



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:27 PM GMT

PDB ID : 2RDZ  
Title : High Resolution Crystal Structure of the Escherichia coli Cytochrome c Nitrite Reductase.  
Authors : Clarke, T.A.; Hemmings, A.M.; Richardson, D.J.  
Deposited on : 2007-09-25  
Resolution : 1.74 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>

---

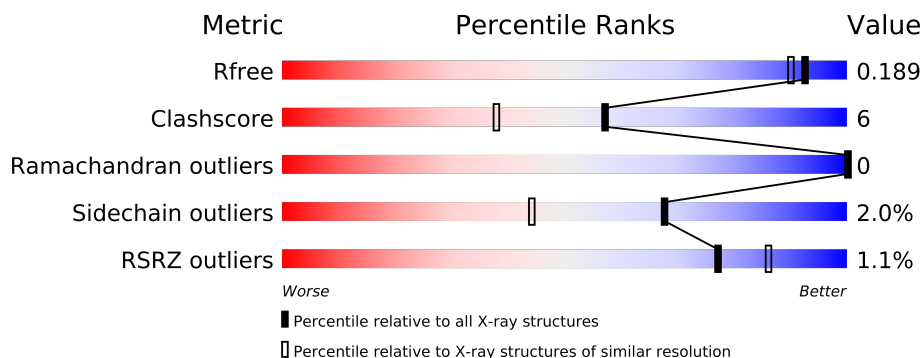
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1657 (1.76-1.72)
Clashscore	79885	1881 (1.76-1.72)
Ramachandran outliers	78287	1859 (1.76-1.72)
Sidechain outliers	78261	1859 (1.76-1.72)
RSRZ outliers	66119	1658 (1.76-1.72)

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	452	
1	B	452	
1	C	452	
1	D	452	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	HEC	A	4	-	X
3	HEC	B	4	-	X
3	HEC	C	4	-	X
4	SO4	D	2001	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	A	11	-	X
5	EDO	A	14	-	X
5	EDO	A	15	-	X
5	EDO	A	22	-	X
5	EDO	B	17	-	X
5	EDO	B	18	-	X
5	EDO	B	19	-	X
5	EDO	B	20	-	X
5	EDO	C	12	-	X
5	EDO	C	21	-	X
5	EDO	C	23	-	X
5	EDO	C	25	-	X
5	EDO	D	21	-	X
5	EDO	D	22	-	X
5	EDO	D	23	-	X
5	EDO	D	24	-	X
5	EDO	D	25	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17176 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.

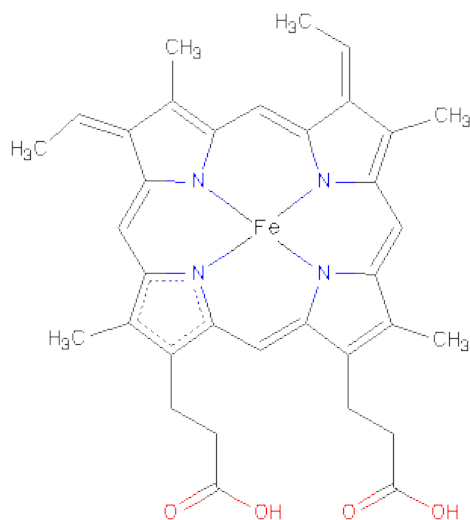
- Molecule 1 is a protein called Cytochrome c-552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	2	0
			3487	2187	619	659	22			
1	B	441	Total	C	N	O	S	0	8	0
			3520	2209	622	667	22			
1	C	441	Total	C	N	O	S	0	5	0
			3502	2197	620	662	23			
1	D	441	Total	C	N	O	S	0	7	0
			3514	2203	623	666	22			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		

- Molecule 3 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



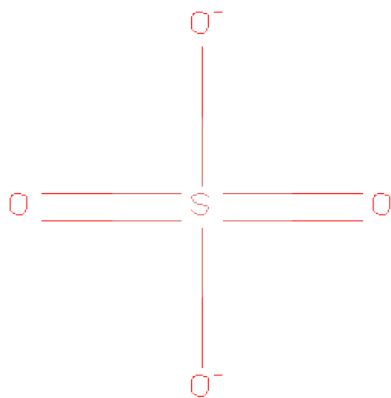
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B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

Continued on next page...

Continued from previous page...

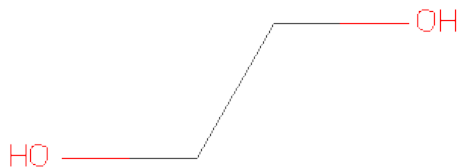
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	547	Total O 548 548	0	1
6	B	553	Total O 554 554	0	1
6	C	490	Total O 491 491	0	1
6	D	559	Total O 560 560	0	1

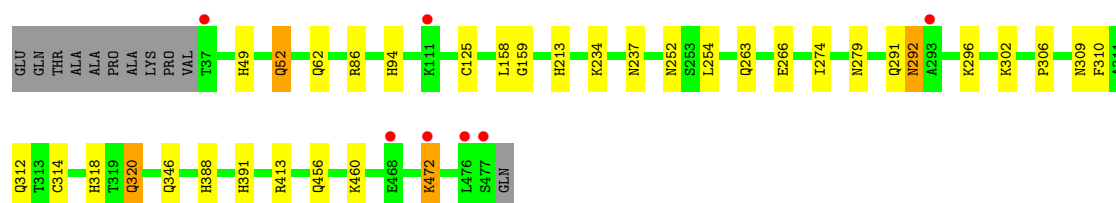


### 3 Residue-property plots

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.

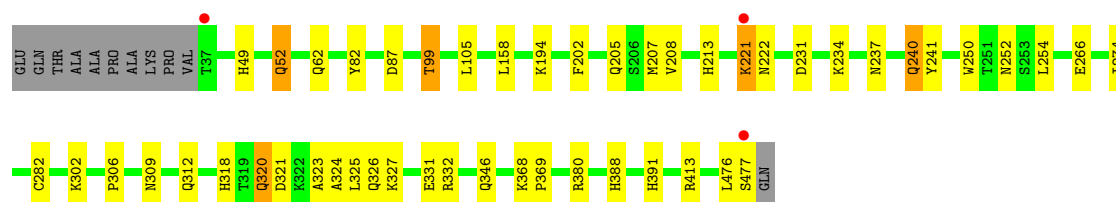
#### • Molecule 1: Cytochrome c-552

Chain A: 



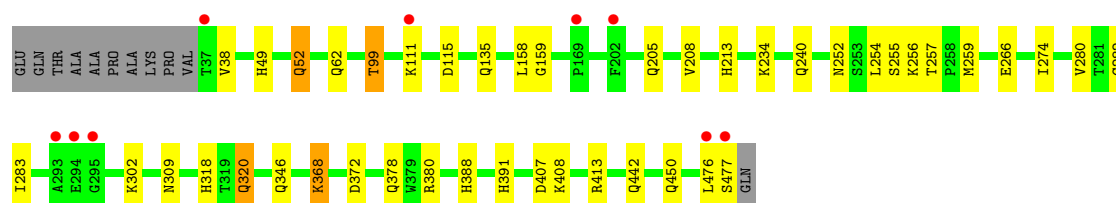
#### • Molecule 1: Cytochrome c-552

Chain B: 



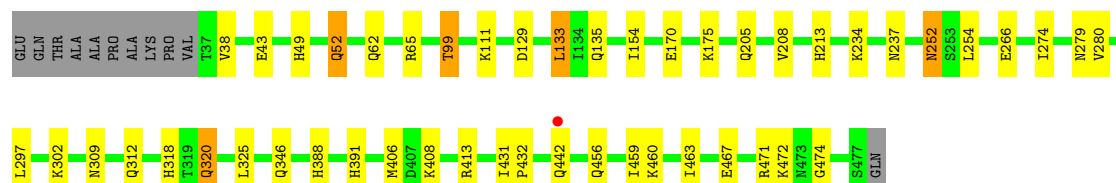
#### • Molecule 1: Cytochrome c-552

Chain C: 



#### • Molecule 1: Cytochrome c-552

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.46Å 79.30Å 137.58Å 90.00° 101.57° 90.00°	Depositor
Resolution (Å)	39.65 – 1.74 39.65 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.65-1.74) 99.1 (39.65-1.74)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.154 , 0.189 0.154 , 0.189	Depositor DCC
$R_{free}$ test set	9756 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 193618 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: CA, HEC, EDO, SO4

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	0.58	0/3577	0.60	0/4839
1	B	0.60	0/3628	0.62	0/4906
1	C	0.56	0/3601	0.59	0/4870
1	D	0.62	0/3619	0.62	0/4895
All	All	0.59	0/14425	0.61	0/19510

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	3487	0	3382	31	0
1	B	3520	0	3422	41	0
1	C	3502	0	3400	42	0
1	D	3514	0	3411	45	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	215	0	151	19	0
3	B	215	0	150	12	0
3	C	215	0	150	13	0
3	D	215	0	150	11	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	32	0	48	4	0
5	B	24	0	36	0	0
5	C	24	0	36	4	0
5	D	32	0	48	2	0
6	A	548	0	0	5	0
6	B	554	0	0	10	0
6	C	491	0	0	10	0
6	D	560	0	0	13	0
All	All	17176	0	14384	188	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 6.

All (188) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:125:CYS:SG	3:A:1:HEC:CAC	2.28	1.20
1:C:476:LEU:HB3	1:C:477:SER:HA	1.20	1.12
5:A:11:EDO:H22	1:B:332:ARG:HH12	1.27	0.99
1:C:476:LEU:HB3	1:C:477:SER:CA	2.00	0.92
1:B:99:THR:HG21	6:B:882:HOH:O	1.70	0.90
1:D:99:THR:HG21	6:D:809:HOH:O	1.76	0.85
1:B:476:LEU:O	1:B:477:SER:HB2	1.82	0.78
3:A:2:HEC:HBC3	3:A:2:HEC:HMC1	1.64	0.77
5:A:11:EDO:H22	1:B:332:ARG:NH1	2.00	0.76
1:D:65:ARG:NH1	6:D:840:HOH:O	2.19	0.75
1:C:442:GLN:HB3	6:C:920:HOH:O	1.85	0.74
3:C:4:HEC:HMC1	3:C:4:HEC:HBC3	1.70	0.74
1:B:62:GLN:HE21	1:B:302:LYS:HZ3	1.36	0.73
1:A:86:ARG:HE	5:A:21:EDO:H21	1.53	0.72
1:A:125:CYS:SG	3:A:1:HEC:C3C	2.78	0.71
3:B:2:HEC:HMC1	3:B:2:HEC:HBC3	1.72	0.71
1:C:476:LEU:CB	1:C:477:SER:HA	2.09	0.71
1:C:99:THR:HG23	6:C:490:HOH:O	1.90	0.71
1:D:65:ARG:HG3	5:D:481:EDO:H21	1.73	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:4:HEC:HMC1	3:A:4:HEC:HBC3	1.73	0.70
1:A:320:GLN:HE21	1:A:320:GLN:H	1.40	0.70
1:D:391:HIS:HE1	3:D:4:HEC:O2D	1.77	0.68
3:C:2:HEC:HBC3	3:C:2:HEC:HMC1	1.76	0.68
1:B:221:LYS:HZ3	1:B:222:ASN:H	1.41	0.67
1:B:99:THR:HG23	6:B:516:HOH:O	1.93	0.67
1:B:62:GLN:HE21	1:B:302:LYS:NZ	1.91	0.67
1:D:133:LEU:CD2	1:D:154:ILE:HD11	2.24	0.66
1:C:49:HIS:HD2	6:C:612:HOH:O	1.78	0.66
1:C:320:GLN:H	1:C:320:GLN:HE21	1.44	0.65
3:D:2:HEC:HMC1	3:D:2:HEC:HBC3	1.78	0.65
1:B:391:HIS:HE1	3:B:4:HEC:O2D	1.80	0.64
3:B:4:HEC:HBC3	3:B:4:HEC:HMC1	1.79	0.64
1:A:391:HIS:HE1	3:A:4:HEC:O2D	1.81	0.64
1:D:320:GLN:H	1:D:320:GLN:HE21	1.45	0.64
1:A:125:CYS:SG	3:A:1:HEC:HAC	2.33	0.63
3:D:4:HEC:HBC3	3:D:4:HEC:HMC1	1.81	0.63
1:D:309:ASN:HD21	1:D:312[A]:GLN:NE2	1.97	0.63
1:D:252:ASN:ND2	1:D:254:LEU:H	1.97	0.62
3:D:4:HEC:HBB3	3:D:4:HEC:HMB1	1.81	0.62
1:C:391:HIS:HE1	3:C:4:HEC:O2D	1.83	0.61
1:D:49:HIS:HD2	6:D:688:HOH:O	1.83	0.61
1:D:62:GLN:HE21	1:D:302:LYS:NZ	1.98	0.61
1:D:320:GLN:H	1:D:320:GLN:NE2	1.99	0.61
3:C:5:HEC:HMC1	3:C:5:HEC:HBC3	1.82	0.61
1:D:309:ASN:HD21	1:D:312[A]:GLN:HE21	1.50	0.60
3:A:1:HEC:HMC1	3:A:1:HEC:HBC3	1.82	0.59
1:A:346:GLN:NE2	1:A:413:ARG:HH11	2.00	0.59
1:C:320:GLN:H	1:C:320:GLN:NE2	2.01	0.59
1:B:346:GLN:NE2	1:B:413:ARG:HH11	2.01	0.58
1:D:99:THR:HG23	6:D:493:HOH:O	2.02	0.58
1:C:52:GLN:H	1:C:52:GLN:NE2	2.01	0.58
3:C:4:HEC:HMB1	3:C:4:HEC:HBB3	1.86	0.58
1:C:388:HIS:HE1	6:C:518:HOH:O	1.84	0.58
1:D:346:GLN:NE2	1:D:413:ARG:HH11	2.02	0.57
1:B:312[B]:GLN:NE2	6:B:1028:HOH:O	2.38	0.57
1:A:320:GLN:NE2	1:A:320:GLN:H	2.03	0.57
1:A:252:ASN:ND2	1:A:254:LEU:H	2.03	0.57
1:D:133:LEU:HD23	1:D:154:ILE:HD11	1.84	0.57
3:B:1:HEC:HMC1	3:B:1:HEC:HBC3	1.87	0.56
1:B:252:ASN:ND2	1:B:254:LEU:H	2.03	0.56
1:A:292:ASN:HD22	1:A:292:ASN:C	2.07	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:292:ASN:ND2	1:A:296:LYS:H	2.04	0.56
1:C:49:HIS:HE1	6:C:634:HOH:O	1.89	0.56
1:B:320:GLN:H	1:B:320:GLN:HE21	1.52	0.56
1:A:49:HIS:HD2	6:A:688:HOH:O	1.88	0.55
1:C:274:ILE:CG2	3:C:5:HEC:HAD1	2.36	0.55
1:D:170:GLU:HB3	1:D:175[B]:LYS:HD3	1.88	0.55
1:B:49:HIS:HD2	6:B:653:HOH:O	1.88	0.55
1:A:125:CYS:SG	3:A:1:HEC:CBC	2.94	0.55
1:B:320:GLN:H	1:B:320:GLN:NE2	2.04	0.55
1:C:346:GLN:NE2	1:C:413:ARG:HH11	2.05	0.55
1:A:388:HIS:HE1	6:A:483:HOH:O	1.90	0.55
3:B:4:HEC:HBB3	3:B:4:HEC:HMB1	1.89	0.54
1:D:274:ILE:CG2	3:D:5:HEC:HAD1	2.37	0.54
1:C:111:LYS:HG2	1:C:115:ASP:OD2	2.07	0.54
1:A:52:GLN:NE2	1:A:52:GLN:H	2.06	0.54
3:C:1:HEC:HMC1	3:C:1:HEC:HBC3	1.90	0.54
1:D:252:ASN:HD22	1:D:254:LEU:H	1.56	0.54
1:A:213:HIS:HB3	1:A:266:GLU:HB2	1.89	0.54
1:B:52:GLN:NE2	1:B:52:GLN:H	2.06	0.53
1:A:274:ILE:CG2	3:A:5:HEC:HAD1	2.39	0.53
1:C:407:ASP:OD2	5:C:21:EDO:H11	2.08	0.53
1:C:240:GLN:HB3	6:C:692:HOH:O	2.08	0.53
1:D:52:GLN:H	1:D:52:GLN:NE2	2.06	0.53
3:A:5:HEC:HBB3	3:A:5:HEC:HMB1	1.89	0.53
1:B:476:LEU:O	1:B:477:SER:CB	2.56	0.52
1:B:240:GLN:HE21	1:B:241:TYR:N	2.07	0.52
1:C:252:ASN:ND2	1:C:254:LEU:H	2.07	0.52
1:D:459:ILE:HA	1:D:463:ILE:HD12	1.91	0.52
1:C:476:LEU:CB	1:C:477:SER:CA	2.80	0.52
3:D:1:HEC:HBC3	3:D:1:HEC:HMC1	1.91	0.52
3:A:5:HEC:HMC1	3:A:5:HEC:HBC3	1.91	0.52
1:D:472:LYS:HG3	6:D:664:HOH:O	2.10	0.51
1:B:274:ILE:CG2	3:B:5:HEC:HAD1	2.41	0.51
1:D:43:GLU:CD	1:D:43:GLU:H	2.14	0.51
1:A:292:ASN:HD21	1:A:296:LYS:H	1.57	0.50
1:C:368:LYS:HE3	1:C:372:ASP:OD2	2.11	0.50
5:A:11:EDO:C2	1:B:332:ARG:HH12	2.12	0.50
1:D:280:VAL:HG13	3:D:5:HEC:HBC2	1.93	0.50
1:D:274:ILE:HG21	3:D:5:HEC:HAD1	1.93	0.50
1:D:234:LYS:HE2	6:D:1039:HOH:O	2.10	0.50
1:A:49:HIS:HE1	6:A:648:HOH:O	1.94	0.50
1:C:408:LYS:NZ	5:C:21:EDO:H12	2.25	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:5:HEC:HMB1	3:D:5:HEC:HBB3	1.94	0.49
1:C:213:HIS:HB3	1:C:266:GLU:HB2	1.95	0.49
3:D:5:HEC:HBC3	3:D:5:HEC:HMC1	1.94	0.49
3:A:4:HEC:HMB1	3:A:4:HEC:HBB3	1.94	0.49
1:D:279[A]:ASN:ND2	6:D:836:HOH:O	2.46	0.49
1:A:234:LYS:H	1:A:237:ASN:HD22	1.60	0.48
1:D:62:GLN:HE21	1:D:302:LYS:HZ1	1.60	0.48
1:C:280:VAL:HG13	3:C:5:HEC:HBC2	1.95	0.48
3:A:1:HEC:CBC	3:A:1:HEC:HMC1	2.44	0.48
1:D:318:HIS:HB3	1:D:320:GLN:NE2	2.29	0.48
1:B:306:PRO:HB2	3:B:5:HEC:HBB1	1.97	0.47
1:D:49:HIS:HE1	6:D:662:HOH:O	1.97	0.47
1:D:472:LYS:CG	6:D:664:HOH:O	2.62	0.47
1:C:205:GLN:HB3	1:C:283:ILE:HD13	1.97	0.47
1:C:282:CYS:HA	3:C:4:HEC:CHC	2.46	0.46
3:B:2:HEC:HBB3	3:B:2:HEC:HMB1	1.96	0.46
1:B:49:HIS:HE1	6:B:583:HOH:O	1.98	0.46
1:B:321[B]:ASP:OD1	1:B:324:ALA:HB2	2.15	0.46
1:C:256:LYS:HE2	6:C:772:HOH:O	2.14	0.46
1:B:380:ARG:NH1	6:B:597:HOH:O	2.47	0.46
1:B:213:HIS:HB3	1:B:266:GLU:HB2	1.97	0.46
1:B:202:PHE:HE1	6:B:958:HOH:O	1.99	0.46
1:D:133:LEU:HD22	1:D:154:ILE:HD11	1.97	0.46
3:B:3:HEC:HMC1	3:B:3:HEC:HBC3	1.98	0.45
1:D:388:HIS:HE1	6:D:555:HOH:O	1.99	0.45
1:C:257:THR:O	1:C:259[B]:MET:HG2	2.15	0.45
1:C:318:HIS:HB3	1:C:320:GLN:NE2	2.31	0.45
1:C:252:ASN:HD22	1:C:255:SER:H	1.65	0.45
1:B:327[A]:LYS:HG3	6:B:851:HOH:O	2.15	0.45
3:C:3:HEC:HMC1	3:C:3:HEC:HBC3	1.97	0.45
1:D:234:LYS:H	1:D:237:ASN:HD22	1.65	0.45
1:B:323:ALA:HA	1:B:326:GLN:HE21	1.81	0.45
1:D:213:HIS:HB3	1:D:266:GLU:HB2	1.97	0.45
1:C:205:GLN:O	1:C:208[B]:VAL:HG12	2.17	0.45
1:B:234:LYS:H	1:B:237:ASN:HD22	1.64	0.44
1:D:474:GLY:HA2	6:D:641:HOH:O	2.18	0.44
1:C:257:THR:HB	1:C:259[A]:MET:SD	2.58	0.44
1:D:205:GLN:O	1:D:208:VAL:HG22	2.18	0.44
1:B:205:GLN:O	1:B:208[B]:VAL:HG22	2.18	0.43
1:C:38:VAL:HG23	1:C:135:GLN:OE1	2.17	0.43
1:C:159:GLY:O	3:C:2:HEC:HMC3	2.19	0.43
3:D:2:HEC:HMB1	3:D:2:HEC:HBB3	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:388:HIS:HE1	6:B:484:HOH:O	2.01	0.43
1:D:467:GLU:O	1:D:471:ARG:HG3	2.18	0.43
1:C:259[B]:MET:CE	1:C:378:GLN:NE2	2.82	0.43
1:B:158:LEU:HG	3:B:3:HEC:HBC2	1.99	0.43
1:B:87:ASP:HB2	1:B:105:LEU:HB2	1.99	0.43
1:B:194:LYS:HE3	1:B:207:MET:CE	2.49	0.43
1:C:408:LYS:HZ3	5:C:21:EDO:H12	1.84	0.43
1:D:52:GLN:HE21	1:D:52:GLN:H	1.65	0.43
1:A:159:GLY:O	3:A:2:HEC:HMC3	2.19	0.42
1:C:274:ILE:HG21	3:C:5:HEC:HAD1	2.01	0.42
1:C:450:GLN:HG3	6:C:854:HOH:O	2.18	0.42
1:C:407:ASP:HB2	1:D:406:MET:HE3	2.01	0.42
1:B:82:TYR:CD1	1:B:250:TRP:HB3	2.54	0.42
1:D:431:ILE:HG22	1:D:432:PRO:O	2.19	0.42
6:C:646:HOH:O	5:D:25:EDO:H22	2.20	0.42
1:C:62:GLN:HE21	1:C:302:LYS:NZ	2.18	0.42
1:B:282:CYS:HA	3:B:4:HEC:CHC	2.50	0.42
1:A:318:HIS:HB3	1:A:320:GLN:NE2	2.35	0.41
1:B:318:HIS:HB3	1:B:320:GLN:NE2	2.35	0.41
1:A:263:GLN:NE2	6:A:1005:HOH:O	2.53	0.41
1:C:407:ASP:OD2	5:C:21:EDO:C1	2.68	0.41
1:D:408:LYS:NZ	6:D:873:HOH:O	2.53	0.41
1:C:380:ARG:NH1	6:C:600:HOH:O	2.53	0.41
1:D:38:VAL:HG23	1:D:135:GLN:CD	2.41	0.41
3:A:2:HEC:CBC	3:A:2:HEC:HMC1	2.44	0.41
1:D:129:ASP:HB3	1:D:154:ILE:HD13	2.02	0.41
1:A:62:GLN:HE21	1:A:302:LYS:NZ	2.17	0.41
1:D:234:LYS:HD3	6:D:1011:HOH:O	2.20	0.41
1:C:158:LEU:HG	3:C:3:HEC:HBC2	2.03	0.41
1:A:94:HIS:CD2	3:A:3:HEC:ND	2.88	0.41
3:A:2:HEC:HMB1	3:A:2:HEC:HBB3	2.02	0.41
1:A:158:LEU:HG	3:A:3:HEC:HBC2	2.02	0.41
1:A:456:GLN:HE21	1:A:460:LYS:HE3	1.85	0.41
1:B:368:LYS:HB3	1:B:369:PRO:HD3	2.02	0.41
1:A:306:PRO:HG2	3:A:4:HEC:CHD	2.51	0.40
1:D:456:GLN:NE2	1:D:460:LYS:HE3	2.36	0.40
1:B:231:ASP:CB	1:B:240:GLN:HE22	2.34	0.40
1:A:291:GLN:NE2	6:A:913:HOH:O	2.53	0.40
3:B:2:HEC:HMC1	3:B:2:HEC:CBC	2.47	0.40
1:B:221:LYS:NZ	6:B:821:HOH:O	2.46	0.40
1:A:310:PHE:CE2	1:A:314:CYS:HB2	2.57	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	441/452 (98%)	432 (98%)	9 (2%)	0	100	100
1	B	447/452 (99%)	437 (98%)	10 (2%)	0	100	100
1	C	444/452 (98%)	432 (97%)	12 (3%)	0	100	100
1	D	446/452 (99%)	436 (98%)	10 (2%)	0	100	100
All	All	1778/1808 (98%)	1737 (98%)	41 (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	364/370 (98%)	357 (98%)	7 (2%)	69	47
1	B	370/370 (100%)	363 (98%)	7 (2%)	69	47
1	C	367/370 (99%)	361 (98%)	6 (2%)	75	56
1	D	369/370 (100%)	359 (97%)	10 (3%)	57	30
All	All	1470/1480 (99%)	1440 (98%)	30 (2%)	68	44

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	279	ASN
1	A	292	ASN
1	A	309	ASN
1	A	312	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	320	GLN
1	A	472	LYS
1	B	52	GLN
1	B	99	THR
1	B	221	LYS
1	B	240	GLN
1	B	309	ASN
1	B	320	GLN
1	B	325	LEU
1	C	52	GLN
1	C	99	THR
1	C	234	LYS
1	C	309	ASN
1	C	320	GLN
1	C	368	LYS
1	D	52	GLN
1	D	99	THR
1	D	111	LYS
1	D	133	LEU
1	D	252	ASN
1	D	297	LEU
1	D	320	GLN
1	D	325	LEU
1	D	442[A]	GLN
1	D	442[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	49	HIS
1	A	52	GLN
1	A	62	GLN
1	A	237	ASN
1	A	252	ASN
1	A	279	ASN
1	A	291	GLN
1	A	292	ASN
1	A	309	ASN
1	A	312	GLN
1	A	320	GLN
1	A	334	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	337	ASN
1	A	346	GLN
1	A	371	GLN
1	A	388	HIS
1	A	391	HIS
1	A	456	GLN
1	B	49	HIS
1	B	52	GLN
1	B	62	GLN
1	B	237	ASN
1	B	240	GLN
1	B	252	ASN
1	B	291	GLN
1	B	309	ASN
1	B	320	GLN
1	B	326	GLN
1	B	334	GLN
1	B	346	GLN
1	B	371	GLN
1	B	388	HIS
1	B	391	HIS
1	B	469	GLN
1	C	49	HIS
1	C	52	GLN
1	C	62	GLN
1	C	237	ASN
1	C	252	ASN
1	C	291	GLN
1	C	309	ASN
1	C	320	GLN
1	C	346	GLN
1	C	371	GLN
1	C	388	HIS
1	C	391	HIS
1	C	469	GLN
1	D	49	HIS
1	D	52	GLN
1	D	62	GLN
1	D	237	ASN
1	D	252	ASN
1	D	291	GLN
1	D	320	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	326	GLN
1	D	346	GLN
1	D	371	GLN
1	D	388	HIS
1	D	391	HIS
1	D	456	GLN
1	D	469	GLN

### 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 ⓘ

Of 60 ligands modelled in this entry, 8 are monoatomic - leaving 52 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	HEC	A	1	1,6	50,50,50	2.92	14 (28%)	56,82,82	1.68	16 (28%)
5	EDO	A	11	-	3,3,3	0.46	0	2,2,2	0.79	0
5	EDO	A	13	-	3,3,3	0.47	0	2,2,2	0.69	0
5	EDO	A	14	-	3,3,3	0.47	0	2,2,2	0.41	0
5	EDO	A	15	-	3,3,3	0.49	0	2,2,2	0.40	0
3	HEC	A	2	1	50,50,50	2.84	14 (28%)	56,82,82	1.80	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	20	-	3,3,3	0.58	0	2,2,2	0.08	0
4	SO4	A	2001	-	4,4,4	0.14	0	6,6,6	0.24	0
5	EDO	A	21	-	3,3,3	0.50	0	2,2,2	0.47	0
5	EDO	A	22	-	3,3,3	0.52	0	2,2,2	0.43	0
3	HEC	A	3	1,2	50,50,50	2.85	15 (30%)	56,82,82	1.85	13 (23%)
3	HEC	A	4	1,2	50,50,50	2.84	14 (28%)	56,82,82	1.86	10 (17%)
5	EDO	A	481	-	3,3,3	0.49	0	2,2,2	0.30	0
3	HEC	A	5	1	50,50,50	2.76	13 (26%)	56,82,82	1.77	14 (25%)
3	HEC	B	1	1,6	50,50,50	2.90	14 (28%)	56,82,82	1.80	12 (21%)
5	EDO	B	16	-	3,3,3	0.60	0	2,2,2	0.33	0
5	EDO	B	17	-	3,3,3	0.52	0	2,2,2	0.46	0
5	EDO	B	18	-	3,3,3	0.51	0	2,2,2	0.38	0
5	EDO	B	19	-	3,3,3	0.55	0	2,2,2	0.20	0
3	HEC	B	2	1	50,50,50	3.59	15 (30%)	56,82,82	3.63	18 (32%)
5	EDO	B	20	-	3,3,3	0.52	0	2,2,2	0.57	0
4	SO4	B	2001	-	4,4,4	0.27	0	6,6,6	0.21	0
3	HEC	B	3	1,2	50,50,50	2.89	14 (28%)	56,82,82	1.77	11 (19%)
3	HEC	B	4	1,2	50,50,50	2.78	15 (30%)	56,82,82	1.80	11 (19%)
5	EDO	B	481	-	3,3,3	0.65	0	2,2,2	0.31	0
3	HEC	B	5	1	50,50,50	2.79	15 (30%)	56,82,82	1.62	11 (19%)
3	HEC	C	1	1,6	50,50,50	2.86	14 (28%)	56,82,82	1.64	11 (19%)
5	EDO	C	12	-	3,3,3	0.49	0	2,2,2	0.78	0
3	HEC	C	2	1	50,50,50	2.84	14 (28%)	56,82,82	1.88	14 (25%)
4	SO4	C	2001	-	4,4,4	0.23	0	6,6,6	0.31	0
5	EDO	C	21	-	3,3,3	0.45	0	2,2,2	0.65	0
5	EDO	C	22	-	3,3,3	0.54	0	2,2,2	0.25	0
5	EDO	C	23	-	3,3,3	0.52	0	2,2,2	0.46	0
5	EDO	C	25	-	3,3,3	0.47	0	2,2,2	0.54	0
3	HEC	C	3	1,2	50,50,50	2.80	14 (28%)	56,82,82	1.90	16 (28%)
3	HEC	C	4	1,2	50,50,50	2.79	14 (28%)	56,82,82	1.76	11 (19%)
5	EDO	C	481	-	3,3,3	0.59	0	2,2,2	0.28	0
3	HEC	C	5	1	50,50,50	2.91	14 (28%)	56,82,82	1.64	11 (19%)
3	HEC	D	1	1,6	50,50,50	2.89	14 (28%)	56,82,82	1.85	13 (23%)
3	HEC	D	2	1	50,50,50	2.81	14 (28%)	56,82,82	1.79	13 (23%)
4	SO4	D	2001	-	4,4,4	0.14	0	6,6,6	0.19	0
5	EDO	D	21	-	3,3,3	0.57	0	2,2,2	0.51	0
5	EDO	D	22	-	3,3,3	0.52	0	2,2,2	0.74	0
5	EDO	D	23	-	3,3,3	0.56	0	2,2,2	0.46	0
5	EDO	D	24	-	3,3,3	0.54	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	D	25	-	3,3,3	0.59	0	2,2,2	0.15	0
3	HEC	D	3	1,2	50,50,50	2.77	15 (30%)	56,82,82	1.85	11 (19%)
3	HEC	D	4	1	50,50,50	2.74	14 (28%)	56,82,82	1.85	13 (23%)
5	EDO	D	481	-	3,3,3	0.42	0	2,2,2	0.40	0
5	EDO	D	482	-	3,3,3	0.58	0	2,2,2	0.25	0
3	HEC	D	5	1	50,50,50	2.85	13 (26%)	56,82,82	1.65	8 (14%)
5	EDO	D	6	-	3,3,3	0.65	0	2,2,2	0.21	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
3	HEC	A	1	1,6	-	0/10/54/54	0/0/8/8
5	EDO	A	11	-	-	0/1/1/1	0/0/0/0
5	EDO	A	13	-	-	0/1/1/1	0/0/0/0
5	EDO	A	14	-	-	0/1/1/1	0/0/0/0
5	EDO	A	15	-	-	0/1/1/1	0/0/0/0
3	HEC	A	2	1	-	0/10/54/54	0/0/8/8
5	EDO	A	20	-	-	0/1/1/1	0/0/0/0
4	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
5	EDO	A	21	-	-	0/1/1/1	0/0/0/0
5	EDO	A	22	-	-	0/1/1/1	0/0/0/0
3	HEC	A	3	1,2	-	0/10/54/54	0/0/8/8
3	HEC	A	4	1,2	-	0/10/54/54	0/0/8/8
5	EDO	A	481	-	-	0/1/1/1	0/0/0/0
3	HEC	A	5	1	-	0/10/54/54	0/0/8/8
3	HEC	B	1	1,6	-	0/10/54/54	0/0/8/8
5	EDO	B	16	-	-	0/1/1/1	0/0/0/0
5	EDO	B	17	-	-	0/1/1/1	0/0/0/0
5	EDO	B	18	-	-	0/1/1/1	0/0/0/0
5	EDO	B	19	-	-	0/1/1/1	0/0/0/0
3	HEC	B	2	1	-	0/10/54/54	0/0/8/8
5	EDO	B	20	-	-	0/1/1/1	0/0/0/0
4	SO4	B	2001	-	-	0/0/0/0	0/0/0/0
3	HEC	B	3	1,2	-	0/10/54/54	0/0/8/8
3	HEC	B	4	1,2	-	0/10/54/54	0/0/8/8
5	EDO	B	481	-	-	0/1/1/1	0/0/0/0
3	HEC	B	5	1	-	0/10/54/54	0/0/8/8
3	HEC	C	1	1,6	-	0/10/54/54	0/0/8/8
5	EDO	C	12	-	-	0/1/1/1	0/0/0/0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	C	2	1	-	0/10/54/54	0/0/8/8
4	SO4	C	2001	-	-	0/0/0/0	0/0/0/0
5	EDO	C	21	-	-	0/1/1/1	0/0/0/0
5	EDO	C	22	-	-	0/1/1/1	0/0/0/0
5	EDO	C	23	-	-	0/1/1/1	0/0/0/0
5	EDO	C	25	-	-	0/1/1/1	0/0/0/0
3	HEC	C	3	1,2	-	0/10/54/54	0/0/8/8
3	HEC	C	4	1,2	-	0/10/54/54	0/0/8/8
5	EDO	C	481	-	-	0/1/1/1	0/0/0/0
3	HEC	C	5	1	-	0/10/54/54	0/0/8/8
3	HEC	D	1	1,6	-	0/10/54/54	0/0/8/8
3	HEC	D	2	1	-	0/10/54/54	0/0/8/8
4	SO4	D	2001	-	-	0/0/0/0	0/0/0/0
5	EDO	D	21	-	-	0/1/1/1	0/0/0/0
5	EDO	D	22	-	-	0/1/1/1	0/0/0/0
5	EDO	D	23	-	-	0/1/1/1	0/0/0/0
5	EDO	D	24	-	-	0/1/1/1	0/0/0/0
5	EDO	D	25	-	-	0/1/1/1	0/0/0/0
3	HEC	D	3	1,2	-	0/10/54/54	0/0/8/8
3	HEC	D	4	1	-	0/10/54/54	0/0/8/8
5	EDO	D	481	-	-	0/1/1/1	0/0/0/0
5	EDO	D	482	-	-	0/1/1/1	0/0/0/0
3	HEC	D	5	1	-	0/10/54/54	0/0/8/8
5	EDO	D	6	-	-	0/1/1/1	0/0/0/0

All (283) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	HEC	C1D-ND	14.77	1.65	1.36
3	C	5	HEC	C3C-CAC	10.68	1.57	1.35
3	A	1	HEC	C3C-CAC	10.35	1.56	1.35
3	B	5	HEC	C3C-CAC	10.33	1.56	1.35
3	C	3	HEC	C3C-CAC	10.28	1.56	1.35
3	A	2	HEC	C3C-CAC	10.22	1.56	1.35
3	D	2	HEC	C3C-CAC	10.21	1.56	1.35
3	A	2	HEC	C3B-CAB	10.19	1.56	1.35
3	D	5	HEC	C3C-CAC	10.18	1.56	1.35
3	B	2	HEC	C3C-CAC	10.12	1.56	1.35
3	B	3	HEC	C3C-CAC	10.10	1.56	1.35
3	D	1	HEC	C3C-CAC	10.08	1.56	1.35
3	B	1	HEC	C3B-CAB	10.08	1.56	1.35
3	A	3	HEC	C3C-CAC	10.06	1.56	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	HEC	C3C-CAC	10.00	1.56	1.35
3	A	4	HEC	C3C-CAC	9.98	1.55	1.35
3	B	1	HEC	C3C-CAC	9.94	1.55	1.35
3	D	3	HEC	C3C-CAC	9.91	1.55	1.35
3	B	3	HEC	C3B-CAB	9.87	1.55	1.35
3	C	1	HEC	C3C-CAC	9.81	1.55	1.35
3	C	4	HEC	C3C-CAC	9.79	1.55	1.35
3	A	5	HEC	C3C-CAC	9.78	1.55	1.35
3	D	1	HEC	C3B-CAB	9.78	1.55	1.35
3	D	3	HEC	C3B-CAB	9.72	1.55	1.35
3	A	1	HEC	C3B-CAB	9.70	1.55	1.35
3	C	5	HEC	C3B-CAB	9.63	1.55	1.35
3	D	5	HEC	C3B-CAB	9.55	1.55	1.35
3	C	2	HEC	C3B-CAB	9.55	1.55	1.35
3	B	4	HEC	C3C-CAC	9.52	1.55	1.35
3	C	4	HEC	C3B-CAB	9.51	1.55	1.35
3	D	4	HEC	C3C-CAC	9.50	1.55	1.35
3	B	2	HEC	C3B-CAB	9.49	1.55	1.35
3	A	3	HEC	C3B-CAB	9.49	1.55	1.35
3	C	1	HEC	C3B-CAB	9.46	1.54	1.35
3	C	3	HEC	C3B-CAB	9.41	1.54	1.35
3	B	4	HEC	C3B-CAB	9.39	1.54	1.35
3	A	4	HEC	C3B-CAB	9.28	1.54	1.35
3	D	4	HEC	C3B-CAB	9.26	1.54	1.35
3	B	5	HEC	C3B-CAB	9.09	1.54	1.35
3	D	2	HEC	C3B-CAB	8.93	1.53	1.35
3	A	5	HEC	C3B-CAB	8.80	1.53	1.35
3	A	1	HEC	C1C-C2C	5.90	1.47	1.40
3	B	1	HEC	C1B-C2B	5.72	1.47	1.40
3	B	4	HEC	C1B-C2B	5.63	1.47	1.40
3	C	1	HEC	C1B-C2B	5.60	1.47	1.40
3	D	5	HEC	C1C-C2C	5.50	1.47	1.40
3	A	4	HEC	C1B-C2B	5.49	1.47	1.40
3	C	1	HEC	C3D-C2D	5.47	1.53	1.37
3	A	1	HEC	C1B-C2B	5.43	1.46	1.40
3	D	4	HEC	C1D-C2D	5.40	1.46	1.40
3	C	2	HEC	C3D-C2D	5.31	1.53	1.37
3	B	3	HEC	C1B-C2B	5.27	1.46	1.40
3	B	2	HEC	C1B-C2B	5.27	1.46	1.40
3	C	4	HEC	C1B-C2B	5.26	1.46	1.40
3	C	5	HEC	C1C-C2C	5.25	1.46	1.40
3	B	2	HEC	C1D-CHD	-5.23	1.25	1.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3	HEC	C1C-C2C	5.19	1.46	1.40
3	D	1	HEC	C1B-C2B	5.18	1.46	1.40
3	C	3	HEC	C3D-C2D	5.18	1.53	1.37
3	C	5	HEC	C3D-C2D	5.15	1.52	1.37
3	B	4	HEC	C3D-C2D	5.15	1.52	1.37
3	D	4	HEC	C1B-C2B	5.13	1.46	1.40
3	A	4	HEC	C3D-C2D	5.13	1.52	1.37
3	D	1	HEC	C3D-C2D	5.07	1.52	1.37
3	A	3	HEC	C3D-C2D	5.02	1.52	1.37
3	D	3	HEC	C1D-C2D	5.00	1.46	1.40
3	A	1	HEC	C3D-C2D	5.00	1.52	1.37
3	D	3	HEC	C1C-C2C	4.99	1.46	1.40
3	B	2	HEC	C1C-C2C	4.99	1.46	1.40
3	D	4	HEC	C3D-C2D	4.98	1.52	1.37
3	D	1	HEC	C3C-C4C	4.96	1.47	1.41
3	A	4	HEC	C1C-C2C	4.95	1.46	1.40
3	B	3	HEC	C3D-C2D	4.93	1.52	1.37
3	D	2	HEC	C1B-C2B	4.91	1.46	1.40
3	C	3	HEC	C1C-C2C	4.91	1.46	1.40
3	B	1	HEC	C3D-C2D	4.90	1.52	1.37
3	B	1	HEC	C1D-C2D	4.90	1.46	1.40
3	B	1	HEC	C1C-C2C	4.90	1.46	1.40
3	B	5	HEC	C1C-C2C	4.89	1.46	1.40
3	A	5	HEC	C1B-C2B	4.88	1.46	1.40
3	D	5	HEC	C3D-C2D	4.87	1.52	1.37
3	C	4	HEC	C3D-C2D	4.86	1.52	1.37
3	C	2	HEC	C1B-C2B	4.86	1.46	1.40
3	A	5	HEC	C3D-C2D	4.83	1.52	1.37
3	A	2	HEC	C1C-C2C	4.82	1.46	1.40
3	B	4	HEC	C1D-C2D	4.81	1.46	1.40
3	C	5	HEC	C1B-C2B	4.80	1.46	1.40
3	D	2	HEC	C3D-C2D	4.79	1.51	1.37
3	B	2	HEC	C3D-C2D	4.79	1.51	1.37
3	B	2	HEC	C3B-C4B	4.78	1.47	1.41
3	C	4	HEC	C1C-C2C	4.75	1.46	1.40
3	D	2	HEC	C1C-C2C	4.75	1.46	1.40
3	C	5	HEC	C3C-C4C	4.74	1.47	1.41
3	D	3	HEC	C3D-C2D	4.70	1.51	1.37
3	D	5	HEC	C3C-C4C	4.66	1.47	1.41
3	A	2	HEC	C3D-C2D	4.62	1.51	1.37
3	C	3	HEC	C1B-C2B	4.62	1.45	1.40
3	B	5	HEC	C3D-C2D	4.61	1.51	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5	HEC	C1D-C2D	4.61	1.45	1.40
3	B	5	HEC	C1D-C2D	4.61	1.45	1.40
3	A	3	HEC	C1D-C2D	4.60	1.45	1.40
3	A	3	HEC	C1C-C2C	4.55	1.45	1.40
3	D	2	HEC	C3C-C4C	4.54	1.47	1.41
3	C	4	HEC	C1D-C2D	4.54	1.45	1.40
3	D	1	HEC	FE-ND	4.52	2.11	1.92
3	A	2	HEC	C1B-C2B	4.52	1.45	1.40
3	A	5	HEC	C3C-C4C	4.49	1.47	1.41
3	D	5	HEC	C1B-C2B	4.49	1.45	1.40
3	B	3	HEC	C1D-C2D	4.47	1.45	1.40
3	A	5	HEC	C1C-C2C	4.46	1.45	1.40
3	A	3	HEC	FE-NC	4.44	2.11	1.92
3	A	1	HEC	C1D-C2D	4.43	1.45	1.40
3	D	5	HEC	C1D-C2D	4.39	1.45	1.40
3	C	1	HEC	FE-ND	4.39	2.11	1.92
3	B	5	HEC	C1B-C2B	4.39	1.45	1.40
3	B	4	HEC	C1C-C2C	4.35	1.45	1.40
3	A	3	HEC	C3C-C4C	4.35	1.47	1.41
3	C	5	HEC	C1D-C2D	4.34	1.45	1.40
3	A	4	HEC	C3C-C4C	4.32	1.47	1.41
3	D	4	HEC	C1C-C2C	4.32	1.45	1.40
3	C	1	HEC	C1D-C2D	4.31	1.45	1.40
3	C	2	HEC	FE-NA	4.26	2.10	1.92
3	A	2	HEC	C1D-C2D	4.23	1.45	1.40
3	A	1	HEC	C3C-C4C	4.18	1.46	1.41
3	C	1	HEC	C1C-C2C	4.17	1.45	1.40
3	D	3	HEC	C1B-C2B	4.13	1.45	1.40
3	A	3	HEC	C1B-C2B	4.12	1.45	1.40
3	B	3	HEC	C3C-C4C	4.12	1.46	1.41
3	C	1	HEC	C3B-C4B	4.11	1.46	1.41
3	B	1	HEC	FE-ND	4.11	2.10	1.92
3	D	2	HEC	FE-ND	4.10	2.10	1.92
3	C	2	HEC	FE-ND	4.09	2.10	1.92
3	A	4	HEC	C1D-C2D	4.08	1.45	1.40
3	D	1	HEC	C1D-C2D	4.08	1.45	1.40
3	C	2	HEC	C3B-C4B	4.02	1.46	1.41
3	C	3	HEC	C1D-C2D	3.98	1.45	1.40
3	A	4	HEC	C3B-C4B	3.96	1.46	1.41
3	C	2	HEC	C1D-C2D	3.93	1.45	1.40
3	A	1	HEC	FE-ND	3.93	2.09	1.92
3	A	5	HEC	FE-ND	3.91	2.09	1.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3	HEC	C3B-C4B	3.87	1.46	1.41
3	C	1	HEC	FE-NB	3.87	2.09	1.92
3	B	5	HEC	C3C-C4C	3.84	1.46	1.41
3	B	2	HEC	FE-NA	3.83	2.08	1.92
3	C	2	HEC	FE-NC	3.82	2.08	1.92
3	B	3	HEC	FE-NC	3.80	2.08	1.92
3	D	1	HEC	C1C-C2C	3.78	1.44	1.40
3	A	2	HEC	FE-NC	3.77	2.08	1.92
3	B	2	HEC	FE-NC	3.77	2.08	1.92
3	A	2	HEC	C3B-C4B	3.77	1.46	1.41
3	D	1	HEC	C3B-C4B	3.76	1.46	1.41
3	C	2	HEC	C1C-C2C	3.71	1.44	1.40
3	B	1	HEC	FE-NB	3.71	2.08	1.92
3	D	2	HEC	FE-NC	3.71	2.08	1.92
3	D	2	HEC	C1D-C2D	3.68	1.44	1.40
3	D	3	HEC	FE-NC	3.66	2.08	1.92
3	A	2	HEC	FE-NB	3.64	2.08	1.92
3	D	2	HEC	C3B-C4B	3.63	1.46	1.41
3	B	2	HEC	FE-ND	3.62	2.08	1.92
3	D	2	HEC	FE-NA	3.61	2.07	1.92
3	C	4	HEC	FE-NC	3.56	2.07	1.92
3	B	5	HEC	C3B-C4B	3.55	1.46	1.41
3	C	1	HEC	C3C-C4C	3.54	1.46	1.41
3	C	3	HEC	FE-NC	3.53	2.07	1.92
3	B	3	HEC	C3B-C2B	-3.52	1.34	1.41
3	C	2	HEC	C3C-C4C	3.51	1.46	1.41
3	D	4	HEC	C3C-C4C	3.50	1.46	1.41
3	B	5	HEC	C3B-C2B	-3.49	1.34	1.41
3	A	5	HEC	C3B-C4B	3.48	1.46	1.41
3	C	3	HEC	FE-NB	3.47	2.07	1.92
3	C	5	HEC	FE-NC	3.47	2.07	1.92
3	B	1	HEC	C3C-C4C	3.46	1.46	1.41
3	D	1	HEC	FE-NA	3.45	2.07	1.92
3	A	3	HEC	FE-NA	3.45	2.07	1.92
3	D	4	HEC	FE-NC	3.45	2.07	1.92
3	B	4	HEC	C3B-C2B	-3.44	1.34	1.41
3	B	2	HEC	C3C-C4C	3.43	1.45	1.41
3	B	1	HEC	C3B-C4B	3.42	1.45	1.41
3	D	5	HEC	C3C-C2C	-3.42	1.34	1.41
3	C	3	HEC	C3B-C4B	3.40	1.45	1.41
3	D	5	HEC	C3B-C2B	-3.39	1.34	1.41
3	B	5	HEC	FE-ND	3.37	2.06	1.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	HEC	C3B-C4B	3.35	1.45	1.41
3	C	4	HEC	C3C-C4C	3.34	1.45	1.41
3	B	2	HEC	C3B-C2B	-3.34	1.34	1.41
3	A	3	HEC	C3B-C4B	3.33	1.45	1.41
3	A	1	HEC	FE-NB	3.33	2.06	1.92
3	A	4	HEC	FE-NA	3.32	2.06	1.92
3	A	4	HEC	C3C-C2C	-3.31	1.34	1.41
3	D	3	HEC	C3B-C4B	3.30	1.45	1.41
3	D	3	HEC	C3C-C4C	3.26	1.45	1.41
3	C	4	HEC	FE-ND	3.26	2.06	1.92
3	C	5	HEC	FE-NB	3.25	2.06	1.92
3	B	4	HEC	FE-ND	3.20	2.06	1.92
3	D	1	HEC	C3C-C2C	-3.20	1.34	1.41
3	A	1	HEC	C3C-C2C	-3.18	1.34	1.41
3	A	2	HEC	FE-NA	3.15	2.05	1.92
3	A	3	HEC	C3C-C2C	-3.15	1.34	1.41
3	C	5	HEC	FE-NA	3.14	2.05	1.92
3	B	4	HEC	FE-NC	3.14	2.05	1.92
3	C	4	HEC	C3B-C2B	-3.12	1.34	1.41
3	D	5	HEC	FE-ND	3.12	2.05	1.92
3	C	3	HEC	C3C-C4C	3.11	1.45	1.41
3	C	3	HEC	C3B-C2B	-3.11	1.34	1.41
3	A	3	HEC	C3B-C2B	-3.10	1.35	1.41
3	A	5	HEC	C3C-C2C	-3.09	1.35	1.41
3	A	1	HEC	FE-NC	3.06	2.05	1.92
3	D	4	HEC	C3B-C2B	-3.05	1.35	1.41
3	D	2	HEC	C3B-C2B	-3.04	1.35	1.41
3	D	3	HEC	FE-NB	3.04	2.05	1.92
3	C	5	HEC	C3B-C4B	3.02	1.45	1.41
3	D	5	HEC	FE-NC	3.02	2.05	1.92
3	B	5	HEC	C3C-C2C	-3.02	1.35	1.41
3	A	1	HEC	C3B-C4B	3.01	1.45	1.41
3	D	1	HEC	C3B-C2B	-3.00	1.35	1.41
3	B	4	HEC	C3C-C4C	3.00	1.45	1.41
3	B	1	HEC	FE-NA	3.00	2.05	1.92
3	B	3	HEC	FE-NB	2.98	2.05	1.92
3	A	5	HEC	C3B-C2B	-2.98	1.35	1.41
3	B	2	HEC	FE-NB	2.96	2.05	1.92
3	D	3	HEC	C3C-C2C	-2.94	1.35	1.41
3	C	1	HEC	C3C-C2C	-2.93	1.35	1.41
3	A	2	HEC	C3B-C2B	-2.93	1.35	1.41
3	A	3	HEC	FE-NB	2.92	2.05	1.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	HEC	FE-NB	2.92	2.04	1.92
3	C	3	HEC	FE-NA	2.91	2.04	1.92
3	A	5	HEC	FE-NB	2.91	2.04	1.92
3	C	4	HEC	C3C-C2C	-2.91	1.35	1.41
3	D	2	HEC	FE-NB	2.91	2.04	1.92
3	A	4	HEC	C3B-C2B	-2.89	1.35	1.41
3	C	2	HEC	C3B-C2B	-2.89	1.35	1.41
3	B	3	HEC	FE-NA	2.89	2.04	1.92
3	D	2	HEC	C3C-C2C	-2.89	1.35	1.41
3	D	4	HEC	C3C-C2C	-2.87	1.35	1.41
3	C	5	HEC	FE-ND	2.87	2.04	1.92
3	B	2	HEC	C3C-C2C	-2.87	1.35	1.41
3	A	4	HEC	FE-NB	2.86	2.04	1.92
3	D	4	HEC	FE-ND	2.86	2.04	1.92
3	A	2	HEC	C3C-C4C	2.86	1.45	1.41
3	B	1	HEC	C3B-C2B	-2.84	1.35	1.41
3	A	4	HEC	FE-ND	2.83	2.04	1.92
3	C	4	HEC	C3B-C4B	2.82	1.45	1.41
3	C	1	HEC	C3B-C2B	-2.82	1.35	1.41
3	B	4	HEC	FE-NA	2.81	2.04	1.92
3	B	5	HEC	FE-NC	2.81	2.04	1.92
3	C	3	HEC	FE-ND	2.80	2.04	1.92
3	C	5	HEC	C3C-C2C	-2.80	1.35	1.41
3	D	3	HEC	C3B-C2B	-2.77	1.35	1.41
3	A	2	HEC	C3C-C2C	-2.73	1.35	1.41
3	B	3	HEC	FE-ND	2.72	2.04	1.92
3	A	2	HEC	FE-ND	2.71	2.04	1.92
3	C	3	HEC	C3C-C2C	-2.70	1.35	1.41
3	B	3	HEC	C3C-C2C	-2.69	1.35	1.41
3	C	2	HEC	C3C-C2C	-2.68	1.35	1.41
3	B	4	HEC	FE-NB	2.64	2.03	1.92
3	B	1	HEC	FE-NC	2.62	2.03	1.92
3	D	4	HEC	C3B-C4B	2.62	1.44	1.41
3	C	5	HEC	C3B-C2B	-2.61	1.36	1.41
3	C	4	HEC	FE-NA	2.60	2.03	1.92
3	B	4	HEC	C3C-C2C	-2.60	1.36	1.41
3	C	4	HEC	FE-NB	2.59	2.03	1.92
3	D	1	HEC	FE-NC	2.59	2.03	1.92
3	D	3	HEC	FE-ND	2.58	2.03	1.92
3	A	3	HEC	FE-ND	2.56	2.03	1.92
3	B	4	HEC	C3B-C4B	2.55	1.44	1.41
3	A	1	HEC	FE-NA	2.54	2.03	1.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5	HEC	FE-NA	2.53	2.03	1.92
3	D	1	HEC	FE-NB	2.51	2.03	1.92
3	D	4	HEC	FE-NB	2.48	2.03	1.92
3	B	5	HEC	FE-NB	2.46	2.03	1.92
3	D	4	HEC	FE-NA	2.42	2.02	1.92
3	B	1	HEC	C3C-C2C	-2.40	1.36	1.41
3	B	5	HEC	FE-NA	2.36	2.02	1.92
3	D	5	HEC	FE-NA	2.26	2.02	1.92
3	D	3	HEC	FE-NA	2.25	2.02	1.92
3	A	4	HEC	FE-NC	2.24	2.02	1.92
3	A	1	HEC	C3B-C2B	-2.18	1.37	1.41
3	A	3	HEC	C1D-ND	2.15	1.40	1.36
3	B	4	HEC	CMD-C2D	2.08	1.56	1.51
3	C	1	HEC	FE-NA	2.07	2.01	1.92
3	C	1	HEC	FE-NC	2.06	2.01	1.92
3	B	5	HEC	C4D-ND	2.04	1.40	1.36
3	D	3	HEC	CMD-C2D	2.02	1.55	1.51

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	HEC	C2D-C1D-ND	-14.91	98.16	109.41
3	B	2	HEC	C1D-C2D-C3D	12.00	115.35	107.00
3	B	2	HEC	C2D-C1D-CHD	9.63	144.26	126.00
3	D	3	HEC	CBB-CAB-C3B	-7.00	108.75	128.44
3	B	2	HEC	CMD-C2D-C1D	-6.98	117.89	128.62
3	B	2	HEC	C4C-CHD-C1D	6.97	136.65	127.47
3	D	1	HEC	CBB-CAB-C3B	-6.65	109.72	128.44
3	A	3	HEC	CBB-CAB-C3B	-6.63	109.79	128.44
3	B	1	HEC	CBB-CAB-C3B	-6.58	109.90	128.44
3	B	3	HEC	CBB-CAB-C3B	-6.36	110.53	128.44
3	A	4	HEC	CBB-CAB-C3B	-6.11	111.23	128.44
3	C	1	HEC	CBB-CAB-C3B	-5.97	111.63	128.44
3	C	3	HEC	CBB-CAB-C3B	-5.93	111.74	128.44
3	A	5	HEC	CBB-CAB-C3B	-5.89	111.86	128.44
3	D	4	HEC	CBB-CAB-C3B	-5.82	112.05	128.44
3	D	2	HEC	CBB-CAB-C3B	-5.72	112.34	128.44
3	A	2	HEC	CBB-CAB-C3B	-5.69	112.42	128.44
3	B	4	HEC	CBB-CAB-C3B	-5.64	112.55	128.44
3	B	2	HEC	CHD-C1D-ND	-5.50	115.39	124.58
3	B	2	HEC	CBB-CAB-C3B	-5.44	113.12	128.44
3	A	1	HEC	CBB-CAB-C3B	-5.37	113.33	128.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	HEC	CBB-CAB-C3B	-5.34	113.42	128.44
3	D	5	HEC	CBB-CAB-C3B	-5.06	114.21	128.44
3	C	4	HEC	CBC-CAC-C3C	-5.02	114.31	128.44
3	C	5	HEC	CBB-CAB-C3B	-4.97	114.44	128.44
3	C	4	HEC	CBB-CAB-C3B	-4.95	114.51	128.44
3	A	2	HEC	CBC-CAC-C3C	-4.74	115.11	128.44
3	C	2	HEC	CBC-CAC-C3C	-4.74	115.11	128.44
3	B	5	HEC	CBB-CAB-C3B	-4.68	115.27	128.44
3	A	4	HEC	CBC-CAC-C3C	-4.66	115.32	128.44
3	B	4	HEC	CMC-C2C-C1C	-4.61	121.53	128.62
3	D	4	HEC	CBC-CAC-C3C	-4.58	115.54	128.44
3	B	1	HEC	CBC-CAC-C3C	-4.51	115.73	128.44
3	C	3	HEC	CBC-CAC-C3C	-4.47	115.84	128.44
3	B	4	HEC	CBC-CAC-C3C	-4.44	115.94	128.44
3	B	4	HEC	C4D-ND-C1D	4.37	112.52	106.76
3	D	2	HEC	CBC-CAC-C3C	-4.33	116.26	128.44
3	D	5	HEC	CBC-CAC-C3C	-4.32	116.27	128.44
3	C	2	HEC	C4D-ND-C1D	4.17	112.25	106.76
3	B	5	HEC	CMC-C2C-C1C	-4.15	122.23	128.62
3	C	5	HEC	CBC-CAC-C3C	-4.15	116.75	128.44
3	A	3	HEC	CBC-CAC-C3C	-4.13	116.82	128.44
3	D	4	HEC	C4D-ND-C1D	4.12	112.19	106.76
3	A	5	HEC	CMC-C2C-C1C	-4.01	122.45	128.62
3	D	3	HEC	CMB-C2B-C1B	-3.92	122.60	128.62
3	A	4	HEC	CMB-C2B-C1B	-3.91	122.60	128.62
3	C	5	HEC	CMC-C2C-C1C	-3.87	122.67	128.62
3	D	2	HEC	C4D-ND-C1D	3.86	111.85	106.76
3	A	2	HEC	CMC-C2C-C1C	-3.85	122.70	128.62
3	B	2	HEC	CMB-C2B-C1B	-3.83	122.73	128.62
3	B	4	HEC	CBA-CAA-C2A	-3.79	105.27	112.35
3	C	4	HEC	C4D-ND-C1D	3.79	111.75	106.76
3	D	5	HEC	CMC-C2C-C1C	-3.77	122.83	128.62
3	D	1	HEC	CBC-CAC-C3C	-3.73	117.95	128.44
3	B	2	HEC	CBC-CAC-C3C	-3.72	117.96	128.44
3	A	3	HEC	C4D-ND-C1D	3.72	111.66	106.76
3	B	3	HEC	CBC-CAC-C3C	-3.71	118.00	128.44
3	D	5	HEC	CMB-C2B-C1B	-3.68	122.96	128.62
3	D	1	HEC	C4D-ND-C1D	3.67	111.60	106.76
3	D	1	HEC	CMC-C2C-C1C	-3.62	123.05	128.62
3	C	3	HEC	C4D-ND-C1D	3.59	111.49	106.76
3	D	4	HEC	CMC-C2C-C1C	-3.59	123.11	128.62
3	B	2	HEC	C4D-ND-C1D	3.58	111.48	106.76

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	HEC	CMB-C2B-C1B	-3.57	123.13	128.62
3	A	4	HEC	C4D-ND-C1D	3.57	111.46	106.76
3	C	1	HEC	CMC-C2C-C1C	-3.55	123.15	128.62
3	A	5	HEC	CBC-CAC-C3C	-3.55	118.44	128.44
3	D	1	HEC	CMB-C2B-C1B	-3.54	123.17	128.62
3	A	4	HEC	CMB-C2B-C3B	3.49	129.57	125.72
3	C	2	HEC	CMB-C2B-C1B	-3.49	123.26	128.62
3	A	1	HEC	CMB-C2B-C1B	-3.47	123.28	128.62
3	A	2	HEC	C2A-C1A-NA	-3.46	107.04	109.64
3	B	3	HEC	C4D-ND-C1D	3.44	111.29	106.76
3	D	3	HEC	CBC-CAC-C3C	-3.42	118.81	128.44
3	C	4	HEC	CMC-C2C-C1C	-3.38	123.43	128.62
3	D	5	HEC	C1D-C2D-C3D	-3.37	104.65	107.00
3	D	2	HEC	CMB-C2B-C1B	-3.36	123.45	128.62
3	C	2	HEC	CMC-C2C-C1C	-3.33	123.49	128.62
3	A	1	HEC	CBC-CAC-C3C	-3.33	119.06	128.44
3	D	3	HEC	CMC-C2C-C1C	-3.30	123.55	128.62
3	D	4	HEC	CMB-C2B-C1B	-3.27	123.59	128.62
3	A	4	HEC	CBA-CAA-C2A	-3.24	106.29	112.35
3	B	5	HEC	CMB-C2B-C1B	-3.24	123.64	128.62
3	C	1	HEC	C1D-C2D-C3D	-3.22	104.76	107.00
3	C	1	HEC	CBC-CAC-C3C	-3.22	119.39	128.44
3	C	5	HEC	CMB-C2B-C1B	-3.19	123.71	128.62
3	D	2	HEC	C1D-C2D-C3D	-3.17	104.79	107.00
3	A	5	HEC	C1D-C2D-C3D	-3.17	104.79	107.00
3	B	5	HEC	CMC-C2C-C3C	3.16	129.21	125.72
3	A	2	HEC	CMB-C2B-C1B	-3.14	123.79	128.62
3	A	4	HEC	CMC-C2C-C1C	-3.14	123.80	128.62
3	A	2	HEC	C4D-ND-C1D	3.13	110.89	106.76
3	D	3	HEC	CMB-C2B-C3B	3.10	129.14	125.72
3	C	3	HEC	CBD-CAD-C3D	-3.10	107.23	112.69
3	B	1	HEC	C4A-C3A-C2A	3.10	108.86	106.89
3	C	3	HEC	CMC-C2C-C1C	-3.09	123.87	128.62
3	D	4	HEC	C2B-C1B-NB	-3.08	107.08	109.41
3	B	5	HEC	CBC-CAC-C3C	-3.08	119.77	128.44
3	D	2	HEC	C2A-C1A-NA	-3.08	107.33	109.64
3	B	1	HEC	C4D-ND-C1D	3.07	110.81	106.76
3	C	3	HEC	CMB-C2B-C1B	-3.05	123.92	128.62
3	A	1	HEC	CMB-C2B-C3B	3.05	129.08	125.72
3	A	1	HEC	C4D-ND-C1D	3.05	110.78	106.76
3	A	5	HEC	CMB-C2B-C1B	-3.04	123.94	128.62
3	C	1	HEC	C4D-ND-C1D	3.04	110.76	106.76

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	HEC	C2A-C1A-NA	-3.01	107.38	109.64
3	C	2	HEC	CBD-CAD-C3D	-3.01	107.40	112.69
3	B	1	HEC	CMC-C2C-C1C	-3.00	124.01	128.62
3	C	2	HEC	C2A-C1A-NA	-2.99	107.39	109.64
3	C	4	HEC	C2A-C1A-NA	-2.97	107.41	109.64
3	B	2	HEC	CMC-C2C-C1C	-2.96	124.07	128.62
3	A	3	HEC	CMC-C2C-C1C	-2.96	124.07	128.62
3	B	3	HEC	C1D-C2D-C3D	-2.94	104.95	107.00
3	D	4	HEC	CMC-C2C-C3C	2.91	128.94	125.72
3	C	2	HEC	C3C-C4C-NC	-2.89	107.34	111.52
3	B	1	HEC	CMB-C2B-C1B	-2.87	124.21	128.62
3	A	3	HEC	CMB-C2B-C1B	-2.86	124.22	128.62
3	A	5	HEC	CMC-C2C-C3C	2.86	128.88	125.72
3	B	3	HEC	CMC-C2C-C1C	-2.85	124.24	128.62
3	C	3	HEC	CBA-CAA-C2A	-2.83	107.05	112.35
3	B	5	HEC	CMB-C2B-C3B	2.81	128.82	125.72
3	A	3	HEC	CBD-CAD-C3D	-2.79	107.77	112.69
3	A	1	HEC	CBA-CAA-C2A	-2.79	107.13	112.35
3	B	1	HEC	C2B-C1B-NB	-2.77	107.32	109.41
3	C	5	HEC	CMC-C2C-C3C	2.77	128.78	125.72
3	D	4	HEC	C4A-CHB-C1B	-2.77	123.83	127.47
3	D	3	HEC	CMC-C2C-C3C	2.76	128.77	125.72
3	B	4	HEC	C4B-C3B-C2B	2.75	108.43	106.68
3	D	5	HEC	CMB-C2B-C3B	2.75	128.76	125.72
3	D	1	HEC	CMB-C2B-C3B	2.74	128.75	125.72
3	A	1	HEC	CMC-C2C-C1C	-2.74	124.41	128.62
3	A	5	HEC	CBD-CAD-C3D	-2.74	107.87	112.69
3	B	2	HEC	CMB-C2B-C3B	2.74	128.74	125.72
3	B	5	HEC	CBA-CAA-C2A	-2.72	107.26	112.35
3	C	2	HEC	C2C-C1C-NC	-2.70	107.37	109.41
3	D	2	HEC	CMB-C2B-C3B	2.69	128.69	125.72
3	D	3	HEC	C4D-ND-C1D	2.69	110.31	106.76
3	D	3	HEC	C1D-C2D-C3D	-2.69	105.13	107.00
3	B	1	HEC	CBA-CAA-C2A	-2.64	107.42	112.35
3	C	1	HEC	CMB-C2B-C3B	2.63	128.62	125.72
3	D	1	HEC	CMC-C2C-C3C	2.61	128.60	125.72
3	C	3	HEC	C3B-C4B-NB	-2.61	107.75	111.52
3	A	5	HEC	C3B-C4B-NB	-2.59	107.77	111.52
3	D	3	HEC	CBA-CAA-C2A	-2.58	107.53	112.35
3	A	5	HEC	C4D-ND-C1D	2.58	110.16	106.76
3	C	4	HEC	CBA-CAA-C2A	-2.58	107.53	112.35
3	C	5	HEC	C4D-C3D-C2D	-2.58	104.25	106.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	HEC	CBD-CAD-C3D	-2.58	108.16	112.69
3	D	5	HEC	CMC-C2C-C3C	2.57	128.56	125.72
3	D	2	HEC	CMC-C2C-C1C	-2.57	124.67	128.62
3	D	4	HEC	O1A-CGA-CBA	-2.57	114.20	123.03
3	B	1	HEC	C1D-C2D-C3D	-2.56	105.22	107.00
3	A	3	HEC	CBA-CAA-C2A	-2.56	107.57	112.35
3	A	5	HEC	CMD-C2D-C3D	2.55	129.75	124.94
3	D	1	HEC	CBA-CAA-C2A	-2.55	107.58	112.35
3	C	3	HEC	C2B-C1B-NB	-2.50	107.52	109.41
3	D	4	HEC	CBD-CAD-C3D	-2.50	108.29	112.69
3	B	5	HEC	CMA-C3A-C2A	2.49	129.63	124.94
3	A	1	HEC	C2A-C1A-NA	-2.49	107.77	109.64
3	C	2	HEC	CMB-C2B-C3B	2.48	128.46	125.72
3	C	1	HEC	C2B-C1B-NB	-2.47	107.55	109.41
3	A	3	HEC	C3C-C4C-NC	-2.47	107.95	111.52
3	A	3	HEC	C2A-C1A-NA	-2.46	107.79	109.64
3	A	2	HEC	C4A-NA-C1A	2.46	109.27	105.58
3	B	2	HEC	CBD-CAD-C3D	-2.46	108.36	112.69
3	D	1	HEC	C3A-C4A-NA	-2.46	107.56	109.41
3	A	5	HEC	CBA-CAA-C2A	-2.45	107.78	112.35
3	A	3	HEC	C2B-C1B-NB	-2.44	107.57	109.41
3	C	3	HEC	CMC-C2C-C3C	2.44	128.41	125.72
3	C	4	HEC	CMC-C2C-C3C	2.43	128.40	125.72
3	C	1	HEC	CBA-CAA-C2A	-2.43	107.81	112.35
3	A	2	HEC	CBA-CAA-C2A	-2.42	107.82	112.35
3	D	4	HEC	CMA-C3A-C2A	2.42	129.51	124.94
3	D	2	HEC	C4A-NA-C1A	2.42	109.21	105.58
3	A	4	HEC	CMC-C2C-C3C	2.40	128.37	125.72
3	B	4	HEC	CMB-C2B-C1B	-2.40	124.92	128.62
3	C	5	HEC	C3B-C4B-NB	-2.40	108.05	111.52
3	B	3	HEC	C3C-C4C-NC	-2.39	108.08	111.52
3	D	4	HEC	C1D-C2D-C3D	-2.38	105.34	107.00
3	C	1	HEC	C4A-C3A-C2A	2.38	108.41	106.89
3	D	3	HEC	C3C-C4C-NC	-2.38	108.08	111.52
3	C	5	HEC	C4A-C3A-C2A	2.37	108.40	106.89
3	B	3	HEC	C2B-C1B-NB	-2.37	107.62	109.41
3	D	1	HEC	C4A-NA-C1A	2.35	109.11	105.58
3	A	2	HEC	C2C-C1C-NC	-2.35	107.64	109.41
3	D	1	HEC	C3C-C4C-NC	-2.34	108.13	111.52
3	A	2	HEC	C3A-C4A-NA	-2.35	107.64	109.41
3	B	5	HEC	C3B-C4B-NB	-2.33	108.15	111.52
3	C	5	HEC	CMB-C2B-C3B	2.33	128.30	125.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	HEC	C2B-C1B-NB	-2.33	107.65	109.41
3	A	1	HEC	C4A-CHB-C1B	-2.33	124.41	127.47
3	A	1	HEC	C3A-C4A-NA	-2.32	107.66	109.41
3	D	2	HEC	C3A-C4A-NA	-2.32	107.66	109.41
3	D	2	HEC	CBA-CAA-C2A	-2.31	108.03	112.35
3	A	2	HEC	C3C-C4C-NC	-2.29	108.21	111.52
3	D	3	HEC	CBD-CAD-C3D	-2.28	108.68	112.69
3	B	2	HEC	C2A-C1A-NA	-2.27	107.93	109.64
3	D	2	HEC	C3C-C4C-NC	-2.27	108.25	111.52
3	C	4	HEC	C3A-C4A-NA	-2.26	107.70	109.41
3	C	2	HEC	C4A-NA-C1A	2.26	108.98	105.58
3	B	4	HEC	C3C-C4C-NC	-2.26	108.26	111.52
3	D	5	HEC	CBA-CAA-C2A	-2.25	108.14	112.35
3	B	2	HEC	C4A-NA-C1A	2.25	108.96	105.58
3	B	1	HEC	C3C-C4C-NC	-2.25	108.27	111.52
3	C	4	HEC	C4A-NA-C1A	2.23	108.92	105.58
3	A	3	HEC	C3B-C4B-NB	-2.23	108.30	111.52
3	B	2	HEC	C3C-C4C-NC	-2.23	108.30	111.52
3	B	1	HEC	CMC-C2C-C3C	2.22	128.18	125.72
3	C	3	HEC	C1D-C2D-C3D	-2.22	105.45	107.00
3	A	3	HEC	CMC-C2C-C3C	2.21	128.16	125.72
3	A	1	HEC	C4A-NA-C1A	2.20	108.88	105.58
3	C	5	HEC	C4D-ND-C1D	2.19	109.64	106.76
3	C	2	HEC	C3B-C4B-NB	-2.19	108.36	111.52
3	A	1	HEC	C1D-C2D-C3D	-2.18	105.48	107.00
3	A	5	HEC	CMB-C2B-C3B	2.18	128.12	125.72
3	B	4	HEC	C2B-C1B-NB	-2.18	107.77	109.41
3	B	3	HEC	C2C-C1C-NC	-2.18	107.77	109.41
3	B	2	HEC	C3A-C4A-NA	-2.17	107.77	109.41
3	A	4	HEC	C3B-C4B-NB	-2.17	108.39	111.52
3	B	5	HEC	C4D-ND-C1D	2.17	109.62	106.76
3	A	5	HEC	C2B-C1B-NB	-2.16	107.78	109.41
3	A	1	HEC	C4D-C3D-C2D	-2.16	104.69	106.92
3	D	2	HEC	CMA-C3A-C2A	2.16	129.00	124.94
3	C	4	HEC	CMB-C2B-C1B	-2.15	125.31	128.62
3	A	2	HEC	CBD-CAD-C3D	-2.15	108.91	112.69
3	A	4	HEC	C4A-NA-C1A	2.15	108.80	105.58
3	A	1	HEC	C3B-C4B-NB	-2.15	108.42	111.52
3	D	1	HEC	C4D-C3D-C2D	-2.14	104.71	106.92
3	B	2	HEC	C2C-C1C-NC	-2.14	107.80	109.41
3	B	4	HEC	C3B-C4B-NB	-2.13	108.44	111.52
3	C	3	HEC	C2A-C1A-NA	-2.13	108.04	109.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	HEC	C3A-C4A-NA	-2.13	107.81	109.41
3	A	3	HEC	C4A-NA-C1A	2.12	108.77	105.58
3	B	4	HEC	O1A-CGA-CBA	-2.12	115.75	123.03
3	A	1	HEC	C1A-C2A-C3A	2.12	108.36	106.69
3	C	3	HEC	C4B-C3B-C2B	2.11	108.02	106.68
3	B	5	HEC	C1D-C2D-C3D	-2.10	105.54	107.00
3	B	3	HEC	C3B-C4B-NB	-2.10	108.49	111.52
3	B	1	HEC	C3A-C4A-NA	-2.08	107.84	109.41
3	C	2	HEC	C1D-C2D-C3D	-2.08	105.55	107.00
3	C	3	HEC	C3C-C4C-NC	-2.07	108.53	111.52
3	C	3	HEC	CMB-C2B-C3B	2.06	128.00	125.72
3	C	5	HEC	C2B-C1B-NB	-2.06	107.85	109.41
3	A	5	HEC	CMD-C2D-C1D	-2.06	125.45	128.62
3	B	3	HEC	CBA-CAA-C2A	-2.06	108.50	112.35
3	C	2	HEC	C4C-NC-C1C	2.04	109.45	106.76
3	D	4	HEC	C3B-C4B-NB	-2.03	108.59	111.52
3	C	3	HEC	C4A-NA-C1A	2.02	108.61	105.58
3	C	4	HEC	C2B-C1B-NB	-2.01	107.89	109.41
3	A	2	HEC	CMB-C2B-C3B	2.01	127.93	125.72

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	441/452 (97%)	-0.28	7 (1%) 68 79	7, 13, 25, 34	8 (1%)
1	B	441/452 (97%)	-0.41	3 (0%) 84 91	6, 13, 22, 28	9 (2%)
1	C	441/452 (97%)	-0.16	9 (2%) 62 72	8, 16, 28, 38	9 (2%)
1	D	441/452 (97%)	-0.38	1 (0%) 93 95	6, 12, 21, 27	8 (1%)
All	All	1764/1808 (97%)	-0.31	20 (1%) 77 86	6, 14, 24, 38	34 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	477	SER	5.1
1	C	476	LEU	3.8
1	A	111	LYS	3.2
1	C	293	ALA	3.2
1	C	477	SER	3.2
1	A	477	SER	3.1
1	C	294	GLU	2.8
1	A	476	LEU	2.7
1	C	37	THR	2.6
1	C	111	LYS	2.5
1	C	202	PHE	2.4
1	A	293	ALA	2.4
1	C	169	PRO	2.2
1	C	295	GLY	2.2
1	D	442[A]	GLN	2.1
1	B	37	THR	2.1
1	A	468[A]	GLU	2.0
1	A	472	LYS	2.0
1	A	37	THR	2.0
1	B	221	LYS	2.0

## 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(Å <sup>2</sup> )	Q<0.9
5	EDO	A	11	4/4	0.17	12.25	26,26,29,30	0
5	EDO	D	21	4/4	0.15	10.85	23,29,32,35	0
5	EDO	B	20	4/4	0.15	10.07	23,28,30,35	0
5	EDO	D	25	4/4	0.16	6.71	27,27,30,30	0
5	EDO	B	19	4/4	0.12	6.52	20,25,25,25	0
5	EDO	C	12	4/4	0.16	6.36	28,29,30,32	0
5	EDO	C	25	4/4	0.14	4.68	23,23,26,28	0
5	EDO	C	21	4/4	0.19	4.40	34,35,35,36	0
5	EDO	D	22	4/4	0.16	4.30	33,33,33,35	0
3	HEC	B	4	43/43	0.09	3.75	6,8,17,25	0
5	EDO	B	18	4/4	0.12	3.57	27,28,28,28	0
5	EDO	C	23	4/4	0.17	3.38	35,35,35,36	0
5	EDO	A	14	4/4	0.11	3.25	30,31,31,33	0
5	EDO	D	24	4/4	0.12	3.11	20,21,22,22	0
4	SO4	D	2001	5/5	0.12	2.93	33,33,34,37	0
5	EDO	D	23	4/4	0.12	2.87	24,28,30,34	0
5	EDO	A	22	4/4	0.13	2.74	20,25,28,31	0
3	HEC	C	4	43/43	0.10	2.44	9,12,20,28	0
3	HEC	A	4	43/43	0.09	2.29	5,9,18,26	0
5	EDO	A	15	4/4	0.10	2.28	27,27,27,27	0
5	EDO	B	17	4/4	0.09	2.16	28,29,30,31	0
3	HEC	D	4	43/43	0.08	1.74	5,8,16,26	0
5	EDO	D	481	4/4	0.16	1.68	34,34,35,35	0
3	HEC	C	1	43/43	0.09	1.53	9,12,13,13	0
5	EDO	A	13	4/4	0.09	1.43	22,23,25,28	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	21	4/4	0.12	1.36	32,32,32,34	0
3	HEC	A	1	43/43	0.09	1.23	7,9,10,11	0
2	CA	A	1502	1/1	0.09	1.21	28,28,28,28	0
3	HEC	D	5	43/43	0.09	1.19	7,11,22,24	0
4	SO4	A	2001	5/5	0.09	1.14	23,25,27,31	0
3	HEC	B	1	43/43	0.08	1.12	6,8,10,11	0
3	HEC	D	3	43/43	0.07	1.08	4,7,9,12	0
2	CA	A	1501	1/1	0.07	0.97	10,10,10,10	0
3	HEC	A	2	43/43	0.09	0.92	10,12,15,16	0
3	HEC	C	2	43/43	0.11	0.80	12,16,17,19	0
4	SO4	C	2001	5/5	0.12	0.74	36,36,38,39	0
3	HEC	A	5	43/43	0.07	0.66	8,10,19,24	0
3	HEC	A	3	43/43	0.07	0.64	7,9,11,13	0
3	HEC	C	5	43/43	0.09	0.61	11,14,22,30	0
5	EDO	B	481	4/4	0.09	0.56	12,14,16,18	0
3	HEC	D	1	43/43	0.07	0.44	5,7,9,10	0
5	EDO	B	16	4/4	0.07	0.40	16,17,17,19	0
3	HEC	B	5	43/43	0.08	0.30	7,10,19,23	0
5	EDO	D	482	4/4	0.07	0.27	17,18,18,19	0
5	EDO	C	481	4/4	0.07	0.23	13,16,18,19	0
3	HEC	B	3	43/43	0.07	0.23	5,7,10,11	0
3	HEC	B	2	43/43	0.07	0.22	7,9,12,12	0
5	EDO	A	481	4/4	0.08	0.11	11,12,14,17	0
3	HEC	C	3	43/43	0.07	0.08	9,11,14,15	0
2	CA	C	1501	1/1	0.08	0.01	11,11,11,11	0
2	CA	D	1502	1/1	0.10	-0.02	16,16,16,16	1
3	HEC	D	2	43/43	0.07	-0.16	7,10,12,14	0
5	EDO	D	6	4/4	0.07	-0.37	12,13,15,18	0
2	CA	C	1502	1/1	0.07	-0.40	31,31,31,31	0
4	SO4	B	2001	5/5	0.07	-0.54	21,21,25,27	0
2	CA	B	1502	1/1	0.05	-0.87	25,25,25,25	0
2	CA	D	1501	1/1	0.07	-0.91	8,8,8,8	0
5	EDO	C	22	4/4	0.06	-1.15	18,18,20,21	0
5	EDO	A	20	4/4	0.07	-1.56	18,19,19,20	0
2	CA	B	1501	1/1	0.04	-4.09	10,10,10,10	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.