



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:26 pm BST

PDB ID : 4C7K
Title : 11b-Hydroxysteroid Dehydrogenase Type I in complex with inhibitor
Authors : Goldberg, F.W.; Dossetter, A.G.; Scott, J.S.; Robb, G.R.; Boyd, S.; Groombridge, S.D.; Kemmitt, P.D.; Sjogren, T.; Morentin Gutierrez, P.; de Schoolmeester, J.; Swales, J.G.; Turnbull, A.V.; Wild, M.J.
Deposited on : 2013-09-23
Resolution : 1.91 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

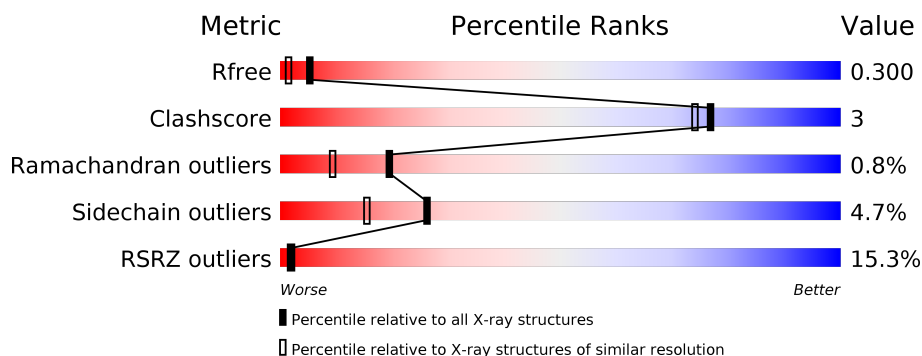
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	269	
1	B	269	
1	C	269	
1	D	269	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8908 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.

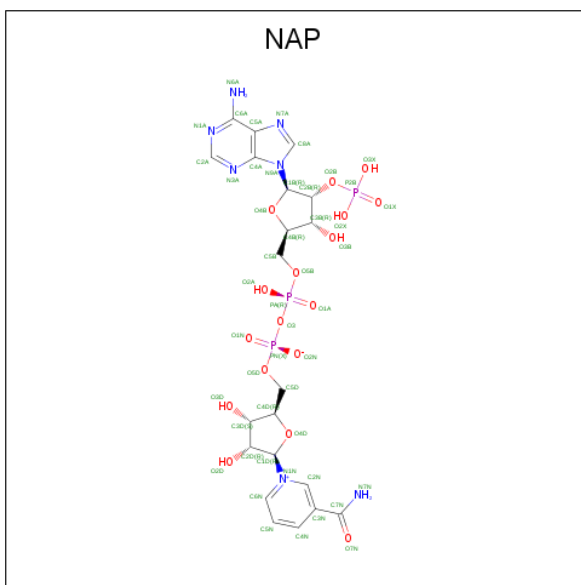
- Molecule 1 is a protein called CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1974	1256	337	367	14			
1	B	258	Total	C	N	O	S	0	0	0
			1973	1256	337	366	14			
1	C	258	Total	C	N	O	S	0	0	0
			1974	1256	337	367	14			
1	D	258	Total	C	N	O	S	0	0	0
			1974	1256	337	367	14			

There are 16 discrepancies between the modelled and reference sequences:

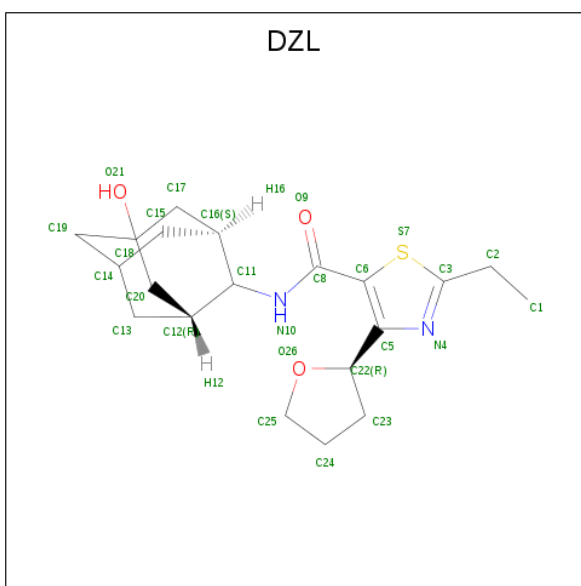
Chain	Residue	Modelled	Actual	Comment	Reference
A	179	LEU	MET	engineered mutation	UNP P28845
A	262	ARG	LEU	engineered mutation	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
A	278	GLU	PHE	engineered mutation	UNP P28845
B	179	LEU	MET	engineered mutation	UNP P28845
B	262	ARG	LEU	engineered mutation	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
B	278	GLU	PHE	engineered mutation	UNP P28845
C	179	LEU	MET	engineered mutation	UNP P28845
C	262	ARG	LEU	engineered mutation	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
C	278	GLU	PHE	engineered mutation	UNP P28845
D	179	LEU	MET	engineered mutation	UNP P28845
D	262	ARG	LEU	engineered mutation	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845
D	278	GLU	PHE	engineered mutation	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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 2-ethyl-N-[(1S,3R)-5-oxidanyl-2-adamantyl]-4-[(2R)-oxolan-2-yl]-1,3-thiazole-5-carboxamide (three-letter code: DZL) (formula: C₂₀H₂₈N₂O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	20	2	3	1		
3	B	1	Total	C	N	O	S	0	0
			26	20	2	3	1		
3	C	1	Total	C	N	O	S	0	0
			26	20	2	3	1		


- Molecule 4 is water.

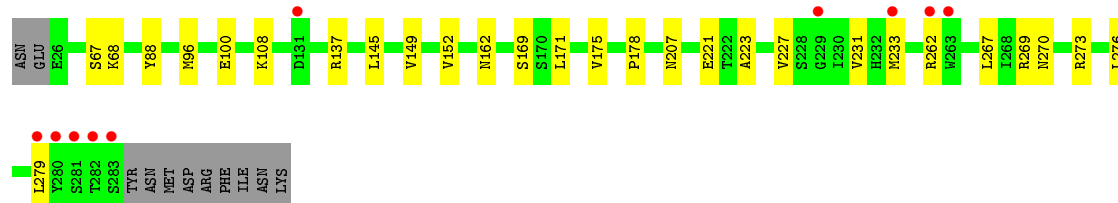
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	243	Total	O	0	0
			243	243		
4	B	226	Total	O	0	0
			226	226		
4	C	137	Total	O	0	0
			137	137		
4	D	137	Total	O	0	0
			137	137		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

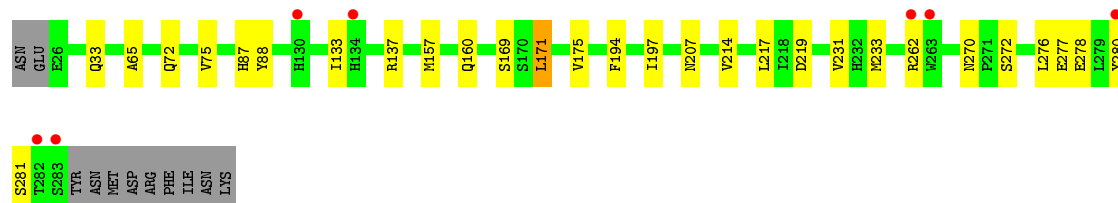
• Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1

Chain A: 



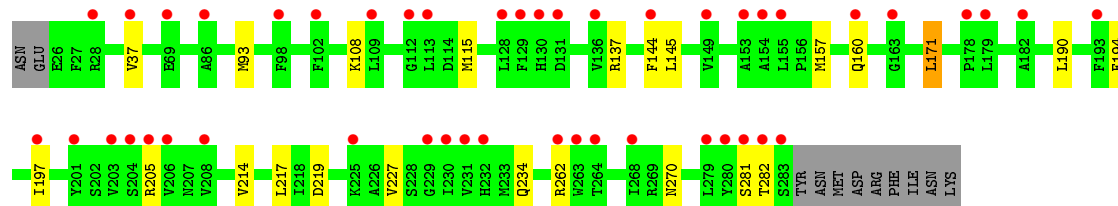
• Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1

Chain B: 




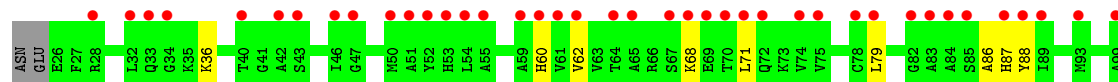
• Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1

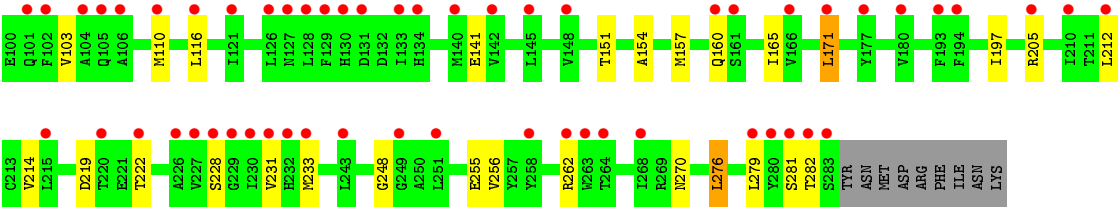
Chain C: 



• Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.33Å 99.25Å 99.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 1.91 49.62 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.63-1.91) 96.0 (49.62-1.91)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.36 (at 1.91Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.240 , 0.290 0.247 , 0.300	Depositor DCC
R_{free} test set	3737 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h 0.020 for -h,-l,-k 0.025 for k,h,-l 0.012 for l,h,k 0.012 for k,l,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8908	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, DZL

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	0.49	0/2006	0.66	0/2708
1	B	0.51	0/2005	0.65	0/2707
1	C	0.47	0/2005	0.65	0/2705
1	D	0.47	0/2006	0.65	0/2708
All	All	0.48	0/8022	0.65	0/10828

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	1974	0	2026	17	0
1	B	1973	0	2023	16	0
1	C	1974	0	2025	7	0
1	D	1974	0	2026	17	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
3	A	26	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	28	0	0
3	C	26	0	28	0	0
4	A	243	0	0	1	0
4	B	226	0	0	2	0
4	C	137	0	0	1	0
4	D	137	0	0	5	0
All	All	8908	0	8284	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (50) 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:207:ASN:HB2	4:B:2156:HOH:O	1.66	0.94
1:D:68:LYS:HA	4:D:2032:HOH:O	1.86	0.74
1:D:197:ILE:HG22	4:D:2100:HOH:O	1.87	0.73
1:A:162:ASN:HD22	1:A:207:ASN:HD22	1.40	0.69
1:D:141:GLU:HB3	4:D:2049:HOH:O	1.95	0.67
1:A:152:VAL:HG21	1:B:133:ILE:HD11	1.81	0.62
1:D:62:VAL:HG22	1:D:87:HIS:HB2	1.88	0.56
1:A:162:ASN:ND2	1:A:207:ASN:HD22	2.05	0.55
1:B:87:HIS:HD2	4:B:2043:HOH:O	1.91	0.54
1:B:217:LEU:HD22	1:B:233:MET:HG3	1.90	0.53
1:C:37:VAL:HG13	1:C:115:MET:HB3	1.91	0.53
1:D:103:VAL:HG11	1:D:154:ALA:HB2	1.91	0.53
1:A:100:GLU:HG3	1:A:149:VAL:HG13	1.90	0.52
1:A:100:GLU:HG3	1:A:149:VAL:CG1	2.41	0.51
1:A:68:LYS:HG3	1:A:88:TYR:HE1	1.75	0.51
1:B:157:MET:O	1:B:160:GLN:HG2	2.11	0.51
1:A:269:ARG:HB2	4:A:2225:HOH:O	2.09	0.50
1:D:171:LEU:HD12	1:D:214:VAL:HG12	1.94	0.49
1:B:194:PHE:HA	1:B:197:ILE:HG12	1.95	0.49
1:D:116:LEU:HD23	1:D:165:ILE:HG23	1.96	0.48
1:A:227:VAL:HG22	1:A:231:VAL:HB	1.97	0.47
1:A:68:LYS:HG3	1:A:88:TYR:CE1	2.50	0.47
1:D:157:MET:O	1:D:160:GLN:HG2	2.14	0.47
1:B:169:SER:O	2:B:1284:NAP:H6N	2.15	0.47
1:D:36:LYS:HA	1:D:60:HIS:HB2	1.97	0.46
1:D:36:LYS:HG2	1:D:110:MET:HB3	1.98	0.46
1:B:171:LEU:HD12	1:B:214:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:PHE:HA	1:C:197:ILE:HG12	2.00	0.44
1:A:175:VAL:HG13	1:B:277:GLU:HG3	1.99	0.44
1:D:222:THR:HB	4:D:2107:HOH:O	2.17	0.44
1:A:178:PRO:HD2	1:B:280:TYR:CE2	2.53	0.44
1:A:273:ARG:HG3	1:B:175:VAL:HG22	2.00	0.44
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.99	0.44
1:C:171:LEU:HD12	1:C:214:VAL:HG12	2.00	0.44
1:D:151:THR:HG23	1:D:165:ILE:HD13	2.00	0.43
1:A:96:MET:HG3	1:B:137:ARG:HH22	1.83	0.43
1:A:267:LEU:O	1:B:272:SER:HB2	2.19	0.42
1:D:212:LEU:HB3	1:D:255:GLU:HG2	2.02	0.42
1:A:223:ALA:O	1:A:227:VAL:HB	2.20	0.41
1:C:93:MET:HG2	2:C:1284:NAP:H2A	2.03	0.41
1:A:169:SER:O	2:A:1284:NAP:H6N	2.20	0.41
1:B:75:VAL:HG21	1:B:88:TYR:HB3	2.01	0.41
1:C:157:MET:O	1:C:160:GLN:HG2	2.20	0.41
1:B:75:VAL:CG2	1:B:88:TYR:HB3	2.50	0.41
1:D:276:LEU:HA	1:D:276:LEU:HD12	1.90	0.41
1:C:144:PHE:HD1	1:C:190:LEU:HD23	1.85	0.41
1:D:79:LEU:HG	1:D:86:ALA:HB3	2.03	0.41
1:C:160:GLN:HB2	4:C:2082:HOH:O	2.21	0.40
1:A:178:PRO:HD2	1:B:280:TYR:HE2	1.86	0.40
1:D:71:LEU:HB2	4:D:2032: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	256/269 (95%)	248 (97%)	8 (3%)	0	100	100
1	B	256/269 (95%)	246 (96%)	7 (3%)	3 (1%)	13	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	254/269 (94%)	244 (96%)	9 (4%)	1 (0%)	34	24
1	D	256/269 (95%)	242 (94%)	10 (4%)	4 (2%)	9	2
All	All	1022/1076 (95%)	980 (96%)	34 (3%)	8 (1%)	19	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281	SER
1	D	231	VAL
1	D	281	SER
1	C	219	ASP
1	D	228	SER
1	B	65	ALA
1	B	219	ASP
1	D	219	ASP

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	215/226 (95%)	204 (95%)	11 (5%)	24	13
1	B	214/226 (95%)	206 (96%)	8 (4%)	34	23
1	C	215/226 (95%)	203 (94%)	12 (6%)	21	10
1	D	215/226 (95%)	206 (96%)	9 (4%)	30	19
All	All	859/904 (95%)	819 (95%)	40 (5%)	26	15

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

Mol	Chain	Res	Type
1	A	67	SER
1	A	108	LYS
1	A	137	ARG
1	A	145	LEU

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Mol	Chain	Res	Type
1	A	171	LEU
1	A	221	GLU
1	A	233	MET
1	A	262	ARG
1	A	270	ASN
1	A	276	LEU
1	A	279	LEU
1	B	33	GLN
1	B	72	GLN
1	B	171	LEU
1	B	231	VAL
1	B	262	ARG
1	B	270	ASN
1	B	276	LEU
1	B	278	GLU
1	C	108	LYS
1	C	137	ARG
1	C	145	LEU
1	C	171	LEU
1	C	205	ARG
1	C	217	LEU
1	C	227	VAL
1	C	234	GLN
1	C	262	ARG
1	C	270	ASN
1	C	281	SER
1	C	282	THR
1	D	88	TYR
1	D	171	LEU
1	D	205	ARG
1	D	233	MET
1	D	262	ARG
1	D	270	ASN
1	D	276	LEU
1	D	279	LEU
1	D	282	THR

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

Mol	Chain	Res	Type
1	A	87	HIS
1	A	101	GLN

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Mol	Chain	Res	Type
1	A	123	ASN
1	A	134	HIS
1	A	162	ASN
1	B	87	HIS
1	B	207	ASN
1	B	270	ASN
1	C	101	GLN
1	C	123	ASN
1	C	270	ASN
1	D	127	ASN
1	D	160	GLN
1	D	207	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
2	NAP	D	1284	-	45,52,52	1.04	3 (6%)	56,80,80	1.03	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	A	1284	-	45,52,52	1.00	3 (6%)	56,80,80	1.10	3 (5%)
2	NAP	B	1284	-	45,52,52	0.99	3 (6%)	56,80,80	1.15	4 (7%)
3	DZL	A	1285	-	25,30,30	1.28	2 (8%)	26,46,46	0.85	1 (3%)
2	NAP	C	1284	-	45,52,52	1.03	3 (6%)	56,80,80	1.04	3 (5%)
3	DZL	C	1285	-	25,30,30	0.99	3 (12%)	26,46,46	0.49	0
3	DZL	B	1285	-	25,30,30	0.95	1 (4%)	26,46,46	0.81	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	D	1284	-	-	3/31/67/67	0/5/5/5
2	NAP	A	1284	-	-	4/31/67/67	0/5/5/5
2	NAP	B	1284	-	-	5/31/67/67	0/5/5/5
3	DZL	A	1285	-	-	0/4/52/52	0/6/5/5
2	NAP	C	1284	-	-	4/31/67/67	0/5/5/5
3	DZL	C	1285	-	-	0/4/52/52	0/6/5/5
3	DZL	B	1285	-	-	0/4/52/52	0/6/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1285	DZL	C2-C3	-4.74	1.46	1.49
2	A	1284	NAP	O4B-C1B	3.27	1.45	1.41
3	B	1285	DZL	C2-C3	-3.15	1.47	1.49
3	C	1285	DZL	C5-C22	-2.98	1.48	1.51
2	B	1284	NAP	O4B-C1B	2.88	1.45	1.41
2	B	1284	NAP	C8A-N7A	-2.81	1.29	1.34
2	D	1284	NAP	O4D-C1D	2.79	1.45	1.41
2	C	1284	NAP	O4D-C1D	2.75	1.44	1.41
2	B	1284	NAP	O4D-C1D	2.54	1.44	1.41
2	C	1284	NAP	O4B-C1B	2.53	1.44	1.41
2	D	1284	NAP	O4B-C1B	2.45	1.44	1.41
3	A	1285	DZL	C5-C22	-2.44	1.49	1.51
2	A	1284	NAP	O4D-C1D	2.38	1.44	1.41
2	D	1284	NAP	C8A-N7A	-2.26	1.30	1.34
2	C	1284	NAP	C8A-N7A	-2.19	1.30	1.34
3	C	1285	DZL	C2-C3	-2.19	1.48	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1284	NAP	C8A-N7A	-2.07	1.31	1.34
3	C	1285	DZL	C8-N10	2.05	1.38	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1284	NAP	N3A-C2A-N1A	-4.40	121.81	128.68
2	C	1284	NAP	N3A-C2A-N1A	-4.23	122.07	128.68
2	A	1284	NAP	N3A-C2A-N1A	-4.21	122.10	128.68
2	B	1284	NAP	N3A-C2A-N1A	-4.12	122.24	128.68
2	B	1284	NAP	C3N-C7N-N7N	3.99	122.53	117.75
2	A	1284	NAP	C3N-C7N-N7N	3.48	121.93	117.75
3	B	1285	DZL	C15-C16-C17	-2.62	105.91	109.34
2	B	1284	NAP	O7N-C7N-N7N	-2.55	118.96	122.58
2	C	1284	NAP	C4A-C5A-N7A	-2.28	107.02	109.40
2	D	1284	NAP	C4A-C5A-N7A	-2.28	107.03	109.40
2	A	1284	NAP	C1B-N9A-C4A	-2.08	122.99	126.64
2	C	1284	NAP	O7N-C7N-N7N	-2.08	119.63	122.58
3	A	1285	DZL	C15-C16-C17	-2.06	106.64	109.34
2	B	1284	NAP	C4A-C5A-N7A	-2.03	107.29	109.40

There are no chirality outliers.

All (16) torsion outliers are listed below:

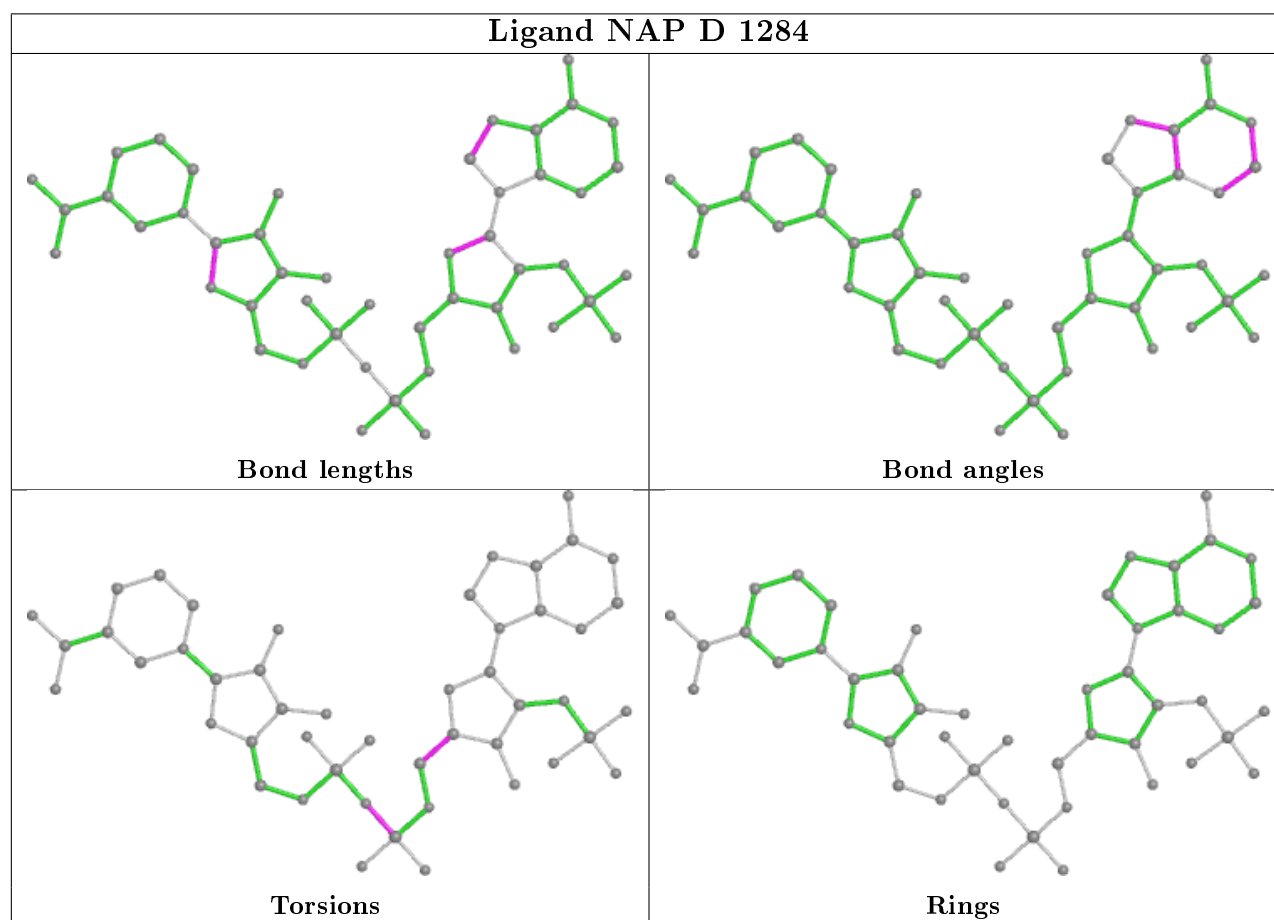
Mol	Chain	Res	Type	Atoms
2	B	1284	NAP	C1B-C2B-O2B-P2B
2	B	1284	NAP	C3B-C2B-O2B-P2B
2	A	1284	NAP	PN-O3-PA-O2A
2	B	1284	NAP	PN-O3-PA-O2A
2	C	1284	NAP	O4D-C4D-C5D-O5D
2	D	1284	NAP	PN-O3-PA-O2A
2	C	1284	NAP	PN-O3-PA-O2A
2	D	1284	NAP	PN-O3-PA-O1A
2	C	1284	NAP	C3D-C4D-C5D-O5D
2	A	1284	NAP	C3B-C2B-O2B-P2B
2	B	1284	NAP	O4B-C4B-C5B-O5B
2	A	1284	NAP	PN-O3-PA-O1A
2	B	1284	NAP	PN-O3-PA-O1A
2	D	1284	NAP	O4B-C4B-C5B-O5B
2	A	1284	NAP	O4B-C4B-C5B-O5B
2	C	1284	NAP	O4B-C4B-C5B-O5B

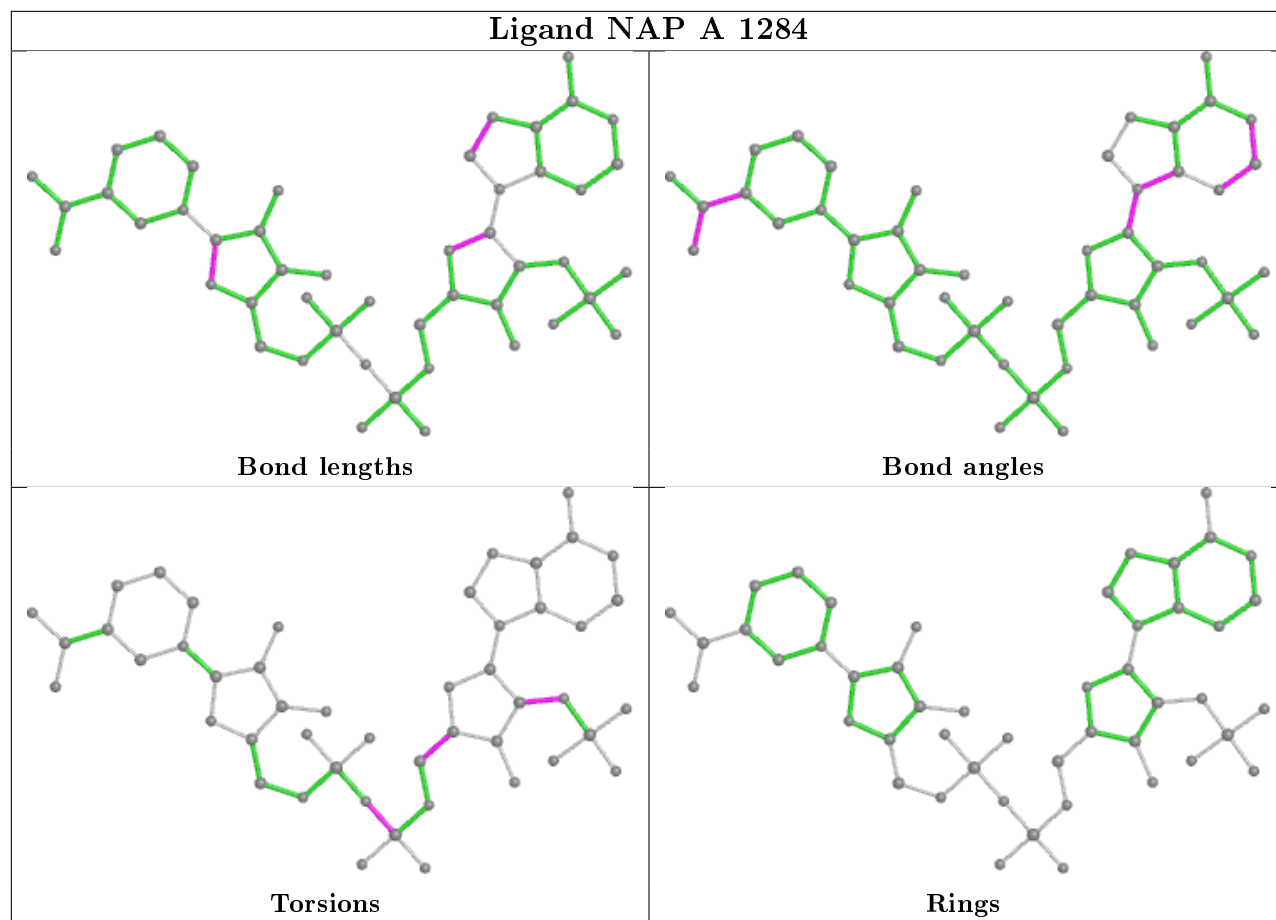
There are no ring outliers.

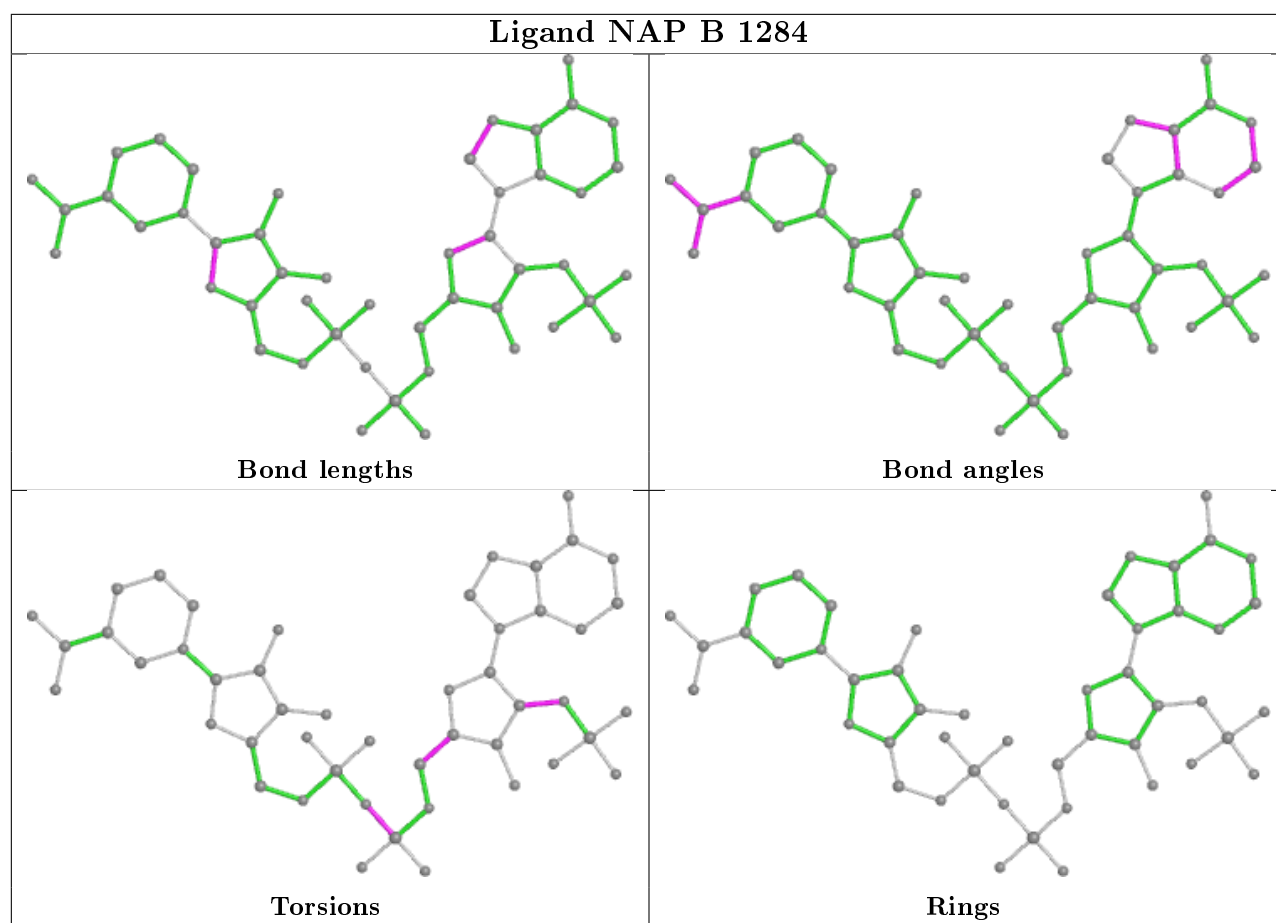
3 monomers are involved in 3 short contacts:

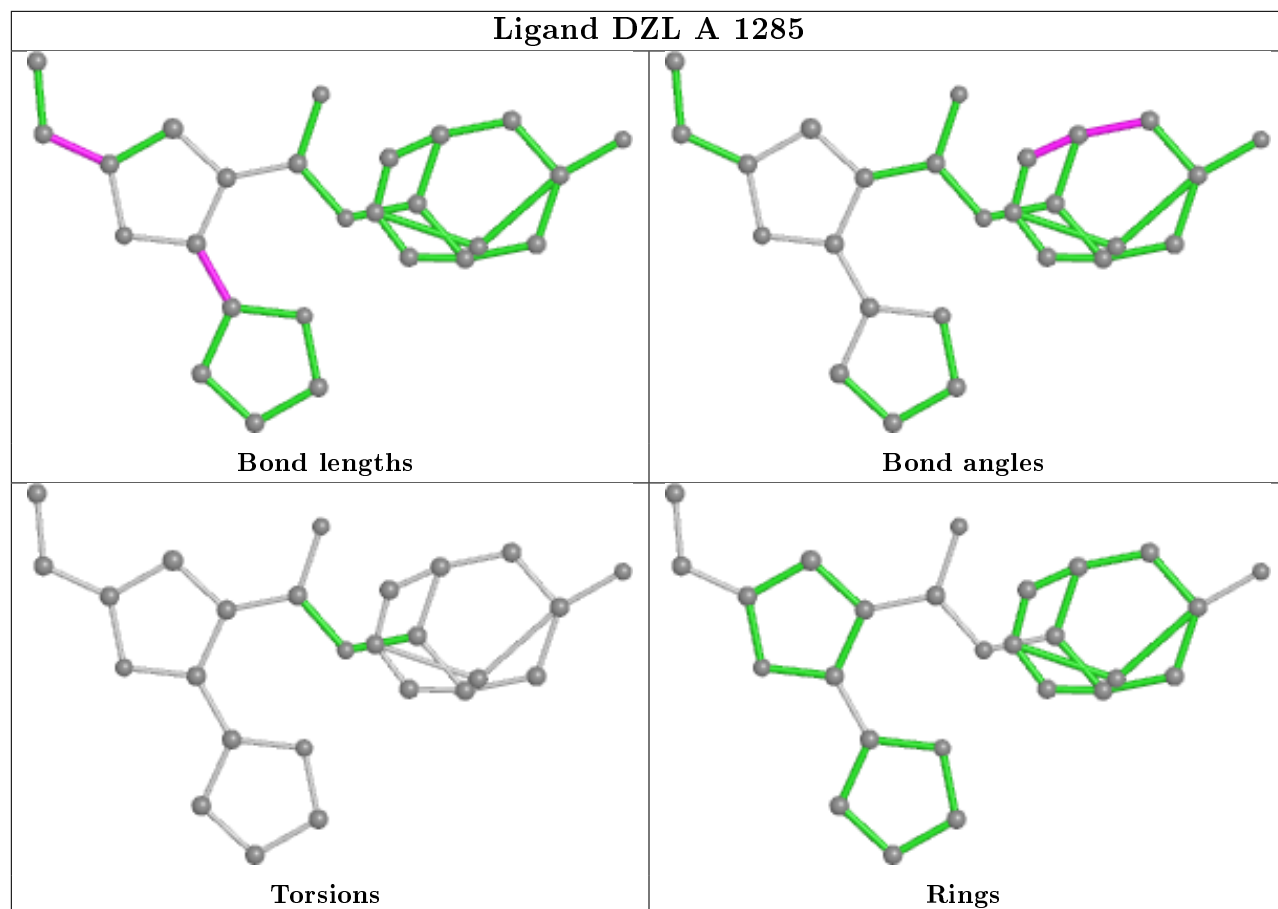
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1284	NAP	1	0
2	B	1284	NAP	1	0
2	C	1284	NAP	1	0

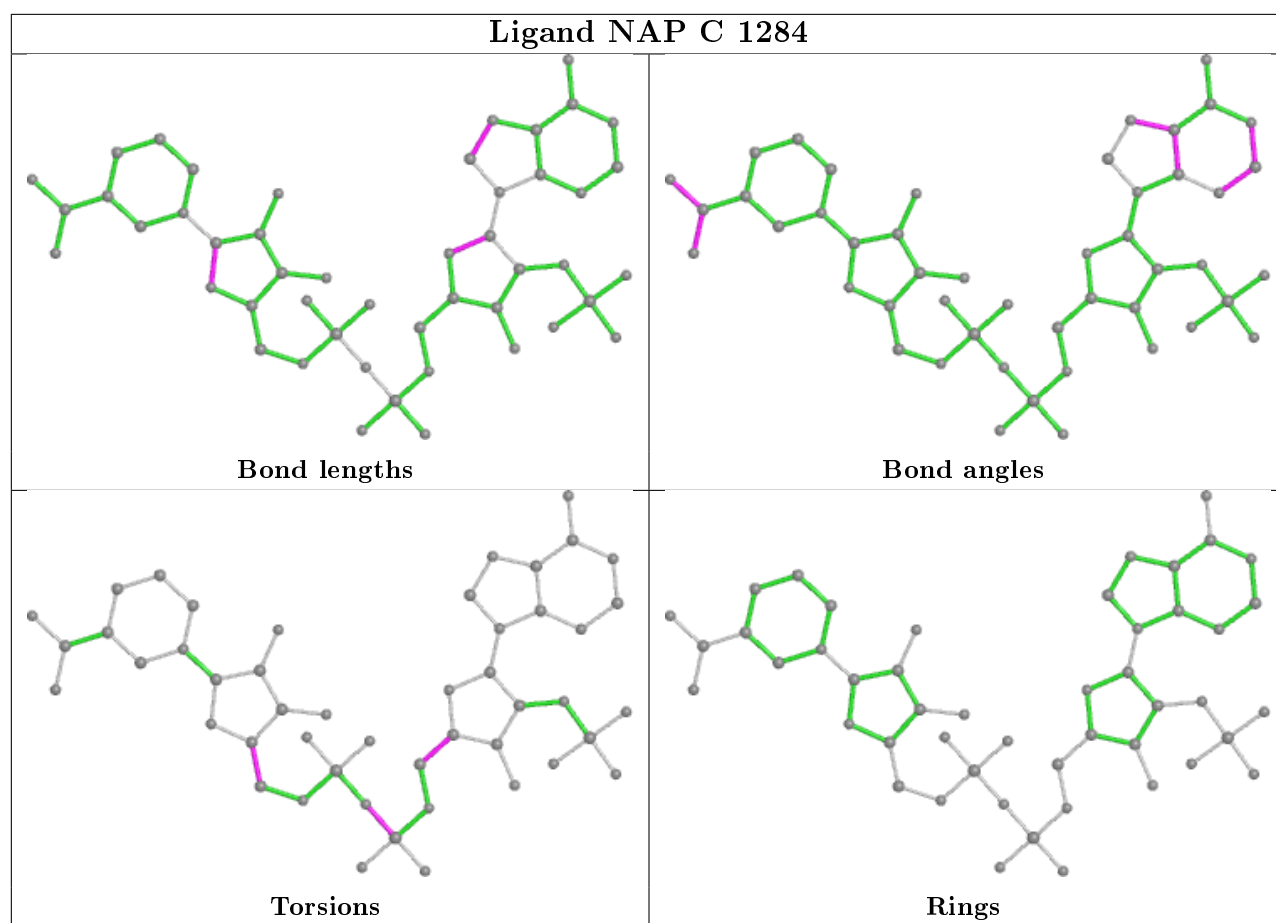
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

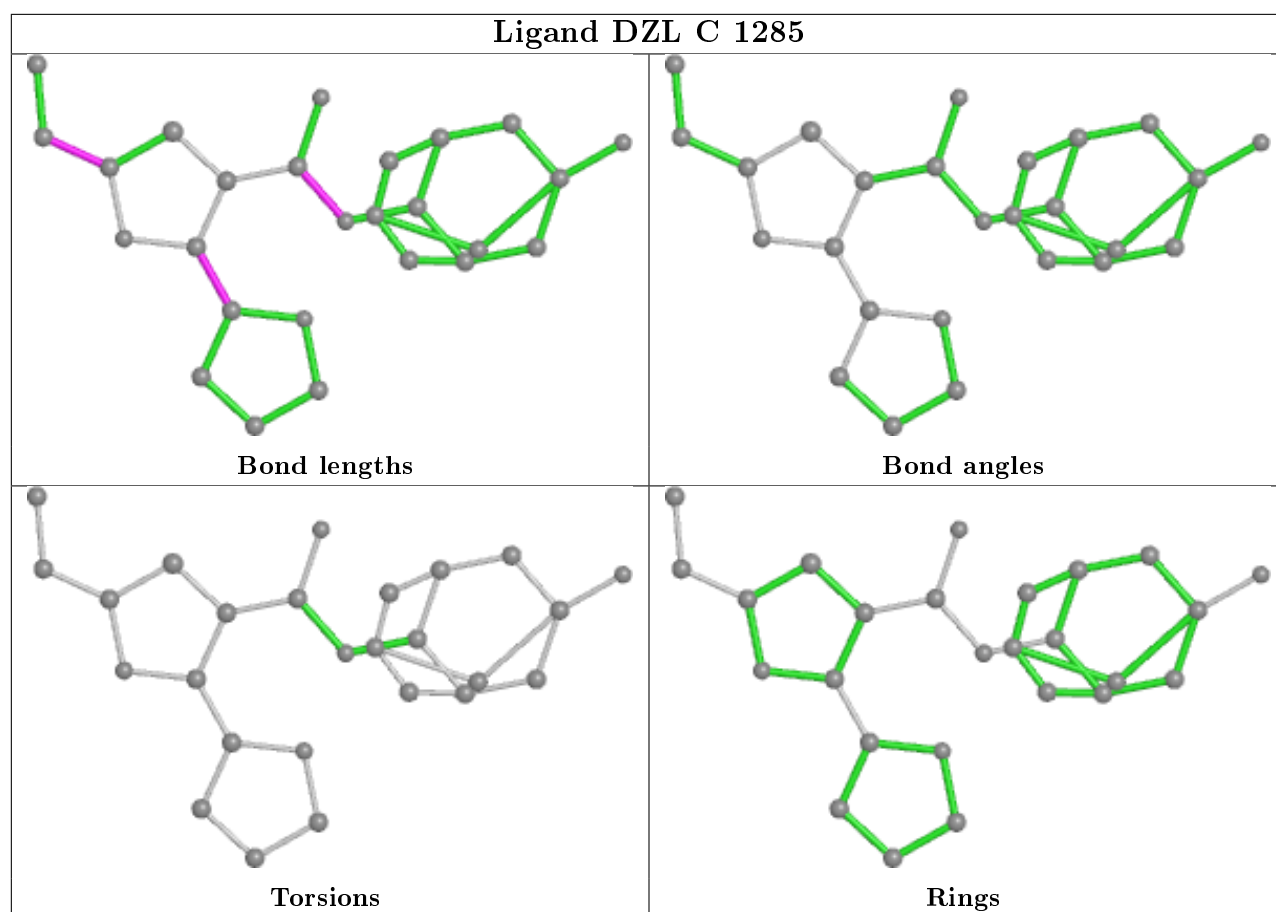


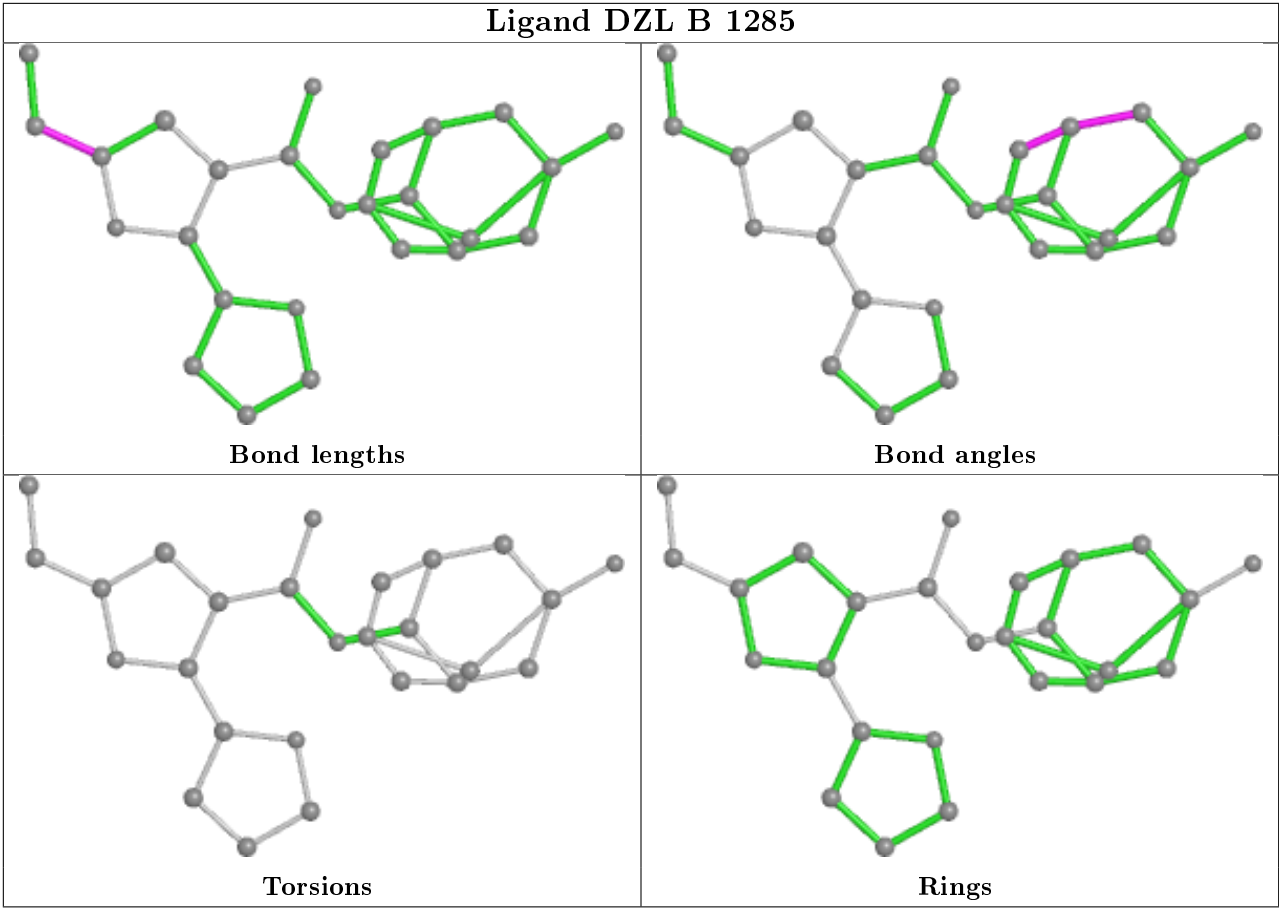












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	232:HIS	C	233:MET	N	3.34

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	258/269 (95%)	0.04	10 (3%) 39 42	6, 14, 45, 91	0
1	B	258/269 (95%)	0.03	7 (2%) 54 57	7, 14, 37, 99	0
1	C	258/269 (95%)	1.08	46 (17%) 1 1	14, 31, 57, 114	0
1	D	258/269 (95%)	1.95	95 (36%) 0 0	20, 39, 73, 118	0
All	All	1032/1076 (95%)	0.77	158 (15%) 2 2	6, 26, 58, 118	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	283	SER	11.0
1	B	283	SER	9.8
1	A	282	THR	8.9
1	D	230	ILE	8.7
1	C	280	TYR	8.2
1	D	282	THR	8.1
1	D	231	VAL	7.6
1	D	232	HIS	7.2
1	D	263	TRP	6.3
1	B	263	TRP	6.2
1	D	61	VAL	5.9
1	C	279	LEU	5.9
1	C	203	VAL	5.7
1	D	233	MET	5.7
1	D	74	VAL	5.7
1	D	67	SER	5.1
1	C	205	ARG	4.9
1	C	206	VAL	4.9
1	D	134	HIS	4.7
1	D	268	ILE	4.7
1	C	232	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	231	VAL	4.7
1	D	99	ALA	4.7
1	D	43	SER	4.6
1	D	101	GLN	4.6
1	D	279	LEU	4.5
1	D	130	HIS	4.4
1	C	263	TRP	4.4
1	A	283	SER	4.2
1	C	197	ILE	4.2
1	D	171	LEU	4.2
1	D	33	GLN	4.1
1	D	89	ILE	4.1
1	D	258	TYR	4.1
1	C	282	THR	4.1
1	D	262	ARG	4.1
1	D	64	THR	4.1
1	A	280	TYR	4.0
1	C	130	HIS	4.0
1	D	128	LEU	3.9
1	C	128	LEU	3.9
1	D	205	ARG	3.8
1	A	229	GLY	3.8
1	D	28	ARG	3.7
1	D	53	HIS	3.7
1	D	52	TYR	3.7
1	D	88	TYR	3.6
1	D	127	ASN	3.6
1	C	163	GLY	3.6
1	D	87	HIS	3.6
1	C	283	SER	3.5
1	D	126	LEU	3.4
1	D	105	GLN	3.4
1	D	51	ALA	3.4
1	D	251	LEU	3.4
1	B	282	THR	3.3
1	D	226	ALA	3.3
1	C	153	ALA	3.3
1	D	47	GLY	3.2
1	C	262	ARG	3.2
1	D	104	ALA	3.2
1	D	60	HIS	3.1
1	D	129	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	54	LEU	3.1
1	C	149	VAL	3.1
1	C	208	VAL	3.1
1	D	116	LEU	3.1
1	B	262	ARG	3.1
1	D	85	SER	3.0
1	A	263	TRP	3.0
1	D	62	VAL	3.0
1	D	264	THR	3.0
1	D	180	VAL	3.0
1	D	34	GLY	3.0
1	D	75	VAL	3.0
1	C	144	PHE	3.0
1	C	230	ILE	2.9
1	D	72	GLN	2.9
1	A	233	MET	2.9
1	D	83	ALA	2.9
1	D	177	TYR	2.9
1	B	280	TYR	2.9
1	D	131	ASP	2.8
1	D	79	LEU	2.8
1	A	281	SER	2.8
1	A	279	LEU	2.8
1	C	102	PHE	2.8
1	D	78	CYS	2.7
1	D	84	ALA	2.7
1	D	82	GLY	2.7
1	D	93	MET	2.7
1	D	133	ILE	2.7
1	C	129	PHE	2.7
1	C	281	SER	2.7
1	C	204	SER	2.7
1	D	228	SER	2.7
1	C	268	ILE	2.6
1	D	32	LEU	2.6
1	D	71	LEU	2.6
1	D	222	THR	2.6
1	A	262	ARG	2.6
1	D	59	ALA	2.6
1	D	193	PHE	2.6
1	D	227	VAL	2.6
1	D	249	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	201	TYR	2.5
1	B	130	HIS	2.5
1	D	145	LEU	2.5
1	D	69	GLU	2.5
1	D	166	VAL	2.5
1	D	106	ALA	2.4
1	D	220	THR	2.4
1	D	42	ALA	2.4
1	D	65	ALA	2.4
1	C	178	PRO	2.4
1	D	229	GLY	2.4
1	D	161	SER	2.4
1	C	229	GLY	2.3
1	A	131	ASP	2.3
1	D	140	MET	2.3
1	C	160	GLN	2.3
1	D	40	THR	2.3
1	C	131	ASP	2.3
1	D	160	GLN	2.3
1	C	182	ALA	2.3
1	C	179	LEU	2.3
1	C	154	ALA	2.3
1	D	70	THR	2.3
1	C	109	LEU	2.3
1	C	155	LEU	2.3
1	D	212	LEU	2.3
1	D	281	SER	2.3
1	D	280	TYR	2.3
1	D	142	VAL	2.3
1	C	98	PHE	2.2
1	D	68	LYS	2.2
1	D	121	ILE	2.2
1	D	210	ILE	2.2
1	D	194	PHE	2.2
1	D	55	ALA	2.2
1	C	112	GLY	2.2
1	C	193	PHE	2.2
1	D	46	ILE	2.1
1	D	215	LEU	2.1
1	D	110	MET	2.1
1	D	243	LEU	2.1
1	C	86	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	37	VAL	2.1
1	C	69	GLU	2.1
1	C	136	VAL	2.1
1	D	148	VAL	2.1
1	C	28	ARG	2.1
1	D	50	MET	2.1
1	C	225	LYS	2.1
1	C	264	THR	2.0
1	D	102	PHE	2.0
1	B	134	HIS	2.0
1	C	113	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

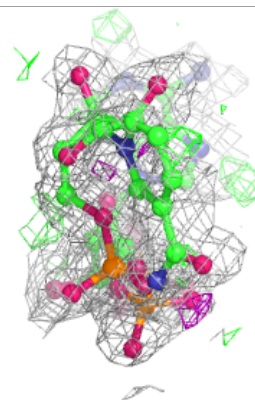
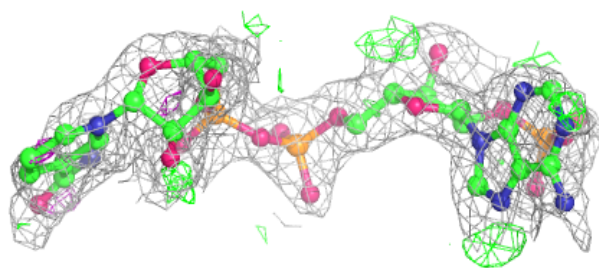
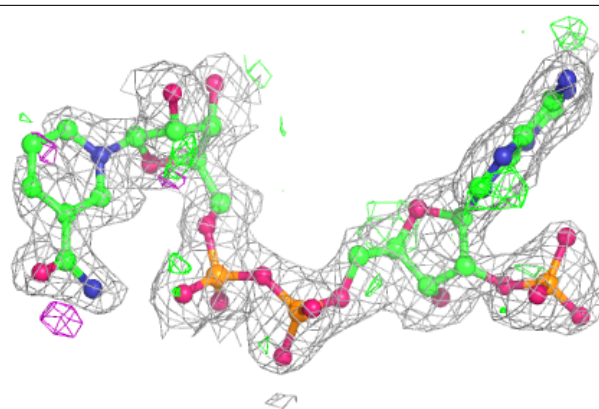
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAP	D	1284	48/48	0.87	0.19	27,32,37,39	0
2	NAP	C	1284	48/48	0.94	0.11	15,23,32,35	0
3	DZL	C	1285	26/26	0.94	0.11	21,25,29,29	0
3	DZL	A	1285	26/26	0.96	0.09	9,13,23,24	0
3	DZL	B	1285	26/26	0.96	0.09	7,12,18,28	0
2	NAP	B	1284	48/48	0.97	0.09	5,11,13,14	0
2	NAP	A	1284	48/48	0.98	0.08	6,11,15,17	0

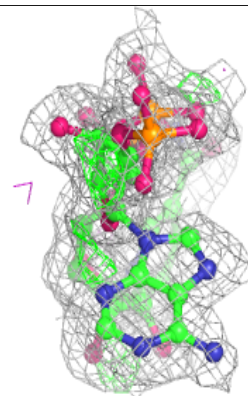
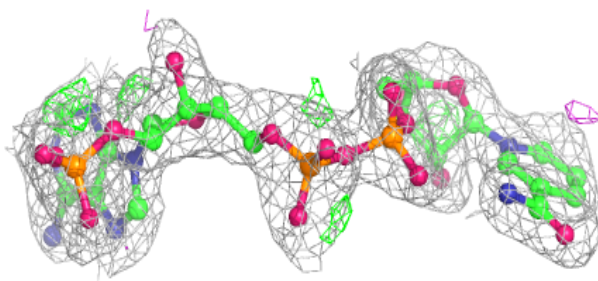
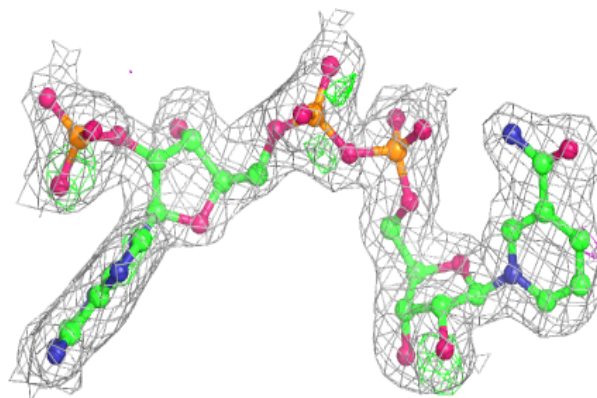
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP D 1284:

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

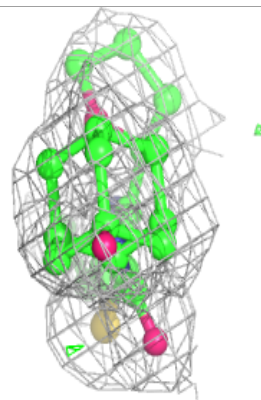
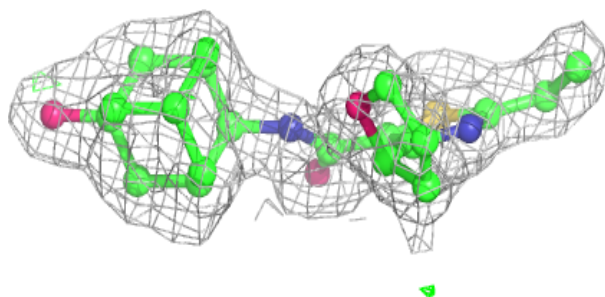
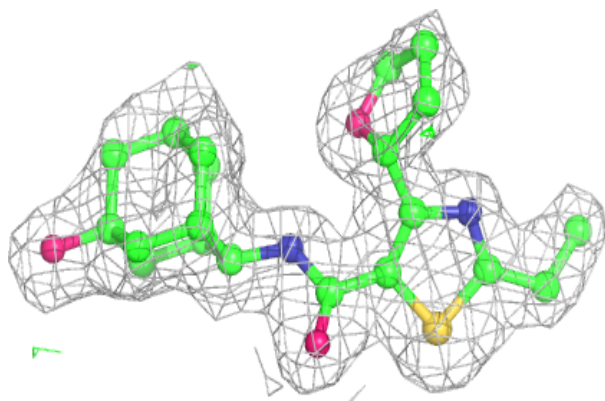
**Electron density around NAP C 1284:**

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

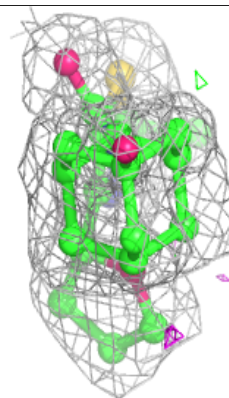
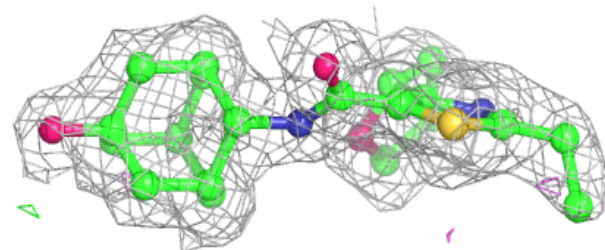
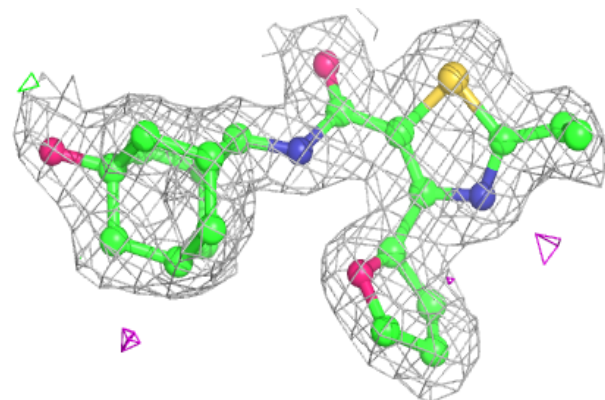


Electron density around DZL C 1285:

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

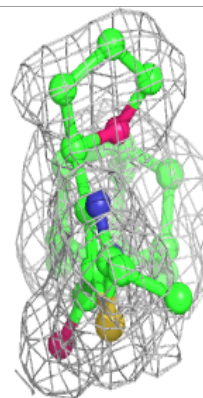
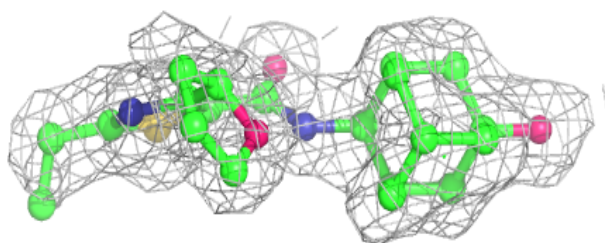
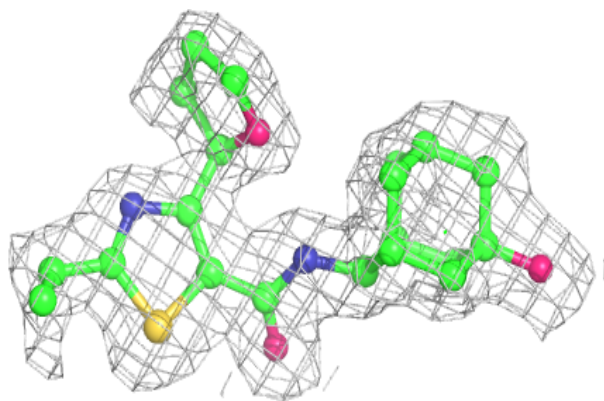
**Electron density around DZL A 1285:**

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

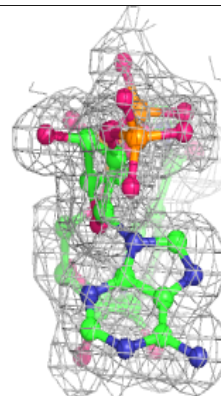
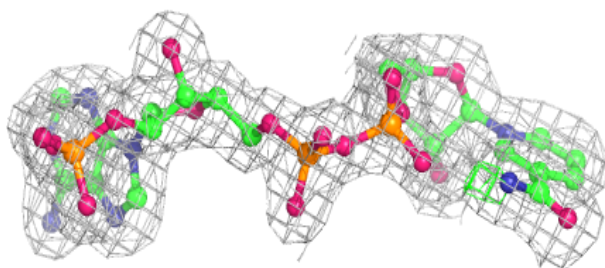
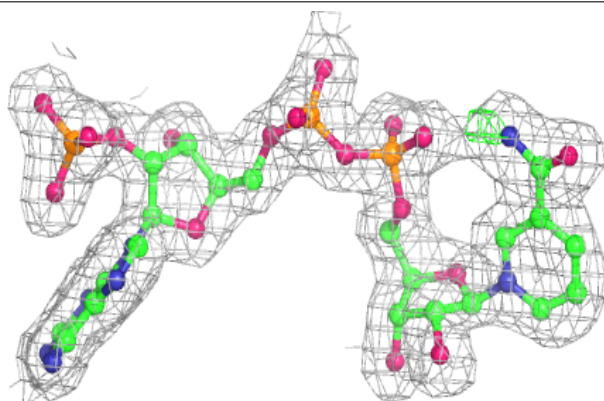


Electron density around DZL B 1285:

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

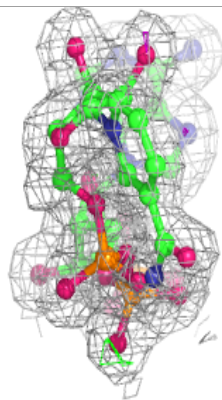
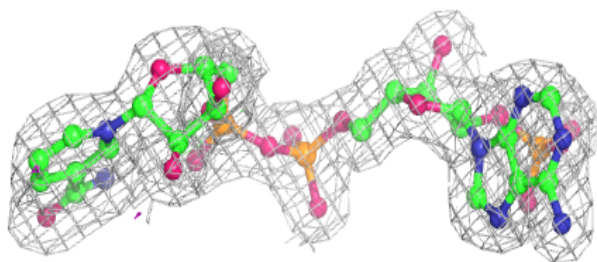
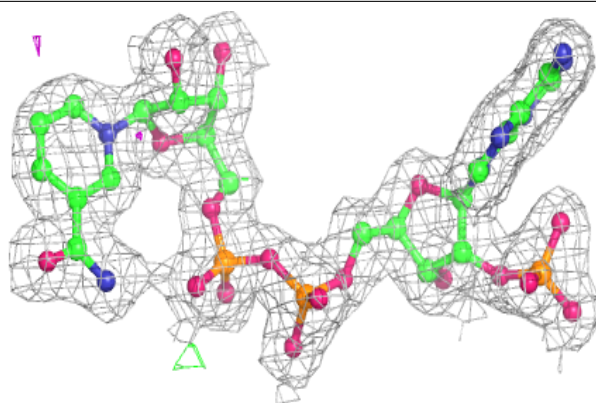
**Electron density around NAP B 1284:**

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



Electron density around NAP A 1284:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.