WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 04:27 am GMT

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PDB ID	:	1K2O
Title	:	Cytochrome P450Cam with Bound BIS(2,2'-BIPYRIDINE)-(5-METHYL-2-2'-BIPYRIDINE)-C2-ADAMANTANE RUTHENIUM (II)
Authors	:	Dunn, A.R.; Dmochowski, I.J.; Bilwes, A.M.; Gray, H.B.; Crane, B.R.
Deposited on	:	2001-09-28
Resolution	:	1.65 Å(reported)

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1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
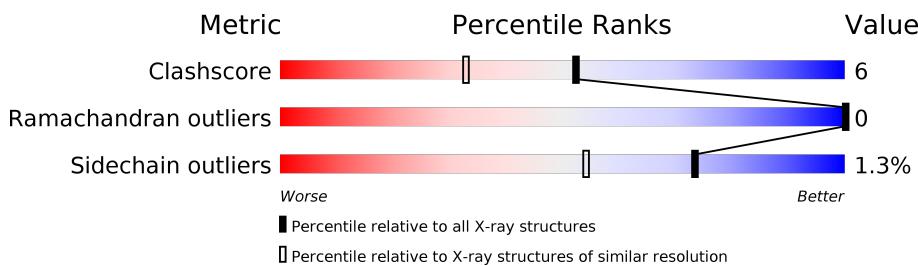
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	414	85% 12% · ·
1	B	414	84% 13% ·
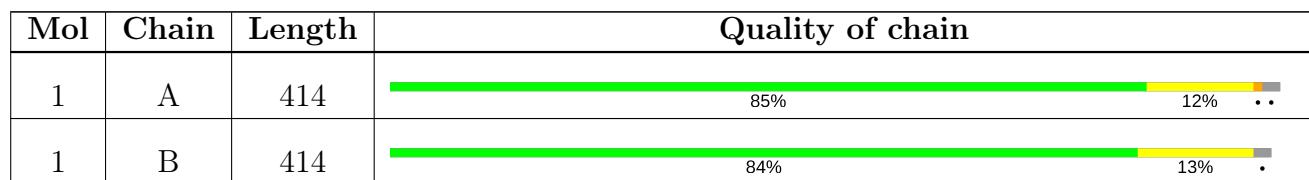
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	RFA	A	900[A]	X	-	-	-
4	RFA	B	902[A]	X	-	-	-
5	RFB	A	901[B]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	RFB	B	903[B]	X	-	-	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7649 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 Cytochrome P450CAM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	12	0
			3311	2094	579	620	18			
1	B	406	Total	C	N	O	S	0	6	0
			3258	2063	568	608	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	ALA	CYS	ENGINEERED	UNP P00183
B	334	ALA	CYS	ENGINEERED	UNP P00183

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).
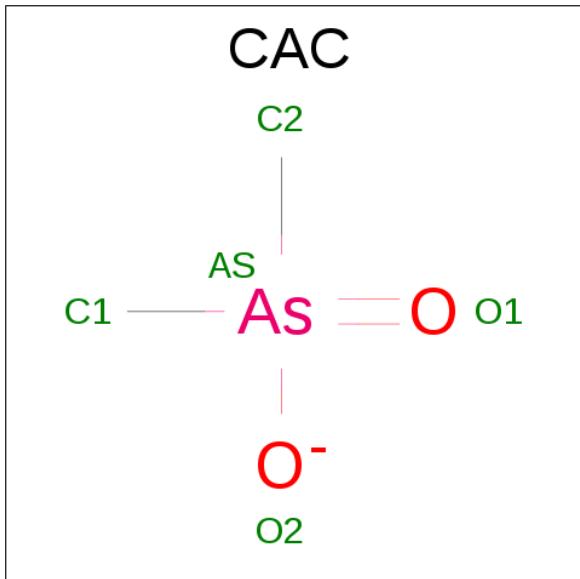
CAC

C2

AS

C1 —— As ══ O   O1

O⁻

O2

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	As	C	O	0	0
			4	1	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 4	As 1	C 2	O 1	0	0
2	B	1	Total 4	As 1	C 2	O 1	0	0
2	A	1	Total 4	As 1	C 2	O 1	0	0
2	B	1	Total 4	As 1	C 2	O 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
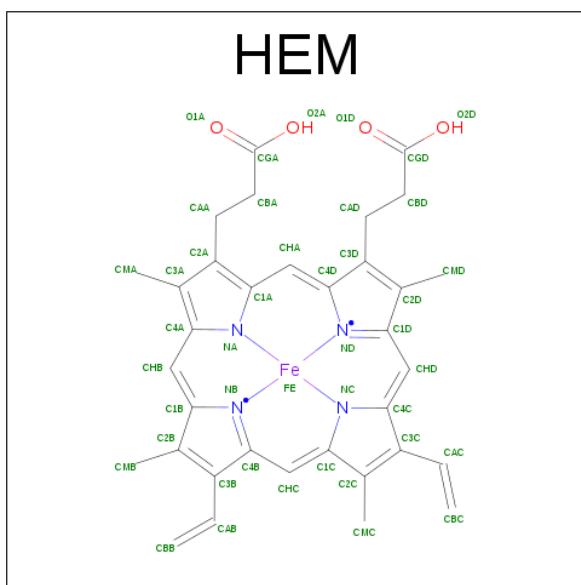
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is DELTA-BIS(2,2'-BIPYRIDINE)-(5-METHYL-2-2'-BIPYRIDINE)-C2-ADA MANTANE RUTHENIUM (II) (three-letter code: RFA) (formula: $C_{54}H_{75}F_8N_7Ru$).
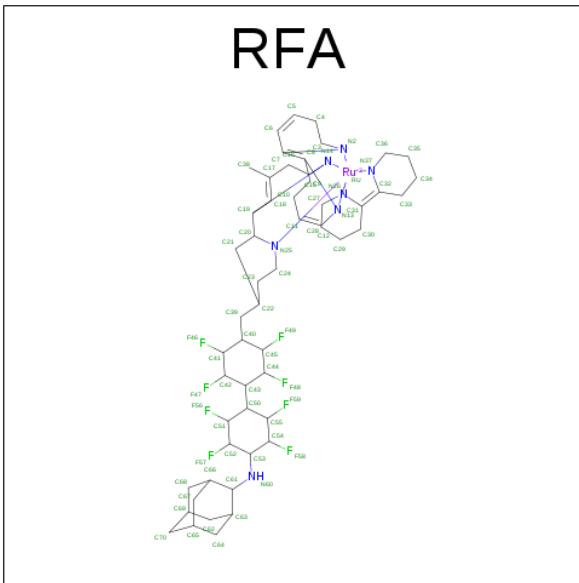
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	Ru	0	1
			70	54	8	7	1		
4	B	1	Total	C	F	N	Ru	0	1
			70	54	8	7	1		

- Molecule 5 is LAMBDA-BIS(2,2'-BIPYRIDINE)-(5-METHYL-2-2'-BIPYRIDINE)-C2-AD
  AMANTANE RUTHENIUM (II) (three-letter code: RFB) (formula: $C_{54}H_{75}F_8N_7Ru$).
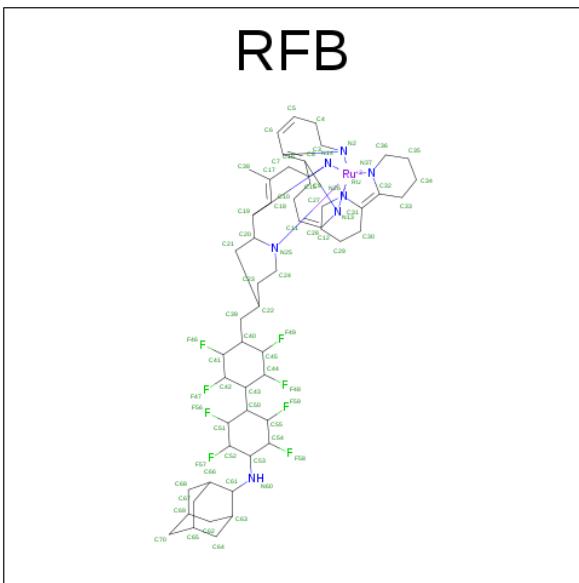
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	Ru	0	1
			70	54	8	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	F	N	Ru	0	1
			70	54	8	7	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	391	Total	O	0	0
			391	391		
6	B	303	Total	O	0	0
			303	303		

3 Residue-property plots ⓘ

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

Note EDS was not executed.

• Molecule 1: Cytochrome P450CAM

Chain A:

• Molecule 1: Cytochrome P450CAM

Chain B:
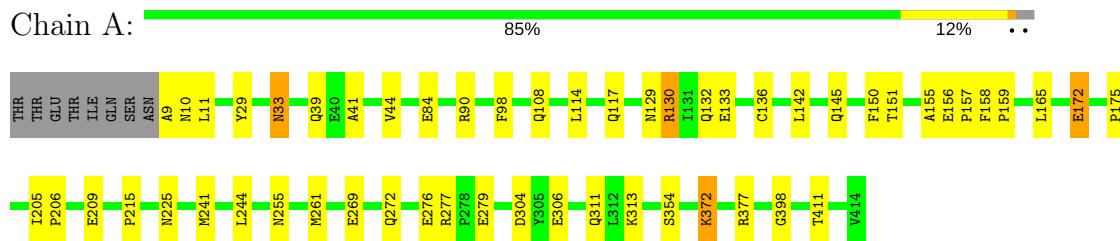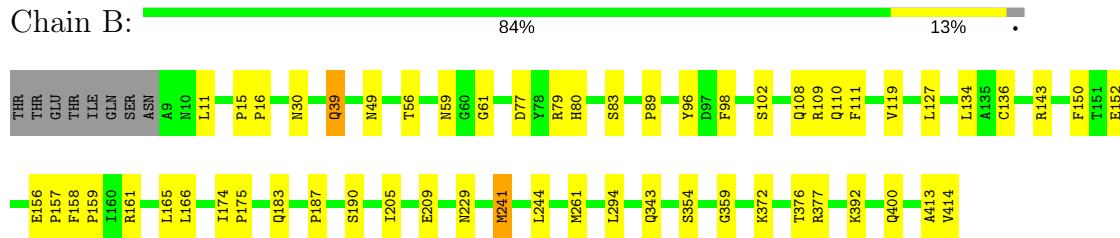
4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.87Å 67.05Å 72.52Å 71.16° 65.20° 62.31°	Depositor
Resolution (Å)	19.81 – 1.65	Depositor
% Data completeness (in resolution range)	97.8 (19.81-1.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.226	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7649	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, HEM, RFA, RFB

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	0.34	0/3390	0.60	0/4605
1	B	0.33	0/3337	0.59	2/4532 (0.0%)
All	All	0.34	0/6727	0.59	2/9137 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	109	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	B	109	ARG	NE-CZ-NH2	5.62	123.11	120.30

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	3311	0	3243	44	0
1	B	3258	0	3196	42	0
2	A	8	0	0	1	0
2	B	12	0	0	5	0
3	A	43	0	30	0	0
3	B	43	0	30	2	0
4	A	70	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	70	0	60	1	0
5	A	70	0	60	1	0
5	B	70	0	60	1	0
6	A	391	0	0	8	0
6	B	303	0	0	4	0
All	All	7649	0	6739	87	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 6.

All (87) 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:110:GLN:HE22	1:B:229:ASN:H	1.13	0.96
1:B:136[A]:CYS:HB3	2:B:504:CAC:AS	2.30	0.92
1:A:306:GLU:HG3	1:A:311:GLN:HE22	1.38	0.89
1:A:306:GLU:CG	1:A:311:GLN:HE22	1.93	0.81
1:A:306:GLU:HG3	1:A:311:GLN:NE2	1.96	0.79
1:A:151[A]:THR:HG22	6:A:1278:HOH:O	1.85	0.76
1:A:132:GLN:NE2	1:A:136:CYS:SG	2.61	0.73
1:A:306:GLU:CD	1:A:311:GLN:HE22	1.94	0.71
1:A:11:LEU:HD23	2:A:503:CAC:C1	2.21	0.70
1:B:158:PHE:HB3	1:B:159:PRO:HD3	1.75	0.69
1:B:136[A]:CYS:CB	2:B:504:CAC:AS	2.98	0.68
1:A:130:ARG:HG2	1:A:130:ARG:HH21	1.59	0.66
1:B:376:THR:CG2	1:B:414:VAL:HG21	2.29	0.63
1:A:241[A]:MET:HG3	6:A:1562:HOH:O	1.99	0.62
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.80	0.62
1:B:110:GLN:NE2	1:B:229:ASN:H	1.91	0.60
1:B:108:GLN:HE22	1:B:354:SER:HB2	1.67	0.60
1:A:255[A]:ASN:OD1	1:A:398:GLY:HA3	2.02	0.59
1:A:313:LYS:HE3	6:A:1617:HOH:O	2.03	0.59
1:B:11:LEU:HD23	2:B:502:CAC:C2	2.33	0.59
1:A:304:ASP:OD1	1:A:313:LYS:HD2	2.04	0.58
1:B:343[A]:GLN:OE1	1:B:343[A]:GLN:HA	2.02	0.58
1:B:119:VAL:HG12	1:B:166:LEU:HD21	1.85	0.58
1:B:136[B]:CYS:SG	1:B:377:ARG:NH2	2.77	0.58
1:A:29:TYR:CD2	5:A:901[B]:RFB:H61	2.40	0.57
1:B:127[A]:LEU:HD11	1:B:165:LEU:HG	1.85	0.57
1:A:84:GLU:CD	1:A:90:ARG:HH12	2.08	0.56
3:B:417:HEM:HHD	3:B:417:HEM:HBC2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.71	0.55
1:A:9:ALA:O	1:A:10:ASN:HB2	2.06	0.55
1:B:134:LEU:HD21	1:B:161:ARG:HB2	1.89	0.55
1:B:136[A]:CYS:HB2	2:B:504:CAC:C2	2.37	0.55
1:A:277:ARG:HD3	1:A:279:GLU:OE1	2.07	0.54
1:B:372:LYS:HD3	6:B:1359:HOH:O	2.07	0.54
1:A:306:GLU:HG2	6:A:1466:HOH:O	2.06	0.54
1:B:376:THR:HG22	1:B:414:VAL:HG21	1.89	0.54
1:B:96:TYR:HB3	2:B:500:CAC:C1	2.39	0.53
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.91	0.53
1:A:130:ARG:NH2	1:A:130:ARG:HG2	2.22	0.53
1:A:44[A]:VAL:HG11	6:A:1503:HOH:O	2.09	0.53
1:A:175:PRO:HG3	1:B:79:ARG:HH11	1.74	0.52
1:A:269[B]:GLU:HG2	6:A:1424:HOH:O	2.10	0.52
1:B:156:GLU:HB2	1:B:157:PRO:HD3	1.91	0.52
1:A:130:ARG:NH2	1:A:165:LEU:HD11	2.26	0.51
1:B:111:PHE:HD2	1:B:241[B]:MET:SD	2.34	0.50
1:B:134:LEU:HD11	1:B:161:ARG:HD2	1.92	0.50
1:B:205:ILE:O	1:B:209[B]:GLU:HG2	2.12	0.50
1:A:41:ALA:O	1:A:44[A]:VAL:HG22	2.11	0.49
1:A:172:GLU:CD	1:A:172:GLU:H	2.17	0.48
1:B:187:PRO:HG3	4:B:902[A]:RFA:H211	1.95	0.48
1:A:129:ASN:O	1:A:133:GLU:HG3	2.13	0.48
1:A:205:ILE:O	1:A:209:GLU:HG2	2.13	0.48
1:A:372:LYS:HB2	1:A:372:LYS:HE3	1.66	0.48
1:B:77:ASP:OD2	1:B:80:HIS:HB2	2.14	0.48
1:B:98:PHE:HB3	1:B:244:LEU:HB2	1.96	0.47
1:A:311:GLN:NE2	1:A:311:GLN:HA	2.31	0.46
1:A:215:PRO:HB3	1:A:225:ASN:OD1	2.15	0.45
1:B:187:PRO:HG3	5:B:903[B]:RFB:H211	1.98	0.45
1:B:56:THR:O	1:B:61:GLY:HA2	2.17	0.44
1:B:392:LYS:HD3	1:B:400:GLN:OE1	2.17	0.44
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.52	0.44
1:B:59:ASN:HB3	1:B:89:PRO:HD3	1.99	0.44
1:A:142:LEU:HA	1:A:145:GLN:NE2	2.33	0.44
1:A:151[A]:THR:HA	1:A:155:ALA:HB3	2.00	0.44
1:B:294:LEU:H	1:B:294:LEU:HD23	1.83	0.43
1:A:151[B]:THR:HA	1:A:155:ALA:HB3	2.01	0.43
1:A:205:ILE:HB	1:A:206:PRO:HD3	2.01	0.42
1:B:39:GLN:NE2	1:B:39:GLN:H	2.16	0.42
1:A:151[B]:THR:HG21	6:A:1594:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:NH2	1:B:413:ALA:HB2	2.35	0.42
1:B:241[A]:MET:HG3	6:B:1203:HOH:O	2.20	0.42
1:A:272[B]:GLN:HE21	1:A:276[B]:GLU:CD	2.23	0.42
1:B:83[A]:SER:O	1:B:102:SER:HA	2.20	0.41
1:B:152:GLU:HG2	6:B:1396:HOH:O	2.20	0.41
1:B:134:LEU:HD11	1:B:161:ARG:CD	2.49	0.41
1:B:183:GLN:OE1	1:B:190:SER:HB2	2.20	0.41
1:B:15:PRO:HA	1:B:16:PRO:HD3	1.86	0.41
4:A:900[A]:RFA:H383	6:B:1597:HOH:O	2.20	0.41
1:B:174:ILE:HB	1:B:175:PRO:HD3	2.03	0.41
1:A:130:ARG:HD3	6:A:1273:HOH:O	2.21	0.41
1:A:33[A]:ASN:O	1:A:33[A]:ASN:CG	2.58	0.41
1:B:150:PHE:CZ	1:B:261:MET:HG3	2.55	0.40
1:B:359:GLY:HA3	3:B:417:HEM:C3C	2.56	0.40
1:A:156:GLU:HB2	1:A:157:PRO:HD3	2.04	0.40
1:B:83[B]:SER:O	1:B:102:SER:HA	2.20	0.40
1:A:114:LEU:O	1:A:117:GLN:HB2	2.21	0.40
1:A:377:ARG:O	1:A:411:THR:HB	2.22	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	416/414 (100%)	398 (96%)	18 (4%)	0	100	100
1	B	410/414 (99%)	396 (97%)	14 (3%)	0	100	100
All	All	826/828 (100%)	794 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/357 (101%)	355 (98%)	6 (2%)	66	43
1	B	355/357 (99%)	350 (99%)	5 (1%)	71	50
All	All	716/714 (100%)	705 (98%)	11 (2%)	73	48

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33[A]	ASN
1	A	33[B]	ASN
1	A	39	GLN
1	A	130	ARG
1	A	172	GLU
1	A	372	LYS
1	B	30	ASN
1	B	39	GLN
1	B	49	ASN
1	B	241[A]	MET
1	B	241[B]	MET

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

Mol	Chain	Res	Type
1	A	39	GLN
1	A	46	GLN
1	A	69	GLN
1	A	108	GLN
1	A	132	GLN
1	A	149	ASN
1	A	210	GLN
1	A	229	ASN
1	A	311	GLN
1	B	17	HIS
1	B	30	ASN

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Mol	Chain	Res	Type
1	B	33	ASN
1	B	39	GLN
1	B	46	GLN
1	B	108	GLN
1	B	110	GLN
1	B	117	GLN
1	B	210	GLN
1	B	227	GLN
1	B	311	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

11 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	HEM	A	417	1,6	28,50,50	1.35	3 (10%)	17,82,82	1.58	3 (17%)
2	CAC	A	501	1	0,3,4	0.00	-	0,3,6	0.00	-
2	CAC	A	503	1	0,3,4	0.00	-	0,3,6	0.00	-
4	RFA	A	900[A]	-	68,83,83	4.97	45 (66%)	62,137,137	5.87	40 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	RFB	A	901[B]	-	68,83,83	4.94	45 (66%)	62,137,137	6.02	43 (69%)
3	HEM	B	417	1,6	28,50,50	1.53	4 (14%)	17,82,82	1.63	5 (29%)
2	CAC	B	500	1	0,3,4	0.00	-	0,3,6	0.00	-
2	CAC	B	502	1	0,3,4	0.00	-	0,3,6	0.00	-
2	CAC	B	504	-	0,3,4	0.00	-	0,3,6	0.00	-
4	RFA	B	902[A]	-	68,83,83	5.01	45 (66%)	62,137,137	6.00	42 (67%)
5	RFB	B	903[B]	-	68,83,83	4.87	44 (64%)	62,137,137	6.03	44 (70%)

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	HEM	A	417	1,6	-	0/6/54/54	0/0/8/8
2	CAC	A	501	1	-	0/0/0/0	0/0/0/0
2	CAC	A	503	1	-	0/0/0/0	0/0/0/0
4	RFA	A	900[A]	-	11/11/32/38	0/12/230/230	0/11/14/14
5	RFB	A	901[B]	-	11/11/32/38	0/12/230/230	0/11/14/14
3	HEM	B	417	1,6	-	0/6/54/54	0/0/8/8
2	CAC	B	500	1	-	0/0/0/0	0/0/0/0
2	CAC	B	502	1	-	0/0/0/0	0/0/0/0
2	CAC	B	504	-	-	0/0/0/0	0/0/0/0
4	RFA	B	902[A]	-	11/11/32/38	0/12/230/230	0/11/14/14
5	RFB	B	903[B]	-	11/11/32/38	0/12/230/230	0/11/14/14

All (186) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901[B]	RFB	C36-N37	-11.28	1.35	1.46
5	B	903[B]	RFB	C27-N26	-11.17	1.35	1.46
4	B	902[A]	RFA	C55-C54	-11.12	1.38	1.52
5	B	903[B]	RFB	C3-N2	-11.12	1.35	1.46
5	A	901[B]	RFB	C3-N2	-11.09	1.35	1.46
4	B	902[A]	RFA	C27-N26	-10.99	1.36	1.46
4	A	900[A]	RFA	C36-N37	-10.98	1.36	1.46
5	A	901[B]	RFB	C27-N26	-10.91	1.36	1.46
4	B	902[A]	RFA	C3-N2	-10.84	1.36	1.46
5	B	903[B]	RFB	C36-N37	-10.80	1.36	1.46
4	A	900[A]	RFA	C3-N2	-10.78	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902[A]	RFA	C36-N37	-10.77	1.36	1.46
5	A	901[B]	RFB	C52-C51	-10.67	1.39	1.52
4	A	900[A]	RFA	C52-C51	-10.56	1.39	1.52
4	A	900[A]	RFA	C27-N26	-10.56	1.36	1.46
4	B	902[A]	RFA	C45-C44	-10.40	1.39	1.52
5	A	901[B]	RFB	C42-C41	-10.25	1.39	1.52
4	B	902[A]	RFA	C42-C41	-10.18	1.39	1.52
4	A	900[A]	RFA	C45-C44	-10.15	1.40	1.52
4	A	900[A]	RFA	C42-C41	-10.10	1.40	1.52
5	B	903[B]	RFB	C52-C51	-9.90	1.40	1.52
5	A	901[B]	RFB	C45-C44	-9.76	1.40	1.52
5	B	903[B]	RFB	C42-C41	-9.67	1.40	1.52
4	A	900[A]	RFA	C55-C54	-9.39	1.40	1.52
5	B	903[B]	RFB	C45-C44	-9.37	1.40	1.52
4	A	900[A]	RFA	C15-N14	-9.34	1.35	1.48
4	B	902[A]	RFA	C15-N14	-9.02	1.35	1.48
5	B	903[B]	RFB	C55-C54	-8.94	1.41	1.52
4	B	902[A]	RFA	C21-C20	-8.77	1.39	1.53
5	A	901[B]	RFB	C55-C54	-8.72	1.41	1.52
4	B	902[A]	RFA	C52-C51	-8.67	1.41	1.52
5	B	903[B]	RFB	C24-N25	-8.55	1.36	1.48
5	A	901[B]	RFB	C24-N25	-8.34	1.36	1.48
4	A	900[A]	RFA	C21-C20	-8.27	1.40	1.53
5	A	901[B]	RFB	C15-N14	-8.09	1.36	1.48
4	A	900[A]	RFA	C24-N25	-7.93	1.37	1.48
4	B	902[A]	RFA	C24-N25	-7.93	1.37	1.48
5	B	903[B]	RFB	C15-N14	-7.62	1.37	1.48
5	A	901[B]	RFB	C21-C20	-7.38	1.41	1.53
5	B	903[B]	RFB	C21-C20	-7.26	1.41	1.53
5	A	901[B]	RFB	C24-C23	-6.67	1.37	1.52
5	B	903[B]	RFB	C24-C23	-6.66	1.37	1.52
4	B	902[A]	RFA	C21-C22	-6.65	1.36	1.52
4	B	902[A]	RFA	C50-C43	-6.65	1.39	1.54
5	A	901[B]	RFB	C33-C32	-6.32	1.39	1.49
4	B	902[A]	RFA	C3-C4	-6.23	1.38	1.51
4	A	900[A]	RFA	C3-C4	-6.22	1.38	1.51
5	B	903[B]	RFB	C3-C4	-6.21	1.38	1.51
4	A	900[A]	RFA	C21-C22	-6.16	1.37	1.52
5	B	903[B]	RFB	C33-C32	-6.14	1.40	1.49
4	A	900[A]	RFA	C53-N60	-6.05	1.36	1.47
5	A	901[B]	RFB	C3-C4	-6.04	1.39	1.51
4	A	900[A]	RFA	C50-C43	-6.02	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901[B]	RFB	C50-C43	-5.96	1.40	1.54
4	B	902[A]	RFA	C9-C8	-5.95	1.40	1.49
4	A	900[A]	RFA	C9-C8	-5.92	1.40	1.49
4	B	902[A]	RFA	C53-N60	-5.87	1.37	1.47
5	A	901[B]	RFB	C21-C22	-5.85	1.38	1.52
5	B	903[B]	RFB	C9-C8	-5.83	1.40	1.49
4	B	902[A]	RFA	C30-C31	-5.82	1.40	1.49
5	B	903[B]	RFB	C21-C22	-5.81	1.38	1.52
5	B	903[B]	RFB	C30-C31	-5.79	1.40	1.49
4	A	900[A]	RFA	C33-C32	-5.77	1.40	1.49
5	B	903[B]	RFB	C53-N60	-5.76	1.37	1.47
4	A	900[A]	RFA	C24-C23	-5.76	1.39	1.52
4	B	902[A]	RFA	C33-C32	-5.73	1.40	1.49
5	A	901[B]	RFB	C39-C40	-5.71	1.47	1.54
4	A	900[A]	RFA	C30-C31	-5.67	1.41	1.49
5	A	901[B]	RFB	C30-C31	-5.65	1.41	1.49
5	A	901[B]	RFB	C9-C8	-5.56	1.41	1.49
4	B	902[A]	RFA	C24-C23	-5.45	1.40	1.52
5	A	901[B]	RFB	C53-N60	-5.43	1.37	1.47
5	A	901[B]	RFB	C9-C10	-5.41	1.37	1.52
5	B	903[B]	RFB	C50-C43	-5.29	1.42	1.54
4	A	900[A]	RFA	C15-C16	-5.24	1.37	1.51
5	B	903[B]	RFB	C9-C10	-5.22	1.37	1.52
4	B	902[A]	RFA	C9-C10	-5.22	1.37	1.52
4	A	900[A]	RFA	C9-C10	-5.21	1.37	1.52
4	B	902[A]	RFA	C15-C16	-5.11	1.37	1.51
5	B	903[B]	RFB	C23-C22	-4.92	1.38	1.52
5	B	903[B]	RFB	C39-C40	-4.92	1.48	1.54
5	A	901[B]	RFB	C23-C22	-4.83	1.38	1.52
4	B	902[A]	RFA	C19-C20	-4.81	1.47	1.54
4	B	902[A]	RFA	C39-C40	-4.61	1.48	1.54
4	B	902[A]	RFA	C23-C22	-4.56	1.39	1.52
4	A	900[A]	RFA	C23-C22	-4.55	1.39	1.52
5	A	901[B]	RFB	C34-C33	-4.44	1.37	1.52
4	B	902[A]	RFA	C29-C30	-4.41	1.37	1.52
5	B	903[B]	RFB	C34-C33	-4.39	1.37	1.52
4	A	900[A]	RFA	C29-C30	-4.38	1.37	1.52
4	A	900[A]	RFA	C34-C33	-4.33	1.37	1.52
5	A	901[B]	RFB	C15-C16	-4.28	1.40	1.51
4	B	902[A]	RFA	C34-C33	-4.25	1.38	1.52
5	A	901[B]	RFB	C29-C30	-4.16	1.38	1.52
3	B	417	HEM	C3C-C2C	-4.14	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	903[B]	RFB	C29-C30	-4.13	1.38	1.52
5	B	903[B]	RFB	C15-C16	-4.04	1.40	1.51
4	A	900[A]	RFA	C39-C40	-4.00	1.49	1.54
4	A	900[A]	RFA	C19-C20	-3.88	1.48	1.54
3	B	417	HEM	C3B-CAB	-3.80	1.40	1.47
3	B	417	HEM	C3C-CAC	-3.65	1.40	1.47
5	B	903[B]	RFB	C19-C20	-3.64	1.49	1.54
5	B	903[B]	RFB	C28-C27	-3.58	1.38	1.51
3	A	417	HEM	C3B-CAB	-3.55	1.40	1.47
5	A	901[B]	RFB	C28-C27	-3.52	1.38	1.51
3	A	417	HEM	C3C-CAC	-3.51	1.40	1.47
4	B	902[A]	RFA	C16-C17	-3.44	1.39	1.49
5	A	901[B]	RFB	C19-C20	-3.44	1.49	1.54
4	A	900[A]	RFA	C16-C17	-3.42	1.39	1.49
3	A	417	HEM	C3C-C2C	-3.42	1.35	1.40
4	B	902[A]	RFA	C28-C27	-3.28	1.39	1.51
4	A	900[A]	RFA	C35-C36	-3.25	1.39	1.51
4	B	902[A]	RFA	C35-C36	-3.24	1.39	1.51
5	B	903[B]	RFB	C16-C17	-3.21	1.39	1.49
5	A	901[B]	RFB	C35-C36	-3.17	1.39	1.51
4	A	900[A]	RFA	C28-C27	-3.17	1.39	1.51
5	A	901[B]	RFB	C16-C17	-3.15	1.39	1.49
5	A	901[B]	RFB	C29-C28	-3.15	1.38	1.51
5	B	903[B]	RFB	C29-C28	-3.14	1.38	1.51
5	B	903[B]	RFB	C35-C36	-3.11	1.39	1.51
4	A	900[A]	RFA	RU-N14	-3.09	2.01	2.12
4	B	902[A]	RFA	C29-C28	-3.08	1.39	1.51
4	B	902[A]	RFA	C35-C34	-3.04	1.39	1.51
4	A	900[A]	RFA	C29-C28	-3.04	1.39	1.51
4	A	900[A]	RFA	C35-C34	-3.03	1.39	1.51
5	B	903[B]	RFB	C35-C34	-2.96	1.39	1.51
5	A	901[B]	RFB	C35-C34	-2.92	1.39	1.51
4	A	900[A]	RFA	C4-C5	-2.80	1.39	1.48
5	A	901[B]	RFB	C4-C5	-2.79	1.39	1.48
5	B	903[B]	RFB	C4-C5	-2.77	1.39	1.48
4	B	902[A]	RFA	C4-C5	-2.76	1.39	1.48
5	B	903[B]	RFB	C10-C11	-2.73	1.39	1.48
4	A	900[A]	RFA	C10-C11	-2.71	1.39	1.48
4	B	902[A]	RFA	C10-C11	-2.68	1.39	1.48
5	A	901[B]	RFB	C10-C11	-2.67	1.39	1.48
4	B	902[A]	RFA	RU-N14	-2.60	2.02	2.12
3	B	417	HEM	C3B-C2B	-2.44	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901[B]	RFB	RU-N25	-2.26	2.04	2.12
4	B	902[A]	RFA	C39-C22	-2.17	1.49	1.53
4	A	900[A]	RFA	RU-N25	-2.09	2.04	2.12
5	B	903[B]	RFB	RU-N25	-2.07	2.04	2.12
5	A	901[B]	RFB	RU-N14	-2.06	2.04	2.12
5	A	901[B]	RFB	C70-C69	2.01	1.57	1.52
4	B	902[A]	RFA	C70-C69	2.03	1.57	1.52
5	A	901[B]	RFB	C68-C69	2.06	1.57	1.52
4	A	900[A]	RFA	C67-C66	2.09	1.58	1.53
4	A	900[A]	RFA	C62-C63	2.10	1.58	1.53
5	B	903[B]	RFB	C68-C69	2.16	1.58	1.52
5	B	903[B]	RFB	C62-C69	2.17	1.58	1.52
4	A	900[A]	RFA	C68-C69	2.17	1.58	1.52
5	B	903[B]	RFB	C62-C63	2.18	1.58	1.53
5	B	903[B]	RFB	C67-C66	2.18	1.58	1.53
4	A	900[A]	RFA	C68-C66	2.21	1.58	1.53
4	A	900[A]	RFA	C62-C69	2.26	1.58	1.52
5	A	901[B]	RFB	C62-C69	2.28	1.58	1.52
5	B	903[B]	RFB	C68-C66	2.29	1.58	1.53
4	B	902[A]	RFA	C67-C65	2.30	1.58	1.52
5	A	901[B]	RFB	C62-C63	2.30	1.58	1.53
5	A	901[B]	RFB	C18-C17	2.32	1.37	1.32
5	A	901[B]	RFB	C68-C66	2.36	1.58	1.53
5	B	903[B]	RFB	C18-C17	2.53	1.37	1.32
4	B	902[A]	RFA	C68-C69	2.59	1.59	1.52
4	B	902[A]	RFA	C62-C69	2.63	1.59	1.52
4	A	900[A]	RFA	C18-C17	2.78	1.37	1.32
4	B	902[A]	RFA	C18-C17	2.79	1.37	1.32
4	B	902[A]	RFA	C12-C11	2.80	1.38	1.33
4	A	900[A]	RFA	C12-C11	2.84	1.38	1.33
4	B	902[A]	RFA	C62-C63	2.97	1.60	1.53
5	B	903[B]	RFB	C12-C11	3.19	1.39	1.33
4	B	902[A]	RFA	C63-C61	3.31	1.58	1.53
5	A	901[B]	RFB	C12-C11	3.35	1.39	1.33
4	B	902[A]	RFA	C66-C61	3.48	1.58	1.53
4	A	900[A]	RFA	C66-C61	3.82	1.58	1.53
4	A	900[A]	RFA	C32-C31	3.85	1.47	1.36
5	B	903[B]	RFB	C66-C61	3.97	1.59	1.53
4	B	902[A]	RFA	C32-C31	3.97	1.48	1.36
5	B	903[B]	RFB	C32-C31	4.14	1.48	1.36
5	A	901[B]	RFB	C32-C31	4.17	1.48	1.36
5	A	901[B]	RFB	C66-C61	4.88	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901[B]	RFB	C63-C61	4.88	1.60	1.53
4	A	900[A]	RFA	C63-C61	5.25	1.60	1.53
5	B	903[B]	RFB	C63-C61	5.60	1.61	1.53
5	A	901[B]	RFB	C7-C8	7.42	1.47	1.37
5	B	903[B]	RFB	C7-C8	7.78	1.48	1.37
4	A	900[A]	RFA	C7-C8	8.05	1.48	1.37
4	B	902[A]	RFA	C7-C8	8.06	1.48	1.37

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	903[B]	RFB	C16-C17-C18	-6.92	115.74	121.57
5	A	901[B]	RFB	C16-C17-C18	-6.62	116.00	121.57
5	A	901[B]	RFB	C38-C17-C18	-4.34	116.33	122.43
5	B	903[B]	RFB	C38-C17-C18	-4.12	116.64	122.43
5	B	903[B]	RFB	C36-N37-C32	-3.90	119.53	124.79
5	B	903[B]	RFB	C6-C7-N2	-3.86	118.58	124.43
5	A	901[B]	RFB	C6-C7-N2	-3.68	118.85	124.43
5	A	901[B]	RFB	C36-N37-C32	-3.67	119.83	124.79
4	A	900[A]	RFA	C27-N26-C31	-3.62	119.91	124.79
4	A	900[A]	RFA	C36-N37-C32	-3.55	120.00	124.79
4	B	902[A]	RFA	C36-N37-C32	-3.53	120.02	124.79
4	B	902[A]	RFA	C6-C7-N2	-3.40	119.27	124.43
4	A	900[A]	RFA	C6-C7-N2	-3.32	119.40	124.43
4	B	902[A]	RFA	C27-N26-C31	-3.16	120.52	124.79
3	B	417	HEM	CMA-C3A-C4A	-3.13	123.65	128.46
3	A	417	HEM	CMA-C3A-C4A	-3.05	123.78	128.46
3	B	417	HEM	CMD-C2D-C1D	-2.86	124.06	128.46
3	A	417	HEM	CMD-C2D-C1D	-2.67	124.36	128.46
5	B	903[B]	RFB	C27-N26-C31	-2.62	121.25	124.79
5	A	901[B]	RFB	C27-N26-C31	-2.60	121.27	124.79
4	B	902[A]	RFA	C16-C17-C18	-2.24	119.68	121.57
3	B	417	HEM	CMD-C2D-C3D	2.10	128.90	124.94
5	B	903[B]	RFB	C63-C61-N60	2.24	115.48	112.10
3	B	417	HEM	C4A-C3A-C2A	2.25	108.56	107.00
3	B	417	HEM	CMB-C2B-C3B	2.46	129.46	124.89
3	A	417	HEM	CMB-C2B-C3B	2.51	129.54	124.89
5	A	901[B]	RFB	C29-C28-C27	2.97	117.13	111.21
4	B	902[A]	RFA	C21-C20-C19	3.03	124.02	117.23
5	B	903[B]	RFB	C29-C28-C27	3.03	117.24	111.21
4	A	900[A]	RFA	C16-C15-N14	3.05	122.47	111.94
4	B	902[A]	RFA	C16-C15-N14	3.12	122.69	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	902[A]	RFA	C29-C28-C27	3.23	117.65	111.21
4	A	900[A]	RFA	C29-C28-C27	3.26	117.70	111.21
4	A	900[A]	RFA	C21-C20-C19	3.34	124.73	117.23
5	A	901[B]	RFB	C34-C33-C32	3.43	118.75	110.67
4	B	902[A]	RFA	C66-C61-N60	3.46	117.32	112.10
5	B	903[B]	RFB	C34-C33-C32	3.47	118.84	110.67
5	A	901[B]	RFB	C19-C20-N25	3.53	114.34	109.07
5	A	901[B]	RFB	C39-C40-C41	3.57	118.12	112.72
4	B	902[A]	RFA	C39-C22-C21	3.59	120.04	111.73
5	B	903[B]	RFB	C39-C40-C41	3.60	118.16	112.72
4	A	900[A]	RFA	C34-C33-C32	3.69	119.36	110.67
4	B	902[A]	RFA	C34-C33-C32	3.70	119.39	110.67
5	B	903[B]	RFB	C19-C20-N25	3.71	114.61	109.07
5	A	901[B]	RFB	C39-C22-C21	3.81	120.54	111.73
4	A	900[A]	RFA	C39-C22-C21	3.85	120.64	111.73
5	B	903[B]	RFB	C29-C30-C31	3.86	119.76	110.67
4	B	902[A]	RFA	C29-C30-C31	3.86	119.76	110.67
5	B	903[B]	RFB	C39-C22-C21	3.86	120.67	111.73
5	A	901[B]	RFB	C29-C30-C31	3.88	119.82	110.67
4	A	900[A]	RFA	C29-C30-C31	3.94	119.96	110.67
4	A	900[A]	RFA	C39-C22-C23	4.00	120.96	111.70
4	B	902[A]	RFA	C34-C35-C36	4.02	119.22	111.21
5	A	901[B]	RFB	C16-C15-N14	4.05	125.93	111.94
4	A	900[A]	RFA	C34-C35-C36	4.07	119.31	111.21
4	A	900[A]	RFA	C19-C20-N25	4.10	115.19	109.07
5	B	903[B]	RFB	C16-C15-N14	4.15	126.26	111.94
5	A	901[B]	RFB	C39-C22-C23	4.19	121.41	111.70
5	B	903[B]	RFB	C39-C22-C23	4.23	121.50	111.70
4	B	902[A]	RFA	C39-C22-C23	4.24	121.52	111.70
5	A	901[B]	RFB	C34-C35-C36	4.25	119.68	111.21
5	B	903[B]	RFB	C34-C35-C36	4.27	119.72	111.21
4	B	902[A]	RFA	C23-C24-N25	4.38	120.15	113.00
4	B	902[A]	RFA	C39-C40-C41	4.49	119.51	112.72
4	B	902[A]	RFA	C19-C20-N25	4.50	115.79	109.07
4	A	900[A]	RFA	C23-C24-N25	4.53	120.38	113.00
4	B	902[A]	RFA	C39-C40-C45	4.65	119.74	112.72
4	A	900[A]	RFA	C39-C40-C45	4.66	119.76	112.72
5	B	903[B]	RFB	C21-C22-C23	4.66	117.82	109.12
5	A	901[B]	RFB	C24-C23-C22	4.73	119.66	110.24
4	A	900[A]	RFA	C39-C40-C41	4.75	119.89	112.72
5	A	901[B]	RFB	C21-C22-C23	4.78	118.05	109.12
4	B	902[A]	RFA	C24-C23-C22	4.88	119.94	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	900[A]	RFA	C24-C23-C22	4.89	119.97	110.24
5	B	903[B]	RFB	C24-C23-C22	4.93	120.06	110.24
4	A	900[A]	RFA	C21-C22-C23	4.97	118.40	109.12
4	B	902[A]	RFA	C21-C22-C23	4.99	118.43	109.12
5	B	903[B]	RFB	C21-C20-C19	5.02	128.49	117.23
5	A	901[B]	RFB	C21-C20-C19	5.15	128.78	117.23
4	B	902[A]	RFA	C55-C54-C53	5.23	118.96	112.09
5	A	901[B]	RFB	C23-C24-N25	5.32	121.67	113.00
5	B	903[B]	RFB	C23-C24-N25	5.39	121.78	113.00
4	B	902[A]	RFA	C51-C52-C53	5.80	119.70	112.09
5	B	903[B]	RFB	C39-C40-C45	5.85	121.56	112.72
5	A	901[B]	RFB	C39-C40-C45	5.91	121.65	112.72
5	B	903[B]	RFB	C38-C17-C16	5.96	127.61	116.35
5	A	901[B]	RFB	C38-C17-C16	5.99	127.68	116.35
5	A	901[B]	RFB	C55-C54-C53	6.02	120.00	112.09
5	B	903[B]	RFB	C55-C54-C53	6.16	120.17	112.09
4	A	900[A]	RFA	C55-C54-C53	6.22	120.25	112.09
5	B	903[B]	RFB	F46-C41-C40	6.66	119.21	109.99
4	B	902[A]	RFA	F46-C41-C40	6.70	119.25	109.99
5	B	903[B]	RFB	F49-C45-C40	6.72	119.28	109.99
4	A	900[A]	RFA	C51-C52-C53	6.87	121.11	112.09
4	B	902[A]	RFA	C4-C3-N2	6.88	121.53	111.19
4	A	900[A]	RFA	C4-C3-N2	6.94	121.62	111.19
5	B	903[B]	RFB	C51-C52-C53	7.02	121.30	112.09
5	A	901[B]	RFB	F56-C51-C52	7.05	117.38	108.56
5	A	901[B]	RFB	F46-C41-C40	7.06	119.75	109.99
4	A	900[A]	RFA	F46-C41-C40	7.09	119.80	109.99
4	A	900[A]	RFA	F56-C51-C52	7.11	117.46	108.56
4	B	902[A]	RFA	F49-C45-C40	7.13	119.85	109.99
5	B	903[B]	RFB	C4-C3-N2	7.20	122.02	111.19
4	A	900[A]	RFA	F49-C45-C40	7.22	119.97	109.99
5	A	901[B]	RFB	F49-C45-C40	7.27	120.04	109.99
5	A	901[B]	RFB	C51-C52-C53	7.27	121.63	112.09
5	A	901[B]	RFB	C4-C3-N2	7.34	122.22	111.19
5	B	903[B]	RFB	F56-C51-C52	7.35	117.75	108.56
4	A	900[A]	RFA	F59-C55-C54	7.46	117.89	108.56
5	B	903[B]	RFB	F47-C42-C41	7.47	117.91	108.56
4	B	902[A]	RFA	C52-C51-C50	7.51	119.77	111.55
4	B	902[A]	RFA	F59-C55-C54	7.52	117.97	108.56
5	A	901[B]	RFB	F47-C42-C41	7.56	118.02	108.56
5	B	903[B]	RFB	F59-C55-C54	7.58	118.04	108.56
4	B	902[A]	RFA	C41-C42-C43	7.58	119.85	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	902[A]	RFA	F56-C51-C52	7.59	118.06	108.56
4	A	900[A]	RFA	F47-C42-C41	7.60	118.07	108.56
5	A	901[B]	RFB	F59-C55-C54	7.72	118.21	108.56
4	B	902[A]	RFA	F47-C42-C41	7.73	118.23	108.56
4	A	900[A]	RFA	F48-C44-C45	7.81	118.33	108.56
5	B	903[B]	RFB	F48-C44-C45	7.84	118.37	108.56
4	B	902[A]	RFA	F48-C44-C45	7.84	118.37	108.56
5	A	901[B]	RFB	F48-C44-C45	8.05	118.63	108.56
4	B	902[A]	RFA	F57-C52-C51	8.09	118.68	108.56
5	A	901[B]	RFB	F58-C54-C55	8.11	118.71	108.56
4	A	900[A]	RFA	F58-C54-C55	8.12	118.72	108.56
4	A	900[A]	RFA	F57-C52-C51	8.16	118.77	108.56
4	B	902[A]	RFA	F59-C55-C50	8.17	120.40	110.02
5	B	903[B]	RFB	F57-C52-C51	8.17	118.78	108.56
5	A	901[B]	RFB	F57-C52-C51	8.17	118.79	108.56
5	B	903[B]	RFB	F58-C54-C55	8.24	118.86	108.56
4	B	902[A]	RFA	F48-C44-C43	8.24	120.49	110.02
5	A	901[B]	RFB	C54-C55-C50	8.29	120.63	111.55
4	A	900[A]	RFA	C54-C55-C50	8.33	120.67	111.55
4	A	900[A]	RFA	C41-C42-C43	8.33	120.67	111.55
5	A	901[B]	RFB	C45-C44-C43	8.34	120.68	111.55
5	B	903[B]	RFB	C45-C44-C43	8.35	120.69	111.55
4	B	902[A]	RFA	F58-C54-C55	8.38	119.05	108.56
5	A	901[B]	RFB	F48-C44-C43	8.40	120.69	110.02
5	A	901[B]	RFB	C41-C42-C43	8.47	120.82	111.55
4	A	900[A]	RFA	C45-C44-C43	8.49	120.84	111.55
4	A	900[A]	RFA	F48-C44-C43	8.50	120.82	110.02
5	B	903[B]	RFB	C41-C42-C43	8.52	120.87	111.55
5	B	903[B]	RFB	F59-C55-C50	8.56	120.90	110.02
5	B	903[B]	RFB	F48-C44-C43	8.59	120.94	110.02
4	A	900[A]	RFA	C52-C51-C50	8.62	120.99	111.55
5	B	903[B]	RFB	C52-C51-C50	8.63	121.00	111.55
5	A	901[B]	RFB	C52-C51-C50	8.67	121.04	111.55
5	B	903[B]	RFB	C54-C55-C50	8.69	121.06	111.55
4	B	902[A]	RFA	C45-C44-C43	8.76	121.14	111.55
5	A	901[B]	RFB	F59-C55-C50	8.76	121.16	110.02
5	A	901[B]	RFB	F47-C42-C43	8.77	121.16	110.02
5	B	903[B]	RFB	F47-C42-C43	8.81	121.22	110.02
5	B	903[B]	RFB	F56-C51-C50	8.83	121.25	110.02
4	A	900[A]	RFA	F47-C42-C43	8.85	121.26	110.02
4	A	900[A]	RFA	F59-C55-C50	8.99	121.44	110.02
4	A	900[A]	RFA	F49-C45-C44	9.01	119.84	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901[B]	RFB	F49-C45-C44	9.02	119.84	108.56
4	A	900[A]	RFA	F56-C51-C50	9.08	121.56	110.02
5	A	901[B]	RFB	F56-C51-C50	9.10	121.58	110.02
5	A	901[B]	RFB	F46-C41-C42	9.17	120.03	108.56
4	B	902[A]	RFA	C54-C55-C50	9.21	121.63	111.55
5	B	903[B]	RFB	F49-C45-C44	9.26	120.14	108.56
4	A	900[A]	RFA	F46-C41-C42	9.26	120.15	108.56
4	B	902[A]	RFA	F47-C42-C43	9.36	121.92	110.02
4	B	902[A]	RFA	F49-C45-C44	9.40	120.32	108.56
5	B	903[B]	RFB	F46-C41-C42	9.40	120.32	108.56
4	B	902[A]	RFA	F46-C41-C42	9.43	120.36	108.56
4	B	902[A]	RFA	F56-C51-C50	9.56	122.17	110.02
5	A	901[B]	RFB	F57-C52-C53	14.28	119.58	108.45
5	B	903[B]	RFB	F57-C52-C53	14.71	119.92	108.45
4	A	900[A]	RFA	F57-C52-C53	14.98	120.13	108.45
5	B	903[B]	RFB	F58-C54-C53	16.05	120.96	108.45
4	A	900[A]	RFA	F58-C54-C53	16.14	121.03	108.45
5	A	901[B]	RFB	F58-C54-C53	16.48	121.29	108.45
4	B	902[A]	RFA	F57-C52-C53	16.89	121.62	108.45
4	B	902[A]	RFA	F58-C54-C53	17.35	121.98	108.45

All (44) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	900[A]	RFA	C42
4	A	900[A]	RFA	C44
4	A	900[A]	RFA	C19
4	A	900[A]	RFA	C45
4	A	900[A]	RFA	C22
4	A	900[A]	RFA	C51
4	A	900[A]	RFA	C54
4	A	900[A]	RFA	C20
4	A	900[A]	RFA	C55
4	A	900[A]	RFA	C41
4	A	900[A]	RFA	C52
5	A	901[B]	RFB	C42
5	A	901[B]	RFB	C44
5	A	901[B]	RFB	C19
5	A	901[B]	RFB	C45
5	A	901[B]	RFB	C22
5	A	901[B]	RFB	C51
5	A	901[B]	RFB	C54

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Mol	Chain	Res	Type	Atom
5	A	901[B]	RFB	C20
5	A	901[B]	RFB	C55
5	A	901[B]	RFB	C41
5	A	901[B]	RFB	C52
5	B	903[B]	RFB	C42
5	B	903[B]	RFB	C44
5	B	903[B]	RFB	C19
5	B	903[B]	RFB	C45
5	B	903[B]	RFB	C22
5	B	903[B]	RFB	C51
5	B	903[B]	RFB	C54
5	B	903[B]	RFB	C20
5	B	903[B]	RFB	C55
5	B	903[B]	RFB	C41
5	B	903[B]	RFB	C52
4	B	902[A]	RFA	C42
4	B	902[A]	RFA	C44
4	B	902[A]	RFA	C19
4	B	902[A]	RFA	C45
4	B	902[A]	RFA	C22
4	B	902[A]	RFA	C51
4	B	902[A]	RFA	C54
4	B	902[A]	RFA	C20
4	B	902[A]	RFA	C55
4	B	902[A]	RFA	C41
4	B	902[A]	RFA	C52

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	CAC	1	0
4	A	900[A]	RFA	1	0
5	A	901[B]	RFB	1	0
3	B	417	HEM	2	0
2	B	500	CAC	1	0
2	B	502	CAC	1	0
2	B	504	CAC	3	0
4	B	902[A]	RFA	1	0
5	B	903[B]	RFB	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.