



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:21 PM GMT

PDB ID : 3TOR
Title : Crystal structure of Escherichia coli NrfA with Europium bound
Authors : Lockwood, C.W.J.; Clarke, T.A.; Butt, J.N.; Hemmings, A.M.; Richardson, D.J.
Deposited on : 2011-09-06
Resolution : 2.00 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

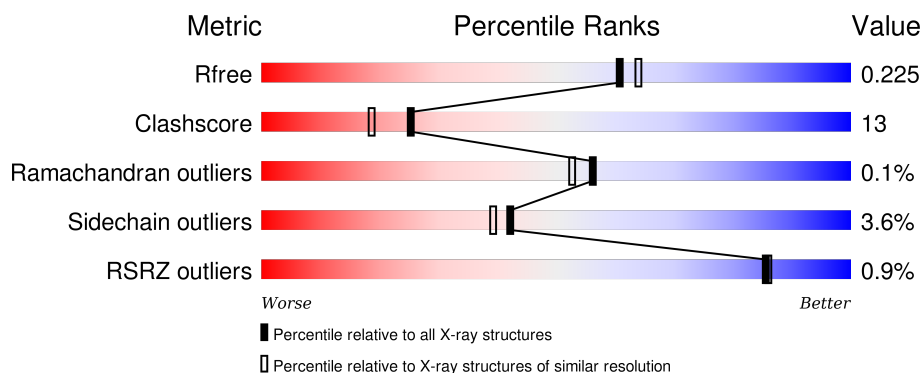
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 82%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 13% • • </div> </div>
1	B	452	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 82%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 14% • • </div> </div>
1	C	452	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 82%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 13% • • </div> </div>
1	D	452	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 81%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% 14% • • </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16846 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 nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	1	0
			3481	2181	619	659	22			
1	B	441	Total	C	N	O	S	0	1	0
			3481	2181	619	659	22			
1	C	441	Total	C	N	O	S	0	1	0
			3481	2181	619	659	22			
1	D	441	Total	C	N	O	S	0	1	0
			3480	2180	619	659	22			

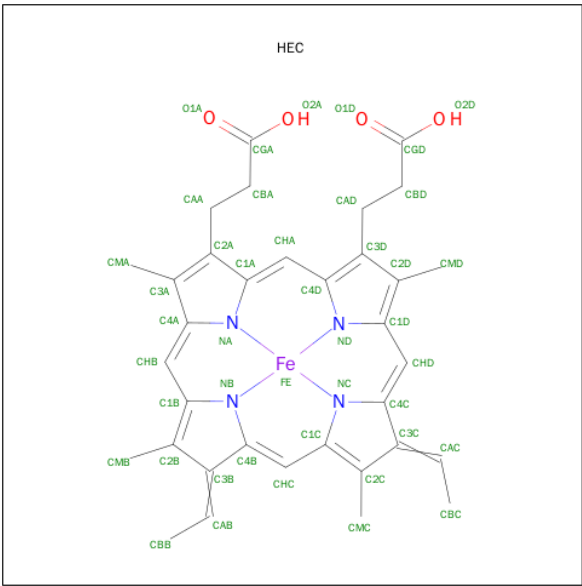
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is EUROPIUM ION (three-letter code: EU) (formula: Eu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Eu	0	0
			3	3		
3	A	3	Total	Eu	0	0
			3	3		
3	D	1	Total	Eu	0	0
			1	1		
3	C	2	Total	Eu	0	0
			2	2		

- Molecule 4 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

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

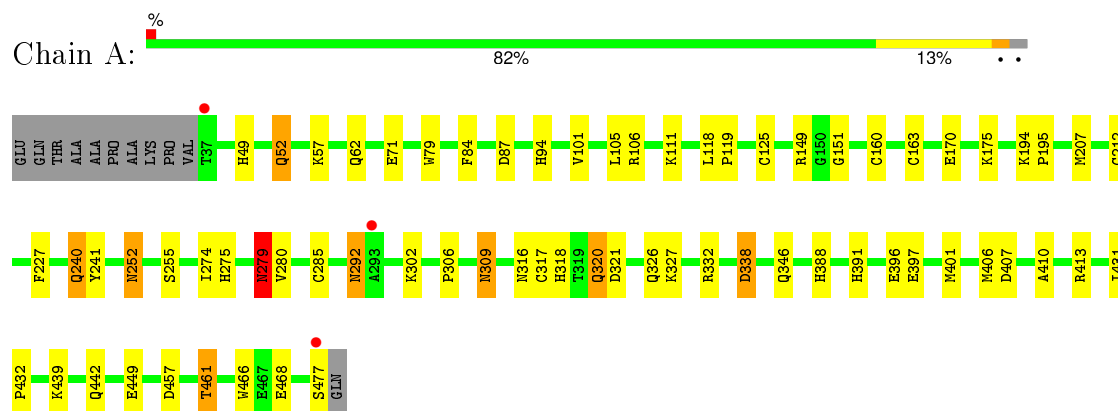
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	524	Total 524	O 524	0	0
5	B	533	Total 533	O 533	0	0
5	C	522	Total 522	O 522	0	0
5	D	471	Total 471	O 471	0	0

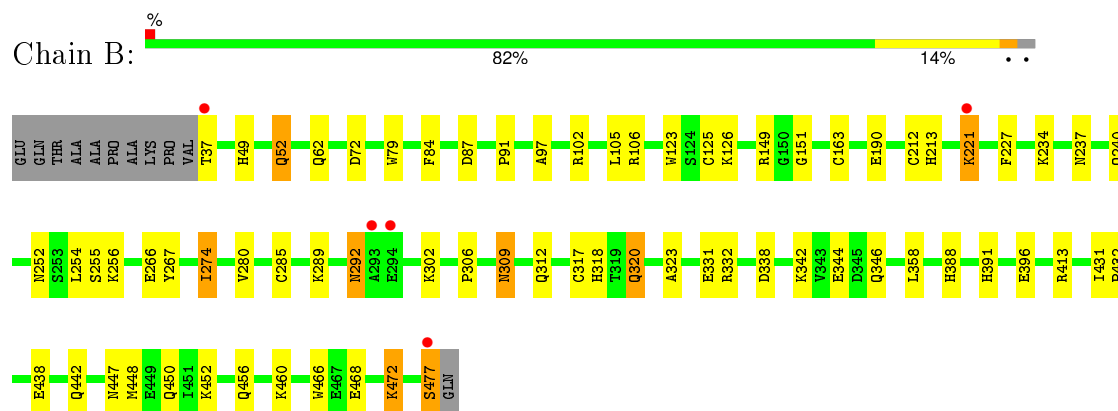
3 Residue-property plots [i](#)

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.

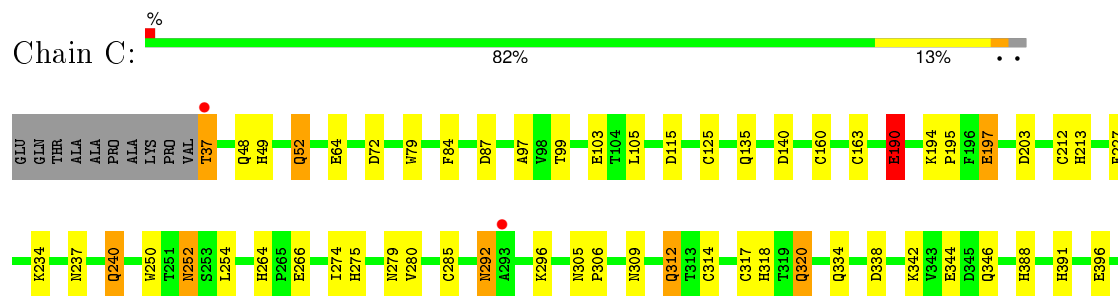
• Molecule 1: Cytochrome c nitrite reductase

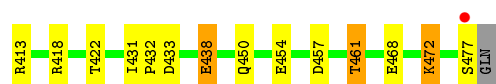


• Molecule 1: Cytochrome c nitrite reductase

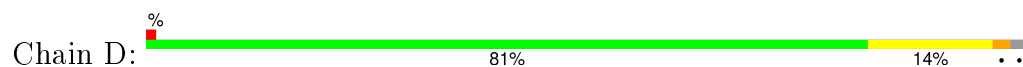


• Molecule 1: Cytochrome c nitrite reductase





● Molecule 1: Cytochrome c nitrite reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.88Å 90.49Å 292.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.10 – 2.00 19.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (146.10-2.00) 98.3 (19.97-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.164 , 0.222 0.166 , 0.225	Depositor DCC
R_{free} test set	6985 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	6 of 139181 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16846	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.66 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.3308e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EU, CA, 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	1.05	2/3569 (0.1%)	0.88	3/4827 (0.1%)
1	B	1.10	4/3569 (0.1%)	0.90	4/4827 (0.1%)
1	C	1.07	4/3569 (0.1%)	0.88	1/4827 (0.0%)
1	D	5.90	8/3569 (0.2%)	2.17	9/4827 (0.2%)
All	All	3.09	18/14276 (0.1%)	1.33	17/19308 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	396[A]	GLU	CD-OE2	213.94	3.60	1.25
1	D	396[B]	GLU	CD-OE2	213.94	3.60	1.25
1	D	396[A]	GLU	CD-OE1	107.80	2.44	1.25
1	D	396[B]	GLU	CD-OE1	107.80	2.44	1.25
1	D	396[A]	GLU	CG-CD	53.70	2.32	1.51
1	D	396[B]	GLU	CG-CD	53.70	2.32	1.51
1	C	190	GLU	CB-CG	12.30	1.75	1.52
1	C	190	GLU	CG-CD	-6.92	1.41	1.51
1	B	97	ALA	CA-CB	6.15	1.65	1.52
1	C	438	GLU	CG-CD	5.85	1.60	1.51
1	A	279	ASN	CB-CG	5.48	1.63	1.51
1	B	323	ALA	CA-CB	5.25	1.63	1.52
1	A	101	VAL	CB-CG2	5.16	1.63	1.52
1	C	97	ALA	CA-CB	5.15	1.63	1.52
1	B	331	GLU	CB-CG	-5.13	1.42	1.52
1	D	412	ALA	CA-CB	5.11	1.63	1.52
1	D	294	GLU	CG-CD	5.06	1.59	1.51
1	B	267	TYR	CD1-CE1	5.06	1.47	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	396[A]	GLU	OE1-CD-OE2	-80.74	26.41	123.30
1	D	396[B]	GLU	OE1-CD-OE2	-80.74	26.41	123.30
1	D	396[A]	GLU	CG-CD-OE2	-42.46	33.38	118.30
1	D	396[B]	GLU	CG-CD-OE2	-42.46	33.38	118.30
1	D	396[A]	GLU	CG-CD-OE1	-33.02	52.25	118.30
1	D	396[B]	GLU	CG-CD-OE1	-33.02	52.25	118.30
1	D	396[A]	GLU	CB-CG-CD	-13.65	77.34	114.20
1	D	396[B]	GLU	CB-CG-CD	-13.65	77.34	114.20
1	B	274	ILE	CG1-CB-CG2	-7.91	93.99	111.40
1	B	102	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	A	106	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	338	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	D	413	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	338	ASP	CB-CG-OD1	5.72	123.44	118.30
1	B	106	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	342	LYS	CD-CE-NZ	-5.06	100.06	111.70
1	C	140	ASP	CB-CG-OD2	-5.06	113.75	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3481	0	3371	80	0
1	B	3481	0	3371	87	0
1	C	3481	0	3371	82	0
1	D	3480	0	3371	88	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	215	0	155	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	215	0	155	35	0
4	C	215	0	155	31	0
4	D	215	0	155	33	0
5	A	524	0	0	20	1
5	B	533	0	0	16	1
5	C	522	0	0	13	0
5	D	471	0	0	14	0
All	All	16846	0	14104	351	1

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 13.

All (351) 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:C:190:GLU:CB	1:C:190:GLU:CG	1.75	1.55
1:B:37:THR:HA	5:B:1763:HOH:O	1.26	1.31
1:D:396[A]:GLU:OE2	1:D:396[A]:GLU:HG2	1.23	1.31
1:C:125:CYS:SG	4:C:3:HEC:CAC	2.21	1.28
1:B:285:CYS:SG	4:B:6:HEC:CAC	2.23	1.27
1:C:163:CYS:SG	4:C:4:HEC:CAC	2.22	1.27
1:A:439:LYS:HG3	5:A:1990:HOH:O	1.20	1.25
1:B:317:CYS:SG	4:B:7:HEC:CAC	2.25	1.24
1:D:212:CYS:SG	4:D:5:HEC:HAC	1.73	1.24
1:B:472:LYS:HB3	5:B:1700:HOH:O	1.10	1.24
1:B:163:CYS:SG	4:B:4:HEC:CAC	2.26	1.23
1:D:317:CYS:SG	4:D:7:HEC:CAC	2.31	1.19
1:D:163:CYS:SG	4:D:4:HEC:CAC	2.31	1.19
1:A:125:CYS:SG	4:A:3:HEC:CAC	2.32	1.18
1:C:317:CYS:SG	4:C:7:HEC:CAC	2.31	1.18
1:B:125:CYS:SG	4:B:3:HEC:HAC	1.77	1.17
1:A:163:CYS:SG	4:A:4:HEC:HAC	1.85	1.07
1:A:338:ASP:HB2	5:A:2013:HOH:O	1.55	1.07
1:C:212:CYS:SG	4:C:5:HEC:HAC	1.91	1.05
1:B:338:ASP:HB2	5:B:1834:HOH:O	1.53	1.05
1:B:212:CYS:SG	4:B:5:HEC:HAC	1.97	1.02
1:D:396[A]:GLU:OE2	1:D:396[A]:GLU:OE1	1.79	1.01
1:D:396[A]:GLU:CG	1:D:396[A]:GLU:OE1	2.10	1.00
1:D:396[A]:GLU:OE2	1:D:396[A]:GLU:CG	2.10	0.98
1:B:396[B]:GLU:HG3	1:C:396[B]:GLU:HG2	1.45	0.98
1:A:396[B]:GLU:HG3	1:D:396[B]:GLU:HG2	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:LYS:HG2	5:D:1474:HOH:O	1.64	0.97
1:A:212:CYS:SG	4:A:5:HEC:HAC	2.00	0.97
1:B:126:LYS:HB2	5:B:1915:HOH:O	1.65	0.94
1:D:396[A]:GLU:HG2	1:D:396[A]:GLU:OE1	1.68	0.93
1:A:317:CYS:SG	4:A:7:HEC:HAC	2.09	0.90
1:C:190:GLU:HG3	1:C:190:GLU:C	1.93	0.89
1:A:309:ASN:CB	5:A:1635:HOH:O	2.19	0.89
1:C:338:ASP:HB2	5:C:1240:HOH:O	1.72	0.88
1:B:285:CYS:SG	4:B:6:HEC:HAC	2.14	0.87
1:B:456:GLN:HG3	1:B:460:LYS:HE3	1.58	0.86
1:A:396[B]:GLU:HG3	1:D:396[B]:GLU:CG	2.06	0.86
1:C:234:LYS:HG2	5:C:1733:HOH:O	1.75	0.86
1:A:309:ASN:HB2	5:A:1635:HOH:O	1.77	0.84
4:C:7:HEC:HBB3	4:C:7:HEC:HMB1	1.58	0.84
1:A:285:CYS:SG	4:A:6:HEC:HAC	2.17	0.83
1:D:125:CYS:SG	4:D:3:HEC:HAC	2.18	0.83
1:D:149:ARG:HD2	5:D:1762:HOH:O	1.79	0.83
1:A:62:GLN:HE21	1:A:302:LYS:NZ	1.75	0.83
1:C:125:CYS:SG	4:C:3:HEC:HAC	2.17	0.82
1:A:62:GLN:HE21	1:A:302:LYS:HZ3	1.28	0.82
1:C:433:ASP:HB2	5:C:1378:HOH:O	1.80	0.81
1:D:285:CYS:SG	4:D:6:HEC:HAC	2.20	0.81
1:D:125:CYS:SG	4:D:3:HEC:C3C	2.70	0.80
1:C:190:GLU:CG	1:C:190:GLU:C	2.50	0.79
1:D:292:ASN:HD22	1:D:292:ASN:C	1.84	0.79
1:A:163:CYS:SG	4:A:4:HEC:C3C	2.71	0.79
1:D:457:ASP:HB2	5:D:1956:HOH:O	1.81	0.79
1:D:223:LYS:HE2	5:D:2019:HOH:O	1.81	0.79
1:C:314:CYS:SG	4:C:7:HEC:CBB	2.70	0.78
1:C:285:CYS:SG	4:C:6:HEC:CBC	2.72	0.77
1:B:62:GLN:HE21	1:B:302:LYS:NZ	1.82	0.77
1:C:212:CYS:SG	4:C:5:HEC:C3C	2.74	0.76
1:B:477:SER:CB	5:B:1375:HOH:O	2.34	0.76
1:C:163:CYS:SG	4:C:4:HEC:HAC	2.25	0.76
1:B:317:CYS:SG	4:B:7:HEC:HAC	2.27	0.75
1:C:285:CYS:SG	4:C:6:HEC:HAC	2.22	0.75
1:C:52:GLN:H	1:C:52:GLN:NE2	1.85	0.75
1:B:396[B]:GLU:CG	1:C:396[B]:GLU:HG2	2.15	0.75
4:A:3:HEC:HMC1	4:A:3:HEC:HBC3	1.69	0.74
1:A:457:ASP:O	1:A:461:THR:HG23	1.87	0.74
1:B:317:CYS:SG	4:B:7:HEC:C3C	2.75	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLN:H	1:A:320:GLN:HE21	1.33	0.74
1:B:125:CYS:SG	4:B:3:HEC:C3C	2.75	0.74
1:A:468:GLU:OE1	5:A:1770:HOH:O	2.05	0.74
1:D:285:CYS:SG	4:D:6:HEC:CBC	2.76	0.73
1:B:468:GLU:O	1:B:472:LYS:CD	2.37	0.73
1:D:391:HIS:HE1	4:D:6:HEC:O2D	1.72	0.73
1:A:212:CYS:SG	4:A:5:HEC:C3C	2.78	0.72
1:A:170:GLU:HB3	1:A:175:LYS:HD3	1.72	0.72
1:D:125:CYS:SG	4:D:3:HEC:CBC	2.77	0.72
1:A:461:THR:HG21	5:A:1514:HOH:O	1.88	0.72
1:C:317:CYS:SG	4:C:7:HEC:C3C	2.78	0.71
1:C:190:GLU:CG	1:C:190:GLU:CA	2.66	0.71
1:A:125:CYS:SG	4:A:3:HEC:C3C	2.77	0.71
1:B:396[B]:GLU:HG3	1:C:396[B]:GLU:CG	2.20	0.71
1:A:449:GLU:HG3	5:A:1449:HOH:O	1.89	0.71
1:C:391:HIS:HE1	4:C:6:HEC:O2D	1.71	0.71
5:B:890:HOH:O	1:C:342:LYS:HE3	1.89	0.71
1:C:125:CYS:SG	4:C:3:HEC:C3C	2.78	0.70
1:B:163:CYS:SG	4:B:4:HEC:HAC	2.29	0.70
1:A:309:ASN:HB3	5:A:1635:HOH:O	1.84	0.70
1:D:346:GLN:NE2	1:D:413:ARG:HH11	1.90	0.70
4:B:7:HEC:HBB3	4:B:7:HEC:HMB1	1.73	0.70
1:B:123:TRP:HE3	5:B:1915:HOH:O	1.75	0.70
1:A:317:CYS:SG	4:A:7:HEC:C3C	2.78	0.70
1:C:194:LYS:NZ	1:C:203:ASP:OD2	2.22	0.70
4:D:7:HEC:HMB1	4:D:7:HEC:HBB3	1.73	0.70
1:C:52:GLN:H	1:C:52:GLN:HE21	1.37	0.69
1:B:468:GLU:O	1:B:472:LYS:HD2	1.91	0.69
1:C:457:ASP:O	1:C:461:THR:HG23	1.91	0.69
1:D:285:CYS:SG	4:D:6:HEC:C3C	2.80	0.69
1:C:285:CYS:SG	4:C:6:HEC:C3C	2.80	0.69
1:A:285:CYS:SG	4:A:6:HEC:CBC	2.81	0.69
1:D:317:CYS:SG	4:D:7:HEC:C3C	2.80	0.69
1:B:477:SER:HB2	5:B:1375:HOH:O	1.90	0.69
1:A:391:HIS:HE1	4:A:6:HEC:O2D	1.75	0.68
1:A:71:GLU:OE2	5:A:1696:HOH:O	2.09	0.68
1:D:457:ASP:CB	5:D:1956:HOH:O	2.40	0.68
1:D:115:ASP:OD1	5:D:1901:HOH:O	2.11	0.68
1:C:292:ASN:C	1:C:292:ASN:HD22	1.98	0.67
1:C:49:HIS:HD2	5:C:1373:HOH:O	1.77	0.67
1:A:320:GLN:NE2	1:A:320:GLN:H	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:4:HEC:HMC1	4:A:4:HEC:HBC3	1.77	0.67
1:D:170:GLU:HB3	1:D:175:LYS:HE2	1.77	0.67
1:C:334:GLN:NE2	5:C:1928:HOH:O	2.27	0.67
1:C:388:HIS:HD2	5:C:1955:HOH:O	1.77	0.66
1:C:197:GLU:CD	1:C:197:GLU:H	1.98	0.66
1:D:163:CYS:SG	4:D:4:HEC:HAC	2.34	0.66
1:D:472:LYS:HA	1:D:472:LYS:HE3	1.78	0.66
1:A:160:CYS:SG	4:A:4:HEC:C3B	2.84	0.66
1:C:163:CYS:SG	4:C:4:HEC:C3C	2.83	0.66
1:D:163:CYS:SG	4:D:4:HEC:C3C	2.84	0.66
1:D:52:GLN:H	1:D:52:GLN:NE2	1.94	0.66
1:C:190:GLU:CD	1:C:190:GLU:CB	2.60	0.65
1:B:477:SER:HB3	5:B:1375:HOH:O	1.96	0.65
1:B:62:GLN:HE21	1:B:302:LYS:HZ3	1.44	0.65
1:B:450:GLN:HG3	5:B:946:HOH:O	1.96	0.65
4:C:4:HEC:HMC1	4:C:4:HEC:HBC3	1.79	0.65
1:C:450:GLN:O	1:C:454:GLU:HG3	1.96	0.65
1:C:163:CYS:SG	4:C:4:HEC:CBC	2.84	0.65
1:C:64:GLU:HG3	5:C:1947:HOH:O	1.97	0.64
1:A:285:CYS:SG	4:A:6:HEC:C3C	2.85	0.64
1:B:212:CYS:SG	4:B:5:HEC:C3C	2.85	0.64
1:D:320:GLN:H	1:D:320:GLN:HE21	1.45	0.64
1:A:388:HIS:HD2	5:A:872:HOH:O	1.80	0.63
1:B:285:CYS:SG	4:B:6:HEC:CBC	2.86	0.63
1:D:212:CYS:SG	4:D:5:HEC:C3C	2.85	0.63
1:C:160:CYS:SG	4:C:4:HEC:C3B	2.87	0.62
1:B:163:CYS:SG	4:B:4:HEC:C3C	2.86	0.62
1:B:163:CYS:SG	4:B:4:HEC:CBC	2.88	0.62
1:D:241:TYR:O	1:D:244:LYS:HG2	2.00	0.62
1:B:320:GLN:H	1:B:320:GLN:HE21	1.48	0.61
1:B:346:GLN:NE2	1:B:413:ARG:HH11	1.98	0.61
1:A:292:ASN:C	1:A:292:ASN:HD22	2.02	0.61
4:A:6:HEC:HMC1	4:A:6:HEC:HBC3	1.81	0.61
1:D:149:ARG:CD	5:D:1762:HOH:O	2.44	0.61
1:D:292:ASN:ND2	1:D:292:ASN:C	2.54	0.61
1:B:456:GLN:HE21	1:B:460:LYS:HE2	1.65	0.60
1:B:49:HIS:HD2	5:B:588:HOH:O	1.83	0.60
1:B:438:GLU:O	1:B:442:GLN:HG3	2.02	0.60
1:C:115:ASP:OD1	5:C:1630:HOH:O	2.17	0.60
1:D:320:GLN:H	1:D:320:GLN:NE2	2.00	0.59
1:B:309:ASN:HD21	1:B:312:GLN:HE22	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ASN:HD22	1:B:292:ASN:C	2.03	0.59
1:C:320:GLN:H	1:C:320:GLN:HE21	1.49	0.59
1:C:312:GLN:NE2	5:C:1820:HOH:O	2.35	0.59
1:A:49:HIS:HD2	5:A:758:HOH:O	1.84	0.59
1:C:317:CYS:SG	4:C:7:HEC:CBC	2.91	0.58
1:A:280:VAL:HG13	4:A:7:HEC:HBC2	1.84	0.58
1:B:468:GLU:OE1	5:B:1920:HOH:O	2.17	0.58
1:B:234:LYS:H	1:B:237:ASN:HD22	1.52	0.58
1:B:72:ASP:OD2	1:B:344:GLU:OE1	2.22	0.58
1:B:285:CYS:SG	4:B:6:HEC:C3C	2.92	0.58
1:D:317:CYS:HG	4:D:7:HEC:CAC	2.17	0.58
1:A:160:CYS:SG	4:A:4:HEC:CBB	2.90	0.58
1:B:456:GLN:HE21	1:B:460:LYS:CE	2.16	0.58
1:D:235:VAL:HB	1:D:401:MET:HE3	1.86	0.57
1:B:87:ASP:HB2	1:B:105:LEU:HB2	1.87	0.57
4:B:7:HEC:HBC3	4:B:7:HEC:HMC1	1.87	0.57
1:C:125:CYS:SG	4:C:3:HEC:CBC	2.92	0.56
4:B:6:HEC:HBC3	4:B:6:HEC:HMC1	1.87	0.56
1:D:292:ASN:ND2	1:D:296:LYS:H	2.03	0.56
1:D:346:GLN:HE22	1:D:413:ARG:HH11	1.53	0.56
1:C:472:LYS:HE3	1:C:472:LYS:HA	1.86	0.56
4:D:6:HEC:HMC1	4:D:6:HEC:HBC3	1.86	0.56
1:A:396[B]:GLU:OE1	1:D:332:ARG:CZ	2.53	0.56
4:A:7:HEC:HBA2	4:D:7:HEC:HBA2	1.86	0.56
1:C:320:GLN:H	1:C:320:GLN:NE2	2.03	0.56
4:D:6:HEC:HMB1	4:D:6:HEC:HBB3	1.87	0.56
1:A:397:GLU:O	1:A:401:MET:HG3	2.05	0.56
1:D:52:GLN:H	1:D:52:GLN:HE21	1.51	0.56
1:B:320:GLN:H	1:B:320:GLN:NE2	2.04	0.56
1:C:314:CYS:SG	4:C:7:HEC:C3B	2.91	0.56
1:A:396[B]:GLU:CG	1:D:396[B]:GLU:CG	2.83	0.55
1:B:391:HIS:HE1	4:B:6:HEC:O2D	1.88	0.55
1:C:234:LYS:H	1:C:237:ASN:HD22	1.53	0.55
1:B:52:GLN:NE2	1:B:52:GLN:H	2.04	0.55
1:D:317:CYS:SG	4:D:7:HEC:HAC	2.38	0.55
1:D:49:HIS:HD2	5:D:1446:HOH:O	1.89	0.55
1:D:283:ILE:HD11	4:D:5:HEC:HBB1	1.89	0.55
1:A:125:CYS:SG	4:A:3:HEC:CBC	2.94	0.55
1:B:318:HIS:HB3	1:B:320:GLN:NE2	2.21	0.55
1:C:346:GLN:NE2	1:C:413:ARG:HH11	2.05	0.55
1:D:317:CYS:SG	4:D:7:HEC:CBC	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:GLU:O	1:C:472:LYS:HD2	2.08	0.55
1:A:240:GLN:HE21	1:A:241:TYR:N	2.05	0.55
1:C:195:PRO:HB2	1:C:197:GLU:OE2	2.08	0.54
1:C:391:HIS:CE1	4:C:6:HEC:O2D	2.58	0.54
1:B:252:ASN:HD21	1:B:254:LEU:HB2	1.73	0.54
1:B:447:ASN:ND2	1:B:450:GLN:NE2	2.56	0.54
1:D:223:LYS:CE	5:D:2019:HOH:O	2.46	0.53
1:A:194:LYS:HE3	1:A:207:MET:HE3	1.88	0.53
1:D:457:ASP:O	1:D:461:THR:HG23	2.08	0.53
1:B:309:ASN:HD21	1:B:312:GLN:NE2	2.06	0.53
1:A:194:LYS:HE3	1:A:207:MET:CE	2.39	0.53
1:A:125:CYS:SG	4:A:3:HEC:HAC	2.42	0.53
1:B:468:GLU:O	1:B:472:LYS:HD3	2.09	0.52
1:B:346:GLN:HE22	1:B:413:ARG:HH11	1.56	0.52
1:C:438:GLU:HG3	5:C:983:HOH:O	2.09	0.52
1:D:163:CYS:SG	4:D:4:HEC:CBC	2.98	0.52
1:C:190:GLU:HG3	1:C:190:GLU:O	2.09	0.52
1:A:212:CYS:SG	4:A:5:HEC:CBC	2.96	0.52
1:B:252:ASN:ND2	1:B:254:LEU:H	2.09	0.51
1:D:290:VAL:HG12	1:D:312:GLN:HG2	1.93	0.51
1:B:289:LYS:HD2	5:B:1892:HOH:O	2.10	0.51
1:A:316:ASN:HB3	5:A:1640:HOH:O	2.10	0.51
4:A:3:HEC:HMC1	4:A:3:HEC:CBC	2.39	0.51
1:C:292:ASN:ND2	1:C:296:LYS:H	2.08	0.51
1:A:396[B]:GLU:HG3	1:D:396[B]:GLU:HG3	1.91	0.51
1:D:234:LYS:H	1:D:237:ASN:HD22	1.59	0.51
1:D:282:CYS:O	1:D:286:HIS:HB2	2.11	0.50
1:A:52:GLN:H	1:A:52:GLN:NE2	2.09	0.50
1:A:317:CYS:SG	4:A:7:HEC:CBC	2.98	0.50
1:A:87:ASP:HB2	1:A:105:LEU:HB2	1.92	0.50
1:B:396[B]:GLU:CG	1:C:396[B]:GLU:CG	2.85	0.50
1:B:280:VAL:HG13	4:B:7:HEC:HBC2	1.93	0.50
1:A:332:ARG:CZ	1:D:396[B]:GLU:OE1	2.60	0.50
4:B:4:HEC:HBC1	4:B:5:HEC:HHC	1.93	0.50
1:C:37:THR:HG23	1:C:135:GLN:NE2	2.26	0.49
1:B:431:ILE:HG22	1:B:432:PRO:O	2.11	0.49
1:B:252:ASN:HD22	1:B:255:SER:H	1.61	0.49
1:A:396[B]:GLU:CG	1:D:396[B]:GLU:HG3	2.43	0.48
5:A:1236:HOH:O	1:D:342:LYS:HE3	2.13	0.48
1:C:292:ASN:HD21	1:C:296:LYS:H	1.61	0.48
1:B:151:GLY:HA3	1:B:466:TRP:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HB3	1:A:207:MET:CE	2.43	0.48
1:C:49:HIS:HE1	5:C:623:HOH:O	1.96	0.48
1:D:391:HIS:CE1	4:D:6:HEC:O2D	2.60	0.48
1:A:227:PHE:N	1:A:227:PHE:CD2	2.81	0.48
1:A:391:HIS:CD2	1:A:391:HIS:H	2.30	0.48
1:D:292:ASN:HD21	1:D:296:LYS:H	1.62	0.48
1:C:213:HIS:HB3	1:C:266:GLU:HB2	1.96	0.47
1:A:346:GLN:NE2	1:A:413:ARG:HH11	2.12	0.47
1:A:118:LEU:HB3	1:A:119:PRO:HD2	1.95	0.47
1:A:407:ASP:HB2	1:D:406:MET:HE3	1.97	0.47
1:D:477:SER:HB2	5:D:574:HOH:O	2.14	0.47
1:D:158:LEU:HG	4:D:5:HEC:HBC2	1.96	0.47
1:B:317:CYS:SG	4:B:7:HEC:CBC	2.99	0.47
1:B:388:HIS:HD2	5:B:921:HOH:O	1.97	0.47
1:A:442:GLN:HG3	5:A:604:HOH:O	2.14	0.47
1:D:91:PRO:HG3	4:D:3:HEC:CGD	2.45	0.47
4:D:4:HEC:HBC3	4:D:4:HEC:HMC1	1.96	0.47
1:C:418:ARG:O	1:C:422:THR:HG23	2.15	0.47
1:B:252:ASN:ND2	1:B:254:LEU:HB2	2.29	0.47
1:A:439:LYS:CG	5:A:1990:HOH:O	2.07	0.47
1:A:79:TRP:CE3	1:A:84:PHE:HB3	2.49	0.47
4:A:7:HEC:HBD1	4:D:7:HEC:HBD1	1.97	0.47
1:A:57:LYS:HE2	5:A:1552:HOH:O	2.14	0.47
1:C:285:CYS:SG	4:C:6:HEC:HBC3	2.52	0.46
1:B:256:LYS:HG2	1:B:358:LEU:HD13	1.96	0.46
1:C:48:GLN:HB2	5:C:614:HOH:O	2.14	0.46
1:A:252:ASN:HD22	1:A:255:SER:H	1.61	0.46
4:C:7:HEC:CBB	4:C:7:HEC:HMB1	2.38	0.46
1:D:381:TRP:O	1:D:385:ILE:HG13	2.15	0.46
1:A:275:HIS:CG	4:A:6:HEC:HBC2	2.51	0.46
1:B:309:ASN:ND2	1:B:312:GLN:NE2	2.64	0.46
1:B:306:PRO:HB2	4:B:7:HEC:HBB1	1.97	0.46
1:A:62:GLN:HE21	1:A:302:LYS:HZ2	1.63	0.46
4:A:5:HEC:HMC1	4:A:5:HEC:HBC3	1.98	0.46
1:B:79:TRP:CE3	1:B:84:PHE:HB3	2.50	0.46
1:A:321:ASP:HB3	5:A:1242:HOH:O	2.16	0.46
1:B:125:CYS:SG	4:B:3:HEC:CBC	3.00	0.45
1:D:257:THR:O	1:D:259:MET:HG2	2.16	0.45
1:C:79:TRP:CE3	1:C:84:PHE:HB3	2.51	0.45
1:A:457:ASP:O	1:A:461:THR:CG2	2.63	0.45
1:B:190:GLU:CD	5:B:1958:HOH:O	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:CYS:SG	4:C:7:HEC:HAC	2.42	0.45
1:D:72:ASP:OD2	1:D:344:GLU:OE1	2.34	0.45
1:A:391:HIS:CE1	4:A:6:HEC:O2D	2.64	0.45
1:B:91:PRO:HG3	4:B:3:HEC:CGD	2.47	0.45
1:B:221:LYS:NZ	5:B:1656:HOH:O	2.50	0.45
1:D:234:LYS:HD2	5:D:2040:HOH:O	2.16	0.45
1:C:305:ASN:HA	1:C:306:PRO:HD3	1.75	0.44
1:B:234:LYS:H	1:B:237:ASN:ND2	2.14	0.44
1:A:151:GLY:HA3	1:A:466:TRP:CE2	2.52	0.44
1:B:332:ARG:CZ	1:C:396[B]:GLU:OE1	2.66	0.44
1:B:256:LYS:HG2	1:B:358:LEU:CD1	2.47	0.44
1:D:263:GLN:O	1:D:264:HIS:C	2.55	0.44
1:C:252:ASN:ND2	1:C:254:LEU:H	2.16	0.44
1:D:51:ASP:OD2	1:D:296:LYS:NZ	2.51	0.44
4:C:3:HEC:HMC1	4:C:3:HEC:HBC3	1.99	0.44
1:D:463:ILE:HB	1:D:464:PRO:HD3	1.99	0.44
1:A:320:GLN:N	1:A:320:GLN:HE21	2.10	0.44
1:B:472:LYS:N	1:B:472:LYS:HD2	2.32	0.43
1:B:213:HIS:HB3	1:B:266:GLU:HB2	2.00	0.43
1:D:62:GLN:HE21	1:D:302:LYS:NZ	2.16	0.43
1:B:317:CYS:HG	4:B:7:HEC:HAC	1.82	0.43
1:D:336:ILE:HD12	1:D:391:HIS:HA	2.00	0.43
1:C:87:ASP:HB2	1:C:105:LEU:HB2	1.99	0.43
1:B:274:ILE:HG23	1:B:274:ILE:HD12	1.39	0.43
1:A:326:GLN:NE2	5:A:1685:HOH:O	2.51	0.43
1:C:72:ASP:OD2	1:C:344:GLU:OE1	2.35	0.43
1:C:212:CYS:SG	4:C:5:HEC:CBC	2.99	0.43
4:B:4:HEC:HMB1	4:B:4:HEC:HBB3	2.00	0.43
1:A:306:PRO:HB2	4:A:7:HEC:HBB1	2.00	0.43
4:A:6:HEC:HMB1	4:A:6:HEC:HBB3	1.99	0.43
1:D:317:CYS:HG	4:D:7:HEC:HAC	1.81	0.43
1:C:318:HIS:HB3	1:C:320:GLN:NE2	2.34	0.43
1:D:368:LYS:HB3	1:D:369:PRO:HD3	2.00	0.43
1:D:227:PHE:N	1:D:227:PHE:CD2	2.87	0.43
1:D:213:HIS:CE1	4:D:3:HEC:HMD1	2.54	0.42
1:B:317:CYS:HG	4:B:7:HEC:CAC	2.23	0.42
1:D:115:ASP:CG	5:D:1901:HOH:O	2.56	0.42
1:C:292:ASN:C	1:C:292:ASN:ND2	2.70	0.42
1:A:449:GLU:CG	5:A:1449:HOH:O	2.58	0.42
4:C:6:HEC:HMC1	4:C:6:HEC:HBC3	2.01	0.42
1:B:391:HIS:H	1:B:391:HIS:CD2	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:THR:O	1:C:103:GLU:HG3	2.20	0.42
1:B:52:GLN:HE21	1:B:52:GLN:H	1.66	0.42
4:B:7:HEC:HBD1	4:C:7:HEC:HBD1	2.02	0.42
1:C:37:THR:HG23	1:C:135:GLN:HE22	1.84	0.42
1:D:349:HIS:O	1:D:353:GLU:HG3	2.20	0.42
1:C:227:PHE:N	1:C:227:PHE:CD2	2.87	0.42
1:A:279:ASN:HD22	1:A:279:ASN:HA	1.80	0.41
1:B:448:MET:O	1:B:452:LYS:HG3	2.20	0.41
4:B:7:HEC:HBA2	4:C:7:HEC:HBA2	2.03	0.41
1:A:318:HIS:HB3	1:A:320:GLN:NE2	2.35	0.41
1:B:62:GLN:HE21	1:B:302:LYS:HZ2	1.61	0.41
1:C:240:GLN:HB3	1:C:240:GLN:HE21	1.62	0.41
1:D:125:CYS:SG	4:D:3:HEC:HBC3	2.59	0.41
1:C:391:HIS:HD2	5:C:572:HOH:O	2.04	0.41
1:A:62:GLN:NE2	1:A:302:LYS:NZ	2.55	0.41
1:A:111:LYS:NZ	5:A:1766:HOH:O	2.53	0.41
1:A:431:ILE:HG22	1:A:432:PRO:O	2.21	0.41
1:A:410:ALA:HB2	1:D:410:ALA:HB2	2.01	0.41
1:A:94:HIS:CD2	4:A:5:HEC:ND	2.88	0.41
4:A:6:HEC:HMC1	4:A:6:HEC:CBC	2.50	0.41
1:C:275:HIS:HB3	1:C:280:VAL:HB	2.02	0.41
1:D:305:ASN:HA	1:D:306:PRO:HD3	1.86	0.41
4:B:4:HEC:HBC1	4:B:5:HEC:CHC	2.51	0.41
4:B:6:HEC:HBB3	4:B:6:HEC:HMB1	2.03	0.41
1:D:384:ALA:HB2	1:D:401:MET:HB2	2.01	0.41
1:D:460:LYS:HD3	5:D:1448:HOH:O	2.21	0.41
1:B:227:PHE:N	1:B:227:PHE:CD2	2.89	0.41
1:C:391:HIS:H	1:C:391:HIS:CD2	2.38	0.41
1:C:431:ILE:HG22	1:C:432:PRO:O	2.21	0.41
1:A:346:GLN:HG3	1:A:406:MET:SD	2.61	0.40
1:B:212:CYS:SG	4:B:5:HEC:CBC	3.02	0.40
1:D:94:HIS:CD2	4:D:5:HEC:ND	2.88	0.40
4:B:4:HEC:HMC1	4:B:4:HEC:HBC3	2.04	0.40
1:D:252:ASN:HD22	1:D:255:SER:H	1.68	0.40
1:D:286:HIS:O	5:D:659:HOH:O	2.22	0.40
1:B:318:HIS:HB3	1:B:320:GLN:HE21	1.87	0.40
1:B:213:HIS:CE1	4:B:3:HEC:HMD1	2.56	0.40
1:D:282:CYS:HA	4:D:6:HEC:CHC	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:498:HOH:O	5:B:1700:HOH:O[4_445]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/452 (97%)	431 (98%)	9 (2%)	0	100	100
1	B	440/452 (97%)	428 (97%)	12 (3%)	0	100	100
1	C	440/452 (97%)	428 (97%)	11 (2%)	1 (0%)	52	48
1	D	440/452 (97%)	429 (98%)	11 (2%)	0	100	100
All	All	1760/1808 (97%)	1716 (98%)	43 (2%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	264	HIS

5.3.2 Protein sidechains [i](#)

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%)	350 (96%)	13 (4%)	42	39
1	B	363/370 (98%)	354 (98%)	9 (2%)	55	55
1	C	363/370 (98%)	347 (96%)	16 (4%)	35	30
1	D	363/370 (98%)	348 (96%)	15 (4%)	37	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1452/1480 (98%)	1399 (96%)	53 (4%)	42	38

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	149	ARG
1	A	195	PRO
1	A	240	GLN
1	A	252	ASN
1	A	274	ILE
1	A	279	ASN
1	A	292	ASN
1	A	309	ASN
1	A	320	GLN
1	A	327	LYS
1	A	461	THR
1	A	477	SER
1	B	52	GLN
1	B	149	ARG
1	B	221	LYS
1	B	240	GLN
1	B	292	ASN
1	B	309	ASN
1	B	320	GLN
1	B	472	LYS
1	B	477	SER
1	C	37	THR
1	C	52	GLN
1	C	190	GLU
1	C	197	GLU
1	C	240	GLN
1	C	250	TRP
1	C	252	ASN
1	C	274	ILE
1	C	279	ASN
1	C	292	ASN
1	C	309	ASN
1	C	312	GLN
1	C	320	GLN
1	C	461	THR
1	C	472	LYS

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Mol	Chain	Res	Type
1	C	477	SER
1	D	52	GLN
1	D	221	LYS
1	D	240	GLN
1	D	244	LYS
1	D	252	ASN
1	D	279	ASN
1	D	292	ASN
1	D	309	ASN
1	D	312	GLN
1	D	320	GLN
1	D	396[A]	GLU
1	D	396[B]	GLU
1	D	461	THR
1	D	472	LYS
1	D	477	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	49	HIS
1	A	52	GLN
1	A	62	GLN
1	A	237	ASN
1	A	240	GLN
1	A	252	ASN
1	A	279	ASN
1	A	291	GLN
1	A	292	ASN
1	A	309	ASN
1	A	312	GLN
1	A	320	GLN
1	A	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	469	GLN
1	B	48	GLN

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Mol	Chain	Res	Type
1	B	49	HIS
1	B	52	GLN
1	B	62	GLN
1	B	237	ASN
1	B	252	ASN
1	B	279	ASN
1	B	291	GLN
1	B	292	ASN
1	B	309	ASN
1	B	312	GLN
1	B	320	GLN
1	B	326	GLN
1	B	346	GLN
1	B	371	GLN
1	B	388	HIS
1	B	391	HIS
1	B	430	GLN
1	B	450	GLN
1	B	456	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	473	ASN
1	D	48	GLN
1	D	49	HIS
1	D	52	GLN
1	D	62	GLN
1	D	144	HIS

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Mol	Chain	Res	Type
1	D	237	ASN
1	D	252	ASN
1	D	279	ASN
1	D	291	GLN
1	D	292	ASN
1	D	309	ASN
1	D	320	GLN
1	D	334	GLN
1	D	346	GLN
1	D	371	GLN
1	D	388	HIS
1	D	391	HIS
1	D	430	GLN
1	D	456	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 13 are monoatomic - leaving 20 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
4	HEC	A	3	1,5	24,50,50	2.29	7 (29%)	19,82,82	3.27	10 (52%)
4	HEC	A	4	1	24,50,50	2.00	6 (25%)	19,82,82	2.94	11 (57%)
4	HEC	A	5	1,3	24,50,50	2.15	8 (33%)	19,82,82	3.08	8 (42%)
4	HEC	A	6	1,3	24,50,50	2.09	7 (29%)	19,82,82	2.83	6 (31%)
4	HEC	A	7	1,3	24,50,50	1.96	6 (25%)	19,82,82	2.74	8 (42%)
4	HEC	B	3	1,5	24,50,50	2.70	12 (50%)	19,82,82	3.01	6 (31%)
4	HEC	B	4	1	24,50,50	2.10	10 (41%)	19,82,82	2.69	4 (21%)
4	HEC	B	5	1,3	24,50,50	1.97	6 (25%)	19,82,82	3.64	9 (47%)
4	HEC	B	6	1,3	24,50,50	2.44	8 (33%)	19,82,82	2.57	7 (36%)
4	HEC	B	7	1,3	24,50,50	2.38	8 (33%)	19,82,82	2.79	7 (36%)
4	HEC	C	3	1,5	24,50,50	2.37	8 (33%)	19,82,82	2.59	8 (42%)
4	HEC	C	4	1	24,50,50	2.33	5 (20%)	19,82,82	2.73	7 (36%)
4	HEC	C	5	1,3	24,50,50	2.15	9 (37%)	19,82,82	3.10	11 (57%)
4	HEC	C	6	1,3	24,50,50	2.40	5 (20%)	19,82,82	3.41	10 (52%)
4	HEC	C	7	1,3	24,50,50	2.60	6 (25%)	19,82,82	2.77	8 (42%)
4	HEC	D	3	1,5	24,50,50	2.33	7 (29%)	19,82,82	2.70	4 (21%)
4	HEC	D	4	1	24,50,50	1.96	8 (33%)	19,82,82	3.36	8 (42%)
4	HEC	D	5	1,3	24,50,50	2.22	6 (25%)	19,82,82	3.25	12 (63%)
4	HEC	D	6	1,3	24,50,50	2.46	6 (25%)	19,82,82	3.18	7 (36%)
4	HEC	D	7	1,3	24,50,50	2.33	8 (33%)	19,82,82	2.74	7 (36%)

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
4	HEC	A	3	1,5	-	0/6/54/54	0/0/8/8
4	HEC	A	4	1	-	0/6/54/54	0/0/8/8
4	HEC	A	5	1,3	-	0/6/54/54	0/0/8/8
4	HEC	A	6	1,3	-	0/6/54/54	0/0/8/8
4	HEC	A	7	1,3	-	0/6/54/54	0/0/8/8
4	HEC	B	3	1,5	-	0/6/54/54	0/0/8/8
4	HEC	B	4	1	-	0/6/54/54	0/0/8/8
4	HEC	B	5	1,3	-	0/6/54/54	0/0/8/8
4	HEC	B	6	1,3	-	0/6/54/54	0/0/8/8
4	HEC	B	7	1,3	-	0/6/54/54	0/0/8/8
4	HEC	C	3	1,5	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	C	4	1	-	0/6/54/54	0/0/8/8
4	HEC	C	5	1,3	-	0/6/54/54	0/0/8/8
4	HEC	C	6	1,3	-	0/6/54/54	0/0/8/8
4	HEC	C	7	1,3	-	0/6/54/54	0/0/8/8
4	HEC	D	3	1,5	-	0/6/54/54	0/0/8/8
4	HEC	D	4	1	-	0/6/54/54	0/0/8/8
4	HEC	D	5	1,3	-	0/6/54/54	0/0/8/8
4	HEC	D	6	1,3	-	0/6/54/54	0/0/8/8
4	HEC	D	7	1,3	-	0/6/54/54	0/0/8/8

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	7	HEC	C3B-C2B	-8.85	1.31	1.40
4	B	3	HEC	C3C-C2C	-7.82	1.32	1.40
4	D	6	HEC	C3C-C2C	-7.53	1.32	1.40
4	D	7	HEC	C3B-C2B	-7.07	1.33	1.40
4	C	6	HEC	C3C-C2C	-6.95	1.33	1.40
4	C	4	HEC	C3B-C2B	-6.77	1.33	1.40
4	D	6	HEC	C3B-C2B	-6.58	1.33	1.40
4	D	3	HEC	C3C-C2C	-6.56	1.33	1.40
4	D	5	HEC	C3B-C2B	-6.55	1.33	1.40
4	C	3	HEC	C3B-C2B	-6.44	1.34	1.40
4	B	6	HEC	C3B-C2B	-6.31	1.34	1.40
4	B	7	HEC	C3C-C2C	-6.24	1.34	1.40
4	A	6	HEC	C3C-C2C	-6.12	1.34	1.40
4	B	6	HEC	C3C-C2C	-5.96	1.34	1.40
4	B	3	HEC	C3B-C2B	-5.67	1.34	1.40
4	C	7	HEC	C3C-C2C	-5.37	1.35	1.40
4	A	3	HEC	C3C-C2C	-5.36	1.35	1.40
4	C	6	HEC	C3B-C2B	-5.16	1.35	1.40
4	A	5	HEC	C3B-C2B	-5.01	1.35	1.40
4	C	5	HEC	C3C-C2C	-4.99	1.35	1.40
4	C	3	HEC	C3C-C2C	-4.86	1.35	1.40
4	D	3	HEC	C3B-C2B	-4.76	1.35	1.40
4	B	7	HEC	C3B-C2B	-4.66	1.35	1.40
4	A	3	HEC	C3B-C2B	-4.59	1.36	1.40
4	A	4	HEC	C3C-C2C	-4.58	1.36	1.40
4	D	5	HEC	C3C-C2C	-4.26	1.36	1.40
4	A	6	HEC	C3B-C2B	-4.15	1.36	1.40
4	C	4	HEC	C3C-C2C	-4.08	1.36	1.40
4	A	7	HEC	C3C-C2C	-4.02	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5	HEC	C3B-C2B	-3.99	1.36	1.40
4	A	4	HEC	C3B-C2B	-3.75	1.36	1.40
4	A	7	HEC	C3B-C2B	-3.54	1.37	1.40
4	B	4	HEC	C3B-C2B	-3.52	1.37	1.40
4	C	5	HEC	C3B-C2B	-3.47	1.37	1.40
4	B	5	HEC	C3C-C2C	-3.37	1.37	1.40
4	D	7	HEC	C3C-C2C	-3.32	1.37	1.40
4	D	4	HEC	C3B-C2B	-3.20	1.37	1.40
4	A	5	HEC	C3C-C2C	-3.07	1.37	1.40
4	B	4	HEC	C3C-C2C	-2.98	1.37	1.40
4	D	4	HEC	C3C-C2C	-2.50	1.38	1.40
4	C	5	HEC	C2A-C3A	-2.47	1.30	1.37
4	A	3	HEC	C4D-CHA	-2.42	1.33	1.39
4	B	3	HEC	C4D-CHA	-2.06	1.34	1.39
4	C	7	HEC	CMC-C2C	2.00	1.56	1.51
4	C	3	HEC	CMC-C2C	2.00	1.56	1.51
4	D	5	HEC	CMA-C3A	2.01	1.56	1.51
4	A	6	HEC	CMA-C3A	2.01	1.56	1.51
4	D	7	HEC	C3C-C4C	2.04	1.47	1.42
4	C	3	HEC	C4B-NB	2.04	1.39	1.36
4	B	3	HEC	CMA-C3A	2.04	1.56	1.51
4	D	6	HEC	CMB-C2B	2.06	1.56	1.51
4	C	5	HEC	CMC-C2C	2.06	1.56	1.51
4	D	7	HEC	C4B-NB	2.06	1.39	1.36
4	D	4	HEC	C1A-NA	2.07	1.39	1.36
4	B	4	HEC	CMD-C2D	2.09	1.56	1.51
4	B	3	HEC	C4A-NA	2.09	1.39	1.36
4	A	5	HEC	C4B-NB	2.10	1.39	1.36
4	C	5	HEC	CBC-CAC	2.11	1.58	1.49
4	D	3	HEC	CAA-C2A	2.11	1.56	1.52
4	C	7	HEC	CMA-C3A	2.12	1.56	1.51
4	C	5	HEC	CMB-C2B	2.13	1.56	1.51
4	D	3	HEC	CAD-C3D	2.13	1.55	1.52
4	B	5	HEC	CMB-C2B	2.14	1.56	1.51
4	D	5	HEC	CMD-C2D	2.14	1.56	1.51
4	A	4	HEC	CMC-C2C	2.14	1.56	1.51
4	B	7	HEC	CMC-C2C	2.15	1.56	1.51
4	B	6	HEC	CAD-C3D	2.16	1.55	1.52
4	C	3	HEC	CBC-CAC	2.17	1.58	1.49
4	A	7	HEC	CMC-C2C	2.18	1.56	1.51
4	D	3	HEC	C1A-NA	2.19	1.39	1.36
4	A	3	HEC	C4A-NA	2.20	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	HEC	C4B-NB	2.20	1.39	1.36
4	A	5	HEC	CMB-C2B	2.21	1.56	1.51
4	B	7	HEC	C4B-NB	2.22	1.39	1.36
4	B	7	HEC	CBB-CAB	2.24	1.58	1.49
4	B	5	HEC	CAA-C2A	2.28	1.56	1.52
4	A	6	HEC	CAD-C3D	2.28	1.55	1.52
4	B	6	HEC	CMC-C2C	2.29	1.56	1.51
4	B	3	HEC	CMB-C2B	2.29	1.56	1.51
4	B	4	HEC	CMB-C2B	2.32	1.56	1.51
4	B	4	HEC	CAA-C2A	2.33	1.56	1.52
4	C	3	HEC	CBB-CAB	2.36	1.59	1.49
4	B	3	HEC	CAD-C3D	2.36	1.56	1.52
4	C	7	HEC	C4C-NC	2.36	1.39	1.36
4	A	6	HEC	CAA-C2A	2.38	1.56	1.52
4	D	7	HEC	CMB-C2B	2.39	1.56	1.51
4	B	3	HEC	CBB-CAB	2.40	1.59	1.49
4	D	6	HEC	CMA-C3A	2.40	1.56	1.51
4	B	6	HEC	CBB-CAB	2.42	1.59	1.49
4	B	3	HEC	CMD-C2D	2.44	1.56	1.51
4	C	3	HEC	CMB-C2B	2.45	1.56	1.51
4	D	4	HEC	CMC-C2C	2.46	1.56	1.51
4	B	3	HEC	CAA-C2A	2.47	1.57	1.52
4	D	7	HEC	CMA-C3A	2.50	1.57	1.51
4	A	3	HEC	CBB-CAB	2.50	1.59	1.49
4	A	4	HEC	CAA-C2A	2.50	1.57	1.52
4	C	4	HEC	C4A-NA	2.52	1.40	1.36
4	B	4	HEC	C4B-NB	2.54	1.40	1.36
4	A	6	HEC	CMB-C2B	2.55	1.57	1.51
4	D	4	HEC	CAD-C3D	2.58	1.56	1.52
4	B	7	HEC	C4A-NA	2.59	1.40	1.36
4	D	6	HEC	CAA-C2A	2.59	1.57	1.52
4	C	5	HEC	CAD-C3D	2.63	1.56	1.52
4	A	7	HEC	CAD-C3D	2.66	1.56	1.52
4	B	3	HEC	CMC-C2C	2.67	1.57	1.51
4	B	6	HEC	C1A-NA	2.70	1.40	1.36
4	D	4	HEC	CMA-C3A	2.72	1.57	1.51
4	A	5	HEC	C1A-NA	2.74	1.40	1.36
4	B	6	HEC	CMB-C2B	2.74	1.57	1.51
4	A	5	HEC	CMA-C3A	2.76	1.57	1.51
4	D	4	HEC	C3B-C4B	2.82	1.49	1.42
4	A	4	HEC	CMA-C3A	2.82	1.57	1.51
4	D	5	HEC	CMC-C2C	2.84	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	7	HEC	CMC-C2C	2.86	1.57	1.51
4	C	6	HEC	C1A-NA	2.90	1.40	1.36
4	C	6	HEC	CAD-C3D	2.90	1.57	1.52
4	B	7	HEC	CAD-C3D	2.90	1.57	1.52
4	A	7	HEC	C4A-NA	2.99	1.40	1.36
4	B	4	HEC	C4A-NA	3.01	1.40	1.36
4	C	5	HEC	CMA-C3A	3.15	1.58	1.51
4	C	4	HEC	CMA-C3A	3.21	1.58	1.51
4	A	5	HEC	CMD-C2D	3.24	1.58	1.51
4	B	4	HEC	CMA-C3A	3.37	1.58	1.51
4	B	5	HEC	C4B-NB	3.55	1.41	1.36
4	A	3	HEC	CAA-C2A	3.57	1.59	1.52
4	C	5	HEC	C3D-C2D	3.73	1.48	1.37
4	B	4	HEC	CMC-C2C	3.77	1.59	1.51
4	A	6	HEC	C3D-C2D	3.80	1.48	1.37
4	B	4	HEC	C3D-C2D	3.86	1.49	1.37
4	C	7	HEC	C3D-C2D	3.88	1.49	1.37
4	D	6	HEC	C3D-C2D	3.89	1.49	1.37
4	D	5	HEC	C3D-C2D	4.05	1.49	1.37
4	B	5	HEC	C3D-C2D	4.21	1.50	1.37
4	A	3	HEC	C3D-C2D	4.27	1.50	1.37
4	B	6	HEC	C3D-C2D	4.40	1.50	1.37
4	D	7	HEC	C3D-C2D	4.42	1.50	1.37
4	A	5	HEC	C3D-C2D	4.46	1.50	1.37
4	A	7	HEC	C3D-C2D	4.48	1.50	1.37
4	B	3	HEC	C3D-C2D	4.67	1.51	1.37
4	A	4	HEC	C3D-C2D	4.71	1.51	1.37
4	C	4	HEC	C3D-C2D	4.71	1.51	1.37
4	D	3	HEC	C3D-C2D	4.91	1.52	1.37
4	C	3	HEC	C3D-C2D	4.98	1.52	1.37
4	D	4	HEC	C3D-C2D	5.06	1.52	1.37
4	B	7	HEC	C3D-C2D	5.18	1.53	1.37
4	C	6	HEC	C3D-C2D	5.24	1.53	1.37

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5	HEC	CBB-CAB-C3B	-9.71	105.78	127.35
4	D	4	HEC	CBB-CAB-C3B	-9.54	106.14	127.35
4	D	3	HEC	CBB-CAB-C3B	-8.92	107.53	127.35
4	D	6	HEC	CBB-CAB-C3B	-8.55	108.35	127.35
4	A	6	HEC	CBB-CAB-C3B	-8.35	108.78	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3	HEC	CBB-CAB-C3B	-8.32	108.87	127.35
4	B	4	HEC	CBB-CAB-C3B	-8.28	108.94	127.35
4	A	7	HEC	CBB-CAB-C3B	-8.20	109.12	127.35
4	A	5	HEC	CBB-CAB-C3B	-8.16	109.23	127.35
4	C	5	HEC	CBB-CAB-C3B	-8.03	109.51	127.35
4	B	7	HEC	CBB-CAB-C3B	-7.80	110.02	127.35
4	B	6	HEC	CBB-CAB-C3B	-7.56	110.56	127.35
4	A	3	HEC	CBC-CAC-C3C	-7.47	110.75	127.35
4	C	7	HEC	CBB-CAB-C3B	-7.19	111.38	127.35
4	C	4	HEC	CBB-CAB-C3B	-7.18	111.39	127.35
4	C	3	HEC	CBB-CAB-C3B	-7.08	111.61	127.35
4	A	4	HEC	CBB-CAB-C3B	-6.70	112.46	127.35
4	C	6	HEC	CBB-CAB-C3B	-6.69	112.48	127.35
4	D	7	HEC	CBB-CAB-C3B	-6.61	112.66	127.35
4	D	5	HEC	CBB-CAB-C3B	-6.55	112.80	127.35
4	C	6	HEC	CBA-CAA-C2A	-6.49	100.89	112.53
4	B	3	HEC	CMB-C2B-C1B	-6.35	117.86	128.36
4	A	3	HEC	CBB-CAB-C3B	-6.26	113.44	127.35
4	A	4	HEC	CBC-CAC-C3C	-6.25	113.47	127.35
4	B	5	HEC	CMC-C2C-C1C	-5.71	118.92	128.36
4	D	6	HEC	CBC-CAC-C3C	-5.65	114.79	127.35
4	C	7	HEC	CMC-C2C-C1C	-5.60	119.10	128.36
4	C	6	HEC	CMC-C2C-C1C	-5.53	119.21	128.36
4	D	4	HEC	CBC-CAC-C3C	-5.52	115.08	127.35
4	D	4	HEC	CMC-C2C-C1C	-5.39	119.44	128.36
4	D	3	HEC	CMB-C2B-C1B	-5.30	119.60	128.36
4	B	5	HEC	CAA-C2A-C1A	-5.28	121.27	127.01
4	C	4	HEC	CBC-CAC-C3C	-5.25	115.68	127.35
4	D	5	HEC	CBA-CAA-C2A	-5.25	103.12	112.53
4	D	7	HEC	CBA-CAA-C2A	-5.21	103.18	112.53
4	A	4	HEC	CMB-C2B-C1B	-5.14	119.86	128.36
4	D	6	HEC	CBA-CAA-C2A	-5.08	103.42	112.53
4	B	7	HEC	CBC-CAC-C3C	-5.07	116.08	127.35
4	C	6	HEC	CBC-CAC-C3C	-5.02	116.19	127.35
4	A	5	HEC	CAA-C2A-C1A	-5.01	121.57	127.01
4	D	5	HEC	CAA-C2A-C1A	-4.98	121.60	127.01
4	A	6	HEC	CBA-CAA-C2A	-4.95	103.65	112.53
4	C	5	HEC	CBC-CAC-C3C	-4.84	116.59	127.35
4	B	5	HEC	CMB-C2B-C1B	-4.77	120.48	128.36
4	D	5	HEC	CBD-CAD-C3D	-4.71	104.09	112.53
4	A	3	HEC	CMB-C2B-C1B	-4.70	120.58	128.36
4	A	5	HEC	CMC-C2C-C1C	-4.59	120.77	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5	HEC	CBC-CAC-C3C	-4.50	117.35	127.35
4	D	4	HEC	CAA-C2A-C1A	-4.42	122.21	127.01
4	B	6	HEC	CBA-CAA-C2A	-4.33	104.77	112.53
4	B	4	HEC	CBC-CAC-C3C	-4.32	117.76	127.35
4	B	4	HEC	CMB-C2B-C1B	-4.30	121.24	128.36
4	A	7	HEC	CMB-C2B-C1B	-4.29	121.26	128.36
4	C	5	HEC	CBD-CAD-C3D	-4.29	104.84	112.53
4	D	6	HEC	CMC-C2C-C1C	-4.18	121.44	128.36
4	C	6	HEC	CAD-CBD-CGD	-4.14	105.17	112.75
4	A	6	HEC	CBC-CAC-C3C	-4.13	118.17	127.35
4	B	7	HEC	CMB-C2B-C1B	-4.13	121.54	128.36
4	C	6	HEC	CAA-C2A-C1A	-4.08	122.58	127.01
4	B	5	HEC	CAA-CBA-CGA	-4.03	105.36	112.75
4	D	7	HEC	CBD-CAD-C3D	-4.01	105.34	112.53
4	D	5	HEC	CBC-CAC-C3C	-4.01	118.44	127.35
4	C	6	HEC	CBD-CAD-C3D	-3.99	105.38	112.53
4	C	7	HEC	CBA-CAA-C2A	-3.94	105.46	112.53
4	B	5	HEC	CBD-CAD-C3D	-3.92	105.50	112.53
4	B	4	HEC	CMC-C2C-C1C	-3.90	121.91	128.36
4	D	6	HEC	CAA-C2A-C1A	-3.90	122.77	127.01
4	C	7	HEC	CMB-C2B-C1B	-3.89	121.93	128.36
4	A	3	HEC	CMC-C2C-C1C	-3.87	121.95	128.36
4	C	4	HEC	CMC-C2C-C1C	-3.84	122.00	128.36
4	B	5	HEC	CAD-CBD-CGD	-3.84	105.71	112.75
4	C	3	HEC	CBA-CAA-C2A	-3.83	105.66	112.53
4	B	7	HEC	CMC-C2C-C1C	-3.64	122.34	128.36
4	B	6	HEC	CMB-C2B-C1B	-3.63	122.36	128.36
4	C	4	HEC	CAD-CBD-CGD	-3.58	106.19	112.75
4	D	5	HEC	CAA-CBA-CGA	-3.52	106.29	112.75
4	C	3	HEC	CMB-C2B-C1B	-3.48	122.61	128.36
4	D	4	HEC	CMB-C2B-C1B	-3.42	122.70	128.36
4	A	7	HEC	CAA-C2A-C1A	-3.42	123.30	127.01
4	C	5	HEC	CAA-C2A-C1A	-3.37	123.35	127.01
4	D	7	HEC	CAA-C2A-C1A	-3.33	123.39	127.01
4	A	7	HEC	CMC-C2C-C1C	-3.30	122.90	128.36
4	C	6	HEC	CMB-C2B-C1B	-3.28	122.93	128.36
4	D	7	HEC	CBC-CAC-C3C	-3.23	120.17	127.35
4	B	3	HEC	CAA-C2A-C1A	-3.20	123.53	127.01
4	A	6	HEC	CMB-C2B-C1B	-3.20	123.07	128.36
4	A	5	HEC	CAD-CBD-CGD	-3.19	106.89	112.75
4	C	5	HEC	CMC-C2C-C1C	-3.14	123.17	128.36
4	B	5	HEC	CBA-CAA-C2A	-3.07	107.03	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4	HEC	CBD-CAD-C3D	-3.04	107.08	112.53
4	B	7	HEC	CAA-C2A-C1A	-3.04	123.71	127.01
4	B	7	HEC	CBA-CAA-C2A	-3.02	107.12	112.53
4	B	5	HEC	CBC-CAC-C3C	-3.00	120.68	127.35
4	A	6	HEC	CMC-C2C-C1C	-3.00	123.41	128.36
4	C	5	HEC	CBA-CAA-C2A	-2.97	107.21	112.53
4	D	7	HEC	CMD-C2D-C1D	-2.96	123.46	128.36
4	C	3	HEC	CAA-C2A-C1A	-2.96	123.79	127.01
4	B	3	HEC	CMC-C2C-C1C	-2.91	123.55	128.36
4	A	5	HEC	CBD-CAD-C3D	-2.91	107.32	112.53
4	D	7	HEC	CMC-C2C-C1C	-2.87	123.61	128.36
4	A	4	HEC	CAD-CBD-CGD	-2.86	107.51	112.75
4	C	4	HEC	CMB-C2B-C1B	-2.82	123.69	128.36
4	C	3	HEC	CBC-CAC-C3C	-2.82	121.08	127.35
4	D	5	HEC	CMC-C2C-C1C	-2.79	123.75	128.36
4	C	5	HEC	CMB-C2B-C1B	-2.76	123.80	128.36
4	A	3	HEC	CBA-CAA-C2A	-2.75	107.60	112.53
4	A	7	HEC	CBC-CAC-C3C	-2.74	121.27	127.35
4	A	6	HEC	CAA-CBA-CGA	-2.72	107.76	112.75
4	C	7	HEC	CAA-C2A-C1A	-2.69	124.09	127.01
4	D	4	HEC	CBD-CAD-C3D	-2.68	107.72	112.53
4	C	5	HEC	CAA-CBA-CGA	-2.67	107.85	112.75
4	D	5	HEC	CAD-CBD-CGD	-2.63	107.92	112.75
4	A	5	HEC	CMB-C2B-C1B	-2.62	124.02	128.36
4	A	3	HEC	C3C-C4C-NC	-2.60	106.03	110.94
4	A	7	HEC	CAD-CBD-CGD	-2.60	107.98	112.75
4	B	6	HEC	CAD-CBD-CGD	-2.56	108.05	112.75
4	D	6	HEC	CAD-CBD-CGD	-2.51	108.15	112.75
4	C	7	HEC	CBC-CAC-C3C	-2.51	121.78	127.35
4	A	7	HEC	CAA-CBA-CGA	-2.46	108.23	112.75
4	B	6	HEC	CBC-CAC-C3C	-2.42	121.98	127.35
4	A	4	HEC	CMC-C2C-C1C	-2.42	124.37	128.36
4	A	4	HEC	CAA-C2A-C1A	-2.41	124.39	127.01
4	B	3	HEC	CBA-CAA-C2A	-2.41	108.21	112.53
4	D	6	HEC	CMB-C2B-C1B	-2.37	124.44	128.36
4	C	4	HEC	C3C-C4C-NC	-2.36	106.49	110.94
4	C	6	HEC	CAA-CBA-CGA	-2.34	108.45	112.75
4	D	4	HEC	CBA-CAA-C2A	-2.30	108.41	112.53
4	B	6	HEC	CBD-CAD-C3D	-2.29	108.43	112.53
4	A	4	HEC	CMD-C2D-C1D	-2.26	124.62	128.36
4	A	5	HEC	CBA-CAA-C2A	-2.26	108.48	112.53
4	C	7	HEC	CMD-C2D-C1D	-2.25	124.64	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5	HEC	CAD-CBD-CGD	-2.18	108.75	112.75
4	C	4	HEC	CMD-C2D-C1D	-2.16	124.79	128.36
4	A	7	HEC	CBD-CAD-C3D	-2.16	108.67	112.53
4	D	5	HEC	C3B-C4B-NB	-2.15	106.88	110.94
4	D	3	HEC	CBA-CAA-C2A	-2.11	108.75	112.53
4	A	4	HEC	CBA-CAA-C2A	-2.10	108.76	112.53
4	D	4	HEC	CMD-C2D-C1D	-2.10	124.89	128.36
4	A	3	HEC	CAA-C2A-C1A	-2.08	124.75	127.01
4	C	7	HEC	CBD-CAD-C3D	-2.07	108.81	112.53
4	D	5	HEC	C3C-C4C-NC	-2.03	107.11	110.94
4	B	7	HEC	CMA-C3A-C2A	2.02	129.46	125.24
4	C	5	HEC	C4C-C3C-C2C	2.03	108.54	106.35
4	B	6	HEC	C4C-C3C-C2C	2.03	108.54	106.35
4	A	4	HEC	CMA-C3A-C2A	2.07	129.57	125.24
4	C	3	HEC	CAD-C3D-C4D	2.08	129.26	127.01
4	C	6	HEC	C4C-C3C-C2C	2.12	108.65	106.35
4	A	4	HEC	CMD-C2D-C3D	2.14	129.70	125.24
4	D	3	HEC	CMD-C2D-C1D	2.16	131.93	128.36
4	C	3	HEC	CMD-C2D-C1D	2.18	131.98	128.36
4	D	5	HEC	C4C-C3C-C2C	2.42	108.96	106.35
4	A	3	HEC	C4C-C3C-C2C	2.61	109.17	106.35
4	C	3	HEC	C4C-C3C-C2C	2.74	109.31	106.35
4	D	5	HEC	CMA-C3A-C2A	3.38	132.30	125.24
4	C	5	HEC	CAD-C3D-C4D	3.49	130.79	127.01
4	A	3	HEC	CAD-CBD-CGD	3.84	119.78	112.75
4	A	3	HEC	CAD-C3D-C4D	4.69	132.09	127.01
4	B	3	HEC	CAD-C3D-C4D	4.87	132.30	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3	HEC	6	0
4	A	4	HEC	5	0
4	A	5	HEC	5	0
4	A	6	HEC	9	0
4	A	7	HEC	7	0
4	B	3	HEC	5	0
4	B	4	HEC	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5	HEC	5	0
4	B	6	HEC	7	0
4	B	7	HEC	12	0
4	C	3	HEC	5	0
4	C	4	HEC	6	0
4	C	5	HEC	3	0
4	C	6	HEC	7	0
4	C	7	HEC	10	0
4	D	3	HEC	6	0
4	D	4	HEC	5	0
4	D	5	HEC	5	0
4	D	6	HEC	8	0
4	D	7	HEC	9	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.50	3 (0%) 89 89	8, 16, 28, 39	0
1	B	441/452 (97%)	-0.46	5 (1%) 82 83	9, 17, 29, 40	0
1	C	441/452 (97%)	-0.45	3 (0%) 89 89	9, 18, 31, 42	0
1	D	441/452 (97%)	-0.33	4 (0%) 85 86	11, 20, 34, 43	0
All	All	1764/1808 (97%)	-0.43	15 (0%) 85 86	8, 18, 31, 43	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	THR	3.6
1	B	293	ALA	3.4
1	D	221	LYS	3.2
1	C	293	ALA	3.1
1	D	37	THR	3.0
1	C	37	THR	2.9
1	B	37	THR	2.7
1	B	477	SER	2.7
1	A	293	ALA	2.6
1	B	221	LYS	2.5
1	D	293	ALA	2.3
1	B	294	GLU	2.2
1	A	477	SER	2.0
1	C	477	SER	2.0
1	D	460	LYS	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 ⓘ

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	HEC	C	6	43/43	0.97	0.11	1.66	5,13,17,25	0
4	HEC	D	6	43/43	0.98	0.10	1.53	9,14,20,31	0
4	HEC	B	7	43/43	0.98	0.11	0.77	10,15,31,40	0
4	HEC	C	7	43/43	0.98	0.11	0.65	10,14,31,39	0
4	HEC	A	6	43/43	0.98	0.09	0.59	6,10,16,24	0
4	HEC	A	7	43/43	0.98	0.11	0.55	12,16,33,44	0
4	HEC	B	6	43/43	0.98	0.09	0.51	5,10,18,25	0
4	HEC	D	7	43/43	0.98	0.11	0.34	11,15,35,41	0
4	HEC	A	4	43/43	0.98	0.10	0.18	8,14,16,21	0
4	HEC	B	3	43/43	0.98	0.08	0.16	4,10,14,15	0
4	HEC	B	4	43/43	0.99	0.09	-0.02	9,12,15,19	0
4	HEC	A	3	43/43	0.99	0.08	-0.04	3,8,12,14	0
4	HEC	C	4	43/43	0.98	0.10	-0.09	11,15,19,23	0
4	HEC	A	5	43/43	0.99	0.07	-0.11	5,10,12,13	0
4	HEC	B	5	43/43	0.99	0.08	-0.14	4,10,12,15	0
4	HEC	C	5	43/43	0.99	0.08	-0.23	4,11,14,16	0
4	HEC	D	4	43/43	0.97	0.10	-0.35	15,20,23,25	0
4	HEC	D	3	43/43	0.98	0.08	-0.43	9,15,18,19	0
4	HEC	D	5	43/43	0.98	0.08	-0.44	8,14,17,25	0
4	HEC	C	3	43/43	0.99	0.07	-0.88	8,13,16,17	0
3	EU	A	480	1/1	0.99	0.07	-1.02	24,24,24,24	1
2	CA	B	1	1/1	1.00	0.07	-1.29	13,13,13,13	0
3	EU	B	480	1/1	0.99	0.07	-1.29	25,25,25,25	1
2	CA	A	1	1/1	1.00	0.05	-2.39	12,12,12,12	0
2	CA	C	1	1/1	1.00	0.04	-2.99	13,13,13,13	0
2	CA	D	1	1/1	0.99	0.03	-3.14	19,19,19,19	0
3	EU	D	2	1/1	1.00	0.04	-	19,19,19,19	0
3	EU	A	479	1/1	1.00	0.07	-	16,16,16,16	1
3	EU	C	479	1/1	1.00	0.02	-	19,19,19,19	0
3	EU	A	2	1/1	1.00	0.03	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EU	B	479	1/1	1.00	0.11	-	13,13,13,13	1
3	EU	B	2	1/1	1.00	0.03	-	15,15,15,15	0
3	EU	C	2	1/1	1.00	0.03	-	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.