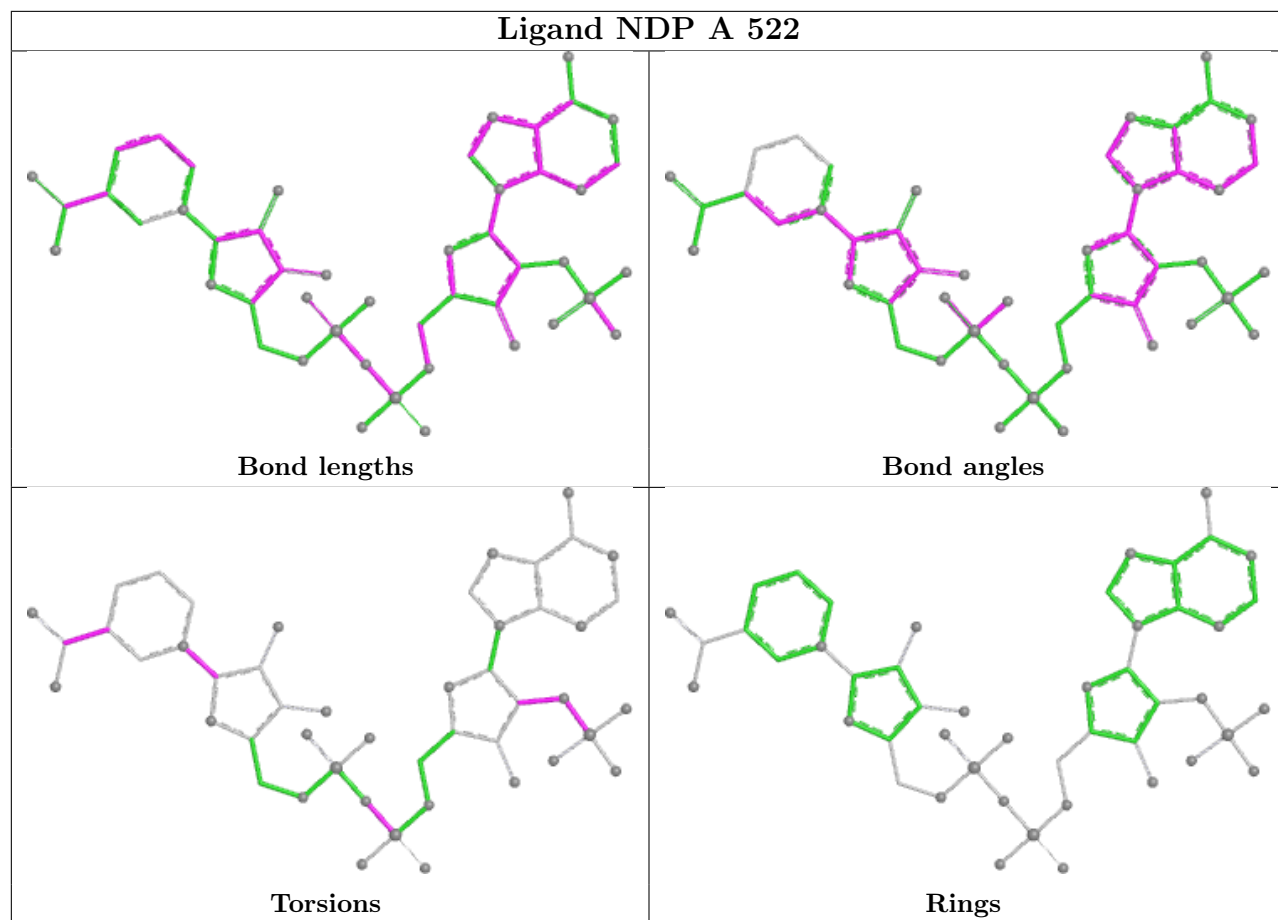
Ligand CPS C 2

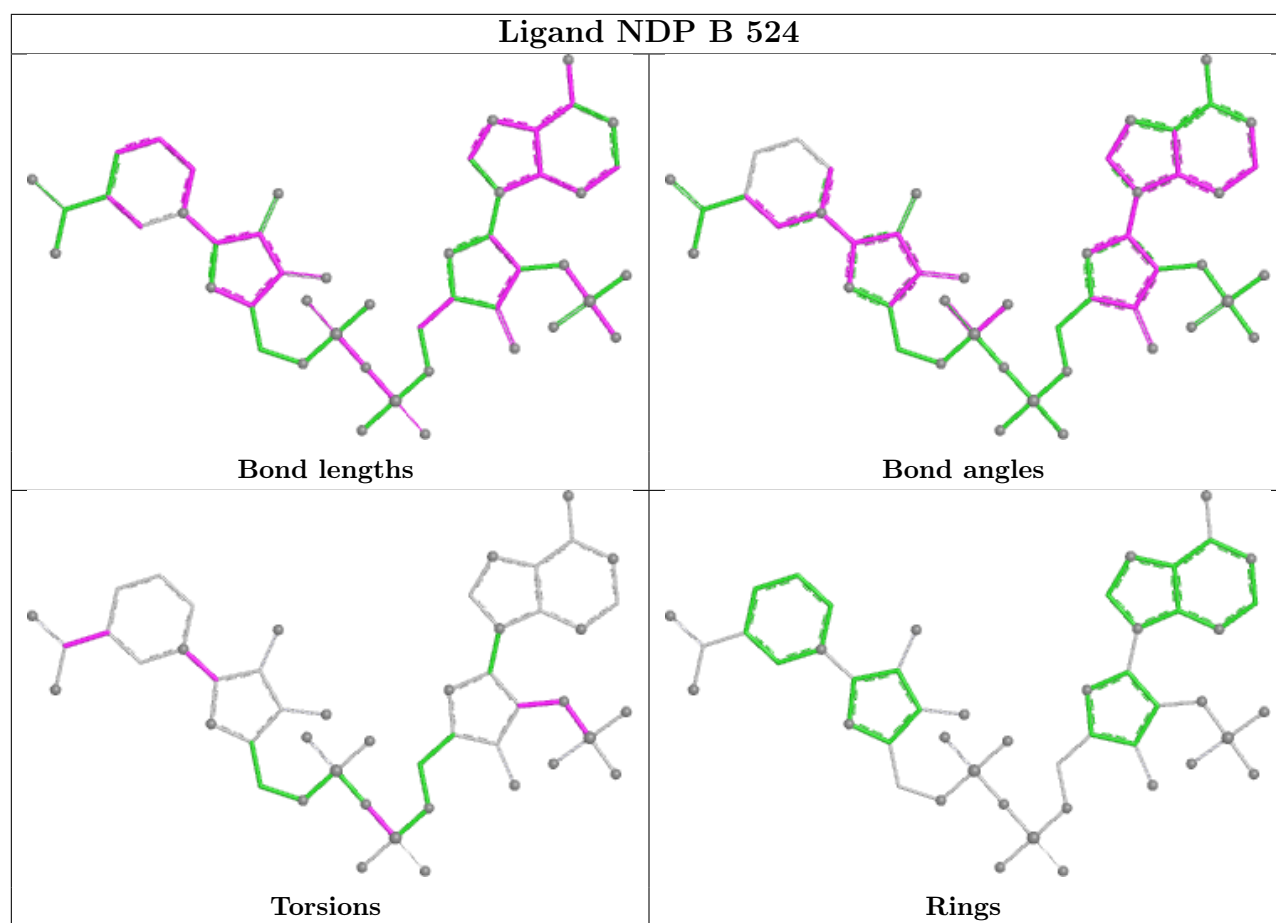


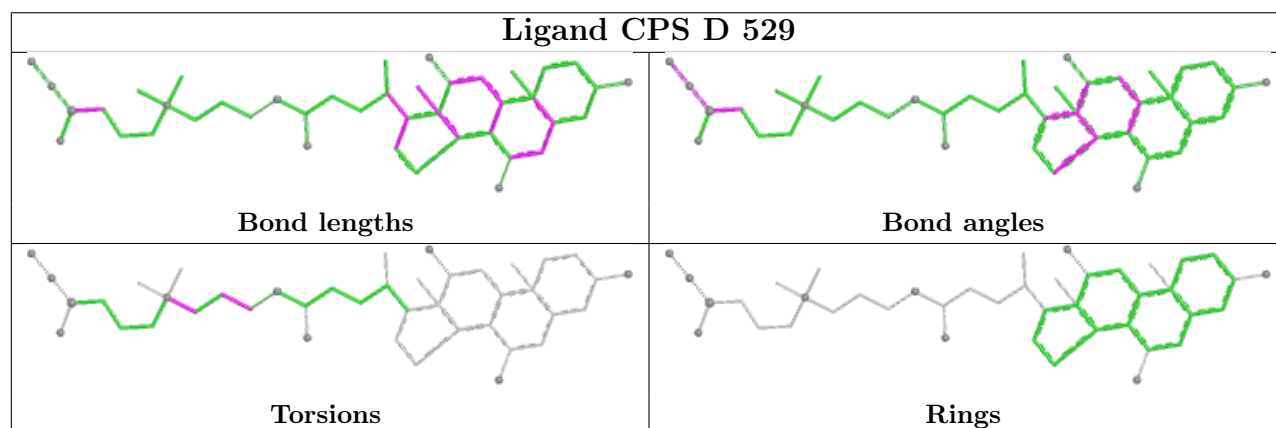
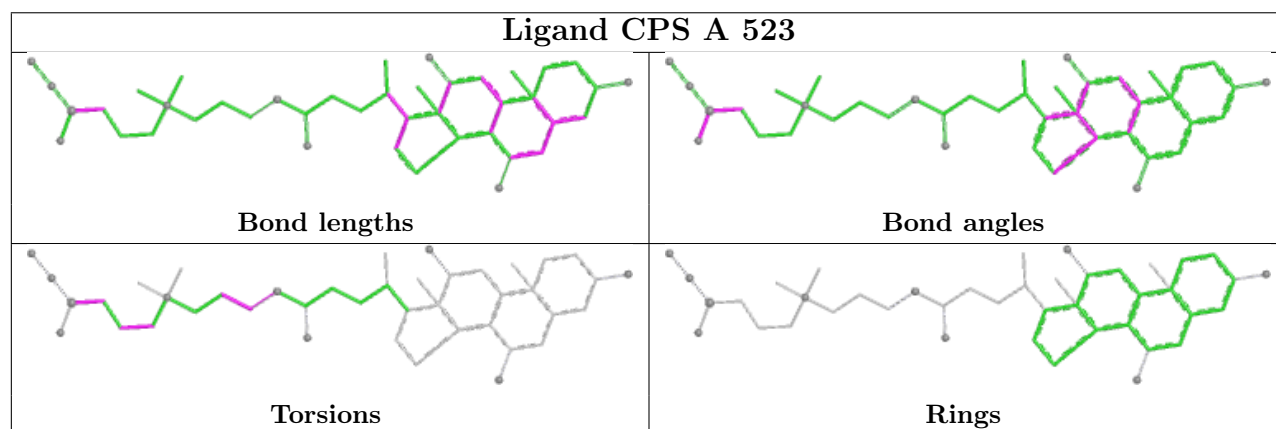
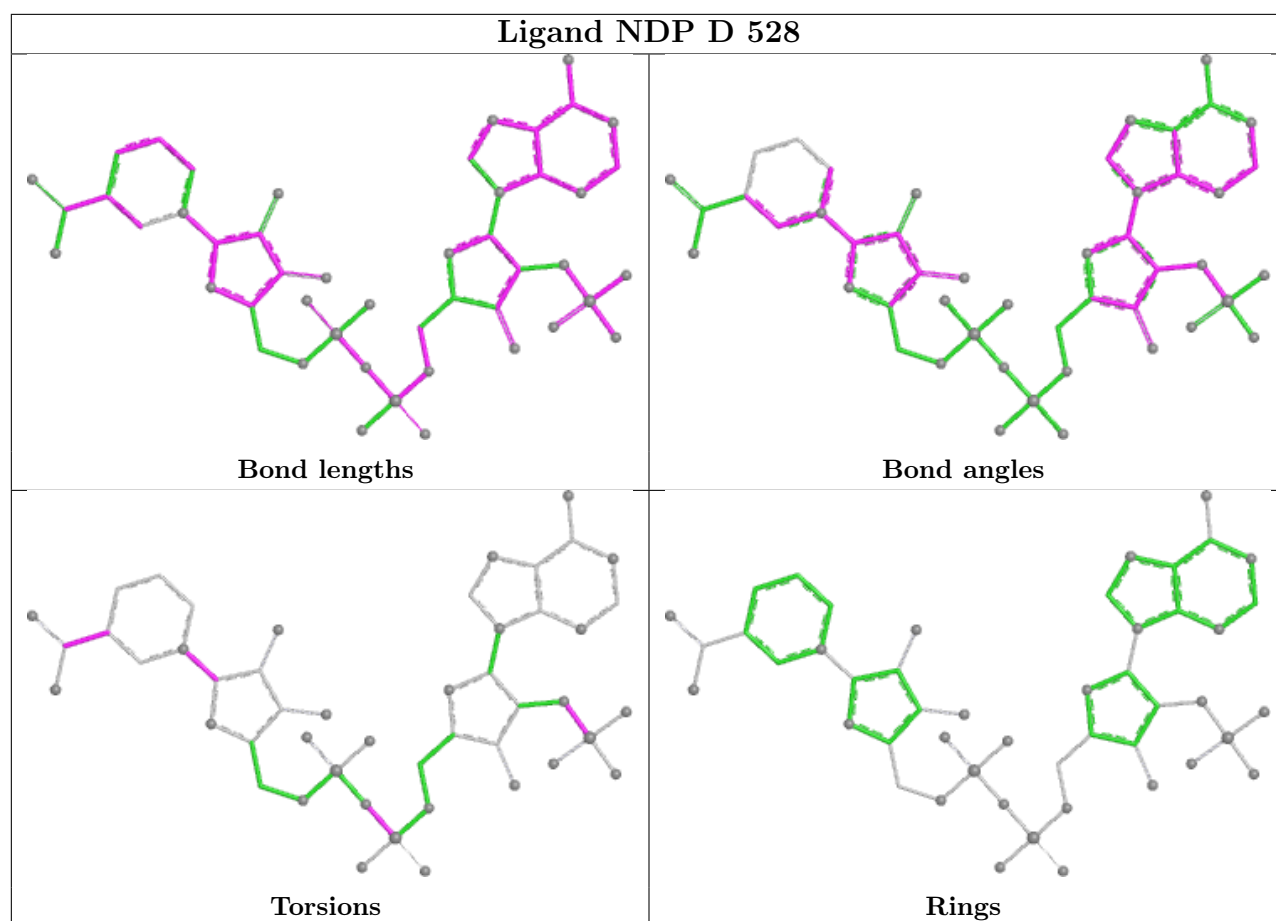
Ligand CPS B 525











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.