



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:52 AM GMT

PDB ID : 2IBZ
Title : Yeast Cytochrome BC1 Complex with Stigmatellin
Authors : Hunte, C.
Deposited on : 2006-09-12
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

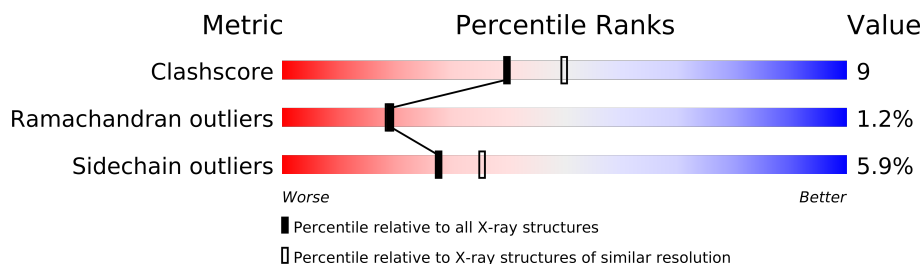
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	
2	B	352	
3	C	385	
4	D	248	
5	E	185	
6	H	74	
7	F	127	
8	G	94	
9	I	66	
10	X	127	
11	Y	107	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 17779 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ubiquinol-cytochrome-c reductase complex core protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	CONFLICT	UNP P07256

- Molecule 2 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3089	2080	484	504	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	122	THR	ILE	CONFLICT	UNP P00163

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total	C	N	O	S	0	0	0
			1933	1232	333	359	9			

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mito-

chondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called Ubiquinol-cytochrome c reductase complex 17 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			

- Molecule 8 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	93	Total	C	N	O	S	98	0	0
			773	510	131	130	2			

- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase complex 7.3 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	55	Total	C	N	O	0	0	0
			448	298	75	75			

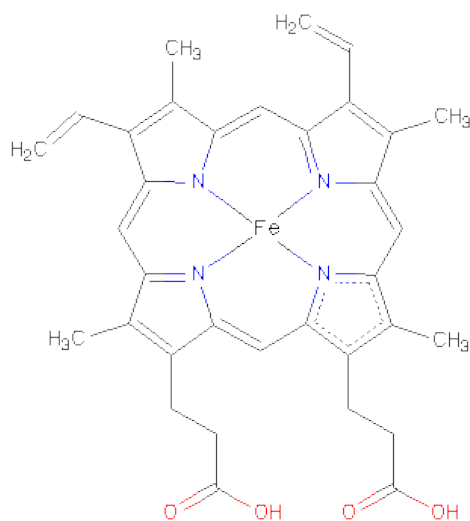
- Molecule 10 is a protein called Variable Heavy chain of antibody fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called Variable Light chain of antibody fragment.

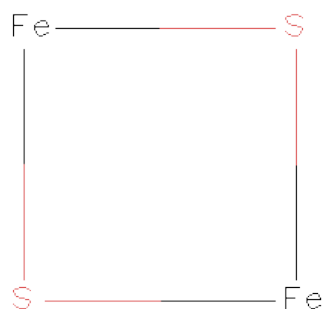
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	Y	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



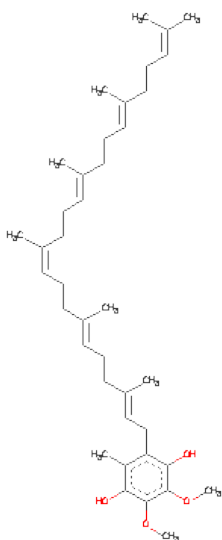
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



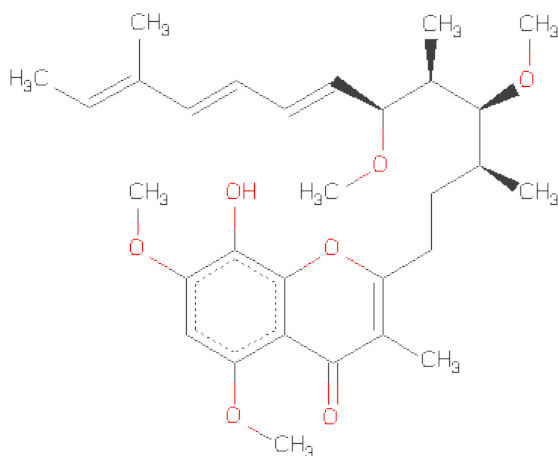
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 14 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			43	39	4		

- Molecule 15 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			37	30	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	49	Total	O	0	0
			49	49		
16	B	11	Total	O	0	0
			11	11		
16	C	111	Total	O	0	0
			111	111		
16	D	68	Total	O	0	0
			68	68		
16	E	32	Total	O	0	0
			32	32		
16	F	36	Total	O	0	0
			36	36		
16	G	19	Total	O	0	0
			19	19		
16	H	6	Total	O	0	0
			6	6		
16	I	1	Total	O	0	0
			1	1		
16	X	5	Total	O	0	0
			5	5		
16	Y	2	Total	O	0	0
			2	2		

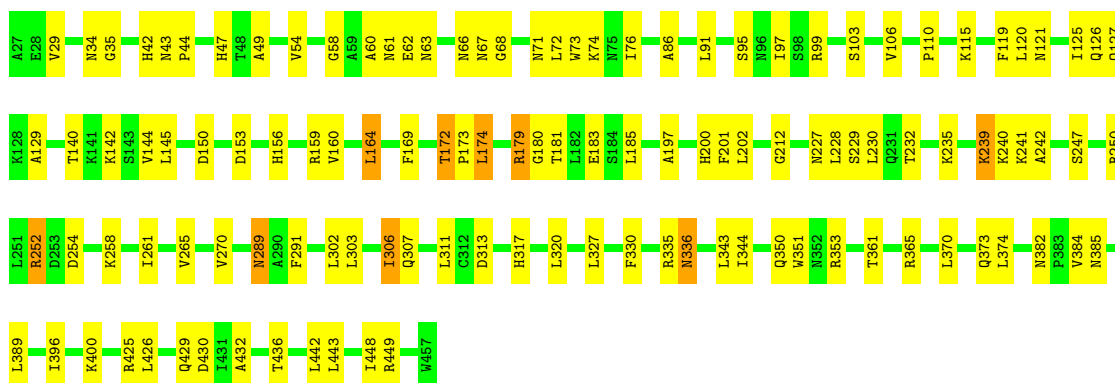
3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein 1

Chain A:



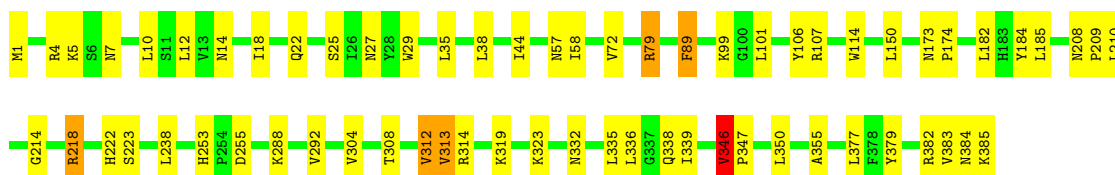
- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2

Chain B:



- Molecule 3: Cytochrome b

Chain C:



- Molecule 4: Cytochrome c1, heme protein, mitochondrial precursor

L283	W286	F302	K306	PRO	ARG	LYS	M62	H67	G68	L69	Y74	H78	Y94	G95	V96	R109	V110	A111	V112	R113	T121	E124	V125	M128	Y134	R147	P148	L151	V154	T155	P156	S178	P203	V206	T243	T244	Y247	V251	N256	H263	K267	S279	L280
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|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| H184 | H185 | D186 | I187 | R190 | I191 | A196 | I202 | Y205 | K211 | G215 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| K31 | M33 | F39 | D40 | L43 | K44 | E45 | M46 | A49 | G52 | Y55 | A56 | Y57 | F58 | M59 | K72 | T85 | M91 | A92 | K93 | P102 | L103 | V107 | P115 | I118 | R119 | H120 | E125 | A129 | R146 | Q151 | I154 | I158 | G168 | D172 | W176 | H181 |

- V74
T75
D76
Q77
L78
R82
K86
G91
L94
V95
E99
E100
C101
V105
L117
L130
A139
L142
K147

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|-----|-----|----|----|----|--|-----|-----|--|-----|--|-----|-----|--|-----|-----|-----|-----|-----|--|-----|--|-----|--|-----|--|-----|-----|-----|--|-----|-----|-----|--|-----|-----|-----|--|------|--|------|
| ME1 | PR0 | Q3 | S4 | F5 | | I15 | L16 | | L21 | | N30 | Q31 | | L41 | G42 | L43 | K44 | F45 | | L48 | | N53 | | M56 | | R71 | A72 | Y73 | | R77 | A78 | H79 | | H86 | L87 | L88 | | K115 | | K127 |
|-----|-----|----|----|----|--|-----|-----|--|-----|--|-----|-----|--|-----|-----|-----|-----|-----|--|-----|--|-----|--|-----|--|-----|-----|-----|--|-----|-----|-----|--|-----|-----|-----|--|------|--|------|

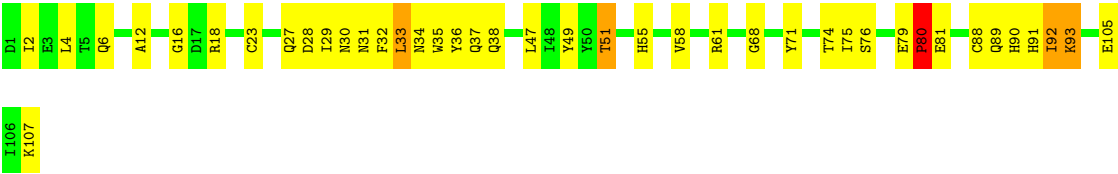
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|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | G2 | M16 | V29 | S30 | P31 | L37 | Q38 | F41 | V45 | F52 | Q55 | F56 | L60 | I61 | P62 | I65 | W70 | N77 | K83 | R86 | E87 | E88 | L89 | N93 | V94 |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | PHE | S4 | S5 | L6 | Y7 | K8 | T9 | K12 | R13 | N14 | V18 | Q29 | L48 | A58 | GLY | ASP | GLY | ASP | ASP | ASP | ASP | GLU |
|-----|-----|-----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- [illegible]

- Molecule 11: Variable Light chain of antibody fragment

Chain Y: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.47Å 163.92Å 147.28Å 90.00° 117.50° 90.00°	Depositor
Resolution (Å)	14.96 – 2.30	Depositor
% Data completeness (in resolution range)	84.7 (14.96-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17779	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FES, SMA, UQ6

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	0.39	0/3405	0.62	0/4614
2	B	0.35	0/2781	0.60	0/3764
3	C	0.53	0/3191	0.71	5/4353 (0.1%)
4	D	0.40	0/1993	0.64	0/2714
5	E	0.39	0/1444	0.66	0/1957
6	H	0.37	0/638	0.54	0/858
7	F	0.42	0/1032	0.69	2/1397 (0.1%)
8	G	0.43	0/804	0.54	0/1088
9	I	0.43	0/461	0.50	0/622
10	X	0.36	0/1043	0.64	0/1422
11	Y	0.32	0/863	0.55	0/1172
All	All	0.41	0/17655	0.63	7/23961 (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
4	D	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	79	ARG	NE-CZ-NH1	-7.80	116.40	120.30
7	F	71	ARG	NE-CZ-NH1	-7.35	116.62	120.30
3	C	314	ARG	NE-CZ-NH1	-5.57	117.52	120.30
3	C	346	VAL	N-CA-C	5.22	125.10	111.00
3	C	107	ARG	NE-CZ-NH1	-5.21	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	71	ARG	NE-CZ-NH2	5.17	122.89	120.30
3	C	79	ARG	NE-CZ-NH2	5.13	122.87	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	94	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3321	74	0
2	B	2735	0	2774	73	0
3	C	3089	0	3125	37	0
4	D	1933	0	1855	23	0
5	E	1411	0	1386	30	0
6	H	624	0	581	11	0
7	F	1012	0	1026	13	0
8	G	773	0	736	13	0
9	I	448	0	445	6	0
10	X	1015	0	959	32	0
11	Y	842	0	820	29	0
12	C	86	0	60	5	0
12	D	43	0	30	0	0
13	E	4	0	0	1	0
14	C	43	0	58	6	0
15	C	37	0	41	0	0
16	A	49	0	0	1	0
16	B	11	0	0	0	0
16	C	111	0	0	1	0
16	D	68	0	0	2	0
16	E	32	0	0	0	0
16	F	36	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	G	19	0	0	0	0
16	H	6	0	0	0	0
16	I	1	0	0	0	0
16	X	5	0	0	1	0
16	Y	2	0	0	0	0
All	All	17779	0	17217	326	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (326) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:H:77:GLN:H	6:H:77:GLN:HE21	1.00	0.98
14:C:506:UQ6:H103	14:C:506:UQ6:H1M1	1.46	0.95
11:Y:31:ASN:HD22	11:Y:51:THR:HG21	1.36	0.90
5:E:72:LYS:HZ3	9:I:29:GLN:HE22	1.16	0.88
2:B:347:LYS:HD3	2:B:347:LYS:H	1.40	0.85
7:F:31:GLN:HE21	7:F:31:GLN:HA	1.41	0.85
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.59	0.85
6:H:77:GLN:H	6:H:77:GLN:NE2	1.75	0.82
3:C:253:HIS:HD2	3:C:255:ASP:H	1.28	0.82
3:C:7:ASN:HD22	3:C:10:LEU:H	1.28	0.81
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.28	0.81
2:B:182:LYS:HB2	2:B:211:ALA:HB2	1.61	0.81
1:A:63:ASN:HB2	1:A:66:ASN:ND2	1.97	0.80
7:F:77:ARG:HD3	7:F:88:LEU:HD11	1.65	0.79
3:C:44:ILE:HD12	14:C:506:UQ6:H202	1.64	0.79
5:E:72:LYS:NZ	9:I:29:GLN:HE22	1.82	0.77
6:H:78:LEU:HD13	6:H:142:LEU:HD22	1.67	0.75
3:C:58:ILE:H	3:C:173:ASN:HD22	1.34	0.74
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.69	0.72
1:A:74:LYS:HG3	1:A:95:SER:HB3	1.71	0.71
11:Y:31:ASN:ND2	11:Y:51:THR:HG21	2.05	0.71
7:F:77:ARG:HD2	16:F:154:HOH:O	1.91	0.71
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.38	0.71
4:D:62:MET:HB3	4:D:67:HIS:NE2	2.06	0.69
2:B:30:THR:HG23	2:B:190:GLU:HB3	1.75	0.69
10:X:54:ASN:HD22	10:X:54:ASN:H	1.41	0.69
6:H:91:GLY:O	6:H:95:VAL:HG13	1.91	0.69
11:Y:37:GLN:HB2	11:Y:47:LEU:HD11	1.76	0.68
6:H:74:VAL:HG12	6:H:75:THR:H	1.57	0.68
2:B:65:LEU:O	2:B:69:ARG:HG2	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:181:THR:HB	2:B:212:GLY:H	1.58	0.67
1:A:73:TRP:CE3	1:A:76:ILE:HD11	2.30	0.66
2:B:300:ASN:O	2:B:304:ILE:HG12	1.96	0.66
3:C:214:GLY:O	3:C:218:ARG:HD2	1.95	0.66
2:B:336:ILE:HG21	2:B:339:ASN:HB2	1.79	0.65
1:A:258:LYS:HG2	1:A:335:ARG:HG3	1.78	0.65
2:B:49:HIS:HD2	2:B:161:TYR:H	1.45	0.65
6:H:77:GLN:N	6:H:77:GLN:HE21	1.84	0.65
4:D:113:ARG:HG2	4:D:151:LEU:O	1.97	0.63
3:C:253:HIS:CD2	3:C:255:ASP:H	2.15	0.63
2:B:44:LYS:HB2	2:B:47:VAL:HG21	1.81	0.63
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.46	0.62
3:C:58:ILE:H	3:C:173:ASN:ND2	1.98	0.62
5:E:107:VAL:HG12	5:E:118:ILE:HB	1.81	0.62
11:Y:32:PHE:HD2	11:Y:92:ILE:HG22	1.63	0.62
2:B:287:LEU:HD21	2:B:304:ILE:HG21	1.83	0.61
11:Y:27:GLN:HG2	11:Y:28:ASP:H	1.65	0.61
11:Y:4:LEU:HD23	11:Y:88:CYS:SG	2.41	0.61
10:X:61:ASN:HD22	10:X:63:SER:H	1.48	0.61
5:E:172:ASP:H	5:E:184:HIS:HD2	1.49	0.61
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.83	0.60
14:C:506:UQ6:H103	14:C:506:UQ6:C1M	2.24	0.60
1:A:29:VAL:HG11	1:A:400:LYS:HB3	1.83	0.60
5:E:172:ASP:H	5:E:184:HIS:CD2	2.19	0.60
3:C:25:SER:OG	7:F:79:HIS:HD2	1.85	0.59
14:C:506:UQ6:H1M1	14:C:506:UQ6:C10	2.25	0.59
5:E:129:ALA:HB2	5:E:187:ILE:HG23	1.83	0.59
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.84	0.59
2:B:241:ILE:HG12	2:B:287:LEU:HB3	1.84	0.59
5:E:44:LYS:NZ	5:E:52:GLY:H	2.00	0.59
11:Y:6:GLN:HG2	11:Y:23:CYS:SG	2.43	0.59
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.18	0.59
1:A:63:ASN:HB2	1:A:66:ASN:HD22	1.66	0.58
3:C:57:ASN:HA	3:C:173:ASN:HD21	1.68	0.58
5:E:72:LYS:NZ	9:I:29:GLN:NE2	2.50	0.58
2:B:336:ILE:CG2	2:B:339:ASN:HB2	2.34	0.58
3:C:1:MET:N	16:C:581:HOH:O	2.36	0.58
2:B:49:HIS:CD2	2:B:161:TYR:H	2.22	0.58
4:D:109:ARG:HG3	4:D:178:SER:CB	2.34	0.57
3:C:22:GLN:HE22	14:C:506:UQ6:H3M3	1.70	0.57
7:F:43:LEU:HD13	7:F:48:LEU:HD11	1.86	0.57
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:Y:29:ILE:HG22	11:Y:92:ILE:HD12	1.86	0.57
10:X:61:ASN:ND2	10:X:63:SER:H	2.03	0.57
3:C:347:PRO:HG3	8:G:77:ASN:HB2	1.86	0.57
1:A:265:VAL:HG21	1:A:426:LEU:HD12	1.87	0.57
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.70	0.57
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.04	0.57
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.40	0.57
12:C:401:HEM:HHD	12:C:401:HEM:HBC2	1.87	0.57
2:B:336:ILE:HD12	2:B:336:ILE:H	1.69	0.57
1:A:68:GLY:HA3	1:A:185:LEU:HD11	1.87	0.57
12:C:402:HEM:HBC2	12:C:402:HEM:HMC2	1.87	0.57
10:X:29:ILE:H	10:X:77:ASN:HD21	1.51	0.57
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.87	0.57
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.86	0.56
7:F:53:ASN:ND2	7:F:56:MET:H	2.02	0.56
5:E:55:TYR:O	5:E:59:MET:HG2	2.05	0.56
3:C:323:LYS:HE3	8:G:55:GLN:HE22	1.69	0.56
3:C:208:ASN:HD22	3:C:210:LEU:H	1.53	0.56
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.05	0.56
3:C:44:ILE:HD12	14:C:506:UQ6:C20	2.36	0.55
1:A:303:LEU:O	1:A:307:GLN:HG3	2.06	0.55
2:B:347:LYS:HG2	2:B:348:LEU:N	2.21	0.55
5:E:107:VAL:CG1	5:E:118:ILE:HB	2.36	0.55
10:X:24:VAL:HG21	10:X:29:ILE:HD11	1.87	0.55
2:B:313:ASP:O	2:B:316:PRO:HD3	2.07	0.55
2:B:232:ARG:HH21	2:B:232:ARG:HB3	1.71	0.55
2:B:252:GLN:O	2:B:255:VAL:HG22	2.07	0.55
1:A:58:GLY:H	1:A:61:ASN:HD22	1.56	0.54
8:G:56:PHE:O	8:G:60:LEU:HB2	2.07	0.54
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.89	0.54
1:A:42:HIS:CD2	1:A:42:HIS:H	2.24	0.54
1:A:270:VAL:HG21	1:A:396:ILE:HD13	1.88	0.54
2:B:68:VAL:O	2:B:72:GLU:HG3	2.07	0.54
7:F:15:ILE:HG23	7:F:21:LEU:HB3	1.89	0.53
10:X:38:ILE:HA	10:X:49:VAL:HG23	1.89	0.53
4:D:247:MET:O	4:D:251:VAL:HG22	2.09	0.53
10:X:87:THR:HG22	10:X:88:THR:N	2.24	0.53
1:A:344:ILE:HG21	1:A:448:ILE:HD12	1.91	0.53
2:B:182:LYS:HB2	2:B:211:ALA:CB	2.37	0.53
1:A:47:HIS:O	1:A:110:PRO:HD3	2.09	0.53
1:A:289:ASN:HD22	1:A:289:ASN:C	2.12	0.53
2:B:52:ASN:ND2	2:B:80:SER:OG	2.42	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:169:PHE:O	1:A:172:THR:HB	2.09	0.52
1:A:156:HIS:HD2	1:A:159:ARG:NH2	2.03	0.52
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.91	0.52
9:I:5:SER:O	9:I:9:THR:HG23	2.10	0.52
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.45	0.52
1:A:172:THR:HG23	1:A:242:ALA:HA	1.91	0.52
1:A:68:GLY:HA3	1:A:185:LEU:CD1	2.39	0.52
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.92	0.52
2:B:43:THR:HG22	2:B:175:PHE:HD1	1.73	0.52
2:B:24:ALA:HB3	2:B:191:ASN:ND2	2.24	0.52
1:A:67:ASN:ND2	1:A:180:GLY:HA2	2.25	0.51
10:X:49:VAL:HG12	10:X:68:LEU:HD23	1.92	0.51
4:D:125:VAL:HA	4:D:128:MET:HE3	1.92	0.51
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.17	0.51
11:Y:4:LEU:CD2	11:Y:88:CYS:SG	2.98	0.51
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.44	0.51
2:B:315:SER:N	2:B:316:PRO:HD3	2.25	0.51
10:X:61:ASN:HD22	10:X:62:PRO:N	2.08	0.51
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.11	0.51
2:B:252:GLN:HB3	2:B:343:VAL:HG21	1.92	0.51
2:B:40:ARG:HB2	2:B:84:ARG:O	2.11	0.51
4:D:74:TYR:CE1	6:H:139:ALA:HA	2.46	0.51
1:A:142:LYS:NZ	1:A:142:LYS:HB2	2.26	0.51
4:D:263:HIS:NE2	4:D:267:LYS:HE3	2.26	0.50
10:X:49:VAL:CG1	10:X:68:LEU:HD23	2.41	0.50
2:B:228:GLU:HA	2:B:353:TYR:O	2.12	0.50
10:X:48:TRP:CZ2	10:X:50:GLY:HA2	2.46	0.50
2:B:294:SER:HB3	2:B:358:ASP:HB3	1.94	0.50
10:X:99:SER:HB3	10:X:109:MET:HG2	1.94	0.50
10:X:32:GLY:O	10:X:54:ASN:HB3	2.11	0.49
2:B:232:ARG:HB3	2:B:232:ARG:NH2	2.27	0.49
11:Y:34:ASN:HD22	11:Y:49:TYR:HA	1.77	0.49
1:A:373:GLN:HG3	1:A:374:LEU:N	2.27	0.49
2:B:46:GLY:O	2:B:49:HIS:HB3	2.13	0.49
5:E:46:ASN:OD1	5:E:49:ALA:HA	2.12	0.49
2:B:44:LYS:HB2	2:B:47:VAL:CG2	2.40	0.49
4:D:147:ARG:HG2	4:D:148:PRO:O	2.12	0.49
8:G:61:ILE:HB	8:G:62:PRO:HD3	1.95	0.49
5:E:103:LEU:O	5:E:120:HIS:HB3	2.13	0.49
2:B:347:LYS:N	2:B:347:LYS:HD3	2.17	0.48
3:C:323:LYS:CE	8:G:55:GLN:HE22	2.26	0.48
10:X:6:GLU:H	10:X:114:GLN:HE21	1.62	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:350:GLN:NE2	1:A:353:ARG:HD3	2.28	0.48
1:A:49:ALA:HA	1:A:212:GLY:HA3	1.95	0.48
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.95	0.48
1:A:179:ARG:HG2	1:A:179:ARG:HH21	1.79	0.48
11:Y:2:ILE:HD12	11:Y:2:ILE:N	2.29	0.48
2:B:267:LEU:HD22	2:B:304:ILE:HD13	1.96	0.48
1:A:91:LEU:HD23	1:A:106:VAL:HG11	1.95	0.48
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.14	0.48
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.29	0.48
1:A:235:LYS:HB2	1:A:235:LYS:NZ	2.29	0.48
2:B:110:TYR:HD1	2:B:209:LEU:HD23	1.79	0.48
11:Y:36:TYR:HE2	11:Y:89:GLN:HG2	1.79	0.48
10:X:51:TYR:CD2	10:X:51:TYR:C	2.88	0.47
5:E:93:LYS:HD3	5:E:215:GLY:HA3	1.95	0.47
1:A:71:ASN:HA	1:A:97:ILE:HG13	1.97	0.47
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.79	0.47
1:A:429:GLN:HE22	9:I:13:ARG:NH2	2.12	0.47
7:F:31:GLN:HE21	7:F:31:GLN:CA	2.16	0.47
10:X:29:ILE:HG12	10:X:77:ASN:ND2	2.30	0.47
1:A:306:ILE:HA	1:A:311:LEU:HD22	1.95	0.47
1:A:229:SER:HB3	1:A:232:THR:HB	1.96	0.47
11:Y:47:LEU:HA	11:Y:58:VAL:HG11	1.97	0.47
10:X:87:THR:HG22	10:X:88:THR:H	1.80	0.47
2:B:43:THR:HG22	2:B:175:PHE:CD1	2.49	0.47
1:A:160:VAL:CG2	1:A:436:THR:HG22	2.45	0.47
5:E:186:ASP:OD2	5:E:190:ARG:HD2	2.15	0.47
2:B:313:ASP:HB3	2:B:344:LYS:O	2.15	0.46
1:A:289:ASN:ND2	1:A:291:PHE:H	2.14	0.46
7:F:31:GLN:NE2	7:F:31:GLN:HA	2.18	0.46
10:X:61:ASN:HD22	10:X:61:ASN:C	2.18	0.46
1:A:365:ARG:HD2	2:B:72:GLU:OE1	2.15	0.46
10:X:38:ILE:HD12	10:X:46:LEU:HD22	1.97	0.46
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.13	0.46
10:X:37:TRP:CZ3	10:X:96:CYS:HB3	2.50	0.46
1:A:72:LEU:HD13	1:A:144:VAL:HG21	1.97	0.46
3:C:335:LEU:HD13	3:C:339:ILE:HG12	1.97	0.46
11:Y:33:LEU:HD22	11:Y:71:TYR:CG	2.51	0.46
3:C:7:ASN:ND2	3:C:10:LEU:H	2.04	0.46
1:A:62:GLU:OE1	1:A:67:ASN:HA	2.15	0.46
1:A:289:ASN:HD22	1:A:291:PHE:H	1.61	0.46
11:Y:55:HIS:O	11:Y:58:VAL:HG22	2.15	0.46
2:B:69:ARG:O	2:B:73:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:26:THR:OG1	2:B:191:ASN:ND2	2.48	0.46
5:E:43:LEU:HD21	8:G:29:VAL:HG11	1.98	0.46
3:C:218:ARG:HG3	8:G:16:MET:CE	2.46	0.46
5:E:125:GLU:HB3	5:E:187:ILE:HG12	1.96	0.46
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.97	0.46
11:Y:36:TYR:OH	11:Y:89:GLN:NE2	2.49	0.46
5:E:38:ASN:HD21	5:E:40:ASP:CG	2.18	0.46
12:C:401:HEM:HHD	12:C:401:HEM:CBC	2.45	0.46
11:Y:33:LEU:HD23	11:Y:35:TRP:HE1	1.81	0.46
5:E:191:ILE:HD13	5:E:196:ALA:HB3	1.98	0.45
1:A:382:ASN:OD1	1:A:384:VAL:HG22	2.17	0.45
2:B:324:LYS:O	2:B:327:VAL:HG22	2.16	0.45
3:C:18:ILE:HA	3:C:222:HIS:HB2	1.98	0.45
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.52	0.45
11:Y:2:ILE:HD12	11:Y:2:ILE:H	1.81	0.45
1:A:385:ASN:O	1:A:389:LEU:HG	2.16	0.45
2:B:182:LYS:HD3	2:B:207:SER:HA	1.97	0.45
3:C:27:ASN:OD1	3:C:29:TRP:HB2	2.17	0.45
8:G:61:ILE:O	8:G:65:ILE:HG13	2.17	0.45
2:B:197:LEU:O	2:B:201:VAL:HG23	2.16	0.45
2:B:308:LEU:HB2	2:B:348:LEU:HD22	1.98	0.45
4:D:286:TRP:CD2	8:G:37:LEU:HD12	2.52	0.45
10:X:11:LEU:HD13	10:X:125:ARG:HD2	1.98	0.45
10:X:7:SER:OG	10:X:21:THR:HG23	2.17	0.45
4:D:111:ALA:HA	4:D:154:TYR:HA	1.98	0.45
2:B:59:THR:HA	2:B:112:THR:HA	1.99	0.45
10:X:14:PRO:O	10:X:15:SER:HB3	2.17	0.45
2:B:347:LYS:HG2	2:B:348:LEU:H	1.81	0.44
1:A:73:TRP:CZ3	1:A:76:ILE:HD11	2.52	0.44
11:Y:37:GLN:HB2	11:Y:47:LEU:CD1	2.44	0.44
1:A:74:LYS:HB2	1:A:97:ILE:HD11	2.00	0.44
8:G:89:LEU:O	8:G:93:ASN:HB2	2.17	0.44
7:F:53:ASN:HD21	7:F:56:MET:H	1.65	0.44
4:D:243:THR:CB	6:H:77:GLN:HE22	2.30	0.44
1:A:127:GLN:C	1:A:129:ALA:H	2.21	0.44
10:X:33:TYR:HB3	10:X:99:SER:O	2.18	0.44
2:B:62:ARG:HH21	2:B:62:ARG:HB2	1.83	0.44
10:X:49:VAL:HG12	10:X:68:LEU:CD2	2.47	0.44
6:H:101:CYS:O	6:H:105:VAL:HG23	2.17	0.44
11:Y:93:LYS:NZ	11:Y:93:LYS:HB3	2.33	0.44
3:C:312:VAL:HG21	7:F:5:PHE:CE1	2.52	0.44
4:D:78:HIS:HD2	16:D:324:HOH:O	2.01	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:350:GLN:NE2	1:A:353:ARG:HH21	2.12	0.43
1:A:200:HIS:C	1:A:202:LEU:H	2.21	0.43
1:A:250:ARG:NH1	1:A:442:LEU:O	2.51	0.43
11:Y:32:PHE:CD2	11:Y:92:ILE:HG22	2.48	0.43
10:X:93:THR:HA	10:X:117:THR:HA	1.99	0.43
2:B:305:VAL:HG11	2:B:368:LEU:HB3	2.00	0.43
2:B:49:HIS:HE1	2:B:130:ASP:OD1	2.02	0.43
4:D:286:TRP:CZ3	5:E:56:ALA:HA	2.54	0.43
10:X:98:ARG:O	10:X:109:MET:HA	2.19	0.43
11:Y:61:ARG:HB2	11:Y:76:SER:HB3	2.00	0.43
2:B:108:VAL:O	2:B:112:THR:HG23	2.19	0.43
2:B:305:VAL:HG21	2:B:368:LEU:HD22	2.01	0.43
1:A:365:ARG:NH1	16:A:483:HOH:O	2.49	0.43
1:A:374:LEU:HD12	1:A:374:LEU:HA	1.87	0.43
1:A:54:VAL:HG13	1:A:103:SER:HB3	2.01	0.43
5:E:146:ARG:CZ	5:E:202:ILE:HD11	2.49	0.43
1:A:197:ALA:O	1:A:201:PHE:HB2	2.19	0.43
3:C:106:TYR:HB3	3:C:114:TRP:CD2	2.54	0.43
12:C:401:HEM:HBC2	12:C:401:HEM:CHD	2.49	0.43
5:E:154:ILE:HD12	5:E:205:TYR:CE2	2.54	0.43
3:C:89:PHE:HE2	12:C:401:HEM:HBB2	1.82	0.43
4:D:286:TRP:CD2	5:E:59:MET:HG3	2.54	0.43
11:Y:34:ASN:ND2	11:Y:91:HIS:HE1	2.17	0.42
1:A:239:LYS:HB2	1:A:240:LYS:H	1.70	0.42
4:D:134:TYR:OH	4:D:156:PRO:HD3	2.19	0.42
4:D:279:SER:O	4:D:283:LEU:HB2	2.19	0.42
3:C:384:ASN:O	3:C:385:LYS:HB2	2.18	0.42
2:B:124:LEU:HB2	2:B:125:PRO:HD3	2.00	0.42
2:B:151:PHE:O	2:B:156:GLY:HA3	2.20	0.42
2:B:252:GLN:HG3	2:B:253:TYR:N	2.34	0.42
11:Y:79:GLU:HA	11:Y:80:PRO:HA	1.78	0.42
2:B:155:LEU:HD12	2:B:155:LEU:N	2.34	0.42
2:B:39:SER:OG	2:B:84:ARG:HD3	2.20	0.42
3:C:346:VAL:HG12	3:C:347:PRO:N	2.35	0.42
10:X:51:TYR:HD2	10:X:51:TYR:C	2.23	0.42
5:E:120:HIS:CD2	5:E:151:GLN:HG2	2.54	0.42
2:B:220:GLU:HA	2:B:221:PRO:HD3	1.88	0.42
2:B:317:ALA:O	2:B:321:THR:HG22	2.20	0.42
4:D:302:PHE:HB2	7:F:73:TYR:CD1	2.54	0.42
1:A:60:ALA:O	1:A:173:PRO:HB3	2.20	0.42
7:F:45:PHE:O	7:F:48:LEU:HB2	2.20	0.42
2:B:321:THR:O	2:B:325:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:57:TYR:HB3	9:I:7:TYR:OH	2.20	0.42
6:H:95:VAL:O	6:H:99:GLU:HB2	2.20	0.41
1:A:306:ILE:C	1:A:306:ILE:HD12	2.40	0.41
10:X:20:LEU:HD22	10:X:116:THR:HG21	2.02	0.41
3:C:379:TYR:CE1	3:C:383:VAL:HG21	2.55	0.41
11:Y:12:ALA:HB2	11:Y:105:GLU:HB2	2.01	0.41
2:B:251:ALA:O	2:B:255:VAL:HG13	2.20	0.41
8:G:30:SER:HA	8:G:31:PRO:HD3	1.95	0.41
8:G:83:LYS:O	8:G:86:ARG:HG2	2.20	0.41
1:A:247:SER:O	1:A:432:ALA:HA	2.20	0.41
4:D:113:ARG:NH1	16:D:369:HOH:O	2.53	0.41
11:Y:32:PHE:O	11:Y:90:HIS:HA	2.20	0.41
2:B:175:PHE:CZ	2:B:179:VAL:HG21	2.55	0.41
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.66	0.41
6:H:82:ARG:O	6:H:86:LYS:HG3	2.21	0.41
4:D:109:ARG:HG3	4:D:178:SER:HB2	2.03	0.41
1:A:58:GLY:H	1:A:61:ASN:ND2	2.17	0.41
16:X:130:HOH:O	11:Y:49:TYR:HB2	2.20	0.41
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.36	0.41
5:E:181:HIS:HB2	13:E:4:FES:S1	2.61	0.41
3:C:338:GLN:HG3	8:G:70:TRP:CH2	2.55	0.41
3:C:304:VAL:HG13	3:C:308:THR:HG23	2.01	0.41
3:C:173:ASN:HB3	3:C:174:PRO:HD3	2.03	0.41
2:B:241:ILE:CG1	2:B:287:LEU:HB3	2.51	0.41
5:E:120:HIS:HD2	5:E:151:GLN:HG2	1.84	0.41
1:A:336:ASN:C	1:A:336:ASN:HD22	2.25	0.41
1:A:164:LEU:HD13	1:A:327:LEU:HD13	2.03	0.41
2:B:241:ILE:HA	2:B:352:ASN:O	2.21	0.41
2:B:146:LEU:HD13	2:B:354:VAL:CG2	2.51	0.41
3:C:313:VAL:HG22	3:C:319:LYS:HE3	2.03	0.41
11:Y:74:THR:HG22	11:Y:75:ILE:N	2.36	0.40
2:B:137:CYS:SG	2:B:139:VAL:HG22	2.60	0.40
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.84	0.40
11:Y:33:LEU:HD23	11:Y:35:TRP:NE1	2.36	0.40
2:B:301:ILE:O	2:B:305:VAL:HG23	2.21	0.40
2:B:114:PHE:O	2:B:169:LEU:HD11	2.21	0.40
3:C:72:VAL:HA	5:E:85:THR:HG22	2.03	0.40
10:X:45:LYS:HG3	10:X:45:LYS:O	2.21	0.40
3:C:288:LYS:O	3:C:292:VAL:HG13	2.21	0.40
10:X:54:ASN:ND2	10:X:54:ASN:H	2.13	0.40
10:X:24:VAL:CG2	10:X:29:ILE:HD11	2.49	0.40
1:A:74:LYS:HG3	1:A:95:SER:CB	2.47	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:76:ILE:HG23	1:A:140:THR:HG21	2.02	0.40
1:A:43:ASN:HA	1:A:44:PRO:HD2	1.88	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	429/431 (100%)	400 (93%)	25 (6%)	4 (1%)	25	26
2	B	350/352 (99%)	308 (88%)	38 (11%)	4 (1%)	21	21
3	C	383/385 (100%)	368 (96%)	13 (3%)	2 (0%)	38	45
4	D	243/248 (98%)	236 (97%)	7 (3%)	0	100	100
5	E	183/185 (99%)	172 (94%)	8 (4%)	3 (2%)	14	12
6	H	72/74 (97%)	69 (96%)	3 (4%)	0	100	100
7	F	123/127 (97%)	121 (98%)	2 (2%)	0	100	100
8	G	91/94 (97%)	80 (88%)	7 (8%)	4 (4%)	4	1
9	I	53/66 (80%)	51 (96%)	0	2 (4%)	5	2
10	X	125/127 (98%)	114 (91%)	9 (7%)	2 (2%)	14	12
11	Y	105/107 (98%)	88 (84%)	12 (11%)	5 (5%)	4	1
All	All	2157/2196 (98%)	2007 (93%)	124 (6%)	26 (1%)	19	19

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	335	PRO
3	C	223	SER
5	E	103	LEU
8	G	93	ASN
10	X	33	TYR
2	B	152	ARG

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Mol	Chain	Res	Type
2	B	153	LYS
5	E	46	ASN
11	Y	51	THR
1	A	227	ASN
8	G	37	LEU
8	G	38	GLN
9	I	13	ARG
11	Y	30	ASN
11	Y	68	GLY
1	A	228	LEU
9	I	12	LYS
1	A	230	LEU
2	B	342	ALA
10	X	90	ASP
11	Y	16	GLY
3	C	346	VAL
5	E	102	PRO
1	A	35	GLY
8	G	45	VAL
11	Y	80	PRO

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	370/370 (100%)	344 (93%)	26 (7%)	21	26
2	B	301/301 (100%)	282 (94%)	19 (6%)	25	32
3	C	338/338 (100%)	318 (94%)	20 (6%)	28	35
4	D	203/206 (98%)	196 (97%)	7 (3%)	49	64
5	E	151/151 (100%)	148 (98%)	3 (2%)	68	84
6	H	67/67 (100%)	63 (94%)	4 (6%)	27	35
7	F	109/111 (98%)	101 (93%)	8 (7%)	20	24
8	G	77/78 (99%)	73 (95%)	4 (5%)	32	42
9	I	45/54 (83%)	41 (91%)	4 (9%)	14	16
10	X	112/112 (100%)	104 (93%)	8 (7%)	21	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Y	93/93 (100%)	85 (91%)	8 (9%)	15	17
All	All	1866/1881 (99%)	1755 (94%)	111 (6%)	28	35

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	115	LYS
1	A	120	LEU
1	A	126	GLN
1	A	145	LEU
1	A	150	ASP
1	A	153	ASP
1	A	164	LEU
1	A	172	THR
1	A	174	LEU
1	A	179	ARG
1	A	183	GLU
1	A	239	LYS
1	A	241	LYS
1	A	252	ARG
1	A	261	ILE
1	A	289	ASN
1	A	306	ILE
1	A	320	LEU
1	A	330	PHE
1	A	336	ASN
1	A	343	LEU
1	A	361	THR
1	A	370	LEU
1	A	425	ARG
1	A	443	LEU
2	B	17	LEU
2	B	30	THR
2	B	31	LEU
2	B	40	ARG
2	B	43	THR
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	107	ASP
2	B	128	ARG

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Mol	Chain	Res	Type
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	215	LEU
2	B	232	ARG
2	B	312	LYS
2	B	338	LEU
2	B	347	LYS
2	B	362	LEU
3	C	5	LYS
3	C	12	LEU
3	C	35	LEU
3	C	38	LEU
3	C	79	ARG
3	C	89	PHE
3	C	99	LYS
3	C	101	LEU
3	C	150	LEU
3	C	182	LEU
3	C	184	TYR
3	C	185	LEU
3	C	218	ARG
3	C	238	LEU
3	C	312	VAL
3	C	313	VAL
3	C	336	LEU
3	C	350	LEU
3	C	377	LEU
3	C	382	ARG
4	D	69	LEU
4	D	113	ARG
4	D	244	THR
4	D	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	283	LEU
5	E	46	ASN
5	E	91	MET
5	E	211	LYS
6	H	77	GLN
6	H	94	LEU
6	H	117	LEU

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Mol	Chain	Res	Type
6	H	130	LEU
7	F	16	LEU
7	F	30	ASN
7	F	31	GLN
7	F	41	LEU
7	F	48	LEU
7	F	86	HIS
7	F	115	LYS
7	F	127	LYS
8	G	41	PHE
8	G	52	PHE
8	G	60	LEU
8	G	88	GLU
9	I	13	ARG
9	I	14	ASN
9	I	18	VAL
9	I	48	LEU
10	X	39	ARG
10	X	51	TYR
10	X	54	ASN
10	X	57	ASP
10	X	61	ASN
10	X	68	LEU
10	X	79	PHE
10	X	89	GLU
11	Y	18	ARG
11	Y	33	LEU
11	Y	38	GLN
11	Y	80	PRO
11	Y	81	GLU
11	Y	92	ILE
11	Y	93	LYS
11	Y	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	61	ASN
1	A	63	ASN
1	A	66	ASN
1	A	67	ASN

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Mol	Chain	Res	Type
1	A	121	ASN
1	A	156	HIS
1	A	171	ASN
1	A	199	ASN
1	A	200	HIS
1	A	274	ASN
1	A	289	ASN
1	A	298	GLN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	385	ASN
1	A	388	ASN
1	A	429	GLN
2	B	49	HIS
2	B	52	ASN
2	B	55	ASN
2	B	191	ASN
2	B	252	GLN
3	C	7	ASN
3	C	14	ASN
3	C	22	GLN
3	C	43	GLN
3	C	173	ASN
3	C	208	ASN
3	C	253	HIS
3	C	332	ASN
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
4	D	256	ASN
5	E	38	ASN
5	E	97	ASN
5	E	106	ASN
5	E	184	HIS
6	H	77	GLN
6	H	111	GLN
7	F	31	GLN
7	F	53	ASN
7	F	57	GLN
7	F	79	HIS
9	I	14	ASN

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Mol	Chain	Res	Type
9	I	29	GLN
10	X	54	ASN
10	X	59	ASN
10	X	61	ASN
10	X	77	ASN
10	X	78	GLN
10	X	114	GLN
11	Y	31	ASN
11	Y	34	ASN
11	Y	89	GLN
11	Y	90	HIS
11	Y	91	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	$\# Z > 2$
12	HEM	C	401	3	49,50,50	2.02	12 (24%)	46,82,82	1.53	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	HEM	C	402	3	49,50,50	1.87	16 (32%)	46,82,82	1.31	3 (6%)
15	SMA	C	505	-	38,38,38	1.40	4 (10%)	50,52,52	2.20	7 (14%)
14	UQ6	C	506	-	43,43,43	2.53	14 (32%)	55,55,55	2.18	18 (32%)
12	HEM	D	3	4	49,50,50	2.02	10 (20%)	46,82,82	1.39	4 (8%)
13	FES	E	4	5	0,4,4	0.00	-	0,4,4	0.00	-

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
12	HEM	C	401	3	-	0/14/114/114	0/0/8/8
12	HEM	C	402	3	-	0/14/114/114	0/0/8/8
15	SMA	C	505	-	-	0/33/34/34	0/0/2/2
14	UQ6	C	506	-	-	0/39/39/39	0/1/1/1
12	HEM	D	3	4	-	0/14/114/114	0/0/8/8
13	FES	E	4	5	-	0/0/4/4	0/0/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	506	UQ6	C7-C6	6.48	1.59	1.51
12	C	401	HEM	C2B-C1B	-6.19	1.43	1.44
15	C	505	SMA	C4-C4A	6.00	1.49	1.40
14	C	506	UQ6	O5-C5	-5.37	1.24	1.37
12	D	3	HEM	C3B-C2B	-5.12	1.34	1.43
14	C	506	UQ6	O2-C2	-5.09	1.24	1.37
12	D	3	HEM	C3C-C2C	-4.94	1.35	1.43
14	C	506	UQ6	C2-C3	4.77	1.47	1.39
12	C	401	HEM	C3C-C2C	-4.69	1.35	1.43
12	C	401	HEM	C3D-C2D	-4.59	1.35	1.43
14	C	506	UQ6	C5-C4	4.42	1.46	1.39
12	D	3	HEM	C3D-C2D	-4.41	1.36	1.43
12	C	401	HEM	C3B-C2B	-4.38	1.36	1.43
12	C	401	HEM	CMC-C2C	4.38	1.61	1.47
12	C	402	HEM	C3C-C2C	-4.31	1.36	1.43
12	D	3	HEM	CBB-CAB	4.29	1.53	1.28
12	C	402	HEM	C3D-C2D	-4.19	1.36	1.43
12	D	3	HEM	CBC-CAC	4.17	1.53	1.28
12	C	402	HEM	C3B-C2B	-4.13	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	3	HEM	C3B-CAB	4.06	1.53	1.40
12	C	402	HEM	C4A-C3A	4.03	1.45	1.40
14	C	506	UQ6	C18-C19	3.87	1.40	1.32
14	C	506	UQ6	C5-C6	3.79	1.46	1.40
14	C	506	UQ6	C23-C24	3.68	1.40	1.32
15	C	505	SMA	O1-C2	3.64	1.40	1.38
12	D	3	HEM	C3C-CAC	3.64	1.51	1.40
14	C	506	UQ6	C13-C14	3.63	1.40	1.32
12	C	401	HEM	C4A-C3A	3.47	1.44	1.40
14	C	506	UQ6	C8-C9	3.47	1.39	1.32
14	C	506	UQ6	C28-C29	3.44	1.39	1.32
12	D	3	HEM	C4A-C3A	3.43	1.44	1.40
12	C	402	HEM	CHB-C1B	3.37	1.40	1.35
12	C	402	HEM	CHA-C4D	3.08	1.40	1.35
12	C	401	HEM	CMB-C2B	2.98	1.56	1.47
12	D	3	HEM	CHA-C4D	2.89	1.40	1.35
12	C	402	HEM	FE-NA	2.88	2.04	1.92
12	D	3	HEM	FE-NA	2.87	2.04	1.92
12	C	402	HEM	CMB-C2B	2.82	1.56	1.47
12	C	402	HEM	C2D-C1D	-2.68	1.43	1.44
14	C	506	UQ6	C2-C1	2.66	1.47	1.40
14	C	506	UQ6	C33-C34	2.55	1.40	1.32
15	C	505	SMA	C4-C3	2.43	1.48	1.41
12	C	401	HEM	CHA-C4D	2.26	1.39	1.35
12	C	401	HEM	CBC-CAC	2.24	1.41	1.28
12	C	402	HEM	CMC-C2C	2.18	1.54	1.47
12	C	401	HEM	CMD-C2D	2.17	1.54	1.47
12	C	401	HEM	CBB-CAB	2.11	1.41	1.28
12	C	402	HEM	FE-NB	2.11	2.05	1.97
15	C	505	SMA	C7-C8	2.11	1.43	1.40
12	C	402	HEM	CBC-CAC	2.10	1.41	1.28
14	C	506	UQ6	O3-C3	2.07	1.42	1.38
12	C	401	HEM	CHD-C4C	2.05	1.40	1.36
12	C	402	HEM	CBB-CAB	2.05	1.40	1.28
12	C	402	HEM	CMD-C2D	2.05	1.53	1.47
12	C	402	HEM	CHC-C1C	2.02	1.39	1.36
12	C	402	HEM	FE-NC	2.00	2.05	1.97

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	505	SMA	C2-O1-C8A	-11.77	118.23	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	506	UQ6	C3M-O3-C3	6.92	133.81	114.90
12	D	3	HEM	C3B-C4B-NB	-6.67	109.23	114.00
12	C	401	HEM	C3B-C4B-NB	-6.28	109.51	114.00
14	C	506	UQ6	C17-C18-C19	6.15	141.07	127.80
12	C	402	HEM	C3B-C4B-NB	-5.82	109.83	114.00
15	C	505	SMA	C9-C2-C3	5.12	126.59	120.42
14	C	506	UQ6	C4M-O4-C4	4.41	126.95	114.90
15	C	505	SMA	C3-C4-C4A	-4.22	115.06	121.65
15	C	505	SMA	C9-C10-C11	-4.08	108.91	114.58
14	C	506	UQ6	C21-C19-C18	3.73	128.27	121.08
14	C	506	UQ6	C11-C12-C13	3.51	121.64	111.62
12	C	401	HEM	C4A-CHB-C1B	-3.44	122.94	127.47
14	C	506	UQ6	C20-C19-C18	-2.96	117.66	123.52
14	C	506	UQ6	C6-C7-C8	2.93	117.12	112.25
14	C	506	UQ6	C27-C28-C29	2.87	134.00	127.80
14	C	506	UQ6	C30-C29-C31	-2.83	111.08	115.39
12	C	402	HEM	C2D-C1D-ND	-2.81	109.61	112.93
12	D	3	HEM	C2D-C1D-ND	-2.80	109.63	112.93
14	C	506	UQ6	C22-C23-C24	2.79	133.81	127.80
15	C	505	SMA	C4-C3-C2	2.75	120.89	116.97
14	C	506	UQ6	C25-C24-C26	-2.67	111.33	115.39
12	C	401	HEM	CMC-C2C-C3C	-2.66	119.89	126.16
12	C	402	HEM	CBD-CAD-C3D	-2.56	108.78	114.37
14	C	506	UQ6	C15-C14-C16	-2.55	111.52	115.39
14	C	506	UQ6	C11-C9-C8	2.52	125.94	121.08
14	C	506	UQ6	C16-C14-C13	2.46	125.82	121.08
14	C	506	UQ6	C1M-C1-C2	-2.38	115.59	120.35
14	C	506	UQ6	C17-C16-C14	2.34	120.48	112.74
12	D	3	HEM	CMA-C3A-C4A	-2.33	125.04	128.62
12	C	401	HEM	C2D-C1D-ND	-2.32	110.19	112.93
12	C	401	HEM	CMD-C2D-C3D	2.23	130.65	125.60
12	C	401	HEM	CHC-C4B-NB	2.22	126.43	124.58
14	C	506	UQ6	C1M-C1-C6	2.20	123.50	120.42
15	C	505	SMA	C3M-C3-C4	-2.13	117.50	120.37
15	C	505	SMA	O8-C8-C7	2.08	124.00	119.35
14	C	506	UQ6	C27-C26-C24	2.08	119.62	112.74
12	D	3	HEM	CMD-C2D-C3D	2.08	130.31	125.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.