



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:40 AM GMT

PDB ID : 3OCD  
Title : Diheme SoxAX - C236M mutant  
Authors : Maher, M.J.  
Deposited on : 2010-08-09  
Resolution : 2.25 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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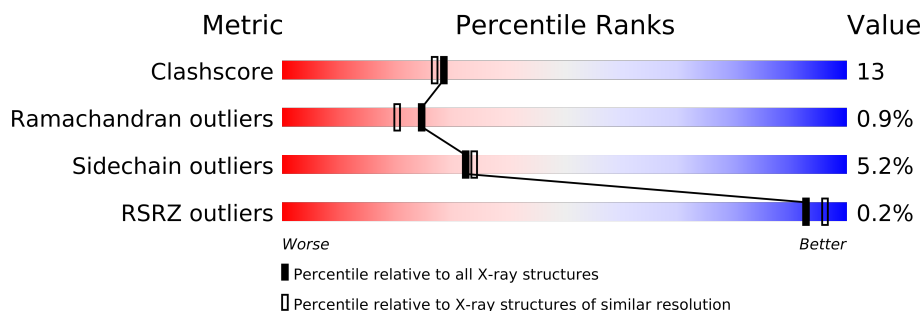
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance





The reported resolution of this entry is 2.25 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	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	275	
1	C	275	
2	B	208	
2	D	208	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6543 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1	0
			1789	1126	316	333	14			
1	C	229	Total	C	N	O	S	0	1	0
			1789	1126	316	333	14			

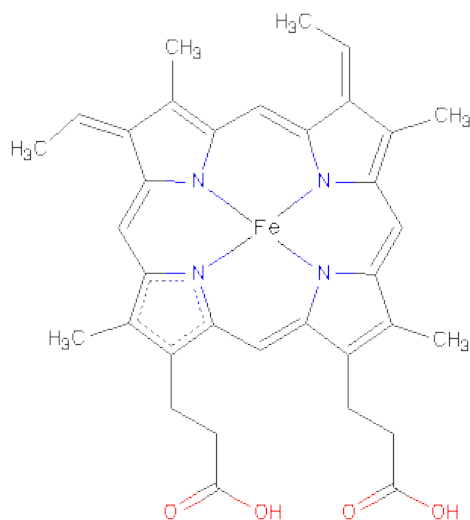
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	MET	CYS	ENGINEERED MUTATION	UNP Q7BQR6
C	236	MET	CYS	ENGINEERED MUTATION	UNP Q7BQR6

- Molecule 2 is a protein called SoxX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	4	4	0
			1373	861	239	267	6			
2	D	180	Total	C	N	O	S	11	5	0
			1377	865	239	267	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		

- Molecule 4 is water.

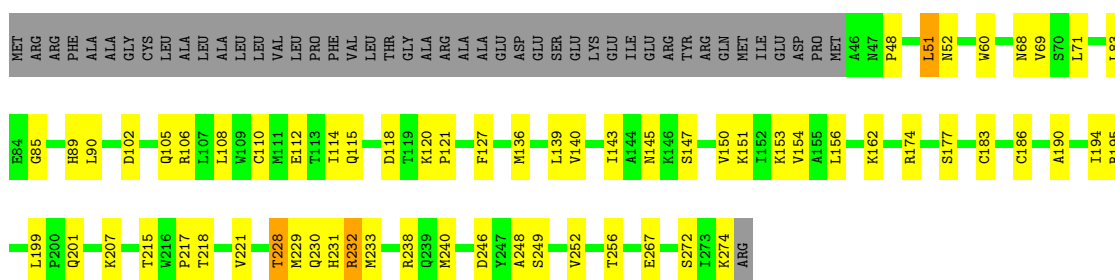
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	9	Total	O	0	0
			9	9		
4	C	11	Total	O	0	0
			11	11		
4	D	10	Total	O	0	0
			10	10		

### 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.

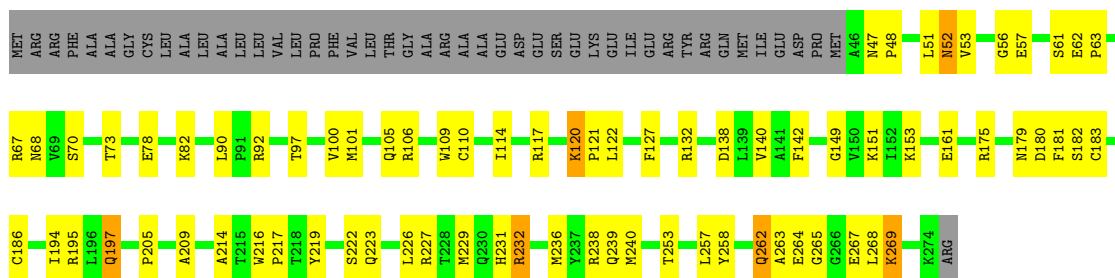
#### • Molecule 1: SoxA

Chain A:



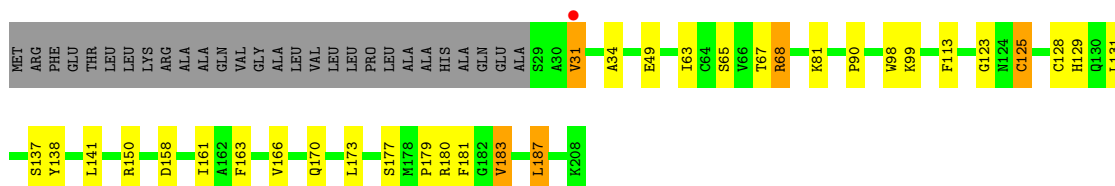
#### • Molecule 1: SoxA

Chain C:



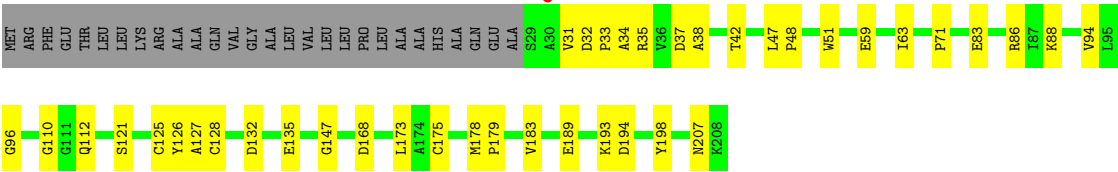
#### • Molecule 2: SoxX

Chain B:



#### • Molecule 2: SoxX

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.50Å 66.03Å 85.89Å 112.59° 94.33° 90.02°	Depositor
Resolution (Å)	41.18 – 2.25 41.18 – 2.25	Depositor EDS
% Data completeness (in resolution range)	90.2 (41.18-2.25) 90.3 (41.18-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.221 , 0.257 0.223 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 13.4	EDS
Estimated twinning fraction	0.508 for H, K, L 0.492 for -H, K, -K-L 0.479 for -h,k,-k-l	Xtriage
Reported twinning fraction	0.508 for H, K, L 0.492 for -H, K, -K-L	Depositor
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 41131 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/1830	0.58	0/2473
1	C	0.41	0/1830	0.57	0/2473
2	B	0.44	0/1414	0.56	0/1919
2	D	0.41	0/1421	0.55	0/1929
All	All	0.42	0/6495	0.57	0/8794

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1789	0	1789	48	0
1	C	1789	0	1789	60	0
2	B	1373	0	1355	24	0
2	D	1377	0	1364	30	0
3	A	43	0	32	9	0
3	B	43	0	32	10	0
3	C	43	0	32	12	0
3	D	43	0	32	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	13	0	0	4	0
4	B	9	0	0	1	0
4	C	11	0	0	1	0
4	D	10	0	0	0	0
All	All	6543	0	6425	161	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (161) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:183:CYS:SG	3:A:401:HEC:HAB	1.50	1.50
1:A:183:CYS:SG	3:A:401:HEC:CAB	2.26	1.22
2:B:125:CYS:SG	3:B:401:HEC:HAB	1.97	1.04
2:D:125:CYS:SG	3:D:401:HEC:CAB	2.48	1.01
1:C:186:CYS:SG	3:C:401:HEC:HAC	2.00	1.00
1:C:183:CYS:SG	3:C:401:HEC:HAB	2.03	0.98
2:D:125:CYS:SG	3:D:401:HEC:HAB	2.04	0.97
1:C:183:CYS:SG	3:C:401:HEC:CAB	2.55	0.94
1:C:186:CYS:SG	3:C:401:HEC:CAC	2.55	0.94
2:B:128:CYS:SG	3:B:401:HEC:CAC	2.62	0.87
2:D:128:CYS:SG	3:D:401:HEC:HAC	2.14	0.87
2:B:125:CYS:HB2	2:B:131:LEU:HD11	1.57	0.86
2:B:125:CYS:SG	3:B:401:HEC:CAB	2.64	0.85
1:C:262:GLN:HA	1:C:262:GLN:HE21	1.41	0.85
1:A:194:ILE:HD12	1:A:199:LEU:HD21	1.60	0.83
1:A:156:LEU:HB3	1:A:162:LYS:HG2	1.62	0.81
2:B:34:ALA:HA	4:B:209:HOH:O	1.81	0.79
1:A:108:LEU:O	1:A:112:GLU:HG2	1.84	0.76
1:A:71:LEU:HD22	1:A:110:CYS:HB3	1.68	0.75
2:D:128:CYS:SG	3:D:401:HEC:CAC	2.80	0.70
2:B:179:PRO:HD3	3:B:401:HEC:HBC2	1.75	0.68
1:A:233:MET:HG3	1:A:252:VAL:HG13	1.74	0.68
1:A:186:CYS:SG	3:A:401:HEC:HAC	2.35	0.67
3:B:401:HEC:HMC1	3:B:401:HEC:HBC3	1.77	0.66
1:A:246:ASP:HB2	1:A:249:SER:HB3	1.77	0.66
1:A:194:ILE:CD1	3:A:401:HEC:HHD	2.27	0.65
2:D:96:GLY:HA3	2:D:194:ASP:OD1	1.98	0.64
1:C:101:MET:HE1	1:C:106:ARG:HH11	1.63	0.63
2:B:98:TRP:CZ2	2:B:99:LYS:HE3	2.34	0.63
2:B:181:PHE:HB3	2:B:187:LEU:HG	1.81	0.62
2:D:147:GLY:HA2	2:D:207:ASN:HD22	1.65	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:195:ARG:NH2	4:C:282:HOH:O	2.33	0.60
2:B:170:GLN:HA	2:B:173:LEU:O	2.01	0.60
1:C:92:ARG:HA	1:C:161:GLU:OE2	2.01	0.60
2:D:179:PRO:HD3	3:D:401:HEC:CBC	2.33	0.59
1:A:230:GLN:NE2	1:A:248:ALA:H	2.02	0.58
2:D:125:CYS:SG	3:D:401:HEC:C3B	2.92	0.58
1:C:101:MET:HE1	1:C:106:ARG:HD2	1.84	0.58
1:A:85:GLY:O	1:A:89:HIS:ND1	2.36	0.57
1:C:101:MET:HE1	1:C:106:ARG:CD	2.34	0.57
2:D:59:GLU:O	2:D:63:ILE:HG13	2.05	0.57
1:A:102:ASP:H	1:A:105:GLN:HE21	1.51	0.57
1:C:262:GLN:CA	1:C:262:GLN:HE21	2.15	0.57
1:C:149:GLY:O	1:C:267:GLU:HG3	2.05	0.56
1:C:52:ASN:H	1:C:52:ASN:HD22	1.51	0.56
1:A:71:LEU:CD2	1:A:110:CYS:HB3	2.34	0.56
1:A:127:PHE:CG	1:A:231:HIS:HD2	2.24	0.56
1:A:140:VAL:HG12	1:A:217:PRO:HG3	1.87	0.55
2:D:38:ALA:O	2:D:42:THR:HG23	2.07	0.55
2:D:125:CYS:HG	3:D:401:HEC:HAB	1.68	0.55
2:D:110:GLY:HA3	2:D:121:SER:HA	1.89	0.55
1:A:186:CYS:SG	3:A:401:HEC:CAC	2.95	0.54
1:C:219:TYR:HA	1:C:226:LEU:HA	1.88	0.54
1:A:190:ALA:HB2	1:A:201:GLN:OE1	2.08	0.53
1:A:174:ARG:HA	2:B:65:SER:HB3	1.90	0.53
2:D:86:ARG:NH2	2:D:183:VAL:HG13	2.24	0.53
2:B:177:SER:HB2	3:B:401:HEC:HMD2	1.90	0.53
1:C:101:MET:CE	1:C:106:ARG:HH11	2.22	0.53
2:B:158:ASP:HA	2:B:161:ILE:HD12	1.91	0.52
3:D:401:HEC:HMB1	3:D:401:HEC:HBB3	1.91	0.52
1:C:238:ARG:O	2:D:112:GLN:HG2	2.09	0.52
2:D:128:CYS:HG	3:D:401:HEC:HAC	1.70	0.52
1:A:232:ARG:HA	1:A:232:ARG:HE	1.73	0.52
1:C:110:CYS:O	1:C:114:ILE:HB	2.09	0.52
1:A:151:LYS:HG3	1:A:267:GLU:HG3	1.91	0.52
1:C:258:TYR:O	1:C:262:GLN:HG2	2.09	0.52
2:D:189:GLU:HG2	2:D:193:LYS:HD2	1.92	0.51
2:B:180:ARG:HB3	2:B:183:VAL:HG12	1.92	0.51
1:A:52:ASN:H	1:A:52:ASN:ND2	2.09	0.51
2:D:71:PRO:HG3	2:D:175:CYS:SG	2.50	0.51
2:D:48:PRO:O	2:D:51:TRP:HB2	2.11	0.51
1:C:78:GLU:HB2	1:C:82:LYS:HB3	1.92	0.50
1:A:194:ILE:HD12	3:A:401:HEC:HHD	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69:VAL:O	1:A:115:GLN:HG2	2.11	0.50
3:D:401:HEC:HBD1	3:D:401:HEC:HHA	1.93	0.50
1:C:53:VAL:HG13	1:C:142:PHE:HA	1.93	0.50
1:C:194:ILE:HA	2:D:127:ALA:O	2.12	0.50
2:D:179:PRO:HD3	3:D:401:HEC:HBC3	1.94	0.49
1:C:67:ARG:HG3	1:C:114:ILE:O	2.12	0.49
1:A:139:LEU:O	1:A:143:ILE:HD12	2.12	0.49
1:C:262:GLN:NE2	1:C:262:GLN:HA	2.18	0.49
1:C:127:PHE:O	1:C:132:ARG:NH1	2.44	0.49
1:A:105:GLN:HG3	1:A:248:ALA:HB1	1.93	0.49
1:A:145:ASN:HB3	4:A:284:HOH:O	2.11	0.49
1:C:101:MET:HA	1:C:105:GLN:HE21	1.78	0.49
1:C:100:VAL:HG11	1:C:257:LEU:HD22	1.94	0.48
1:C:183:CYS:HA	3:C:401:HEC:CHC	2.43	0.48
1:A:150:VAL:HG12	1:A:151:LYS:N	2.28	0.48
2:B:128:CYS:SG	3:B:401:HEC:HAC	2.52	0.48
1:A:105:GLN:CG	1:A:248:ALA:HB1	2.44	0.48
3:A:401:HEC:HHA	3:A:401:HEC:HBA1	1.96	0.48
2:D:179:PRO:HD3	3:D:401:HEC:HBC2	1.94	0.48
1:C:183:CYS:SG	3:C:401:HEC:C3B	3.01	0.48
1:A:228:THR:CG2	4:A:276:HOH:O	2.61	0.48
1:C:216:TRP:CG	1:C:229:MET:HE2	2.48	0.48
1:C:101:MET:HB3	1:C:105:GLN:HB3	1.96	0.48
1:C:61:SER:HA	1:C:70:SER:HB2	1.94	0.48
1:A:215:THR:O	1:A:218:THR:HB	2.13	0.48
1:C:197:GLN:HE21	1:C:197:GLN:HA	1.80	0.47
1:A:89:HIS:HD2	1:A:153:LYS:O	1.98	0.47
2:D:33:PRO:C	2:D:35:ARG:H	2.18	0.47
1:A:118:ASP:O	1:A:121:PRO:HD2	2.14	0.47
1:A:238:ARG:HA	2:B:113:PHE:CE2	2.50	0.47
1:C:205:PRO:HG3	1:C:262:GLN:HE22	1.80	0.47
1:A:136:MET:O	1:A:140:VAL:HG23	2.15	0.47
1:C:239:GLN:CD	3:C:401:HEC:HBC2	2.35	0.46
1:A:194:ILE:HG13	1:A:199:LEU:HD11	1.98	0.46
1:C:214:ALA:HA	1:C:268:LEU:HD23	1.97	0.46
1:A:229:MET:HG2	1:A:256:THR:HG23	1.96	0.46
1:A:194:ILE:HD13	3:A:401:HEC:HHD	1.97	0.46
1:A:240:MET:HG3	3:A:401:HEC:HMC2	1.97	0.46
1:A:228:THR:HG21	4:A:276:HOH:O	2.16	0.46
1:C:236:MET:HB2	3:C:401:HEC:HBB2	1.98	0.46
1:C:175:ARG:NE	1:C:180:ASP:O	2.44	0.46
1:C:179:ASN:HA	2:D:179:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:216:TRP:CZ2	1:C:232:ARG:HD2	2.51	0.45
2:B:123:GLY:HA3	3:B:401:HEC:HBB1	1.99	0.45
1:A:195:ARG:HD2	2:B:137:SER:OG	2.16	0.45
1:C:223:GLN:HE22	1:C:231:HIS:HE1	1.65	0.45
2:B:129:HIS:O	2:B:138:TYR:HB2	2.16	0.44
2:B:81:LYS:HB2	2:B:81:LYS:HE3	1.90	0.44
2:D:178:MET:HA	3:D:401:HEC:HBC2	1.98	0.44
1:C:151:LYS:HD2	1:C:265:GLY:O	2.17	0.44
2:D:126:TYR:OH	2:D:198:TYR:OH	2.18	0.44
1:C:62:GLU:HA	1:C:63:PRO:HD3	1.92	0.44
1:C:47:ASN:HA	1:C:48:PRO:HD3	1.79	0.43
1:C:232:ARG:HD3	3:C:401:HEC:C2A	2.48	0.43
1:C:105:GLN:NE2	1:C:253:THR:OG1	2.51	0.43
1:A:52:ASN:H	1:A:52:ASN:HD22	1.64	0.43
2:D:132:ASP:HB3	2:D:135:GLU:HB2	2.00	0.43
1:C:232:ARG:HH11	3:C:401:HEC:C1A	2.31	0.43
1:A:60:TRP:CZ2	1:A:83:LEU:HD21	2.52	0.43
1:C:209:ALA:O	1:C:263:ALA:HB2	2.18	0.43
2:B:128:CYS:SG	3:B:401:HEC:C3C	3.07	0.43
2:D:88:LYS:HA	2:D:88:LYS:HD3	1.79	0.43
1:C:120:LYS:N	1:C:121:PRO:HD2	2.34	0.43
1:A:106:ARG:HD2	1:A:106:ARG:HA	1.88	0.43
1:C:140:VAL:HG12	1:C:217:PRO:HG3	2.01	0.42
1:C:175:ARG:HG2	1:C:182:SER:HB3	2.01	0.42
1:C:101:MET:HA	1:C:105:GLN:NE2	2.34	0.42
1:C:56:GLY:HA3	1:C:138:ASP:O	2.19	0.42
1:C:181:PHE:HB3	1:C:240:MET:HG2	2.00	0.42
1:A:218:THR:HG21	1:A:274:LYS:HD2	2.01	0.42
3:D:401:HEC:CBD	3:D:401:HEC:HHA	2.50	0.42
2:D:83:GLU:HB3	2:D:168:ASP:CG	2.40	0.42
1:A:154:VAL:HG22	4:A:280:HOH:O	2.19	0.42
1:C:267:GLU:HG2	1:C:269:LYS:HE2	2.00	0.42
2:D:168:ASP:OD2	2:D:183:VAL:HG21	2.20	0.41
1:C:97:THR:HG22	1:C:109:TRP:CE2	2.55	0.41
2:B:90:PRO:HD3	2:B:163:PHE:CZ	2.54	0.41
2:D:173:LEU:HD23	3:D:401:HEC:HBD2	2.03	0.41
1:C:227:ARG:HD2	1:C:231:HIS:CG	2.56	0.41
2:B:67:THR:O	2:B:68:ARG:HG2	2.21	0.41
2:B:67:THR:C	2:B:68:ARG:HG2	2.40	0.41
1:A:48:PRO:O	1:A:51:LEU:HG	2.21	0.40
1:C:183:CYS:HA	3:C:401:HEC:HHC	2.03	0.40
1:C:205:PRO:HG3	1:C:262:GLN:NE2	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:117:ARG:NH2	1:C:122:LEU:HD11	2.37	0.40
2:B:166:VAL:CG2	3:B:401:HEC:HMB2	2.51	0.40
1:C:232:ARG:NH1	3:C:401:HEC:CHA	2.84	0.40
1:A:102:ASP:H	1:A:105:GLN:NE2	2.19	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/275 (83%)	212 (93%)	13 (6%)	3 (1%)	18	11
1	C	228/275 (83%)	207 (91%)	19 (8%)	2 (1%)	25	20
2	B	182/208 (88%)	169 (93%)	12 (7%)	1 (0%)	38	38
2	D	183/208 (88%)	170 (93%)	12 (7%)	1 (0%)	38	38
All	All	821/966 (85%)	758 (92%)	56 (7%)	7 (1%)	25	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	LYS
2	B	31	VAL
1	A	177	SER
2	D	34	ALA
1	C	264	GLU
1	C	222	SER
1	A	114	ILE

### 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	190/226 (84%)	181 (95%)	9 (5%)	36	40
1	C	190/226 (84%)	178 (94%)	12 (6%)	25	24
2	B	149/165 (90%)	140 (94%)	9 (6%)	27	26
2	D	150/165 (91%)	144 (96%)	6 (4%)	42	49
All	All	679/782 (87%)	643 (95%)	36 (5%)	32	33

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	68	ASN
1	A	90	LEU
1	A	120	LYS
1	A	147	SER
1	A	221	VAL
1	A	228	THR
1	A	232	ARG
1	A	272	SER
2	B	31	VAL
2	B	49	GLU
2	B	63	ILE
2	B	68	ARG
2	B	125	CYS
2	B	141	LEU
2	B	150	ARG
2	B	183	VAL
2	B	187	LEU
1	C	51	LEU
1	C	52	ASN
1	C	57	GLU
1	C	68	ASN
1	C	73	THR
1	C	90	LEU
1	C	120	LYS
1	C	153	LYS
1	C	197	GLN
1	C	232	ARG
1	C	262	GLN
1	C	269	LYS
2	D	31	VAL

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Mol	Chain	Res	Type
2	D	32	ASP
2	D	37	ASP
2	D	47	LEU
2	D	94[A]	VAL
2	D	94[B]	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	68	ASN
1	A	105	GLN
1	A	115	GLN
1	A	230	GLN
1	A	231	HIS
1	A	262	GLN
2	B	112	GLN
2	B	207	ASN
1	C	52	ASN
1	C	68	ASN
1	C	105	GLN
1	C	197	GLN
1	C	230	GLN
1	C	231	HIS
1	C	262	GLN
2	D	207	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	HEC	A	401	1	50,50,50	2.80	14 (28%)	56,82,82	1.98	15 (26%)
3	HEC	B	401	2	50,50,50	2.91	14 (28%)	56,82,82	1.85	13 (23%)
3	HEC	C	401	1	50,50,50	2.88	15 (30%)	56,82,82	1.72	9 (16%)
3	HEC	D	401	2	50,50,50	2.86	15 (30%)	56,82,82	1.94	16 (28%)

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	-	0/10/54/54	0/0/8/8
3	HEC	B	401	2	-	0/10/54/54	0/0/8/8
3	HEC	C	401	1	-	0/10/54/54	0/0/8/8
3	HEC	D	401	2	-	0/10/54/54	0/0/8/8

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	HEC	C3C-CAC	10.11	1.56	1.35
3	D	401	HEC	C3B-CAB	10.06	1.56	1.35
3	C	401	HEC	C3C-CAC	10.02	1.56	1.35
3	C	401	HEC	C3B-CAB	9.83	1.55	1.35
3	B	401	HEC	C3B-CAB	9.76	1.55	1.35
3	A	401	HEC	C3C-CAC	9.73	1.55	1.35
3	D	401	HEC	C3C-CAC	9.59	1.55	1.35
3	A	401	HEC	C3B-CAB	9.50	1.55	1.35
3	D	401	HEC	C3D-C2D	5.87	1.55	1.37
3	B	401	HEC	C3D-C2D	5.63	1.54	1.37
3	A	401	HEC	C3D-C2D	5.37	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	HEC	C3D-C2D	5.35	1.53	1.37
3	B	401	HEC	FE-NB	4.88	2.13	1.92
3	B	401	HEC	FE-ND	4.81	2.13	1.92
3	A	401	HEC	FE-ND	4.77	2.13	1.92
3	C	401	HEC	FE-NB	4.76	2.12	1.92
3	C	401	HEC	C1C-C2C	4.57	1.45	1.40
3	D	401	HEC	C1D-C2D	4.57	1.45	1.40
3	D	401	HEC	FE-NB	4.55	2.12	1.92
3	A	401	HEC	C1D-C2D	4.51	1.45	1.40
3	C	401	HEC	FE-ND	4.48	2.11	1.92
3	D	401	HEC	C1B-C2B	4.35	1.45	1.40
3	B	401	HEC	C1C-C2C	4.25	1.45	1.40
3	A	401	HEC	C1C-C2C	4.19	1.45	1.40
3	D	401	HEC	C1C-C2C	4.16	1.45	1.40
3	B	401	HEC	C1D-C2D	4.03	1.45	1.40
3	B	401	HEC	FE-NA	4.02	2.09	1.92
3	C	401	HEC	C1B-C2B	4.02	1.45	1.40
3	B	401	HEC	C1B-C2B	3.90	1.45	1.40
3	B	401	HEC	C3B-C4B	3.75	1.46	1.41
3	D	401	HEC	C3C-C4C	3.62	1.46	1.41
3	C	401	HEC	C3B-C4B	3.60	1.46	1.41
3	D	401	HEC	FE-ND	3.56	2.07	1.92
3	C	401	HEC	C1D-C2D	3.54	1.44	1.40
3	A	401	HEC	C1B-C2B	3.54	1.44	1.40
3	A	401	HEC	C3C-C2C	-3.53	1.34	1.41
3	A	401	HEC	C3B-C2B	-3.47	1.34	1.41
3	C	401	HEC	FE-NC	3.42	2.07	1.92
3	A	401	HEC	FE-NB	3.41	2.07	1.92
3	D	401	HEC	FE-NA	3.38	2.06	1.92
3	C	401	HEC	C3B-C2B	-3.28	1.34	1.41
3	C	401	HEC	C3C-C2C	-3.20	1.34	1.41
3	D	401	HEC	C3B-C2B	-3.14	1.34	1.41
3	B	401	HEC	C3C-C4C	3.14	1.45	1.41
3	A	401	HEC	FE-NC	3.11	2.05	1.92
3	B	401	HEC	C3B-C2B	-3.02	1.35	1.41
3	A	401	HEC	C3B-C4B	2.96	1.45	1.41
3	D	401	HEC	C3C-C2C	-2.93	1.35	1.41
3	B	401	HEC	C3C-C2C	-2.64	1.36	1.41
3	D	401	HEC	CAD-C3D	2.63	1.56	1.52
3	A	401	HEC	C3C-C4C	2.63	1.44	1.41
3	D	401	HEC	C3B-C4B	2.58	1.44	1.41
3	C	401	HEC	C3C-C4C	2.48	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	HEC	CAD-C3D	2.45	1.56	1.52
3	D	401	HEC	FE-NC	2.40	2.02	1.92
3	A	401	HEC	FE-NA	2.37	2.02	1.92
3	C	401	HEC	FE-NA	2.30	2.02	1.92
3	C	401	HEC	CAD-C3D	2.18	1.55	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	HEC	CBB-CAB-C3B	-7.01	108.69	128.44
3	B	401	HEC	CBB-CAB-C3B	-6.39	110.44	128.44
3	A	401	HEC	CBC-CAC-C3C	-6.28	110.75	128.44
3	D	401	HEC	CBC-CAC-C3C	-6.03	111.47	128.44
3	D	401	HEC	CBB-CAB-C3B	-5.18	113.84	128.44
3	C	401	HEC	CBB-CAB-C3B	-5.09	114.10	128.44
3	C	401	HEC	CBC-CAC-C3C	-4.68	115.26	128.44
3	B	401	HEC	CBC-CAC-C3C	-4.43	115.97	128.44
3	B	401	HEC	C4D-ND-C1D	4.28	112.40	106.76
3	D	401	HEC	C4D-ND-C1D	4.22	112.32	106.76
3	C	401	HEC	C4D-ND-C1D	3.55	111.44	106.76
3	A	401	HEC	C4B-C3B-C2B	3.51	108.92	106.68
3	A	401	HEC	C2C-C1C-NC	-3.25	106.95	109.41
3	A	401	HEC	C4D-ND-C1D	3.25	111.05	106.76
3	A	401	HEC	C3B-C4B-NB	-3.25	106.83	111.52
3	D	401	HEC	C4A-CHB-C1B	-3.18	123.28	127.47
3	D	401	HEC	CMB-C2B-C1B	-3.15	123.78	128.62
3	B	401	HEC	CMC-C2C-C1C	-3.13	123.80	128.62
3	C	401	HEC	C2A-C1A-NA	-3.10	107.31	109.64
3	D	401	HEC	CMC-C2C-C1C	-3.03	123.97	128.62
3	D	401	HEC	C4A-C3A-C2A	2.95	108.77	106.89
3	D	401	HEC	C3C-C4C-NC	-2.91	107.31	111.52
3	B	401	HEC	C3B-C4B-NB	-2.90	107.33	111.52
3	D	401	HEC	CBD-CAD-C3D	-2.82	107.72	112.69
3	A	401	HEC	C3C-C2C-C1C	2.77	108.91	107.07
3	B	401	HEC	C3C-C4C-NC	-2.75	107.54	111.52
3	D	401	HEC	C4C-C3C-C2C	2.71	108.40	106.68
3	B	401	HEC	CBA-CAA-C2A	-2.65	107.40	112.35
3	D	401	HEC	C3A-C4A-NA	-2.62	107.43	109.41
3	C	401	HEC	CMB-C2B-C1B	-2.59	124.63	128.62
3	A	401	HEC	C3C-C4C-NC	-2.49	107.92	111.52
3	B	401	HEC	CMB-C2B-C1B	-2.44	124.86	128.62
3	C	401	HEC	CMC-C2C-C1C	-2.41	124.92	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	HEC	C3A-C4A-NA	-2.36	107.63	109.41
3	C	401	HEC	C3B-C4B-NB	-2.34	108.14	111.52
3	B	401	HEC	C2C-C1C-NC	-2.29	107.68	109.41
3	B	401	HEC	C1D-C2D-C3D	-2.28	105.41	107.00
3	C	401	HEC	C1A-C2A-C3A	2.24	108.45	106.69
3	A	401	HEC	C4A-CHB-C1B	-2.19	124.59	127.47
3	A	401	HEC	C1D-C2D-C3D	-2.18	105.48	107.00
3	B	401	HEC	C4B-C3B-C2B	2.18	108.06	106.68
3	A	401	HEC	C4D-C3D-C2D	-2.18	104.67	106.92
3	A	401	HEC	C2B-C1B-NB	-2.16	107.78	109.41
3	D	401	HEC	C4D-C3D-C2D	-2.13	104.72	106.92
3	A	401	HEC	CBD-CAD-C3D	-2.12	108.95	112.69
3	D	401	HEC	O2D-CGD-CBD	2.11	121.67	114.22
3	A	401	HEC	C2A-C1A-NA	-2.11	108.05	109.64
3	D	401	HEC	CMB-C2B-C3B	2.10	128.04	125.72
3	B	401	HEC	C2A-C1A-NA	-2.02	108.12	109.64
3	C	401	HEC	C3C-C4C-NC	-2.01	108.61	111.52
3	B	401	HEC	C4C-C3C-C2C	2.01	107.96	106.68
3	D	401	HEC	C1D-C2D-C3D	-2.01	105.60	107.00
3	D	401	HEC	O1D-CGD-CBD	-2.01	116.13	123.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	229/275 (83%)	-0.31	0	100 100	21, 32, 38, 42	0
1	C	229/275 (83%)	-0.25	0	100 100	25, 33, 41, 50	0
2	B	180/208 (86%)	-0.24	1 (0%)	86 91	19, 33, 45, 53	0
2	D	180/208 (86%)	-0.18	1 (0%)	86 91	22, 34, 47, 51	0
All	All	818/966 (84%)	-0.25	2 (0%)	93 96	19, 33, 43, 53	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	30	ALA	3.0
2	B	31	VAL	2.2

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	D	401	43/43	0.16	1.73	19,33,37,37	0
3	HEC	C	401	43/43	0.14	0.60	29,34,36,37	0
3	HEC	A	401	43/43	0.14	0.58	24,28,35,39	0
3	HEC	B	401	43/43	0.13	0.48	15,23,26,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.