



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:25 PM UTC

PDB ID : 4C7K / pdb_00004c7k
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 types of validation reports are described at

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

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

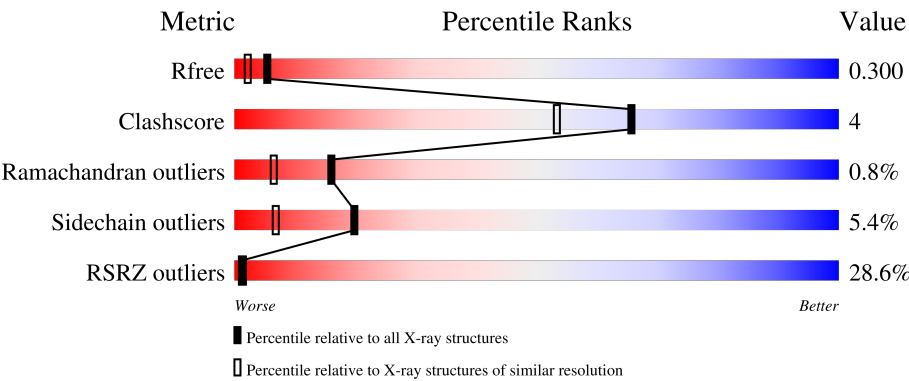
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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

Mol	Chain	Length	Quality of chain
1	A	269	8% 84% 11%
1	B	269	6% 82% 13%
1	C	269	35% 85% 11%
1	D	269	61% 76% 19%

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.

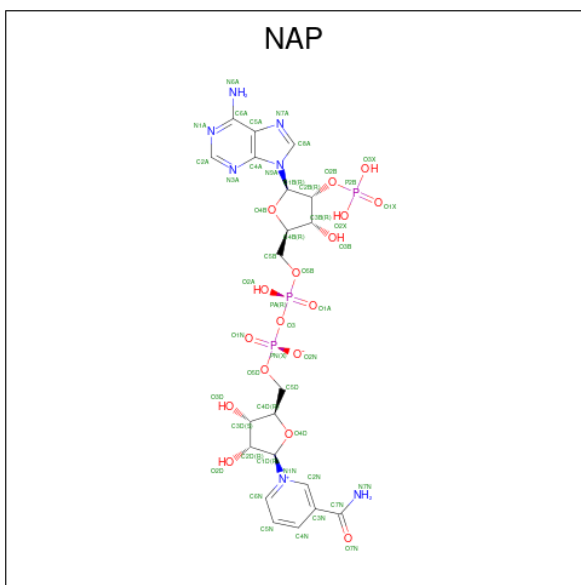
- Molecule 1 is a protein called CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1.

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:

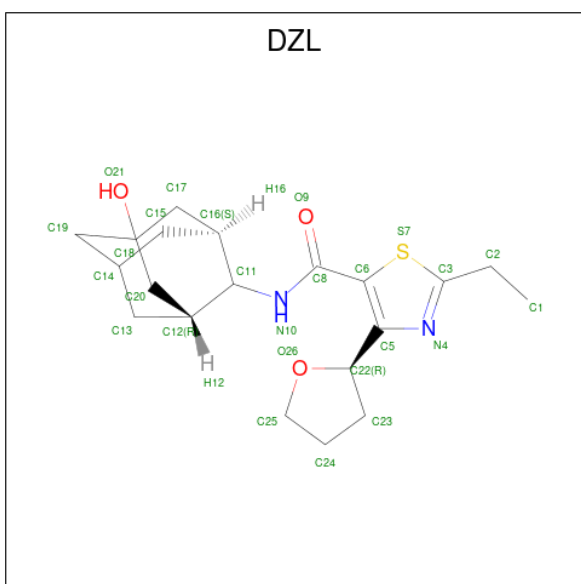
Chain	Residue	Modelled	Actual	Comment	Reference
A	179	LEU	MET	engineered mutation	UNP P28845
A	262	ARG	LEU	engineered mutation	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
A	278	GLU	PHE	engineered mutation	UNP P28845
B	179	LEU	MET	engineered mutation	UNP P28845
B	262	ARG	LEU	engineered mutation	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 (CCD ID: 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 (CCD ID: 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.

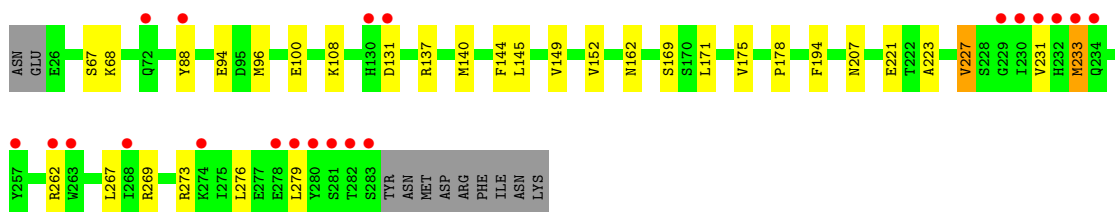
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	243	Total	O	0	0
			243	243		
4	B	226	Total	O	0	0
			226	226		
4	C	137	Total	O	0	0
			137	137		
4	D	137	Total	O	0	0
			137	137		

3 Residue-property plots

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

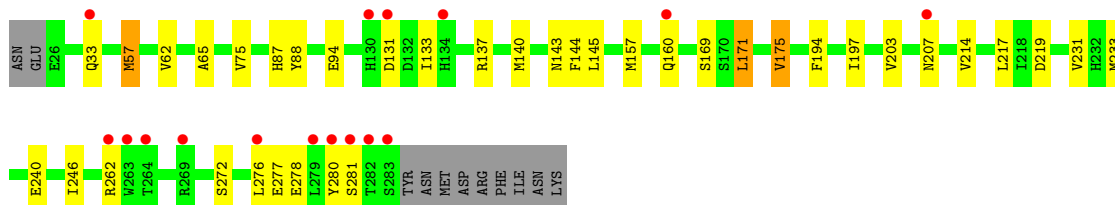
• Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1

Chain A: 



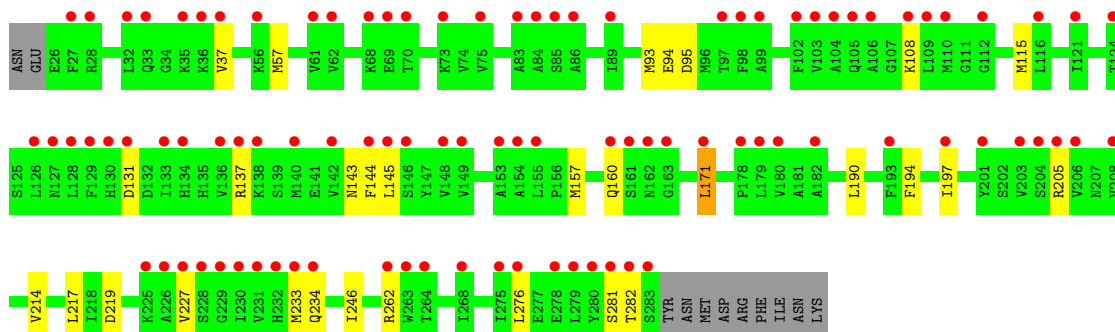
• Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1

Chain B: 



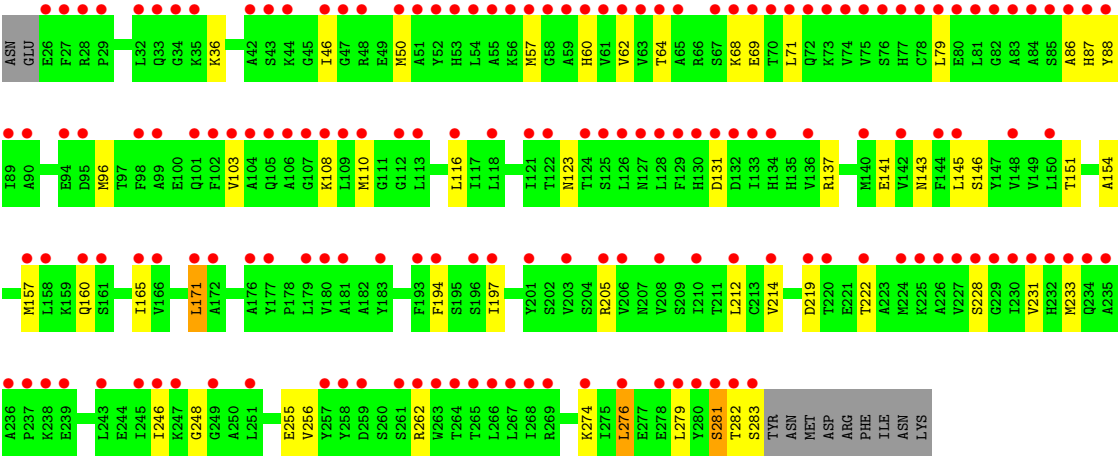
• Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1

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 49.63 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.63-1.91) 96.0 (49.63-1.91)	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 , 50.1	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

5.1 Standard geometry

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	0.85	0/2006	1.28	3/2708 (0.1%)
1	B	0.89	1/2005 (0.0%)	1.28	5/2707 (0.2%)
1	C	0.84	0/2005	1.38	3/2705 (0.1%)
1	D	0.83	0/2006	1.38	5/2708 (0.2%)
All	All	0.85	1/8022 (0.0%)	1.33	16/10828 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	MET	SD-CE	-5.45	1.66	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	ASP	CA-CB-CG	8.14	120.74	112.60
1	B	94	GLU	N-CA-C	-6.19	105.22	112.89
1	C	94	GLU	N-CA-C	-6.10	105.09	112.54
1	B	240	GLU	CB-CG-CD	6.01	122.82	112.60
1	D	64	THR	CA-C-N	5.99	132.97	121.54
1	D	64	THR	C-N-CA	5.99	132.97	121.54
1	A	194	PHE	CA-CB-CG	-5.75	108.05	113.80
1	B	143	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	131	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	62	VAL	N-CA-CB	5.31	118.90	112.10
1	B	131	ASP	CA-CB-CG	5.30	117.90	112.60
1	D	123	ASN	CA-CB-CG	5.28	117.88	112.60
1	D	194	PHE	CA-CB-CG	-5.20	108.60	113.80
1	C	95	ASP	CA-CB-CG	5.14	117.74	112.60
1	D	131	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	94	GLU	N-CA-C	-5.04	105.88	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	22	0
1	B	1973	0	2023	21	0
1	C	1974	0	2025	9	0
1	D	1974	0	2026	22	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
3	B	26	0	28	0	0
3	C	26	0	28	1	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	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (63) 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:C:57:MET:HE1	1:C:246:ILE:HG21	1.78	0.65
1:A:231:VAL:HG13	1:A:233:MET:HE3	1.79	0.63
1:A:152:VAL:HG21	1:B:133:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:MET:HE1	1:B:246:ILE:HG21	1.83	0.61
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:A:144:PHE:CE2	1:B:140:MET:HE3	2.41	0.55
1:B:87:HIS:HD2	4:B:2043:HOH:O	1.91	0.54
1:A:233:MET:HE1	1:B:280:TYR:HE1	1.73	0.54
1:D:46:ILE:HG22	1:D:50:MET:HE2	1.90	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:C:233:MET:HE1	3:C:1285:DZL:H13C	1.90	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:D:57:MET:HE1	1:D:246:ILE:HG21	1.95	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:68:LYS:HG3	1:A:88:TYR:CE1	2.50	0.47
1:A:227:VAL:HG22	1:A:231:VAL:HB	1.97	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:A:233:MET:HE1	1:B:280:TYR:CE1	2.50	0.46
1:D:36:LYS:HG2	1:D:110:MET:HB3	1.98	0.46
1:D:96:MET:HE1	1:D:146:SER:HB3	1.98	0.45
1:B:171:LEU:HD12	1:B:214:VAL:HG12	1.98	0.45
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:D:88:TYR:C	1:D:88:TYR:CD1	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:HE3	1:B:144:PHE:CE2	2.56	0.41
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:D:281:SER:C	1:D:283:SER:H	2.28	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:HD12	1:D:276:LEU:HA	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%)	10	3
1	C	254/269 (94%)	244 (96%)	9 (4%)	1 (0%)	30	19
1	D	256/269 (95%)	242 (94%)	10 (4%)	4 (2%)	7	2
All	All	1022/1076 (95%)	980 (96%)	34 (3%)	8 (1%)	16	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281	SER

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Mol	Chain	Res	Type
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%)	21	8
1	B	214/226 (95%)	205 (96%)	9 (4%)	26	11
1	C	215/226 (95%)	202 (94%)	13 (6%)	17	5
1	D	215/226 (95%)	202 (94%)	13 (6%)	17	5
All	All	859/904 (95%)	813 (95%)	46 (5%)	20	7

All (46) 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
1	A	171	LEU
1	A	221	GLU
1	A	227	VAL
1	A	233	MET
1	A	262	ARG
1	A	276	LEU
1	A	279	LEU
1	B	33	GLN
1	B	145	LEU
1	B	171	LEU

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Mol	Chain	Res	Type
1	B	175	VAL
1	B	203	VAL
1	B	231	VAL
1	B	262	ARG
1	B	276	LEU
1	B	278	GLU
1	C	108	LYS
1	C	137	ARG
1	C	143	ASN
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	276	LEU
1	C	281	SER
1	C	282	THR
1	D	69	GLU
1	D	108	LYS
1	D	137	ARG
1	D	143	ASN
1	D	145	LEU
1	D	171	LEU
1	D	205	ARG
1	D	233	MET
1	D	262	ARG
1	D	274	LYS
1	D	276	LEU
1	D	279	LEU
1	D	282	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	134	HIS
1	A	162	ASN
1	A	270	ASN
1	B	87	HIS
1	B	123	ASN

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Mol	Chain	Res	Type
1	B	160	GLN
1	B	207	ASN
1	B	253	GLN
1	B	270	ASN
1	C	101	GLN
1	C	105	GLN
1	C	130	HIS
1	C	270	ASN
1	D	101	GLN
1	D	127	ASN
1	D	160	GLN
1	D	207	ASN
1	D	253	GLN
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 oligosaccharides 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	B	1284	-	50,52,52	0.92	1 (2%)	71,80,80	1.56	10 (14%)
3	DZL	B	1285	-	28,30,30	0.86	1 (3%)	33,46,46	0.82	2 (6%)
2	NAP	C	1284	-	50,52,52	1.00	2 (4%)	71,80,80	1.46	8 (11%)
2	NAP	A	1284	-	50,52,52	0.89	2 (4%)	71,80,80	1.39	8 (11%)
3	DZL	A	1285	-	28,30,30	0.89	1 (3%)	33,46,46	0.93	2 (6%)
3	DZL	C	1285	-	28,30,30	0.83	2 (7%)	33,46,46	0.66	0
2	NAP	D	1284	-	50,52,52	1.03	1 (2%)	71,80,80	1.46	7 (9%)

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	B	1284	-	-	4/35/67/67	0/5/5/5
3	DZL	B	1285	-	-	1/10/52/52	0/6/5/5
2	NAP	C	1284	-	-	3/35/67/67	0/5/5/5
2	NAP	A	1284	-	-	3/35/67/67	0/5/5/5
3	DZL	A	1285	-	-	0/10/52/52	0/6/5/5
3	DZL	C	1285	-	-	0/10/52/52	0/6/5/5
2	NAP	D	1284	-	-	2/35/67/67	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1284	NAP	O4D-C1D	3.11	1.45	1.40
2	C	1284	NAP	O4D-C1D	3.07	1.44	1.40
2	B	1284	NAP	O4D-C1D	2.85	1.44	1.40
3	A	1285	DZL	C8-C6	-2.73	1.44	1.49
2	A	1284	NAP	O4D-C1D	2.67	1.44	1.40
3	B	1285	DZL	C8-C6	-2.62	1.44	1.49
3	C	1285	DZL	C8-C6	-2.37	1.44	1.49
2	C	1284	NAP	PN-O3	2.17	1.61	1.59
3	C	1285	DZL	C8-N10	2.13	1.38	1.34
2	A	1284	NAP	C5A-C4A	2.04	1.42	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1284	NAP	C5A-C4A-N3A	-5.23	119.52	126.72
2	C	1284	NAP	C5A-C4A-N3A	-5.12	119.67	126.72
2	D	1284	NAP	C5A-C4A-N3A	-5.09	119.70	126.72
2	D	1284	NAP	N3A-C2A-N1A	-4.48	121.81	128.58
2	B	1284	NAP	N3A-C4A-N9A	4.46	134.76	127.17
2	A	1284	NAP	C5A-C4A-N3A	-4.32	120.76	126.72
2	C	1284	NAP	N3A-C2A-N1A	-4.30	122.07	128.58
2	A	1284	NAP	N3A-C2A-N1A	-4.28	122.10	128.58
2	B	1284	NAP	N3A-C2A-N1A	-4.19	122.24	128.58
2	D	1284	NAP	N3A-C4A-N9A	4.11	134.16	127.17
2	B	1284	NAP	C3N-C7N-N7N	3.89	122.53	117.74
2	C	1284	NAP	N3A-C4A-N9A	3.83	133.69	127.17
2	A	1284	NAP	N3A-C4A-N9A	3.77	133.57	127.17
2	D	1284	NAP	C5A-N7A-C8A	3.76	109.36	103.45
2	C	1284	NAP	C2A-N3A-C4A	3.69	120.83	111.83
2	B	1284	NAP	C2A-N3A-C4A	3.68	120.83	111.83
2	D	1284	NAP	C2A-N3A-C4A	3.65	120.76	111.83
2	C	1284	NAP	C5A-N7A-C8A	3.52	108.99	103.45
2	B	1284	NAP	C5A-N7A-C8A	3.43	108.84	103.45
2	A	1284	NAP	C3N-C7N-N7N	3.40	121.93	117.74
2	A	1284	NAP	C2A-N3A-C4A	3.26	119.78	111.83
2	C	1284	NAP	C4A-C5A-N7A	-3.12	107.02	110.58
2	D	1284	NAP	C4A-C5A-N7A	-3.11	107.03	110.58
2	B	1284	NAP	C4A-C5A-N7A	-2.88	107.29	110.58
2	A	1284	NAP	C5A-N7A-C8A	2.78	107.82	103.45
2	D	1284	NAP	N9A-C8A-N7A	-2.64	110.19	113.94
2	B	1284	NAP	O7N-C7N-N7N	-2.53	118.96	122.62
2	C	1284	NAP	N9A-C8A-N7A	-2.51	110.38	113.94
2	B	1284	NAP	N9A-C8A-N7A	-2.34	110.62	113.94
3	B	1285	DZL	C6-C8-N10	-2.31	113.00	115.99
2	A	1284	NAP	C4A-C5A-N7A	-2.27	107.98	110.58
3	B	1285	DZL	C15-C16-C17	-2.27	105.91	109.25
2	A	1284	NAP	N9A-C8A-N7A	-2.25	110.75	113.94
2	B	1284	NAP	C4D-O4D-C1D	-2.19	107.92	109.92
3	A	1285	DZL	O9-C8-C6	2.14	123.93	120.15
2	C	1284	NAP	O7N-C7N-N7N	-2.07	119.63	122.62
3	A	1285	DZL	C6-C8-N10	-2.02	113.37	115.99

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1284	NAP	C1B-C2B-O2B-P2B

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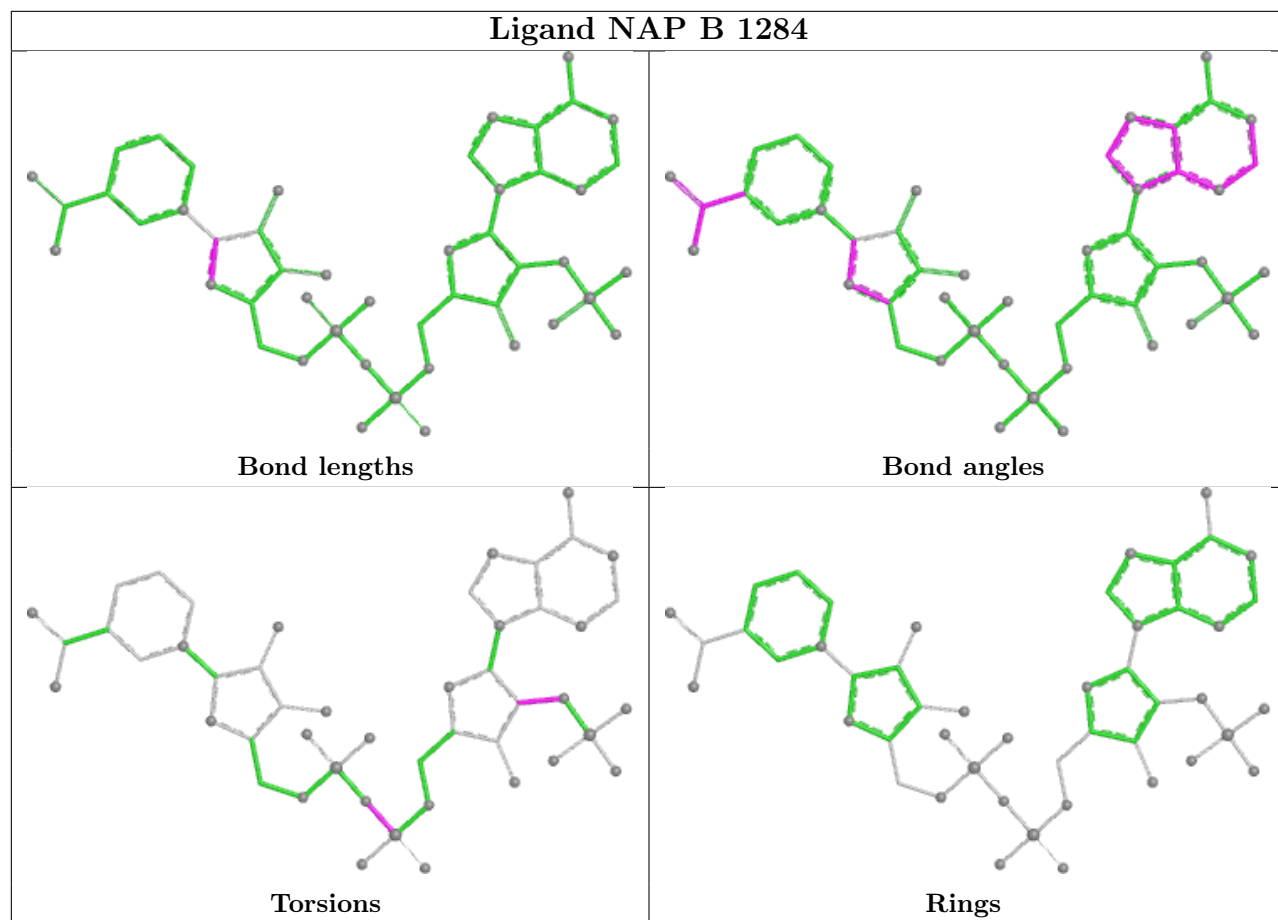
Mol	Chain	Res	Type	Atoms
2	B	1284	NAP	C3B-C2B-O2B-P2B
2	A	1284	NAP	PN-O3-PA-O2A
2	B	1284	NAP	PN-O3-PA-O2A
2	C	1284	NAP	O4D-C4D-C5D-O5D
2	C	1284	NAP	PN-O3-PA-O2A
2	D	1284	NAP	PN-O3-PA-O2A
2	D	1284	NAP	PN-O3-PA-O1A
3	B	1285	DZL	C1-C2-C3-N4
2	A	1284	NAP	C3B-C2B-O2B-P2B
2	A	1284	NAP	PN-O3-PA-O1A
2	B	1284	NAP	PN-O3-PA-O1A
2	C	1284	NAP	C3D-C4D-C5D-O5D

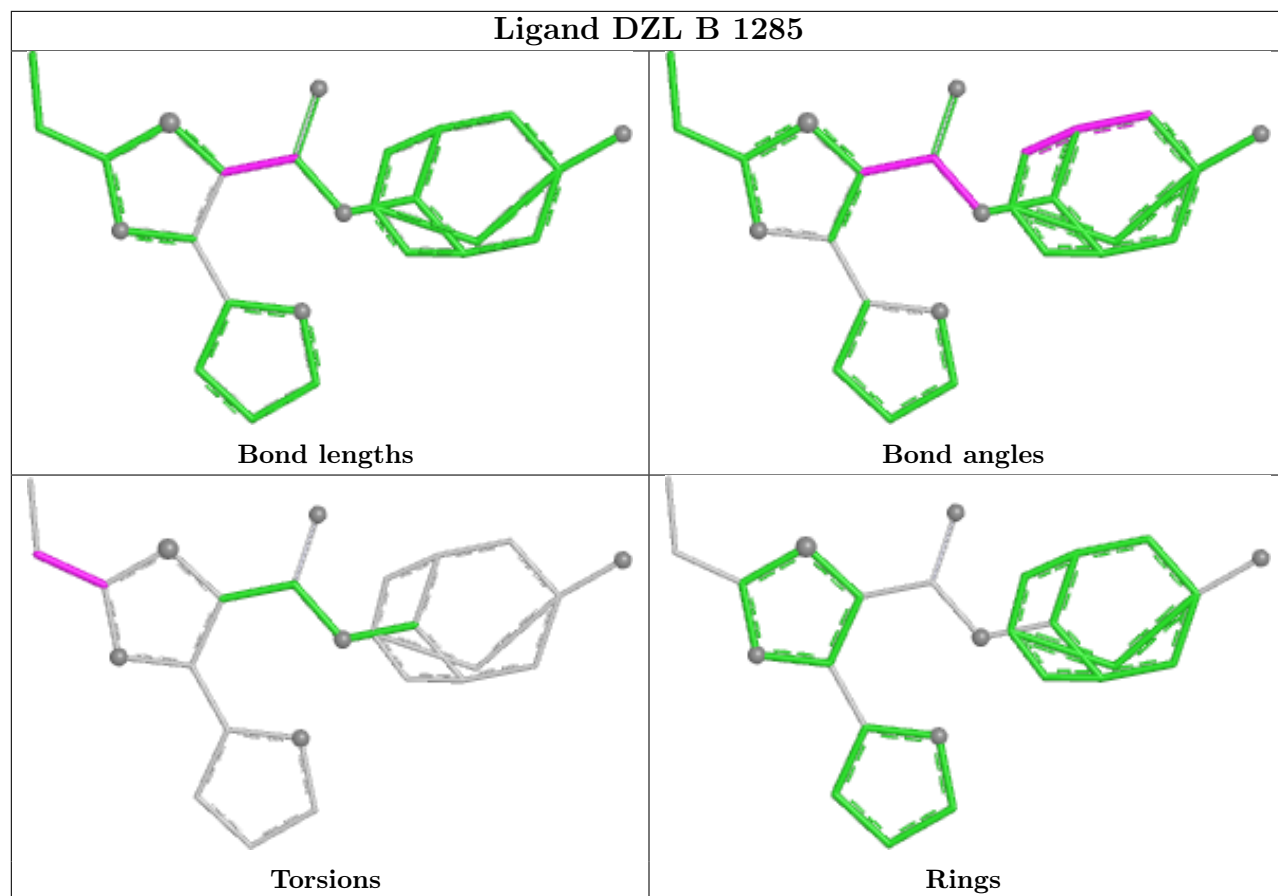
There are no ring outliers.

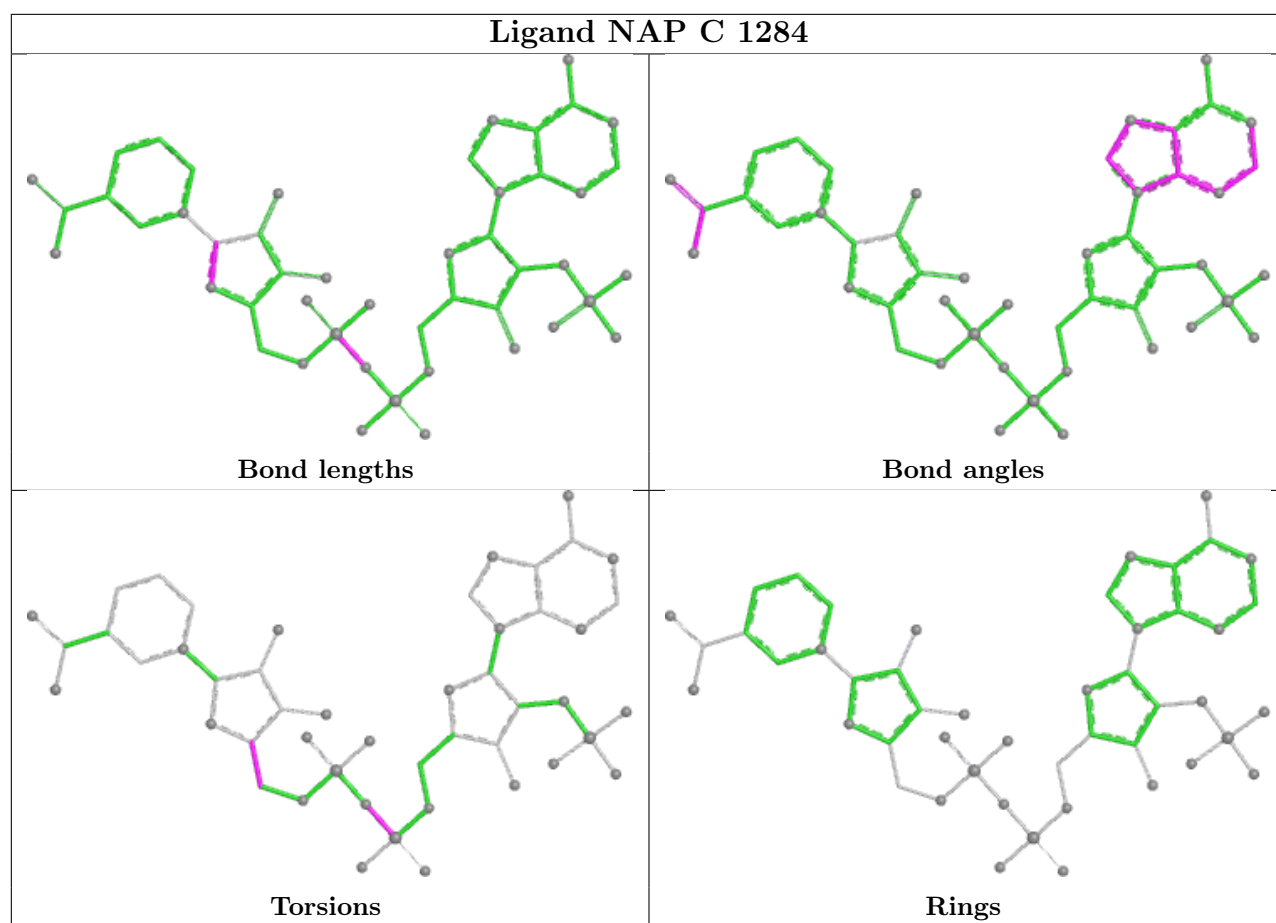
4 monomers are involved in 4 short contacts:

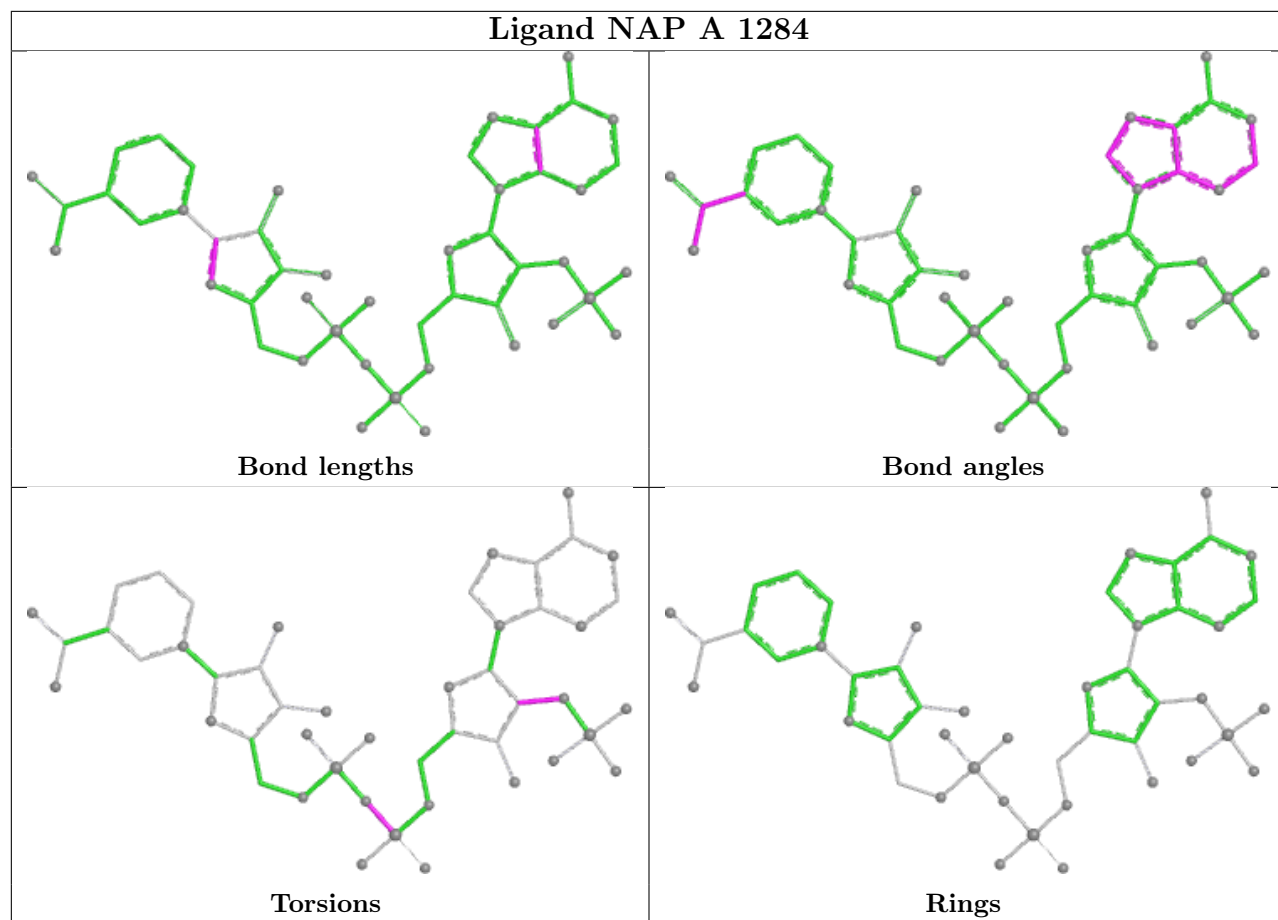
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1284	NAP	1	0
2	C	1284	NAP	1	0
2	A	1284	NAP	1	0
3	C	1285	DZL	1	0

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

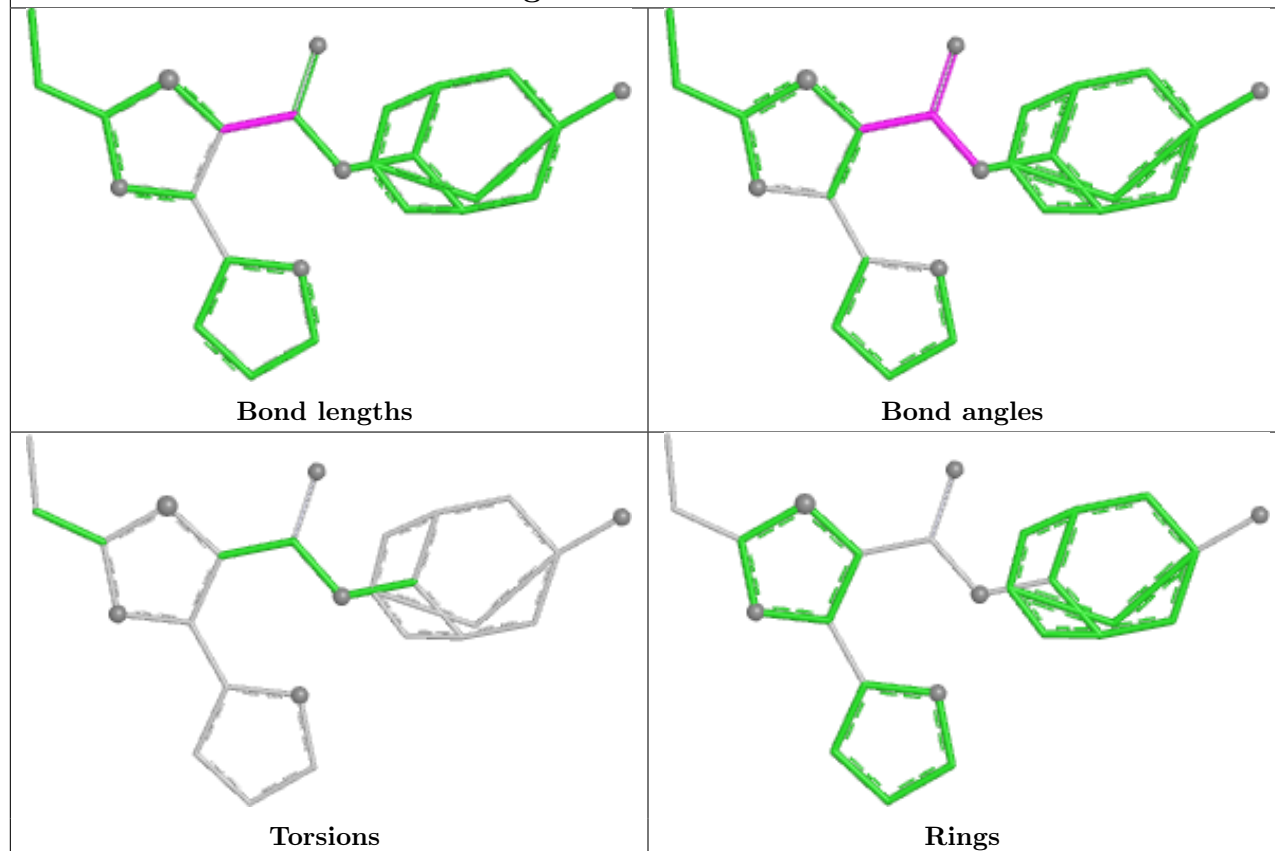




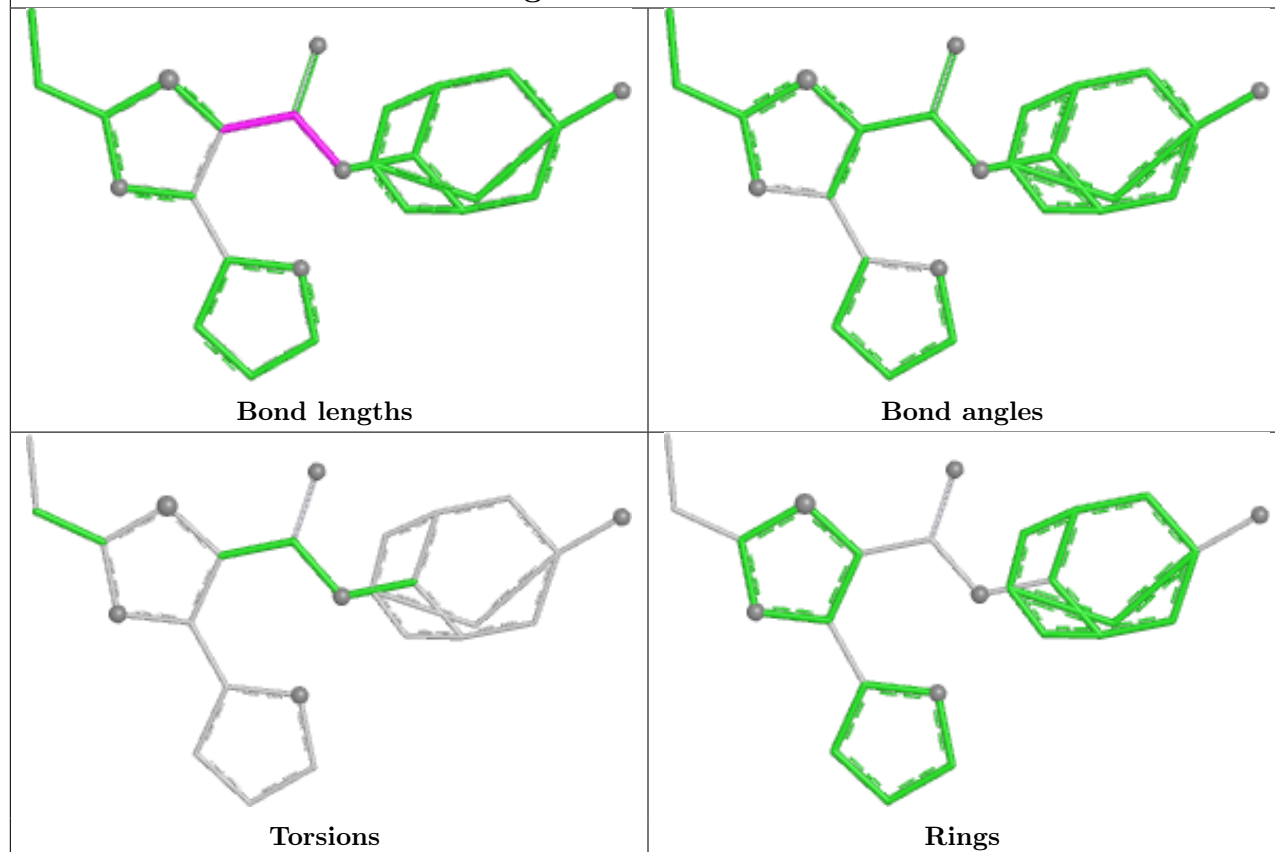


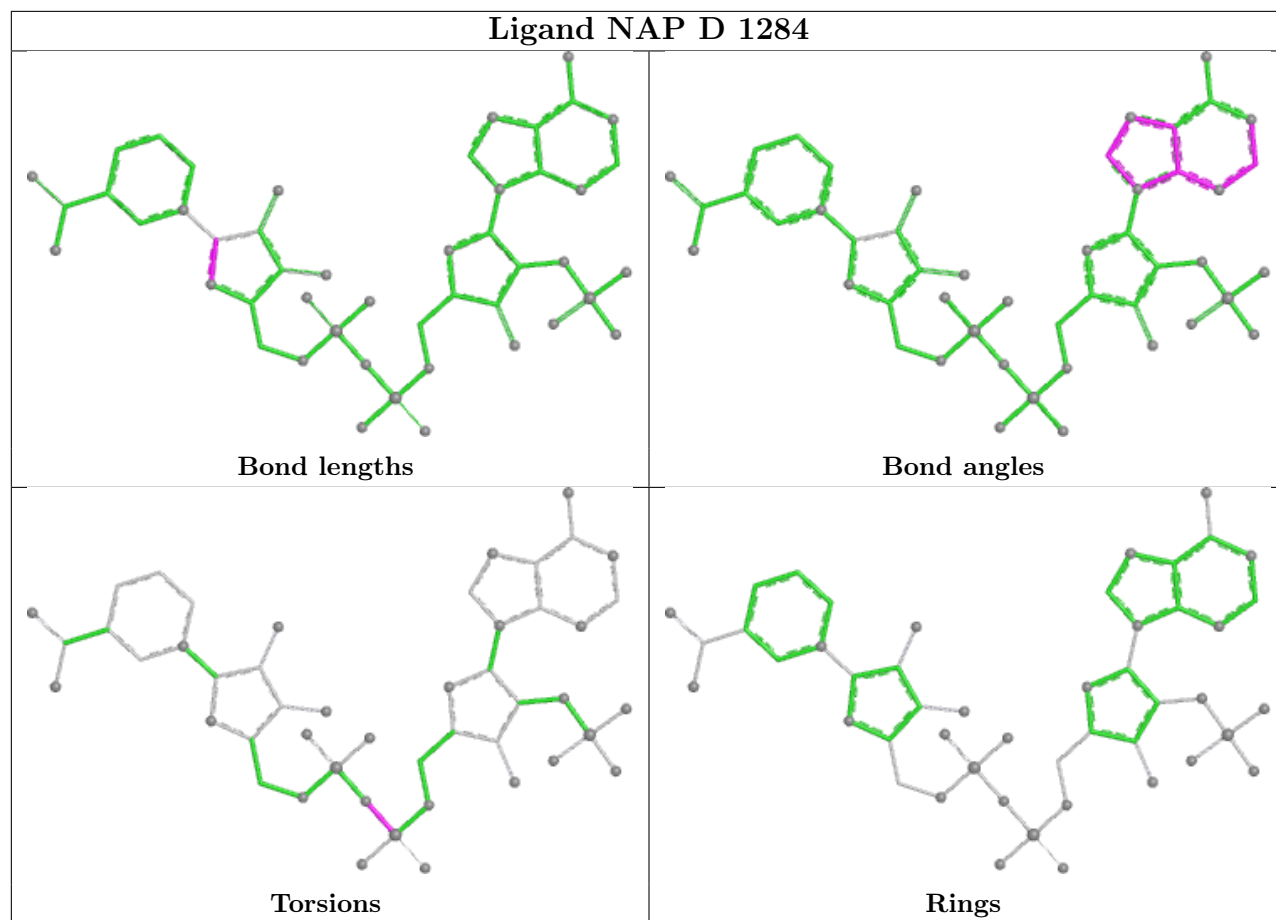


Ligand DZL A 1285



Ligand DZL C 1285





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.21	21 (8%)	18 22	6, 14, 45, 91	0
1	B	258/269 (95%)	0.15	16 (6%)	26 31	7, 14, 37, 99	0
1	C	258/269 (95%)	1.69	95 (36%)	1 0	14, 31, 57, 114	0
1	D	258/269 (95%)	2.57	163 (63%)	0 0	20, 39, 73, 118	0
All	All	1032/1076 (95%)	1.16	295 (28%)	1 1	6, 26, 58, 118	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	SER	8.6
1	A	282	THR	8.5
1	D	230	ILE	7.9
1	D	231	VAL	7.8
1	D	61	VAL	6.6
1	C	231	VAL	6.5
1	C	279	LEU	6.3
1	A	283	SER	6.1
1	D	283	SER	6.1
1	D	74	VAL	6.1
1	D	279	LEU	6.0
1	C	280	TYR	5.7
1	B	263	TRP	5.6
1	D	71	LEU	5.6
1	D	229	GLY	5.4
1	D	263	TRP	5.4
1	C	283	SER	5.4
1	D	282	THR	5.4
1	C	232	HIS	5.4
1	C	230	ILE	5.3
1	D	232	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	89	ILE	5.2
1	D	52	TYR	5.1
1	A	280	TYR	5.0
1	C	203	VAL	5.0
1	C	128	LEU	4.9
1	D	128	LEU	4.9
1	C	263	TRP	4.8
1	D	75	VAL	4.8
1	D	67	SER	4.7
1	B	280	TYR	4.6
1	D	262	ARG	4.6
1	D	264	THR	4.5
1	D	99	ALA	4.5
1	D	129	PHE	4.5
1	C	129	PHE	4.5
1	C	206	VAL	4.4
1	D	227	VAL	4.4
1	A	233	MET	4.4
1	D	228	SER	4.4
1	D	233	MET	4.3
1	C	197	ILE	4.2
1	B	282	THR	4.2
1	D	126	LEU	4.2
1	D	88	TYR	4.2
1	D	56	LYS	4.2
1	A	281	SER	4.1
1	A	229	GLY	4.1
1	D	65	ALA	4.0
1	D	27	PHE	4.0
1	D	130	HIS	4.0
1	D	70	THR	3.9
1	C	130	HIS	3.9
1	D	81	LEU	3.9
1	D	33	GLN	3.9
1	D	226	ALA	3.9
1	C	204	SER	3.9
1	D	281	SER	3.9
1	D	29	PRO	3.9
1	D	57	MET	3.8
1	D	59	ALA	3.8
1	C	262	ARG	3.8
1	D	160	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	282	THR	3.7
1	D	280	TYR	3.7
1	D	46	ILE	3.7
1	D	63	VAL	3.7
1	D	268	ILE	3.7
1	A	279	LEU	3.7
1	C	205	ARG	3.7
1	D	258	TYR	3.7
1	D	131	ASP	3.7
1	C	133	ILE	3.6
1	D	105	GLN	3.6
1	D	235	ALA	3.6
1	C	225	LYS	3.6
1	A	131	ASP	3.6
1	D	79	LEU	3.6
1	D	171	LEU	3.6
1	C	153	ALA	3.6
1	B	262	ARG	3.6
1	C	264	THR	3.6
1	D	54	LEU	3.6
1	D	32	LEU	3.5
1	D	51	ALA	3.5
1	D	55	ALA	3.5
1	D	106	ALA	3.5
1	D	43	SER	3.5
1	C	102	PHE	3.5
1	A	232	HIS	3.5
1	D	134	HIS	3.5
1	D	225	LYS	3.5
1	D	62	VAL	3.4
1	C	109	LEU	3.4
1	D	109	LEU	3.4
1	D	85	SER	3.4
1	D	127	ASN	3.4
1	C	229	GLY	3.4
1	D	116	LEU	3.4
1	C	160	GLN	3.4
1	A	263	TRP	3.4
1	C	144	PHE	3.3
1	D	132	ASP	3.3
1	A	231	VAL	3.3
1	D	72	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	101	GLN	3.3
1	D	205	ARG	3.3
1	B	207	ASN	3.3
1	D	249	GLY	3.3
1	D	206	VAL	3.2
1	D	60	HIS	3.2
1	A	262	ARG	3.2
1	C	108	LYS	3.2
1	B	131	ASP	3.2
1	C	83	ALA	3.2
1	D	69	GLU	3.2
1	D	121	ILE	3.2
1	D	133	ILE	3.2
1	D	53	HIS	3.2
1	D	68	LYS	3.1
1	D	208	VAL	3.1
1	B	130	HIS	3.1
1	D	102	PHE	3.1
1	C	182	ALA	3.1
1	C	149	VAL	3.1
1	D	234	GLN	3.1
1	D	222	THR	3.1
1	C	179	LEU	3.1
1	D	140	MET	3.1
1	D	83	ALA	3.1
1	C	268	ILE	3.0
1	D	78	CYS	3.0
1	B	279	LEU	3.0
1	D	276	LEU	3.0
1	D	58	GLY	3.0
1	A	230	ILE	3.0
1	D	238	LYS	2.9
1	C	163	GLY	2.9
1	D	110	MET	2.9
1	D	144	PHE	2.9
1	D	278	GLU	2.9
1	D	86	ALA	2.9
1	D	251	LEU	2.9
1	C	28	ARG	2.9
1	D	265	THR	2.9
1	C	86	ALA	2.9
1	A	268	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	61	VAL	2.9
1	C	37	VAL	2.8
1	D	257	TYR	2.8
1	D	28	ARG	2.8
1	D	98	PHE	2.8
1	D	145	LEU	2.8
1	D	64	THR	2.8
1	B	160	GLN	2.8
1	D	166	VAL	2.8
1	C	154	ALA	2.8
1	C	98	PHE	2.8
1	D	47	GLY	2.8
1	C	89	ILE	2.8
1	C	281	SER	2.8
1	C	112	GLY	2.8
1	D	77	HIS	2.8
1	D	266	LEU	2.8
1	D	237	PRO	2.8
1	D	84	ALA	2.7
1	D	82	GLY	2.7
1	B	264	THR	2.7
1	D	236	ALA	2.7
1	D	158	LEU	2.7
1	C	178	PRO	2.7
1	D	197	ILE	2.7
1	C	137	ARG	2.7
1	D	108	LYS	2.7
1	D	181	ALA	2.6
1	A	234	GLN	2.6
1	C	69	GLU	2.6
1	D	180	VAL	2.6
1	C	131	ASP	2.6
1	C	201	TYR	2.6
1	C	138	LYS	2.6
1	D	44	LYS	2.6
1	D	161	SER	2.6
1	A	72	GLN	2.6
1	D	104	ALA	2.6
1	C	70	THR	2.6
1	D	76	SER	2.6
1	D	107	GLY	2.6
1	D	73	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	274	LYS	2.6
1	C	155	LEU	2.5
1	D	34	GLY	2.5
1	D	42	ALA	2.5
1	D	35	LYS	2.5
1	D	113	LEU	2.5
1	A	130	HIS	2.5
1	B	134	HIS	2.5
1	C	180	VAL	2.5
1	C	227	VAL	2.5
1	D	183	TYR	2.4
1	C	126	LEU	2.4
1	C	134	HIS	2.4
1	C	145	LEU	2.4
1	C	68	LYS	2.4
1	C	84	ALA	2.4
1	D	220	THR	2.4
1	C	208	VAL	2.4
1	D	136	VAL	2.4
1	D	179	LEU	2.4
1	D	165	ILE	2.4
1	D	103	VAL	2.4
1	D	118	LEU	2.4
1	C	193	PHE	2.4
1	D	194	PHE	2.4
1	C	97	THR	2.4
1	D	210	ILE	2.4
1	D	90	ALA	2.4
1	C	278	GLU	2.4
1	D	87	HIS	2.4
1	D	148	VAL	2.4
1	C	140	MET	2.4
1	C	233	MET	2.4
1	B	269	ARG	2.3
1	D	124	THR	2.3
1	C	226	ALA	2.3
1	C	275	ILE	2.3
1	C	36	LYS	2.3
1	C	56	LYS	2.3
1	C	85	SER	2.3
1	C	161	SER	2.3
1	D	26	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	32	LEU	2.3
1	C	105	GLN	2.3
1	C	276	LEU	2.3
1	D	267	LEU	2.3
1	A	274	LYS	2.3
1	C	35	LYS	2.3
1	C	33	GLN	2.3
1	C	116	LEU	2.3
1	D	150	LEU	2.3
1	C	110	MET	2.3
1	A	88	TYR	2.3
1	C	27	PHE	2.3
1	D	245	ILE	2.3
1	C	75	VAL	2.3
1	C	103	VAL	2.3
1	D	142	VAL	2.3
1	D	203	VAL	2.3
1	A	278	GLU	2.2
1	D	176	ALA	2.2
1	D	193	PHE	2.2
1	D	50	MET	2.2
1	D	247	LYS	2.2
1	D	243	LEU	2.2
1	B	33	GLN	2.2
1	C	162	ASN	2.2
1	D	94	GLU	2.2
1	D	122	THR	2.2
1	D	259	ASP	2.2
1	C	104	ALA	2.2
1	D	172	ALA	2.2
1	D	177	TYR	2.2
1	D	201	TYR	2.2
1	D	246	ILE	2.2
1	D	80	GLU	2.2
1	C	146	SER	2.2
1	C	234	GLN	2.1
1	D	95	ASP	2.1
1	B	281	SER	2.1
1	D	219	ASP	2.1
1	C	62	VAL	2.1
1	C	136	VAL	2.1
1	C	142	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	239	GLU	2.1
1	C	171	LEU	2.1
1	C	106	ALA	2.1
1	A	257	TYR	2.1
1	C	228	SER	2.1
1	D	48	ARG	2.1
1	D	261	SER	2.1
1	C	124	THR	2.1
1	D	112	GLY	2.1
1	C	148	VAL	2.1
1	D	214	VAL	2.1
1	D	212	LEU	2.1
1	C	99	ALA	2.1
1	D	269	ARG	2.1
1	C	73	LYS	2.0
1	D	125	SER	2.0
1	D	196	SER	2.0
1	C	127	ASN	2.0
1	B	276	LEU	2.0
1	D	157	MET	2.0
1	D	224	MET	2.0
1	C	121	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	D	1284	48/48	0.84	0.12	27,32,37,39	0

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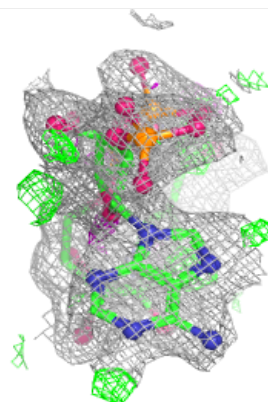
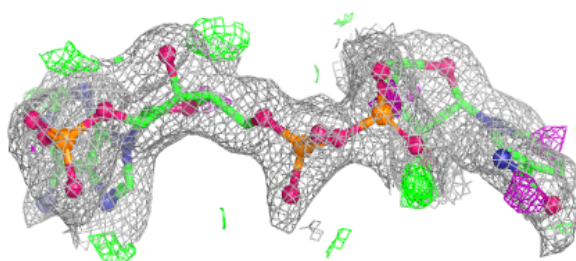
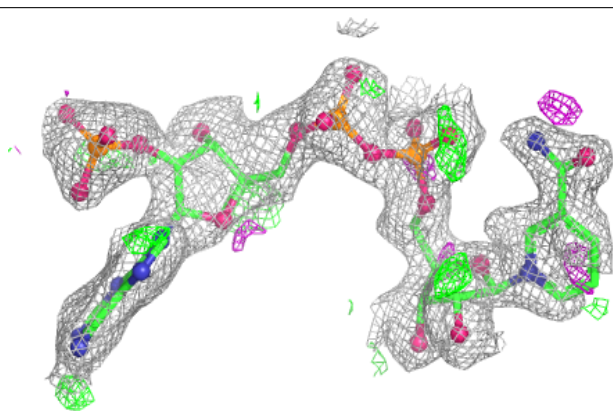
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	C	1284	48/48	0.92	0.09	15,23,32,35	0
3	DZL	C	1285	26/26	0.94	0.08	21,25,29,29	0
3	DZL	A	1285	26/26	0.95	0.07	9,13,23,24	0
3	DZL	B	1285	26/26	0.96	0.07	7,12,18,28	0
2	NAP	B	1284	48/48	0.97	0.05	5,11,13,14	0
2	NAP	A	1284	48/48	0.98	0.05	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.

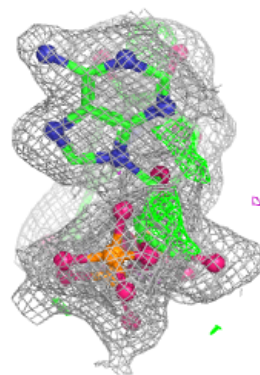
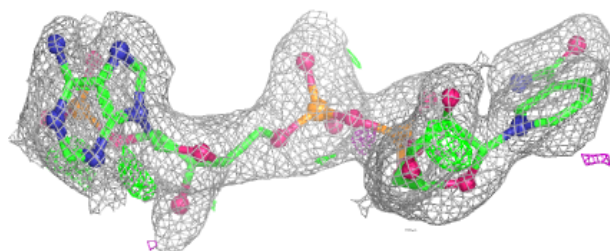
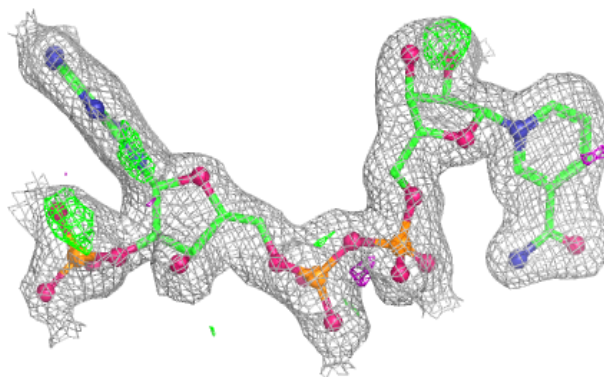
Electron density around NAP D 1284:

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

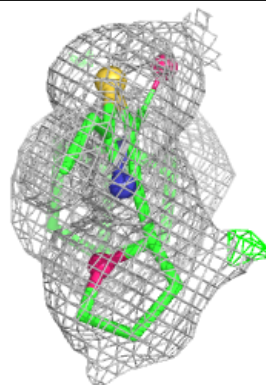
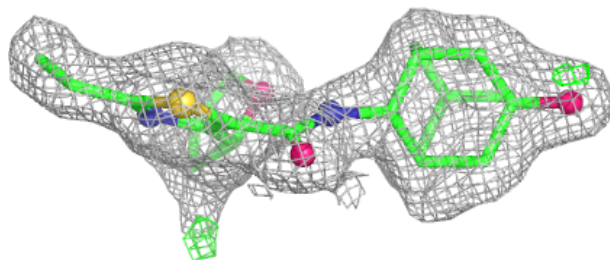
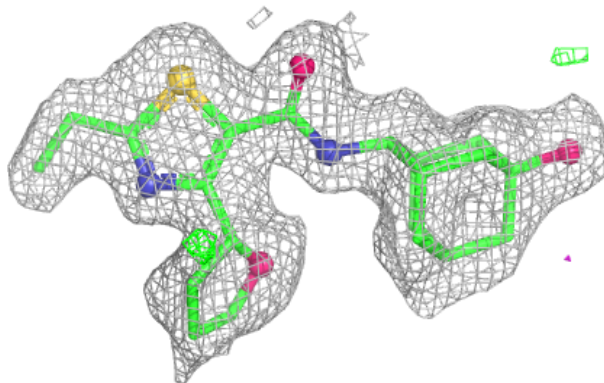


Electron density around NAP C 1284:

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

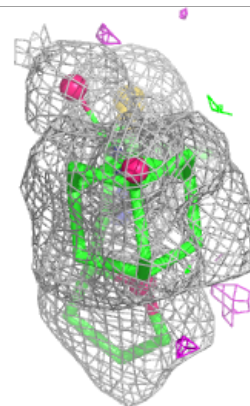
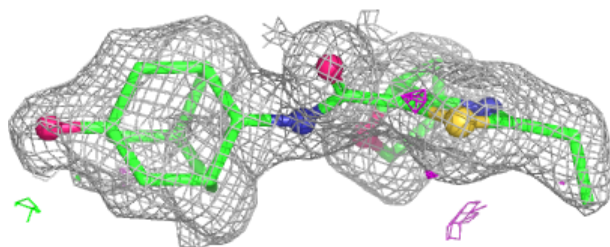
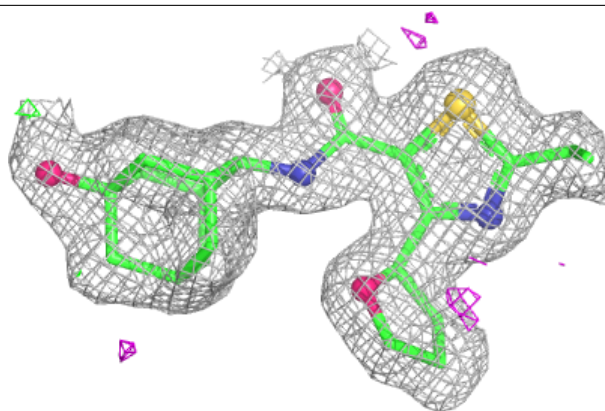
**Electron density around DZL C 1285:**

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and green (positive)

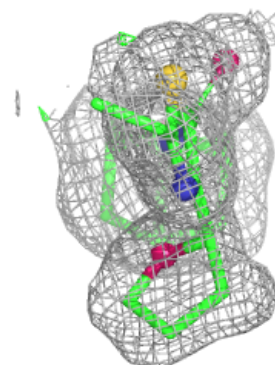
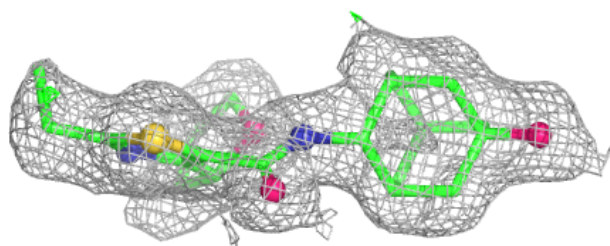
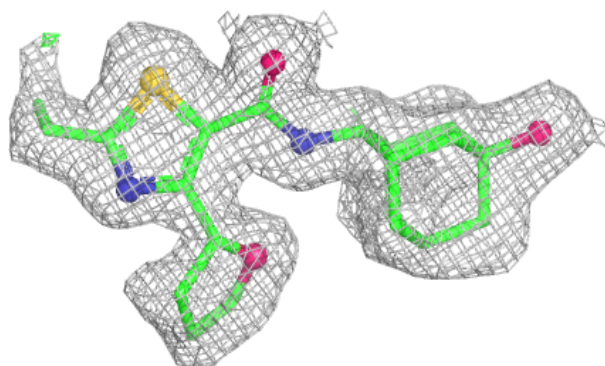


Electron density around DZL A 1285:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

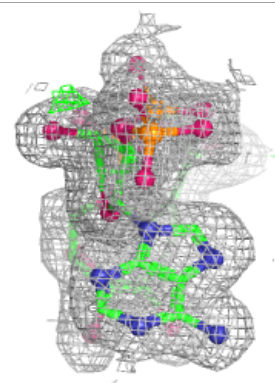
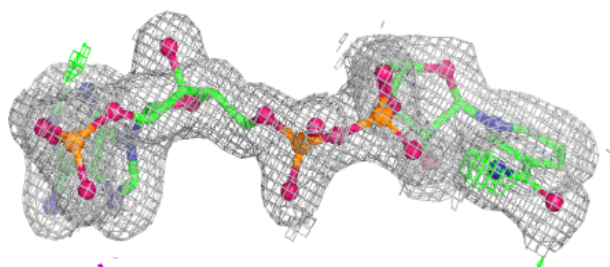
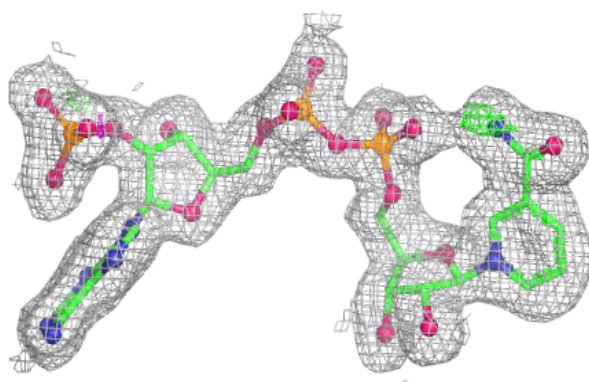
**Electron density around DZL B 1285:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

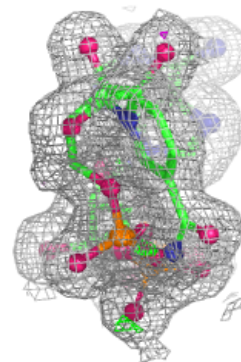
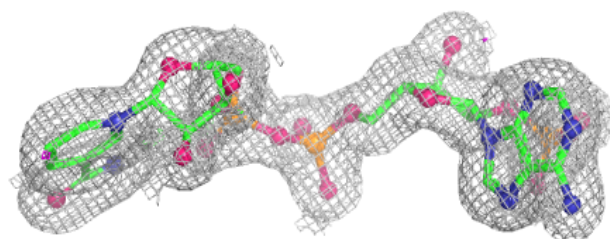
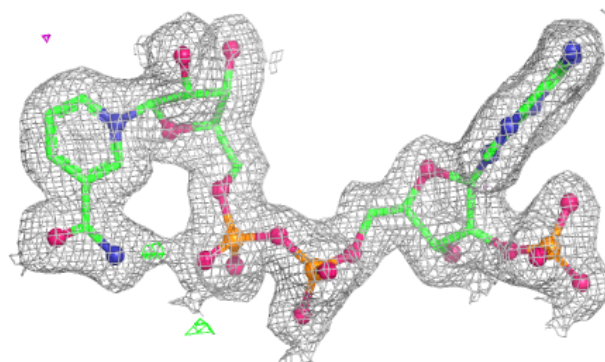


Electron density around NAP B 1284:

$2mF_o-DF_c$ (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.