



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:36 AM UTC

PDB ID : 1MXH / pdb_00001mxh
Title : Crystal Structure of Substrate Complex of Putative Pteridine Reductase 2 (PTR2) from Trypanosoma cruzi
Authors : Schormann, N.; Pal, B.; Senkovich, O.; Carson, M.; Howard, A.; Smith, C.; Delucas, L.; Chattopadhyay, D.
Deposited on : 2002-10-02
Resolution : 2.20 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

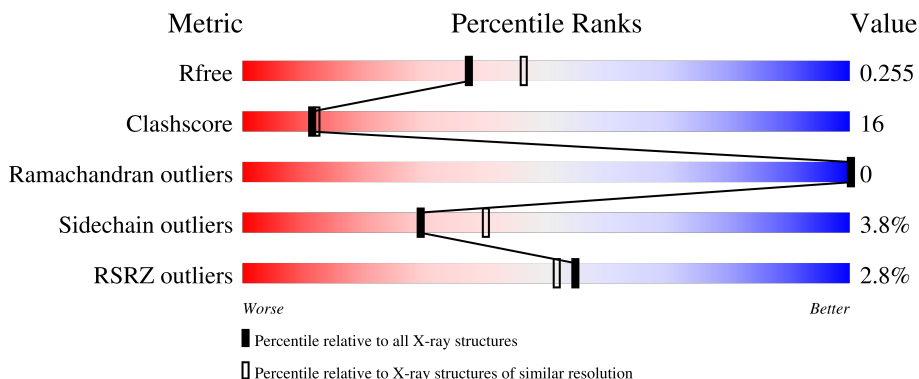
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	276	2% 62% 25% • 10%
1	B	276	2% 55% 32% • 10%
1	C	276	3% 61% 25% • 10%
1	D	276	4% 63% 23% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

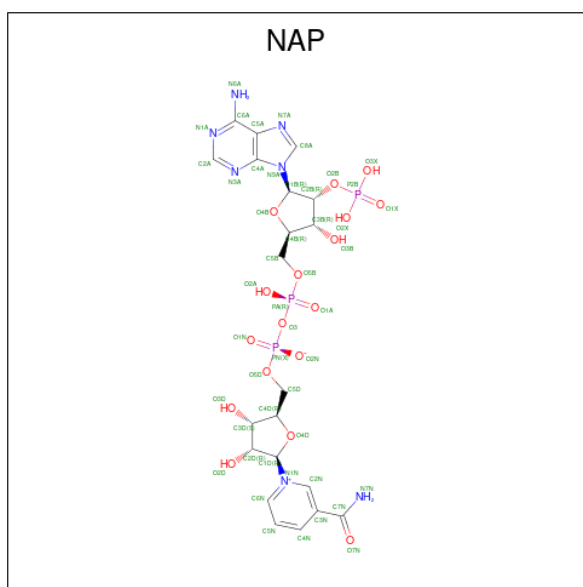
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DHF	A	1278	-	X	-	-
3	DHF	B	2278	-	X	-	-
3	DHF	D	4278	-	X	-	-

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 PTERIDINE REDUCTASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total 1845	C 1161	N 338	O 335	S 11	0	0	0
1	B	248	Total 1845	C 1161	N 338	O 335	S 11	0	0	0
1	C	248	Total 1845	C 1161	N 338	O 335	S 11	0	0	0
1	D	248	Total 1845	C 1161	N 338	O 335	S 11	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



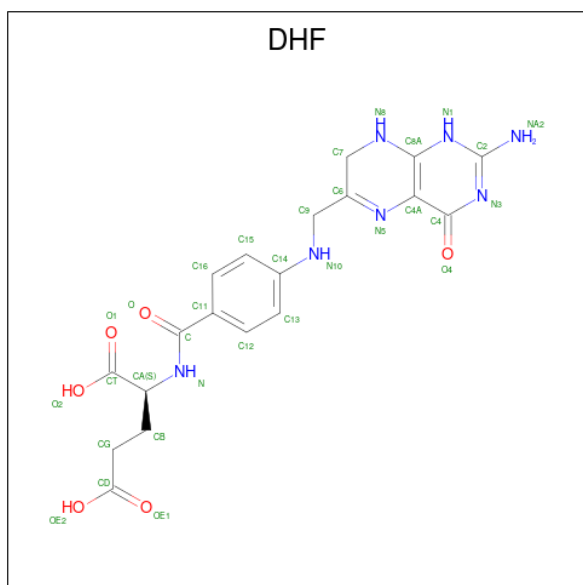
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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

- Molecule 3 is DIHYDROFOLIC ACID (CCD ID: DHF) (formula: $C_{19}H_{21}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	18	7	4		
3	B	1	Total	C	N	O	0	0
			29	18	7	4		
3	C	1	Total	C	N	O	0	0
			29	18	7	4		
3	D	1	Total	C	N	O	0	0
			29	18	7	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total	O	0	0
			95	95		
4	B	89	Total	O	0	0
			89	89		
4	C	133	Total	O	0	0
			133	133		

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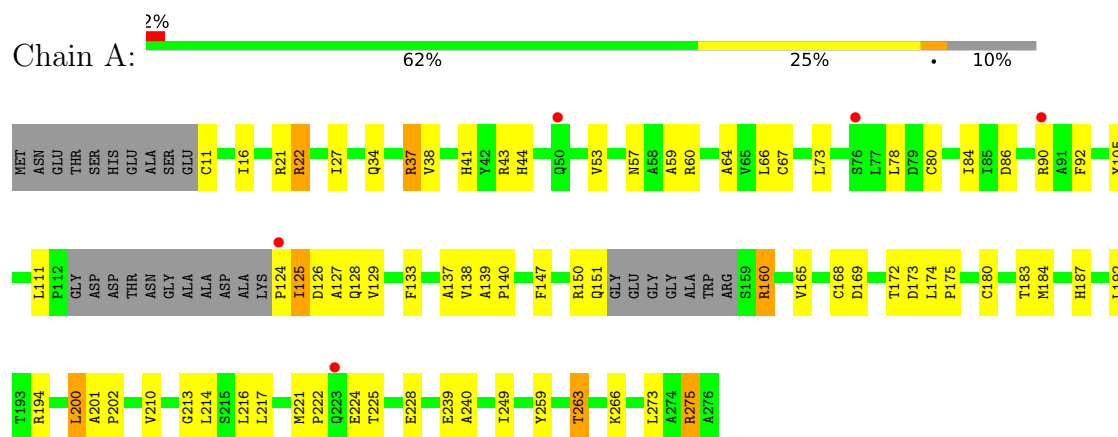
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	140	Total	O	0	0
			140	140		

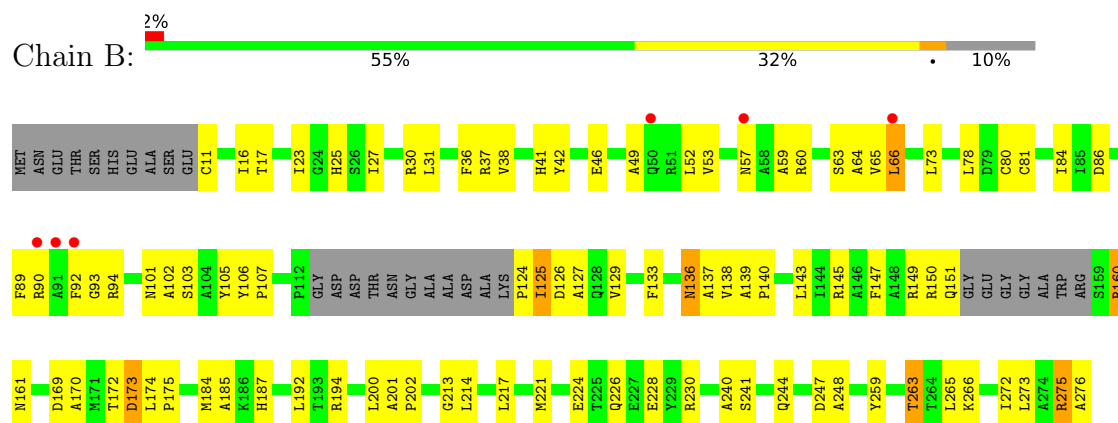
3 Residue-property plots [i](#)

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 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.

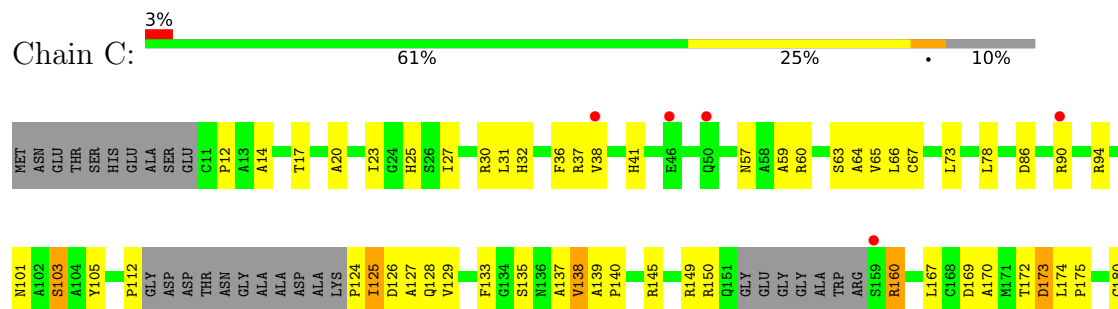
• Molecule 1: PTERIDINE REDUCTASE 2

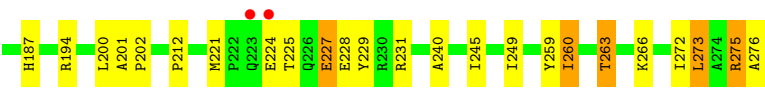


• Molecule 1: PTERIDINE REDUCTASE 2

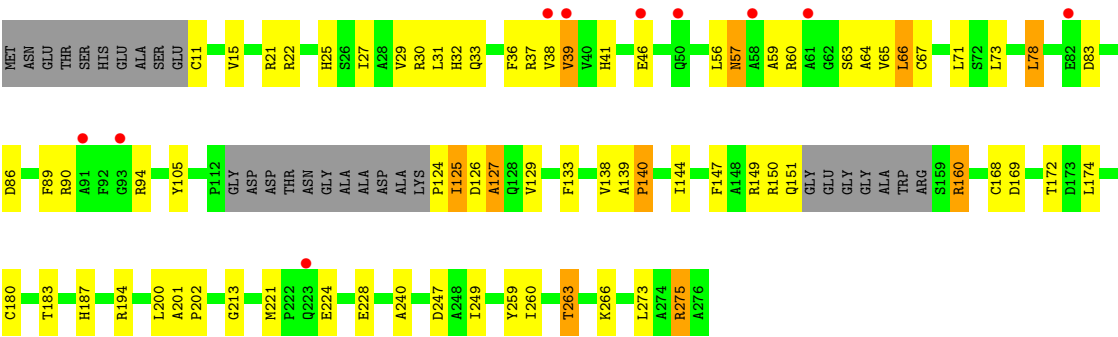


• Molecule 1: PTERIDINE REDUCTASE 2





● Molecule 1: PTERIDINE REDUCTASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	74.61Å 74.61Å 181.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.45 – 2.20 19.45 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (19.45-2.20) 97.7 (19.45-2.20)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 1.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.205 , 0.251 0.207 , 0.255	Depositor DCC
R_{free} test set	4343 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l 0.057 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8145	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, DHF

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	0.44	0/1876	0.95	5/2546 (0.2%)
1	B	0.42	0/1876	0.94	6/2546 (0.2%)
1	C	0.46	0/1876	0.99	8/2546 (0.3%)
1	D	0.47	0/1876	0.98	4/2546 (0.2%)
All	All	0.45	0/7504	0.96	23/10184 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	ILE	N-CA-C	8.67	119.24	110.23
1	B	38	VAL	N-CA-C	8.60	120.99	108.53
1	D	39	VAL	O-C-N	-7.83	113.06	122.77
1	B	125	ILE	N-CA-C	7.77	118.31	110.23
1	A	38	VAL	N-CA-C	7.68	120.68	108.85
1	C	125	ILE	N-CA-C	7.36	117.88	110.23
1	A	125	ILE	N-CA-C	6.79	117.30	110.23
1	A	213	GLY	N-CA-C	-6.42	104.37	110.21
1	B	213	GLY	N-CA-C	-6.12	104.64	110.21
1	D	127	ALA	N-CA-C	-5.75	104.99	112.23
1	D	180	CYS	N-CA-C	5.65	117.89	111.11
1	C	138	VAL	N-CA-C	5.56	116.34	110.72
1	A	22	ARG	N-CA-C	5.53	116.72	108.31
1	B	103	SER	N-CA-C	5.37	117.13	108.32
1	C	135	SER	N-CA-C	5.30	117.06	111.28
1	B	136	ASN	N-CA-C	5.22	119.70	113.23
1	C	37	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	C	103	SER	N-CA-C	5.16	116.78	108.32
1	B	173	ASP	N-CA-C	-5.12	106.54	112.89
1	C	128	GLN	N-CA-C	-5.12	105.78	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	ILE	N-CA-C	5.07	115.98	108.23
1	C	173	ASP	N-CA-C	-5.03	106.65	112.89
1	A	37	ARG	CD-NE-CZ	-5.01	117.38	124.40

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	1845	0	1880	62	0
1	B	1845	0	1880	78	0
1	C	1845	0	1878	70	0
1	D	1845	0	1880	66	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	2	0
2	D	48	0	25	3	0
3	A	29	0	14	1	0
3	B	29	0	14	5	0
3	C	29	0	14	3	0
3	D	29	0	14	3	0
4	A	95	0	0	5	0
4	B	89	0	0	2	0
4	C	133	0	0	1	0
4	D	140	0	0	4	0
All	All	8145	0	7674	247	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 16.

All (247) 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:221:MET:CE	3:B:2278:DHF:H12	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:O	1:C:275:ARG:HD3	1.59	1.02
1:B:221:MET:HE1	3:B:2278:DHF:H12	1.42	0.99
1:B:86:ASP:OD2	1:B:90:ARG:HD2	1.67	0.94
1:B:57:ASN:HD21	1:B:64:ALA:H	1.17	0.91
1:C:31:LEU:O	1:C:36:PHE:HB2	1.74	0.86
1:C:194:ARG:HH21	1:D:187:HIS:HE1	1.23	0.86
1:A:86:ASP:OD1	1:A:90:ARG:HD2	1.75	0.85
1:B:37:ARG:HH21	1:B:92:PHE:HB3	1.44	0.82
1:B:275:ARG:HD3	1:C:174:LEU:O	1.78	0.82
1:A:275:ARG:HD3	1:D:174:LEU:O	1.80	0.81
1:B:263:THR:HG22	1:D:266:LYS:HE3	1.61	0.81
1:A:174:LEU:O	1:D:275:ARG:HD3	1.82	0.80
1:D:31:LEU:O	1:D:36:PHE:HB2	1.81	0.80
1:D:66:LEU:H	1:D:66:LEU:HD23	1.49	0.77
1:B:53:VAL:HG21	1:B:66:LEU:HB3	1.66	0.77
1:B:221:MET:HE3	3:B:2278:DHF:H12	1.66	0.77
1:A:169:ASP:HB3	1:A:172:THR:HG23	1.67	0.77
1:A:57:ASN:HD21	1:A:64:ALA:H	1.33	0.76
1:B:221:MET:HE1	3:B:2278:DHF:C12	2.14	0.76
1:D:57:ASN:ND2	1:D:63:SER:H	1.86	0.74
1:B:276:ALA:HA	1:C:276:ALA:HA	1.72	0.71
1:C:57:ASN:HD21	1:C:64:ALA:H	1.38	0.71
1:B:73:LEU:HD21	1:B:138:VAL:HG21	1.71	0.71
1:C:86:ASP:OD2	1:C:90:ARG:HD2	1.91	0.70
1:C:105:TYR:OH	3:C:3278:DHF:H15	1.91	0.70
1:C:187:HIS:HE1	1:D:194:ARG:HH21	1.40	0.70
1:C:194:ARG:HH21	1:D:187:HIS:CE1	2.09	0.69
1:A:66:LEU:HD23	1:A:66:LEU:H	1.58	0.68
1:D:11:CYS:O	1:D:37:ARG:NH1	2.26	0.68
1:C:124:PRO:HG2	1:C:127:ALA:HB3	1.76	0.68
1:A:125:ILE:HG23	1:A:126:ASP:H	1.59	0.67
1:B:275:ARG:HG2	4:B:2282:HOH:O	1.94	0.67
1:A:139:ALA:HB3	1:A:140:PRO:HD3	1.77	0.67
1:D:46:GLU:HG3	4:D:4297:HOH:O	1.93	0.67
1:D:86:ASP:OD1	1:D:90:ARG:HD2	1.95	0.66
1:B:57:ASN:HD21	1:B:64:ALA:N	1.93	0.64
1:B:169:ASP:HB3	1:B:172:THR:HG23	1.78	0.64
1:B:66:LEU:H	1:B:66:LEU:HD23	1.61	0.64
1:C:66:LEU:HD23	1:C:66:LEU:H	1.62	0.64
1:B:31:LEU:O	1:B:36:PHE:HB2	1.96	0.64
1:B:240:ALA:HB2	1:D:259:TYR:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ILE:CD1	1:A:249:ILE:HD13	2.28	0.63
1:A:37:ARG:HH21	1:A:92:PHE:HB3	1.64	0.63
1:A:173:ASP:O	1:A:175:PRO:HD3	1.98	0.63
1:A:160:ARG:HB2	4:A:1312:HOH:O	1.98	0.63
1:B:137:ALA:C	1:B:140:PRO:HD2	2.24	0.63
1:A:125:ILE:HG23	1:A:126:ASP:N	2.13	0.63
1:C:221:MET:HE1	3:C:3278:DHF:H12	1.79	0.62
1:D:105:TYR:OH	3:D:4278:DHF:H15	1.99	0.62
1:B:11:CYS:HB2	1:B:37:ARG:HH11	1.65	0.62
1:B:139:ALA:HB3	1:B:140:PRO:HD3	1.81	0.62
1:A:214:LEU:HD11	1:A:217:LEU:HD21	1.82	0.62
1:D:57:ASN:HD21	1:D:63:SER:N	1.99	0.60
1:B:214:LEU:HD11	1:B:217:LEU:HD21	1.83	0.60
1:D:140:PRO:O	1:D:144:ILE:HG13	2.00	0.60
1:A:57:ASN:HD21	1:A:64:ALA:N	1.98	0.60
1:D:139:ALA:HB3	1:D:140:PRO:HD3	1.84	0.59
1:D:224:GLU:O	1:D:228:GLU:HG3	2.02	0.59
1:B:147:PHE:O	1:B:151:GLN:HG2	2.02	0.59
1:B:105:TYR:OH	3:B:2278:DHF:H15	2.02	0.59
1:C:139:ALA:HB3	1:C:140:PRO:HD3	1.83	0.59
1:C:194:ARG:NH2	1:D:187:HIS:HE1	1.98	0.58
1:D:221:MET:HE1	3:D:4278:DHF:H12	1.86	0.58
1:A:53:VAL:HG21	1:A:66:LEU:HB3	1.84	0.58
1:A:210:VAL:HG21	1:A:249:ILE:HG13	1.84	0.58
1:C:221:MET:CE	3:C:3278:DHF:H12	2.34	0.57
1:A:194:ARG:NH2	1:B:173:ASP:HA	2.20	0.57
1:A:180:CYS:HB2	4:B:2302:HOH:O	2.05	0.57
1:A:263:THR:HG22	1:C:266:LYS:HE3	1.87	0.57
1:B:42:TYR:CE2	1:B:46:GLU:HA	2.39	0.57
1:B:86:ASP:HA	1:B:150:ARG:NH1	2.19	0.56
1:B:201:ALA:HB3	1:B:202:PRO:HD3	1.85	0.56
1:A:168:CYS:SG	4:A:1341:HOH:O	2.25	0.56
1:B:259:TYR:CE2	1:D:240:ALA:HB2	2.41	0.56
1:B:125:ILE:HG23	1:B:126:ASP:N	2.20	0.55
1:A:169:ASP:HB3	1:A:172:THR:CG2	2.35	0.55
1:B:16:ILE:N	1:B:16:ILE:HD12	2.21	0.55
1:D:57:ASN:ND2	1:D:63:SER:N	2.55	0.55
1:A:59:ALA:O	1:A:60:ARG:HG3	2.06	0.55
1:C:94:ARG:CZ	1:C:160:ARG:HH21	2.20	0.55
1:B:226:GLN:NE2	1:B:230:ARG:HH22	2.05	0.54
1:B:263:THR:HG21	1:D:266:LYS:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ILE:HG23	1:C:126:ASP:N	2.23	0.54
1:A:124:PRO:HG2	1:A:127:ALA:HB3	1.90	0.53
1:B:173:ASP:O	1:B:175:PRO:HD3	2.09	0.53
1:D:57:ASN:HD21	1:D:64:ALA:H	1.56	0.53
1:A:86:ASP:HA	1:A:150:ARG:NH1	2.24	0.53
1:D:94:ARG:CZ	1:D:160:ARG:HH21	2.22	0.53
1:D:41:HIS:HA	1:D:67:CYS:O	2.08	0.53
1:D:160:ARG:HB2	4:D:4303:HOH:O	2.09	0.53
1:A:129:VAL:O	1:A:133:PHE:HB2	2.09	0.52
1:A:266:LYS:O	1:C:263:THR:HG21	2.09	0.52
1:C:38:VAL:HG23	1:C:38:VAL:O	2.08	0.52
1:A:224:GLU:O	1:A:228:GLU:HG3	2.10	0.52
1:B:124:PRO:HG2	1:B:127:ALA:HB3	1.92	0.52
1:A:173:ASP:C	1:A:175:PRO:HD3	2.35	0.51
1:D:125:ILE:HG23	1:D:126:ASP:N	2.25	0.51
1:A:34:GLN:NE2	4:A:1306:HOH:O	2.41	0.51
1:B:226:GLN:HE21	1:B:230:ARG:HH22	1.58	0.51
1:D:86:ASP:HA	1:D:150:ARG:NH1	2.26	0.51
1:C:112:PRO:HG3	1:D:149:ARG:NH1	2.25	0.51
1:D:15:VAL:HA	1:D:39:VAL:HB	1.92	0.51
1:C:212:PRO:HG3	1:C:245:ILE:HD12	1.93	0.51
1:C:227:GLU:HB3	1:C:231:ARG:HH21	1.76	0.51
1:B:145:ARG:O	1:B:149:ARG:HG3	2.11	0.51
1:B:266:LYS:HE3	1:D:263:THR:HG22	1.93	0.51
1:A:105:TYR:OH	3:A:1278:DHF:H15	2.12	0.50
1:A:73:LEU:HD21	1:A:138:VAL:HG21	1.93	0.50
1:B:248:ALA:HB1	1:B:265:LEU:HD23	1.93	0.50
1:B:266:LYS:O	1:D:263:THR:HG21	2.11	0.50
1:A:80:CYS:O	1:A:84:ILE:HG13	2.11	0.50
1:D:221:MET:CE	3:D:4278:DHF:H12	2.41	0.50
1:B:224:GLU:O	1:B:228:GLU:HG3	2.12	0.49
1:B:106:TYR:HB2	1:B:107:PRO:HD2	1.93	0.49
1:C:73:LEU:HD21	1:C:138:VAL:HG21	1.93	0.49
1:D:59:ALA:O	1:D:60:ARG:HG3	2.11	0.49
1:A:27:ILE:HD13	1:A:249:ILE:HD13	1.93	0.49
1:B:59:ALA:O	1:B:60:ARG:HG3	2.13	0.49
1:C:59:ALA:O	1:C:60:ARG:HG3	2.12	0.49
1:A:11:CYS:HB2	1:A:37:ARG:HH11	1.74	0.49
1:B:25:HIS:CD2	1:B:52:LEU:HD22	2.48	0.49
1:B:80:CYS:O	1:B:84:ILE:HG13	2.12	0.49
1:C:101:ASN:HD22	1:C:167:LEU:HG	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ILE:HG23	1:B:126:ASP:H	1.76	0.49
1:D:201:ALA:N	1:D:202:PRO:CD	2.75	0.49
1:B:170:ALA:O	1:B:272:ILE:HD12	2.12	0.49
1:C:65:VAL:HG22	1:C:66:LEU:N	2.27	0.49
1:B:66:LEU:HD23	1:B:66:LEU:N	2.26	0.49
1:A:147:PHE:O	1:A:151:GLN:HG2	2.13	0.48
1:B:17:THR:HA	1:B:41:HIS:HB3	1.94	0.48
1:C:23:ILE:O	1:C:27:ILE:HG13	2.14	0.48
1:C:260:ILE:HG23	1:C:263:THR:CG2	2.43	0.48
1:D:32:HIS:CG	1:D:56:LEU:HD22	2.49	0.48
1:C:125:ILE:HG23	1:C:126:ASP:H	1.78	0.48
1:A:21:ARG:HB3	4:A:1324:HOH:O	2.12	0.48
1:C:57:ASN:ND2	1:C:64:ALA:H	2.08	0.48
1:D:147:PHE:O	1:D:151:GLN:HG2	2.14	0.47
1:C:137:ALA:C	1:C:140:PRO:HD2	2.40	0.47
1:C:31:LEU:C	1:C:36:PHE:HB2	2.40	0.47
1:A:21:ARG:HD3	4:A:1311:HOH:O	2.14	0.47
1:C:201:ALA:HB3	1:C:202:PRO:HD3	1.96	0.47
1:C:173:ASP:C	1:C:175:PRO:HD3	2.40	0.47
1:B:86:ASP:OD1	1:B:150:ARG:NH1	2.47	0.47
1:A:124:PRO:O	1:A:128:GLN:HG3	2.15	0.47
1:B:11:CYS:O	1:B:94:ARG:HD3	2.15	0.47
1:B:81:CYS:HB3	1:B:143:LEU:HD23	1.97	0.47
1:C:124:PRO:HG2	1:C:127:ALA:CB	2.42	0.47
1:C:125:ILE:CG2	1:D:78:LEU:HD11	2.45	0.47
1:C:272:ILE:HG23	1:C:273:LEU:HD13	1.97	0.47
1:C:169:ASP:HB3	1:C:172:THR:HG23	1.96	0.47
1:C:41:HIS:HA	1:C:67:CYS:O	2.15	0.46
1:A:137:ALA:C	1:A:140:PRO:HD2	2.41	0.46
1:C:27:ILE:HD13	1:C:249:ILE:HD13	1.96	0.46
1:D:38:VAL:HG23	1:D:38:VAL:O	2.16	0.46
1:B:65:VAL:HG22	1:B:66:LEU:N	2.31	0.46
1:B:275:ARG:HD2	1:C:174:LEU:HB2	1.98	0.46
1:D:201:ALA:HB3	1:D:202:PRO:HD3	1.98	0.46
1:C:32:HIS:O	1:C:60:ARG:NH1	2.45	0.46
1:D:125:ILE:HG23	1:D:126:ASP:H	1.81	0.46
1:D:29:VAL:O	1:D:33:GLN:HG3	2.16	0.45
1:D:183:THR:O	1:D:187:HIS:HD2	2.00	0.45
1:D:83:ASP:HB3	4:D:4392:HOH:O	2.16	0.45
1:C:12:PRO:HB2	1:C:36:PHE:CE1	2.51	0.45
1:A:201:ALA:N	1:A:202:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:O	1:B:133:PHE:HB2	2.16	0.45
1:D:260:ILE:HG23	1:D:263:THR:CG2	2.46	0.45
1:C:170:ALA:O	1:C:272:ILE:HD12	2.15	0.45
1:B:94:ARG:CZ	1:B:160:ARG:HH21	2.30	0.45
1:A:221:MET:HE2	1:A:225:THR:CG2	2.47	0.45
1:A:259:TYR:CE2	1:C:240:ALA:HB2	2.51	0.45
1:B:37:ARG:NH2	1:B:92:PHE:HB3	2.23	0.45
1:B:57:ASN:ND2	1:B:64:ALA:H	2.00	0.45
1:C:225:THR:O	1:C:229:TYR:HD1	2.00	0.45
1:D:169:ASP:HB3	1:D:172:THR:HG23	1.98	0.45
1:D:260:ILE:HG23	1:D:263:THR:HG21	1.99	0.44
1:A:22:ARG:HB3	1:A:216:LEU:HD12	1.98	0.44
1:A:240:ALA:HB2	1:C:259:TYR:CE2	2.52	0.44
1:C:20:ALA:O	1:C:25:HIS:HD2	2.01	0.44
1:A:16:ILE:HD12	1:A:16:ILE:N	2.32	0.44
1:A:43:ARG:HG2	1:A:44:HIS:CD2	2.53	0.44
1:B:173:ASP:C	1:B:175:PRO:HD3	2.42	0.44
1:C:145:ARG:O	1:C:149:ARG:HG3	2.16	0.44
1:C:173:ASP:O	1:C:175:PRO:HD3	2.18	0.44
1:D:71:LEU:HD22	1:D:139:ALA:HB1	1.99	0.44
1:A:41:HIS:HA	1:A:67:CYS:O	2.18	0.44
1:B:136:ASN:HB2	1:B:185:ALA:HB1	1.99	0.44
1:C:224:GLU:O	1:C:228:GLU:HG3	2.17	0.44
1:A:187:HIS:HE1	1:B:194:ARG:HH21	1.64	0.44
1:D:57:ASN:HD21	1:D:64:ALA:N	2.16	0.44
1:D:57:ASN:HD22	1:D:57:ASN:HA	1.55	0.44
1:D:168:CYS:O	2:D:4277:NAP:H6N	2.18	0.44
1:C:14:ALA:O	1:C:38:VAL:HA	2.18	0.43
1:C:86:ASP:OD1	1:C:150:ARG:NH1	2.51	0.43
1:B:23:ILE:O	1:B:27:ILE:HG13	2.18	0.43
1:B:160:ARG:HB2	1:B:161:ASN:H	1.69	0.43
1:D:89:PHE:CE1	1:D:94:ARG:HA	2.53	0.43
1:A:184:MET:HE3	1:B:192:LEU:HB2	2.00	0.43
1:C:272:ILE:HG23	1:C:273:LEU:CD1	2.48	0.43
1:B:124:PRO:HG2	1:B:127:ALA:CB	2.48	0.43
1:C:17:THR:HA	1:C:41:HIS:HB3	2.00	0.43
1:D:57:ASN:HA	1:D:60:ARG:O	2.18	0.43
1:D:66:LEU:HD23	1:D:66:LEU:N	2.25	0.43
1:D:73:LEU:HD21	1:D:138:VAL:HG21	2.00	0.43
1:A:180:CYS:O	1:A:184:MET:HG3	2.19	0.43
1:A:239:GLU:OE1	1:A:239:GLU:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD21	1:B:138:VAL:CG2	2.43	0.43
1:C:57:ASN:ND2	1:C:63:SER:H	2.16	0.43
1:D:27:ILE:HG12	1:D:249:ILE:HD12	2.01	0.43
1:D:213:GLY:O	2:D:4277:NAP:H4N	2.18	0.43
1:A:11:CYS:HB2	1:A:37:ARG:NH1	2.34	0.42
1:B:49:ALA:O	1:B:53:VAL:HG23	2.18	0.42
1:C:57:ASN:HD22	1:C:63:SER:H	1.68	0.42
1:A:221:MET:HA	1:A:222:PRO:HD3	1.90	0.42
1:B:89:PHE:O	1:B:93:GLY:HA2	2.18	0.42
1:D:66:LEU:H	1:D:66:LEU:CD2	2.27	0.42
1:A:221:MET:HE2	1:A:225:THR:HG21	1.99	0.42
1:C:201:ALA:N	1:C:202:PRO:CD	2.82	0.42
1:B:30:ARG:HH12	1:B:247:ASP:HA	1.84	0.42
1:C:30:ARG:NH1	4:C:3335:HOH:O	2.52	0.42
1:C:103:SER:O	2:C:3277:NAP:H51A	2.20	0.42
1:C:260:ILE:HG23	1:C:263:THR:HG23	2.01	0.42
1:A:192:LEU:HB2	1:B:184:MET:HE3	2.02	0.42
1:B:17:THR:O	1:B:101:ASN:HB3	2.20	0.42
1:B:41:HIS:ND1	1:B:41:HIS:C	2.78	0.41
1:B:241:SER:OG	1:B:244:GLN:HG3	2.20	0.41
1:C:180:CYS:HB2	4:D:4290:HOH:O	2.20	0.41
1:B:17:THR:HB	1:B:102:ALA:HB2	2.01	0.41
1:C:27:ILE:CD1	1:C:249:ILE:HD13	2.51	0.41
1:D:129:VAL:O	1:D:133:PHE:HB2	2.20	0.41
1:A:263:THR:HG21	1:C:266:LYS:O	2.20	0.41
1:D:124:PRO:HG2	1:D:127:ALA:CB	2.50	0.41
1:D:124:PRO:HG2	1:D:127:ALA:HB3	2.01	0.41
1:B:57:ASN:ND2	1:B:63:SER:H	2.18	0.41
1:D:21:ARG:CA	1:D:25:HIS:HB2	2.50	0.41
1:D:22:ARG:NE	2:D:4277:NAP:O2A	2.49	0.41
1:A:111:LEU:HD13	1:B:149:ARG:HG2	2.03	0.40
1:A:165:VAL:HG11	1:A:249:ILE:HG12	2.04	0.40
1:A:183:THR:O	1:A:187:HIS:HD2	2.03	0.40
1:C:23:ILE:HB	2:C:3277:NAP:H51N	2.03	0.40
1:C:66:LEU:HD23	1:C:66:LEU:N	2.32	0.40
1:D:65:VAL:HG22	1:D:66:LEU:N	2.36	0.40
1:A:194:ARG:HH21	1:B:187:HIS:CE1	2.40	0.40
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.96	0.40
1:C:129:VAL:O	1:C:133:PHE:HB2	2.22	0.40
1:C:272:ILE:CG2	1:C:273:LEU:HD13	2.52	0.40
1:D:30:ARG:NH1	1:D:247:ASP:OD1	2.49	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	242/276 (88%)	229 (95%)	13 (5%)	0	100	100
1	B	242/276 (88%)	232 (96%)	10 (4%)	0	100	100
1	C	242/276 (88%)	230 (95%)	12 (5%)	0	100	100
1	D	242/276 (88%)	230 (95%)	12 (5%)	0	100	100
All	All	968/1104 (88%)	921 (95%)	47 (5%)	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	191/209 (91%)	185 (97%)	6 (3%)	35	48
1	B	191/209 (91%)	184 (96%)	7 (4%)	30	41
1	C	191/209 (91%)	184 (96%)	7 (4%)	30	41
1	D	191/209 (91%)	182 (95%)	9 (5%)	23	31
All	All	764/836 (91%)	735 (96%)	29 (4%)	29	40

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	160	ARG
1	A	200	LEU
1	A	263	THR
1	A	273	LEU
1	A	275	ARG
1	B	66	LEU
1	B	78	LEU
1	B	160	ARG
1	B	200	LEU
1	B	263	THR
1	B	273	LEU
1	B	275	ARG
1	C	78	LEU
1	C	160	ARG
1	C	200	LEU
1	C	227	GLU
1	C	263	THR
1	C	273	LEU
1	C	275	ARG
1	D	57	ASN
1	D	66	LEU
1	D	78	LEU
1	D	140	PRO
1	D	160	ARG
1	D	200	LEU
1	D	263	THR
1	D	273	LEU
1	D	275	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	34	GLN
1	A	44	HIS
1	A	50	GLN
1	A	57	ASN
1	A	151	GLN
1	A	187	HIS
1	A	223	GLN
1	A	226	GLN
1	B	25	HIS

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Mol	Chain	Res	Type
1	B	33	GLN
1	B	34	GLN
1	B	44	HIS
1	B	50	GLN
1	B	57	ASN
1	B	100	ASN
1	B	101	ASN
1	B	151	GLN
1	B	187	HIS
1	B	223	GLN
1	B	226	GLN
1	B	237	GLN
1	C	33	GLN
1	C	34	GLN
1	C	50	GLN
1	C	57	ASN
1	C	101	ASN
1	C	151	GLN
1	C	187	HIS
1	C	204	HIS
1	C	223	GLN
1	C	226	GLN
1	D	33	GLN
1	D	50	GLN
1	D	57	ASN
1	D	151	GLN
1	D	187	HIS
1	D	223	GLN
1	D	226	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 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	DHF	C	3278	-	29,31,34	5.46	17 (58%)	34,43,47	2.62	15 (44%)
2	NAP	A	1277	-	50,52,52	2.08	13 (26%)	71,80,80	1.50	16 (22%)
2	NAP	B	2277	-	50,52,52	2.03	11 (22%)	71,80,80	1.47	15 (21%)
3	DHF	A	1278	-	29,31,34	5.53	17 (58%)	34,43,47	2.66	15 (44%)
2	NAP	D	4277	-	50,52,52	2.02	12 (24%)	71,80,80	1.63	14 (19%)
3	DHF	B	2278	-	29,31,34	5.62	19 (65%)	34,43,47	2.66	16 (47%)
3	DHF	D	4278	-	29,31,34	5.44	17 (58%)	34,43,47	2.64	15 (44%)
2	NAP	C	3277	-	50,52,52	2.03	12 (24%)	71,80,80	1.56	14 (19%)

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	DHF	C	3278	-	-	8/17/28/31	0/3/3/3
2	NAP	A	1277	-	-	4/35/67/67	0/5/5/5
2	NAP	B	2277	-	-	2/35/67/67	0/5/5/5
3	DHF	A	1278	-	-	10/17/28/31	0/3/3/3
2	NAP	D	4277	-	-	4/35/67/67	0/5/5/5
3	DHF	B	2278	-	-	10/17/28/31	0/3/3/3
3	DHF	D	4278	-	-	10/17/28/31	0/3/3/3
2	NAP	C	3277	-	-	1/35/67/67	0/5/5/5

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1278	DHF	C16-C15	14.15	1.61	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3278	DHF	C16-C15	14.09	1.61	1.38
3	B	2278	DHF	C16-C15	14.05	1.61	1.38
3	D	4278	DHF	C16-C15	13.86	1.61	1.38
3	B	2278	DHF	C16-C11	13.08	1.59	1.39
3	A	1278	DHF	C16-C11	12.85	1.58	1.39
3	C	3278	DHF	C16-C11	12.35	1.58	1.39
3	D	4278	DHF	C16-C11	12.13	1.57	1.39
3	B	2278	DHF	C13-C12	10.60	1.55	1.38
3	D	4278	DHF	C13-C12	10.30	1.55	1.38
3	C	3278	DHF	C13-C12	10.21	1.55	1.38
3	A	1278	DHF	C13-C12	10.18	1.55	1.38
3	B	2278	DHF	C13-C14	8.40	1.53	1.39
3	A	1278	DHF	C13-C14	7.93	1.52	1.39
3	D	4278	DHF	C13-C14	7.75	1.52	1.39
3	C	3278	DHF	C13-C14	7.59	1.52	1.39
2	A	1277	NAP	C2N-N1N	7.55	1.43	1.35
2	D	4277	NAP	C2N-N1N	7.34	1.43	1.35
2	B	2277	NAP	C2N-N1N	7.28	1.43	1.35
3	A	1278	DHF	C8A-N1	6.98	1.47	1.37
3	C	3278	DHF	C8A-N1	6.98	1.47	1.37
3	B	2278	DHF	C8A-N1	6.95	1.47	1.37
3	D	4278	DHF	C2-NA2	-6.85	1.18	1.34
3	A	1278	DHF	C2-NA2	-6.71	1.18	1.34
3	D	4278	DHF	C8A-N1	6.66	1.47	1.37
2	C	3277	NAP	C2N-N1N	6.40	1.42	1.35
3	B	2278	DHF	C7-C6	-6.38	1.42	1.49
3	B	2278	DHF	C2-NA2	-6.37	1.19	1.34
3	A	1278	DHF	C7-C6	-6.30	1.42	1.49
3	B	2278	DHF	C2-N3	6.27	1.48	1.33
3	C	3278	DHF	C12-C11	6.26	1.48	1.39
3	D	4278	DHF	C7-C6	-6.22	1.42	1.49
3	C	3278	DHF	C2-N3	6.21	1.48	1.33
3	C	3278	DHF	C7-C6	-6.20	1.42	1.49
3	B	2278	DHF	C12-C11	6.17	1.48	1.39
3	D	4278	DHF	C-N	-6.15	1.20	1.34
3	C	3278	DHF	C2-NA2	-6.10	1.19	1.34
3	D	4278	DHF	C12-C11	6.05	1.48	1.39
3	A	1278	DHF	C-N	-6.02	1.20	1.34
3	B	2278	DHF	C-N	-6.00	1.20	1.34
3	A	1278	DHF	C2-N3	5.92	1.47	1.33
3	A	1278	DHF	C12-C11	5.89	1.48	1.39
3	C	3278	DHF	C-N	-5.87	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4278	DHF	C2-N3	5.82	1.47	1.33
3	C	3278	DHF	C4A-N5	5.42	1.49	1.37
3	B	2278	DHF	C4A-N5	5.40	1.49	1.37
2	A	1277	NAP	C4N-C3N	5.30	1.47	1.39
3	B	2278	DHF	C9-N10	5.27	1.53	1.45
3	A	1278	DHF	C4A-N5	5.25	1.49	1.37
3	D	4278	DHF	C4A-N5	5.21	1.49	1.37
2	C	3277	NAP	C4N-C3N	5.12	1.47	1.39
2	B	2277	NAP	C4N-C3N	5.02	1.47	1.39
2	C	3277	NAP	O4D-C1D	4.95	1.47	1.40
3	C	3278	DHF	C9-N10	4.93	1.53	1.45
3	A	1278	DHF	C9-N10	4.92	1.53	1.45
3	D	4278	DHF	C9-N10	4.88	1.53	1.45
2	A	1277	NAP	O4D-C1D	4.86	1.47	1.40
2	D	4277	NAP	C4N-C3N	4.68	1.46	1.39
2	B	2277	NAP	O4D-C1D	4.45	1.46	1.40
2	D	4277	NAP	O4D-C1D	4.20	1.46	1.40
2	B	2277	NAP	C2A-N1A	3.98	1.41	1.33
2	D	4277	NAP	C2A-N1A	3.87	1.40	1.33
2	C	3277	NAP	C2A-N1A	3.83	1.40	1.33
2	C	3277	NAP	PN-O3	-3.78	1.55	1.59
2	A	1277	NAP	C2A-N1A	3.51	1.40	1.33
2	A	1277	NAP	C6N-N1N	3.48	1.43	1.35
2	B	2277	NAP	C6N-N1N	3.41	1.43	1.35
2	C	3277	NAP	C6N-N1N	3.39	1.43	1.35
2	B	2277	NAP	PN-O3	-3.38	1.55	1.59
3	D	4278	DHF	C7-N8	-3.32	1.40	1.45
3	A	1278	DHF	C7-N8	-3.32	1.40	1.45
3	B	2278	DHF	C7-N8	-3.24	1.40	1.45
2	D	4277	NAP	C6N-N1N	3.14	1.42	1.35
3	C	3278	DHF	CA-CT	3.14	1.60	1.52
3	C	3278	DHF	C7-N8	-3.07	1.40	1.45
3	A	1278	DHF	CA-CT	3.05	1.60	1.52
3	D	4278	DHF	CA-CT	3.04	1.60	1.52
3	B	2278	DHF	CA-CT	3.03	1.60	1.52
3	C	3278	DHF	C8A-N8	-3.03	1.29	1.32
2	A	1277	NAP	PN-O3	-3.02	1.56	1.59
2	C	3277	NAP	PA-O1A	-3.02	1.40	1.50
3	D	4278	DHF	C4A-C8A	-2.92	1.38	1.43
2	B	2277	NAP	PA-O1A	-2.89	1.40	1.50
2	A	1277	NAP	C2A-N3A	2.88	1.39	1.33
3	A	1278	DHF	C4A-C8A	-2.86	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3278	DHF	C4A-C8A	-2.85	1.38	1.43
2	A	1277	NAP	PA-O1A	-2.85	1.40	1.50
2	C	3277	NAP	C2A-N3A	2.83	1.39	1.33
3	D	4278	DHF	C8A-N8	-2.81	1.29	1.32
3	B	2278	DHF	C8A-N8	-2.78	1.29	1.32
2	C	3277	NAP	C4A-N3A	2.76	1.39	1.34
3	A	1278	DHF	C8A-N8	-2.74	1.29	1.32
2	D	4277	NAP	PA-O1A	-2.74	1.41	1.50
2	A	1277	NAP	C4A-N3A	2.72	1.39	1.34
2	B	2277	NAP	C2A-N3A	2.68	1.38	1.33
2	A	1277	NAP	C5N-C4N	2.66	1.43	1.38
2	D	4277	NAP	C2A-N3A	2.66	1.38	1.33
3	B	2278	DHF	C4A-C8A	-2.65	1.39	1.43
2	D	4277	NAP	C3N-C7N	2.60	1.54	1.50
2	B	2277	NAP	C4A-N3A	2.59	1.39	1.34
2	D	4277	NAP	C4A-N3A	2.57	1.39	1.34
3	D	4278	DHF	O1-CT	2.54	1.29	1.22
3	A	1278	DHF	O1-CT	2.54	1.29	1.22
3	B	2278	DHF	O1-CT	2.52	1.29	1.22
2	D	4277	NAP	C5N-C4N	2.52	1.43	1.38
2	D	4277	NAP	PN-O3	-2.48	1.56	1.59
3	C	3278	DHF	O1-CT	2.46	1.29	1.22
2	A	1277	NAP	C3N-C7N	2.37	1.54	1.50
2	B	2277	NAP	C5N-C4N	2.37	1.43	1.38
2	B	2277	NAP	P2B-O2B	2.36	1.63	1.59
2	C	3277	NAP	P2B-O2B	2.31	1.63	1.59
2	D	4277	NAP	P2B-O2B	2.25	1.63	1.59
2	C	3277	NAP	C5N-C4N	2.25	1.42	1.38
3	B	2278	DHF	C4-C4A	2.21	1.51	1.45
2	A	1277	NAP	C6N-C5N	2.13	1.43	1.38
3	B	2278	DHF	C4-N3	2.11	1.41	1.38
2	A	1277	NAP	P2B-O2B	2.11	1.63	1.59
2	C	3277	NAP	C3N-C7N	2.02	1.53	1.50

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4278	DHF	O-C-C11	7.50	135.75	120.90
3	B	2278	DHF	O-C-C11	7.43	135.62	120.90
3	A	1278	DHF	O-C-C11	7.39	135.54	120.90
3	C	3278	DHF	O-C-C11	7.27	135.30	120.90
2	D	4277	NAP	O4B-C1B-N9A	5.01	117.72	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3278	DHF	C6-C7-N8	4.80	129.20	114.16
3	A	1278	DHF	C6-C7-N8	4.79	129.17	114.16
3	B	2278	DHF	C6-C7-N8	4.76	129.08	114.16
3	D	4278	DHF	C6-C7-N8	4.75	129.03	114.16
3	D	4278	DHF	C11-C-N	-4.37	108.93	117.04
3	B	2278	DHF	C11-C-N	-4.33	109.01	117.04
3	A	1278	DHF	C11-C-N	-4.26	109.15	117.04
2	D	4277	NAP	C2B-C1B-N9A	-4.21	106.83	113.75
3	C	3278	DHF	NA2-C2-N1	4.09	125.39	116.76
3	A	1278	DHF	NA2-C2-N1	3.98	125.16	116.76
3	D	4278	DHF	NA2-C2-N1	3.96	125.12	116.76
3	C	3278	DHF	O-C-N	-3.95	114.95	122.47
3	C	3278	DHF	C11-C-N	-3.93	109.75	117.04
3	C	3278	DHF	C4A-C8A-N1	3.88	123.87	115.89
3	A	1278	DHF	C7-N8-C8A	-3.87	115.26	123.81
3	D	4278	DHF	C7-N8-C8A	-3.85	115.30	123.81
2	C	3277	NAP	O4B-C1B-N9A	3.85	115.48	108.09
2	C	3277	NAP	O5B-C5B-C4B	-3.83	95.94	108.99
2	C	3277	NAP	N3A-C2A-N1A	-3.82	122.79	128.58
3	B	2278	DHF	C7-N8-C8A	-3.80	115.41	123.81
2	A	1277	NAP	N3A-C2A-N1A	-3.78	122.86	128.58
2	D	4277	NAP	N3A-C2A-N1A	-3.78	122.87	128.58
3	B	2278	DHF	NA2-C2-N1	3.77	124.72	116.76
3	A	1278	DHF	O-C-N	-3.77	115.30	122.47
3	D	4278	DHF	O-C-N	-3.76	115.32	122.47
3	C	3278	DHF	C7-N8-C8A	-3.76	115.51	123.81
3	B	2278	DHF	C4A-C8A-N1	3.75	123.59	115.89
3	B	2278	DHF	O-C-N	-3.73	115.37	122.47
3	D	4278	DHF	C4A-C8A-N1	3.72	123.54	115.89
3	A	1278	DHF	C4A-C8A-N1	3.70	123.48	115.89
2	D	4277	NAP	O5B-C5B-C4B	-3.65	96.57	108.99
3	B	2278	DHF	C4A-C8A-N8	3.60	123.28	115.89
3	C	3278	DHF	C16-C11-C12	-3.54	114.06	118.57
2	B	2277	NAP	C6N-N1N-C1D	-3.52	112.82	119.73
2	B	2277	NAP	N3A-C2A-N1A	-3.50	123.28	128.58
3	D	4278	DHF	C4A-C8A-N8	3.50	123.08	115.89
2	A	1277	NAP	C6N-N1N-C1D	-3.46	112.93	119.73
3	A	1278	DHF	C4A-C8A-N8	3.45	122.97	115.89
2	D	4277	NAP	C6N-N1N-C1D	-3.43	113.00	119.73
2	C	3277	NAP	C6N-N1N-C1D	-3.39	113.07	119.73
3	A	1278	DHF	C16-C11-C12	-3.36	114.29	118.57
3	B	2278	DHF	C16-C11-C12	-3.26	114.42	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3278	DHF	C4A-C8A-N8	3.26	122.59	115.89
3	D	4278	DHF	C16-C11-C12	-3.21	114.49	118.57
2	B	2277	NAP	O5B-C5B-C4B	-3.19	98.12	108.99
3	B	2278	DHF	CA-N-C	3.16	129.15	121.56
3	A	1278	DHF	CA-N-C	3.12	129.05	121.56
3	D	4278	DHF	CA-N-C	3.06	128.91	121.56
2	A	1277	NAP	O5B-C5B-C4B	-3.06	98.59	108.99
3	B	2278	DHF	C12-C13-C14	3.05	123.81	120.30
3	A	1278	DHF	C12-C13-C14	3.02	123.77	120.30
2	A	1277	NAP	C3N-C7N-N7N	3.01	121.45	117.74
2	A	1277	NAP	O2A-PA-O1A	3.01	126.46	112.44
2	A	1277	NAP	O4B-C1B-N9A	3.00	113.84	108.09
2	B	2277	NAP	C3N-C7N-N7N	2.98	121.41	117.74
3	C	3278	DHF	CA-N-C	2.97	128.69	121.56
2	C	3277	NAP	C2B-C1B-N9A	-2.97	108.87	113.75
2	B	2277	NAP	O2A-PA-O1A	2.95	126.15	112.44
2	D	4277	NAP	C3N-C7N-N7N	2.94	121.36	117.74
3	C	3278	DHF	N1-C2-N3	-2.82	118.16	123.32
2	C	3277	NAP	C2N-C3N-C4N	2.82	121.53	118.26
2	D	4277	NAP	C1B-N9A-C8A	2.81	133.32	127.09
2	C	3277	NAP	C3N-C7N-N7N	2.81	121.19	117.74
2	B	2277	NAP	O7N-C7N-C3N	-2.80	116.17	119.60
3	D	4278	DHF	C12-C11-C	2.80	129.67	120.60
2	C	3277	NAP	O2A-PA-O1A	2.78	125.36	112.44
2	A	1277	NAP	C2N-C3N-C4N	2.76	121.47	118.26
3	B	2278	DHF	N1-C2-N3	-2.76	118.27	123.32
2	B	2277	NAP	O4B-C1B-N9A	2.74	113.35	108.09
3	B	2278	DHF	C12-C11-C	2.73	129.44	120.60
3	A	1278	DHF	N1-C2-N3	-2.72	118.34	123.32
2	B	2277	NAP	C2N-C3N-C4N	2.72	121.42	118.26
2	D	4277	NAP	O2A-PA-O1A	2.71	125.05	112.44
3	A	1278	DHF	C12-C11-C	2.70	129.35	120.60
3	C	3278	DHF	C12-C11-C	2.69	129.32	120.60
2	D	4277	NAP	C4A-N9A-C1B	-2.68	120.36	126.63
2	C	3277	NAP	O7N-C7N-C3N	-2.67	116.33	119.60
3	D	4278	DHF	C12-C13-C14	2.66	123.36	120.30
2	C	3277	NAP	C4A-N9A-C1B	-2.65	120.45	126.63
3	D	4278	DHF	N1-C2-N3	-2.64	118.49	123.32
2	A	1277	NAP	O7N-C7N-C3N	-2.63	116.39	119.60
3	C	3278	DHF	C12-C13-C14	2.62	123.31	120.30
2	C	3277	NAP	C1B-N9A-C8A	2.57	132.81	127.09
3	A	1278	DHF	C13-C14-N10	-2.57	115.16	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4277	NAP	O7N-C7N-C3N	-2.54	116.49	119.60
2	B	2277	NAP	C2B-C1B-N9A	-2.45	109.71	113.75
2	D	4277	NAP	C2N-C3N-C4N	2.40	121.05	118.26
3	B	2278	DHF	C13-C14-N10	-2.36	115.63	120.96
2	D	4277	NAP	O3X-P2B-O2X	2.32	116.51	107.80
2	B	2277	NAP	C2B-C3B-C4B	2.30	106.94	101.99
2	A	1277	NAP	C2B-C3B-C4B	2.30	106.93	101.99
2	C	3277	NAP	O3X-P2B-O2X	2.29	116.38	107.80
2	B	2277	NAP	C2N-N1N-C1D	2.28	124.16	119.13
2	A	1277	NAP	C1B-N9A-C8A	2.27	132.13	127.09
3	C	3278	DHF	C13-C14-N10	-2.26	115.85	120.96
2	A	1277	NAP	C4A-N9A-C1B	-2.26	121.35	126.63
2	A	1277	NAP	O3X-P2B-O2X	2.26	116.26	107.80
2	C	3277	NAP	C5N-C4N-C3N	-2.25	118.15	120.36
3	A	1278	DHF	C15-C14-N10	2.23	126.01	120.96
2	A	1277	NAP	C5N-C4N-C3N	-2.21	118.19	120.36
3	B	2278	DHF	N1-C8A-N8	-2.21	113.13	117.28
3	D	4278	DHF	C13-C14-N10	-2.21	115.97	120.96
2	B	2277	NAP	O3X-P2B-O2X	2.21	116.07	107.80
2	B	2277	NAP	C1B-N9A-C8A	2.19	131.96	127.09
2	A	1277	NAP	C2N-N1N-C1D	2.16	123.90	119.13
2	D	4277	NAP	C5N-C6N-N1N	-2.15	117.44	120.38
2	A	1277	NAP	C2B-C1B-N9A	-2.09	110.31	113.75
2	A	1277	NAP	C4B-O4B-C1B	2.09	114.07	109.47
3	D	4278	DHF	N1-C8A-N8	-2.07	113.39	117.28
3	B	2278	DHF	C15-C14-N10	2.07	125.63	120.96
2	D	4277	NAP	C2N-N1N-C1D	2.06	123.67	119.13
2	B	2277	NAP	C5N-C4N-C3N	-2.04	118.36	120.36
2	C	3277	NAP	C5N-C6N-N1N	-2.03	117.62	120.38
2	B	2277	NAP	C4A-N9A-C1B	-2.03	121.89	126.63
3	C	3278	DHF	C15-C14-N10	2.01	125.50	120.96

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4277	NAP	O4D-C1D-N1N-C2N
3	A	1278	DHF	N-C-C11-C12
3	D	4278	DHF	N-C-C11-C12
3	A	1278	DHF	O-C-C11-C12
3	D	4278	DHF	O-C-C11-C12
3	D	4278	DHF	O-C-C11-C16

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Mol	Chain	Res	Type	Atoms
3	A	1278	DHF	O-C-C11-C16
3	D	4278	DHF	N-C-C11-C16
3	A	1278	DHF	N-C-C11-C16
3	C	3278	DHF	O-C-C11-C12
3	C	3278	DHF	N-C-C11-C12
3	C	3278	DHF	N-C-C11-C16
3	C	3278	DHF	O-C-C11-C16
3	B	2278	DHF	N-C-C11-C12
3	B	2278	DHF	O-C-C11-C12
3	B	2278	DHF	O-C-C11-C16
3	B	2278	DHF	N-C-C11-C16
3	C	3278	DHF	N-CA-CT-O2
3	A	1278	DHF	N-CA-CT-O1
3	B	2278	DHF	N-CA-CT-O1
3	B	2278	DHF	N-CA-CT-O2
3	C	3278	DHF	N-CA-CT-O1
3	D	4278	DHF	N-CA-CT-O1
3	D	4278	DHF	N-CA-CT-O2
3	A	1278	DHF	N-CA-CT-O2
3	A	1278	DHF	N-CA-CB-CG
3	B	2278	DHF	N-CA-CB-CG
3	D	4278	DHF	N-CA-CB-CG
3	A	1278	DHF	CB-CA-CT-O2
3	C	3278	DHF	CB-CA-CT-O2
3	D	4278	DHF	CB-CA-CT-O2
3	B	2278	DHF	CB-CA-CT-O2
3	A	1278	DHF	CT-CA-CB-CG
3	B	2278	DHF	CT-CA-CB-CG
3	D	4278	DHF	CT-CA-CB-CG
3	A	1278	DHF	CB-CA-CT-O1
3	C	3278	DHF	CB-CA-CT-O1
3	D	4278	DHF	CB-CA-CT-O1
3	B	2278	DHF	CB-CA-CT-O1
2	A	1277	NAP	O4D-C1D-N1N-C2N
2	A	1277	NAP	O4D-C1D-N1N-C6N
2	D	4277	NAP	O4D-C1D-N1N-C6N
2	A	1277	NAP	PN-O3-PA-O2A
2	B	2277	NAP	PN-O3-PA-O2A
2	B	2277	NAP	O4B-C4B-C5B-O5B
2	C	3277	NAP	O4B-C4B-C5B-O5B
2	D	4277	NAP	O4B-C4B-C5B-O5B
2	A	1277	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	4277	NAP	PN-O3-PA-O1A

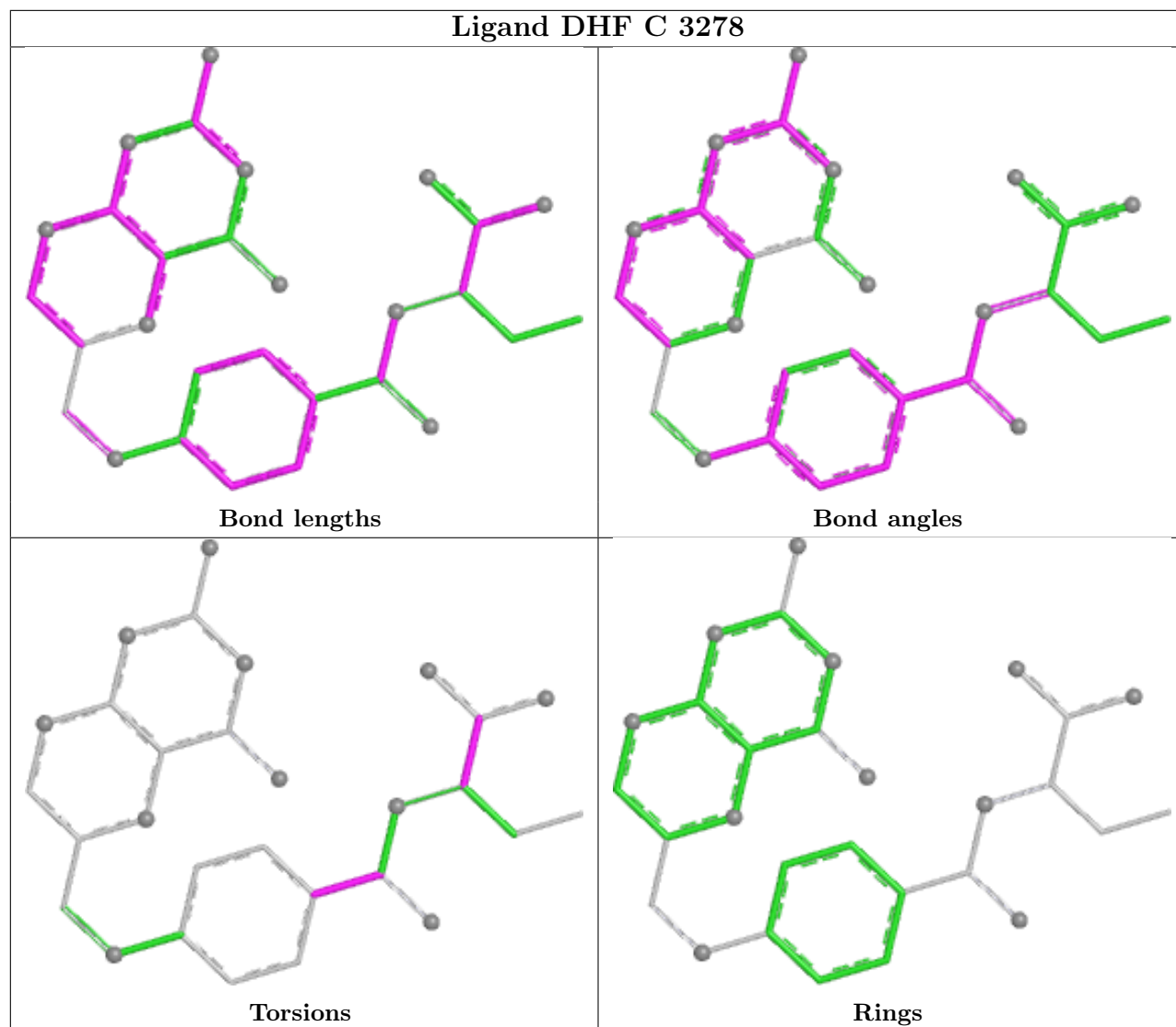
There are no ring outliers.

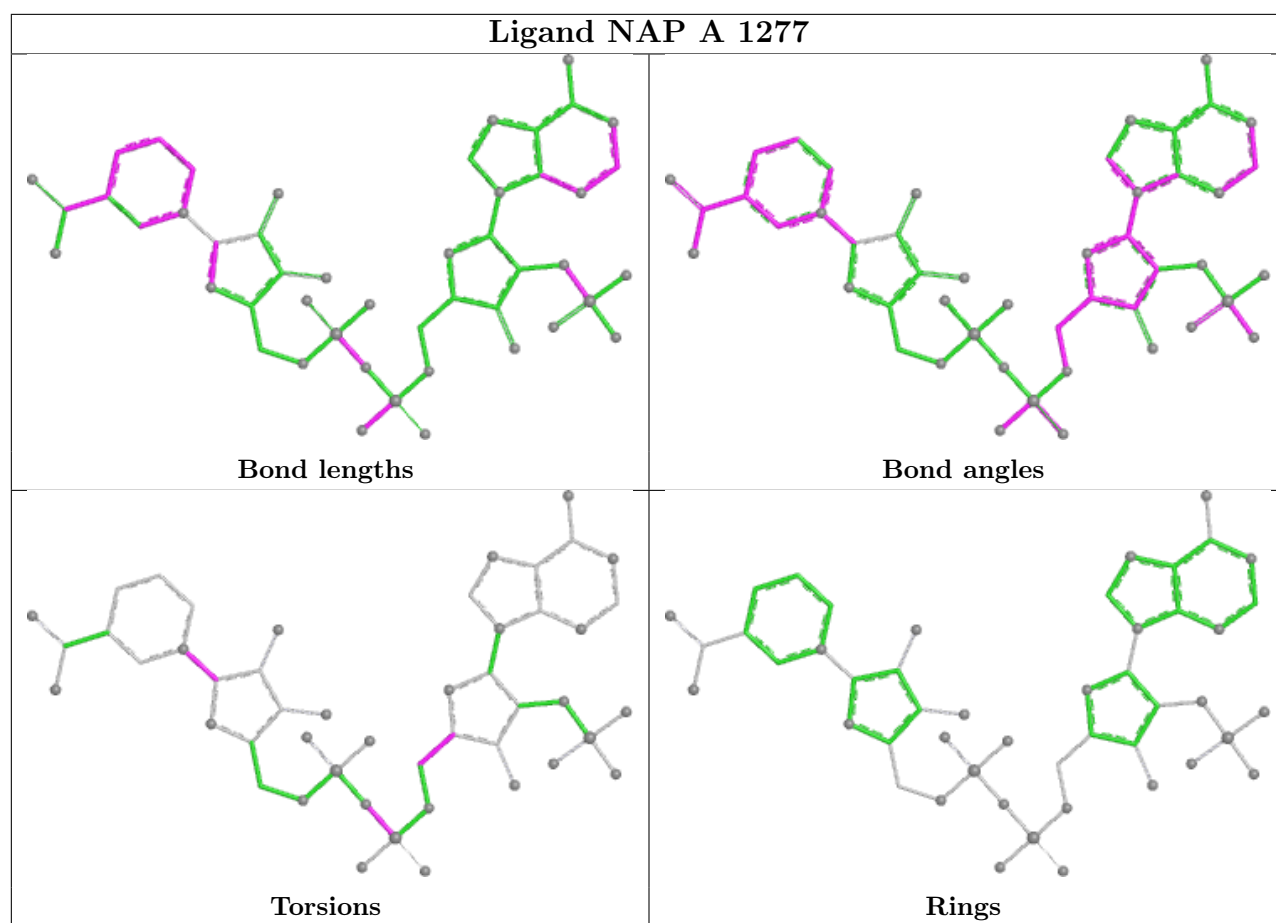
6 monomers are involved in 17 short contacts:

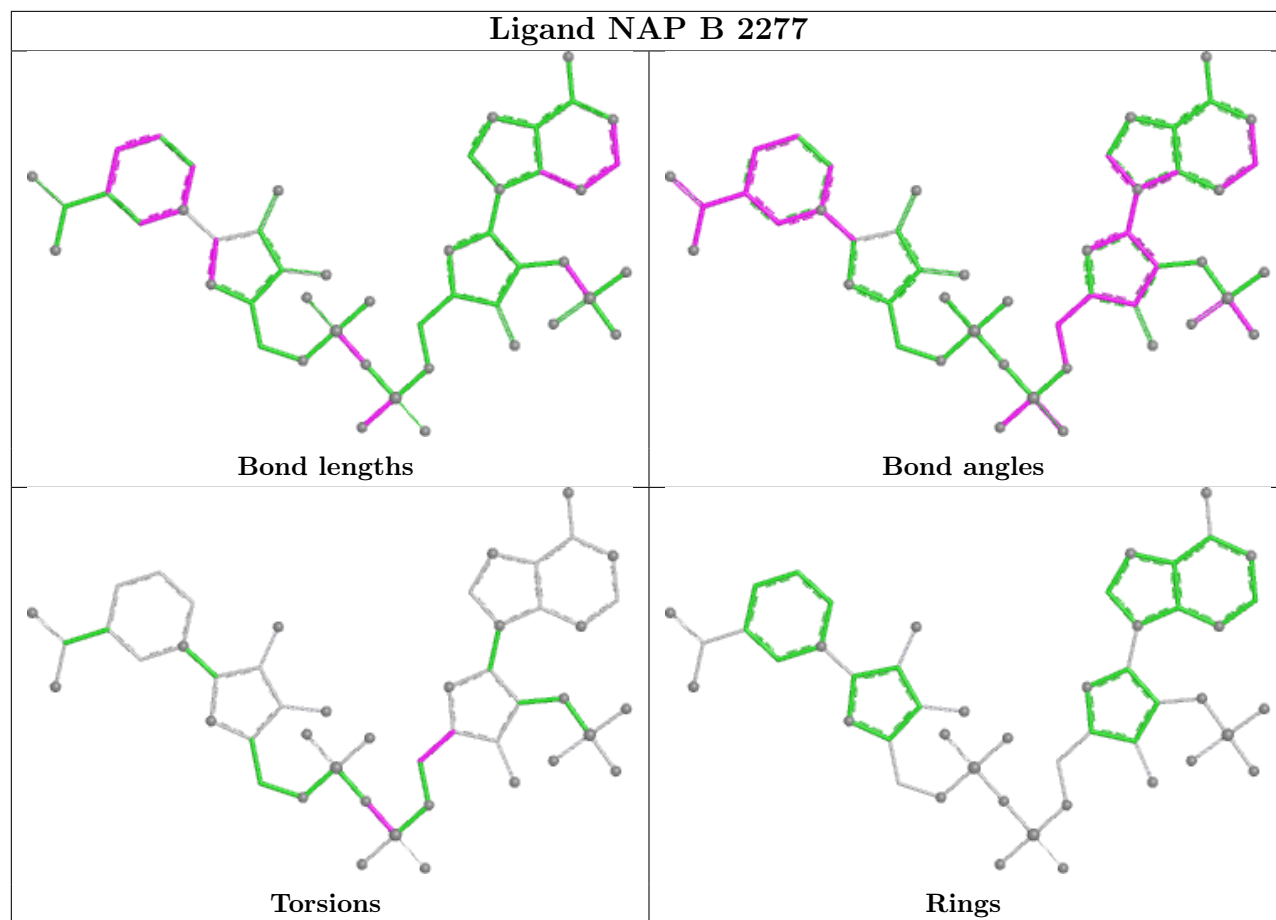
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3278	DHF	3	0
3	A	1278	DHF	1	0
2	D	4277	NAP	3	0
3	B	2278	DHF	5	0
3	D	4278	DHF	3	0
2	C	3277	NAP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

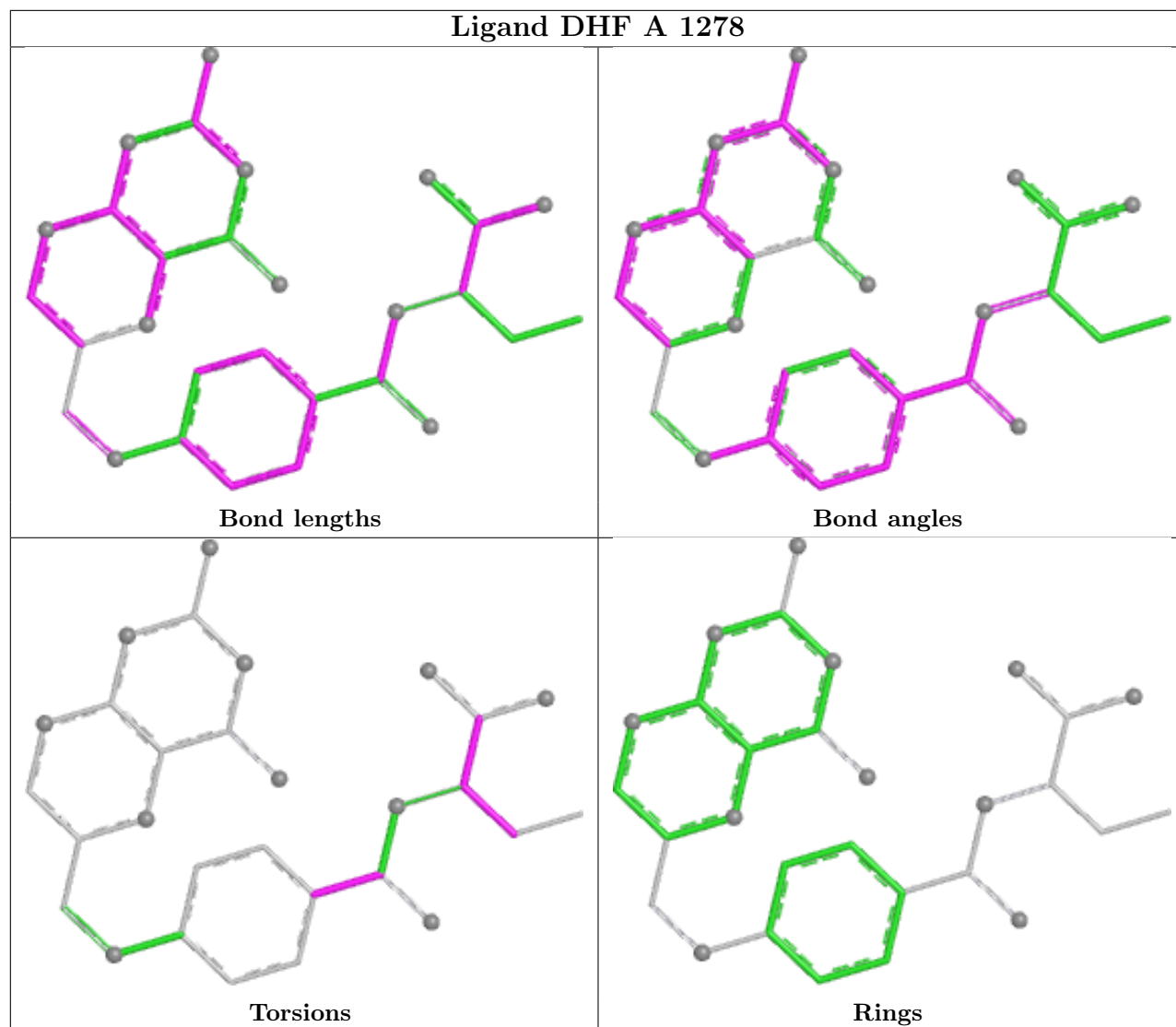
Ligand DHF C 3278

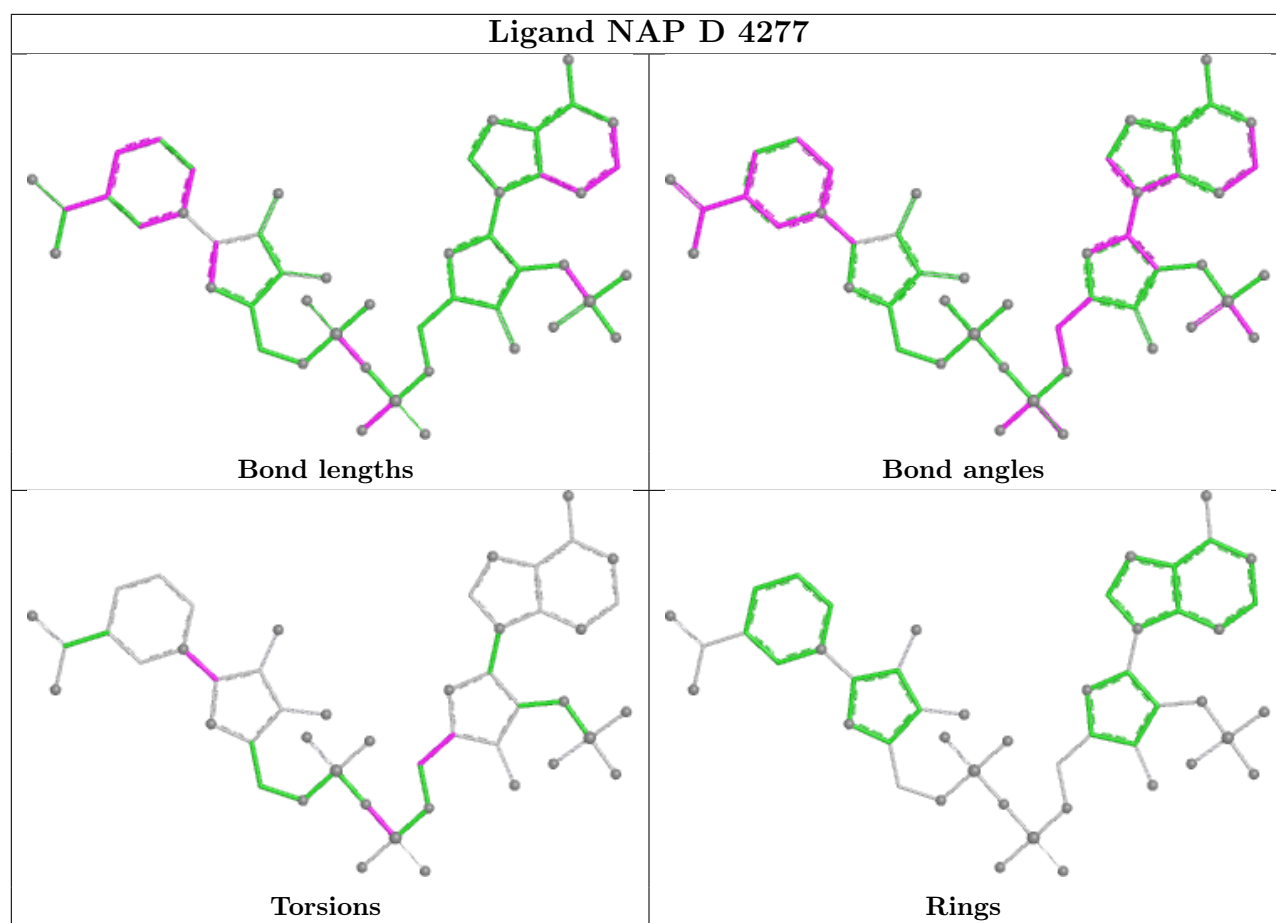




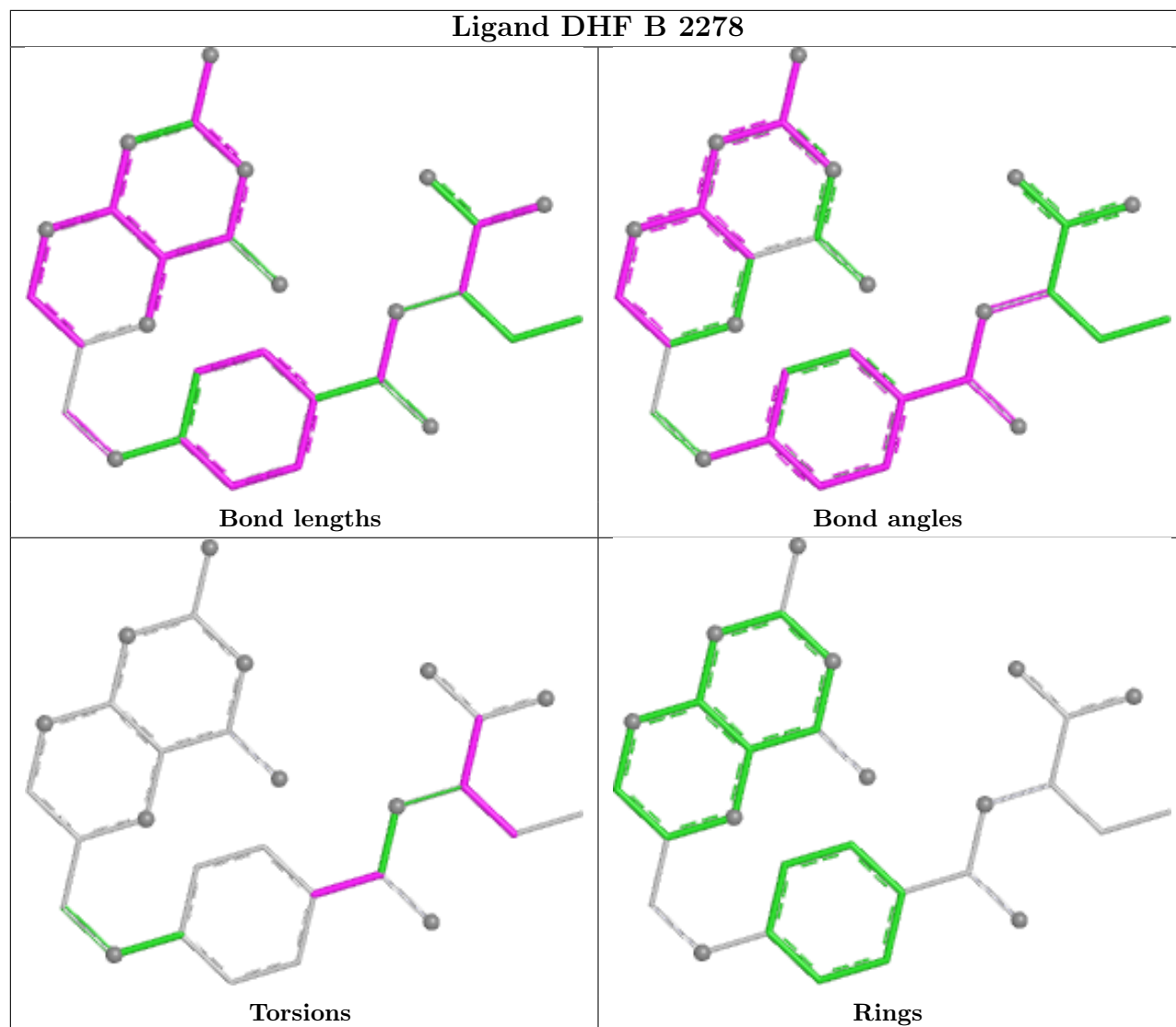


Ligand DHF A 1278

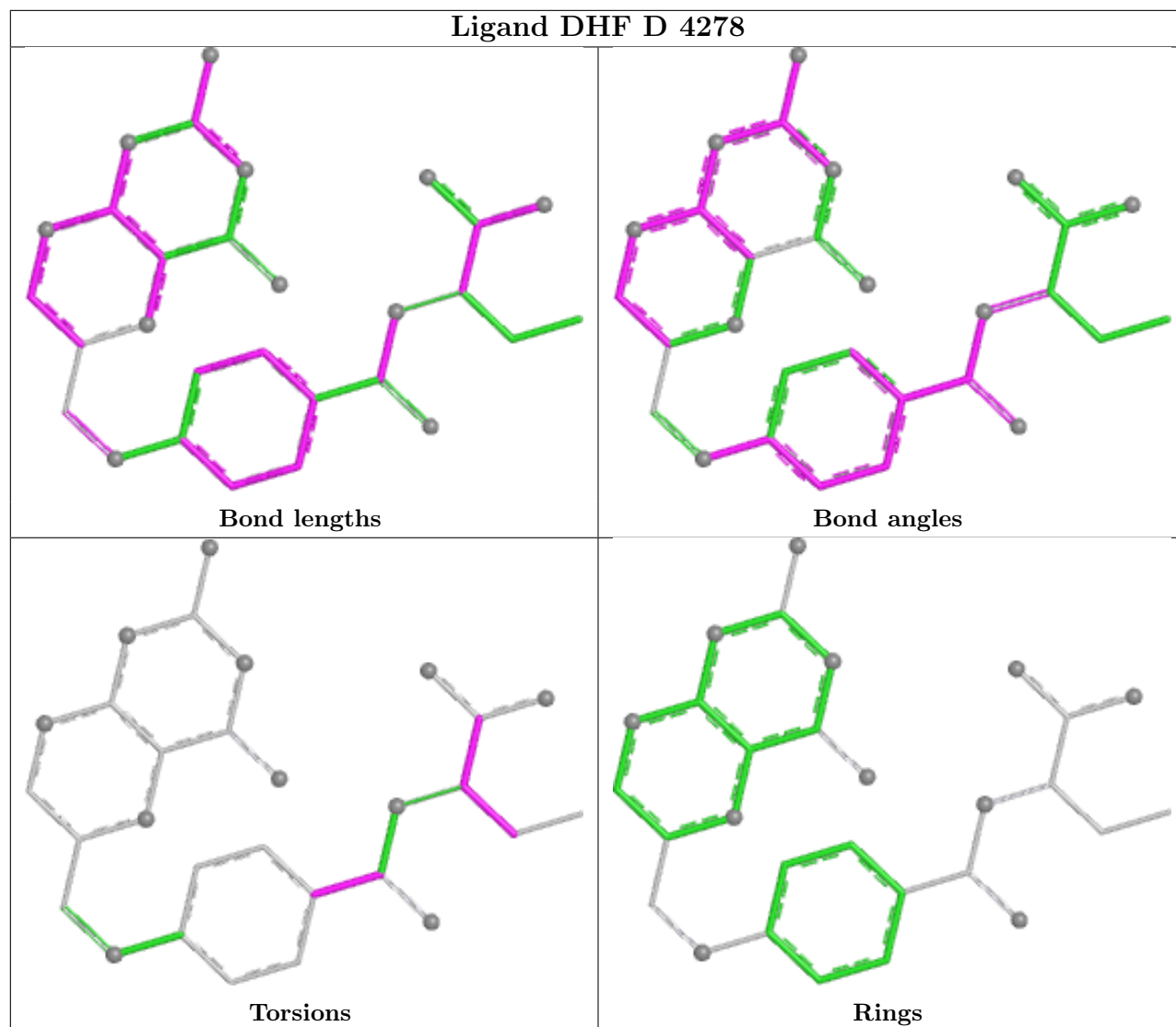


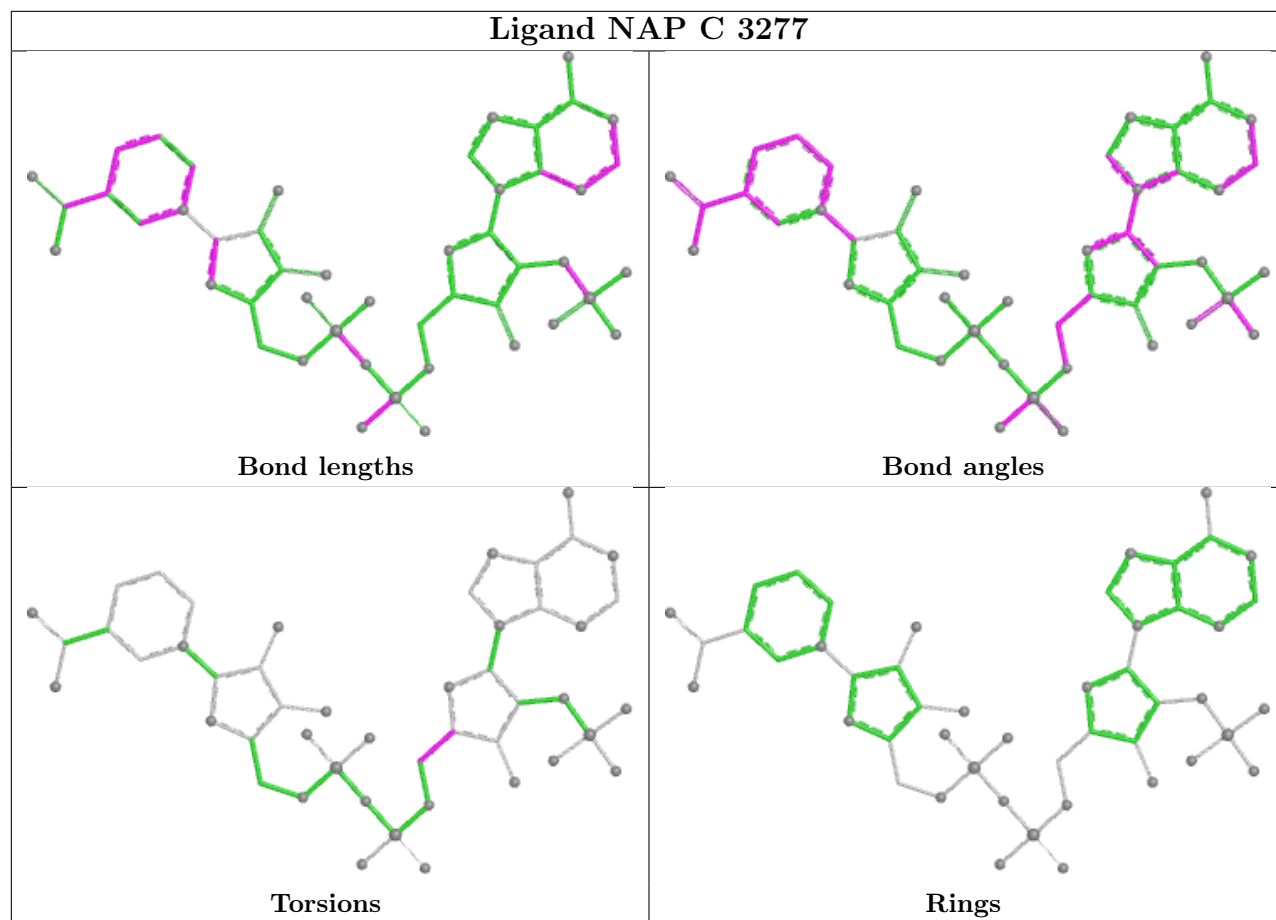


Ligand DHF B 2278



Ligand DHF D 4278





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	248/276 (89%)	0.14	5 (2%) 65 62	15, 30, 48, 61	0
1	B	248/276 (89%)	0.29	6 (2%) 59 56	16, 32, 51, 61	0
1	C	248/276 (89%)	-0.10	7 (2%) 55 52	11, 24, 45, 57	0
1	D	248/276 (89%)	0.00	10 (4%) 42 39	8, 24, 48, 56	0
All	All	992/1104 (89%)	0.08	28 (2%) 55 52	8, 28, 49, 61	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	GLN	3.7
1	D	38	VAL	3.6
1	C	90	ARG	3.5
1	C	50	GLN	3.3
1	C	38	VAL	3.1
1	B	90	ARG	3.1
1	D	82	GLU	3.1
1	B	91	ALA	3.0
1	A	124	PRO	3.0
1	D	46	GLU	2.8
1	D	93	GLY	2.7
1	A	90	ARG	2.7
1	B	92	PHE	2.6
1	C	46	GLU	2.5
1	C	159	SER	2.5
1	D	58	ALA	2.4
1	D	91	ALA	2.3
1	A	223	GLN	2.3
1	A	76	SER	2.3
1	D	39	VAL	2.3
1	D	223	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	66	LEU	2.2
1	C	224	GLU	2.2
1	D	61	ALA	2.2
1	A	50	GLN	2.2
1	B	50	GLN	2.2
1	B	57	ASN	2.1
1	C	223	GLN	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](#)

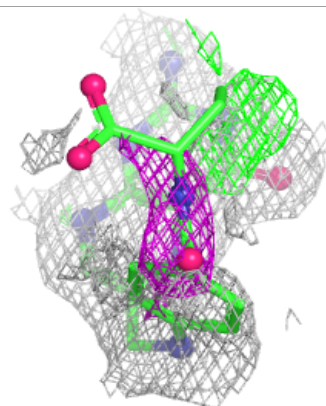
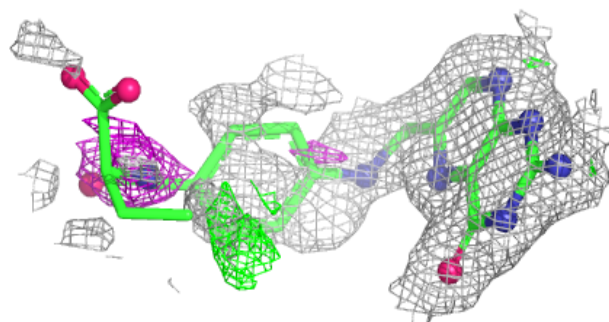
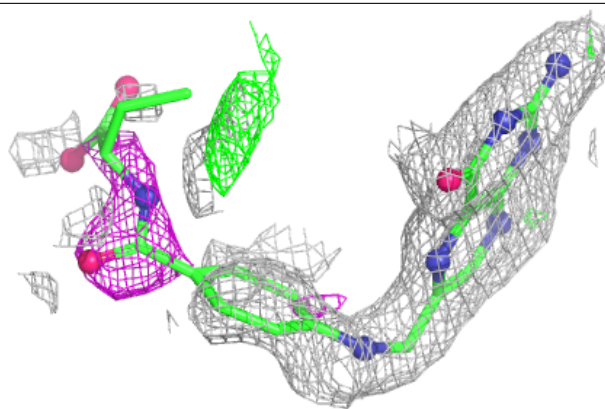
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	DHF	B	2278	29/32	0.80	0.17	24,55,82,82	0
3	DHF	A	1278	29/32	0.81	0.16	27,50,73,73	0
3	DHF	C	3278	29/32	0.83	0.18	16,47,75,75	0
3	DHF	D	4278	29/32	0.85	0.18	18,46,77,77	0
2	NAP	A	1277	48/48	0.95	0.08	20,24,28,29	0
2	NAP	B	2277	48/48	0.95	0.08	20,28,34,35	0
2	NAP	D	4277	48/48	0.96	0.06	13,18,23,24	0
2	NAP	C	3277	48/48	0.97	0.06	13,17,21,23	0

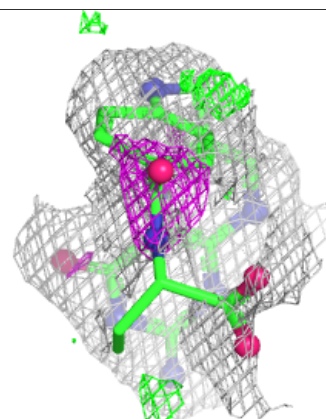
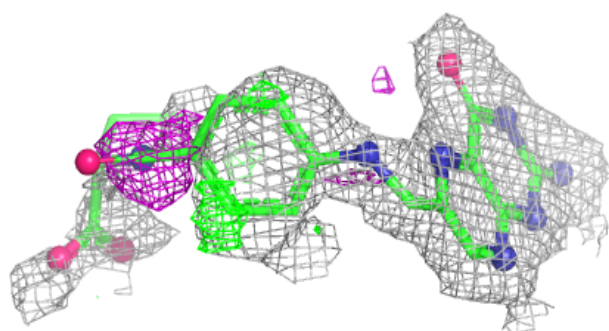
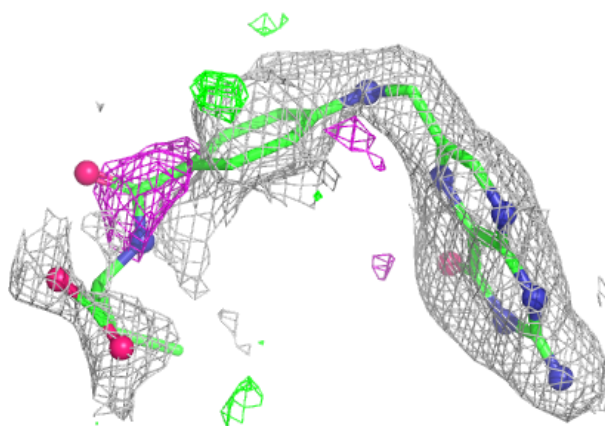
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DHF B 2278:

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

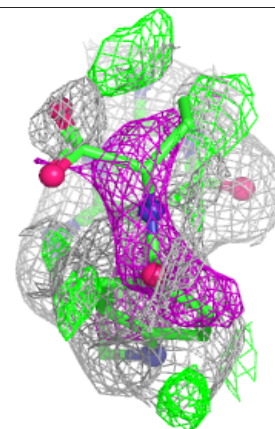
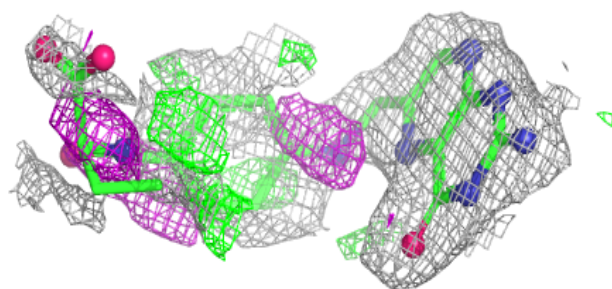
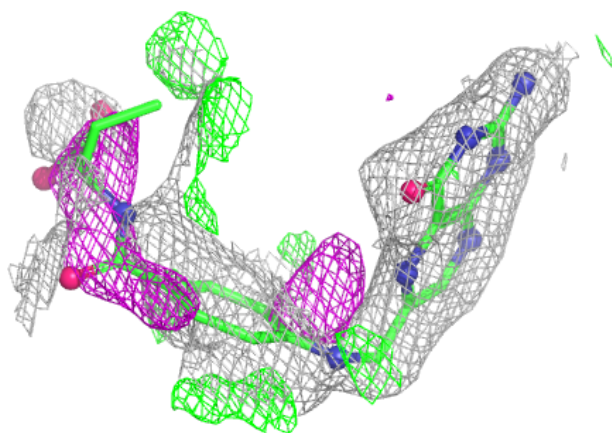
**Electron density around DHF A 1278:**

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



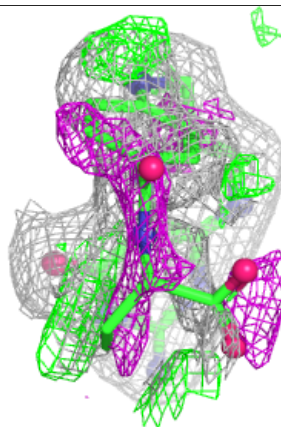
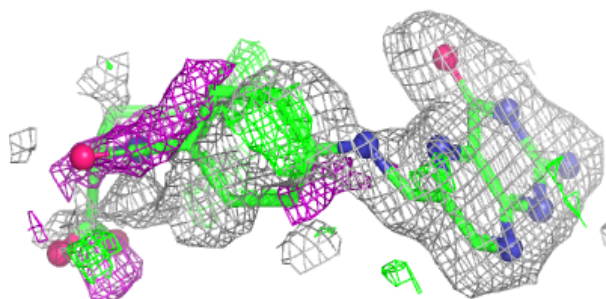
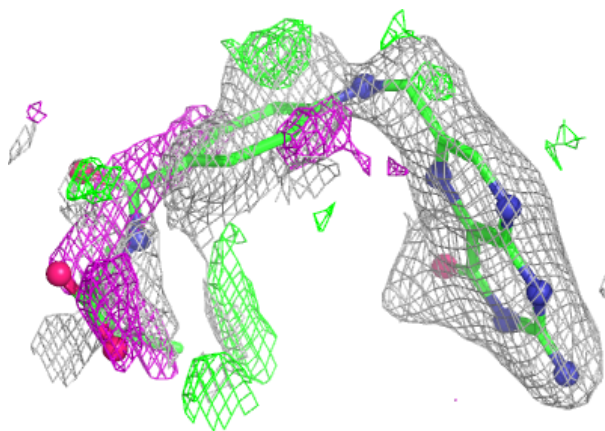
Electron density around DHF C 3278:

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

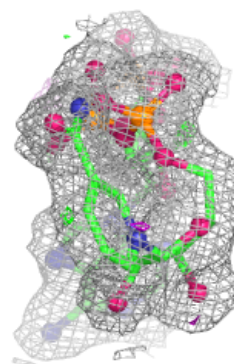
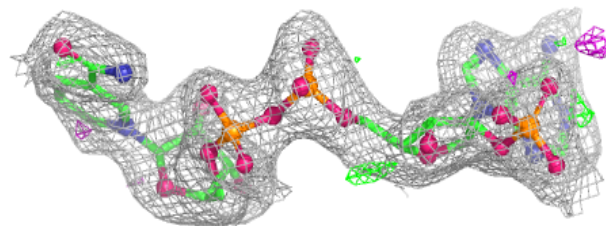
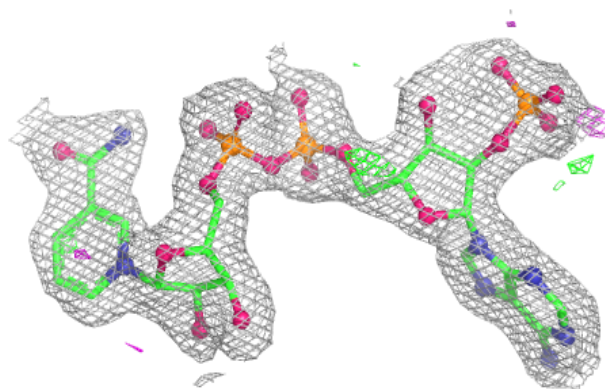


Electron density around DHF D 4278:

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

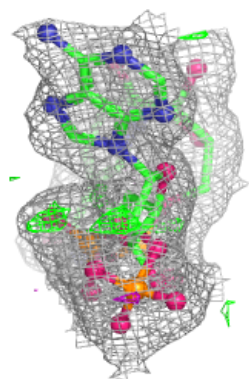
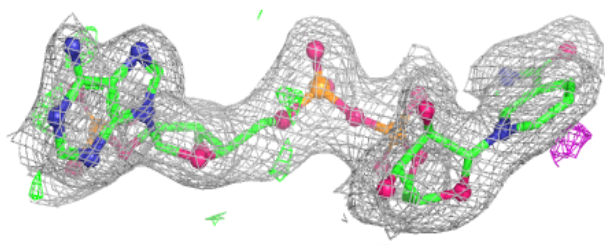
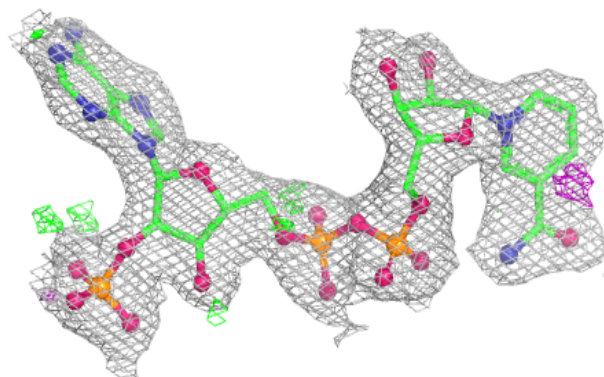
**Electron density around NAP A 1277:**

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

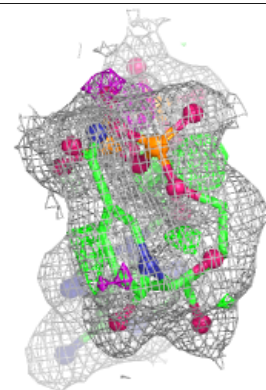
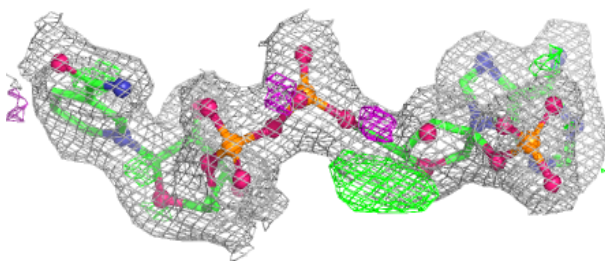
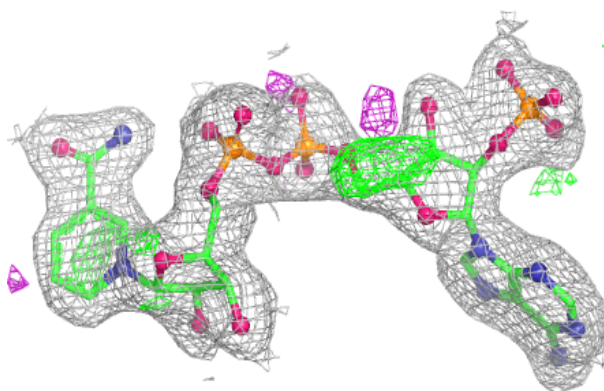


Electron density around NAP B 2277:

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

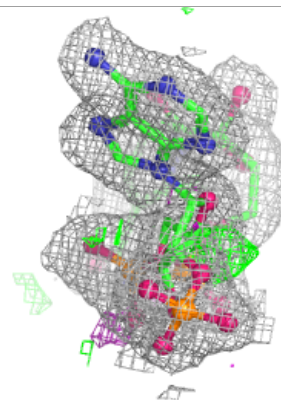
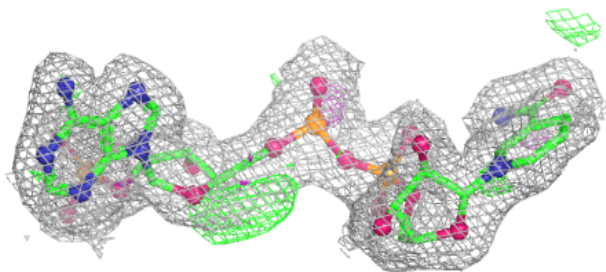
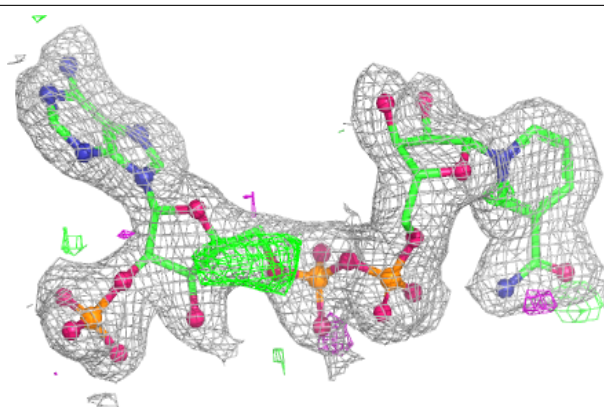
**Electron density around NAP D 4277:**

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



Electron density around NAP C 3277:

$2mF_o-DF_c$ (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.