



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:19 PM EDT

PDB ID : 2MTA / pdb_00002mta
Title : CRYSTAL STRUCTURE OF A TERNARY ELECTRON TRANSFER COM-
PLEX 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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

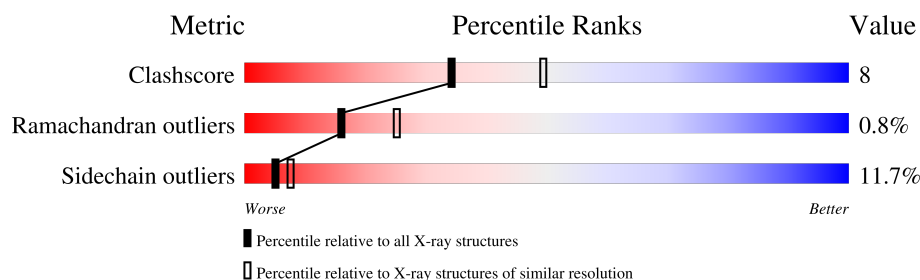
1 Overall quality at a glance

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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	373	
2	L	125	
3	A	105	
4	C	147	

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	-
7	HEC	C	200	X	-	-	-

2 Entry composition

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

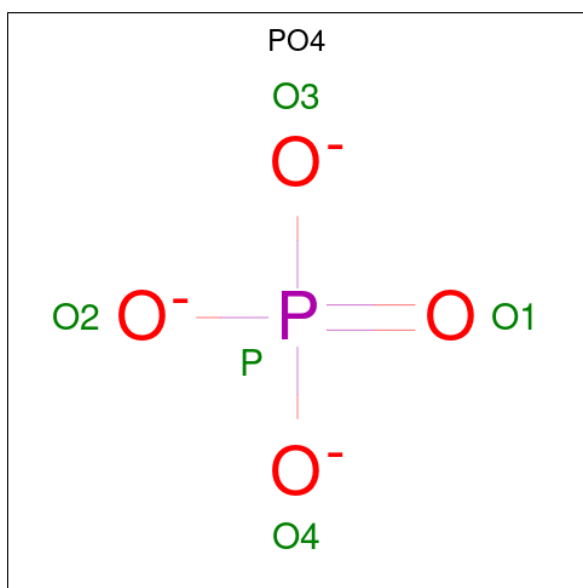
- Molecule 3 is a protein called AMICYANIN.

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 (CCD ID: PO4) (formula: O_4P).

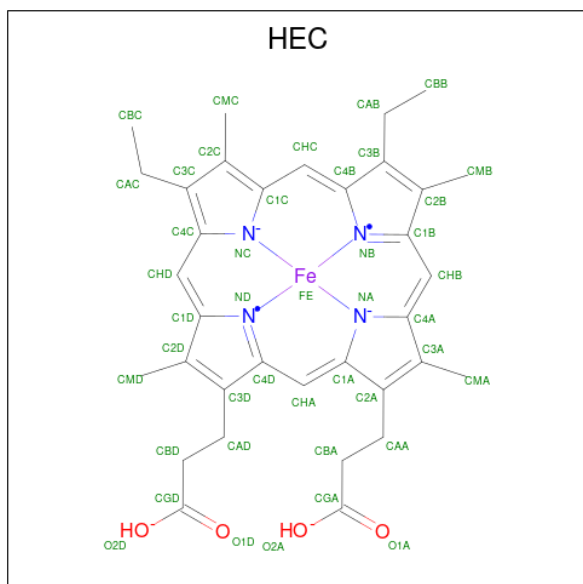


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	O	P	0	0
			3	2	1		

- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

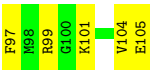
- Molecule 7 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



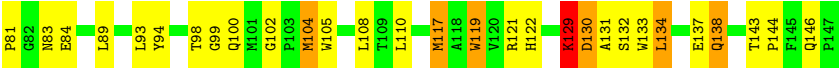
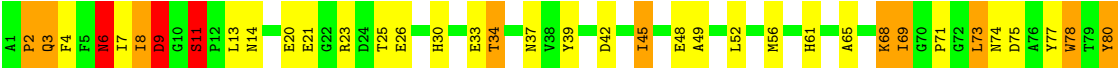
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 8 is water.

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



● Molecule 4: CYTOCHROME C551I



4 Data and refinement statistics

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: CU, HEC, PO4, TRQ

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	1.43	20/2976 (0.7%)	2.12	117/4055 (2.9%)
2	L	1.34	5/964 (0.5%)	2.19	42/1315 (3.2%)
3	A	1.40	13/828 (1.6%)	2.11	34/1124 (3.0%)
4	C	1.29	5/1180 (0.4%)	2.25	59/1605 (3.7%)
All	All	1.38	43/5948 (0.7%)	2.16	252/8099 (3.1%)

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 (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	362	HIS	CD2-NE2	-8.61	1.28	1.37
2	L	107	ILE	CA-CB	8.43	1.62	1.53
1	H	67	LEU	CA-C	8.22	1.59	1.53
1	H	318	HIS	CD2-NE2	-7.42	1.29	1.37
3	A	92	CYS	CA-CB	-7.17	1.43	1.53
3	A	95	HIS	CG-ND1	-7.16	1.30	1.38
1	H	208	HIS	CD2-NE2	-7.09	1.30	1.37
2	L	120	HIS	CD2-NE2	-6.96	1.30	1.37
3	A	91	HIS	CD2-NE2	-6.93	1.30	1.37
3	A	4	THR	CA-CB	6.93	1.64	1.53
2	L	28	HIS	CD2-NE2	-6.60	1.30	1.37
1	H	218	PRO	CA-CB	-6.44	1.44	1.53
1	H	203	HIS	CD2-NE2	-6.43	1.30	1.37
3	A	36	HIS	CD2-NE2	-6.42	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	275	HIS	CD2-NE2	-6.30	1.30	1.37
1	H	362	HIS	CG-ND1	-6.22	1.31	1.38
1	H	293	HIS	CG-ND1	-6.10	1.31	1.38
3	A	53	HIS	CG-ND1	-6.09	1.31	1.38
1	H	81	HIS	CD2-NE2	-6.00	1.31	1.37
1	H	300	LEU	CB-CG	-5.92	1.41	1.53
4	C	30	HIS	CD2-NE2	-5.85	1.31	1.37
4	C	122	HIS	CD2-NE2	-5.83	1.31	1.37
1	H	217	HIS	CD2-NE2	-5.76	1.31	1.37
1	H	182	HIS	CG-ND1	-5.75	1.31	1.38
1	H	149	VAL	CA-C	-5.48	1.46	1.52
1	H	300	LEU	CA-CB	-5.36	1.43	1.53
4	C	98	THR	CA-CB	5.33	1.62	1.53
3	A	56	HIS	CD2-NE2	-5.29	1.32	1.37
3	A	53	HIS	CD2-NE2	-5.21	1.32	1.37
3	A	95	HIS	CD2-NE2	-5.16	1.32	1.37
4	C	30	HIS	CG-ND1	-5.15	1.32	1.38
1	H	314	PHE	CA-CB	-5.13	1.45	1.53
3	A	101	LYS	CA-CB	-5.10	1.45	1.53
1	H	182	HIS	CD2-NE2	-5.09	1.32	1.37
1	H	81	HIS	CG-ND1	-5.09	1.32	1.38
3	A	35	LEU	CA-CB	-5.08	1.45	1.53
3	A	37	VAL	CA-CB	5.06	1.61	1.54
1	H	237	HIS	CD2-NE2	-5.06	1.32	1.37
2	L	26	TRP	NE1-CE2	-5.04	1.31	1.37
1	H	275	HIS	CG-ND1	-5.03	1.32	1.38
2	L	82	VAL	CA-CB	-5.02	1.49	1.54
3	A	91	HIS	CG-ND1	-5.02	1.32	1.38
4	C	78	TRP	CG-CD2	-5.00	1.34	1.43

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	81	HIS	CA-CB-CG	12.02	125.82	113.80
1	H	328	ASP	CA-CB-CG	11.43	124.03	112.60
4	C	117	MET	CG-SD-CE	-11.35	75.93	100.90
4	C	11	SER	CA-C-O	-10.84	105.31	120.16
4	C	138	GLN	OE1-CD-NE2	-10.65	111.95	122.60
1	H	165	VAL	N-CA-CB	-10.57	100.24	111.87
1	H	211	ASP	CA-CB-CG	10.38	122.97	112.60
2	L	45	ASN	OD1-CG-ND2	-10.09	112.52	122.60
1	H	359	GLN	OE1-CD-NE2	-9.88	112.72	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	104	ASN	CA-CB-CG	9.71	122.31	112.60
2	L	75	ARG	CB-CG-CD	-9.15	90.26	111.30
2	L	13	TRP	CE2-CD2-CE3	9.11	127.91	118.80
2	L	24	ASP	CA-CB-CG	8.88	121.47	112.60
2	L	18	ASN	CA-CB-CG	8.81	121.41	112.60
1	H	165	VAL	CB-CA-C	8.73	119.32	109.89
1	H	195	THR	N-CA-C	-8.72	94.68	108.63
4	C	74	ASN	N-CA-C	8.68	122.62	112.72
4	C	34	THR	N-CA-CB	-8.55	99.52	110.90
3	A	76	GLN	OE1-CD-NE2	-8.48	114.11	122.60
3	A	18	ASP	CA-CB-CG	8.36	120.95	112.60
4	C	9	ASP	N-CA-C	8.30	128.48	110.80
1	H	12	ASP	CA-CB-CG	8.13	120.73	112.60
2	L	19	ASP	CA-CB-CG	8.13	120.73	112.60
4	C	138	GLN	CG-CD-NE2	8.04	128.47	116.40
4	C	14	ASN	CA-CB-CG	-8.00	104.60	112.60
2	L	82	VAL	CB-CA-C	-7.91	99.46	111.08
1	H	272	VAL	CB-CA-C	-7.89	98.06	110.69
1	H	319	GLU	CA-CB-CG	-7.82	98.47	114.10
2	L	28	HIS	CB-CG-CD2	-7.80	121.06	131.20
3	A	56	HIS	CA-CB-CG	7.79	121.59	113.80
1	H	194	GLY	N-CA-C	-7.79	103.69	114.67
1	H	275	HIS	CB-CG-CD2	-7.68	121.22	131.20
3	A	53	HIS	ND1-CG-CD2	7.66	113.76	106.10
1	H	358	ASN	OD1-CG-ND2	-7.65	114.95	122.60
4	C	7	ILE	N-CA-C	7.63	120.63	111.09
1	H	372	MET	N-CA-C	7.63	121.81	110.52
1	H	67	LEU	CA-C-O	7.61	125.72	120.47
1	H	125	TYR	CB-CA-C	-7.60	101.74	110.17
2	L	8	ASP	CA-CB-CG	7.58	120.18	112.60
4	C	130	ASP	N-CA-C	-7.56	94.55	108.24
1	H	372	MET	CA-C-O	7.53	130.60	121.72
1	H	17	GLN	N-CA-C	7.42	120.60	109.25
4	C	74	ASN	CA-CB-CG	7.39	120.00	112.60
2	L	55	ALA	N-CA-C	7.39	121.22	110.28
3	A	53	HIS	CG-CD2-NE2	-7.38	99.82	107.20
1	H	30	ASP	CA-CB-CG	7.35	119.95	112.60
1	H	119	ARG	NE-CZ-NH1	7.32	128.82	121.50
2	L	45	ASN	CB-CG-ND2	7.30	127.35	116.40
4	C	105	TRP	CG-CD2-CE3	7.23	141.13	133.90
2	L	105	ASP	N-CA-C	-7.18	104.12	113.17
1	H	72	VAL	O-C-N	-7.16	115.52	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	83	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	H	339	GLY	O-C-N	-7.08	114.74	122.24
1	H	196	GLU	N-CA-C	7.06	121.59	113.19
1	H	52	ASP	CA-CB-CG	7.02	119.62	112.60
1	H	248	PHE	CA-CB-CG	-6.95	106.85	113.80
1	H	217	HIS	CA-CB-CG	-6.93	106.87	113.80
4	C	13	LEU	CA-C-N	-6.93	113.83	122.84
4	C	13	LEU	C-N-CA	-6.93	113.83	122.84
1	H	102	ASP	CA-CB-CG	6.91	119.51	112.60
2	L	18	ASN	OD1-CG-ND2	-6.89	115.71	122.60
4	C	25	THR	N-CA-C	6.88	119.21	110.33
4	C	102	GLY	CA-C-N	6.88	126.85	119.76
4	C	102	GLY	C-N-CA	6.88	126.85	119.76
1	H	212	GLU	N-CA-C	-6.87	98.01	109.07
1	H	359	GLN	CG-CD-NE2	6.86	126.69	116.40
2	L	34	ASN	OD1-CG-ND2	-6.85	115.75	122.60
1	H	371	ASP	CA-CB-CG	6.84	119.44	112.60
4	C	37	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	H	275	HIS	CB-CG-ND1	6.82	132.92	122.70
3	A	16	VAL	O-C-N	6.81	130.37	122.81
1	H	165	VAL	N-CA-C	-6.77	101.36	109.01
1	H	19	ASP	CA-C-O	-6.72	112.94	120.54
4	C	2	PRO	N-CA-C	6.72	126.32	112.47
2	L	32	ASP	CA-CB-CG	6.69	119.29	112.60
1	H	362	HIS	CB-CG-CD2	-6.67	122.53	131.20
4	C	131	ALA	N-CA-C	-6.63	96.71	109.24
1	H	48	GLN	OE1-CD-NE2	-6.57	116.03	122.60
3	A	45	TRP	CG-CD2-CE3	6.57	140.47	133.90
1	H	351	GLY	CA-C-O	6.55	127.12	119.13
4	C	129	LYS	CA-CB-CG	6.55	127.20	114.10
4	C	61	HIS	CA-CB-CG	-6.55	107.25	113.80
2	L	13	TRP	CD2-CE3-CZ3	-6.50	110.15	118.60
1	H	185	ASP	CA-CB-CG	6.50	119.10	112.60
1	H	72	VAL	N-CA-CB	-6.49	102.46	111.41
1	H	167	ASP	CA-CB-CG	-6.48	106.12	112.60
4	C	9	ASP	CA-CB-CG	-6.48	106.12	112.60
1	H	338	THR	CA-CB-OG1	-6.40	100.00	109.60
3	A	95	HIS	CG-CD2-NE2	-6.39	100.81	107.20
1	H	318	HIS	CB-CG-CD2	-6.39	122.90	131.20
1	H	355	ARG	CG-CD-NE	-6.39	97.95	112.00
1	H	122	VAL	CB-CA-C	-6.37	99.53	110.30
1	H	164	ASP	CA-CB-CG	-6.36	106.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	45	TRP	CB-CG-CD1	-6.36	117.36	126.90
2	L	63	ASN	CA-C-N	6.35	126.04	119.82
2	L	63	ASN	C-N-CA	6.35	126.04	119.82
1	H	252	VAL	N-CA-CB	-6.33	99.75	111.91
3	A	5	ILE	O-C-N	-6.32	117.06	121.55
3	A	73	LYS	N-CA-CB	-6.31	101.34	110.87
1	H	203	HIS	CB-CG-CD2	-6.30	123.00	131.20
1	H	71	VAL	CA-CB-CG2	-6.30	99.70	110.40
1	H	120	PHE	CA-CB-CG	6.29	120.09	113.80
4	C	80	TYR	CB-CA-C	6.28	117.37	110.15
1	H	357	VAL	N-CA-C	-6.27	96.70	107.24
1	H	318	HIS	ND1-CG-CD2	6.26	112.36	106.10
4	C	99	GLY	O-C-N	6.24	129.55	122.62
1	H	119	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	H	132	THR	O-C-N	-6.17	115.06	121.60
1	H	325	VAL	CG1-CB-CG2	-6.16	97.25	110.80
3	A	73	LYS	N-CA-C	-6.13	100.86	109.69
1	H	265	ARG	O-C-N	-6.12	117.18	121.65
1	H	100	VAL	CA-C-O	-6.12	113.51	120.67
2	L	10	ARG	NE-CZ-NH2	-6.12	113.70	119.20
3	A	68	LYS	N-CA-C	-6.10	99.26	108.96
3	A	7	SER	N-CA-C	-6.09	98.46	108.76
2	L	26	TRP	CB-CG-CD1	-6.09	117.77	126.90
3	A	16	VAL	CA-CB-CG2	-6.08	100.07	110.40
4	C	122	HIS	CB-CG-CD2	-6.08	123.30	131.20
1	H	67	LEU	N-CA-CB	-6.07	101.93	111.70
1	H	197	GLY	N-CA-C	-6.06	98.82	113.18
3	A	25	ILE	N-CA-C	-6.04	98.93	107.75
1	H	279	ASP	CA-CB-CG	6.03	118.63	112.60
1	H	131	LEU	N-CA-CB	-6.02	100.47	110.23
1	H	170	HIS	CB-CG-CD2	-6.01	123.38	131.20
4	C	3	GLN	CB-CG-CD	6.00	122.80	112.60
1	H	210	GLU	CB-CG-CD	5.93	122.69	112.60
4	C	74	ASN	OD1-CG-ND2	-5.93	116.67	122.60
4	C	105	TRP	CB-CG-CD1	-5.92	118.03	126.90
3	A	24	ASP	CA-C-N	-5.91	115.24	123.10
3	A	24	ASP	C-N-CA	-5.91	115.24	123.10
1	H	346	HIS	CA-CB-CG	5.88	119.68	113.80
3	A	6	PRO	N-CA-C	5.88	121.88	113.47
1	H	237	HIS	O-C-N	-5.87	116.08	123.01
2	L	104	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	H	109	THR	CA-CB-OG1	-5.78	100.93	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	26	ALA	CA-C-O	5.78	126.49	120.25
1	H	244	GLY	N-CA-C	-5.76	106.57	114.64
1	H	82	ALA	N-CA-C	-5.75	100.33	109.76
2	L	20	ILE	N-CA-C	5.74	121.28	109.34
2	L	10	ARG	CB-CG-CD	-5.74	98.11	111.30
1	H	224	ALA	O-C-N	-5.73	115.44	122.25
1	H	217	HIS	CG-CD2-NE2	-5.72	101.48	107.20
4	C	56	MET	CA-CB-CG	-5.72	102.66	114.10
1	H	6	ALA	CA-C-O	-5.71	114.80	120.80
4	C	119	TRP	CG-CD2-CE3	5.71	139.61	133.90
1	H	50	VAL	CA-C-O	-5.67	114.41	120.59
2	L	25	TYR	N-CA-C	-5.67	101.46	109.96
4	C	71	PRO	N-CA-C	5.67	119.57	111.13
3	A	47	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	H	318	HIS	CG-CD2-NE2	-5.64	101.56	107.20
4	C	94	TYR	O-C-N	5.64	128.18	122.09
2	L	84	GLY	N-CA-C	-5.61	107.89	115.36
4	C	2	PRO	CA-N-CD	-5.61	104.14	112.00
3	A	55	VAL	CB-CA-C	-5.61	101.86	110.50
1	H	289	ASP	CA-CB-CG	5.60	118.20	112.60
1	H	333	LEU	N-CA-C	-5.59	99.41	108.52
1	H	308	GLY	N-CA-C	-5.59	107.55	115.43
1	H	111	ASP	N-CA-C	-5.58	98.14	107.80
1	H	245	ASP	O-C-N	5.57	129.73	123.27
1	H	50	VAL	N-CA-CB	-5.55	104.72	111.21
1	H	329	GLU	CA-C-N	-5.55	115.97	123.46
1	H	329	GLU	C-N-CA	-5.55	115.97	123.46
1	H	250	PRO	N-CA-C	5.54	119.17	110.80
1	H	289	ASP	N-CA-C	-5.54	103.21	110.53
3	A	76	GLN	CG-CD-NE2	5.53	124.69	116.40
4	C	137	GLU	N-CA-C	-5.53	104.89	111.69
2	L	66	ASP	CA-CB-CG	5.49	118.09	112.60
3	A	95	HIS	ND1-CG-CD2	5.49	111.58	106.10
1	H	129	THR	CA-CB-OG1	-5.48	101.38	109.60
1	H	216	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	H	67	LEU	O-C-N	-5.47	115.03	121.32
1	H	114	LEU	CA-C-N	5.47	125.39	119.76
1	H	114	LEU	C-N-CA	5.47	125.39	119.76
2	L	26	TRP	CG-CD2-CE3	5.46	139.36	133.90
1	H	207	PHE	CA-CB-CG	5.46	119.26	113.80
3	A	91	HIS	CB-CG-CD2	-5.45	124.12	131.20
2	L	77	CYS	O-C-N	-5.43	117.14	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	57	PHE	O-C-N	-5.42	116.85	123.19
2	L	75	ARG	NE-CZ-NH2	-5.42	114.33	119.20
4	C	74	ASN	CB-CG-ND2	5.39	124.48	116.40
3	A	55	VAL	N-CA-CB	5.38	120.26	111.44
1	H	326	SER	O-C-N	-5.37	116.67	122.79
1	H	225	GLY	O-C-N	-5.37	118.16	122.51
1	H	229	TRP	CE2-CD2-CG	-5.36	100.76	107.20
2	L	43	LEU	CB-CA-C	-5.36	101.89	110.79
1	H	71	VAL	O-C-N	-5.36	117.10	123.05
4	C	80	TYR	N-CA-C	-5.36	100.20	109.15
1	H	20	GLU	CB-CG-CD	5.35	121.70	112.60
4	C	14	ASN	N-CA-C	5.35	117.34	108.20
1	H	129	THR	N-CA-C	-5.34	98.86	108.48
1	H	144	SER	N-CA-C	-5.34	100.14	109.48
1	H	71	VAL	N-CA-CB	-5.34	102.69	111.45
2	L	8	ASP	N-CA-C	-5.33	102.94	109.65
2	L	30	SER	CA-CB-OG	-5.33	100.45	111.10
3	A	9	SER	N-CA-C	-5.33	101.95	110.10
3	A	105	GLU	CA-CB-CG	5.31	124.72	114.10
2	L	101	GLU	CB-CG-CD	5.30	121.62	112.60
4	C	30	HIS	CA-CB-CG	-5.30	108.50	113.80
4	C	11	SER	N-CA-C	5.29	121.50	109.81
1	H	305	ALA	N-CA-C	5.29	118.89	112.23
3	A	8	GLU	CB-CG-CD	5.28	121.58	112.60
1	H	336	LEU	CA-C-O	5.28	126.14	120.38
2	L	21	GLN	CA-C-O	5.28	125.53	119.35
3	A	54	ASN	CA-CB-CG	5.26	117.86	112.60
1	H	35	TYR	O-C-N	-5.25	117.24	123.22
1	H	123	GLY	O-C-N	-5.25	115.88	122.70
4	C	9	ASP	CA-C-O	5.23	127.99	120.51
3	A	66	ALA	CA-C-O	-5.23	115.86	121.56
2	L	54	THR	N-CA-CB	-5.23	102.47	110.26
4	C	138	GLN	N-CA-C	-5.23	105.66	111.36
4	C	26	GLU	N-CA-C	-5.22	105.67	111.36
1	H	238	GLN	O-C-N	-5.22	117.20	123.31
1	H	41	HIS	CB-CG-CD2	-5.21	124.43	131.20
4	C	37	ASN	CB-CG-ND2	5.20	124.20	116.40
4	C	33	GLU	CB-CG-CD	5.20	121.43	112.60
4	C	143	THR	CA-C-N	5.19	125.49	119.93
4	C	143	THR	C-N-CA	5.19	125.49	119.93
1	H	291	TRP	CE2-CD2-CG	-5.19	100.97	107.20
4	C	34	THR	CB-CA-C	5.19	117.74	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	105	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	H	67	LEU	CB-CA-C	5.18	115.58	110.71
1	H	122	VAL	CA-C-O	-5.17	116.51	121.63
2	L	81	ASN	CA-C-O	-5.16	115.88	121.87
1	H	174	THR	N-CA-C	-5.16	107.66	114.31
1	H	71	VAL	CA-CB-CG1	5.15	119.15	110.40
4	C	9	ASP	CB-CA-C	-5.12	100.22	110.42
4	C	75	ASP	CA-CB-CG	5.12	117.72	112.60
4	C	61	HIS	ND1-CE1-NE2	5.12	113.52	108.40
1	H	172	PHE	CA-C-N	5.11	125.51	119.99
1	H	172	PHE	C-N-CA	5.11	125.51	119.99
4	C	61	HIS	ND1-CG-CD2	5.11	111.20	106.10
4	C	129	LYS	N-CA-C	-5.10	99.93	110.80
4	C	4	PHE	N-CA-C	5.10	117.01	107.99
2	L	72	ILE	O-C-N	-5.09	117.38	123.03
1	H	367	ILE	CA-C-O	-5.09	114.92	120.72
4	C	30	HIS	CB-CG-CD2	-5.09	124.59	131.20
3	A	41	ASP	CA-CB-CG	5.08	117.68	112.60
1	H	340	ASP	N-CA-C	-5.06	107.16	113.38
1	H	102	ASP	CB-CA-C	5.05	116.68	109.26
1	H	112	ILE	CB-CG1-CD1	-5.04	103.21	113.80
3	A	45	TRP	CE2-CD2-CG	-5.04	101.15	107.20
3	A	99	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	H	324	ASN	CA-C-O	-5.04	115.76	121.25
4	C	78	TRP	CE2-CD2-CE3	5.04	123.83	118.80
1	H	169	TYR	CA-C-O	-5.03	115.22	121.06
1	H	259	GLU	O-C-N	-5.03	116.89	122.07
4	C	6	ASN	CA-C-O	-5.02	115.19	120.92
2	L	40	GLY	CA-C-N	-5.01	117.48	122.69
2	L	40	GLY	C-N-CA	-5.01	117.48	122.69
2	L	63	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	H	363	GLY	CA-C-O	-5.01	114.36	121.52
2	L	104	ASN	CA-C-O	-5.00	114.05	119.95

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 ⓘ

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	43	0
2	L	956	0	857	15	0
3	A	807	0	794	9	0
4	C	1145	0	1038	22	0
5	H	3	0	0	0	2
6	A	1	0	0	0	0
7	C	43	0	30	2	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	86	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 (86) 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)
4:C:93:LEU:HD12	4:C:117:MET:HE2	1.68	0.75
3:A:4:THR:O	3:A:6:PRO:HD3	1.91	0.70
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
4:C:104:MET:HE3	7:C:200:HEC:HBB2	1.79	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
8:L:142:HOH:O	3:A:71:MET:HE2	2.02	0.60
1:H:76:GLY:HA2	8:H:431:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
4:C:93:LEU:HD12	4:C:117:MET:CE	2.35	0.54
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
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
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
1:H:319:GLU:CD	2:L:10:ARG:HH22	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:316:MET:HE1	1:H:333:LEU:HD13	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
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:193:PHE:C	1:H:195:THR:H	2.26	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
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
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
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%)	2	2
All	All	741/750 (99%)	683 (92%)	52 (7%)	6 (1%)	16	25

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
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%)	266 (88%)	35 (12%)	5	8
2	L	104/104 (100%)	95 (91%)	9 (9%)	9	16
3	A	85/85 (100%)	78 (92%)	7 (8%)	10	18
4	C	118/118 (100%)	98 (83%)	20 (17%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	608/608 (100%)	537 (88%)	71 (12%)	5 7

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	H	24	LEU
1	H	48	GLN
1	H	62	ILE
1	H	67	LEU
1	H	71	VAL
1	H	102	ASP
1	H	103	PRO
1	H	109	THR
1	H	113	GLU
1	H	122	VAL
1	H	131	LEU
1	H	149	VAL
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	205	GLU
1	H	226	ARG
1	H	227	LEU
1	H	241	LEU
1	H	249	LEU
1	H	252	VAL
1	H	272	VAL
1	H	280	ARG
1	H	300	LEU
1	H	303	LEU
1	H	313	LYS
1	H	329	GLU
1	H	330	LYS
1	H	332	LEU
1	H	333	LEU
1	H	360	LEU
2	L	7	THR
2	L	30	SER

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Mol	Chain	Res	Type
2	L	82	VAL
2	L	85	ARG
2	L	87	PRO
2	L	91	THR
2	L	95	LEU
2	L	104	ASN
2	L	131	SER
3	A	1	ASP
3	A	6	PRO
3	A	16	VAL
3	A	27	LYS
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	20	GLU
4	C	45	ILE
4	C	48	GLU
4	C	52	LEU
4	C	69	ILE
4	C	73	LEU
4	C	84	GLU
4	C	89	LEU
4	C	104	MET
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	37	ASN
1	H	41	HIS
1	H	69	ASN
1	H	208	HIS

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Mol	Chain	Res	Type
1	H	222	GLN
1	H	271	GLN
1	H	318	HIS
1	H	365	GLN
2	L	18	ASN
2	L	28	HIS
2	L	34	ASN
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	16,17,18	1.85	6 (37%)	16,24,26	3.82	10 (62%)

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	-	0/5/19/21	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	57	TRQ	CZ3-CH2	-3.21	1.37	1.45
2	L	57	TRQ	CH2-CZ2	-3.13	1.39	1.53
2	L	57	TRQ	CD1-NE1	-3.12	1.29	1.36
2	L	57	TRQ	CE2-CZ2	-2.77	1.40	1.50
2	L	57	TRQ	CD2-CG	-2.20	1.38	1.42
2	L	57	TRQ	CE2-NE1	-2.20	1.34	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	57	TRQ	CD1-CG-CD2	9.65	114.66	105.95
2	L	57	TRQ	CE2-CD2-CG	-7.27	97.52	107.16
2	L	57	TRQ	CB-CG-CD1	-4.40	118.39	126.97
2	L	57	TRQ	O7-CZ2-CH2	4.21	123.76	118.39
2	L	57	TRQ	CD2-CE2-NE1	3.20	113.02	107.20
2	L	57	TRQ	CE3-CD2-CG	3.13	146.60	131.15
2	L	57	TRQ	CG-CD1-NE1	-2.90	105.49	109.22
2	L	57	TRQ	O6-CH2-CZ3	-2.40	117.26	121.58
2	L	57	TRQ	CZ3-CH2-CZ2	2.31	122.01	118.68
2	L	57	TRQ	CZ2-CE2-NE1	-2.28	121.70	127.25

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 oligosaccharides 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	$\# Z > 2$
5	PO4	H	0	-	0,2,4	-	-	0,1,6	-	-
7	HEC	C	200	4	50,50,50	0.88	2 (4%)	68,82,82	1.19	6 (8%)

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	1/1/3/7	1/14/54/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	200	HEC	O2A-CGA	-2.21	1.23	1.30
7	C	200	HEC	O2D-CGD	-2.17	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	200	HEC	CBC-CAC-C3C	3.12	120.87	112.42
7	C	200	HEC	O2D-CGD-CBD	2.38	121.51	114.00
7	C	200	HEC	C1D-C2D-C3D	-2.28	104.58	106.98
7	C	200	HEC	C3C-C4C-NC	2.25	112.65	110.15
7	C	200	HEC	C1C-C2C-C3C	2.07	109.19	106.82
7	C	200	HEC	C4C-C3C-C2C	-2.03	103.72	106.87

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	200	HEC	NA

All (1) torsion outliers are listed below:

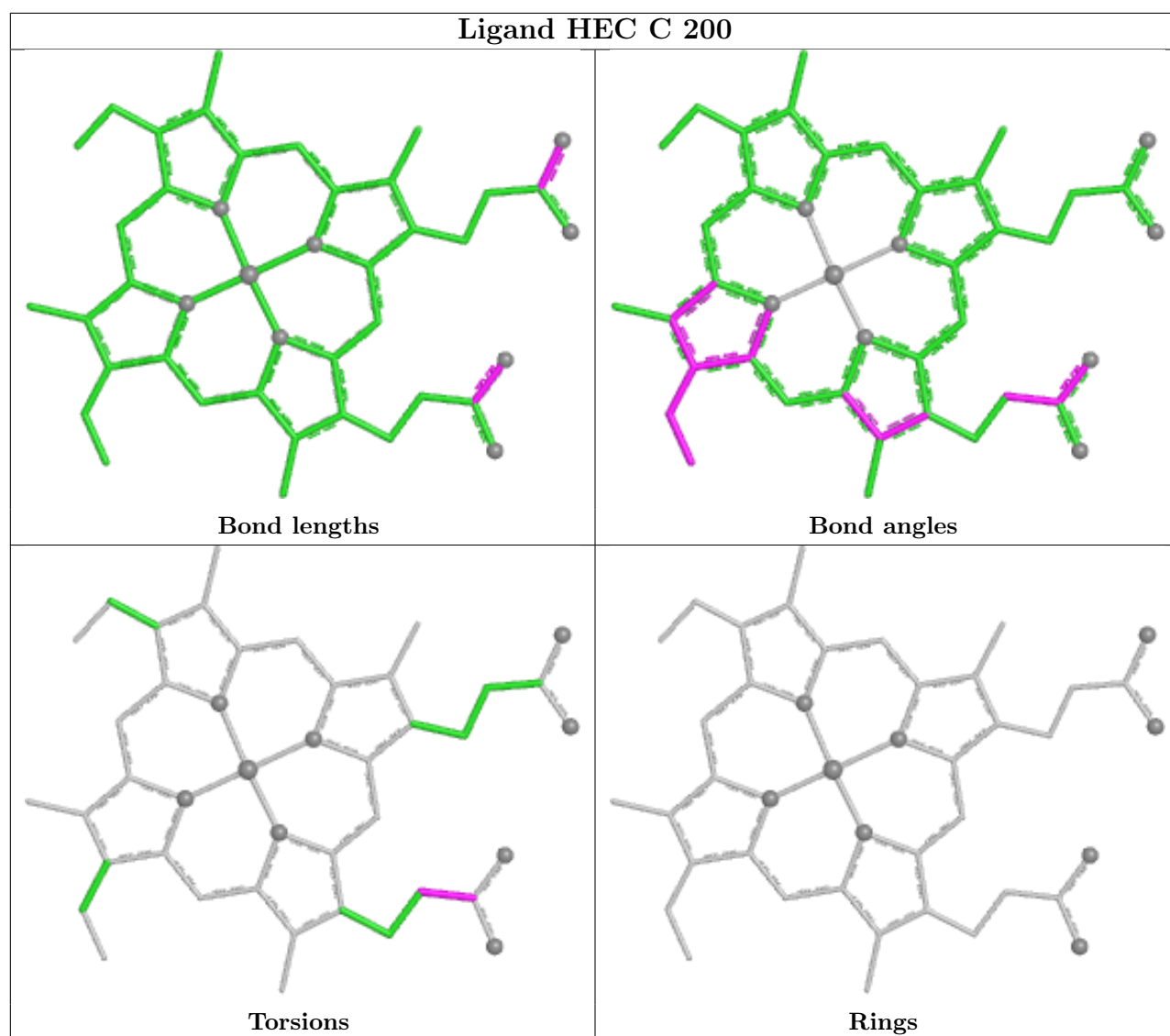
Mol	Chain	Res	Type	Atoms
7	C	200	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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



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.