



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:25 am BST

PDB ID : 3TTV
Title : Structure of the F413E variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2011-09-15
Resolution : 1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

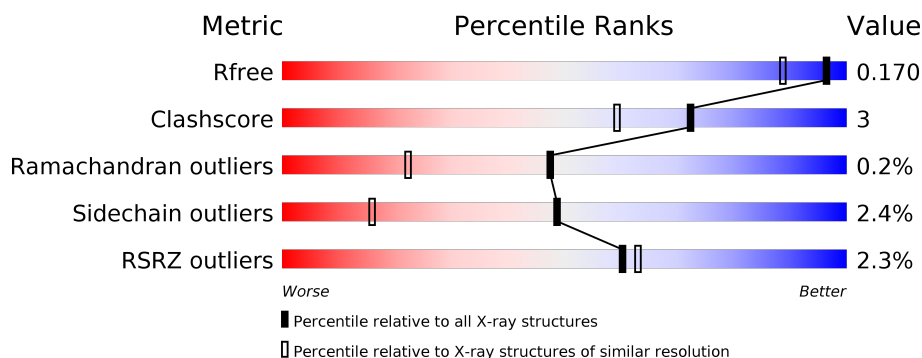
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 on 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	A	753	<div> <div> <div>0%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	753	<div> <div>3%</div> <div>81%</div> <div>14%</div> <div>• • •</div> </div>
1	C	753	<div> <div>3%</div> <div>83%</div> <div>12%</div> <div>• • •</div> </div>
1	D	753	<div> <div>2%</div> <div>83%</div> <div>12%</div> <div>• •</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26511 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 Catalase HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	3	0
			5755	3652	1006	1085	12			
1	B	726	Total	C	N	O	S	0	3	0
			5758	3654	1006	1086	12			
1	C	726	Total	C	N	O	S	0	2	0
			5750	3649	1006	1083	12			
1	D	726	Total	C	N	O	S	0	2	0
			5750	3649	1006	1083	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	ALA	THR	ENGINEERED MUTATION	UNP P21179
A	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179
B	115	ALA	THR	ENGINEERED MUTATION	UNP P21179
B	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179
C	115	ALA	THR	ENGINEERED MUTATION	UNP P21179
C	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179
D	115	ALA	THR	ENGINEERED MUTATION	UNP P21179
D	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

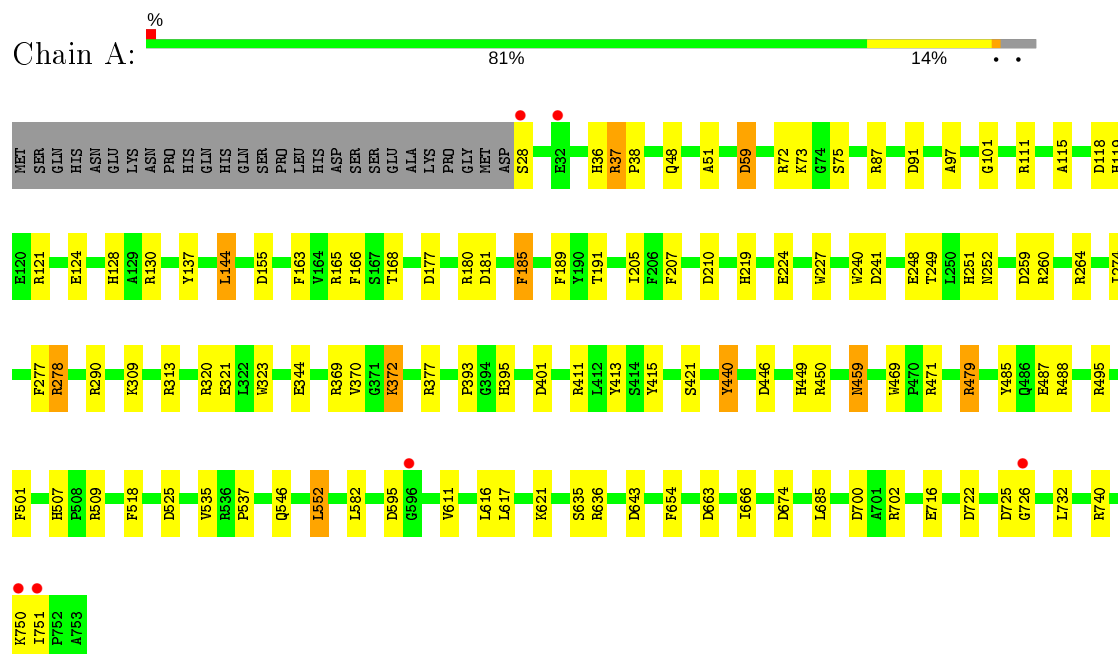
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	864	Total	O	0	0
			864	864		
3	B	775	Total	O	0	0
			775	775		
3	C	797	Total	O	0	0
			797	797		
3	D	890	Total	O	0	0
			890	890		

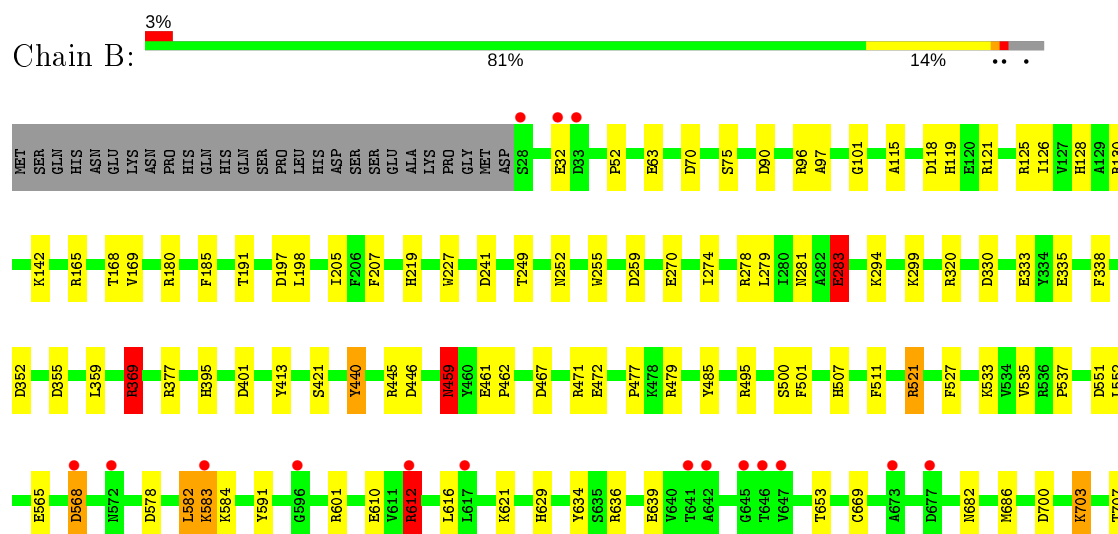
3 Residue-property plots

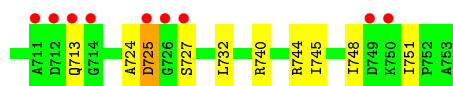
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

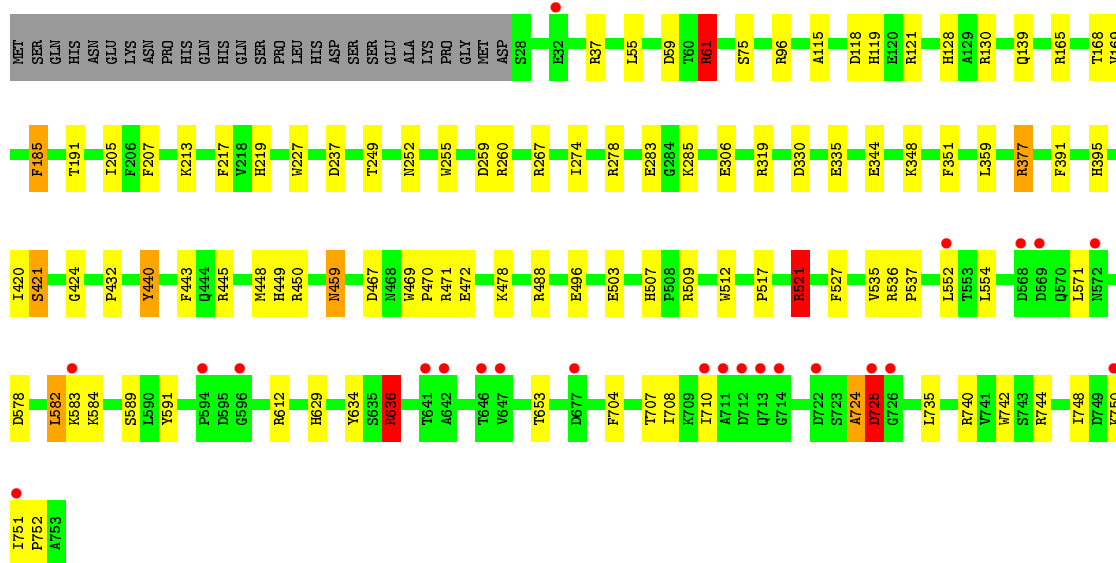
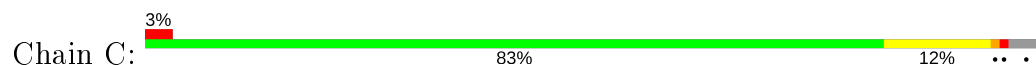


• Molecule 1: Catalase HPII

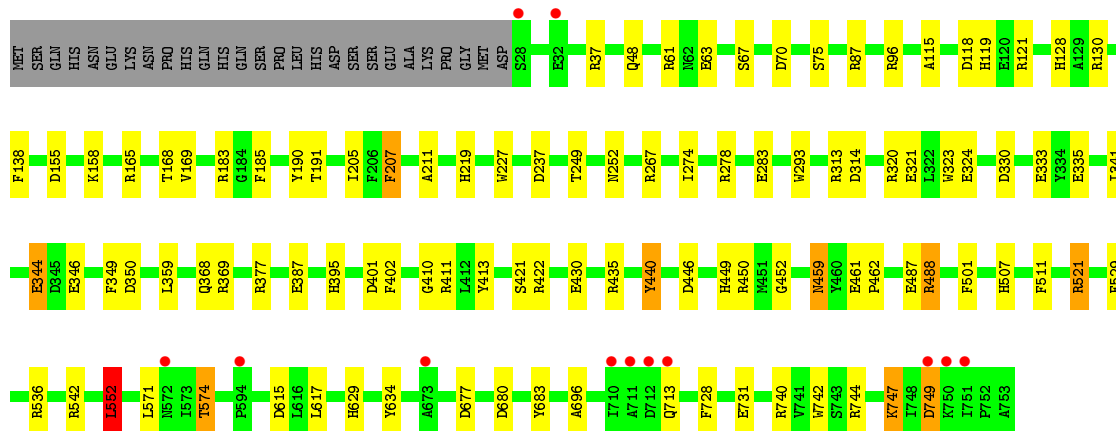
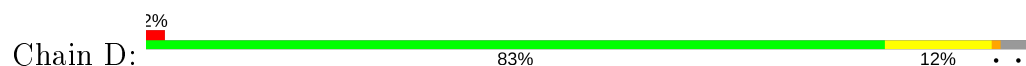




• Molecule 1: Catalase HP11



• Molecule 1: Catalase HP11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.56Å 133.05Å 122.64Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	32.16 – 1.45 32.16 – 1.45	Depositor EDS
% Data completeness (in resolution range)	96.8 (32.16-1.45) 96.8 (32.16-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.145 , 0.172 0.144 , 0.170	Depositor DCC
R_{free} test set	24236 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	26511	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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 ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.35	14/5911 (0.2%)	1.39	72/8035 (0.9%)
1	B	1.29	12/5914 (0.2%)	1.30	53/8040 (0.7%)
1	C	1.31	24/5903 (0.4%)	1.29	39/8024 (0.5%)
1	D	1.37	22/5903 (0.4%)	1.33	46/8024 (0.6%)
All	All	1.33	72/23631 (0.3%)	1.33	210/32123 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	3
All	All	0	4

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	GLU	CD-OE1	10.68	1.37	1.25
1	D	321	GLU	CD-OE1	9.68	1.36	1.25
1	A	440	TYR	CE1-CZ	8.67	1.49	1.38
1	C	59	ASP	CB-CG	8.35	1.69	1.51
1	D	440	TYR	CE1-CZ	8.06	1.49	1.38
1	A	716	GLU	CD-OE1	7.51	1.33	1.25
1	C	440	TYR	CE1-CZ	7.38	1.48	1.38
1	D	344	GLU	CD-OE2	7.07	1.33	1.25
1	A	344	GLU	CD-OE1	6.78	1.33	1.25
1	D	377	ARG	CZ-NH1	6.75	1.41	1.33
1	B	568	ASP	CB-CG	6.51	1.65	1.51
1	B	333	GLU	CD-OE1	-6.35	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	391	PHE	CG-CD1	6.30	1.48	1.38
1	D	37	ARG	CZ-NH1	6.29	1.41	1.33
1	C	377	ARG	CZ-NH1	6.21	1.41	1.33
1	A	469	TRP	CD2-CE2	6.19	1.48	1.41
1	C	742	TRP	CD2-CE2	6.15	1.48	1.41
1	D	368	GLN	CD-OE1	6.12	1.37	1.24
1	A	377	ARG	CZ-NH1	6.08	1.41	1.33
1	A	87	ARG	CZ-NH1	-6.03	1.25	1.33
1	A	323	TRP	CD2-CE2	5.96	1.48	1.41
1	C	255	TRP	CD2-CE2	5.83	1.48	1.41
1	B	472	GLU	CD-OE2	5.79	1.32	1.25
1	A	124	GLU	CD-OE1	5.78	1.32	1.25
1	A	635	SER	CB-OG	5.76	1.49	1.42
1	C	589	SER	CA-CB	5.72	1.61	1.52
1	C	377	ARG	CZ-NH2	5.67	1.40	1.33
1	A	180	ARG	CZ-NH1	5.66	1.40	1.33
1	C	591	TYR	CB-CG	5.65	1.60	1.51
1	D	430	GLU	CD-OE2	-5.63	1.19	1.25
1	B	255	TRP	CD2-CE2	5.62	1.48	1.41
1	B	63	GLU	CD-OE2	5.60	1.31	1.25
1	B	471	ARG	CZ-NH2	5.58	1.40	1.33
1	D	387	GLU	CD-OE2	-5.58	1.19	1.25
1	D	87	ARG	CZ-NH1	-5.56	1.25	1.33
1	D	165	ARG	CZ-NH2	5.54	1.40	1.33
1	C	512	TRP	CD2-CE2	5.53	1.48	1.41
1	C	469	TRP	CD2-CE2	5.50	1.48	1.41
1	C	527	PHE	CG-CD1	5.46	1.47	1.38
1	D	742	TRP	CD2-CE2	5.41	1.47	1.41
1	D	413	TYR	CG-CD1	5.41	1.46	1.39
1	C	744	ARG	CZ-NH1	5.40	1.40	1.33
1	D	346	GLU	CD-OE1	5.39	1.31	1.25
1	C	344	GLU	CD-OE1	5.37	1.31	1.25
1	C	503	GLU	CG-CD	5.35	1.59	1.51
1	C	472	GLU	CD-OE2	5.32	1.31	1.25
1	D	63	GLU	CD-OE2	5.32	1.31	1.25
1	D	323	TRP	CD2-CE2	5.30	1.47	1.41
1	B	459	ASN	CG-OD1	5.29	1.35	1.24
1	B	283	GLU	CG-CD	5.27	1.59	1.51
1	B	270	GLU	CD-OE2	5.27	1.31	1.25
1	D	333	GLU	CD-OE2	-5.25	1.19	1.25
1	B	744	ARG	CZ-NH1	5.24	1.39	1.33
1	A	189	PHE	CE1-CZ	5.19	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	335	GLU	CG-CD	5.18	1.59	1.51
1	A	240	TRP	CD2-CE2	5.14	1.47	1.41
1	A	320	ARG	CZ-NH1	5.12	1.39	1.33
1	C	59	ASP	CG-OD1	5.12	1.37	1.25
1	C	496	GLU	CD-OE2	5.10	1.31	1.25
1	C	344	GLU	CD-OE2	5.10	1.31	1.25
1	B	335	GLU	CB-CG	-5.07	1.42	1.52
1	D	293	TRP	CG-CD1	5.07	1.43	1.36
1	D	452	GLY	C-O	5.06	1.31	1.23
1	D	67	SER	CB-OG	5.05	1.48	1.42
1	C	421	SER	CB-OG	5.05	1.48	1.42
1	C	306	GLU	CD-OE2	5.04	1.31	1.25
1	B	500	SER	CB-OG	5.04	1.48	1.42
1	D	411	ARG	CZ-NH1	5.03	1.39	1.33
1	C	424	GLY	N-CA	5.03	1.53	1.46
1	D	683	TYR	CG-CD1	5.02	1.45	1.39
1	D	377	ARG	CZ-NH2	5.02	1.39	1.33
1	C	351	PHE	CG-CD2	5.01	1.46	1.38

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	A	130	ARG	NE-CZ-NH2	-12.87	113.87	120.30
1	B	495	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	636	ARG	NE-CZ-NH2	10.75	125.67	120.30
1	A	740	ARG	NE-CZ-NH2	-10.61	114.99	120.30
1	D	422	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	B	521	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	C	59	ASP	CB-CG-OD1	10.42	127.68	118.30
1	A	118	ASP	CB-CG-OD1	-9.92	109.37	118.30
1	B	70	ASP	CB-CG-OD1	9.88	127.19	118.30
1	A	377	ARG	NE-CZ-NH2	-9.85	115.37	120.30
1	C	445	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	D	96	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	D	118	ASP	CB-CG-OD1	-9.43	109.81	118.30
1	B	740	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	A	501	PHE	CB-CG-CD2	-9.26	114.32	120.80
1	B	198	LEU	CB-CG-CD1	9.22	126.68	111.00
1	C	521	ARG	CG-CD-NE	9.05	130.81	111.80
1	C	471	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	D	313	ARG	NE-CZ-NH1	8.93	124.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	377	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	A	501	PHE	CB-CG-CD1	8.89	127.03	120.80
1	A	130	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	B	445	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	B	369	ARG	NE-CZ-NH1	-8.66	115.97	120.30
1	C	278	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	A	488	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	A	509	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	B	377	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	B	352	ASP	CB-CG-OD2	8.47	125.92	118.30
1	D	542	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	D	411	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	C	185	PHE	CB-CG-CD2	-8.32	114.98	120.80
1	B	165	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	C	61	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	C	59	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	D	130	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	B	130	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	D	96	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	B	197	ASP	CB-CG-OD1	-7.94	111.15	118.30
1	D	344	GLU	CA-CB-CG	7.81	130.58	113.40
1	D	70	ASP	CB-CG-OD1	7.72	125.25	118.30
1	B	485	TYR	CB-CG-CD1	-7.63	116.42	121.00
1	C	740	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	D	313	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	260	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	B	130	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	411	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	471	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	C	536	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	A	278	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	A	518	PHE	CB-CG-CD1	-7.31	115.68	120.80
1	C	509	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	A	552	LEU	CB-CG-CD2	7.28	123.38	111.00
1	A	411	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	D	435	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	D	634	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	A	166	PHE	CB-CG-CD1	-7.17	115.78	120.80
1	D	501	PHE	CB-CG-CD2	-7.12	115.81	120.80
1	C	260	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	165	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	740	ARG	NE-CZ-NH1	7.09	123.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	180	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	D	207	PHE	CB-CG-CD1	-7.02	115.89	120.80
1	D	617	LEU	CB-CG-CD1	-6.97	99.15	111.00
1	C	285	LYS	CD-CE-NZ	-6.89	95.85	111.70
1	B	527	PHE	CB-CG-CD1	-6.84	116.01	120.80
1	C	319	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	259	ASP	CB-CG-OD1	-6.84	112.14	118.30
1	A	372	LYS	CD-CE-NZ	-6.83	95.99	111.70
1	D	61	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	B	401	ASP	CB-CG-OD2	6.81	124.43	118.30
1	D	488	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	D	350	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	B	369	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	A	313	ARG	NE-CZ-NH1	-6.77	116.91	120.30
1	B	467	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	D	552	LEU	CB-CG-CD2	6.76	122.49	111.00
1	A	525	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	A	259	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	A	488	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	C	217	PHE	CB-CG-CD2	-6.61	116.17	120.80
1	B	142	LYS	CD-CE-NZ	-6.61	96.50	111.70
1	B	601	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	D	740	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	259	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	177	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	A	290	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	C	118	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	A	248	GLU	OE1-CD-OE2	-6.44	115.57	123.30
1	D	450	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	B	241	ASP	CB-CG-OD2	6.35	124.02	118.30
1	B	501	PHE	CB-CG-CD1	6.35	125.25	120.80
1	A	485	TYR	CB-CG-CD1	-6.34	117.19	121.00
1	A	663	ASP	CB-CG-OD1	6.33	123.99	118.30
1	D	138	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	D	377	ARG	CG-CD-NE	-6.31	98.55	111.80
1	B	521	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	37	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	680	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	495	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	118	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	C	450	ARG	NE-CZ-NH2	-6.24	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	LYS	CD-CE-NZ	-6.23	97.38	111.70
1	B	90	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	446	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	450	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	471	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	722	ASP	CB-CG-OD2	6.13	123.82	118.30
1	D	401	ASP	CB-CG-OD2	6.12	123.81	118.30
1	B	278	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	267	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	D	37	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	D	446	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	111	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	D	617	LEU	CB-CG-CD2	6.03	121.25	111.00
1	D	121	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	518	PHE	CB-CG-CD2	5.99	124.99	120.80
1	B	479	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	654	PHE	CB-CG-CD1	-5.99	116.61	120.80
1	A	616	LEU	CB-CG-CD2	-5.95	100.88	111.00
1	A	259	ASP	CB-CG-OD2	5.94	123.65	118.30
1	C	96	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	582	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	A	72	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	A	185	PHE	CB-CG-CD2	-5.92	116.65	120.80
1	D	183	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	C	554	LEU	CB-CG-CD2	-5.89	100.99	111.00
1	A	260	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	125	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	139	GLN	N-CA-CB	-5.85	100.08	110.60
1	C	377	ARG	CA-CB-CG	-5.85	100.53	113.40
1	C	582	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	A	277	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	B	471	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	479	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	C	467	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	B	96	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	D	615	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	501	PHE	CB-CG-CD2	-5.75	116.78	120.80
1	C	37	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	348	LYS	CA-CB-CG	-5.72	100.81	113.40
1	C	260	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	C	213	LYS	CD-CE-NZ	-5.69	98.62	111.70
1	A	124	GLU	OE1-CD-OE2	-5.68	116.48	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	A	264	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	180	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	155	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	B	636	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	595	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	674	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	A	137	TYR	CZ-CE2-CD2	-5.58	114.77	119.80
1	A	210	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	224	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	B	551	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	D	61	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	C	735	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	A	155	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	495	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	377	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	338	PHE	CB-CG-CD1	-5.52	116.93	120.80
1	C	259	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	D	511	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	A	144	LEU	CB-CG-CD1	-5.43	101.76	111.00
1	B	355	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	702	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	C	636	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	A	166	PHE	CB-CG-CD2	5.40	124.58	120.80
1	D	377	ARG	NH1-CZ-NH2	5.40	125.33	119.40
1	A	59	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	C	185	PHE	CB-CG-CD1	5.38	124.56	120.80
1	C	335	GLU	OE1-CD-OE2	5.34	129.71	123.30
1	C	509	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	B	612	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	165	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	D	529	PHE	CB-CG-CD1	-5.31	117.09	120.80
1	B	279	LEU	CB-CG-CD1	-5.30	101.98	111.00
1	A	241	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	A	446	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	536	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	324	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	A	479	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	401	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	165	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	320	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	55	LEU	CB-CG-CD2	5.19	119.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	314	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	591	TYR	CZ-CE2-CD2	-5.16	115.16	119.80
1	A	611	VAL	CG1-CB-CG2	-5.16	102.65	110.90
1	A	621	LYS	CD-CE-NZ	-5.15	99.84	111.70
1	B	377	ARG	CG-CD-NE	-5.15	100.98	111.80
1	D	521	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	685	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	B	511	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	A	121	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	299	LYS	CD-CE-NZ	-5.10	99.97	111.70
1	A	582	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	D	349	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	D	402	PHE	CD1-CE1-CZ	-5.08	114.01	120.10
1	A	700	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	643	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	320	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	568	ASP	N-CA-CB	-5.04	101.54	110.60
1	A	91	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	C	130	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	181	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	477	PRO	N-CD-CG	-5.01	95.68	103.20
1	D	190	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	121	ARG	Sidechain
1	C	121	ARG	Sidechain
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

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	A	5755	0	5587	37	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5758	0	5589	53	2
1	C	5750	0	5583	35	0
1	D	5750	0	5583	41	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	1	0
3	A	864	0	0	9	1
3	B	775	0	0	15	0
3	C	797	0	0	9	0
3	D	890	0	0	16	1
All	All	26511	0	22462	153	3

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 3.

All (153) 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:B:521:ARG:HD3	3:B:3047:HOH:O	1.27	1.33
1:B:533:LYS:HE3	3:C:2623:HOH:O	1.28	1.26
1:D:449[B]:HIS:NE2	3:D:2501:HOH:O	1.65	1.24
1:A:546:GLN:HG3	3:A:3434:HOH:O	1.45	1.16
1:A:479:ARG:NH2	3:A:2607:HOH:O	1.89	1.05
1:B:294:LYS:HD2	3:B:3483:HOH:O	1.55	1.03
1:A:369:ARG:HD3	3:A:2403:HOH:O	1.61	1.00
1:D:341:ILE:HG13	3:D:3022:HOH:O	1.60	1.00
1:B:521:ARG:NH2	1:B:745:ILE:HD13	1.88	0.89
1:A:546:GLN:CG	3:A:3434:HOH:O	2.12	0.84
1:C:283:GLU:OE1	3:C:2292:HOH:O	1.95	0.84
1:D:521:ARG:HD3	3:D:3213:HOH:O	1.78	0.83
1:B:521:ARG:HH22	1:B:745:ILE:HD13	1.45	0.80
1:C:636:ARG:NH1	3:C:2717:HOH:O	2.17	0.77
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.73	0.70
1:D:731:GLU:OE2	3:D:3028:HOH:O	2.09	0.69
1:D:574:THR:HG22	3:D:1614:HOH:O	1.93	0.67
1:D:449[B]:HIS:CE1	3:D:2501:HOH:O	2.27	0.67
1:D:283:GLU:OE1	3:D:2496:HOH:O	2.12	0.67
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.78	0.66
1:D:341:ILE:CG1	3:D:3022:HOH:O	2.27	0.66
1:B:294:LYS:CE	3:B:3483:HOH:O	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:LYS:NZ	1:B:583:LYS:H	1.96	0.64
1:C:751:ILE:HG13	1:C:752:PRO:HD2	1.80	0.62
1:A:546:GLN:CD	3:A:3434:HOH:O	2.33	0.62
1:A:36:HIS:CD2	1:A:36:HIS:H	2.17	0.62
1:D:488:ARG:NE	3:D:2698:HOH:O	1.63	0.62
1:D:158:LYS:HB3	3:D:3454:HOH:O	2.00	0.61
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.84	0.60
1:B:521:ARG:HH22	1:B:745:ILE:CD1	2.15	0.60
1:B:583:LYS:O	1:B:584:LYS:HB3	2.03	0.59
1:C:521:ARG:HD2	1:C:521:ARG:O	2.01	0.59
1:B:119:HIS:CE1	1:C:421:SER:HB2	2.38	0.59
1:B:629:HIS:HD2	3:B:1057:HOH:O	1.86	0.58
1:B:748:ILE:O	1:B:751:ILE:HG22	2.02	0.58
1:D:629:HIS:HD2	3:D:1554:HOH:O	1.87	0.58
1:A:751:ILE:HD12	1:A:751:ILE:O	2.05	0.57
1:C:629:HIS:HD2	3:C:1129:HOH:O	1.87	0.57
1:B:359:LEU:H	1:B:507:HIS:HD2	1.51	0.57
1:B:294:LYS:NZ	3:B:2778:HOH:O	2.37	0.56
1:D:359:LEU:H	1:D:507:HIS:HD2	1.52	0.56
1:D:574:THR:HG23	3:D:3354:HOH:O	2.06	0.56
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.20	0.56
1:A:119:HIS:CE1	1:D:421:SER:HB2	2.42	0.55
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.88	0.55
1:B:32:GLU:HG2	3:B:2850:HOH:O	2.06	0.54
1:B:621:LYS:HG2	3:B:2721:HOH:O	2.07	0.54
1:A:421:SER:HB2	1:D:119:HIS:CE1	2.43	0.54
1:B:669:OCS:OD1	1:B:700:ASP:HB2	2.07	0.54
1:A:28:SER:N	3:A:3144:HOH:O	2.41	0.53
1:C:535:VAL:O	1:C:537:PRO:HD3	2.08	0.53
1:B:578:ASP:HB2	1:B:582:LEU:O	2.09	0.53
1:C:583:LYS:O	1:C:584:LYS:HB3	2.09	0.53
1:A:395:HIS:HE1	3:A:3225:HOH:O	1.91	0.52
1:D:341:ILE:CD1	3:D:3022:HOH:O	2.55	0.52
1:B:552:LEU:HB2	3:B:3202:HOH:O	2.10	0.52
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.92	0.52
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.91	0.51
1:B:724:ALA:O	1:B:725:ASP:O	2.28	0.51
1:B:294:LYS:HE3	3:B:3483:HOH:O	2.08	0.50
1:C:359:LEU:H	1:C:507:HIS:HD2	1.60	0.50
1:C:395:HIS:HE1	3:C:3337:HOH:O	1.93	0.50
1:D:488:ARG:NH2	3:D:2698:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:TYR:O	1:B:653:THR:HA	2.11	0.50
1:A:369:ARG:HH21	1:A:369:ARG:HG3	1.77	0.50
1:B:610:GLU:HG2	3:B:3191:HOH:O	2.12	0.49
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.28	0.48
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.43	0.48
1:B:359:LEU:H	1:B:507:HIS:CD2	2.30	0.48
1:C:115:ALA:O	1:C:119:HIS:HD2	1.96	0.48
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.29	0.47
1:A:372:LYS:NZ	3:A:2965:HOH:O	2.47	0.47
1:D:713:GLN:O	1:D:713:GLN:HG2	2.15	0.47
1:A:535:VAL:O	1:A:537:PRO:HD3	2.14	0.47
1:B:421:SER:HB2	1:C:119:HIS:CE1	2.50	0.47
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.97	0.47
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.30	0.47
1:A:207:PHE:O	1:A:249:THR:HA	2.15	0.46
1:B:535:VAL:O	1:B:537:PRO:HD3	2.15	0.46
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.31	0.46
1:A:552:LEU:HD12	3:A:2786:HOH:O	2.16	0.46
1:A:115:ALA:O	1:A:119:HIS:HD2	1.99	0.46
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.16	0.46
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.98	0.46
1:A:97:ALA:O	1:A:101:GLY:HA3	2.16	0.46
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.51	0.46
1:A:750:LYS:NZ	1:D:677:ASP:HB3	2.31	0.46
1:C:552:LEU:HD11	1:C:571:LEU:HD23	1.97	0.45
1:D:749:ASP:OD1	1:D:749:ASP:N	2.44	0.45
1:C:61:ARG:HG3	3:C:2648:HOH:O	2.15	0.45
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.51	0.45
1:D:552:LEU:HD11	1:D:571:LEU:HA	1.98	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.36	0.45
1:C:724:ALA:O	1:C:725:ASP:HB2	2.18	0.44
1:B:369:ARG:HG3	3:B:778:HOH:O	2.17	0.44
1:B:395:HIS:HE1	3:B:3281:HOH:O	2.00	0.44
1:D:335:GLU:OE1	1:D:369:ARG:HG2	2.17	0.44
1:C:448:MET:O	1:C:449[B]:HIS:HB2	2.18	0.44
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.98	0.44
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	2.00	0.44
1:C:634:TYR:O	1:C:653:THR:HA	2.18	0.44
1:A:36:HIS:HD2	1:A:36:HIS:H	1.64	0.44
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.40	0.44
1:B:745:ILE:O	1:B:748:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:HIS:HA	1:C:168:THR:O	2.17	0.43
1:B:294:LYS:CD	3:B:3483:HOH:O	2.27	0.43
1:D:359:LEU:H	1:D:507:HIS:CD2	2.35	0.43
1:B:369:ARG:HH11	1:B:369:ARG:HD3	1.50	0.43
1:D:128:HIS:HA	1:D:168:THR:O	2.18	0.43
1:D:459:ASN:H	1:D:459:ASN:HD22	1.67	0.43
1:B:583:LYS:HZ2	1:B:583:LYS:H	1.65	0.43
3:B:1038:HOH:O	1:D:449[B]:HIS:HD2	2.01	0.43
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.54	0.43
1:B:128:HIS:HA	1:B:168:THR:O	2.19	0.43
1:D:461:GLU:HA	1:D:462:PRO:C	2.39	0.43
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.54	0.42
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.99	0.42
1:D:207:PHE:O	1:D:249:THR:HA	2.19	0.42
1:C:552:LEU:HB2	3:C:3296:HOH:O	2.19	0.42
1:D:115:ALA:O	1:D:119:HIS:HD2	2.02	0.42
1:A:128:HIS:HA	1:A:168:THR:O	2.20	0.42
1:A:666:ILE:HD11	1:A:732:LEU:CD2	2.50	0.42
1:B:533:LYS:CE	3:C:2623:HOH:O	2.14	0.42
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.55	0.42
1:B:725:ASP:OD2	1:B:727:SER:N	2.53	0.42
1:D:395:HIS:HE1	3:D:3312:HOH:O	2.03	0.42
1:A:725:ASP:HB2	1:A:726:GLY:H	1.66	0.41
1:C:704:PHE:O	1:C:707:THR:HG22	2.19	0.41
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.01	0.41
1:A:38:PRO:HA	1:A:48:GLN:OE1	2.21	0.41
1:C:612:ARG:HG3	3:C:3087:HOH:O	2.19	0.41
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.24	0.41
1:A:750:LYS:HZ3	1:D:677:ASP:HB3	1.84	0.41
1:B:703:LYS:HD3	1:B:703:LYS:N	2.36	0.41
1:C:521:ARG:HD3	1:C:521:ARG:HA	1.25	0.41
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.55	0.41
1:B:461:GLU:HA	1:B:462:PRO:C	2.39	0.41
1:B:97:ALA:O	1:B:101:GLY:HA3	2.20	0.41
1:D:267:ARG:HH21	1:D:267:ARG:HD2	1.75	0.41
1:B:440:TYR:C	1:B:440:TYR:CD2	2.94	0.41
1:B:52:PRO:HG3	3:D:1451:HOH:O	2.21	0.41
1:C:748:ILE:O	1:C:751:ILE:HG22	2.20	0.41
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.56	0.41
1:D:744:ARG:HA	1:D:747:LYS:HD3	2.02	0.41
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.96	0.40
1:B:126:ILE:HG12	3:B:928:HOH:O	2.21	0.40
1:B:207:PHE:O	1:B:249:THR:HA	2.21	0.40
1:C:207:PHE:O	1:C:249:THR:HA	2.21	0.40
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.56	0.40
1:B:115:ALA:O	1:B:119:HIS:HD2	2.04	0.40
1:A:413:TYR:CE2	1:B:413:TYR:HE2	2.39	0.40
1:C:578:ASP:HB3	1:C:582:LEU:O	2.21	0.40

All (3) 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)
3:A:2805:HOH:O	3:D:2468:HOH:O[1_455]	1.97	0.23
1:A:59:ASP:OD1	1:B:369:ARG:NH2[2_545]	1.97	0.23
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_545]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	726/753 (96%)	709 (98%)	16 (2%)	1 (0%)	51 24
1	B	726/753 (96%)	706 (97%)	17 (2%)	3 (0%)	34 13
1	C	725/753 (96%)	705 (97%)	18 (2%)	2 (0%)	41 18
1	D	725/753 (96%)	708 (98%)	16 (2%)	1 (0%)	51 24
All	All	2902/3012 (96%)	2828 (98%)	67 (2%)	7 (0%)	47 22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	C	75	SER
1	A	75	SER
1	B	75	SER
1	C	725	ASP
1	B	612	ARG
1	D	75	SER

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	A	612/634 (96%)	603 (98%)	9 (2%)	65	35
1	B	612/634 (96%)	594 (97%)	18 (3%)	42	10
1	C	611/634 (96%)	593 (97%)	18 (3%)	42	10
1	D	611/634 (96%)	597 (98%)	14 (2%)	50	17
All	All	2446/2536 (96%)	2387 (98%)	59 (2%)	49	16

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	440	TYR
1	A	459	ASN
1	A	617	LEU
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	252	ASN
1	B	283	GLU

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Mol	Chain	Res	Type
1	B	369	ARG
1	B	440	TYR
1	B	459	ASN
1	B	565	GLU
1	B	568	ASP
1	B	583	LYS
1	B	612	ARG
1	B	616	LEU
1	B	639	GLU
1	B	703	LYS
1	B	713	GLN
1	B	732	LEU
1	C	61	ARG
1	C	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	377	ARG
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	517	PRO
1	C	521	ARG
1	C	636	ARG
1	C	725	ASP
1	C	750	LYS
1	D	48	GLN
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	344	GLU
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	574	THR

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Mol	Chain	Res	Type
1	D	747	LYS
1	D	749	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OCS	A	669	1	7,8,9	2.20	2 (28%)	6,11,13	1.74	2 (33%)
1	OCS	D	669	1	7,8,9	2.14	2 (28%)	6,11,13	2.10	2 (33%)
1	OCS	B	669	1	7,8,9	1.96	1 (14%)	6,11,13	4.22	3 (50%)
1	OCS	C	669	1	7,8,9	1.58	2 (28%)	6,11,13	2.10	2 (33%)

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
1	OCS	A	669	1	-	3/4/7/9	-
1	OCS	D	669	1	-	1/4/7/9	-
1	OCS	B	669	1	-	3/4/7/9	-
1	OCS	C	669	1	-	1/4/7/9	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	OCS	OD2-SG	4.71	1.64	1.47
1	D	669	OCS	CB-CA	4.43	1.58	1.53
1	A	669	OCS	OD2-SG	4.42	1.63	1.47
1	D	669	OCS	OD2-SG	3.05	1.58	1.47
1	C	669	OCS	OD2-SG	2.88	1.57	1.47
1	A	669	OCS	CB-CA	2.76	1.56	1.53
1	C	669	OCS	CB-CA	2.24	1.55	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	OCS	OD1-SG-CB	7.33	115.65	106.94
1	B	669	OCS	OD3-SG-CB	-5.80	100.04	106.94
1	C	669	OCS	OD1-SG-CB	-4.40	101.72	106.94
1	D	669	OCS	OD3-SG-CB	-4.15	102.01	106.94
1	B	669	OCS	OD2-SG-CB	-4.03	99.32	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	OCS	OD3-SG-CB	-2.56	103.90	106.94
1	C	669	OCS	OD2-SG-CB	2.49	109.70	105.74
1	D	669	OCS	OD2-SG-OD3	2.38	117.09	111.27
1	A	669	OCS	OD2-SG-OD1	2.26	116.79	111.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	669	OCS	N-CA-CB-SG
1	D	669	OCS	N-CA-CB-SG
1	B	669	OCS	N-CA-CB-SG
1	C	669	OCS	N-CA-CB-SG
1	A	669	OCS	CA-CB-SG-OD2
1	B	669	OCS	CA-CB-SG-OD2
1	B	669	OCS	CA-CB-SG-OD1
1	A	669	OCS	CA-CB-SG-OD3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	669	OCS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	760	1	27,50,50	1.35	4 (14%)	17,82,82	2.90	6 (35%)
2	HEM	A	760	1	27,50,50	1.90	6 (22%)	17,82,82	3.48	9 (52%)
2	HEM	C	760	1	27,50,50	1.60	6 (22%)	17,82,82	2.66	6 (35%)
2	HEM	B	760	1	27,50,50	1.68	7 (25%)	17,82,82	2.54	8 (47%)

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	HEM	D	760	1	-	0/6/54/54	-
2	HEM	A	760	1	-	0/6/54/54	-
2	HEM	C	760	1	-	0/6/54/54	-
2	HEM	B	760	1	-	0/6/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C4A-NA	5.33	1.47	1.36
2	A	760	HEM	C1A-NA	4.57	1.45	1.36
2	B	760	HEM	C4A-NA	3.67	1.43	1.36
2	B	760	HEM	C1A-NA	3.44	1.43	1.36
2	C	760	HEM	C4A-NA	3.43	1.43	1.36
2	D	760	HEM	C1B-C2B	3.18	1.49	1.42
2	A	760	HEM	C1B-C2B	2.99	1.49	1.42
2	C	760	HEM	C4D-C3D	2.95	1.49	1.42
2	B	760	HEM	CAA-C2A	-2.78	1.48	1.52
2	A	760	HEM	C3D-C2D	2.67	1.45	1.37
2	C	760	HEM	C1B-C2B	2.65	1.48	1.42
2	A	760	HEM	C2A-C3A	2.64	1.45	1.37
2	D	760	HEM	C1A-NA	2.63	1.41	1.36
2	B	760	HEM	C1D-ND	2.61	1.41	1.36
2	D	760	HEM	CMA-C3A	-2.52	1.46	1.51
2	B	760	HEM	C1C-C2C	2.50	1.48	1.42
2	C	760	HEM	C1A-NA	2.49	1.41	1.36
2	D	760	HEM	C4A-NA	2.37	1.41	1.36
2	C	760	HEM	C3B-CAB	2.34	1.52	1.47
2	A	760	HEM	CMB-C2B	-2.31	1.46	1.51
2	C	760	HEM	C3C-C2C	2.27	1.43	1.40
2	B	760	HEM	C3C-C2C	-2.20	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	760	HEM	C4D-C3D	2.15	1.47	1.42

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	C1D-C2D-C3D	-8.01	101.42	107.00
2	A	760	HEM	CBD-CAD-C3D	-6.41	100.67	112.48
2	A	760	HEM	CAA-CBA-CGA	-5.83	102.89	112.67
2	B	760	HEM	CAA-CBA-CGA	-5.79	102.95	112.67
2	D	760	HEM	CBD-CAD-C3D	-5.73	101.92	112.48
2	D	760	HEM	CAA-CBA-CGA	-5.55	103.36	112.67
2	C	760	HEM	CBD-CAD-C3D	-5.48	102.38	112.48
2	C	760	HEM	CMB-C2B-C3B	5.19	134.39	124.68
2	D	760	HEM	CMB-C2B-C3B	4.86	133.76	124.68
2	B	760	HEM	CBD-CAD-C3D	-4.73	103.75	112.48
2	A	760	HEM	CMB-C2B-C3B	4.72	133.51	124.68
2	C	760	HEM	CAA-CBA-CGA	-4.68	104.82	112.67
2	D	760	HEM	C4C-C3C-C2C	-4.53	103.73	106.90
2	C	760	HEM	C1D-C2D-C3D	-4.31	103.99	107.00
2	A	760	HEM	C4C-C3C-C2C	-4.04	104.08	106.90
2	B	760	HEM	CMB-C2B-C3B	3.09	130.47	124.68
2	B	760	HEM	CMA-C3A-C2A	2.85	130.32	124.94
2	B	760	HEM	CMA-C3A-C4A	-2.75	124.24	128.46
2	D	760	HEM	CMA-C3A-C4A	-2.73	124.27	128.46
2	A	760	HEM	CAD-CBD-CGD	-2.69	108.16	112.67
2	B	760	HEM	CMD-C2D-C1D	-2.67	124.36	128.46
2	B	760	HEM	CMC-C2C-C3C	2.57	129.49	124.68
2	D	760	HEM	CMA-C3A-C2A	2.56	129.76	124.94
2	C	760	HEM	C3B-C4B-NB	2.39	112.30	109.21
2	B	760	HEM	C4A-C3A-C2A	-2.29	105.41	107.00
2	A	760	HEM	CMD-C2D-C3D	2.21	129.10	124.94
2	A	760	HEM	CMA-C3A-C4A	-2.15	125.17	128.46
2	A	760	HEM	C3C-C4C-NC	2.12	114.94	110.94
2	C	760	HEM	CMA-C3A-C4A	-2.11	125.22	128.46

There are no chirality outliers.

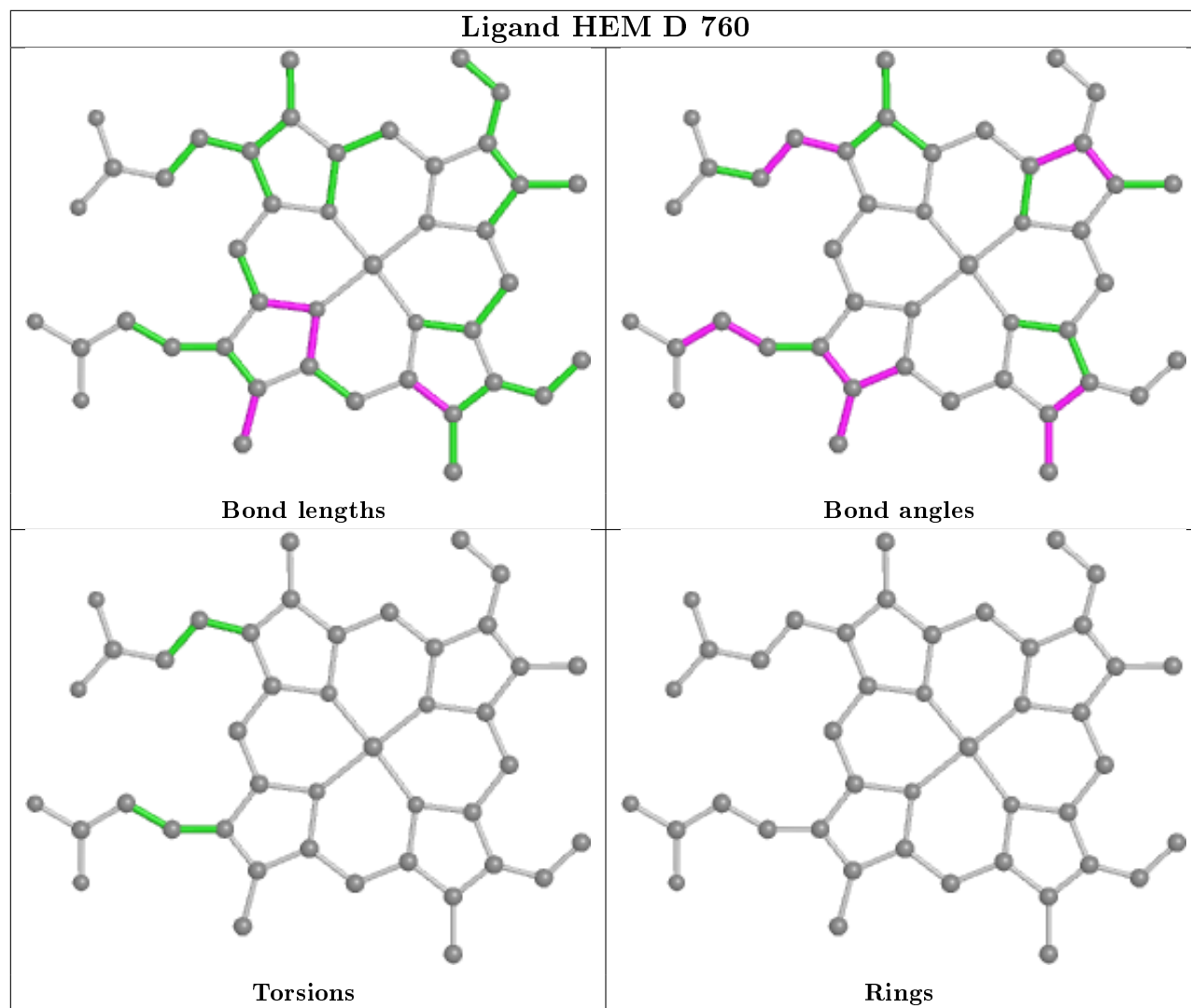
There are no torsion outliers.

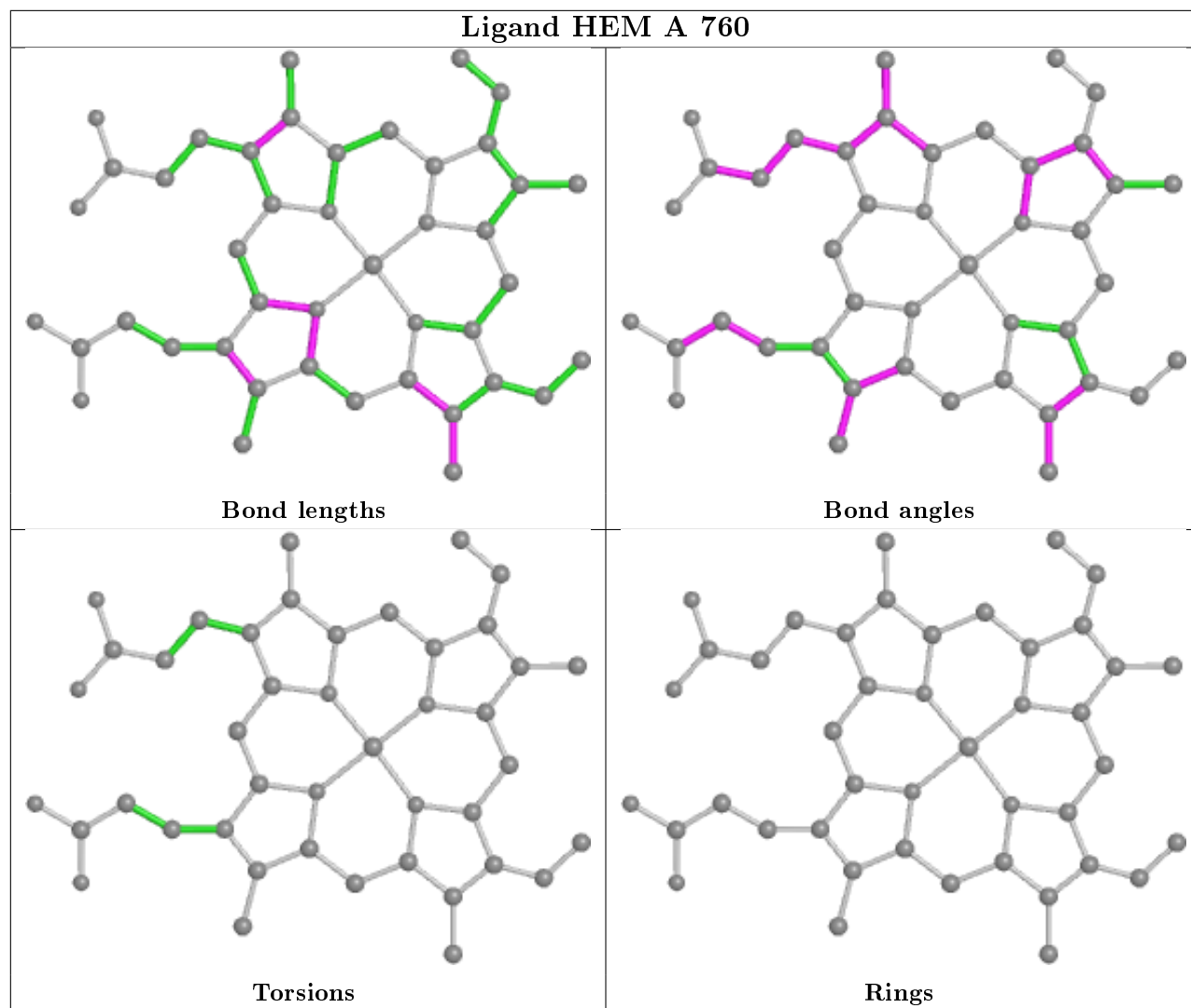
There are no ring outliers.

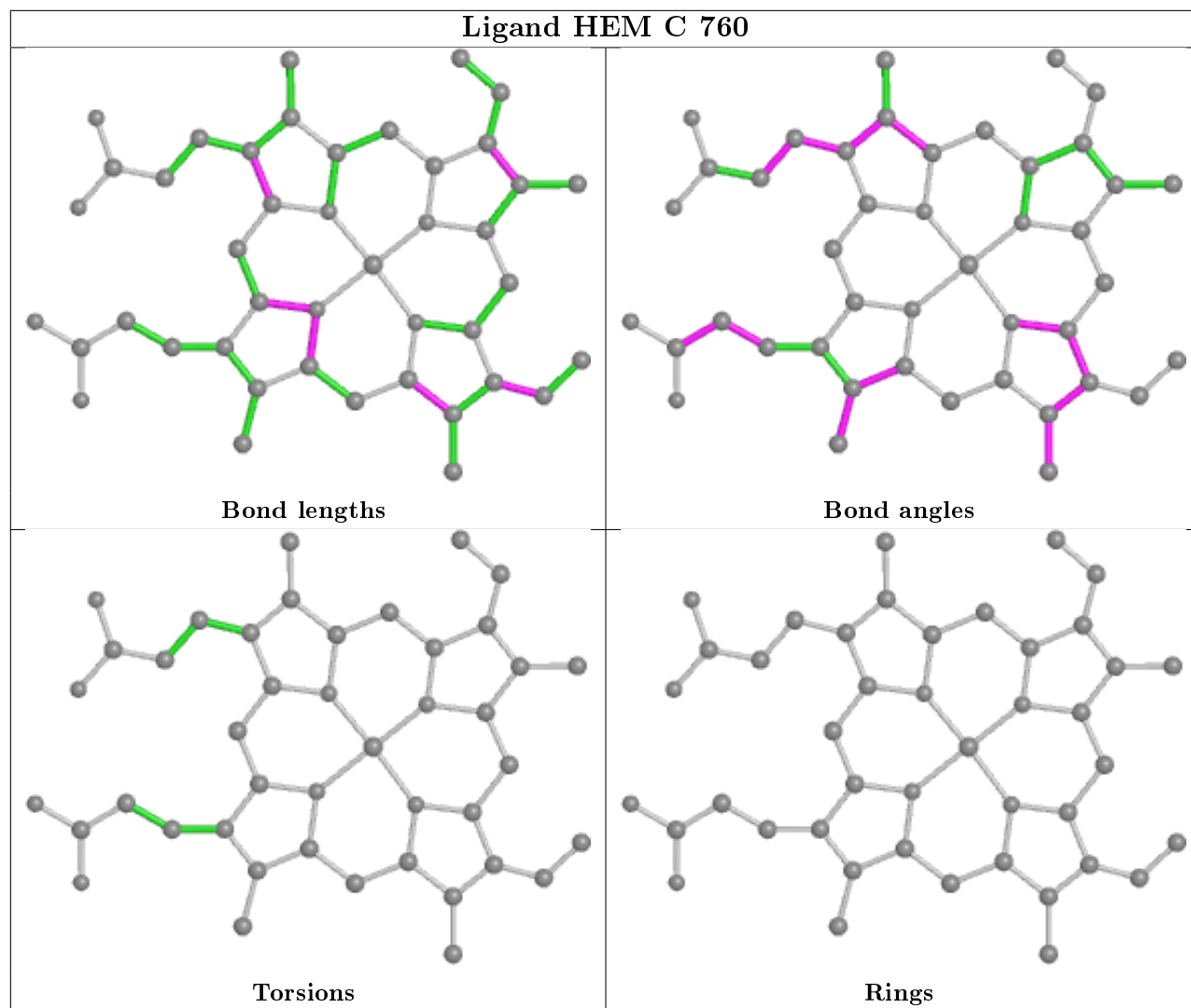
4 monomers are involved in 4 short contacts:

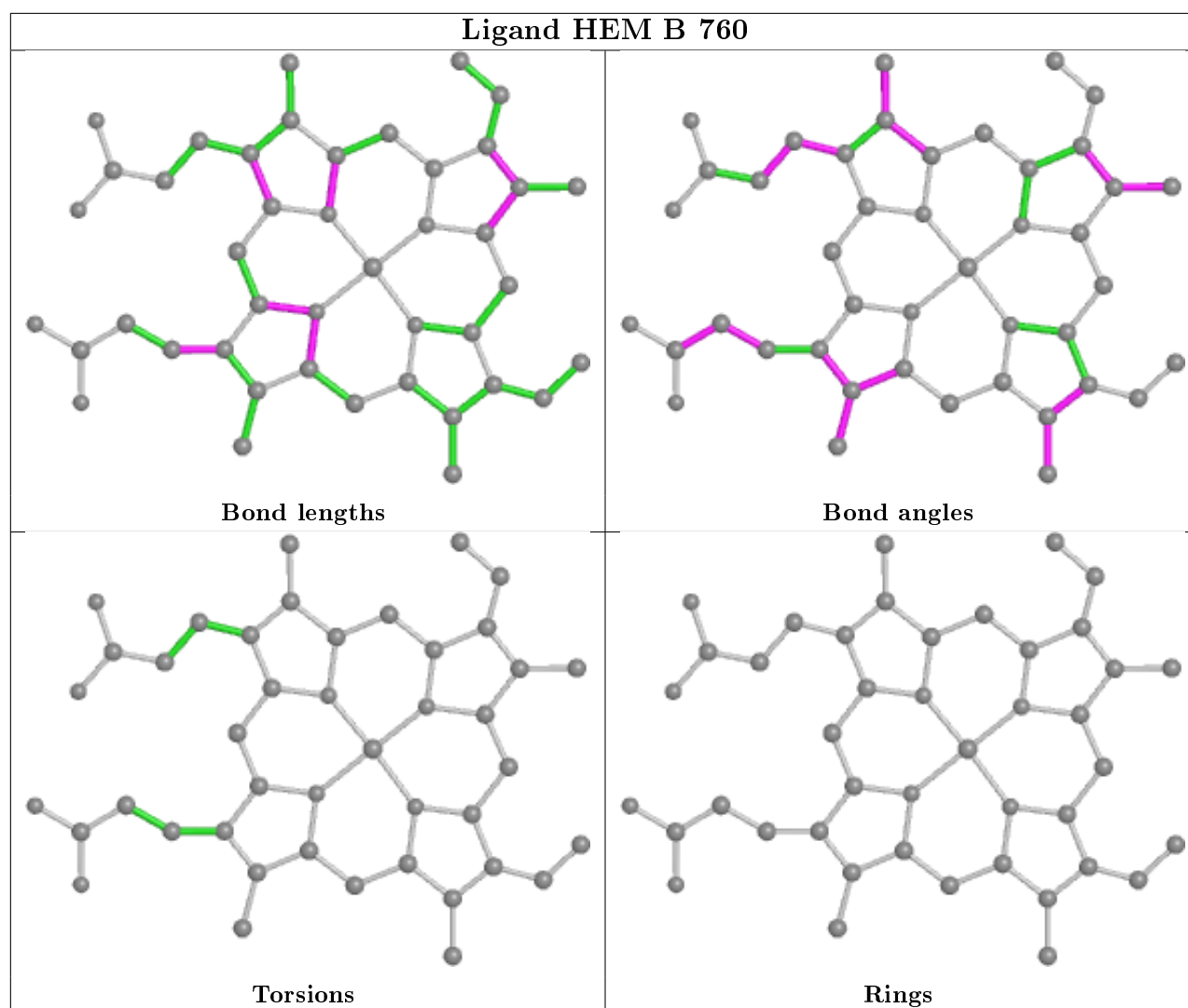
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	760	HEM	1	0
2	A	760	HEM	1	0
2	C	760	HEM	1	0
2	B	760	HEM	1	0

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	A	725/753 (96%)	-0.35	6 (0%) 86 87	6, 11, 25, 52	1 (0%)
1	B	725/753 (96%)	-0.20	25 (3%) 45 48	7, 13, 34, 57	1 (0%)
1	C	725/753 (96%)	-0.25	23 (3%) 47 50	7, 13, 33, 53	1 (0%)
1	D	725/753 (96%)	-0.31	12 (1%) 70 70	6, 11, 27, 56	1 (0%)
All	All	2900/3012 (96%)	-0.28	66 (2%) 60 63	6, 12, 31, 57	4 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	5.6
1	D	750	LYS	4.4
1	C	726	GLY	4.3
1	B	713	GLN	4.2
1	C	711	ALA	4.0
1	B	647	VAL	3.8
1	B	28	SER	3.7
1	B	750	LYS	3.7
1	B	711	ALA	3.7
1	C	751	ILE	3.6
1	D	749	ASP	3.5
1	A	32	GLU	3.4
1	D	712	ASP	3.3
1	B	32	GLU	3.3
1	B	712	ASP	3.3
1	A	28	SER	3.2
1	D	713	GLN	3.1
1	B	673	ALA	3.1
1	D	28	SER	3.1
1	C	712	ASP	3.0
1	B	583	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	594	PRO	2.9
1	C	646	THR	2.9
1	B	645	GLY	2.9
1	C	641	THR	2.9
1	B	568	ASP	2.8
1	D	572	ASN	2.8
1	C	714	GLY	2.8
1	C	583	LYS	2.8
1	C	750	LYS	2.8
1	C	713	GLN	2.7
1	D	711	ALA	2.7
1	B	596	GLY	2.7
1	D	594	PRO	2.7
1	D	751	ILE	2.7
1	B	677	ASP	2.7
1	A	726	GLY	2.5
1	B	646	THR	2.5
1	C	642	ALA	2.4
1	D	673	ALA	2.4
1	A	750	LYS	2.4
1	B	725	ASP	2.4
1	B	749	ASP	2.4
1	C	710	ILE	2.4
1	B	572	ASN	2.3
1	C	725	ASP	2.3
1	C	568	ASP	2.3
1	C	32	GLU	2.3
1	B	642	ALA	2.2
1	A	751	ILE	2.2
1	C	552	LEU	2.2
1	B	612	ARG	2.2
1	B	33	ASP	2.2
1	B	727	SER	2.2
1	D	710	ILE	2.2
1	C	677	ASP	2.2
1	C	572	ASN	2.2
1	A	596	GLY	2.2
1	C	569	ASP	2.2
1	B	641	THR	2.2
1	B	714	GLY	2.2
1	C	647	VAL	2.1
1	C	596	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	722	ASP	2.1
1	D	32	GLU	2.1
1	B	617	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	B	669	9/10	0.93	0.13	27,28,33,38	0
1	OCS	D	669	9/10	0.94	0.12	19,21,27,29	0
1	OCS	C	669	9/10	0.94	0.14	27,30,36,39	0
1	OCS	A	669	9/10	0.95	0.11	16,19,26,29	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

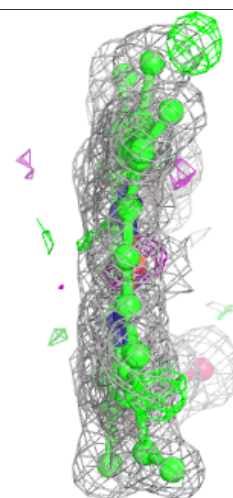
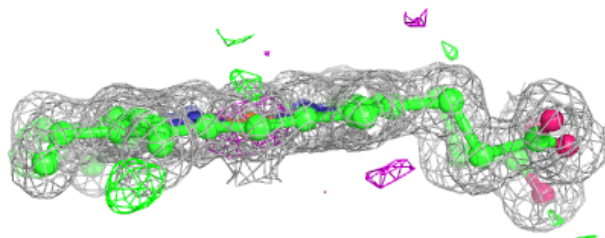
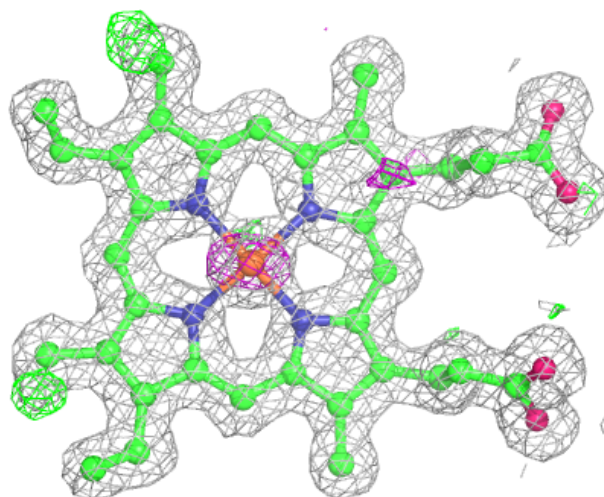
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	D	760	43/43	0.99	0.05	5,7,8,14	0
2	HEM	A	760	43/43	0.99	0.06	5,7,9,15	0
2	HEM	C	760	43/43	0.99	0.05	6,8,10,17	0
2	HEM	B	760	43/43	0.99	0.06	6,8,10,16	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.

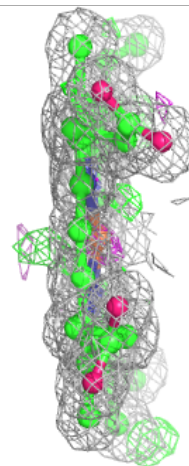
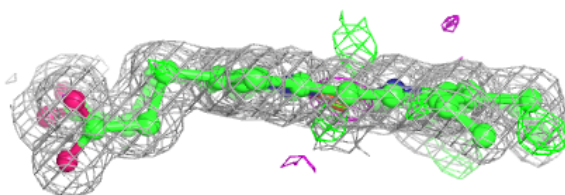
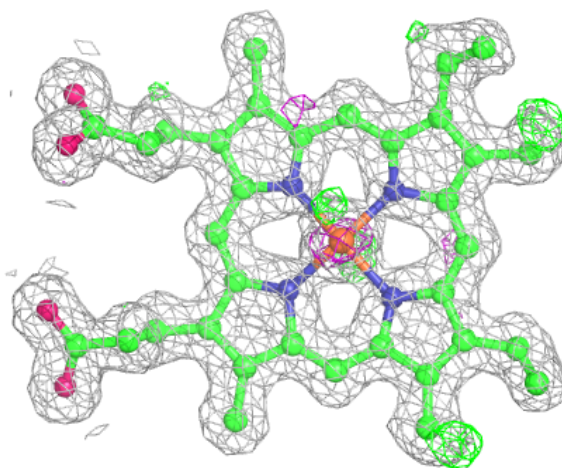
Electron density around HEM D 760:

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



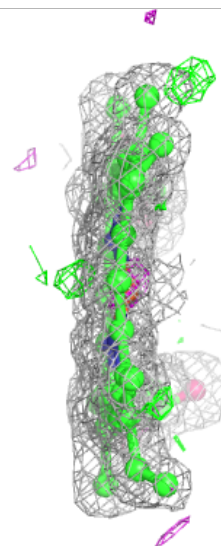
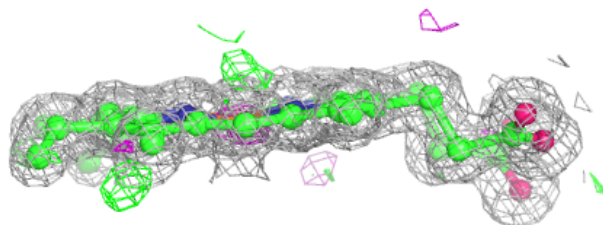
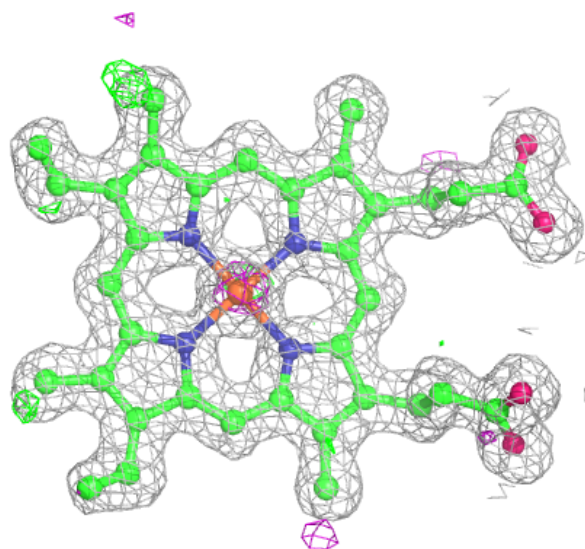
Electron density around HEM A 760:

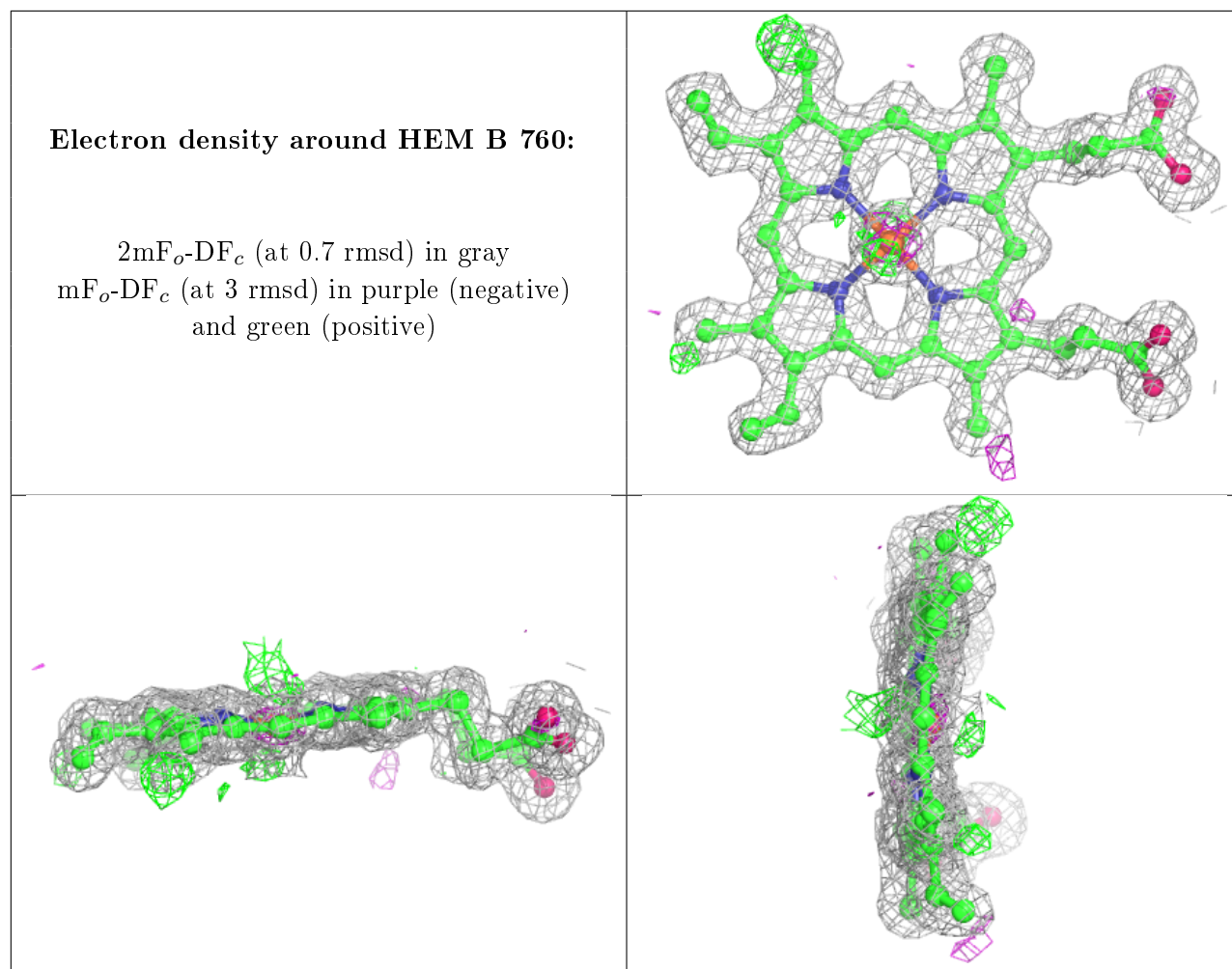
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 760:

$2mF_o-DF_c$ (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.