Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 08:34 am BST

PDB ID	:	3OA8
Title	:	Diheme SoxAX
Authors	:	Maher, M.J.
Deposited on	:	2010-08-04
Resolution	:	1.77 Å(reported)

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

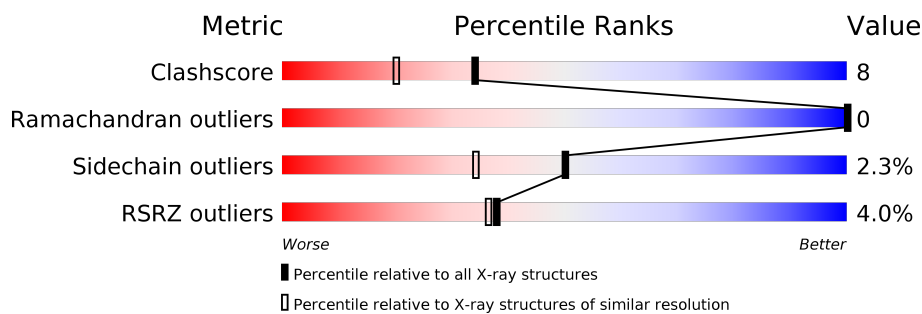|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0
Sidechain outliers		2.3%
RSRZ outliers		4.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 <=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	275	3% / 76% / 7% · 17%
1	C	275	72% / 11% · 17%
1	E	275	3% / 71% / 13% / 17%
2	B	208	6% / 75% / 12% / 13%
2	D	208	5% / 76% / 11% / 13%
2	F	208	5% / 74% / 12% / 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10596 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 SoxA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	2	0
			1794	1127	317	334	16			
1	C	229	Total	C	N	O	S	0	3	0
			1798	1130	317	335	16			
1	E	229	Total	C	N	O	S	0	4	0
			1805	1135	319	335	16			

- Molecule 2 is a protein called SoxX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	5	0
			1377	865	239	267	6			
2	D	180	Total	C	N	O	S	0	0	0
			1358	847	239	266	6			
2	F	180	Total	C	N	O	S	0	3	0
			1368	855	239	268	6			

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).
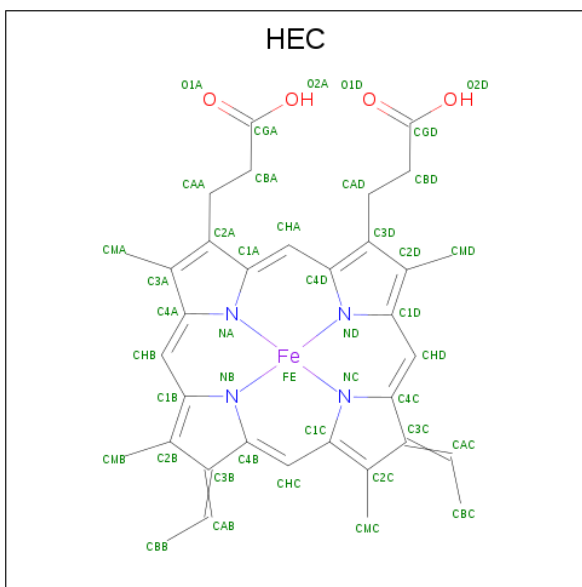
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

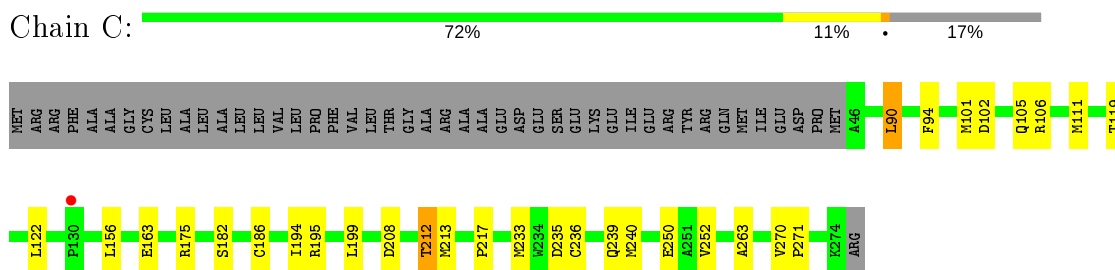| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	140	Total 140	O 140	0	0
5	B	152	Total 152	O 152	0	0
5	C	151	Total 151	O 151	0	0
5	D	148	Total 148	O 148	0	0
5	E	122	Total 122	O 122	0	0
5	F	120	Total 120	O 120	0	0

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.
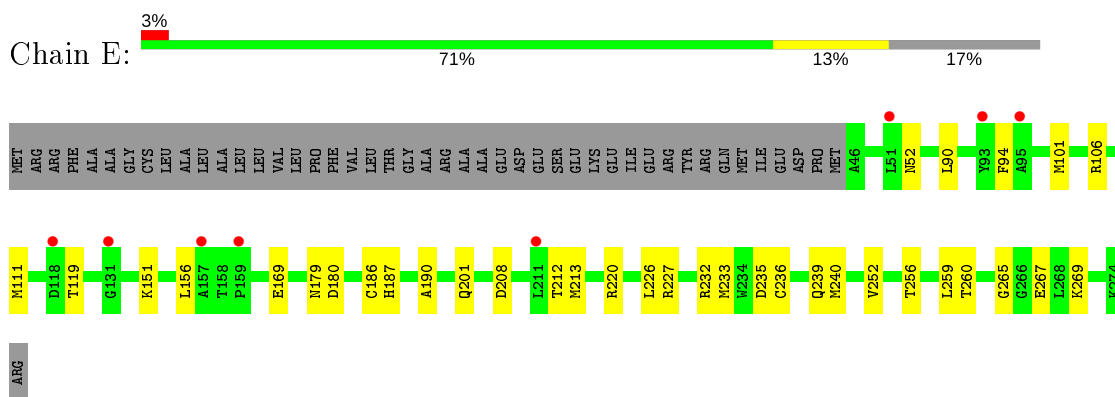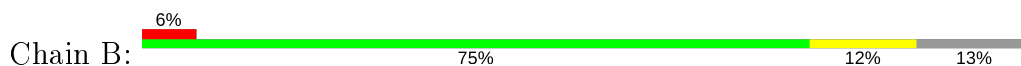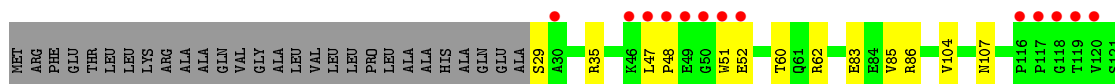
- Molecule 1: SoxA
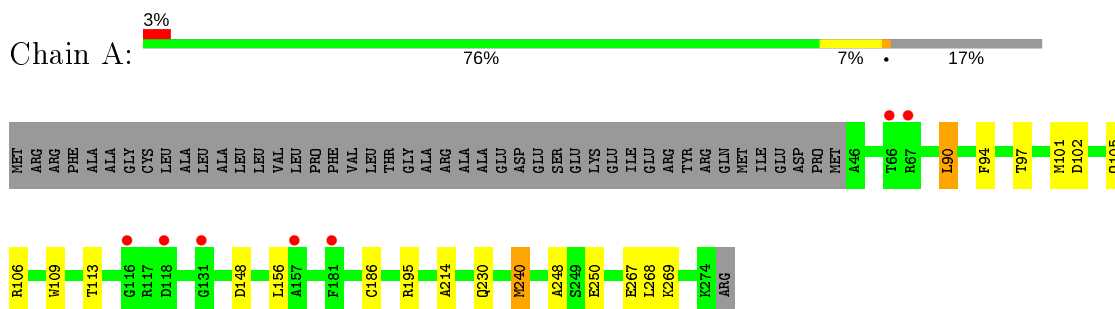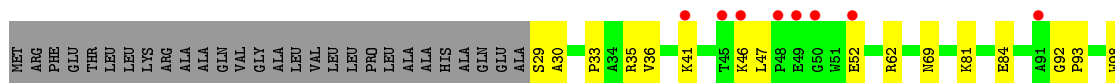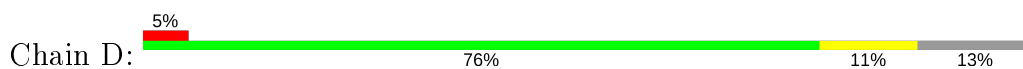

- Molecule 1: SoxA

- Molecule 1: SoxA

- Molecule 2: SoxX

MET ARG PHE GLU THR LEU LEU LYS ARG ALA ALA GLN VAL GLY ALA LEU VAL LEU LEU PRO LEU ALA ALA HIS ALA GLN GLU ALA S29 A30 R35 K46 L47 P48 E49 G50 W51 E52 T60 Q61 R62 E83 E84 V85 R86 V104 N107 P116 P117 G118 T119 V120 S121

G122 Y126 A127 C128 D132 E135 V136 S137 R150 V183 I192 V195 V196 N207 K208

• Molecule 2: SoxX

Chain D:

MET ARG PHE GLU THR LEU LEU LYS ARG ALA ALA GLN VAL GLY ALA LEU VAL LEU LEU PRO LEU ALA ALA HIS ALA GLN GLU ALA S29 A30 P33 A34 R35 V36 K41 T45 K46 L47 P48 E49 G50 W51 E52 R62 N69 K81 E84 A91 Q92 P93 W98

Q112 P117 C128 L131 S137 V195 E203 K208

• Molecule 2: SoxX

Chain F:

MET ARG PHE GLU THR LEU LEU LYS ARG ALA ALA GLN VAL GLY ALA LEU VAL LEU LEU PRO LEU ALA ALA HIS ALA GLN GLU ALA S29 A30 D37 K46 Q57 Q61 R62 I63 V66 T67 R68 A77 K81 E84 A91 I95 W98 D115 P116 P117

G118 T119 V120 A127 C128 G139 G149 R150 V183 V195 E203 N207 K208

4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.17Å　　74.63Å　　74.30Å 110.02°　　108.08°　　108.54°	Depositor
Resolution (Å)	35.31　−　1.77 35.31　−　1.77	Depositor EDS
% Data completeness (in resolution range)	92.2 (35.31-1.77) 92.2 (35.31-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.19 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183　,　　　0.230 0.186　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.4	EDS
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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Property	Value	Source
Estimated twinning fraction	0.013 for -k,-l,h+k+l 0.013 for h+k+l,-h,-k 0.014 for h+k+l,-l,-h 0.014 for -l,h+k+l,-k 0.014 for -k,h+k+l,-h 0.014 for -l,-h,h+k+l 0.086 for h,-h-k-l,k 0.086 for h,l,-h-k-l 0.014 for -h-k-l,h,l 0.014 for k,-h-k-l,l 0.013 for l,k,-h-k-l 0.013 for -h-k-l,k,h 0.016 for l,h,k 0.016 for k,l,h 0.026 for l,-h-k-l,h 0.021 for -l,-k,-h 0.023 for k,h,-h-k-l 0.020 for -k,-h,-l 0.025 for -h-k-l,l,k 0.023 for -h,-l,-k 0.020 for -h,h+k+l,-l 0.018 for -h,-k,h+k+l 0.019 for h+k+l,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10596	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, CSS, 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	A	0.65	0/1821	0.72	2/2460 (0.1%)
1	C	0.66	0/1828	0.71	0/2471
1	E	0.59	0/1838	0.69	0/2484
2	B	0.68	0/1421	0.68	1/1929 (0.1%)
2	D	0.71	0/1387	0.69	0/1881
2	F	0.63	0/1406	0.66	0/1907
All	All	0.65	0/9701	0.69	3/13132 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	MET	CG-SD-CE	-7.29	88.54	100.20
1	A	90	LEU	CA-CB-CG	5.74	128.50	115.30
2	B	132	ASP	CB-CG-OD1	5.14	122.93	118.30

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	1794	0	1786	23	0
1	C	1798	0	1790	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1805	0	1804	33	0
2	B	1377	0	1363	27	0
2	D	1358	0	1322	21	0
2	F	1368	0	1341	26	0
3	A	43	0	31	8	0
3	B	43	0	31	6	0
3	C	43	0	31	11	0
3	D	43	0	31	3	0
3	E	43	0	31	10	0
3	F	43	0	31	5	0
4	B	5	0	0	0	0
5	A	140	0	0	0	0
5	B	152	0	0	10	0
5	C	151	0	0	1	0
5	D	148	0	0	2	0
5	E	122	0	0	1	0
5	F	120	0	0	2	0
All	All	10596	0	9592	163	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 (163) 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)
2:F:77:ALA:O	2:F:81:LYS:HD3	1.26	1.35
1:E:169:GLU:CD	2:F:68:ARG:HH22	1.43	1.21
2:B:128:CYS:SG	3:B:401:HEC:CAC	2.36	1.13
1:C:217:PRO:HD2	1:C:270:VAL:HG21	1.31	1.09
1:C:186:CYS:SG	3:C:401:HEC:CAC	2.40	1.09
2:D:128:CYS:SG	3:D:401:HEC:CAC	2.41	1.08
1:E:186:CYS:SG	3:E:401:HEC:CAC	2.44	1.06
2:F:128:CYS:SG	3:F:401:HEC:CAC	2.49	1.01
1:A:186:CYS:SG	3:A:401:HEC:CAC	2.48	1.00
2:D:47:LEU:HD13	2:D:52:GLU:HG3	1.45	0.99
1:E:169:GLU:CD	2:F:68:ARG:NH2	2.26	0.89
2:B:60:THR:HG21	2:B:83:GLU:OE1	1.76	0.84
1:E:239:GLN:HB2	5:E:374:HOH:O	1.82	0.80
2:F:77:ALA:O	2:F:81:LYS:CD	2.21	0.79
3:E:401:HEC:HMC1	3:E:401:HEC:HBC3	1.64	0.77
1:A:94:PHE:HB2	1:A:101:MET:HE2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:VAL:HG23	1:C:271:PRO:HA	1.70	0.72
1:A:94:PHE:HB2	1:A:101:MET:CE	2.19	0.71
1:C:217:PRO:HD2	1:C:270:VAL:CG2	2.17	0.70
2:F:98:TRP:NE1	2:F:203:GLU:HG3	2.06	0.69
1:A:186:CYS:SG	3:A:401:HEC:CBC	2.81	0.68
2:B:35:ARG:CZ	5:B:853:HOH:O	2.41	0.68
1:E:52:ASN:HB2	1:E:226[B]:LEU:HD23	1.77	0.67
1:C:111:MET:HE1	1:C:119:THR:HG22	1.75	0.67
1:C:208:ASP:O	1:C:212:THR:HG23	1.97	0.65
1:C:194:ILE:HD12	1:C:199:LEU:HD21	1.79	0.65
1:C:101:MET:CE	1:C:106:ARG:HH11	2.10	0.64
1:C:186:CYS:SG	3:C:401:HEC:CBC	2.85	0.64
1:A:240:MET:HG2	3:A:401:HEC:HMC2	1.80	0.64
1:E:52:ASN:CB	1:E:226[B]:LEU:HD23	2.28	0.63
2:B:128:CYS:SG	3:B:401:HEC:C3C	2.86	0.63
1:C:240:MET:HG2	3:C:401:HEC:HMC2	1.80	0.63
1:C:194:ILE:HG13	1:C:199:LEU:HD11	1.82	0.62
2:B:128:CYS:SG	3:B:401:HEC:CBC	2.86	0.62
1:C:101:MET:HE3	1:C:106:ARG:HD3	1.82	0.62
1:A:186:CYS:SG	3:A:401:HEC:HBC3	2.40	0.62
1:C:163:GLU:OE2	2:D:35:ARG:HD3	2.00	0.62
1:C:250:GLU:CD	2:D:35:ARG:HH22	2.03	0.60
2:F:128:CYS:SG	3:F:401:HEC:CBC	2.89	0.60
2:D:128:CYS:SG	3:D:401:HEC:HAC	2.37	0.59
2:D:52:GLU:H	2:D:52:GLU:CD	2.05	0.59
1:E:169:GLU:CG	2:F:68:ARG:NH2	2.65	0.59
1:E:169:GLU:CG	2:F:68:ARG:HH22	2.16	0.59
1:E:169:GLU:HG2	2:F:68:ARG:NH2	2.19	0.58
1:E:213:MET:HE1	1:E:259:LEU:HD13	1.86	0.58
1:E:240:MET:HG2	3:E:401:HEC:HMC2	1.86	0.57
2:D:128:CYS:SG	3:D:401:HEC:C3C	2.93	0.57
2:B:52:GLU:N	5:B:501:HOH:O	2.36	0.57
1:C:186:CYS:SG	3:C:401:HEC:C3C	2.92	0.57
1:E:94:PHE:CD2	1:E:101:MET:HE3	2.40	0.56
1:E:240:MET:CG	3:E:401:HEC:HMC2	2.35	0.56
2:F:62:ARG:O	2:F:66[A]:VAL:HG23	2.06	0.56
2:F:63:ILE:HD13	5:F:216:HOH:O	2.05	0.55
1:C:239:GLN:HA	2:D:112:GLN:HE21	1.72	0.55
1:A:186:CYS:SG	3:A:401:HEC:C3C	2.95	0.55
1:C:194:ILE:HD13	3:C:401:HEC:HAC	1.89	0.55
1:E:208:ASP:O	1:E:212:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:MET:HE1	1:C:122:LEU:HD12	1.88	0.55
1:C:270:VAL:CG2	1:C:271:PRO:HA	2.37	0.55
2:F:98:TRP:HE1	2:F:203:GLU:HG3	1.69	0.55
1:C:111:MET:CE	1:C:122:LEU:HD12	2.38	0.54
2:D:29:SER:HB3	2:F:68:ARG:NH1	2.22	0.54
1:C:101:MET:HE1	1:C:106:ARG:HH11	1.72	0.54
1:C:194:ILE:CD1	3:C:401:HEC:HAC	2.38	0.54
2:B:51:TRP:C	5:B:501:HOH:O	2.45	0.54
1:E:151:LYS:HD2	1:E:265:GLY:O	2.08	0.54
3:E:401:HEC:HMC1	3:E:401:HEC:CBC	2.37	0.54
2:D:29:SER:N	5:D:389:HOH:O	2.39	0.53
1:C:94:PHE:HB2	1:C:101:MET:HE2	1.90	0.53
1:E:186:CYS:SG	3:E:401:HEC:C3C	2.96	0.53
2:F:128:CYS:SG	3:F:401:HEC:C3C	2.97	0.53
2:B:86:ARG:NH1	2:B:183:VAL:HG11	2.24	0.52
3:A:401:HEC:HBC3	3:A:401:HEC:HMC1	1.91	0.52
2:B:104:VAL:HB	2:B:195[B]:VAL:HG23	1.91	0.52
2:B:47:LEU:HD22	5:B:501:HOH:O	2.10	0.52
2:B:48:PRO:HB2	2:B:51:TRP:CD1	2.45	0.51
1:C:102:ASP:H	1:C:105:GLN:HE21	1.56	0.51
1:A:94:PHE:CG	1:A:101:MET:HE3	2.45	0.51
1:A:101:MET:CE	1:A:106:ARG:HH11	2.24	0.51
1:C:194:ILE:CD1	1:C:199:LEU:HD11	2.40	0.50
2:D:62:ARG:HH22	1:E:201:GLN:HE22	1.58	0.50
1:E:220:ARG:HD3	1:E:227:ARG:HG3	1.93	0.50
1:A:148:ASP:OD1	1:A:269:LYS:HA	2.12	0.50
2:F:128:CYS:SG	3:F:401:HEC:HBC3	2.52	0.50
1:C:186:CYS:SG	3:C:401:HEC:HBC3	2.52	0.50
1:E:220:ARG:HH12	1:E:232:ARG:HH11	1.60	0.50
1:E:111:MET:HE1	1:E:119:THR:HG22	1.94	0.49
3:F:401:HEC:HMB1	3:F:401:HEC:HBB3	1.93	0.49
2:B:52:GLU:CA	5:B:501:HOH:O	2.61	0.49
2:B:62:ARG:HD3	5:B:518:HOH:O	2.13	0.49
2:F:98:TRP:NE1	2:F:203:GLU:CG	2.73	0.49
1:E:186:CYS:SG	3:E:401:HEC:CBC	3.00	0.49
2:B:52:GLU:HA	5:B:501:HOH:O	2.12	0.48
1:C:194:ILE:CG1	1:C:199:LEU:HD11	2.43	0.48
2:B:35:ARG:NE	5:B:853:HOH:O	2.47	0.47
1:A:214:ALA:HA	1:A:268:LEU:HD23	1.96	0.47
2:B:86:ARG:CZ	2:B:183:VAL:CG1	2.92	0.47
1:A:94:PHE:CD2	1:A:101:MET:HE3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:MET:HB2	1:C:263:ALA:CB	2.45	0.47
1:E:212:THR:HG22	3:E:401:HEC:O2A	2.15	0.47
1:E:52:ASN:CG	1:E:226[B]:LEU:HD23	2.35	0.46
1:A:94:PHE:CB	1:A:101:MET:CE	2.92	0.46
1:E:233:MET:HG3	1:E:252:VAL:HG13	1.98	0.46
1:C:111:MET:CE	1:C:119:THR:HG22	2.43	0.46
2:F:149:GLY:H	2:F:207:ASN:HD21	1.63	0.46
1:A:195:ARG:HD2	2:B:137:SER:OG	2.16	0.46
2:B:29:SER:HA	2:D:30:ALA:HB2	1.98	0.45
2:D:62:ARG:CZ	1:E:190:ALA:HB2	2.47	0.45
1:E:186:CYS:SG	3:E:401:HEC:HAC	2.49	0.45
1:A:102:ASP:H	1:A:105:GLN:HE21	1.64	0.45
1:C:101:MET:HE3	1:C:106:ARG:HH11	1.78	0.45
2:B:47:LEU:HB3	5:B:501:HOH:O	2.15	0.45
2:D:69:ASN:ND2	5:D:276:HOH:O	2.50	0.45
1:C:90:LEU:HD13	5:C:289:HOH:O	2.16	0.45
1:A:267:GLU:HG2	1:A:269:LYS:HE2	1.98	0.44
3:B:401:HEC:HMC1	3:B:401:HEC:HBC3	1.99	0.44
1:C:212:THR:HB	3:C:401:HEC:CGA	2.48	0.44
1:A:101:MET:HE3	1:A:106:ARG:HH11	1.82	0.44
2:B:128:CYS:SG	3:B:401:HEC:HBC3	2.57	0.44
1:E:232:ARG:NH2	1:E:236[A]:CSS:SD	2.90	0.44
1:C:217:PRO:CD	1:C:270:VAL:HG21	2.23	0.44
1:A:109:TRP:CE2	1:A:113:THR:HG21	2.53	0.44
2:D:98:TRP:NE1	2:D:203:GLU:HG3	2.33	0.44
1:E:179:ASN:O	1:E:180:ASP:HB2	2.18	0.44
2:F:57:GLN:HA	2:F:61:GLN:OE1	2.18	0.44
2:F:81:LYS:CD	2:F:81:LYS:N	2.81	0.43
2:D:92:GLY:HA3	2:D:93:PRO:HD2	1.78	0.43
2:F:98:TRP:HE1	2:F:203:GLU:CG	2.32	0.43
1:C:195:ARG:HD2	2:D:137:SER:OG	2.19	0.43
1:C:233:MET:HG3	1:C:252:VAL:HG13	2.00	0.43
1:C:111:MET:HB3	1:C:111:MET:HE2	1.81	0.43
3:C:401:HEC:HBB3	3:C:401:HEC:HMB1	2.01	0.43
3:C:401:HEC:HMC1	3:C:401:HEC:HBC3	2.00	0.43
2:F:127:ALA:O	2:F:139:GLY:HA3	2.19	0.43
1:A:240:MET:CG	3:A:401:HEC:HMC2	2.49	0.43
1:C:236[B]:CSS:HA	1:C:239:GLN:HG2	2.00	0.42
2:B:150:ARG:H	2:B:207:ASN:ND2	2.17	0.42
2:B:85:VAL:HG13	5:B:253:HOH:O	2.19	0.42
1:E:267:GLU:OE2	1:E:269:LYS:NZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLN:NE2	1:A:248:ALA:H	2.17	0.42
2:D:62:ARG:HH22	1:E:201:GLN:NE2	2.18	0.42
1:A:97:THR:OG1	1:A:101:MET:CE	2.67	0.42
2:B:192:ILE:O	2:B:196[A]:VAL:HG23	2.20	0.42
2:B:107:ASN:HB3	2:B:122:GLY:HA3	2.02	0.42
3:A:401:HEC:HBB3	3:A:401:HEC:HMB1	2.01	0.42
2:D:41:LYS:HD2	2:D:41:LYS:HA	1.90	0.41
1:E:256:THR:O	1:E:260[A]:THR:HG23	2.20	0.41
1:C:101:MET:HE1	1:C:106:ARG:NH1	2.34	0.41
2:F:208:LYS:HB2	5:F:619:HOH:O	2.21	0.41
2:D:29:SER:CB	2:F:68:ARG:NH1	2.84	0.41
1:C:175:ARG:HG2	1:C:182:SER:HB3	2.03	0.41
1:E:101:MET:CE	1:E:106:ARG:HH11	2.34	0.41
2:B:86:ARG:NH2	2:B:183:VAL:HG13	2.35	0.41
1:C:94:PHE:HB2	1:C:101:MET:CE	2.50	0.41
2:B:128:CYS:SG	3:B:401:HEC:HAC	2.48	0.41
2:B:126:TYR:CE2	2:B:135:GLU:HG2	2.56	0.41
2:F:150:ARG:H	2:F:207:ASN:ND2	2.19	0.41
2:F:115:ASP:HA	2:F:116:PRO:HD3	1.93	0.41
1:C:240:MET:CG	3:C:401:HEC:HMC2	2.50	0.40
1:A:101:MET:HA	1:A:105:GLN:NE2	2.36	0.40
2:D:33:PRO:O	2:D:36:VAL:HG23	2.21	0.40
1:E:187:HIS:CD2	3:E:401:HEC:NB	2.88	0.40
1:A:97:THR:CG2	1:A:101:MET:HE1	2.52	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	227/275 (82%)	223 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	228/275 (83%)	225 (99%)	3 (1%)	0	100	100
1	E	229/275 (83%)	226 (99%)	3 (1%)	0	100	100
2	B	183/208 (88%)	178 (97%)	5 (3%)	0	100	100
2	D	178/208 (86%)	174 (98%)	4 (2%)	0	100	100
2	F	181/208 (87%)	177 (98%)	4 (2%)	0	100	100
All	All	1226/1449 (85%)	1203 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	189/225 (84%)	186 (98%)	3 (2%)	62	51
1	C	190/225 (84%)	186 (98%)	4 (2%)	53	38
1	E	191/225 (85%)	188 (98%)	3 (2%)	62	51
2	B	150/165 (91%)	150 (100%)	0	100	100
2	D	145/165 (88%)	140 (97%)	5 (3%)	37	20
2	F	148/165 (90%)	140 (95%)	8 (5%)	22	8
All	All	1013/1170 (87%)	990 (98%)	23 (2%)	50	34

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	156	LEU
1	A	250	GLU
1	C	90	LEU
1	C	156	LEU
1	C	212	THR
1	C	235	ASP
2	D	46	LYS

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Mol	Chain	Res	Type
2	D	81	LYS
2	D	84	GLU
2	D	131	LEU
2	D	195	VAL
1	E	90	LEU
1	E	156	LEU
1	E	235	ASP
2	F	29	SER
2	F	37	ASP
2	F	46	LYS
2	F	84	GLU
2	F	95	LEU
2	F	183	VAL
2	F	195	VAL
2	F	208	LYS

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

Mol	Chain	Res	Type
1	A	52	ASN
1	A	68	ASN
1	A	105	GLN
1	A	230	GLN
1	A	262	GLN
2	B	112	GLN
2	B	207	ASN
1	C	52	ASN
1	C	105	GLN
1	C	230	GLN
2	D	112	GLN
2	D	207	ASN
1	E	52	ASN
1	E	68	ASN
1	E	105	GLN
1	E	230	GLN
2	F	112	GLN
2	F	207	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	CSS	C	236[B]	1,3	4,5,7	0.89	0	1,5,8	0.04	0
1	CSS	C	236[A]	1,3	4,6,7	0.68	0	1,6,8	1.27	0
1	CSS	A	236[A]	1,3	4,6,7	0.69	0	1,6,8	1.08	0
1	CSS	E	236[A]	1,3	4,6,7	0.60	0	1,6,8	1.04	0
1	CSS	A	236[B]	1,3	4,5,7	0.77	0	1,5,8	0.88	0
1	CSS	E	236[B]	1,3	4,5,7	0.70	0	1,5,8	0.41	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSS	C	236[B]	1,3	-	0/1/4/7	-
1	CSS	C	236[A]	1,3	-	0/1/5/7	-
1	CSS	A	236[A]	1,3	-	0/1/5/7	-
1	CSS	E	236[A]	1,3	-	0/1/5/7	-
1	CSS	A	236[B]	1,3	-	0/1/4/7	-
1	CSS	E	236[B]	1,3	-	0/1/4/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	236[B]	CSS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	236[A]	CSS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 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	#$\|Z\|>2$
4	SO4	B	209	-	4,4,4	0.66	0	6,6,6	0.62	0
3	HEC	A	401	1	26,50,50	2.02	6 (23%)	18,82,82	2.09	6 (33%)
3	HEC	B	401	2	26,50,50	2.36	5 (19%)	18,82,82	2.22	7 (38%)
3	HEC	C	401	1	26,50,50	2.52	8 (30%)	18,82,82	1.91	5 (27%)
3	HEC	D	401	2	26,50,50	2.24	5 (19%)	18,82,82	2.29	6 (33%)
3	HEC	E	401	1	26,50,50	2.50	4 (15%)	18,82,82	2.39	7 (38%)
3	HEC	F	401	2	26,50,50	2.24	5 (19%)	18,82,82	2.46	8 (44%)

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
3	HEC	A	401	1	-	0/6/54/54	-
3	HEC	B	401	2	-	0/6/54/54	-
3	HEC	C	401	1	-	0/6/54/54	-
3	HEC	D	401	2	-	0/6/54/54	-
3	HEC	E	401	1	-	0/6/54/54	-
3	HEC	F	401	2	-	0/6/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	HEC	C3B-C2B	-7.12	1.33	1.40
3	B	401	HEC	C3B-C2B	-6.99	1.33	1.40
3	F	401	HEC	C3C-C2C	-6.85	1.33	1.40
3	C	401	HEC	C3C-C2C	-6.78	1.33	1.40
3	D	401	HEC	C3B-C2B	-6.78	1.33	1.40
3	C	401	HEC	C3B-C2B	-6.75	1.33	1.40
3	E	401	HEC	C3C-C2C	-6.75	1.33	1.40
3	B	401	HEC	C3C-C2C	-5.64	1.34	1.40
3	D	401	HEC	C3C-C2C	-4.94	1.35	1.40
3	E	401	HEC	C3D-C2D	4.80	1.51	1.37
3	C	401	HEC	C3D-C2D	4.78	1.51	1.37
3	B	401	HEC	C3D-C2D	4.75	1.51	1.37
3	F	401	HEC	C3D-C2D	4.62	1.51	1.37
3	D	401	HEC	C3D-C2D	4.53	1.51	1.37
3	A	401	HEC	C3B-C2B	-4.52	1.36	1.40
3	A	401	HEC	C3C-C2C	-4.51	1.36	1.40
3	A	401	HEC	C3D-C2D	4.31	1.50	1.37
3	F	401	HEC	C3B-C2B	-4.20	1.36	1.40
3	B	401	HEC	CMD-C2D	2.55	1.56	1.51
3	F	401	HEC	C3B-C4B	2.28	1.47	1.43
3	B	401	HEC	C1A-C2A	2.24	1.47	1.42
3	C	401	HEC	CAD-C3D	2.22	1.55	1.52
3	A	401	HEC	C4A-C3A	2.18	1.47	1.42
3	D	401	HEC	C1D-ND	2.18	1.40	1.36
3	A	401	HEC	C1D-CHD	-2.16	1.35	1.41
3	E	401	HEC	CAD-C3D	2.12	1.55	1.52
3	C	401	HEC	CBB-CAB	2.11	1.57	1.49
3	C	401	HEC	C4D-CHA	-2.10	1.35	1.41
3	C	401	HEC	C1D-CHD	-2.05	1.35	1.41
3	C	401	HEC	C4A-C3A	2.04	1.47	1.42
3	D	401	HEC	CMB-C2B	2.03	1.56	1.51
3	A	401	HEC	CAA-C2A	2.03	1.55	1.52
3	F	401	HEC	C4A-C3A	2.01	1.47	1.42

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	HEC	CMB-C2B-C3B	4.98	131.68	125.82
3	E	401	HEC	CMB-C2B-C1B	-4.84	121.02	128.46
3	D	401	HEC	CMC-C2C-C1C	-4.84	121.02	128.46
3	D	401	HEC	CMC-C2C-C3C	4.77	131.43	125.82
3	F	401	HEC	CMB-C2B-C1B	-4.36	121.77	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	HEC	CMC-C2C-C1C	-4.36	121.77	128.46
3	F	401	HEC	CMC-C2C-C3C	4.09	130.63	125.82
3	C	401	HEC	CMB-C2B-C1B	-4.08	122.20	128.46
3	A	401	HEC	CBD-CAD-C3D	-4.07	104.98	112.49
3	C	401	HEC	C1D-C2D-C3D	-4.01	104.21	107.00
3	B	401	HEC	CMC-C2C-C1C	-3.87	122.52	128.46
3	A	401	HEC	C1D-C2D-C3D	-3.65	104.46	107.00
3	B	401	HEC	C1D-C2D-C3D	-3.65	104.46	107.00
3	B	401	HEC	CMB-C2B-C1B	-3.61	122.92	128.46
3	D	401	HEC	CAA-CBA-CGA	-3.54	106.73	112.67
3	E	401	HEC	CAD-CBD-CGD	-3.48	106.84	112.67
3	A	401	HEC	CMC-C2C-C3C	3.38	129.80	125.82
3	B	401	HEC	CBA-CAA-C2A	-3.23	106.52	112.48
3	B	401	HEC	CMC-C2C-C3C	3.18	129.56	125.82
3	A	401	HEC	CMB-C2B-C1B	-3.14	123.64	128.46
3	B	401	HEC	CMB-C2B-C3B	3.07	129.44	125.82
3	F	401	HEC	CMB-C2B-C3B	3.04	129.40	125.82
3	D	401	HEC	CBA-CAA-C2A	-3.02	106.91	112.48
3	F	401	HEC	CAD-CBD-CGD	-2.94	107.73	112.67
3	C	401	HEC	CMB-C2B-C3B	2.89	129.22	125.82
3	F	401	HEC	CBA-CAA-C2A	-2.88	107.17	112.48
3	E	401	HEC	CMA-C3A-C2A	2.84	130.30	124.94
3	A	401	HEC	CMC-C2C-C1C	-2.77	124.20	128.46
3	C	401	HEC	CBD-CAD-C3D	-2.71	107.49	112.49
3	B	401	HEC	CAD-CBD-CGD	-2.69	108.16	112.67
3	D	401	HEC	C1D-C2D-C3D	-2.69	105.13	107.00
3	E	401	HEC	C1D-C2D-C3D	-2.68	105.13	107.00
3	F	401	HEC	CMD-C2D-C1D	-2.60	124.47	128.46
3	F	401	HEC	CMD-C2D-C3D	2.57	129.79	124.94
3	E	401	HEC	CBD-CAD-C3D	-2.55	107.78	112.49
3	C	401	HEC	CMC-C2C-C1C	-2.52	124.59	128.46
3	D	401	HEC	CBD-CAD-C3D	-2.21	108.40	112.49
3	A	401	HEC	CMB-C2B-C3B	2.20	128.41	125.82
3	E	401	HEC	CMD-C2D-C3D	2.11	128.93	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 43 short contacts:

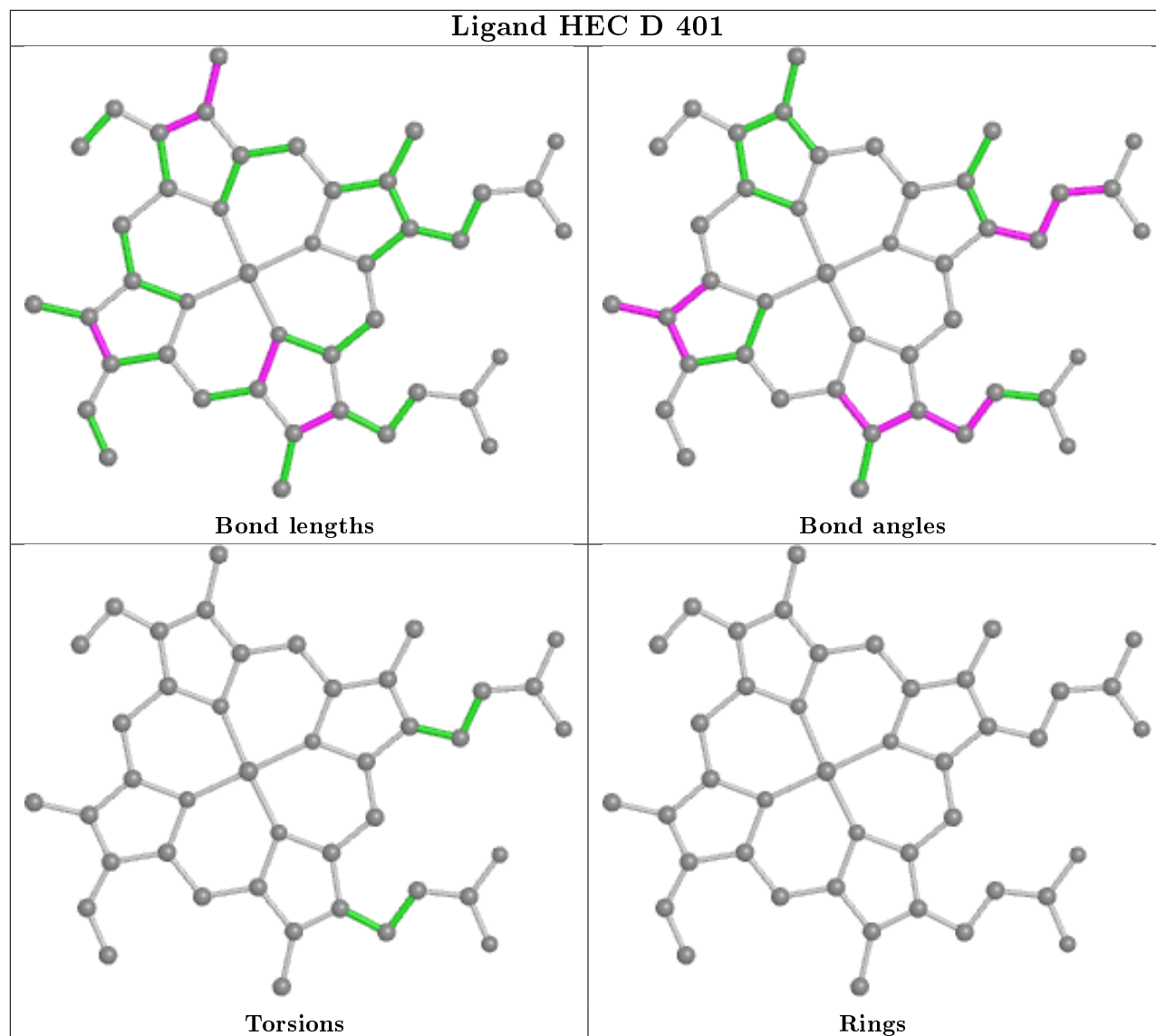| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	HEC	8	0
3	B	401	HEC	6	0
3	C	401	HEC	11	0
3	D	401	HEC	3	0
3	E	401	HEC	10	0
3	F	401	HEC	5	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEC A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC F 401

Bond lengths

Bond angles

Torsions

Rings
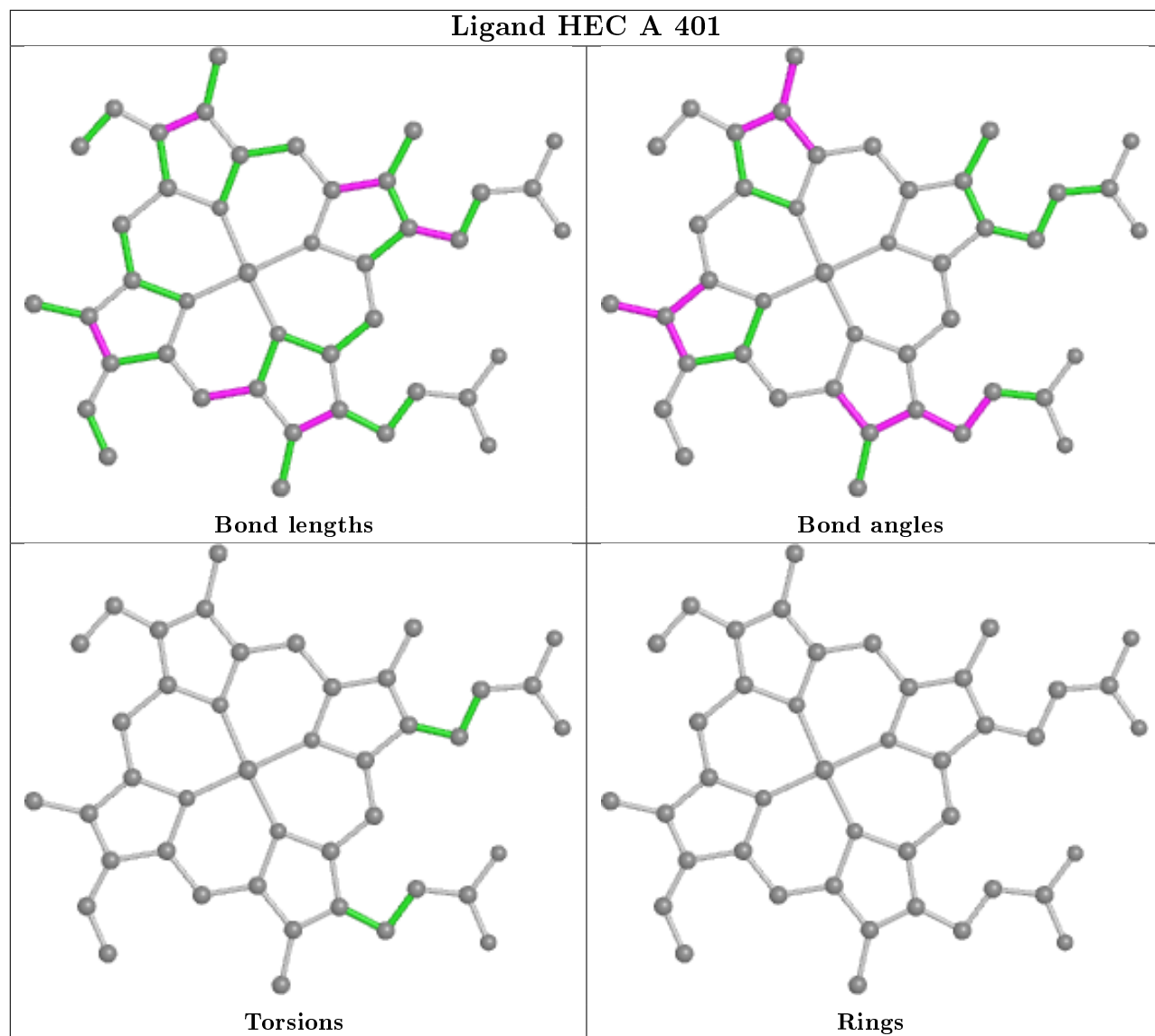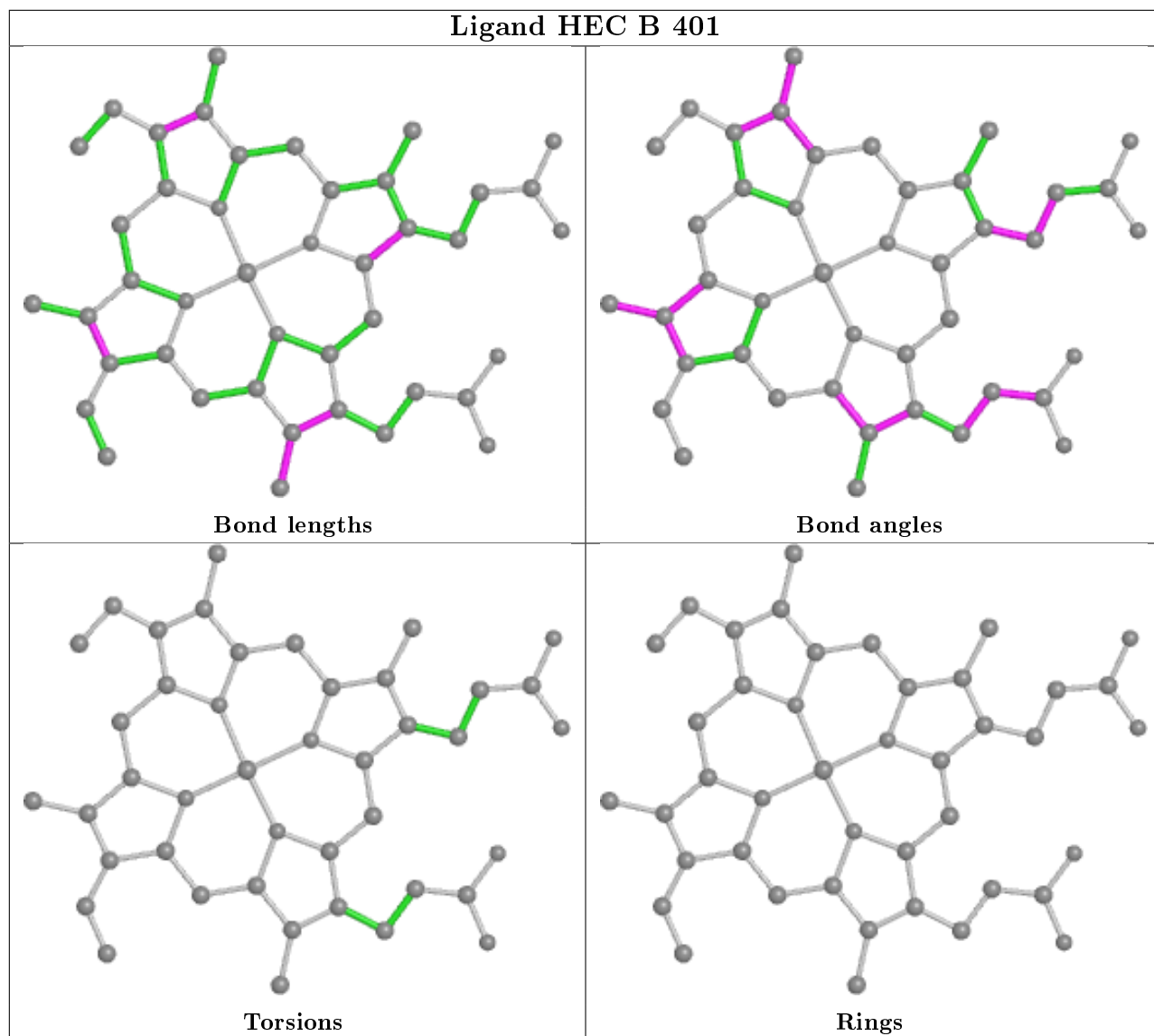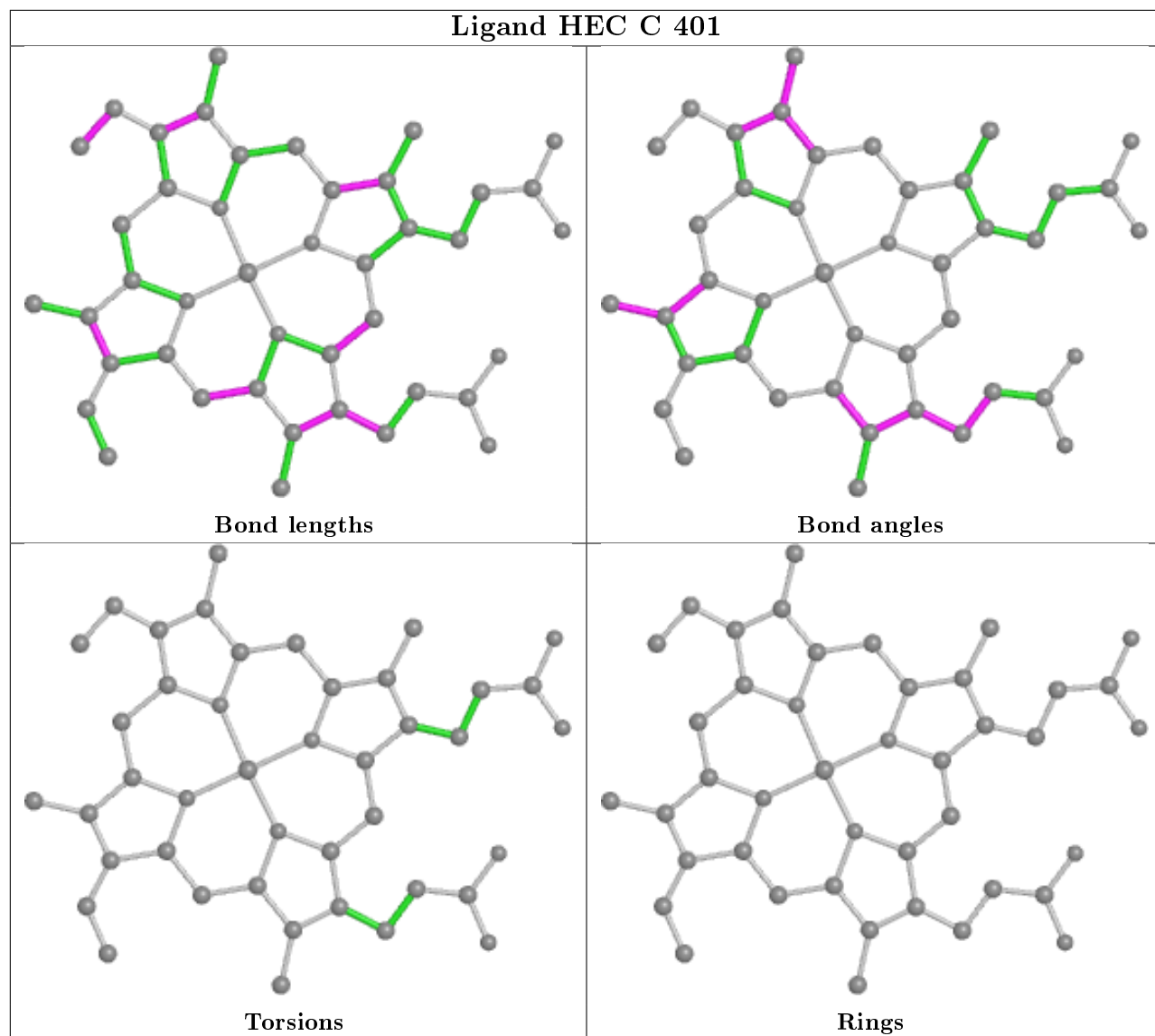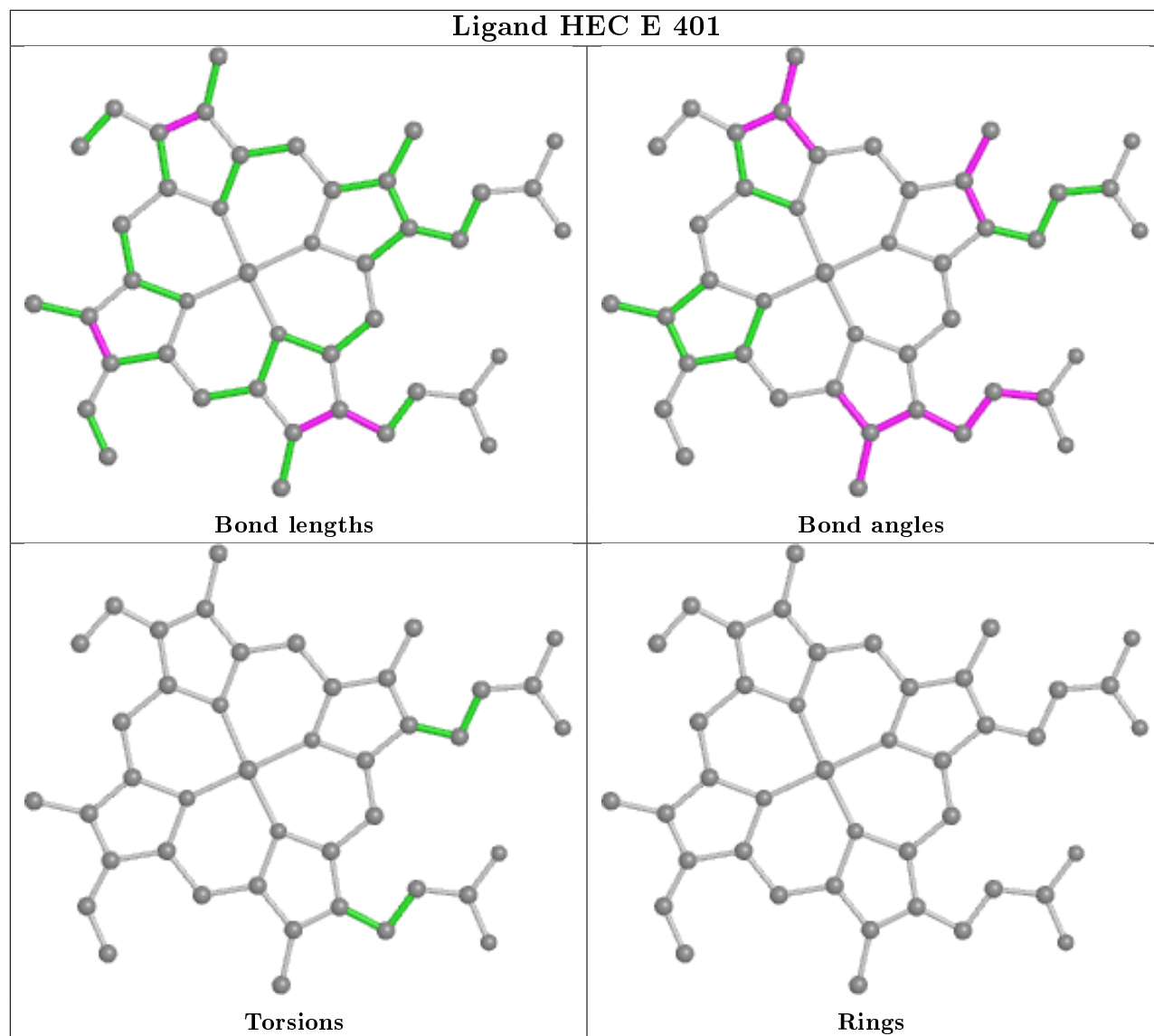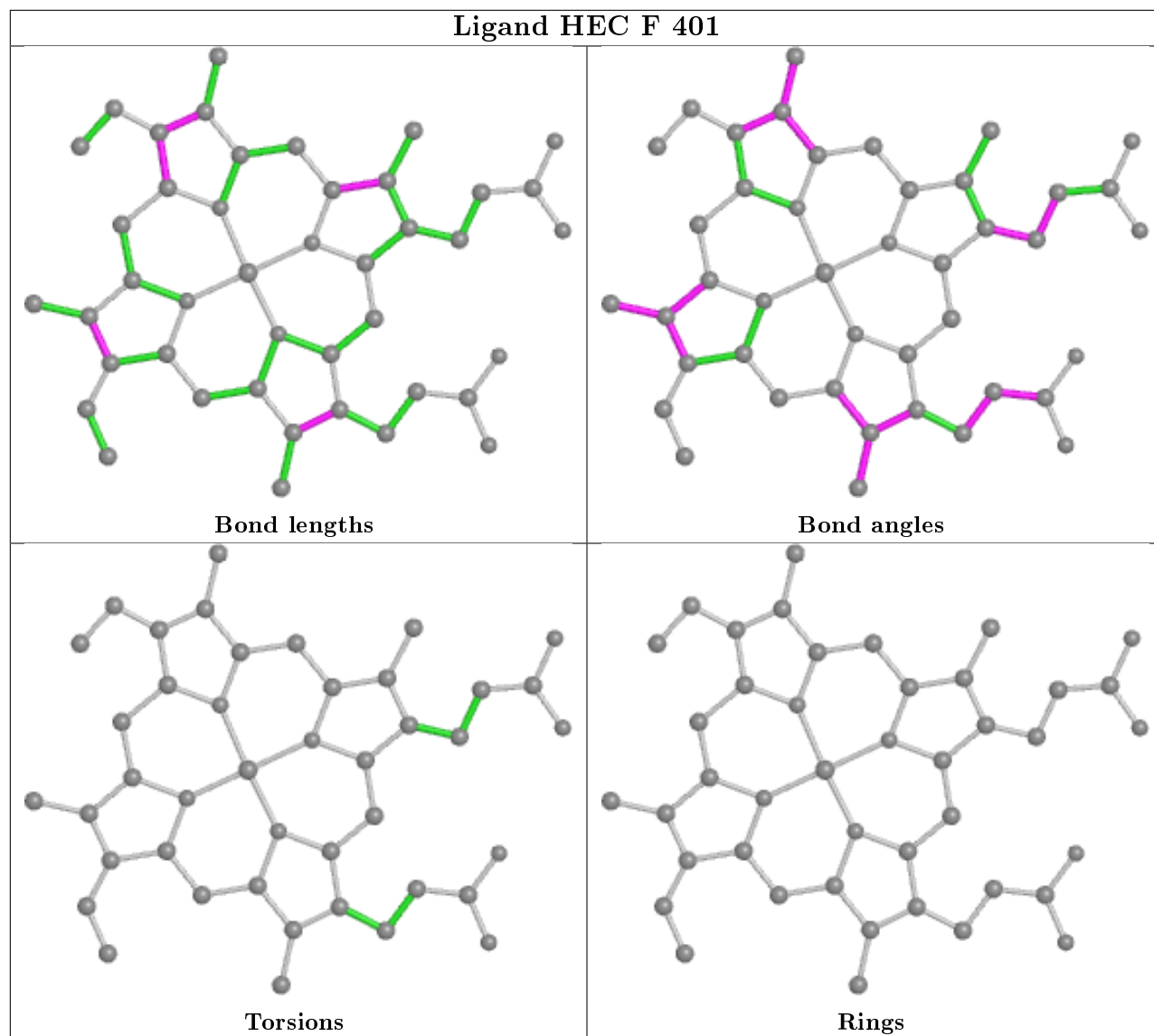
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	228/275 (82%)	0.03	7 (3%)	49	47	15, 27, 42, 53	0
1	C	228/275 (82%)	-0.05	1 (0%)	92	92	17, 26, 37, 46	0
1	E	228/275 (82%)	0.28	8 (3%)	44	42	18, 31, 54, 70	0
2	B	180/208 (86%)	0.18	13 (7%)	15	15	15, 26, 45, 61	0
2	D	180/208 (86%)	0.09	10 (5%)	24	23	16, 27, 41, 52	0
2	F	180/208 (86%)	0.22	10 (5%)	24	23	17, 30, 51, 63	0
All	All	1224/1449 (84%)	0.12	49 (4%)	38	36	15, 27, 46, 70	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	50	GLY	4.9
1	E	95	ALA	4.9
2	D	117	PRO	4.7
2	B	48	PRO	4.6
2	F	117	PRO	4.4
2	D	50	GLY	4.2
2	D	91	ALA	4.1
2	B	118	GLY	4.0
2	F	91	ALA	3.9
2	D	208	LYS	3.9
2	F	29	SER	3.6
2	F	208	LYS	3.6
2	F	46	LYS	3.6
2	F	119	THR	3.3
1	E	157	ALA	3.3
2	D	48	PRO	3.1
1	A	118	ASP	3.0
2	B	52	GLU	3.0
2	B	117	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	118	GLY	3.0
2	F	30	ALA	2.9
2	B	119	THR	2.9
2	B	47	LEU	2.8
2	D	45	THR	2.8
1	E	118	ASP	2.7
2	F	120	VAL	2.7
2	B	30	ALA	2.6
1	A	116	GLY	2.5
2	B	46	LYS	2.5
1	E	93	TYR	2.5
1	E	211	LEU	2.5
2	B	116	PRO	2.4
2	F	116	PRO	2.4
1	A	181	PHE	2.3
1	A	131	GLY	2.3
2	D	52	GLU	2.3
1	A	157	ALA	2.3
1	C	130	PRO	2.3
1	E	159	PRO	2.3
2	B	49	GLU	2.3
1	A	67	ARG	2.2
2	D	49	GLU	2.2
2	D	41	LYS	2.2
2	B	51	TRP	2.2
1	E	51	LEU	2.1
2	D	46	LYS	2.1
1	E	131	GLY	2.1
1	A	66	THR	2.0
2	B	120	VAL	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	CSS	A	236[A]	7/8	0.97	0.11	17,19,20,21	7
1	CSS	A	236[B]	6/8	0.97	0.11	19,20,20,21	6
1	CSS	E	236[A]	7/8	0.98	0.12	22,22,25,26	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSS	E	236[B]	6/8	0.98	0.12	15,20,20,21	6
1	CSS	C	236[B]	6/8	0.99	0.07	20,20,20,21	6
1	CSS	C	236[A]	7/8	0.99	0.07	18,20,21,22	7

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
4	SO4	B	209	5/5	0.89	0.11	27,33,34,38	0
3	HEC	B	401	43/43	0.97	0.11	12,15,23,34	0
3	HEC	E	401	43/43	0.97	0.14	14,18,30,39	0
3	HEC	C	401	43/43	0.98	0.11	16,20,34,40	0
3	HEC	D	401	43/43	0.98	0.13	12,16,23,28	0
3	HEC	A	401	43/43	0.98	0.15	14,18,35,45	0
3	HEC	F	401	43/43	0.98	0.11	15,18,25,33	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.
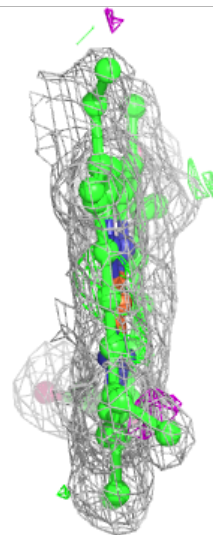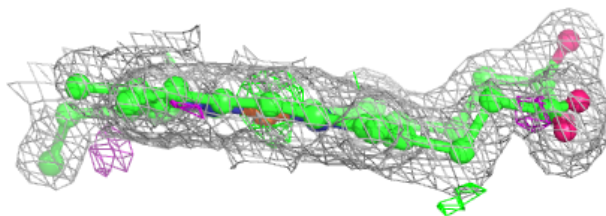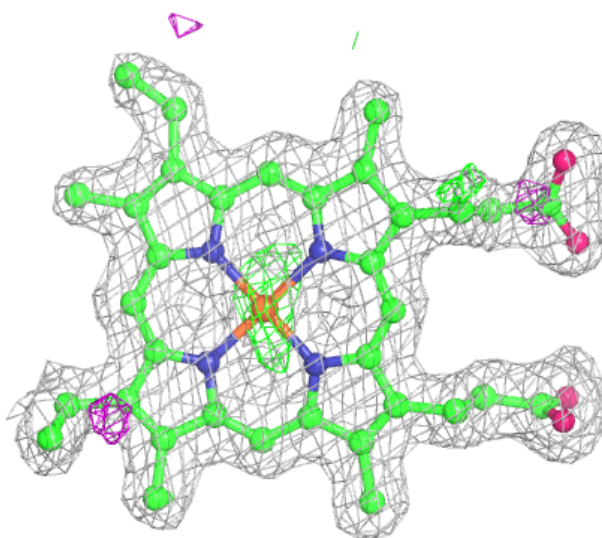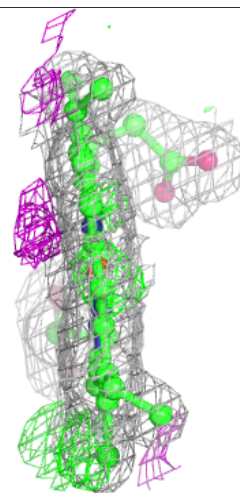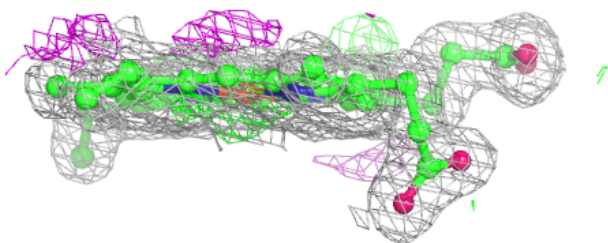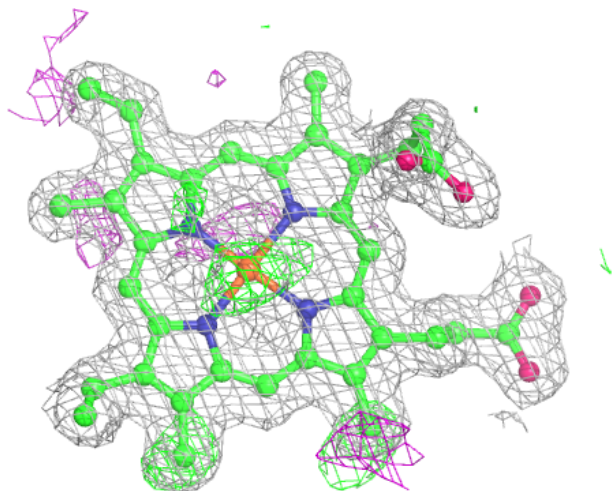
Electron density around HEC B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
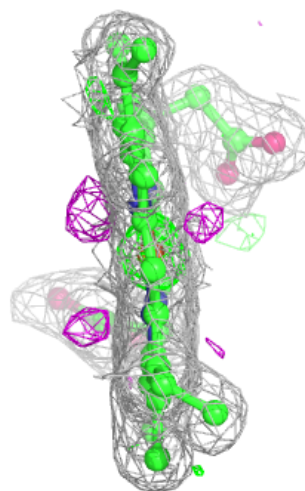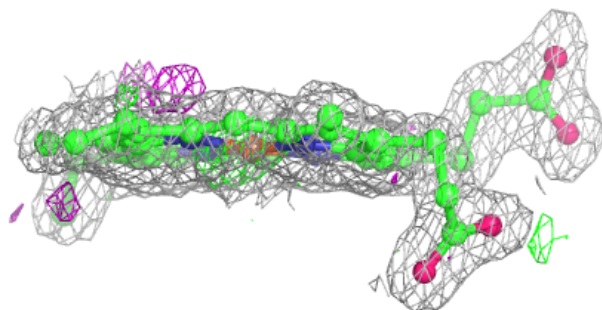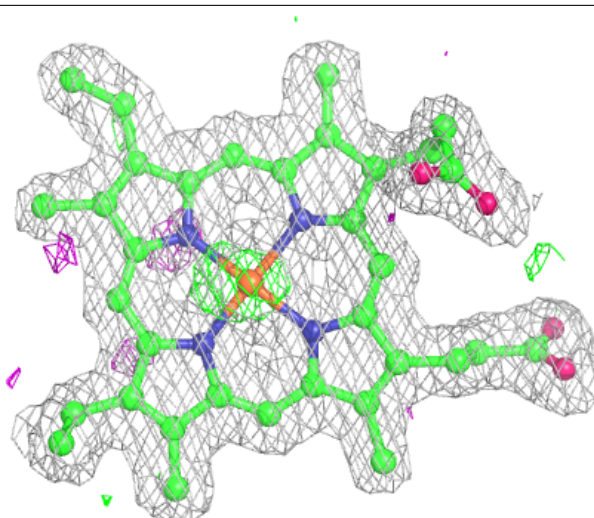
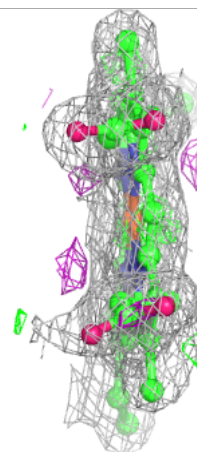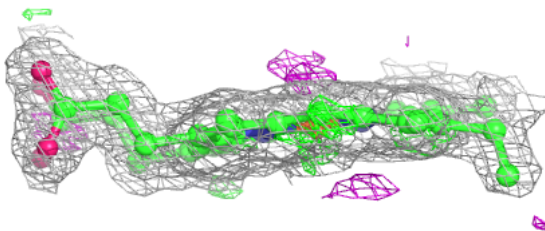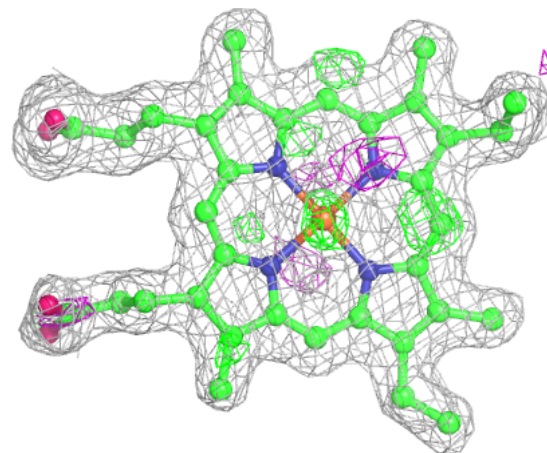Electron density around HEC E 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
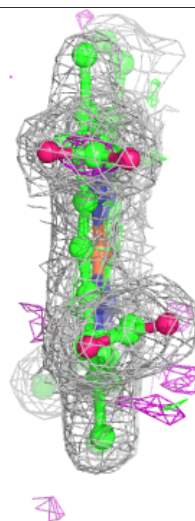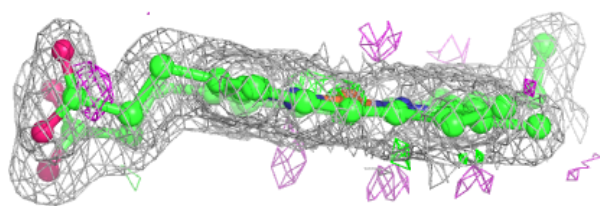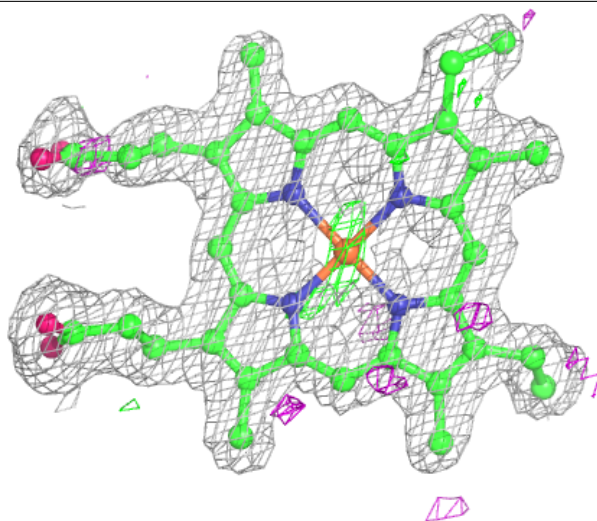
Electron density around HEC C 401:

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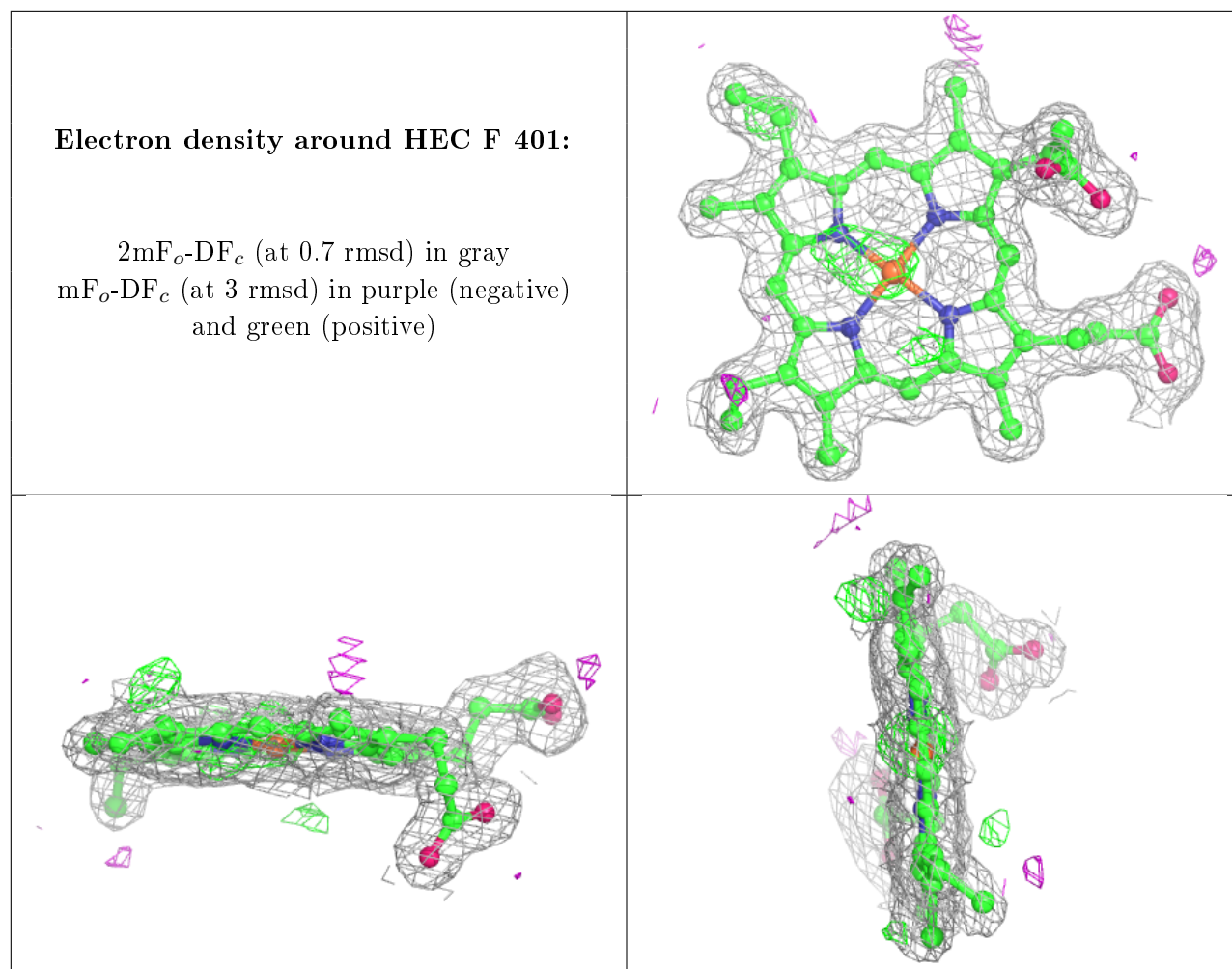and green (positive)

Electron density around HEC D 401:

$2mF_o$-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 A 401:

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

Electron density around HEC F 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.