



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 4, 2018 – 08:24 PM EST

PDB ID : 6FO0
EMDB ID: : EMD-4286
Title : CryoEM structure of bovine cytochrome bc1 in complex with the anti-malarial compound GSK932121
Authors : Johnson, R.M.; Ampornpanai, K.; O'Neil, P.M.; Fishwick, C.W.G.; Jamson, A.H.; Rawson, S.D.; Hasnain, S.S.; Antonyuk, S.V.; Muench, S.P.
Deposited on : 2018-02-05
Resolution : 4.10 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

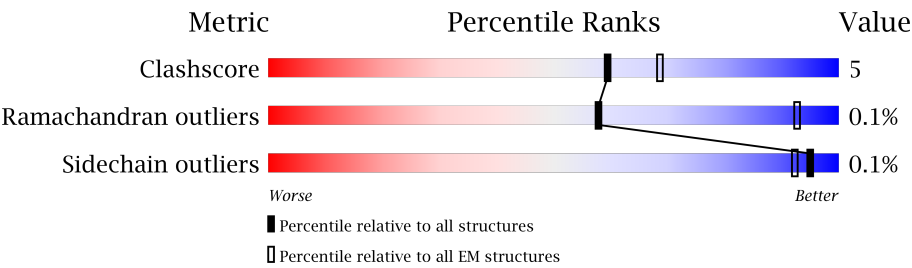
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	480	79% 14% 8%
1	N	480	79% 14% 8%
2	B	453	78% 14% 9%
2	O	453	77% 14% 9%
3	C	379	83% 14% .
3	P	379	84% 13% .
4	D	325	61% 12% 26%
4	Q	325	63% 11% 26%
5	E	274	59% 6% 35%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	R	274	
6	F	111	
6	S	111	
7	G	82	
7	T	82	
8	H	91	
8	U	91	
9	I	17	
9	V	17	
10	J	64	
10	W	64	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 61356 atoms, of which 30362 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	N	443	Total	C	H	N	O	S	0	0
			6753	2142	3325	603	663	20		
1	A	443	Total	C	H	N	O	S	0	0
			6753	2142	3325	603	663	20		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	O	414	Total	C	H	N	O	S	0	0
			6206	1955	3094	549	601	7		
2	B	414	Total	C	H	N	O	S	0	0
			6206	1955	3094	549	601	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	305	GLU	GLN	conflict	UNP P23004
B	305	GLU	GLN	conflict	UNP P23004

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	P	370	Total	C	H	N	O	S	0	0
			5933	1973	2997	456	489	18		
3	C	370	Total	C	H	N	O	S	0	0
			5933	1973	2997	456	489	18		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Q	239	Total	C	H	N	O	S	0	0
			3751	1216	1848	327	345	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	239	Total	C	H	N	O	S	0	0
			3751	1216	1848	327	345	15		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	R	178	Total	C	H	N	O	S	0	0
			2658	848	1311	231	260	8		
5	E	178	Total	C	H	N	O	S	0	0
			2658	848	1311	231	260	8		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	S	98	Total	C	H	N	O	S	0	0
			1710	547	850	154	157	2		
6	F	98	Total	C	H	N	O	S	0	0
			1710	547	850	154	157	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	56	ASP	ASN	conflict	UNP P00129
F	56	ASP	ASN	conflict	UNP P00129

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	T	74	Total	C	H	N	O	S	0	0
			1255	408	631	117	98	1		
7	G	74	Total	C	H	N	O	S	0	0
			1255	408	631	117	98	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	U	65	Total	C	H	N	O	S	0	0
			1041	321	512	96	107	5		
8	H	65	Total	C	H	N	O	S	0	0
			1041	321	512	96	107	5		

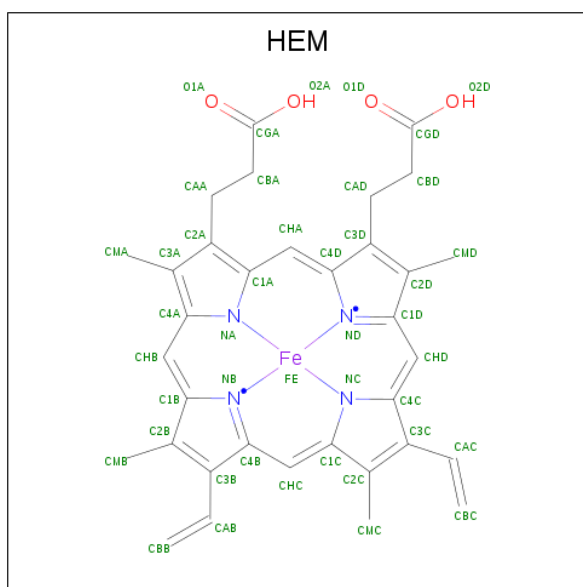
- Molecule 9 is a protein called Chain I/V.

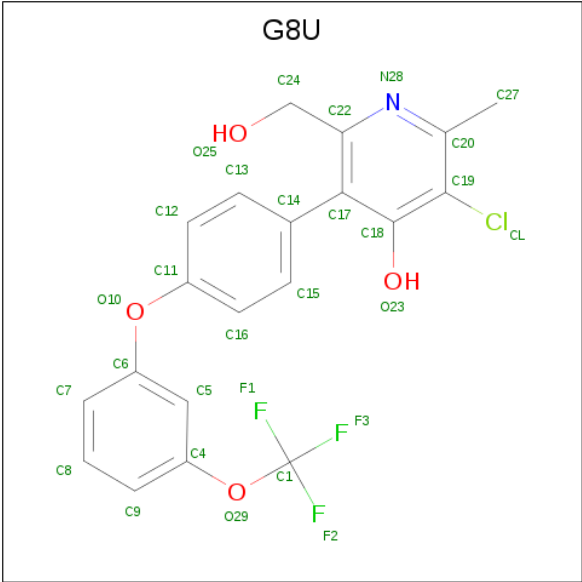
Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	17	Total	C	H	N	O	0	0
			263	81	136	24	22		
9	I	17	Total	C	H	N	O	0	0
			263	81	136	24	22		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	57	Total	C	H	N	O	0	0
			950	312	477	82	79		
10	J	57	Total	C	H	N	O	0	0
			950	312	477	82	79		

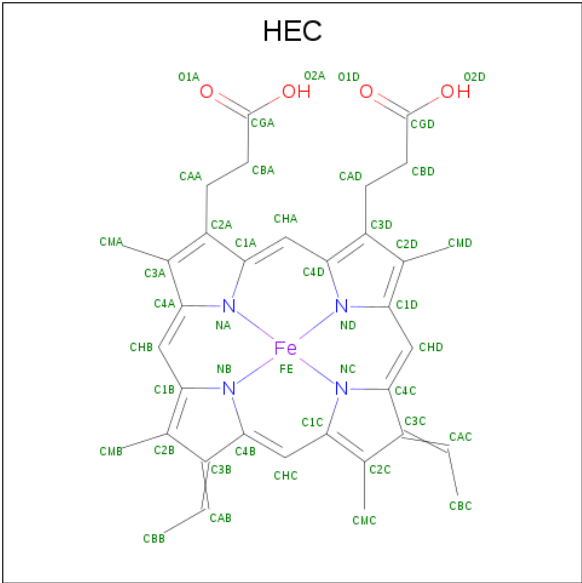
- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms						AltConf
12	P	1	Total	C	Cl	F	N	O	0
			29	20	1	3	1	4	
12	C	1	Total	C	Cl	F	N	O	0
			29	20	1	3	1	4	

- Molecule 13 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

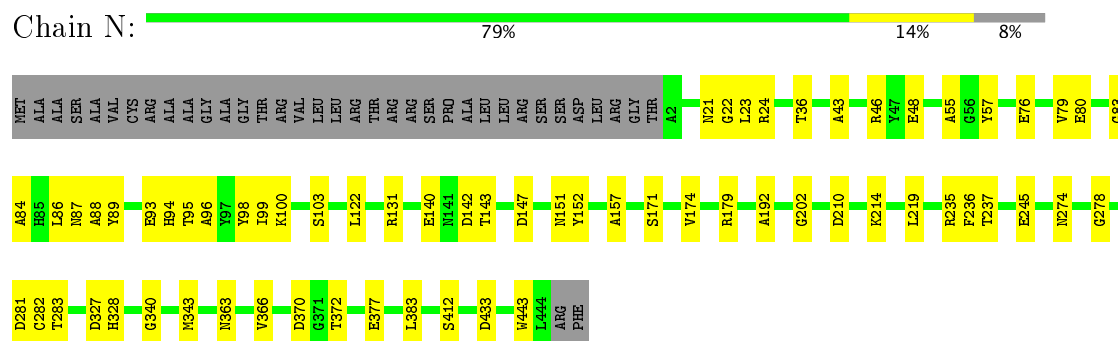


Mol	Chain	Residues	Atoms					AltConf
13	Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

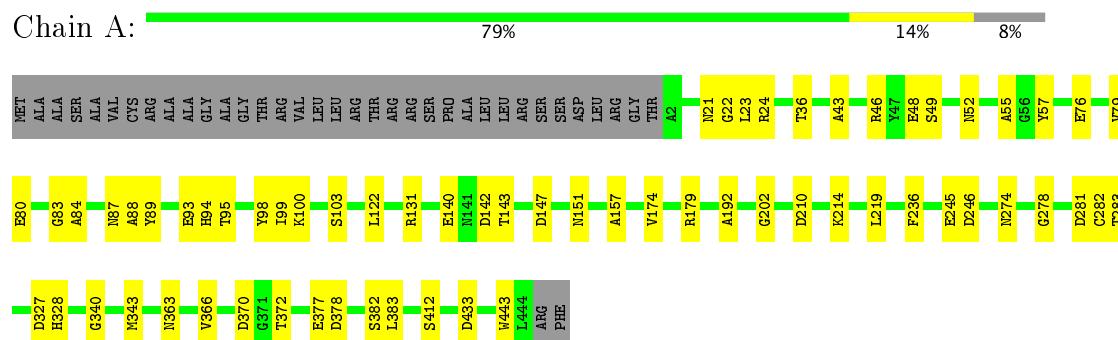
3 Residue-property plots

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

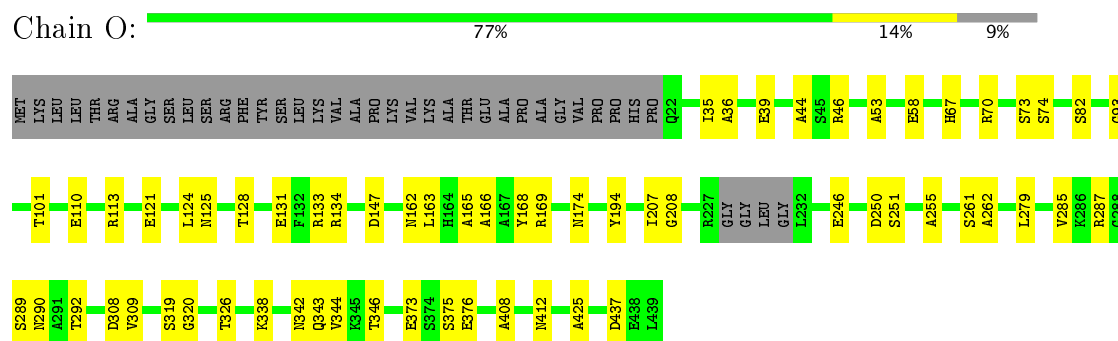
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial




- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

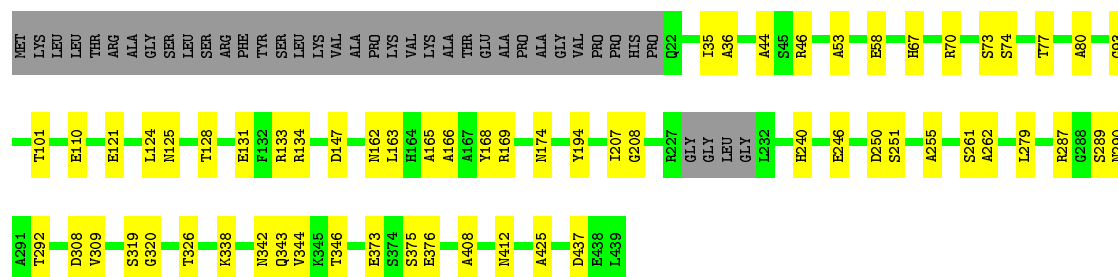


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial




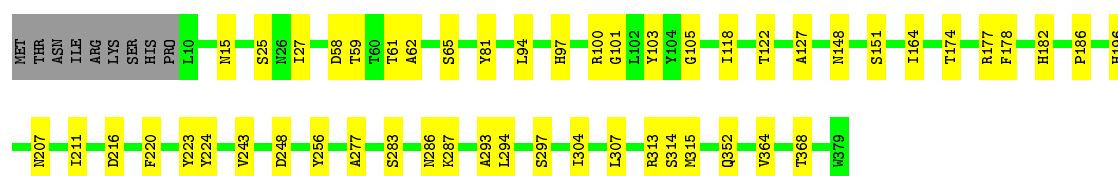
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:  78% 14% 9%




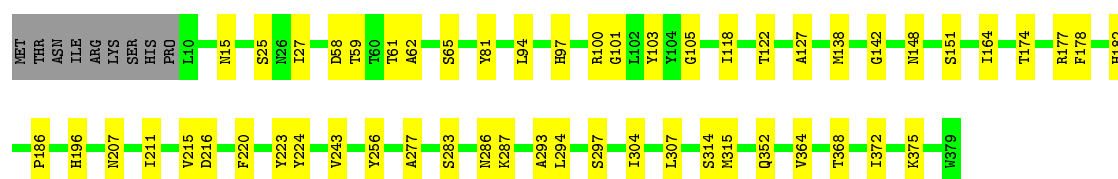
• Molecule 3: Cytochrome b

Chain P:  84% 13% •



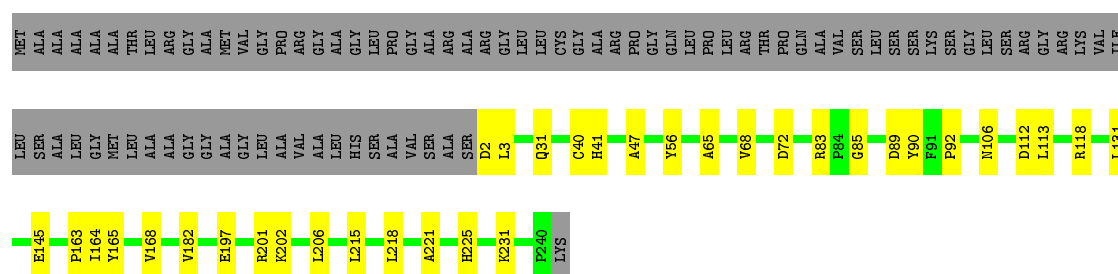
• Molecule 3: Cytochrome b

Chain C:  83% 14% •



• Molecule 4: Cytochrome c1, heme protein, mitochondrial

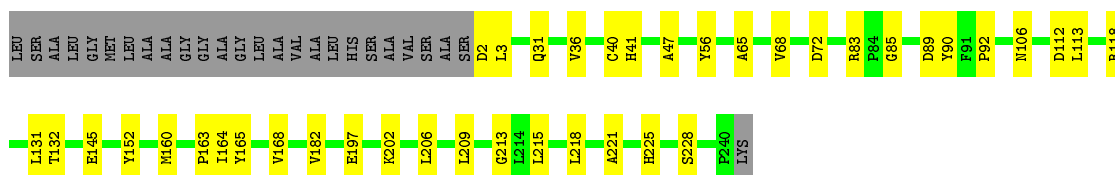
Chain Q:  63% 11% 26%



• Molecule 4: Cytochrome c1, heme protein, mitochondrial

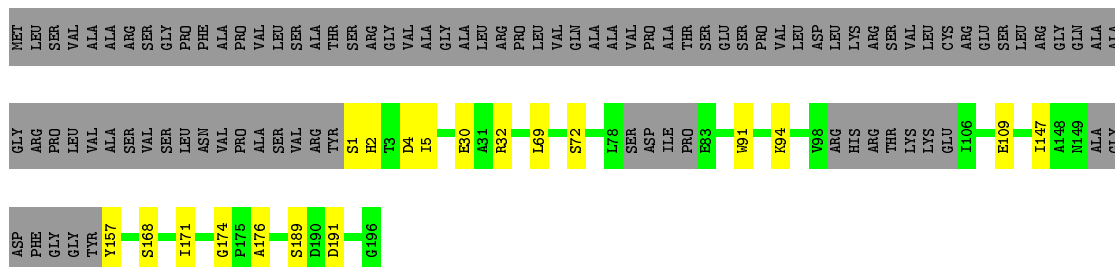
Chain D:  61% 12% 26%





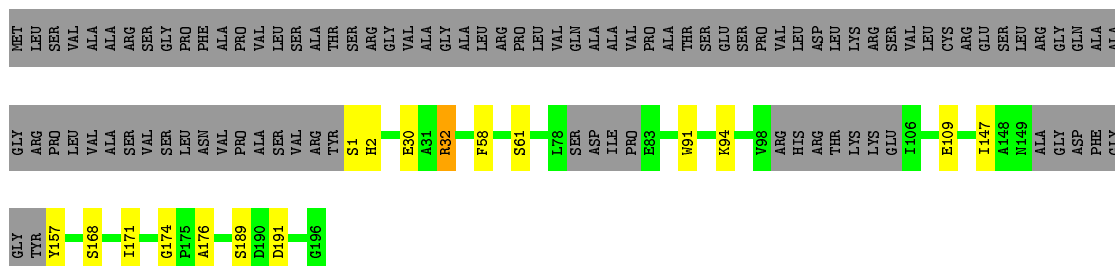
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R: 58% 7% 35%



- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 59% 6% 35%



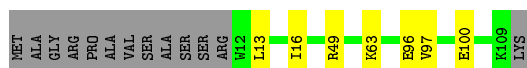
- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain S: 82% 6% 12%



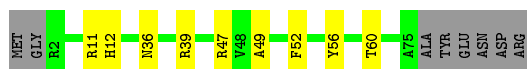
- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F: 82% 6% 12%




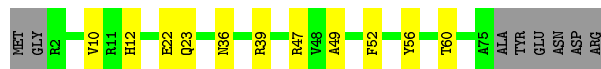
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain T: 79% 11% 10%



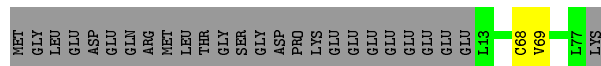
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G:  77% 13% 10%



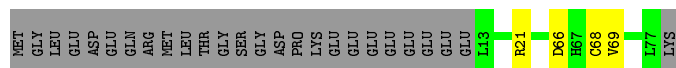
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain U:  69% . 29%




- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:  67% . 29%



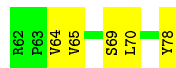
- Molecule 9: Chain I/V

Chain V:  71% 29%



- Molecule 9: Chain I/V

Chain I:  71% 29%




- Molecule 10: Cytochrome b-c1 complex subunit 9

Chain W:  86% . 11%



- Molecule 10: Cytochrome b-c1 complex subunit 9

Chain J:  86% . 11%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	232910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	79000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G8U, HEC, HEM

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 >2	RMSZ	# Z >2
1	A	0.53	0/3500	0.59	0/4752
1	N	0.53	0/3500	0.59	0/4752
10	J	0.52	0/486	0.56	0/655
10	W	0.52	0/486	0.56	0/655
2	B	0.52	0/3166	0.62	2/4291 (0.0%)
2	O	0.52	0/3166	0.62	2/4291 (0.0%)
3	C	0.59	0/3031	0.57	0/4150
3	P	0.59	0/3031	0.57	0/4150
4	D	0.57	0/1962	0.60	0/2665
4	Q	0.57	0/1962	0.60	0/2665
5	E	0.43	0/1373	0.59	1/1861 (0.1%)
5	R	0.43	0/1373	0.59	1/1861 (0.1%)
6	F	0.55	0/879	0.58	0/1180
6	S	0.55	0/879	0.58	0/1180
7	G	0.53	0/645	0.63	0/873
7	T	0.53	0/645	0.64	0/873
8	H	0.39	0/534	0.53	0/718
8	U	0.39	0/534	0.53	0/718
9	I	0.50	0/129	0.79	0/177
9	V	0.50	0/129	0.79	0/177
All	All	0.54	0/31410	0.59	6/42644 (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
3	C	0	1
3	P	0	1
5	E	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
5	R	0	1
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	32	ARG	NE-CZ-NH1	5.91	123.26	120.30
2	O	70	ARG	NE-CZ-NH2	-5.91	117.35	120.30
2	B	70	ARG	NE-CZ-NH2	-5.90	117.35	120.30
5	E	32	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	O	70	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	B	70	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	15	ASN	Peptide
5	E	174	GLY	Peptide
3	P	15	ASN	Peptide
5	R	174	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3428	3325	3324	43	0
1	N	3428	3325	3324	46	0
2	B	3112	3094	3090	41	0
2	O	3112	3094	3090	44	0
3	C	2936	2997	2996	37	0
3	P	2936	2997	2996	36	0
4	D	1903	1848	1849	28	0
4	Q	1903	1848	1849	24	0
5	E	1347	1311	1310	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	1347	1311	1310	11	0
6	F	860	850	849	6	0
6	S	860	850	849	5	0
7	G	624	631	630	7	0
7	T	624	631	630	5	0
8	H	529	512	511	3	0
8	U	529	512	511	1	0
9	I	127	136	135	3	0
9	V	127	136	135	3	0
10	J	473	477	477	2	0
10	W	473	477	477	3	0
11	C	86	0	60	19	0
11	P	86	0	60	19	0
12	C	29	0	15	3	0
12	P	29	0	15	3	0
13	D	43	0	32	9	0
13	Q	43	0	32	6	0
All	All	30994	30362	30556	338	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 5.

All (338) 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)
11:P:501:HEM:HBA1	11:P:501:HEM:HHA	1.65	0.79
13:D:501:HEC:HHA	13:D:501:HEC:HBD1	1.65	0.78
13:Q:501:HEC:HBD1	13:Q:501:HEC:HHA	1.65	0.78
11:C:501:HEM:HHA	11:C:501:HEM:HBA1	1.66	0.77
1:N:412:SER:OG	10:W:15:ARG:NH2	2.18	0.77
1:A:89:TYR:OH	1:A:377:GLU:OE1	2.04	0.76
1:N:89:TYR:OH	1:N:377:GLU:OE1	2.04	0.76
8:H:68:CYS:SG	8:H:69:VAL:N	2.59	0.75
8:U:68:CYS:SG	8:U:69:VAL:N	2.59	0.75
2:O:134:ARG:NH2	6:F:49:ARG:O	2.21	0.74
4:D:152:TYR:OH	8:H:66:ASP:OD2	2.06	0.74
1:N:122:LEU:O	1:N:179:ARG:NH1	2.23	0.72
4:Q:41:HIS:NE2	13:Q:501:HEC:NB	2.38	0.72
2:O:162:ASN:ND2	2:O:246:GLU:OE2	2.23	0.71
1:N:57:TYR:OH	2:O:287:ARG:NH2	2.23	0.71
2:B:162:ASN:ND2	2:B:246:GLU:OE2	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:O	1:A:179:ARG:NH1	2.23	0.71
1:N:372:THR:OG1	2:O:373:GLU:OE2	2.07	0.70
1:N:80:GLU:OE1	2:O:292:THR:OG1	2.05	0.70
1:N:131:ARG:NH1	1:N:174:VAL:O	2.24	0.70
1:A:131:ARG:NH1	1:A:174:VAL:O	2.24	0.70
1:A:57:TYR:OH	2:B:287:ARG:NH2	2.25	0.69
2:B:343:GLN:O	2:B:346:THR:OG1	2.09	0.69
1:N:43:ALA:O	1:N:95:THR:OG1	2.11	0.69
11:C:502:HEM:HMA1	12:C:503:G8U:H15	1.75	0.68
1:N:142:ASP:OD1	5:R:1:SER:OG	2.11	0.68
4:Q:40:CYS:SG	13:Q:501:HEC:HAC	2.33	0.68
2:O:343:GLN:O	2:O:346:THR:OG1	2.10	0.68
1:A:36:THR:OG1	1:A:99:ILE:O	2.07	0.67
2:B:408:ALA:O	2:B:412:ASN:ND2	2.26	0.67
1:A:43:ALA:O	1:A:95:THR:OG1	2.11	0.67
1:N:87:ASN:ND2	1:N:98:TYR:OH	2.27	0.67
11:C:502:HEM:HBC2	11:C:502:HEM:HHD	1.77	0.67
2:O:168:TYR:OH	2:O:320:GLY:O	2.13	0.67
1:A:87:ASN:ND2	1:A:98:TYR:OH	2.27	0.67
3:P:174:THR:OG1	3:P:177:ARG:NH2	2.28	0.67
3:P:256:TYR:OH	4:Q:118:ARG:NH2	2.28	0.67
3:C:174:THR:OG1	3:C:177:ARG:NH2	2.28	0.66
11:P:502:HEM:HBC2	11:P:502:HEM:HHD	1.77	0.66
2:O:408:ALA:O	2:O:412:ASN:ND2	2.26	0.66
1:N:36:THR:OG1	1:N:99:ILE:O	2.06	0.66
2:B:168:TYR:OH	2:B:320:GLY:O	2.13	0.66
7:T:56:TYR:O	7:T:60:THR:OG1	2.11	0.65
1:N:366:VAL:HG11	2:O:44:ALA:HB2	1.78	0.65
1:A:80:GLU:OE1	2:B:292:THR:OG1	2.11	0.65
6:S:49:ARG:O	2:B:134:ARG:NH2	2.30	0.65
3:P:364:VAL:O	3:P:368:THR:OG1	2.12	0.64
13:Q:501:HEC:HMB1	13:Q:501:HEC:HBB3	1.80	0.64
1:A:412:SER:OG	10:J:15:ARG:NH2	2.30	0.64
1:N:370:ASP:OD2	2:O:375:SER:OG	2.14	0.64
3:P:294:LEU:O	3:P:297:SER:OG	2.08	0.63
11:P:502:HEM:HMA1	12:P:503:G8U:H15	1.80	0.63
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.32	0.62
1:N:343:MET:SD	1:N:443:TRP:N	2.72	0.62
3:P:164:ILE:O	3:P:177:ARG:NH2	2.32	0.62
3:C:256:TYR:OH	4:D:118:ARG:NH2	2.31	0.62
13:D:501:HEC:HMB1	13:D:501:HEC:HBB3	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MET:SD	1:A:443:TRP:N	2.72	0.62
3:C:164:ILE:O	3:C:177:ARG:NH2	2.32	0.62
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.32	0.62
11:P:502:HEM:HBD2	11:P:502:HEM:HHA	1.81	0.62
4:D:112:ASP:OD1	4:D:113:LEU:N	2.32	0.61
4:Q:112:ASP:OD1	4:Q:113:LEU:N	2.32	0.61
1:A:142:ASP:OD1	5:E:1:SER:OG	2.18	0.61
4:D:47:ALA:HB2	4:D:90:TYR:HD1	1.65	0.60
2:O:58:GLU:O	2:O:174:ASN:ND2	2.33	0.60
2:B:58:GLU:O	2:B:174:ASN:ND2	2.33	0.60
7:T:36:ASN:OD1	7:T:39:ARG:NH2	2.34	0.60
7:G:36:ASN:OD1	7:G:39:ARG:NH2	2.34	0.60
5:R:147:ILE:O	5:R:157:TYR:N	2.34	0.60
4:Q:163:PRO:HG2	13:Q:501:HEC:HBB2	1.82	0.60
2:O:124:LEU:O	2:O:128:THR:OG1	2.13	0.60
5:E:147:ILE:O	5:E:157:TYR:N	2.34	0.60
3:C:364:VAL:O	3:C:368:THR:OG1	2.11	0.59
11:C:502:HEM:HBD2	11:C:502:HEM:HHA	1.83	0.59
3:C:207:ASN:ND2	3:C:211:ILE:O	2.36	0.59
1:A:246:ASP:OD2	7:G:10:VAL:N	2.35	0.59
4:Q:47:ALA:HB2	4:Q:90:TYR:HD1	1.65	0.59
3:P:207:ASN:ND2	3:P:211:ILE:O	2.36	0.59
1:A:23:LEU:N	1:A:192:ALA:HB1	2.18	0.58
4:D:131:LEU:HD11	13:D:501:HEC:HMB2	1.86	0.58
1:N:23:LEU:N	1:N:192:ALA:HB1	2.18	0.58
11:P:501:HEM:HMC2	11:P:501:HEM:HBC2	1.85	0.58
5:R:30:GLU:OE2	10:W:11:SER:OG	2.22	0.58
9:V:69:SER:OG	9:V:70:LEU:N	2.37	0.58
1:N:366:VAL:CG1	2:O:44:ALA:HB2	2.34	0.57
7:G:56:TYR:O	7:G:60:THR:OG1	2.11	0.57
9:I:69:SER:OG	9:I:70:LEU:N	2.37	0.57
5:R:189:SER:OG	5:R:191:ASP:OD1	2.22	0.57
1:N:76:GLU:OE2	2:O:289:SER:N	2.38	0.57
11:C:502:HEM:HMB2	11:C:502:HEM:HBB2	1.86	0.57
1:A:370:ASP:OD2	2:B:375:SER:OG	2.18	0.56
3:C:294:LEU:O	3:C:297:SER:OG	2.08	0.56
5:E:189:SER:OG	5:E:191:ASP:OD1	2.22	0.56
1:A:366:VAL:HG11	2:B:44:ALA:HB2	1.87	0.56
2:B:124:LEU:O	2:B:128:THR:OG1	2.13	0.56
11:C:501:HEM:HBC2	11:C:501:HEM:HMC2	1.87	0.56
11:P:502:HEM:HMB2	11:P:502:HEM:HBB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:48:GLU:OE2	1:N:55:ALA:N	2.39	0.56
3:P:58:ASP:OD1	3:P:59:THR:N	2.40	0.55
4:Q:221:ALA:O	4:Q:225:HIS:N	2.39	0.55
1:A:48:GLU:OE2	1:A:55:ALA:N	2.39	0.55
5:E:58:PHE:O	5:E:61:SER:OG	2.12	0.55
1:A:87:ASN:OD1	1:A:88:ALA:N	2.40	0.55
2:B:121:GLU:O	2:B:125:ASN:ND2	2.40	0.55
3:C:58:ASP:OD1	3:C:59:THR:N	2.40	0.55
4:D:40:CYS:SG	13:D:501:HEC:HAC	2.47	0.54
4:D:160:MET:SD	13:D:501:HEC:C4D	2.95	0.54
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.37	0.54
1:A:103:SER:OG	1:A:202:GLY:O	2.19	0.54
3:C:81:TYR:HB2	3:C:243:VAL:HG23	1.89	0.54
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.37	0.54
1:A:327:ASP:OD1	1:A:328:HIS:N	2.41	0.54
2:O:121:GLU:O	2:O:125:ASN:ND2	2.40	0.54
3:P:81:TYR:HB2	3:P:243:VAL:HG23	1.89	0.54
7:G:49:ALA:O	7:G:52:PHE:N	2.41	0.54
3:C:94:LEU:O	3:C:97:HIS:N	2.41	0.54
1:N:87:ASN:OD1	1:N:88:ALA:N	2.40	0.54
7:T:49:ALA:O	7:T:52:PHE:N	2.41	0.54
1:N:412:SER:O	10:W:15:ARG:NH2	2.41	0.53
4:D:221:ALA:O	4:D:225:HIS:N	2.38	0.53
5:E:109:GLU:OE2	5:E:168:SER:OG	2.23	0.53
3:P:277:ALA:HB1	3:P:294:LEU:HD11	1.91	0.53
1:N:327:ASP:OD1	1:N:328:HIS:N	2.41	0.53
3:P:94:LEU:O	3:P:97:HIS:N	2.41	0.53
2:O:250:ASP:OD1	2:O:251:SER:N	2.42	0.53
3:P:81:TYR:CB	3:P:243:VAL:HG23	2.40	0.52
2:B:46:ARG:NH1	2:B:376:GLU:OE1	2.42	0.52
3:C:148:ASN:O	3:C:151:SER:OG	2.27	0.52
3:C:25:SER:OG	3:C:216:ASP:OD2	2.16	0.52
3:P:25:SER:OG	3:P:216:ASP:OD2	2.16	0.52
11:P:502:HEM:HBD2	11:P:502:HEM:O2A	2.10	0.52
3:C:277:ALA:HB1	3:C:294:LEU:HD11	1.91	0.52
2:B:250:ASP:OD1	2:B:251:SER:N	2.42	0.52
2:O:46:ARG:NH1	2:O:376:GLU:OE1	2.42	0.52
1:A:76:GLU:OE2	2:B:289:SER:N	2.43	0.51
2:O:74:SER:O	2:O:82:SER:OG	2.11	0.51
11:C:501:HEM:HMB2	11:C:501:HEM:HBB2	1.92	0.51
3:P:314:SER:OG	3:P:315:MET:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:433:ASP:OD2	3:P:223:TYR:OH	2.28	0.51
2:O:319:SER:OG	2:O:320:GLY:N	2.43	0.51
4:D:72:ASP:OD2	4:D:83:ARG:NH2	2.44	0.51
1:N:245:GLU:OE2	7:T:11:ARG:NE	2.31	0.51
3:P:118:ILE:O	3:P:122:THR:OG1	2.18	0.51
3:P:148:ASN:O	3:P:151:SER:OG	2.27	0.51
11:P:501:HEM:HBB2	11:P:501:HEM:HMB2	1.93	0.51
4:Q:2:ASP:OD1	4:Q:3:LEU:N	2.44	0.51
3:C:118:ILE:O	3:C:122:THR:OG1	2.18	0.51
3:C:81:TYR:CB	3:C:243:VAL:HG23	2.40	0.51
2:B:319:SER:OG	2:B:320:GLY:N	2.43	0.51
3:P:178:PHE:O	3:P:182:HIS:N	2.44	0.51
4:Q:72:ASP:OD2	4:Q:83:ARG:NH2	2.44	0.51
5:R:1:SER:OG	5:R:2:HIS:N	2.44	0.51
3:C:127:ALA:CB	11:C:501:HEM:HMB1	2.41	0.50
2:O:437:ASP:OD2	2:B:169:ARG:NH2	2.44	0.50
3:C:314:SER:OG	3:C:315:MET:N	2.43	0.50
5:R:109:GLU:OE2	5:R:168:SER:OG	2.23	0.50
4:Q:215:LEU:O	4:Q:218:LEU:N	2.45	0.50
11:C:502:HEM:O2A	11:C:502:HEM:HBD2	2.12	0.50
4:Q:106:ASN:ND2	4:Q:145:GLU:O	2.45	0.50
3:C:178:PHE:O	3:C:182:HIS:N	2.44	0.50
3:C:283:SER:O	3:C:352:GLN:NE2	2.45	0.50
4:D:215:LEU:O	4:D:218:LEU:N	2.45	0.50
6:F:13:LEU:O	6:F:16:ILE:HG22	2.12	0.50
3:P:127:ALA:CB	11:P:501:HEM:HMB1	2.42	0.50
4:D:2:ASP:OD1	4:D:3:LEU:N	2.44	0.50
1:N:76:GLU:OE2	2:O:290:ASN:N	2.44	0.50
11:P:501:HEM:HBC2	11:P:501:HEM:CMC	2.42	0.50
3:C:127:ALA:HB2	11:C:501:HEM:HMB1	1.94	0.49
3:P:286:ASN:OD1	3:P:287:LYS:N	2.45	0.49
5:E:1:SER:OG	5:E:2:HIS:N	2.43	0.49
2:O:279:LEU:HD11	2:O:344:VAL:HG22	1.93	0.49
2:O:73:SER:O	2:O:74:SER:OG	2.24	0.49
6:S:13:LEU:O	6:S:16:ILE:HG22	2.12	0.49
2:B:261:SER:OG	2:B:262:ALA:N	2.45	0.49
4:D:106:ASN:ND2	4:D:145:GLU:O	2.45	0.49
2:B:279:LEU:HD11	2:B:344:VAL:HG22	1.93	0.49
3:P:283:SER:O	3:P:352:GLN:NE2	2.45	0.49
1:N:171:SER:N	5:R:4:ASP:OD1	2.43	0.49
2:B:131:GLU:OE1	2:B:133:ARG:NE	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:VAL:CG1	2:B:44:ALA:HB2	2.41	0.49
3:C:286:ASN:OD1	3:C:287:LYS:N	2.45	0.49
2:O:261:SER:OG	2:O:262:ALA:N	2.45	0.49
2:O:163:LEU:HD12	2:O:425:ALA:HB3	1.95	0.49
3:P:248:ASP:OD1	4:Q:118:ARG:NH2	2.42	0.49
3:P:293:ALA:O	3:P:297:SER:N	2.45	0.49
1:N:192:ALA:HB2	1:N:219:LEU:HD23	1.95	0.49
2:B:163:LEU:HD12	2:B:425:ALA:HB3	1.95	0.49
3:C:101:GLY:O	3:C:105:GLY:N	2.46	0.48
2:O:131:GLU:OE1	2:O:133:ARG:NE	2.45	0.48
3:C:293:ALA:O	3:C:297:SER:N	2.45	0.48
4:D:41:HIS:NE2	13:D:501:HEC:NB	2.61	0.48
11:C:501:HEM:HBC2	11:C:501:HEM:CMC	2.43	0.48
9:I:64:VAL:HG22	9:I:78:TYR:O	2.14	0.48
1:N:245:GLU:OE1	7:T:12:HIS:N	2.43	0.48
4:D:164:ILE:HD13	4:D:182:VAL:HG11	1.94	0.48
1:A:245:GLU:OE1	7:G:12:HIS:N	2.44	0.48
2:O:162:ASN:O	2:O:166:ALA:N	2.44	0.48
3:P:101:GLY:O	3:P:105:GLY:N	2.46	0.48
3:P:127:ALA:HB2	11:P:501:HEM:HMB1	1.95	0.48
11:P:502:HEM:O2A	11:P:502:HEM:HHA	2.14	0.48
2:B:308:ASP:OD1	2:B:309:VAL:N	2.47	0.47
3:C:186:PRO:HG2	11:C:501:HEM:HMC1	1.96	0.47
1:A:192:ALA:HB2	1:A:219:LEU:HD23	1.95	0.47
1:A:94:HIS:O	1:A:95:THR:OG1	2.32	0.47
4:Q:164:ILE:HD13	4:Q:182:VAL:HG11	1.94	0.47
1:A:79:VAL:O	1:A:83:GLY:N	2.48	0.47
1:A:433:ASP:OD2	3:C:223:TYR:OH	2.32	0.47
1:N:94:HIS:O	1:N:95:THR:OG1	2.32	0.47
1:A:340:GLY:HA2	1:A:343:MET:HE3	1.97	0.47
9:V:64:VAL:HG22	9:V:78:TYR:O	2.14	0.47
2:B:67:HIS:NE2	2:B:147:ASP:OD2	2.43	0.47
4:Q:202:LYS:O	4:Q:206:LEU:N	2.48	0.47
3:C:27:ILE:HD12	3:C:224:TYR:CZ	2.50	0.47
4:D:202:LYS:O	4:D:206:LEU:N	2.48	0.47
1:N:86:LEU:HD23	2:O:285:VAL:HG13	1.97	0.47
11:C:501:HEM:HHA	11:C:501:HEM:CGD	2.45	0.47
2:O:53:ALA:O	2:O:194:TYR:OH	2.33	0.47
4:D:164:ILE:CD1	4:D:182:VAL:HG11	2.45	0.46
1:N:21:ASN:OD1	1:N:22:GLY:N	2.49	0.46
2:B:338:LYS:O	2:B:342:ASN:ND2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:502:HEM:O2A	11:C:502:HEM:HHA	2.15	0.46
4:D:197:GLU:N	4:D:197:GLU:OE1	2.48	0.46
1:N:84:ALA:HB1	1:N:100:LYS:O	2.15	0.46
3:P:27:ILE:HD12	3:P:224:TYR:CZ	2.50	0.46
4:D:163:PRO:HG2	13:D:501:HEC:HBB2	1.97	0.46
5:R:69:LEU:O	5:R:72:SER:OG	2.28	0.46
3:P:186:PRO:HG2	11:P:501:HEM:HMC1	1.96	0.46
3:P:220:PHE:CZ	12:P:503:G8U:H13	2.51	0.46
1:A:84:ALA:HB1	1:A:100:LYS:O	2.15	0.46
11:C:502:HEM:CMA	12:C:503:G8U:H15	2.43	0.46
1:N:140:GLU:O	1:N:143:THR:OG1	2.20	0.46
1:N:363:ASN:ND2	2:O:93:GLY:O	2.48	0.46
3:P:61:THR:O	3:P:65:SER:N	2.47	0.46
2:B:73:SER:O	2:B:74:SER:OG	2.24	0.46
4:D:228:SER:O	7:G:23:GLN:NE2	2.49	0.46
2:O:338:LYS:O	2:O:342:ASN:ND2	2.49	0.46
6:S:97:VAL:O	6:S:100:GLU:N	2.49	0.46
2:B:162:ASN:HA	2:B:165:ALA:HB3	1.98	0.46
2:B:162:ASN:O	2:B:166:ALA:N	2.44	0.46
1:A:372:THR:OG1	2:B:373:GLU:OE2	2.15	0.46
4:D:83:ARG:NH2	4:D:89:ASP:OD2	2.49	0.46
4:Q:197:GLU:OE1	4:Q:197:GLU:N	2.49	0.46
4:Q:31:GLN:NE2	4:Q:56:TYR:OH	2.49	0.46
1:A:274:ASN:O	1:A:278:GLY:N	2.50	0.45
1:N:340:GLY:HA2	1:N:343:MET:HE3	1.97	0.45
1:A:21:ASN:OD1	1:A:22:GLY:N	2.49	0.45
4:Q:165:TYR:CE1	4:Q:168:VAL:HG23	2.52	0.45
2:B:46:ARG:NH1	2:B:110:GLU:OE2	2.49	0.45
1:N:79:VAL:O	1:N:83:GLY:N	2.48	0.45
2:O:279:LEU:HD11	2:O:344:VAL:CG2	2.47	0.45
4:Q:164:ILE:CD1	4:Q:182:VAL:HG11	2.45	0.45
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.44	0.45
2:B:279:LEU:HD11	2:B:344:VAL:CG2	2.47	0.45
4:D:165:TYR:CE1	4:D:168:VAL:HG23	2.51	0.45
6:F:97:VAL:O	6:F:100:GLU:N	2.48	0.45
2:B:53:ALA:O	2:B:194:TYR:OH	2.33	0.45
4:D:31:GLN:NE2	4:D:56:TYR:OH	2.49	0.45
4:Q:131:LEU:HD11	13:Q:501:HEC:HMB2	1.98	0.45
4:D:132:THR:O	8:H:21:ARG:NH2	2.49	0.45
4:Q:65:ALA:HB1	4:Q:85:GLY:C	2.37	0.45
2:B:101:THR:HG22	9:I:65:VAL:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:308:ASP:OD1	2:O:309:VAL:N	2.47	0.44
11:C:501:HEM:CGD	11:C:501:HEM:HBA1	2.47	0.44
4:D:65:ALA:HB1	4:D:85:GLY:C	2.37	0.44
3:P:100:ARG:O	3:P:103:TYR:N	2.50	0.44
1:N:103:SER:OG	1:N:202:GLY:O	2.19	0.44
4:Q:83:ARG:NH2	4:Q:89:ASP:OD2	2.49	0.44
1:N:274:ASN:O	1:N:278:GLY:N	2.49	0.44
3:P:313:ARG:HE	6:S:38:HIS:CD2	2.35	0.44
1:A:140:GLU:O	1:A:143:THR:OG1	2.20	0.44
1:A:147:ASP:O	1:A:151:ASN:ND2	2.50	0.44
2:O:162:ASN:HA	2:O:165:ALA:HB3	1.98	0.44
3:P:196:HIS:NE2	11:P:502:HEM:ND	2.66	0.44
1:A:157:ALA:HB1	1:A:236:PHE:CE1	2.53	0.44
3:C:196:HIS:NE2	11:C:502:HEM:ND	2.66	0.44
1:N:147:ASP:O	1:N:151:ASN:ND2	2.50	0.44
1:N:157:ALA:HB1	1:N:236:PHE:CE1	2.53	0.43
11:C:502:HEM:CMB	11:C:502:HEM:HBB2	2.48	0.43
2:B:255:ALA:O	2:B:326:THR:N	2.49	0.43
3:C:100:ARG:O	3:C:103:TYR:N	2.50	0.43
5:R:171:ILE:HD13	5:R:176:ALA:HB3	2.00	0.43
1:A:363:ASN:ND2	2:B:93:GLY:O	2.51	0.43
1:N:210:ASP:O	1:N:214:LYS:N	2.51	0.43
3:C:220:PHE:CZ	12:C:503:G8U:H13	2.53	0.43
5:E:30:GLU:OE2	10:J:11:SER:OG	2.12	0.43
2:O:46:ARG:NH1	2:O:110:GLU:OE2	2.49	0.43
1:A:281:ASP:O	1:A:283:THR:N	2.52	0.43
5:E:171:ILE:HD13	5:E:176:ALA:HB3	2.00	0.43
2:O:133:ARG:NH1	6:F:96:GLU:OE2	2.51	0.43
1:N:24:ARG:NH1	1:N:383:LEU:O	2.52	0.43
11:P:501:HEM:HBA1	11:P:501:HEM:CGD	2.49	0.43
3:C:61:THR:O	3:C:65:SER:N	2.47	0.43
11:P:501:HEM:CGD	11:P:501:HEM:HHA	2.48	0.43
4:D:36:VAL:HG11	13:D:501:HEC:HAB	2.00	0.43
2:O:169:ARG:NH2	2:B:437:ASP:OD2	2.52	0.43
3:C:372:ILE:O	3:C:375:LYS:N	2.50	0.42
3:P:304:ILE:O	3:P:307:LEU:N	2.47	0.42
2:O:133:ARG:NH2	6:F:96:GLU:OE2	2.51	0.42
5:E:91:TRP:N	5:E:94:LYS:O	2.49	0.42
2:O:35:ILE:HG22	2:O:36:ALA:N	2.34	0.42
2:B:35:ILE:HG22	2:B:36:ALA:N	2.34	0.42
3:C:304:ILE:O	3:C:307:LEU:N	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:502:HEM:CMB	11:P:502:HEM:HBB2	2.49	0.42
5:R:91:TRP:N	5:R:94:LYS:O	2.49	0.42
1:A:24:ARG:NH1	1:A:383:LEU:O	2.52	0.42
1:A:49:SER:N	1:A:52:ASN:OD1	2.52	0.42
3:P:182:HIS:NE2	11:P:501:HEM:NB	2.68	0.42
2:B:77:THR:OG1	2:B:80:ALA:O	2.25	0.42
3:C:58:ASP:O	3:C:62:ALA:HB2	2.20	0.42
2:B:207:ILE:HG22	2:B:208:GLY:N	2.35	0.42
4:D:36:VAL:CG1	13:D:501:HEC:HAB	2.50	0.42
3:P:58:ASP:O	3:P:62:ALA:HB2	2.20	0.42
4:Q:231:LYS:O	6:S:71:ARG:NH2	2.53	0.42
3:C:182:HIS:NE2	11:C:501:HEM:NB	2.68	0.42
2:O:207:ILE:HG22	2:O:208:GLY:N	2.35	0.41
4:Q:68:VAL:HG11	4:Q:92:PRO:HG2	2.02	0.41
1:A:210:ASP:O	1:A:214:LYS:N	2.51	0.41
1:N:152:TYR:CE1	5:R:5:ILE:HD13	2.55	0.41
11:P:502:HEM:CMA	12:P:503:G8U:H15	2.48	0.41
4:D:209:LEU:O	4:D:213:GLY:N	2.44	0.41
5:E:32:ARG:NH1	7:G:22:GLU:OE2	2.52	0.41
1:N:235:ARG:NH1	1:N:237:THR:OG1	2.51	0.41
1:N:281:ASP:O	1:N:283:THR:N	2.52	0.41
1:A:76:GLU:OE2	2:B:290:ASN:N	2.54	0.41
2:O:67:HIS:NE2	2:O:147:ASP:OD2	2.43	0.41
3:P:27:ILE:HD12	3:P:224:TYR:OH	2.21	0.41
4:Q:197:GLU:O	4:Q:201:ARG:N	2.48	0.41
2:O:101:THR:HG22	9:V:65:VAL:HG13	2.03	0.41
2:B:169:ARG:HE	2:B:240:HIS:HB2	1.87	0.40
4:D:68:VAL:HG11	4:D:92:PRO:HG2	2.03	0.40
1:A:378:ASP:O	1:A:382:SER:OG	2.23	0.40
3:C:215:VAL:O	6:F:63:LYS:NZ	2.44	0.40
1:N:95:THR:HG22	1:N:96:ALA:N	2.36	0.40
2:O:255:ALA:O	2:O:326:THR:N	2.49	0.40
3:C:138:MET:O	3:C:142:GLY:N	2.48	0.40
2:O:39:GLU:OE2	2:O:113:ARG:NH2	2.49	0.40
3:C:27:ILE:HD12	3:C:224:TYR:OH	2.21	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 PDB entries followed by that with respect to all EM entries.

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	441/480 (92%)	398 (90%)	42 (10%)	1 (0%)	51	84
1	N	441/480 (92%)	398 (90%)	42 (10%)	1 (0%)	51	84
2	B	408/453 (90%)	360 (88%)	48 (12%)	0	100	100
2	O	408/453 (90%)	360 (88%)	48 (12%)	0	100	100
3	C	368/379 (97%)	330 (90%)	38 (10%)	0	100	100
3	P	368/379 (97%)	330 (90%)	38 (10%)	0	100	100
4	D	237/325 (73%)	215 (91%)	22 (9%)	0	100	100
4	Q	237/325 (73%)	216 (91%)	21 (9%)	0	100	100
5	E	170/274 (62%)	151 (89%)	19 (11%)	0	100	100
5	R	170/274 (62%)	151 (89%)	19 (11%)	0	100	100
6	F	96/111 (86%)	91 (95%)	5 (5%)	0	100	100
6	S	96/111 (86%)	90 (94%)	6 (6%)	0	100	100
7	G	72/82 (88%)	64 (89%)	8 (11%)	0	100	100
7	T	72/82 (88%)	64 (89%)	8 (11%)	0	100	100
8	H	63/91 (69%)	58 (92%)	5 (8%)	0	100	100
8	U	63/91 (69%)	58 (92%)	5 (8%)	0	100	100
9	I	15/17 (88%)	8 (53%)	7 (47%)	0	100	100
9	V	15/17 (88%)	8 (53%)	7 (47%)	0	100	100
10	J	55/64 (86%)	53 (96%)	2 (4%)	0	100	100
10	W	55/64 (86%)	53 (96%)	2 (4%)	0	100	100
All	All	3850/4552 (85%)	3456 (90%)	392 (10%)	2 (0%)	58	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	282	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	282	CYS

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 PDB entries followed by that with respect to all EM entries.

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	367/394 (93%)	367 (100%)	0	100	100
1	N	367/394 (93%)	367 (100%)	0	100	100
2	B	325/355 (92%)	325 (100%)	0	100	100
2	O	325/355 (92%)	325 (100%)	0	100	100
3	C	318/327 (97%)	318 (100%)	0	100	100
3	P	318/327 (97%)	318 (100%)	0	100	100
4	D	204/257 (79%)	204 (100%)	0	100	100
4	Q	204/257 (79%)	204 (100%)	0	100	100
5	E	147/228 (64%)	147 (100%)	0	100	100
5	R	147/228 (64%)	147 (100%)	0	100	100
6	F	90/99 (91%)	90 (100%)	0	100	100
6	S	90/99 (91%)	90 (100%)	0	100	100
7	G	66/72 (92%)	65 (98%)	1 (2%)	70	86
7	T	66/72 (92%)	65 (98%)	1 (2%)	70	86
8	H	62/85 (73%)	62 (100%)	0	100	100
8	U	62/85 (73%)	62 (100%)	0	100	100
9	I	15/15 (100%)	15 (100%)	0	100	100
9	V	15/15 (100%)	15 (100%)	0	100	100
10	J	48/54 (89%)	48 (100%)	0	100	100
10	W	48/54 (89%)	48 (100%)	0	100	100
All	All	3284/3772 (87%)	3282 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	T	47	ARG
7	G	47	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	252	HIS
2	O	343	GLN
4	Q	31	GLN
5	R	141	HIS
5	R	161	HIS
1	A	87	ASN
1	A	252	HIS
2	B	343	GLN
4	D	31	GLN
5	E	141	HIS
5	E	161	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	HEM	C	501	-	28,50,50	1.93	5 (17%)	17,82,82	2.08	7 (41%)
11	HEM	C	502	3	28,50,50	2.10	4 (14%)	17,82,82	1.78	4 (23%)
12	G8U	C	503	-	31,31,31	0.98	1 (3%)	39,45,45	1.14	5 (12%)
13	HEC	D	501	4	28,50,50	2.50	3 (10%)	16,82,82	2.09	5 (31%)
11	HEM	P	501	3	28,50,50	1.94	5 (17%)	17,82,82	2.13	7 (41%)
11	HEM	P	502	3	28,50,50	2.10	4 (14%)	17,82,82	1.75	4 (23%)
12	G8U	P	503	-	31,31,31	0.97	1 (3%)	39,45,45	1.12	4 (10%)
13	HEC	Q	501	4	28,50,50	2.50	3 (10%)	16,82,82	2.09	5 (31%)

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
11	HEM	C	501	-	-	0/6/54/54	0/0/8/8
11	HEM	C	502	3	-	0/6/54/54	0/0/8/8
12	G8U	C	503	-	-	0/15/15/15	0/3/3/3
13	HEC	D	501	4	-	0/6/54/54	0/0/8/8
11	HEM	P	501	3	-	0/6/54/54	0/0/8/8
11	HEM	P	502	3	-	0/6/54/54	0/0/8/8
12	G8U	P	503	-	-	0/15/15/15	0/3/3/3
13	HEC	Q	501	4	-	0/6/54/54	0/0/8/8

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	501	HEC	C3C-C2C	-8.40	1.31	1.40
13	Q	501	HEC	C3C-C2C	-8.38	1.31	1.40
13	D	501	HEC	C3B-C2B	-7.17	1.33	1.40
13	Q	501	HEC	C3B-C2B	-7.17	1.33	1.40
11	P	502	HEM	C3C-C2C	-6.60	1.31	1.40
11	C	502	HEM	C3C-C2C	-6.60	1.31	1.40
11	C	501	HEM	C3C-C2C	-5.44	1.33	1.40
11	P	501	HEM	C3C-C2C	-5.39	1.33	1.40
11	P	502	HEM	C3B-C2B	-4.99	1.33	1.40
11	C	502	HEM	C3B-C2B	-4.95	1.33	1.40
11	P	501	HEM	C3B-C2B	-4.57	1.34	1.40
11	C	501	HEM	C3B-C2B	-4.50	1.34	1.40
11	P	501	HEM	C4B-CHC	-2.19	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	501	HEM	C4B-CHC	-2.17	1.34	1.40
12	P	503	G8U	C19-CL	2.74	1.78	1.72
12	C	503	G8U	C19-CL	2.77	1.78	1.72
11	C	501	HEM	C3C-CAC	3.05	1.53	1.47
11	P	501	HEM	C3C-CAC	3.13	1.54	1.47
11	C	502	HEM	C3B-CAB	3.29	1.54	1.47
11	P	502	HEM	C3B-CAB	3.32	1.54	1.47
11	P	502	HEM	C3C-CAC	3.42	1.54	1.47
11	C	502	HEM	C3C-CAC	3.43	1.54	1.47
11	C	501	HEM	C3B-CAB	3.84	1.55	1.47
11	P	501	HEM	C3B-CAB	3.85	1.55	1.47
13	Q	501	HEC	C3D-C2D	5.14	1.52	1.37
13	D	501	HEC	C3D-C2D	5.16	1.53	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	501	HEC	CAA-CBA-CGA	-4.02	105.79	112.66
13	Q	501	HEC	CAA-CBA-CGA	-4.01	105.81	112.66
11	C	501	HEM	CBD-CAD-C3D	-3.48	105.83	112.47
11	P	501	HEM	CAA-CBA-CGA	-3.40	106.85	112.66
11	P	501	HEM	CBD-CAD-C3D	-3.34	106.09	112.47
11	C	501	HEM	CAA-CBA-CGA	-3.32	106.99	112.66
12	C	503	G8U	C27-C20-C19	-3.29	119.55	123.35
12	P	503	G8U	C27-C20-C19	-3.28	119.56	123.35
13	D	501	HEC	CAD-CBD-CGD	-3.26	107.09	112.66
13	Q	501	HEC	CAD-CBD-CGD	-3.24	107.13	112.66
11	C	502	HEM	CBA-CAA-C2A	-3.01	106.72	112.48
11	P	502	HEM	CBA-CAA-C2A	-3.01	106.73	112.48
13	Q	501	HEC	C1D-C2D-C3D	-2.98	104.93	107.00
11	C	502	HEM	CAA-CBA-CGA	-2.91	107.69	112.66
13	D	501	HEC	C1D-C2D-C3D	-2.91	104.97	107.00
11	P	502	HEM	CAD-C3D-C2D	-2.68	121.35	129.00
11	P	501	HEM	CAA-C2A-C3A	-2.68	121.35	129.00
11	C	502	HEM	CAD-C3D-C2D	-2.67	121.37	129.00
11	P	502	HEM	CAA-CBA-CGA	-2.63	108.17	112.66
13	D	501	HEC	CMB-C2B-C1B	-2.62	124.43	128.46
11	P	501	HEM	CMA-C3A-C4A	-2.62	124.44	128.46
13	Q	501	HEC	CMB-C2B-C1B	-2.62	124.44	128.46
11	C	501	HEM	CAA-C2A-C3A	-2.57	121.66	129.00
11	C	501	HEM	CMA-C3A-C4A	-2.45	124.69	128.46
12	C	503	G8U	C17-C22-N28	-2.20	120.95	123.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	503	G8U	C17-C22-N28	-2.17	120.99	123.71
12	C	503	G8U	C24-C22-C17	-2.15	119.59	122.27
12	C	503	G8U	O25-C24-C22	-2.07	107.72	112.20
12	P	503	G8U	O25-C24-C22	-2.04	107.78	112.20
12	P	503	G8U	C27-C20-N28	2.16	119.74	116.52
12	C	503	G8U	C27-C20-N28	2.21	119.82	116.52
11	C	501	HEM	C3B-C4B-NB	2.35	112.25	109.21
11	P	501	HEM	C3B-C4B-NB	2.38	112.29	109.21
13	Q	501	HEC	C4C-C3C-C2C	2.57	109.12	106.35
13	D	501	HEC	C4C-C3C-C2C	2.60	109.16	106.35
11	C	501	HEM	C4A-C3A-C2A	2.88	109.00	107.00
11	C	502	HEM	C1D-C2D-C3D	2.89	109.01	107.00
11	P	501	HEM	C4A-C3A-C2A	3.00	109.09	107.00
11	P	502	HEM	C1D-C2D-C3D	3.05	109.12	107.00
11	C	501	HEM	CMC-C2C-C3C	3.58	131.53	124.89
11	P	501	HEM	CMC-C2C-C3C	3.62	131.61	124.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	501	HEM	10	0
11	C	502	HEM	9	0
12	C	503	G8U	3	0
13	D	501	HEC	9	0
11	P	501	HEM	10	0
11	P	502	HEM	9	0
12	P	503	G8U	3	0
13	Q	501	HEC	6	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.