Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2023 – 12:56 AM EST

PDB ID	:	1B86
Title	:	HUMAN DEOXYHAEMOGLOBIN-2,3-DIPHOSPHOGLYCERATE COMPLEX
Authors	:	Richard, V.; Dodson, G.G.; Mauguen, Y.
Deposited on	:	1999-02-08
Resolution	:	2.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

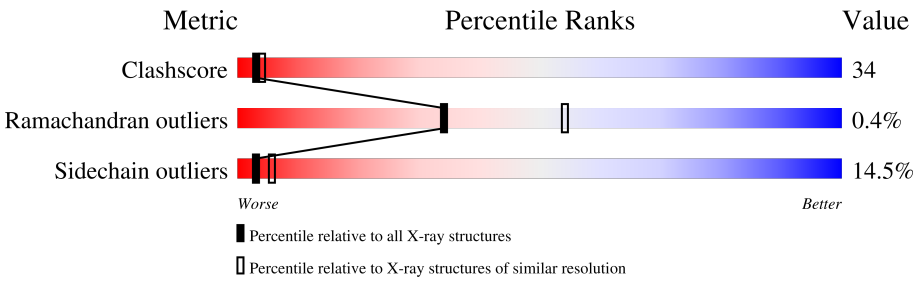
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	141	32% 44% 18% 6%
1	C	141	33% 48% 15% •
2	B	146	32% 40% 23% 5%
2	D	146	25% 36% 32% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DG2	D	701	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4715 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.

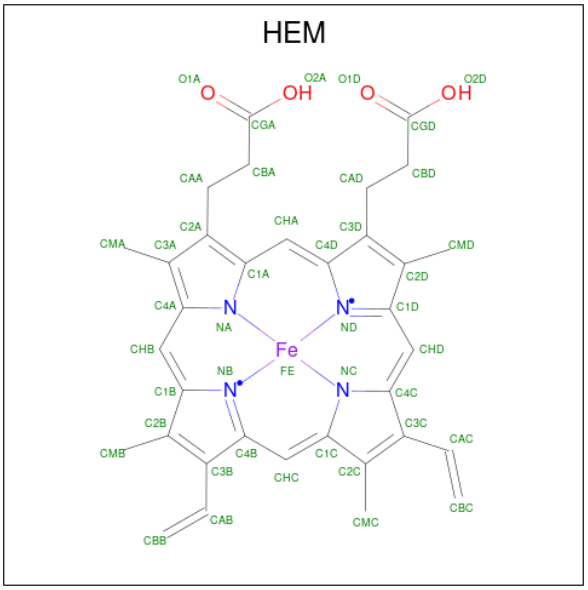
- Molecule 1 is a protein called PROTEIN (HEMOGLOBIN; ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1069	685	187	194	3	0	0	0
1	C	141	1069	685	187	194	3	0	0	0

- Molecule 2 is a protein called PROTEIN (HEMOGLOBIN; BETA CHAIN).

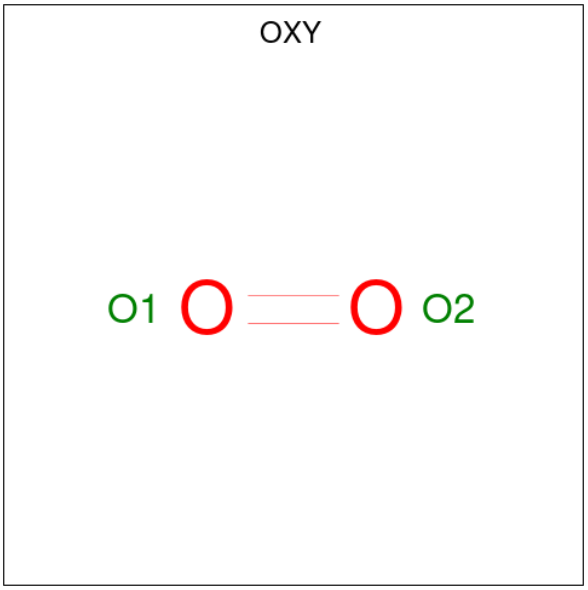
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1123	724	195	201	3	0	0	0
2	D	146	1127	727	196	201	3	0	1	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



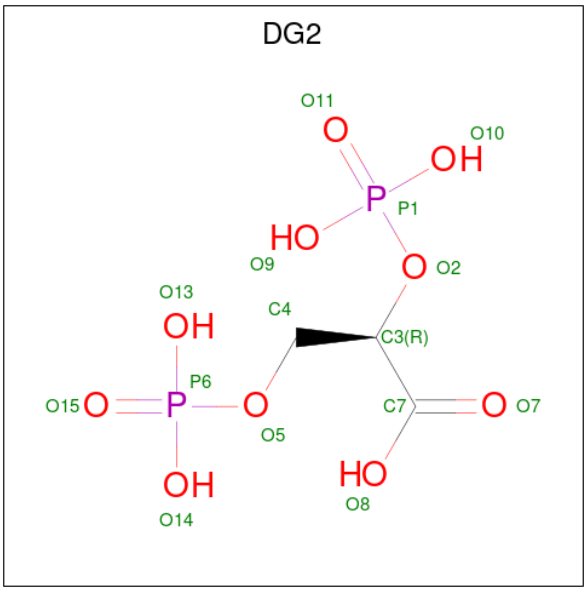
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
3	B	1	43	34	1	4	4	0	0
3	C	1	43	34	1	4	4	0	0
3	D	1	43	34	1	4	4	0	0

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	2	2	0	0
4	C	1	2	2	0	0

- Molecule 5 is (2R)-2,3-diphosphoglyceric acid (three-letter code: DG2) (formula: $C_3H_8O_{10}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	D	1	15	3	10	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	29	29	29	0	0
			Total	O		
6	B	46	46	46	0	0
			Total	O		
6	C	16	16	16	0	0
			Total	O		
6	D	45	45	45	0	0

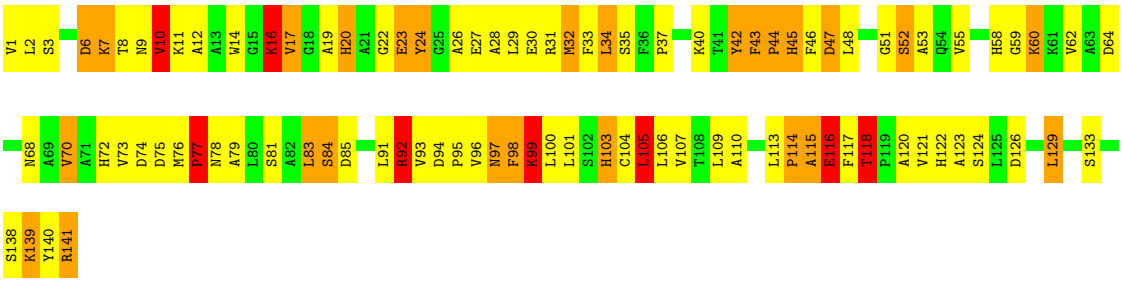
3 Residue-property plots (i)

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.

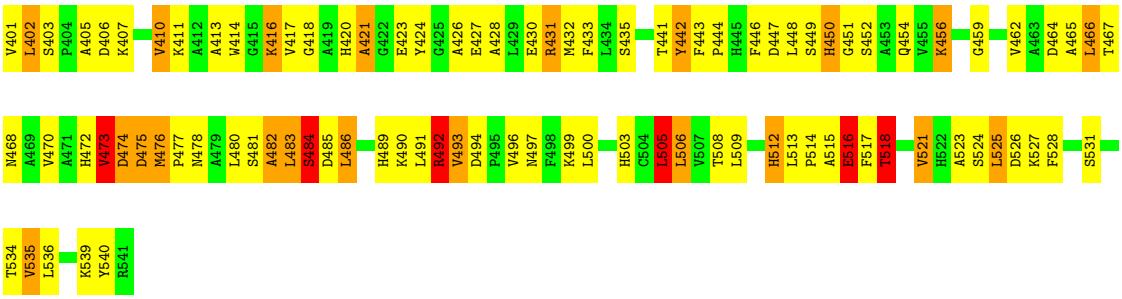
• Molecule 1: PROTEIN (HEMOGLOBIN; ALPHA CHAIN)

Chain A: 32% 44% 18% 6%



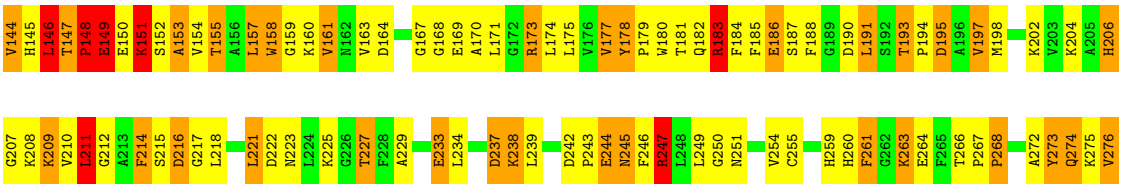
• Molecule 1: PROTEIN (HEMOGLOBIN; ALPHA CHAIN)

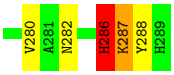
Chain C: 33% 48% 15% •



• Molecule 2: PROTEIN (HEMOGLOBIN; BETA CHAIN)

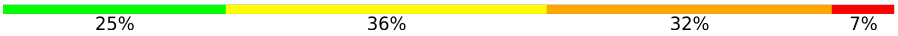
Chain B: 32% 40% 23% 5%

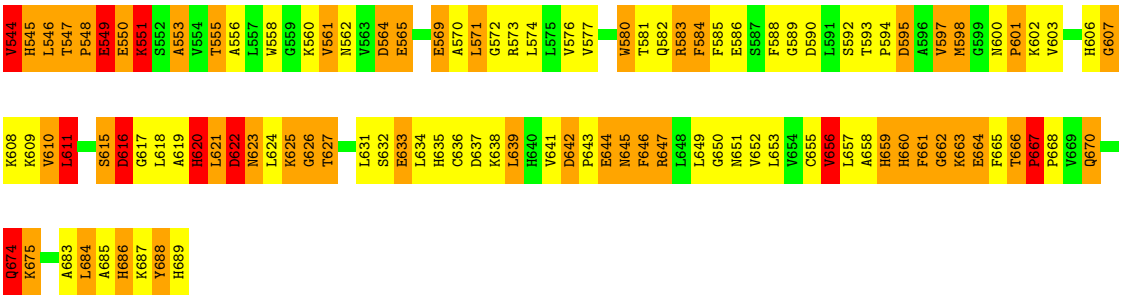




• Molecule 2: PROTEIN (HEMOGLOBIN; BETA CHAIN)

Chain D:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	96.30Å 98.08Å 65.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.0 (10.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.13	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4715	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, OXY, DG2

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	1.10	2/1097 (0.2%)	2.97	120/1491 (8.0%)
1	C	1.10	0/1097	2.83	98/1491 (6.6%)
2	B	1.13	1/1153 (0.1%)	2.85	112/1566 (7.2%)
2	D	1.14	2/1162 (0.2%)	2.85	118/1577 (7.5%)
All	All	1.12	5/4509 (0.1%)	2.88	448/6125 (7.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	B	0	2
2	D	1	0
All	All	1	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	626	GLY	N-CA	6.77	1.56	1.46
2	B	212	GLY	N-CA	6.00	1.55	1.46
2	D	650	GLY	N-CA	5.55	1.54	1.46
1	A	27	GLU	CD-OE2	-5.35	1.19	1.25
1	A	124	SER	CB-OG	5.03	1.48	1.42

All (448) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	ARG	NE-CZ-NH2	25.57	133.09	120.30
1	C	492	ARG	NE-CZ-NH2	-22.38	109.11	120.30
1	C	526	ASP	CB-CG-OD1	18.50	134.95	118.30
2	B	286	HIS	CA-CB-CG	18.29	144.69	113.60
1	C	431	ARG	NE-CZ-NH2	-17.40	111.60	120.30
1	A	11	LYS	CD-CE-NZ	16.06	148.64	111.70
1	C	431	ARG	NE-CZ-NH1	15.51	128.05	120.30
1	C	423	GLU	CA-CB-CG	15.17	146.77	113.40
2	B	145	HIS	N-CA-CB	14.62	136.91	110.60
2	B	145	HIS	CA-CB-CG	-14.44	89.05	113.60
2	D	545	HIS	N-CA-CB	14.37	136.47	110.60
2	D	590	ASP	CB-CG-OD1	-14.05	105.66	118.30
2	B	233	GLU	OE1-CD-OE2	14.04	140.15	123.30
2	B	173	ARG	NE-CZ-NH1	13.76	127.18	120.30
2	B	222	ASP	CB-CG-OD1	13.49	130.44	118.30
2	B	288	TYR	CB-CG-CD2	-13.33	113.00	121.00
2	B	286	HIS	CB-CA-C	-13.31	83.78	110.40
2	D	564	ASP	CB-CG-OD1	13.19	130.17	118.30
2	B	145	HIS	CB-CA-C	-13.18	84.03	110.40
2	B	286	HIS	N-CA-CB	13.10	134.18	110.60
1	A	92	ARG	CD-NE-CZ	13.04	141.86	123.60
1	C	518	THR	N-CA-CB	-12.99	85.63	110.30
2	D	545	HIS	CA-CB-CG	-12.88	91.70	113.60
1	A	114	PRO	O-C-N	12.76	143.12	122.70
2	D	595	ASP	CB-CG-OD1	-12.66	106.91	118.30
1	C	475	ASP	CB-CG-OD2	-12.32	107.21	118.30
1	A	126	ASP	CB-CG-OD1	12.14	129.22	118.30
1	A	31	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	42	TYR	CB-CG-CD1	12.03	128.22	121.00
2	D	610	VAL	CA-CB-CG2	12.02	128.92	110.90
2	B	216	ASP	CB-CG-OD1	11.79	128.91	118.30
1	A	27	GLU	CG-CD-OE2	11.68	141.67	118.30
2	D	644	GLU	OE1-CD-OE2	11.68	137.31	123.30
2	D	569	GLU	OE1-CD-OE2	11.60	137.22	123.30
1	A	92	ARG	NE-CZ-NH1	-11.41	114.59	120.30
1	A	118	THR	N-CA-CB	-11.37	88.70	110.30
2	B	222	ASP	CB-CG-OD2	-11.34	108.10	118.30
2	D	595	ASP	CB-CG-OD2	11.26	128.44	118.30
2	B	264	GLU	CA-CB-CG	11.17	137.97	113.40
1	C	430	GLU	OE1-CD-OE2	11.15	136.68	123.30
1	A	23	GLU	CA-CB-CG	11.13	137.89	113.40
2	D	583	ARG	NE-CZ-NH2	10.95	125.77	120.30
2	D	564	ASP	CB-CG-OD2	-10.84	108.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	149	GLU	OE1-CD-OE2	-10.83	110.31	123.30
2	D	565	GLU	CA-CB-CG	10.66	136.85	113.40
1	A	126	ASP	CB-CG-OD2	-10.56	108.79	118.30
2	D	551	LYS	CB-CA-C	-10.07	90.25	110.40
2	B	264	GLU	CB-CG-CD	9.99	141.16	114.20
2	D	545	HIS	O-C-N	9.81	138.40	122.70
2	B	210	VAL	CA-CB-CG1	9.77	125.56	110.90
1	C	423	GLU	OE1-CD-OE2	-9.74	111.61	123.30
2	B	169	GLU	OE1-CD-OE2	9.70	134.94	123.30
1	C	447	ASP	CB-CG-OD2	-9.68	109.59	118.30
1	A	118	THR	CA-CB-CG2	9.55	125.77	112.40
1	A	140	TYR	O-C-N	9.51	137.92	122.70
1	A	72	HIS	CA-CB-CG	-9.42	97.59	113.60
2	B	149	GLU	CG-CD-OE1	9.39	137.07	118.30
1	A	60	LYS	CA-CB-CG	9.30	133.85	113.40
1	A	97	ASN	CB-CG-OD1	-9.04	103.52	121.60
2	D	617	GLY	O-C-N	9.02	137.13	122.70
1	C	413	ALA	N-CA-CB	-9.00	97.50	110.10
2	B	146	LEU	CA-CB-CG	8.90	135.76	115.30
2	D	642	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	A	27	GLU	OE1-CD-OE2	-8.87	112.66	123.30
1	A	46	PHE	O-C-N	8.76	136.72	122.70
2	B	242	ASP	CB-CG-OD1	-8.76	110.42	118.30
1	A	70	VAL	CA-CB-CG2	8.74	124.00	110.90
1	C	492	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	C	462	VAL	CG1-CB-CG2	8.67	124.77	110.90
2	B	153	ALA	N-CA-CB	-8.63	98.02	110.10
1	A	30	GLU	OE1-CD-OE2	8.62	133.65	123.30
1	A	7	LYS	CA-C-O	8.40	137.75	120.10
2	B	247	ARG	NE-CZ-NH2	-8.37	116.12	120.30
2	D	582	GLN	CG-CD-OE1	8.36	138.33	121.60
1	C	418	GLY	CA-C-O	8.35	135.63	120.60
2	D	655	CYS	CA-CB-SG	8.28	128.91	114.00
1	C	431	ARG	CD-NE-CZ	-8.20	112.12	123.60
1	C	531	SER	CB-CA-C	8.18	125.64	110.10
1	C	536	LEU	CB-CA-C	8.16	125.70	110.20
1	A	99	LYS	CG-CD-CE	8.15	136.35	111.90
1	C	418	GLY	CA-C-N	-8.11	99.36	117.20
2	D	544	VAL	CA-CB-CG2	8.11	123.06	110.90
1	A	47	ASP	CB-CG-OD1	-8.05	111.06	118.30
1	A	31	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	A	140	TYR	CZ-CE2-CD2	-8.03	112.58	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	ASP	CB-CG-OD1	7.95	125.45	118.30
2	B	237	ASP	CB-CG-OD1	-7.91	111.18	118.30
1	C	427	GLU	CA-CB-CG	7.91	130.79	113.40
2	D	616	ASP	CB-CG-OD2	7.87	125.39	118.30
1	A	77	PRO	O-C-N	7.84	135.25	122.70
1	A	32	MET	CA-CB-CG	-7.84	99.98	113.30
2	B	238	LYS	N-CA-CB	-7.81	96.55	110.60
1	A	8	THR	O-C-N	7.80	135.18	122.70
2	B	287	LYS	CB-CA-C	-7.79	94.81	110.40
2	B	266	THR	CA-CB-CG2	7.77	123.28	112.40
1	A	105	LEU	CA-CB-CG	7.72	133.06	115.30
1	C	526	ASP	OD1-CG-OD2	-7.71	108.65	123.30
1	C	492	ARG	CD-NE-CZ	-7.70	112.82	123.60
2	D	617	GLY	CA-C-O	-7.69	106.76	120.60
1	A	115	ALA	N-CA-CB	-7.68	99.35	110.10
2	B	263	LYS	CA-CB-CG	7.67	130.28	113.40
1	C	476	MET	CA-CB-CG	-7.66	100.28	113.30
1	A	59	GLY	CA-C-O	7.63	134.34	120.60
1	C	482	ALA	N-CA-CB	-7.59	99.47	110.10
2	B	183	ARG	NE-CZ-NH1	7.59	124.09	120.30
2	D	688	TYR	CB-CG-CD2	7.58	125.55	121.00
1	C	474	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	C	462	VAL	CA-CB-CG2	-7.53	99.61	110.90
1	C	516	GLU	OE1-CD-OE2	7.52	132.32	123.30
2	D	647	ARG	NE-CZ-NH1	-7.51	116.54	120.30
2	B	250	GLY	O-C-N	-7.51	110.69	122.70
1	A	96	VAL	CA-C-O	-7.50	104.36	120.10
1	C	497	ASN	CB-CG-OD1	7.47	136.55	121.60
1	A	34	LEU	CA-CB-CG	7.44	132.40	115.30
1	C	459	GLY	O-C-N	-7.43	110.81	122.70
2	B	264	GLU	CG-CD-OE2	7.39	133.09	118.30
2	D	663	LYS	CA-CB-CG	7.38	129.64	113.40
2	B	151	LYS	O-C-N	-7.37	110.91	122.70
1	A	7	LYS	N-CA-CB	-7.37	97.34	110.60
2	B	184	PHE	CG-CD1-CE1	7.36	128.90	120.80
2	B	255	CYS	CA-CB-SG	7.35	127.23	114.00
2	D	615	SER	O-C-N	-7.34	110.95	122.70
2	D	659	HIS	CA-C-O	7.33	135.49	120.10
2	B	216	ASP	CA-C-N	7.32	130.84	116.20
2	B	177	VAL	CA-C-O	-7.31	104.74	120.10
2	D	565	GLU	CB-CG-CD	7.31	133.93	114.20
2	D	583	ARG	CG-CD-NE	-7.30	96.47	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	638	LYS	CB-CA-C	-7.30	95.80	110.40
2	B	190	ASP	CB-CG-OD1	-7.29	111.74	118.30
1	A	7	LYS	O-C-N	-7.28	111.05	122.70
1	A	24	TYR	CB-CG-CD1	7.26	125.36	121.00
1	C	433	PHE	O-C-N	7.21	134.24	122.70
2	B	197	VAL	CA-CB-CG2	7.19	121.68	110.90
1	A	129	LEU	O-C-N	7.19	134.20	122.70
2	D	548	PRO	N-CD-CG	-7.17	92.45	103.20
2	D	590	ASP	CB-CG-OD2	7.17	124.75	118.30
1	C	402	LEU	O-C-N	7.16	134.16	122.70
2	B	260	HIS	N-CA-CB	-7.15	97.73	110.60
1	A	64	ASP	CA-CB-CG	7.15	129.12	113.40
2	B	245	ASN	CB-CG-OD1	7.14	135.88	121.60
1	C	465	ALA	CB-CA-C	7.12	120.77	110.10
1	A	2	LEU	CB-CG-CD1	-7.11	98.92	111.00
1	A	24	TYR	CA-CB-CG	7.10	126.88	113.40
2	D	663	LYS	CB-CG-CD	7.09	130.05	111.60
1	C	531	SER	N-CA-CB	-7.07	99.90	110.50
1	C	450	HIS	CA-C-N	-7.06	102.09	116.20
2	B	244	GLU	OE1-CD-OE2	7.05	131.76	123.30
2	D	571	LEU	CB-CG-CD2	-7.05	99.02	111.00
2	B	264	GLU	OE1-CD-OE2	-6.96	114.95	123.30
2	B	198	MET	CG-SD-CE	6.95	111.32	100.20
2	D	684	LEU	CB-CG-CD2	-6.93	99.21	111.00
1	A	46	PHE	CB-CG-CD1	-6.88	115.98	120.80
1	A	74	ASP	CB-CG-OD1	-6.87	112.11	118.30
2	D	684	LEU	CA-C-O	6.87	134.53	120.10
1	A	117	PHE	CA-C-O	6.87	134.52	120.10
2	B	288	TYR	CB-CG-CD1	6.86	125.11	121.00
1	A	107	VAL	CG1-CB-CG2	-6.86	99.93	110.90
2	D	580	TRP	CA-C-O	-6.83	105.75	120.10
1	C	494	ASP	CB-CG-OD1	-6.82	112.16	118.30
2	D	603	VAL	CA-C-O	6.81	134.40	120.10
1	C	414	TRP	CH2-CZ2-CE2	-6.81	110.59	117.40
2	D	553	ALA	O-C-N	6.80	133.59	122.70
1	C	505	LEU	CB-CG-CD2	-6.79	99.45	111.00
1	A	10	VAL	O-C-N	6.79	133.56	122.70
1	A	29	LEU	CA-CB-CG	6.75	130.83	115.30
1	C	459	GLY	CA-C-O	6.75	132.74	120.60
1	C	427	GLU	CB-CG-CD	6.75	132.41	114.20
2	D	656	VAL	CB-CA-C	6.72	124.17	111.40
2	D	666	THR	O-C-N	6.68	133.80	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	274	GLN	CB-CG-CD	6.66	128.92	111.60
1	C	421	ALA	CB-CA-C	6.66	120.09	110.10
2	B	239	LEU	N-CA-CB	-6.63	97.14	110.40
2	D	622	ASP	CB-CG-OD1	6.61	124.25	118.30
2	B	222	ASP	O-C-N	6.60	133.26	122.70
1	C	448	LEU	CA-CB-CG	-6.60	100.12	115.30
2	B	282	ASN	O-C-N	6.59	133.25	122.70
2	D	625[A]	LYS	N-CA-CB	6.59	122.46	110.60
2	D	625[B]	LYS	N-CA-CB	6.59	122.46	110.60
1	C	505	LEU	C-N-CA	6.59	138.18	121.70
2	D	660	HIS	CA-C-O	-6.59	106.27	120.10
2	B	216	ASP	OD1-CG-OD2	-6.58	110.80	123.30
1	C	450	HIS	CB-CA-C	6.58	123.56	110.40
2	B	246	PHE	CB-CG-CD1	-6.56	116.21	120.80
1	C	454	GLN	N-CA-CB	-6.53	98.84	110.60
2	B	210	VAL	CA-CB-CG2	-6.53	101.11	110.90
1	A	116	GLU	CG-CD-OE1	-6.48	105.34	118.30
2	D	601	PRO	CA-C-N	-6.47	102.96	117.20
1	A	138	SER	O-C-N	6.47	133.05	122.70
1	A	92	ARG	NH1-CZ-NH2	-6.44	112.31	119.40
2	B	204	LYS	CD-CE-NZ	6.44	126.52	111.70
2	D	601	PRO	O-C-N	6.43	132.99	122.70
2	B	170	ALA	CB-CA-C	6.43	119.75	110.10
2	D	572	GLY	CA-C-N	6.43	131.34	117.20
1	A	20	HIS	CA-CB-CG	-6.42	102.69	113.60
1	C	531	SER	O-C-N	-6.41	112.44	122.70
2	B	266	THR	CA-CB-OG1	-6.41	95.53	109.00
1	A	47	ASP	O-C-N	6.41	132.95	122.70
2	D	615	SER	CA-CB-OG	6.41	128.49	111.20
1	C	449	SER	CA-C-N	-6.40	103.13	117.20
2	B	286	HIS	O-C-N	6.39	132.93	122.70
1	A	27	GLU	CG-CD-OE1	-6.39	105.53	118.30
1	A	114	PRO	CA-C-O	-6.38	104.88	120.20
2	D	586	GLU	O-C-N	6.38	132.91	122.70
2	D	561	VAL	CG1-CB-CG2	-6.37	100.70	110.90
2	D	547	THR	CA-CB-CG2	6.36	121.30	112.40
1	A	19	ALA	N-CA-CB	-6.33	101.23	110.10
2	B	276	VAL	N-CA-CB	-6.32	97.60	111.50
2	B	158	TRP	CA-C-O	6.31	133.34	120.10
2	B	268	PRO	CA-C-O	-6.28	105.14	120.20
2	D	570	ALA	N-CA-CB	6.28	118.89	110.10
1	C	524	SER	O-C-N	-6.27	112.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	646	PHE	O-C-N	6.26	132.72	122.70
2	D	657	LEU	CB-CG-CD1	6.26	121.64	111.00
1	A	1	VAL	CA-CB-CG2	-6.24	101.54	110.90
1	C	492	ARG	NH1-CZ-NH2	6.22	126.24	119.40
2	B	184	PHE	CB-CG-CD1	6.22	125.15	120.80
2	D	583	ARG	O-C-N	-6.20	112.78	122.70
2	B	233	GLU	CG-CD-OE2	-6.20	105.91	118.30
2	D	659	HIS	CA-CB-CG	-6.18	103.09	113.60
2	B	187	SER	N-CA-CB	-6.15	101.27	110.50
2	D	686	HIS	N-CA-CB	-6.15	99.54	110.60
2	B	209	LYS	N-CA-CB	6.13	121.64	110.60
2	D	658	ALA	N-CA-CB	-6.13	101.52	110.10
2	B	186	GLU	OE1-CD-OE2	6.12	130.65	123.30
1	C	516	GLU	CG-CD-OE1	-6.12	106.07	118.30
2	D	569	GLU	CG-CD-OE2	-6.12	106.07	118.30
1	A	99	LYS	CA-C-N	6.11	130.65	117.20
2	D	661	PHE	CB-CG-CD2	6.11	125.07	120.80
2	B	273	TYR	CB-CG-CD2	6.09	124.66	121.00
1	A	104	CYS	CA-CB-SG	-6.08	103.05	114.00
1	A	14	TRP	O-C-N	-6.06	112.90	123.20
1	C	474	ASP	OD1-CG-OD2	6.05	134.80	123.30
1	C	423	GLU	N-CA-CB	6.05	121.49	110.60
2	D	651	ASN	CB-CG-OD1	6.04	133.68	121.60
2	B	282	ASN	CB-CG-OD1	6.04	133.68	121.60
2	D	589	GLY	CA-C-O	6.04	131.47	120.60
1	A	83	LEU	CB-CG-CD2	-6.03	100.75	111.00
2	B	170	ALA	N-CA-CB	-6.02	101.67	110.10
2	B	158	TRP	CA-C-N	-6.01	104.18	116.20
2	D	601	PRO	N-CD-CG	-6.00	94.20	103.20
1	C	427	GLU	N-CA-CB	-5.99	99.82	110.60
2	B	227	THR	OG1-CB-CG2	-5.99	96.23	110.00
2	D	620	HIS	CB-CA-C	-5.97	98.45	110.40
1	A	114	PRO	N-CA-CB	5.97	110.47	103.30
1	A	140	TYR	CG-CD2-CE2	5.97	126.08	121.30
1	C	499	LYS	CB-CA-C	-5.97	98.47	110.40
1	A	83	LEU	CA-CB-CG	5.96	129.02	115.30
1	A	23	GLU	CA-C-O	5.95	132.60	120.10
2	D	595	ASP	O-C-N	5.95	132.22	122.70
1	A	79	ALA	CB-CA-C	5.95	119.02	110.10
1	C	405	ALA	CB-CA-C	-5.94	101.18	110.10
2	B	173	ARG	CG-CD-NE	-5.93	99.35	111.80
2	D	638	LYS	CG-CD-CE	5.92	129.65	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	486	LEU	O-C-N	-5.91	113.24	122.70
1	C	420	HIS	O-C-N	5.91	132.16	122.70
1	A	98	PHE	CA-C-O	5.90	132.49	120.10
2	B	148	PRO	C-N-CA	-5.90	106.96	121.70
1	A	47	ASP	CA-C-O	-5.89	107.73	120.10
2	D	615	SER	CA-C-O	5.88	132.46	120.10
1	C	446	PHE	CB-CG-CD1	-5.88	116.68	120.80
2	D	670	GLN	CA-CB-CG	-5.88	100.48	113.40
1	A	96	VAL	CA-CB-CG2	5.87	119.71	110.90
2	D	666	THR	CA-C-O	-5.87	107.77	120.10
1	A	138	SER	CA-C-O	-5.87	107.78	120.10
2	D	675	LYS	O-C-N	5.86	132.08	122.70
2	D	684	LEU	O-C-N	-5.86	113.32	122.70
2	D	550	GLU	CG-CD-OE1	-5.86	106.58	118.30
1	A	122	HIS	CA-C-O	5.83	132.34	120.10
1	C	527	LYS	O-C-N	5.83	132.02	122.70
1	C	414	TRP	CB-CG-CD2	5.82	134.17	126.60
2	B	245	ASN	CA-C-O	5.82	132.32	120.10
1	C	462	VAL	CA-CB-CG1	-5.82	102.17	110.90
2	B	186	GLU	CA-CB-CG	5.81	126.17	113.40
1	C	456	LYS	CA-CB-CG	5.81	126.17	113.40
2	D	576	VAL	CA-CB-CG1	5.79	119.58	110.90
2	B	280	VAL	CG1-CB-CG2	5.79	120.16	110.90
1	A	47	ASP	CA-CB-CG	-5.78	100.68	113.40
2	D	545	HIS	C-N-CA	-5.77	107.27	121.70
2	B	249	LEU	CA-C-N	5.75	127.71	116.20
1	A	94	ASP	CB-CG-OD1	-5.75	113.12	118.30
2	B	170	ALA	O-C-N	-5.75	113.50	122.70
2	B	173	ARG	NH1-CZ-NH2	-5.75	113.07	119.40
1	C	446	PHE	CD1-CE1-CZ	-5.75	113.20	120.10
2	B	148	PRO	O-C-N	5.75	131.90	122.70
1	C	485	ASP	CA-CB-CG	5.73	126.01	113.40
1	A	60	LYS	CG-CD-CE	5.72	129.07	111.90
2	D	647	ARG	O-C-N	5.72	131.86	122.70
2	B	204	LYS	C-N-CA	5.72	136.00	121.70
2	D	667	PRO	O-C-N	5.72	131.97	121.10
2	B	157	LEU	CB-CG-CD2	5.71	120.71	111.00
1	A	96	VAL	CG1-CB-CG2	-5.71	101.77	110.90
1	A	96	VAL	O-C-N	5.70	131.82	122.70
2	D	545	HIS	CB-CA-C	-5.70	99.00	110.40
1	A	26	ALA	O-C-N	-5.70	113.59	122.70
2	B	268	PRO	CA-C-N	5.69	129.71	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	489	HIS	CB-CA-C	-5.69	99.03	110.40
2	B	216	ASP	O-C-N	-5.68	113.54	123.20
1	A	17	VAL	CA-C-N	-5.68	104.84	116.20
2	D	598	MET	C-N-CA	5.68	134.22	122.30
2	D	623	ASN	O-C-N	5.68	131.79	122.70
1	C	517	PHE	O-C-N	-5.67	113.62	122.70
2	B	273	TYR	CB-CG-CD1	-5.67	117.60	121.00
2	B	185	PHE	CB-CG-CD2	5.65	124.75	120.80
1	A	75	ASP	C-N-CA	-5.64	107.60	121.70
1	C	517	PHE	CA-C-O	5.63	131.92	120.10
2	D	569	GLU	CA-CB-CG	5.63	125.78	113.40
2	B	177	VAL	CA-CB-CG1	5.62	119.33	110.90
2	B	211	LEU	C-N-CA	-5.62	110.49	122.30
1	C	450	HIS	CA-CB-CG	-5.62	104.05	113.60
1	A	29	LEU	CB-CA-C	5.61	120.86	110.20
1	C	492	ARG	CB-CG-CD	-5.61	97.01	111.60
2	B	251	ASN	CB-CG-OD1	5.61	132.82	121.60
2	D	625[A]	LYS	CB-CA-C	5.61	121.61	110.40
2	D	625[B]	LYS	CB-CA-C	5.61	121.61	110.40
2	D	657	LEU	O-C-N	-5.60	113.73	122.70
1	A	12	ALA	CA-C-N	5.59	129.50	117.20
1	A	78	ASN	OD1-CG-ND2	5.58	134.73	121.90
1	C	512	HIS	CA-C-N	5.58	129.47	117.20
2	D	574	LEU	CA-CB-CG	5.58	128.12	115.30
2	B	209	LYS	O-C-N	5.57	131.62	122.70
1	C	426	ALA	N-CA-CB	5.57	117.90	110.10
2	D	659	HIS	CA-C-N	-5.57	104.94	117.20
2	D	544	VAL	N-CA-CB	5.55	123.72	111.50
1	A	46	PHE	CD1-CG-CD2	5.55	125.51	118.30
2	D	645	ASN	O-C-N	5.54	131.57	122.70
2	D	562	ASN	O-C-N	-5.54	113.84	122.70
2	B	247	ARG	CD-NE-CZ	-5.53	115.86	123.60
1	A	9	ASN	CB-CG-ND2	-5.52	103.46	116.70
1	A	43	PHE	CB-CG-CD2	5.51	124.66	120.80
1	A	98	PHE	O-C-N	-5.51	113.88	122.70
2	B	177	VAL	O-C-N	5.51	131.52	122.70
1	C	493	VAL	CG1-CB-CG2	5.51	119.72	110.90
2	D	611	LEU	CA-C-O	5.51	131.67	120.10
1	A	24	TYR	CA-C-O	-5.51	108.53	120.10
1	A	43	PHE	CB-CG-CD1	-5.51	116.94	120.80
2	B	214	PHE	CB-CG-CD2	-5.50	116.95	120.80
1	A	97	ASN	CB-CG-ND2	5.50	129.90	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	SER	CA-C-N	-5.50	105.11	117.20
2	B	238	LYS	CA-CB-CG	-5.49	101.32	113.40
2	D	633	GLU	CA-C-N	5.49	129.27	117.20
2	D	638	LYS	CA-CB-CG	5.48	125.46	113.40
2	B	206	HIS	O-C-N	-5.47	113.91	123.20
1	C	441	THR	CA-CB-OG1	-5.46	97.53	109.00
1	A	10	VAL	CA-C-O	-5.46	108.64	120.10
2	B	147	THR	CA-CB-OG1	-5.46	97.54	109.00
2	B	212	GLY	O-C-N	5.46	131.43	122.70
2	D	636	CYS	C-N-CA	5.45	135.33	121.70
1	A	11	LYS	CB-CG-CD	5.45	125.77	111.60
2	B	195	ASP	CA-C-O	-5.45	108.65	120.10
2	D	685	ALA	N-CA-CB	-5.44	102.49	110.10
1	A	77	PRO	N-CD-CG	-5.43	95.05	103.20
1	A	68	ASN	CB-CG-OD1	-5.43	110.74	121.60
2	D	556	ALA	N-CA-CB	-5.43	102.50	110.10
1	C	467	THR	CA-CB-CG2	-5.41	104.82	112.40
2	D	569	GLU	CB-CG-CD	-5.41	99.59	114.20
1	A	22	GLY	O-C-N	5.41	131.35	122.70
1	A	53	ALA	N-CA-CB	-5.40	102.53	110.10
2	D	601	PRO	CB-CA-C	-5.39	98.52	112.00
2	D	642	ASP	O-C-N	5.39	131.34	121.10
2	B	263	LYS	CD-CE-NZ	5.39	124.09	111.70
1	C	414	TRP	CB-CG-CD1	-5.39	120.00	127.00
2	D	622	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	C	534	THR	O-C-N	-5.38	114.09	122.70
2	B	282	ASN	CB-CG-ND2	-5.37	103.82	116.70
1	C	464	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	C	535	VAL	CA-CB-CG1	5.35	118.92	110.90
1	C	525	LEU	N-CA-CB	-5.35	99.71	110.40
1	A	93	VAL	CA-CB-CG2	5.34	118.90	110.90
1	A	8	THR	CA-CB-CG2	-5.33	104.93	112.40
1	A	68	ASN	OD1-CG-ND2	5.33	134.16	121.90
1	A	139	LYS	CD-CE-NZ	-5.33	99.45	111.70
2	B	149	GLU	CB-CA-C	5.33	121.05	110.40
1	C	416	LYS	CB-CA-C	-5.32	99.77	110.40
1	C	491	LEU	CB-CG-CD1	5.32	120.04	111.00
2	D	549	GLU	CA-C-N	-5.32	105.50	117.20
2	B	288	TYR	CG-CD1-CE1	-5.32	117.05	121.30
2	D	607	GLY	O-C-N	-5.31	114.20	122.70
1	C	432	MET	CG-SD-CE	5.31	108.69	100.20
2	B	209	LYS	CD-CE-NZ	-5.30	99.50	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	ASP	CB-CG-OD2	5.30	123.07	118.30
2	D	585	PHE	CZ-CE2-CD2	-5.29	113.75	120.10
2	D	548	PRO	O-C-N	5.29	131.17	122.70
2	B	260	HIS	CA-CB-CG	-5.29	104.61	113.60
1	A	23	GLU	CB-CA-C	-5.29	99.82	110.40
1	C	442	TYR	CA-C-O	-5.29	109.00	120.10
1	C	430	GLU	CG-CD-OE1	-5.29	107.73	118.30
1	C	442	TYR	CA-CB-CG	-5.29	103.36	113.40
2	D	665	PHE	CB-CA-C	5.25	120.91	110.40
2	D	597	VAL	CA-CB-CG1	-5.25	103.02	110.90
2	D	674	GLN	N-CA-CB	5.24	120.04	110.60
2	D	584	PHE	CZ-CE2-CD2	5.24	126.39	120.10
2	D	611	LEU	O-C-N	-5.24	114.29	123.20
1	A	46	PHE	CA-C-N	-5.22	105.72	117.20
1	C	512	HIS	CA-C-O	-5.21	109.15	120.10
1	C	483	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	C	484	SER	O-C-N	5.21	131.03	122.70
2	B	169	GLU	N-CA-CB	-5.19	101.26	110.60
1	C	473	VAL	CG1-CB-CG2	5.19	119.20	110.90
1	A	16	LYS	CB-CG-CD	-5.18	98.12	111.60
2	D	627	THR	N-CA-CB	5.18	120.15	110.30
1	A	6	ASP	O-C-N	5.18	130.99	122.70
1	A	72	HIS	CA-C-O	-5.18	109.22	120.10
2	D	646	PHE	N-CA-CB	5.18	119.92	110.60
1	A	42	TYR	CD1-CG-CD2	-5.16	112.22	117.90
2	B	188	PHE	CZ-CE2-CD2	-5.16	113.91	120.10
2	D	641	VAL	N-CA-CB	-5.14	100.18	111.50
2	D	647	ARG	NE-CZ-NH2	5.13	122.87	120.30
2	D	639	LEU	O-C-N	5.13	130.91	122.70
1	A	122	HIS	CA-CB-CG	5.13	122.32	113.60
1	A	14	TRP	CD1-NE1-CE2	-5.13	104.39	109.00
2	D	688	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	47	ASP	C-N-CA	-5.12	108.91	121.70
2	B	261	PHE	CA-CB-CG	-5.12	101.62	113.90
2	B	197	VAL	N-CA-CB	-5.12	100.25	111.50
1	C	414	TRP	CA-CB-CG	-5.12	103.98	113.70
2	B	149	GLU	O-C-N	5.11	130.88	122.70
1	C	506	LEU	O-C-N	5.11	130.88	122.70
1	A	91	LEU	O-C-N	-5.11	114.53	122.70
2	B	178	TYR	N-CA-CB	5.10	119.78	110.60
1	C	474	ASP	CB-CG-OD1	-5.10	113.71	118.30
2	B	191	LEU	CA-CB-CG	5.10	127.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	603	VAL	N-CA-CB	-5.10	100.28	111.50
1	A	116	GLU	CG-CD-OE2	5.10	128.49	118.30
2	B	158	TRP	CB-CG-CD1	5.10	133.62	127.00
1	A	103	HIS	CG-ND1-CE1	5.09	115.33	108.20
1	C	500	LEU	CB-CG-CD2	-5.09	102.34	111.00
2	D	652	VAL	CG1-CB-CG2	5.08	119.03	110.90
1	C	493	VAL	CA-CB-CG1	-5.08	103.29	110.90
2	D	664	GLU	N-CA-CB	-5.07	101.47	110.60
1	A	68	ASN	N-CA-CB	-5.07	101.47	110.60
2	B	223	ASN	CB-CG-OD1	-5.07	111.46	121.60
2	B	168	GLY	CA-C-O	5.07	129.72	120.60
1	A	123	ALA	N-CA-CB	-5.06	103.01	110.10
1	C	528	PHE	CB-CG-CD1	-5.06	117.26	120.80
2	D	616	ASP	CB-CA-C	5.06	120.52	110.40
1	A	20	HIS	O-C-N	5.06	130.79	122.70
2	B	160	LYS	CB-CG-CD	-5.05	98.46	111.60
1	C	475	ASP	OD1-CG-OD2	5.05	132.90	123.30
1	A	7	LYS	CD-CE-NZ	-5.05	100.09	111.70
2	B	157	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	A	99	LYS	O-C-N	-5.03	114.66	122.70
1	A	123	ALA	CB-CA-C	5.03	117.64	110.10
1	C	467	THR	CA-CB-OG1	5.03	119.56	109.00
1	C	521	VAL	O-C-N	5.02	130.73	122.70
1	C	508	THR	OG1-CB-CG2	5.02	121.55	110.00
2	D	553	ALA	CA-C-N	-5.01	106.17	117.20
1	C	534	THR	C-N-CA	5.01	134.22	121.70
1	A	70	VAL	CG1-CB-CG2	-5.01	102.89	110.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	545	HIS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
2	B	183	ARG	Sidechain
2	B	247	ARG	Sidechain
1	C	492	ARG	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	1069	0	1073	58	1
1	C	1069	0	1070	54	0
2	B	1123	0	1115	92	0
2	D	1127	0	1124	107	0
3	A	43	0	30	2	0
3	B	43	0	30	6	0
3	C	43	0	30	0	0
3	D	43	0	30	12	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	D	15	0	3	2	0
6	A	29	0	0	1	1
6	B	46	0	0	9	1
6	C	16	0	0	0	0
6	D	45	0	0	9	1
All	All	4715	0	4505	308	2

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 34.

All (308) 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)
2:D:686:HIS:NE2	6:D:102:HOH:O	1.57	1.28
2:D:571:LEU:HD22	6:D:128:HOH:O	1.12	1.24
2:B:153:ALA:HA	6:B:49:HOH:O	1.38	1.17
2:D:649:LEU:HD23	3:D:691:HEM:HBB2	1.25	1.14
1:A:118:THR:HG22	1:A:121:VAL:H	1.09	1.13
2:D:547:THR:HG22	2:D:549:GLU:N	1.64	1.12
2:B:217:GLY:HA3	6:B:44:HOH:O	1.46	1.11
2:D:686:HIS:CD2	6:D:102:HOH:O	1.85	1.09
2:B:147:THR:HG22	2:B:149:GLU:H	1.11	1.09
2:D:571:LEU:HB2	6:D:128:HOH:O	1.45	1.08
2:B:147:THR:HG23	2:B:148:PRO:HD2	1.25	1.07
2:D:549:GLU:OE1	2:D:549:GLU:HA	1.53	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:291:HEM:HHC	3:B:291:HEM:HBB2	1.39	1.01
2:D:547:THR:HG22	2:D:549:GLU:H	0.90	1.01
2:D:667:PRO:HB2	2:D:668:PRO:HD3	1.42	0.99
2:B:147:THR:CG2	2:B:148:PRO:HD2	1.94	0.98
1:C:513:LEU:HB3	1:C:516:GLU:HG3	1.46	0.97
2:D:548:PRO:HA	2:D:551:LYS:HG3	1.47	0.96
2:D:544:VAL:HA	6:D:104:HOH:O	1.66	0.95
2:B:147:THR:HG22	2:B:149:GLU:N	1.81	0.94
2:B:147:THR:C	2:B:151:LYS:HE3	1.87	0.93
2:B:153:ALA:CA	6:B:49:HOH:O	2.05	0.90
1:C:513:LEU:HB3	1:C:516:GLU:CG	2.03	0.89
2:B:164:ASP:HA	2:B:208:LYS:HG2	1.54	0.88
2:D:649:LEU:HD23	3:D:691:HEM:CBB	2.04	0.86
1:A:103:HIS:HE1	2:B:274:GLN:OE1	1.56	0.86
2:B:147:THR:CG2	2:B:149:GLU:H	1.89	0.86
2:B:148:PRO:CA	2:B:151:LYS:HE3	2.06	0.86
1:A:6:ASP:O	1:A:10:VAL:HG13	1.79	0.83
1:C:496:VAL:O	1:C:496:VAL:HG22	1.77	0.82
2:D:547:THR:CG2	2:D:549:GLU:H	1.85	0.82
2:B:148:PRO:N	2:B:151:LYS:HE3	1.95	0.81
2:B:147:THR:O	2:B:151:LYS:HE3	1.81	0.80
1:A:118:THR:HG22	1:A:121:VAL:N	1.94	0.79
1:C:484:SER:HB2	1:C:539:LYS:HD2	1.66	0.78
2:D:616:ASP:O	2:D:620:HIS:CD2	2.37	0.78
5:D:701:DG2:C7	5:D:701:DG2:O11	2.31	0.78
2:D:632:SER:HB3	2:D:687:LYS:HG3	1.65	0.77
1:C:417:VAL:CG1	1:C:421:ALA:HB2	2.13	0.77
1:A:42:TYR:C	1:A:44:PRO:HD3	2.05	0.77
1:A:43:PHE:N	1:A:44:PRO:HD3	2.00	0.77
2:B:167:GLY:HA2	2:B:211:LEU:HD23	1.65	0.77
2:D:547:THR:O	2:D:551:LYS:HG2	1.85	0.76
1:A:76:MET:N	1:A:77:PRO:CD	2.49	0.76
2:D:607:GLY:HA2	6:D:128:HOH:O	1.84	0.76
2:D:600:ASN:OD1	2:D:602:LYS:HB2	1.86	0.76
1:C:417:VAL:HG12	1:C:421:ALA:HB2	1.68	0.75
1:A:45:HIS:ND1	1:A:45:HIS:N	2.29	0.74
2:B:146:LEU:HD23	2:B:151:LYS:CA	2.18	0.73
1:A:17:VAL:HG13	1:A:24:TYR:CD2	2.23	0.73
1:A:76:MET:N	1:A:77:PRO:HD3	2.03	0.73
2:B:180:TRP:O	2:B:183:ARG:HG2	1.88	0.73
1:A:114:PRO:O	2:B:259:HIS:NE2	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:547:THR:HB	2:D:550:GLU:HG3	1.70	0.71
2:D:649:LEU:CD2	3:D:691:HEM:HBB2	2.15	0.71
1:C:401:VAL:HG13	1:C:401:VAL:O	1.90	0.70
2:B:286:HIS:ND1	2:B:287:LYS:HE2	2.05	0.70
1:A:43:PHE:HA	1:A:45:HIS:CE1	2.27	0.69
2:B:193:THR:HG22	2:B:194:PRO:HD2	1.74	0.69
2:B:148:PRO:HA	2:B:151:LYS:CE	2.22	0.69
1:A:20:HIS:O	1:A:23:GLU:HB2	1.93	0.68
1:C:496:VAL:O	1:C:496:VAL:CG2	2.40	0.68
2:D:545:HIS:O	2:D:675:LYS:HE2	1.93	0.68
2:D:618:LEU:HA	2:D:621:LEU:HD13	1.75	0.68
2:B:148:PRO:HB3	2:B:151:LYS:NZ	2.09	0.67
2:D:639:LEU:HD13	3:D:691:HEM:C3D	2.30	0.67
2:B:148:PRO:HB3	2:B:151:LYS:HZ1	1.60	0.67
2:B:287:LYS:HE3	6:B:42:HOH:O	1.94	0.67
2:D:667:PRO:CB	2:D:668:PRO:HD3	2.17	0.67
2:B:148:PRO:CA	2:B:151:LYS:CE	2.73	0.66
2:B:148:PRO:HA	2:B:151:LYS:HZ2	1.59	0.66
2:B:147:THR:HG23	2:B:148:PRO:CD	2.16	0.66
2:D:620:HIS:CD2	2:D:620:HIS:N	2.63	0.66
2:B:181:THR:HG22	2:B:245:ASN:HD21	1.60	0.66
1:A:32:MET:SD	1:A:101:LEU:HB2	2.36	0.65
2:B:229:ALA:O	2:B:233:GLU:HG3	1.95	0.65
2:D:667:PRO:N	2:D:668:PRO:CD	2.59	0.65
1:C:431:ARG:HD3	2:D:670:GLN:OE1	1.96	0.65
2:D:546:LEU:HD23	2:D:550:GLU:CB	2.27	0.65
2:B:148:PRO:HA	2:B:151:LYS:HE3	1.79	0.64
2:D:621:LEU:HD12	2:D:624:LEU:HD11	1.77	0.64
2:B:148:PRO:CD	2:B:149:GLU:H	2.11	0.64
2:B:148:PRO:CB	2:B:151:LYS:NZ	2.62	0.63
1:C:443:PHE:N	1:C:444:PRO:CD	2.62	0.63
1:A:47:ASP:OD1	1:A:47:ASP:C	2.33	0.63
2:B:217:GLY:HA2	2:B:227:THR:HG21	1.80	0.63
2:D:581:THR:HG22	2:D:645:ASN:ND2	2.14	0.62
2:D:661:PHE:HB3	2:D:664:GLU:HB3	1.80	0.62
2:B:147:THR:CG2	2:B:148:PRO:CD	2.75	0.62
1:A:58:HIS:O	1:A:62:VAL:HG23	1.99	0.62
1:A:28:ALA:HB1	1:A:105:LEU:HD13	1.80	0.62
1:C:505:LEU:O	1:C:509:LEU:HG	2.00	0.62
3:B:291:HEM:NC	6:B:126:HOH:O	2.31	0.62
2:B:146:LEU:HD23	2:B:151:LYS:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:581:THR:HG22	2:D:645:ASN:HD22	1.65	0.61
2:D:624:LEU:O	2:D:683:ALA:HB1	2.00	0.61
1:C:503:HIS:HE1	2:D:674:GLN:OE1	1.84	0.61
2:B:148:PRO:HA	2:B:151:LYS:HG2	1.83	0.60
1:A:99:LYS:HD2	1:A:99:LYS:N	2.17	0.60
2:B:146:LEU:HD23	2:B:151:LYS:HB3	1.83	0.60
2:B:148:PRO:HA	2:B:151:LYS:NZ	2.17	0.59
2:B:148:PRO:CD	2:B:149:GLU:N	2.62	0.59
1:C:450:HIS:ND1	1:C:451:GLY:N	2.51	0.59
1:C:476:MET:HB2	1:C:477:PRO:HD3	1.84	0.59
2:B:234:LEU:CD2	3:B:291:HEM:HBA2	2.32	0.59
1:A:43:PHE:N	1:A:44:PRO:CD	2.66	0.59
1:A:103:HIS:CE1	2:B:274:GLN:OE1	2.47	0.59
1:A:113:LEU:HB3	1:A:116:GLU:HG2	1.84	0.58
1:A:44:PRO:HD2	1:A:45:HIS:ND1	2.17	0.58
2:B:153:ALA:C	6:B:49:HOH:O	2.37	0.58
3:D:691:HEM:HBB2	3:D:691:HEM:HHC	1.85	0.58
2:D:583:ARG:HD3	2:D:584:PHE:CZ	2.38	0.58
1:A:92:ARG:HG3	1:A:92:ARG:HH11	1.69	0.57
2:B:254:VAL:HG11	2:B:274:GLN:OE1	2.05	0.57
2:D:558:TRP:HH2	2:D:611:LEU:HD11	1.70	0.57
2:D:667:PRO:N	2:D:668:PRO:HD2	2.20	0.56
2:D:588:PHE:HA	2:D:602:LYS:HE3	1.86	0.56
1:C:480:LEU:HD12	1:C:535:VAL:HG11	1.86	0.56
2:D:546:LEU:HD23	2:D:550:GLU:HB2	1.88	0.56
1:A:43:PHE:HA	1:A:45:HIS:HE1	1.71	0.56
2:D:600:ASN:OD1	2:D:602:LYS:CB	2.54	0.56
2:B:148:PRO:CB	2:B:151:LYS:HZ2	2.17	0.56
1:A:3:SER:O	1:A:7:LYS:HG3	2.06	0.56
1:C:452:SER:O	1:C:456:LYS:HG3	2.06	0.56
2:B:148:PRO:CA	2:B:151:LYS:HZ2	2.19	0.55
2:D:547:THR:CG2	2:D:548:PRO:CD	2.85	0.55
2:D:667:PRO:HB2	2:D:668:PRO:CD	2.27	0.55
2:B:148:PRO:CA	2:B:151:LYS:NZ	2.70	0.54
2:B:150:GLU:OE1	2:B:275:LYS:NZ	2.40	0.54
1:A:37:PRO:O	1:A:40:LYS:HG3	2.07	0.54
2:B:233:GLU:O	2:B:237:ASP:HB2	2.07	0.54
1:A:52:SER:OG	1:A:55:VAL:HG23	2.07	0.54
2:D:639:LEU:CD1	3:D:691:HEM:C3D	2.91	0.54
2:B:147:THR:O	2:B:151:LYS:CE	2.55	0.53
2:B:183:ARG:HB3	1:C:492:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:LEU:HD23	2:B:151:LYS:CB	2.37	0.53
1:A:28:ALA:CB	1:A:105:LEU:HD13	2.38	0.53
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.43	0.53
2:D:667:PRO:CB	2:D:668:PRO:CD	2.86	0.53
2:D:558:TRP:HA	2:D:561:VAL:HG23	1.91	0.53
2:D:616:ASP:O	2:D:620:HIS:HD2	1.86	0.53
1:C:481:SER:OG	1:C:482:ALA:N	2.40	0.52
2:D:546:LEU:HD23	2:D:550:GLU:HB3	1.91	0.52
2:D:633:GLU:O	2:D:637:ASP:HB2	2.09	0.52
2:B:148:PRO:HD2	2:B:149:GLU:H	1.75	0.52
1:C:512:HIS:O	1:C:513:LEU:HD23	2.10	0.52
2:D:684:LEU:HD12	3:D:691:HEM:HAB	1.92	0.52
2:B:157:LEU:C	2:B:159:GLY:N	2.62	0.51
3:B:291:HEM:HBB2	3:B:291:HEM:CHC	2.20	0.51
2:B:193:THR:CG2	2:B:194:PRO:HD2	2.40	0.51
1:A:115:ALA:HB3	1:A:116:GLU:OE2	2.11	0.51
1:C:401:VAL:O	1:C:401:VAL:CG1	2.58	0.51
2:B:211:LEU:O	2:B:215:SER:HB2	2.11	0.51
1:A:16:LYS:O	1:A:17:VAL:C	2.49	0.51
2:D:594:PRO:O	2:D:598:MET:HG2	2.10	0.51
2:D:592:SER:O	2:D:593:THR:HG23	2.11	0.51
1:C:403:SER:O	1:C:406:ASP:HB2	2.12	0.50
1:C:435:SER:HB3	2:D:674:GLN:HG3	1.93	0.50
1:A:98:PHE:HB3	1:A:133:SER:HB3	1.92	0.50
2:B:161:VAL:HG12	2:B:261:PHE:CZ	2.47	0.50
2:B:244:GLU:O	2:B:244:GLU:HG3	2.12	0.50
1:C:468:ASN:O	1:C:472:HIS:HD2	1.95	0.50
2:D:571:LEU:CD2	6:D:128:HOH:O	1.90	0.50
2:B:151:LYS:O	2:B:155:THR:HB	2.11	0.50
1:C:476:MET:O	1:C:477:PRO:C	2.47	0.50
2:D:624:LEU:O	2:D:683:ALA:CB	2.60	0.50
2:D:548:PRO:CA	2:D:551:LYS:HG3	2.33	0.49
1:A:113:LEU:HB3	1:A:116:GLU:CG	2.43	0.49
1:C:466:LEU:O	1:C:470:VAL:HG23	2.13	0.49
2:B:193:THR:HG22	2:B:194:PRO:CD	2.42	0.49
2:B:181:THR:HG22	2:B:245:ASN:ND2	2.27	0.49
1:A:118:THR:CG2	1:A:120:ALA:HB3	2.43	0.49
3:D:691:HEM:CBB	3:D:691:HEM:HHC	2.43	0.49
2:B:146:LEU:CD2	2:B:151:LYS:HB3	2.43	0.49
2:D:549:GLU:OE1	2:D:549:GLU:CA	2.41	0.49
1:A:40:LYS:NZ	2:D:689:HIS:O	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:616:ASP:O	2:D:619:ALA:HB3	2.13	0.49
2:D:620:HIS:HB2	2:D:627:THR:OG1	2.13	0.49
2:D:623:ASN:ND2	2:D:626:GLY:H	2.11	0.49
2:D:550:GLU:O	2:D:553:ALA:HB3	2.13	0.48
1:C:428:ALA:HB2	1:C:505:LEU:HD13	1.95	0.48
1:C:476:MET:N	1:C:477:PRO:HD2	2.28	0.48
2:D:684:LEU:CD1	3:D:691:HEM:HAB	2.43	0.48
2:B:144:VAL:HG23	2:B:146:LEU:HD13	1.95	0.48
1:C:410:VAL:HG23	1:C:470:VAL:HG13	1.96	0.48
2:D:609:LYS:HD3	3:D:691:HEM:CAA	2.43	0.48
2:B:157:LEU:C	2:B:159:GLY:H	2.16	0.48
1:A:17:VAL:HG13	1:A:24:TYR:HD2	1.78	0.48
2:B:193:THR:CB	2:B:194:PRO:CD	2.91	0.48
2:D:661:PHE:O	2:D:664:GLU:HB2	2.14	0.48
1:A:28:ALA:CB	1:A:105:LEU:CD1	2.92	0.48
1:A:58:HIS:HE1	3:A:143:HEM:CHA	2.25	0.48
1:A:84:SER:HB2	1:A:139:LYS:HD2	1.95	0.48
1:A:97:ASN:ND2	6:A:148:HOH:O	2.31	0.48
2:D:593:THR:O	2:D:597:VAL:HG23	2.14	0.48
2:D:666:THR:HB	2:D:668:PRO:HD2	1.96	0.48
2:D:547:THR:CB	2:D:550:GLU:HG3	2.40	0.48
2:B:218:LEU:O	2:B:221:LEU:HD22	2.14	0.47
2:B:272:ALA:O	2:B:276:VAL:HG23	2.13	0.47
2:D:684:LEU:HD23	2:D:684:LEU:HA	1.66	0.47
1:C:407:LYS:NZ	1:C:474:ASP:OD1	2.30	0.47
2:D:544:VAL:HG13	2:D:546:LEU:HD12	1.97	0.47
1:A:17:VAL:HG13	1:A:24:TYR:CE2	2.49	0.47
2:B:147:THR:HG22	2:B:150:GLU:H	1.79	0.47
2:D:639:LEU:HD13	3:D:691:HEM:C2D	2.49	0.47
1:C:480:LEU:HD12	1:C:535:VAL:CG1	2.43	0.47
1:C:513:LEU:O	1:C:516:GLU:HG2	2.14	0.47
2:D:642:ASP:OD1	2:D:643:PRO:HD2	2.13	0.47
2:B:163:VAL:HG13	2:B:211:LEU:HB3	1.96	0.47
1:A:44:PRO:HD2	1:A:45:HIS:CE1	2.50	0.46
1:A:35:SER:C	1:A:37:PRO:HD3	2.35	0.46
1:C:486:LEU:HD11	1:C:490:LYS:HD3	1.97	0.46
2:D:547:THR:O	2:D:551:LYS:CG	2.60	0.46
2:B:167:GLY:HA3	2:B:207:GLY:O	2.16	0.46
1:C:483:LEU:HD12	1:C:483:LEU:HA	1.65	0.46
2:D:571:LEU:HD21	2:D:606:HIS:HD2	1.80	0.46
1:A:113:LEU:N	1:A:114:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:O	1:A:73:VAL:HB	2.15	0.46
2:D:632:SER:CB	2:D:687:LYS:HG3	2.42	0.46
2:D:551:LYS:O	2:D:555:THR:HB	2.16	0.46
2:D:644:GLU:OE1	2:D:647:ARG:NH1	2.49	0.45
1:A:16:LYS:NZ	1:A:16:LYS:HB3	2.20	0.45
2:B:173:ARG:O	2:B:177:VAL:HG23	2.16	0.45
2:D:611:LEU:HD22	2:D:611:LEU:HA	1.65	0.45
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.80	0.45
1:C:518:THR:HG22	1:C:521:VAL:HG23	1.99	0.45
2:D:620:HIS:C	2:D:622:ASP:H	2.19	0.45
2:B:217:GLY:CA	6:B:44:HOH:O	2.28	0.45
1:C:475:ASP:OD2	1:C:478:ASN:HB2	2.17	0.45
1:C:417:VAL:HG11	1:C:421:ALA:HB2	1.94	0.45
2:B:182:GLN:O	2:B:183:ARG:C	2.53	0.44
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.70	0.44
2:B:178:TYR:N	2:B:179:PRO:CD	2.80	0.44
1:C:514:PRO:O	1:C:515:ALA:C	2.54	0.44
2:B:267:PRO:N	2:B:268:PRO:CD	2.81	0.44
1:C:513:LEU:HB3	1:C:516:GLU:HG2	1.92	0.44
2:B:191:LEU:HB3	2:B:197:VAL:HG22	2.00	0.44
2:D:558:TRP:CE3	2:D:561:VAL:HG21	2.53	0.44
1:A:92:ARG:NH1	2:D:583:ARG:HB2	2.33	0.44
1:C:493:VAL:O	1:C:540:TYR:HE2	2.01	0.44
1:C:523:ALA:HA	2:D:577:VAL:HG13	1.98	0.44
2:D:573:ARG:O	2:D:577:VAL:HG23	2.17	0.44
1:C:417:VAL:CG1	1:C:421:ALA:CB	2.91	0.44
2:D:546:LEU:CD2	2:D:550:GLU:HB3	2.47	0.44
3:A:143:HEM:HBC2	3:A:143:HEM:HMC1	2.00	0.44
2:B:225:LYS:HD3	2:B:286:HIS:CD2	2.53	0.44
2:B:148:PRO:CG	2:B:149:GLU:N	2.82	0.43
2:D:548:PRO:HA	2:D:551:LYS:NZ	2.33	0.43
2:D:573:ARG:HD2	2:D:656:VAL:CG2	2.49	0.43
2:B:164:ASP:CA	2:B:208:LYS:HG2	2.37	0.43
2:D:661:PHE:O	2:D:662:GLY:C	2.56	0.43
1:A:109:LEU:O	1:A:110:ALA:C	2.54	0.43
1:C:476:MET:N	1:C:477:PRO:CD	2.82	0.43
2:D:656:VAL:O	2:D:659:HIS:HB3	2.18	0.43
2:B:153:ALA:O	2:B:154:VAL:C	2.56	0.43
2:B:272:ALA:O	2:B:275:LYS:HB2	2.18	0.43
2:D:571:LEU:CB	6:D:128:HOH:O	2.20	0.43
2:D:684:LEU:CD1	3:D:691:HEM:CAB	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PHE:HD1	1:A:33:PHE:HA	1.58	0.43
1:C:466:LEU:HD12	1:C:466:LEU:HA	1.34	0.43
2:D:547:THR:HG23	2:D:548:PRO:CD	2.49	0.43
2:D:548:PRO:CB	2:D:551:LYS:HZ2	2.31	0.43
2:B:158:TRP:HE3	2:B:273:TYR:OH	2.02	0.43
2:B:206:HIS:NE2	6:B:126:HOH:O	2.36	0.42
1:C:407:LYS:O	1:C:411:LYS:HG3	2.19	0.42
1:C:406:ASP:O	1:C:410:VAL:HG13	2.19	0.42
1:C:424:TYR:N	1:C:424:TYR:CD1	2.86	0.42
2:B:146:LEU:HD21	2:B:154:VAL:HG21	2.02	0.42
1:C:442:TYR:C	1:C:444:PRO:HD2	2.39	0.42
2:D:631:LEU:HD23	2:D:631:LEU:HA	1.91	0.42
1:A:47:ASP:OD1	1:A:48:LEU:N	2.53	0.42
2:B:146:LEU:HD23	2:B:151:LYS:N	2.34	0.42
2:D:558:TRP:CH2	2:D:611:LEU:HD11	2.51	0.42
2:D:569:GLU:HG2	2:D:656:VAL:HG22	2.01	0.42
2:D:661:PHE:O	2:D:664:GLU:CB	2.67	0.42
1:A:34:LEU:HD12	2:B:267:PRO:C	2.40	0.42
2:B:193:THR:CB	2:B:194:PRO:HD2	2.50	0.42
2:B:147:THR:O	2:B:151:LYS:CD	2.67	0.41
1:C:402:LEU:HD23	1:C:402:LEU:HA	1.85	0.41
1:C:470:VAL:O	1:C:473:VAL:HB	2.20	0.41
1:C:516:GLU:HG2	1:C:516:GLU:H	1.31	0.41
2:B:161:VAL:HG12	2:B:261:PHE:HZ	1.85	0.41
1:A:51:GLY:O	1:A:52:SER:C	2.55	0.41
1:C:476:MET:HB2	1:C:477:PRO:CD	2.50	0.41
2:D:600:ASN:HA	2:D:601:PRO:HD2	1.52	0.41
2:D:653:LEU:O	2:D:656:VAL:N	2.52	0.41
1:A:141:ARG:HD3	2:D:580:TRP:HZ3	1.86	0.41
2:B:209:LYS:HE3	3:B:291:HEM:HAA2	2.01	0.41
1:C:505:LEU:HD13	1:C:505:LEU:HA	1.83	0.41
2:D:545:HIS:O	2:D:675:LYS:CE	2.66	0.41
2:D:548:PRO:CA	2:D:551:LYS:HZ2	2.34	0.41
2:D:601:PRO:HG2	2:D:602:LYS:H	1.86	0.41
2:D:635:HIS:HB3	2:D:688:TYR:OH	2.20	0.41
2:B:211:LEU:HA	2:B:214:PHE:HB3	2.03	0.41
2:B:243:PRO:HB2	2:B:247:ARG:HH22	1.86	0.41
2:D:644:GLU:O	2:D:644:GLU:HG3	2.21	0.41
1:A:100:LEU:HA	1:A:100:LEU:HD23	1.83	0.41
2:B:171:LEU:O	2:B:174:LEU:HB3	2.21	0.41
2:D:588:PHE:O	2:D:602:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:HB3	1:A:16:LYS:HZ1	1.85	0.40
3:B:291:HEM:HAA1	6:B:65:HOH:O	2.21	0.40
1:C:525:LEU:HA	1:C:525:LEU:HD23	1.89	0.40
2:D:548:PRO:HA	2:D:551:LYS:HZ2	1.86	0.40
1:C:442:TYR:C	1:C:444:PRO:CD	2.89	0.40
5:D:701:DG2:H41	6:D:106:HOH:O	2.21	0.40
1:A:20:HIS:CD2	1:A:20:HIS:N	2.88	0.40
2:D:547:THR:HG22	2:D:549:GLU:CA	2.44	0.40
2:D:643:PRO:HA	2:D:646:PHE:CD2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:170:HOH:O	6:D:132:HOH:O[4_554]	0.01	2.19
1:A:23:GLU:OE1	6:B:28:HOH:O[3_445]	1.65	0.55

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	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
1	C	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
2	B	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
2	D	145/146 (99%)	133 (92%)	10 (7%)	2 (1%)	11	20
All	All	567/574 (99%)	528 (93%)	37 (6%)	2 (0%)	34	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	662	GLY
2	D	564	ASP

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	113/113 (100%)	98 (87%)	15 (13%)	4 7
1	C	113/113 (100%)	104 (92%)	9 (8%)	12 23
2	B	118/118 (100%)	98 (83%)	20 (17%)	2 3
2	D	119/118 (101%)	95 (80%)	24 (20%)	1 2
All	All	463/462 (100%)	395 (85%)	68 (15%)	3 5

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	16	LYS
1	A	44	PRO
1	A	45	HIS
1	A	52	SER
1	A	60	LYS
1	A	77	PRO
1	A	83	LEU
1	A	84	SER
1	A	92	ARG
1	A	95	PRO
1	A	99	LYS
1	A	105	LEU
1	A	116	GLU
1	A	118	THR
2	B	144	VAL
2	B	146	LEU
2	B	148	PRO
2	B	149	GLU
2	B	151	LYS

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Mol	Chain	Res	Type
2	B	152	SER
2	B	155	THR
2	B	161	VAL
2	B	175	LEU
2	B	183	ARG
2	B	186	GLU
2	B	193	THR
2	B	195	ASP
2	B	202	LYS
2	B	211	LEU
2	B	216	ASP
2	B	221	LEU
2	B	238	LYS
2	B	263	LYS
2	B	286	HIS
1	C	410	VAL
1	C	416	LYS
1	C	466	LEU
1	C	473	VAL
1	C	484	SER
1	C	505	LEU
1	C	506	LEU
1	C	516	GLU
1	C	518	THR
2	D	544	VAL
2	D	546	LEU
2	D	549	GLU
2	D	551	LYS
2	D	555	THR
2	D	560	LYS
2	D	565	GLU
2	D	595	ASP
2	D	608	LYS
2	D	610	VAL
2	D	611	LEU
2	D	615	SER
2	D	616	ASP
2	D	620	HIS
2	D	621	LEU
2	D	622	ASP
2	D	625[A]	LYS
2	D	625[B]	LYS

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Mol	Chain	Res	Type
2	D	634	LEU
2	D	656	VAL
2	D	660	HIS
2	D	663	LYS
2	D	667	PRO
2	D	674	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	78	ASN
1	A	103	HIS
2	B	223	ASN
2	B	245	ASN
1	C	420	HIS
1	C	472	HIS
1	C	497	ASN
1	C	503	HIS
2	D	620	HIS
2	D	623	ASN
2	D	645	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
3	HEM	A	143	1,4	41,50,50	1.57	5 (12%)	45,82,82	2.48	19 (42%)
3	HEM	C	543	1,4	41,50,50	1.52	9 (21%)	45,82,82	2.18	14 (31%)
5	DG2	D	701	-	13,14,14	2.00	3 (23%)	18,21,21	5.67	9 (50%)
3	HEM	D	691	2,6	41,50,50	1.54	8 (19%)	45,82,82	2.32	15 (33%)
4	OXY	A	144	3	1,1,1	0.39	0	-		
3	HEM	B	291	2,6	41,50,50	1.66	8 (19%)	45,82,82	1.80	9 (20%)
4	OXY	C	544	3	1,1,1	0.54	0	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	143	1,4	-	2/12/54/54	-
3	HEM	C	543	1,4	-	6/12/54/54	-
5	DG2	D	701	-	1/1/4/4	7/15/15/15	-
3	HEM	D	691	2,6	-	4/12/54/54	-
3	HEM	B	291	2,6	-	3/12/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	291	HEM	C3C-C2C	-5.32	1.33	1.40
5	D	701	DG2	O5-C4	-4.79	1.26	1.44
3	A	143	HEM	C3C-C2C	-4.71	1.33	1.40
3	D	691	HEM	C3C-C2C	-4.67	1.33	1.40
3	C	543	HEM	C3C-C2C	-4.40	1.34	1.40
3	B	291	HEM	C2A-C3A	-3.51	1.27	1.37
3	A	143	HEM	C3C-CAC	3.35	1.54	1.47
3	B	291	HEM	C3C-CAC	3.16	1.54	1.47
5	D	701	DG2	P6-O15	-3.11	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	701	DG2	P1-O11	-3.05	1.40	1.50
3	D	691	HEM	CAB-C3B	2.94	1.55	1.47
3	B	291	HEM	CAB-C3B	2.72	1.54	1.47
3	C	543	HEM	CAB-C3B	2.69	1.54	1.47
3	C	543	HEM	CHA-C4D	2.65	1.41	1.35
3	A	143	HEM	CHA-C4D	2.53	1.41	1.35
3	B	291	HEM	CHB-C1B	2.46	1.41	1.35
3	A	143	HEM	CMB-C2B	2.45	1.56	1.50
3	B	291	HEM	CMB-C2B	2.42	1.55	1.50
3	C	543	HEM	C4A-NA	2.42	1.41	1.36
3	C	543	HEM	CMD-C2D	2.39	1.55	1.50
3	D	691	HEM	CAA-C2A	2.36	1.55	1.52
3	B	291	HEM	CAA-C2A	2.36	1.55	1.52
3	C	543	HEM	CMB-C2B	2.32	1.55	1.50
3	C	543	HEM	CHB-C1B	2.30	1.40	1.35
3	C	543	HEM	C3B-C2B	-2.30	1.32	1.37
3	D	691	HEM	C3C-CAC	2.14	1.52	1.47
3	D	691	HEM	CHA-C4D	2.13	1.40	1.35
3	D	691	HEM	C3B-C2B	-2.06	1.33	1.37
3	D	691	HEM	C3D-C2D	-2.06	1.32	1.36
3	C	543	HEM	C3C-CAC	2.04	1.52	1.47
3	D	691	HEM	C2A-C3A	-2.02	1.31	1.37
3	B	291	HEM	O2A-CGA	-2.01	1.24	1.30
3	A	143	HEM	C2C-C1C	2.00	1.47	1.42

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	701	DG2	O2-C3-C4	18.31	136.61	106.56
5	D	701	DG2	O13-P6-O5	7.57	126.89	106.73
5	D	701	DG2	P6-O5-C4	7.34	138.50	118.30
3	A	143	HEM	CAD-CBD-CGD	7.32	129.36	113.60
5	D	701	DG2	P1-O2-C3	-7.30	106.30	123.04
3	D	691	HEM	O1D-CGD-CBD	-6.94	100.79	123.08
5	D	701	DG2	O14-P6-O5	-6.46	89.54	106.73
3	D	691	HEM	O2D-CGD-O1D	6.33	139.07	123.30
3	C	543	HEM	CMA-C3A-C4A	-5.47	120.05	128.46
3	A	143	HEM	CHB-C1B-NB	5.29	130.92	124.38
3	C	543	HEM	O2D-CGD-O1D	5.14	136.12	123.30
3	C	543	HEM	O1D-CGD-CBD	-5.01	106.98	123.08
3	D	691	HEM	CMA-C3A-C4A	-4.82	121.05	128.46
3	B	291	HEM	CBA-CAA-C2A	-4.82	104.40	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	143	HEM	CHA-C4D-ND	-4.62	118.67	124.38
3	B	291	HEM	O2A-CGA-O1A	4.28	133.96	123.30
3	C	543	HEM	CMB-C2B-C1B	-4.18	118.67	125.04
3	A	143	HEM	CMB-C2B-C1B	-4.03	118.90	125.04
3	C	543	HEM	CMA-C3A-C2A	3.99	132.47	124.94
3	C	543	HEM	C4C-CHD-C1D	-3.93	117.37	122.56
3	B	291	HEM	C4B-CHC-C1C	3.90	127.71	122.56
3	A	143	HEM	CHA-C4D-C3D	3.89	132.62	125.33
3	D	691	HEM	CHD-C1D-ND	3.67	128.42	124.43
3	D	691	HEM	CMA-C3A-C2A	3.60	131.72	124.94
3	A	143	HEM	O2A-CGA-O1A	3.58	132.23	123.30
3	D	691	HEM	C3D-C4D-ND	-3.44	106.33	110.17
3	A	143	HEM	O2D-CGD-O1D	3.40	131.78	123.30
3	A	143	HEM	CBB-CAB-C3B	3.38	144.46	127.62
3	C	543	HEM	C4B-CHC-C1C	-3.30	118.21	122.56
3	D	691	HEM	CBA-CAA-C2A	-3.25	107.08	112.62
3	B	291	HEM	CMA-C3A-C4A	-3.15	123.62	128.46
3	B	291	HEM	CHD-C1D-ND	3.12	127.82	124.43
3	A	143	HEM	C3B-C2B-C1B	3.04	108.74	106.49
3	D	691	HEM	CHA-C4D-ND	3.03	128.12	124.38
5	D	701	DG2	O8-C7-O7	-3.01	117.25	124.09
3	C	543	HEM	CBA-CAA-C2A	2.97	117.69	112.62
3	D	691	HEM	CAD-CBD-CGD	-2.93	107.30	113.60
3	C	543	HEM	C3B-C2B-C1B	2.82	108.58	106.49
3	C	543	HEM	O1A-CGA-CBA	-2.80	114.08	123.08
3	C	543	HEM	CHB-C1B-NB	2.78	127.82	124.38
3	D	691	HEM	CHB-C1B-NB	2.77	127.80	124.38
5	D	701	DG2	O8-C7-C3	2.73	120.83	113.03
3	B	291	HEM	CMD-C2D-C1D	-2.73	120.88	125.04
3	A	143	HEM	C4D-C3D-C2D	2.73	110.87	106.90
3	A	143	HEM	CBA-CAA-C2A	2.67	117.17	112.62
3	A	143	HEM	C1D-C2D-C3D	-2.64	104.18	106.96
3	B	291	HEM	C4B-C3B-C2B	2.46	109.07	107.11
3	A	143	HEM	CHD-C1D-C2D	-2.45	121.15	124.98
3	D	691	HEM	C4D-C3D-C2D	2.42	110.43	106.90
3	A	143	HEM	O1A-CGA-CBA	-2.42	115.30	123.08
3	D	691	HEM	CAD-C3D-C2D	-2.42	123.38	127.88
3	A	143	HEM	O1D-CGD-CBD	-2.39	115.39	123.08
3	A	143	HEM	CMD-C2D-C1D	2.38	128.66	125.04
5	D	701	DG2	O10-P1-O9	-2.37	98.60	107.64
3	D	691	HEM	O2A-CGA-O1A	2.34	129.13	123.30
3	D	691	HEM	CBD-CAD-C3D	-2.34	106.14	112.63

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	143	HEM	CHB-C1B-C2B	-2.30	120.36	126.72
3	A	143	HEM	CMA-C3A-C4A	2.26	131.94	128.46
3	D	691	HEM	C4D-ND-C1D	2.24	107.39	105.07
3	B	291	HEM	CMA-C3A-C2A	2.24	129.16	124.94
3	C	543	HEM	CHD-C1D-ND	2.18	126.80	124.43
3	A	143	HEM	C2D-C1D-ND	2.15	112.45	109.88
3	C	543	HEM	CHC-C4B-NB	2.10	126.71	124.43
3	B	291	HEM	CHC-C4B-C3B	2.10	127.78	124.57
5	D	701	DG2	O10-P1-O2	2.06	115.22	105.99
3	C	543	HEM	O2A-CGA-CBA	2.00	120.46	114.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	701	DG2	C3

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	701	DG2	C7-C3-C4-O5
5	D	701	DG2	C7-C3-O2-P1
5	D	701	DG2	O2-C3-C7-O7
5	D	701	DG2	C3-C4-O5-P6
5	D	701	DG2	C4-O5-P6-O15
5	D	701	DG2	C4-O5-P6-O14
5	D	701	DG2	O2-C3-C7-O8
3	B	291	HEM	C4B-C3B-CAB-CBB
3	C	543	HEM	C4D-C3D-CAD-CBD
3	D	691	HEM	CAD-CBD-CGD-O1D
3	D	691	HEM	CAD-CBD-CGD-O2D
3	A	143	HEM	CAA-CBA-CGA-O1A
3	C	543	HEM	CAD-CBD-CGD-O1D
3	A	143	HEM	CAA-CBA-CGA-O2A
3	C	543	HEM	CAA-CBA-CGA-O2A
3	C	543	HEM	CAD-CBD-CGD-O2D
3	C	543	HEM	C2D-C3D-CAD-CBD
3	C	543	HEM	CAA-CBA-CGA-O1A
3	B	291	HEM	CAD-CBD-CGD-O2D
3	B	291	HEM	CAD-CBD-CGD-O1D
3	D	691	HEM	CAA-CBA-CGA-O2A
3	D	691	HEM	CAA-CBA-CGA-O1A

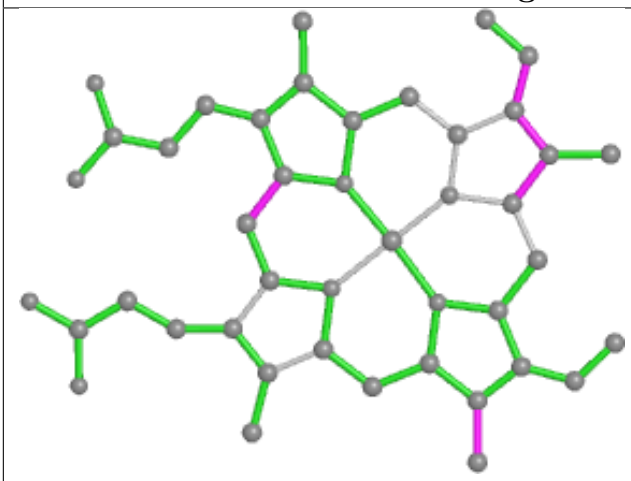
There are no ring outliers.

4 monomers are involved in 22 short contacts:

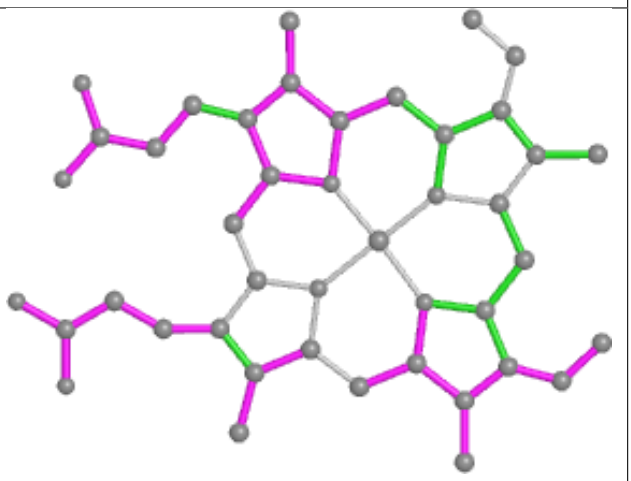
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	143	HEM	2	0
5	D	701	DG2	2	0
3	D	691	HEM	12	0
3	B	291	HEM	6	0

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.

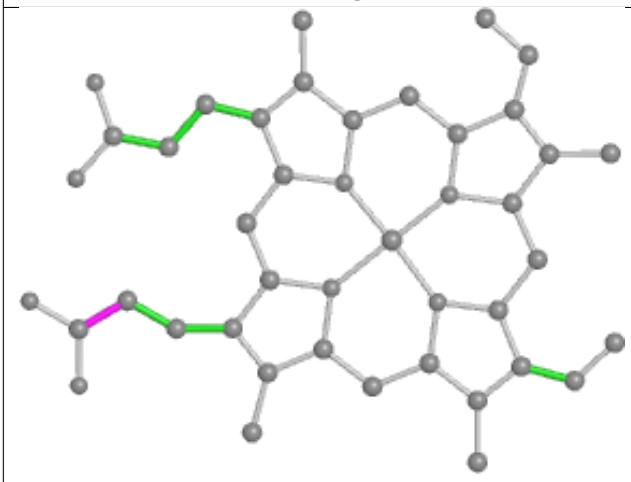
Ligand HEM A 143



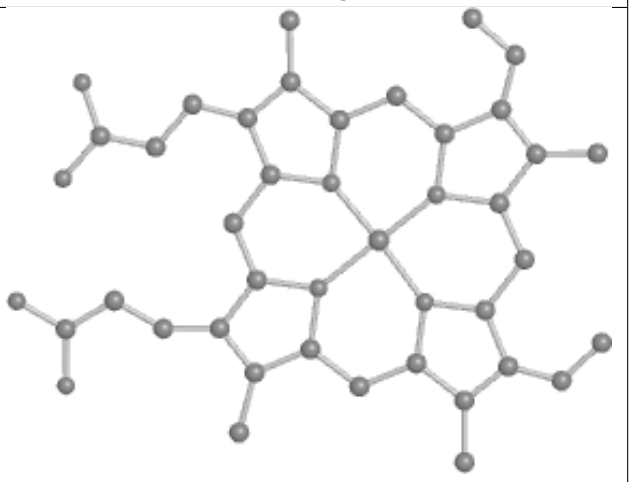
Bond lengths



Bond angles

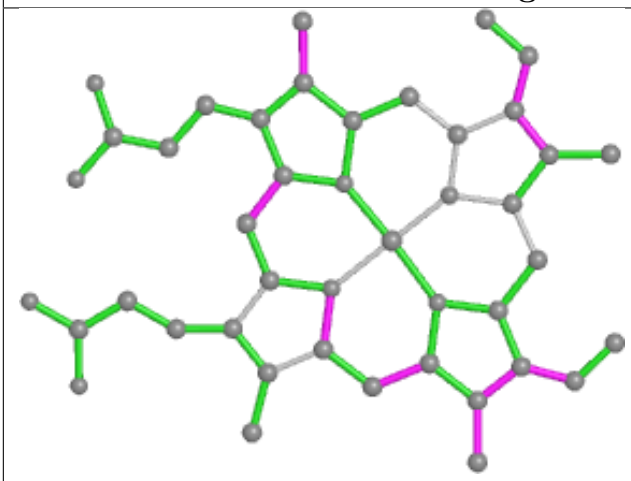


Torsions

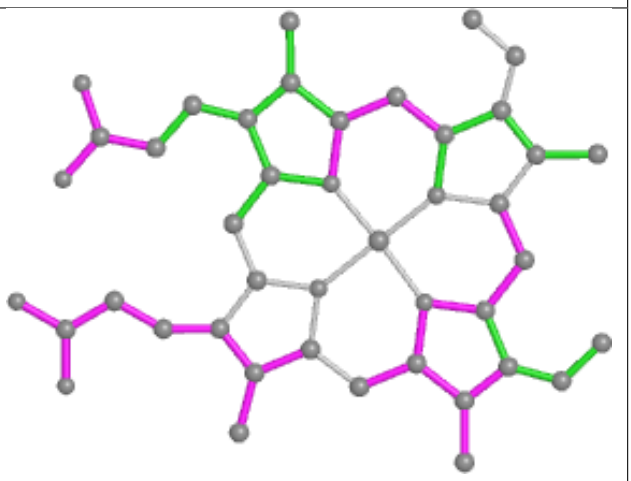


Rings

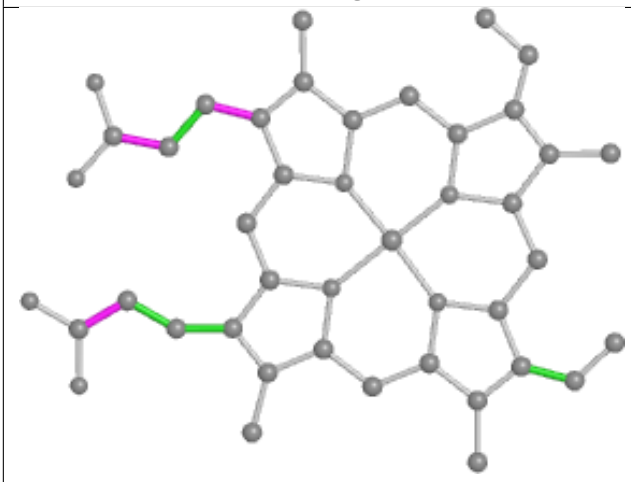
Ligand HEM C 543



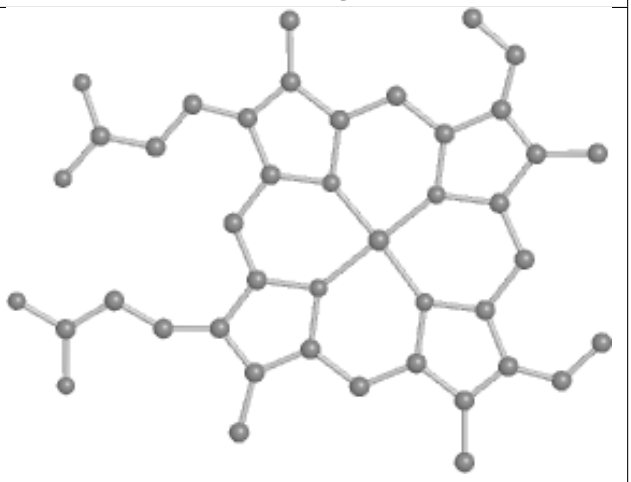
Bond lengths



Bond angles

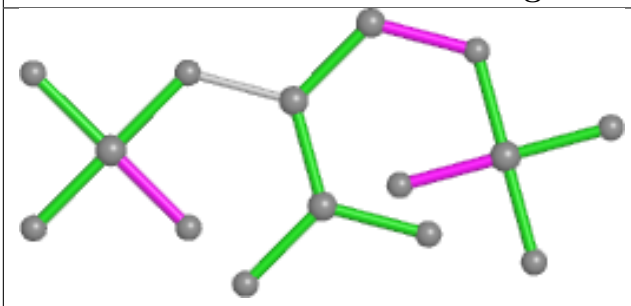


Torsions

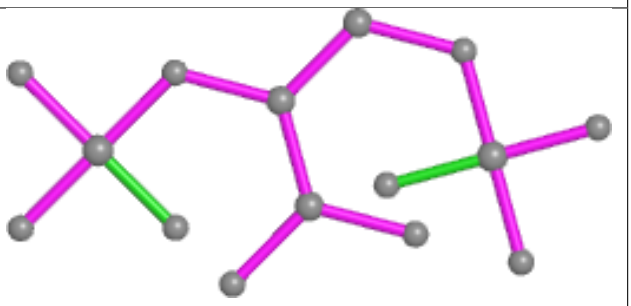


Rings

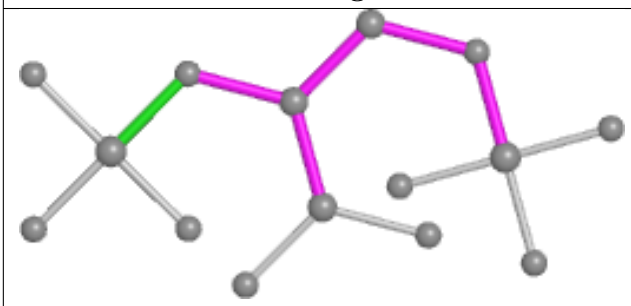
Ligand DG2 D 701



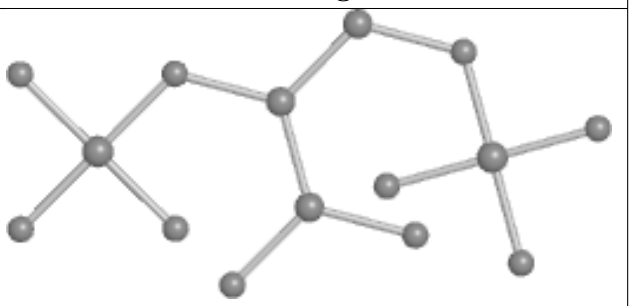
Bond lengths



Bond angles

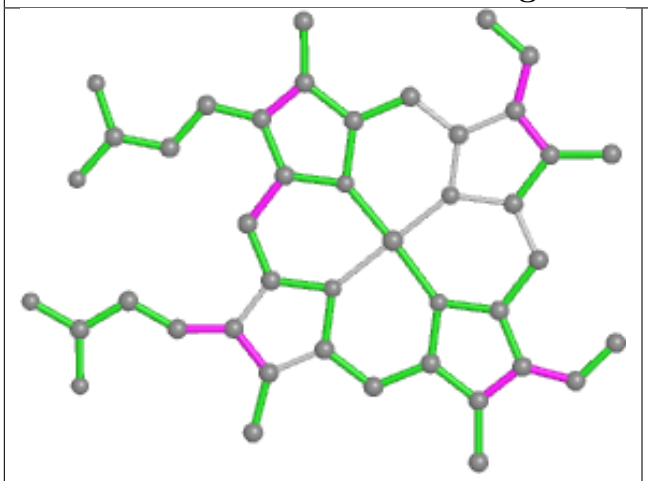


Torsions

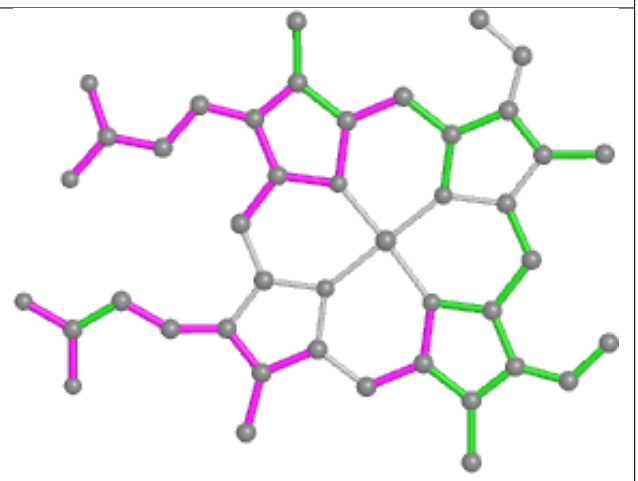


Rings

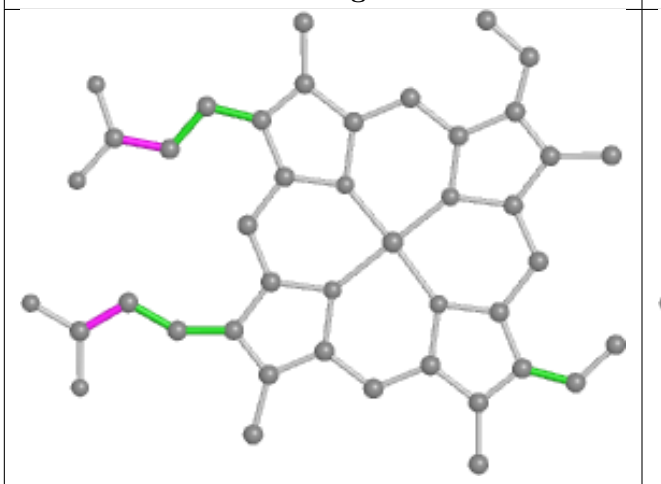
Ligand HEM D 691



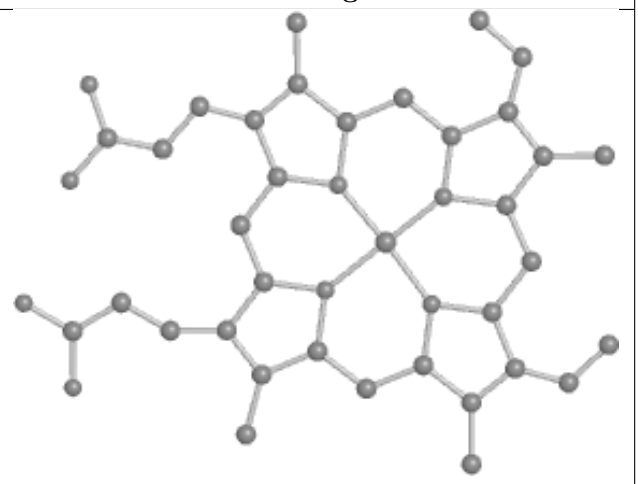
Bond lengths



Bond angles

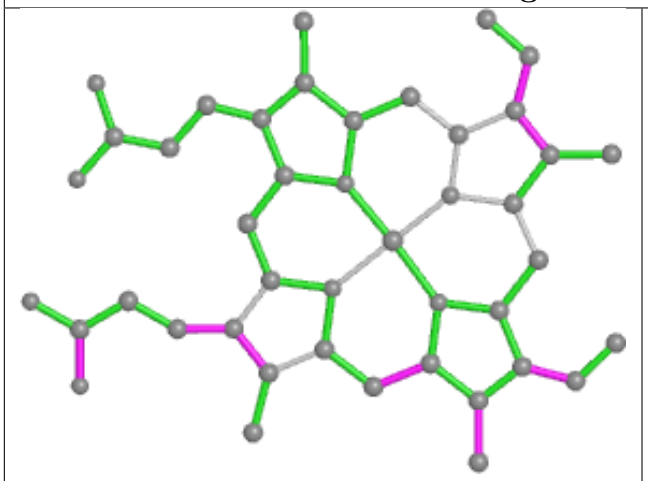


Torsions

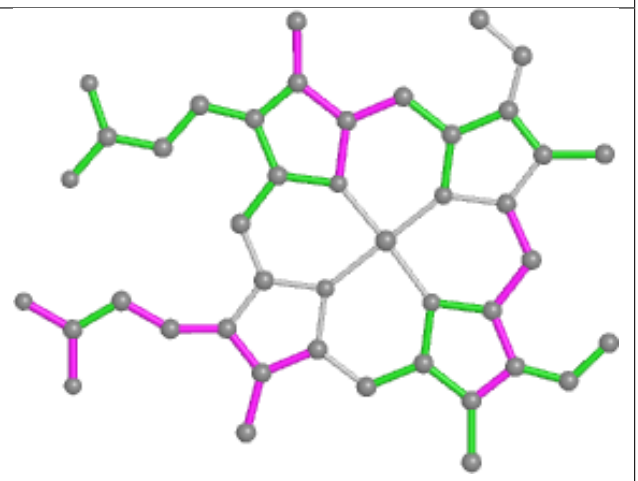


Rings

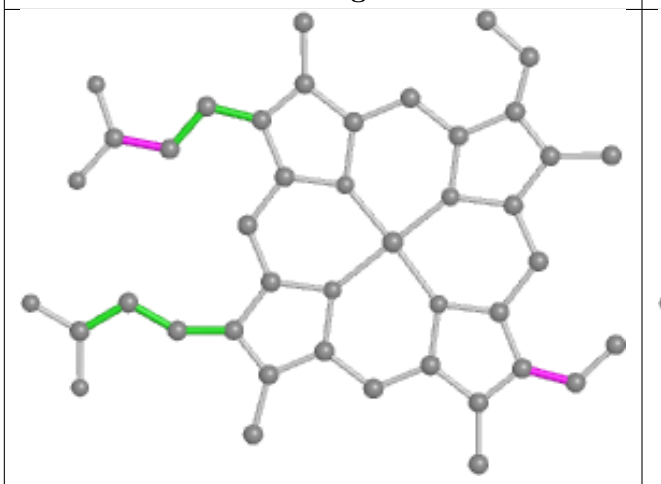
Ligand HEM B 291



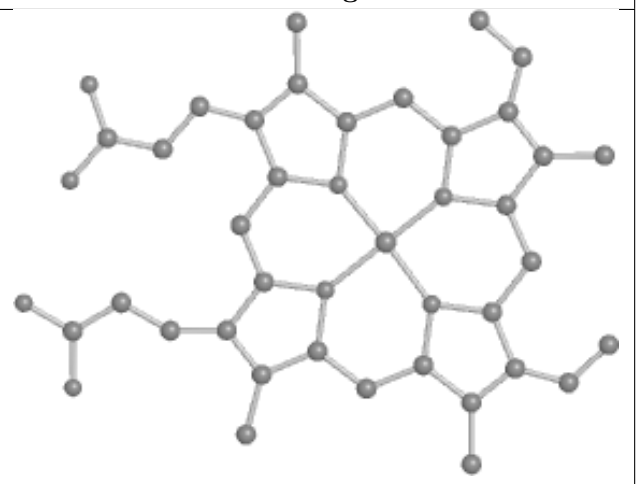
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.