Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 02:59 AM EDT

PDB ID	:	7SMZ
Title	:	X-ray crystal structure of CYP142A3 from Mycobacterium Marinum in complex with 4-cholesten-3-one
Authors	:	Ghith, A.; Bruning, J.B.; Bell, S.G.
Deposited on	:	2021-10-27
Resolution	:	2.04 Å(reported)

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

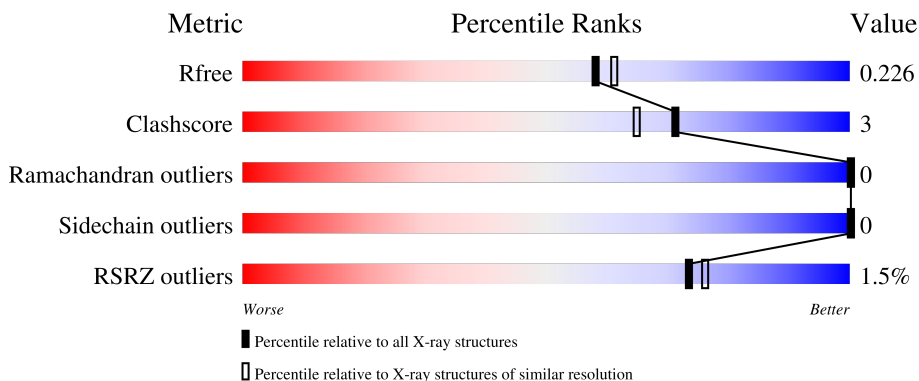|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	405	89% 8% •
1	B	405	90% 7% •

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
2	K2B	A	501	X	-	-	-
2	K2B	B	502	X	-	-	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6860 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.
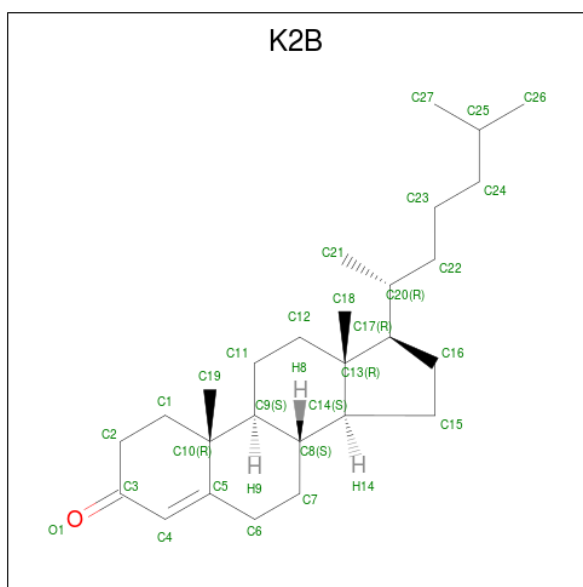
- Molecule 1 is a protein called Cytochrome P450 142A3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	1	0
			3122	1948	552	602	20			
1	B	395	Total	C	N	O	S	0	1	0
			3130	1952	557	601	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	GLY	-	expression tag	UNP A0A2Z5YMP0
A	403	GLY	-	expression tag	UNP A0A2Z5YMP0
A	404	SER	-	expression tag	UNP A0A2Z5YMP0
A	405	GLY	-	expression tag	UNP A0A2Z5YMP0
B	402	GLY	-	expression tag	UNP A0A2Z5YMP0
B	403	GLY	-	expression tag	UNP A0A2Z5YMP0
B	404	SER	-	expression tag	UNP A0A2Z5YMP0
B	405	GLY	-	expression tag	UNP A0A2Z5YMP0

- Molecule 2 is (8ALPHA,9BETA)-CHOLEST-4-EN-3-ONE (three-letter code: K2B) (formula: $C_{27}H_{44}O$) (labeled as "Ligand of Interest" by depositor).

K2B

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 28	C 27	O 1	0	0
2	B	1	Total 28	C 27	O 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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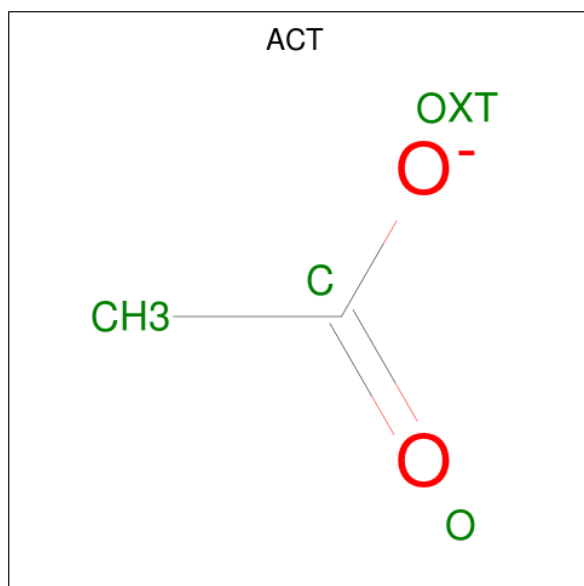
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Na 1	0	0
5	B	3	Total 3	Na 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	211	Total 211	O 211	0	0
6	B	219	Total 219	O 219	0	0

3 Residue-property plots ⓘ

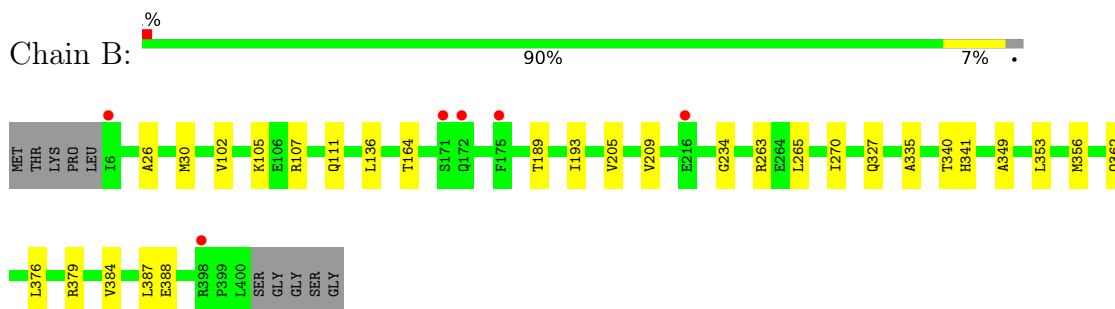These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cytochrome P450 142A3

• Molecule 1: Cytochrome P450 142A3

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.31Å 50.40Å 82.58Å 82.32° 75.59° 72.05°	Depositor
Resolution (Å)	46.69 – 2.04 46.69 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.69-2.04) 98.0 (46.69-2.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.180 , 0.225 0.181 , 0.226	Depositor DCC
R_{free} test set	1989 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.1	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6860	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.75% 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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K2B, ACT, HEM, NA

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	0.26	0/3179	0.45	0/4307
1	B	0.29	0/3187	0.47	0/4317
All	All	0.27	0/6366	0.46	0/8624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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	3122	0	3056	21	0
1	B	3130	0	3073	21	0
2	A	28	0	44	1	0
2	B	28	0	44	4	0
3	A	43	0	30	0	0
3	B	43	0	30	3	0
4	A	16	0	12	2	0
4	B	16	0	12	0	0
5	A	1	0	0	0	0
5	B	3	0	0	0	0
6	A	211	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	219	0	0	0	0
All	All	6860	0	6301	44	0

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

All (44) 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:263:ARG:HH22	1:B:362:GLN:HB2	1.49	0.76
1:B:234:GLY:HA2	3:B:501:HEM:HAB	1.76	0.68
1:B:379[A]:ARG:HH12	1:B:384:VAL:HG23	1.62	0.64
1:A:189:THR:O	1:A:193:ILE:HG12	1.98	0.64
1:B:263:ARG:NH1	1:B:362:GLN:OE1	2.34	0.60
1:A:379:ARG:HD3	1:A:380:PRO:HD2	1.89	0.55
1:B:164:THR:HA	1:B:379[A]:ARG:HD3	1.89	0.55
1:B:270:ILE:HD12	1:B:353:LEU:HB3	1.89	0.54
1:A:99:ARG:O	1:A:103:LYS:HG2	2.08	0.53
1:B:349:ALA:HB2	3:B:501:HEM:HBB2	1.90	0.53
1:A:136:LEU:HB3	1:A:137:PRO:HD3	1.91	0.53
1:B:335:ALA:HB1	3:B:501:HEM:HBC1	1.91	0.51
1:B:263:ARG:NH2	1:B:362:GLN:HB2	2.24	0.50
1:B:340:THR:HG23	1:B:341:HIS:CD2	2.46	0.50
1:A:189:THR:HA	4:A:504:ACT:H1	1.94	0.50
1:A:197:ARG:HG2	1:A:209:VAL:HG11	1.93	0.48
1:B:26:ALA:O	1:B:30:MET:HG3	2.13	0.48
2:B:502:K2B:H193	2:B:502:K2B:H111	1.42	0.48
1:B:136:LEU:HD22	1:B:356:MET:HB2	1.95	0.47
1:A:196:ARG:HD2	1:A:206:SER:HB2	1.95	0.47
2:B:502:K2B:H182	2:B:502:K2B:H8	1.71	0.47
1:A:265:LEU:HD21	1:B:265:LEU:HD21	1.95	0.47
1:B:189:THR:O	1:B:193:ILE:HG12	2.16	0.46
1:A:101:ARG:HA	1:A:104:ASP:OD2	2.15	0.46
1:A:229:LEU:HA	2:A:501:K2B:H211	1.97	0.46
1:A:299:SER:O	1:A:302:GLU:HG2	2.16	0.45
1:B:376:LEU:HB2	1:B:387:LEU:HD22	1.99	0.45
1:B:102:VAL:HA	1:B:105:LYS:HE2	2.00	0.44
1:A:262:ASP:OD2	1:B:327:GLN:NE2	2.41	0.44
1:A:136:LEU:HD22	1:A:356:MET:HB2	1.98	0.44
1:A:43:LEU:HD13	4:A:503:ACT:H2	2.00	0.42
1:A:379:ARG:HD3	1:A:379:ARG:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:CG	1:A:317:VAL:HG21	2.54	0.42
1:A:282:ASN:HA	1:A:306:LEU:O	2.20	0.42
2:B:502:K2B:H8	2:B:502:K2B:H191	1.72	0.42
1:A:18:TYR:CD2	1:A:382:ASN:HA	2.55	0.41
1:B:107:ARG:O	1:B:111:GLN:HG3	2.20	0.41
1:A:242:LEU:HG	1:A:353:LEU:HD23	2.02	0.41
1:B:205:VAL:O	1:B:209:VAL:HG23	2.21	0.41
1:B:379[A]:ARG:NH1	1:B:384:VAL:O	2.54	0.41
1:B:379[B]:ARG:HG3	1:B:388:GLU:HG2	2.04	0.40
1:A:110:ALA:HB1	1:A:359:ARG:NH2	2.36	0.40
1:A:259:LEU:HD23	1:A:361:VAL:HG21	2.03	0.40
2:B:502:K2B:H152	2:B:502:K2B:H181	1.90	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	394/405 (97%)	383 (97%)	11 (3%)	0	100	100
1	B	394/405 (97%)	383 (97%)	11 (3%)	0	100	100
All	All	788/810 (97%)	766 (97%)	22 (3%)	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	339/346 (98%)	339 (100%)	0	100	100
1	B	340/346 (98%)	340 (100%)	0	100	100
All	All	679/692 (98%)	679 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#|Z| > 2$
2	K2B	A	501	-	31,31,31	4.23	18 (58%)	48,48,48	6.95	24 (50%)
4	ACT	B	503	-	3,3,3	1.29	0	3,3,3	1.51	0
4	ACT	A	503	-	3,3,3	1.33	0	3,3,3	1.37	0
4	ACT	A	505	-	3,3,3	1.29	0	3,3,3	1.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	ACT	B	505	-	3,3,3	1.30	0	3,3,3	1.52	0
4	ACT	B	504	-	3,3,3	1.17	0	3,3,3	1.55	0
3	HEM	A	502	1	41,50,50	1.46	7 (17%)	45,82,82	1.79	8 (17%)
3	HEM	B	501	1	41,50,50	1.48	6 (14%)	45,82,82	1.90	11 (24%)
4	ACT	B	506	-	3,3,3	1.31	0	3,3,3	1.52	0
4	ACT	A	504	-	3,3,3	1.07	0	3,3,3	1.45	0
2	K2B	B	502	-	31,31,31	4.27	18 (58%)	48,48,48	6.60	20 (41%)
4	ACT	A	506	-	3,3,3	1.31	0	3,3,3	1.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	K2B	A	501	-	5/5/10/11	8/10/68/68	0/4/4/4
3	HEM	B	501	1	-	0/12/54/54	-
2	K2B	B	502	-	4/4/10/11	8/10/68/68	0/4/4/4
3	HEM	A	502	1	-	0/12/54/54	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	K2B	C4-C3	9.15	1.65	1.45
2	A	501	K2B	C4-C3	8.95	1.64	1.45
2	B	502	K2B	C6-C5	7.51	1.63	1.50
2	A	501	K2B	C1-C2	7.11	1.67	1.53
2	B	502	K2B	C1-C2	7.05	1.67	1.53
2	B	502	K2B	C13-C14	-6.96	1.41	1.55
2	A	501	K2B	C6-C5	6.90	1.62	1.50
2	A	501	K2B	C13-C14	-6.83	1.42	1.55
2	B	502	K2B	C4-C5	6.83	1.44	1.34
2	B	502	K2B	C1-C10	-6.74	1.41	1.54
2	A	501	K2B	C4-C5	6.74	1.44	1.34
2	A	501	K2B	C10-C5	6.53	1.65	1.52
2	A	501	K2B	C1-C10	-6.47	1.41	1.54
2	A	501	K2B	C16-C17	-6.42	1.41	1.54
2	B	502	K2B	C10-C5	6.36	1.65	1.52
2	B	502	K2B	C16-C17	-6.30	1.41	1.54
2	B	502	K2B	C10-C9	5.75	1.65	1.56
2	B	502	K2B	C13-C17	5.56	1.65	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	K2B	C13-C17	5.50	1.65	1.55
2	A	501	K2B	C10-C9	5.43	1.65	1.56
2	A	501	K2B	C8-C14	5.13	1.63	1.53
2	B	502	K2B	C8-C9	-4.69	1.44	1.53
3	B	501	HEM	C1B-NB	-4.26	1.33	1.40
3	A	502	HEM	C1B-NB	-4.24	1.33	1.40
2	B	502	K2B	C8-C14	4.05	1.61	1.53
2	A	501	K2B	C8-C9	-3.93	1.46	1.53
3	A	502	HEM	C4D-ND	-3.25	1.34	1.40
2	A	501	K2B	C15-C14	3.21	1.61	1.54
3	B	501	HEM	C4D-ND	-3.17	1.34	1.40
2	B	502	K2B	C15-C14	3.07	1.60	1.54
3	B	501	HEM	FE-NB	3.06	2.12	1.96
2	A	501	K2B	C11-C9	-2.96	1.48	1.53
3	A	502	HEM	FE-NB	2.87	2.11	1.96
3	A	502	HEM	C4B-NB	-2.85	1.32	1.38
2	B	502	K2B	C20-C17	2.78	1.59	1.54
2	A	501	K2B	C20-C17	2.73	1.59	1.54
2	A	501	K2B	C16-C15	2.70	1.61	1.54
2	B	502	K2B	C16-C15	2.67	1.61	1.54
3	B	501	HEM	C1D-ND	-2.55	1.33	1.38
2	B	502	K2B	C11-C9	-2.54	1.49	1.53
3	B	501	HEM	C4B-NB	-2.50	1.33	1.38
3	A	502	HEM	O2D-CGD	-2.46	1.22	1.30
3	A	502	HEM	C1D-ND	-2.24	1.34	1.38
2	B	502	K2B	C7-C6	2.19	1.57	1.52
3	B	501	HEM	C3B-C4B	2.13	1.49	1.44
2	A	501	K2B	C7-C8	2.10	1.57	1.53
2	B	502	K2B	O1-C3	-2.07	1.19	1.23
2	A	501	K2B	O1-C3	-2.05	1.19	1.23
3	A	502	HEM	O2A-CGA	-2.02	1.24	1.30

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	K2B	C19-C10-C9	-23.75	83.37	111.68
2	B	502	K2B	C18-C13-C12	-19.31	80.09	110.59
2	A	501	K2B	C18-C13-C17	-18.57	77.08	111.71
2	B	502	K2B	C19-C10-C9	-18.04	90.17	111.68
2	A	501	K2B	C18-C13-C12	-17.15	83.51	110.59
2	B	502	K2B	C18-C13-C17	-16.57	80.81	111.71
2	B	502	K2B	C19-C10-C1	-16.56	83.27	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	K2B	C19-C10-C1	-15.82	84.44	109.43
2	B	502	K2B	C19-C10-C5	-14.96	84.13	108.34
2	A	501	K2B	C19-C10-C5	-14.86	84.30	108.34
2	A	501	K2B	C17-C13-C14	11.07	113.18	100.07
2	B	502	K2B	C17-C13-C14	10.00	111.92	100.07
2	B	502	K2B	C18-C13-C14	-9.97	93.12	111.71
2	A	501	K2B	C18-C13-C14	-9.04	94.86	111.71
2	B	502	K2B	C12-C13-C14	8.95	121.16	107.27
2	B	502	K2B	C1-C10-C9	8.12	120.08	108.73
2	A	501	K2B	C12-C13-C14	7.40	118.75	107.27
2	A	501	K2B	C9-C10-C5	6.91	120.49	109.65
2	A	501	K2B	C1-C10-C9	6.88	118.34	108.73
2	B	502	K2B	C9-C10-C5	6.68	120.13	109.65
2	B	502	K2B	C10-C5-C4	-6.13	112.77	122.68
2	A	501	K2B	C7-C8-C14	-6.07	101.70	112.08
2	A	501	K2B	C12-C13-C17	6.05	125.62	116.57
2	A	501	K2B	C14-C8-C9	5.97	117.09	109.09
2	A	501	K2B	C11-C9-C10	-5.50	105.83	113.08
2	B	502	K2B	C15-C14-C8	5.42	128.00	119.08
3	B	501	HEM	C1B-NB-C4B	5.25	110.50	105.07
2	A	501	K2B	C5-C4-C3	-5.23	115.23	123.67
2	B	502	K2B	C1-C10-C5	5.19	118.26	108.75
2	A	501	K2B	C1-C10-C5	5.04	117.97	108.75
3	A	502	HEM	C1B-NB-C4B	5.03	110.27	105.07
2	B	502	K2B	C12-C13-C17	5.01	124.07	116.57
2	B	502	K2B	C5-C4-C3	-4.95	115.69	123.67
2	A	501	K2B	C10-C5-C4	-4.69	115.08	122.68
2	B	502	K2B	C13-C17-C20	-4.47	112.48	119.49
3	B	501	HEM	CBA-CAA-C2A	-4.34	105.21	112.62
2	A	501	K2B	C6-C5-C10	-4.33	108.78	116.77
2	A	501	K2B	C15-C14-C8	4.26	126.10	119.08
3	A	502	HEM	CHC-C4B-NB	4.24	129.04	124.43
3	A	502	HEM	CHD-C1D-ND	4.19	128.99	124.43
2	B	502	K2B	C7-C8-C14	-4.09	105.09	112.08
2	A	501	K2B	C13-C17-C20	-3.60	113.85	119.49
3	A	502	HEM	CHA-C4D-ND	3.37	128.54	124.38
3	B	501	HEM	CHB-C1B-NB	3.34	128.50	124.38
3	B	501	HEM	CHC-C4B-NB	3.31	128.03	124.43
3	A	502	HEM	CHB-C1B-NB	3.20	128.33	124.38
3	B	501	HEM	CHD-C1D-ND	3.18	127.88	124.43
3	A	502	HEM	CHD-C1D-C2D	-3.17	120.02	124.98
2	B	502	K2B	C7-C6-C5	3.04	117.66	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	HEM	O2A-CGA-CBA	3.04	123.80	114.03
3	B	501	HEM	CMA-C3A-C4A	-3.04	123.79	128.46
3	B	501	HEM	CHD-C1D-C2D	-2.83	120.56	124.98
2	B	502	K2B	C6-C5-C4	-2.83	116.14	120.87
2	A	501	K2B	C6-C5-C4	-2.64	116.46	120.87
3	A	502	HEM	O2A-CGA-CBA	2.62	122.44	114.03
3	B	501	HEM	CAD-C3D-C4D	2.40	128.85	124.66
2	B	502	K2B	C6-C5-C10	-2.37	112.39	116.77
3	B	501	HEM	CHA-C4D-ND	2.30	127.22	124.38
2	A	501	K2B	C10-C9-C8	2.26	116.13	112.73
2	A	501	K2B	C7-C8-C9	2.17	113.18	110.49
3	A	502	HEM	CHA-C4D-C3D	-2.15	121.28	125.33
3	B	501	HEM	O1A-CGA-CBA	-2.07	116.44	123.08
2	A	501	K2B	C11-C12-C13	-2.00	109.35	112.78

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	K2B	C9
2	A	501	K2B	C10
2	A	501	K2B	C17
2	A	501	K2B	C13
2	A	501	K2B	C20
2	B	502	K2B	C17
2	B	502	K2B	C13
2	B	502	K2B	C20
2	B	502	K2B	C10

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	K2B	C21-C20-C22-C23
2	B	502	K2B	C13-C17-C20-C22
2	A	501	K2B	C17-C20-C22-C23
2	B	502	K2B	C17-C20-C22-C23
2	B	502	K2B	C21-C20-C22-C23
2	B	502	K2B	C23-C24-C25-C27
2	A	501	K2B	C13-C17-C20-C22
2	B	502	K2B	C13-C17-C20-C21
2	A	501	K2B	C13-C17-C20-C21
2	B	502	K2B	C16-C17-C20-C22
2	B	502	K2B	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	A	501	K2B	C23-C24-C25-C26
2	B	502	K2B	C16-C17-C20-C21
2	A	501	K2B	C23-C24-C25-C27
2	A	501	K2B	C16-C17-C20-C22
2	A	501	K2B	C16-C17-C20-C21

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	K2B	1	0
4	A	503	ACT	1	0
3	B	501	HEM	3	0
4	A	504	ACT	1	0
2	B	502	K2B	4	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 K2B A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand K2B B 502

Bond lengths

Bond angles

Torsions

Rings

5.7   Other polymers ⓘ

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(Å²)	Q<0.9
1	A	395/405 (97%)	-0.12	6 (1%)	73	76	14, 27, 45, 64	0
1	B	395/405 (97%)	-0.17	6 (1%)	73	76	14, 26, 44, 64	0
All	All	790/810 (97%)	-0.14	12 (1%)	73	76	14, 27, 45, 64	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ILE	4.0
1	A	173	GLU	3.1
1	B	172	GLN	3.1
1	B	398	ARG	3.0
1	A	214	ASP	2.9
1	B	216	GLU	2.9
1	A	198	ALA	2.8
1	B	175	PHE	2.3
1	B	6	ILE	2.3
1	A	372	GLN	2.2
1	A	209	VAL	2.1
1	B	171	SER	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 ⓘ

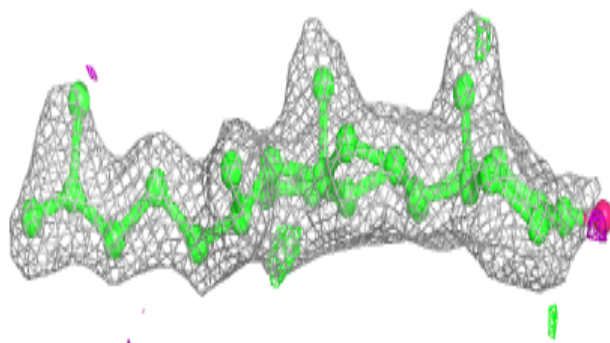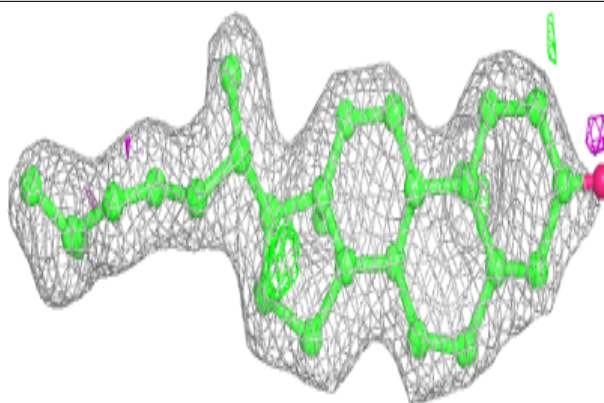There are no monosaccharides in this entry.

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.

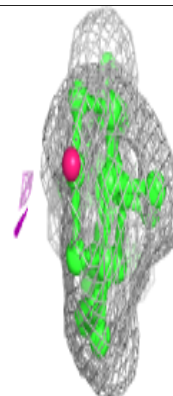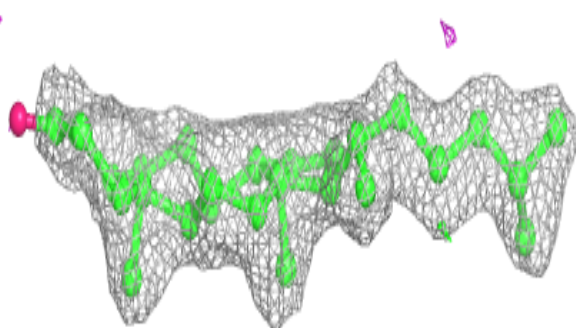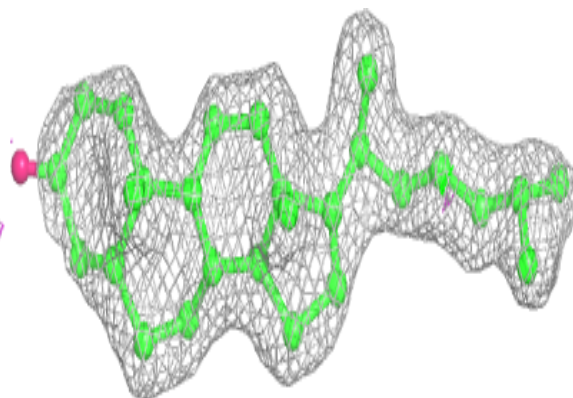| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	K2B	B	502	28/28	0.85	0.17	18,34,43,57	0
2	K2B	A	501	28/28	0.86	0.15	18,31,45,60	0
5	NA	B	508	1/1	0.87	0.15	47,47,47,47	0
4	ACT	A	504	4/4	0.88	0.17	30,35,38,41	0
4	ACT	A	506	4/4	0.89	0.14	42,43,45,54	0
5	NA	B	509	1/1	0.89	0.20	44,44,44,44	0
4	ACT	B	505	4/4	0.91	0.11	44,47,47,52	0
5	NA	B	507	1/1	0.91	0.12	33,33,33,33	0
4	ACT	B	503	4/4	0.92	0.16	38,41,43,44	0
4	ACT	B	504	4/4	0.94	0.23	27,34,37,42	0
4	ACT	A	505	4/4	0.95	0.17	40,43,49,51	0
4	ACT	A	503	4/4	0.96	0.09	33,35,40,40	0
3	HEM	B	501	43/43	0.97	0.11	13,17,22,25	0
3	HEM	A	502	43/43	0.97	0.11	11,17,21,30	0
4	ACT	B	506	4/4	0.97	0.11	31,35,36,37	0
5	NA	A	507	1/1	0.99	0.06	29,29,29,29	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 K2B B 502:

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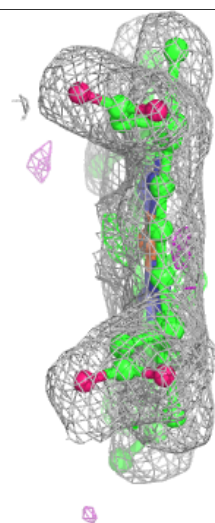mF_o-DF_c (at 3 rmsd) in purple (negative)
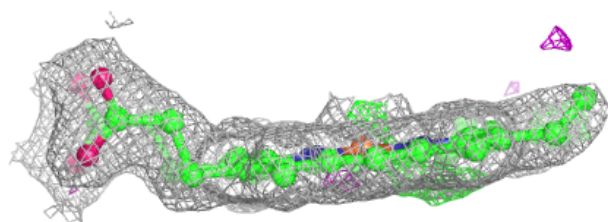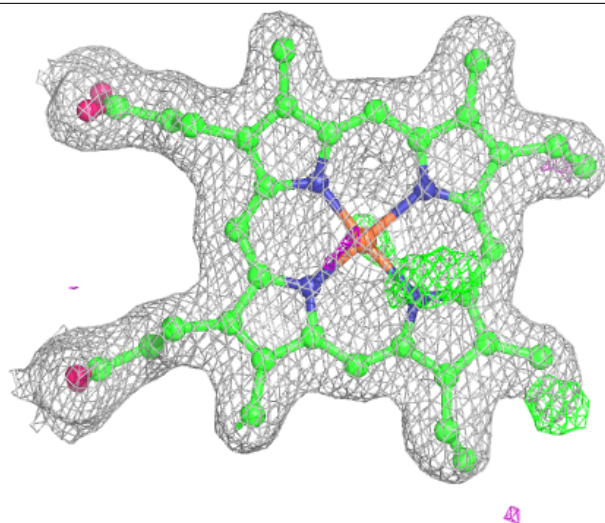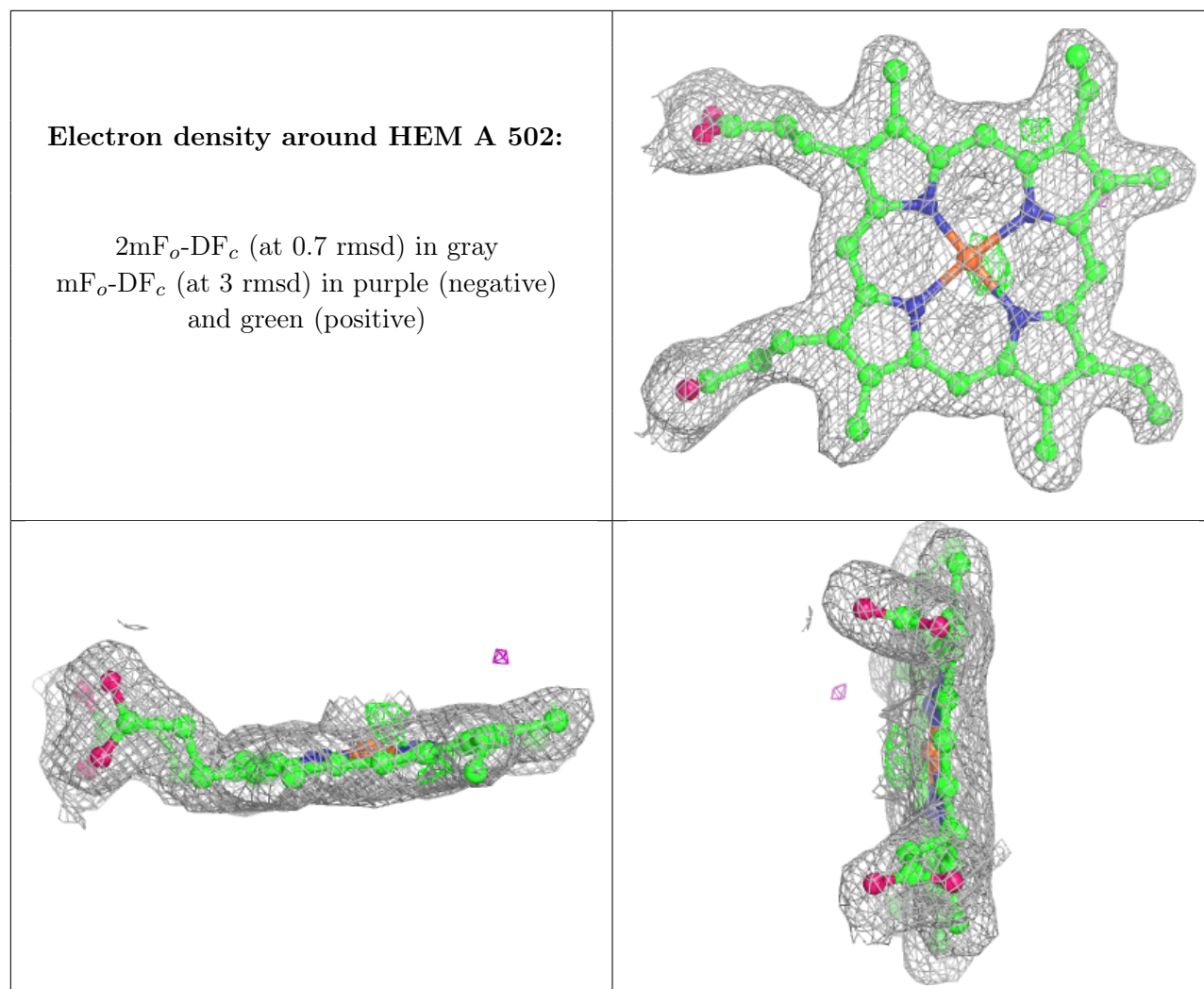and green (positive)

Electron density around K2B A 501:

$2mF_o$-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 B 501:

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

Electron density around HEM A 502:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.