



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:03 AM GMT

PDB ID : 2FBW  
Title : Avian respiratory complex II with carboxin bound  
Authors : Huang, L.S.; Sun, G.; Cobessi, D.; Wang, A.C.; Shen, J.T.; Tung, E.Y.; Anderson, V.E.; Berry, E.A.  
Deposited on : 2005-12-10  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

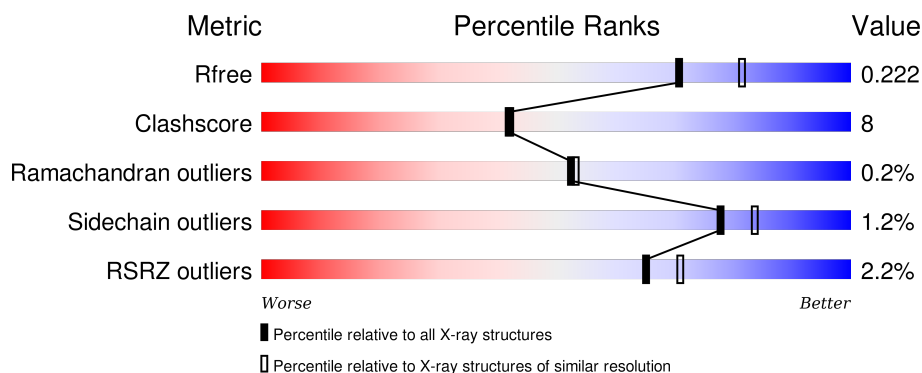
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



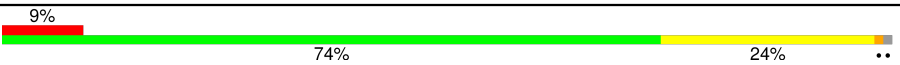

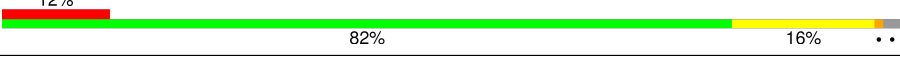
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	621	<div> <div>87%</div> <div>12% •</div> </div>
1	N	621	<div> <div>85%</div> <div>13% •</div> </div>
2	B	252	<div> <div>84%</div> <div>10% • 5%</div> </div>
2	O	252	<div> <div>84%</div> <div>10% • 5%</div> </div>
3	C	141	<div> <div>4%</div> <div>74%</div> <div>23% ••</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	141	
4	D	103	
4	Q	103	

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
11	F3S	O	1004	-	-	-	X
13	CBE	C	144	-	-	X	X
13	CBE	P	202	-	-	X	X
14	TEO	A	1002	X	-	-	-
14	TEO	N	1002	X	-	-	-
15	PEE	D	109	-	-	-	X
15	PEE	Q	210	-	-	-	X
16	UNL	A	1003	-	-	X	-
16	UNL	A	1004	-	-	X	-
16	UNL	B	1005	-	-	X	-
16	UNL	C	145	-	-	X	-
16	UNL	C	214	-	-	X	X
16	UNL	C	272	-	-	-	X
16	UNL	N	1003	-	-	X	-
16	UNL	O	1005	-	-	X	-
16	UNL	P	211	-	-	X	X
17	GOL	B	1010	-	-	-	X
17	GOL	C	294	-	-	-	X
17	GOL	O	1009	-	-	-	X
17	GOL	P	208	-	-	-	X
5	BHG	C	142	X	-	-	X
5	BHG	P	204	X	-	-	-

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 19494 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 Succinate dehydrogenase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4731	2959	844	899	29			
1	N	612	Total	C	N	O	S	0	0	0
			4725	2956	843	897	29			

- Molecule 2 is a protein called succinate dehydrogenase Ip subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1918	1213	325	358	22			
2	O	239	Total	C	N	O	S	0	0	0
			1918	1213	325	358	22			

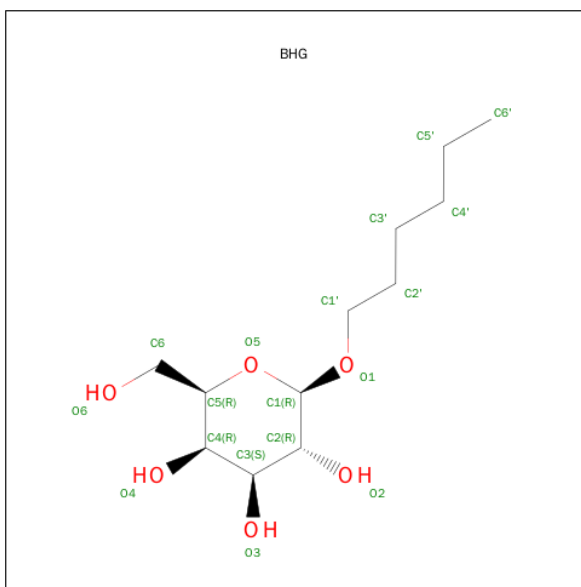
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome B, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	140	Total	C	N	O	S	0	0	0
			1078	708	179	187	4			
3	P	140	Total	C	N	O	S	0	0	0
			1078	708	179	187	4			

- Molecule 4 is a protein called Succinate dehydrogenase cytochrome B, small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	101	Total	C	N	O	S	0	0	0
			765	505	121	136	3			
4	Q	101	Total	C	N	O	S	0	0	0
			765	505	121	136	3			

- Molecule 5 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>6</sub>).

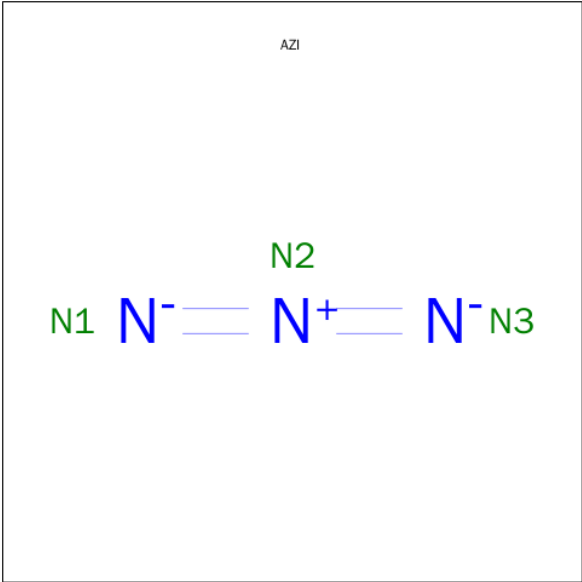


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			18	12	6		
5	P	1	Total	C	O	0	0
			18	12	6		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

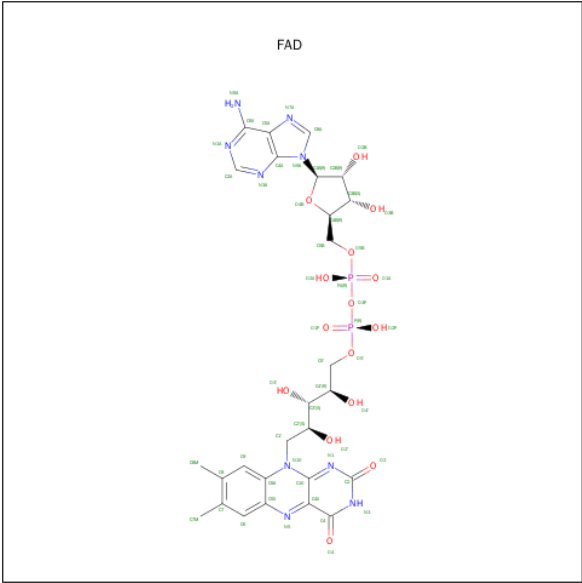
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	O	1	Total	K	0	0
			1	1		
6	B	1	Total	K	0	0
			1	1		
6	A	1	Total	K	0	0
			1	1		
6	N	1	Total	K	0	0
			1	1		

- Molecule 7 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



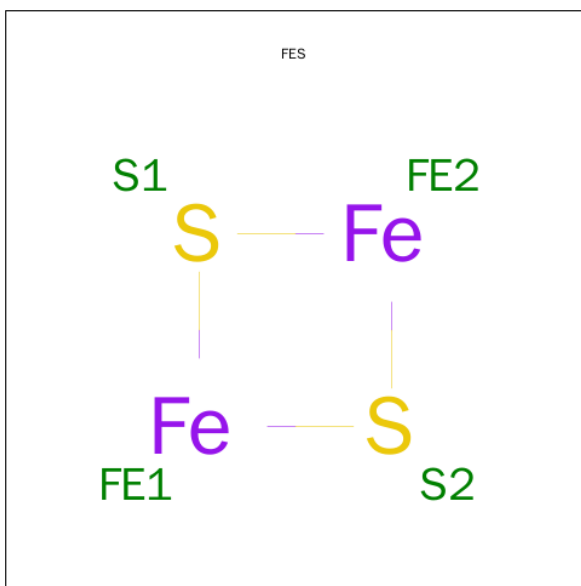
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total N 3 3	0	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



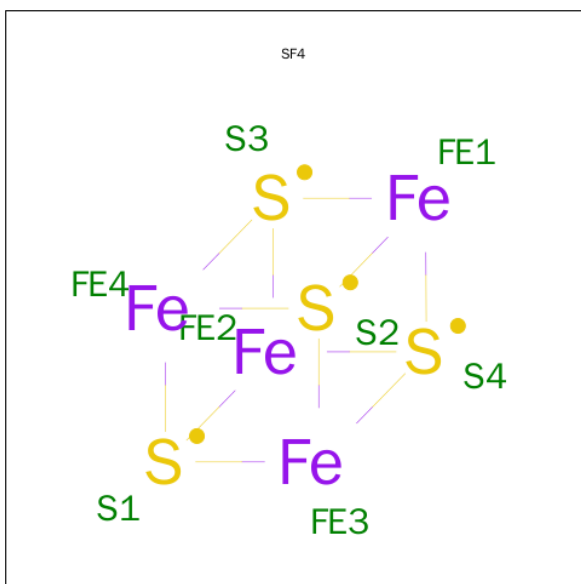
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O P 53 27 9 15 2	0	0
8	N	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			4	2	2		
9	O	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



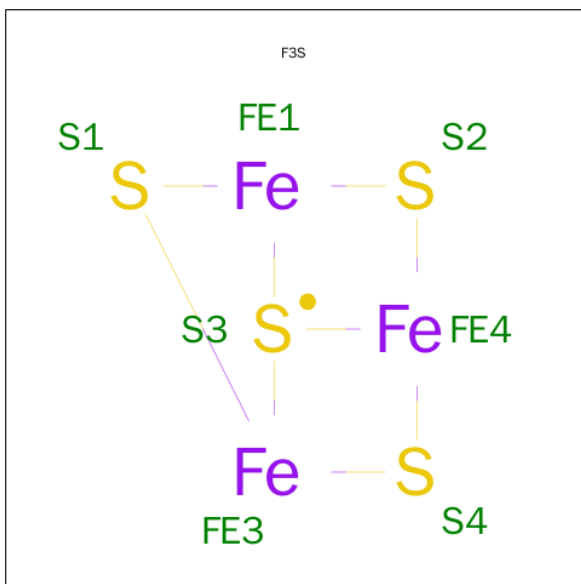
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	O	1	Total	Fe	S	0	0
			8	4	4		

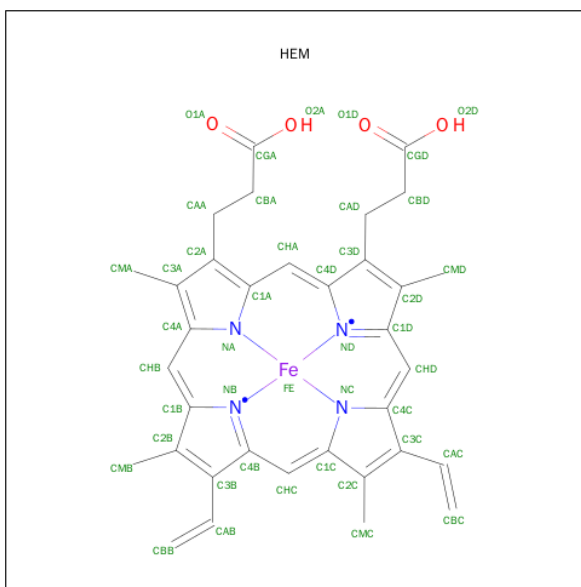
- Molecule 11 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			7	3	4		
11	O	1	Total	Fe	S	0	0
			7	3	4		

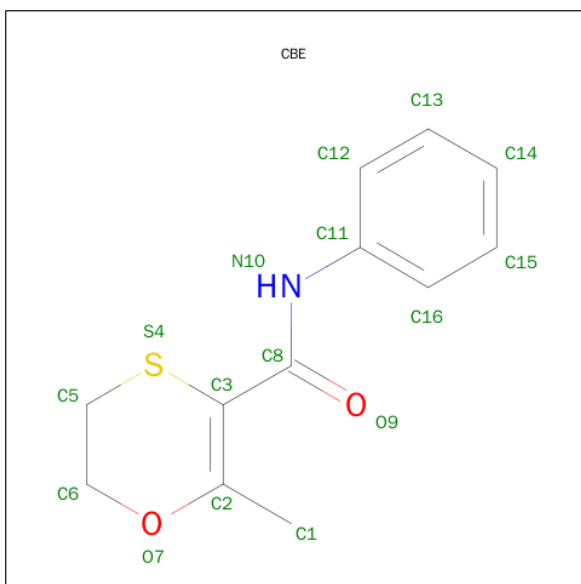
- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 41	C 32	Fe 1	N 4	O 4	0	0
12	P	1	Total 41	C 32	Fe 1	N 4	O 4	0	0

- Molecule 13 is 2-METHYL-N-PHENYL-5,6-DIHYDRO-1,4-OXATHIINE-3-CARBOXAMIDE (three-letter code: CBE) (formula:  $C_{12}H_{13}NO_2S$ ).



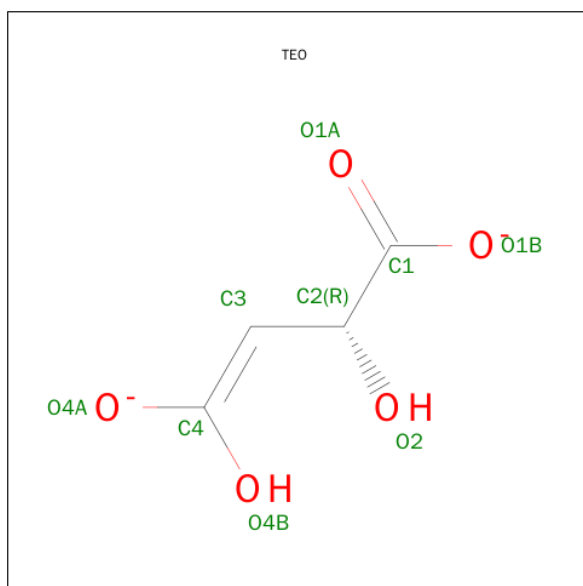
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

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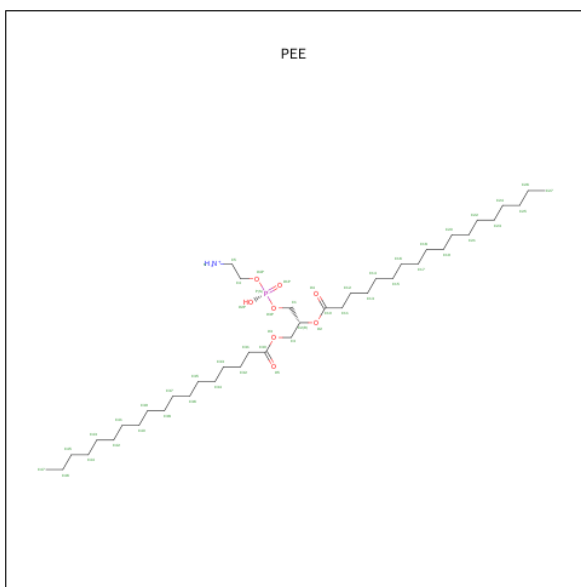
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	P	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

- Molecule 14 is MALATE LIKE INTERMEDIATE (three-letter code: TEO) (formula:  $C_4H_4O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			9	4	5		
14	N	1	Total	C	O	0	0
			9	4	5		

- Molecule 15 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	1	Total C 24 24	0	0
15	Q	1	Total C 24 24	0	0

- Molecule 16 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	P	7	Total O 11 11	0	0
16	Q	6	Total O 6 6	0	0
16	D	9	Total O 9 9	0	0
16	B	10	Total O 14 14	0	0
16	C	15	Total O 22 22	0	0
16	A	21	Total O 29 29	0	0
16	N	21	Total O 24 24	0	0
16	O	6	Total O 10 10	0	0

- Molecule 17 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

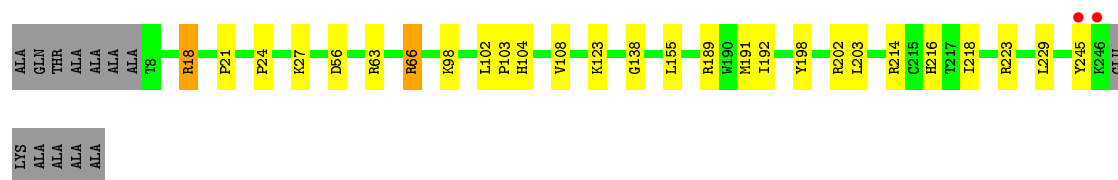
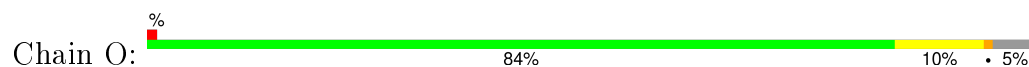


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			6	3	3		
17	B	1	Total	C	O	0	0
			6	3	3		
17	O	1	Total	C	O	0	0
			6	3	3		
17	P	1	Total	C	O	0	0
			6	3	3		

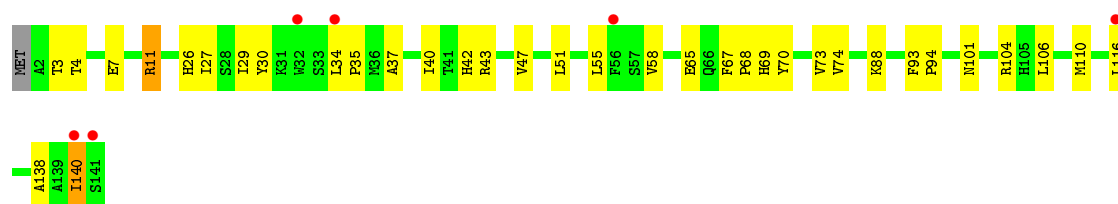
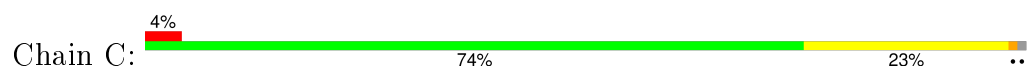
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	550	Total	O	0	0
			550	550		
18	B	299	Total	O	0	0
			299	299		
18	C	109	Total	O	0	0
			109	109		
18	D	57	Total	O	0	0
			57	57		
18	N	545	Total	O	0	0
			545	545		
18	O	285	Total	O	0	0
			285	285		
18	P	90	Total	O	0	0
			90	90		
18	Q	65	Total	O	0	0
			65	65		

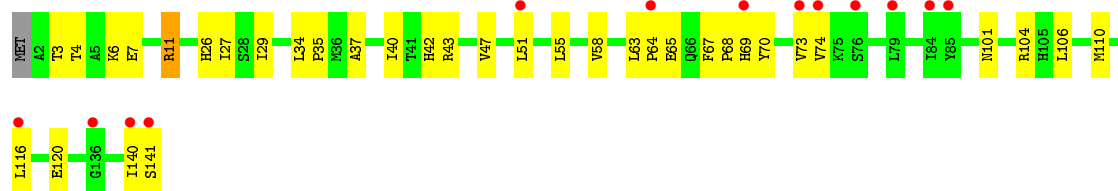




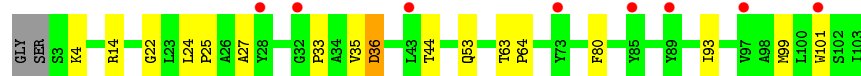
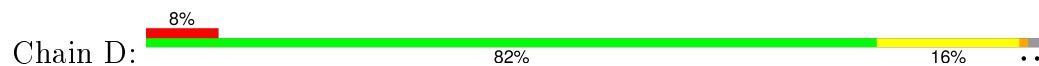
- Molecule 3: Succinate dehydrogenase cytochrome B, large subunit



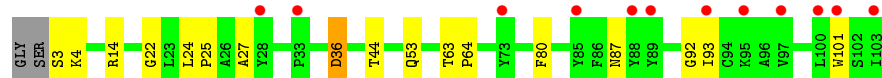
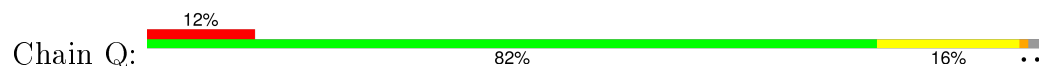
- Molecule 3: Succinate dehydrogenase cytochrome B, large subunit



- Molecule 4: Succinate dehydrogenase cytochrome B, small subunit



- Molecule 4: Succinate dehydrogenase cytochrome B, small subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.70Å 200.75Å 67.63Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	64.09 – 2.10 64.09 – 2.06	Depositor EDS
% Data completeness (in resolution range)	88.2 (64.09-2.10) 85.1 (64.09-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.62 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.187 , 0.227 0.182 , 0.222	Depositor DCC
$R_{free}$ test set	8009 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.3	EDS
Estimated twinning fraction	0.287 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 166892 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: AZI, GOL, CBE, SF4, TEO, BHG, F3S, FES, PEE, HEM, UNL, K, FAD

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	0.65	0/4832	0.81	5/6543 (0.1%)
1	N	0.66	0/4826	0.81	5/6535 (0.1%)
2	B	0.66	0/1959	0.81	2/2641 (0.1%)
2	O	0.64	0/1959	0.80	2/2641 (0.1%)
3	C	0.51	0/1107	0.61	0/1506
3	P	0.49	0/1107	0.60	0/1506
4	D	0.44	0/788	0.60	0/1082
4	Q	0.43	0/788	0.59	0/1082
All	All	0.62	0/17366	0.77	14/23536 (0.1%)

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
3	C	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	N	469	ARG	NE-CZ-NH2	-7.86	116.37	120.30
2	O	18	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	469	ARG	NE-CZ-NH2	-6.79	116.91	120.30
2	O	18	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	B	18	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	N	360	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	360	LEU	CA-CB-CG	5.64	128.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	256	GLY	N-CA-C	-5.62	99.04	113.10
1	A	256	GLY	N-CA-C	-5.52	99.31	113.10
1	N	140	GLY	N-CA-C	5.23	126.18	113.10
1	A	140	GLY	N-CA-C	5.17	126.04	113.10
1	N	54	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	54	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	30	TYR	Sidechain

## 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	4731	0	4614	53	0
1	N	4725	0	4609	62	0
2	B	1918	0	1910	31	0
2	O	1918	0	1909	31	0
3	C	1078	0	1118	39	0
3	P	1078	0	1118	39	0
4	D	765	0	761	17	0
4	Q	765	0	761	14	0
5	C	18	0	24	0	0
5	P	18	0	24	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
7	A	3	0	0	0	0
8	A	53	0	29	3	0
8	N	53	0	29	3	0
9	B	4	0	0	0	0
9	O	4	0	0	0	0
10	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	O	8	0	0	0	0
11	B	7	0	0	0	0
11	O	7	0	0	0	0
12	C	41	0	24	1	0
12	P	41	0	24	0	0
13	C	16	0	13	12	0
13	P	16	0	13	10	0
14	A	9	0	2	3	0
14	N	9	0	2	2	0
15	D	24	0	40	0	0
15	Q	24	0	40	2	0
16	A	29	0	0	7	0
16	B	14	0	0	3	0
16	C	22	0	0	4	0
16	D	9	0	0	0	0
16	N	24	0	0	2	0
16	O	10	0	0	3	0
16	P	11	0	0	2	0
16	Q	6	0	0	0	0
17	B	6	0	8	0	0
17	C	6	0	8	1	0
17	O	6	0	8	2	0
17	P	6	0	8	0	0
18	A	550	0	0	8	0
18	B	299	0	0	5	0
18	C	109	0	0	4	0
18	D	57	0	0	1	0
18	N	545	0	0	18	0
18	O	285	0	0	5	0
18	P	90	0	0	5	0
18	Q	65	0	0	1	0
All	All	19494	0	17096	289	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 (289) 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)
13:C:144:CBE:O7	13:C:144:CBE:C2	1.73	1.36
13:P:202:CBE:C2	13:P:202:CBE:O7	1.73	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:144:CBE:O7	13:C:144:CBE:C6	1.81	1.26
13:P:202:CBE:C6	13:P:202:CBE:O7	1.82	1.26
16:B:1005:UNL:O5	16:B:1005:UNL:O6	1.55	1.25
16:A:1003:UNL:O5	16:A:1003:UNL:O6	1.54	1.25
16:O:1005:UNL:O6	16:O:1005:UNL:O5	1.54	1.24
16:A:1004:UNL:O5	16:A:1004:UNL:O6	1.55	1.23
16:P:211:UNL:O5	16:P:211:UNL:O1	1.57	1.22
16:C:214:UNL:O6	16:C:214:UNL:O5	1.56	1.22
16:O:1005:UNL:O1	16:O:1005:UNL:O5	1.57	1.22
16:C:145:UNL:O5	16:C:145:UNL:O6	1.55	1.22
16:P:211:UNL:O5	16:P:211:UNL:O6	1.55	1.22
16:C:145:UNL:O5	16:C:145:UNL:O1	1.57	1.22
16:N:1003:UNL:O1	16:N:1003:UNL:O5	1.58	1.21
16:N:1003:UNL:O5	16:N:1003:UNL:O6	1.56	1.21
16:A:1003:UNL:O5	16:A:1003:UNL:O1	1.57	1.20
16:B:1005:UNL:O5	16:B:1005:UNL:O1	1.57	1.18
16:A:1004:UNL:O5	16:A:1004:UNL:O1	1.59	1.16
16:C:214:UNL:O5	16:C:214:UNL:O1	1.59	1.15
2:O:66:ARG:HB2	2:O:66:ARG:HH11	1.22	1.03
2:B:66:ARG:HH11	2:B:66:ARG:HB2	1.24	1.02
1:N:189:ARG:HD3	1:N:439:PRO:HB2	1.42	1.01
1:A:189:ARG:HD3	1:A:439:PRO:HB2	1.43	1.00
1:A:112:ASN:HD22	2:B:138:GLY:H	1.13	0.95
1:N:280:GLY:HA2	18:N:1552:HOH:O	1.68	0.93
1:N:96:ILE:HG21	18:N:1568:HOH:O	1.68	0.91
1:N:112:ASN:HD22	2:O:138:GLY:H	1.22	0.86
16:A:1003:UNL:O5	16:A:1003:UNL:O4	1.94	0.85
16:O:1005:UNL:O3	16:O:1005:UNL:O5	1.95	0.85
3:P:40:ILE:HA	13:P:202:CBE:H11	1.60	0.83
1:A:297:ARG:HH22	14:A:1002:TEO:C3	1.92	0.82
1:N:96:ILE:HD13	18:N:1568:HOH:O	1.78	0.82
3:P:40:ILE:HA	13:P:202:CBE:C1	2.11	0.81
3:C:40:ILE:HA	13:C:144:CBE:H11	1.62	0.81
2:O:66:ARG:CB	2:O:66:ARG:HH11	1.94	0.79
2:B:66:ARG:HH11	2:B:66:ARG:CB	1.95	0.79
2:O:214:ARG:HH22	4:Q:53:GLN:HE22	1.31	0.79
1:A:507:LYS:HE3	18:A:2803:HOH:O	1.83	0.79
2:B:214:ARG:HH22	4:D:53:GLN:HE22	1.29	0.78
1:A:112:ASN:ND2	2:B:138:GLY:H	1.81	0.78
3:C:101:ASN:HD21	3:C:104:ARG:HH11	1.30	0.78
1:N:297:ARG:HH22	14:N:1002:TEO:C3	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:24:LEU:HB2	4:Q:25:PRO:HD3	1.66	0.77
3:C:26:HIS:CD2	3:C:27:ILE:H	2.03	0.77
4:D:24:LEU:HB2	4:D:25:PRO:HD3	1.66	0.77
3:P:26:HIS:CD2	3:P:27:ILE:H	2.04	0.76
3:P:101:ASN:HD21	3:P:104:ARG:HH11	1.32	0.75
2:B:216:HIS:HD2	13:C:144:CBE:H51	1.51	0.75
1:A:181:LEU:HD21	1:A:211:ILE:HD11	1.67	0.75
1:A:13:PRO:HA	18:A:2907:HOH:O	1.87	0.74
3:P:7:GLU:O	3:P:11:ARG:HG2	1.88	0.74
3:P:3:THR:CG2	3:P:7:GLU:HB2	2.16	0.74
3:C:40:ILE:HA	13:C:144:CBE:C1	2.16	0.74
2:O:216:HIS:HD2	13:P:202:CBE:H51	1.52	0.74
1:N:181:LEU:HD21	1:N:211:ILE:HD11	1.68	0.73
3:C:7:GLU:O	3:C:11:ARG:HG2	1.88	0.73
3:C:3:THR:CG2	3:C:7:GLU:HB2	2.18	0.72
3:P:141:SER:HB2	15:Q:210:PEE:H27	1.72	0.70
1:N:112:ASN:ND2	2:O:138:GLY:H	1.91	0.67
2:O:18:ARG:NH2	2:O:56:ASP:OD2	2.28	0.67
1:A:216:TYR:H	1:A:366:ASN:ND2	1.93	0.67
1:A:486:GLY:O	1:A:490:GLN:HG3	1.96	0.66
1:N:486:GLY:O	1:N:490:GLN:HG3	1.96	0.65
1:A:18:GLU:OE1	1:A:438:VAL:HG11	1.96	0.65
1:N:277:ASN:O	18:N:1552:HOH:O	2.15	0.65
3:C:43:ARG:CZ	13:C:144:CBE:H61	2.26	0.65
13:P:202:CBE:C6	13:P:202:CBE:C2	2.75	0.64
13:C:144:CBE:C2	13:C:144:CBE:C6	2.75	0.64
3:C:40:ILE:HG22	13:C:144:CBE:H12A	1.79	0.64
1:A:72:GLU:OE1	1:A:144:HIS:HD2	1.81	0.64
1:N:84:VAL:N	18:N:1568:HOH:O	2.30	0.64
1:N:72:GLU:OE1	1:N:144:HIS:HD2	1.80	0.64
1:N:216:TYR:H	1:N:366:ASN:ND2	1.96	0.64
2:B:18:ARG:NH2	2:B:56:ASP:OD2	2.31	0.64
3:P:40:ILE:HG22	13:P:202:CBE:H12A	1.80	0.64
1:N:276:ILE:HB	18:N:1552:HOH:O	1.98	0.63
16:A:1003:UNL:O5	16:A:1003:UNL:O3	2.17	0.63
2:O:214:ARG:HH12	4:Q:53:GLN:NE2	1.97	0.62
1:N:60:ALA:HB3	1:N:154:GLY:HA3	1.82	0.62
1:N:121:GLU:HG2	18:N:1145:HOH:O	1.99	0.62
1:N:276:ILE:HD12	18:N:1552:HOH:O	1.99	0.62
3:C:37:ALA:O	3:C:40:ILE:HG12	2.00	0.61
3:P:37:ALA:O	3:P:40:ILE:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:ARG:HH12	4:D:53:GLN:NE2	1.98	0.60
1:A:573:ARG:HD3	18:A:2910:HOH:O	2.00	0.60
4:Q:63:THR:HB	4:Q:64:PRO:HD3	1.82	0.60
2:O:218:ILE:HD11	13:P:202:CBE:H52	1.83	0.60
1:N:207:LYS:NZ	1:N:436:GLU:HB2	2.16	0.60
4:D:22:GLY:O	4:D:25:PRO:HD2	2.01	0.60
4:D:63:THR:HB	4:D:64:PRO:HD3	1.83	0.59
3:C:34:LEU:HB3	3:C:35:PRO:HD3	1.83	0.59
1:N:401:ALA:N	1:N:402:SER:HA	2.18	0.59
3:P:69:HIS:O	3:P:73:VAL:HG23	2.03	0.59
1:A:401:ALA:N	1:A:402:SER:HA	2.18	0.59
3:C:69:HIS:O	3:C:73:VAL:HG23	2.02	0.59
4:Q:22:GLY:O	4:Q:25:PRO:HD2	2.02	0.59
1:N:18:GLU:OE1	1:N:438:VAL:HG11	2.02	0.58
3:C:34:LEU:HD23	18:C:1715:HOH:O	2.04	0.58
1:A:297:ARG:HH22	14:A:1002:TEO:C4	2.17	0.58
17:O:1009:GOL:H32	18:O:1055:HOH:O	2.03	0.58
3:P:34:LEU:HB3	3:P:35:PRO:HD3	1.84	0.57
1:A:207:LYS:NZ	1:A:436:GLU:HB2	2.20	0.57
16:A:1003:UNL:O5	16:A:1003:UNL:O2	2.21	0.57
3:P:43:ARG:CZ	13:P:202:CBE:H61	2.34	0.57
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.86	0.57
2:O:21:PRO:O	2:O:24:PRO:HD3	2.05	0.56
1:N:207:LYS:HZ1	1:N:436:GLU:HB2	1.71	0.56
1:A:112:ASN:HD22	2:B:138:GLY:N	1.93	0.56
3:P:4:THR:OG1	3:P:7:GLU:HG3	2.05	0.56
3:P:55:LEU:O	3:P:58:VAL:HG12	2.06	0.56
3:P:106:LEU:O	3:P:110:MET:HG3	2.05	0.56
3:C:106:LEU:O	3:C:110:MET:HG3	2.06	0.55
1:A:417:LEU:HD21	8:A:1001:FAD:H5'2	1.88	0.55
1:N:112:ASN:HD22	2:O:138:GLY:N	2.00	0.55
1:N:263:LEU:HG	1:N:264:ILE:N	2.22	0.55
3:C:55:LEU:O	3:C:58:VAL:HG12	2.07	0.55
3:C:68:PRO:HA	4:D:99:MET:HE1	1.88	0.54
4:D:36:ASP:OD2	4:D:93:ILE:N	2.39	0.54
2:B:218:ILE:HD11	13:C:144:CBE:H52	1.89	0.54
18:N:1307:HOH:O	2:O:66:ARG:HB3	2.07	0.54
1:A:263:LEU:HG	1:A:264:ILE:N	2.21	0.54
2:B:66:ARG:CG	2:B:66:ARG:NH1	2.71	0.54
3:C:101:ASN:ND2	3:C:104:ARG:HH11	2.04	0.54
4:Q:36:ASP:OD2	4:Q:93:ILE:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:507:LYS:HE3	18:N:1183:HOH:O	2.07	0.54
4:Q:3:SER:HA	18:Q:2973:HOH:O	2.08	0.54
3:C:42:HIS:HD2	3:C:101:ASN:HB3	1.73	0.54
2:O:198:TYR:O	2:O:202:ARG:HG3	2.08	0.54
2:O:223:ARG:HA	3:P:116:LEU:HD21	1.90	0.54
3:C:4:THR:OG1	3:C:7:GLU:HG3	2.06	0.53
3:P:47:VAL:O	3:P:51:LEU:HG	2.09	0.53
2:O:223:ARG:HD3	18:P:1197:HOH:O	2.09	0.53
3:P:3:THR:HG22	3:P:7:GLU:HB2	1.89	0.53
1:A:331:GLN:HB3	18:A:2596:HOH:O	2.09	0.53
1:N:297:ARG:HH22	14:N:1002:TEO:C4	2.21	0.52
2:B:66:ARG:HH11	2:B:66:ARG:CG	2.23	0.52
3:C:47:VAL:O	3:C:51:LEU:HG	2.09	0.52
1:A:50:LEU:HD21	1:A:228:THR:HG21	1.91	0.52
3:C:26:HIS:CG	3:C:27:ILE:H	2.27	0.52
2:O:66:ARG:NH1	2:O:66:ARG:HB2	2.07	0.52
3:P:42:HIS:HD2	3:P:101:ASN:HB3	1.74	0.52
3:C:3:THR:HG23	3:C:7:GLU:HB2	1.92	0.51
2:O:66:ARG:NH1	2:O:66:ARG:CG	2.73	0.51
2:B:58:THR:HB	18:B:2575:HOH:O	2.09	0.51
2:O:27:LYS:HD3	18:O:1219:HOH:O	2.09	0.51
1:N:155:HIS:HD2	18:O:1154:HOH:O	1.94	0.51
3:P:26:HIS:CG	3:P:27:ILE:H	2.29	0.51
1:N:496:LEU:HD12	1:N:536:ILE:HG21	1.92	0.51
1:N:50:LEU:HD21	1:N:228:THR:HG21	1.93	0.51
2:B:214:ARG:NH2	4:D:53:GLN:HE22	2.04	0.51
1:N:280:GLY:CA	18:N:1552:HOH:O	2.44	0.50
1:N:417:LEU:HD21	8:N:1001:FAD:H5'2	1.92	0.50
2:O:66:ARG:CG	2:O:66:ARG:HH11	2.23	0.50
3:C:70:TYR:O	3:C:74:VAL:HG23	2.12	0.50
1:N:87:SER:HB2	1:N:405:GLY:HA3	1.93	0.50
3:P:3:THR:HG23	3:P:7:GLU:OE1	2.11	0.50
3:P:101:ASN:ND2	3:P:104:ARG:HH11	2.05	0.50
18:C:1528:HOH:O	3:P:40:ILE:HD11	2.11	0.49
2:B:223:ARG:HA	3:C:116:LEU:HD21	1.94	0.49
1:N:83:THR:C	18:N:1568:HOH:O	2.51	0.49
2:O:214:ARG:NH2	4:Q:53:GLN:HE22	2.06	0.49
2:B:198:TYR:O	2:B:202:ARG:HG3	2.12	0.49
1:A:87:SER:HB2	1:A:405:GLY:HA3	1.94	0.49
3:P:70:TYR:O	3:P:74:VAL:HG23	2.11	0.49
16:B:1005:UNL:O5	16:B:1005:UNL:O3	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:326:HIS:HE1	18:N:1240:HOH:O	1.95	0.49
4:D:44:THR:HG21	4:D:80:PHE:HB2	1.95	0.49
3:P:3:THR:HG23	3:P:7:GLU:HB2	1.92	0.49
3:C:3:THR:HG22	3:C:7:GLU:HB2	1.91	0.49
1:A:496:LEU:HD12	1:A:536:ILE:HG21	1.95	0.49
1:N:83:THR:HB	18:N:1568:HOH:O	2.12	0.48
4:Q:44:THR:HG21	4:Q:80:PHE:HB2	1.95	0.48
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.48	0.48
1:N:431:THR:HG22	1:N:432:CYS:SG	2.53	0.48
3:C:3:THR:HG23	3:C:7:GLU:OE1	2.12	0.48
4:D:33:PRO:HG2	18:D:2339:HOH:O	2.13	0.48
1:A:431:THR:HG22	1:A:432:CYS:SG	2.54	0.48
1:A:155:HIS:HD2	18:B:2145:HOH:O	1.97	0.48
18:B:1949:HOH:O	4:D:4:LYS:HE3	2.14	0.48
1:A:61:GLN:OE1	1:A:265:THR:HB	2.14	0.48
1:A:369:GLY:HA2	18:A:2554:HOH:O	2.13	0.47
4:Q:27:ALA:HB1	15:Q:210:PEE:H63	1.96	0.47
1:A:205:ARG:NH2	1:A:438:VAL:HG13	2.29	0.47
1:A:453:LEU:C	1:A:453:LEU:HD23	2.35	0.47
3:P:67:PHE:HB3	3:P:68:PRO:HD3	1.96	0.47
2:B:216:HIS:HD2	13:C:144:CBE:C5	2.25	0.47
1:N:205:ARG:NH2	1:N:438:VAL:HG13	2.29	0.47
2:O:155:LEU:CD1	2:O:192:ILE:HD11	2.45	0.47
1:N:253:HIS:NE2	1:N:263:LEU:HD11	2.29	0.47
2:B:245:TYR:O	4:D:4:LYS:NZ	2.48	0.47
1:N:515:TRP:CD1	2:O:108:VAL:HG11	2.50	0.47
3:C:67:PHE:HB3	3:C:68:PRO:HD3	1.96	0.47
1:N:174:VAL:HG12	1:N:175:GLU:HG3	1.97	0.47
2:O:245:TYR:O	4:Q:4:LYS:NZ	2.48	0.47
17:C:294:GOL:O3	4:D:93:ILE:HG23	2.15	0.47
1:N:61:GLN:OE1	1:N:265:THR:HB	2.15	0.47
1:A:515:TRP:CD1	2:B:108:VAL:HG11	2.50	0.46
3:P:116:LEU:HA	3:P:116:LEU:HD12	1.81	0.46
2:B:214:ARG:HH12	4:D:53:GLN:HE21	1.64	0.46
2:O:155:LEU:HD11	2:O:192:ILE:HD11	1.98	0.46
2:B:155:LEU:HD11	2:B:192:ILE:HD11	1.98	0.46
3:C:88:LYS:NZ	3:C:140:ILE:HG12	2.30	0.46
2:B:66:ARG:HB2	2:B:66:ARG:NH1	2.09	0.46
1:A:253:HIS:NE2	1:A:263:LEU:HD11	2.31	0.46
3:C:68:PRO:HA	4:D:99:MET:CE	2.45	0.46
1:A:253:HIS:O	1:A:361:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:124:LYS:NZ	18:N:1327:HOH:O	2.48	0.46
18:O:1175:HOH:O	3:P:6:LYS:HE2	2.15	0.46
3:P:34:LEU:HD23	18:P:1034:HOH:O	2.16	0.46
1:N:462:THR:HG21	18:N:1439:HOH:O	2.16	0.46
3:C:65:GLU:HG3	3:C:69:HIS:CD2	2.51	0.45
1:N:375:LYS:HE2	18:N:1371:HOH:O	2.15	0.45
2:B:216:HIS:CD2	13:C:144:CBE:H51	2.42	0.45
2:B:98:LYS:HE3	18:C:2293:HOH:O	2.16	0.45
2:O:104:HIS:O	17:O:1009:GOL:H12	2.17	0.45
1:N:453:LEU:HD23	1:N:453:LEU:C	2.37	0.45
1:A:197:GLU:HB2	18:A:2047:HOH:O	2.16	0.45
3:C:101:ASN:ND2	3:C:104:ARG:HD3	2.32	0.45
1:N:220:TYR:CG	1:N:363:VAL:HG21	2.52	0.45
1:A:381:HIS:ND1	1:A:386:ASP:OD1	2.46	0.45
2:O:191:MET:CE	2:O:203:LEU:HD21	2.46	0.45
1:N:381:HIS:ND1	1:N:386:ASP:OD1	2.47	0.44
2:O:216:HIS:CD2	13:P:202:CBE:H51	2.42	0.44
2:B:155:LEU:CD1	2:B:192:ILE:HD11	2.46	0.44
2:O:123:LYS:NZ	3:P:3:THR:O	2.47	0.44
1:N:72:GLU:OE1	1:N:144:HIS:CD2	2.66	0.44
2:B:121:GLN:NE2	2:B:171:TYR:OH	2.49	0.44
3:P:63:LEU:HA	3:P:64:PRO:HD3	1.81	0.44
1:A:155:HIS:HE1	2:B:156:TYR:O	2.00	0.44
2:B:191:MET:CE	2:B:203:LEU:HD21	2.48	0.44
3:P:120:GLU:HG3	18:P:1252:HOH:O	2.18	0.44
3:C:116:LEU:HA	3:C:116:LEU:HD12	1.83	0.44
1:N:567:LEU:HD23	1:N:570:GLN:NE2	2.32	0.44
1:A:174:VAL:HG12	1:A:175:GLU:HG3	2.00	0.44
1:A:72:GLU:OE1	1:A:144:HIS:CD2	2.67	0.43
1:N:463:ILE:O	1:N:506:LEU:HA	2.18	0.43
3:P:65:GLU:HG3	3:P:69:HIS:CD2	2.53	0.43
1:N:189:ARG:HH11	1:N:189:ARG:HG2	1.83	0.43
3:P:42:HIS:CD2	3:P:101:ASN:HB3	2.53	0.43
1:N:60:ALA:HA	8:N:1001:FAD:N5	2.34	0.43
1:A:567:LEU:HD23	1:A:570:GLN:NE2	2.33	0.43
1:N:71:MET:HG2	1:N:127:GLN:HB2	2.00	0.43
1:A:213:THR:OG1	1:A:233:GLY:HA3	2.18	0.43
1:A:121:GLU:HG2	18:A:1907:HOH:O	2.18	0.43
3:C:42:HIS:CD2	3:C:101:ASN:HB3	2.53	0.43
1:N:155:HIS:CD2	18:O:1154:HOH:O	2.71	0.43
1:A:220:TYR:CD2	1:A:363:VAL:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:268:CYS:HB3	1:N:325:LEU:HD21	2.00	0.43
1:N:96:ILE:CG2	18:N:1568:HOH:O	2.46	0.43
2:B:53:ASN:HA	18:B:1848:HOH:O	2.18	0.43
2:O:214:ARG:HH12	4:Q:53:GLN:HE21	1.65	0.43
1:A:268:CYS:HB3	1:A:325:LEU:HD21	2.00	0.43
3:P:101:ASN:ND2	3:P:104:ARG:HD3	2.34	0.43
1:A:189:ARG:HH11	1:A:189:ARG:HG2	1.83	0.43
3:C:11:ARG:HG3	18:C:2021:HOH:O	2.18	0.43
1:A:189:ARG:NE	18:A:2471:HOH:O	2.30	0.42
4:Q:53:GLN:HA	4:Q:53:GLN:NE2	2.34	0.42
4:D:53:GLN:NE2	4:D:53:GLN:HA	2.34	0.42
1:A:39:GLU:HB3	1:A:168:TYR:CE2	2.54	0.42
2:O:98:LYS:HE3	18:P:1629:HOH:O	2.18	0.42
1:N:60:ALA:HA	8:N:1001:FAD:C5X	2.49	0.42
1:N:253:HIS:O	1:N:361:PRO:HA	2.18	0.42
1:A:60:ALA:HA	8:A:1001:FAD:C5X	2.50	0.42
3:C:29:ILE:HD12	3:C:29:ILE:C	2.40	0.42
3:C:43:ARG:HE	12:C:143:HEM:CGA	2.32	0.42
3:P:11:ARG:HG3	18:P:1350:HOH:O	2.19	0.41
1:A:297:ARG:HH22	14:A:1002:TEO:C2	2.34	0.41
2:B:123:LYS:NZ	3:C:3:THR:O	2.51	0.41
1:A:71:MET:HG2	1:A:127:GLN:HB2	2.01	0.41
1:N:382:VAL:O	1:N:385:GLU:HG3	2.20	0.41
1:A:382:VAL:O	1:A:385:GLU:HG3	2.20	0.41
3:C:93:PHE:HB3	3:C:94:PRO:CD	2.50	0.41
3:P:55:LEU:HD23	3:P:55:LEU:HA	1.84	0.41
3:P:29:ILE:HD12	3:P:29:ILE:C	2.41	0.41
3:P:55:LEU:HA	3:P:58:VAL:HG12	2.02	0.41
1:N:213:THR:OG1	1:N:233:GLY:HA3	2.20	0.41
1:N:39:GLU:HB3	1:N:168:TYR:CE2	2.56	0.41
1:A:207:LYS:HZ1	1:A:436:GLU:HB2	1.85	0.41
1:A:60:ALA:HA	8:A:1001:FAD:N5	2.35	0.41
1:N:305:THR:O	1:N:309:ARG:HG3	2.20	0.41
2:O:102:LEU:HA	2:O:103:PRO:HD3	1.94	0.41
3:C:138:ALA:C	3:C:140:ILE:H	2.24	0.40
4:Q:87:ASN:HA	4:Q:92:GLY:HA2	2.04	0.40
1:N:182:LEU:HD23	1:N:182:LEU:HA	1.88	0.40
4:D:27:ALA:HA	4:D:35:VAL:HG11	2.04	0.40
3:C:27:ILE:HG13	13:C:144:CBE:H14	2.03	0.40
1:A:63:GLY:HA2	1:A:153:THR:HG21	2.04	0.40
2:B:227:LYS:HE3	18:B:2787:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	611/621 (98%)	590 (97%)	21 (3%)	0	100	100
1	N	610/621 (98%)	590 (97%)	20 (3%)	0	100	100
2	B	237/252 (94%)	228 (96%)	8 (3%)	1 (0%)	39	37
2	O	237/252 (94%)	229 (97%)	7 (3%)	1 (0%)	39	37
3	C	138/141 (98%)	135 (98%)	2 (1%)	1 (1%)	26	21
3	P	138/141 (98%)	135 (98%)	2 (1%)	1 (1%)	26	21
4	D	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
4	Q	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
All	All	2169/2234 (97%)	2101 (97%)	64 (3%)	4 (0%)	52	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	66	ARG
2	O	66	ARG
3	C	140	ILE
3	P	140	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	498/506 (98%)	495 (99%)	3 (1%)	90	94
1	N	497/506 (98%)	493 (99%)	4 (1%)	86	91
2	B	214/219 (98%)	211 (99%)	3 (1%)	74	80
2	O	214/219 (98%)	211 (99%)	3 (1%)	74	80
3	C	118/119 (99%)	117 (99%)	1 (1%)	86	91
3	P	118/119 (99%)	117 (99%)	1 (1%)	86	91
4	D	78/79 (99%)	75 (96%)	3 (4%)	40	40
4	Q	78/79 (99%)	75 (96%)	3 (4%)	40	40
All	All	1815/1846 (98%)	1794 (99%)	21 (1%)	78	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	73	ASP
1	A	130	PHE
2	B	63	ARG
2	B	189	ARG
2	B	229	LEU
3	C	11	ARG
4	D	14	ARG
4	D	36	ASP
4	D	101	TRP
1	N	10	THR
1	N	72	GLU
1	N	73	ASP
1	N	130	PHE
2	O	63	ARG
2	O	189	ARG
2	O	229	LEU
3	P	11	ARG
4	Q	14	ARG
4	Q	36	ASP
4	Q	101	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN

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Mol	Chain	Res	Type
1	A	112	ASN
1	A	144	HIS
1	A	155	HIS
1	A	185	ASN
1	A	326	HIS
1	A	366	ASN
1	A	383	ASN
1	A	534	GLN
1	A	571	GLN
2	B	121	GLN
3	C	26	HIS
3	C	42	HIS
3	C	69	HIS
3	C	101	ASN
4	D	9	HIS
4	D	53	GLN
1	N	43	ASN
1	N	112	ASN
1	N	144	HIS
1	N	155	HIS
1	N	185	ASN
1	N	366	ASN
1	N	383	ASN
1	N	534	GLN
1	N	571	GLN
2	O	121	GLN
2	O	216	HIS
3	P	26	HIS
3	P	42	HIS
3	P	69	HIS
3	P	101	ASN
4	Q	9	HIS
4	Q	53	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 122 ligands modelled in this entry, 95 are unknown and 4 are monoatomic - leaving 23 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
8	FAD	A	1001	1	48,58,58	2.27	15 (31%)	54,89,89	2.77	15 (27%)
14	TEO	A	1002	-	0,8,8	0.00	-	1,10,10	6.30	1 (100%)
7	AZI	A	623	-	0,2,2	0.00	-	0,1,1	0.00	-
9	FES	B	1002	2	0,4,4	0.00	-	0,4,4	0.00	-
10	SF4	B	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
11	F3S	B	1004	2	0,9,9	0.00	-	0,15,15	0.00	-
17	GOL	B	1010	-	5,5,5	1.05	0	5,5,5	0.57	0
5	BHG	C	142	-	18,18,18	1.85	5 (27%)	23,23,23	0.78	0
12	HEM	C	143	3,4	29,48,50	2.42	10 (34%)	24,80,82	2.47	8 (33%)
13	CBE	C	144	-	15,17,17	6.05	10 (66%)	17,22,22	2.29	3 (17%)
17	GOL	C	294	-	5,5,5	1.17	0	5,5,5	0.63	0
15	PEE	D	109	-	22,22,50	0.86	1 (4%)	20,20,55	0.97	2 (10%)
8	FAD	N	1001	1	48,58,58	2.27	15 (31%)	54,89,89	2.73	13 (24%)
14	TEO	N	1002	-	0,8,8	0.00	-	1,10,10	6.21	1 (100%)
9	FES	O	1002	2	0,4,4	0.00	-	0,4,4	0.00	-
10	SF4	O	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
11	F3S	O	1004	2	0,9,9	0.00	-	0,15,15	0.00	-
17	GOL	O	1009	-	5,5,5	1.02	0	5,5,5	0.60	0
12	HEM	P	201	3,4	29,48,50	2.53	10 (34%)	24,80,82	2.49	8 (33%)
13	CBE	P	202	-	15,17,17	6.19	10 (66%)	17,22,22	2.24	3 (17%)
5	BHG	P	204	-	18,18,18	1.53	3 (16%)	23,23,23	0.68	0
17	GOL	P	208	-	5,5,5	1.23	0	5,5,5	0.65	0
15	PEE	Q	210	-	22,22,50	0.87	1 (4%)	20,20,55	0.95	2 (10%)

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
8	FAD	A	1001	1	-	0/30/50/50	0/6/6/6
14	TEO	A	1002	-	1/1/3/4	0/1/8/8	0/0/0/0
7	AZI	A	623	-	-	0/0/0/0	0/0/0/0
9	FES	B	1002	2	-	0/0/4/4	0/1/1/1
10	SF4	B	1003	2	-	0/0/48/48	0/6/5/5
11	F3S	B	1004	2	-	0/0/24/24	0/0/3/3
17	GOL	B	1010	-	-	0/4/4/4	0/0/0/0
5	BHG	C	142	-	1/1/5/5	0/9/29/29	0/1/1/1
12	HEM	C	143	3,4	-	0/6/50/54	0/0/8/8
13	CBE	C	144	-	-	0/6/19/19	0/1/2/2
17	GOL	C	294	-	-	0/4/4/4	0/0/0/0
15	PEE	D	109	-	-	0/18/18/54	0/0/0/0
8	FAD	N	1001	1	-	0/30/50/50	0/6/6/6
14	TEO	N	1002	-	1/1/3/4	0/1/8/8	0/0/0/0
9	FES	O	1002	2	-	0/0/4/4	0/1/1/1
10	SF4	O	1003	2	-	0/0/48/48	0/6/5/5
11	F3S	O	1004	2	-	0/0/24/24	0/0/3/3
17	GOL	O	1009	-	-	0/4/4/4	0/0/0/0
12	HEM	P	201	3,4	-	0/6/50/54	0/0/8/8
13	CBE	P	202	-	-	0/6/19/19	0/1/2/2
5	BHG	P	204	-	1/1/5/5	0/9/29/29	0/1/1/1
17	GOL	P	208	-	-	0/4/4/4	0/0/0/0
15	PEE	Q	210	-	-	0/18/18/54	0/0/0/0

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	202	CBE	C3-S4	-18.28	1.39	1.74
13	C	144	CBE	C3-S4	-17.73	1.40	1.74
13	P	202	CBE	C5-S4	-8.79	1.45	1.80
13	C	144	CBE	C5-S4	-8.77	1.45	1.80
12	P	201	HEM	C2D-C3D	-6.17	1.36	1.54
12	P	201	HEM	CAB-C3B	-5.87	1.39	1.53
12	C	143	HEM	C2D-C3D	-5.82	1.37	1.54
12	C	143	HEM	CAB-C3B	-5.67	1.40	1.53
12	P	201	HEM	CAC-C3C	-4.62	1.42	1.53
12	C	143	HEM	C3D-C4D	-4.42	1.45	1.51
8	A	1001	FAD	PA-O2A	-4.21	1.37	1.54
8	N	1001	FAD	PA-O1A	-4.19	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	143	HEM	CAC-C3C	-4.14	1.43	1.53
12	P	201	HEM	C3C-C4C	-4.12	1.44	1.52
8	N	1001	FAD	PA-O2A	-4.09	1.37	1.54
12	P	201	HEM	C3D-C4D	-3.95	1.46	1.51
12	P	201	HEM	C2C-C1C	-3.89	1.45	1.52
8	A	1001	FAD	PA-O1A	-3.86	1.37	1.51
12	C	143	HEM	C3C-C4C	-3.83	1.45	1.52
13	C	144	CBE	C11-N10	-3.78	1.34	1.41
13	P	202	CBE	C11-N10	-3.61	1.34	1.41
12	C	143	HEM	C2C-C1C	-3.48	1.46	1.52
15	Q	210	PEE	C19-C18	-2.86	1.35	1.51
15	D	109	PEE	C19-C18	-2.67	1.36	1.51
12	C	143	HEM	CAD-C3D	-2.36	1.49	1.54
8	A	1001	FAD	O4B-C1B	-2.25	1.38	1.41
8	A	1001	FAD	C5A-N7A	-2.05	1.32	1.39
12	P	201	HEM	CAD-C3D	-2.04	1.50	1.54
12	P	201	HEM	C2D-C1D	-2.04	1.45	1.51
12	C	143	HEM	C2D-C1D	-2.02	1.45	1.51
8	N	1001	FAD	C9-C9A	2.01	1.45	1.40
13	C	144	CBE	C12-C11	2.08	1.42	1.39
5	C	142	BHG	O5-C5	2.08	1.49	1.44
12	P	201	HEM	C4C-NC	2.18	1.38	1.36
5	C	142	BHG	C3-C2	2.19	1.58	1.52
8	A	1001	FAD	C5X-N5	2.21	1.38	1.35
8	N	1001	FAD	C4A-N3A	2.22	1.38	1.35
13	C	144	CBE	C15-C16	2.25	1.43	1.38
13	P	202	CBE	C13-C12	2.29	1.43	1.38
5	P	204	BHG	C4-C5	2.36	1.58	1.53
5	C	142	BHG	C4-C5	2.37	1.58	1.53
8	N	1001	FAD	C6-C7	2.37	1.44	1.37
8	N	1001	FAD	C4'-C3'	2.37	1.58	1.53
13	C	144	CBE	C13-C12	2.44	1.43	1.38
8	A	1001	FAD	C2A-N1A	2.46	1.38	1.33
13	P	202	CBE	C15-C14	2.49	1.44	1.38
8	A	1001	FAD	C6-C7	2.49	1.44	1.37
13	P	202	CBE	C15-C16	2.52	1.44	1.38
8	N	1001	FAD	C9A-N10	2.56	1.42	1.38
13	C	144	CBE	C15-C14	2.58	1.44	1.38
8	A	1001	FAD	C8-C7	2.62	1.48	1.41
13	C	144	CBE	C14-C13	2.67	1.44	1.38
12	C	143	HEM	C1C-NC	2.71	1.39	1.36
8	N	1001	FAD	C2A-N1A	2.76	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	1001	FAD	C6-C5X	2.78	1.46	1.41
8	N	1001	FAD	C8-C7	2.84	1.48	1.41
5	P	204	BHG	O5-C1	2.88	1.49	1.41
13	P	202	CBE	C12-C11	2.89	1.44	1.39
13	P	202	CBE	C14-C13	2.89	1.45	1.38
12	C	143	HEM	C4C-NC	3.15	1.39	1.36
5	C	142	BHG	O5-C1	3.24	1.50	1.41
8	A	1001	FAD	C4-C4X	3.26	1.47	1.41
8	A	1001	FAD	C1'-N10	3.28	1.51	1.48
12	P	201	HEM	C1C-NC	3.46	1.40	1.36
8	N	1001	FAD	C2A-N3A	3.53	1.38	1.32
8	A	1001	FAD	C9A-N10	3.69	1.43	1.38
13	P	202	CBE	C16-C11	3.96	1.45	1.39
8	A	1001	FAD	C4-N3	4.01	1.40	1.33
5	P	204	BHG	O1-C1	4.02	1.47	1.40
8	N	1001	FAD	C4-N3	4.04	1.40	1.33
8	A	1001	FAD	C2A-N3A	4.12	1.39	1.32
13	C	144	CBE	C16-C11	4.54	1.46	1.39
8	N	1001	FAD	C4-C4X	4.67	1.50	1.41
5	C	142	BHG	O1-C1	5.07	1.49	1.40
8	N	1001	FAD	C4X-N5	5.14	1.41	1.33
8	A	1001	FAD	C4X-N5	5.42	1.41	1.33
8	A	1001	FAD	C10-N10	6.59	1.46	1.39
8	N	1001	FAD	C10-N10	6.87	1.47	1.39
13	C	144	CBE	O7-C6	9.53	1.81	1.44
13	P	202	CBE	O7-C6	9.86	1.82	1.44

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1001	FAD	N3A-C2A-N1A	-12.50	119.32	128.89
8	N	1001	FAD	N3A-C2A-N1A	-12.22	119.54	128.89
8	N	1001	FAD	C4X-C10-N10	-6.27	116.82	120.52
8	A	1001	FAD	C4X-C10-N10	-6.03	116.97	120.52
8	A	1001	FAD	C4-C4X-C10	-4.97	116.76	119.94
8	N	1001	FAD	C4-C4X-C10	-4.61	116.99	119.94
8	N	1001	FAD	C1B-N9A-C4A	-3.45	121.73	126.94
8	A	1001	FAD	C1B-N9A-C4A	-3.36	121.86	126.94
8	N	1001	FAD	O3P-PA-O5B	-3.15	94.59	102.94
8	A	1001	FAD	O3P-PA-O5B	-3.09	94.74	102.94
8	N	1001	FAD	C4X-C4-N3	-3.07	119.39	123.59
8	A	1001	FAD	C4X-C4-N3	-2.72	119.87	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1001	FAD	O3P-P-O5'	-2.44	96.47	102.94
13	P	202	CBE	C3-C8-N10	-2.24	111.54	115.61
13	C	144	CBE	C3-C8-N10	-2.22	111.58	115.61
8	N	1001	FAD	O3P-P-O5'	-2.15	97.23	102.94
8	A	1001	FAD	O3'-C3'-C2'	-2.05	103.57	108.75
8	A	1001	FAD	C8M-C8-C7	2.02	125.16	120.73
8	N	1001	FAD	C1'-C2'-C3'	2.43	116.77	109.82
15	Q	210	PEE	C19-C18-C17	2.56	127.75	114.53
8	N	1001	FAD	O2P-P-O3P	2.57	116.74	105.09
8	A	1001	FAD	C1'-C2'-C3'	2.60	117.25	109.82
15	D	109	PEE	C19-C18-C17	2.65	128.23	114.53
15	Q	210	PEE	C20-C19-C18	2.67	128.33	114.53
15	D	109	PEE	C20-C19-C18	2.79	128.92	114.53
8	A	1001	FAD	O2P-P-O3P	2.95	118.49	105.09
12	C	143	HEM	CAD-C3D-C2D	3.21	122.43	113.22
12	C	143	HEM	CMD-C2D-C3D	3.31	128.97	114.35
12	P	201	HEM	CAD-C3D-C2D	3.38	122.94	113.22
12	P	201	HEM	CMD-C2D-C3D	3.38	129.31	114.35
8	N	1001	FAD	P-O3P-PA	3.49	142.52	132.73
8	A	1001	FAD	P-O3P-PA	3.58	142.78	132.73
12	C	143	HEM	CMC-C2C-C3C	3.64	124.91	116.20
12	P	201	HEM	CMC-C2C-C3C	3.74	125.16	116.20
12	C	143	HEM	CMB-C2B-C3B	3.94	125.63	116.20
12	P	201	HEM	C2D-C3D-C4D	4.07	108.40	101.50
12	C	143	HEM	CAB-C3B-C2B	4.15	126.14	116.20
12	P	201	HEM	CAB-C3B-C2B	4.18	126.22	116.20
12	P	201	HEM	CMB-C2B-C3B	4.22	126.31	116.20
12	C	143	HEM	C2D-C3D-C4D	4.23	108.66	101.50
8	A	1001	FAD	C4-C4X-N5	4.44	124.11	118.72
8	N	1001	FAD	C4-C4X-N5	4.46	124.13	118.72
12	P	201	HEM	CAD-C3D-C4D	4.59	128.66	112.47
12	C	143	HEM	CAD-C3D-C4D	4.66	128.90	112.47
12	P	201	HEM	CAC-C3C-C2C	4.98	128.13	116.20
13	P	202	CBE	O7-C2-C1	5.07	115.31	109.44
12	C	143	HEM	CAC-C3C-C2C	5.08	128.37	116.20
13	C	144	CBE	O7-C2-C1	5.43	115.72	109.44
8	A	1001	FAD	C4-N3-C2	5.64	120.12	115.25
8	N	1001	FAD	C4-N3-C2	5.67	120.15	115.25
14	N	1002	TEO	O2-C2-C3	6.21	122.44	109.53
8	N	1001	FAD	C4X-N5-C5X	6.23	123.93	116.76
8	A	1001	FAD	C4X-N5-C5X	6.28	123.98	116.76
14	A	1002	TEO	O2-C2-C3	6.30	122.64	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
13	C	144	CBE	C5-S4-C3	6.98	120.12	101.11
13	P	202	CBE	C5-S4-C3	7.08	120.39	101.11

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	142	BHG	C4
14	A	1002	TEO	C2
5	P	204	BHG	C4
14	N	1002	TEO	C2

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1001	FAD	3	0
14	A	1002	TEO	3	0
12	C	143	HEM	1	0
13	C	144	CBE	12	0
17	C	294	GOL	1	0
8	N	1001	FAD	3	0
14	N	1002	TEO	2	0
17	O	1009	GOL	2	0
13	P	202	CBE	10	0
15	Q	210	PEE	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	613/621 (98%)	-0.07	4 (0%) 89 91	11, 23, 45, 85	0
1	N	612/621 (98%)	-0.06	2 (0%) 94 95	10, 22, 42, 81	0
2	B	239/252 (94%)	-0.09	2 (0%) 87 90	15, 22, 38, 67	0
2	O	239/252 (94%)	-0.10	2 (0%) 87 90	13, 22, 37, 68	0
3	C	140/141 (99%)	0.21	6 (4%) 39 48	19, 34, 52, 75	0
3	P	140/141 (99%)	0.49	13 (9%) 11 15	18, 37, 77, 87	0
4	D	101/103 (98%)	0.53	8 (7%) 15 21	21, 41, 59, 62	0
4	Q	101/103 (98%)	0.79	12 (11%) 6 8	26, 47, 67, 75	0
All	All	2185/2234 (97%)	0.05	49 (2%) 65 71	10, 24, 53, 87	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	10	THR	9.1
3	P	140	ILE	8.2
3	P	141	SER	8.1
4	Q	93	ILE	6.6
3	C	140	ILE	6.2
4	Q	101	TRP	6.1
1	A	10	THR	6.1
1	A	9	SER	6.0
4	Q	103	ILE	5.9
3	C	141	SER	5.5
4	Q	73	TYR	5.0
4	D	73	TYR	4.8
2	O	245	TYR	4.2
4	Q	97	VAL	3.7
4	Q	88	TYR	3.6
2	O	246	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
4	D	89	TYR	3.5
4	Q	100	LEU	3.4
4	Q	28	TYR	3.3
4	D	97	VAL	3.3
3	P	79	LEU	3.2
4	D	32	GLY	2.9
4	D	43	LEU	2.9
4	D	85	TYR	2.8
3	C	34	LEU	2.8
3	P	116	LEU	2.7
4	Q	33	PRO	2.7
4	Q	85	TYR	2.6
1	A	11	GLN	2.6
3	P	136	GLY	2.6
3	C	32	TRP	2.5
4	D	101	TRP	2.5
3	P	76	SER	2.4
3	P	85	TYR	2.4
3	P	69	HIS	2.4
3	P	73	VAL	2.3
1	A	383	ASN	2.3
2	B	118	PHE	2.3
4	D	28	TYR	2.2
3	P	64	PRO	2.2
4	Q	95	LYS	2.2
3	C	116	LEU	2.2
3	C	56	PHE	2.2
3	P	74	VAL	2.2
3	P	51	LEU	2.1
2	B	48	LEU	2.1
4	Q	89	TYR	2.1
3	P	84	ILE	2.0
1	N	383	ASN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
16	UNL	C	214	5/-	0.63	0.48	24.12	90,91,92,93	0
17	GOL	P	208	6/6	0.32	1.66	15.84	155,156,156,157	0
17	GOL	C	294	6/6	0.84	0.85	10.38	132,132,133,133	0
17	GOL	O	1009	6/6	0.90	0.19	8.79	29,30,33,33	0
16	UNL	P	211	5/-	0.47	0.92	6.44	119,119,120,121	0
16	UNL	C	272	1/-	0.91	0.19	4.28	54,54,54,54	0
15	PEE	D	109	24/51	0.62	0.53	3.60	48,64,74,75	0
5	BHG	C	142	18/18	0.81	0.34	3.00	49,67,79,79	0
15	PEE	Q	210	24/51	0.58	0.61	2.75	70,82,95,95	0
13	CBE	C	144	16/16	0.75	0.25	2.64	23,29,37,46	0
11	F3S	O	1004	7/7	0.99	0.14	2.55	15,20,22,22	0
17	GOL	B	1010	6/6	0.96	0.13	2.13	26,29,32,32	0
13	CBE	P	202	16/16	0.89	0.21	2.10	21,30,36,49	0
16	UNL	A	1020	1/-	0.94	0.28	1.83	34,34,34,34	0
5	BHG	P	204	18/18	0.91	0.18	1.60	38,45,58,59	0
14	TEO	N	1002	9/9	0.95	0.12	1.54	13,17,22,23	0
8	FAD	N	1001	53/53	0.97	0.12	1.20	4,13,21,24	0
16	UNL	N	1015	1/-	0.93	0.19	1.02	42,42,42,42	0
8	FAD	A	1001	53/53	0.97	0.12	0.69	9,14,22,25	0
16	UNL	N	1003	4/-	0.87	0.15	0.55	57,58,59,59	0
14	TEO	A	1002	9/9	0.96	0.11	0.12	19,21,24,26	0
12	HEM	P	201	41/43	0.97	0.13	-0.06	29,32,43,48	0
10	SF4	O	1003	8/8	0.99	0.12	-0.17	14,18,20,20	0
12	HEM	C	143	41/43	0.98	0.12	-0.26	23,32,40,49	0
11	F3S	B	1004	7/7	0.99	0.11	-0.27	17,19,20,25	0
9	FES	B	1002	4/4	0.99	0.12	-0.38	14,16,16,17	0
9	FES	O	1002	4/4	0.99	0.11	-0.48	14,16,16,19	0
6	K	N	622	1/1	0.99	0.10	-0.59	19,19,19,19	0
10	SF4	B	1003	8/8	0.99	0.10	-0.63	16,17,19,21	0
6	K	A	622	1/1	0.99	0.09	-1.35	24,24,24,24	0
6	K	B	253	1/1	0.99	0.07	-1.87	38,38,38,38	0
6	K	O	253	1/1	0.96	0.08	-1.91	39,39,39,39	0
16	UNL	D	247	1/-	0.74	0.17	-	68,68,68,68	0
16	UNL	Q	288	1/-	0.80	0.25	-	44,44,44,44	0
16	UNL	P	274	1/-	0.78	0.24	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	UNL	A	1008	1/-	0.81	1.06	-	62,62,62,62	0
16	UNL	N	1019	1/-	0.92	0.24	-	49,49,49,49	0
16	UNL	A	1007	1/-	0.61	0.25	-	66,66,66,66	0
16	UNL	N	1016	1/-	0.55	0.21	-	62,62,62,62	0
16	UNL	N	1014	1/-	0.35	0.34	-	76,76,76,76	0
16	UNL	C	293	1/-	0.73	0.27	-	62,62,62,62	0
16	UNL	N	1013	1/-	0.78	0.28	-	57,57,57,57	0
16	UNL	N	1023	1/-	0.71	0.15	-	45,45,45,45	0
16	UNL	C	259	1/-	0.35	0.25	-	64,64,64,64	0
16	UNL	P	233	1/-	0.82	0.21	-	44,44,44,44	0
16	UNL	B	1006	1/-	0.47	0.60	-	76,76,76,76	0
16	UNL	Q	219	1/-	0.93	0.17	-	45,45,45,45	0
16	UNL	O	276	1/-	0.52	0.26	-	65,65,65,65	0
16	UNL	C	145	4/-	0.87	0.11	-	70,70,70,70	0
16	UNL	N	1010	1/-	0.91	0.22	-	63,63,63,63	0
16	UNL	A	1005	1/-	0.32	0.76	-	66,66,66,66	0
16	UNL	C	292	1/-	0.70	0.30	-	64,64,64,64	0
16	UNL	D	245	1/-	0.88	0.15	-	58,58,58,58	0
16	UNL	O	1008	1/-	0.86	0.29	-	47,47,47,47	0
16	UNL	Q	221	1/-	0.84	0.17	-	56,56,56,56	0
16	UNL	A	1003	6/-	0.67	0.30	-	135,136,136,137	0
16	UNL	N	1011	1/-	0.91	0.14	-	38,38,38,38	0
16	UNL	A	1014	1/-	0.84	0.23	-	47,47,47,47	0
16	UNL	C	240	1/-	0.93	0.20	-	45,45,45,45	0
16	UNL	B	258	1/-	0.84	0.21	-	57,57,57,57	0
16	UNL	A	1018	1/-	0.91	0.23	-	45,45,45,45	0
16	UNL	P	285	1/-	0.82	0.17	-	50,50,50,50	0
16	UNL	D	265	1/-	0.61	0.71	-	103,103,103,103	0
16	UNL	P	236	1/-	0.90	0.16	-	53,53,53,53	0
16	UNL	C	254	1/-	0.68	0.18	-	55,55,55,55	0
16	UNL	A	1012	1/-	0.80	0.38	-	69,69,69,69	0
16	UNL	Q	234	1/-	0.88	0.40	-	53,53,53,53	0
16	UNL	A	1010	1/-	0.67	0.37	-	67,67,67,67	0
16	UNL	C	256	1/-	0.87	0.19	-	61,61,61,61	0
16	UNL	B	1005	5/-	0.60	0.40	-	92,93,93,94	0
16	UNL	B	268	1/-	0.76	0.21	-	51,51,51,51	0
16	UNL	N	1007	1/-	0.80	0.19	-	59,59,59,59	0
16	UNL	O	282	1/-	0.77	0.17	-	52,52,52,52	0
16	UNL	O	1005	5/-	0.70	0.38	-	146,146,147,147	0
16	UNL	B	297	1/-	0.85	0.38	-	51,51,51,51	0
16	UNL	A	1021	1/-	0.88	0.16	-	37,37,37,37	0
16	UNL	A	1013	1/-	0.85	0.12	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	UNL	N	1009	1/-	0.81	0.19	-	50,50,50,50	0
16	UNL	A	1004	4/-	0.74	0.21	-	55,60,60,61	0
16	UNL	O	1007	1/-	0.84	0.15	-	69,69,69,69	0
16	UNL	N	1020	1/-	0.85	0.13	-	56,56,56,56	0
16	UNL	C	248	1/-	0.59	0.52	-	57,57,57,57	0
16	UNL	N	1008	1/-	0.90	0.14	-	39,39,39,39	0
16	UNL	D	263	1/-	0.78	0.25	-	53,53,53,53	0
16	UNL	A	1006	1/-	0.92	0.10	-	47,47,47,47	0
16	UNL	N	1005	1/-	0.10	0.88	-	76,76,76,76	0
16	UNL	C	289	1/-	0.86	0.15	-	57,57,57,57	0
16	UNL	C	251	1/-	0.83	0.32	-	53,53,53,53	0
16	UNL	N	1004	1/-	0.90	0.17	-	45,45,45,45	0
16	UNL	A	1019	1/-	0.94	0.24	-	37,37,37,37	0
16	UNL	Q	237	1/-	0.82	0.23	-	47,47,47,47	0
16	UNL	B	280	1/-	0.84	0.15	-	53,53,53,53	0
16	UNL	D	250	1/-	0.92	0.19	-	53,53,53,53	0
16	UNL	N	1022	1/-	0.48	0.39	-	72,72,72,72	0
16	UNL	A	1017	1/-	0.93	0.17	-	48,48,48,48	0
16	UNL	B	1007	1/-	0.17	1.00	-	74,74,74,74	0
16	UNL	N	1021	1/-	0.79	0.18	-	42,42,42,42	0
16	UNL	A	1011	1/-	0.80	0.24	-	55,55,55,55	0
16	UNL	C	267	1/-	0.89	0.21	-	52,52,52,52	0
16	UNL	O	1006	1/-	0.86	0.20	-	66,66,66,66	0
16	UNL	N	1006	1/-	0.61	0.28	-	52,52,52,52	0
16	UNL	A	1015	1/-	0.66	0.51	-	69,69,69,69	0
16	UNL	D	255	1/-	0.95	0.07	-	35,35,35,35	0
16	UNL	D	266	1/-	0.63	0.32	-	62,62,62,62	0
16	UNL	D	291	1/-	0.75	0.17	-	58,58,58,58	0
16	UNL	A	1022	1/-	0.58	0.27	-	51,51,51,51	0
16	UNL	N	1017	1/-	0.92	0.12	-	30,30,30,30	0
16	UNL	P	218	1/-	0.90	0.16	-	57,57,57,57	0
16	UNL	P	224	1/-	0.47	0.29	-	71,71,71,71	0
16	UNL	A	1016	1/-	0.80	0.38	-	50,50,50,50	0
16	UNL	B	277	1/-	0.77	0.18	-	46,46,46,46	0
16	UNL	C	235	1/-	0.66	0.23	-	71,71,71,71	0
16	UNL	B	1009	1/-	0.69	0.26	-	73,73,73,73	0
16	UNL	A	1009	1/-	0.84	0.37	-	50,50,50,50	0
16	UNL	B	1008	1/-	0.88	0.44	-	61,61,61,61	0
7	AZI	A	623	3/3	0.81	0.18	-	56,56,64,64	0
16	UNL	Q	287	1/-	0.21	0.50	-	75,75,75,75	0
16	UNL	D	262	1/-	0.81	0.21	-	59,59,59,59	0
16	UNL	C	241	1/-	0.92	0.15	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	UNL	A	1023	1/-	0.70	0.28	-	53,53,53,53	0
16	UNL	N	1012	1/-	0.15	0.99	-	94,94,94,94	0
16	UNL	N	1018	1/-	0.71	0.21	-	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.