Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2021 – 02:10 PM EST

PDB ID	:	2MTA
Title	:	CRYSTAL STRUCTURE OF A TERNARY ELECTRON TRANSFER COMPLEX BETWEEN METHYLAMINE DEHYDROGENASE, AMICYANIN AND A C-TYPE CYTOCHROME
Authors	:	Chen, L.; Mathews, F.S.
Deposited on	:	1993-10-26
Resolution	:	2.40 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:

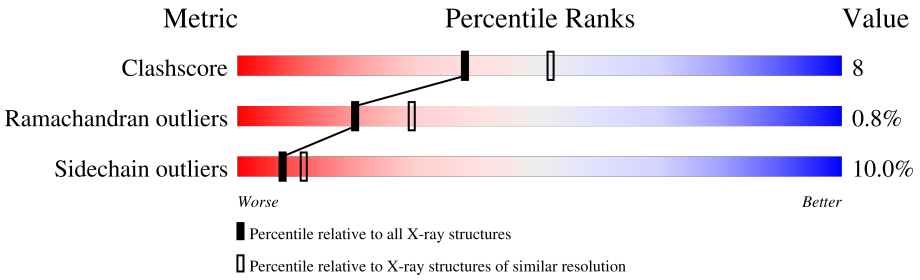
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	H	373	70% 24% 6% ·
2	L	125	76% 18% 6%
3	A	105	76% 21% ·
4	C	147	67% 21% 10% ·

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	PO4	H	0	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5981 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 METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	373	Total	C	N	O	S	0	0	0
			2899	1840	498	553	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	299	PHE	LEU	conflict	UNP P29894

- Molecule 2 is a protein called METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	57	TRQ	TRP	conflict	UNP P22619

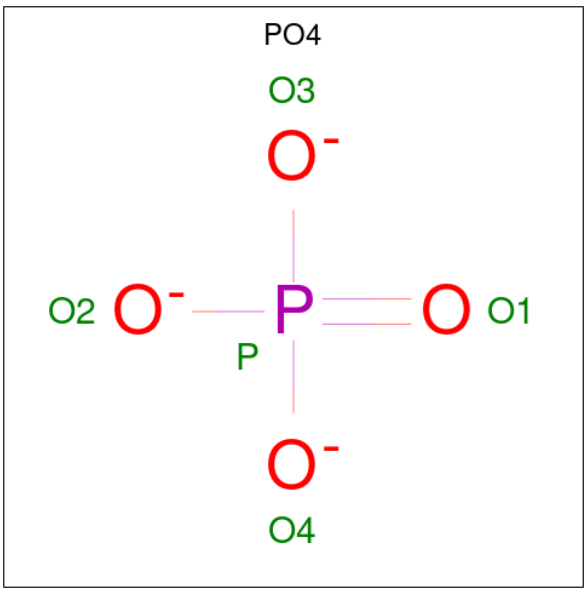
- Molecule 3 is a protein called AMICYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	105	Total	C	N	O	S	0	0	0
			807	516	133	152	6			

- Molecule 4 is a protein called CYTOCHROME C551I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	147	Total	C	N	O	S	0	0	0
			1145	724	182	231	8			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

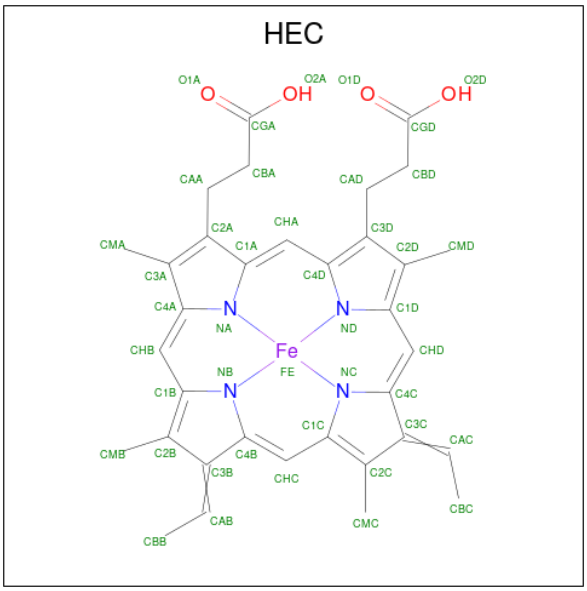


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total O P 3 2 1	0	0

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cu 1 1	0	0

- Molecule 7 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	73	Total	O	0	0
			73	73		
8	L	17	Total	O	0	0
			17	17		
8	A	14	Total	O	0	0
			14	14		
8	C	23	Total	O	0	0
			23	23		

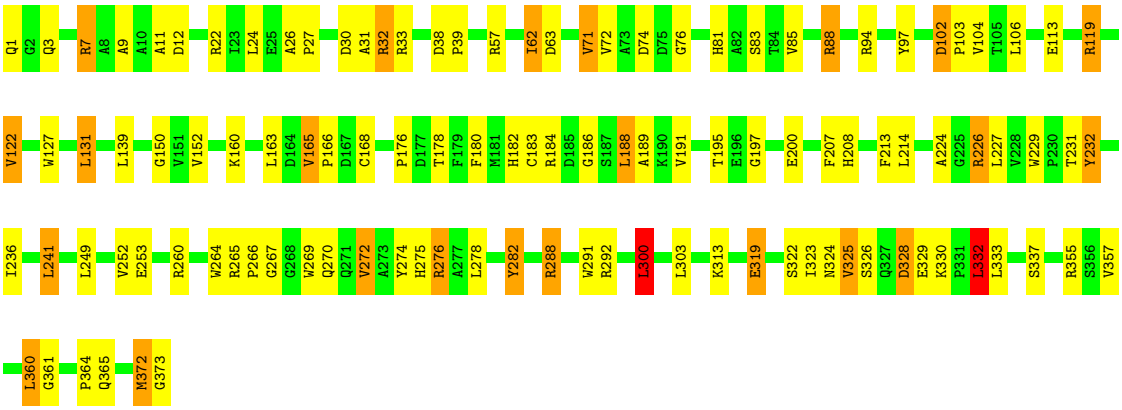
3 Residue-property plots (i)

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.

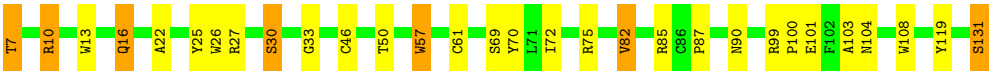
• Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)

Chain H:



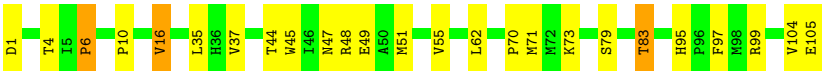
• Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

Chain L:



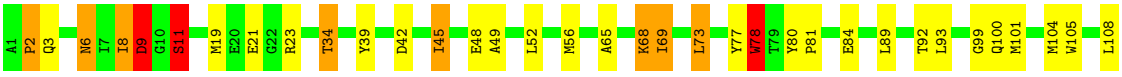
• Molecule 3: AMICYANIN

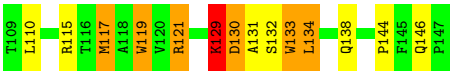
Chain A:



• Molecule 4: CYTOCHROME C551I

Chain C:




T109
L110
R115
T116
M117
A118
W119
V120
R121
K129
D130
A131
S132
W133
L134
Q138
P144
F145
Q146
P147

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	148.81Å 68.85Å 187.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5981	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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: TRQ, PO4, CU, HEC

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	H	1.05	0/2976	1.84	69/4055 (1.7%)
2	L	1.04	0/964	1.87	20/1315 (1.5%)
3	A	1.04	0/828	1.79	14/1124 (1.2%)
4	C	1.05	1/1180 (0.1%)	1.92	34/1605 (2.1%)
All	All	1.05	1/5948 (0.0%)	1.85	137/8099 (1.7%)

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	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	78	TRP	CG-CD2	-5.24	1.34	1.43

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	119	ARG	NE-CZ-NH1	17.03	128.82	120.30
4	C	117	MET	CG-SD-CE	-15.17	75.93	100.20
1	H	119	ARG	NE-CZ-NH2	-13.32	113.64	120.30
2	L	10	ARG	NE-CZ-NH2	-13.21	113.70	120.30
3	A	99	ARG	NE-CZ-NH1	12.48	126.54	120.30
4	C	121	ARG	NE-CZ-NH1	12.29	126.45	120.30
2	L	75	ARG	NE-CZ-NH2	-11.95	114.33	120.30
3	A	99	ARG	NE-CZ-NH2	-11.06	114.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	94	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	H	7	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	H	291	TRP	CD1-CG-CD2	9.39	113.81	106.30
1	H	94	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	H	33	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	H	226	ARG	NE-CZ-NH2	-9.10	115.75	120.30
3	A	45	TRP	CD1-CG-CD2	9.04	113.53	106.30
1	H	229	TRP	CD1-CG-CD2	8.93	113.45	106.30
1	H	57	ARG	NE-CZ-NH1	8.78	124.69	120.30
4	C	105	TRP	CD1-CG-CD2	8.63	113.21	106.30
1	H	325	VAL	CG1-CB-CG2	-8.53	97.25	110.90
1	H	274	TYR	CB-CG-CD2	-8.52	115.89	121.00
1	H	288	ARG	NE-CZ-NH1	8.25	124.42	120.30
2	L	75	ARG	CB-CG-CD	-8.21	90.26	111.60
1	H	229	TRP	CE2-CD2-CG	-8.17	100.76	107.30
4	C	105	TRP	CG-CD2-CE3	8.04	141.13	133.90
2	L	10	ARG	NE-CZ-NH1	7.98	124.29	120.30
4	C	121	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	H	291	TRP	CE2-CD2-CG	-7.91	100.97	107.30
4	C	105	TRP	CE2-CD2-CG	-7.91	100.97	107.30
3	A	45	TRP	CE2-CD2-CG	-7.69	101.15	107.30
2	L	13	TRP	CE2-CD2-CE3	7.68	127.91	118.70
2	L	75	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	H	264	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	H	372	MET	CA-C-N	-7.60	100.99	116.20
4	C	119	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	H	71	VAL	CA-CB-CG2	-7.47	99.70	110.90
3	A	45	TRP	CB-CG-CD1	-7.41	117.36	127.00
1	H	269	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	H	241	LEU	CA-CB-CG	7.33	132.17	115.30
2	L	99	ARG	NE-CZ-NH1	7.30	123.95	120.30
3	A	45	TRP	CG-CD2-CE3	7.29	140.47	133.90
4	C	115	ARG	NE-CZ-NH1	7.29	123.95	120.30
2	L	26	TRP	CD1-CG-CD2	7.27	112.12	106.30
3	A	16	VAL	CA-CB-CG2	-7.22	100.07	110.90
2	L	26	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	H	81	HIS	CA-CB-CG	7.19	125.82	113.60
1	H	265	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	H	232	TYR	CB-CG-CD2	-7.14	116.72	121.00
2	L	26	TRP	CB-CG-CD1	-7.10	117.77	127.00
4	C	11	SER	CA-C-O	-7.04	105.31	120.10
1	H	272	VAL	CB-CA-C	-7.02	98.06	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	133	TRP	CD1-CG-CD2	6.91	111.82	106.30
4	C	105	TRP	CB-CG-CD1	-6.90	118.03	127.00
1	H	276	ARG	NE-CZ-NH1	6.88	123.74	120.30
4	C	78	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	H	319	GLU	CA-CB-CG	-6.79	98.47	113.40
1	H	355	ARG	NE-CZ-NH2	-6.76	116.92	120.30
4	C	119	TRP	CD1-CG-CD2	6.75	111.70	106.30
4	C	11	SER	CA-C-N	6.74	135.97	117.10
1	H	127	TRP	CD1-CG-CD2	6.73	111.68	106.30
2	L	13	TRP	CD2-CE3-CZ3	-6.66	110.15	118.80
1	H	102	ASP	CB-CG-OD1	6.63	124.27	118.30
4	C	9	ASP	CB-CG-OD1	6.61	124.25	118.30
1	H	355	ARG	CG-CD-NE	-6.60	97.95	111.80
1	H	184	ARG	NE-CZ-NH1	6.52	123.56	120.30
4	C	9	ASP	N-CA-C	6.47	128.48	111.00
1	H	30	ASP	CB-CG-OD1	6.46	124.11	118.30
4	C	133	TRP	CE2-CD2-CG	-6.38	102.20	107.30
4	C	119	TRP	CG-CD2-CE3	6.34	139.61	133.90
2	L	82	VAL	CB-CA-C	-6.28	99.46	111.40
3	A	45	TRP	CG-CD1-NE1	-6.28	103.82	110.10
4	C	129	LYS	CA-CB-CG	6.27	127.20	113.40
4	C	56	MET	CA-CB-CG	-6.26	102.66	113.30
1	H	122	VAL	CB-CA-C	-6.25	99.53	111.40
4	C	99	GLY	CA-C-N	-6.21	103.55	117.20
4	C	9	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	H	57	ARG	NE-CZ-NH2	-6.15	117.23	120.30
4	C	130	ASP	N-CA-C	-6.09	94.55	111.00
4	C	19	MET	CG-SD-CE	6.08	109.93	100.20
2	L	26	TRP	CG-CD2-CE3	6.07	139.36	133.90
1	H	127	TRP	CE2-CD2-CG	-6.07	102.45	107.30
1	H	269	TRP	CE2-CD2-CG	-6.07	102.45	107.30
1	H	195	THR	N-CA-C	-6.05	94.68	111.00
1	H	152	VAL	CG1-CB-CG2	-6.03	101.25	110.90
4	C	2	PRO	CA-C-N	-5.90	104.22	117.20
1	H	264	TRP	CE2-CD2-CG	-5.88	102.59	107.30
1	H	291	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	H	88	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	H	332	LEU	CA-CB-CG	5.74	128.50	115.30
1	H	63	ASP	CB-CG-OD1	5.73	123.46	118.30
1	H	213	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	H	226	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	H	197	GLY	N-CA-C	-5.71	98.82	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	51	MET	CA-CB-CG	5.69	122.98	113.30
1	H	31	ALA	CB-CA-C	-5.69	101.57	110.10
4	C	34	THR	N-CA-CB	-5.67	99.52	110.30
1	H	328	ASP	CB-CG-OD1	5.62	123.36	118.30
1	H	282	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	H	131	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	H	355	ARG	NE-CZ-NH1	5.59	123.09	120.30
4	C	78	TRP	CE2-CD2-CG	-5.58	102.83	107.30
2	L	13	TRP	CD1-CG-CD2	5.58	110.76	106.30
1	H	33	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	H	71	VAL	CA-CB-CG1	5.50	119.15	110.90
1	H	72	VAL	CA-CB-CG2	-5.48	102.67	110.90
2	L	13	TRP	CE2-CD2-CG	-5.48	102.91	107.30
1	H	292	ARG	NE-CZ-NH2	-5.47	117.56	120.30
4	C	2	PRO	N-CA-C	5.47	126.32	112.10
4	C	101	MET	CG-SD-CE	-5.46	91.46	100.20
1	H	104	VAL	CG1-CB-CG2	-5.37	102.31	110.90
4	C	105	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	H	252	VAL	N-CA-CB	-5.34	99.75	111.50
3	A	83	THR	CA-CB-CG2	-5.33	104.94	112.40
1	H	229	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	H	357	VAL	N-CA-C	-5.29	96.70	111.00
4	C	131	ALA	N-CA-C	-5.29	96.71	111.00
2	L	13	TRP	CG-CD2-CE3	-5.26	129.16	133.90
4	C	2	PRO	CA-N-CD	-5.25	104.14	111.50
1	H	224	ALA	CA-C-N	5.23	126.66	116.20
1	H	373	GLY	N-CA-C	-5.22	100.04	113.10
1	H	119	ARG	CD-NE-CZ	5.22	130.90	123.60
1	H	11	ALA	N-CA-CB	-5.21	102.80	110.10
2	L	10	ARG	CB-CG-CD	-5.19	98.11	111.60
4	C	133	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	H	300	LEU	CA-CB-CG	-5.17	103.42	115.30
3	A	105	GLU	CA-CB-CG	5.15	124.72	113.40
3	A	73	LYS	N-CA-CB	-5.15	101.34	110.60
1	H	165	VAL	N-CA-CB	-5.12	100.24	111.50
1	H	22	ARG	NE-CZ-NH2	-5.11	117.75	120.30
4	C	9	ASP	CB-CA-C	-5.09	100.22	110.40
2	L	7	THR	CA-C-N	5.08	128.37	117.20
2	L	26	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	H	360	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	H	291	TRP	CB-CG-CD1	-5.04	120.44	127.00
1	H	337	SER	N-CA-CB	-5.04	102.93	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	70	TYR	CB-CG-CD2	-5.03	117.98	121.00
3	A	55	VAL	CB-CA-C	-5.02	101.86	111.40
3	A	48	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	C	146	GLN	Peptide
4	C	77	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	H	2899	0	2792	41	0
2	L	956	0	857	15	0
3	A	807	0	794	9	0
4	C	1145	0	1038	25	0
5	H	3	0	0	0	2
6	A	1	0	0	0	0
7	C	43	0	30	4	0
8	A	14	0	0	0	0
8	C	23	0	0	3	0
8	H	73	0	0	4	0
8	L	17	0	0	2	0
All	All	5981	0	5511	87	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 8.

All (87) 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)
3:A:4:THR:O	3:A:6:PRO:HD3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:282:TYR:HB3	1:H:300:LEU:HD21	1.73	0.69
4:C:34:THR:HB	8:C:220:HOH:O	1.93	0.68
4:C:65:ALA:HB1	4:C:73:LEU:HB2	1.76	0.67
1:H:325:VAL:HG12	1:H:326:SER:O	1.93	0.67
4:C:68:LYS:HD2	4:C:69:ILE:HD13	1.77	0.67
1:H:270:GLN:HB2	1:H:322:SER:HB3	1.77	0.67
1:H:39:PRO:HG3	1:H:365:GLN:HE21	1.61	0.64
1:H:275:HIS:CD2	1:H:278:LEU:H	2.16	0.63
2:L:69:SER:HB2	2:L:131:SER:HA	1.81	0.62
1:H:85:VAL:HA	8:H:414:HOH:O	1.99	0.62
4:C:8:ILE:HG12	4:C:9:ASP:H	1.65	0.60
1:H:76:GLY:HA2	8:H:431:HOH:O	2.01	0.60
1:H:253:GLU:HG2	1:H:260:ARG:NH2	2.17	0.59
1:H:119:ARG:HD2	8:H:403:HOH:O	2.01	0.59
1:H:182:HIS:NE2	1:H:208:HIS:HE1	2.02	0.58
1:H:214:LEU:HD12	1:H:231:THR:HG22	1.86	0.58
1:H:188:LEU:HD13	1:H:207:PHE:CE1	2.39	0.57
8:L:142:HOH:O	3:A:71:MET:HE2	2.03	0.57
4:C:8:ILE:O	4:C:9:ASP:HB2	2.04	0.57
2:L:57:TRQ:HB2	2:L:108:TRP:NE1	2.20	0.57
4:C:93:LEU:HD12	4:C:117:MET:CE	2.35	0.57
4:C:134:LEU:HG	4:C:138:GLN:HB3	1.85	0.57
1:H:83:SER:HB3	1:H:97:TYR:CZ	2.41	0.56
1:H:300:LEU:HD11	1:H:323:ILE:HD13	1.88	0.56
4:C:42:ASP:HB3	4:C:45:ILE:HB	1.89	0.55
1:H:166:PRO:HG2	1:H:168:CYS:SG	2.47	0.54
1:H:188:LEU:HD13	1:H:207:PHE:HE1	1.74	0.52
4:C:49:ALA:HB1	4:C:119:TRP:HB2	1.91	0.52
4:C:129:LYS:HD2	4:C:130:ASP:N	2.25	0.51
4:C:93:LEU:HD12	4:C:117:MET:HE2	1.91	0.51
1:H:182:HIS:NE2	1:H:208:HIS:CE1	2.79	0.51
4:C:39:TYR:HB3	4:C:45:ILE:HG21	1.94	0.50
2:L:46:CYS:HB3	2:L:50:THR:OG1	2.12	0.50
1:H:275:HIS:HE1	1:H:328:ASP:O	1.94	0.50
1:H:38:ASP:HA	1:H:364:PRO:HA	1.93	0.49
2:L:108:TRP:HA	2:L:108:TRP:CE3	2.47	0.49
2:L:100:PRO:HG2	3:A:97:PHE:HE1	1.77	0.49
1:H:32:ARG:HH21	1:H:332:LEU:HD13	1.78	0.49
1:H:74:ASP:O	1:H:372:MET:HG2	2.12	0.49
2:L:57:TRQ:HB2	2:L:108:TRP:HE1	1.77	0.49
4:C:133:TRP:CD1	4:C:134:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:GLN:O	1:H:7:ARG:HG2	2.13	0.49
2:L:101:GLU:HB3	3:A:95:HIS:CD2	2.47	0.48
4:C:6:ASN:HA	8:C:212:HOH:O	2.12	0.48
1:H:32:ARG:HE	1:H:332:LEU:HD22	1.79	0.47
1:H:186:GLY:HA2	1:H:208:HIS:CE1	2.50	0.47
1:H:253:GLU:HG3	8:H:413:HOH:O	2.14	0.47
2:L:103:ALA:HB1	8:L:136:HOH:O	2.14	0.47
1:H:26:ALA:HA	1:H:27:PRO:HD2	1.70	0.46
4:C:6:ASN:HD21	4:C:8:ILE:HD13	1.80	0.46
4:C:100:GLN:HB3	7:C:200:HEC:HBC2	1.97	0.46
1:H:139:LEU:HA	1:H:150:GLY:O	2.16	0.46
3:A:37:VAL:CG2	3:A:104:VAL:HG22	2.46	0.46
1:H:178:THR:HA	1:H:191:VAL:O	2.15	0.45
1:H:88:ARG:HD3	1:H:88:ARG:HA	1.82	0.45
4:C:23:ARG:HB3	4:C:110:LEU:HD22	1.98	0.45
1:H:267:GLY:HA3	1:H:288:ARG:CZ	2.47	0.45
4:C:11:SER:HB3	8:C:210:HOH:O	2.16	0.45
1:H:9:ALA:O	1:H:12:ASP:HB2	2.16	0.45
3:A:16:VAL:HG21	3:A:44:THR:HG21	1.98	0.45
2:L:61:CYS:SG	2:L:72:ILE:HG13	2.57	0.44
1:H:62:ILE:HD11	1:H:106:LEU:HG	1.99	0.44
4:C:92:THR:HG21	7:C:200:HEC:HMA2	1.99	0.44
1:H:180:PHE:HA	1:H:189:ALA:O	2.18	0.43
2:L:61:CYS:O	2:L:69:SER:HA	2.17	0.43
4:C:78:TRP:HB3	4:C:80:TYR:O	2.18	0.43
1:H:168:CYS:HA	1:H:183:CYS:HA	2.00	0.43
1:H:275:HIS:HD2	1:H:278:LEU:H	1.63	0.43
1:H:324:ASN:OD1	1:H:325:VAL:N	2.50	0.43
4:C:133:TRP:HD1	4:C:134:LEU:HD13	1.83	0.42
2:L:16:GLN:NE2	2:L:22:ALA:HB3	2.35	0.42
4:C:104:MET:CE	7:C:200:HEC:HBB2	2.50	0.42
1:H:232:TYR:O	1:H:266:PRO:HD2	2.19	0.42
3:A:47:ASN:ND2	3:A:49:GLU:H	2.18	0.42
4:C:8:ILE:HG12	4:C:9:ASP:N	2.33	0.42
4:C:93:LEU:HD21	7:C:200:HEC:HMB2	2.01	0.41
1:H:319:GLU:CD	2:L:10:ARG:HH22	2.23	0.41
1:H:236:ILE:HG21	1:H:236:ILE:HD13	1.82	0.41
3:A:10:PRO:HD3	3:A:70:PRO:HB2	2.03	0.41
2:L:25:TYR:CE2	2:L:27:ARG:HG3	2.55	0.41
1:H:330:LYS:HD2	1:H:330:LYS:HA	1.75	0.41
2:L:30:SER:HA	2:L:90:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:33:GLY:HA3	2:L:119:TYR:OH	2.21	0.41
3:A:62:LEU:HD23	3:A:62:LEU:HA	1.85	0.41
1:H:38:ASP:OD2	1:H:361:GLY:HA3	2.20	0.40
4:C:80:TYR:HA	4:C:81:PRO:HD3	1.89	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)
5:H:0:PO4:P	5:H:0:PO4:O2[4_555]	1.52	0.68
5:H:0:PO4:P	5:H:0:PO4:O3[4_555]	1.52	0.68

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	H	371/373 (100%)	348 (94%)	23 (6%)	0	100	100
2	L	122/125 (98%)	110 (90%)	12 (10%)	0	100	100
3	A	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
4	C	145/147 (99%)	128 (88%)	11 (8%)	6 (4%)	3	2
All	All	741/750 (99%)	683 (92%)	52 (7%)	6 (1%)	19	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	11	SER
4	C	3	GLN
4	C	9	ASP
4	C	21	GLU
4	C	68	LYS

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Mol	Chain	Res	Type
4	C	129	LYS

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	H	301/301 (100%)	272 (90%)	29 (10%)	8 12
2	L	104/104 (100%)	96 (92%)	8 (8%)	13 20
3	A	85/85 (100%)	80 (94%)	5 (6%)	19 32
4	C	118/118 (100%)	99 (84%)	19 (16%)	2 3
All	All	608/608 (100%)	547 (90%)	61 (10%)	7 11

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	H	24	LEU
1	H	32	ARG
1	H	62	ILE
1	H	71	VAL
1	H	102	ASP
1	H	103	PRO
1	H	113	GLU
1	H	122	VAL
1	H	131	LEU
1	H	160	LYS
1	H	163	LEU
1	H	165	VAL
1	H	176	PRO
1	H	188	LEU
1	H	200	GLU
1	H	226	ARG
1	H	227	LEU
1	H	241	LEU
1	H	249	LEU

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Mol	Chain	Res	Type
1	H	272	VAL
1	H	276	ARG
1	H	300	LEU
1	H	303	LEU
1	H	313	LYS
1	H	329	GLU
1	H	332	LEU
1	H	333	LEU
1	H	360	LEU
2	L	7	THR
2	L	16	GLN
2	L	30	SER
2	L	82	VAL
2	L	85	ARG
2	L	87	PRO
2	L	104	ASN
2	L	131	SER
3	A	1	ASP
3	A	6	PRO
3	A	35	LEU
3	A	79	SER
3	A	83	THR
4	C	2	PRO
4	C	6	ASN
4	C	8	ILE
4	C	9	ASP
4	C	11	SER
4	C	45	ILE
4	C	48	GLU
4	C	52	LEU
4	C	69	ILE
4	C	73	LEU
4	C	78	TRP
4	C	84	GLU
4	C	89	LEU
4	C	108	LEU
4	C	121	ARG
4	C	129	LYS
4	C	132	SER
4	C	134	LEU
4	C	144	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	H	69	ASN
1	H	170	HIS
1	H	208	HIS
1	H	222	GLN
1	H	271	GLN
1	H	275	HIS
1	H	318	HIS
1	H	365	GLN
2	L	104	ASN
3	A	47	ASN
4	C	6	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
2	TRQ	L	57	2	13,17,18	4.57	4 (30%)	14,24,26	3.36	9 (64%)

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
2	TRQ	L	57	2	-	0/4/19/21	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	57	TRQ	CH2-CZ2	-13.38	1.39	1.54
2	L	57	TRQ	CE2-CZ2	-7.31	1.40	1.50
2	L	57	TRQ	CD1-NE1	-4.29	1.29	1.36
2	L	57	TRQ	CZ3-CH2	-3.19	1.37	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	57	TRQ	CB-CG-CD1	-7.75	118.39	127.97
2	L	57	TRQ	CG-CB-CA	5.83	123.53	114.53
2	L	57	TRQ	O7-CZ2-CH2	4.04	123.76	119.00
2	L	57	TRQ	O6-CH2-CZ2	3.24	120.71	118.51
2	L	57	TRQ	CE3-CZ3-CH2	2.91	123.28	121.08
2	L	57	TRQ	CE2-CD2-CE3	-2.66	115.84	119.15
2	L	57	TRQ	CZ3-CH2-CZ2	2.41	122.01	118.72
2	L	57	TRQ	O6-CH2-CZ3	-2.35	117.26	121.51
2	L	57	TRQ	CD2-CE2-NE1	2.09	113.02	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	57	TRQ	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	HEC	C	200	4	26,50,50	1.53	3 (11%)	18,82,82	2.11	9 (50%)
5	PO4	H	0	-	0,2,4	0.00	-	0,1,6	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEC	C	200	4	-	0/6/54/54	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	200	HEC	C3B-C2B	-5.30	1.35	1.40
7	C	200	HEC	C3C-C2C	-3.86	1.36	1.40
7	C	200	HEC	C1D-ND	2.35	1.41	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	200	HEC	CMB-C2B-C3B	3.65	130.11	125.82
7	C	200	HEC	C1D-C2D-C3D	-3.47	104.58	107.00
7	C	200	HEC	CMB-C2B-C1B	-3.21	123.53	128.46
7	C	200	HEC	CMC-C2C-C1C	-3.20	123.54	128.46
7	C	200	HEC	CMA-C3A-C2A	2.71	130.06	124.94
7	C	200	HEC	CAA-CBA-CGA	2.57	116.98	112.67
7	C	200	HEC	C4C-C3C-C2C	-2.44	103.72	106.35
7	C	200	HEC	CBA-CAA-C2A	-2.24	108.35	112.48
7	C	200	HEC	CBD-CAD-C3D	2.19	116.53	112.49

There are no chirality outliers.

There are no torsion outliers.

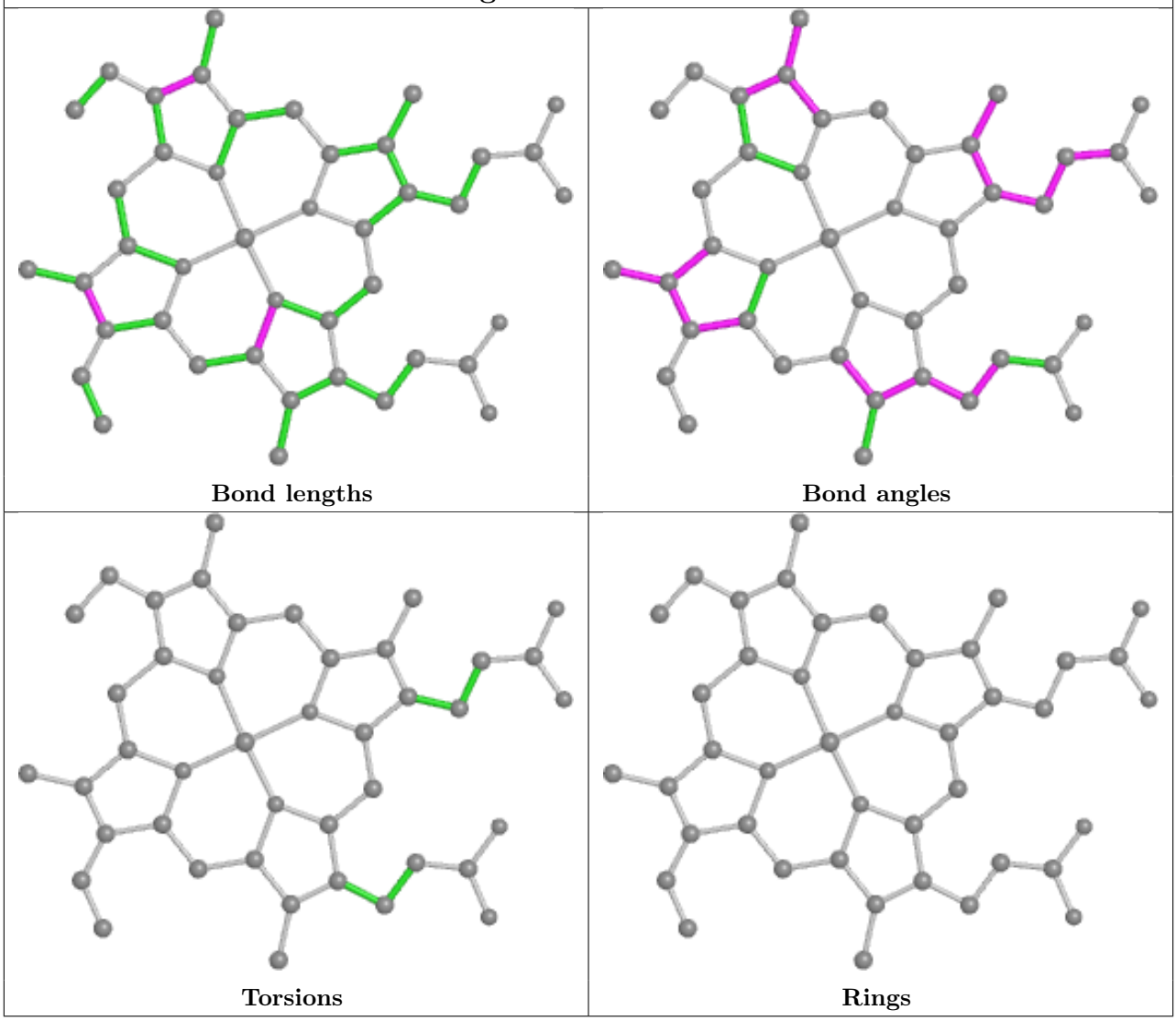
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	200	HEC	4	0
5	H	0	PO4	0	2

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 200



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.