



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:16 AM GMT

PDB ID : 3OA8  
Title : Diheme SoxAX  
Authors : Maher, M.J.  
Deposited on : 2010-08-04  
Resolution : 1.77 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

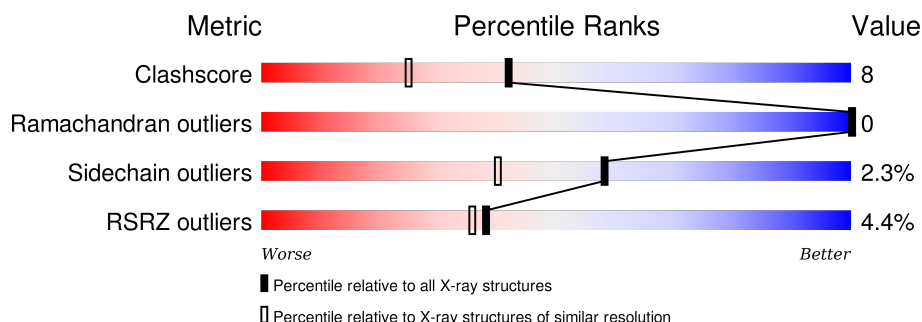
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	275	<div> <div>3%</div> <div>76% 7% 17%</div> </div>
1	C	275	<div> <div>%</div> <div>72% 11% 17%</div> </div>
1	E	275	<div> <div>3%</div> <div>71% 13% 17%</div> </div>
2	B	208	<div> <div>7%</div> <div>75% 12% 13%</div> </div>
2	D	208	<div> <div>6%</div> <div>76% 11% 13%</div> </div>
2	F	208	<div> <div>5%</div> <div>74% 12% 13%</div> </div>

## 2 Entry composition

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.

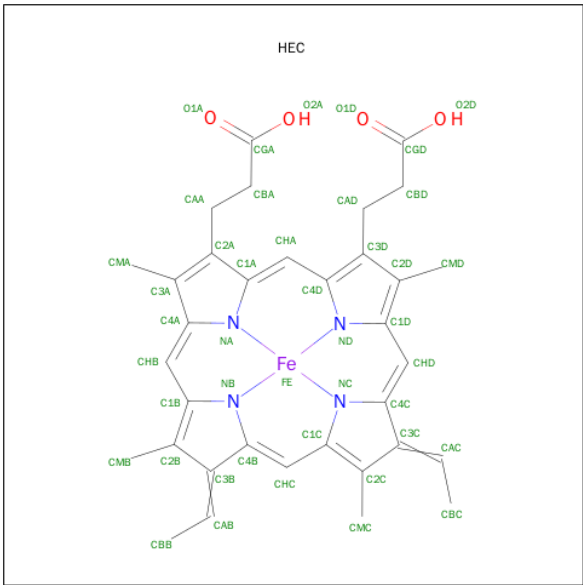
- Molecule 1 is a protein called SoxA.

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 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

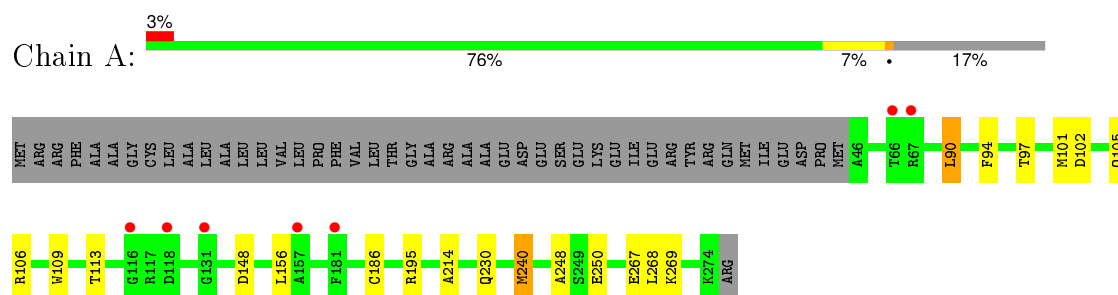
- Molecule 5 is water.

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

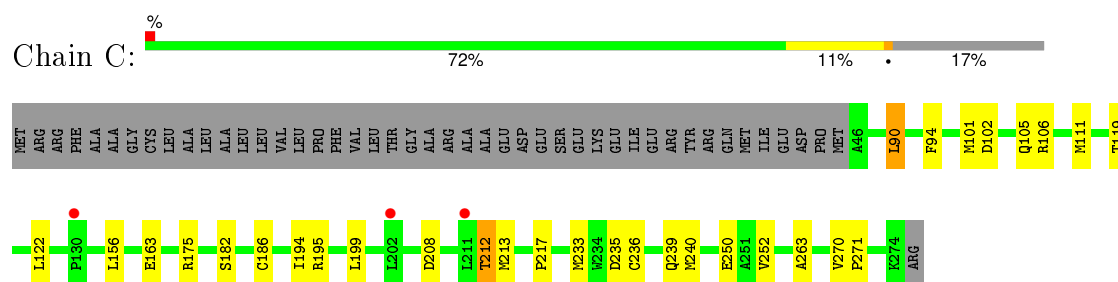
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

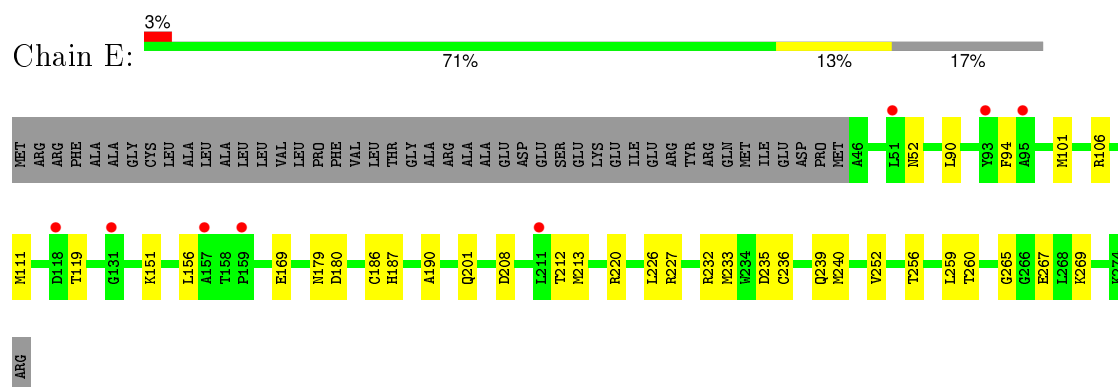
- Molecule 1: SoxA



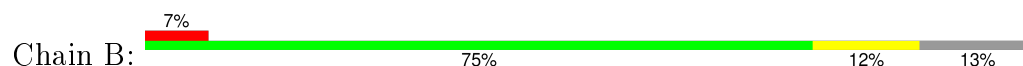
- Molecule 1: SoxA

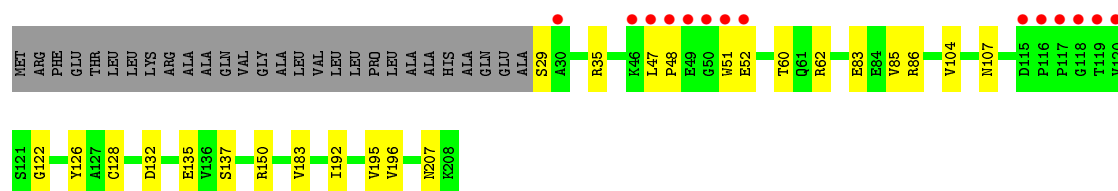


- Molecule 1: SoxA

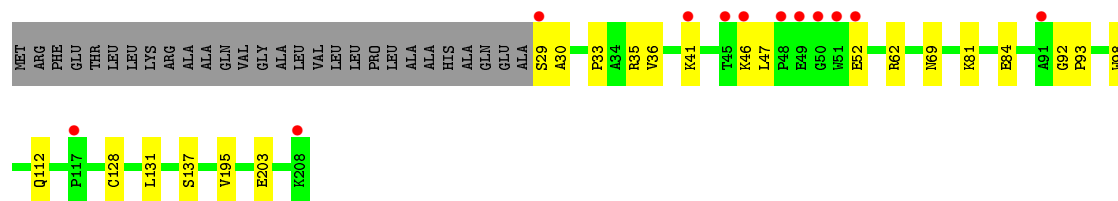
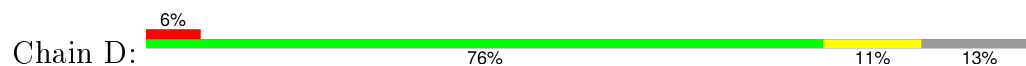


- Molecule 2: SoxX

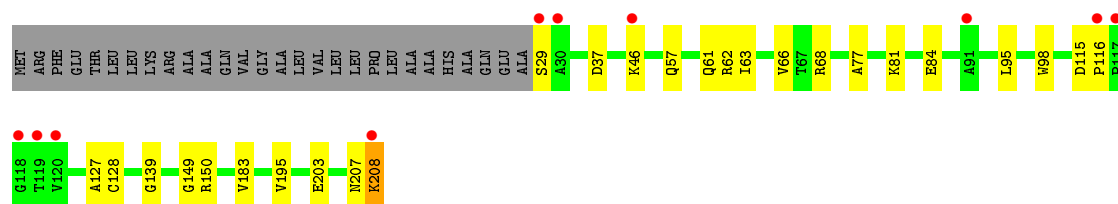
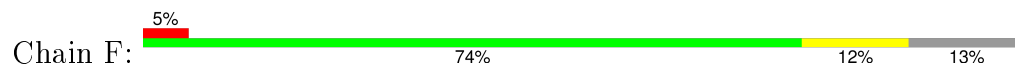




• Molecule 2: SoxX



• Molecule 2: SoxX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 76.8 (35.31-1.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.6	EDS
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

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<sup>1</sup>Intensities estimated from amplitudes.



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Property	Value	Source
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47, \langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 110854 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10596	wwPDB-VP
Average B, all atoms ( $\text{\AA}^2$ )	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.*

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<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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(°)	Ideal(°)
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
1:E:169:GLU:CG	2:F:68:ARG:NH2	2.65	0.59
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: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
2:D:29:SER:HB3	2:F:68:ARG:NH1	2.22	0.54
1:C:111:MET:CE	1:C:122:LEU:HD12	2.38	0.54
1:C:194:ILE:CD1	3:C:401:HEC:HAC	2.38	0.54
1:C:101:MET:HE1	1:C:106:ARG:HH11	1.72	0.54
3:E:401:HEC:HMC1	3:E:401:HEC:CBC	2.37	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
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:47:LEU:HD22	5:B:501:HOH:O	2.10	0.52
2:B:104:VAL:HB	2:B:195[B]:VAL:HG23	1.91	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
3:F:401:HEC:HMB1	3:F:401:HEC:HBB3	1.93	0.49
1:E:111:MET:HE1	1:E:119:THR:HG22	1.94	0.49
2:F:98:TRP:NE1	2:F:203:GLU:CG	2.73	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
1:E:186:CYS:SG	3:E:401:HEC:CBC	3.00	0.49
1:C:194:ILE:CG1	1:C:199:LEU:HD11	2.43	0.48
2:B:52:GLU:HA	5:B:501:HOH:O	2.12	0.48
2:B:35:ARG:NE	5:B:853:HOH:O	2.47	0.47
2:B:86:ARG:CZ	2:B:183:VAL:CG1	2.92	0.47
1:A:214:ALA:HA	1:A:268:LEU:HD23	1.96	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
2:B:128:CYS:SG	3:B:401:HEC:HBC3	2.57	0.44
1:A:101:MET:HE3	1:A:106:ARG:HH11	1.82	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:E:179:ASN:O	1:E:180:ASP:HB2	2.18	0.44
2:D:98:TRP:NE1	2:D:203:GLU:HG3	2.33	0.44
1:A:109:TRP:CE2	1:A:113:THR:HG21	2.53	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:F:98:TRP:HE1	2:F:203:GLU:CG	2.32	0.43
2:D:92:GLY:HA3	2:D:93:PRO:HD2	1.78	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
3:C:401:HEC:HMB1	3:C:401:HEC:HBB3	2.01	0.43
3:C:401:HEC:HBC3	3:C:401:HEC:HMC1	2.00	0.43
1:C:111:MET:HB3	1:C:111:MET:HE2	1.81	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
1:E:267:GLU:OE2	1:E:269:LYS:NZ	2.50	0.42
2:B:85:VAL:HG13	5:B:253:HOH:O	2.19	0.42
2:B:150:ARG:H	2:B:207:ASN:ND2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:ARG:HH22	1:E:201:GLN:NE2	2.18	0.42
1:A:230:GLN:NE2	1:A:248:ALA:H	2.17	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:E:101:MET:CE	1:E:106:ARG:HH11	2.34	0.41
1:C:175:ARG:HG2	1:C:182:SER:HB3	2.03	0.41
1:C:94:PHE:HB2	1:C:101:MET:CE	2.50	0.41
2:B:86:ARG:NH2	2:B:183:VAL:HG13	2.35	0.41
2:B:128:CYS:SG	3:B:401:HEC:HAC	2.48	0.41
2:F:150:ARG:H	2:F:207:ASN:ND2	2.19	0.41
2:B:126:TYR:CE2	2:B:135:GLU:HG2	2.56	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:E:187:HIS:CD2	3:E:401:HEC:NB	2.88	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: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%)	70	57
1	C	190/225 (84%)	186 (98%)	4 (2%)	61	44
1	E	191/225 (85%)	188 (98%)	3 (2%)	70	57
2	B	150/165 (91%)	150 (100%)	0	100	100
2	D	145/165 (88%)	140 (97%)	5 (3%)	44	24
2	F	148/165 (90%)	140 (95%)	8 (5%)	27	10
All	All	1013/1170 (87%)	990 (98%)	23 (2%)	58	40

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 ⓘ

There are no RNA molecules in this entry.

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

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	A	236[A]	1,3	4,6,7	0.61	0	3,6,8	1.52	1 (33%)
1	CSS	A	236[B]	1,3	4,5,7	1.07	0	3,5,8	1.90	1 (33%)
1	CSS	C	236[A]	1,3	4,6,7	0.61	0	3,6,8	1.29	0
1	CSS	C	236[B]	1,3	4,5,7	1.45	1 (25%)	3,5,8	1.75	1 (33%)
1	CSS	E	236[A]	1,3	4,6,7	0.54	0	3,6,8	1.71	1 (33%)
1	CSS	E	236[B]	1,3	4,5,7	0.91	0	3,5,8	1.32	1 (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	CSS	A	236[A]	1,3	-	0/1/5/7	0/0/0/0
1	CSS	A	236[B]	1,3	-	0/1/4/7	0/0/0/0
1	CSS	C	236[A]	1,3	-	0/1/5/7	0/0/0/0
1	CSS	C	236[B]	1,3	-	0/1/4/7	0/0/0/0
1	CSS	E	236[A]	1,3	-	0/1/5/7	0/0/0/0
1	CSS	E	236[B]	1,3	-	0/1/4/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236[B]	CSS	CB-CA	2.25	1.55	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236[B]	CSS	O-C-CA	-2.75	118.34	125.49
1	C	236[B]	CSS	O-C-CA	-2.75	118.34	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	236[A]	CSS	CB-SG-SD	-2.37	99.30	103.94
1	E	236[B]	CSS	O-C-CA	-2.16	119.87	125.49
1	A	236[A]	CSS	O-C-CA	-2.14	119.92	125.49

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
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	$\# Z  > 2$
3	HEC	A	401	1	24,50,50	2.02	5 (20%)	19,82,82	2.35	5 (26%)
4	SO4	B	209	-	4,4,4	0.87	0	6,6,6	0.40	0
3	HEC	B	401	2	24,50,50	2.38	4 (16%)	19,82,82	2.32	6 (31%)
3	HEC	C	401	1	24,50,50	2.54	3 (12%)	19,82,82	2.17	6 (31%)
3	HEC	D	401	2	24,50,50	2.22	4 (16%)	19,82,82	2.59	7 (36%)
3	HEC	E	401	1	24,50,50	2.50	3 (12%)	19,82,82	2.77	6 (31%)
3	HEC	F	401	2	24,50,50	2.23	4 (16%)	19,82,82	2.73	8 (42%)

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	0/0/8/8
4	SO4	B	209	-	-	0/0/0/0	0/0/0/0
3	HEC	B	401	2	-	0/6/54/54	0/0/8/8
3	HEC	C	401	1	-	0/6/54/54	0/0/8/8
3	HEC	D	401	2	-	0/6/54/54	0/0/8/8
3	HEC	E	401	1	-	0/6/54/54	0/0/8/8
3	HEC	F	401	2	-	0/6/54/54	0/0/8/8

All (23) 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	-6.74	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	A	401	HEC	C3B-C2B	-4.52	1.36	1.40
3	A	401	HEC	C3C-C2C	-4.51	1.36	1.40
3	F	401	HEC	C3B-C2B	-4.20	1.36	1.40
3	A	401	HEC	CMB-C2B	2.06	1.56	1.51
3	D	401	HEC	CMB-C2B	2.21	1.56	1.51
3	F	401	HEC	C4C-NC	2.25	1.39	1.36
3	A	401	HEC	C4B-NB	2.29	1.39	1.36
3	B	401	HEC	CMD-C2D	2.57	1.56	1.51
3	A	401	HEC	C3D-C2D	4.31	1.50	1.37
3	D	401	HEC	C3D-C2D	4.53	1.51	1.37
3	F	401	HEC	C3D-C2D	4.62	1.51	1.37
3	B	401	HEC	C3D-C2D	4.75	1.51	1.37
3	C	401	HEC	C3D-C2D	4.78	1.51	1.37
3	E	401	HEC	C3D-C2D	4.80	1.51	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	HEC	CBB-CAB-C3B	-7.85	109.90	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	HEC	CBB-CAB-C3B	-7.50	110.69	127.35
3	D	401	HEC	CBB-CAB-C3B	-7.16	111.43	127.35
3	C	401	HEC	CBB-CAB-C3B	-6.55	112.80	127.35
3	A	401	HEC	CBB-CAB-C3B	-6.46	113.00	127.35
3	B	401	HEC	CBB-CAB-C3B	-6.34	113.27	127.35
3	E	401	HEC	CBC-CAC-C3C	-5.39	115.38	127.35
3	E	401	HEC	CMB-C2B-C1B	-4.44	121.02	128.36
3	D	401	HEC	CMC-C2C-C1C	-4.44	121.02	128.36
3	A	401	HEC	CBD-CAD-C3D	-4.21	104.98	112.53
3	F	401	HEC	CMB-C2B-C1B	-3.99	121.77	128.36
3	F	401	HEC	CMC-C2C-C1C	-3.99	121.77	128.36
3	A	401	HEC	CBC-CAC-C3C	-3.74	119.03	127.35
3	C	401	HEC	CMB-C2B-C1B	-3.73	122.20	128.36
3	D	401	HEC	CBC-CAC-C3C	-3.55	119.46	127.35
3	B	401	HEC	CMC-C2C-C1C	-3.53	122.52	128.36
3	B	401	HEC	CBA-CAA-C2A	-3.35	106.52	112.53
3	B	401	HEC	CMB-C2B-C1B	-3.29	122.92	128.36
3	D	401	HEC	CAA-CBA-CGA	-3.28	106.73	112.75
3	E	401	HEC	CAD-CBD-CGD	-3.22	106.84	112.75
3	D	401	HEC	CBA-CAA-C2A	-3.13	106.91	112.53
3	F	401	HEC	CBA-CAA-C2A	-2.99	107.17	112.53
3	A	401	HEC	CMB-C2B-C1B	-2.86	123.64	128.36
3	C	401	HEC	CBD-CAD-C3D	-2.81	107.49	112.53
3	F	401	HEC	CAD-CBD-CGD	-2.73	107.73	112.75
3	F	401	HEC	CBC-CAC-C3C	-2.71	121.32	127.35
3	E	401	HEC	CBD-CAD-C3D	-2.65	107.78	112.53
3	A	401	HEC	CMC-C2C-C1C	-2.51	124.20	128.36
3	B	401	HEC	CAD-CBD-CGD	-2.50	108.16	112.75
3	B	401	HEC	CAA-C2A-C1A	-2.46	124.34	127.01
3	F	401	HEC	CMD-C2D-C1D	-2.36	124.47	128.36
3	D	401	HEC	CBD-CAD-C3D	-2.30	108.40	112.53
3	C	401	HEC	CMC-C2C-C1C	-2.28	124.59	128.36
3	C	401	HEC	CBC-CAC-C3C	-2.24	122.38	127.35
3	C	401	HEC	CAA-C2A-C1A	-2.21	124.61	127.01
3	D	401	HEC	CAA-C2A-C1A	-2.16	124.67	127.01
3	F	401	HEC	CMD-C2D-C3D	2.18	129.79	125.24
3	E	401	HEC	CMA-C3A-C2A	2.42	130.30	125.24

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	228/275 (82%)	0.09	7 (3%)	52	50	15, 27, 42, 53	0
1	C	228/275 (82%)	0.01	3 (1%)	79	79	17, 26, 37, 46	0
1	E	228/275 (82%)	0.33	8 (3%)	48	46	18, 31, 54, 70	0
2	B	180/208 (86%)	0.23	14 (7%)	16	15	15, 26, 45, 61	0
2	D	180/208 (86%)	0.14	12 (6%)	21	20	16, 27, 41, 52	0
2	F	180/208 (86%)	0.27	10 (5%)	28	26	17, 30, 51, 63	0
All	All	1224/1449 (84%)	0.17	54 (4%)	38	36	15, 27, 46, 70	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	50	GLY	5.1
1	E	95	ALA	5.0
2	B	48	PRO	4.8
2	D	117	PRO	4.7
2	F	117	PRO	4.5
2	D	91	ALA	4.2
2	D	50	GLY	4.2
2	D	208	LYS	4.1
2	B	118	GLY	4.0
2	F	91	ALA	4.0
2	F	208	LYS	3.6
2	F	46	LYS	3.6
2	F	29	SER	3.6
2	F	119	THR	3.5
2	F	118	GLY	3.3
1	E	157	ALA	3.2
2	B	52	GLU	3.2
2	D	48	PRO	3.1
2	B	117	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	118	ASP	3.0
2	B	47	LEU	2.9
2	B	119	THR	2.9
2	F	120	VAL	2.8
2	F	30	ALA	2.8
2	D	45	THR	2.7
1	E	118	ASP	2.7
2	B	30	ALA	2.7
1	E	211	LEU	2.6
2	B	46	LYS	2.5
1	C	130	PRO	2.5
2	B	116	PRO	2.5
2	F	116	PRO	2.5
1	A	116	GLY	2.5
1	A	181	PHE	2.5
1	E	93	TYR	2.4
2	B	49	GLU	2.4
1	A	157	ALA	2.4
1	A	131	GLY	2.4
2	D	49	GLU	2.3
2	D	52	GLU	2.3
2	D	41	LYS	2.3
1	E	159	PRO	2.3
2	B	51	TRP	2.3
1	A	67	ARG	2.2
1	C	211	LEU	2.2
2	D	46	LYS	2.2
1	A	66	THR	2.2
1	E	131	GLY	2.1
2	D	51	TRP	2.1
1	E	51	LEU	2.1
2	D	29	SER	2.1
2	B	115	ASP	2.1
2	B	120	VAL	2.0
1	C	202	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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
1	CSS	A	236[A]	7/8	0.97	0.11	-	17,19,20,21	7
1	CSS	E	236[A]	7/8	0.98	0.12	-	22,22,25,26	7
1	CSS	A	236[B]	6/8	0.97	0.11	-	19,20,20,21	6
1	CSS	E	236[B]	6/8	0.98	0.12	-	15,20,20,21	6

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	209	5/5	0.89	0.11	1.89	27,33,34,38	0
3	HEC	A	401	43/43	0.98	0.15	1.69	14,18,35,45	0
3	HEC	D	401	43/43	0.98	0.13	1.28	12,16,23,28	0
3	HEC	E	401	43/43	0.96	0.15	1.24	14,18,30,39	0
3	HEC	B	401	43/43	0.97	0.12	0.66	12,15,23,34	0
3	HEC	F	401	43/43	0.98	0.11	0.59	15,18,25,33	0
3	HEC	C	401	43/43	0.97	0.11	0.39	16,20,34,40	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.