



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:29 AM GMT

PDB ID : 2H88
Title : Avian Mitochondrial Respiratory Complex II at 1.8 Angstrom Resolution
Authors : Huang, L.S.; Shen, J.T.; Wang, A.C.; Berry, E.A.
Deposited on : 2006-06-06
Resolution : 1.74 Å(reported)

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

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

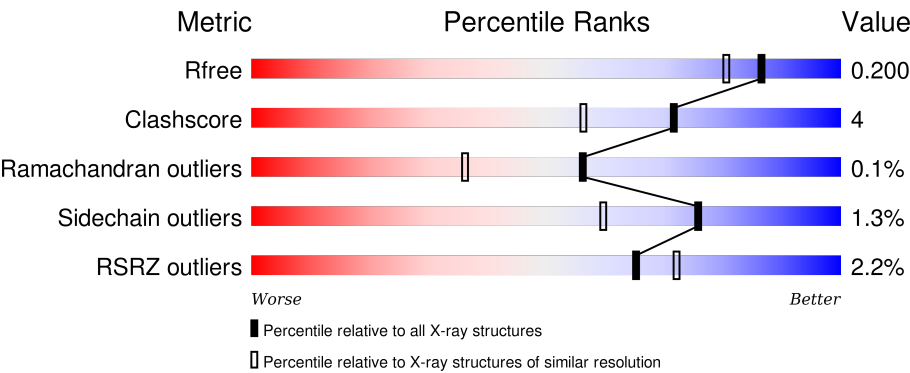
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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 $\leq 5\%$. 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></div><div><div></div><div></div><div></div><div></div></div><div>90%8%</div></div>
1	N	621	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>91%7%</div></div>
2	B	252	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>89%6%5%</div></div>
2	O	252	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>90%5%</div></div>
3	C	140	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>81%18%</div></div>

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Mol	Chain	Length	Quality of chain
3	P	140	
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
13	GOL	B	1009	-	-	-	X
13	GOL	O	1009	-	-	-	X
14	BHG	C	141	X	-	-	-
14	BHG	P	205	X	-	-	-
8	TEO	A	1002	X	-	-	-
8	TEO	N	1002	X	-	-	-
9	UNL	B	1007	-	-	-	X
9	UNL	C	145	-	-	-	X
9	UNL	D	107	-	-	-	X
9	UNL	D	116	-	-	-	X
9	UNL	N	1007	-	-	X	-
9	UNL	O	1006	-	-	X	-
9	UNL	P	208	-	-	X	-
9	UNL	P	209	-	-	X	-
9	UNL	P	220	-	-	-	X
9	UNL	Q	212	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 19414 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	612	Total	C	N	O	S	0	0	0
			4726	2956	843	898	29			
1	N	612	Total	C	N	O	S	0	0	0
			4726	2956	843	898	29			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	ARG	CYS	CONFLICT	UNP Q9YHT1
A	556	LEU	PHE	CONFLICT	UNP Q9YHT1
A	560	GLU	ASP	CONFLICT	UNP Q9YHT1
N	501	ARG	CYS	CONFLICT	UNP Q9YHT1
N	556	LEU	PHE	CONFLICT	UNP Q9YHT1
N	560	GLU	ASP	CONFLICT	UNP Q9YHT1

- 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
			1916	1213	325	356	22			
2	O	239	Total	C	N	O	S	0	0	0
			1916	1213	325	356	22			

- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total	C	N	O	S	0	0	0
			1077	706	178	189	4			
3	P	139	Total	C	N	O	S	0	0	0
			1077	706	178	189	4			

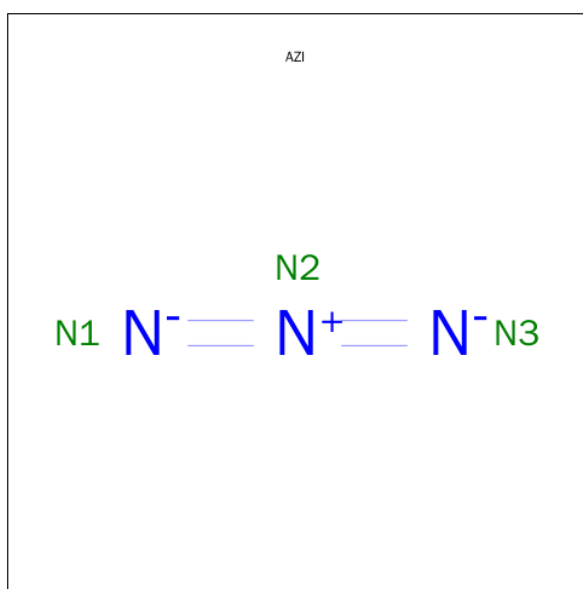
- Molecule 4 is a protein called Succinate dehydrogenase cytochrome B, small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	101	Total	C	N	O	S	0	0	0
			766	505	121	137	3			
4	Q	101	Total	C	N	O	S	0	0	0
			766	505	121	137	3			

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

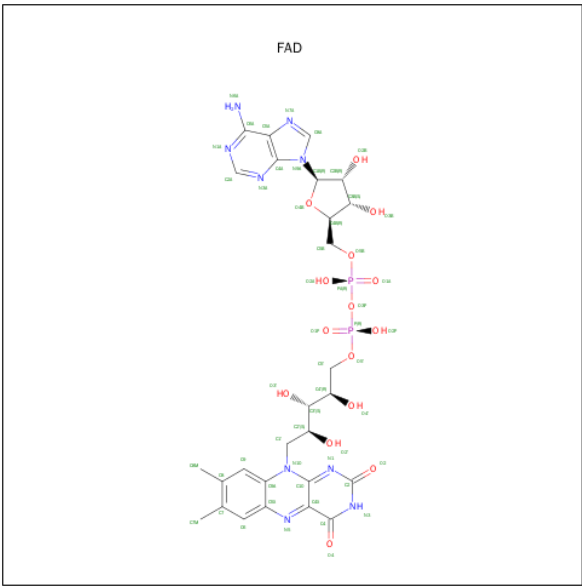
- Molecule 6 is AZIDE ION (three-letter code: AZI) (formula: N₃).



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

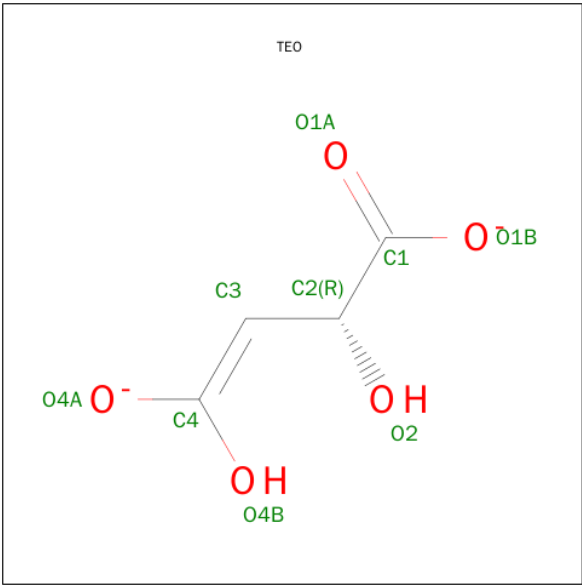
- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:

C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 8 is MALATE LIKE INTERMEDIATE (three-letter code: TEO) (formula: C₄H₄O₅).



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

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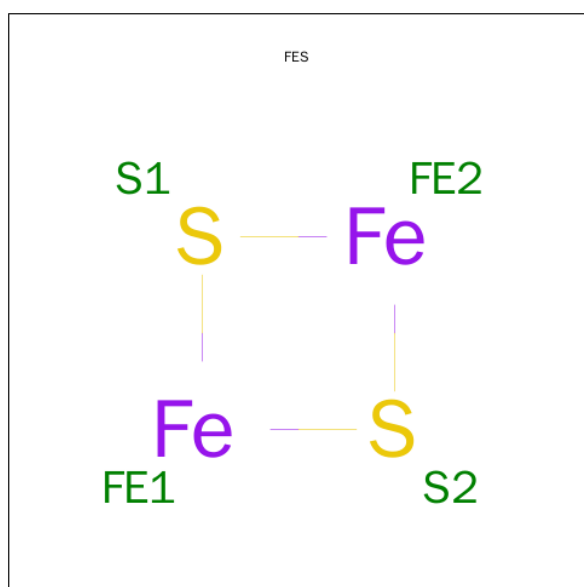
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	C	O	0	0
			9	4	5		

- Molecule 9 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

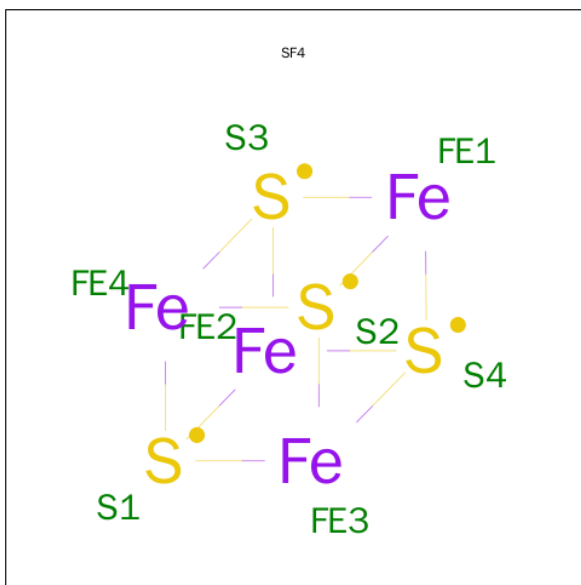
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	P	14	Total	C	O	0	0
			22	6	16		
9	Q	6	Total	C	O	0	0
			16	12	4		
9	D	11	Total	C	O	0	0
			32	21	11		
9	B	4	Total	O		0	0
			4	4			
9	C	9	Total	C	O	0	0
			16	6	10		
9	A	6	Total	O		0	0
			7	7			
9	N	10	Total	O		0	0
			11	11			
9	O	4	Total	O		0	0
			4	4			

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



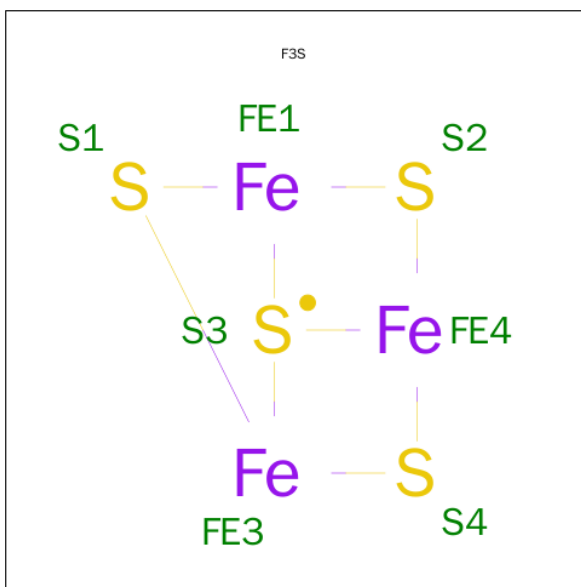
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			4	2	2		
10	O	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



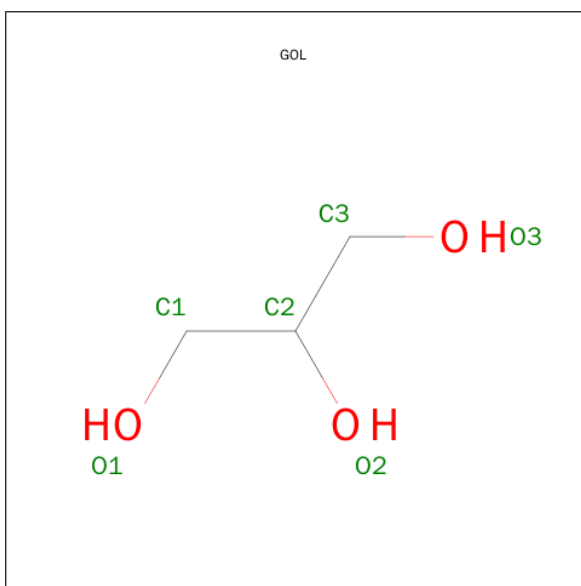
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



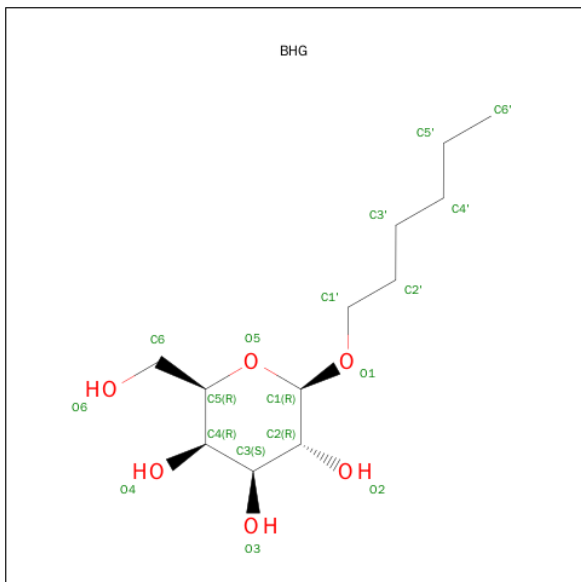
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			7	3	4		
12	O	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



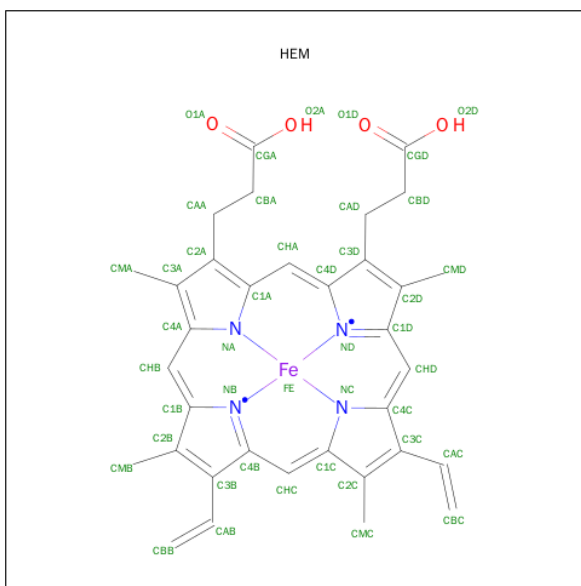
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			6	3	3		
13	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 14 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula: $C_{12}H_{24}O_6$).



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

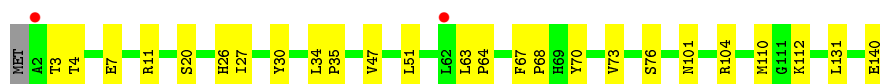
- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



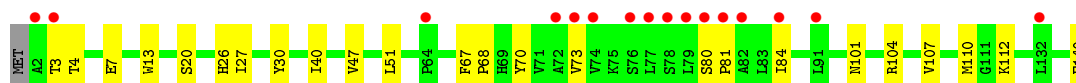
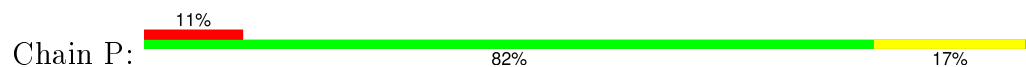
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total 41	C 32	Fe 1	N 4	O 4	0	0
15	P	1	Total 41	C 32	Fe 1	N 4	O 4	0	0

- Molecule 16 is water.

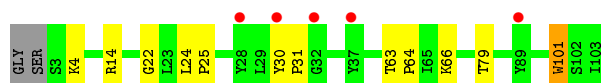
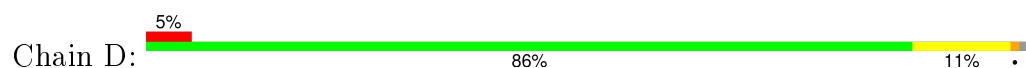
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	579	Total 579	O 579	0	0
16	B	296	Total 296	O 296	0	0
16	C	104	Total 104	O 104	0	0
16	D	51	Total 51	O 51	0	0
16	N	569	Total 569	O 569	0	0
16	O	281	Total 281	O 281	0	0
16	P	99	Total 99	O 99	0	0
16	Q	51	Total 51	O 51	0	0



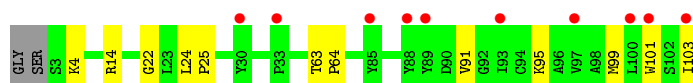
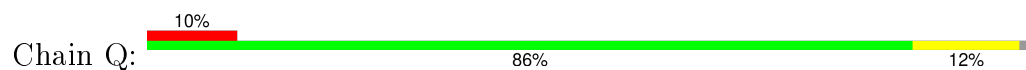
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT



- 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, α , β , γ	119.97Å 199.39Å 68.06Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	45.14 – 1.74 45.14 – 1.70	Depositor EDS
% Data completeness (in resolution range)	89.2 (45.14-1.74) 86.9 (45.14-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.206 0.175 , 0.200	Depositor DCC
R_{free} test set	14646 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.0	EDS
Estimated twinning fraction	0.227 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 304101 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19414	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, TEO, SF4, BHG, F3S, FES, 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	0.99	1/4827 (0.0%)	0.86	2/6535 (0.0%)
1	N	1.01	1/4827 (0.0%)	0.87	1/6535 (0.0%)
2	B	0.99	2/1958 (0.1%)	0.83	0/2640
2	O	1.00	1/1958 (0.1%)	0.84	0/2640
3	C	0.73	0/1106	0.68	0/1503
3	P	0.73	0/1106	0.68	0/1503
4	D	0.60	0/789	0.64	0/1082
4	Q	0.54	0/789	0.62	0/1082
All	All	0.94	5/17360 (0.0%)	0.82	3/23520 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
3	C	0	1
3	P	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	84	ALA	CA-CB	6.40	1.65	1.52
2	B	142	TYR	CD1-CE1	6.09	1.48	1.39
1	A	103	ALA	CA-CB	5.94	1.65	1.52
2	B	84	ALA	CA-CB	5.23	1.63	1.52
1	N	148	CYS	CB-SG	5.16	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLY	N-CA-C	6.00	128.10	113.10
1	N	140	GLY	N-CA-C	5.91	127.87	113.10
1	A	318	LYS	CD-CE-NZ	5.25	123.78	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	TYR	Sidechain
3	C	30	TYR	Sidechain
1	N	172	TYR	Sidechain
3	P	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	4726	0	4609	33	0
1	N	4726	0	4609	34	0
2	B	1916	0	1913	10	0
2	O	1916	0	1913	8	0
3	C	1077	0	1112	22	0
3	P	1077	0	1112	20	0
4	D	766	0	761	10	0
4	Q	766	0	761	10	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
6	A	3	0	0	0	0
6	N	3	0	0	0	0
7	A	53	0	30	3	0
7	N	53	0	30	3	0
8	A	9	0	2	3	0
8	N	9	0	2	1	0
9	A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	4	0	0	1	0
9	C	16	0	0	0	0
9	D	32	0	0	1	0
9	N	11	0	0	3	0
9	O	4	0	0	2	0
9	P	22	0	0	4	0
9	Q	16	0	0	0	0
10	B	4	0	0	0	0
10	O	4	0	0	0	0
11	B	8	0	0	0	0
11	O	8	0	0	0	0
12	B	7	0	0	0	0
12	O	7	0	0	0	0
13	B	6	0	8	1	0
13	O	6	0	8	1	0
14	C	18	0	24	0	0
14	P	18	0	24	0	0
15	C	41	0	24	0	0
15	P	41	0	24	0	0
16	A	579	0	0	8	0
16	B	296	0	0	3	0
16	C	104	0	0	3	0
16	D	51	0	0	1	0
16	N	569	0	0	7	0
16	O	281	0	0	0	0
16	P	99	0	0	0	0
16	Q	51	0	0	0	0
All	All	19414	0	16966	146	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 4.

All (146) 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)
9:O:1005:UNL:O1	9:O:1006:UNL:O1	1.69	1.09
1:N:13:PRO:O	9:N:1011:UNL:O1	1.75	1.04
9:B:1005:UNL:O1	9:B:1006:UNL:O1	1.84	0.96
4:Q:91:VAL:HG11	4:Q:99:MET:HE1	1.56	0.85
3:P:101:ASN:HD21	3:P:104:ARG:HH11	1.27	0.82
3:C:3:THR:HG22	3:C:7:GLU:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:3:THR:HG22	3:P:7:GLU:HB2	1.63	0.78
3:C:101:ASN:HD21	3:C:104:ARG:HH11	1.29	0.78
1:N:471:ASN:HB3	9:N:1007:UNL:O1	1.84	0.78
4:D:24:LEU:HB2	4:D:25:PRO:HD3	1.68	0.75
16:N:1533:HOH:O	2:O:88:LYS:HE2	1.86	0.75
4:Q:24:LEU:HB2	4:Q:25:PRO:HD3	1.67	0.74
3:C:26:HIS:CD2	3:C:27:ILE:H	2.05	0.74
1:N:205:ARG:NH2	1:N:440:SER:HA	2.02	0.74
1:A:207:LYS:NZ	1:A:436:GLU:OE1	2.21	0.74
1:N:205:ARG:HB3	16:N:1514:HOH:O	1.89	0.72
3:P:26:HIS:CD2	3:P:27:ILE:H	2.07	0.71
9:P:208:UNL:O1	9:P:209:UNL:O1	2.10	0.70
1:A:189:ARG:HD3	1:A:439:PRO:HB2	1.75	0.68
1:N:189:ARG:HD3	1:N:439:PRO:HB2	1.76	0.67
4:Q:22:GLY:O	4:Q:25:PRO:HD2	1.95	0.66
3:C:70:TYR:O	3:C:73:VAL:HG12	1.95	0.66
3:P:70:TYR:O	3:P:73:VAL:HG12	1.96	0.66
1:N:507:LYS:HE3	16:N:1170:HOH:O	1.95	0.66
1:N:471:ASN:CB	9:N:1007:UNL:O1	2.45	0.64
1:N:207:LYS:NZ	1:N:436:GLU:OE1	2.31	0.63
2:O:192:ILE:C	2:O:192:ILE:HD12	2.20	0.62
4:D:22:GLY:O	4:D:25:PRO:HD2	1.98	0.62
2:O:245:TYR:O	4:Q:4:LYS:NZ	2.32	0.62
1:A:387:LYS:HD3	16:A:2193:HOH:O	1.99	0.61
1:N:205:ARG:HH21	1:N:440:SER:HA	1.65	0.61
2:O:152:LEU:HD23	2:O:192:ILE:HD11	1.83	0.61
2:B:192:ILE:C	2:B:192:ILE:HD12	2.21	0.61
1:N:207:LYS:NZ	1:N:436:GLU:HB2	2.15	0.61
3:P:67:PHE:HB3	3:P:68:PRO:HD3	1.83	0.60
1:A:401:ALA:N	1:A:402:SER:HA	2.16	0.60
3:C:67:PHE:HB3	3:C:68:PRO:HD3	1.84	0.60
4:Q:95:LYS:HG3	4:Q:99:MET:CE	2.31	0.59
2:B:152:LEU:HD23	2:B:192:ILE:HD11	1.84	0.58
1:N:401:ALA:N	1:N:402:SER:HA	2.18	0.58
2:B:245:TYR:O	4:D:4:LYS:NZ	2.36	0.58
1:N:207:LYS:HZ1	1:N:436:GLU:HB2	1.70	0.57
1:A:507:LYS:HE3	16:A:2733:HOH:O	2.05	0.55
2:O:152:LEU:HD23	2:O:192:ILE:CD1	2.36	0.55
3:C:140:GLU:OXT	4:D:101:TRP:HD1	1.90	0.55
3:C:140:GLU:OXT	4:D:101:TRP:CD1	2.60	0.55
2:B:152:LEU:HD23	2:B:192:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:THR:HB	4:D:64:PRO:HD3	1.90	0.54
1:A:169:ASP:HB2	16:A:2502:HOH:O	2.07	0.54
4:Q:63:THR:HB	4:Q:64:PRO:HD3	1.90	0.54
3:P:101:ASN:ND2	3:P:104:ARG:HH11	2.03	0.53
3:C:110:MET:HE3	3:C:112:LYS:HD2	1.91	0.53
1:A:455:LYS:NZ	16:A:2885:HOH:O	2.41	0.53
4:Q:95:LYS:HG3	4:Q:99:MET:HE3	1.90	0.53
1:A:207:LYS:NZ	1:A:436:GLU:HB2	2.25	0.52
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.90	0.52
2:B:104:HIS:O	13:B:1009:GOL:H12	2.11	0.51
3:P:110:MET:HE3	3:P:112:LYS:HD2	1.92	0.51
3:P:4:THR:OG1	3:P:7:GLU:HG3	2.11	0.51
3:C:4:THR:OG1	3:C:7:GLU:HG3	2.10	0.51
1:A:593:LYS:HE3	16:A:2370:HOH:O	2.12	0.50
1:N:381:HIS:O	1:N:597:LYS:NZ	2.44	0.50
3:C:70:TYR:HA	3:C:73:VAL:HG12	1.93	0.50
3:P:70:TYR:HA	3:P:73:VAL:HG12	1.92	0.49
1:A:297:ARG:HH22	8:A:1002:TEO:C3	2.26	0.49
9:P:208:UNL:O1	9:P:209:UNL:O2	2.31	0.48
1:N:60:ALA:HB3	1:N:154:GLY:HA3	1.95	0.48
1:A:263:LEU:HG	1:A:264:ILE:N	2.28	0.48
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.47	0.48
1:A:381:HIS:O	1:A:597:LYS:NZ	2.47	0.48
1:N:496:LEU:HD12	1:N:536:ILE:HG21	1.95	0.47
4:Q:95:LYS:HG3	4:Q:99:MET:HE2	1.96	0.47
1:N:574:PRO:HD2	1:N:577:GLU:HB2	1.97	0.47
3:C:3:THR:CG2	3:C:7:GLU:HB2	2.41	0.47
1:N:243:PRO:HB3	1:N:586:TYR:CZ	2.49	0.47
2:B:98:LYS:HE3	16:C:2230:HOH:O	2.15	0.47
1:A:496:LEU:HD12	1:A:536:ILE:HG21	1.96	0.47
1:N:263:LEU:HG	1:N:264:ILE:N	2.29	0.47
2:O:104:HIS:O	13:O:1009:GOL:H12	2.14	0.47
3:P:84:ILE:HD13	4:Q:103:ILE:HG22	1.97	0.47
1:N:121:GLU:HG2	16:N:1133:HOH:O	2.15	0.46
4:Q:91:VAL:CG1	4:Q:99:MET:HE1	2.39	0.46
4:D:66:LYS:HG3	16:D:2127:HOH:O	2.16	0.46
4:D:79:THR:HG21	9:D:107:UNL:C1	2.46	0.46
1:N:189:ARG:NH1	1:N:440:SER:O	2.38	0.46
1:A:297:ARG:HH22	8:A:1002:TEO:C4	2.30	0.45
1:A:243:PRO:HB3	1:A:586:TYR:CZ	2.51	0.45
1:A:11:GLN:HG3	16:A:2932:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:326:HIS:HD2	16:N:1422:HOH:O	1.99	0.45
3:C:101:ASN:ND2	3:C:104:ARG:HH11	2.05	0.45
3:C:70:TYR:O	3:C:73:VAL:CG1	2.64	0.45
1:N:414:LEU:HG	7:N:1001:FAD:C2	2.47	0.45
1:A:574:PRO:HD2	1:A:577:GLU:HB2	1.98	0.45
1:A:381:HIS:ND1	1:A:386:ASP:OD1	2.47	0.45
3:P:70:TYR:O	3:P:73:VAL:CG1	2.65	0.45
2:O:192:ILE:C	2:O:192:ILE:CD1	2.85	0.45
1:A:60:ALA:HA	7:A:1001:FAD:C5X	2.48	0.44
1:A:470:LEU:HD11	1:A:474:LYS:HE3	2.00	0.44
1:N:381:HIS:ND1	1:N:386:ASP:OD1	2.46	0.44
1:A:181:LEU:HD21	1:A:211:ILE:HD11	2.00	0.44
3:P:80:SER:HA	3:P:81:PRO:HD3	1.81	0.44
3:P:101:ASN:HD21	3:P:104:ARG:NH1	2.06	0.44
1:N:87:SER:HB2	1:N:405:GLY:HA3	1.98	0.44
1:N:60:ALA:HA	7:N:1001:FAD:C6	2.48	0.43
3:C:26:HIS:CG	3:C:27:ILE:H	2.37	0.43
1:N:507:LYS:HE2	1:N:509:PHE:CZ	2.53	0.43
1:N:60:ALA:HA	7:N:1001:FAD:C5X	2.47	0.43
9:O:1006:UNL:O1	9:P:208:UNL:O1	2.36	0.43
16:B:2845:HOH:O	4:D:4:LYS:CE	2.67	0.43
3:P:3:THR:CG2	3:P:7:GLU:HB2	2.41	0.43
3:C:63:LEU:HA	3:C:64:PRO:HD3	1.86	0.43
2:B:95:LYS:NZ	16:B:2777:HOH:O	2.47	0.43
3:C:11:ARG:HD2	16:C:2556:HOH:O	2.18	0.43
1:A:326:HIS:HE1	16:A:2021:HOH:O	2.01	0.42
1:N:297:ARG:HH22	8:N:1002:TEO:C3	2.32	0.42
3:P:140:GLU:HG3	3:P:140:GLU:OXT	2.19	0.42
3:C:140:GLU:HG3	3:C:140:GLU:OXT	2.19	0.42
3:C:131:LEU:HD23	3:C:131:LEU:HA	1.90	0.42
3:P:107:VAL:HA	3:P:110:MET:HE2	2.01	0.42
1:N:170:THR:HB	1:N:172:TYR:CE1	2.54	0.42
3:P:47:VAL:O	3:P:51:LEU:HG	2.20	0.42
1:A:87:SER:HB2	1:A:405:GLY:HA3	2.01	0.42
1:A:507:LYS:HE2	1:A:509:PHE:CZ	2.54	0.42
1:N:289:PRO:HD2	16:N:1215:HOH:O	2.19	0.42
2:B:192:ILE:C	2:B:192:ILE:CD1	2.87	0.42
1:N:326:HIS:HE1	16:N:1226:HOH:O	2.03	0.42
3:C:34:LEU:HB3	3:C:35:PRO:HD3	2.01	0.42
3:C:101:ASN:ND2	3:C:104:ARG:HD3	2.35	0.41
1:N:470:LEU:HD11	1:N:474:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:HA	7:A:1001:FAD:C6	2.49	0.41
1:A:170:THR:HB	1:A:172:TYR:CE1	2.54	0.41
3:C:47:VAL:O	3:C:51:LEU:HG	2.19	0.41
3:P:40:ILE:CG2	9:P:209:UNL:O2	2.69	0.41
2:B:102:LEU:HA	2:B:103:PRO:HD3	1.86	0.41
3:C:76:SER:HB3	16:C:2741:HOH:O	2.20	0.41
2:B:150:GLN:HG2	16:B:2054:HOH:O	2.19	0.41
1:N:181:LEU:HD21	1:N:211:ILE:HD11	2.03	0.41
1:A:354:LYS:NZ	16:A:2177:HOH:O	2.52	0.41
1:A:462:THR:O	1:A:462:THR:CG2	2.68	0.41
4:D:30:TYR:N	4:D:31:PRO:HD3	2.37	0.40
1:N:453:LEU:C	1:N:453:LEU:HD23	2.41	0.40
3:P:101:ASN:ND2	3:P:104:ARG:HD3	2.36	0.40
1:A:414:LEU:HG	7:A:1001:FAD:C2	2.52	0.40
1:A:253:HIS:O	1:A:361:PRO:HA	2.21	0.40
2:O:176:ASP:HB3	3:P:13:TRP:CZ2	2.57	0.40
1:A:297:ARG:HH22	8:A:1002:TEO:C2	2.35	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	610/621 (98%)	591 (97%)	19 (3%)	0	100	100
1	N	610/621 (98%)	591 (97%)	19 (3%)	0	100	100
2	B	237/252 (94%)	231 (98%)	5 (2%)	1 (0%)	39	20
2	O	237/252 (94%)	232 (98%)	4 (2%)	1 (0%)	39	20
3	C	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
3	P	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
4	D	99/103 (96%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	99/103 (96%)	98 (99%)	1 (1%)	0	100	100
All	All	2166/2232 (97%)	2113 (98%)	51 (2%)	2 (0%)	56	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	66	ARG
2	O	66	ARG

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	497/506 (98%)	493 (99%)	4 (1%)	86	77
1	N	497/506 (98%)	493 (99%)	4 (1%)	86	77
2	B	214/219 (98%)	210 (98%)	4 (2%)	65	42
2	O	214/219 (98%)	209 (98%)	5 (2%)	58	33
3	C	118/119 (99%)	117 (99%)	1 (1%)	86	77
3	P	118/119 (99%)	117 (99%)	1 (1%)	86	77
4	D	78/79 (99%)	76 (97%)	2 (3%)	54	28
4	Q	78/79 (99%)	76 (97%)	2 (3%)	54	28
All	All	1814/1846 (98%)	1791 (99%)	23 (1%)	76	60

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	72	GLU
1	A	73	ASP
1	A	130	PHE
2	B	63	ARG
2	B	66	ARG

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Mol	Chain	Res	Type
2	B	67	GLU
2	B	189	ARG
3	C	20	SER
4	D	14	ARG
4	D	101	TRP
1	N	48	THR
1	N	72	GLU
1	N	73	ASP
1	N	130	PHE
2	O	63	ARG
2	O	66	ARG
2	O	67	GLU
2	O	189	ARG
2	O	217	THR
3	P	20	SER
4	Q	14	ARG
4	Q	101	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	HIS
1	A	534	GLN
2	B	121	GLN
2	B	137	GLN
3	C	26	HIS
3	C	66	GLN
3	C	101	ASN
1	N	326	HIS
1	N	534	GLN
2	O	121	GLN
2	O	137	GLN
3	P	26	HIS
3	P	66	GLN
3	P	101	ASN

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 ⓘ

Of 86 ligands modelled in this entry, 64 are unknown and 4 are monoatomic - leaving 18 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$
7	FAD	A	1001	1	48,58,58	1.88	16 (33%)	54,89,89	2.90	13 (24%)
8	TEO	A	1002	-	0,8,8	0.00	-	1,10,10	12.37	1 (100%)
6	AZI	A	623	-	0,2,2	0.00	-	0,1,1	0.00	-
10	FES	B	1002	2	0,4,4	0.00	-	0,4,4	0.00	-
11	SF4	B	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
12	F3S	B	1004	2	0,9,9	0.00	-	0,15,15	0.00	-
13	GOL	B	1009	-	5,5,5	1.12	0	5,5,5	0.58	0
14	BHG	C	141	-	18,18,18	1.73	4 (22%)	23,23,23	0.78	1 (4%)
15	HEM	C	142	3,4	29,48,50	2.20	9 (31%)	24,80,82	2.77	10 (41%)
7	FAD	N	1001	1	48,58,58	2.07	15 (31%)	54,89,89	2.96	13 (24%)
8	TEO	N	1002	-	0,8,8	0.00	-	1,10,10	13.17	1 (100%)
6	AZI	N	623	-	0,2,2	0.00	-	0,1,1	0.00	-
10	FES	O	1002	2	0,4,4	0.00	-	0,4,4	0.00	-
11	SF4	O	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
12	F3S	O	1004	2	0,9,9	0.00	-	0,15,15	0.00	-
13	GOL	O	1009	-	5,5,5	1.15	0	5,5,5	0.73	0
15	HEM	P	201	3,4	29,48,50	2.24	9 (31%)	24,80,82	2.76	10 (41%)
14	BHG	P	205	-	18,18,18	1.34	2 (11%)	23,23,23	0.66	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
7	FAD	A	1001	1	-	0/30/50/50	0/6/6/6
8	TEO	A	1002	-	1/1/3/4	0/1/8/8	0/0/0/0
6	AZI	A	623	-	-	0/0/0/0	0/0/0/0
10	FES	B	1002	2	-	0/0/4/4	0/1/1/1
11	SF4	B	1003	2	-	0/0/48/48	0/6/5/5
12	F3S	B	1004	2	-	0/0/24/24	0/0/3/3
13	GOL	B	1009	-	-	0/4/4/4	0/0/0/0
14	BHG	C	141	-	1/1/5/5	0/9/29/29	0/1/1/1
15	HEM	C	142	3,4	-	0/6/50/54	0/0/8/8
7	FAD	N	1001	1	-	0/30/50/50	0/6/6/6
8	TEO	N	1002	-	1/1/3/4	0/1/8/8	0/0/0/0
6	AZI	N	623	-	-	0/0/0/0	0/0/0/0
10	FES	O	1002	2	-	0/0/4/4	0/1/1/1
11	SF4	O	1003	2	-	0/0/48/48	0/6/5/5
12	F3S	O	1004	2	-	0/0/24/24	0/0/3/3
13	GOL	O	1009	-	-	0/4/4/4	0/0/0/0
15	HEM	P	201	3,4	-	0/6/50/54	0/0/8/8
14	BHG	P	205	-	1/1/5/5	0/9/29/29	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	201	HEM	C2D-C3D	-4.98	1.39	1.54
15	C	142	HEM	CAB-C3B	-4.75	1.42	1.53
15	C	142	HEM	C2D-C3D	-4.71	1.40	1.54
15	P	201	HEM	CAB-C3B	-4.68	1.42	1.53
7	A	1001	FAD	PA-O2A	-3.63	1.39	1.54
15	P	201	HEM	CAC-C3C	-3.48	1.45	1.53
15	C	142	HEM	C2C-C1C	-3.44	1.46	1.52
15	C	142	HEM	C3D-C4D	-3.39	1.47	1.51
7	N	1001	FAD	PA-O1A	-3.19	1.39	1.51
7	N	1001	FAD	PA-O2A	-3.19	1.41	1.54
7	A	1001	FAD	PA-O1A	-3.08	1.39	1.51
15	C	142	HEM	C3C-C4C	-2.97	1.46	1.52
15	P	201	HEM	C2C-C1C	-2.81	1.47	1.52
15	C	142	HEM	CAC-C3C	-2.66	1.47	1.53
15	P	201	HEM	C3D-C4D	-2.51	1.48	1.51
15	P	201	HEM	C3C-C4C	-2.50	1.47	1.52
7	A	1001	FAD	C2'-C3'	-2.26	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1001	FAD	C2B-C3B	2.03	1.58	1.53
7	A	1001	FAD	C2A-N1A	2.04	1.37	1.33
7	A	1001	FAD	C4-N3	2.06	1.36	1.33
7	A	1001	FAD	C7M-C7	2.07	1.55	1.51
7	N	1001	FAD	C10-N10	2.07	1.41	1.39
7	N	1001	FAD	C4-N3	2.08	1.37	1.33
15	C	142	HEM	C4C-NC	2.17	1.38	1.36
7	A	1001	FAD	C6-C7	2.32	1.44	1.37
14	C	141	BHG	C3-C2	2.34	1.58	1.52
7	A	1001	FAD	C5X-N5	2.35	1.39	1.35
14	C	141	BHG	C4-C5	2.45	1.58	1.53
14	P	205	BHG	C4-C5	2.48	1.58	1.53
7	N	1001	FAD	C10-N1	2.61	1.40	1.35
7	N	1001	FAD	C1'-N10	2.61	1.51	1.48
7	A	1001	FAD	C4-C4X	2.64	1.46	1.41
7	A	1001	FAD	O2'-C2'	2.66	1.49	1.43
15	C	142	HEM	CAA-C2A	2.69	1.56	1.52
7	A	1001	FAD	C10-N1	2.69	1.40	1.35
7	N	1001	FAD	O2'-C2'	2.73	1.49	1.43
7	N	1001	FAD	C2B-C3B	2.79	1.61	1.53
7	N	1001	FAD	C4'-C3'	2.80	1.59	1.53
7	A	1001	FAD	C4'-C3'	2.85	1.59	1.53
14	C	141	BHG	O5-C1	3.03	1.49	1.41
7	N	1001	FAD	C4X-C10	3.20	1.47	1.41
7	A	1001	FAD	C2A-N3A	3.27	1.38	1.32
7	N	1001	FAD	C4-C4X	3.30	1.47	1.41
15	P	201	HEM	C4C-NC	3.39	1.40	1.36
14	P	205	BHG	O1-C1	3.64	1.46	1.40
15	P	201	HEM	CAA-C2A	3.82	1.58	1.52
7	A	1001	FAD	C10-N10	3.87	1.43	1.39
7	N	1001	FAD	C4X-N5	4.02	1.39	1.33
7	N	1001	FAD	C2A-N1A	4.43	1.42	1.33
7	N	1001	FAD	C5X-N5	4.46	1.42	1.35
14	C	141	BHG	O1-C1	4.55	1.48	1.40
15	P	201	HEM	C1C-NC	4.60	1.41	1.36
15	C	142	HEM	C1C-NC	5.07	1.42	1.36
7	N	1001	FAD	C2A-N3A	5.08	1.41	1.32
7	A	1001	FAD	C4X-N5	5.27	1.41	1.33

All (49) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	1001	FAD	N3A-C2A-N1A	-13.41	118.62	128.89
7	A	1001	FAD	N3A-C2A-N1A	-13.13	118.84	128.89
7	N	1001	FAD	C4X-C10-N10	-7.15	116.31	120.52
7	A	1001	FAD	C4X-C10-N10	-6.85	116.48	120.52
7	N	1001	FAD	C4-C4X-C10	-5.80	116.23	119.94
7	A	1001	FAD	C4-C4X-C10	-5.44	116.46	119.94
7	A	1001	FAD	C1B-N9A-C4A	-3.70	121.36	126.94
7	N	1001	FAD	C1B-N9A-C4A	-3.57	121.55	126.94
7	A	1001	FAD	O3P-PA-O5B	-3.15	94.59	102.94
7	N	1001	FAD	C4X-C4-N3	-3.03	119.44	123.59
7	N	1001	FAD	O3P-PA-O5B	-2.90	95.24	102.94
7	A	1001	FAD	C4X-C4-N3	-2.73	119.86	123.59
7	A	1001	FAD	O2'-C2'-C3'	-2.37	103.05	109.02
7	N	1001	FAD	O2'-C2'-C3'	-2.37	103.07	109.02
7	N	1001	FAD	O3'-C3'-C2'	-2.34	102.84	108.75
7	N	1001	FAD	O3P-P-O5'	-2.13	97.29	102.94
7	A	1001	FAD	O3'-C3'-C2'	-2.08	103.52	108.75
7	A	1001	FAD	O2P-P-O3P	2.11	114.69	105.09
14	C	141	BHG	C1'-O1-C1	2.12	117.65	113.94
15	C	142	HEM	C3C-C4C-NC	2.51	114.44	110.21
15	P	201	HEM	C3C-C4C-NC	2.55	114.50	110.21
15	C	142	HEM	C4B-CHC-C1C	2.61	130.18	125.82
15	P	201	HEM	C4B-CHC-C1C	2.91	130.69	125.82
15	P	201	HEM	C2D-C3D-C4D	3.14	106.83	101.50
15	C	142	HEM	C2D-C3D-C4D	3.26	107.03	101.50
7	A	1001	FAD	P-O3P-PA	3.28	141.95	132.73
15	C	142	HEM	CAD-C3D-C2D	3.41	123.02	113.22
15	P	201	HEM	CAD-C3D-C2D	3.53	123.35	113.22
7	N	1001	FAD	P-O3P-PA	3.69	143.08	132.73
15	P	201	HEM	CMD-C2D-C3D	3.76	130.97	114.35
15	C	142	HEM	CMD-C2D-C3D	3.84	131.35	114.35
7	N	1001	FAD	C4-C4X-N5	3.85	123.39	118.72
7	A	1001	FAD	C4-C4X-N5	3.93	123.49	118.72
15	P	201	HEM	CAB-C3B-C2B	4.06	125.92	116.20
15	C	142	HEM	CAB-C3B-C2B	4.08	125.97	116.20
15	P	201	HEM	CMB-C2B-C3B	4.11	126.03	116.20
7	N	1001	FAD	C4X-N5-C5X	4.20	121.60	116.76
15	C	142	HEM	CMB-C2B-C3B	4.55	127.11	116.20
15	C	142	HEM	CMC-C2C-C3C	4.80	127.69	116.20
15	P	201	HEM	CMC-C2C-C3C	4.81	127.72	116.20
7	A	1001	FAD	C4X-N5-C5X	4.85	122.34	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	201	HEM	CAD-C3D-C4D	4.90	129.74	112.47
15	C	142	HEM	CAD-C3D-C4D	4.94	129.91	112.47
15	C	142	HEM	CAC-C3C-C2C	6.06	130.71	116.20
15	P	201	HEM	CAC-C3C-C2C	6.18	131.01	116.20
7	A	1001	FAD	C4-N3-C2	8.20	122.34	115.25
7	N	1001	FAD	C4-N3-C2	8.77	122.83	115.25
8	A	1002	TEO	O2-C2-C3	12.37	135.25	109.53
8	N	1002	TEO	O2-C2-C3	13.17	136.92	109.53

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	141	BHG	C4
14	P	205	BHG	C4
8	A	1002	TEO	C2
8	N	1002	TEO	C2

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1001	FAD	3	0
8	A	1002	TEO	3	0
13	B	1009	GOL	1	0
7	N	1001	FAD	3	0
8	N	1002	TEO	1	0
13	O	1009	GOL	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	612/621 (98%)	-0.38	6 (0%) 84 89	14, 23, 45, 74	0
1	N	612/621 (98%)	-0.38	5 (0%) 87 91	12, 22, 43, 69	0
2	B	239/252 (94%)	-0.46	2 (0%) 87 91	15, 24, 41, 70	0
2	O	239/252 (94%)	-0.43	3 (1%) 79 85	14, 23, 37, 69	0
3	C	139/140 (99%)	-0.15	2 (1%) 78 84	21, 35, 50, 61	0
3	P	139/140 (99%)	0.34	16 (11%) 6 8	21, 37, 81, 92	0
4	D	101/103 (98%)	0.14	5 (4%) 32 37	26, 42, 58, 66	0
4	Q	101/103 (98%)	0.51	10 (9%) 9 11	27, 47, 69, 79	0
All	All	2182/2232 (97%)	-0.27	49 (2%) 65 72	12, 25, 54, 92	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	79	LEU	6.6
3	P	78	SER	4.6
1	A	10	THR	4.6
3	P	64	PRO	4.3
4	Q	88	TYR	4.1
2	O	8	THR	3.9
4	Q	85	TYR	3.9
3	P	74	VAL	3.8
3	P	76	SER	3.6
4	Q	103	ILE	3.5
2	B	8	THR	3.5
3	P	77	LEU	3.5
4	Q	33	PRO	3.4
1	A	568	GLN	3.3
4	D	32	GLY	3.1
3	P	2	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
4	Q	93	ILE	3.0
4	D	30	TYR	3.0
3	P	73	VAL	2.9
3	P	81	PRO	2.8
3	C	62	LEU	2.8
1	N	10	THR	2.7
1	N	568	GLN	2.7
2	O	246	LYS	2.6
1	A	566	PRO	2.6
3	P	132	LEU	2.6
3	P	3	THR	2.6
3	P	84	ILE	2.6
1	A	13	PRO	2.6
3	P	82	ALA	2.5
4	Q	30	TYR	2.5
4	Q	89	TYR	2.5
1	N	185	ASN	2.4
1	A	567	LEU	2.3
3	C	2	ALA	2.3
4	Q	101	TRP	2.3
3	P	91	LEU	2.3
3	P	72	ALA	2.3
1	A	571	GLN	2.3
2	O	245	TYR	2.3
4	D	37	TYR	2.2
2	B	246	LYS	2.2
4	D	89	TYR	2.2
4	Q	97	VAL	2.2
3	P	80	SER	2.1
4	D	28	TYR	2.0
4	Q	100	LEU	2.0
1	N	13	PRO	2.0
1	N	571	GLN	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, 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	LLDF	B-factors(Å ²)	Q<0.9
9	UNL	D	107	6/-	0.92	0.29	9.44	66,68,69,70	0
9	UNL	Q	212	7/-	0.63	0.51	9.19	74,75,76,76	0
9	UNL	B	1007	1/-	0.79	0.19	7.74	61,61,61,61	0
9	UNL	P	220	2/-	0.77	0.28	5.96	81,81,81,81	0
13	GOL	O	1009	6/6	0.94	0.10	5.36	35,40,41,43	0
9	UNL	C	145	4/-	0.92	0.20	4.56	100,100,100,100	0
9	UNL	D	116	10/-	0.79	0.22	4.16	65,66,69,69	0
13	GOL	B	1009	6/6	0.94	0.09	3.44	33,36,38,38	0
9	UNL	D	114	8/-	0.93	0.16	1.93	61,63,64,65	0
9	UNL	P	209	2/-	0.82	0.15	1.80	49,49,49,49	0
9	UNL	P	229	1/-	0.89	0.11	1.75	54,54,54,54	0
12	F3S	B	1004	7/7	0.99	0.08	1.53	18,20,21,22	0
14	BHG	P	205	18/18	0.95	0.12	1.35	36,42,59,61	0
14	BHG	C	141	18/18	0.86	0.16	1.32	48,70,75,75	0
9	UNL	Q	219	1/-	0.74	0.12	1.11	60,60,60,60	0
11	SF4	O	1003	8/8	1.00	0.09	0.98	16,17,18,18	0
9	UNL	O	1006	1/-	0.82	0.12	0.97	54,54,54,54	0
6	AZI	A	623	3/3	0.90	0.11	0.95	62,62,63,64	0
12	F3S	O	1004	7/7	0.99	0.09	0.92	19,20,21,22	0
15	HEM	P	201	41/43	0.97	0.11	0.83	28,33,50,53	0
11	SF4	B	1003	8/8	1.00	0.08	0.81	17,19,19,19	0
9	UNL	Q	213	5/-	0.86	0.19	0.72	74,74,74,74	0
9	UNL	N	1011	1/-	0.89	0.13	0.67	37,37,37,37	0
9	UNL	B	1006	1/-	0.76	0.10	0.38	60,60,60,60	0
10	FES	O	1002	4/4	1.00	0.09	0.32	13,14,14,15	0
15	HEM	C	142	41/43	0.98	0.09	0.27	27,32,49,52	0
7	FAD	N	1001	53/53	0.98	0.08	0.19	11,14,18,21	0
7	FAD	A	1001	53/53	0.98	0.07	0.15	12,14,18,22	0
10	FES	B	1002	4/4	1.00	0.08	0.12	14,16,16,16	0
5	K	A	622	1/1	0.98	0.07	-0.28	24,24,24,24	0
5	K	N	622	1/1	0.98	0.07	-0.29	25,25,25,25	0
8	TEO	N	1002	9/9	0.97	0.06	-0.37	17,18,19,20	1
5	K	B	253	1/1	0.99	0.06	-0.38	38,38,38,38	0
5	K	O	253	1/1	0.99	0.06	-0.38	39,39,39,39	0
8	TEO	A	1002	9/9	0.99	0.06	-0.97	18,20,23,24	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	UNL	C	237	1/-	0.84	0.14	-	66,66,66,66	0
9	UNL	C	147	1/-	0.85	0.14	-	59,59,59,59	0
9	UNL	A	1005	1/-	0.78	0.13	-	63,63,63,63	0
9	UNL	Q	228	1/-	0.88	0.11	-	64,64,64,64	0
9	UNL	C	144	1/-	0.84	0.21	-	62,62,62,62	0
9	UNL	P	215	4/-	0.65	0.17	-	74,74,75,76	0
9	UNL	N	1009	1/-	0.85	0.17	-	54,54,54,54	0
9	UNL	A	1004	1/-	0.78	0.23	-	61,61,61,61	0
9	UNL	P	216	1/-	0.87	0.19	-	53,53,53,53	0
9	UNL	A	1008	1/-	0.84	0.25	-	64,64,64,64	0
9	UNL	N	1004	1/-	0.90	0.14	-	60,60,60,60	0
9	UNL	N	1007	1/-	0.95	0.18	-	44,44,44,44	0
9	UNL	N	1010	1/-	0.79	0.11	-	60,60,60,60	0
9	UNL	P	242	1/-	0.82	0.17	-	57,57,57,57	0
9	UNL	D	249	1/-	0.65	0.31	-	72,72,72,72	0
9	UNL	N	1006	1/-	0.90	0.14	-	54,54,54,54	0
6	AZI	N	623	3/3	0.82	0.09	-	68,68,70,71	0
9	UNL	C	238	1/-	0.77	0.10	-	59,59,59,59	0
9	UNL	D	108	1/-	0.46	0.14	-	63,63,63,63	0
9	UNL	D	250	1/-	0.75	0.12	-	73,73,73,73	0
9	UNL	Q	218	1/-	0.95	0.11	-	53,53,53,53	0
9	UNL	Q	256	1/-	0.66	0.20	-	84,84,84,84	0
9	UNL	P	217	1/-	-0.03	0.43	-	113,113,113,113	0
9	UNL	N	1005	1/-	0.77	0.25	-	76,76,76,76	0
9	UNL	N	1012	1/-	0.92	0.12	-	53,53,53,53	0
9	UNL	D	252	1/-	0.49	0.12	-	73,73,73,73	0
9	UNL	C	149	1/-	0.88	0.17	-	81,81,81,81	0
9	UNL	N	1003	2/-	0.32	0.39	-	114,114,114,114	0
9	UNL	P	231	1/-	0.67	0.21	-	74,74,74,74	0
9	UNL	P	240	1/-	0.85	0.12	-	56,56,56,56	0
9	UNL	O	1008	1/-	0.50	0.20	-	63,63,63,63	0
9	UNL	B	1008	1/-	0.65	0.20	-	69,69,69,69	0
9	UNL	P	230	1/-	0.81	0.18	-	69,69,69,69	0
9	UNL	P	241	1/-	0.81	0.23	-	59,59,59,59	0
9	UNL	P	214	4/-	0.60	0.76	-	94,94,94,95	0
9	UNL	A	1006	1/-	0.74	0.35	-	63,63,63,63	0
9	UNL	A	1003	1/-	0.88	0.25	-	69,69,69,69	0
9	UNL	N	1008	1/-	0.77	0.15	-	65,65,65,65	0
9	UNL	A	1007	2/-	0.62	0.33	-	65,65,65,66	0
9	UNL	O	1007	1/-	0.68	0.16	-	59,59,59,59	0
9	UNL	D	119	1/-	0.97	0.18	-	63,63,63,63	0
9	UNL	O	1005	1/-	0.98	0.10	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	UNL	C	146	4/-	0.76	0.46	-	108,109,109,109	0
9	UNL	C	148	1/-	0.96	0.14	-	56,56,56,56	0
9	UNL	D	254	1/-	0.67	0.10	-	67,67,67,67	0
9	UNL	B	1005	1/-	0.97	0.07	-	39,39,39,39	0
9	UNL	P	232	1/-	0.91	0.29	-	61,61,61,61	0
9	UNL	D	251	1/-	0.86	0.10	-	73,73,73,73	0
9	UNL	D	253	1/-	0.81	0.15	-	72,72,72,72	0
9	UNL	P	208	1/-	0.94	0.09	-	44,44,44,44	0
9	UNL	C	143	2/-	0.54	0.17	-	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.