



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:29 AM GMT

PDB ID : 3L1T
Title : E. coli NrfA sulfite ocmplex
Authors : Clarke, T.A.; Hemmings, A.M.; Butt, J.N.
Deposited on : 2009-12-14
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

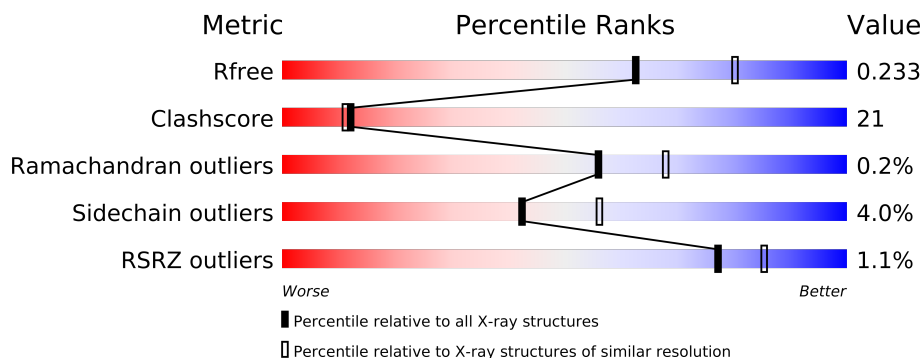
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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
2	CA	B	2	-	X
2	CA	C	2	-	X
4	SO3	B	482	-	X
5	EDO	B	483	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	C	482	-	X
5	EDO	C	483	-	X
5	EDO	C	484	-	X
5	EDO	C	7	-	X
5	EDO	C	9	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15858 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.

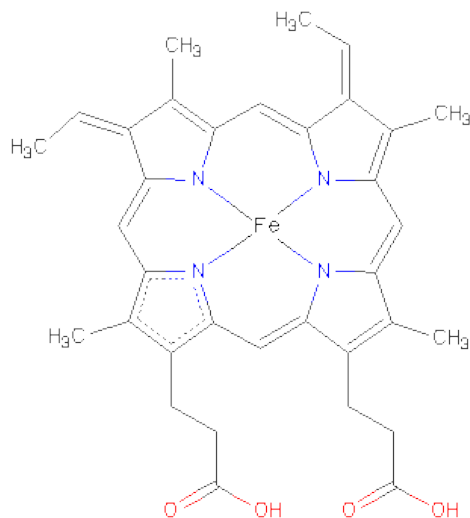
- Molecule 1 is a protein called Cytochrome c-552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	1	1	0
			3485	2183	620	660	22			
1	B	441	Total	C	N	O	S	0	2	0
			3491	2188	622	659	22			
1	C	441	Total	C	N	O	S	1	4	0
			3502	2195	621	664	22			
1	D	441	Total	C	N	O	S	0	2	0
			3487	2185	619	661	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: C₃₄H₃₄FeN₄O₄).



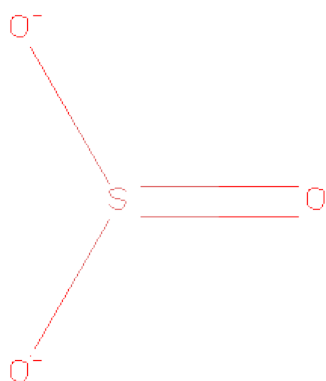
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B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

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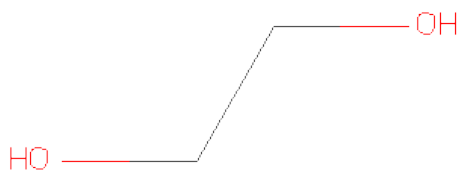
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 4 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O S		
			4	3 1	0	0
4	B	1	Total	O S		
			4	3 1	0	0
4	B	1	Total	O S		
			4	3 1	0	0
4	C	1	Total	O S		
			4	3 1	0	0
4	D	1	Total	O S		
			4	3 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

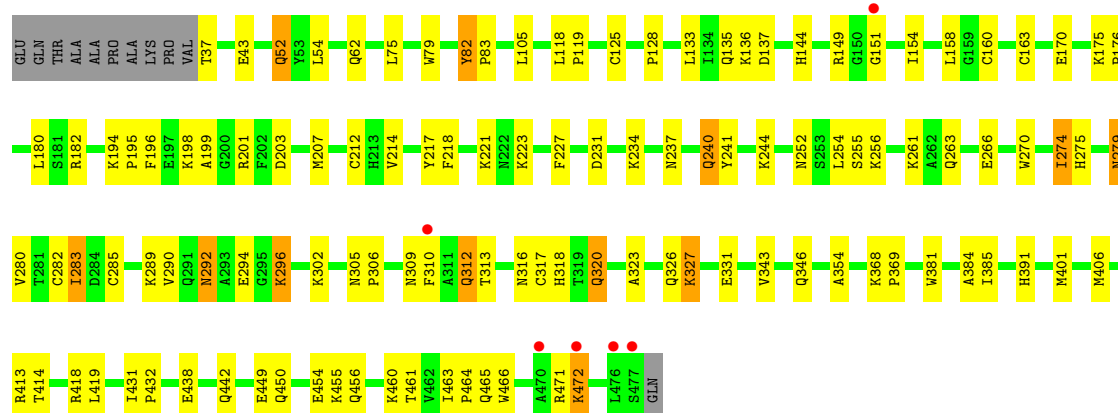
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	222	Total 222	O 222	0	0
6	B	291	Total 291	O 291	0	0
6	C	292	Total 292	O 292	0	0
6	D	152	Total 152	O 152	0	0

3 Residue-property plots

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

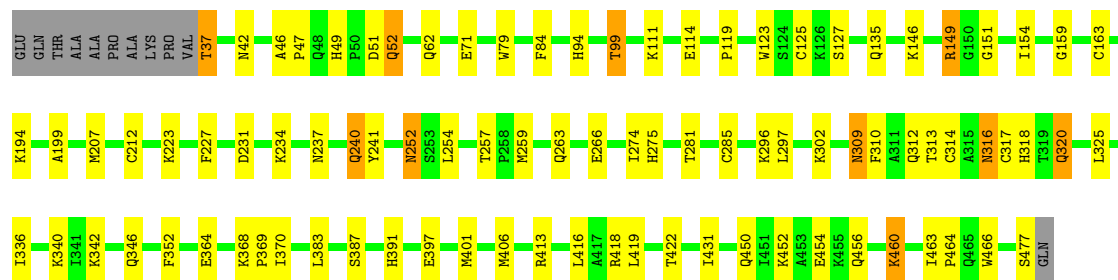
• Molecule 1: Cytochrome c-552

Chain A: 



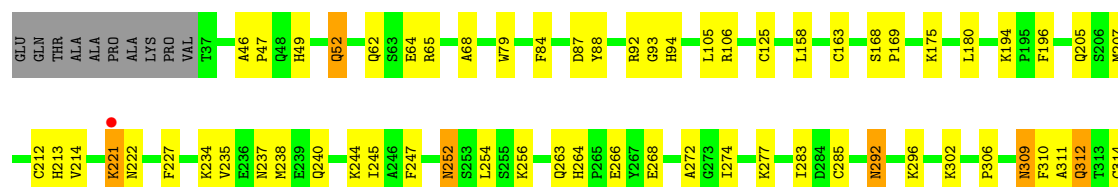
• Molecule 1: Cytochrome c-552

Chain B: 



• Molecule 1: Cytochrome c-552

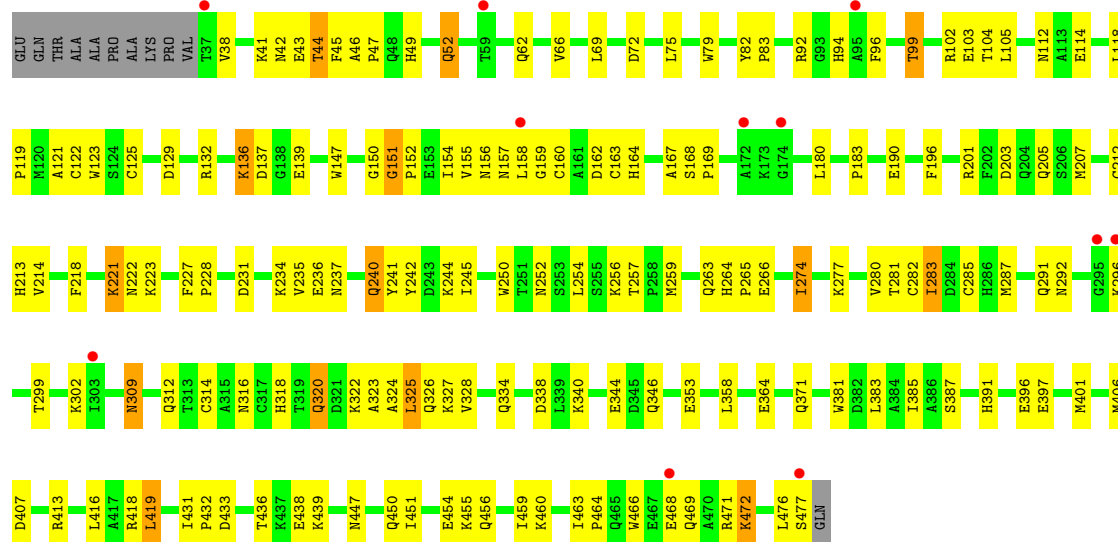
Chain C: 





• 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, α , β , γ	90.52Å 82.23Å 142.17Å 90.00° 101.08° 90.00°	Depositor
Resolution (Å)	50.36 – 2.30 50.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.36-2.30) 99.7 (50.36-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.177 , 0.238 0.176 , 0.233	Depositor DCC
R_{free} test set	4553 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 90970 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15858	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: SO3, CA, EDO, 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	0.50	1/3569 (0.0%)	0.58	0/4827
1	B	0.52	0/3578	0.60	0/4838
1	C	0.53	0/3595	0.59	0/4861
1	D	0.41	0/3577	0.52	0/4838
All	All	0.49	1/14319 (0.0%)	0.57	0/19364

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	442	GLN	CD-NE2	-6.21	1.17	1.32

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	3485	0	3374	139	0
1	B	3491	0	3389	115	0
1	C	3502	0	3396	122	0
1	D	3487	0	3378	189	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	A	215	0	155	53	0
3	B	215	0	155	42	0
3	C	215	0	155	44	0
3	D	215	0	155	52	0
4	A	4	0	0	0	0
4	B	8	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	8	0	12	0	0
5	B	8	0	12	10	0
5	C	24	0	36	8	0
5	D	8	0	12	8	0
6	A	222	0	0	16	0
6	B	291	0	0	22	0
6	C	292	0	0	18	0
6	D	152	0	0	25	0
All	All	15858	0	14229	622	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 21.

All (622) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:296:LYS:HE2	5:B:483:EDO:C1	1.27	1.57
1:B:296:LYS:CE	5:B:483:EDO:H11	1.29	1.53
1:C:125:CYS:SG	3:C:479:HEC:CAC	2.02	1.47
1:A:160:CYS:SG	3:A:480:HEC:CAB	2.02	1.47
1:D:122:CYS:SG	3:D:479:HEC:CAB	2.01	1.47
1:D:212:CYS:SG	3:D:3:HEC:CAC	2.03	1.46
1:A:125:CYS:SG	3:A:479:HEC:CAC	2.08	1.41
1:B:125:CYS:SG	3:B:479:HEC:CAC	2.07	1.40
1:A:198:LYS:HE2	1:C:65:ARG:NH1	1.31	1.40
1:D:52:GLN:H	1:D:52:GLN:NE2	1.21	1.36
1:B:212:CYS:SG	3:B:3:HEC:CAC	2.14	1.35
1:D:125:CYS:SG	3:D:479:HEC:CAC	2.13	1.34
1:A:456:GLN:NE2	1:A:460:LYS:HE3	1.41	1.34
1:B:163:CYS:SG	3:B:480:HEC:CAC	2.18	1.31
1:C:212:CYS:SG	3:C:3:HEC:CAC	2.18	1.31

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:314:CYS:SG	3:D:5:HEC:CAB	2.19	1.31
1:A:317:CYS:SG	3:A:5:HEC:CAC	2.19	1.29
1:B:285:CYS:SG	3:B:4:HEC:CAC	2.19	1.28
1:A:163:CYS:SG	3:A:480:HEC:CAC	2.22	1.27
1:A:212:CYS:SG	3:A:3:HEC:CAC	2.27	1.23
1:C:285:CYS:SG	3:C:4:HEC:CAC	2.29	1.20
1:A:285:CYS:SG	3:A:4:HEC:CAC	2.29	1.20
1:B:317:CYS:SG	3:B:5:HEC:CAC	2.30	1.19
1:A:198:LYS:CE	1:C:65:ARG:NH1	2.07	1.16
1:A:52:GLN:H	1:A:52:GLN:NE2	1.45	1.15
1:A:456:GLN:HE21	1:A:460:LYS:CE	1.61	1.13
1:C:221:LYS:HE3	1:C:221:LYS:N	1.64	1.13
1:D:163:CYS:SG	3:D:480:HEC:CAC	2.37	1.13
1:D:285:CYS:SG	3:D:4:HEC:CAC	2.37	1.13
3:A:5:HEC:HMB1	3:A:5:HEC:HBB3	1.28	1.10
1:C:317:CYS:SG	3:C:5:HEC:CAC	2.39	1.10
1:C:163:CYS:SG	3:C:480:HEC:CAC	2.40	1.09
1:C:221:LYS:HE3	1:C:221:LYS:H	0.97	1.08
3:D:5:HEC:HBB3	3:D:5:HEC:HMB1	1.34	1.05
1:D:52:GLN:N	1:D:52:GLN:NE2	2.05	1.04
1:D:49:HIS:HD2	6:D:643:HOH:O	1.41	1.04
3:D:480:HEC:HBC3	3:D:480:HEC:HMC1	1.42	1.02
1:D:125:CYS:SG	3:D:479:HEC:C3C	2.48	1.01
1:D:52:GLN:N	1:D:52:GLN:HE21	1.59	1.00
1:B:309:ASN:HB3	6:B:543:HOH:O	1.61	0.99
1:C:125:CYS:SG	3:C:479:HEC:C3C	2.50	0.99
1:C:221:LYS:CE	1:C:221:LYS:H	1.76	0.97
3:C:4:HEC:HMC1	3:C:4:HEC:HBC3	1.43	0.97
1:B:309:ASN:CB	6:B:543:HOH:O	2.12	0.97
1:B:212:CYS:SG	3:B:3:HEC:HAC	2.02	0.97
1:C:309:ASN:ND2	1:C:312:GLN:HE22	1.62	0.97
3:D:479:HEC:HMC1	3:D:479:HEC:CBC	1.95	0.96
1:C:345:ASP:OD1	5:C:9:EDO:H11	1.65	0.96
1:D:38:VAL:HG11	1:D:132:ARG:HA	1.45	0.95
3:B:480:HEC:HMC1	3:B:480:HEC:HBC3	1.49	0.94
3:D:480:HEC:HMC1	3:D:480:HEC:CBC	1.99	0.93
3:D:479:HEC:HBC3	3:D:479:HEC:HMC1	1.45	0.93
1:C:320:GLN:HG2	5:C:484:EDO:H22	1.50	0.93
1:A:198:LYS:HE2	1:C:65:ARG:HH12	1.27	0.93
1:A:52:GLN:N	1:A:52:GLN:HE21	1.67	0.92
1:A:125:CYS:SG	3:A:479:HEC:C3C	2.58	0.92
3:B:5:HEC:HMB1	3:B:5:HEC:HBB3	1.52	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:436:THR:OG1	1:D:439:LYS:HG3	1.70	0.91
1:C:125:CYS:SG	3:C:479:HEC:HAC	2.08	0.91
1:C:317:CYS:SG	3:C:5:HEC:HBC3	2.11	0.91
3:A:480:HEC:HMB1	3:A:480:HEC:HBB3	1.53	0.91
1:A:125:CYS:SG	3:A:479:HEC:HAC	2.11	0.91
1:C:317:CYS:SG	3:C:5:HEC:CBC	2.59	0.90
1:B:125:CYS:SG	3:B:479:HEC:CBC	2.58	0.90
1:D:125:CYS:SG	3:D:479:HEC:CBC	2.58	0.90
1:B:125:CYS:SG	3:B:479:HEC:C3C	2.60	0.89
1:A:198:LYS:HE2	1:C:65:ARG:HH11	1.29	0.89
1:B:37:THR:HA	6:B:924:HOH:O	1.73	0.89
1:D:52:GLN:H	1:D:52:GLN:HE21	0.90	0.89
1:C:309:ASN:ND2	1:C:312:GLN:NE2	2.21	0.89
1:A:212:CYS:SG	3:A:3:HEC:CBC	2.60	0.88
1:C:391:HIS:HE1	3:C:4:HEC:O2D	1.55	0.88
3:A:479:HEC:HMC1	3:A:479:HEC:HBC3	1.54	0.88
1:D:221:LYS:H	1:D:221:LYS:HZ2	1.17	0.88
3:A:5:HEC:HMB1	3:A:5:HEC:CBB	2.03	0.88
3:C:3:HEC:HBC3	3:C:3:HEC:HMC1	1.56	0.88
3:A:4:HEC:HMC1	3:A:4:HEC:HBC3	1.56	0.88
3:D:5:HEC:CBB	3:D:5:HEC:HMB1	2.05	0.87
1:A:292:ASN:C	1:A:292:ASN:HD22	1.75	0.86
1:A:52:GLN:H	1:A:52:GLN:HE21	0.91	0.86
3:A:3:HEC:HMC1	3:A:3:HEC:HBC3	1.57	0.86
1:D:472:LYS:NZ	1:D:472:LYS:HB3	1.89	0.86
1:B:99:THR:HG22	6:B:506:HOH:O	1.77	0.85
1:A:198:LYS:CE	1:C:65:ARG:HH12	1.80	0.84
3:C:4:HEC:HMC1	3:C:4:HEC:CBC	2.06	0.84
3:B:4:HEC:HBC3	3:B:4:HEC:HMC1	1.59	0.84
1:B:234:LYS:HE2	6:B:876:HOH:O	1.75	0.84
1:A:163:CYS:SG	3:A:480:HEC:CBC	2.65	0.84
1:C:296:LYS:CE	6:C:534:HOH:O	2.26	0.84
1:A:317:CYS:SG	3:A:5:HEC:C3C	2.65	0.83
1:A:317:CYS:SG	3:A:5:HEC:HAC	2.18	0.83
1:B:163:CYS:SG	3:B:480:HEC:HAC	2.18	0.83
1:D:364:GLU:HG2	6:D:531:HOH:O	1.77	0.83
1:A:292:ASN:ND2	1:A:296:LYS:H	1.77	0.83
1:D:212:CYS:SG	3:D:3:HEC:C3C	2.66	0.83
3:A:480:HEC:HBC3	3:A:480:HEC:HMC1	1.60	0.82
3:D:4:HEC:HBC3	3:D:4:HEC:HMC1	1.61	0.81
1:B:312:GLN:HG3	6:B:638:HOH:O	1.80	0.81
1:D:364:GLU:CG	6:D:531:HOH:O	2.26	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:52:GLN:N	1:A:52:GLN:NE2	2.28	0.81
1:C:221:LYS:HD2	6:C:674:HOH:O	1.80	0.80
1:C:296:LYS:HE2	6:C:534:HOH:O	1.82	0.80
1:B:364:GLU:HG3	6:B:981:HOH:O	1.81	0.79
1:D:125:CYS:SG	3:D:479:HEC:HBC3	2.23	0.79
1:D:231:ASP:OD2	1:D:240:GLN:NE2	2.16	0.78
3:A:480:HEC:HMC1	3:A:480:HEC:CBC	2.13	0.78
1:B:37:THR:CA	6:B:924:HOH:O	2.30	0.78
1:B:317:CYS:SG	3:B:5:HEC:CBC	2.72	0.77
1:D:256:LYS:HG3	1:D:358:LEU:HD13	1.67	0.77
1:C:212:CYS:SG	3:C:3:HEC:CBC	2.73	0.77
1:B:163:CYS:SG	3:B:480:HEC:C3C	2.74	0.76
1:B:346:GLN:NE2	1:B:413:ARG:HH11	1.83	0.76
1:B:312:GLN:CD	6:B:638:HOH:O	2.23	0.76
1:D:327:LYS:CE	6:D:1034:HOH:O	2.33	0.76
1:A:212:CYS:SG	3:A:3:HEC:HBC3	2.25	0.76
1:B:52:GLN:NE2	1:B:52:GLN:H	1.84	0.76
3:C:5:HEC:HBB3	3:C:5:HEC:HMB1	1.66	0.75
1:D:334:GLN:HE21	1:D:338[B]:ASP:CG	1.89	0.75
1:A:320:GLN:H	1:A:320:GLN:HE21	1.31	0.75
1:D:314:CYS:SG	3:D:5:HEC:CBB	2.75	0.74
1:C:212:CYS:SG	3:C:3:HEC:C3C	2.75	0.74
1:D:314:CYS:SG	3:D:5:HEC:HAB	2.22	0.74
1:B:352:PHE:CD2	1:B:431:ILE:HD12	2.22	0.74
1:D:256:LYS:HG3	1:D:358:LEU:CD1	2.18	0.74
1:B:296:LYS:CD	5:B:483:EDO:H11	2.17	0.74
1:B:296:LYS:HE2	5:B:483:EDO:C2	2.15	0.74
1:B:391:HIS:HE1	3:B:4:HEC:O2D	1.71	0.74
1:C:163:CYS:SG	3:C:480:HEC:CBC	2.75	0.74
1:D:292:ASN:HD21	1:D:296:LYS:HB2	1.52	0.73
3:C:479:HEC:HBC3	3:C:479:HEC:HMC1	1.69	0.73
1:B:285:CYS:SG	3:B:4:HEC:CBC	2.76	0.73
1:A:62:GLN:HE21	1:A:302:LYS:NZ	1.87	0.73
1:C:328:VAL:HG21	5:C:484:EDO:H12	1.70	0.73
1:D:334:GLN:NE2	1:D:338[B]:ASP:OD1	2.22	0.73
1:A:163:CYS:SG	3:A:480:HEC:C3C	2.77	0.73
1:A:456:GLN:HE21	1:A:460:LYS:HE3	0.67	0.73
3:B:5:HEC:HBC3	3:B:5:HEC:HMC1	1.70	0.72
1:D:221:LYS:H	1:D:221:LYS:NZ	1.86	0.72
1:D:240:GLN:HB3	6:D:540:HOH:O	1.88	0.72
1:A:198:LYS:CE	1:C:65:ARG:HH11	1.89	0.72
1:B:285:CYS:SG	3:B:4:HEC:HAC	2.27	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:CYS:SG	3:A:480:HEC:C3B	2.77	0.71
1:B:312:GLN:CG	6:B:638:HOH:O	2.37	0.71
1:A:449:GLU:HG3	6:A:770:HOH:O	1.90	0.71
1:D:45:PHE:HA	6:D:757:HOH:O	1.90	0.71
5:C:483:EDO:H21	6:C:544:HOH:O	1.90	0.71
1:D:69:LEU:HD12	6:D:499:HOH:O	1.91	0.71
1:D:163:CYS:SG	3:D:480:HEC:CBC	2.78	0.71
1:B:99:THR:CG2	6:B:506:HOH:O	2.35	0.71
1:D:122:CYS:SG	3:D:479:HEC:CBB	2.79	0.71
1:D:201:ARG:O	1:D:205:GLN:HG3	1.89	0.71
1:D:158:LEU:HG	3:D:3:HEC:HBC2	1.73	0.71
1:A:292:ASN:HD21	1:A:296:LYS:H	1.36	0.71
1:D:240:GLN:CB	6:D:540:HOH:O	2.39	0.71
1:B:285:CYS:SG	3:B:4:HEC:C3C	2.79	0.70
1:D:221:LYS:N	1:D:221:LYS:NZ	2.40	0.70
3:D:5:HEC:HBC3	3:D:5:HEC:HMC1	1.73	0.70
1:B:37:THR:HG22	1:B:135:GLN:OE1	1.92	0.70
1:D:163:CYS:SG	3:D:480:HEC:C3C	2.80	0.70
1:D:92:ARG:NH2	1:D:96:PHE:CD1	2.59	0.70
1:A:231:ASP:OD2	1:A:240:GLN:NE2	2.24	0.70
1:B:125:CYS:SG	3:B:479:HEC:HAC	2.28	0.70
1:B:212:CYS:SG	3:B:3:HEC:C3C	2.78	0.70
1:C:175:LYS:HE3	6:C:563:HOH:O	1.91	0.70
1:B:125:CYS:SG	3:B:479:HEC:HBC3	2.31	0.70
1:C:212:CYS:SG	3:C:3:HEC:HAC	2.30	0.70
1:D:456:GLN:HE21	1:D:456:GLN:HA	1.57	0.69
1:C:368:LYS:HB3	1:C:369:PRO:HD3	1.73	0.69
1:D:328:VAL:CG2	5:D:482:EDO:H21	2.22	0.69
1:C:125:CYS:SG	3:C:479:HEC:CBC	2.80	0.69
1:A:163:CYS:SG	3:A:480:HEC:HBC3	2.32	0.69
1:C:62:GLN:HE21	1:C:302:LYS:HZ3	1.39	0.69
3:B:480:HEC:HMC1	3:B:480:HEC:CBC	2.23	0.69
3:B:4:HEC:CBC	3:B:4:HEC:HMC1	2.23	0.69
1:C:52:GLN:H	1:C:52:GLN:NE2	1.91	0.68
3:A:3:HEC:HMC1	3:A:3:HEC:CBC	2.22	0.68
1:D:203:ASP:O	1:D:207:MET:HG3	1.93	0.68
1:B:199:ALA:HA	6:B:600:HOH:O	1.93	0.67
1:D:285:CYS:SG	3:D:4:HEC:HAC	2.34	0.67
1:A:419:LEU:HA	6:A:648:HOH:O	1.94	0.67
1:C:163:CYS:SG	3:C:480:HEC:HBC3	2.34	0.67
1:D:292:ASN:ND2	1:D:296:LYS:HB2	2.10	0.67
1:D:418:ARG:HD3	6:D:490:HOH:O	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:43:GLU:N	1:D:43:GLU:OE2	2.21	0.66
1:B:146:LYS:O	1:B:149:ARG:HB2	1.94	0.66
1:C:87:ASP:HB2	1:C:105:LEU:HB2	1.76	0.66
1:D:391:HIS:HD2	6:D:804:HOH:O	1.79	0.66
1:C:391:HIS:CE1	3:C:4:HEC:O2D	2.45	0.66
1:C:163:CYS:SG	3:C:480:HEC:C3C	2.84	0.66
1:B:317:CYS:SG	3:B:5:HEC:C3C	2.83	0.66
1:C:345:ASP:CG	5:C:9:EDO:H11	2.16	0.66
1:A:62:GLN:HE21	1:A:302:LYS:HZ3	1.42	0.65
1:C:62:GLN:HE21	1:C:302:LYS:NZ	1.94	0.65
1:A:252:ASN:HD21	1:A:254:LEU:HB2	1.60	0.65
1:B:52:GLN:HE21	1:B:52:GLN:H	1.44	0.65
3:D:479:HEC:CBC	3:D:479:HEC:CMC	2.73	0.65
1:C:285:CYS:SG	3:C:4:HEC:C3C	2.85	0.65
1:A:320:GLN:NE2	1:A:320:GLN:H	1.95	0.65
1:D:328:VAL:CG2	5:D:482:EDO:C2	2.75	0.65
1:A:212:CYS:SG	3:A:3:HEC:C3C	2.84	0.64
1:A:431:ILE:HG22	1:A:432:PRO:O	1.97	0.64
1:D:123:TRP:CG	1:D:154:ILE:HD13	2.33	0.64
3:A:5:HEC:CMB	3:A:5:HEC:HBB3	2.17	0.64
3:A:4:HEC:HMB1	3:A:4:HEC:HBB3	1.79	0.64
1:C:277[B]:LYS:NZ	6:C:629:HOH:O	2.21	0.64
1:D:324:ALA:HB1	5:D:482:EDO:H11	1.80	0.64
1:B:49:HIS:HE1	6:B:572:HOH:O	1.81	0.64
1:A:256:LYS:HD2	6:A:849:HOH:O	1.96	0.64
1:C:49:HIS:HD2	6:C:656:HOH:O	1.81	0.64
3:A:5:HEC:HMC1	3:A:5:HEC:HBC3	1.81	0.63
6:A:581:HOH:O	1:B:342:LYS:HE3	1.98	0.63
1:C:205:GLN:HB3	1:C:283:ILE:HD13	1.79	0.63
1:D:320:GLN:H	1:D:320:GLN:HE21	1.45	0.63
1:C:345:ASP:OD1	5:C:9:EDO:C1	2.43	0.63
3:B:480:HEC:HMB1	3:B:480:HEC:HBB3	1.79	0.63
1:C:309:ASN:HD21	1:C:312:GLN:HE22	1.46	0.63
1:B:320:GLN:H	1:B:320:GLN:HE21	1.47	0.62
1:D:285:CYS:SG	3:D:4:HEC:C3C	2.87	0.62
1:A:285:CYS:SG	3:A:4:HEC:C3C	2.87	0.62
1:A:285:CYS:SG	3:A:4:HEC:CBC	2.87	0.62
3:A:480:HEC:HBB3	3:A:480:HEC:CMB	2.28	0.62
1:B:234:LYS:H	1:B:237:ASN:HD22	1.47	0.62
1:D:450:GLN:O	1:D:454:GLU:HG3	1.99	0.62
1:C:318:HIS:HB3	1:C:320:GLN:NE2	2.14	0.62
1:D:235:VAL:HG13	1:D:236:GLU:N	2.15	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:383:LEU:HD23	1:D:401:MET:HE3	1.82	0.62
1:D:455:LYS:O	1:D:459:ILE:HG13	2.00	0.62
1:C:285:CYS:SG	3:C:4:HEC:HAC	2.34	0.62
1:C:317:CYS:SG	3:C:5:HEC:C3C	2.87	0.61
1:A:450:GLN:O	1:A:454:GLU:HG3	2.01	0.61
3:A:479:HEC:HMC1	3:A:479:HEC:CBC	2.27	0.61
3:A:4:HEC:HMC1	3:A:4:HEC:CBC	2.29	0.61
1:B:252:ASN:ND2	1:B:254:LEU:H	1.97	0.61
1:A:125:CYS:SG	3:A:479:HEC:CBC	2.86	0.61
1:B:317:CYS:SG	3:B:5:HEC:HBC3	2.39	0.61
1:D:472:LYS:HB3	1:D:472:LYS:HZ2	1.61	0.61
1:C:406:MET:CE	1:D:407:ASP:HB2	2.30	0.61
1:D:163:CYS:SG	3:D:480:HEC:HBC3	2.40	0.61
1:B:352:PHE:HB2	1:B:431:ILE:HD11	1.83	0.60
1:C:52:GLN:H	1:C:52:GLN:HE21	1.48	0.60
1:A:285:CYS:SG	3:A:4:HEC:HAC	2.36	0.60
1:B:317:CYS:HG	3:B:5:HEC:CAC	2.12	0.60
3:B:5:HEC:CBC	3:B:5:HEC:HMC1	2.30	0.60
1:A:292:ASN:C	1:A:292:ASN:ND2	2.49	0.60
1:D:314:CYS:SG	3:D:5:HEC:C3B	2.88	0.60
3:C:480:HEC:HMC1	3:C:480:HEC:HBC3	1.82	0.60
1:D:221:LYS:N	1:D:221:LYS:HZ2	1.92	0.60
1:D:327:LYS:HE3	6:D:1034:HOH:O	2.01	0.60
1:D:456:GLN:NE2	1:D:456:GLN:HA	2.17	0.60
1:B:123:TRP:CG	1:B:154:ILE:HD13	2.37	0.60
1:A:327:LYS:HE3	1:A:331[B]:GLU:OE2	2.02	0.60
1:D:136:LYS:HG2	1:D:137:ASP:OD1	2.02	0.60
1:D:38:VAL:CG1	1:D:132:ARG:HA	2.25	0.60
1:A:214:VAL:HG21	1:A:227:PHE:CZ	2.37	0.60
1:C:320:GLN:NE2	6:C:933:HOH:O	2.30	0.60
1:C:320:GLN:H	1:C:320:GLN:NE2	1.99	0.59
1:C:285:CYS:SG	3:C:4:HEC:CBC	2.91	0.59
3:C:4:HEC:CMC	3:C:4:HEC:CBC	2.80	0.59
1:A:346:GLN:NE2	1:A:413:ARG:HH11	2.00	0.59
1:D:391:HIS:HE1	3:D:4:HEC:O2D	1.85	0.59
1:B:352:PHE:CB	1:B:431:ILE:HD11	2.31	0.59
1:B:346:GLN:HE22	1:B:413:ARG:HH11	1.49	0.59
1:A:176:PRO:HD2	6:A:513:HOH:O	2.01	0.59
1:D:476:LEU:HG	1:D:477:SER:H	1.68	0.59
3:B:5:HEC:HBB3	3:B:5:HEC:CMB	2.29	0.59
1:D:62:GLN:HE21	1:D:302:LYS:NZ	2.01	0.59
1:C:296:LYS:HD3	6:C:534:HOH:O	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:433:ASP:OD1	1:D:439:LYS:HD3	2.03	0.58
1:A:252:ASN:ND2	1:A:254:LEU:HB2	2.17	0.58
1:D:320:GLN:H	1:D:320:GLN:NE2	2.01	0.58
1:A:280:VAL:HG13	3:A:5:HEC:HBC2	1.85	0.57
1:D:119:PRO:HG3	1:D:223:LYS:HD2	1.86	0.57
1:C:406:MET:HE3	1:D:407:ASP:HB2	1.85	0.57
1:B:194:LYS:HB3	1:B:207:MET:HE1	1.86	0.57
3:B:5:HEC:HBD2	6:B:627:HOH:O	2.04	0.57
1:A:182:ARG:HG3	6:A:584:HOH:O	2.03	0.57
1:A:201:ARG:HA	6:A:905:HOH:O	2.03	0.57
1:A:406:MET:HG2	1:B:406:MET:HB3	1.86	0.57
3:C:3:HEC:HMC1	3:C:3:HEC:CBC	2.31	0.57
3:B:4:HEC:HMB1	3:B:4:HEC:HBB3	1.85	0.57
1:A:318:HIS:HB3	1:A:320:GLN:NE2	2.19	0.57
1:B:320:GLN:H	1:B:320:GLN:NE2	2.03	0.57
1:D:41:LYS:HA	1:D:156:ASN:OD1	2.05	0.57
1:D:257:THR:O	1:D:259:MET:HG2	2.05	0.56
3:C:480:HEC:HMC1	3:C:480:HEC:CBC	2.35	0.56
1:B:364:GLU:N	6:B:895:HOH:O	2.38	0.56
1:D:235:VAL:HB	1:D:401:MET:HE3	1.87	0.56
3:C:4:HEC:HMB1	3:C:4:HEC:HBB3	1.88	0.56
1:D:312:GLN:HA	1:D:312:GLN:OE1	2.04	0.56
1:A:52:GLN:HG2	3:A:480:HEC:C4A	2.36	0.56
1:B:391:HIS:CE1	3:B:4:HEC:O2D	2.58	0.56
1:A:256:LYS:CD	6:A:849:HOH:O	2.53	0.56
1:A:418:ARG:HD3	6:A:585:HOH:O	2.04	0.56
1:C:296:LYS:CD	6:C:534:HOH:O	2.53	0.56
1:B:163:CYS:SG	3:B:480:HEC:CBC	2.91	0.56
1:C:194:LYS:HB3	1:C:207:MET:HE1	1.87	0.56
1:C:312:GLN:H	1:C:312:GLN:NE2	2.04	0.55
1:A:43:GLU:CD	1:A:43:GLU:H	2.10	0.55
1:D:151:GLY:HA3	1:D:466:TRP:CE2	2.41	0.55
1:C:431:ILE:HG22	1:C:432:PRO:O	2.07	0.55
1:B:212:CYS:SG	3:B:3:HEC:CBC	2.93	0.55
3:A:5:HEC:CBB	3:A:5:HEC:CMB	2.79	0.55
1:A:290:VAL:HG12	1:A:312:GLN:HG2	1.89	0.55
3:B:3:HEC:HBC3	3:B:3:HEC:HMC1	1.89	0.54
1:A:456:GLN:NE2	1:A:460:LYS:CE	2.37	0.54
1:A:133:LEU:HD12	1:A:154:ILE:HD11	1.89	0.54
1:B:194:LYS:HB3	1:B:207:MET:CE	2.38	0.54
1:B:296:LYS:NZ	5:B:483:EDO:H22	2.21	0.54
3:B:479:HEC:HBC3	3:B:479:HEC:HMC1	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:292:ASN:C	1:C:292:ASN:HD22	2.11	0.54
1:B:252:ASN:HD22	1:B:254:LEU:H	1.55	0.54
1:D:281:THR:HG22	6:D:500:HOH:O	2.08	0.54
1:C:320:GLN:H	1:C:320:GLN:HE21	1.55	0.54
1:C:240:GLN:O	1:C:244:LYS:HG3	2.07	0.54
1:B:383:LEU:HD23	1:B:401:MET:HE3	1.90	0.54
1:D:43:GLU:O	1:D:45:PHE:N	2.41	0.53
1:D:456:GLN:O	1:D:460:LYS:HG2	2.08	0.53
1:A:263:GLN:NE2	6:A:812:HOH:O	2.41	0.53
1:C:292:ASN:HD21	1:C:296:LYS:H	1.55	0.53
1:A:144:HIS:HD2	6:A:597:HOH:O	1.92	0.53
3:D:479:HEC:HMB1	3:D:479:HEC:HBB3	1.90	0.53
3:C:5:HEC:CBC	3:C:5:HEC:HMC1	2.39	0.53
1:D:364:GLU:CD	6:D:531:HOH:O	2.46	0.53
1:B:309:ASN:HB2	6:B:543:HOH:O	1.95	0.53
1:D:472:LYS:HB3	1:D:472:LYS:HZ3	1.71	0.53
3:D:479:HEC:HMC1	3:D:479:HEC:HBC2	1.83	0.53
1:A:198:LYS:HD2	6:A:778:HOH:O	2.08	0.53
1:D:157:ASN:O	1:D:158:LEU:C	2.47	0.53
1:C:212:CYS:SG	3:C:3:HEC:HBC3	2.49	0.52
1:A:151:GLY:HA3	1:A:466:TRP:CD2	2.44	0.52
1:D:328:VAL:HG21	5:D:482:EDO:H21	1.91	0.52
1:A:343:VAL:HG22	1:A:406:MET:HE2	1.91	0.52
1:A:194:LYS:HB3	1:A:207:MET:CE	2.39	0.52
1:D:381:TRP:O	1:D:385:ILE:HG13	2.10	0.52
1:D:94:HIS:CD2	3:D:3:HEC:ND	2.77	0.52
1:A:463:ILE:HB	1:A:464:PRO:HD3	1.90	0.52
1:C:463:ILE:HB	1:C:464:PRO:HD3	1.92	0.52
1:B:234:LYS:H	1:B:237:ASN:ND2	2.06	0.52
1:A:151:GLY:HA3	1:A:466:TRP:CE2	2.44	0.52
3:D:480:HEC:CMC	3:D:480:HEC:CBC	2.76	0.52
3:D:5:HEC:HBB3	3:D:5:HEC:CMB	2.23	0.51
1:D:42:ASN:ND2	6:D:530:HOH:O	2.42	0.51
1:B:37:THR:HA	1:B:135:GLN:HE22	1.76	0.51
1:B:368:LYS:HB3	1:B:369:PRO:HD3	1.92	0.51
1:A:343:VAL:HG22	1:A:406:MET:CE	2.40	0.51
1:C:49:HIS:HE1	6:C:709:HOH:O	1.93	0.51
1:D:235:VAL:CG1	1:D:236:GLU:N	2.73	0.51
1:A:461:THR:O	1:A:465:GLN:HG3	2.10	0.51
1:C:346:GLN:NE2	1:C:413:ARG:HH11	2.08	0.51
1:C:252:ASN:ND2	1:C:254:LEU:H	2.09	0.51
3:D:4:HEC:HMC1	3:D:4:HEC:CBC	2.38	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:218:PHE:HB2	6:A:578:HOH:O	2.11	0.51
1:D:265:PRO:HD2	1:D:387:SER:HB2	1.93	0.51
3:D:479:HEC:HBC3	3:D:479:HEC:CMC	2.31	0.51
1:B:94:HIS:CD2	3:B:3:HEC:ND	2.79	0.51
1:D:346:GLN:NE2	1:D:413:ARG:HH11	2.08	0.51
1:A:282:CYS:HA	3:A:4:HEC:CHC	2.41	0.51
1:A:252:ASN:HD22	1:A:255:SER:H	1.57	0.51
1:D:252:ASN:ND2	1:D:254:LEU:H	2.08	0.51
1:D:46:ALA:N	1:D:47:PRO:CD	2.74	0.51
1:A:198:LYS:HE3	1:C:65:ARG:NH1	2.15	0.50
1:D:436:THR:HG1	1:D:439:LYS:HG3	1.75	0.50
1:D:240:GLN:HB2	6:D:540:HOH:O	2.09	0.50
1:A:170:GLU:OE1	1:A:175:LYS:HD3	2.11	0.50
1:D:323:ALA:HA	1:D:326:GLN:HE21	1.75	0.50
1:D:245:ILE:HD12	6:D:775:HOH:O	2.11	0.50
1:A:283:ILE:HD11	3:A:3:HEC:HBB1	1.93	0.50
1:D:472:LYS:CB	1:D:472:LYS:NZ	2.69	0.50
1:D:105:LEU:HD23	1:D:455:LYS:HG2	1.94	0.50
3:C:479:HEC:CBC	3:C:479:HEC:HMC1	2.41	0.50
3:B:479:HEC:HMC1	3:B:479:HEC:CBC	2.42	0.50
1:D:256:LYS:HG3	1:D:358:LEU:HD11	1.94	0.50
1:D:125:CYS:SG	3:D:479:HEC:C2C	2.98	0.50
1:C:175:LYS:CE	6:C:563:HOH:O	2.55	0.50
1:D:151:GLY:HA2	1:D:466:TRP:CE3	2.46	0.50
1:C:312:GLN:N	1:C:312:GLN:NE2	2.59	0.49
1:D:252:ASN:HD22	1:D:254:LEU:H	1.59	0.49
1:B:450:GLN:O	1:B:454:GLU:HG3	2.12	0.49
1:A:323:ALA:HA	1:A:326:GLN:HE21	1.77	0.49
1:A:255:SER:HB3	1:A:354:ALA:HB3	1.95	0.49
1:D:312:GLN:O	1:D:316:ASN:ND2	2.46	0.49
3:D:3:HEC:HBC3	3:D:3:HEC:HMC1	1.93	0.49
1:A:62:GLN:NE2	1:A:302:LYS:NZ	2.58	0.49
1:D:371:GLN:NE2	6:D:528:HOH:O	2.46	0.49
1:C:94:HIS:CD2	3:C:3:HEC:ND	2.80	0.49
3:C:5:HEC:HBC3	3:C:5:HEC:HMC1	1.95	0.49
1:D:129:ASP:CB	1:D:154:ILE:HA	2.43	0.49
1:C:397:GLU:OE2	1:C:397:GLU:HA	2.12	0.49
1:D:280:VAL:HG13	3:D:5:HEC:HBC2	1.93	0.49
1:D:151:GLY:CA	1:D:466:TRP:CD2	2.96	0.49
1:D:66:VAL:HG13	6:D:903:HOH:O	2.12	0.49
3:D:5:HEC:CMB	3:D:5:HEC:CBB	2.81	0.48
1:D:291:GLN:HA	1:D:296:LYS:O	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:397:GLU:O	1:D:401:MET:HG3	2.12	0.48
1:D:282:CYS:HA	3:D:4:HEC:CHC	2.43	0.48
1:C:331[B]:GLU:OE1	1:D:277:LYS:NZ	2.42	0.48
1:D:167:ALA:O	1:D:168:SER:C	2.52	0.48
3:A:3:HEC:CBC	3:A:3:HEC:CMC	2.90	0.48
1:D:235:VAL:HB	1:D:401:MET:CE	2.43	0.48
1:C:68:ALA:HB3	1:C:88:TYR:CD2	2.49	0.48
1:D:309:ASN:OD1	1:D:312:GLN:CG	2.61	0.48
1:D:322:LYS:HE2	6:D:871:HOH:O	2.13	0.48
1:B:285:CYS:SG	3:B:4:HEC:HBC3	2.54	0.48
1:B:418:ARG:O	1:B:422:THR:HG23	2.13	0.48
1:A:471:ARG:O	1:A:472:LYS:C	2.52	0.48
1:D:419:LEU:HD22	1:D:419:LEU:O	2.14	0.48
1:A:234:LYS:H	1:A:237:ASN:ND2	2.11	0.48
1:D:213:HIS:HB3	1:D:266:GLU:HB2	1.96	0.48
1:D:468:GLU:O	1:D:472:LYS:HG2	2.14	0.48
1:A:234:LYS:H	1:A:237:ASN:HD22	1.60	0.47
1:B:352:PHE:CB	1:B:431:ILE:CD1	2.92	0.47
1:D:328:VAL:CG2	5:D:482:EDO:H22	2.44	0.47
1:C:227:PHE:N	1:C:227:PHE:CD2	2.82	0.47
1:D:447:ASN:O	1:D:451:ILE:HG13	2.15	0.47
1:D:44:THR:O	1:D:44:THR:HG22	2.14	0.47
1:C:292:ASN:C	1:C:292:ASN:ND2	2.68	0.47
1:D:328:VAL:HG23	5:D:482:EDO:C2	2.44	0.47
1:A:252:ASN:ND2	1:A:254:LEU:H	2.12	0.47
1:A:414:THR:HG22	1:A:418:ARG:NH1	2.29	0.47
1:D:99:THR:CG2	6:D:483:HOH:O	2.62	0.47
1:D:328:VAL:HG21	5:D:482:EDO:C2	2.43	0.47
1:C:274:ILE:HD12	1:C:277[B]:LYS:HD2	1.96	0.47
1:A:227:PHE:N	1:A:227:PHE:CD2	2.82	0.47
1:A:62:GLN:NE2	1:A:302:LYS:HZ2	2.11	0.47
1:A:256:LYS:CE	6:A:849:HOH:O	2.62	0.47
1:B:297:LEU:HB2	6:B:592:HOH:O	2.14	0.47
1:C:194:LYS:HB3	1:C:207:MET:CE	2.44	0.47
1:C:245:ILE:HG13	1:C:247:PHE:HB2	1.97	0.47
1:B:370:ILE:HD13	1:B:416:LEU:HD23	1.95	0.47
1:D:99:THR:HG22	6:D:483:HOH:O	2.16	0.47
1:A:368:LYS:HB3	1:A:369:PRO:HD3	1.97	0.47
3:D:480:HEC:HBC2	3:D:480:HEC:HMC1	1.94	0.46
1:C:272:ALA:O	1:C:277[B]:LYS:HE3	2.15	0.46
1:C:421:ALA:C	1:C:423:LYS:H	2.19	0.46
1:B:266:GLU:OE1	1:B:387:SER:CB	2.63	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:155:VAL:HB	6:D:533:HOH:O	2.14	0.46
1:B:296:LYS:CE	5:B:483:EDO:C2	2.83	0.46
1:C:309:ASN:HD21	1:C:312:GLN:NE2	2.06	0.46
1:B:352:PHE:CG	1:B:431:ILE:CD1	2.98	0.46
1:B:352:PHE:CG	1:B:431:ILE:HD12	2.49	0.46
1:D:383:LEU:HD23	1:D:401:MET:CE	2.44	0.46
1:A:119:PRO:HG3	1:A:223:LYS:HD3	1.97	0.46
1:C:235:VAL:HB	1:C:401:MET:HE3	1.97	0.46
1:C:158:LEU:HD11	3:C:3:HEC:C3C	2.45	0.46
1:B:391:HIS:H	1:B:391:HIS:CD2	2.33	0.46
1:D:150:GLY:O	1:D:151:GLY:C	2.54	0.46
1:B:227:PHE:N	1:B:227:PHE:CD2	2.83	0.46
1:C:318:HIS:HB3	1:C:320:GLN:HE21	1.79	0.46
1:D:391:HIS:CE1	3:D:4:HEC:O2D	2.67	0.46
1:C:321:ASP:HB2	6:C:642:HOH:O	2.15	0.46
1:C:234:LYS:H	1:C:237:ASN:HD22	1.64	0.46
1:A:195:PRO:HG3	6:A:541:HOH:O	2.15	0.46
1:D:160:CYS:O	1:D:164:HIS:HB2	2.16	0.46
1:A:105:LEU:HD23	1:A:455:LYS:HG2	1.97	0.46
1:A:79:TRP:CE2	1:A:261:LYS:HE2	2.51	0.46
1:B:318:HIS:HB3	1:B:320:GLN:NE2	2.31	0.46
1:A:214:VAL:HG21	1:A:227:PHE:CE1	2.51	0.46
1:A:274:ILE:HG13	3:B:5:HEC:HAA2	1.97	0.46
1:C:309:ASN:CG	1:C:312:GLN:NE2	2.67	0.46
1:D:43:GLU:C	1:D:45:PHE:H	2.19	0.46
1:B:149:ARG:HG3	6:B:516:HOH:O	2.16	0.46
1:D:151:GLY:HA3	1:D:466:TRP:CD2	2.52	0.45
1:C:310:PHE:CE2	1:C:314:CYS:HB2	2.51	0.45
1:D:283:ILE:CG2	6:D:519:HOH:O	2.64	0.45
1:B:397:GLU:O	1:B:401:MET:HG3	2.17	0.45
1:D:318:HIS:HB3	1:D:320:GLN:NE2	2.32	0.45
1:C:406:MET:HB3	1:D:406:MET:HG2	1.98	0.45
1:C:292:ASN:ND2	1:C:296:LYS:H	2.15	0.45
1:B:310:PHE:CE2	1:B:314:CYS:HB2	2.51	0.45
1:B:51:ASP:OD2	5:B:483:EDO:O1	2.35	0.45
1:A:163:CYS:SG	3:A:480:HEC:HAC	2.43	0.45
1:D:43:GLU:C	1:D:45:PHE:N	2.69	0.45
1:A:391:HIS:HE1	3:A:4:HEC:O2D	1.98	0.45
1:B:42:ASN:OD1	1:B:159:GLY:HA3	2.17	0.45
1:D:227:PHE:N	1:D:227:PHE:CD2	2.85	0.45
1:C:477:SER:HB2	6:C:554:HOH:O	2.17	0.45
1:C:238:MET:CE	1:C:268:GLU:HG2	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:125:CYS:HG	3:A:479:HEC:CAC	2.22	0.44
1:A:231:ASP:HB3	1:A:240:GLN:HE22	1.82	0.44
1:D:62:GLN:HE21	1:D:302:LYS:HZ1	1.63	0.44
1:D:152:PRO:HG3	1:D:466:TRP:CD1	2.52	0.44
1:D:158:LEU:CG	3:D:3:HEC:HBC2	2.44	0.44
1:C:194:LYS:HE3	1:C:207:MET:HE3	1.99	0.44
1:A:194:LYS:HE2	6:A:548:HOH:O	2.17	0.44
1:C:252:ASN:HD22	1:C:254:LEU:H	1.65	0.44
1:B:79:TRP:CE3	1:B:84:PHE:HB3	2.53	0.44
1:A:217:TYR:HH	1:A:241:TYR:HH	1.58	0.44
1:A:292:ASN:OD1	1:A:296:LYS:CB	2.65	0.44
1:A:381:TRP:CE2	1:A:385:ILE:HD11	2.53	0.44
1:D:309:ASN:OD1	1:D:312:GLN:HB2	2.18	0.44
1:A:472:LYS:HE3	1:A:472:LYS:HA	1.98	0.44
1:C:163:CYS:HG	3:C:480:HEC:CAC	2.26	0.44
5:C:9:EDO:H12	6:C:788:HOH:O	2.17	0.44
1:D:221:LYS:N	1:D:221:LYS:HZ3	2.15	0.44
1:B:151:GLY:HA3	1:B:466:TRP:CE2	2.53	0.44
1:B:46:ALA:N	1:B:47:PRO:CD	2.80	0.44
1:D:328:VAL:HG23	5:D:482:EDO:H22	2.00	0.44
1:C:180:LEU:HG	1:C:196:PHE:CD1	2.53	0.44
1:B:309:ASN:ND2	1:B:312:GLN:HG2	2.33	0.44
1:B:383:LEU:HD23	1:B:401:MET:CE	2.48	0.44
1:A:279:ASN:HD22	1:A:279:ASN:HA	1.66	0.44
1:D:180:LEU:HG	1:D:196:PHE:CD1	2.53	0.44
1:D:228:PRO:HG3	1:D:242:TYR:OH	2.18	0.43
1:B:281:THR:HG22	6:B:493:HOH:O	2.17	0.43
3:A:480:HEC:CBC	3:A:480:HEC:CMC	2.92	0.43
1:C:125:CYS:SG	3:C:479:HEC:C2C	3.04	0.43
1:C:406:MET:HE2	1:D:407:ASP:HB2	1.99	0.43
1:D:476:LEU:O	1:D:477:SER:C	2.57	0.43
1:D:121:ALA:HB3	1:D:218:PHE:CZ	2.54	0.43
1:D:72:ASP:OD2	1:D:344:GLU:OE1	2.35	0.43
1:B:460:LYS:HA	1:B:460:LYS:HD3	1.52	0.43
1:C:213:HIS:HB3	1:C:266:GLU:HB2	2.00	0.43
1:D:433:ASP:OD1	1:D:439:LYS:CD	2.66	0.43
1:B:49:HIS:HD2	6:B:706:HOH:O	2.02	0.43
1:A:310:PHE:HA	1:A:313:THR:OG1	2.19	0.43
1:C:64:GLU:OE1	6:C:1022:HOH:O	2.22	0.43
3:D:480:HEC:HMB1	3:D:480:HEC:HBB3	2.01	0.43
1:C:397:GLU:O	1:C:401:MET:HG3	2.18	0.43
1:A:384:ALA:N	1:A:401:MET:HE2	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:314:CYS:SG	3:D:5:HEC:HBB3	2.56	0.43
1:A:317:CYS:SG	3:A:5:HEC:CBC	3.02	0.43
1:B:370:ILE:HD13	1:B:416:LEU:CD2	2.49	0.43
1:A:75:LEU:HB3	1:A:79:TRP:CZ3	2.54	0.43
1:C:168:SER:HA	1:C:169:PRO:HD3	1.88	0.43
1:A:199:ALA:HB1	1:A:203:ASP:HB2	2.01	0.43
1:C:467:GLU:O	1:C:471:ARG:HG3	2.19	0.43
1:B:296:LYS:CE	5:B:483:EDO:C1	2.22	0.42
1:C:306:PRO:HG2	3:C:4:HEC:CHD	2.49	0.42
1:B:463:ILE:HB	1:B:464:PRO:HD3	2.01	0.42
1:A:275:HIS:CE1	3:A:5:HEC:NA	2.86	0.42
1:D:75:LEU:HB3	1:D:79:TRP:CZ3	2.54	0.42
1:A:305:ASN:HA	1:A:306:PRO:HD3	1.83	0.42
1:A:289:LYS:NZ	3:A:480:HEC:O1D	2.48	0.42
1:D:104:THR:HG21	3:D:479:HEC:HMA1	2.02	0.42
1:D:94:HIS:CD2	3:D:3:HEC:C4D	3.03	0.42
1:B:37:THR:CG2	1:B:135:GLN:OE1	2.66	0.42
1:A:320:GLN:N	1:A:320:GLN:HE21	2.09	0.42
1:D:214:VAL:HG21	1:D:227:PHE:CZ	2.54	0.42
1:A:313:THR:O	1:A:316:ASN:HB2	2.18	0.42
1:B:452:LYS:O	1:B:456:GLN:HG2	2.19	0.42
1:D:244:LYS:HD2	1:D:244:LYS:HA	1.53	0.42
1:D:263:GLN:O	1:D:264:HIS:C	2.57	0.42
1:B:296:LYS:NZ	5:B:483:EDO:C2	2.82	0.42
3:A:4:HEC:CMB	3:A:4:HEC:HBB3	2.48	0.42
1:D:102:ARG:HD3	1:D:463:ILE:HD12	2.01	0.42
1:B:240:GLN:HE21	1:B:241:TYR:N	2.17	0.42
1:D:221:LYS:HE2	1:D:222:ASN:HB2	2.02	0.42
1:D:139:GLU:OE1	1:D:183:PRO:HB2	2.20	0.42
1:D:391:HIS:CD2	6:D:804:HOH:O	2.62	0.42
1:B:336:ILE:O	1:B:340[A]:LYS:HB3	2.19	0.42
1:D:159:GLY:O	1:D:162:ASP:HB2	2.20	0.42
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.85	0.42
1:C:106:ARG:NE	6:C:673:HOH:O	2.36	0.42
3:D:3:HEC:HMB1	3:D:3:HEC:HBB3	2.02	0.42
1:B:275:HIS:CG	3:B:4:HEC:HBC2	2.54	0.42
1:D:252:ASN:ND2	1:D:254:LEU:HB2	2.34	0.42
1:D:463:ILE:N	1:D:464:PRO:CD	2.83	0.42
1:B:231:ASP:OD2	1:B:240:GLN:NE2	2.53	0.42
1:D:438:GLU:CD	1:D:438:GLU:H	2.22	0.42
3:C:3:HEC:CMC	3:C:3:HEC:CBC	2.97	0.41
1:B:52:GLN:NE2	1:B:52:GLN:N	2.62	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:LEU:HB3	1:A:119:PRO:HD2	2.02	0.41
1:A:180:LEU:HG	1:A:196:PHE:CD1	2.55	0.41
1:A:158:LEU:HD11	3:A:3:HEC:C3C	2.49	0.41
1:C:346:GLN:HG3	1:C:406:MET:SD	2.60	0.41
1:A:266:GLU:O	1:A:270:TRP:HB3	2.20	0.41
1:B:263:GLN:HA	6:B:1042:HOH:O	2.19	0.41
1:C:325:LEU:HD23	5:C:484:EDO:H11	2.01	0.41
1:D:123:TRP:CE2	1:D:147:TRP:CD1	3.09	0.41
1:B:127:SER:HB3	1:B:154:ILE:HG23	2.03	0.41
1:D:340:LYS:CE	6:D:501:HOH:O	2.69	0.41
1:A:37:THR:OG1	1:A:135:GLN:NE2	2.52	0.41
1:B:313:THR:O	1:B:316:ASN:HB2	2.20	0.41
1:B:296:LYS:CE	5:B:483:EDO:H22	2.50	0.41
1:D:125:CYS:HB3	1:D:212:CYS:HB3	2.03	0.41
1:C:65:ARG:NE	6:C:633:HOH:O	2.54	0.41
1:A:274:ILE:HA	1:A:274:ILE:HD13	1.83	0.41
1:A:292:ASN:OD1	1:A:296:LYS:HB3	2.20	0.41
1:C:311:ALA:O	1:C:315:ALA:HB3	2.21	0.41
1:D:353:GLU:HB2	1:D:416:LEU:HD13	2.02	0.41
1:C:46:ALA:N	1:C:47:PRO:CD	2.84	0.41
1:A:82:TYR:CD1	1:A:83:PRO:HD2	2.55	0.41
1:D:469:GLN:HA	1:D:469:GLN:NE2	2.36	0.41
1:B:71:GLU:OE2	6:B:636:HOH:O	2.21	0.41
1:D:122:CYS:SG	3:D:479:HEC:C3B	3.00	0.41
1:A:292:ASN:ND2	1:A:294:GLU:H	2.19	0.41
1:D:468:GLU:HA	1:D:471:ARG:NH1	2.36	0.41
3:C:5:HEC:HBB3	3:C:5:HEC:CMB	2.44	0.41
1:D:240:GLN:NE2	1:D:241:TYR:N	2.68	0.41
1:D:168:SER:HA	1:D:169:PRO:HD3	1.81	0.41
1:D:274:ILE:HA	1:D:274:ILE:HD13	1.92	0.41
1:D:325:LEU:HD12	1:D:325:LEU:HA	1.72	0.41
1:A:128:PRO:HD3	1:A:158:LEU:HA	2.03	0.41
1:C:391:HIS:CD2	1:C:391:HIS:H	2.39	0.41
1:A:292:ASN:ND2	1:A:294:GLU:N	2.69	0.41
1:B:352:PHE:CD2	1:B:431:ILE:CD1	3.00	0.41
1:A:133:LEU:HA	1:A:133:LEU:HD23	1.78	0.41
1:C:92:ARG:HB2	1:C:93:GLY:H	1.77	0.41
1:A:136:LYS:HE2	1:A:137:ASP:OD1	2.20	0.41
1:D:287:MET:HE1	1:D:299:THR:HG21	2.02	0.41
1:C:79:TRP:CE3	1:C:84:PHE:HB3	2.56	0.41
1:A:283:ILE:HD11	3:A:3:HEC:CBB	2.50	0.41
1:D:118:LEU:HB3	1:D:119:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:151:GLY:HA2	1:D:466:TRP:CZ3	2.56	0.41
1:D:82:TYR:CD1	1:D:83:PRO:HD2	2.56	0.41
1:B:119:PRO:HG3	1:B:223:LYS:HD2	2.03	0.41
1:D:103:GLU:O	1:D:455:LYS:HE2	2.20	0.40
1:B:123:TRP:CB	1:B:154:ILE:HD13	2.51	0.40
1:A:144:HIS:O	1:A:149:ARG:NH2	2.48	0.40
1:A:381:TRP:CZ2	1:A:385:ILE:HD11	2.56	0.40
1:B:62:GLN:HE21	1:B:302:LYS:NZ	2.18	0.40
3:A:480:HEC:HMB1	3:A:480:HEC:CBB	2.35	0.40
1:D:396:GLU:HG2	1:D:397:GLU:N	2.36	0.40
1:D:213:HIS:CE1	3:D:479:HEC:HMD1	2.56	0.40
1:A:198:LYS:HE3	1:C:65:ARG:HH11	1.77	0.40
1:C:158:LEU:HD11	3:C:3:HEC:C4C	2.52	0.40
1:D:431:ILE:HG22	1:D:432:PRO:O	2.21	0.40
1:A:438:GLU:H	1:A:438:GLU:CD	2.24	0.40
1:C:214:VAL:HG21	1:C:227:PHE:CZ	2.57	0.40
1:B:257:THR:O	1:B:259:MET:HG2	2.21	0.40
1:D:234:LYS:H	1:D:237:ASN:HD22	1.70	0.40
1:C:263:GLN:O	1:C:264:HIS:C	2.60	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	440/452 (97%)	423 (96%)	17 (4%)	0	100	100
1	B	441/452 (98%)	427 (97%)	14 (3%)	0	100	100
1	C	443/452 (98%)	434 (98%)	8 (2%)	1 (0%)	56	68
1	D	441/452 (98%)	413 (94%)	25 (6%)	3 (1%)	30	34
All	All	1765/1808 (98%)	1697 (96%)	64 (4%)	4 (0%)	56	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	44	THR
1	C	422	THR
1	D	136	LYS
1	D	151	GLY

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	363/370 (98%)	348 (96%)	15 (4%)	41	55
1	B	364/370 (98%)	348 (96%)	16 (4%)	39	51
1	C	366/370 (99%)	354 (97%)	12 (3%)	50	66
1	D	364/370 (98%)	349 (96%)	15 (4%)	41	55
All	All	1457/1480 (98%)	1399 (96%)	58 (4%)	42	56

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	82	TYR
1	A	221	LYS
1	A	240	GLN
1	A	244	LYS
1	A	274	ILE
1	A	279	ASN
1	A	283	ILE
1	A	292	ASN
1	A	296	LYS
1	A	309	ASN
1	A	312	GLN
1	A	320	GLN
1	A	327	LYS
1	A	472	LYS
1	B	37	THR
1	B	52	GLN
1	B	99	THR
1	B	111	LYS

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Mol	Chain	Res	Type
1	B	114	GLU
1	B	149	ARG
1	B	240	GLN
1	B	252	ASN
1	B	274	ILE
1	B	309	ASN
1	B	316	ASN
1	B	320	GLN
1	B	325	LEU
1	B	419	LEU
1	B	460	LYS
1	B	477	SER
1	C	52	GLN
1	C	221	LYS
1	C	222	ASN
1	C	252	ASN
1	C	256	LYS
1	C	292	ASN
1	C	309	ASN
1	C	312	GLN
1	C	320	GLN
1	C	340	LYS
1	C	385	ILE
1	C	477	SER
1	D	52	GLN
1	D	99	THR
1	D	112	ASN
1	D	114	GLU
1	D	190	GLU
1	D	221	LYS
1	D	240	GLN
1	D	250	TRP
1	D	274	ILE
1	D	283	ILE
1	D	309	ASN
1	D	320	GLN
1	D	325	LEU
1	D	419	LEU
1	D	472	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	62	GLN
1	A	135	GLN
1	A	237	ASN
1	A	240	GLN
1	A	252	ASN
1	A	279	ASN
1	A	291	GLN
1	A	292	ASN
1	A	309	ASN
1	A	320	GLN
1	A	326	GLN
1	A	334	GLN
1	A	346	GLN
1	A	371	GLN
1	A	388	HIS
1	A	391	HIS
1	A	427	HIS
1	A	456	GLN
1	A	469	GLN
1	B	49	HIS
1	B	52	GLN
1	B	62	GLN
1	B	222	ASN
1	B	237	ASN
1	B	240	GLN
1	B	252	ASN
1	B	309	ASN
1	B	320	GLN
1	B	337	ASN
1	B	346	GLN
1	B	371	GLN
1	B	388	HIS
1	B	391	HIS
1	B	469	GLN
1	C	48	GLN
1	C	49	HIS
1	C	52	GLN
1	C	62	GLN
1	C	237	ASN
1	C	240	GLN
1	C	252	ASN
1	C	279	ASN

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Mol	Chain	Res	Type
1	C	291	GLN
1	C	292	ASN
1	C	309	ASN
1	C	312	GLN
1	C	320	GLN
1	C	326	GLN
1	C	346	GLN
1	C	371	GLN
1	C	388	HIS
1	C	391	HIS
1	C	427	HIS
1	C	450	GLN
1	C	469	GLN
1	D	42	ASN
1	D	52	GLN
1	D	62	GLN
1	D	144	HIS
1	D	237	ASN
1	D	240	GLN
1	D	252	ASN
1	D	291	GLN
1	D	320	GLN
1	D	326	GLN
1	D	334	GLN
1	D	346	GLN
1	D	371	GLN
1	D	388	HIS
1	D	391	HIS
1	D	427	HIS
1	D	456	GLN
1	D	469	GLN
1	D	473	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

Of 45 ligands modelled in this entry, 8 are monoatomic - leaving 37 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	3	1,2	50,50,50	2.71	12 (24%)	56,82,82	2.08	15 (26%)
3	HEC	A	4	1,2	50,50,50	2.75	11 (22%)	56,82,82	2.06	13 (23%)
3	HEC	A	479	1,4	50,50,50	2.86	14 (28%)	56,82,82	1.81	11 (19%)
3	HEC	A	480	1	50,50,50	2.75	14 (28%)	56,82,82	1.86	10 (17%)
4	SO3	A	481	3	3,3,3	1.21	0	2,3,3	0.63	0
3	HEC	A	5	1	50,50,50	2.74	13 (26%)	56,82,82	1.82	13 (23%)
5	EDO	A	6	-	3,3,3	0.44	0	2,2,2	0.90	0
5	EDO	A	8	-	3,3,3	0.57	0	2,2,2	0.29	0
5	EDO	B	12	-	3,3,3	0.58	0	2,2,2	0.46	0
3	HEC	B	3	1,2	50,50,50	2.81	14 (28%)	56,82,82	1.87	13 (23%)
3	HEC	B	4	1,2	50,50,50	2.74	15 (30%)	56,82,82	2.12	21 (37%)
3	HEC	B	479	1,4	50,50,50	2.79	13 (26%)	56,82,82	1.75	11 (19%)
3	HEC	B	480	1	50,50,50	2.73	14 (28%)	56,82,82	1.92	14 (25%)
4	SO3	B	481	-	3,3,3	1.02	0	2,3,3	0.57	0
4	SO3	B	482	3	3,3,3	1.19	0	2,3,3	0.62	0
5	EDO	B	483	-	3,3,3	0.62	0	2,2,2	0.21	0
3	HEC	B	5	1	50,50,50	2.72	12 (24%)	56,82,82	1.97	13 (23%)
5	EDO	C	10	-	3,3,3	0.52	0	2,2,2	0.47	0
3	HEC	C	3	1,2	50,50,50	2.67	13 (26%)	56,82,82	1.97	11 (19%)
3	HEC	C	4	1,2	50,50,50	2.67	13 (26%)	56,82,82	2.08	14 (25%)
3	HEC	C	479	1,4	50,50,50	2.81	14 (28%)	56,82,82	1.76	12 (21%)
3	HEC	C	480	1	50,50,50	2.73	12 (24%)	56,82,82	1.83	13 (23%)
4	SO3	C	481	3	3,3,3	1.06	0	2,3,3	0.60	0
5	EDO	C	482	-	3,3,3	0.49	0	2,2,2	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	483	-	3,3,3	0.51	0	2,2,2	0.47	0
5	EDO	C	484	-	3,3,3	0.55	0	2,2,2	0.29	0
3	HEC	C	5	1	50,50,50	2.82	12 (24%)	56,82,82	1.90	14 (25%)
5	EDO	C	7	-	3,3,3	0.47	0	2,2,2	0.60	0
5	EDO	C	9	-	3,3,3	0.54	0	2,2,2	0.75	0
5	EDO	D	11	-	3,3,3	0.41	0	2,2,2	0.81	0
3	HEC	D	3	1,2	50,50,50	2.75	16 (32%)	56,82,82	1.94	15 (26%)
3	HEC	D	4	1,2	50,50,50	2.64	12 (24%)	56,82,82	1.96	12 (21%)
3	HEC	D	479	1,4	50,50,50	2.77	15 (30%)	56,82,82	2.03	13 (23%)
3	HEC	D	480	1	50,50,50	2.80	13 (26%)	56,82,82	1.87	15 (26%)
4	SO3	D	481	3	3,3,3	1.14	0	2,3,3	0.56	0
5	EDO	D	482	-	3,3,3	0.56	0	2,2,2	0.38	0
3	HEC	D	5	1	50,50,50	2.74	14 (28%)	56,82,82	1.97	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	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
3	HEC	A	479	1,4	-	0/10/54/54	0/0/8/8
3	HEC	A	480	1	-	0/10/54/54	0/0/8/8
4	SO3	A	481	3	-	0/0/0/0	0/0/0/0
3	HEC	A	5	1	-	0/10/54/54	0/0/8/8
5	EDO	A	6	-	-	0/1/1/1	0/0/0/0
5	EDO	A	8	-	-	0/1/1/1	0/0/0/0
5	EDO	B	12	-	-	0/1/1/1	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
3	HEC	B	479	1,4	-	0/10/54/54	0/0/8/8
3	HEC	B	480	1	-	0/10/54/54	0/0/8/8
4	SO3	B	481	-	-	0/0/0/0	0/0/0/0
4	SO3	B	482	3	-	0/0/0/0	0/0/0/0
5	EDO	B	483	-	-	0/1/1/1	0/0/0/0
3	HEC	B	5	1	-	0/10/54/54	0/0/8/8
5	EDO	C	10	-	-	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
3	HEC	C	479	1,4	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	C	480	1	-	0/10/54/54	0/0/8/8
4	SO3	C	481	3	-	0/0/0/0	0/0/0/0
5	EDO	C	482	-	-	0/1/1/1	0/0/0/0
5	EDO	C	483	-	-	0/1/1/1	0/0/0/0
5	EDO	C	484	-	-	0/1/1/1	0/0/0/0
3	HEC	C	5	1	-	0/10/54/54	0/0/8/8
5	EDO	C	7	-	-	0/1/1/1	0/0/0/0
5	EDO	C	9	-	-	0/1/1/1	0/0/0/0
5	EDO	D	11	-	-	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	1,2	-	0/10/54/54	0/0/8/8
3	HEC	D	479	1,4	-	0/10/54/54	0/0/8/8
3	HEC	D	480	1	-	0/10/54/54	0/0/8/8
4	SO3	D	481	3	-	0/0/0/0	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

All (266) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	HEC	C3C-CAC	10.86	1.57	1.35
3	A	4	HEC	C3C-CAC	10.65	1.57	1.35
3	D	5	HEC	C3C-CAC	10.36	1.56	1.35
3	A	5	HEC	C3C-CAC	10.29	1.56	1.35
3	B	479	HEC	C3C-CAC	10.15	1.56	1.35
3	B	3	HEC	C3C-CAC	10.13	1.56	1.35
3	B	5	HEC	C3C-CAC	10.11	1.56	1.35
3	A	480	HEC	C3C-CAC	10.04	1.56	1.35
3	C	479	HEC	C3C-CAC	9.98	1.56	1.35
3	A	3	HEC	C3C-CAC	9.95	1.55	1.35
3	D	4	HEC	C3C-CAC	9.94	1.55	1.35
3	C	480	HEC	C3C-CAC	9.93	1.55	1.35
3	C	479	HEC	C3B-CAB	9.90	1.55	1.35
3	B	4	HEC	C3B-CAB	9.85	1.55	1.35
3	B	479	HEC	C3B-CAB	9.82	1.55	1.35
3	C	4	HEC	C3B-CAB	9.78	1.55	1.35
3	C	480	HEC	C3B-CAB	9.75	1.55	1.35
3	C	5	HEC	C3B-CAB	9.73	1.55	1.35
3	C	3	HEC	C3C-CAC	9.72	1.55	1.35
3	C	4	HEC	C3C-CAC	9.72	1.55	1.35
3	D	3	HEC	C3C-CAC	9.70	1.55	1.35
3	A	4	HEC	C3B-CAB	9.68	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	HEC	C3B-CAB	9.67	1.55	1.35
3	D	480	HEC	C3C-CAC	9.64	1.55	1.35
3	D	479	HEC	C3B-CAB	9.63	1.55	1.35
3	D	480	HEC	C3B-CAB	9.54	1.55	1.35
3	B	480	HEC	C3C-CAC	9.54	1.55	1.35
3	D	479	HEC	C3C-CAC	9.52	1.55	1.35
3	B	4	HEC	C3C-CAC	9.48	1.54	1.35
3	A	479	HEC	C3B-CAB	9.47	1.54	1.35
3	B	480	HEC	C3B-CAB	9.47	1.54	1.35
3	D	3	HEC	C3B-CAB	9.41	1.54	1.35
3	B	3	HEC	C3B-CAB	9.37	1.54	1.35
3	A	479	HEC	C3C-CAC	9.36	1.54	1.35
3	B	5	HEC	C3B-CAB	9.24	1.54	1.35
3	D	5	HEC	C3B-CAB	9.17	1.54	1.35
3	A	480	HEC	C3B-CAB	9.04	1.54	1.35
3	A	5	HEC	C3B-CAB	9.03	1.54	1.35
3	A	3	HEC	C3B-CAB	8.91	1.53	1.35
3	D	4	HEC	C3B-CAB	8.90	1.53	1.35
3	C	5	HEC	C1C-C2C	5.73	1.47	1.40
3	D	479	HEC	C3D-C2D	5.63	1.54	1.37
3	D	480	HEC	C3D-C2D	5.61	1.54	1.37
3	A	4	HEC	C3D-C2D	5.61	1.54	1.37
3	D	5	HEC	C3D-C2D	5.54	1.54	1.37
3	A	479	HEC	C3D-C2D	5.52	1.54	1.37
3	B	3	HEC	C3D-C2D	5.50	1.54	1.37
3	C	479	HEC	C1C-C2C	5.50	1.47	1.40
3	C	3	HEC	C3D-C2D	5.47	1.53	1.37
3	D	4	HEC	C3D-C2D	5.43	1.53	1.37
3	B	3	HEC	C1C-C2C	5.40	1.46	1.40
3	D	3	HEC	C3D-C2D	5.36	1.53	1.37
3	A	480	HEC	C3D-C2D	5.34	1.53	1.37
3	C	480	HEC	C3D-C2D	5.34	1.53	1.37
3	B	5	HEC	C3D-C2D	5.29	1.53	1.37
3	B	479	HEC	C1C-C2C	5.28	1.46	1.40
3	C	5	HEC	C3D-C2D	5.28	1.53	1.37
3	B	4	HEC	C3D-C2D	5.21	1.53	1.37
3	A	3	HEC	C3D-C2D	5.15	1.52	1.37
3	A	479	HEC	C1B-C2B	5.12	1.46	1.40
3	A	5	HEC	C3D-C2D	5.10	1.52	1.37
3	A	479	HEC	FE-ND	5.02	2.14	1.92
3	C	479	HEC	C3D-C2D	5.01	1.52	1.37
3	B	479	HEC	C3D-C2D	4.99	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	HEC	C3D-C2D	4.94	1.52	1.37
3	A	479	HEC	C1C-C2C	4.91	1.46	1.40
3	A	480	HEC	C1C-C2C	4.89	1.46	1.40
3	B	480	HEC	C3D-C2D	4.84	1.52	1.37
3	B	5	HEC	FE-ND	4.84	2.13	1.92
3	D	5	HEC	C1C-C2C	4.79	1.46	1.40
3	D	3	HEC	C1B-C2B	4.70	1.46	1.40
3	B	5	HEC	C1C-C2C	4.68	1.46	1.40
3	A	3	HEC	C1C-C2C	4.67	1.46	1.40
3	B	5	HEC	C1B-C2B	4.64	1.46	1.40
3	B	480	HEC	FE-ND	4.64	2.12	1.92
3	A	3	HEC	C1B-C2B	4.61	1.45	1.40
3	B	480	HEC	C1D-C2D	4.60	1.45	1.40
3	A	480	HEC	C1B-C2B	4.57	1.45	1.40
3	A	5	HEC	C1B-C2B	4.55	1.45	1.40
3	D	480	HEC	C1B-C2B	4.53	1.45	1.40
3	B	4	HEC	C1C-C2C	4.53	1.45	1.40
3	D	479	HEC	FE-ND	4.49	2.11	1.92
3	C	480	HEC	C1B-C2B	4.46	1.45	1.40
3	C	4	HEC	C1C-C2C	4.45	1.45	1.40
3	A	5	HEC	FE-ND	4.45	2.11	1.92
3	D	480	HEC	C1C-C2C	4.41	1.45	1.40
3	A	3	HEC	C3B-C2B	-4.40	1.32	1.41
3	B	3	HEC	C3C-C4C	4.39	1.47	1.41
3	D	3	HEC	C1C-C2C	4.38	1.45	1.40
3	C	480	HEC	C1C-C2C	4.35	1.45	1.40
3	D	480	HEC	FE-ND	4.34	2.11	1.92
3	B	480	HEC	C1B-C2B	4.33	1.45	1.40
3	A	5	HEC	C1D-C2D	4.30	1.45	1.40
3	A	4	HEC	FE-ND	4.29	2.10	1.92
3	B	3	HEC	FE-NC	4.26	2.10	1.92
3	B	3	HEC	C1D-C2D	4.25	1.45	1.40
3	D	4	HEC	C1C-C2C	4.24	1.45	1.40
3	D	4	HEC	C1B-C2B	4.23	1.45	1.40
3	D	479	HEC	C1C-C2C	4.23	1.45	1.40
3	A	3	HEC	C1D-C2D	4.20	1.45	1.40
3	C	480	HEC	FE-NA	4.16	2.10	1.92
3	A	479	HEC	FE-NC	4.15	2.10	1.92
3	D	480	HEC	C1D-C2D	4.08	1.45	1.40
3	A	480	HEC	FE-ND	4.07	2.09	1.92
3	C	3	HEC	C1C-C2C	4.06	1.45	1.40
3	B	479	HEC	C1B-C2B	4.04	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	HEC	FE-NA	4.00	2.09	1.92
3	C	3	HEC	C1B-C2B	4.00	1.45	1.40
3	A	4	HEC	C1C-C2C	3.98	1.45	1.40
3	C	479	HEC	C1D-C2D	3.98	1.45	1.40
3	A	479	HEC	C1D-C2D	3.95	1.45	1.40
3	C	5	HEC	C3B-C4B	3.85	1.46	1.41
3	D	479	HEC	FE-NA	3.84	2.08	1.92
3	A	479	HEC	C3C-C4C	3.83	1.46	1.41
3	D	4	HEC	FE-ND	3.82	2.08	1.92
3	A	5	HEC	FE-NC	3.82	2.08	1.92
3	D	480	HEC	FE-NA	3.80	2.08	1.92
3	D	3	HEC	C1D-C2D	3.80	1.44	1.40
3	C	479	HEC	C1B-C2B	3.76	1.44	1.40
3	B	479	HEC	C1D-C2D	3.75	1.44	1.40
3	A	479	HEC	C3B-C4B	3.71	1.46	1.41
3	D	4	HEC	C1D-C2D	3.71	1.44	1.40
3	B	480	HEC	C1C-C2C	3.70	1.44	1.40
3	B	4	HEC	C1B-C2B	3.68	1.44	1.40
3	D	479	HEC	C1B-C2B	3.66	1.44	1.40
3	C	4	HEC	C1D-C2D	3.63	1.44	1.40
3	A	4	HEC	C3B-C2B	-3.62	1.33	1.41
3	B	4	HEC	C3C-C4C	3.60	1.46	1.41
3	A	5	HEC	C1C-C2C	3.60	1.44	1.40
3	D	5	HEC	C1B-C2B	3.60	1.44	1.40
3	C	479	HEC	FE-NB	3.58	2.07	1.92
3	C	5	HEC	FE-ND	3.58	2.07	1.92
3	C	479	HEC	FE-ND	3.58	2.07	1.92
3	C	480	HEC	C3B-C2B	-3.57	1.33	1.41
3	C	4	HEC	C1B-C2B	3.56	1.44	1.40
3	B	479	HEC	FE-NB	3.55	2.07	1.92
3	A	480	HEC	C1D-C2D	3.54	1.44	1.40
3	B	4	HEC	C1D-C2D	3.53	1.44	1.40
3	D	3	HEC	FE-NA	3.51	2.07	1.92
3	D	479	HEC	C3C-C2C	-3.51	1.34	1.41
3	C	3	HEC	FE-NA	3.51	2.07	1.92
3	C	5	HEC	C1B-C2B	3.50	1.44	1.40
3	C	5	HEC	C3B-C2B	-3.50	1.34	1.41
3	B	479	HEC	FE-NA	3.49	2.07	1.92
3	D	480	HEC	C3B-C2B	-3.49	1.34	1.41
3	D	5	HEC	FE-NB	3.49	2.07	1.92
3	C	4	HEC	C3B-C2B	-3.48	1.34	1.41
3	B	4	HEC	C3B-C2B	-3.47	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4	HEC	C3B-C4B	3.47	1.46	1.41
3	C	479	HEC	C3B-C2B	-3.46	1.34	1.41
3	D	479	HEC	C3C-C4C	3.45	1.45	1.41
3	B	480	HEC	FE-NC	3.44	2.07	1.92
3	D	4	HEC	C3B-C2B	-3.43	1.34	1.41
3	D	3	HEC	C3B-C2B	-3.43	1.34	1.41
3	A	479	HEC	C3B-C2B	-3.43	1.34	1.41
3	A	4	HEC	C3C-C4C	3.42	1.45	1.41
3	A	480	HEC	C3C-C2C	-3.42	1.34	1.41
3	B	480	HEC	C3B-C2B	-3.41	1.34	1.41
3	C	3	HEC	FE-ND	3.41	2.07	1.92
3	A	3	HEC	FE-NC	3.40	2.07	1.92
3	D	480	HEC	C3C-C2C	-3.40	1.34	1.41
3	C	3	HEC	C1D-C2D	3.39	1.44	1.40
3	B	5	HEC	C3B-C2B	-3.38	1.34	1.41
3	B	5	HEC	C1D-C2D	3.37	1.44	1.40
3	A	480	HEC	C3B-C2B	-3.36	1.34	1.41
3	A	4	HEC	C1B-C2B	3.36	1.44	1.40
3	D	5	HEC	C1D-C2D	3.32	1.44	1.40
3	B	479	HEC	C3B-C4B	3.31	1.45	1.41
3	B	4	HEC	FE-NC	3.30	2.06	1.92
3	C	479	HEC	C3B-C4B	3.30	1.45	1.41
3	C	5	HEC	FE-NC	3.30	2.06	1.92
3	D	5	HEC	C3B-C2B	-3.29	1.34	1.41
3	C	4	HEC	C3C-C2C	-3.28	1.34	1.41
3	B	5	HEC	C3C-C2C	-3.28	1.34	1.41
3	C	4	HEC	FE-NC	3.26	2.06	1.92
3	A	5	HEC	C3B-C2B	-3.26	1.34	1.41
3	A	479	HEC	C3C-C2C	-3.25	1.34	1.41
3	D	5	HEC	C3C-C4C	3.25	1.45	1.41
3	B	3	HEC	C3B-C2B	-3.24	1.34	1.41
3	B	479	HEC	FE-ND	3.23	2.06	1.92
3	A	480	HEC	FE-NC	3.18	2.06	1.92
3	D	479	HEC	C3B-C2B	-3.18	1.34	1.41
3	A	4	HEC	C1D-C2D	3.18	1.44	1.40
3	B	479	HEC	C3B-C2B	-3.17	1.34	1.41
3	D	4	HEC	C3C-C2C	-3.17	1.34	1.41
3	B	4	HEC	FE-NB	3.16	2.06	1.92
3	B	3	HEC	FE-NA	3.15	2.05	1.92
3	D	480	HEC	FE-NB	3.12	2.05	1.92
3	C	479	HEC	C3C-C2C	-3.12	1.34	1.41
3	C	480	HEC	C3B-C4B	3.11	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	480	HEC	C1D-C2D	3.10	1.44	1.40
3	C	3	HEC	C3B-C2B	-3.08	1.35	1.41
3	D	3	HEC	C3C-C2C	-3.06	1.35	1.41
3	B	4	HEC	C3C-C2C	-3.05	1.35	1.41
3	D	479	HEC	C1D-C2D	3.04	1.44	1.40
3	B	480	HEC	C3C-C2C	-3.02	1.35	1.41
3	A	4	HEC	C3B-C4B	3.01	1.45	1.41
3	C	480	HEC	FE-ND	2.97	2.05	1.92
3	A	5	HEC	C3C-C4C	2.97	1.45	1.41
3	A	480	HEC	C3B-C4B	2.97	1.45	1.41
3	A	4	HEC	C3C-C2C	-2.96	1.35	1.41
3	A	5	HEC	C3C-C2C	-2.95	1.35	1.41
3	B	3	HEC	FE-NB	2.94	2.05	1.92
3	C	5	HEC	C3C-C2C	-2.93	1.35	1.41
3	C	5	HEC	C1D-C2D	2.91	1.43	1.40
3	A	3	HEC	C3B-C4B	2.91	1.45	1.41
3	C	3	HEC	C3C-C2C	-2.89	1.35	1.41
3	C	480	HEC	FE-NB	2.88	2.04	1.92
3	A	3	HEC	C3C-C2C	-2.87	1.35	1.41
3	D	3	HEC	C3B-C4B	2.85	1.45	1.41
3	C	4	HEC	FE-NB	2.83	2.04	1.92
3	D	479	HEC	C3B-C4B	2.79	1.45	1.41
3	D	5	HEC	FE-ND	2.79	2.04	1.92
3	C	480	HEC	C3C-C2C	-2.78	1.35	1.41
3	D	480	HEC	C3B-C4B	2.78	1.45	1.41
3	D	480	HEC	C3C-C4C	2.78	1.45	1.41
3	B	479	HEC	C3C-C2C	-2.76	1.35	1.41
3	C	3	HEC	FE-NC	2.76	2.04	1.92
3	B	5	HEC	C3C-C4C	2.72	1.45	1.41
3	B	3	HEC	C1B-C2B	2.70	1.43	1.40
3	C	479	HEC	C3C-C4C	2.70	1.45	1.41
3	D	5	HEC	C3C-C2C	-2.69	1.35	1.41
3	C	4	HEC	FE-ND	2.68	2.03	1.92
3	A	3	HEC	FE-ND	2.67	2.03	1.92
3	A	5	HEC	C3B-C4B	2.67	1.45	1.41
3	A	480	HEC	FE-NA	2.66	2.03	1.92
3	B	4	HEC	FE-NA	2.64	2.03	1.92
3	B	3	HEC	C3C-C2C	-2.63	1.36	1.41
3	C	479	HEC	FE-NA	2.63	2.03	1.92
3	A	479	HEC	FE-NB	2.56	2.03	1.92
3	D	3	HEC	C3C-C4C	2.53	1.44	1.41
3	B	4	HEC	FE-ND	2.52	2.03	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	HEC	C3C-C4C	2.49	1.44	1.41
3	B	3	HEC	C3B-C4B	2.49	1.44	1.41
3	B	480	HEC	C3B-C4B	2.49	1.44	1.41
3	B	4	HEC	CMD-C2D	2.49	1.56	1.51
3	D	4	HEC	C3C-C4C	2.47	1.44	1.41
3	D	3	HEC	FE-ND	2.47	2.03	1.92
3	C	4	HEC	C3B-C4B	2.46	1.44	1.41
3	C	4	HEC	C3C-C4C	2.44	1.44	1.41
3	B	479	HEC	C3C-C4C	2.42	1.44	1.41
3	C	5	HEC	C3C-C4C	2.41	1.44	1.41
3	A	480	HEC	C3C-C4C	2.37	1.44	1.41
3	D	4	HEC	C3B-C4B	2.36	1.44	1.41
3	D	479	HEC	FE-NB	2.36	2.02	1.92
3	D	3	HEC	CAD-C3D	2.32	1.56	1.52
3	B	3	HEC	CAD-C3D	2.31	1.56	1.52
3	B	480	HEC	FE-NA	2.26	2.02	1.92
3	B	480	HEC	C3C-C4C	2.26	1.44	1.41
3	D	3	HEC	C4B-NB	2.24	1.40	1.37
3	A	3	HEC	C3C-C4C	2.24	1.44	1.41
3	A	5	HEC	CAD-C3D	2.22	1.55	1.52
3	B	480	HEC	FE-NB	2.22	2.01	1.92
3	B	5	HEC	CAD-C3D	2.21	1.55	1.52
3	D	4	HEC	FE-NC	2.20	2.01	1.92
3	D	3	HEC	FE-NB	2.19	2.01	1.92
3	D	3	HEC	FE-NC	2.19	2.01	1.92
3	D	5	HEC	C3B-C4B	2.18	1.44	1.41
3	D	479	HEC	FE-NC	2.13	2.01	1.92
3	C	3	HEC	C3B-C4B	2.12	1.44	1.41
3	C	479	HEC	FE-NC	2.10	2.01	1.92
3	D	5	HEC	FE-NC	2.09	2.01	1.92
3	A	480	HEC	FE-NB	2.09	2.01	1.92
3	D	479	HEC	CAD-C3D	2.02	1.55	1.52
3	B	5	HEC	C4A-NA	2.01	1.39	1.37
3	A	479	HEC	FE-NA	2.01	2.01	1.92

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5	HEC	CBB-CAB-C3B	-7.46	107.44	128.44
3	B	479	HEC	CBB-CAB-C3B	-7.46	107.45	128.44
3	A	4	HEC	CBB-CAB-C3B	-7.40	107.59	128.44
3	D	479	HEC	CBB-CAB-C3B	-7.39	107.63	128.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	479	HEC	CBB-CAB-C3B	-7.17	108.26	128.44
3	A	480	HEC	CBB-CAB-C3B	-7.12	108.39	128.44
3	A	5	HEC	CBB-CAB-C3B	-7.06	108.57	128.44
3	C	4	HEC	CBB-CAB-C3B	-7.04	108.61	128.44
3	C	3	HEC	CBB-CAB-C3B	-6.85	109.16	128.44
3	A	3	HEC	CBB-CAB-C3B	-6.80	109.30	128.44
3	D	5	HEC	CBB-CAB-C3B	-6.72	109.53	128.44
3	D	4	HEC	CBB-CAB-C3B	-6.68	109.63	128.44
3	D	3	HEC	CBB-CAB-C3B	-6.68	109.63	128.44
3	B	4	HEC	CBB-CAB-C3B	-6.63	109.76	128.44
3	B	480	HEC	CBB-CAB-C3B	-6.60	109.85	128.44
3	D	479	HEC	CBC-CAC-C3C	-6.49	110.18	128.44
3	A	3	HEC	CBC-CAC-C3C	-6.41	110.38	128.44
3	D	3	HEC	CBC-CAC-C3C	-6.38	110.47	128.44
3	C	480	HEC	CBB-CAB-C3B	-6.37	110.51	128.44
3	C	5	HEC	CBB-CAB-C3B	-6.34	110.58	128.44
3	D	480	HEC	CBC-CAC-C3C	-6.14	111.15	128.44
3	D	480	HEC	CBB-CAB-C3B	-6.14	111.15	128.44
3	C	3	HEC	CBC-CAC-C3C	-6.13	111.18	128.44
3	A	479	HEC	CBB-CAB-C3B	-6.12	111.21	128.44
3	C	4	HEC	CBC-CAC-C3C	-6.07	111.34	128.44
3	A	3	HEC	CBD-CAD-C3D	-5.96	102.19	112.69
3	B	3	HEC	CBB-CAB-C3B	-5.92	111.76	128.44
3	B	480	HEC	CBC-CAC-C3C	-5.84	112.00	128.44
3	A	4	HEC	CBC-CAC-C3C	-5.50	112.95	128.44
3	D	4	HEC	CBC-CAC-C3C	-5.43	113.14	128.44
3	A	480	HEC	CBC-CAC-C3C	-5.38	113.30	128.44
3	A	479	HEC	CBC-CAC-C3C	-5.13	114.01	128.44
3	B	4	HEC	CBC-CAC-C3C	-4.94	114.53	128.44
3	B	5	HEC	CBC-CAC-C3C	-4.87	114.72	128.44
3	C	480	HEC	CBC-CAC-C3C	-4.85	114.80	128.44
3	D	5	HEC	CBC-CAC-C3C	-4.78	114.98	128.44
3	B	5	HEC	CBA-CAA-C2A	-4.75	103.47	112.35
3	A	5	HEC	CBC-CAC-C3C	-4.52	115.70	128.44
3	C	3	HEC	CMC-C2C-C1C	-4.49	121.71	128.62
3	A	4	HEC	CBA-CAA-C2A	-4.39	104.15	112.35
3	A	3	HEC	CMC-C2C-C1C	-4.35	121.93	128.62
3	B	4	HEC	C4D-ND-C1D	4.32	112.46	106.76
3	B	4	HEC	CBA-CAA-C2A	-4.20	104.50	112.35
3	C	479	HEC	CBC-CAC-C3C	-4.16	116.74	128.44
3	C	5	HEC	CBC-CAC-C3C	-4.09	116.92	128.44
3	A	5	HEC	CMC-C2C-C1C	-4.05	122.39	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	HEC	CBC-CAC-C3C	-4.01	117.16	128.44
3	A	4	HEC	C4D-ND-C1D	3.85	111.84	106.76
3	D	4	HEC	CMC-C2C-C1C	-3.85	122.69	128.62
3	D	4	HEC	C4B-CHC-C1C	-3.83	122.43	127.47
3	A	479	HEC	C4D-ND-C1D	3.80	111.77	106.76
3	D	479	HEC	C4D-ND-C1D	3.78	111.74	106.76
3	C	5	HEC	CMC-C2C-C1C	-3.77	122.82	128.62
3	C	4	HEC	C4D-ND-C1D	3.72	111.67	106.76
3	B	480	HEC	CMC-C2C-C1C	-3.70	122.93	128.62
3	D	479	HEC	C4A-CHB-C1B	-3.68	122.62	127.47
3	C	4	HEC	C4B-CHC-C1C	-3.62	122.71	127.47
3	B	479	HEC	CBC-CAC-C3C	-3.61	118.28	128.44
3	B	3	HEC	CBD-CAD-C3D	-3.60	106.35	112.69
3	C	4	HEC	CMC-C2C-C1C	-3.58	123.12	128.62
3	D	5	HEC	CMC-C2C-C1C	-3.52	123.20	128.62
3	A	5	HEC	CBA-CAA-C2A	-3.48	105.84	112.35
3	A	4	HEC	CMC-C2C-C1C	-3.48	123.28	128.62
3	B	5	HEC	C1A-C2A-C3A	3.47	109.42	106.69
3	B	3	HEC	CMB-C2B-C1B	-3.47	123.29	128.62
3	C	480	HEC	C4D-ND-C1D	3.46	111.32	106.76
3	D	480	HEC	C4D-ND-C1D	3.44	111.30	106.76
3	C	4	HEC	CMB-C2B-C1B	-3.41	123.38	128.62
3	A	479	HEC	C2A-C1A-NA	-3.39	107.09	109.64
3	C	3	HEC	C4D-ND-C1D	3.38	111.21	106.76
3	B	4	HEC	C1D-C2D-C3D	-3.37	104.65	107.00
3	D	4	HEC	C1A-CHA-C4D	-3.37	123.04	127.47
3	A	4	HEC	C4B-CHC-C1C	-3.37	123.04	127.47
3	B	3	HEC	CMC-C2C-C1C	-3.36	123.46	128.62
3	B	479	HEC	CMB-C2B-C1B	-3.35	123.47	128.62
3	B	4	HEC	CBD-CAD-C3D	-3.33	106.83	112.69
3	C	480	HEC	CMC-C2C-C1C	-3.31	123.54	128.62
3	B	480	HEC	C4D-ND-C1D	3.30	111.11	106.76
3	A	479	HEC	C1D-C2D-C3D	-3.28	104.71	107.00
3	D	480	HEC	C2B-C1B-NB	-3.28	106.94	109.41
3	C	5	HEC	C1D-C2D-C3D	-3.26	104.73	107.00
3	B	3	HEC	C4D-ND-C1D	3.25	111.05	106.76
3	A	480	HEC	C4D-ND-C1D	3.23	111.02	106.76
3	D	5	HEC	C4D-ND-C1D	3.22	111.01	106.76
3	D	3	HEC	CBA-CAA-C2A	-3.16	106.44	112.35
3	D	3	HEC	CMC-C2C-C1C	-3.15	123.78	128.62
3	D	479	HEC	C2A-C1A-NA	-3.15	107.28	109.64
3	A	3	HEC	C1D-C2D-C3D	-3.12	104.83	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	HEC	C4A-CHB-C1B	-3.11	123.38	127.47
3	A	4	HEC	C1D-C2D-C3D	-3.10	104.84	107.00
3	D	4	HEC	C4D-ND-C1D	3.09	110.83	106.76
3	B	4	HEC	CMB-C2B-C1B	-3.08	123.88	128.62
3	C	479	HEC	CMC-C2C-C1C	-3.06	123.91	128.62
3	B	480	HEC	C4A-C3A-C2A	3.05	108.83	106.89
3	C	479	HEC	C4D-ND-C1D	3.04	110.77	106.76
3	C	3	HEC	CBA-CAA-C2A	-3.03	106.69	112.35
3	A	479	HEC	CMC-C2C-C1C	-3.00	124.00	128.62
3	B	3	HEC	CMB-C2B-C3B	3.00	129.03	125.72
3	B	479	HEC	C4D-ND-C1D	2.99	110.70	106.76
3	D	5	HEC	CMB-C2B-C1B	-2.98	124.04	128.62
3	A	4	HEC	CMB-C2B-C1B	-2.96	124.07	128.62
3	C	3	HEC	CBD-CAD-C3D	-2.95	107.49	112.69
3	D	5	HEC	C4A-CHB-C1B	-2.94	123.61	127.47
3	B	3	HEC	CBA-CAA-C2A	-2.93	106.87	112.35
3	C	5	HEC	C4B-C3B-C2B	2.92	108.54	106.68
3	B	4	HEC	CMC-C2C-C1C	-2.92	124.13	128.62
3	C	5	HEC	CMD-C2D-C3D	2.92	130.44	124.94
3	A	480	HEC	C2B-C1B-NB	-2.92	107.21	109.41
3	D	5	HEC	C1D-C2D-C3D	-2.91	104.97	107.00
3	D	4	HEC	CBA-CAA-C2A	-2.91	106.92	112.35
3	A	5	HEC	CMC-C2C-C3C	2.89	128.91	125.72
3	B	479	HEC	C4A-CHB-C1B	-2.87	123.70	127.47
3	C	479	HEC	CMB-C2B-C1B	-2.85	124.24	128.62
3	B	479	HEC	CMC-C2C-C1C	-2.84	124.26	128.62
3	C	4	HEC	C2B-C1B-NB	-2.83	107.27	109.41
3	B	479	HEC	C2C-C1C-NC	-2.81	107.29	109.41
3	B	5	HEC	CMC-C2C-C1C	-2.81	124.30	128.62
3	D	479	HEC	CMC-C2C-C1C	-2.80	124.32	128.62
3	A	3	HEC	C4B-C3B-C2B	2.78	108.45	106.68
3	C	5	HEC	C3B-C4B-NB	-2.78	107.51	111.52
3	A	5	HEC	CAD-CBD-CGD	-2.76	104.60	113.47
3	B	3	HEC	C4B-C3B-C2B	2.75	108.43	106.68
3	C	4	HEC	C3B-C2B-C1B	2.74	108.89	107.07
3	C	5	HEC	CMB-C2B-C1B	-2.74	124.41	128.62
3	D	3	HEC	C3A-C4A-NA	-2.72	107.36	109.41
3	A	3	HEC	C4D-ND-C1D	2.71	110.34	106.76
3	B	5	HEC	C2A-C1A-NA	-2.70	107.61	109.64
3	B	4	HEC	C2A-C1A-NA	-2.70	107.61	109.64
3	D	5	HEC	CBA-CAA-C2A	-2.69	107.32	112.35
3	A	480	HEC	C3B-C4B-NB	-2.69	107.64	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5	HEC	C4B-CHC-C1C	-2.68	123.94	127.47
3	A	479	HEC	CMB-C2B-C1B	-2.67	124.52	128.62
3	A	4	HEC	C1A-CHA-C4D	-2.66	123.97	127.47
3	C	4	HEC	C1D-C2D-C3D	-2.65	105.15	107.00
3	C	479	HEC	C3B-C4B-NB	-2.65	107.69	111.52
3	D	4	HEC	CMB-C2B-C1B	-2.65	124.55	128.62
3	D	5	HEC	C3B-C4B-NB	-2.64	107.70	111.52
3	A	480	HEC	C1D-C2D-C3D	-2.64	105.16	107.00
3	D	4	HEC	C2B-C1B-NB	-2.64	107.42	109.41
3	A	3	HEC	C4B-CHC-C1C	-2.62	124.03	127.47
3	B	3	HEC	C3B-C4B-NB	-2.62	107.74	111.52
3	D	3	HEC	C4D-ND-C1D	2.61	110.20	106.76
3	D	3	HEC	C4B-CHC-C1C	-2.61	124.04	127.47
3	D	3	HEC	C4A-C3A-C2A	2.60	108.55	106.89
3	D	480	HEC	C4A-C3A-C2A	2.60	108.55	106.89
3	B	3	HEC	CMC-C2C-C3C	2.59	128.58	125.72
3	D	480	HEC	C3B-C2B-C1B	2.59	108.79	107.07
3	B	5	HEC	C4D-ND-C1D	2.58	110.16	106.76
3	D	5	HEC	C4B-C3B-C2B	2.58	108.32	106.68
3	C	4	HEC	C3B-C4B-NB	-2.56	107.82	111.52
3	A	3	HEC	CBA-CAA-C2A	-2.55	107.58	112.35
3	A	3	HEC	C3C-C2C-C1C	-2.54	105.38	107.07
3	D	479	HEC	CMB-C2B-C1B	-2.54	124.72	128.62
3	B	480	HEC	C3A-C4A-NA	-2.52	107.51	109.41
3	A	480	HEC	CMC-C2C-C1C	-2.52	124.75	128.62
3	D	480	HEC	C1A-CHA-C4D	-2.51	124.16	127.47
3	C	480	HEC	C1D-C2D-C3D	-2.51	105.25	107.00
3	C	480	HEC	CMB-C2B-C1B	-2.51	124.76	128.62
3	B	4	HEC	C3B-C4B-NB	-2.51	107.90	111.52
3	C	480	HEC	C3B-C4B-NB	-2.50	107.91	111.52
3	D	5	HEC	CMD-C2D-C3D	2.50	129.65	124.94
3	A	5	HEC	C4D-C3D-C2D	-2.48	104.35	106.92
3	B	479	HEC	CMB-C2B-C3B	2.48	128.46	125.72
3	D	479	HEC	CMD-C2D-C3D	2.47	129.60	124.94
3	C	5	HEC	CMD-C2D-C1D	-2.47	124.82	128.62
3	D	480	HEC	C1D-C2D-C3D	-2.47	105.28	107.00
3	B	4	HEC	C4A-CHB-C1B	-2.46	124.23	127.47
3	A	480	HEC	C4B-C3B-C2B	2.46	108.25	106.68
3	B	5	HEC	C1D-C2D-C3D	-2.43	105.31	107.00
3	A	3	HEC	C4C-C3C-C2C	2.43	108.22	106.68
3	D	479	HEC	C1D-C2D-C3D	-2.42	105.31	107.00
3	D	5	HEC	C1A-C2A-C3A	2.42	108.59	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	480	HEC	C2B-C1B-NB	-2.41	107.59	109.41
3	C	4	HEC	CAD-CBD-CGD	-2.39	105.78	113.47
3	C	5	HEC	C4D-ND-C1D	2.38	109.89	106.76
3	B	480	HEC	CMB-C2B-C1B	-2.38	124.97	128.62
3	D	480	HEC	C3A-C4A-NA	-2.36	107.63	109.41
3	B	479	HEC	C3B-C4B-NB	-2.36	108.12	111.52
3	A	480	HEC	C1A-CHA-C4D	-2.35	124.38	127.47
3	D	479	HEC	C3B-C4B-NB	-2.35	108.13	111.52
3	D	4	HEC	C4D-C3D-C2D	-2.34	104.50	106.92
3	A	4	HEC	C3B-C4B-NB	-2.33	108.15	111.52
3	A	480	HEC	CAD-CBD-CGD	-2.33	105.99	113.47
3	C	4	HEC	C4A-CHB-C1B	-2.32	124.41	127.47
3	C	479	HEC	C1D-C2D-C3D	-2.32	105.38	107.00
3	A	4	HEC	CAD-CBD-CGD	-2.32	106.00	113.47
3	B	4	HEC	CMB-C2B-C3B	2.32	128.28	125.72
3	A	479	HEC	C3B-C4B-NB	-2.32	108.17	111.52
3	B	5	HEC	C4D-C3D-C2D	-2.31	104.52	106.92
3	C	3	HEC	C2B-C1B-NB	-2.31	107.67	109.41
3	B	480	HEC	C3C-C4C-NC	-2.31	108.18	111.52
3	D	479	HEC	CMD-C2D-C1D	-2.30	125.09	128.62
3	D	3	HEC	C4D-C3D-C2D	-2.29	104.55	106.92
3	C	4	HEC	CBA-CAA-C2A	-2.29	108.07	112.35
3	A	3	HEC	C3B-C4B-NB	-2.28	108.22	111.52
3	D	480	HEC	C3C-C4C-NC	-2.28	108.23	111.52
3	B	480	HEC	CMC-C2C-C3C	2.27	128.23	125.72
3	B	5	HEC	C1A-CHA-C4D	-2.27	124.49	127.47
3	B	480	HEC	C3B-C4B-NB	-2.26	108.25	111.52
3	D	480	HEC	C3B-C4B-NB	-2.26	108.26	111.52
3	D	480	HEC	CMB-C2B-C1B	-2.26	125.15	128.62
3	C	3	HEC	CHD-C1D-ND	2.25	128.34	124.58
3	C	5	HEC	C4A-CHB-C1B	-2.25	124.52	127.47
3	B	480	HEC	C2B-C1B-NB	-2.24	107.72	109.41
3	B	4	HEC	CAD-CBD-CGD	-2.24	106.27	113.47
3	B	479	HEC	C3C-C2C-C1C	2.24	108.56	107.07
3	A	479	HEC	C1A-C2A-C3A	2.24	108.45	106.69
3	C	5	HEC	CBA-CAA-C2A	-2.24	108.17	112.35
3	B	479	HEC	C1D-C2D-C3D	-2.23	105.44	107.00
3	B	4	HEC	C4B-CHC-C1C	-2.23	124.54	127.47
3	C	479	HEC	C2C-C1C-NC	-2.22	107.73	109.41
3	D	480	HEC	C4C-C3C-C2C	2.22	108.09	106.68
3	D	5	HEC	C2B-C1B-NB	-2.21	107.74	109.41
3	B	4	HEC	C3A-C4A-NA	-2.21	107.74	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	HEC	C3B-C4B-NB	-2.21	108.33	111.52
3	D	479	HEC	C1A-C2A-C3A	2.20	108.42	106.69
3	D	3	HEC	C3C-C4C-NC	-2.19	108.35	111.52
3	C	479	HEC	CBD-CAD-C3D	-2.19	108.83	112.69
3	B	4	HEC	C4B-C3B-C2B	2.19	108.07	106.68
3	A	479	HEC	C4A-NA-C1A	2.18	108.85	105.58
3	D	480	HEC	CMC-C2C-C1C	-2.17	125.28	128.62
3	B	4	HEC	C4A-C3A-C2A	2.17	108.28	106.89
3	C	5	HEC	CMB-C2B-C3B	2.16	128.11	125.72
3	D	3	HEC	C3B-C2B-C1B	2.16	108.50	107.07
3	C	480	HEC	C4B-C3B-C2B	2.15	108.05	106.68
3	A	3	HEC	C3C-C4C-NC	-2.14	108.43	111.52
3	B	4	HEC	C3C-C4C-NC	-2.14	108.43	111.52
3	C	479	HEC	C4A-CHB-C1B	-2.14	124.66	127.47
3	B	480	HEC	C4A-CHB-C1B	-2.14	124.66	127.47
3	B	5	HEC	CMD-C2D-C3D	2.14	128.97	124.94
3	C	3	HEC	CMD-C2D-C3D	2.13	128.97	124.94
3	B	480	HEC	C4D-C3D-C2D	-2.12	104.72	106.92
3	D	480	HEC	C4B-CHC-C1C	-2.12	124.68	127.47
3	D	479	HEC	C4B-C3B-C2B	2.12	108.03	106.68
3	A	3	HEC	C4C-CHD-C1D	-2.12	124.69	127.47
3	B	4	HEC	O1A-CGA-CBA	-2.11	115.76	123.03
3	C	480	HEC	C4C-CHD-C1D	-2.11	124.69	127.47
3	D	5	HEC	CMD-C2D-C1D	-2.11	125.38	128.62
3	B	5	HEC	C2B-C1B-NB	-2.11	107.82	109.41
3	C	3	HEC	CMD-C2D-C1D	-2.11	125.38	128.62
3	B	4	HEC	C4C-C3C-C2C	2.10	108.02	106.68
3	A	479	HEC	C3A-C4A-NA	-2.10	107.82	109.41
3	A	5	HEC	C4D-ND-C1D	2.10	109.53	106.76
3	B	3	HEC	C4D-C3D-C2D	-2.10	104.75	106.92
3	C	4	HEC	C4A-C3A-C2A	2.09	108.22	106.89
3	A	3	HEC	C1A-CHA-C4D	-2.09	124.73	127.47
3	D	3	HEC	C2A-C1A-NA	-2.08	108.07	109.64
3	D	3	HEC	C4B-C3B-C2B	2.09	108.01	106.68
3	A	5	HEC	C4B-CHC-C1C	-2.08	124.74	127.47
3	D	4	HEC	C3B-C2B-C1B	2.07	108.45	107.07
3	C	480	HEC	C3A-C4A-NA	-2.08	107.84	109.41
3	D	5	HEC	C2A-C1A-NA	-2.07	108.08	109.64
3	A	5	HEC	C4B-C3B-C2B	2.07	108.00	106.68
3	B	4	HEC	O1D-CGD-CBD	-2.07	115.90	123.03
3	C	479	HEC	CMB-C2B-C3B	2.07	128.00	125.72
3	C	480	HEC	C3B-C2B-C1B	2.06	108.44	107.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4	HEC	O2A-CGA-CBA	2.06	121.51	114.22
3	B	480	HEC	C2A-C1A-NA	-2.06	108.09	109.64
3	A	4	HEC	O1D-CGD-CBD	-2.06	115.94	123.03
3	C	5	HEC	C2D-C1D-CHD	-2.06	122.10	126.00
3	D	5	HEC	CBD-CAD-C3D	-2.05	109.08	112.69
3	A	5	HEC	C1A-C2A-C3A	2.05	108.30	106.69
3	C	3	HEC	C2A-C1A-NA	-2.04	108.10	109.64
3	D	3	HEC	C3B-C4B-NB	-2.04	108.57	111.52
3	C	480	HEC	CBD-CAD-C3D	-2.04	109.11	112.69
3	D	3	HEC	C2B-C1B-NB	-2.02	107.88	109.41
3	C	479	HEC	C4B-C3B-C2B	2.02	107.97	106.68
3	A	5	HEC	CMB-C2B-C1B	-2.00	125.54	128.62
3	A	5	HEC	C1A-CHA-C4D	-2.00	124.84	127.47

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	441/452 (97%)	0.01	6 (1%) 72 80	15, 27, 42, 53	2 (0%)
1	B	441/452 (97%)	-0.30	0 100 100	12, 23, 35, 41	2 (0%)
1	C	441/452 (97%)	-0.29	1 (0%) 93 97	14, 24, 34, 41	3 (0%)
1	D	441/452 (97%)	0.21	11 (2%) 54 65	23, 39, 56, 62	0
All	All	1764/1808 (97%)	-0.09	18 (1%) 77 87	12, 27, 48, 62	7 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	LEU	3.5
1	A	477	SER	3.1
1	D	158	LEU	2.9
1	A	472	LYS	2.9
1	D	296	LYS	2.9
1	D	37	THR	2.5
1	A	151	GLY	2.5
1	D	95	ALA	2.5
1	D	172	ALA	2.3
1	D	295	GLY	2.3
1	C	221	LYS	2.3
1	D	174	GLY	2.2
1	A	470	ALA	2.2
1	D	477	SER	2.2
1	D	59	THR	2.1
1	A	310	PHE	2.1
1	D	468	GLU	2.0
1	D	303	ILE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	B	483	4/4	0.41	21.81	44,45,46,47	0
2	CA	B	2	1/1	0.13	18.37	62,62,62,62	0
5	EDO	C	7	4/4	0.19	12.15	50,50,50,51	0
5	EDO	C	484	4/4	0.19	7.01	51,51,51,53	0
2	CA	C	2	1/1	0.20	3.85	81,81,81,81	0
5	EDO	C	482	4/4	0.22	3.35	40,40,42,45	0
5	EDO	C	483	4/4	0.18	3.02	38,39,39,39	0
5	EDO	C	9	4/4	0.22	2.71	42,44,44,44	0
4	SO3	B	482	4/4	0.12	2.47	28,28,30,33	0
5	EDO	C	10	4/4	0.13	0.85	23,26,27,29	0
3	HEC	C	4	43/43	0.13	0.83	13,17,25,27	0
3	HEC	A	4	43/43	0.12	0.74	16,21,30,32	0
3	HEC	D	5	43/43	0.14	0.63	28,30,38,43	0
3	HEC	B	5	43/43	0.13	0.60	14,18,28,33	0
3	HEC	B	479	43/43	0.12	0.58	10,15,17,18	0
3	HEC	C	3	43/43	0.12	0.54	9,13,17,19	0
3	HEC	D	479	43/43	0.15	0.51	25,32,36,37	0
3	HEC	D	4	43/43	0.14	0.44	24,27,35,41	0
3	HEC	B	4	43/43	0.11	0.36	10,16,21,27	0
3	HEC	C	479	43/43	0.12	0.35	12,15,18,21	0
3	HEC	B	480	43/43	0.12	0.31	13,16,19,20	0
3	HEC	B	3	43/43	0.11	0.26	9,14,20,23	0
5	EDO	B	12	4/4	0.14	0.23	33,35,36,38	0
3	HEC	C	480	43/43	0.12	0.22	14,17,21,22	0
3	HEC	C	5	43/43	0.12	0.19	16,20,30,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HEC	A	5	43/43	0.13	0.18	18,23,32,40	0
2	CA	A	1	1/1	0.12	0.17	18,18,18,18	0
3	HEC	A	480	43/43	0.13	-0.05	24,30,32,35	0
3	HEC	A	3	43/43	0.11	-0.08	16,21,27,30	0
3	HEC	A	479	43/43	0.12	-0.13	15,23,26,27	0
3	HEC	D	3	43/43	0.16	-0.19	25,30,33,35	0
3	HEC	D	480	43/43	0.16	-0.27	42,45,47,49	0
5	EDO	D	482	4/4	0.12	-0.31	52,53,53,54	0
5	EDO	D	11	4/4	0.14	-0.38	43,44,45,46	0
4	SO3	B	481	4/4	0.12	-0.48	48,49,49,50	0
2	CA	A	2	1/1	0.12	-0.71	93,93,93,93	0
4	SO3	D	481	4/4	0.12	-0.90	45,46,46,47	0
5	EDO	A	6	4/4	0.17	-0.92	37,37,37,37	0
2	CA	C	1	1/1	0.10	-1.03	19,19,19,19	0
4	SO3	C	481	4/4	0.10	-1.19	23,23,27,27	0
5	EDO	A	8	4/4	0.10	-1.89	37,37,38,38	0
2	CA	B	1	1/1	0.10	-3.21	19,19,19,19	0
2	CA	D	1	1/1	0.09	-3.83	29,29,29,29	0
4	SO3	A	481	4/4	0.10	-3.93	28,29,30,31	0
2	CA	D	2	1/1	0.08	-4.47	82,82,82,82	0

6.5 Other polymers ⓘ

There are no such residues in this entry.