



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 04:35 PM EST

PDB ID : 8SMU
Title : Integral fusion of the HtaA CR2 domain from *Corynebacterium diphtheriae* within EGFP
Authors : Mahoney, B.J.; Cascio, D.; Clubb, R.T.
Deposited on : 2023-04-26
Resolution : 2.45 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 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

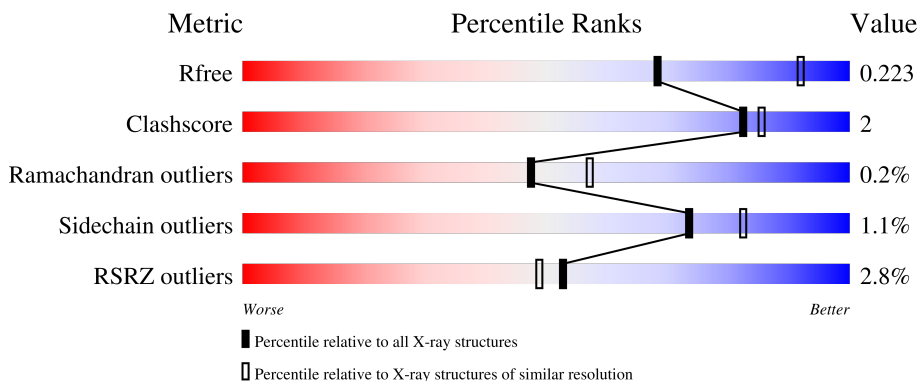
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	A	403	 92% 5% .
1	B	403	 93% 5% .
1	C	403	 91% 6% .
1	D	403	 91% 6% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12400 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 HtaACR2 integral fusion within enhanced green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			2985	1887	505	584	9			
1	B	394	Total	C	N	O	S	0	0	0
			2980	1884	501	585	10			
1	C	393	Total	C	N	O	S	0	0	0
			2993	1892	507	585	9			
1	D	395	Total	C	N	O	S	0	0	0
			2988	1886	503	589	10			

There are 36 discrepancies between the modelled and reference sequences:

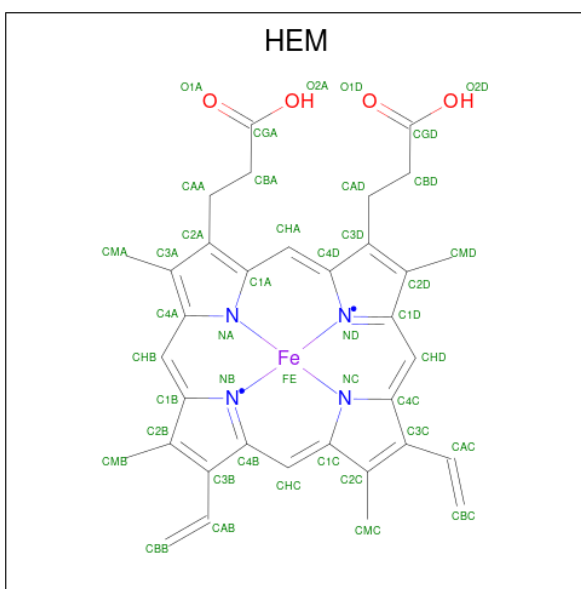
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLY	-	linker	UNP P42212
A	41	GLY	-	linker	UNP P42212
A	42	SER	-	linker	UNP P42212
A	231	LEU	PHE	conflict	UNP P42212
A	233	CRO	SER	chromophore	UNP P42212
A	233	CRO	TYR	chromophore	UNP P42212
A	233	CRO	GLY	chromophore	UNP P42212
A	388	LYS	LEU	conflict	UNP P42212
A	398	LEU	HIS	conflict	UNP P42212
B	40	GLY	-	linker	UNP P42212
B	41	GLY	-	linker	UNP P42212
B	42	SER	-	linker	UNP P42212
B	231	LEU	PHE	conflict	UNP P42212
B	233	CRO	SER	chromophore	UNP P42212
B	233	CRO	TYR	chromophore	UNP P42212
B	233	CRO	GLY	chromophore	UNP P42212
B	388	LYS	LEU	conflict	UNP P42212
B	398	LEU	HIS	conflict	UNP P42212
C	40	GLY	-	linker	UNP P42212
C	41	GLY	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	42	SER	-	linker	UNP P42212
C	231	LEU	PHE	conflict	UNP P42212
C	233	CRO	SER	chromophore	UNP P42212
C	233	CRO	TYR	chromophore	UNP P42212
C	233	CRO	GLY	chromophore	UNP P42212
C	388	LYS	LEU	conflict	UNP P42212
C	398	LEU	HIS	conflict	UNP P42212
D	40	GLY	-	linker	UNP P42212
D	41	GLY	-	linker	UNP P42212
D	42	SER	-	linker	UNP P42212
D	231	LEU	PHE	conflict	UNP P42212
D	233	CRO	SER	chromophore	UNP P42212
D	233	CRO	TYR	chromophore	UNP P42212
D	233	CRO	GLY	chromophore	UNP P42212
D	388	LYS	LEU	conflict	UNP P42212
D	398	LEU	HIS	conflict	UNP P42212

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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		

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



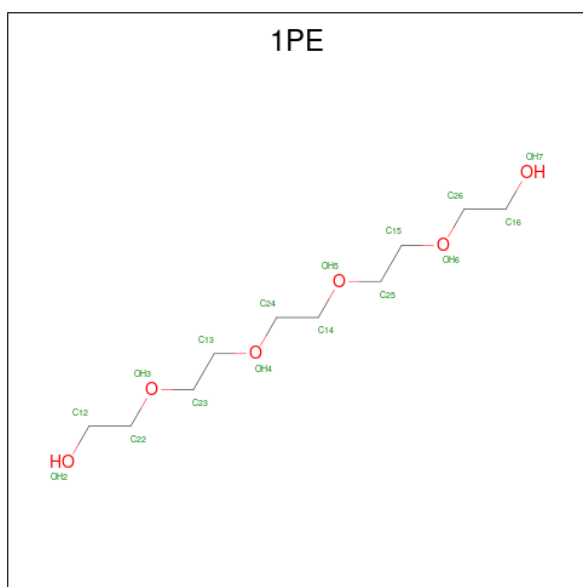
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			16	10 6		
4	B	1	Total	C O	0	0
			16	10 6		
4	C	1	Total	C O	0	0
			16	10 6		
4	D	1	Total	C O	0	0
			16	10 6		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		

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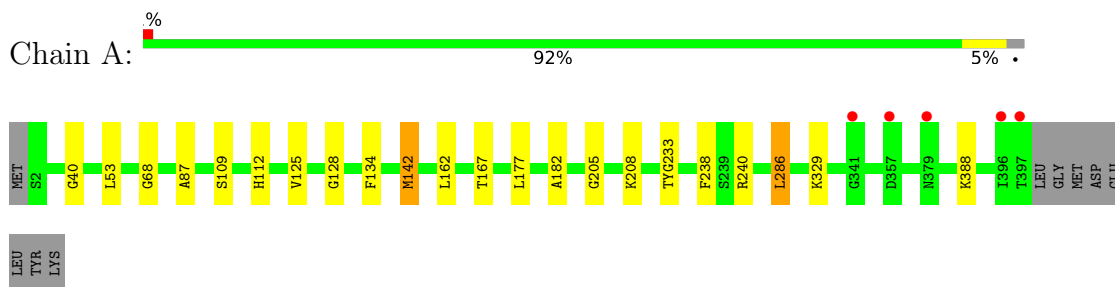
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	14	Total 14	O 14	0	0
6	C	25	Total 25	O 25	0	0
6	D	17	Total 17	O 17	0	0

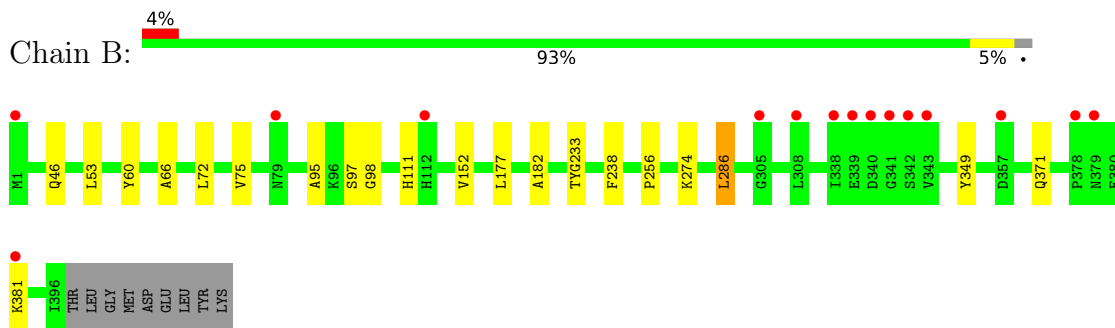
3 Residue-property plots [i](#)

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

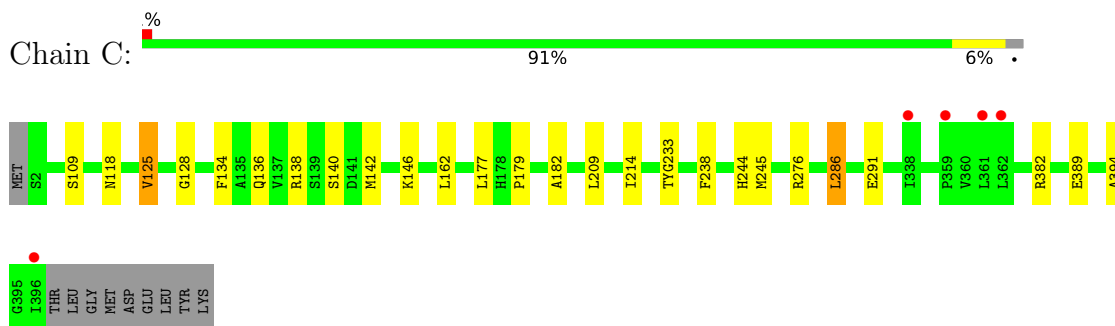
- Molecule 1: HtaACR2 integral fusion within enhanced green fluorescent protein



- Molecule 1: HtaACR2 integral fusion within enhanced green fluorescent protein

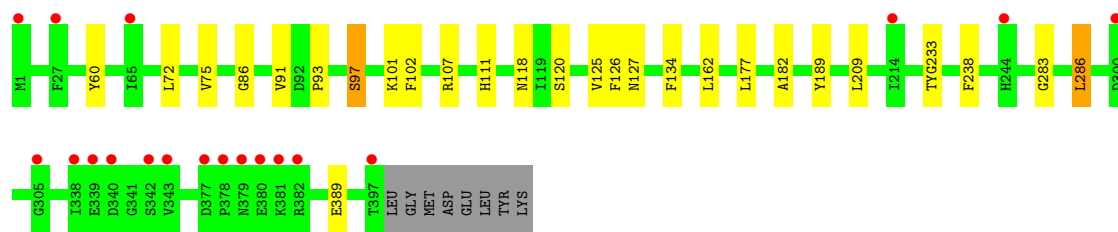


- Molecule 1: HtaACR2 integral fusion within enhanced green fluorescent protein



- Molecule 1: HtaACR2 integral fusion within enhanced green fluorescent protein





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.83Å 272.78Å 73.52Å 90.00° 114.22° 90.00°	Depositor
Resolution (Å)	48.32 – 2.45 48.32 – 2.45	Depositor EDS
% Data completeness (in resolution range)	67.5 (48.32-2.45) 67.5 (48.32-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.45Å)	Xtrriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.209 , 0.233 0.205 , 0.223	Depositor DCC
R_{free} test set	2792 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtrriage
Anisotropy	0.140	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12400	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: CL, CRO, GOL, 1PE, HEM

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	0.38	0/3031	0.62	0/4103
1	B	0.35	0/3026	0.59	0/4097
1	C	0.37	0/3039	0.61	0/4110
1	D	0.35	0/3034	0.59	0/4110
All	All	0.36	0/12130	0.60	0/16420

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2985	0	2816	18	0
1	B	2980	0	2803	14	0
1	C	2993	0	2839	17	0
1	D	2988	0	2801	15	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
3	A	42	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	32	1	0
3	C	42	0	56	1	0
3	D	30	0	40	2	0
4	A	16	0	22	0	0
4	B	16	0	22	4	0
4	C	16	0	22	2	0
4	D	16	0	22	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	20	0	0	1	0
6	B	14	0	0	0	0
6	C	25	0	0	0	0
6	D	17	0	0	0	0
All	All	12400	0	11651	60	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 2.

All (60) 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:A:142:MET:HG3	1:C:142:MET:HG3	1.58	0.86
1:A:125:VAL:HG23	1:A:134:PHE:HE2	1.48	0.78
1:B:256:PRO:HB2	1:D:283:GLY:HA3	1.71	0.72
1:C:125:VAL:HG23	1:C:134:PHE:HE2	1.56	0.70
1:A:208:LYS:HZ2	1:A:388:LYS:HE3	1.60	0.66
1:A:142:MET:CG	1:C:142:MET:HG3	2.27	0.63
1:B:274:LYS:CE	4:B:505:1PE:H141	2.28	0.63
1:B:274:LYS:HE2	4:B:505:1PE:H141	1.81	0.60
1:A:128:GLY:HA2	1:A:162:LEU:HD23	1.83	0.60
1:B:66:ALA:HA	1:B:111:HIS:CE1	2.37	0.59
1:D:238:PHE:HE2	1:D:286:LEU:HD22	1.68	0.59
1:A:238:PHE:HE2	1:A:286:LEU:HD22	1.68	0.59
1:B:72:LEU:HB3	1:B:75:VAL:HB	1.84	0.58
1:B:238:PHE:HE2	1:B:286:LEU:HD22	1.69	0.58
1:C:238:PHE:HE2	1:C:286:LEU:HD22	1.68	0.57
1:A:167:THR:HG22	1:A:240:ARG:HE	1.70	0.57
1:C:128:GLY:HA2	1:C:162:LEU:HD23	1.86	0.56
1:A:208:LYS:NZ	1:A:388:LYS:HE3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:MET:HE1	1:C:394:ALA:HA	1.89	0.54
1:D:97:SER:HB2	1:D:127:ASN:OD1	2.10	0.52
1:B:238:PHE:CE2	1:B:286:LEU:HD22	2.45	0.52
1:C:238:PHE:CE2	1:C:286:LEU:HD22	2.45	0.51
1:A:238:PHE:CE2	1:A:286:LEU:HD22	2.45	0.51
1:D:60:TYR:OH	1:D:111:HIS:NE2	2.38	0.51
1:B:46:GLN:HE21	1:B:371:GLN:HE21	1.59	0.50
1:B:60:TYR:OH	1:B:111:HIS:NE2	2.30	0.50
1:B:95:ALA:O	3:B:506:GOL:H32	2.13	0.49
1:C:136:GLN:NE2	3:C:508:GOL:O2	2.40	0.49
1:B:349:TYR:HB3	4:B:505:1PE:H162	1.94	0.49
1:A:128:GLY:HA2	1:A:162:LEU:CD2	2.42	0.49
1:B:274:LYS:HE3	4:B:505:1PE:H141	1.94	0.48
1:D:238:PHE:CE2	1:D:286:LEU:HD22	2.46	0.48
1:A:329:LYS:NZ	6:A:602:HOH:O	2.47	0.47
1:D:101:LYS:HE2	3:D:507:GOL:H11	1.97	0.47
1:C:118:ASN:HB2	1:C:138:ARG:HB2	1.96	0.46
1:C:125:VAL:CG2	1:C:134:PHE:HE2	2.26	0.46
1:D:72:LEU:HB3	1:D:75:VAL:HB	1.98	0.46
1:D:107:ARG:HG3	1:D:118:ASN:HD21	1.80	0.46
1:A:68:GLY:HA3	1:A:109:SER:O	2.16	0.46
1:D:91:VAL:O	1:D:93:PRO:HD3	2.17	0.45
1:A:125:VAL:HG21	1:B:98:GLY:HA2	1.99	0.45
1:A:208:LYS:NZ	1:A:388:LYS:CE	2.79	0.45
1:D:126:PHE:CD1	1:D:162:LEU:HD21	2.51	0.45
1:A:177:LEU:HD21	1:A:182:ALA:HA	1.99	0.44
1:D:125:VAL:HG23	1:D:134:PHE:HE2	1.83	0.43
1:C:291:GLU:HB3	4:C:505:1PE:H152	1.99	0.43
1:B:177:LEU:HD21	1:B:182:ALA:HA	2.01	0.43
1:A:142:MET:HE3	1:A:142:MET:HB3	1.92	0.43
1:D:86:GLY:HA3	1:D:102:PHE:HA	2.00	0.43
1:C:209:LEU:HB2	1:C:389:GLU:HB2	2.00	0.43
1:A:40:GLY:HA2	1:A:205:GLY:HA3	2.01	0.43
1:D:177:LEU:HD21	1:D:182:ALA:HA	2.01	0.43
1:C:244:HIS:CE1	1:C:245:MET:HE3	2.54	0.42
1:A:208:LYS:HZ2	1:A:388:LYS:CE	2.29	0.42
1:C:140:SER:HB3	1:C:146:LYS:HD3	2.00	0.42
1:D:189:TYR:HD1	3:D:505:GOL:H32	1.84	0.42
1:C:177:LEU:HD21	1:C:182:ALA:HA	2.01	0.41
1:C:276:ARG:HB2	4:C:505:1PE:H241	2.02	0.41
1:D:209:LEU:HB2	1:D:389:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ILE:HD13	1:C:382:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

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	389/403 (96%)	377 (97%)	10 (3%)	2 (0%)	29	34
1	B	389/403 (96%)	380 (98%)	8 (2%)	1 (0%)	41	49
1	C	388/403 (96%)	379 (98%)	9 (2%)	0	100	100
1	D	390/403 (97%)	384 (98%)	6 (2%)	0	100	100
All	All	1556/1612 (96%)	1520 (98%)	33 (2%)	3 (0%)	47	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ALA
1	B	53	LEU
1	A	53	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/326 (94%)	304 (99%)	3 (1%)	76	84
1	B	306/326 (94%)	302 (99%)	4 (1%)	69	79
1	C	310/326 (95%)	306 (99%)	4 (1%)	69	79
1	D	307/326 (94%)	304 (99%)	3 (1%)	76	84
All	All	1230/1304 (94%)	1216 (99%)	14 (1%)	73	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	142	MET
1	A	286	LEU
1	B	97	SER
1	B	152	VAL
1	B	286	LEU
1	B	381	LYS
1	C	109	SER
1	C	125	VAL
1	C	179	PRO
1	C	286	LEU
1	D	97	SER
1	D	120	SER
1	D	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	203	GLN
1	B	46	GLN
1	B	69	GLN
1	B	118	ASN
1	B	203	GLN
1	C	69	GLN
1	D	118	ASN

5.3.3 RNA [i](#)

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	CRO	B	233	1	23,23,24	1.56	4 (17%)	30,32,34	2.42	8 (26%)
1	CRO	A	233	1	23,23,24	1.61	2 (8%)	30,32,34	2.64	8 (26%)
1	CRO	C	233	1	23,23,24	1.73	5 (21%)	30,32,34	2.98	8 (26%)
1	CRO	D	233	1	23,23,24	1.74	2 (8%)	30,32,34	2.51	8 (26%)

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	CRO	B	233	1	-	0/12/31/32	0/2/2/2
1	CRO	A	233	1	-	0/12/31/32	0/2/2/2
1	CRO	C	233	1	-	0/12/31/32	0/2/2/2
1	CRO	D	233	1	-	0/12/31/32	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	233	CRO	CB2-CA2	6.39	1.40	1.35
1	A	233	CRO	CB2-CA2	6.13	1.40	1.35
1	B	233	CRO	CB2-CA2	5.09	1.39	1.35
1	C	233	CRO	CB2-CA2	4.55	1.38	1.35
1	C	233	CRO	CA2-C2	-4.13	1.44	1.48
1	D	233	CRO	C2-N3	-2.73	1.33	1.39
1	A	233	CRO	C2-N3	-2.47	1.34	1.39
1	B	233	CRO	C2-N3	-2.46	1.34	1.39
1	B	233	CRO	CD1-CG2	2.27	1.43	1.39
1	C	233	CRO	CD2-CG2	2.24	1.43	1.39
1	C	233	CRO	CD1-CG2	2.19	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	233	CRO	C2-N3	-2.16	1.34	1.39
1	B	233	CRO	C1-N2	-2.13	1.29	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	CRO	O2-C2-CA2	-7.72	126.63	130.96
1	C	233	CRO	CA2-N2-C1	7.50	111.30	105.77
1	C	233	CRO	C2-CA2-N2	-7.28	103.83	108.93
1	C	233	CRO	CA2-C2-N3	6.80	106.58	103.37
1	D	233	CRO	O2-C2-CA2	-6.64	127.23	130.96
1	A	233	CRO	C2-CA2-N2	-6.62	104.29	108.93
1	A	233	CRO	CA2-N2-C1	6.35	110.45	105.77
1	A	233	CRO	O2-C2-CA2	-6.30	127.42	130.96
1	B	233	CRO	CA2-N2-C1	6.27	110.39	105.77
1	B	233	CRO	C2-CA2-N2	-6.01	104.72	108.93
1	A	233	CRO	CA2-C2-N3	5.86	106.14	103.37
1	D	233	CRO	C2-CA2-N2	-5.85	104.83	108.93
1	D	233	CRO	CA2-C2-N3	5.85	106.14	103.37
1	D	233	CRO	CA2-N2-C1	5.64	109.93	105.77
1	B	233	CRO	O2-C2-CA2	-5.60	127.81	130.96
1	B	233	CRO	C2-N3-C1	4.25	110.12	107.97
1	C	233	CRO	N3-C1-N2	-3.57	108.98	111.45
1	B	233	CRO	CA2-C2-N3	3.53	105.04	103.37
1	D	233	CRO	O3-C3-CA3	-3.09	117.07	126.39
1	A	233	CRO	C2-N3-C1	3.00	109.48	107.97
1	B	233	CRO	O3-C3-CA3	-2.80	117.93	126.39
1	A	233	CRO	N3-C1-N2	-2.74	109.56	111.45
1	B	233	CRO	N3-C1-N2	-2.62	109.64	111.45
1	C	233	CRO	C2-N3-C1	2.54	109.25	107.97
1	A	233	CRO	O3-C3-CA3	-2.54	118.73	126.39
1	C	233	CRO	O3-C3-CA3	-2.49	118.87	126.39
1	D	233	CRO	C2-N3-C1	2.43	109.20	107.97
1	D	233	CRO	N3-C1-N2	-2.39	109.80	111.45
1	A	233	CRO	C1-CA1-N1	-2.37	106.12	109.96
1	B	233	CRO	CB2-CA2-N2	2.07	131.70	128.83
1	C	233	CRO	CB2-CA2-N2	2.06	131.68	128.83
1	D	233	CRO	C1-CA1-N1	-2.05	106.64	109.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 4 are monoatomic - leaving 31 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
4	1PE	C	505	-	15,15,15	0.32	0	14,14,14	0.19	0
4	1PE	A	507	-	15,15,15	0.31	0	14,14,14	0.15	0
3	GOL	C	503	-	5,5,5	0.13	0	5,5,5	0.26	0
3	GOL	D	503	-	5,5,5	0.08	0	5,5,5	0.27	0
3	GOL	D	507	-	5,5,5	0.08	0	5,5,5	0.37	0
4	1PE	D	504	-	15,15,15	0.25	0	14,14,14	0.15	0
2	HEM	B	501	1	41,50,50	0.92	3 (7%)	45,82,82	1.09	3 (6%)
2	HEM	A	501	1	41,50,50	0.94	2 (4%)	45,82,82	1.00	3 (6%)
2	HEM	C	501	1	41,50,50	0.95	2 (4%)	45,82,82	1.06	4 (8%)
3	GOL	A	508	-	5,5,5	0.15	0	5,5,5	0.26	0
3	GOL	C	508	-	5,5,5	0.12	0	5,5,5	0.19	0
3	GOL	D	506	-	5,5,5	0.09	0	5,5,5	0.26	0
3	GOL	A	502	-	5,5,5	0.06	0	5,5,5	0.26	0
3	GOL	C	506	-	5,5,5	0.11	0	5,5,5	0.33	0
3	GOL	D	505	-	5,5,5	0.16	0	5,5,5	0.41	0
3	GOL	B	506	-	5,5,5	0.08	0	5,5,5	0.36	0
3	GOL	A	505	-	5,5,5	0.06	0	5,5,5	0.23	0
4	1PE	B	505	-	15,15,15	0.20	0	14,14,14	0.15	0
3	GOL	B	504	-	5,5,5	0.06	0	5,5,5	0.23	0
3	GOL	C	502	-	5,5,5	0.10	0	5,5,5	0.38	0
3	GOL	D	502	-	5,5,5	0.08	0	5,5,5	0.25	0
3	GOL	C	507	-	5,5,5	0.17	0	5,5,5	0.42	0
2	HEM	D	501	1	41,50,50	0.89	2 (4%)	45,82,82	1.08	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	502	-	5,5,5	0.04	0	5,5,5	0.18	0
3	GOL	A	506	-	5,5,5	0.14	0	5,5,5	0.28	0
3	GOL	B	503	-	5,5,5	0.10	0	5,5,5	0.21	0
3	GOL	A	503	-	5,5,5	0.15	0	5,5,5	0.27	0
3	GOL	C	509	-	5,5,5	0.10	0	5,5,5	0.30	0
3	GOL	A	509	-	5,5,5	0.26	0	5,5,5	0.47	0
3	GOL	C	504	-	5,5,5	0.05	0	5,5,5	0.24	0
3	GOL	A	504	-	5,5,5	0.16	0	5,5,5	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	C	505	-	-	4/13/13/13	-
4	1PE	A	507	-	-	4/13/13/13	-
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	D	503	-	-	0/4/4/4	-
3	GOL	D	507	-	-	0/4/4/4	-
4	1PE	D	504	-	-	2/13/13/13	-
2	HEM	B	501	1	-	5/12/54/54	-
2	HEM	A	501	1	-	7/12/54/54	-
2	HEM	C	501	1	-	3/12/54/54	-
3	GOL	A	508	-	-	1/4/4/4	-
3	GOL	C	508	-	-	0/4/4/4	-
3	GOL	D	506	-	-	0/4/4/4	-
3	GOL	A	502	-	-	1/4/4/4	-
3	GOL	C	506	-	-	2/4/4/4	-
3	GOL	D	505	-	-	1/4/4/4	-
3	GOL	B	506	-	-	0/4/4/4	-
3	GOL	A	505	-	-	0/4/4/4	-
4	1PE	B	505	-	-	3/13/13/13	-
3	GOL	B	504	-	-	0/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
3	GOL	D	502	-	-	4/4/4/4	-
3	GOL	C	507	-	-	0/4/4/4	-
2	HEM	D	501	1	-	6/12/54/54	-
3	GOL	B	502	-	-	0/4/4/4	-
3	GOL	A	506	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	503	-	-	1/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-
3	GOL	C	509	-	-	1/4/4/4	-
3	GOL	A	509	-	-	2/4/4/4	-
3	GOL	C	504	-	-	1/4/4/4	-
3	GOL	A	504	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CHB-C1B	2.59	1.41	1.35
2	C	501	HEM	CHB-C1B	2.58	1.41	1.35
2	B	501	HEM	CHB-C1B	2.45	1.41	1.35
2	D	501	HEM	CHB-C1B	2.34	1.41	1.35
2	A	501	HEM	FE-NB	2.26	2.08	1.96
2	D	501	HEM	C1B-NB	-2.24	1.36	1.40
2	C	501	HEM	FE-NB	2.21	2.07	1.96
2	B	501	HEM	FE-ND	2.19	2.07	1.96
2	B	501	HEM	C1B-NB	-2.06	1.36	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C4B-CHC-C1C	3.55	127.25	122.56
2	C	501	HEM	C4B-CHC-C1C	3.44	127.10	122.56
2	A	501	HEM	C4B-CHC-C1C	3.32	126.94	122.56
2	B	501	HEM	C4B-CHC-C1C	3.24	126.84	122.56
2	B	501	HEM	C4C-CHD-C1D	2.94	126.44	122.56
2	C	501	HEM	C4C-CHD-C1D	2.93	126.42	122.56
2	D	501	HEM	C4C-CHD-C1D	2.92	126.41	122.56
2	B	501	HEM	CMC-C2C-C3C	2.75	129.83	124.68
2	A	501	HEM	C4C-CHD-C1D	2.74	126.17	122.56
2	D	501	HEM	CMC-C2C-C3C	2.40	129.17	124.68
2	C	501	HEM	CMC-C2C-C3C	2.32	129.02	124.68
2	A	501	HEM	CMC-C2C-C3C	2.31	129.00	124.68
2	D	501	HEM	C3B-C2B-C1B	-2.22	104.84	106.49
2	C	501	HEM	CMA-C3A-C4A	-2.03	125.34	128.46

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C1A-C2A-CAA-CBA
3	A	509	GOL	O2-C2-C3-O3
3	A	506	GOL	O1-C1-C2-C3
3	A	509	GOL	C1-C2-C3-O3
3	C	503	GOL	O1-C1-C2-C3
3	C	506	GOL	O1-C1-C2-C3
2	A	501	HEM	C2A-CAA-CBA-CGA
2	C	501	HEM	C2A-CAA-CBA-CGA
2	D	501	HEM	C2A-CAA-CBA-CGA
3	A	502	GOL	O2-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3
3	C	502	GOL	O1-C1-C2-O2
3	C	506	GOL	O1-C1-C2-O2
4	A	507	1PE	OH6-C15-C25-OH5
3	C	502	GOL	O2-C2-C3-O3
3	D	502	GOL	O1-C1-C2-O2
3	D	502	GOL	O2-C2-C3-O3
3	D	505	GOL	O2-C2-C3-O3
4	B	505	1PE	OH4-C13-C23-OH3
2	B	501	HEM	C2A-CAA-CBA-CGA
2	A	501	HEM	C3A-C2A-CAA-CBA
2	D	501	HEM	C1A-C2A-CAA-CBA
3	A	506	GOL	O1-C1-C2-O2
4	B	505	1PE	OH6-C15-C25-OH5
2	A	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O1A
3	C	504	GOL	O2-C2-C3-O3
2	D	501	HEM	CAA-CBA-CGA-O2A
4	C	505	1PE	C14-C24-OH4-C13
2	A	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D
3	A	508	GOL	O1-C1-C2-C3
3	C	509	GOL	C1-C2-C3-O3
4	C	505	1PE	OH6-C15-C25-OH5
2	C	501	HEM	CAD-CBD-CGD-O1D
4	C	505	1PE	OH4-C13-C23-OH3
2	C	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O1D

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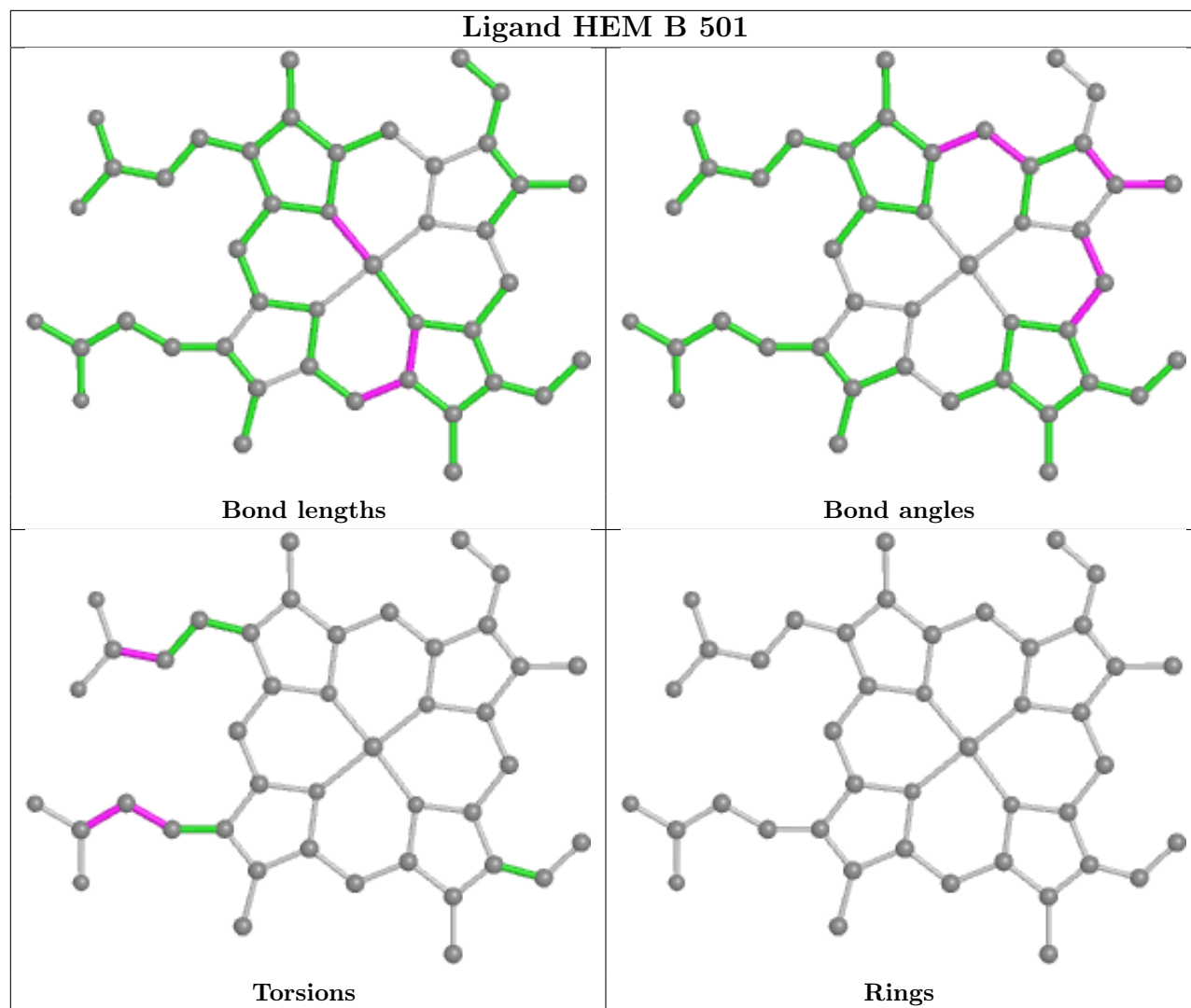
Mol	Chain	Res	Type	Atoms
2	B	501	HEM	CAA-CBA-CGA-O1A
3	C	503	GOL	O1-C1-C2-O2
4	A	507	1PE	C24-C14-OH5-C25
4	D	504	1PE	OH5-C14-C24-OH4
3	D	502	GOL	O1-C1-C2-C3
3	D	502	GOL	C1-C2-C3-O3
4	D	504	1PE	OH4-C13-C23-OH3
4	C	505	1PE	OH5-C14-C24-OH4
4	A	507	1PE	OH5-C14-C24-OH4
4	A	507	1PE	OH4-C13-C23-OH3
4	B	505	1PE	OH5-C14-C24-OH4

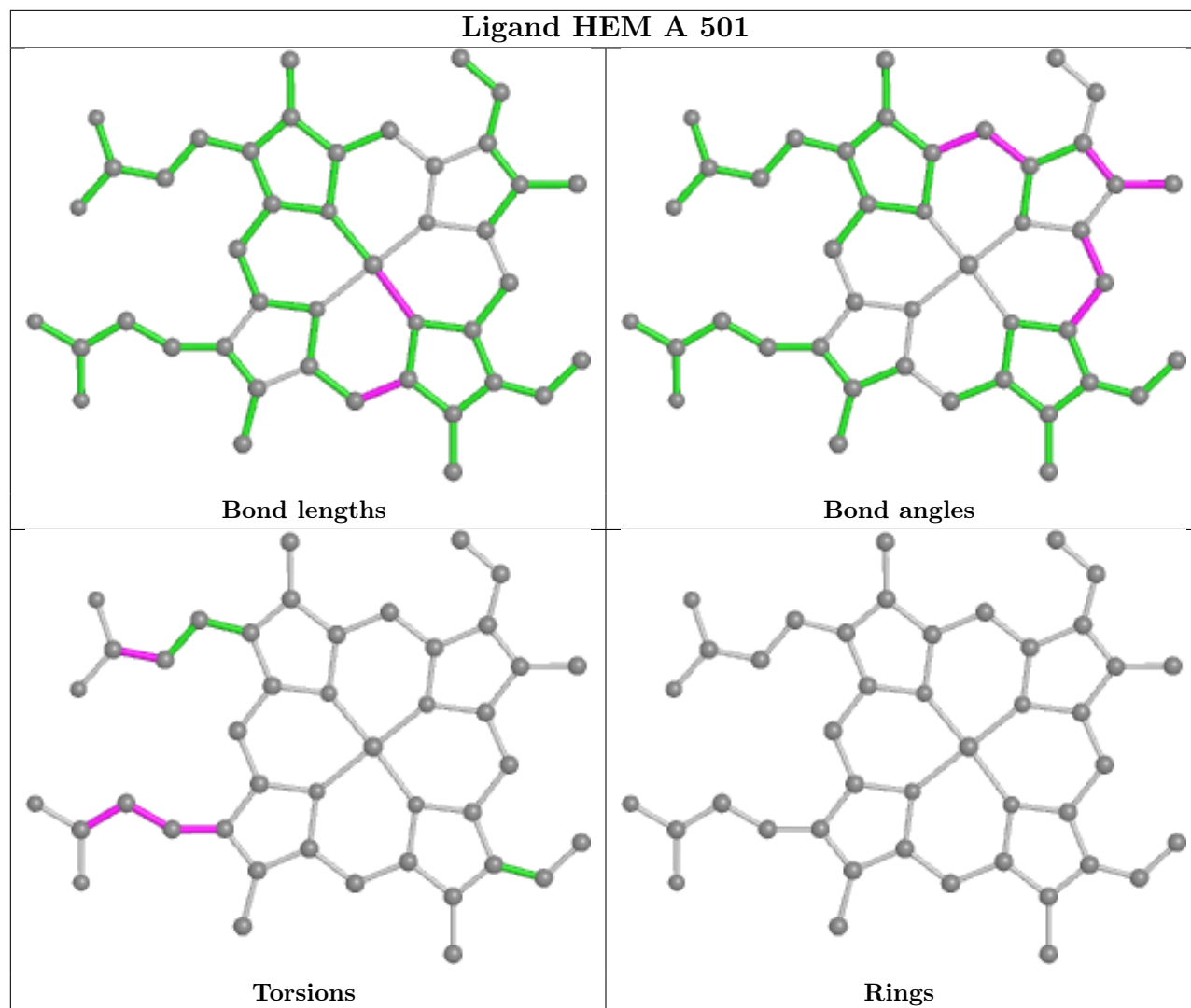
There are no ring outliers.

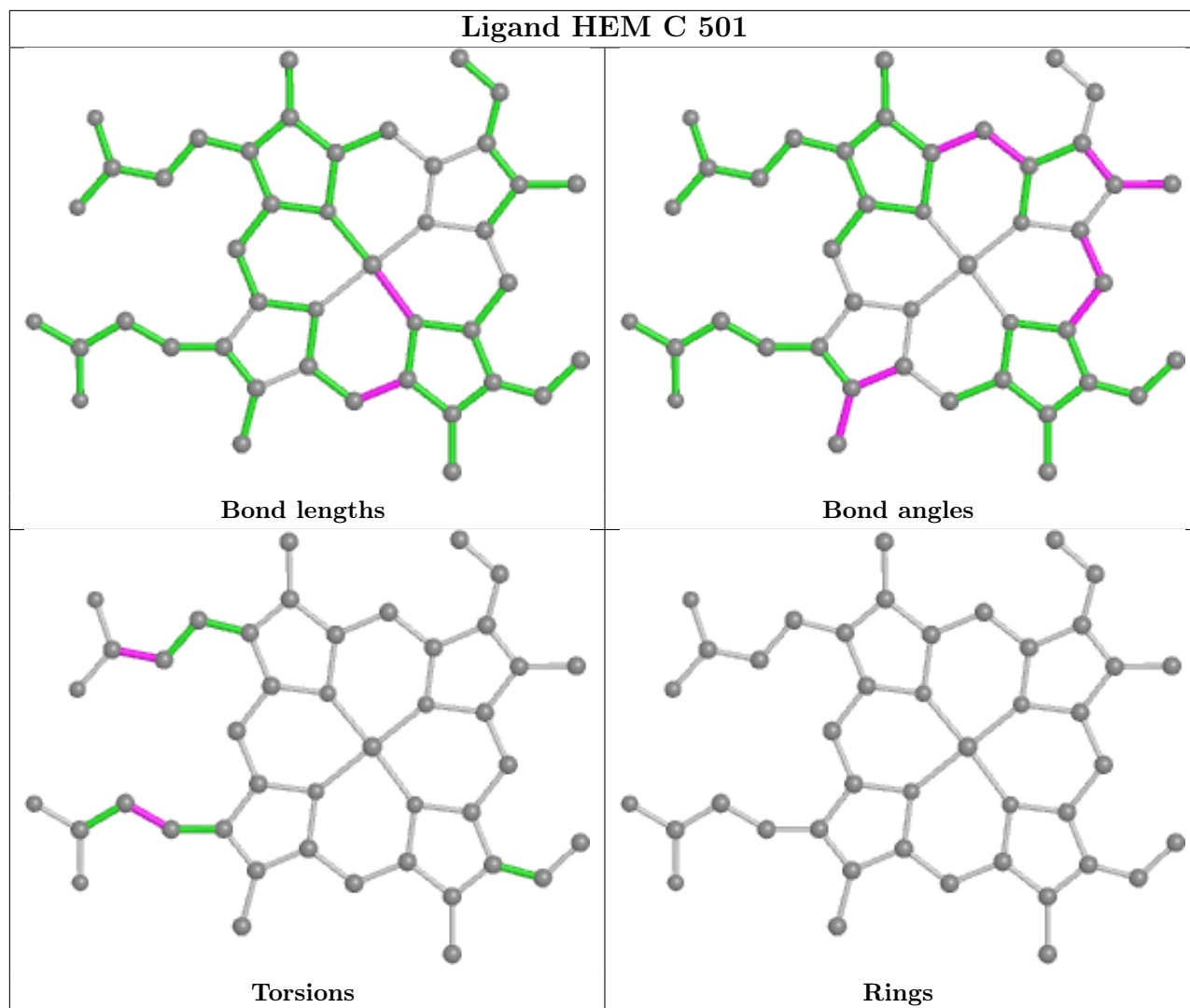
6 monomers are involved in 10 short contacts:

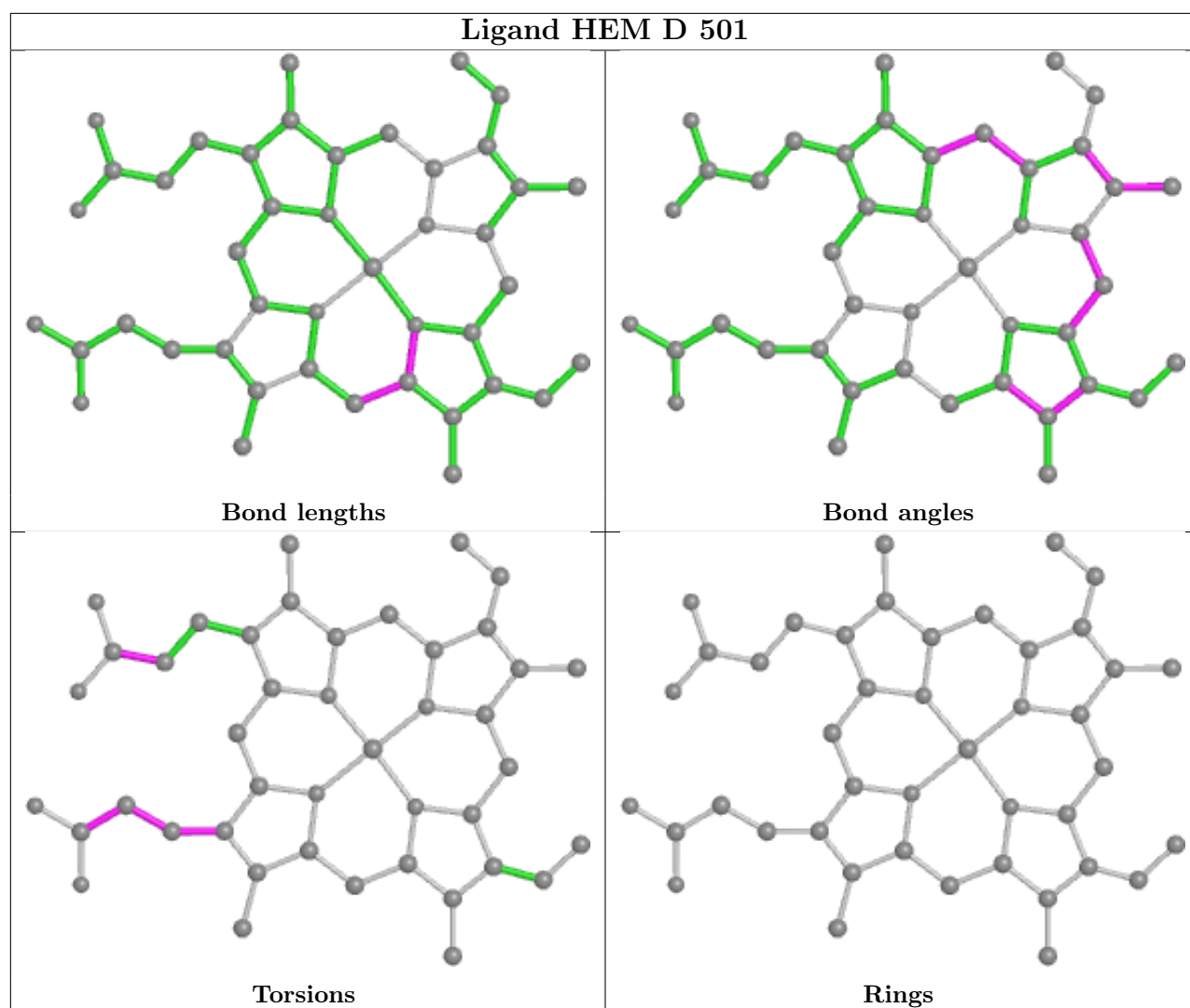
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	505	1PE	2	0
3	D	507	GOL	1	0
3	C	508	GOL	1	0
3	D	505	GOL	1	0
3	B	506	GOL	1	0
4	B	505	1PE	4	0

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	393/403 (97%)	-0.07	5 (1%) 77 76	33, 54, 78, 93	0
1	B	393/403 (97%)	0.09	15 (3%) 40 37	35, 65, 87, 105	0
1	C	392/403 (97%)	0.05	5 (1%) 77 76	34, 55, 84, 98	0
1	D	394/403 (97%)	0.18	19 (4%) 30 28	38, 67, 96, 112	0
All	All	1572/1612 (97%)	0.06	44 (2%) 53 49	33, 60, 87, 112	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	396	ILE	5.3
1	D	378	PRO	5.2
1	D	379	ASN	4.9
1	B	340	ASP	4.8
1	D	338	ILE	4.5
1	B	341	GLY	3.6
1	D	300	ASP	3.5
1	D	27	PHE	3.4
1	D	381	LYS	3.4
1	D	339	GLU	3.3
1	B	378	PRO	3.3
1	B	379	ASN	3.3
1	D	340	ASP	3.3
1	A	397	THR	3.2
1	D	305	GLY	3.2
1	B	381	LYS	3.1
1	B	339	GLU	3.1
1	B	342	SER	3.1
1	D	342	SER	3.1
1	B	305	GLY	2.8
1	B	112	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	357	ASP	2.8
1	D	343	VAL	2.7
1	A	396	ILE	2.7
1	C	362	LEU	2.7
1	D	244	HIS	2.6
1	D	382	ARG	2.6
1	D	397	THR	2.6
1	C	359	PRO	2.6
1	B	1	MET	2.4
1	A	379	ASN	2.3
1	D	1	MET	2.3
1	D	214	ILE	2.2
1	B	357	ASP	2.2
1	D	377	ASP	2.2
1	B	79	ASN	2.1
1	A	341	GLY	2.1
1	C	361	LEU	2.1
1	D	380	GLU	2.1
1	D	65	ILE	2.1
1	B	343	VAL	2.0
1	B	338	ILE	2.0
1	B	308	LEU	2.0
1	C	338	ILE	2.0

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	CRO	B	233	22/23	0.95	0.17	54,55,56,57	0
1	CRO	C	233	22/23	0.96	0.17	43,44,44,45	0
1	CRO	D	233	22/23	0.96	0.15	53,56,58,59	0
1	CRO	A	233	22/23	0.97	0.15	40,41,42,43	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

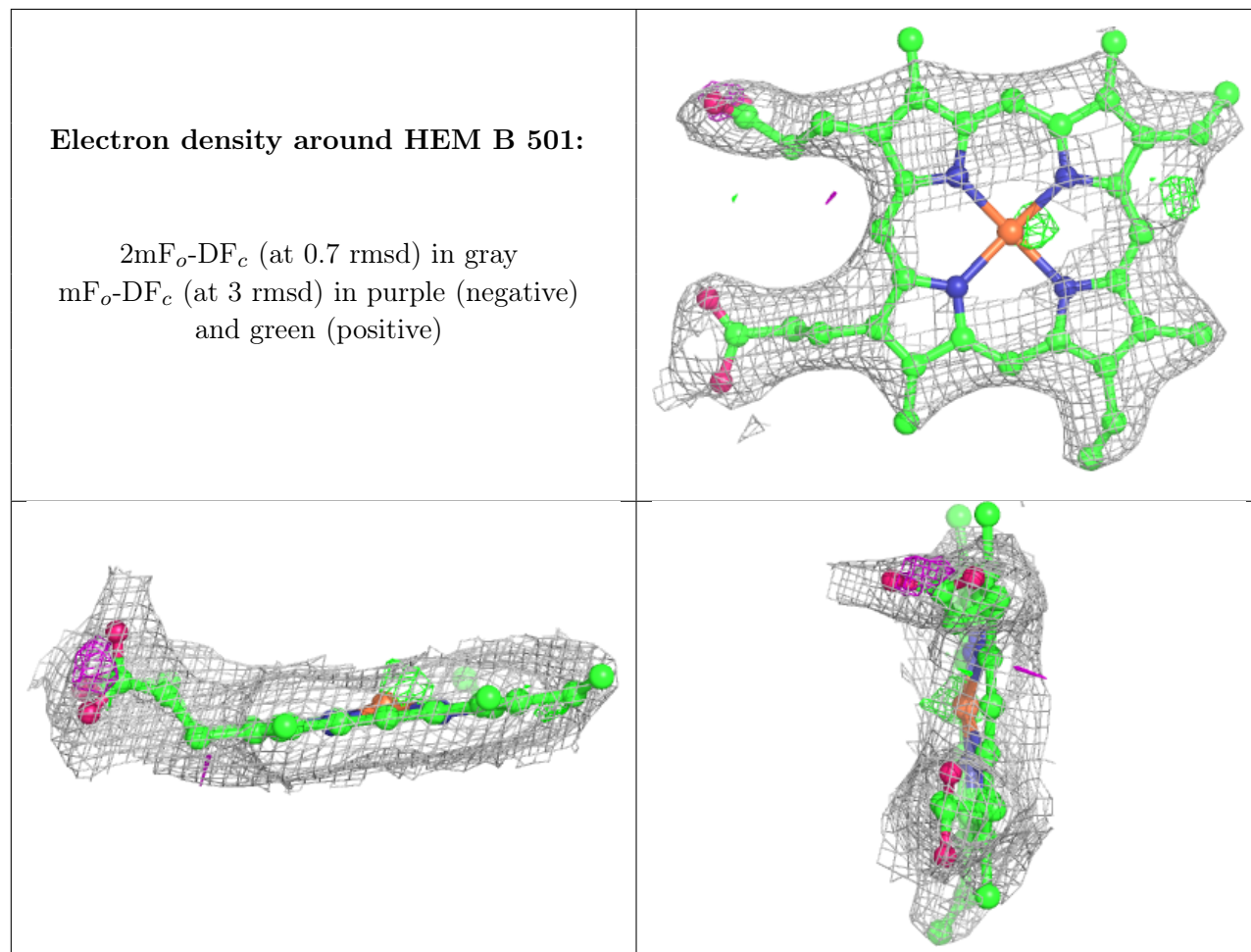
6.4 Ligands [i](#)

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
4	1PE	C	505	16/16	0.49	0.39	79,83,84,84	0
4	1PE	A	507	16/16	0.58	0.29	68,71,72,72	0
4	1PE	D	504	16/16	0.58	0.31	73,79,82,82	0
3	GOL	D	505	6/6	0.63	0.26	81,82,82,82	0
3	GOL	A	509	6/6	0.65	0.32	52,54,55,55	0
4	1PE	B	505	16/16	0.71	0.32	77,82,84,84	0
3	GOL	C	509	6/6	0.72	0.30	74,75,75,75	0
3	GOL	A	506	6/6	0.76	0.24	68,69,70,70	0
3	GOL	C	507	6/6	0.76	0.39	72,73,73,73	0
3	GOL	A	508	6/6	0.82	0.20	63,64,65,65	0
3	GOL	D	506	6/6	0.82	0.22	76,76,77,77	0
3	GOL	C	503	6/6	0.82	0.27	72,72,73,73	0
3	GOL	D	503	6/6	0.83	0.20	76,77,77,78	0
3	GOL	C	502	6/6	0.84	0.29	66,66,66,67	0
3	GOL	C	506	6/6	0.85	0.19	85,86,86,86	0
3	GOL	B	504	6/6	0.86	0.29	84,84,85,85	0
3	GOL	D	507	6/6	0.87	0.18	71,72,72,72	0
3	GOL	B	503	6/6	0.88	0.24	71,72,72,73	0
3	GOL	D	502	6/6	0.88	0.21	73,73,73,74	0
3	GOL	A	503	6/6	0.89	0.28	65,65,65,66	0
3	GOL	B	506	6/6	0.89	0.17	67,68,68,68	0
3	GOL	A	504	6/6	0.90	0.17	59,60,61,61	0
3	GOL	C	508	6/6	0.90	0.27	72,73,73,73	0
5	CL	D	508	1/1	0.90	0.07	73,73,73,73	0
3	GOL	C	504	6/6	0.92	0.12	63,64,64,65	0
5	CL	A	510	1/1	0.93	0.13	61,61,61,61	0
3	GOL	B	502	6/6	0.93	0.35	73,73,73,73	0
3	GOL	A	505	6/6	0.95	0.16	66,67,67,67	0
3	GOL	A	502	6/6	0.95	0.20	52,52,53,53	0
5	CL	B	507	1/1	0.96	0.07	72,72,72,72	0
2	HEM	B	501	43/43	0.96	0.17	64,65,70,73	0
2	HEM	A	501	43/43	0.97	0.17	51,53,54,55	0
5	CL	C	510	1/1	0.97	0.18	55,55,55,55	0
2	HEM	D	501	43/43	0.97	0.17	67,71,74,75	0
2	HEM	C	501	43/43	0.98	0.13	50,52,54,56	0

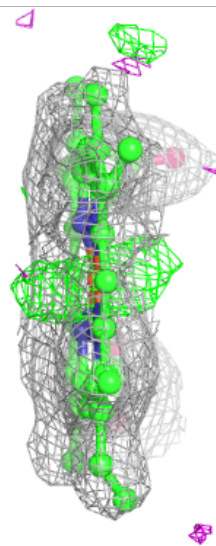
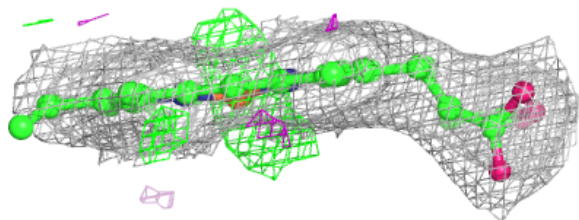
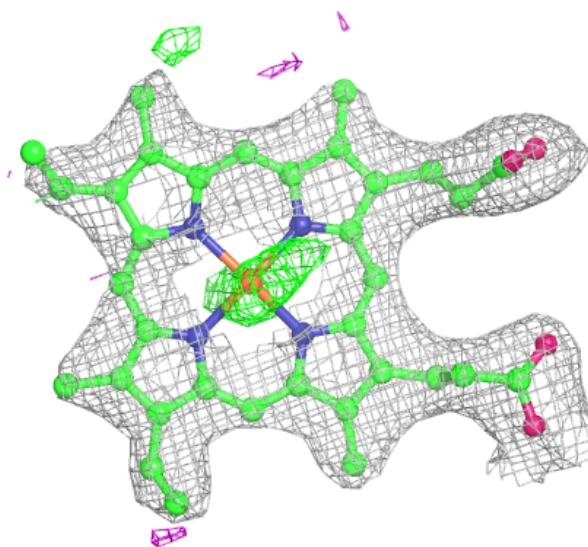
The following is a graphical depiction of the model fit to experimental electron density of all

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.



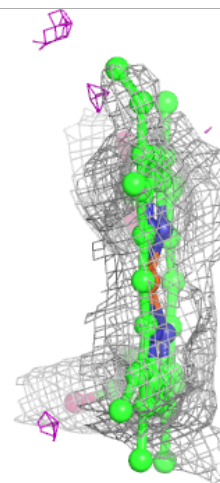
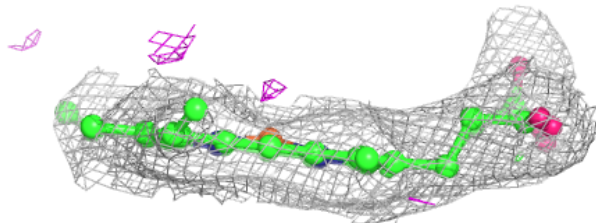
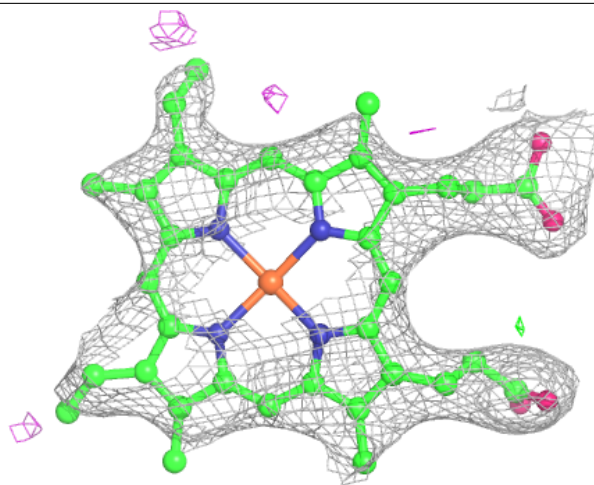
Electron density around HEM A 501:

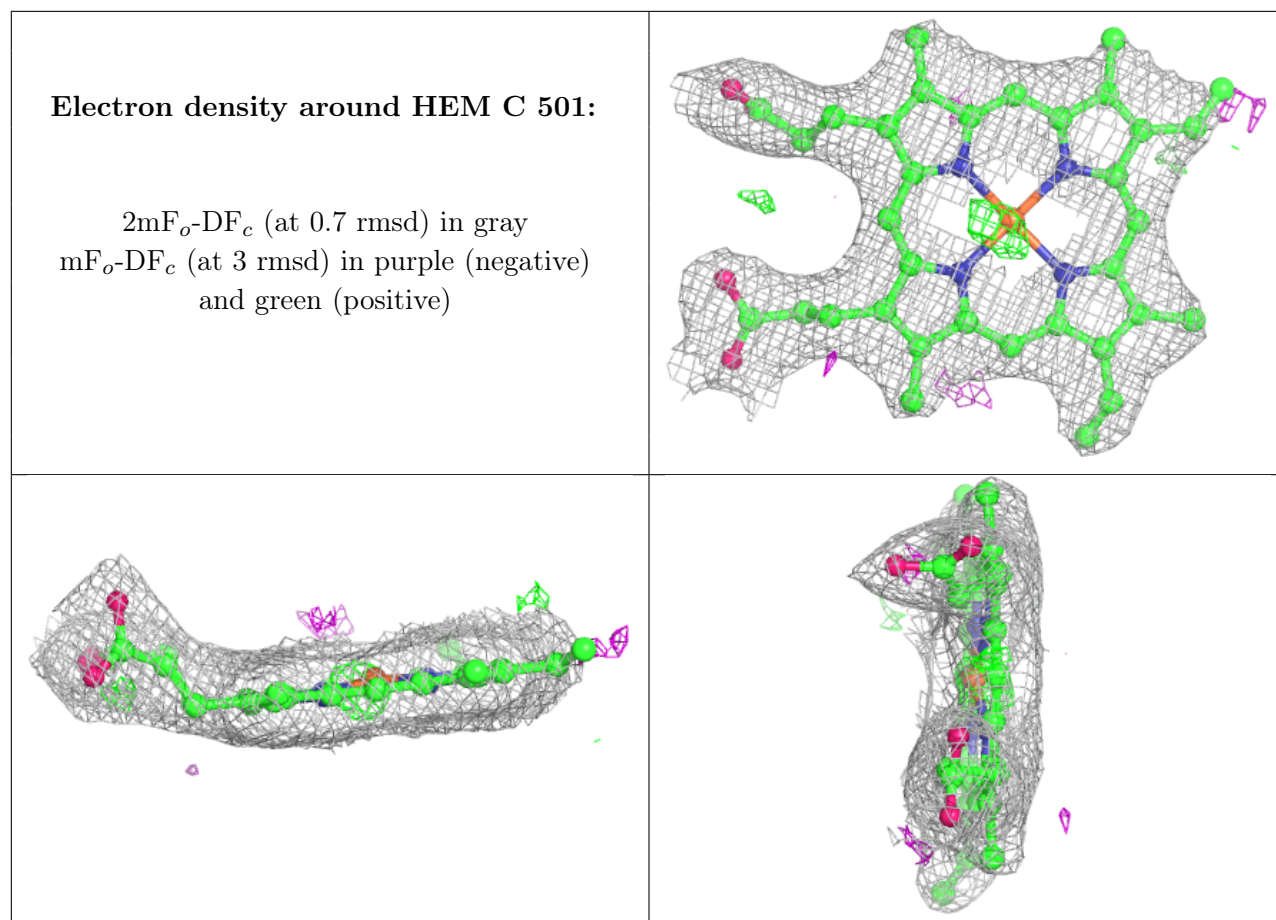
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.