



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:41 PM UTC

PDB ID : 1ZRT / pdb_00001zrt
Title : Rhodobacter capsulatus cytochrome bc1 complex with stigmatellin bound
Authors : Berry, E.A.; Huang, L.S.; Saechao, L.K.; Pon, N.G.; Valkova-Valchanov, M.; Daldal, F.
Deposited on : 2005-05-22
Resolution : 3.51 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 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:

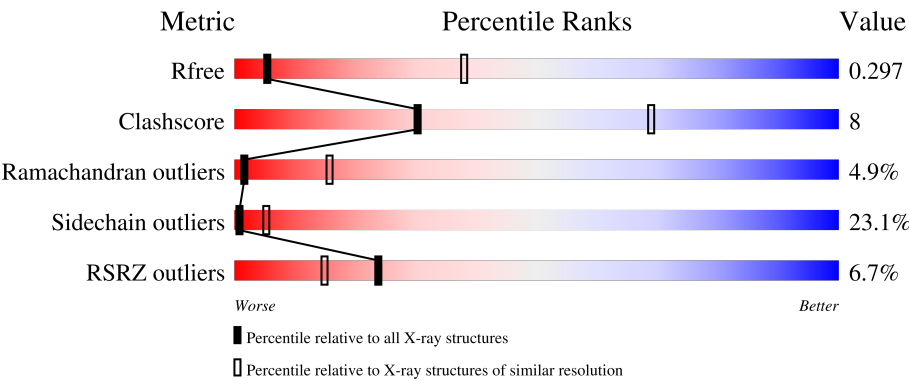
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.51 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))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	437	
1	P	437	
2	D	258	
2	Q	258	
3	E	191	

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Mol	Chain	Length	Quality of chain
3	R	191	5% 57% 30% 7%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13919 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 Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	431	Total	C	N	O	S	0	1	0
			3472	2345	543	570	14			
1	P	431	Total	C	N	O	S	0	1	0
			3468	2342	542	570	14			

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	248	Total	C	N	O	S	0	0	0
			1908	1213	319	359	17			
2	Q	248	Total	C	N	O	S	0	0	0
			1904	1210	318	359	17			

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	183	Total	C	N	O	S	0	0	0
			1372	859	248	257	8			
3	R	183	Total	C	N	O	S	0	0	0
			1376	861	248	259	8			

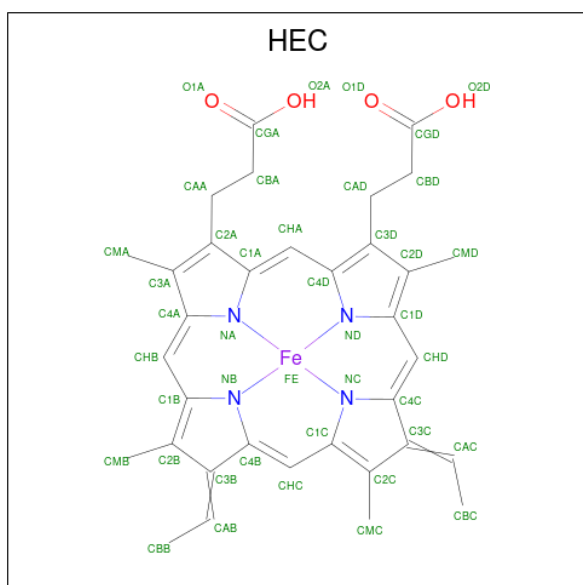
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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

- Molecule 6 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

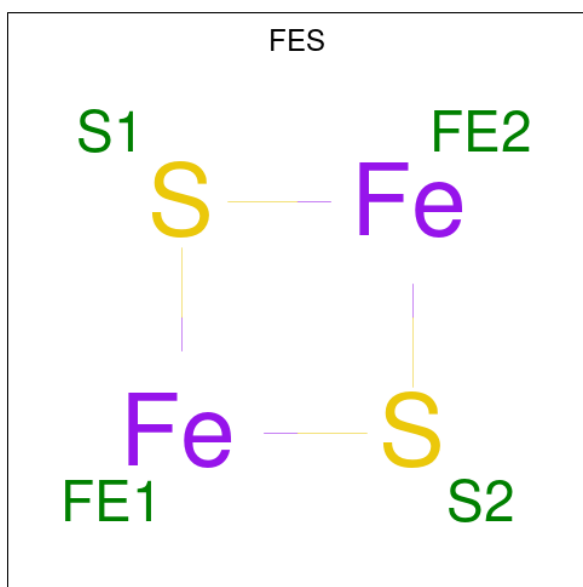
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	2	Total	C	O	0	0
			25	18	7		
6	P	2	Total	C	O	0	0
			36	27	9		

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



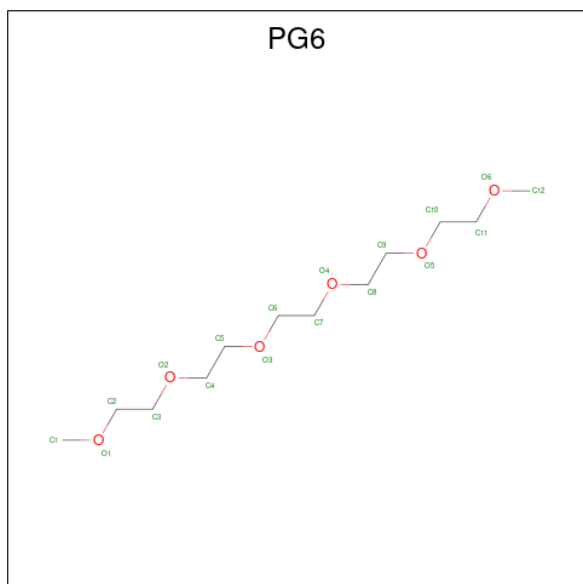
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 9 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (CCD ID: PG6) (formula: C₁₂H₂₆O₆).

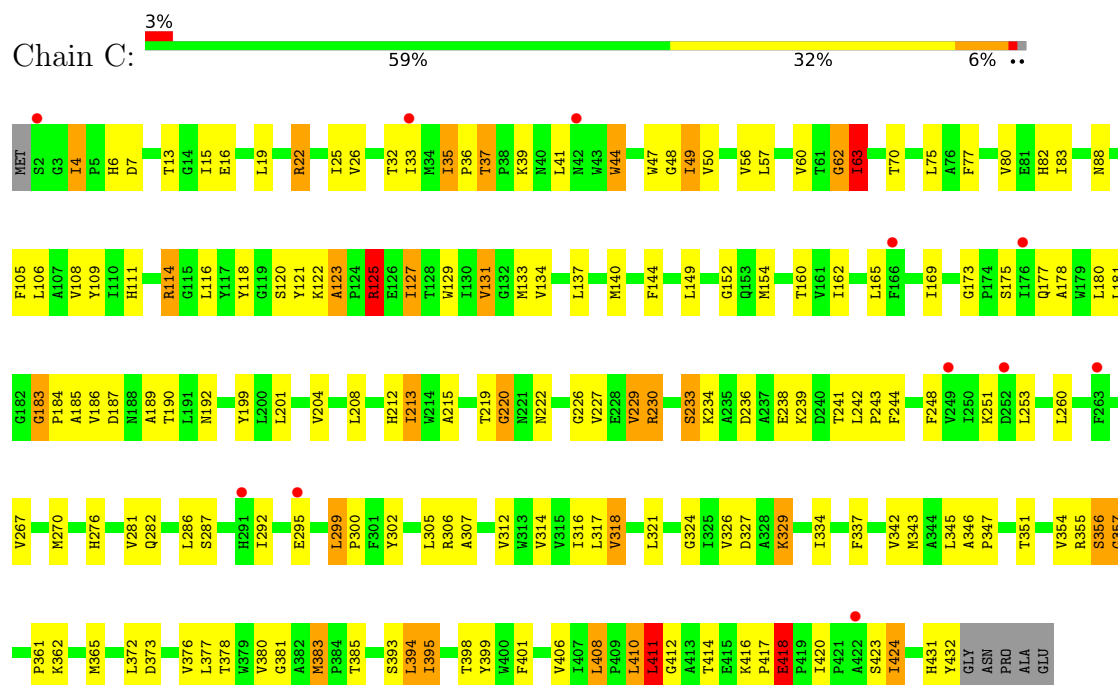


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	Q	1	Total	C	O	0	0
			18	12	6		

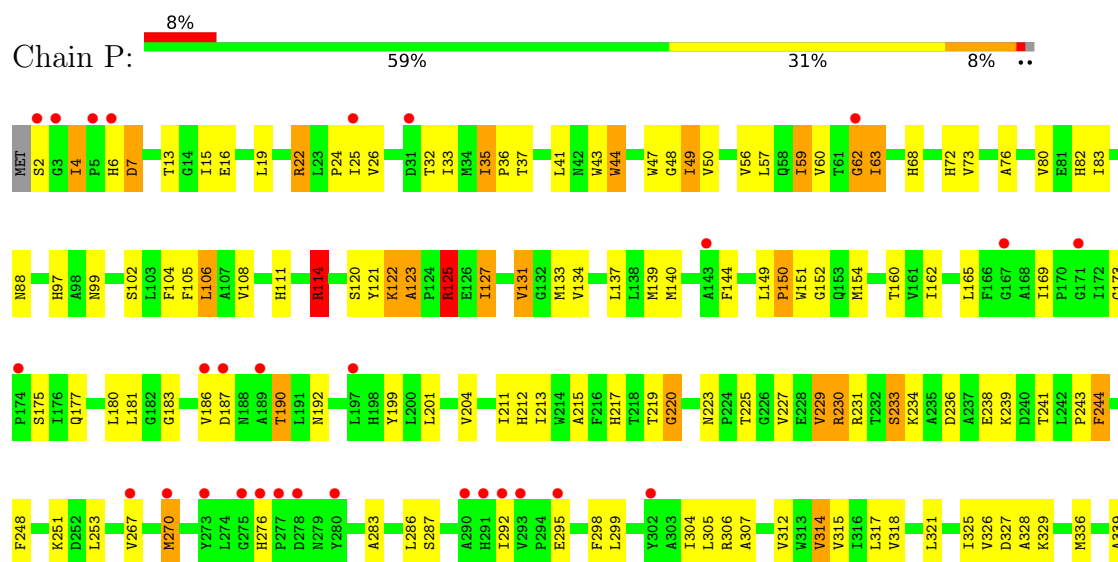
3 Residue-property plots

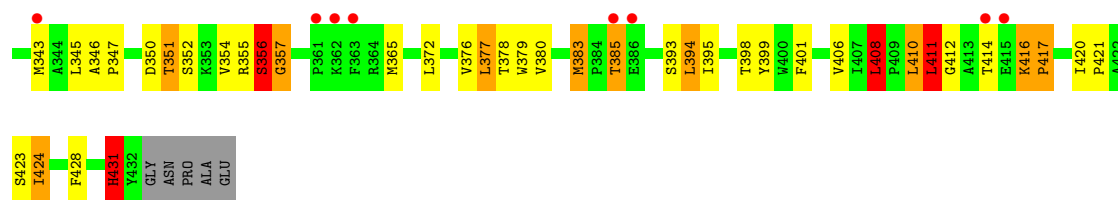
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cytochrome b

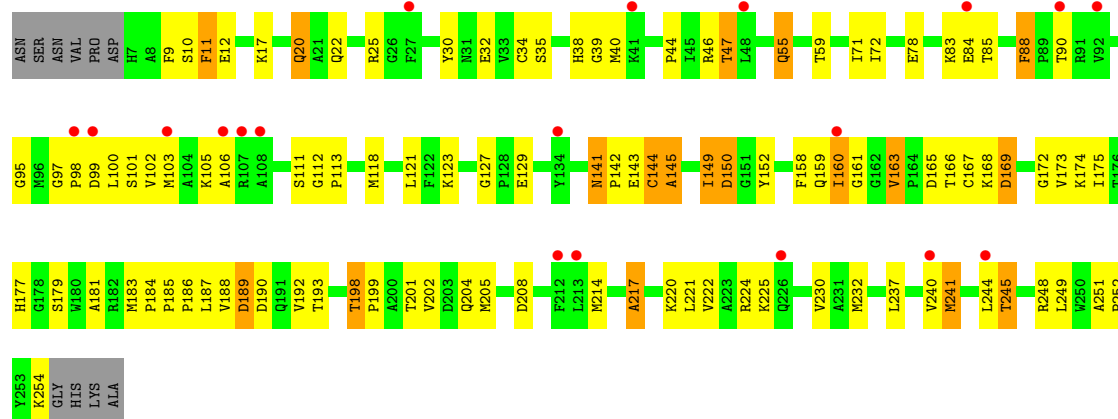


• Molecule 1: Cytochrome b

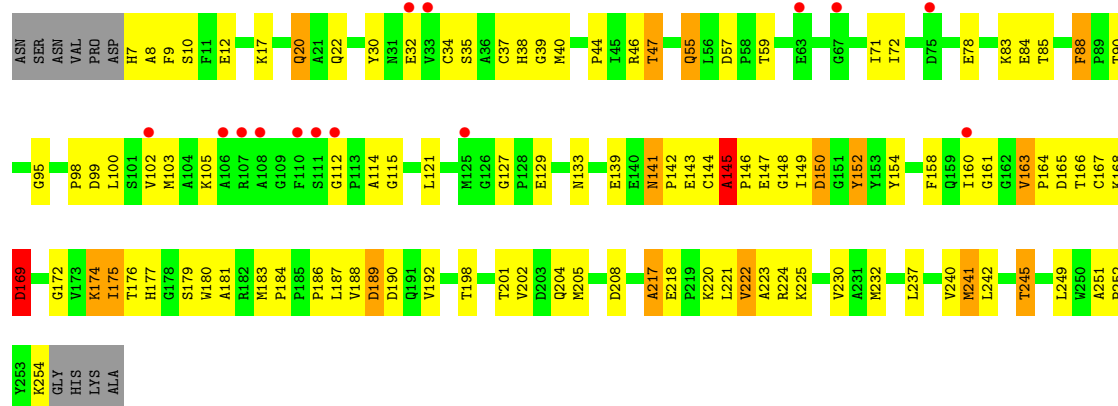




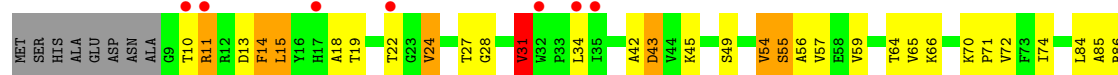
• Molecule 2: Cytochrome c1

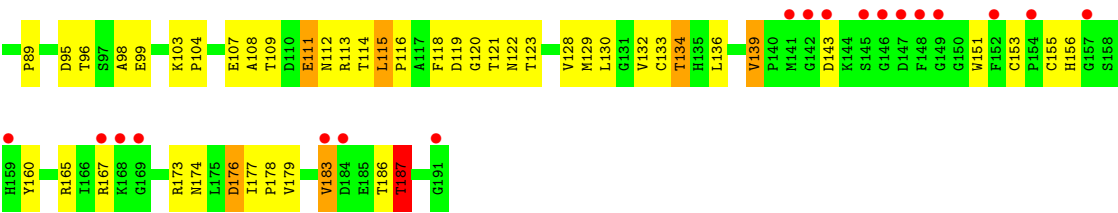


• Molecule 2: Cytochrome c1

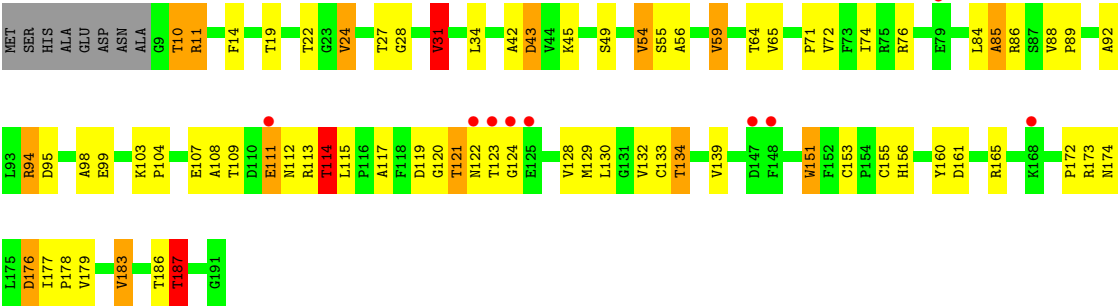


• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit





● Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.63Å 154.36Å 103.06Å 90.00° 113.57° 90.00°	Depositor
Resolution (Å)	59.77 – 3.51 59.77 – 3.51	Depositor EDS
% Data completeness (in resolution range)	96.5 (59.77-3.51) 96.9 (59.77-3.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 3.49Å)	Xtriage
Refinement program	PHENIX dev_3885, CNS 1.1	Depositor
R, R_{free}	0.221 , 0.289 0.228 , 0.297	Depositor DCC
R_{free} test set	1661 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	99.0	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13919	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: UNL, PG6, HEM, SMA, FES, 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	C	1.11	5/3608 (0.1%)	1.54	59/4955 (1.2%)
1	P	1.21	9/3604 (0.2%)	1.55	47/4951 (0.9%)
2	D	0.93	4/1956 (0.2%)	1.35	9/2647 (0.3%)
2	Q	0.90	1/1952 (0.1%)	1.35	11/2643 (0.4%)
3	E	1.01	2/1402 (0.1%)	1.40	12/1905 (0.6%)
3	R	1.01	1/1406 (0.1%)	1.33	6/1910 (0.3%)
All	All	1.07	22/13928 (0.2%)	1.46	144/19011 (0.8%)

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	P	0	1
2	D	0	1
2	Q	0	2
All	All	0	4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	167	ARG	CA-C	6.78	1.56	1.52
2	D	145	ALA	C-O	-6.65	1.20	1.23
1	P	385	THR	CA-C	6.49	1.63	1.52
1	P	215	ALA	CA-CB	-6.32	1.43	1.53
3	R	85	ALA	CA-CB	-6.00	1.44	1.53
1	P	283	ALA	CA-CB	-5.75	1.44	1.53
2	D	145	ALA	CA-CB	-5.69	1.48	1.52
1	P	223	ASN	CA-C	5.62	1.58	1.52
3	E	70	LYS	CA-C	5.61	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	102	VAL	CA-CB	5.58	1.62	1.54
1	C	213	ILE	CA-CB	5.56	1.61	1.54
1	C	185	ALA	CA-CB	-5.56	1.45	1.53
2	D	149	ILE	CA-CB	5.55	1.62	1.54
2	Q	223	ALA	CA-CB	-5.52	1.44	1.53
1	P	339	ALA	CA-C	-5.51	1.45	1.52
1	P	24	PRO	CA-C	5.49	1.57	1.52
1	P	211	ILE	CA-C	5.45	1.59	1.52
1	C	342	VAL	CA-CB	5.30	1.61	1.54
1	C	373	ASP	CA-C	-5.16	1.46	1.52
1	C	149	LEU	C-N	5.14	1.38	1.33
1	P	411	LEU	CA-C	5.05	1.59	1.52
1	P	104	PHE	CA-C	-5.02	1.46	1.52

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	220	GLY	N-CA-C	-9.25	99.60	111.72
1	P	173	GLY	N-CA-C	8.95	126.01	115.09
1	C	416	LYS	CA-C-N	8.23	130.13	119.84
1	C	416	LYS	C-N-CA	8.23	130.13	119.84
1	C	201	LEU	CA-C-N	-8.15	111.40	120.45
1	C	201	LEU	C-N-CA	-8.15	111.40	120.45
1	C	276	HIS	CA-C-N	8.08	129.94	119.84
1	C	276	HIS	C-N-CA	8.08	129.94	119.84
1	C	129	TRP	N-CA-C	7.99	119.68	110.97
1	P	276	HIS	CA-C-N	7.89	129.70	119.84
1	P	276	HIS	C-N-CA	7.89	129.70	119.84
1	P	152	GLY	N-CA-C	-7.78	101.92	112.57
1	P	60	VAL	N-CA-C	7.76	118.51	110.36
1	P	416	LYS	CA-C-N	7.69	129.45	119.84
1	P	416	LYS	C-N-CA	7.69	129.45	119.84
1	C	307	ALA	N-CA-C	-7.66	102.27	111.69
1	P	399	TYR	O-C-N	7.55	130.25	122.09
1	C	183	GLY	CA-C-N	7.31	128.97	119.84
1	C	183	GLY	C-N-CA	7.31	128.97	119.84
1	C	173	GLY	N-CA-C	7.30	127.23	112.34
2	Q	39	GLY	N-CA-C	7.26	124.56	113.02
1	C	118	TYR	N-CA-C	7.15	120.55	112.97
1	C	60	VAL	N-CA-C	7.14	117.86	110.36
2	D	39	GLY	N-CA-C	7.13	124.36	113.02
3	E	115	LEU	CA-C-N	7.06	128.67	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	115	LEU	C-N-CA	7.06	128.67	119.84
3	E	155	CYS	CA-C-N	-7.04	112.68	123.17
3	E	155	CYS	C-N-CA	-7.04	112.68	123.17
1	C	149	LEU	CA-C-N	-7.02	113.67	120.83
1	C	149	LEU	C-N-CA	-7.02	113.67	120.83
1	P	201	LEU	CA-C-N	-7.00	112.35	120.12
1	P	201	LEU	C-N-CA	-7.00	112.35	120.12
1	P	37	THR	CA-C-N	6.98	127.02	119.90
1	P	37	THR	C-N-CA	6.98	127.02	119.90
1	P	44	TRP	N-CA-C	-6.98	104.76	113.28
1	C	152	GLY	N-CA-C	-6.95	103.04	112.57
1	P	243	PRO	CA-C-O	-6.60	113.81	121.86
2	Q	161	GLY	N-CA-C	6.59	120.96	112.13
2	D	144	CYS	O-C-N	6.57	126.83	122.03
1	P	183	GLY	CA-C-N	6.56	128.04	119.84
1	P	183	GLY	C-N-CA	6.56	128.04	119.84
1	C	63	ILE	N-CA-C	6.52	118.11	111.00
2	D	161	GLY	N-CA-C	6.41	120.71	112.13
1	C	281	VAL	N-CA-C	-6.38	98.44	107.75
1	C	318	VAL	N-CA-C	-6.36	106.34	111.81
1	C	243	PRO	CA-C-O	-6.35	114.11	121.86
1	P	346	ALA	N-CA-C	6.35	123.85	109.81
1	C	346	ALA	CA-C-N	-6.33	113.24	119.64
1	C	346	ALA	C-N-CA	-6.33	113.24	119.64
1	C	408	LEU	CA-C-N	-6.31	111.95	119.84
1	C	408	LEU	C-N-CA	-6.31	111.95	119.84
1	P	354	VAL	N-CA-C	-6.30	101.42	109.30
1	C	37	THR	CA-C-N	6.26	126.28	119.90
1	C	37	THR	C-N-CA	6.26	126.28	119.90
1	P	346	ALA	CA-C-N	-6.26	113.32	119.64
1	P	346	ALA	C-N-CA	-6.26	113.32	119.64
3	R	31	VAL	N-CA-C	-6.26	106.61	113.43
1	P	220	GLY	N-CA-C	-6.25	103.80	112.18
1	P	76	ALA	N-CA-C	6.22	118.61	111.02
2	Q	175	ILE	N-CA-C	-6.20	105.32	111.77
1	C	316	ILE	O-C-N	6.15	127.84	121.87
1	P	225	THR	N-CA-C	-6.15	105.60	113.23
1	P	408	LEU	CA-C-N	-6.15	112.16	119.84
1	P	408	LEU	C-N-CA	-6.15	112.16	119.84
1	C	346	ALA	N-CA-C	6.10	123.28	109.81
3	E	31	VAL	N-CA-C	-6.08	106.80	113.43
1	C	411	LEU	N-CA-C	6.06	123.71	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	354	VAL	N-CA-C	-6.04	101.75	109.30
1	P	99	ASN	CA-C-N	6.01	126.66	119.98
1	P	99	ASN	C-N-CA	6.01	126.66	119.98
2	Q	169	ASP	N-CA-C	6.00	117.01	108.74
1	P	351	THR	N-CA-C	-5.98	106.52	113.88
3	R	187	THR	N-CA-C	5.98	119.23	109.06
3	R	155	CYS	CA-C-N	-5.93	113.23	123.25
3	R	155	CYS	C-N-CA	-5.93	113.23	123.25
1	C	77	PHE	N-CA-C	-5.86	104.85	112.23
1	P	149	LEU	CA-C-N	-5.85	112.53	119.84
1	P	149	LEU	C-N-CA	-5.85	112.53	119.84
1	C	399	TYR	O-C-N	5.84	128.08	122.07
1	P	343	MET	N-CA-C	-5.83	106.50	113.97
1	C	299	LEU	CA-C-N	-5.73	112.68	119.84
1	C	299	LEU	C-N-CA	-5.73	112.68	119.84
1	C	316	ILE	CA-C-N	5.72	128.22	120.38
1	C	316	ILE	C-N-CA	5.72	128.22	120.38
2	D	88	PHE	CA-C-N	-5.72	114.08	120.14
2	D	88	PHE	C-N-CA	-5.72	114.08	120.14
2	Q	88	PHE	CA-C-N	-5.70	114.09	120.14
2	Q	88	PHE	C-N-CA	-5.70	114.09	120.14
2	Q	57	ASP	CA-C-N	5.67	125.14	119.24
2	Q	57	ASP	C-N-CA	5.67	125.14	119.24
1	C	343	MET	N-CA-C	-5.67	106.72	113.97
1	P	411	LEU	N-CA-C	5.63	122.80	110.80
1	C	395	ILE	N-CA-C	-5.63	104.87	111.00
2	D	169	ASP	N-CA-C	5.61	116.48	108.74
1	C	406	VAL	CA-C-O	-5.60	115.94	120.70
1	P	139	MET	N-CA-C	5.58	118.90	111.75
3	E	167	ARG	N-CA-C	5.58	117.69	108.48
1	P	307	ALA	N-CA-C	-5.58	104.60	111.40
1	C	282	GLN	CA-CB-CG	5.55	125.21	114.10
1	C	118	TYR	CB-CA-C	-5.55	102.68	111.17
2	Q	95	GLY	CA-C-O	5.52	125.14	119.01
1	P	62	GLY	CA-C-O	-5.50	115.41	120.80
1	C	213	ILE	N-CA-C	-5.50	104.07	111.44
1	P	406	VAL	CA-C-O	-5.50	116.03	120.70
1	P	298	PHE	N-CA-C	-5.47	106.51	114.12
3	R	114	THR	N-CA-C	5.47	117.38	109.07
1	C	242	LEU	CA-C-N	-5.43	114.39	120.14
1	C	242	LEU	C-N-CA	-5.43	114.39	120.14
1	C	44	TRP	N-CA-C	-5.42	106.51	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	189	ALA	CA-C-N	5.42	127.48	120.44
1	C	189	ALA	C-N-CA	5.42	127.48	120.44
2	D	95	GLY	N-CA-C	-5.38	107.69	115.27
1	P	73	VAL	N-CA-C	5.33	116.69	110.62
1	C	63	ILE	CB-CA-C	-5.32	105.11	112.24
1	P	150	PRO	CA-C-N	5.31	129.95	122.46
1	P	150	PRO	C-N-CA	5.31	129.95	122.46
1	C	215	ALA	CA-C-O	-5.30	115.23	121.07
1	P	299	LEU	CA-C-N	-5.30	114.21	119.56
1	P	299	LEU	C-N-CA	-5.30	114.21	119.56
1	P	378	THR	N-CA-CB	5.28	117.88	110.12
1	C	373	ASP	O-C-N	5.23	127.45	122.07
2	D	106	ALA	N-CA-C	-5.22	106.86	114.12
1	C	109	TYR	CA-C-O	-5.22	115.53	120.90
1	C	302	TYR	N-CA-C	-5.20	105.52	111.14
2	Q	145	ALA	CA-C-N	5.19	126.32	119.84
2	Q	145	ALA	C-N-CA	5.19	126.32	119.84
1	C	418	GLU	CA-C-N	-5.18	113.36	119.84
1	C	418	GLU	C-N-CA	-5.18	113.36	119.84
3	E	177	ILE	N-CA-C	-5.18	101.94	108.05
3	E	89	PRO	CA-C-O	-5.17	115.84	121.27
1	P	59	ILE	N-CA-C	-5.17	105.67	110.53
1	C	282	GLN	CB-CG-CD	-5.13	103.88	112.60
3	E	187	THR	N-CA-C	5.12	117.75	109.06
3	R	151	TRP	N-CA-C	5.11	116.75	108.26
1	C	324	GLY	N-CA-C	5.07	121.70	114.85
1	C	337	PHE	N-CA-C	-5.06	105.66	111.07
3	E	139	VAL	CA-C-O	5.05	122.47	119.19
3	E	14	PHE	CA-C-N	5.04	127.75	120.38
3	E	14	PHE	C-N-CA	5.04	127.75	120.38
2	D	159	GLN	N-CA-C	5.04	117.50	111.71
1	C	62	GLY	CA-C-O	-5.03	115.87	120.80
1	P	114	ARG	N-CA-C	-5.03	105.71	111.14
1	P	72	HIS	CA-C-N	5.02	127.61	120.53
1	P	72	HIS	C-N-CA	5.02	127.61	120.53

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	167	CYS	Peptide
1	P	356	SER	Peptide

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Mol	Chain	Res	Type	Group
2	Q	148	GLY	Peptide
2	Q	167	CYS	Peptide

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	C	3472	0	3424	53	0
1	P	3468	0	3413	60	0
2	D	1908	0	1840	31	0
2	Q	1904	0	1829	34	0
3	E	1372	0	1346	28	0
3	R	1376	0	1350	27	0
4	C	86	0	60	2	0
4	P	86	0	60	3	0
5	C	37	0	42	4	0
5	P	37	0	42	3	0
6	C	25	0	0	0	0
6	P	36	0	0	1	0
7	D	43	0	30	5	0
7	Q	43	0	30	7	0
8	E	4	0	0	0	0
8	R	4	0	0	1	0
9	Q	18	0	26	0	0
All	All	13919	0	13492	230	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (230) 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)
1:C:44:TRP:HB3	1:C:114:ARG:HG3	1.72	0.71
1:P:4:ILE:HG13	1:P:231:ARG:HE	1.56	0.69
1:C:162:ILE:HA	1:C:165:LEU:HD12	1.76	0.68
1:P:44:TRP:HB3	1:P:114:ARG:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ALA:O	1:C:355:ARG:NH1	2.28	0.67
3:E:74:ILE:HG23	3:E:128:VAL:HG22	1.77	0.67
1:P:123:ALA:O	1:P:355:ARG:NH1	2.27	0.66
1:P:356:SER:OG	1:P:357:GLY:N	2.29	0.66
2:Q:37:CYS:SG	7:Q:501:HEC:C3C	2.83	0.66
2:D:22:GLN:HE21	2:D:208:ASP:HA	1.61	0.64
1:P:6:HIS:HB3	1:P:36:PRO:HG3	1.80	0.62
2:D:165:ASP:HA	2:D:168:LYS:HB2	1.82	0.62
3:R:98:ALA:O	3:R:113:ARG:NH1	2.32	0.62
3:E:31:VAL:HA	3:E:34:LEU:HD12	1.82	0.61
1:C:356:SER:OG	1:C:357:GLY:N	2.32	0.61
2:Q:165:ASP:HA	2:Q:168:LYS:HB2	1.81	0.61
1:P:4:ILE:HB	1:P:36:PRO:HG2	1.82	0.61
3:R:108:ALA:O	3:R:165:ARG:NH1	2.31	0.61
1:C:180:LEU:HD22	5:C:503:SMA:H28	1.83	0.60
2:Q:139:GLU:HB2	2:Q:154:TYR:HD2	1.66	0.60
1:P:144:PHE:HE2	5:P:503:SMA:H25	1.66	0.60
1:P:162:ILE:HA	1:P:165:LEU:HD12	1.82	0.60
1:C:4:ILE:HB	1:C:36:PRO:HG2	1.83	0.59
1:C:121:TYR:HB2	1:C:347:PRO:HG3	1.84	0.59
3:E:55:SER:OG	3:E:56:ALA:N	2.36	0.59
1:C:131:VAL:HG12	1:C:212:HIS:HD1	1.67	0.59
2:D:168:LYS:HA	2:D:174:LYS:HA	1.84	0.59
3:E:134:THR:HG21	3:E:173:ARG:HB2	1.85	0.58
1:C:47:TRP:O	1:C:111:HIS:ND1	2.36	0.58
3:R:74:ILE:HG23	3:R:128:VAL:HG22	1.84	0.58
1:P:131:VAL:HG12	1:P:212:HIS:HD1	1.68	0.58
1:C:361:PRO:HD3	1:C:418:GLU:HG3	1.86	0.58
1:C:70:THR:HG21	1:C:75:LEU:HD13	1.84	0.57
3:R:156:HIS:N	8:R:501:FES:S1	2.76	0.57
2:D:141:ASN:OD1	2:D:141:ASN:N	2.36	0.57
2:D:44:PRO:O	2:D:47:THR:OG1	2.20	0.57
1:P:306:ARG:NH2	1:P:383:MET:O	2.38	0.57
1:P:41:LEU:O	1:P:251:LYS:NZ	2.38	0.57
2:Q:22:GLN:HE21	2:Q:208:ASP:HA	1.70	0.57
1:C:286:LEU:HD23	3:R:71:PRO:HB3	1.85	0.57
3:R:31:VAL:HA	3:R:34:LEU:HD12	1.85	0.57
1:P:121:TYR:HB2	1:P:347:PRO:HG3	1.85	0.56
1:P:428:PHE:O	1:P:431:HIS:ND1	2.32	0.56
2:D:163:VAL:HG23	2:D:179:SER:HB2	1.86	0.56
3:E:108:ALA:O	3:E:165:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:154:MET:HE1	1:P:292:ILE:HA	1.87	0.55
3:R:134:THR:HG21	3:R:173:ARG:HB2	1.88	0.55
1:C:230:ARG:NH2	1:C:423:SER:OG	2.39	0.55
1:C:306:ARG:NH2	1:C:383:MET:O	2.39	0.55
3:E:103:LYS:NZ	3:E:111:GLU:O	2.37	0.55
1:P:233:SER:OG	1:P:234:LYS:N	2.40	0.55
1:P:180:LEU:HD13	5:P:503:SMA:H28	1.89	0.55
2:D:244:LEU:HB3	3:E:15:LEU:HD11	1.88	0.55
3:E:134:THR:HG22	3:E:173:ARG:HH21	1.71	0.54
2:Q:40:MET:HB2	2:Q:88:PHE:HB2	1.89	0.54
3:R:99:GLU:HB3	3:R:176:ASP:HA	1.88	0.54
3:R:42:ALA:HA	3:R:45:LYS:HB2	1.90	0.54
2:Q:187:LEU:HD13	2:Q:205:MET:HE3	1.89	0.54
2:D:165:ASP:OD1	2:D:165:ASP:N	2.40	0.54
3:R:10:THR:HG22	3:R:14:PHE:HB2	1.90	0.54
3:E:99:GLU:HB3	3:E:176:ASP:HA	1.90	0.53
3:R:151:TRP:HB2	3:R:160:TYR:HB2	1.90	0.53
3:E:85:ALA:O	3:E:165:ARG:NH2	2.40	0.53
1:C:233:SER:OG	1:C:234:LYS:N	2.41	0.53
1:P:230:ARG:NH2	1:P:423:SER:OG	2.41	0.53
3:E:10:THR:HG22	3:E:11:ARG:HH21	1.74	0.53
2:D:144:CYS:SG	2:D:145:ALA:N	2.77	0.53
3:E:98:ALA:O	3:E:113:ARG:NH1	2.35	0.53
3:E:109:THR:OG1	3:E:112:ASN:ND2	2.42	0.53
1:P:102:SER:O	1:P:106:LEU:N	2.35	0.53
2:Q:184:PRO:HD2	7:Q:501:HEC:HBC2	1.91	0.53
2:D:187:LEU:HD13	2:D:205:MET:HE3	1.90	0.53
2:D:40:MET:HB2	2:D:88:PHE:HB2	1.90	0.53
2:Q:112:GLY:HA2	2:Q:115:GLY:H	1.75	0.52
1:P:144:PHE:CE2	5:P:503:SMA:H25	2.45	0.52
3:E:151:TRP:HB2	3:E:160:TYR:HB2	1.92	0.52
2:Q:141:ASN:N	2:Q:141:ASN:OD1	2.43	0.52
1:C:312:VAL:HG13	1:C:394:LEU:HD11	1.91	0.52
3:E:43:ASP:OD1	3:E:43:ASP:N	2.40	0.52
1:P:80:VAL:HG21	1:P:150:PRO:HB3	1.93	0.51
3:E:71:PRO:HB3	1:P:286:LEU:HD23	1.92	0.51
3:R:85:ALA:O	3:R:165:ARG:NH2	2.43	0.51
3:R:103:LYS:NZ	3:R:111:GLU:O	2.39	0.51
1:C:6:HIS:HB3	1:C:36:PRO:HG3	1.91	0.51
3:E:14:PHE:O	3:E:18:ALA:N	2.41	0.51
1:P:379:TRP:HE1	2:Q:114:ALA:HB1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:44:PRO:O	2:Q:47:THR:OG1	2.26	0.51
2:Q:30:TYR:HD1	2:Q:34:CYS:HB2	1.76	0.51
3:R:54:VAL:O	3:R:56:ALA:N	2.45	0.50
3:E:66:LYS:HB2	1:P:286:LEU:HD21	1.91	0.50
1:C:410:LEU:O	1:C:412:GLY:N	2.45	0.50
1:C:178:ALA:HA	1:C:181:LEU:HB2	1.94	0.49
2:D:251:ALA:HA	2:D:254:LYS:HB3	1.94	0.49
1:C:219:THR:OG1	1:C:220:GLY:O	2.29	0.49
2:Q:251:ALA:HA	2:Q:254:LYS:HB3	1.94	0.49
3:R:109:THR:OG1	3:R:112:ASN:ND2	2.44	0.49
2:D:184:PRO:HD2	7:D:501:HEC:HBC2	1.94	0.49
1:C:41:LEU:O	1:C:251:LYS:NZ	2.45	0.49
1:C:244:PHE:HA	1:C:248:PHE:HB2	1.94	0.49
2:Q:189:ASP:OD1	2:Q:202:VAL:N	2.45	0.49
7:D:501:HEC:HBA1	7:D:501:HEC:HBD2	1.94	0.49
1:P:236:ASP:HA	1:P:239:LYS:HE2	1.94	0.49
1:P:230:ARG:HD2	1:P:236:ASP:HB2	1.95	0.49
2:Q:102:VAL:HG23	2:Q:217:ALA:HA	1.95	0.49
1:P:318:VAL:HG12	1:P:326:VAL:HB	1.95	0.48
2:Q:164:PRO:O	2:Q:168:LYS:N	2.46	0.48
2:D:30:TYR:HD1	2:D:34:CYS:HB2	1.77	0.48
2:Q:37:CYS:CB	7:Q:501:HEC:C3C	2.92	0.48
2:D:241:MET:O	2:D:245:THR:OG1	2.31	0.48
1:C:154:MET:HE1	1:C:292:ILE:HA	1.96	0.48
7:Q:501:HEC:HHA	7:Q:501:HEC:HBD2	1.95	0.48
3:R:183:VAL:HG23	3:R:187:THR:HB	1.96	0.48
3:E:143:ASP:O	2:Q:168:LYS:NZ	2.46	0.48
1:C:120:SER:HA	1:C:125:ARG:HD3	1.97	0.47
2:D:38:HIS:HE1	2:D:98:PRO:HD2	1.79	0.47
1:C:39:LYS:HA	1:C:248:PHE:HZ	1.80	0.47
1:C:318:VAL:HG12	1:C:326:VAL:HB	1.97	0.47
1:P:7:ASP:OD1	1:P:7:ASP:N	2.43	0.47
7:Q:501:HEC:HBD2	7:Q:501:HEC:HBA1	1.97	0.47
1:P:229:VAL:HG13	1:P:424:ILE:HD12	1.97	0.47
2:D:9:PHE:HE2	2:D:129:GLU:HG3	1.80	0.47
1:P:219:THR:OG1	1:P:220:GLY:O	2.31	0.47
2:Q:241:MET:O	2:Q:245:THR:OG1	2.34	0.46
1:C:22:ARG:HH11	1:C:22:ARG:HB2	1.80	0.46
1:P:63:ILE:H	1:P:63:ILE:HG12	1.56	0.46
3:R:43:ASP:OD1	3:R:43:ASP:N	2.37	0.46
1:C:144:PHE:HE2	5:C:503:SMA:H25	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:9:PHE:HE2	2:Q:129:GLU:HG3	1.80	0.46
2:D:105:LYS:HG3	2:D:217:ALA:HB1	1.97	0.46
2:Q:165:ASP:OD1	2:Q:165:ASP:N	2.40	0.46
2:Q:139:GLU:HB2	2:Q:154:TYR:CD2	2.48	0.46
2:D:189:ASP:OD1	2:D:202:VAL:N	2.44	0.46
1:P:410:LEU:O	1:P:412:GLY:N	2.49	0.46
2:Q:183:MET:HE3	2:Q:186:PRO:HG3	1.98	0.46
3:E:42:ALA:HA	3:E:45:LYS:HB2	1.98	0.46
1:P:244:PHE:HA	1:P:248:PHE:HB2	1.97	0.46
1:P:47:TRP:O	1:P:111:HIS:ND1	2.49	0.45
1:P:304:ILE:HD11	1:P:377:LEU:HD21	1.98	0.45
2:D:20:GLN:HE22	2:D:55:GLN:HB2	1.81	0.45
2:D:141:ASN:HA	2:D:142:PRO:HD3	1.79	0.45
2:Q:17:LYS:HD2	2:Q:222:VAL:HG12	1.98	0.45
2:Q:152:TYR:HB3	2:Q:180:TRP:HB3	1.98	0.45
1:C:226:GLY:HA3	1:C:356:SER:HB2	1.99	0.45
1:C:49:ILE:HD13	1:C:49:ILE:HA	1.84	0.45
3:E:95:ASP:OD2	3:E:174:ASN:ND2	2.50	0.45
1:C:236:ASP:HA	1:C:239:LYS:HE2	1.99	0.45
1:P:22:ARG:HB2	1:P:22:ARG:HH11	1.82	0.45
3:E:183:VAL:HG23	3:E:187:THR:HB	1.98	0.45
2:Q:38:HIS:HE1	2:Q:98:PRO:HD2	1.82	0.45
3:E:54:VAL:O	3:E:57:VAL:N	2.50	0.44
2:Q:38:HIS:CD2	7:Q:501:HEC:NB	2.85	0.44
2:D:248:ARG:HH22	3:E:11:ARG:NH1	2.15	0.44
1:P:312:VAL:HG13	1:P:394:LEU:HD11	1.98	0.44
1:P:352:SER:HB2	1:P:412:GLY:HA2	2.00	0.44
2:Q:168:LYS:HB3	2:Q:169:ASP:H	1.57	0.44
7:Q:501:HEC:HHA	7:Q:501:HEC:HBA1	1.99	0.44
2:D:174:LYS:HB2	2:D:174:LYS:HE3	1.79	0.44
1:C:229:VAL:HG13	1:C:424:ILE:HD12	1.99	0.44
2:Q:163:VAL:HG13	2:Q:179:SER:HB2	2.00	0.44
1:C:230:ARG:HD2	1:C:236:ASP:HB2	1.99	0.44
1:C:35:ILE:HA	1:C:36:PRO:HD3	1.88	0.43
7:D:501:HEC:HBD2	7:D:501:HEC:HHA	2.00	0.43
1:P:315:VAL:HG11	1:P:328:ALA:HB2	2.01	0.43
3:E:54:VAL:O	3:E:56:ALA:N	2.51	0.43
1:P:181:LEU:HA	1:P:190:THR:HG23	2.01	0.43
1:P:336:MET:HE2	1:P:336:MET:HB3	1.88	0.43
1:C:22:ARG:HG2	1:P:219:THR:HG22	2.00	0.43
1:C:62:GLY:O	4:C:501:HEM:HBC2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:97:HIS:HE1	4:P:501:HEM:NC	2.17	0.43
1:C:63:ILE:H	1:C:63:ILE:HG12	1.61	0.43
3:R:117:ALA:H	3:R:121:THR:HG23	1.83	0.43
1:C:127:ILE:HD12	1:C:127:ILE:HA	1.82	0.43
6:P:504:UNL:O4	2:Q:220:LYS:NZ	2.46	0.43
1:P:105:PHE:CZ	1:P:140:MET:HG2	2.53	0.42
1:P:122:LYS:NZ	1:P:350:ASP:OD2	2.40	0.42
1:C:180:LEU:HD13	5:C:503:SMA:H28	2.01	0.42
2:D:17:LYS:HD2	2:D:222:VAL:HG12	2.00	0.42
1:C:299:LEU:HD23	1:C:299:LEU:HA	1.87	0.42
2:D:38:HIS:CE1	2:D:97:GLY:HA3	2.54	0.42
1:P:127:ILE:HD12	1:P:127:ILE:HA	1.80	0.42
1:P:416:LYS:HA	1:P:417:PRO:HD2	1.80	0.42
2:Q:174:LYS:HB2	2:Q:174:LYS:HE3	1.75	0.42
3:R:59:VAL:HG22	3:R:76:ARG:HH12	1.83	0.42
1:C:80:VAL:HA	1:C:83:ILE:HD12	2.00	0.42
3:E:136:LEU:HD12	3:E:156:HIS:CE1	2.54	0.42
1:C:114:ARG:HE	1:C:114:ARG:HB3	1.68	0.42
1:P:35:ILE:HG13	1:P:217:HIS:CD2	2.55	0.42
1:P:35:ILE:HG13	1:P:217:HIS:HD2	1.85	0.42
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.88	0.42
1:C:199:TYR:CE2	4:C:501:HEM:HBC1	2.54	0.42
1:C:105:PHE:CZ	1:C:140:MET:HG2	2.55	0.42
7:D:501:HEC:HBA1	7:D:501:HEC:HHA	2.01	0.42
1:P:270:MET:HE2	1:P:270:MET:HB3	1.99	0.41
1:P:408:LEU:HD13	1:P:408:LEU:HA	1.89	0.41
1:C:306:ARG:NH2	1:C:381:GLY:O	2.53	0.41
1:P:49:ILE:HD13	1:P:49:ILE:HA	1.80	0.41
3:R:114:THR:HG21	3:R:124:GLY:HA2	2.01	0.41
2:D:198:THR:HA	2:D:199:PRO:HD2	1.97	0.41
1:P:120:SER:HA	1:P:125:ARG:HD3	2.03	0.41
1:C:4:ILE:H	1:C:4:ILE:HG13	1.42	0.41
1:C:125:ARG:HE	1:C:222:ASN:HB2	1.85	0.41
1:P:62:GLY:O	4:P:501:HEM:HBC2	2.21	0.41
1:P:199:TYR:CE2	4:P:501:HEM:HBC1	2.55	0.41
3:R:88:VAL:HA	3:R:89:PRO:HD2	1.77	0.41
3:R:94:ARG:HB2	3:R:95:ASP:H	1.71	0.41
1:P:35:ILE:HA	1:P:36:PRO:HD3	1.87	0.41
1:P:312:VAL:HG12	1:P:314:VAL:HG13	2.01	0.41
1:C:219:THR:HG22	1:P:22:ARG:HG2	2.03	0.41
1:C:295[A]:GLU:OE1	5:C:503:SMA:O8	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:68:HIS:HB3	1:P:83:ILE:HG12	2.03	0.41
3:R:95:ASP:OD2	3:R:174:ASN:ND2	2.54	0.41
2:Q:20:GLN:HE22	2:Q:55:GLN:HB2	1.86	0.41
1:C:260:LEU:HD23	1:C:260:LEU:HA	1.92	0.41
2:D:11:PHE:CE1	2:D:214:MET:HG2	2.56	0.41
2:D:183:MET:HE3	2:D:186:PRO:HG3	2.03	0.41
1:P:114:ARG:HE	1:P:114:ARG:HB3	1.75	0.41
3:R:89:PRO:HG2	3:R:92:ALA:HB3	2.03	0.41
1:C:300:PRO:HD3	1:C:378:THR:HG22	2.03	0.41
2:Q:105:LYS:HD3	2:Q:218:GLU:HG2	2.03	0.41
2:Q:144:CYS:SG	2:Q:145:ALA:N	2.92	0.41
2:D:160:ILE:H	2:D:160:ILE:HG13	1.69	0.40
3:E:99:GLU:HG3	3:E:174:ASN:HB2	2.03	0.40
3:E:99:GLU:HB2	3:E:113:ARG:HH12	1.86	0.40
1:C:183:GLY:HA3	1:C:184:PRO:HD2	1.79	0.40
2:D:22:GLN:HG3	2:D:25:ARG:NH2	2.36	0.40
3:R:11:ARG:H	3:R:11:ARG:HE	1.69	0.40
3:R:172:PRO:HG2	3:R:173:ARG:HD3	2.03	0.40
2:D:38:HIS:CD2	7:D:501:HEC:NB	2.90	0.40
1:P:424:ILE:H	1:P:424:ILE:HG12	1.55	0.40
3:R:165:ARG:HA	3:R:174:ASN:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	430/437 (98%)	363 (84%)	55 (13%)	12 (3%)	4	25
1	P	430/437 (98%)	359 (84%)	58 (14%)	13 (3%)	3	25
2	D	246/258 (95%)	195 (79%)	32 (13%)	19 (8%)	1	8
2	Q	246/258 (95%)	195 (79%)	32 (13%)	19 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	181/191 (95%)	146 (81%)	24 (13%)	11 (6%)	1	12
3	R	181/191 (95%)	142 (78%)	29 (16%)	10 (6%)	1	13
All	All	1714/1772 (97%)	1400 (82%)	230 (13%)	84 (5%)	1	16

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	ALA
1	C	125	ARG
1	C	411	LEU
1	C	417	PRO
2	D	12	GLU
3	E	55	SER
3	E	119	ASP
1	P	125	ARG
1	P	411	LEU
1	P	417	PRO
1	P	431	HIS
2	Q	12	GLU
2	Q	145	ALA
2	Q	181	ALA
3	R	55	SER
1	C	356	SER
1	C	431	HIS
2	D	72	ILE
2	D	143	GLU
2	D	152	TYR
2	D	172	GLY
2	D	177	HIS
2	D	181	ALA
3	E	13	ASP
3	E	118	PHE
1	P	230	ARG
1	P	356	SER
2	Q	72	ILE
2	Q	143	GLU
2	Q	146	PRO
2	Q	150	ASP
2	Q	152	TYR
2	Q	158	PHE
1	C	35	ILE

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Mol	Chain	Res	Type
1	C	230	ARG
2	D	46	ARG
2	D	150	ASP
2	D	158	PHE
2	D	189	ASP
2	D	217	ALA
3	E	24	VAL
3	E	104	PRO
3	E	116	PRO
3	E	122	ASN
1	P	35	ILE
1	P	357	GLY
2	Q	8	ALA
2	Q	142	PRO
2	Q	147	GLU
2	Q	189	ASP
2	Q	217	ALA
3	R	24	VAL
3	R	104	PRO
3	R	119	ASP
3	R	122	ASN
1	C	48	GLY
1	C	329	LYS
2	D	55	GLN
2	D	198	THR
3	E	178	PRO
1	P	123	ALA
2	Q	198	THR
3	R	94	ARG
1	C	187	ASP
1	C	357	GLY
2	D	111	SER
2	D	113	PRO
1	P	43	TRP
1	P	187	ASP
1	P	329	LYS
2	Q	46	ARG
2	Q	55	GLN
3	R	161	ASP
3	R	178	PRO
2	D	112	GLY
3	E	120	GLY

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Mol	Chain	Res	Type
1	P	48	GLY
3	R	28	GLY
3	E	28	GLY
2	Q	127	GLY
2	Q	172	GLY
2	D	127	GLY
3	R	120	GLY
2	D	185	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	356/360 (99%)	278 (78%)	78 (22%)	1	6
1	P	355/360 (99%)	275 (78%)	80 (22%)	1	5
2	D	197/206 (96%)	150 (76%)	47 (24%)	1	4
2	Q	196/206 (95%)	149 (76%)	47 (24%)	1	4
3	E	142/149 (95%)	107 (75%)	35 (25%)	1	4
3	R	143/149 (96%)	108 (76%)	35 (24%)	1	4
All	All	1389/1430 (97%)	1067 (77%)	322 (23%)	1	5

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4	ILE
1	C	7	ASP
1	C	13	THR
1	C	15	ILE
1	C	16	GLU
1	C	19	LEU
1	C	22	ARG
1	C	25	ILE
1	C	26	VAL
1	C	32	THR

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Mol	Chain	Res	Type
1	C	33	ILE
1	C	37	THR
1	C	49	ILE
1	C	50	VAL
1	C	56	VAL
1	C	57	LEU
1	C	63	ILE
1	C	82	HIS
1	C	88	ASN
1	C	106	LEU
1	C	108	VAL
1	C	114	ARG
1	C	122	LYS
1	C	125	ARG
1	C	127	ILE
1	C	131	VAL
1	C	133	MET
1	C	134	VAL
1	C	137	LEU
1	C	160	THR
1	C	169	ILE
1	C	175	SER
1	C	177	GLN
1	C	186	VAL
1	C	190	THR
1	C	192	ASN
1	C	204	VAL
1	C	208	LEU
1	C	213	ILE
1	C	227	VAL
1	C	229	VAL
1	C	233	SER
1	C	238	GLU
1	C	241	THR
1	C	253	LEU
1	C	267	VAL
1	C	270	MET
1	C	287	SER
1	C	305	LEU
1	C	314	VAL
1	C	317	LEU
1	C	321	LEU

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Mol	Chain	Res	Type
1	C	327	ASP
1	C	329	LYS
1	C	334	ILE
1	C	345	LEU
1	C	351	THR
1	C	362	LYS
1	C	365	MET
1	C	372	LEU
1	C	376	VAL
1	C	377	LEU
1	C	380	VAL
1	C	383	MET
1	C	385	THR
1	C	393	SER
1	C	394	LEU
1	C	395	ILE
1	C	398	THR
1	C	401	PHE
1	C	408	LEU
1	C	410	LEU
1	C	411	LEU
1	C	414	THR
1	C	418	GLU
1	C	420	ILE
1	C	424	ILE
1	C	432	TYR
2	D	10	SER
2	D	11	PHE
2	D	20	GLN
2	D	32	GLU
2	D	35	SER
2	D	47	THR
2	D	59	THR
2	D	71	ILE
2	D	78	GLU
2	D	83	LYS
2	D	84	GLU
2	D	85	THR
2	D	90	THR
2	D	99	ASP
2	D	100	LEU
2	D	101	SER

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Mol	Chain	Res	Type
2	D	103	MET
2	D	118	MET
2	D	121	LEU
2	D	123	LYS
2	D	141	ASN
2	D	149	ILE
2	D	150	ASP
2	D	160	ILE
2	D	163	VAL
2	D	166	THR
2	D	169	ASP
2	D	173	VAL
2	D	175	ILE
2	D	188	VAL
2	D	190	ASP
2	D	192	VAL
2	D	193	THR
2	D	201	THR
2	D	204	GLN
2	D	220	LYS
2	D	221	LEU
2	D	224	ARG
2	D	225	LYS
2	D	230	VAL
2	D	232	MET
2	D	237	LEU
2	D	240	VAL
2	D	241	MET
2	D	245	THR
2	D	249	LEU
2	D	252	PRO
3	E	11	ARG
3	E	15	LEU
3	E	19	THR
3	E	22	THR
3	E	24	VAL
3	E	27	THR
3	E	31	VAL
3	E	43	ASP
3	E	49	SER
3	E	54	VAL
3	E	59	VAL

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Mol	Chain	Res	Type
3	E	64	THR
3	E	65	VAL
3	E	72	VAL
3	E	84	LEU
3	E	86	ARG
3	E	96	THR
3	E	107	GLU
3	E	111	GLU
3	E	114	THR
3	E	115	LEU
3	E	121	THR
3	E	123	THR
3	E	129	MET
3	E	130	LEU
3	E	132	VAL
3	E	133	CYS
3	E	134	THR
3	E	139	VAL
3	E	153	CYS
3	E	176	ASP
3	E	179	VAL
3	E	183	VAL
3	E	186	THR
3	E	187	THR
1	P	2	SER
1	P	4	ILE
1	P	7	ASP
1	P	13	THR
1	P	15	ILE
1	P	16	GLU
1	P	19	LEU
1	P	22	ARG
1	P	25	ILE
1	P	26	VAL
1	P	32	THR
1	P	33	ILE
1	P	49	ILE
1	P	50	VAL
1	P	56	VAL
1	P	57	LEU
1	P	59	ILE
1	P	63	ILE

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Mol	Chain	Res	Type
1	P	82	HIS
1	P	88	ASN
1	P	106	LEU
1	P	108	VAL
1	P	114	ARG
1	P	122	LYS
1	P	125	ARG
1	P	127	ILE
1	P	131	VAL
1	P	133	MET
1	P	134	VAL
1	P	137	LEU
1	P	151	TRP
1	P	160	THR
1	P	169	ILE
1	P	175	SER
1	P	177	GLN
1	P	186	VAL
1	P	190	THR
1	P	192	ASN
1	P	204	VAL
1	P	213	ILE
1	P	227	VAL
1	P	229	VAL
1	P	233	SER
1	P	238	GLU
1	P	241	THR
1	P	244	PHE
1	P	253	LEU
1	P	267	VAL
1	P	270	MET
1	P	287	SER
1	P	295[A]	GLU
1	P	295[B]	GLU
1	P	305	LEU
1	P	314	VAL
1	P	317	LEU
1	P	321	LEU
1	P	325	ILE
1	P	327	ASP
1	P	345	LEU
1	P	351	THR

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Mol	Chain	Res	Type
1	P	365	MET
1	P	372	LEU
1	P	376	VAL
1	P	377	LEU
1	P	380	VAL
1	P	383	MET
1	P	385	THR
1	P	393	SER
1	P	394	LEU
1	P	395	ILE
1	P	398	THR
1	P	401	PHE
1	P	408	LEU
1	P	410	LEU
1	P	411	LEU
1	P	414	THR
1	P	420	ILE
1	P	421	PRO
1	P	424	ILE
1	P	431	HIS
2	Q	7	HIS
2	Q	10	SER
2	Q	20	GLN
2	Q	32	GLU
2	Q	35	SER
2	Q	47	THR
2	Q	59	THR
2	Q	71	ILE
2	Q	78	GLU
2	Q	83	LYS
2	Q	84	GLU
2	Q	85	THR
2	Q	90	THR
2	Q	99	ASP
2	Q	100	LEU
2	Q	103	MET
2	Q	121	LEU
2	Q	133	ASN
2	Q	141	ASN
2	Q	149	ILE
2	Q	150	ASP
2	Q	160	ILE

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Mol	Chain	Res	Type
2	Q	163	VAL
2	Q	166	THR
2	Q	169	ASP
2	Q	174	LYS
2	Q	175	ILE
2	Q	176	THR
2	Q	177	HIS
2	Q	188	VAL
2	Q	190	ASP
2	Q	192	VAL
2	Q	201	THR
2	Q	204	GLN
2	Q	221	LEU
2	Q	222	VAL
2	Q	224	ARG
2	Q	225	LYS
2	Q	230	VAL
2	Q	232	MET
2	Q	237	LEU
2	Q	240	VAL
2	Q	241	MET
2	Q	242	LEU
2	Q	245	THR
2	Q	249	LEU
2	Q	252	PRO
3	R	10	THR
3	R	11	ARG
3	R	19	THR
3	R	22	THR
3	R	24	VAL
3	R	27	THR
3	R	31	VAL
3	R	43	ASP
3	R	49	SER
3	R	54	VAL
3	R	59	VAL
3	R	64	THR
3	R	65	VAL
3	R	72	VAL
3	R	84	LEU
3	R	86	ARG
3	R	107	GLU

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Mol	Chain	Res	Type
3	R	111	GLU
3	R	114	THR
3	R	115	LEU
3	R	121	THR
3	R	123	THR
3	R	129	MET
3	R	130	LEU
3	R	132	VAL
3	R	133	CYS
3	R	134	THR
3	R	139	VAL
3	R	153	CYS
3	R	176	ASP
3	R	177	ILE
3	R	179	VAL
3	R	183	VAL
3	R	186	THR
3	R	187	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	88	ASN
2	D	20	GLN
2	D	22	GLN
2	D	133	ASN
2	D	204	GLN
3	E	36	ASN
3	E	39	ASN
3	E	102	ASN
3	E	112	ASN
3	E	159	HIS
1	P	88	ASN
2	Q	20	GLN
2	Q	22	GLN
2	Q	204	GLN
3	R	36	ASN
3	R	39	ASN
3	R	102	ASN
3	R	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 4 are unknown - leaving 11 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	SMA	P	503	-	38,38,38	2.27	6 (15%)	47,52,52	2.16	17 (36%)
5	SMA	C	503	-	38,38,38	2.35	6 (15%)	47,52,52	2.38	15 (31%)
4	HEM	P	502	1	50,50,50	1.43	6 (12%)	67,82,82	1.72	15 (22%)
4	HEM	P	501	1	50,50,50	1.63	8 (16%)	67,82,82	1.59	19 (28%)
8	FES	R	501	3	0,4,4	-	-	-	-	-
7	HEC	D	501	2	46,50,50	1.96	5 (10%)	58,82,82	2.35	19 (32%)
4	HEM	C	502	1	50,50,50	1.56	10 (20%)	67,82,82	1.80	17 (25%)
7	HEC	Q	501	2	46,50,50	2.04	8 (17%)	58,82,82	2.12	16 (27%)
4	HEM	C	501	1	50,50,50	2.14	10 (20%)	67,82,82	1.56	11 (16%)
9	PG6	Q	502	-	17,17,17	0.72	0	16,16,16	0.57	0
8	FES	E	501	3	0,4,4	-	-	-	-	-

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
5	SMA	P	503	-	-	15/34/34/34	0/2/2/2
5	SMA	C	503	-	-	14/34/34/34	0/2/2/2
4	HEM	P	502	1	-	5/14/54/54	-
4	HEM	P	501	1	-	3/14/54/54	-
8	FES	R	501	3	-	-	0/1/1/1
7	HEC	D	501	2	-	11/14/54/54	-
4	HEM	C	502	1	-	3/14/54/54	-
7	HEC	Q	501	2	-	11/14/54/54	-
4	HEM	C	501	1	-	3/14/54/54	-
9	PG6	Q	502	-	-	3/15/15/15	-
8	FES	E	501	3	-	-	0/1/1/1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	HEM	FE-NB	11.09	2.29	1.94
5	P	503	SMA	C3-C2	9.04	1.51	1.34
5	C	503	SMA	C8-C8A	8.21	1.52	1.39
5	C	503	SMA	C3-C2	7.13	1.48	1.34
5	P	503	SMA	C7-C8	6.91	1.50	1.40
7	D	501	HEC	CAC-C3C	6.87	1.57	1.35
7	Q	501	HEC	CAC-C3C	6.58	1.56	1.35
7	D	501	HEC	CAB-C3B	6.57	1.56	1.35
7	Q	501	HEC	CAB-C3B	6.29	1.55	1.35
4	P	501	HEM	FE-NB	5.91	2.13	1.94
7	Q	501	HEC	C3D-C2D	5.58	1.53	1.38
4	C	502	HEM	FE-NA	5.34	2.12	1.95
5	C	503	SMA	C4A-C5	5.24	1.49	1.40
7	D	501	HEC	C3D-C2D	4.92	1.51	1.38
5	C	503	SMA	C7-C8	4.85	1.47	1.40
4	P	502	HEM	FE-NB	4.81	2.09	1.94
5	P	503	SMA	C4A-C5	4.65	1.48	1.40
4	P	501	HEM	FE-NC	4.55	2.10	1.95
4	C	502	HEM	CAC-C3C	4.55	1.59	1.47
5	C	503	SMA	C4A-C8A	4.48	1.50	1.40
5	P	503	SMA	C8-C8A	4.05	1.46	1.39
4	P	501	HEM	FE-ND	3.57	2.05	1.94
4	P	502	HEM	CAC-C3C	3.49	1.56	1.47
5	P	503	SMA	C4A-C8A	3.39	1.48	1.40
4	C	501	HEM	FE-NA	3.39	2.06	1.95
7	D	501	HEC	CAD-C3D	3.20	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	HEM	CMB-C2B	3.07	1.57	1.50
4	C	501	HEM	FE-ND	-3.06	1.85	1.94
4	P	501	HEM	CMB-C2B	2.92	1.56	1.50
4	C	501	HEM	CMC-C2C	2.92	1.56	1.50
7	Q	501	HEC	CAD-C3D	2.75	1.58	1.51
4	C	502	HEM	FE-NB	2.75	2.03	1.94
4	P	501	HEM	CMD-C2D	2.70	1.56	1.50
4	C	501	HEM	CAC-C3C	2.68	1.54	1.47
4	P	502	HEM	FE-NA	2.67	2.04	1.95
7	Q	501	HEC	CHA-C4D	-2.67	1.33	1.39
4	C	502	HEM	CAB-C3B	2.61	1.54	1.47
4	C	502	HEM	C3B-C2B	-2.59	1.31	1.37
4	P	501	HEM	C3C-C2C	-2.48	1.32	1.37
4	C	501	HEM	CAB-C3B	2.45	1.53	1.47
4	C	501	HEM	FE-NC	2.44	2.03	1.95
7	Q	501	HEC	CMB-C2B	2.42	1.55	1.50
4	P	501	HEM	CAC-C3C	2.41	1.53	1.47
7	D	501	HEC	CMC-C2C	2.39	1.55	1.50
5	C	503	SMA	C4A-C4	2.35	1.52	1.46
4	C	501	HEM	C2A-C3A	-2.33	1.32	1.38
4	P	502	HEM	CAB-C3B	2.31	1.53	1.47
7	Q	501	HEC	CAA-C2A	2.25	1.57	1.51
4	P	502	HEM	C3B-C2B	-2.23	1.32	1.37
4	C	501	HEM	CMD-C2D	2.18	1.55	1.50
4	C	502	HEM	CAD-C3D	2.16	1.56	1.51
5	P	503	SMA	O1-C8A	-2.16	1.35	1.38
4	C	502	HEM	O1D-CGD	2.15	1.29	1.22
4	C	502	HEM	CMC-C2C	2.13	1.55	1.50
4	C	502	HEM	FE-ND	2.10	2.01	1.94
7	Q	501	HEC	C3B-C2B	-2.08	1.34	1.41
4	P	502	HEM	CAD-C3D	2.06	1.56	1.51
4	C	502	HEM	C1C-NC	-2.05	1.35	1.39
4	P	501	HEM	C2A-C3A	-2.05	1.33	1.38

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	503	SMA	C14-C15-C16	-8.40	108.86	125.88
7	D	501	HEC	CBB-CAB-C3B	-6.19	115.05	127.43
7	D	501	HEC	CBC-CAC-C3C	-6.15	115.14	127.43
7	Q	501	HEC	CBB-CAB-C3B	-6.13	115.18	127.43
5	P	503	SMA	O7-C7-C8	5.89	120.70	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	501	HEC	CMC-C2C-C1C	-5.76	116.64	125.42
4	C	502	HEM	C3B-C2B-C1B	5.37	110.44	106.41
4	C	501	HEM	C4C-C3C-C2C	5.11	111.25	106.81
7	Q	501	HEC	CAD-C3D-C4D	4.99	134.69	124.94
5	P	503	SMA	C14-C15-C16	-4.85	116.06	125.88
7	D	501	HEC	CAD-C3D-C4D	4.84	134.39	124.94
5	C	503	SMA	C17-C18-C19	-4.80	113.20	126.36
7	Q	501	HEC	CBD-CAD-C3D	4.77	125.72	112.53
7	D	501	HEC	CBD-CAD-C3D	4.69	125.50	112.53
7	Q	501	HEC	CMC-C2C-C1C	-4.64	118.35	125.42
4	C	502	HEM	C1D-C2D-C3D	4.47	111.68	106.98
5	C	503	SMA	O1-C2-C9	4.40	119.46	110.12
4	C	502	HEM	CMD-C2D-C1D	-4.39	118.18	125.03
7	Q	501	HEC	CAA-C2A-C1A	4.24	133.46	124.85
5	P	503	SMA	C16-C17-C18	-4.04	115.09	124.65
7	D	501	HEC	CAA-C2A-C1A	4.03	133.04	124.85
5	C	503	SMA	C7M-O7-C7	4.00	123.38	117.51
7	Q	501	HEC	CBC-CAC-C3C	-3.93	119.59	127.43
4	P	502	HEM	CMB-C2B-C1B	3.86	131.06	125.03
7	Q	501	HEC	C4D-C3D-C2D	-3.85	100.92	106.87
5	P	503	SMA	C22-C11-C12	3.82	117.39	111.14
5	C	503	SMA	C22-C11-C10	3.82	116.25	110.34
5	C	503	SMA	O1-C8A-C8	3.82	123.85	116.28
5	C	503	SMA	O5-C5-C6	-3.75	117.62	124.08
4	P	502	HEM	CMC-C2C-C1C	-3.69	118.23	124.73
5	P	503	SMA	C9-C10-C11	-3.67	107.60	114.46
4	C	502	HEM	CMB-C2B-C3B	-3.67	119.56	128.43
5	P	503	SMA	C7M-O7-C7	3.56	122.73	117.51
4	P	501	HEM	C4C-C3C-C2C	3.54	109.89	106.81
5	C	503	SMA	O4-C4-C3	-3.51	115.84	120.45
4	P	502	HEM	CMB-C2B-C3B	-3.50	119.95	128.43
7	D	501	HEC	CAA-C2A-C3A	-3.47	121.37	127.87
4	P	502	HEM	CHD-C4C-NC	-3.45	120.70	124.45
7	D	501	HEC	C4D-C3D-C2D	-3.44	101.55	106.87
4	P	502	HEM	C3B-C2B-C1B	3.43	108.98	106.41
4	C	501	HEM	CMC-C2C-C1C	3.41	130.73	124.73
5	P	503	SMA	O5-C5-C4A	3.35	120.59	115.84
5	P	503	SMA	O8-C8-C7	3.34	126.40	119.21
7	Q	501	HEC	CAA-C2A-C3A	-3.30	121.69	127.87
7	D	501	HEC	CMD-C2D-C1D	3.22	130.32	125.42
4	C	502	HEM	CMB-C2B-C1B	3.18	130.00	125.03
5	C	503	SMA	C4A-C8A-C8	-3.16	117.14	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	502	HEM	C1D-C2D-C3D	3.08	110.22	106.98
7	D	501	HEC	CBA-CAA-C2A	3.05	120.96	112.53
4	C	502	HEM	C4C-CHD-C1D	-3.05	119.54	126.02
7	D	501	HEC	O1A-CGA-CBA	-2.99	113.60	123.09
5	C	503	SMA	O8-C8-C7	-2.98	112.81	119.21
7	Q	501	HEC	C3D-C4D-ND	2.96	113.44	110.15
4	C	501	HEM	CAA-CBA-CGA	-2.96	105.82	113.67
4	P	502	HEM	CMD-C2D-C1D	-2.94	120.44	125.03
4	C	501	HEM	CAC-C3C-C2C	-2.89	119.03	128.43
4	C	502	HEM	C2D-C1D-ND	-2.87	106.58	109.90
4	C	502	HEM	C2B-C1B-NB	-2.85	106.56	109.84
7	D	501	HEC	CHA-C1A-C2A	2.84	129.34	124.86
4	P	502	HEM	C2B-C1B-NB	-2.84	106.58	109.84
4	P	501	HEM	CAC-C3C-C2C	-2.81	119.31	128.43
4	P	501	HEM	C3B-C4B-NB	-2.80	107.46	109.47
4	P	502	HEM	CHD-C4C-C3C	2.78	129.89	125.21
5	C	503	SMA	O8-C8-C8A	2.78	126.10	119.86
5	P	503	SMA	C7-C6-C5	2.75	124.29	118.98
4	P	501	HEM	CMB-C2B-C1B	-2.75	120.74	125.03
7	Q	501	HEC	CBA-CAA-C2A	2.73	120.09	112.53
5	P	503	SMA	O5-C5-C6	-2.72	119.40	124.08
4	P	501	HEM	C4B-C3B-C2B	2.70	109.76	107.28
4	C	501	HEM	CBD-CAD-C3D	-2.70	105.08	112.53
4	C	501	HEM	CHC-C4B-NB	2.69	127.32	124.42
7	D	501	HEC	C4D-CHA-C1A	2.65	132.85	124.66
5	C	503	SMA	C16-C17-C18	-2.59	118.51	124.65
7	D	501	HEC	CHA-C1A-NA	-2.59	121.64	124.45
4	P	501	HEM	CBA-CAA-C2A	-2.58	105.39	112.53
5	C	503	SMA	O12-C12-C13	2.57	111.77	107.97
7	Q	501	HEC	O1A-CGA-CBA	-2.57	114.94	123.09
4	P	502	HEM	O1D-CGD-CBD	-2.56	114.97	123.09
7	D	501	HEC	C3D-C4D-ND	2.56	112.99	110.15
4	P	501	HEM	CBD-CAD-C3D	-2.53	105.55	112.53
4	C	501	HEM	CBA-CAA-C2A	-2.50	105.62	112.53
4	C	501	HEM	C4B-C3B-C2B	2.48	109.56	107.28
4	P	501	HEM	CAC-C3C-C4C	2.47	130.72	124.82
5	C	503	SMA	O4-C4-C4A	2.47	126.53	122.06
5	P	503	SMA	C22-C11-C10	2.46	114.14	110.34
4	P	502	HEM	C1B-NB-C4B	2.43	108.09	105.21
4	P	501	HEM	CHC-C1C-NC	2.42	127.09	124.45
4	P	502	HEM	C4A-CHB-C1B	-2.41	120.58	126.25
7	Q	501	HEC	C4D-CHA-C1A	2.39	132.03	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	501	HEM	CAA-CBA-CGA	-2.39	107.34	113.67
4	P	502	HEM	C4C-CHD-C1D	-2.36	120.99	126.02
4	C	502	HEM	C4A-CHB-C1B	-2.36	120.69	126.25
7	Q	501	HEC	C4A-C3A-C2A	2.36	110.47	106.97
7	Q	501	HEC	CHA-C1A-NA	-2.34	121.91	124.45
4	P	501	HEM	C4A-C3A-C2A	2.34	109.49	106.82
4	C	502	HEM	C1C-CHC-C4B	2.33	130.97	126.02
7	D	501	HEC	CHC-C1C-NC	2.30	128.03	123.86
4	P	501	HEM	CHD-C1D-C2D	2.28	128.63	125.03
7	D	501	HEC	C4A-C3A-C2A	2.26	110.33	106.97
7	Q	501	HEC	CHA-C1A-C2A	2.25	128.41	124.86
5	P	503	SMA	C13-C14-C15	2.22	116.91	112.11
4	C	502	HEM	C4D-ND-C1D	2.21	107.82	105.21
4	P	501	HEM	CMC-C2C-C3C	-2.19	123.12	128.43
4	C	502	HEM	CHD-C4C-C3C	2.19	128.89	125.21
7	Q	501	HEC	C4D-ND-C1D	2.18	109.38	105.82
5	C	503	SMA	C25-O14-C14	2.17	117.96	112.99
4	P	501	HEM	C1B-NB-C4B	2.17	107.77	105.21
5	P	503	SMA	O4-C4-C3	-2.16	117.60	120.45
4	C	502	HEM	C1B-NB-C4B	2.15	107.76	105.21
5	P	503	SMA	O8-C8-C8A	-2.15	115.03	119.86
4	C	502	HEM	CAB-C3B-C2B	-2.14	121.46	128.43
7	D	501	HEC	C4D-ND-C1D	2.14	109.31	105.82
4	P	501	HEM	CMC-C2C-C1C	2.13	128.47	124.73
4	P	502	HEM	CAB-C3B-C2B	-2.12	121.52	128.43
7	D	501	HEC	CHD-C4C-NC	2.11	126.75	124.45
5	P	503	SMA	O7-C7-C6	-2.11	120.45	124.08
4	C	501	HEM	CMC-C2C-C3C	-2.10	123.35	128.43
5	P	503	SMA	C11-C12-C13	-2.07	108.76	114.29
4	C	501	HEM	CAB-C3B-C4B	-2.06	115.31	124.39
5	P	503	SMA	C17-C18-C19	-2.05	120.73	126.36
4	C	502	HEM	O1D-CGD-CBD	-2.05	116.60	123.09
4	P	501	HEM	C4D-ND-C1D	2.04	107.63	105.21
4	C	501	HEM	CAC-C3C-C4C	2.04	129.70	124.82
4	C	502	HEM	O2A-CGA-CBA	2.04	120.44	114.00
4	C	502	HEM	CAD-C3D-C2D	2.02	131.65	127.87
4	P	502	HEM	C3C-C2C-C1C	2.01	108.94	107.05
4	P	501	HEM	CAD-CBD-CGD	-2.01	108.35	113.67
4	P	501	HEM	CMB-C2B-C3B	2.00	133.27	128.43
4	P	501	HEM	CHC-C4B-NB	2.00	126.58	124.42

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	503	SMA	C13-C14-O14-C25
5	C	503	SMA	C17-C18-C19-C20
5	C	503	SMA	C17-C18-C19-C26
5	P	503	SMA	C3-C2-C9-C10
5	P	503	SMA	O1-C2-C9-C10
5	P	503	SMA	C17-C18-C19-C20
5	P	503	SMA	C17-C18-C19-C26
7	D	501	HEC	C1A-C2A-CAA-CBA
7	D	501	HEC	C3A-C2A-CAA-CBA
7	D	501	HEC	C2B-C3B-CAB-CBB
7	D	501	HEC	C2C-C3C-CAC-CBC
7	D	501	HEC	C4C-C3C-CAC-CBC
7	Q	501	HEC	C1A-C2A-CAA-CBA
7	Q	501	HEC	C3A-C2A-CAA-CBA
7	Q	501	HEC	C2B-C3B-CAB-CBB
7	Q	501	HEC	C2C-C3C-CAC-CBC
7	Q	501	HEC	C4C-C3C-CAC-CBC
5	C	503	SMA	C9-C10-C11-C22
7	D	501	HEC	C4D-C3D-CAD-CBD
7	Q	501	HEC	C4D-C3D-CAD-CBD
4	C	501	HEM	C3D-CAD-CBD-CGD
4	P	501	HEM	C3D-CAD-CBD-CGD
5	C	503	SMA	C6-C5-O5-C5M
5	P	503	SMA	C6-C5-O5-C5M
7	D	501	HEC	C2D-C3D-CAD-CBD
7	Q	501	HEC	C2D-C3D-CAD-CBD
4	C	502	HEM	C2A-CAA-CBA-CGA
4	P	502	HEM	C2A-CAA-CBA-CGA
5	P	503	SMA	C4A-C5-O5-C5M
5	C	503	SMA	C4A-C5-O5-C5M
5	C	503	SMA	C15-C14-O14-C25
9	Q	502	PG6	O3-C6-C7-O4
5	P	503	SMA	C24-C13-C14-O14
5	P	503	SMA	C12-C13-C14-O14
5	P	503	SMA	C15-C16-C17-C18
5	C	503	SMA	C8-C7-O7-C7M
5	P	503	SMA	C15-C14-O14-C25
5	C	503	SMA	C11-C10-C9-C2
7	Q	501	HEC	C3D-CAD-CBD-CGD
5	C	503	SMA	C6-C7-O7-C7M
5	C	503	SMA	C24-C13-C14-C15
5	P	503	SMA	C24-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
5	P	503	SMA	C12-C13-C14-C15
5	P	503	SMA	C13-C14-O14-C25
7	D	501	HEC	C4B-C3B-CAB-CBB
7	Q	501	HEC	C4B-C3B-CAB-CBB
5	P	503	SMA	O14-C14-C15-C16
7	D	501	HEC	C3D-CAD-CBD-CGD
5	C	503	SMA	C12-C13-C14-C15
7	D	501	HEC	CAD-CBD-CGD-O2D
7	Q	501	HEC	CAD-CBD-CGD-O2D
7	Q	501	HEC	CAD-CBD-CGD-O1D
4	C	501	HEM	CAA-CBA-CGA-O1A
7	D	501	HEC	CAD-CBD-CGD-O1D
4	P	502	HEM	C3D-CAD-CBD-CGD
4	P	501	HEM	CAA-CBA-CGA-O1A
9	Q	502	PG6	O4-C8-C9-O5
4	C	502	HEM	CAA-CBA-CGA-O2A
4	P	502	HEM	CAA-CBA-CGA-O2A
4	P	502	HEM	CAA-CBA-CGA-O1A
4	C	502	HEM	CAA-CBA-CGA-O1A
5	C	503	SMA	C24-C13-C14-O14
5	P	503	SMA	C13-C14-C15-C16
5	C	503	SMA	C12-C13-C14-O14
4	C	501	HEM	CAA-CBA-CGA-O2A
4	P	501	HEM	CAA-CBA-CGA-O2A
9	Q	502	PG6	O2-C4-C5-O3
4	P	502	HEM	CAD-CBD-CGD-O2D

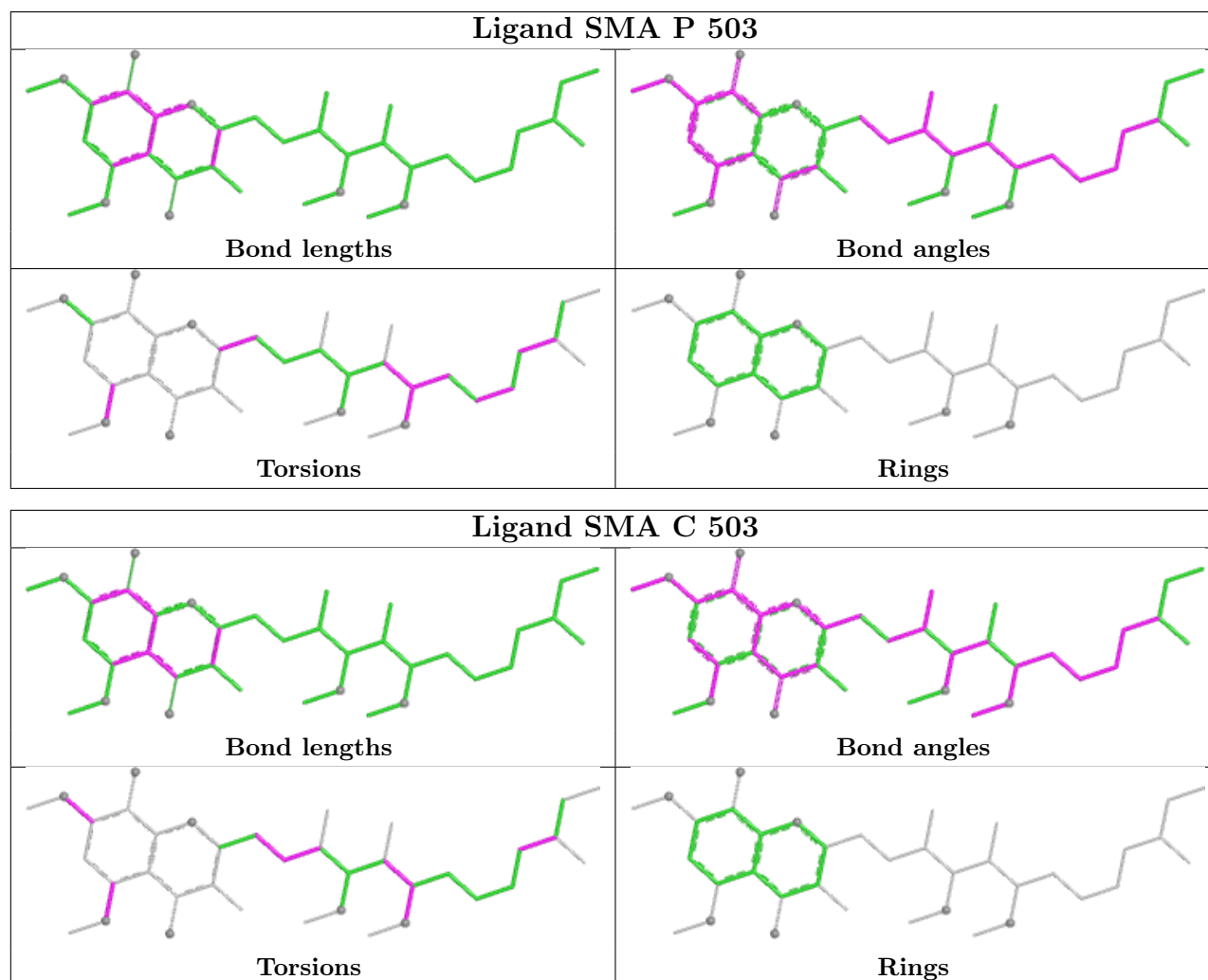
There are no ring outliers.

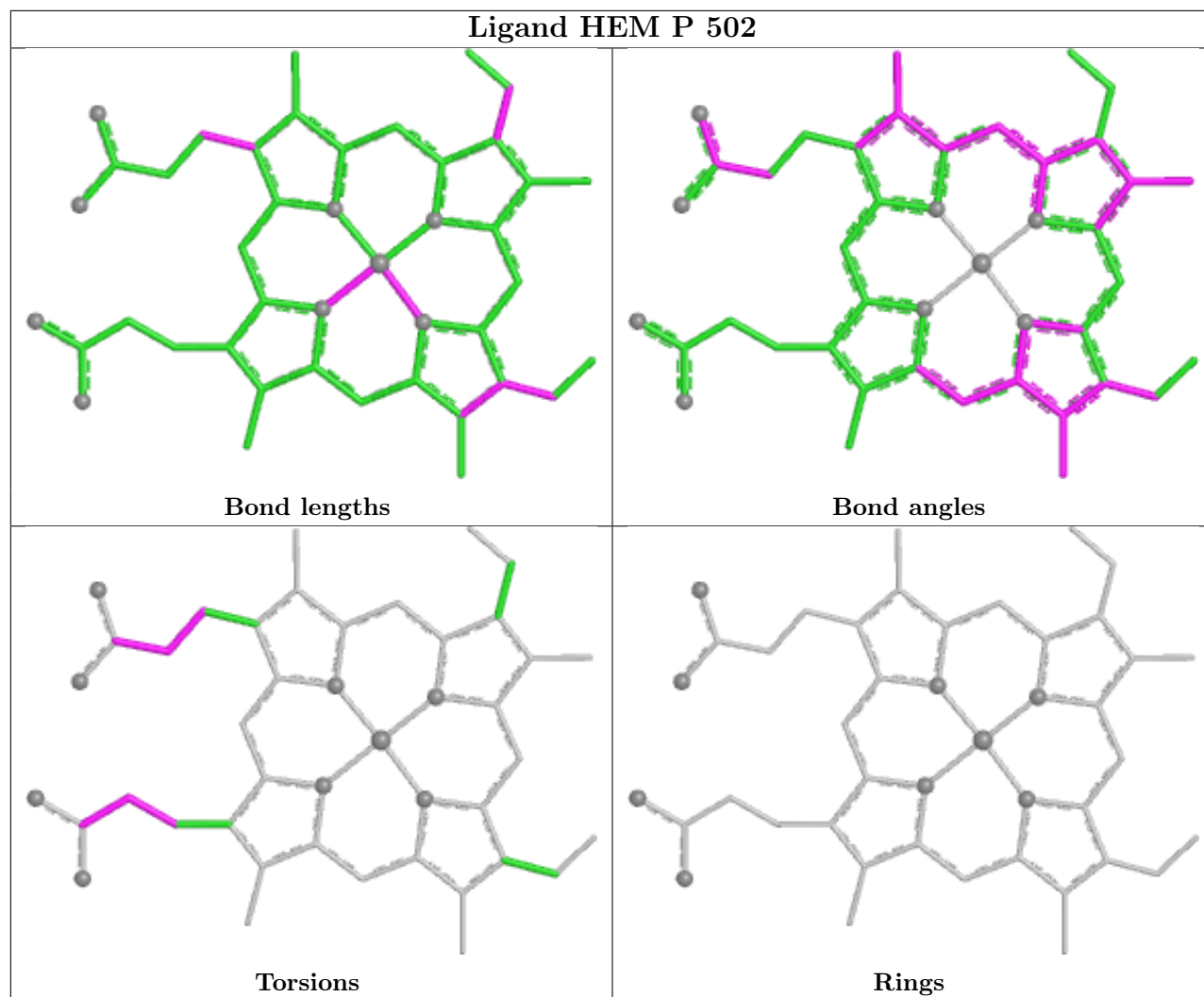
7 monomers are involved in 25 short contacts:

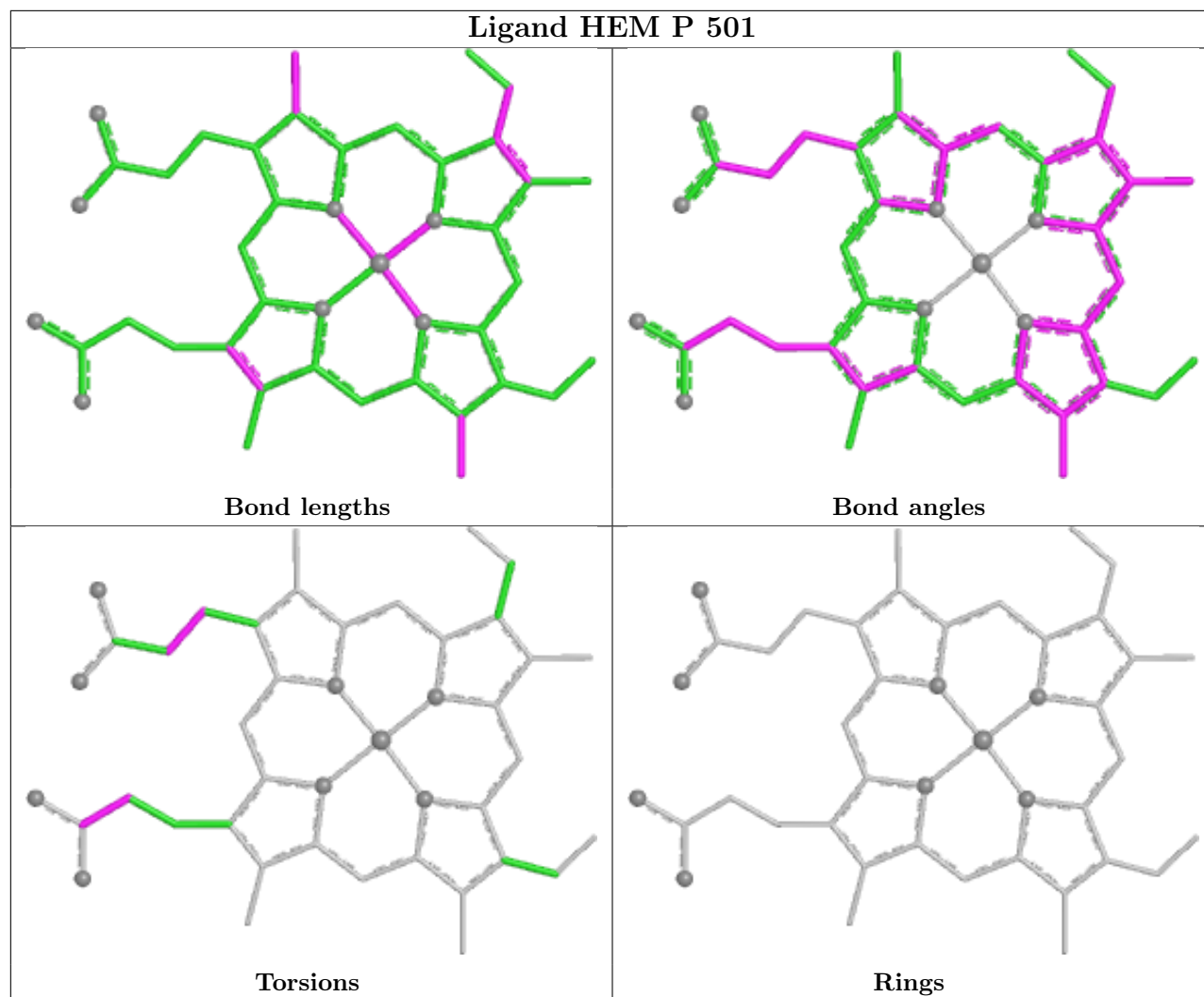
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	503	SMA	3	0
5	C	503	SMA	4	0
4	P	501	HEM	3	0
8	R	501	FES	1	0
7	D	501	HEC	5	0
7	Q	501	HEC	7	0
4	C	501	HEM	2	0

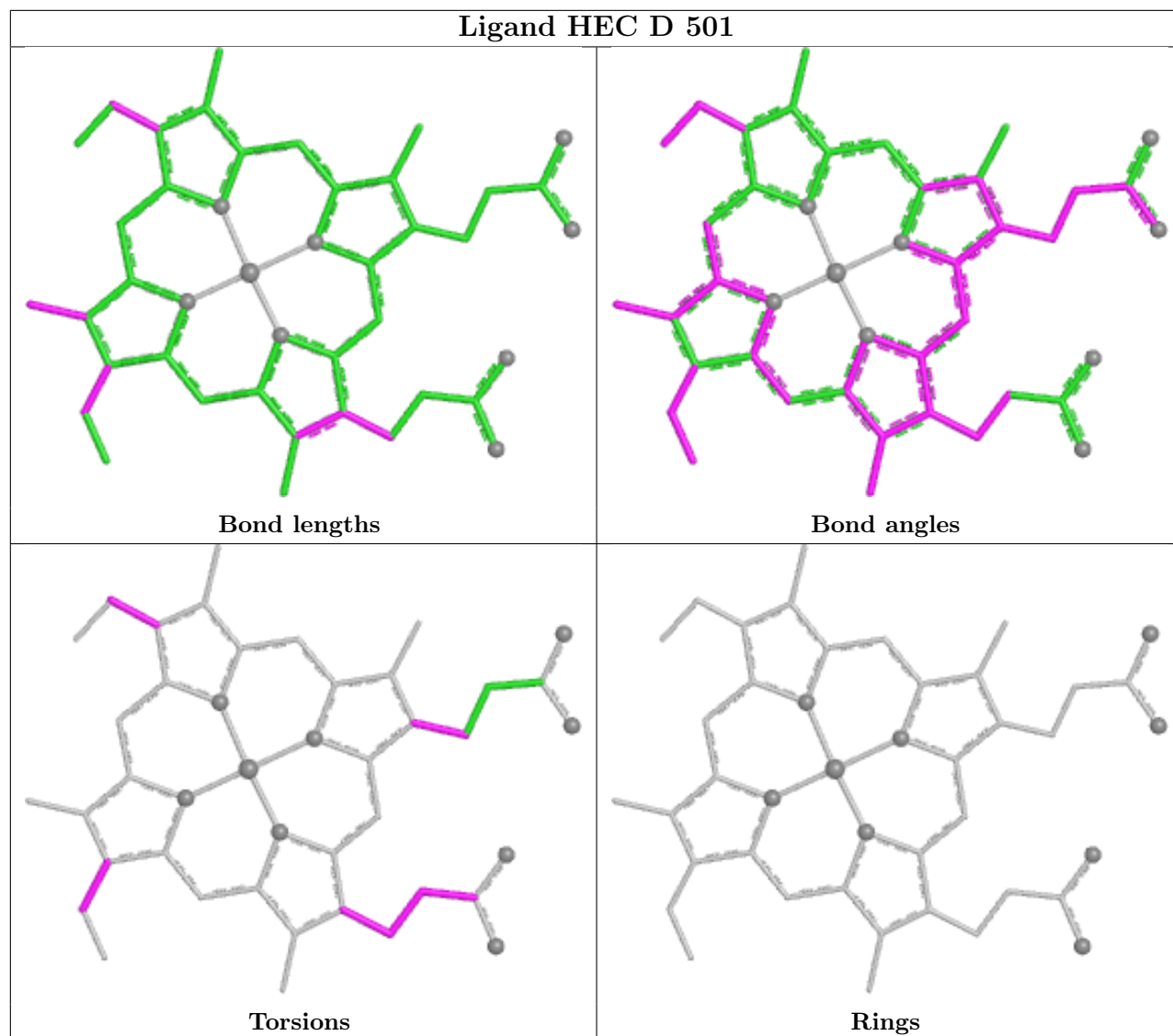
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

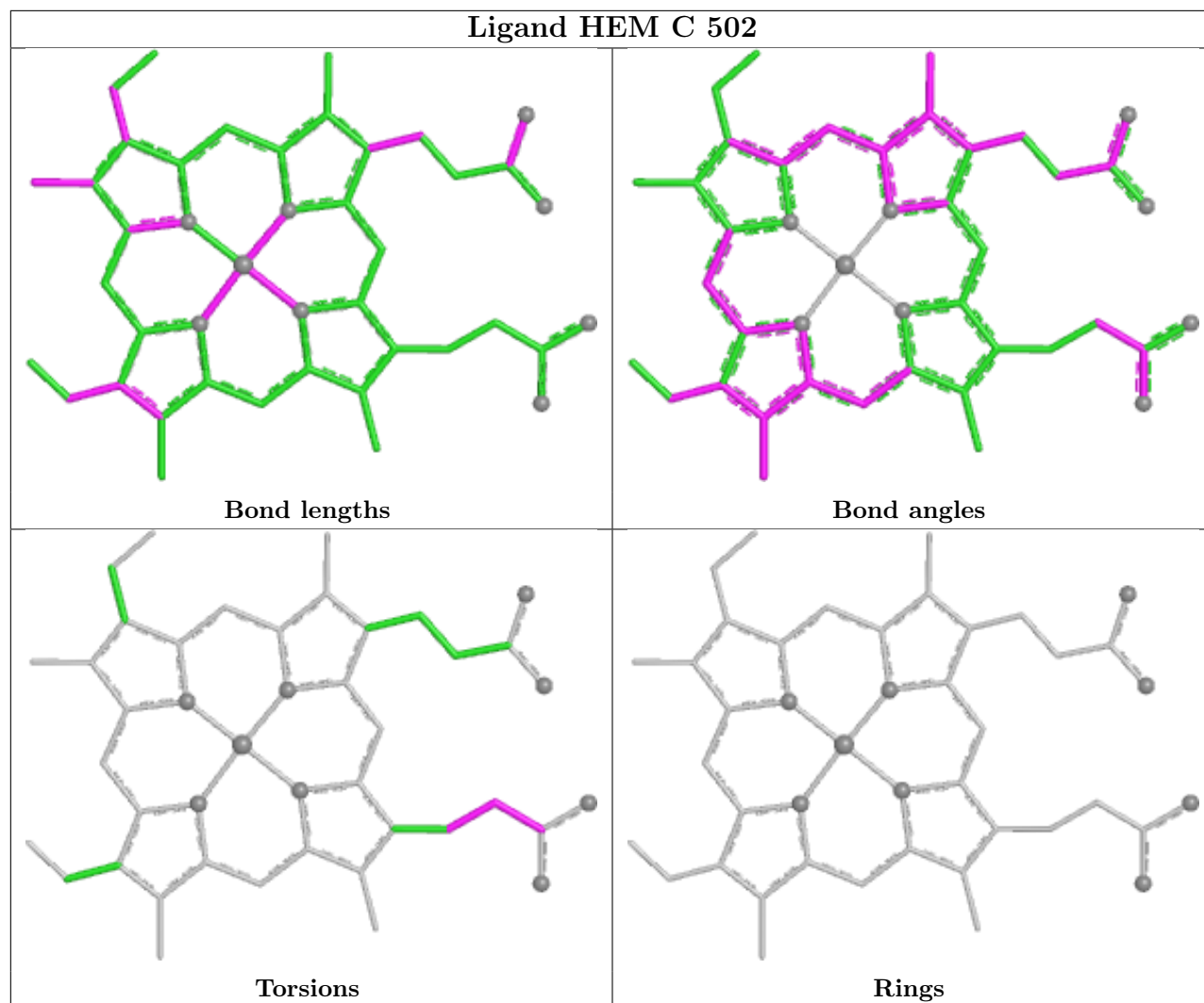
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

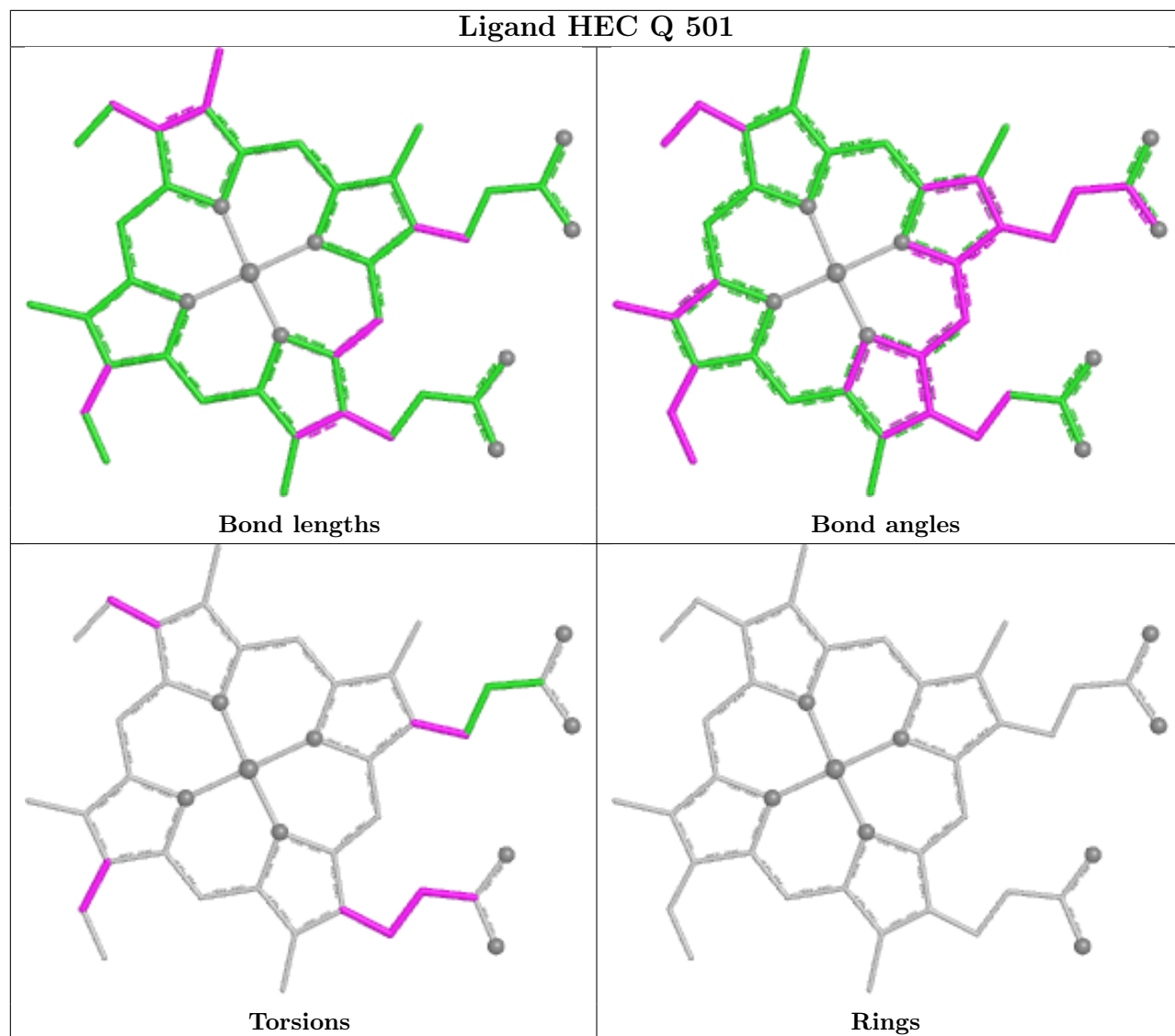


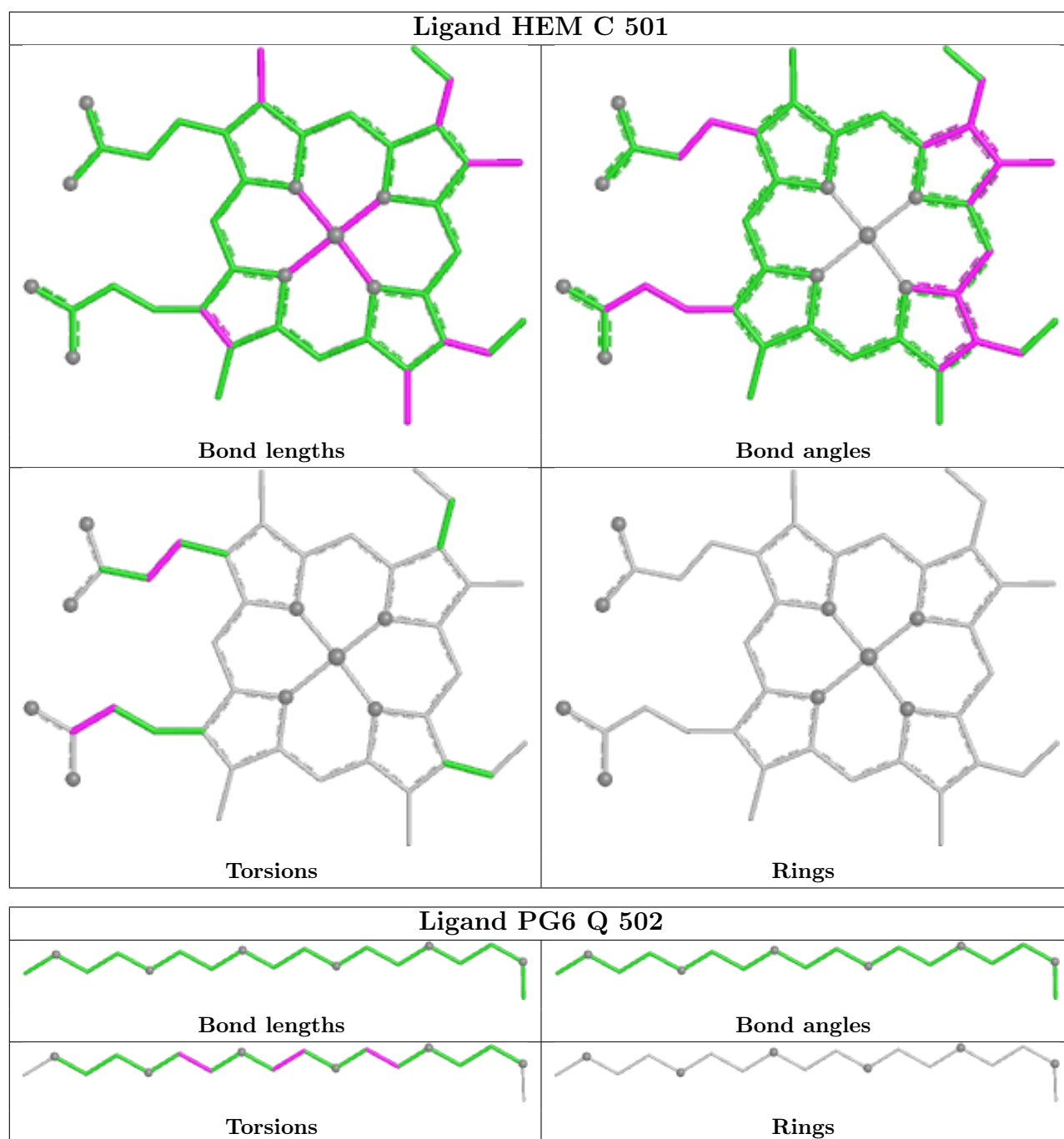












5.7 Other polymers [i](#)

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	431/437 (98%)	0.07	11 (2%) 57 32	48, 101, 141, 197	1 (0%)
1	P	431/437 (98%)	0.39	37 (8%) 16 11	48, 101, 141, 170	1 (0%)
2	D	248/258 (96%)	0.22	19 (7%) 19 13	97, 140, 179, 228	0
2	Q	248/258 (96%)	0.25	14 (5%) 30 17	95, 139, 181, 230	0
3	E	183/191 (95%)	0.72	25 (13%) 6 5	84, 126, 167, 185	0
3	R	183/191 (95%)	0.19	9 (4%) 35 19	88, 129, 170, 190	0
All	All	1724/1772 (97%)	0.28	115 (6%) 24 15	48, 118, 167, 230	2 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	290	ALA	10.3
1	P	291	HIS	7.2
3	E	152	PHE	6.7
1	P	276	HIS	6.6
3	E	147	ASP	6.3
3	E	141	MET	6.0
3	E	168	LYS	5.7
3	R	122	ASN	5.7
3	E	148	PHE	5.4
3	E	154	PRO	5.3
1	P	278	ASP	5.2
2	Q	106	ALA	4.9
3	E	10	THR	4.9
1	P	414	THR	4.7
3	E	146	GLY	4.5
3	R	124	GLY	4.5
2	D	160	ILE	4.4
1	P	277	PRO	4.4
3	E	157	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	P	362	LYS	4.3
1	P	5	PRO	4.3
1	P	171	GLY	4.3
3	R	123	THR	4.2
1	P	295[A]	GLU	4.2
2	D	212	PHE	4.1
1	C	42	ASN	4.1
1	P	386	GLU	3.9
3	E	11	ARG	3.9
2	D	99	ASP	3.8
2	D	213	LEU	3.8
3	E	159	HIS	3.7
2	D	244	LEU	3.6
1	C	252	ASP	3.6
1	P	197	LEU	3.6
2	D	108	ALA	3.5
2	Q	108	ALA	3.5
2	Q	67	GLY	3.5
2	Q	32	GLU	3.4
1	C	249	VAL	3.4
1	P	6	HIS	3.4
2	D	103	MET	3.4
2	D	106	ALA	3.4
1	C	166	PHE	3.3
1	C	295[A]	GLU	3.3
1	C	33	ILE	3.3
1	P	275	GLY	3.3
1	C	291	HIS	3.3
2	Q	107	ARG	3.3
3	E	149	GLY	3.2
1	C	176	ILE	3.2
2	D	98	PRO	3.2
1	P	361	PRO	3.2
3	R	79	GLU	3.2
3	E	17	HIS	3.2
3	E	143	ASP	3.1
3	E	167	ARG	3.1
1	P	293	VAL	3.1
1	P	302	TYR	3.1
3	R	111	GLU	3.1
1	P	3	GLY	3.1
1	P	270	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	P	273	TYR	3.0
2	D	107	ARG	3.0
3	E	145	SER	3.0
1	P	267	VAL	2.9
1	P	25	ILE	2.9
3	R	125	GLU	2.8
1	P	415	GLU	2.8
2	D	226	GLN	2.8
3	E	34	LEU	2.8
3	E	32	TRP	2.8
1	P	363	PHE	2.7
1	P	174	PRO	2.7
1	P	280	TYR	2.7
3	E	191	GLY	2.7
1	P	292	ILE	2.7
2	D	48	LEU	2.7
2	D	92	VAL	2.6
1	P	143	ALA	2.6
1	C	2	SER	2.6
1	P	2	SER	2.6
3	R	148	PHE	2.6
2	D	84	GLU	2.6
3	E	22	THR	2.5
2	Q	102	VAL	2.5
2	D	90	THR	2.5
1	P	187	ASP	2.5
2	Q	111	SER	2.5
2	Q	125	MET	2.5
3	E	183	VAL	2.4
2	D	41	LYS	2.4
2	Q	160	ILE	2.4
2	Q	75	ASP	2.3
1	P	189	ALA	2.3
2	Q	112	GLY	2.3
2	D	134	TYR	2.3
2	D	240	VAL	2.2
1	P	385	THR	2.2
2	D	27	PHE	2.2
3	E	35	ILE	2.2
1	P	31	ASP	2.2
1	P	343	MET	2.2
3	R	147	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	169	GLY	2.1
2	Q	63	GLU	2.1
2	Q	33	VAL	2.1
1	P	62	GLY	2.1
1	C	422	ALA	2.1
2	Q	110	PHE	2.1
1	P	186	VAL	2.1
1	P	167	GLY	2.0
3	E	184	ASP	2.0
3	R	168	LYS	2.0
3	E	142	GLY	2.0
1	C	263	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	UNL	C	505	8/-	0.69	0.14	99,113,116,122	0
6	UNL	C	504	17/-	0.74	0.21	97,127,136,148	17
9	PG6	Q	502	18/18	0.76	0.17	71,114,137,139	0
6	UNL	P	505	8/-	0.81	0.11	82,94,101,110	0
6	UNL	P	504	28/-	0.87	0.19	72,136,156,165	0
5	SMA	P	503	37/37	0.91	0.20	85,102,111,117	0
7	HEC	D	501	43/43	0.92	0.13	100,114,130,135	0
5	SMA	C	503	37/37	0.95	0.14	78,98,110,112	0
4	HEM	C	502	43/43	0.95	0.11	80,107,117,126	0
7	HEC	Q	501	43/43	0.96	0.10	100,113,129,136	0
4	HEM	P	502	43/43	0.96	0.10	79,106,117,128	0

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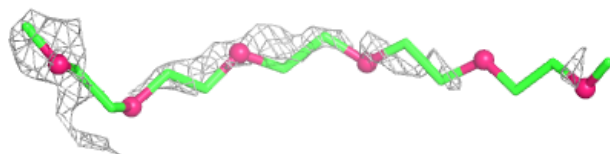
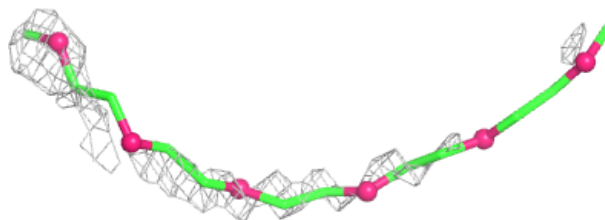
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	HEM	C	501	43/43	0.97	0.11	80,92,112,124	0
8	FES	E	501	4/4	0.97	0.04	88,99,112,114	0
4	HEM	P	501	43/43	0.97	0.14	73,91,105,129	0
8	FES	R	501	4/4	0.99	0.03	102,103,110,120	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

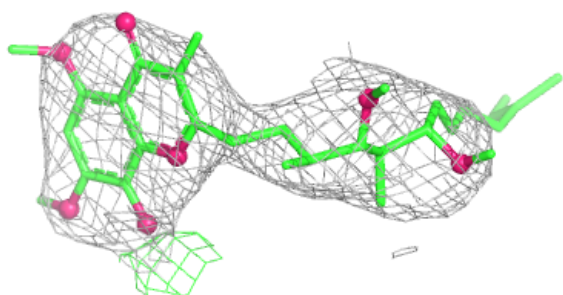
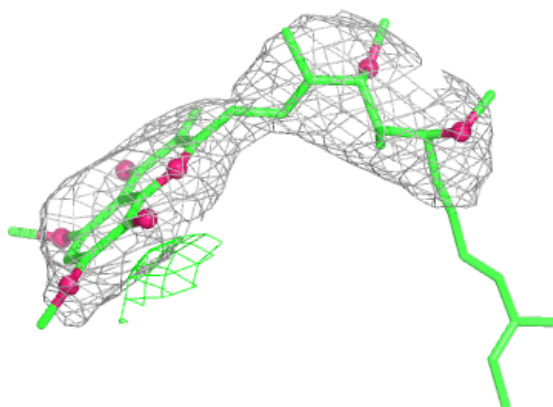
Electron density around PG6 Q 502:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



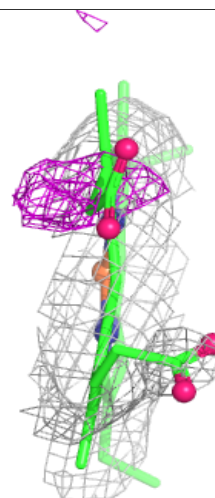
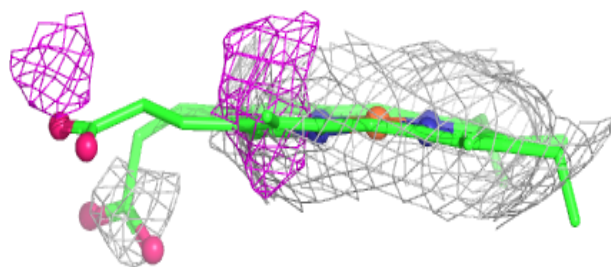
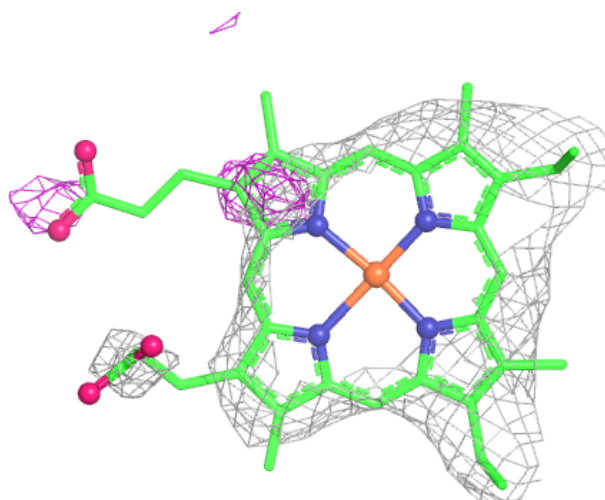
Electron density around SMA P 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



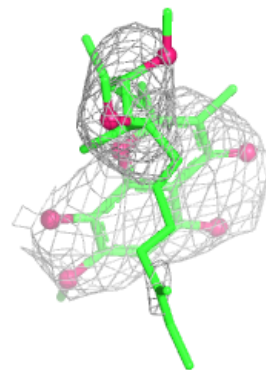
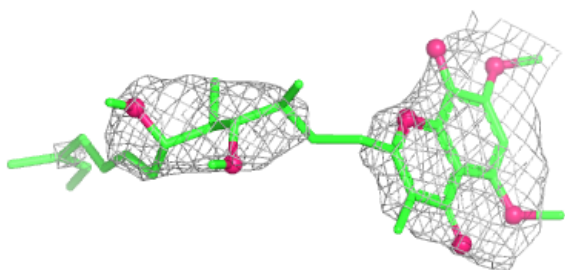
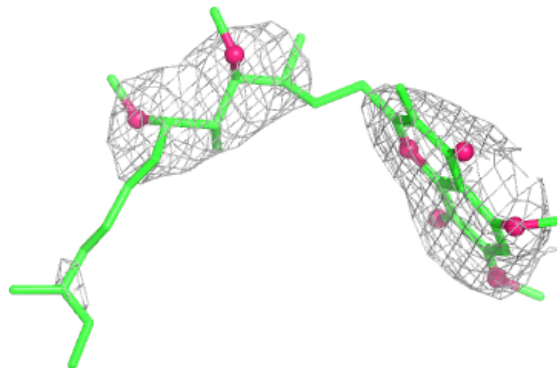
Electron density around HEC D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



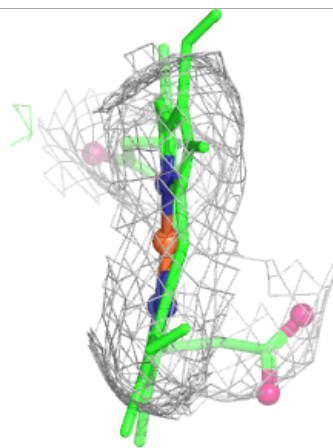
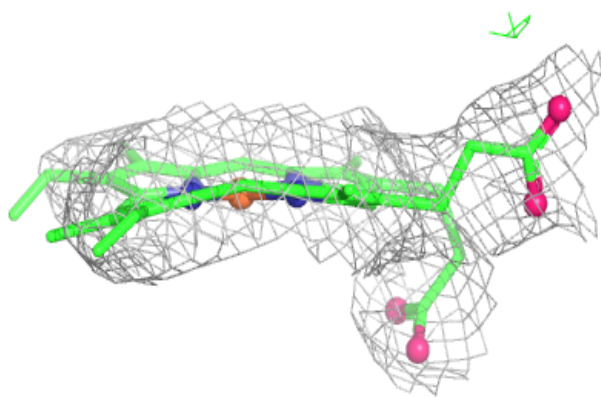
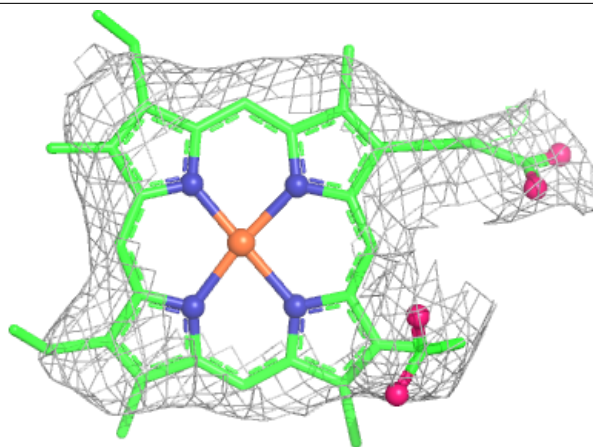
Electron density around SMA C 503:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



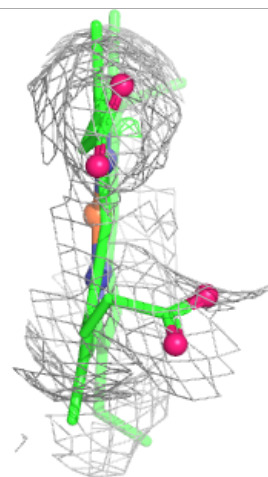
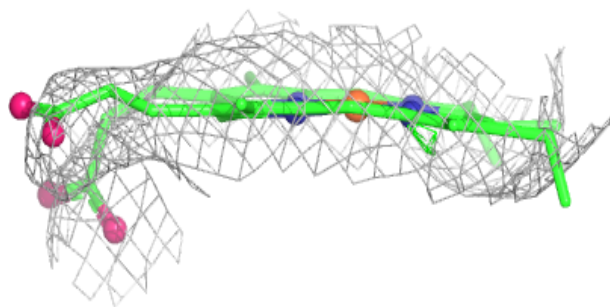
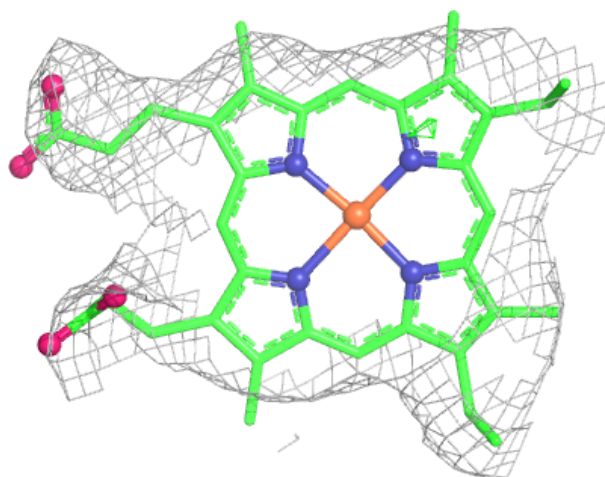
Electron density around HEM C 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



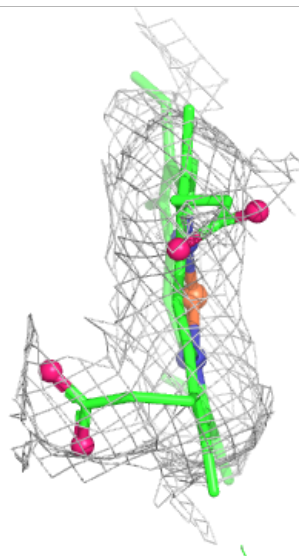
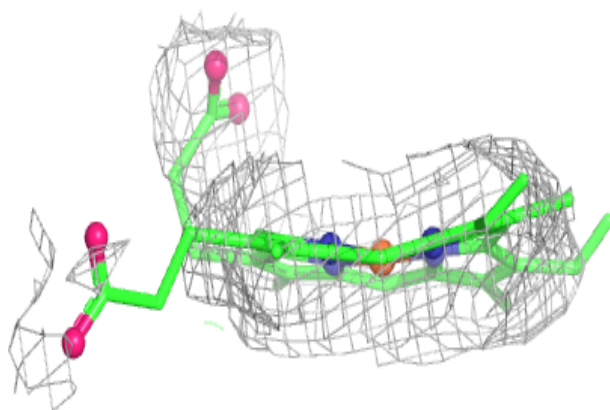
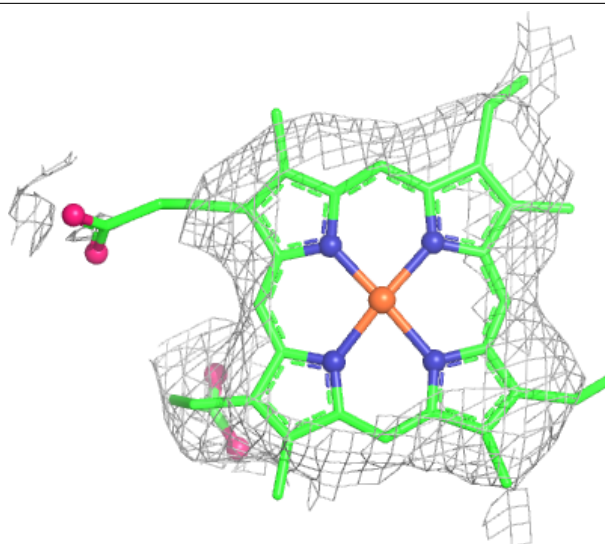
Electron density around HEC Q 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



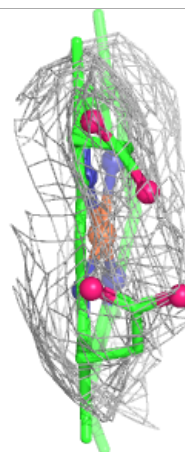
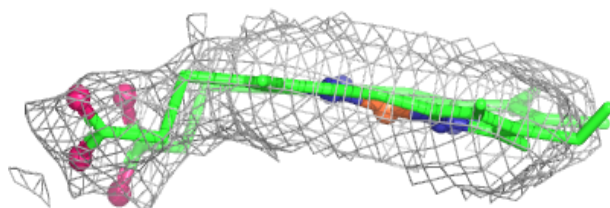
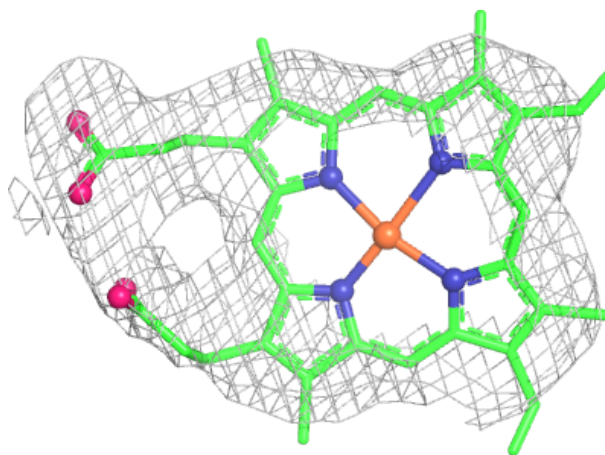
Electron density around HEM P 502:

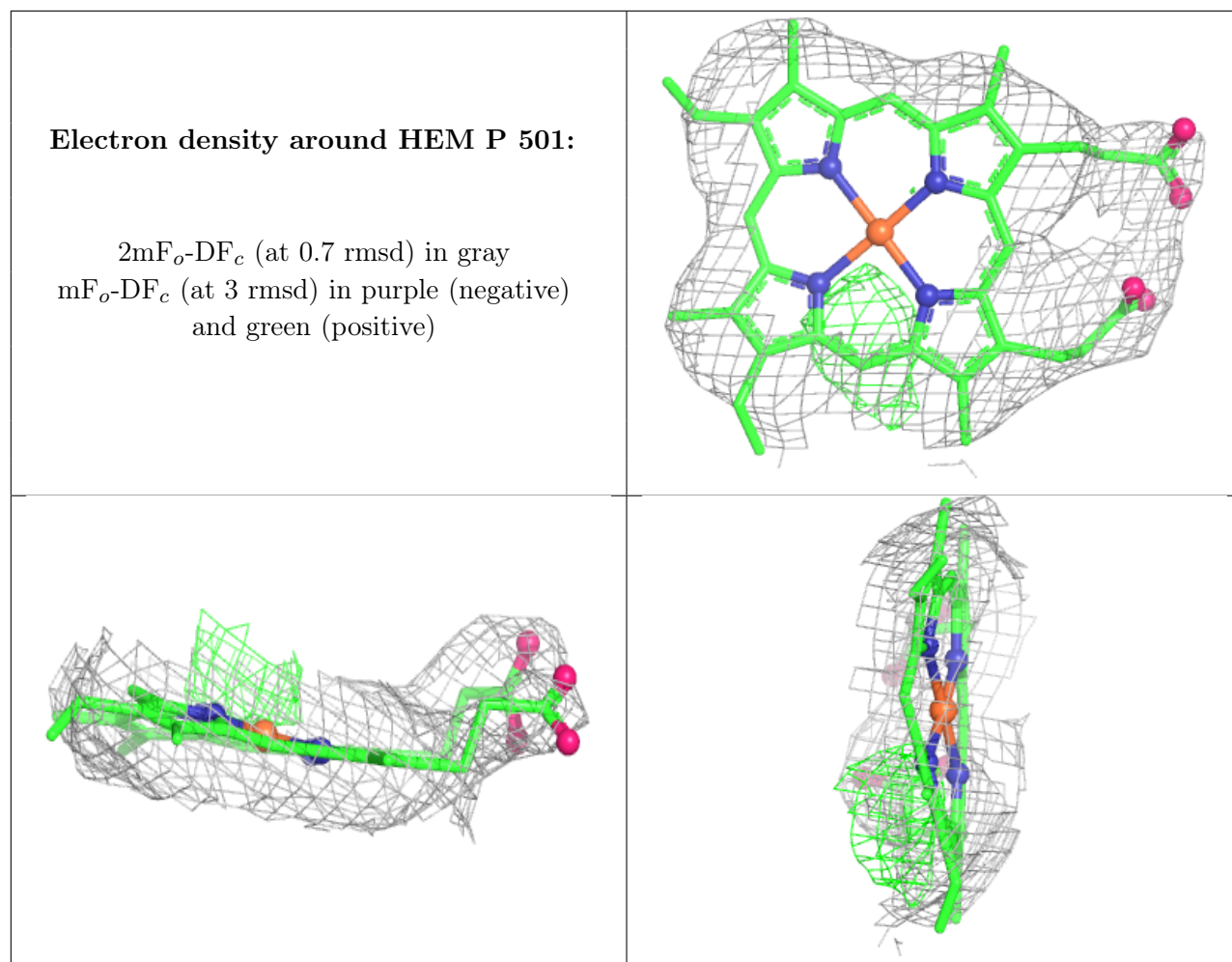
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.