



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:09 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

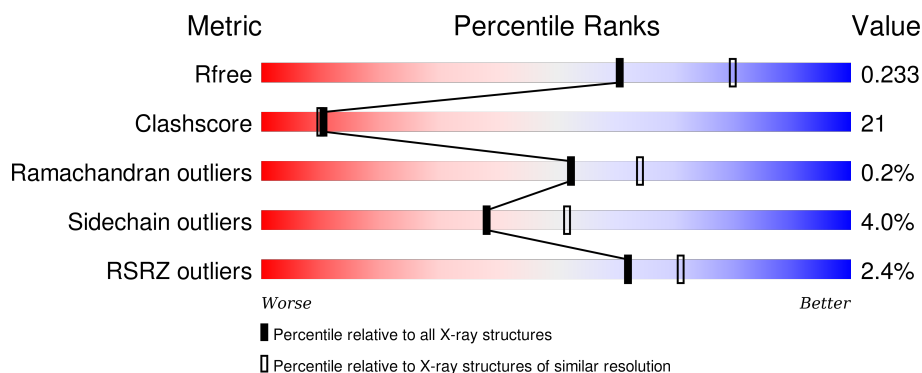
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	452	<div> <div>4%</div> <div>71%</div> <div>23%</div> <div>• •</div> </div>
1	B	452	<div> <div>78%</div> <div>18%</div> <div>• •</div> </div>
1	C	452	<div> <div>77%</div> <div>19%</div> <div>• •</div> </div>
1	D	452	<div> <div>5%</div> <div>61%</div> <div>33%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO3	B	482	-	-	-	X
5	EDO	B	483	-	-	X	X
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	-
5	EDO	D	482	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15858 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

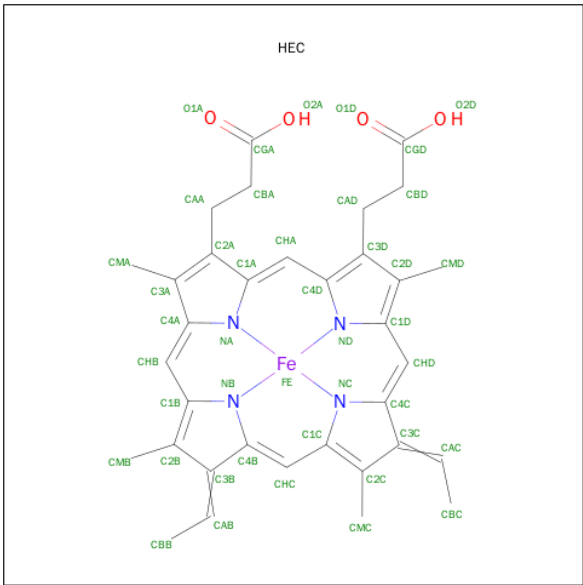
- Molecule 1 is a protein called Cytochrome c-552.

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).



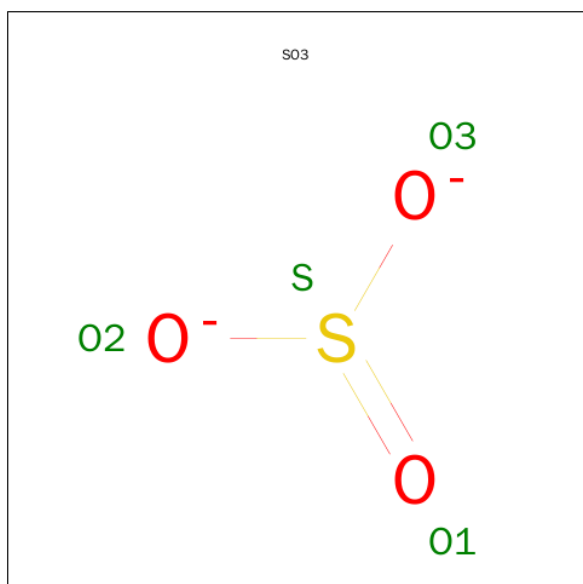
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0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

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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	

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

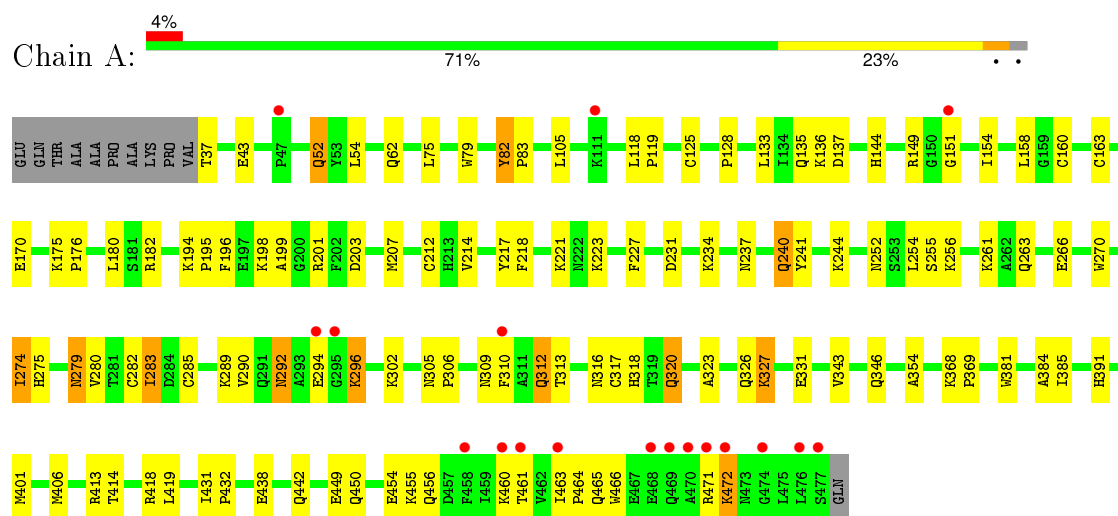
- Molecule 6 is water.

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

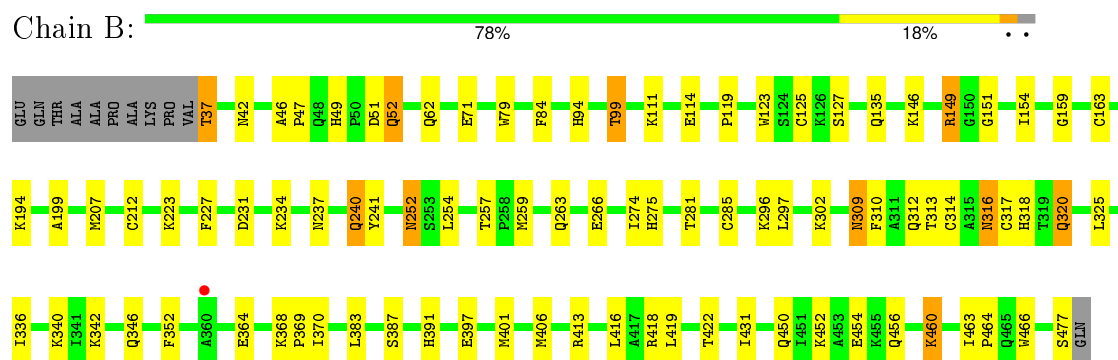
3 Residue-property plots

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.

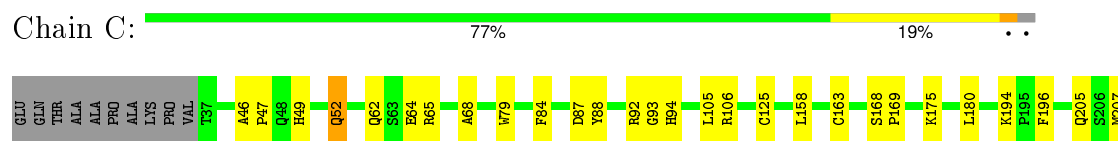
• Molecule 1: Cytochrome c-552

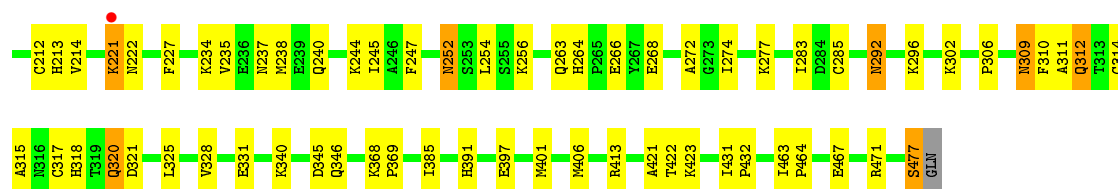


• Molecule 1: Cytochrome c-552

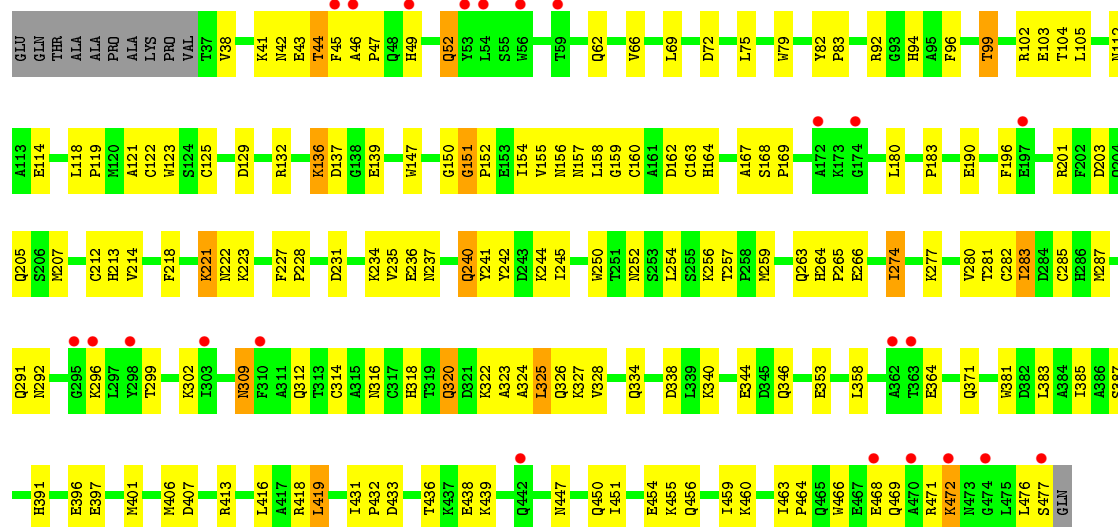


• Molecule 1: Cytochrome c-552





• Molecule 1: Cytochrome c-552



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)	0.35 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (622) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:5:HEC:HMB1	3:B:5:HEC:HBB3	1.52	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	52	64
1	D	441/452 (98%)	413 (94%)	25 (6%)	3 (1%)	26	31
All	All	1765/1808 (98%)	1697 (96%)	64 (4%)	4 (0%)	52	64

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%)	37	50
1	B	364/370 (98%)	348 (96%)	16 (4%)	35	46
1	C	366/370 (99%)	354 (97%)	12 (3%)	45	61
1	D	364/370 (98%)	349 (96%)	15 (4%)	37	50
All	All	1457/1480 (98%)	1399 (96%)	58 (4%)	38	52

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
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

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Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 molecules 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	24,50,50	2.56	5 (20%)	19,82,82	3.25	6 (31%)
3	HEC	A	4	1,2	24,50,50	2.39	3 (12%)	19,82,82	3.14	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	A	479	1,4	24,50,50	2.36	3 (12%)	19,82,82	2.52	4 (21%)
3	HEC	A	480	1	24,50,50	2.38	3 (12%)	19,82,82	2.82	4 (21%)
4	SO3	A	481	3	1,3,3	0.84	0	0,3,3	0.00	-
3	HEC	A	5	1	24,50,50	2.29	4 (16%)	19,82,82	2.95	6 (31%)
5	EDO	A	6	-	3,3,3	0.37	0	2,2,2	0.94	0
5	EDO	A	8	-	3,3,3	0.50	0	2,2,2	0.34	0
5	EDO	B	12	-	3,3,3	0.51	0	2,2,2	0.51	0
3	HEC	B	3	1,2	24,50,50	2.21	5 (20%)	19,82,82	2.68	7 (36%)
3	HEC	B	4	1,2	24,50,50	2.37	5 (20%)	19,82,82	2.98	7 (36%)
3	HEC	B	479	1,4	24,50,50	2.13	4 (16%)	19,82,82	2.53	4 (21%)
3	HEC	B	480	1	24,50,50	2.29	5 (20%)	19,82,82	2.77	5 (26%)
4	SO3	B	481	-	1,3,3	0.52	0	0,3,3	0.00	-
4	SO3	B	482	3	1,3,3	0.46	0	0,3,3	0.00	-
5	EDO	B	483	-	3,3,3	0.55	0	2,2,2	0.26	0
3	HEC	B	5	1	24,50,50	2.40	5 (20%)	19,82,82	3.00	5 (26%)
5	EDO	C	10	-	3,3,3	0.45	0	2,2,2	0.52	0
3	HEC	C	3	1,2	24,50,50	2.16	3 (12%)	19,82,82	3.06	5 (26%)
3	HEC	C	4	1,2	24,50,50	2.33	3 (12%)	19,82,82	3.04	6 (31%)
3	HEC	C	479	1,4	24,50,50	2.33	3 (12%)	19,82,82	2.65	5 (26%)
3	HEC	C	480	1	24,50,50	2.29	4 (16%)	19,82,82	2.64	6 (31%)
4	SO3	C	481	3	1,3,3	0.33	0	0,3,3	0.00	-
5	EDO	C	482	-	3,3,3	0.43	0	2,2,2	0.69	0
5	EDO	C	483	-	3,3,3	0.44	0	2,2,2	0.52	0
5	EDO	C	484	-	3,3,3	0.48	0	2,2,2	0.34	0
3	HEC	C	5	1	24,50,50	2.29	3 (12%)	19,82,82	2.72	9 (47%)
5	EDO	C	7	-	3,3,3	0.40	0	2,2,2	0.64	0
5	EDO	C	9	-	3,3,3	0.47	0	2,2,2	0.79	0
5	EDO	D	11	-	3,3,3	0.35	0	2,2,2	0.85	0
3	HEC	D	3	1,2	24,50,50	2.40	5 (20%)	19,82,82	2.93	5 (26%)
3	HEC	D	4	1,2	24,50,50	2.37	3 (12%)	19,82,82	2.87	6 (31%)
3	HEC	D	479	1,4	24,50,50	2.43	4 (16%)	19,82,82	3.03	5 (26%)
3	HEC	D	480	1	24,50,50	2.44	4 (16%)	19,82,82	2.68	3 (15%)
4	SO3	D	481	3	1,3,3	0.60	0	0,3,3	0.00	-
5	EDO	D	482	-	3,3,3	0.48	0	2,2,2	0.43	0
3	HEC	D	5	1	24,50,50	2.25	3 (12%)	19,82,82	2.76	6 (31%)

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. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	A	3	1,2	-	0/6/54/54	0/0/8/8
3	HEC	A	4	1,2	-	0/6/54/54	0/0/8/8
3	HEC	A	479	1,4	-	0/6/54/54	0/0/8/8
3	HEC	A	480	1	-	0/6/54/54	0/0/8/8
4	SO3	A	481	3	-	0/0/0/0	0/0/0/0
3	HEC	A	5	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
3	HEC	B	4	1,2	-	0/6/54/54	0/0/8/8
3	HEC	B	479	1,4	-	0/6/54/54	0/0/8/8
3	HEC	B	480	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
5	EDO	C	10	-	-	0/1/1/1	0/0/0/0
3	HEC	C	3	1,2	-	0/6/54/54	0/0/8/8
3	HEC	C	4	1,2	-	0/6/54/54	0/0/8/8
3	HEC	C	479	1,4	-	0/6/54/54	0/0/8/8
3	HEC	C	480	1	-	0/6/54/54	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	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
3	HEC	D	4	1,2	-	0/6/54/54	0/0/8/8
3	HEC	D	479	1,4	-	0/6/54/54	0/0/8/8
3	HEC	D	480	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3	HEC	C3B-C2B	-8.32	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4	HEC	C3B-C2B	-6.65	1.33	1.40
3	C	480	HEC	C3B-C2B	-6.56	1.33	1.40
3	D	479	HEC	C3C-C2C	-6.42	1.34	1.40
3	C	5	HEC	C3B-C2B	-6.39	1.34	1.40
3	D	480	HEC	C3B-C2B	-6.37	1.34	1.40
3	C	4	HEC	C3B-C2B	-6.36	1.34	1.40
3	B	4	HEC	C3B-C2B	-6.34	1.34	1.40
3	C	479	HEC	C3B-C2B	-6.31	1.34	1.40
3	D	4	HEC	C3B-C2B	-6.26	1.34	1.40
3	D	3	HEC	C3B-C2B	-6.25	1.34	1.40
3	A	479	HEC	C3B-C2B	-6.24	1.34	1.40
3	A	480	HEC	C3C-C2C	-6.23	1.34	1.40
3	B	480	HEC	C3B-C2B	-6.21	1.34	1.40
3	D	480	HEC	C3C-C2C	-6.17	1.34	1.40
3	B	5	HEC	C3B-C2B	-6.13	1.34	1.40
3	A	480	HEC	C3B-C2B	-6.10	1.34	1.40
3	D	5	HEC	C3B-C2B	-5.95	1.34	1.40
3	C	4	HEC	C3C-C2C	-5.93	1.34	1.40
3	B	5	HEC	C3C-C2C	-5.92	1.34	1.40
3	A	5	HEC	C3B-C2B	-5.88	1.34	1.40
3	A	479	HEC	C3C-C2C	-5.87	1.34	1.40
3	B	3	HEC	C3B-C2B	-5.83	1.34	1.40
3	D	479	HEC	C3B-C2B	-5.71	1.34	1.40
3	D	4	HEC	C3C-C2C	-5.69	1.34	1.40
3	B	479	HEC	C3B-C2B	-5.69	1.34	1.40
3	C	479	HEC	C3C-C2C	-5.58	1.34	1.40
3	C	3	HEC	C3B-C2B	-5.50	1.35	1.40
3	D	3	HEC	C3C-C2C	-5.46	1.35	1.40
3	B	4	HEC	C3C-C2C	-5.43	1.35	1.40
3	B	480	HEC	C3C-C2C	-5.37	1.35	1.40
3	A	4	HEC	C3C-C2C	-5.25	1.35	1.40
3	A	5	HEC	C3C-C2C	-5.23	1.35	1.40
3	C	5	HEC	C3C-C2C	-5.17	1.35	1.40
3	C	3	HEC	C3C-C2C	-5.09	1.35	1.40
3	A	3	HEC	C3C-C2C	-5.06	1.35	1.40
3	C	480	HEC	C3C-C2C	-4.86	1.35	1.40
3	B	479	HEC	C3C-C2C	-4.83	1.35	1.40
3	D	5	HEC	C3C-C2C	-4.67	1.35	1.40
3	B	3	HEC	C3C-C2C	-4.54	1.36	1.40
3	B	3	HEC	C4B-NB	2.01	1.39	1.36
3	C	480	HEC	CMC-C2C	2.04	1.56	1.51
3	B	480	HEC	C4A-NA	2.07	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	479	HEC	CAD-C3D	2.08	1.55	1.52
3	A	3	HEC	C4B-NB	2.10	1.39	1.36
3	D	480	HEC	C4A-NA	2.11	1.39	1.36
3	B	479	HEC	C4B-NB	2.18	1.39	1.36
3	A	3	HEC	CMC-C2C	2.24	1.56	1.51
3	B	5	HEC	CAD-C3D	2.28	1.55	1.52
3	A	5	HEC	CAD-C3D	2.29	1.55	1.52
3	B	480	HEC	C1A-NA	2.29	1.39	1.36
3	B	3	HEC	CAD-C3D	2.38	1.56	1.52
3	D	3	HEC	CAD-C3D	2.38	1.56	1.52
3	B	5	HEC	C4A-NA	2.40	1.39	1.36
3	B	4	HEC	CMB-C2B	2.47	1.57	1.51
3	B	4	HEC	CMD-C2D	2.53	1.56	1.51
3	D	3	HEC	C4B-NB	2.64	1.40	1.36
3	B	480	HEC	C3D-C2D	4.84	1.52	1.37
3	C	4	HEC	C3D-C2D	4.94	1.52	1.37
3	B	479	HEC	C3D-C2D	4.99	1.52	1.37
3	C	479	HEC	C3D-C2D	5.01	1.52	1.37
3	A	5	HEC	C3D-C2D	5.10	1.52	1.37
3	A	3	HEC	C3D-C2D	5.15	1.52	1.37
3	B	4	HEC	C3D-C2D	5.21	1.53	1.37
3	C	5	HEC	C3D-C2D	5.28	1.53	1.37
3	B	5	HEC	C3D-C2D	5.29	1.53	1.37
3	C	480	HEC	C3D-C2D	5.34	1.53	1.37
3	A	480	HEC	C3D-C2D	5.34	1.53	1.37
3	D	3	HEC	C3D-C2D	5.36	1.53	1.37
3	D	4	HEC	C3D-C2D	5.43	1.53	1.37
3	C	3	HEC	C3D-C2D	5.47	1.53	1.37
3	B	3	HEC	C3D-C2D	5.50	1.54	1.37
3	A	479	HEC	C3D-C2D	5.52	1.54	1.37
3	D	5	HEC	C3D-C2D	5.54	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	479	HEC	C3D-C2D	5.63	1.54	1.37

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5	HEC	CBB-CAB-C3B	-8.96	107.44	127.35
3	B	479	HEC	CBB-CAB-C3B	-8.96	107.45	127.35
3	A	4	HEC	CBB-CAB-C3B	-8.89	107.59	127.35
3	D	479	HEC	CBB-CAB-C3B	-8.87	107.63	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	479	HEC	CBB-CAB-C3B	-8.59	108.26	127.35
3	A	480	HEC	CBB-CAB-C3B	-8.53	108.39	127.35
3	A	5	HEC	CBB-CAB-C3B	-8.45	108.57	127.35
3	C	4	HEC	CBB-CAB-C3B	-8.43	108.61	127.35
3	C	3	HEC	CBB-CAB-C3B	-8.19	109.16	127.35
3	A	3	HEC	CBB-CAB-C3B	-8.12	109.30	127.35
3	D	5	HEC	CBB-CAB-C3B	-8.02	109.53	127.35
3	D	4	HEC	CBB-CAB-C3B	-7.97	109.63	127.35
3	D	3	HEC	CBB-CAB-C3B	-7.97	109.63	127.35
3	B	4	HEC	CBB-CAB-C3B	-7.92	109.76	127.35
3	B	480	HEC	CBB-CAB-C3B	-7.87	109.85	127.35
3	D	479	HEC	CBC-CAC-C3C	-7.73	110.18	127.35
3	A	3	HEC	CBC-CAC-C3C	-7.64	110.38	127.35
3	D	3	HEC	CBC-CAC-C3C	-7.60	110.47	127.35
3	C	480	HEC	CBB-CAB-C3B	-7.58	110.51	127.35
3	C	5	HEC	CBB-CAB-C3B	-7.55	110.58	127.35
3	D	480	HEC	CBC-CAC-C3C	-7.29	111.15	127.35
3	D	480	HEC	CBB-CAB-C3B	-7.29	111.15	127.35
3	C	3	HEC	CBC-CAC-C3C	-7.28	111.18	127.35
3	A	479	HEC	CBB-CAB-C3B	-7.26	111.21	127.35
3	C	4	HEC	CBC-CAC-C3C	-7.20	111.34	127.35
3	B	3	HEC	CBB-CAB-C3B	-7.02	111.76	127.35
3	B	480	HEC	CBC-CAC-C3C	-6.91	112.00	127.35
3	A	4	HEC	CBC-CAC-C3C	-6.48	112.95	127.35
3	D	4	HEC	CBC-CAC-C3C	-6.39	113.14	127.35
3	A	480	HEC	CBC-CAC-C3C	-6.32	113.30	127.35
3	A	479	HEC	CBC-CAC-C3C	-6.00	114.01	127.35
3	B	4	HEC	CBC-CAC-C3C	-5.77	114.53	127.35
3	A	3	HEC	CBD-CAD-C3D	-5.77	102.19	112.53
3	B	5	HEC	CBC-CAC-C3C	-5.68	114.72	127.35
3	C	480	HEC	CBC-CAC-C3C	-5.65	114.80	127.35
3	D	5	HEC	CBC-CAC-C3C	-5.57	114.98	127.35
3	A	5	HEC	CBC-CAC-C3C	-5.24	115.70	127.35
3	B	5	HEC	CBA-CAA-C2A	-5.06	103.47	112.53
3	C	479	HEC	CBC-CAC-C3C	-4.78	116.74	127.35
3	C	5	HEC	CBC-CAC-C3C	-4.70	116.92	127.35
3	A	4	HEC	CBA-CAA-C2A	-4.67	104.15	112.53
3	B	3	HEC	CBC-CAC-C3C	-4.59	117.16	127.35
3	B	4	HEC	CBA-CAA-C2A	-4.48	104.50	112.53
3	A	5	HEC	CAD-CBD-CGD	-4.45	104.60	112.75
3	B	479	HEC	CBC-CAC-C3C	-4.08	118.28	127.35
3	C	3	HEC	CMC-C2C-C1C	-4.02	121.71	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3	HEC	CMC-C2C-C1C	-3.89	121.93	128.36
3	C	4	HEC	CAD-CBD-CGD	-3.80	105.78	112.75
3	A	5	HEC	CBA-CAA-C2A	-3.73	105.84	112.53
3	A	480	HEC	CAD-CBD-CGD	-3.69	105.99	112.75
3	A	4	HEC	CAD-CBD-CGD	-3.68	106.00	112.75
3	A	5	HEC	CMC-C2C-C1C	-3.61	122.39	128.36
3	B	4	HEC	CAD-CBD-CGD	-3.53	106.27	112.75
3	B	3	HEC	CBD-CAD-C3D	-3.45	106.35	112.53
3	D	4	HEC	CMC-C2C-C1C	-3.43	122.69	128.36
3	D	3	HEC	CBA-CAA-C2A	-3.40	106.44	112.53
3	C	5	HEC	CMC-C2C-C1C	-3.35	122.82	128.36
3	B	480	HEC	CMC-C2C-C1C	-3.28	122.93	128.36
3	C	3	HEC	CBA-CAA-C2A	-3.26	106.69	112.53
3	B	4	HEC	CBD-CAD-C3D	-3.18	106.83	112.53
3	C	4	HEC	CMC-C2C-C1C	-3.17	123.12	128.36
3	B	3	HEC	CBA-CAA-C2A	-3.16	106.87	112.53
3	D	4	HEC	CBA-CAA-C2A	-3.13	106.92	112.53
3	D	5	HEC	CMC-C2C-C1C	-3.12	123.20	128.36
3	C	5	HEC	CAD-CBD-CGD	-3.11	107.04	112.75
3	A	4	HEC	CMC-C2C-C1C	-3.08	123.28	128.36
3	B	3	HEC	CMB-C2B-C1B	-3.07	123.29	128.36
3	C	4	HEC	CMB-C2B-C1B	-3.01	123.38	128.36
3	D	4	HEC	CAA-CBA-CGA	-2.99	107.26	112.75
3	B	3	HEC	CAA-C2A-C1A	-2.99	123.77	127.01
3	B	3	HEC	CMC-C2C-C1C	-2.96	123.46	128.36
3	B	479	HEC	CMB-C2B-C1B	-2.96	123.47	128.36
3	C	480	HEC	CMC-C2C-C1C	-2.92	123.54	128.36
3	D	5	HEC	CBA-CAA-C2A	-2.91	107.32	112.53
3	D	480	HEC	CAD-CBD-CGD	-2.88	107.46	112.75
3	C	3	HEC	CBD-CAD-C3D	-2.81	107.49	112.53
3	D	3	HEC	CMC-C2C-C1C	-2.77	123.78	128.36
3	A	3	HEC	CBA-CAA-C2A	-2.76	107.58	112.53
3	B	4	HEC	CMB-C2B-C1B	-2.71	123.88	128.36
3	C	479	HEC	CMC-C2C-C1C	-2.69	123.91	128.36
3	A	479	HEC	CMC-C2C-C1C	-2.64	124.00	128.36
3	D	5	HEC	CMB-C2B-C1B	-2.61	124.04	128.36
3	B	5	HEC	CAA-C2A-C1A	-2.60	124.19	127.01
3	A	4	HEC	CMB-C2B-C1B	-2.60	124.07	128.36
3	C	480	HEC	CAA-C2A-C1A	-2.59	124.20	127.01
3	B	4	HEC	CMC-C2C-C1C	-2.56	124.13	128.36
3	C	479	HEC	CMB-C2B-C1B	-2.49	124.24	128.36
3	C	4	HEC	CBA-CAA-C2A	-2.49	108.07	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	479	HEC	CMC-C2C-C1C	-2.48	124.26	128.36
3	B	5	HEC	CMC-C2C-C1C	-2.46	124.30	128.36
3	D	479	HEC	CMC-C2C-C1C	-2.44	124.32	128.36
3	C	5	HEC	CBA-CAA-C2A	-2.43	108.17	112.53
3	A	5	HEC	CAA-CBA-CGA	-2.41	108.34	112.75
3	C	5	HEC	CMB-C2B-C1B	-2.39	124.41	128.36
3	B	480	HEC	CAD-CBD-CGD	-2.36	108.42	112.75
3	C	480	HEC	CAD-CBD-CGD	-2.34	108.46	112.75
3	A	479	HEC	CMB-C2B-C1B	-2.32	124.52	128.36
3	D	4	HEC	CMB-C2B-C1B	-2.31	124.55	128.36
3	D	479	HEC	CMB-C2B-C1B	-2.20	124.72	128.36
3	A	480	HEC	CMC-C2C-C1C	-2.18	124.75	128.36
3	C	480	HEC	CMB-C2B-C1B	-2.18	124.76	128.36
3	C	5	HEC	CMD-C2D-C1D	-2.14	124.82	128.36
3	A	3	HEC	CAA-C2A-C1A	-2.13	124.69	127.01
3	C	479	HEC	CBD-CAD-C3D	-2.07	108.83	112.53
3	B	480	HEC	CMB-C2B-C1B	-2.05	124.97	128.36
3	C	5	HEC	C4B-C3B-C2B	2.03	108.54	106.35
3	D	479	HEC	CMD-C2D-C3D	2.09	129.60	125.24
3	D	5	HEC	CMD-C2D-C3D	2.11	129.65	125.24
3	C	5	HEC	CMD-C2D-C3D	2.49	130.44	125.24
3	D	3	HEC	CAD-C3D-C4D	2.68	129.92	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 217 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	HEC	10	0
3	A	4	HEC	10	0
3	A	479	HEC	7	0
3	A	480	HEC	15	0
3	A	5	HEC	11	0
3	B	3	HEC	6	0
3	B	4	HEC	11	0
3	B	479	HEC	7	0
3	B	480	HEC	7	0
5	B	483	EDO	10	0
3	B	5	HEC	11	0
3	C	3	HEC	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	HEC	11	0
3	C	479	HEC	7	0
3	C	480	HEC	7	0
5	C	483	EDO	1	0
5	C	484	EDO	3	0
3	C	5	HEC	8	0
5	C	9	EDO	4	0
3	D	3	HEC	8	0
3	D	4	HEC	8	0
3	D	479	HEC	16	0
3	D	480	HEC	9	0
5	D	482	EDO	8	0
3	D	5	HEC	11	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.29	18 (4%) 41 50	15, 27, 42, 53	2 (0%)
1	B	441/452 (97%)	-0.00	1 (0%) 95 97	12, 23, 35, 41	2 (0%)
1	C	441/452 (97%)	-0.04	1 (0%) 95 97	14, 24, 34, 41	3 (0%)
1	D	441/452 (97%)	0.48	23 (5%) 31 39	23, 39, 56, 62	0
All	All	1764/1808 (97%)	0.18	43 (2%) 62 71	12, 27, 48, 62	7 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	LYS	3.9
1	A	476	LEU	3.8
1	A	477	SER	3.8
1	D	295	GLY	3.7
1	D	296	LYS	3.4
1	D	362	ALA	3.2
1	A	461	THR	3.1
1	D	174	GLY	3.0
1	D	468	GLU	3.0
1	C	221	LYS	2.8
1	D	477	SER	2.8
1	D	45	PHE	2.8
1	A	468	GLU	2.7
1	A	460	LYS	2.7
1	D	442	GLN	2.6
1	D	474	GLY	2.6
1	D	472	LYS	2.5
1	A	310	PHE	2.5
1	D	363	THR	2.5
1	D	197	GLU	2.5
1	B	360	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	303	ILE	2.4
1	A	458	PHE	2.4
1	A	463	ILE	2.4
1	A	151	GLY	2.3
1	A	470	ALA	2.3
1	D	56	TRP	2.3
1	D	298	TYR	2.3
1	D	54	LEU	2.3
1	D	172	ALA	2.2
1	A	295	GLY	2.2
1	D	46	ALA	2.2
1	D	59	THR	2.2
1	A	47	PRO	2.2
1	A	474	GLY	2.1
1	A	469	GLN	2.1
1	D	470	ALA	2.1
1	D	49	HIS	2.1
1	A	111	LYS	2.1
1	D	310	PHE	2.0
1	A	294	GLU	2.0
1	A	471	ARG	2.0
1	D	53	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	B	483	4/4	0.88	0.55	16.58	44,45,46,47	0
5	EDO	C	7	4/4	0.92	0.22	9.43	50,50,50,51	0
5	EDO	C	484	4/4	0.92	0.23	7.34	51,51,51,53	0
5	EDO	C	483	4/4	0.94	0.22	4.25	38,39,39,39	0
4	SO3	B	482	4/4	0.98	0.15	3.45	28,28,30,33	0
5	EDO	C	482	4/4	0.90	0.21	2.33	40,40,42,45	0
5	EDO	C	9	4/4	0.91	0.18	1.56	42,44,44,44	0
3	HEC	B	3	43/43	0.98	0.14	0.87	9,14,20,23	0
3	HEC	D	5	43/43	0.97	0.17	0.84	28,30,38,43	0
3	HEC	C	4	43/43	0.97	0.15	0.83	13,17,25,27	0
3	HEC	C	5	43/43	0.98	0.15	0.81	16,20,30,32	0
3	HEC	D	479	43/43	0.97	0.16	0.78	25,32,36,37	0
3	HEC	C	3	43/43	0.99	0.14	0.57	9,13,17,19	0
3	HEC	A	480	43/43	0.96	0.19	0.52	24,30,32,35	0
3	HEC	B	479	43/43	0.99	0.13	0.50	10,15,17,18	0
3	HEC	A	4	43/43	0.97	0.13	0.42	16,21,30,32	0
3	HEC	B	4	43/43	0.98	0.14	0.42	10,16,21,27	0
3	HEC	B	480	43/43	0.98	0.14	0.40	13,16,19,20	0
3	HEC	A	479	43/43	0.98	0.14	0.39	15,23,26,27	0
3	HEC	C	479	43/43	0.98	0.14	0.36	12,15,18,21	0
3	HEC	D	4	43/43	0.97	0.15	0.27	24,27,35,41	0
3	HEC	B	5	43/43	0.98	0.15	0.26	14,18,28,33	0
3	HEC	C	480	43/43	0.98	0.14	0.23	14,17,21,22	0
3	HEC	A	3	43/43	0.98	0.15	0.22	16,21,27,30	0
5	EDO	C	10	4/4	0.97	0.14	0.21	23,26,27,29	0
3	HEC	A	5	43/43	0.97	0.14	0.02	18,23,32,40	0
3	HEC	D	3	43/43	0.97	0.17	-0.01	25,30,33,35	0
3	HEC	D	480	43/43	0.94	0.21	-0.01	42,45,47,49	0
4	SO3	D	481	4/4	0.94	0.15	-0.07	45,46,46,47	0
5	EDO	D	482	4/4	0.91	0.14	-0.31	52,53,53,54	0
5	EDO	A	6	4/4	0.94	0.18	-0.60	37,37,37,37	0
4	SO3	A	481	4/4	0.98	0.13	-0.72	28,29,30,31	0
5	EDO	B	12	4/4	0.95	0.12	-0.95	33,35,36,38	0
4	SO3	B	481	4/4	0.96	0.13	-0.96	48,49,49,50	0
4	SO3	C	481	4/4	0.98	0.11	-0.97	23,23,27,27	0
2	CA	A	1	1/1	0.99	0.12	-1.05	18,18,18,18	0
5	EDO	D	11	4/4	0.94	0.14	-1.05	43,44,45,46	0
2	CA	C	1	1/1	0.98	0.11	-1.15	19,19,19,19	0
5	EDO	A	8	4/4	0.96	0.11	-3.30	37,37,38,38	0
2	CA	B	1	1/1	0.99	0.10	-3.39	19,19,19,19	0
2	CA	D	1	1/1	0.99	0.09	-4.00	29,29,29,29	0
2	CA	A	2	1/1	0.65	0.12	-	93,93,93,93	0
2	CA	C	2	1/1	0.38	0.21	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	B	2	1/1	0.89	0.17	-	62,62,62,62	0
2	CA	D	2	1/1	0.91	0.07	-	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.