Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 06:38 AM EDT

PDB ID	:	4QI7
Title	:	Cellobiose dehydrogenase from Neurospora crassa, NcCDH
Authors	:	Tan, T.C.; Gandini, R.; Sygmund, C.; Kittl, R.; Haltrich, D.; Ludwig, R.; Hallberg, B.M.; Divne, C.
Deposited on	:	2014-05-30
Resolution	:	2.90 Å(reported)

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	:	2.37.1
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)	:	2.37.1

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 2.90 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.
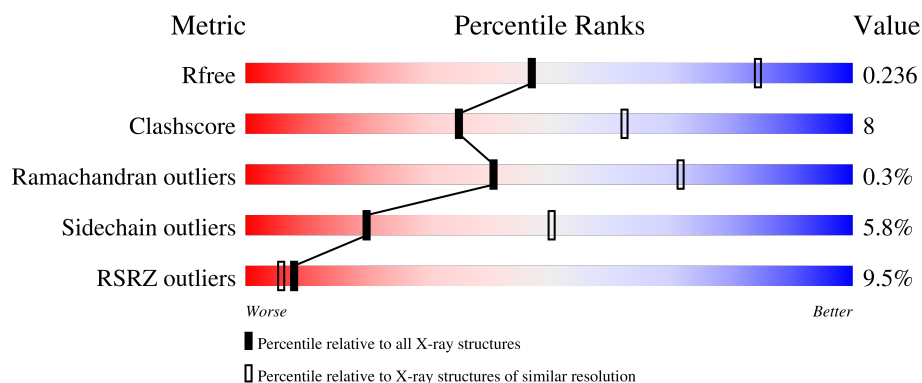
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	806	6% / 77% / 22% / •
1	B	806	13% / 76% / 21% / • •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12482 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 Cellobiose dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	805	Total	C	N	O	S	0	0	0
			6061	3810	1042	1182	27			
1	B	792	Total	C	N	O	S	0	0	0
			5979	3762	1029	1162	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	-	expression tag	UNP Q7RXM0
B	1	PCA	-	expression tag	UNP Q7RXM0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

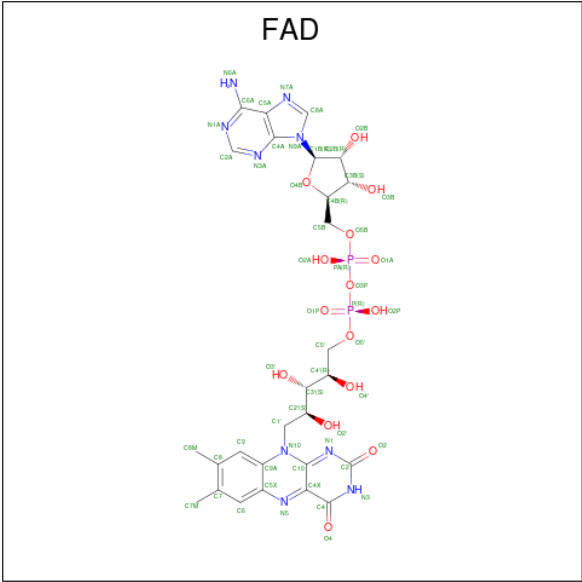HEM

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

O6
OH

O1
HO

O5
O

C6

C1(R) C5(R)

C2(R) C4(S)
C3(R)

N2
HN

OH
O4

C7

OH
O3

C8

O
O7

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

MAN

C6   O5   O1

HO

O6

C5(R)   C1(S)

C4(S)   C2(S)

C3(S)

HO

O4

OH

O3

OH

O2

OH

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 11	C 6	O 5	0	0
5	A	1	Total 11	C 6	O 5	0	0
5	B	1	Total 11	C 6	O 5	0	0
5	B	1	Total 11	C 6	O 5	0	0

- Molecule 6 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total 12	Pt 12	0	0
6	B	8	Total 8	Pt 8	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total 3	Mg 3	0	0
7	B	1	Total 1	Mg 1	0	0

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: Cellobiose dehydrogenase
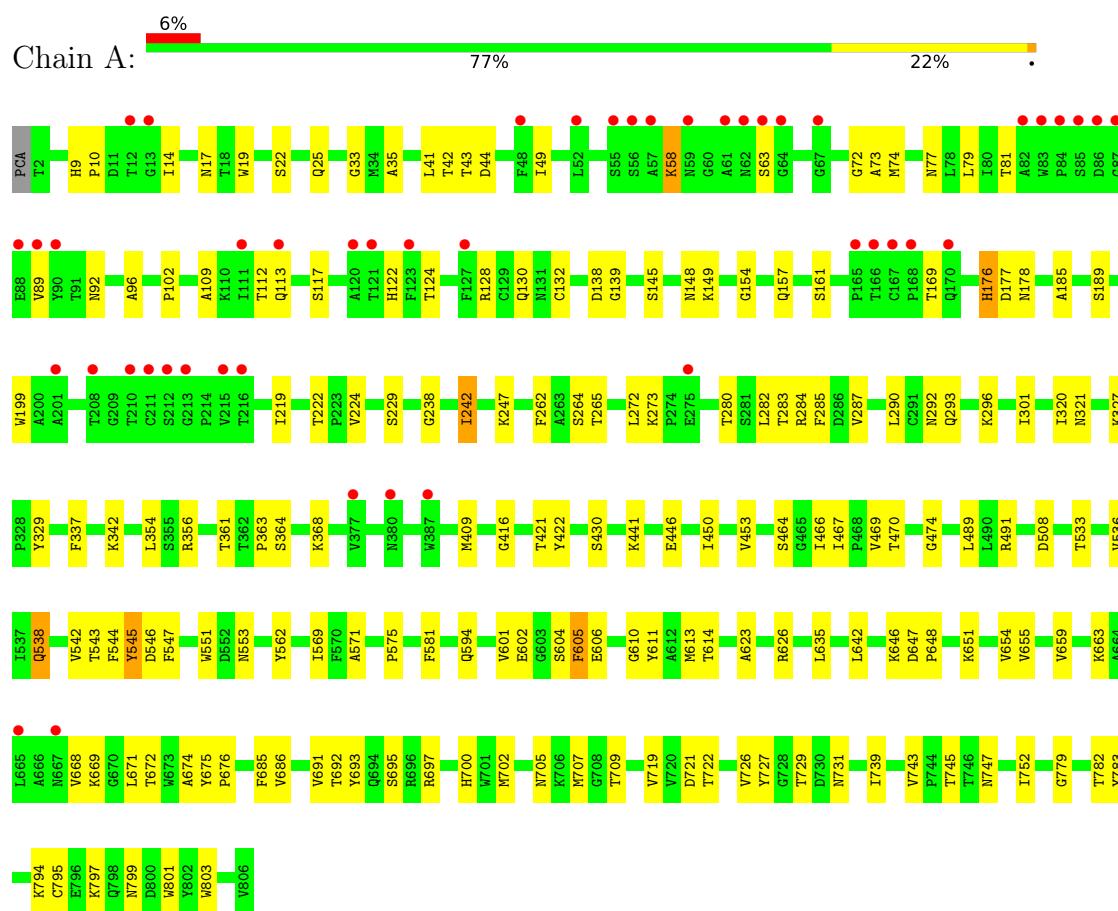
● Molecule 1: Cellobiose dehydrogenase
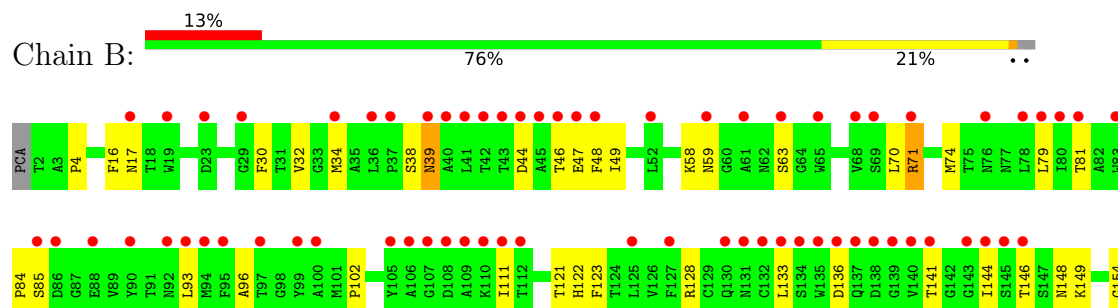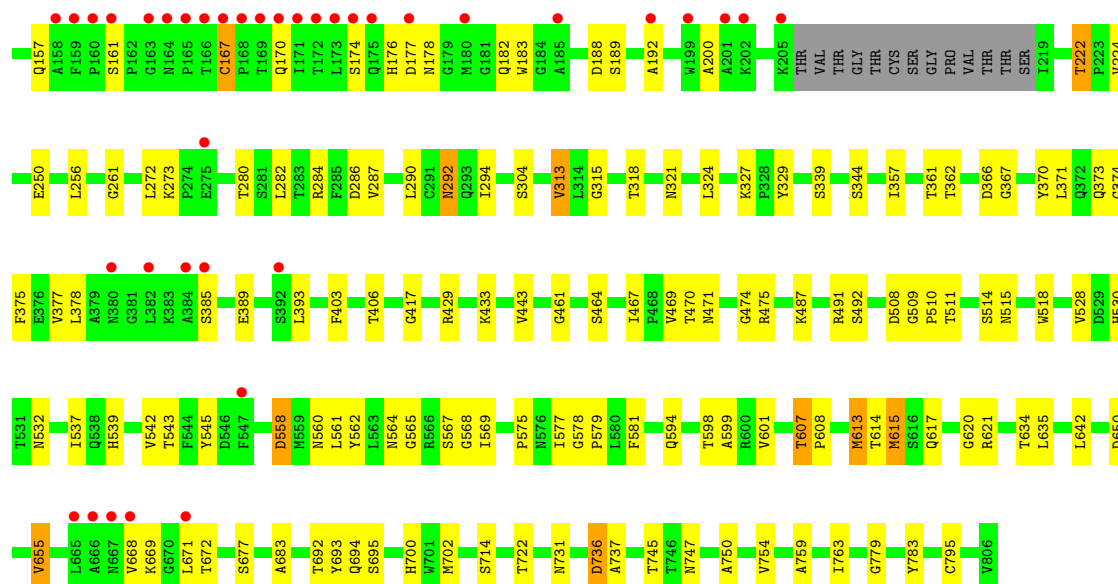
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	133.60Å 141.85Å 147.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.04 – 2.90 58.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (51.04-2.90) 99.9 (58.64-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1477)	Depositor
R, R_{free}	0.185 , 0.235 0.188 , 0.236	Depositor DCC
R_{free} test set	1995 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.2	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.068 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12482	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, PT, HEM, FAD, NAG, MAN

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	0.47	0/6214	0.67	0/8481
1	B	0.46	1/6130 (0.0%)	0.66	0/8362
All	All	0.47	1/12344 (0.0%)	0.66	0/16843

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	THR	C-N	-5.71	1.23	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	604	SER	Peptide
1	B	470	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6061	0	5828	99	0
1	B	5979	0	5749	100	0
2	A	43	0	30	6	0
2	B	43	0	30	9	0
3	A	53	0	31	5	0
3	B	53	0	31	3	0
4	A	98	0	91	5	0
4	B	84	0	78	0	0
5	A	22	0	20	0	0
5	B	22	0	20	0	0
6	A	12	0	0	0	0
6	B	8	0	0	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
All	All	12482	0	11908	201	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 8.

All (201) 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:4:PRO:HB2	1:B:17:ASN:HD22	1.41	0.83
1:B:176:HIS:CE1	2:B:901:HEM:NA	2.48	0.81
1:A:79:LEU:HD22	2:A:901:HEM:HAC	1.67	0.76
1:A:63:SER:HA	1:A:161:SER:HB3	1.67	0.76
1:B:133:LEU:HD22	1:B:144:ILE:HD11	1.68	0.73
1:A:176:HIS:H	1:A:176:HIS:CD2	2.06	0.73
1:B:176:HIS:CD2	2:B:901:HEM:NC	2.58	0.71
1:B:374:GLY:HA3	1:B:613:MET:HE1	1.73	0.71
1:B:491:ARG:HD3	1:B:635:LEU:HD13	1.72	0.70
1:B:287:VAL:HB	1:B:290:LEU:HD12	1.72	0.70
1:A:265:THR:HA	1:A:283:THR:HG21	1.75	0.68
1:B:469:VAL:HB	1:B:474:GLY:HA3	1.75	0.67
1:A:35:ALA:HB3	1:A:49:ILE:HB	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:THR:HG23	1:B:695:SER:H	1.60	0.66
1:B:47:GLU:OE2	1:B:128:ARG:NE	2.27	0.66
1:B:96:ALA:HB2	1:B:102:PRO:HB3	1.78	0.65
1:B:44:ASP:HA	1:B:146:THR:HG22	1.78	0.65
1:B:594:GLN:HG2	1:B:745:THR:HG23	1.78	0.65
1:A:601:VAL:HG12	1:A:613:MET:HG2	1.79	0.64
1:B:39:ASN:N	1:B:39:ASN:OD1	2.30	0.64
1:A:117:SER:HB2	1:A:124:THR:HB	1.80	0.63
1:A:575:PRO:HB3	1:A:602:GLU:OE2	1.98	0.63
1:A:96:ALA:HB2	1:A:102:PRO:HB3	1.81	0.63
2:A:901:HEM:HBA2	2:A:901:HEM:HMA2	1.81	0.63
1:B:128:ARG:HD2	1:B:200:ALA:HB1	1.83	0.61
1:B:177:ASP:OD1	1:B:178:ASN:N	2.34	0.61
1:A:41:LEU:HD22	1:A:149:LYS:HD3	1.84	0.60
1:A:450:ILE:O	1:A:731:ASN:ND2	2.35	0.60
1:A:491:ARG:HD3	1:A:635:LEU:HD13	1.85	0.58
1:B:63:SER:HA	1:B:161:SER:HB3	1.84	0.58
1:B:121:THR:HG22	1:B:122:HIS:CE1	2.38	0.58
1:B:136:ASP:OD1	1:B:141:THR:HA	2.03	0.58
1:B:250:GLU:HG2	1:B:429:ARG:NH2	2.17	0.58
4:A:904:NAG:H82	1:B:461:GLY:HA3	1.86	0.58
1:B:594:GLN:OE1	1:B:621:ARG:NH2	2.36	0.58
1:A:157:GLN:HB3	1:A:178:ASN:HB3	1.86	0.57
1:B:373:GLN:HB2	1:B:543:THR:HG22	1.85	0.57
1:B:46:THR:HG23	1:B:47:GLU:HB3	1.85	0.57
1:A:536:VAL:HB	1:A:674:ALA:HB3	1.87	0.57
1:B:389:GLU:HB2	1:B:403:PHE:CZ	2.40	0.57
1:A:81:THR:HG22	1:A:92:ASN:O	2.05	0.57
1:B:375:PHE:CE1	1:B:579:PRO:HB3	2.40	0.56
1:B:71:ARG:HD3	1:B:144:ILE:HG22	1.88	0.56
1:B:366:ASP:OD1	1:B:367:GLY:N	2.37	0.56
1:A:327:LYS:HG3	1:A:354:LEU:HD11	1.88	0.55
1:A:224:VAL:HG23	1:A:464:SER:O	2.07	0.55
1:A:469:VAL:HB	1:A:474:GLY:HA3	1.89	0.55
1:B:545:TYR:CE1	1:B:569:ILE:HG21	2.41	0.55
1:B:564:ASN:OD1	1:B:565:GLY:N	2.39	0.55
1:A:676:PRO:HB3	1:A:685:PHE:HB2	1.88	0.55
1:A:148:ASN:N	1:A:149:LYS:HA	2.22	0.55
1:B:642:LEU:HD21	1:B:693:TYR:HB3	1.88	0.55
1:A:283:THR:HG23	1:A:285:PHE:H	1.72	0.54
4:A:906:NAG:O7	4:A:906:NAG:O3	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ALA:HB1	1:A:132:CYS:SG	2.48	0.54
1:A:542:VAL:HB	1:A:611:TYR:HA	1.89	0.54
1:A:752:ILE:HD13	3:A:902:FAD:H5'2	1.90	0.54
1:A:176:HIS:HE1	2:A:901:HEM:C4D	2.26	0.53
1:A:337:PHE:HD1	1:A:707:MET:HE1	1.74	0.53
1:B:702:MET:HG2	1:B:737:ALA:HB1	1.90	0.53
1:A:321:ASN:HB2	3:A:902:FAD:N5	2.24	0.53
1:A:747:ASN:HB3	3:A:902:FAD:C2	2.38	0.53
1:B:542:VAL:HG22	1:B:613:MET:HE3	1.89	0.53
1:A:726:VAL:O	1:A:729:THR:OG1	2.23	0.52
1:B:287:VAL:HG22	1:B:562:TYR:HE2	1.74	0.52
1:A:692:THR:HG22	1:A:695:SER:HB2	1.91	0.52
1:B:537:ILE:HD12	1:B:671:LEU:HD11	1.92	0.52
1:B:558:ASP:OD1	1:B:558:ASP:N	2.35	0.52
1:B:38:SER:HA	1:B:192:ALA:HB1	1.92	0.52
1:A:693:TYR:O	1:A:697:ARG:HB3	2.10	0.51
1:A:44:ASP:OD1	1:A:145:SER:OG	2.28	0.51
1:B:47:GLU:HG2	1:B:48:PHE:N	2.25	0.51
1:B:575:PRO:O	1:B:577:ILE:HG13	2.10	0.51
1:A:17:ASN:O	1:A:33:GLY:HA2	2.11	0.51
1:A:89:VAL:O	1:A:113:GLN:NE2	2.39	0.51
1:A:229:SER:OG	1:A:470:THR:HG22	2.11	0.51
1:B:371:LEU:HD11	1:B:545:TYR:HD1	1.76	0.51
1:B:93:LEU:HD11	1:B:111:ILE:HG13	1.93	0.50
1:A:654:VAL:HG12	1:A:686:VAL:HG21	1.93	0.50
1:A:721:ASP:HB3	1:A:727:TYR:CZ	2.47	0.50
1:B:601:VAL:HG23	1:B:601:VAL:O	2.11	0.50
1:B:321:ASN:HB2	3:B:902:FAD:C4X	2.42	0.50
1:B:406:THR:OG1	1:B:577:ILE:O	2.22	0.50
1:A:544:PHE:HB2	1:A:610:GLY:HA2	1.93	0.50
1:A:72:GLY:HA2	1:A:154:GLY:H	1.77	0.50
1:B:79:LEU:HD22	2:B:901:HEM:HAC	1.93	0.49
1:A:321:ASN:HB2	3:A:902:FAD:C4X	2.42	0.49
1:A:642:LEU:O	1:A:646:LYS:HE3	2.13	0.49
1:B:515:ASN:HA	1:B:518:TRP:CD1	2.48	0.49
1:B:81:THR:HG22	2:B:901:HEM:HBC2	1.95	0.49
1:A:293:GLN:HE22	1:A:296:LYS:HD3	1.78	0.49
1:A:700:HIS:O	1:A:702:MET:HG3	2.13	0.49
1:A:262:PHE:HZ	1:A:301:ILE:HD13	1.76	0.48
1:B:273:LYS:HD3	1:B:282:LEU:O	2.12	0.48
1:B:562:TYR:HA	1:B:567:SER:H	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:SER:OG	1:A:25:GLN:HG3	2.13	0.48
1:A:747:ASN:HB3	3:A:902:FAD:O2	2.14	0.48
1:B:747:ASN:HB3	3:B:902:FAD:C2	2.44	0.48
1:B:272:LEU:O	1:B:284:ARG:HG2	2.14	0.48
1:A:72:GLY:HA2	1:A:154:GLY:N	2.29	0.48
1:A:601:VAL:HG23	1:A:601:VAL:O	2.14	0.47
1:B:44:ASP:HA	1:B:146:THR:CG2	2.44	0.47
1:A:128:ARG:CZ	1:A:130:GLN:HE21	2.27	0.47
1:B:327:LYS:HB2	1:B:393:LEU:O	2.14	0.47
1:A:797:LYS:HB2	1:A:803:TRP:CE2	2.50	0.47
1:B:74:MET:HB2	2:B:901:HEM:C1D	2.49	0.47
1:B:167:CYS:HB3	1:B:170:GLN:HB2	1.97	0.47
1:B:176:HIS:CE1	2:B:901:HEM:C1A	3.03	0.47
1:B:375:PHE:HE1	1:B:579:PRO:HB3	1.79	0.47
1:A:293:GLN:HG3	1:A:551:TRP:CE3	2.50	0.46
1:A:19:TRP:CE2	1:A:185:ALA:HB1	2.49	0.46
1:B:224:VAL:HG23	1:B:464:SER:O	2.15	0.46
1:B:491:ARG:HD2	1:B:508:ASP:OD2	2.16	0.46
1:B:176:HIS:CD2	2:B:901:HEM:C1C	3.04	0.46
1:B:578:GLY:N	1:B:599:ALA:O	2.49	0.46
1:B:759:ALA:O	1:B:763:ILE:HG13	2.15	0.46
1:A:122:HIS:HD2	4:A:903:NAG:H5	1.81	0.46
1:B:750:ALA:O	1:B:754:VAL:HG23	2.16	0.46
1:B:315:GLY:O	1:B:318:THR:OG1	2.29	0.46
1:A:287:VAL:HB	1:A:290:LEU:HD12	1.98	0.45
1:A:176:HIS:CE1	2:A:901:HEM:C4D	3.04	0.45
1:A:659:VAL:HG12	1:A:663:LYS:HE2	1.99	0.45
1:A:272:LEU:O	1:A:284:ARG:HG2	2.16	0.45
1:A:668:VAL:HG12	1:A:671:LEU:HB2	1.98	0.45
1:A:176:HIS:CD2	2:A:901:HEM:NC	2.84	0.45
1:A:238:GLY:H	1:A:242:ILE:HD12	1.81	0.45
1:B:154:GLY:HA2	1:B:182:GLN:HA	1.99	0.45
1:B:601:VAL:HG12	1:B:613:MET:HE2	1.97	0.45
1:A:287:VAL:HG22	1:A:562:TYR:HE2	1.81	0.45
1:B:378:LEU:HD21	1:B:537:ILE:CD1	2.46	0.45
1:A:676:PRO:HB3	1:A:685:PHE:CB	2.46	0.45
1:B:560:ASN:O	1:B:564:ASN:ND2	2.50	0.45
1:B:357:ILE:HD13	1:B:417:GLY:HA2	1.99	0.44
1:B:370:TYR:CE2	1:B:568:GLY:HA2	2.52	0.44
1:A:138:ASP:HB3	1:A:139:GLY:H	1.67	0.44
1:B:528:VAL:HG12	1:B:702:MET:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PRO:HB2	1:A:571:ALA:O	2.18	0.44
1:B:30:PHE:HB2	1:B:157:GLN:NE2	2.31	0.44
1:B:509:GLY:N	1:B:510:PRO:HD2	2.32	0.44
1:A:705:ASN:HB3	1:A:719:VAL:HG11	1.99	0.43
1:B:176:HIS:HE1	2:B:901:HEM:C1A	2.35	0.43
1:B:558:ASP:HA	1:B:561:LEU:HB3	1.99	0.43
1:A:73:ALA:O	1:A:77:ASN:ND2	2.48	0.43
1:B:779:GLY:HA2	1:B:783:TYR:CD2	2.53	0.43
1:B:530:HIS:CD2	1:B:620:GLY:HA2	2.53	0.43
1:B:539:HIS:HB3	1:B:542:VAL:HG23	2.01	0.43
1:A:538:GLN:HG3	1:A:672:THR:HB	2.01	0.43
1:B:84:PRO:HD3	1:B:123:PHE:CZ	2.53	0.43
1:B:487:LYS:O	1:B:491:ARG:HG3	2.18	0.43
1:B:443:VAL:HG22	1:B:492:SER:OG	2.19	0.43
1:A:14:ILE:HG23	1:A:199:TRP:CE3	2.53	0.43
1:A:491:ARG:HD2	1:A:508:ASP:OD1	2.18	0.43
1:A:606:GLU:HB2	1:A:675:TYR:OH	2.19	0.43
1:A:409:MET:O	1:A:416:GLY:HA3	2.19	0.42
1:B:148:ASN:O	1:B:149:LYS:HG2	2.18	0.42
1:B:692:THR:OG1	1:B:694:GLN:OE1	2.29	0.42
1:A:446:GLU:OE2	1:A:794:LYS:NZ	2.45	0.42
1:A:647:ASP:HA	1:A:648:PRO:HD2	1.79	0.42
1:A:273:LYS:HE2	1:A:282:LEU:O	2.19	0.42
1:A:9:HIS:HA	1:A:10:PRO:HD3	1.91	0.42
1:A:594:GLN:HG2	1:A:745:THR:HG23	2.00	0.42
1:B:256:LEU:HD12	1:B:433:LYS:O	2.19	0.42
1:A:651:LYS:O	1:A:655:VAL:HG23	2.18	0.42
1:A:669:LYS:HG2	4:A:908:NAG:H83	2.01	0.42
1:A:779:GLY:HA2	1:A:783:TYR:CD2	2.54	0.42
1:B:581:PHE:HZ	1:B:615:MET:HE2	1.84	0.42
1:B:16:PHE:HE2	1:B:49:ILE:HG22	1.85	0.42
1:B:176:HIS:HD2	2:B:901:HEM:C1C	2.38	0.42
1:A:177:ASP:N	1:A:177:ASP:OD1	2.52	0.42
1:A:238:GLY:N	1:A:242:ILE:HD12	2.34	0.42
1:A:290:LEU:HD22	1:A:551:TRP:HE3	1.84	0.42
1:A:337:PHE:O	1:A:342:LYS:HE2	2.19	0.42
1:A:623:ALA:O	1:A:626:ARG:NH2	2.53	0.42
1:B:188:ASP:OD1	1:B:189:SER:N	2.49	0.42
1:B:261:GLY:HA3	1:B:313:VAL:HA	2.01	0.42
1:B:607:THR:HA	1:B:608:PRO:HD3	1.84	0.42
1:A:705:ASN:O	1:A:739:ILE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HA	1:B:70:LEU:HD23	1.74	0.41
1:B:292:ASN:OD1	1:B:575:PRO:HD3	2.20	0.41
1:A:285:PHE:HZ	1:A:301:ILE:HD12	1.85	0.41
1:A:247:LYS:HA	1:A:247:LYS:HD2	1.90	0.41
1:A:264:SER:OG	1:A:265:THR:N	2.54	0.41
1:A:122:HIS:CD2	4:A:903:NAG:H5	2.55	0.41
1:B:475:ARG:HA	1:B:731:ASN:HB2	2.03	0.41
1:A:575:PRO:HG2	1:A:602:GLU:HG3	2.02	0.41
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.71	0.41
1:B:736:ASP:HB2	3:B:902:FAD:O2P	2.20	0.41
1:A:42:THR:OG1	1:A:43:THR:N	2.54	0.41
1:A:545:TYR:CE1	1:A:569:ILE:HD13	2.56	0.41
1:A:489:LEU:HD12	1:A:705:ASN:ND2	2.36	0.41
1:B:58:LYS:HE2	1:B:59:ASN:OD1	2.21	0.41
1:B:655:VAL:HG11	1:B:683:ALA:HA	2.03	0.41
1:A:421:THR:OG1	1:A:422:TYR:N	2.53	0.40
1:A:546:ASP:O	1:A:547:PHE:HB2	2.20	0.40
1:B:599:ALA:HA	1:B:614:THR:O	2.21	0.40
1:B:700:HIS:O	1:B:702:MET:HG3	2.21	0.40
1:A:58:LYS:HA	1:A:58:LYS:HD2	1.86	0.40
1:A:74:MET:HB2	2:A:901:HEM:C1D	2.56	0.40
1:A:441:LYS:HE2	1:A:441:LYS:HB3	1.71	0.40
1:B:532:ASN:HA	1:B:617:GLN:O	2.22	0.40
1:A:799:ASN:HB2	1:A:801:TRP:H	1.87	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	803/806 (100%)	766 (95%)	35 (4%)	2 (0%)	47	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	788/806 (98%)	752 (95%)	34 (4%)	2 (0%)	41	71
All	All	1591/1612 (99%)	1518 (95%)	69 (4%)	4 (0%)	41	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	471	ASN
1	A	605	PHE
1	B	736	ASP
1	A	219	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	643/643 (100%)	610 (95%)	33 (5%)	24	56
1	B	632/643 (98%)	591 (94%)	41 (6%)	17	45
All	All	1275/1286 (99%)	1201 (94%)	74 (6%)	20	50

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	112	THR
1	A	169	THR
1	A	176	HIS
1	A	189	SER
1	A	222	THR
1	A	242	ILE
1	A	280	THR
1	A	292	ASN
1	A	320	ILE
1	A	329	TYR
1	A	356	ARG

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Mol	Chain	Res	Type
1	A	361	THR
1	A	364	SER
1	A	368	LYS
1	A	430	SER
1	A	453	VAL
1	A	466	ILE
1	A	467	ILE
1	A	533	THR
1	A	538	GLN
1	A	543	THR
1	A	545	TYR
1	A	553	ASN
1	A	581	PHE
1	A	605	PHE
1	A	614	THR
1	A	691	VAL
1	A	709	THR
1	A	722	THR
1	A	743	VAL
1	A	782	THR
1	A	795	CYS
1	B	32	VAL
1	B	34	MET
1	B	39	ASN
1	B	71	ARG
1	B	85	SER
1	B	167	CYS
1	B	174	SER
1	B	183	TRP
1	B	222	THR
1	B	280	THR
1	B	286	ASP
1	B	292	ASN
1	B	294	ILE
1	B	304	SER
1	B	313	VAL
1	B	324	LEU
1	B	329	TYR
1	B	339	SER
1	B	344	SER
1	B	361	THR
1	B	362	THR

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Mol	Chain	Res	Type
1	B	377	VAL
1	B	385	SER
1	B	467	ILE
1	B	511	THR
1	B	514	SER
1	B	558	ASP
1	B	598	THR
1	B	607	THR
1	B	613	MET
1	B	615	MET
1	B	634	THR
1	B	650	ASP
1	B	655	VAL
1	B	668	VAL
1	B	669	LYS
1	B	672	THR
1	B	677	SER
1	B	714	SER
1	B	722	THR
1	B	795	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	705	ASN
1	B	17	ASN
1	B	182	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 24 are monoatomic - leaving 21 for Mogul analysis.

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	#$|Z| > 2$
4	NAG	B	904	1	14,14,15	0.39	0	17,19,21	0.62	0
3	FAD	A	902	-	53,58,58	1.24	5 (9%)	68,89,89	1.43	12 (17%)
4	NAG	B	907	1	14,14,15	0.54	0	17,19,21	0.64	0
4	NAG	A	904	1	14,14,15	0.33	0	17,19,21	0.58	0
4	NAG	A	907	1	14,14,15	0.26	0	17,19,21	0.83	1 (5%)
4	NAG	A	905	1	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	B	908	1	14,14,15	0.63	1 (7%)	17,19,21	0.60	0
2	HEM	B	901	1	41,50,50	2.66	14 (34%)	45,82,82	3.26	21 (46%)
4	NAG	B	906	1	14,14,15	0.21	0	17,19,21	0.73	1 (5%)
5	MAN	A	910	1	11,11,12	1.11	2 (18%)	15,15,17	1.56	3 (20%)
4	NAG	B	903	1	14,14,15	0.22	0	17,19,21	0.67	0
4	NAG	A	903	1	14,14,15	0.33	0	17,19,21	0.32	0
5	MAN	B	909	1	11,11,12	1.99	2 (18%)	15,15,17	1.09	0
5	MAN	A	911	1	11,11,12	1.94	5 (45%)	15,15,17	1.01	0
4	NAG	B	905	1	14,14,15	0.36	0	17,19,21	0.46	0
3	FAD	B	902	-	53,58,58	1.18	4 (7%)	68,89,89	1.53	15 (22%)
4	NAG	A	909	1	14,14,15	0.30	0	17,19,21	0.50	0
4	NAG	A	908	1	14,14,15	0.42	0	17,19,21	0.70	1 (5%)
5	MAN	B	910	1	11,11,12	2.45	6 (54%)	15,15,17	1.23	1 (6%)
2	HEM	A	901	1	41,50,50	2.49	15 (36%)	45,82,82	3.40	24 (53%)
4	NAG	A	906	1	14,14,15	0.87	1 (7%)	17,19,21	1.49	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	904	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	902	-	-	6/30/50/50	0/6/6/6
4	NAG	B	907	1	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1	-	4/6/23/26	0/1/1/1
4	NAG	A	907	1	-	2/6/23/26	0/1/1/1
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1
4	NAG	B	908	1	-	0/6/23/26	0/1/1/1
2	HEM	B	901	1	-	2/12/54/54	-
4	NAG	B	906	1	-	0/6/23/26	0/1/1/1
5	MAN	A	910	1	-	2/2/19/22	0/1/1/1
4	NAG	B	903	1	-	0/6/23/26	0/1/1/1
4	NAG	A	903	1	-	2/6/23/26	0/1/1/1
5	MAN	B	909	1	-	2/2/19/22	0/1/1/1
5	MAN	A	911	1	-	2/2/19/22	0/1/1/1
4	NAG	B	905	1	-	2/6/23/26	0/1/1/1
3	FAD	B	902	-	-	3/30/50/50	0/6/6/6
4	NAG	A	909	1	-	0/6/23/26	0/1/1/1
4	NAG	A	908	1	-	2/6/23/26	0/1/1/1
5	MAN	B	910	1	-	2/2/19/22	0/1/1/1
2	HEM	A	901	1	-	5/12/54/54	-
4	NAG	A	906	1	-	4/6/23/26	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	HEM	C1A-NA	6.41	1.49	1.36
2	B	901	HEM	C4A-NA	6.36	1.49	1.36
2	A	901	HEM	C1A-NA	6.09	1.48	1.36
2	B	901	HEM	C3C-C2C	6.02	1.48	1.40
2	A	901	HEM	C4A-NA	5.46	1.47	1.36
5	B	910	MAN	C2-C3	5.09	1.60	1.52
2	A	901	HEM	C3C-C2C	4.70	1.46	1.40
5	B	909	MAN	C1-C2	4.65	1.62	1.52
2	B	901	HEM	C3D-C2D	4.64	1.46	1.36
2	B	901	HEM	C3B-C2B	4.52	1.46	1.37
2	B	901	HEM	CHA-C4D	4.41	1.46	1.35
2	A	901	HEM	C3B-C2B	4.33	1.46	1.37
2	A	901	HEM	C3D-C2D	4.29	1.45	1.36
3	A	902	FAD	C2A-N3A	4.29	1.39	1.32
2	A	901	HEM	CHA-C4D	4.27	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	909	MAN	O2-C2	3.83	1.51	1.43
2	B	901	HEM	FE-NB	3.79	2.15	1.96
3	A	902	FAD	C4X-N5	3.71	1.38	1.30
2	B	901	HEM	FE-ND	3.66	2.15	1.96
3	B	902	FAD	C2A-N3A	3.66	1.38	1.32
5	A	911	MAN	C2-C3	3.66	1.57	1.52
3	B	902	FAD	C4X-N5	3.59	1.37	1.30
2	A	901	HEM	C2A-C3A	3.57	1.48	1.37
2	B	901	HEM	CHB-C1B	3.55	1.44	1.35
2	A	901	HEM	CHB-C1B	3.52	1.44	1.35
2	A	901	HEM	C2C-C1C	3.39	1.50	1.42
5	B	910	MAN	C4-C5	3.35	1.60	1.53
2	B	901	HEM	C2A-C3A	3.34	1.47	1.37
2	A	901	HEM	FE-ND	3.19	2.12	1.96
2	A	901	HEM	FE-NB	2.95	2.11	1.96
2	B	901	HEM	C2C-C1C	2.84	1.49	1.42
5	B	910	MAN	C4-C3	2.83	1.59	1.52
5	B	910	MAN	C1-C2	2.81	1.58	1.52
5	A	911	MAN	C4-C3	2.73	1.59	1.52
3	A	902	FAD	C2B-C1B	-2.73	1.49	1.53
4	A	906	NAG	O5-C1	2.66	1.48	1.43
2	A	901	HEM	C1B-NB	-2.63	1.35	1.40
2	B	901	HEM	C4D-C3D	2.62	1.49	1.45
3	B	902	FAD	C2A-N1A	2.59	1.38	1.33
2	A	901	HEM	C4D-ND	-2.55	1.35	1.40
3	A	902	FAD	C2A-N1A	2.46	1.38	1.33
5	B	910	MAN	O3-C3	2.35	1.48	1.43
5	B	910	MAN	O5-C5	2.29	1.48	1.43
3	A	902	FAD	C10-N1	2.28	1.37	1.33
2	B	901	HEM	C4D-ND	-2.28	1.36	1.40
3	B	902	FAD	C10-N1	2.19	1.37	1.33
4	B	908	NAG	C1-C2	2.18	1.55	1.52
5	A	910	MAN	O5-C1	-2.11	1.40	1.43
2	B	901	HEM	C1B-C2B	2.09	1.48	1.44
2	A	901	HEM	C4D-C3D	2.04	1.48	1.45
2	A	901	HEM	CHC-C4B	2.04	1.46	1.41
5	A	911	MAN	O2-C2	2.03	1.47	1.43
5	A	911	MAN	C1-C2	2.02	1.56	1.52
5	A	911	MAN	O5-C1	-2.02	1.40	1.43
5	A	910	MAN	C1-C2	2.01	1.56	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	HEM	C3B-C2B-C1B	-9.60	99.36	106.49
2	B	901	HEM	C3B-C2B-C1B	-8.88	99.90	106.49
2	A	901	HEM	C2B-C1B-NB	8.45	119.85	109.84
2	B	901	HEM	C2B-C1B-NB	8.30	119.68	109.84
2	A	901	HEM	C2D-C1D-ND	7.64	119.04	109.88
2	B	901	HEM	C2D-C1D-ND	7.64	119.04	109.88
2	A	901	HEM	C3D-C4D-ND	7.27	118.26	110.17
2	B	901	HEM	C3D-C4D-ND	6.48	117.38	110.17
2	A	901	HEM	C4D-ND-C1D	-5.87	99.01	105.07
2	B	901	HEM	C4D-ND-C1D	-5.37	99.52	105.07
2	B	901	HEM	C1D-C2D-C3D	-5.30	101.39	106.96
4	A	906	NAG	C1-O5-C5	5.22	119.27	112.19
2	B	901	HEM	C1B-NB-C4B	-5.21	99.69	105.07
2	A	901	HEM	C1D-C2D-C3D	-5.14	101.55	106.96
3	B	902	FAD	N3A-C2A-N1A	-4.84	121.11	128.68
2	A	901	HEM	C1B-NB-C4B	-4.64	100.28	105.07
3	A	902	FAD	N3A-C2A-N1A	-4.50	121.64	128.68
2	B	901	HEM	CHD-C1D-C2D	-4.29	118.28	124.98
2	A	901	HEM	CHD-C1D-C2D	-4.04	118.66	124.98
5	A	910	MAN	O5-C1-C2	3.58	116.29	110.77
3	A	902	FAD	P-O3P-PA	-3.50	120.81	132.83
5	B	910	MAN	O3-C3-C2	3.43	116.56	109.99
2	A	901	HEM	CMA-C3A-C2A	3.42	131.38	124.94
2	A	901	HEM	CMA-C3A-C4A	-3.29	123.40	128.46
2	A	901	HEM	C4D-C3D-C2D	-3.29	102.10	106.90
3	B	902	FAD	C4X-C10-N10	3.28	121.27	116.48
2	B	901	HEM	C4A-C3A-C2A	-3.28	104.72	107.00
2	B	901	HEM	CMC-C2C-C3C	3.19	130.64	124.68
3	B	902	FAD	C4'-C3'-C2'	-3.17	106.76	113.36
3	A	902	FAD	C4'-C3'-C2'	-3.13	106.85	113.36
2	B	901	HEM	CBA-CAA-C2A	-3.12	107.30	112.62
2	A	901	HEM	CHA-C4D-C3D	-3.08	119.55	125.33
2	A	901	HEM	CHB-C1B-C2B	-3.04	118.32	126.72
3	A	902	FAD	C4X-C10-N10	3.01	120.88	116.48
2	B	901	HEM	C4B-C3B-C2B	-2.99	104.74	107.11
2	B	901	HEM	CHC-C4B-C3B	-2.93	120.09	124.57
2	B	901	HEM	C4D-C3D-C2D	-2.92	102.64	106.90
3	B	902	FAD	O4B-C1B-C2B	-2.88	102.72	106.93
3	B	902	FAD	C4-N3-C2	-2.86	120.35	125.64
4	A	907	NAG	C1-O5-C5	2.86	116.07	112.19
3	B	902	FAD	P-O3P-PA	-2.86	123.02	132.83
3	A	902	FAD	C4A-C5A-N7A	-2.85	106.42	109.40
3	A	902	FAD	C4-N3-C2	-2.83	120.41	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	HEM	CHB-C1B-C2B	-2.78	119.04	126.72
3	B	902	FAD	C1'-N10-C9A	-2.71	115.99	120.51
3	A	902	FAD	O4-C4-C4X	-2.71	119.41	126.60
2	A	901	HEM	CAD-C3D-C4D	2.69	129.36	124.66
2	B	901	HEM	CMB-C2B-C1B	2.68	129.12	125.04
3	B	902	FAD	O4-C4-C4X	-2.61	119.67	126.60
5	A	910	MAN	C1-C2-C3	2.60	112.86	109.67
2	B	901	HEM	CAD-C3D-C4D	2.57	129.15	124.66
2	A	901	HEM	C4A-C3A-C2A	-2.56	105.21	107.00
3	B	902	FAD	C4A-C5A-N7A	-2.56	106.73	109.40
4	B	906	NAG	C1-O5-C5	2.56	115.66	112.19
2	B	901	HEM	CHB-C1B-NB	-2.55	121.23	124.38
2	A	901	HEM	CBA-CAA-C2A	2.55	116.97	112.62
3	A	902	FAD	C4X-C4-N3	2.48	119.49	113.19
2	A	901	HEM	C4B-C3B-C2B	-2.46	105.17	107.11
2	A	901	HEM	CMD-C2D-C1D	2.45	128.78	125.04
2	B	901	HEM	CHA-C4D-C3D	-2.45	120.73	125.33
2	B	901	HEM	CMD-C2D-C1D	2.42	128.72	125.04
5	A	910	MAN	O2-C2-C3	-2.38	105.36	110.14
3	B	902	FAD	C4X-C4-N3	2.38	119.23	113.19
2	A	901	HEM	CMB-C2B-C1B	2.38	128.66	125.04
4	A	908	NAG	C1-O5-C5	2.32	115.33	112.19
3	A	902	FAD	C1'-N10-C9A	-2.32	116.65	120.51
3	B	902	FAD	C4X-C10-N1	-2.32	119.36	124.73
3	B	902	FAD	C10-C4X-N5	-2.31	119.95	124.86
3	A	902	FAD	C10-C4X-N5	-2.25	120.08	124.86
3	A	902	FAD	C4X-C10-N1	-2.20	119.62	124.73
2	A	901	HEM	C3C-C4C-NC	2.15	115.00	110.94
3	B	902	FAD	C4-C4X-C10	2.13	120.38	116.79
3	B	902	FAD	C10-N1-C2	2.11	121.12	116.90
2	A	901	HEM	CHB-C1B-NB	-2.11	121.78	124.38
2	A	901	HEM	CHC-C4B-C3B	-2.09	121.37	124.57
2	A	901	HEM	CBD-CAD-C3D	-2.06	106.91	112.63
2	B	901	HEM	CHA-C4D-ND	-2.06	121.84	124.38
3	B	902	FAD	O3B-C3B-C4B	-2.05	105.12	111.05
2	A	901	HEM	CHD-C1D-ND	-2.02	122.23	124.43
3	A	902	FAD	C10-N1-C2	2.01	120.91	116.90

There are no chirality outliers.
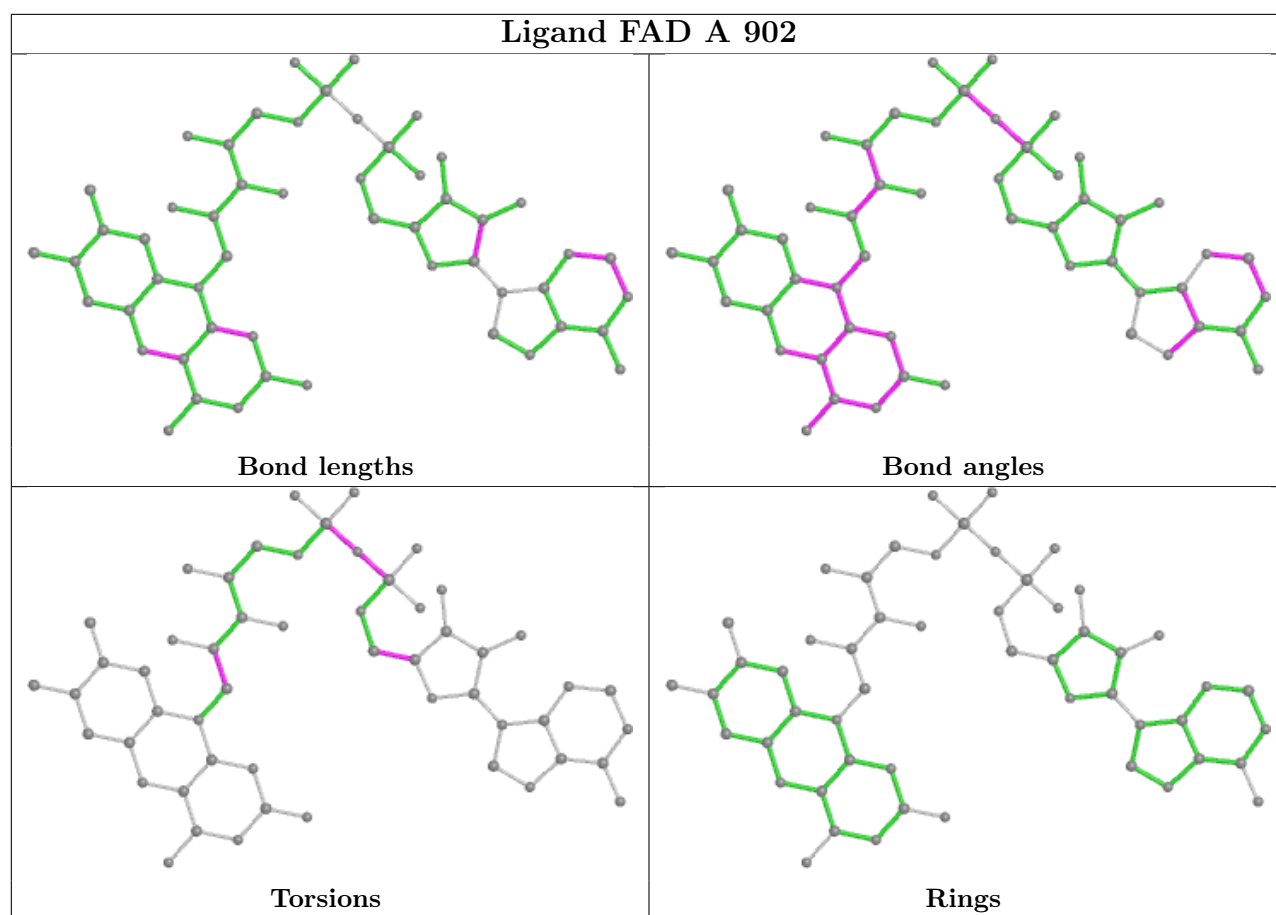
All (41) torsion outliers are listed below:

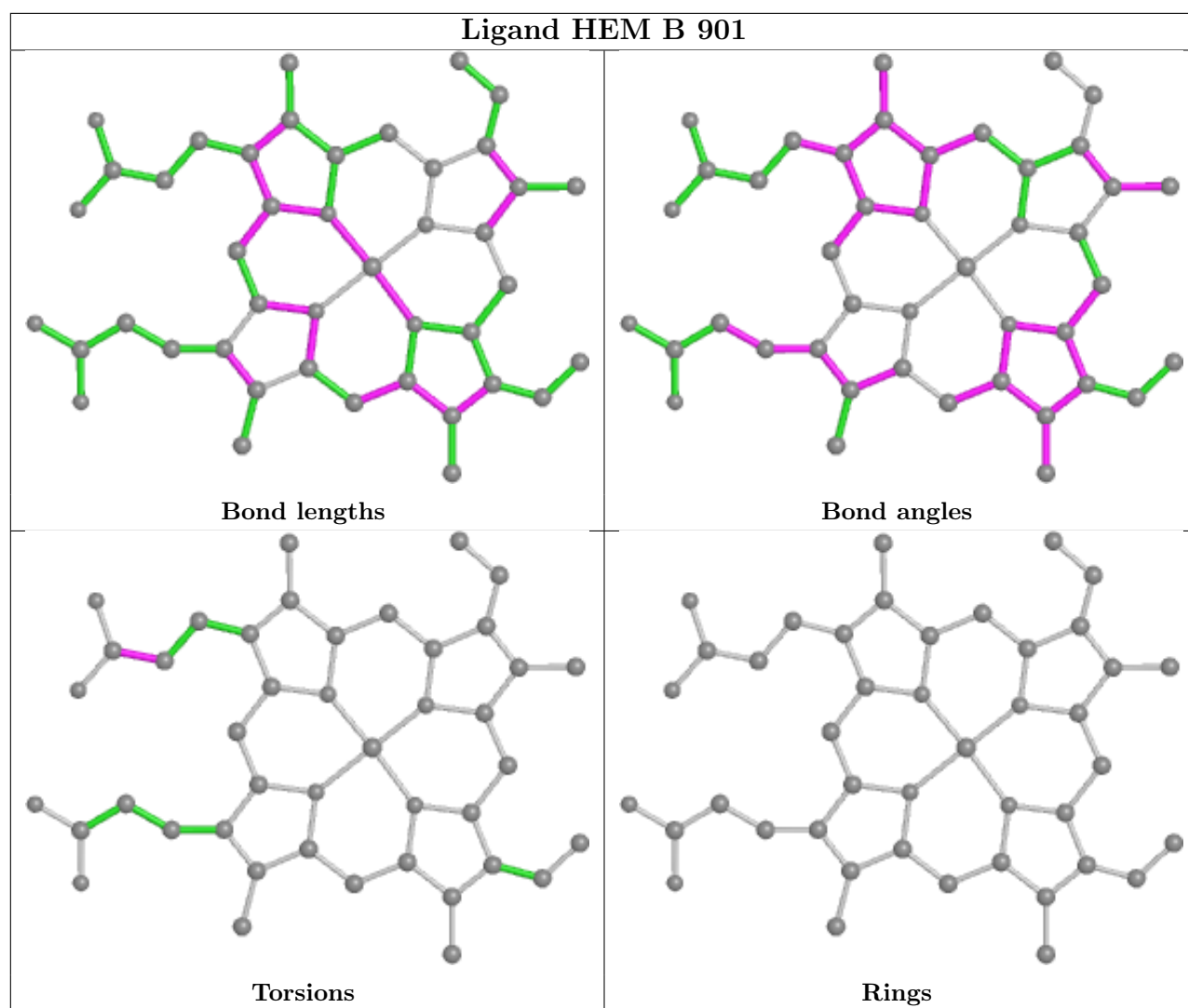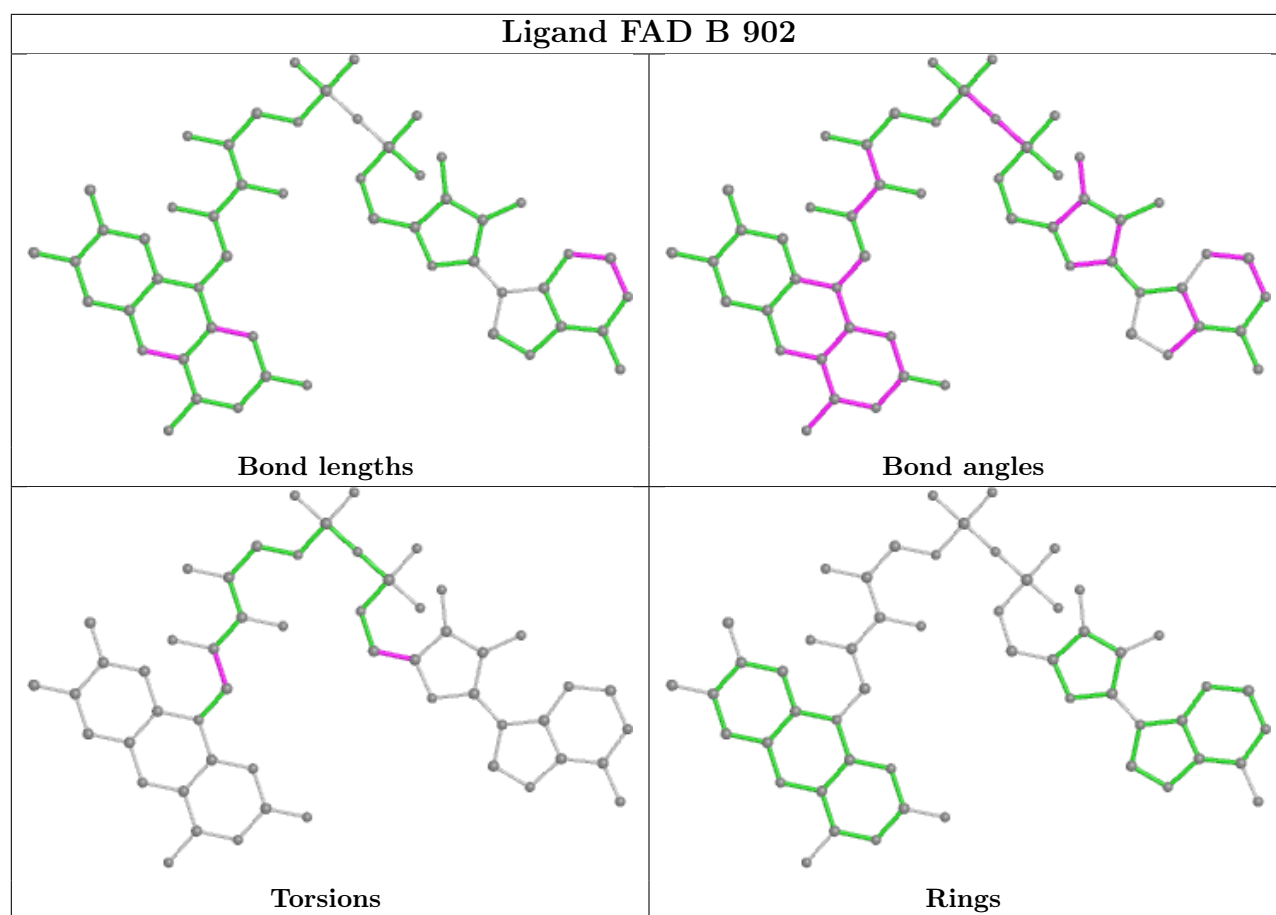| Mol	Chain	Res	Type	Atoms
2	A	901	HEM	C1A-C2A-CAA-CBA
2	A	901	HEM	C3A-C2A-CAA-CBA
3	A	902	FAD	N10-C1'-C2'-O2'
3	A	902	FAD	N10-C1'-C2'-C3'
3	B	902	FAD	N10-C1'-C2'-O2'
4	A	906	NAG	C1-C2-N2-C7
4	A	904	NAG	C4-C5-C6-O6
4	A	904	NAG	O5-C5-C6-O6
4	A	903	NAG	O5-C5-C6-O6
4	A	906	NAG	O5-C5-C6-O6
3	B	902	FAD	O4B-C4B-C5B-O5B
3	B	902	FAD	C3B-C4B-C5B-O5B
4	A	908	NAG	O5-C5-C6-O6
5	B	910	MAN	O5-C5-C6-O6
4	A	903	NAG	C4-C5-C6-O6
5	A	911	MAN	O5-C5-C6-O6
4	B	905	NAG	O5-C5-C6-O6
4	A	906	NAG	C4-C5-C6-O6
4	A	904	NAG	C8-C7-N2-C2
4	A	904	NAG	O7-C7-N2-C2
5	B	909	MAN	C4-C5-C6-O6
4	A	908	NAG	C4-C5-C6-O6
5	B	910	MAN	C4-C5-C6-O6
5	A	910	MAN	C4-C5-C6-O6
2	A	901	HEM	C2A-CAA-CBA-CGA
4	B	905	NAG	C4-C5-C6-O6
5	A	911	MAN	C4-C5-C6-O6
5	B	909	MAN	O5-C5-C6-O6
5	A	910	MAN	O5-C5-C6-O6
4	A	907	NAG	O5-C5-C6-O6
3	A	902	FAD	PA-O3P-P-O5'
3	A	902	FAD	O4B-C4B-C5B-O5B
4	A	906	NAG	C3-C2-N2-C7
2	A	901	HEM	CAD-CBD-CGD-O1D
2	B	901	HEM	CAD-CBD-CGD-O1D
2	A	901	HEM	CAD-CBD-CGD-O2D
2	B	901	HEM	CAD-CBD-CGD-O2D
4	A	907	NAG	C4-C5-C6-O6
3	A	902	FAD	P-O3P-PA-O1A
3	A	902	FAD	C3B-C4B-C5B-O5B
4	B	904	NAG	C4-C5-C6-O6

There are no ring outliers.

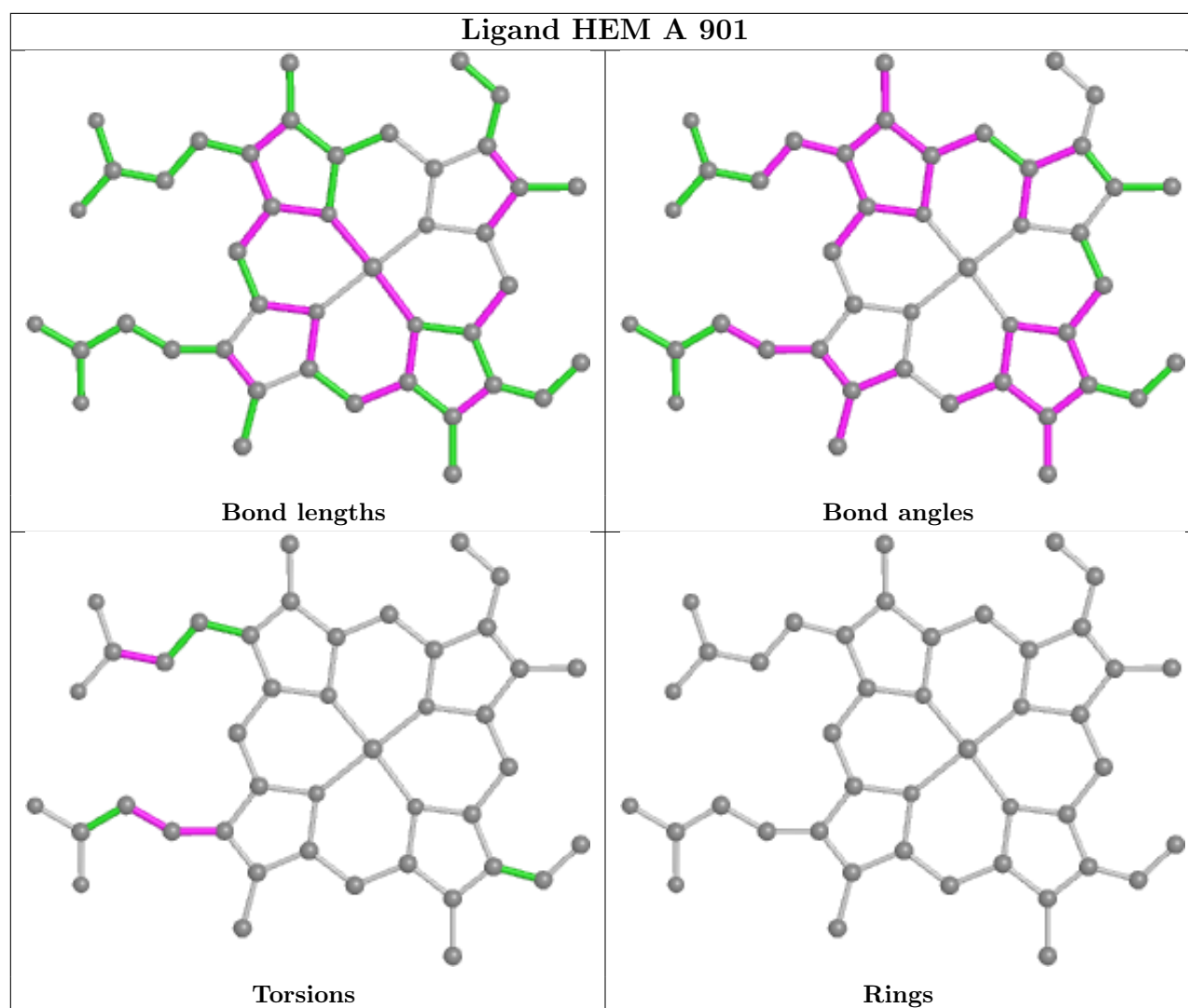8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	FAD	5	0
4	A	904	NAG	1	0
2	B	901	HEM	9	0
4	A	903	NAG	2	0
3	B	902	FAD	3	0
4	A	908	NAG	1	0
2	A	901	HEM	6	0
4	A	906	NAG	1	0

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

Ligand FAD A 902

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 901

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 902

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 901

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	805/806 (99%)	0.27	47 (5%)	23	19	22, 69, 122, 179	0
1	B	792/806 (98%)	0.61	105 (13%)	3	2	25, 75, 149, 196	0
All	All	1597/1612 (99%)	0.44	152 (9%)	8	6	22, 71, 138, 196	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	ASP	8.0
1	B	136	ASP	6.6
1	B	132	CYS	6.2
1	B	171	ILE	6.1
1	B	140	VAL	5.9
1	B	92	ASN	5.5
1	B	138	ASP	5.2
1	B	168	PRO	5.2
1	B	42	THR	5.1
1	A	90	TYR	5.1
1	B	34	MET	5.1
1	A	88	GLU	5.0
1	B	85	SER	4.9
1	A	167	CYS	4.6
1	A	86	ASP	4.6
1	A	12	THR	4.5
1	B	95	PHE	4.5
1	B	41	LEU	4.5
1	A	212	SER	4.5
1	B	43	THR	4.4
1	A	166	THR	4.4
1	B	146	THR	4.4
1	B	141	THR	4.2
1	B	137	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	36	LEU	4.1
1	B	164	ASN	4.1
1	A	211	CYS	4.1
1	A	64	GLY	4.1
1	A	168	PRO	4.0
1	B	167	CYS	4.0
1	B	47	GLU	4.0
1	B	159	PHE	4.0
1	B	174	SER	4.0
1	B	133	LEU	4.0
1	B	158	ALA	4.0
1	B	44	ASP	4.0
1	B	65	TRP	3.9
1	A	13	GLY	3.9
1	B	97	THR	3.9
1	B	37	PRO	3.9
1	B	160	PRO	3.9
1	B	81	THR	3.8
1	B	667	ASN	3.7
1	B	111	ILE	3.7
1	B	99	TYR	3.7
1	B	94	MET	3.6
1	B	175	GLN	3.5
1	B	52	LEU	3.5
1	B	145	SER	3.5
1	B	108	ASP	3.5
1	B	105	TYR	3.4
1	B	385	SER	3.4
1	B	170	GLN	3.4
1	B	169	THR	3.4
1	A	120	ALA	3.3
1	B	665	LEU	3.3
1	A	55	SER	3.3
1	A	85	SER	3.3
1	B	109	ALA	3.2
1	B	68	VAL	3.2
1	B	106	ALA	3.2
1	B	76	ASN	3.2
1	B	78	LEU	3.2
1	B	125	LEU	3.2
1	A	170	GLN	3.1
1	B	48	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	380	ASN	3.1
1	B	110	LYS	3.1
1	B	139	GLY	3.0
1	B	185	ALA	3.0
1	B	384	ALA	3.0
1	A	61	ALA	3.0
1	A	84	PRO	2.9
1	B	127	PHE	2.9
1	B	19	TRP	2.9
1	B	69	SER	2.9
1	A	215	VAL	2.9
1	B	23	ASP	2.9
1	B	80	ILE	2.9
1	B	173	LEU	2.9
1	B	144	ILE	2.9
1	B	46	THR	2.8
1	B	166	THR	2.8
1	A	275	GLU	2.8
1	B	666	ALA	2.8
1	B	134	SER	2.7
1	B	17	ASN	2.7
1	A	665	LEU	2.7
1	B	90	TYR	2.7
1	B	93	LEU	2.7
1	B	135	TRP	2.7
1	B	130	GLN	2.6
1	B	45	ALA	2.6
1	A	59	ASN	2.6
1	A	56	SER	2.6
1	B	40	ALA	2.6
1	A	121	THR	2.6
1	A	63	SER	2.6
1	A	62	ASN	2.6
1	B	59	ASN	2.5
1	A	89	VAL	2.5
1	B	275	GLU	2.5
1	B	201	ALA	2.5
1	A	208	THR	2.4
1	B	161	SER	2.4
1	A	82	ALA	2.4
1	B	165	PRO	2.4
1	A	210	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	172	THR	2.4
1	B	392	SER	2.4
1	B	29	GLY	2.4
1	A	387	TRP	2.4
1	B	131	ASN	2.3
1	B	671	LEU	2.3
1	A	213	GLY	2.3
1	B	39	ASN	2.3
1	B	61	ALA	2.3
1	B	71	ARG	2.3
1	A	87	GLY	2.3
1	A	667	ASN	2.3
1	B	180	MET	2.3
1	A	57	ALA	2.2
1	B	382	LEU	2.2
1	A	216	THR	2.2
1	B	79	LEU	2.2
1	A	123	PHE	2.2
1	B	177	ASP	2.2
1	A	52	LEU	2.2
1	A	127	PHE	2.2
1	A	83	TRP	2.2
1	B	83	TRP	2.2
1	B	100	ALA	2.2
1	B	668	VAL	2.2
1	A	201	ALA	2.2
1	B	112	THR	2.2
1	A	165	PRO	2.1
1	A	111	ILE	2.1
1	B	88	GLU	2.1
1	B	143	GLY	2.1
1	B	107	GLY	2.1
1	B	163	GLY	2.1
1	B	199	TRP	2.1
1	B	63	SER	2.1
1	A	48	PHE	2.1
1	A	67	GLY	2.1
1	B	547	PHE	2.1
1	A	113	GLN	2.0
1	A	380	ASN	2.0
1	B	192	ALA	2.0
1	A	377	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	202	LYS	2.0
1	B	205	LYS	2.0

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

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

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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(Å²)	Q<0.9
4	NAG	A	906	14/15	0.76	0.37	72,105,123,124	0
6	PT	B	915	1/1	0.78	0.15	164,164,164,164	1
7	MG	A	924	1/1	0.82	0.62	73,73,73,73	0
6	PT	B	912	1/1	0.84	0.21	147,147,147,147	1
4	NAG	A	904	14/15	0.84	0.41	90,104,121,121	0
4	NAG	B	903	14/15	0.84	0.22	98,111,115,117	0
4	NAG	B	904	14/15	0.86	0.24	85,104,111,123	0
4	NAG	B	907	14/15	0.86	0.28	86,119,129,129	0
5	MAN	B	910	11/12	0.86	0.30	61,92,106,106	0
6	PT	A	921	1/1	0.87	0.42	282,282,282,282	0
5	MAN	B	909	11/12	0.88	0.29	73,81,96,96	0
6	PT	A	914	1/1	0.89	0.19	156,156,156,156	1
4	NAG	A	903	14/15	0.90	0.30	96,105,116,123	0
4	NAG	B	908	14/15	0.90	0.22	75,91,103,106	0
5	MAN	A	911	11/12	0.90	0.30	89,101,108,109	0
6	PT	A	915	1/1	0.90	0.07	155,155,155,155	1
5	MAN	A	910	11/12	0.91	0.17	91,100,115,119	0
4	NAG	A	908	14/15	0.91	0.25	83,106,124,129	0
6	PT	A	920	1/1	0.92	0.15	114,114,114,114	1
7	MG	B	919	1/1	0.92	0.24	54,54,54,54	0
6	PT	B	913	1/1	0.93	0.07	146,146,146,146	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
7	MG	A	925	1/1	0.94	0.43	54,54,54,54	0
4	NAG	B	906	14/15	0.94	0.15	59,75,109,118	0
4	NAG	B	905	14/15	0.95	0.22	81,99,103,107	0
6	PT	B	914	1/1	0.95	0.15	134,134,134,134	1
6	PT	A	918	1/1	0.95	0.17	123,123,123,123	1
6	PT	B	918	1/1	0.95	0.19	132,132,132,132	0
4	NAG	A	907	14/15	0.95	0.12	63,76,109,116	0
6	PT	A	913	1/1	0.95	0.19	120,120,120,120	0
7	MG	A	926	1/1	0.95	0.25	56,56,56,56	0
4	NAG	A	909	14/15	0.95	0.27	66,83,98,100	0
6	PT	A	916	1/1	0.96	0.15	117,117,117,117	1
2	HEM	B	901	43/43	0.96	0.33	60,86,110,126	0
6	PT	B	916	1/1	0.96	0.18	106,106,106,106	1
2	HEM	A	901	43/43	0.96	0.24	55,78,100,129	0
6	PT	A	917	1/1	0.97	0.14	151,151,151,151	1
3	FAD	A	902	53/53	0.97	0.19	20,52,93,102	0
3	FAD	B	902	53/53	0.97	0.18	20,54,90,97	0
4	NAG	A	905	14/15	0.97	0.15	79,96,105,113	0
6	PT	A	922	1/1	0.97	0.23	133,133,133,133	0
6	PT	B	917	1/1	0.98	0.19	102,102,102,102	0
6	PT	A	919	1/1	0.98	0.18	107,107,107,107	0
6	PT	A	923	1/1	0.99	0.12	92,92,92,92	1
6	PT	A	912	1/1	0.99	0.25	84,84,84,84	0
6	PT	B	911	1/1	1.00	0.22	71,71,71,71	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.
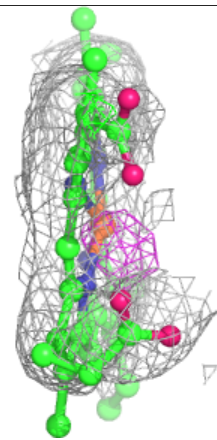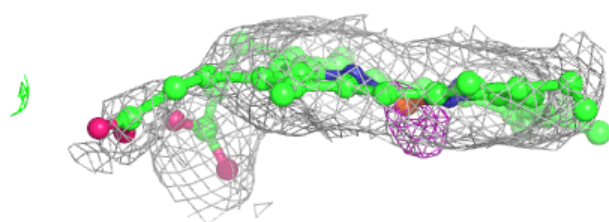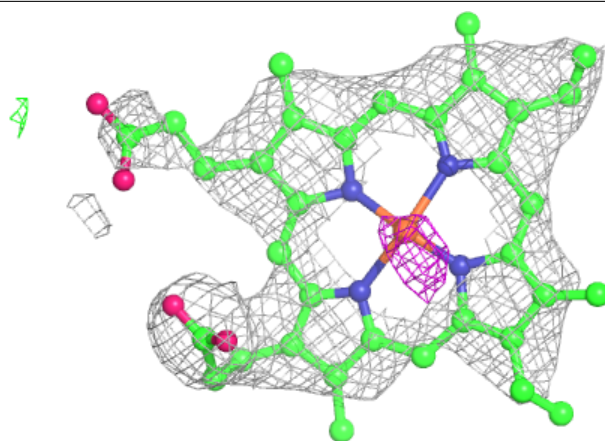
Electron density around HEM B 901:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
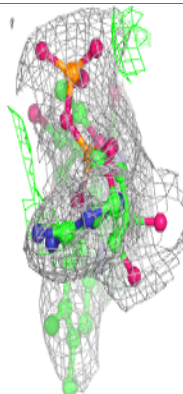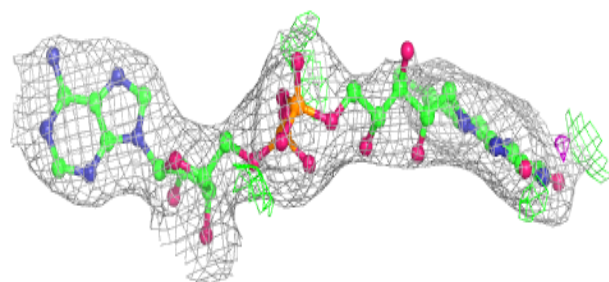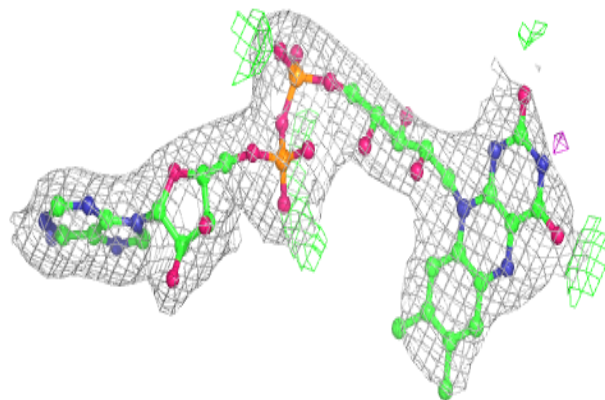mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
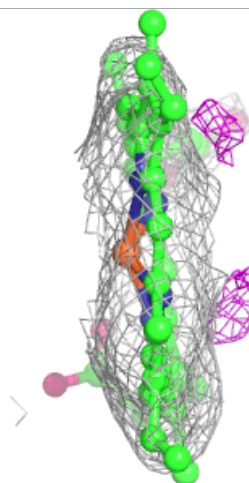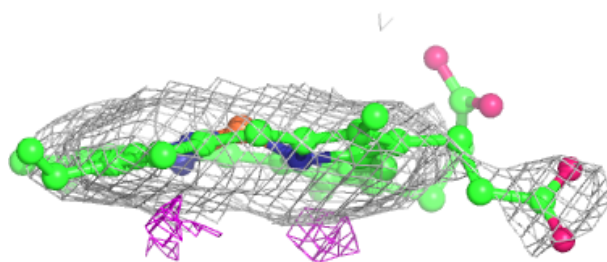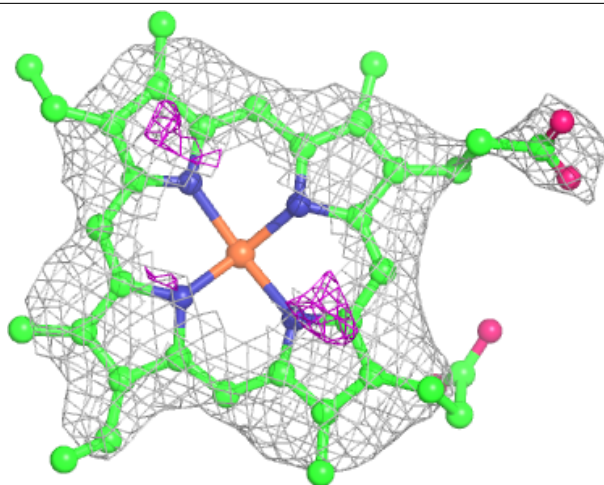
Electron density around HEM A 901:

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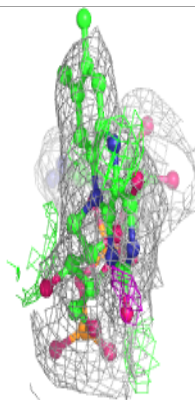mF_o-DF_c (at 3 rmsd) in purple (negative)
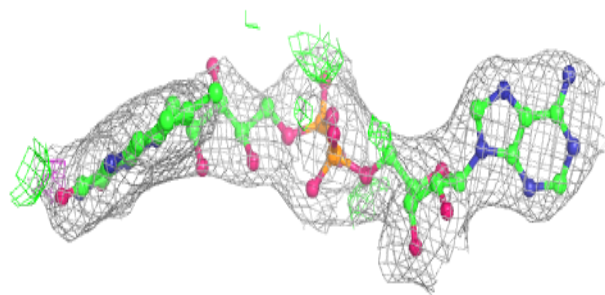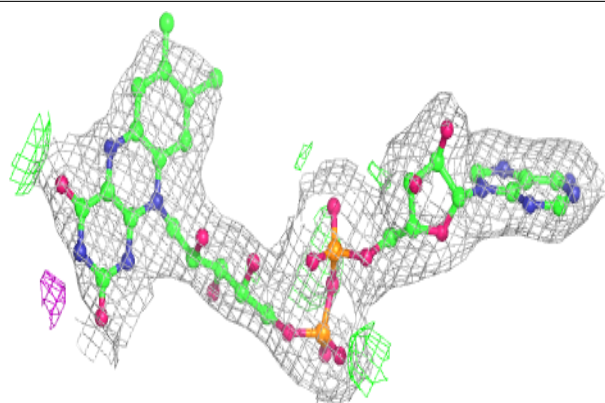and green (positive)

Electron density around FAD A 902:

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

Electron density around FAD B 902:

$2mF_o$-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 ⓘ

There are no such residues in this entry.