Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2021 – 09:38 PM EST

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 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
https://www.wwpdb.org/validation/2017/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:

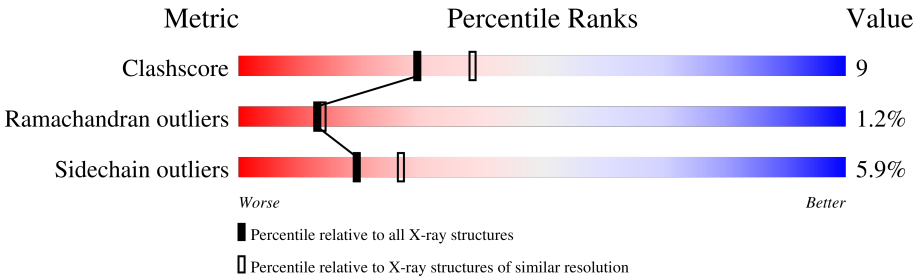
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	72% 26% •
2	B	352	70% 28% •
3	C	385	83% 16% •
4	D	248	85% 13% ••
5	E	185	78% 21% ••
6	H	74	78% 20% •
7	F	127	83% 14% • •
8	G	94	76% 20% • •

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Mol	Chain	Length	Quality of chain
9	I	66	
10	X	127	
11	Y	107	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 17779 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 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			

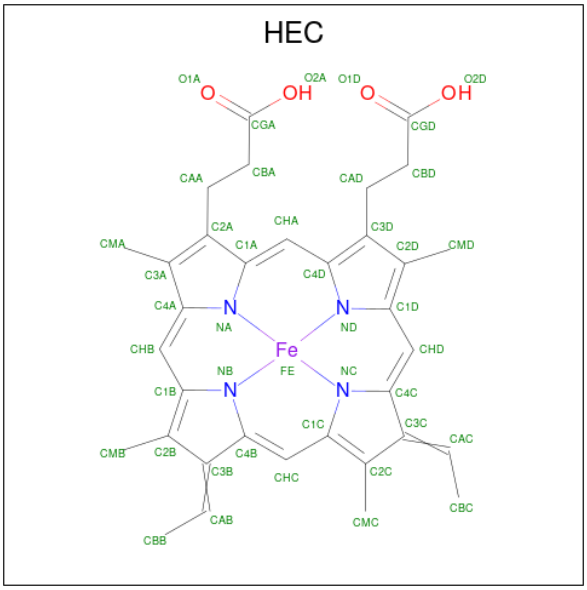
- Molecule 10 is a protein called Variable Heavy chain of antibody fragment.

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.

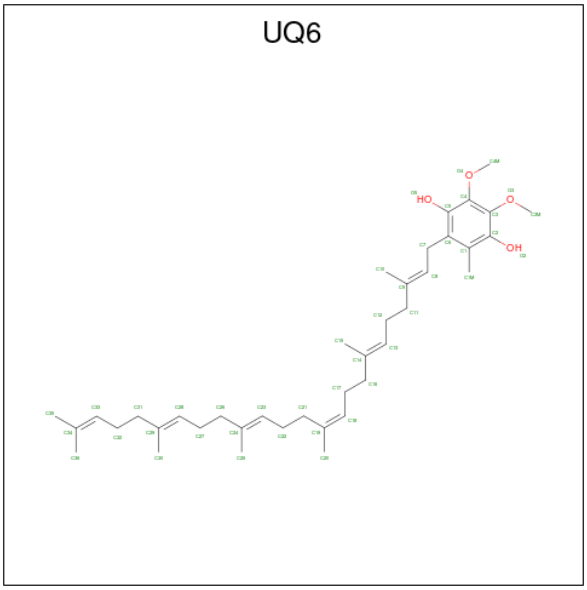
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	Y	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



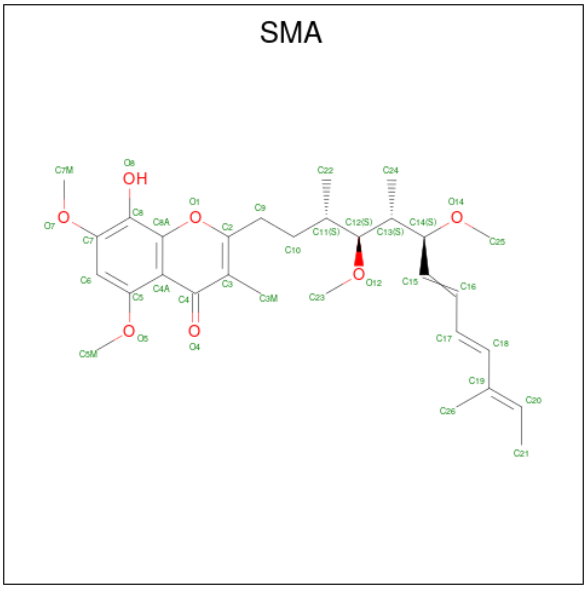
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is 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: $C_{39}H_{60}O_4$).



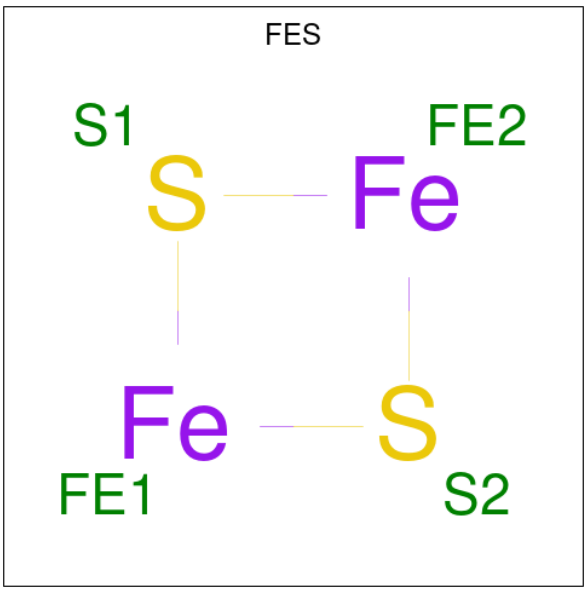
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 43 39 4	0	0

- Molecule 14 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



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

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 16 is water.

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

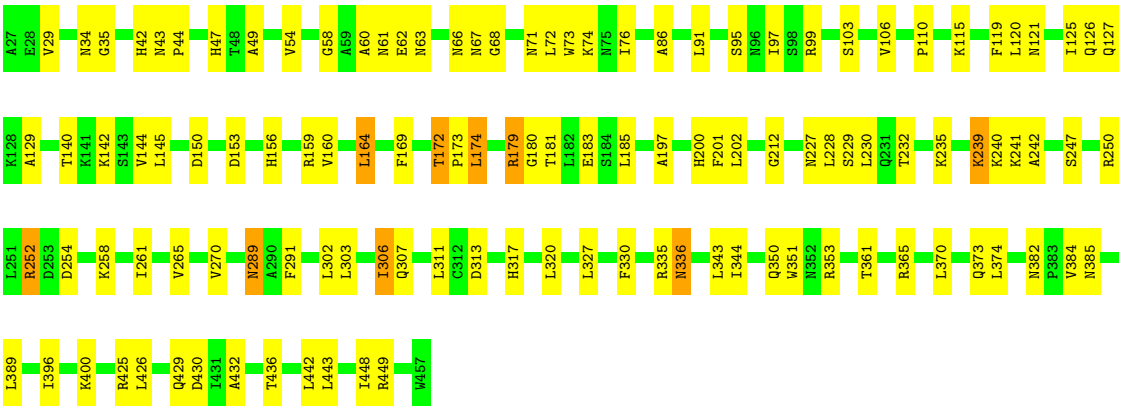
3 Residue-property plots (i)

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

Note EDS was not executed.

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

Chain A:

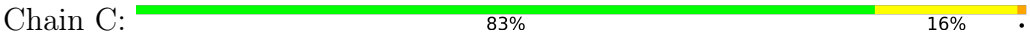


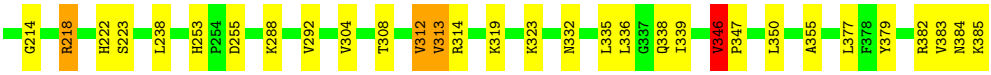
• Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2

Chain B:

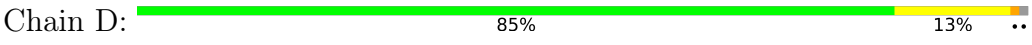
• Molecule 3: Cytochrome b

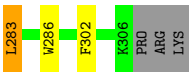
Chain C:



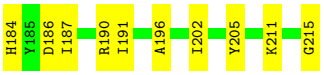


• Molecule 4: Cytochrome c1, heme protein, mitochondrial precursor

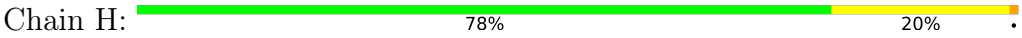


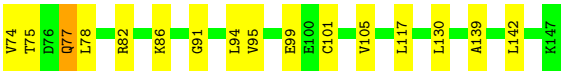


• Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor

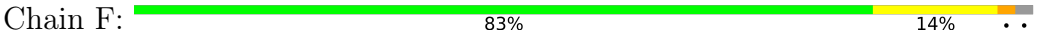


• Molecule 6: Ubiquinol-cytochrome c reductase complex 17 kDa protein

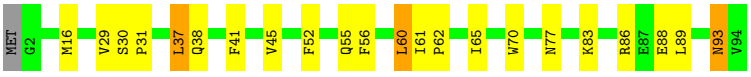




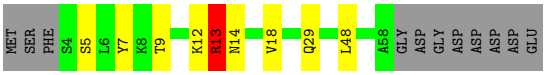
• Molecule 7: Ubiquinol-cytochrome c reductase complex 14 kDa protein



• Molecule 8: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

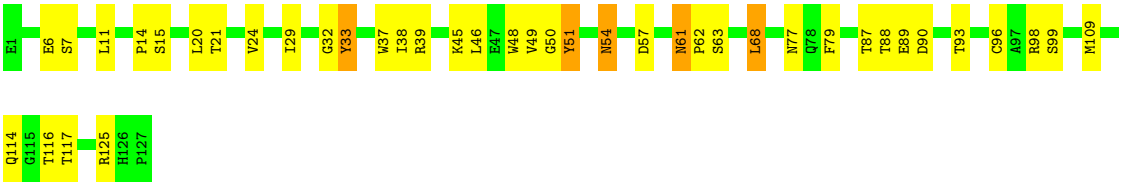


• Molecule 9: Ubiquinol-cytochrome c reductase complex 7.3 kDa protein



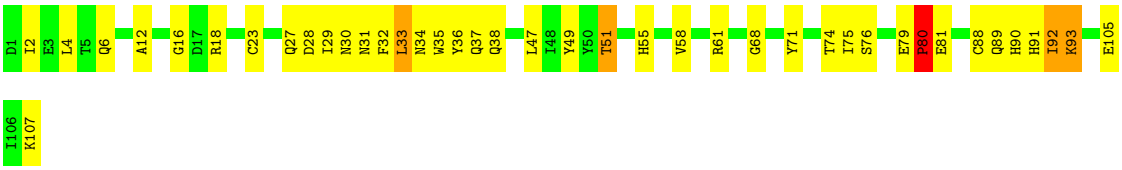
• Molecule 10: Variable Heavy chain of antibody fragment

Chain X:



• Molecule 11: Variable Light chain of antibody fragment

Chain Y:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore 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: FES, UQ6, HEC, SMA

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 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	3344	0	3321	74	0
2	B	2735	0	2774	73	0
3	C	3089	0	3125	36	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	64	4	0
12	D	43	0	30	1	0
13	C	43	0	58	6	0
14	C	37	0	41	0	0
15	E	4	0	0	1	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
16	G	19	0	0	0	0
16	H	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	17221	326	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 9.

All (326) 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)
6:H:77:GLN:HE21	6:H:77:GLN:H	1.00	0.98
13:C:506:UQ6:H103	13: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:H	2:B:347:LYS:HD3	1.40	0.85
7:F:31:GLN:HA	7:F:31:GLN:HE21	1.41	0.85
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.59	0.85
3:C:253:HIS:HD2	3:C:255:ASP:H	1.28	0.82
6:H:77:GLN:H	6:H:77:GLN:NE2	1.75	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	13:C:506:UQ6:H202	1.64	0.79
12:C:401:HEC:HBC3	12:C:401:HEC:HHD	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
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.38	0.71
7:F:77:ARG:HD2	16:F:154:HOH:O	1.91	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
6:H:91:GLY:O	6:H:95:VAL:HG13	1.91	0.69
10:X:54:ASN:HD22	10:X:54:ASN:H	1.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LEU:O	2:B:69:ARG:HG2	1.94	0.68
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:HE21	6:H:77:GLN:N	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
1:A:29:VAL:HG11	1:A:400:LYS:HB3	1.83	0.60
13:C:506:UQ6:H103	13:C:506:UQ6:C1M	2.24	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
13:C:506:UQ6:H1M1	13: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
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:GLN:HE22	13:C:506:UQ6:H3M3	1.70	0.57
7:F:43:LEU:HD13	7:F:48:LEU:HD11	1.86	0.57
10:X:61:ASN:ND2	10:X:63:SER:H	2.03	0.57
11:Y:29:ILE:HG22	11:Y:92:ILE:HD12	1.86	0.57
1:A:265:VAL:HG21	1:A:426:LEU:HD12	1.87	0.57
3:C:347:PRO:HG3	8:G:77:ASN:HB2	1.86	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
1:A:68:GLY:HA3	1:A:185:LEU:HD11	1.87	0.57
2:B:336:ILE:HD12	2:B:336:ILE:H	1.69	0.57
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.87	0.57
10:X:29:ILE:H	10:X:77:ASN:HD21	1.51	0.57
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.86	0.56
5:E:55:TYR:O	5:E:59:MET:HG2	2.05	0.56
7:F:53:ASN:ND2	7:F:56:MET:H	2.02	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
1:A:303:LEU:O	1:A:307:GLN:HG3	2.06	0.55
3:C:44:ILE:HD12	13:C:506:UQ6:C20	2.36	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
2:B:313:ASP:O	2:B:316:PRO:HD3	2.07	0.55
10:X:24:VAL:HG21	10:X:29:ILE:HD11	1.87	0.55
2:B:232:ARG:HB3	2:B:232:ARG:HH21	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
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.89	0.54
8:G:56:PHE:O	8:G:60:LEU:HB2	2.07	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:C	1:A:289:ASN:HD22	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:ASN:ND2	2:B:80:SER:OG	2.42	0.53
1:A:169:PHE:O	1:A:172:THR:HB	2.09	0.52
12:C:402:HEC:HMC1	12:C:402:HEC:HBC2	1.91	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
1:A:172:THR:HG23	1:A:242:ALA:HA	1.91	0.52
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.45	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:24:ALA:HB3	2:B:191:ASN:ND2	2.24	0.52
2:B:43:THR:HG22	2:B:175:PHE:HD1	1.73	0.52
1:A:67:ASN:ND2	1:A:180:GLY:HA2	2.25	0.51
4:D:125:VAL:HA	4:D:128:MET:HE3	1.92	0.51
10:X:49:VAL:HG12	10:X:68:LEU:HD23	1.92	0.51
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.17	0.51
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.44	0.51
11:Y:4:LEU:CD2	11:Y:88:CYS:SG	2.98	0.51
2:B:315:SER:N	2:B:316:PRO:HD3	2.25	0.51
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.11	0.51
10:X:61:ASN:HD22	10:X:62:PRO:N	2.08	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:HB2	1:A:142:LYS:NZ	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
2:B:232:ARG:HB3	2:B:232:ARG:NH2	2.27	0.49
10:X:32:GLY:O	10:X:54:ASN:HB3	2.11	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
12:C:401:HEC:HMB1	12:C:401:HEC:HBB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:103:LEU:O	5:E:120:HIS:HB3	2.13	0.49
2:B:347:LYS:HD3	2:B:347:LYS:N	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
1:A:49:ALA:HA	1:A:212:GLY:HA3	1.95	0.48
1:A:350:GLN:NE2	1:A:353:ARG:HD3	2.28	0.48
1:A:179:ARG:HH21	1:A:179:ARG:HG2	1.79	0.48
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.95	0.48
11:Y:2:ILE:N	11:Y:2:ILE:HD12	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:C	10:X:51:TYR:CD2	2.88	0.47
12:D:3:HEC:HBB3	12:D:3:HEC:HMB1	1.96	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
1:A:429:GLN:HE22	9:I:13:ARG:NH2	2.12	0.47
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.79	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:229:SER:HB3	1:A:232:THR:HB	1.96	0.47
1:A:306:ILE:HA	1:A:311:LEU:HD22	1.95	0.47
1:A:160:VAL:CG2	1:A:436:THR:HG22	2.45	0.47
2:B:43:THR:HG22	2:B:175:PHE:CD1	2.49	0.47
10:X:87:THR:HG22	10:X:88:THR:H	1.80	0.47
11:Y:47:LEU:HA	11:Y:58:VAL:HG11	1.97	0.47
5:E:186:ASP:OD2	5:E:190:ARG:HD2	2.15	0.47
1:A:289:ASN:ND2	1:A:291:PHE:H	2.14	0.46
2:B:313:ASP:HB3	2:B:344:LYS:O	2.15	0.46
1:A:72:LEU:HD13	1:A:144:VAL:HG21	1.97	0.46
1:A:365:ARG:HD2	2:B:72:GLU:OE1	2.15	0.46
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.13	0.46
7:F:31:GLN:HA	7:F:31:GLN:NE2	2.18	0.46
10:X:37:TRP:CZ3	10:X:96:CYS:HB3	2.50	0.46
10:X:38:ILE:HD12	10:X:46:LEU:HD22	1.97	0.46
10:X:61:ASN:HD22	10:X:61:ASN:C	2.18	0.46
3:C:335:LEU:HD13	3:C:339:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:33:LEU:HD22	11:Y:71:TYR:CG	2.51	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
3:C:7:ASN:ND2	3:C:10:LEU:H	2.04	0.46
2:B:26:THR:OG1	2:B:191:ASN:ND2	2.48	0.46
2:B:69:ARG:O	2:B:73:LEU:HD23	2.15	0.46
5:E:43:LEU:HD21	8:G:29:VAL:HG11	1.98	0.46
11:Y:55:HIS:O	11:Y:58:VAL:HG22	2.15	0.46
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.97	0.46
3:C:218:ARG:HG3	8:G:16:MET:CE	2.46	0.46
5:E:38:ASN:HD21	5:E:40:ASP:CG	2.18	0.46
5:E:125:GLU:HB3	5:E:187:ILE:HG12	1.96	0.46
11:Y:36:TYR:OH	11:Y:89:GLN:NE2	2.49	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
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.52	0.45
3:C:18:ILE:HA	3:C:222:HIS:HB2	1.98	0.45
1:A:385:ASN:O	1:A:389:LEU:HG	2.16	0.45
11:Y:2:ILE:HD12	11:Y:2:ILE:H	1.81	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
2:B:197:LEU:O	2:B:201:VAL:HG23	2.16	0.45
8:G:61:ILE:O	8:G:65:ILE:HG13	2.17	0.45
2:B:308:LEU:HB2	2:B:348:LEU:HD22	1.98	0.45
4:D:111:ALA:HA	4:D:154:TYR:HA	1.98	0.45
4:D:286:TRP:CD2	8:G:37:LEU:HD12	2.52	0.45
10:X:7:SER:OG	10:X:21:THR:HG23	2.17	0.45
10:X:11:LEU:HD13	10:X:125:ARG:HD2	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
1:A:73:TRP:CZ3	1:A:76:ILE:HD11	2.52	0.44
2:B:347:LYS:HG2	2:B:348:LEU:H	1.81	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
2:B:62:ARG:HH21	2:B:62:ARG:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:33:TYR:HB3	10:X:99:SER:O	2.18	0.44
6:H:101:CYS:O	6:H:105:VAL:HG23	2.17	0.44
10:X:49:VAL:HG12	10:X:68:LEU:CD2	2.47	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
11:Y:93:LYS:NZ	11:Y:93:LYS:HB3	2.33	0.44
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
1:A:350:GLN:NE2	1:A:353:ARG:HH21	2.12	0.43
11:Y:32:PHE:CD2	11:Y:92:ILE:HG22	2.48	0.43
2:B:305:VAL:HG11	2:B:368:LEU:HB3	2.00	0.43
10:X:93:THR:HA	10:X:117:THR:HA	1.99	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:54:VAL:HG13	1:A:103:SER:HB3	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
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
5:E:154:ILE:HD12	5:E:205:TYR:CE2	2.54	0.43
4:D:286:TRP:CD2	5:E:59:MET:HG3	2.54	0.43
1:A:239:LYS:HB2	1:A:240:LYS:H	1.70	0.42
11:Y:34:ASN:ND2	11:Y:91:HIS:HE1	2.17	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:39:SER:OG	2:B:84:ARG:HD3	2.20	0.42
2:B:155:LEU:N	2:B:155:LEU:HD12	2.34	0.42
3:C:346:VAL:HG12	3:C:347:PRO:N	2.35	0.42
10:X:51:TYR:C	10:X:51:TYR:HD2	2.23	0.42
2:B:220:GLU:HA	2:B:221:PRO:HD3	1.88	0.42
5:E:120:HIS:CD2	5:E:151:GLN:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:321:THR:O	2:B:325:ASN:HB2	2.19	0.42
5:E:57:TYR:HB3	9:I:7:TYR:OH	2.20	0.42
7:F:45:PHE:O	7:F:48:LEU:HB2	2.20	0.42
1:A:306:ILE:C	1:A:306:ILE:HD12	2.40	0.41
3:C:379:TYR:CE1	3:C:383:VAL:HG21	2.55	0.41
6:H:95:VAL:O	6:H:99:GLU:HB2	2.20	0.41
10:X:20:LEU:HD22	10:X:116:THR:HG21	2.02	0.41
11:Y:12:ALA:HB2	11:Y:105:GLU:HB2	2.01	0.41
1:A:247:SER:O	1:A:432:ALA:HA	2.20	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
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
4:D:113:ARG:NH1	16:D:369:HOH:O	2.53	0.41
6:H:82:ARG:O	6:H:86:LYS:HG3	2.21	0.41
11:Y:32:PHE:O	11:Y:90:HIS:HA	2.20	0.41
1:A:58:GLY:H	1:A:61:ASN:ND2	2.17	0.41
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.36	0.41
4:D:109:ARG:HG3	4:D:178:SER:HB2	2.03	0.41
5:E:181:HIS:HB2	15:E:4:FES:S1	2.61	0.41
16:X:130:HOH:O	11:Y:49:TYR:HB2	2.20	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
12:C:401:HEC:HHD	12:C:401:HEC:CBC	2.43	0.41
1:A:164:LEU:HD13	1:A:327:LEU:HD13	2.03	0.41
1:A:336:ASN:C	1:A:336:ASN:HD22	2.25	0.41
2:B:241:ILE:CG1	2:B:287:LEU:HB3	2.51	0.41
3:C:173:ASN:HB3	3:C:174:PRO:HD3	2.03	0.41
5:E:120:HIS:HD2	5:E:151:GLN:HG2	1.84	0.41
2:B:146:LEU:HD13	2:B:354:VAL:CG2	2.51	0.41
2:B:241:ILE:HA	2:B:352:ASN:O	2.21	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:HA	1:A:72:LEU:HD12	1.84	0.40
2:B:114:PHE:O	2:B:169:LEU:HD11	2.21	0.40
2:B:301:ILE:O	2:B:305:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:VAL:HA	5:E:85:THR:HG22	2.03	0.40
3:C:288:LYS:O	3:C:292:VAL:HG13	2.21	0.40
10:X:45:LYS:HG3	10:X:45:LYS:O	2.21	0.40
11:Y:33:LEU:HD23	11:Y:35:TRP:NE1	2.36	0.40
10:X:24:VAL:CG2	10:X:29:ILE:HD11	2.49	0.40
10:X:54:ASN:H	10:X:54:ASN:ND2	2.13	0.40
1:A:43:ASN:HA	1:A:44:PRO:HD2	1.88	0.40
1:A:74:LYS:HG3	1:A:95:SER:CB	2.47	0.40
1:A:76:ILE:HG23	1:A:140:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	429/431 (100%)	400 (93%)	25 (6%)	4 (1%)	17 20
2	B	350/352 (99%)	308 (88%)	38 (11%)	4 (1%)	14 15
3	C	383/385 (100%)	368 (96%)	13 (3%)	2 (0%)	29 35
4	D	243/248 (98%)	236 (97%)	7 (3%)	0	100 100
5	E	183/185 (99%)	172 (94%)	8 (4%)	3 (2%)	9 9
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%)	2 1
9	I	53/66 (80%)	51 (96%)	0	2 (4%)	3 1
10	X	125/127 (98%)	114 (91%)	9 (7%)	2 (2%)	9 9
11	Y	105/107 (98%)	88 (84%)	12 (11%)	5 (5%)	2 1
All	All	2157/2196 (98%)	2007 (93%)	124 (6%)	26 (1%)	13 14

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
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	344 (93%)	26 (7%)	15	19
2	B	301/301 (100%)	282 (94%)	19 (6%)	18	24
3	C	338/338 (100%)	318 (94%)	20 (6%)	19	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	203/206 (98%)	196 (97%)	7 (3%)	37 51
5	E	151/151 (100%)	148 (98%)	3 (2%)	55 72
6	H	67/67 (100%)	63 (94%)	4 (6%)	19 26
7	F	109/111 (98%)	101 (93%)	8 (7%)	14 18
8	G	77/78 (99%)	73 (95%)	4 (5%)	23 32
9	I	45/54 (83%)	41 (91%)	4 (9%)	9 11
10	X	112/112 (100%)	104 (93%)	8 (7%)	14 19
11	Y	93/93 (100%)	85 (91%)	8 (9%)	10 12
All	All	1866/1881 (99%)	1755 (94%)	111 (6%)	19 27

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
11	Y	107	LYS

Sometimes 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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	HEC	C	402	3	26,50,50	1.61	4 (15%)	18,82,82	2.10	7 (38%)
12	HEC	D	3	4	26,50,50	1.73	2 (7%)	18,82,82	1.49	3 (16%)
14	SMA	C	505	-	35,38,38	1.10	4 (11%)	46,52,52	1.60	6 (13%)
12	HEC	C	401	3	26,50,50	1.88	6 (23%)	18,82,82	2.22	6 (33%)
15	FES	E	4	5	0,4,4	0.00	-	-		
13	UQ6	C	506	-	43,43,43	2.58	17 (39%)	51,55,55	2.16	19 (37%)

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	HEC	C	402	3	-	0/6/54/54	-
12	HEC	D	3	4	-	0/6/54/54	-
14	SMA	C	505	-	-	3/33/34/34	0/2/2/2
12	HEC	C	401	3	-	0/6/54/54	-
15	FES	E	4	5	-	-	0/1/1/1
13	UQ6	C	506	-	-	10/39/39/39	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	506	UQ6	C7-C6	7.19	1.59	1.51
12	D	3	HEC	C3B-C2B	-5.69	1.34	1.40
13	C	506	UQ6	O5-C5	-5.57	1.24	1.37
12	D	3	HEC	C3C-C2C	-5.38	1.35	1.40
13	C	506	UQ6	O2-C2	-5.28	1.24	1.37
12	C	401	HEC	C3C-C2C	-4.96	1.35	1.40
13	C	506	UQ6	C2-C3	4.88	1.47	1.39
13	C	506	UQ6	C5-C4	4.52	1.46	1.39
12	C	401	HEC	C3B-C2B	-4.45	1.36	1.40
13	C	506	UQ6	C5-C6	4.35	1.46	1.40
12	C	402	HEC	C3C-C2C	-4.34	1.36	1.40
12	C	402	HEC	C3B-C2B	-4.03	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	401	HEC	CMC-C2C	3.99	1.61	1.51
14	C	505	SMA	O1-C2	3.66	1.40	1.35
13	C	506	UQ6	C2-C1	3.34	1.47	1.40
13	C	506	UQ6	C18-C19	3.24	1.40	1.33
13	C	506	UQ6	C23-C24	3.07	1.40	1.33
13	C	506	UQ6	C13-C14	3.04	1.40	1.33
13	C	506	UQ6	C8-C9	2.90	1.39	1.33
13	C	506	UQ6	C28-C29	2.87	1.39	1.33
13	C	506	UQ6	C33-C34	2.85	1.40	1.32
14	C	505	SMA	C4-C3	2.43	1.48	1.41
12	C	402	HEC	CBB-CAB	-2.36	1.40	1.49
13	C	506	UQ6	C11-C9	2.30	1.56	1.51
13	C	506	UQ6	C21-C19	2.29	1.56	1.51
12	C	402	HEC	CBC-CAC	-2.28	1.41	1.49
12	C	401	HEC	CBB-CAB	-2.26	1.41	1.49
14	C	505	SMA	C7-C8	2.18	1.43	1.40
14	C	505	SMA	C20-C19	2.17	1.35	1.33
12	C	401	HEC	CMB-C2B	2.15	1.56	1.51
13	C	506	UQ6	O3-C3	2.13	1.42	1.38
13	C	506	UQ6	C31-C29	2.06	1.55	1.51
12	C	401	HEC	CBC-CAC	-2.06	1.41	1.49

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	506	UQ6	C3M-O3-C3	6.95	133.81	114.78
13	C	506	UQ6	C17-C18-C19	5.57	141.07	127.66
14	C	505	SMA	C3-C4-C4A	-5.48	115.06	120.58
12	C	401	HEC	CMC-C2C-C3C	-5.04	119.89	125.82
13	C	506	UQ6	C4M-O4-C4	4.44	126.95	114.78
14	C	505	SMA	C9-C2-C3	4.38	126.59	120.39
14	C	505	SMA	C9-C10-C11	-4.31	108.91	114.72
12	C	401	HEC	CMD-C2D-C1D	-4.14	122.10	128.46
12	D	3	HEC	CMD-C2D-C1D	-3.95	122.39	128.46
14	C	505	SMA	C4-C3-C2	3.89	120.89	116.63
12	C	402	HEC	CMB-C2B-C1B	-3.87	122.51	128.46
12	C	402	HEC	CMD-C2D-C1D	-3.59	122.94	128.46
12	C	402	HEC	CMC-C2C-C3C	3.56	130.00	125.82
12	C	402	HEC	CMB-C2B-C3B	3.55	130.00	125.82
12	C	402	HEC	CMC-C2C-C1C	-3.54	123.02	128.46
13	C	506	UQ6	C21-C19-C18	3.53	128.27	121.12
12	C	401	HEC	CMB-C2B-C3B	3.29	129.69	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	401	HEC	CMC-C2C-C1C	3.16	133.32	128.46
13	C	506	UQ6	C6-C7-C8	3.13	117.12	112.17
12	C	401	HEC	CMD-C2D-C3D	3.03	130.65	124.94
12	C	401	HEC	CMB-C2B-C1B	-2.99	123.87	128.46
13	C	506	UQ6	C11-C12-C13	2.97	121.64	111.88
13	C	506	UQ6	C1M-C1-C2	-2.89	115.59	120.50
12	D	3	HEC	CMD-C2D-C3D	2.85	130.31	124.94
13	C	506	UQ6	C27-C28-C29	2.63	134.00	127.66
12	C	402	HEC	CMD-C2D-C3D	2.58	129.80	124.94
13	C	506	UQ6	C22-C23-C24	2.55	133.81	127.66
13	C	506	UQ6	C30-C29-C31	-2.49	111.08	115.27
13	C	506	UQ6	C11-C9-C8	2.38	125.94	121.12
14	C	505	SMA	O1-C8A-C4A	2.36	123.29	120.87
13	C	506	UQ6	C20-C19-C18	-2.35	117.66	123.68
13	C	506	UQ6	C25-C24-C26	-2.34	111.33	115.27
13	C	506	UQ6	C16-C14-C13	2.32	125.82	121.12
13	C	506	UQ6	C17-C16-C14	2.28	120.48	112.98
13	C	506	UQ6	C15-C14-C16	-2.23	111.52	115.27
14	C	505	SMA	O8-C8-C7	2.18	124.00	119.25
13	C	506	UQ6	C1M-C1-C6	2.12	123.50	120.42
12	D	3	HEC	CBD-CAD-C3D	2.08	116.33	112.49
13	C	506	UQ6	C36-C34-C35	-2.06	110.05	114.60
13	C	506	UQ6	C27-C26-C24	2.02	119.62	112.98
12	C	402	HEC	CBD-CAD-C3D	-2.01	108.78	112.49

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	506	UQ6	C13-C14-C16-C17
13	C	506	UQ6	C15-C14-C16-C17
13	C	506	UQ6	C18-C19-C21-C22
13	C	506	UQ6	C20-C19-C21-C22
13	C	506	UQ6	C24-C26-C27-C28
13	C	506	UQ6	C4-C3-O3-C3M
13	C	506	UQ6	C12-C11-C9-C10
13	C	506	UQ6	C12-C11-C9-C8
13	C	506	UQ6	C19-C21-C22-C23
13	C	506	UQ6	C2-C3-O3-C3M
14	C	505	SMA	C4A-C5-O5-C5M
14	C	505	SMA	C6-C5-O5-C5M
14	C	505	SMA	C9-C10-C11-C22

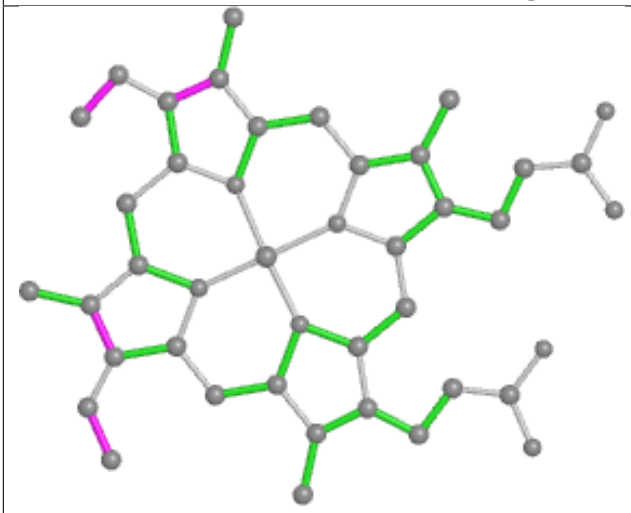
There are no ring outliers.

5 monomers are involved in 12 short contacts:

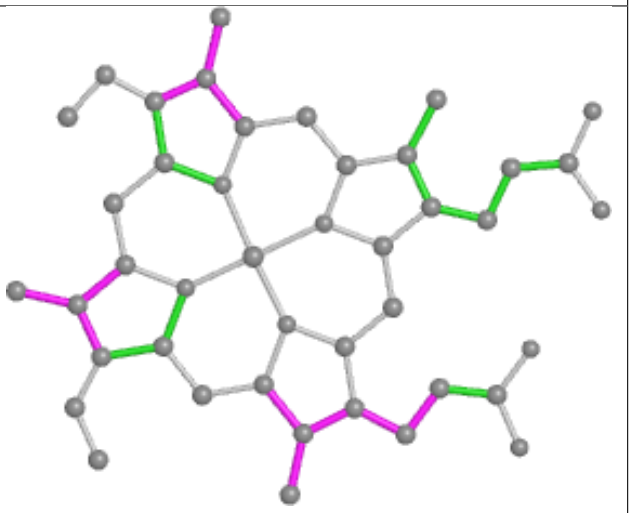
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	402	HEC	1	0
12	D	3	HEC	1	0
12	C	401	HEC	3	0
15	E	4	FES	1	0
13	C	506	UQ6	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

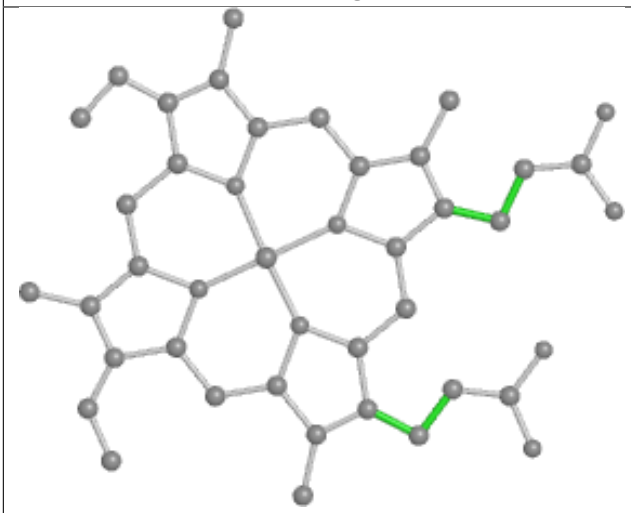
Ligand HEC C 402



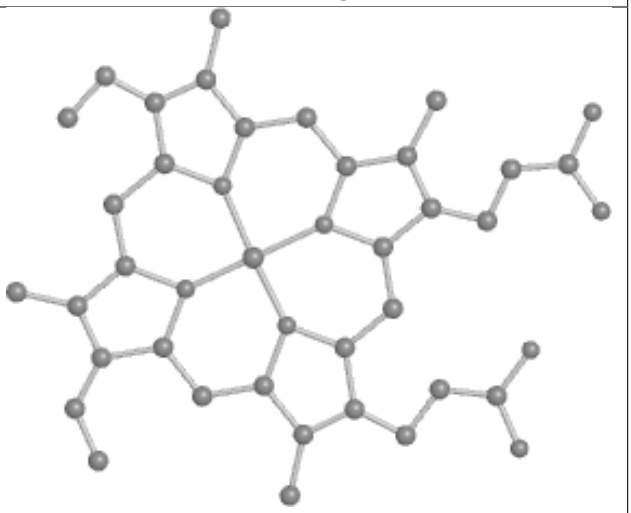
Bond lengths



Bond angles

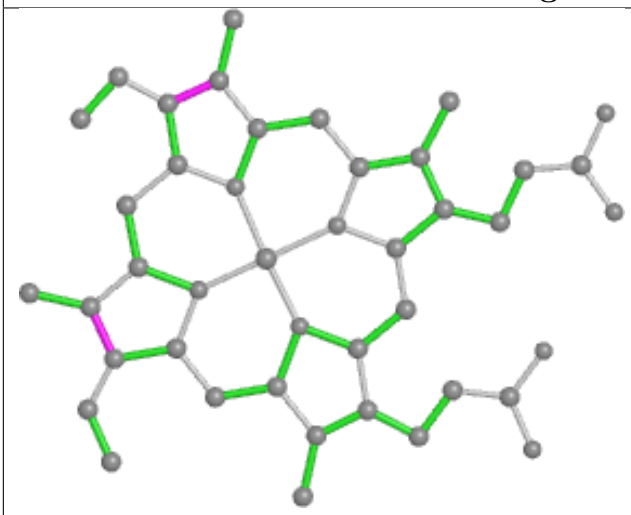


Torsions

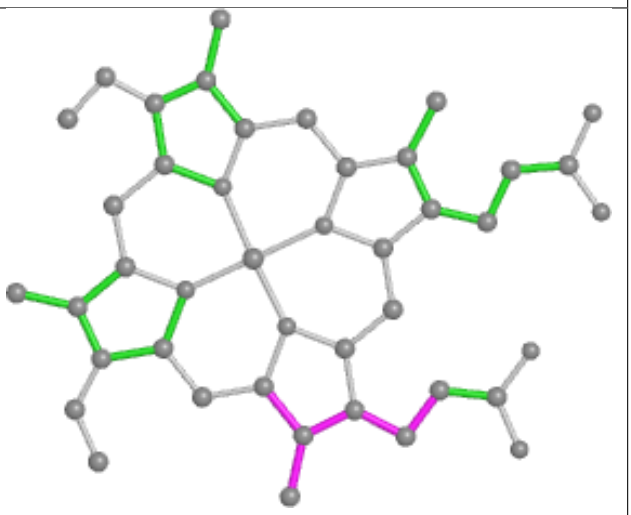


Rings

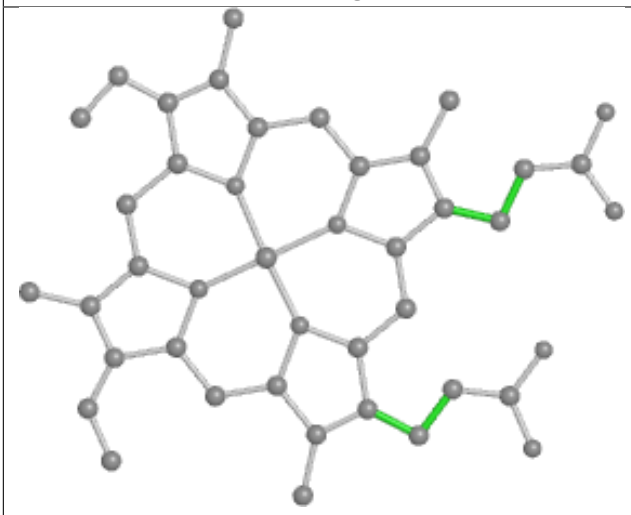
Ligand HEC D 3



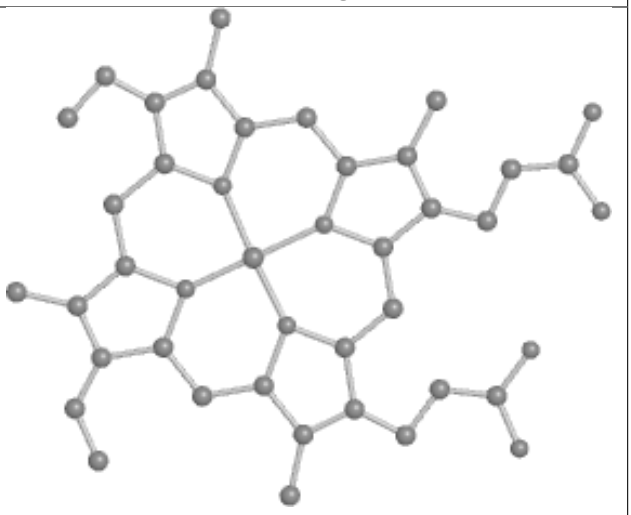
Bond lengths



Bond angles

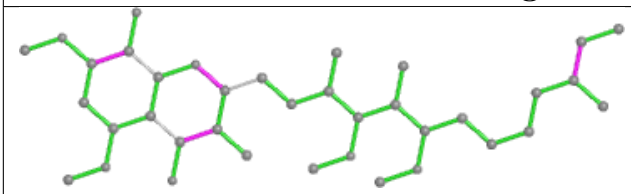


Torsions

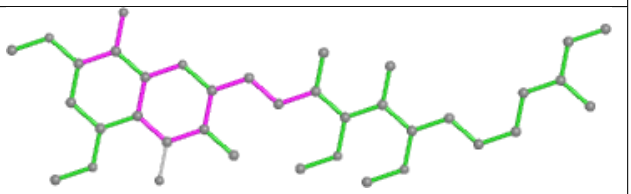


Rings

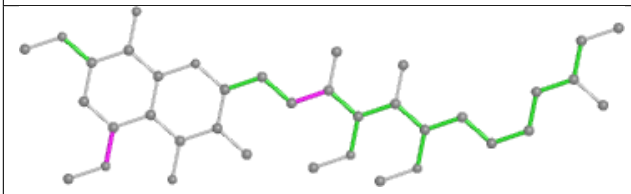
Ligand SMA C 505



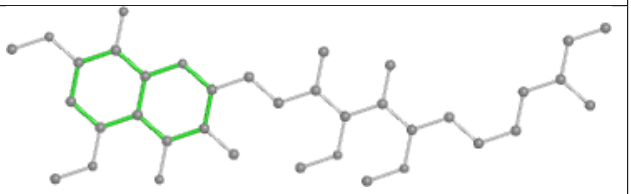
Bond lengths



Bond angles

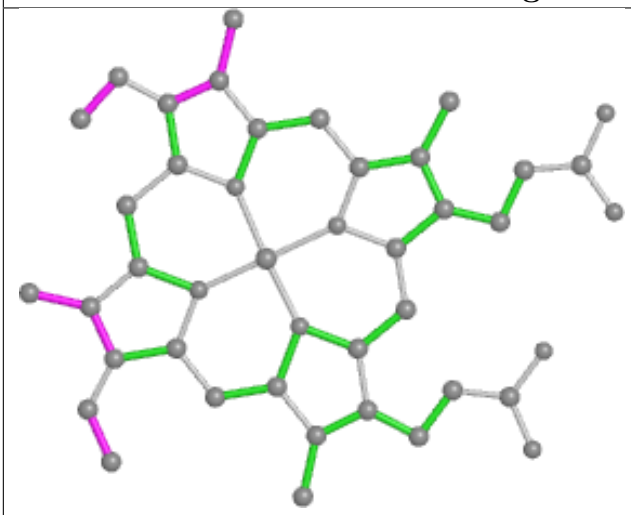


Torsions

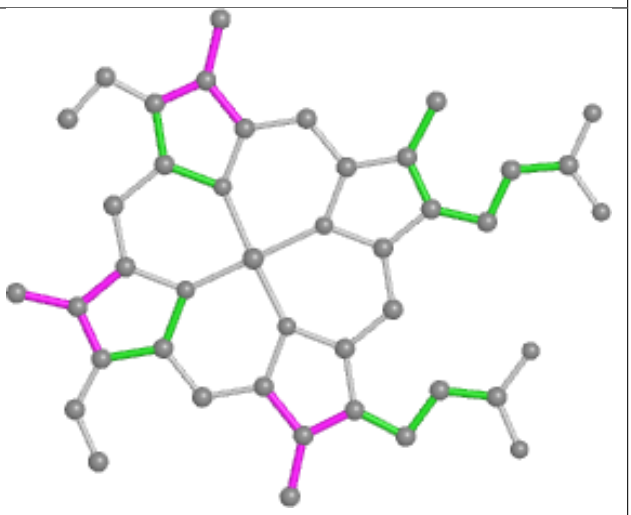


Rings

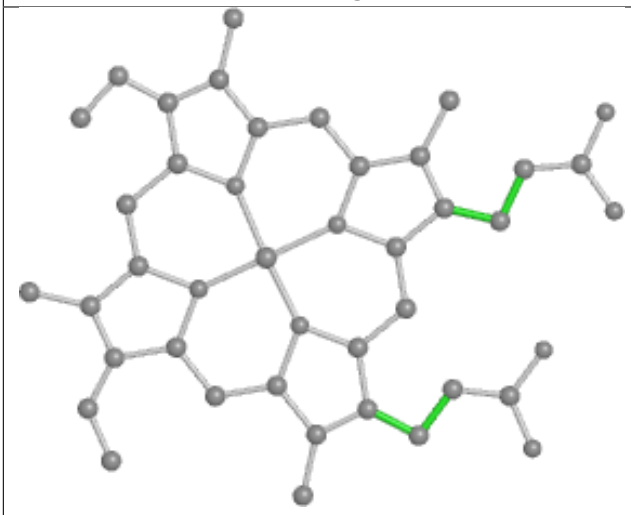
Ligand HEC C 401



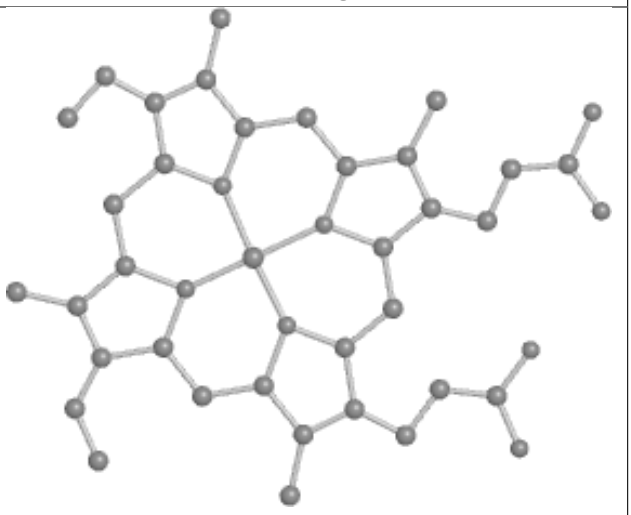
Bond lengths



Bond angles

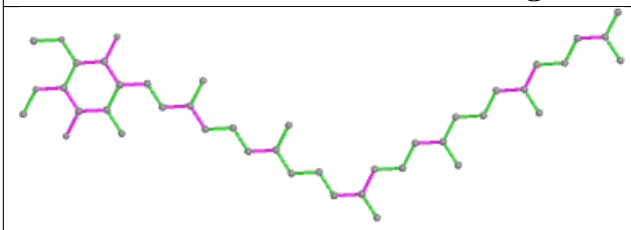


Torsions

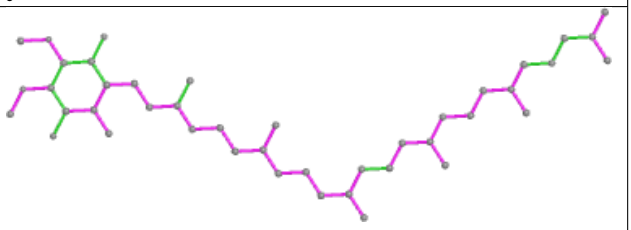


Rings

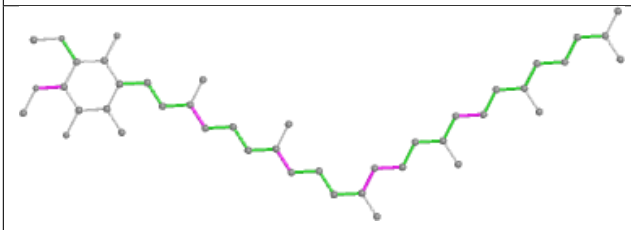
Ligand UQ6 C 506



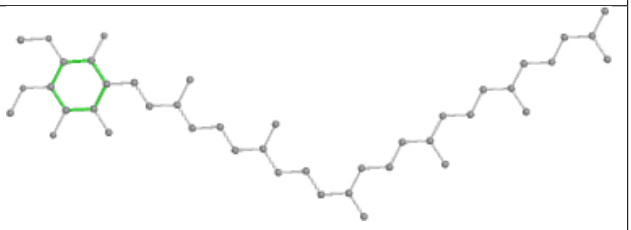
Bond lengths



Bond angles



Torsions



Rings

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.