Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:56 PM GMT

PDB ID	:	1HV4
Title	:	CRYSTAL STRUCTURE ANALYSIS OF BAR-HEAD GOOSE HEMOGLOBIN (DEOXY FORM)
Authors	:	Liang, Y.; Hua, Z.; Liang, X.; Xu, Q.; Lu, G.
Deposited on	:	2001-01-07
Resolution	:	2.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

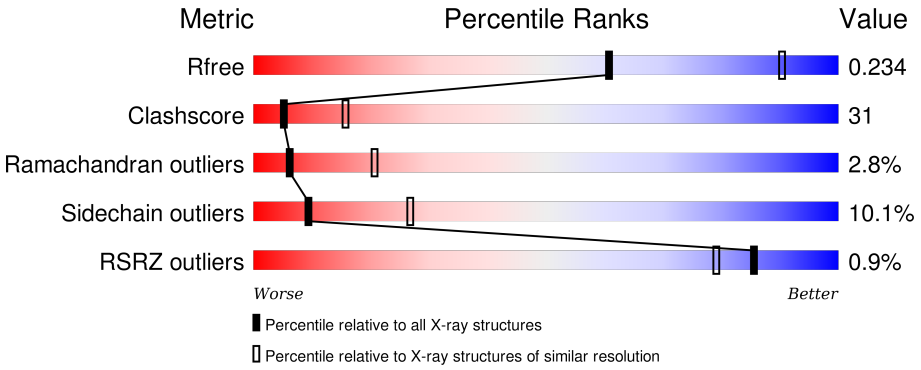
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	141	62% 30% 7%
1	C	141	58% 35% 7%
1	E	141	60% 33% 7%
1	G	141	60% 33% 7%
2	B	146	59% 32% 8%

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Mol	Chain	Length	Quality of chain
2	D	146	59% 32% 8%
2	F	146	57% 34% 8%
2	H	146	58% 33% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9288 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.

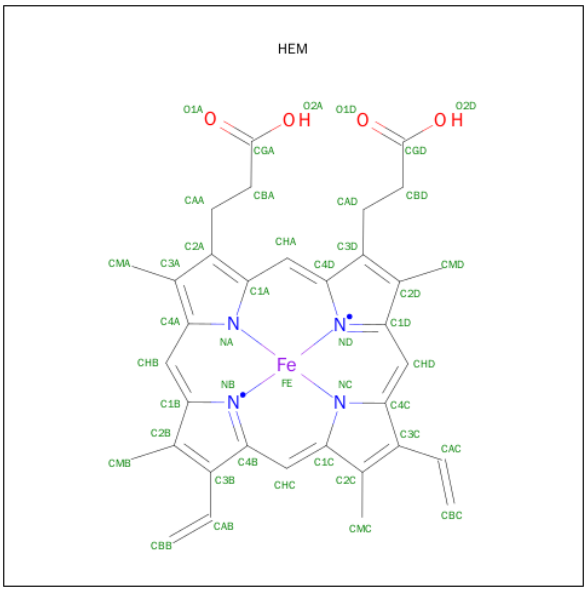
- Molecule 1 is a protein called HEMOGLOBIN ALPHA-A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1084	697	189	195	3			
1	C	141	Total	C	N	O	S	0	0	0
			1084	697	189	195	3			
1	E	141	Total	C	N	O	S	0	0	0
			1084	697	189	195	3			
1	G	141	Total	C	N	O	S	0	0	0
			1084	697	189	195	3			

- Molecule 2 is a protein called HEMOGLOBIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1152	744	204	200	4			
2	D	146	Total	C	N	O	S	0	0	0
			1152	744	204	200	4			
2	F	146	Total	C	N	O	S	0	0	0
			1152	744	204	200	4			
2	H	146	Total	C	N	O	S	0	0	0
			1152	744	204	200	4			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



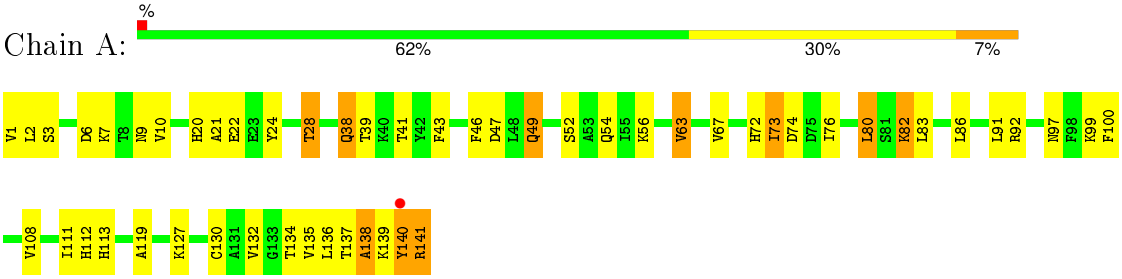
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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.

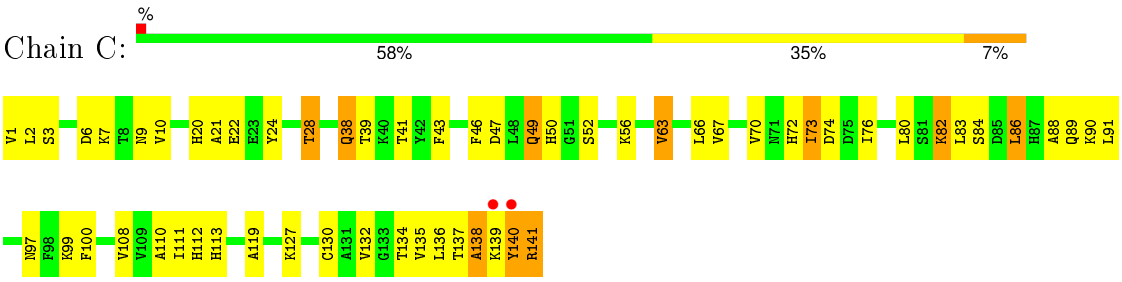
- Molecule 1: HEMOGLOBIN ALPHA-A CHAIN

Chain A:



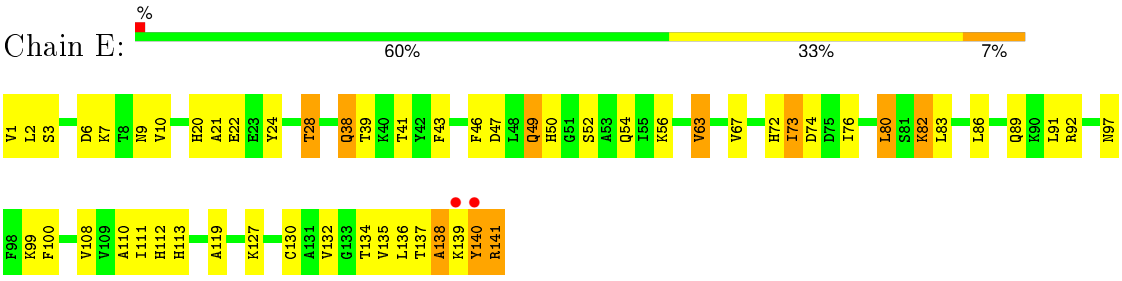
- Molecule 1: HEMOGLOBIN ALPHA-A CHAIN

Chain C:



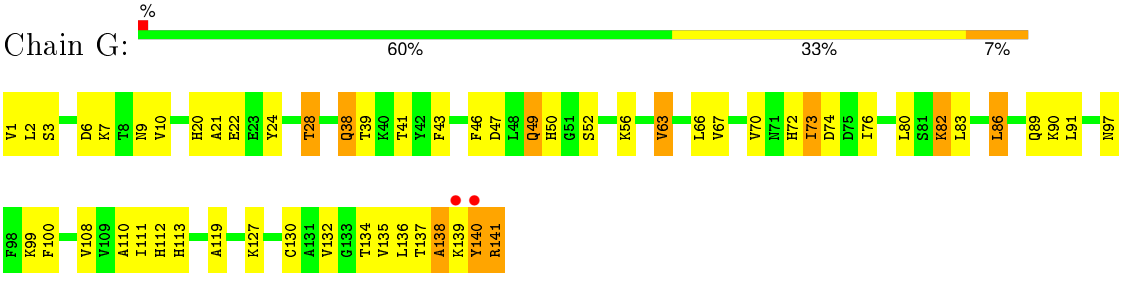
- Molecule 1: HEMOGLOBIN ALPHA-A CHAIN

Chain E:



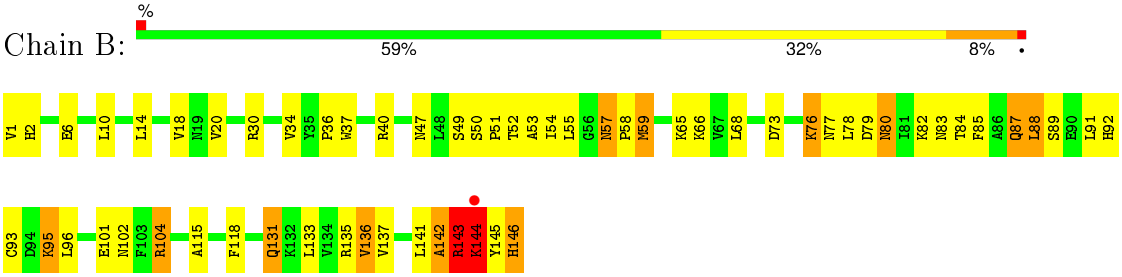
- Molecule 1: HEMOGLOBIN ALPHA-A CHAIN

Chain G:



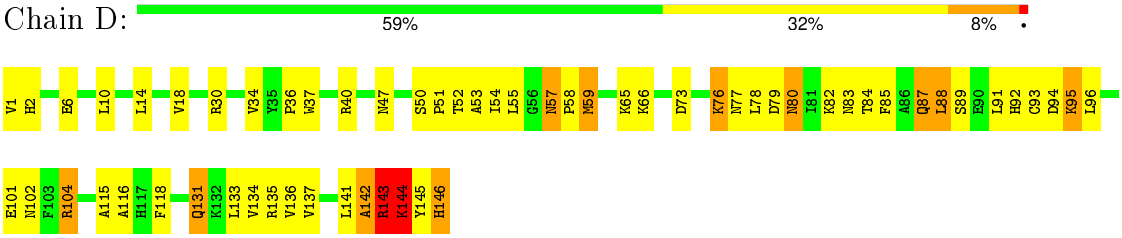
• Molecule 2: HEMOGLOBIN BETA CHAIN

Chain B:



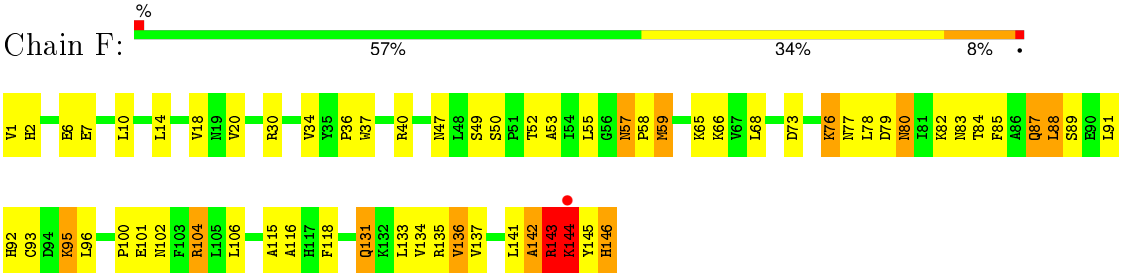
• Molecule 2: HEMOGLOBIN BETA CHAIN

Chain D:



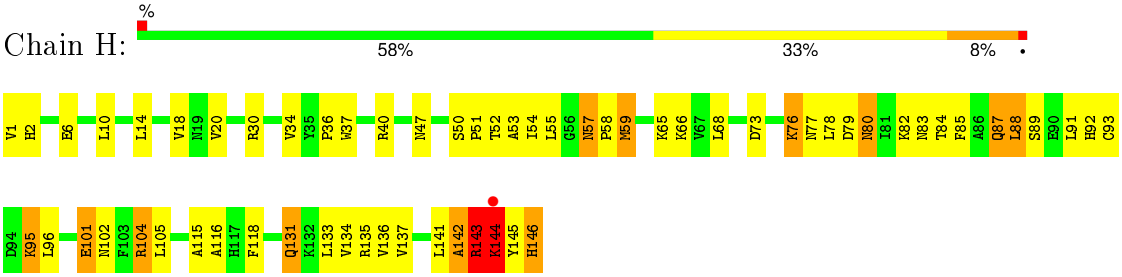
• Molecule 2: HEMOGLOBIN BETA CHAIN

Chain F:



• Molecule 2: HEMOGLOBIN BETA CHAIN

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.66Å 94.10Å 59.23Å 71.55° 65.10° 83.10°	Depositor
Resolution (Å)	36.89 – 2.80 36.89 – 2.55	Depositor EDS
% Data completeness (in resolution range)	84.0 (36.89-2.80) 70.9 (36.89-2.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.05 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.243 0.190 , 0.234	Depositor DCC
R_{free} test set	2752 reflections (11.28%)	DCC
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 25.1	EDS
Estimated twinning fraction	0.457 for -h+l,-k+l,l 0.000 for h-l,-k,-l 0.000 for -h,k-l,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 30654 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9288	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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 48.29 % 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 8.7905e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

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	0.46	0/1109	0.63	0/1501
1	C	0.49	0/1109	0.64	0/1501
1	E	0.47	0/1109	0.64	0/1501
1	G	0.50	0/1109	0.64	0/1501
2	B	0.44	0/1181	0.63	0/1602
2	D	0.43	0/1181	0.63	0/1602
2	F	0.45	0/1181	0.64	0/1602
2	H	0.43	0/1181	0.63	0/1602
All	All	0.46	0/9160	0.63	0/12412

There are no bond length outliers.

There are no bond angle outliers.

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	1084	0	1095	71	0
1	C	1084	0	1095	75	0
1	E	1084	0	1095	75	0
1	G	1084	0	1095	74	0
2	B	1152	0	1163	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1152	0	1163	77	0
2	F	1152	0	1163	76	0
2	H	1152	0	1163	77	0
3	A	43	0	30	0	0
3	B	43	0	30	2	0
3	C	43	0	30	0	0
3	D	43	0	30	1	0
3	E	43	0	30	0	0
3	F	43	0	30	3	0
3	G	43	0	30	0	0
3	H	43	0	30	1	0
All	All	9288	0	9272	568	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 31.

All (568) 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)
2:H:76:LYS:HA	2:H:76:LYS:NZ	1.60	1.15
2:F:76:LYS:HZ2	2:F:76:LYS:HA	0.98	1.15
2:B:76:LYS:HA	2:B:76:LYS:NZ	1.62	1.14
2:D:76:LYS:HA	2:D:76:LYS:NZ	1.60	1.14
2:F:76:LYS:HA	2:F:76:LYS:NZ	1.61	1.14
2:D:76:LYS:HA	2:D:76:LYS:HZ2	0.97	1.11
2:H:76:LYS:HA	2:H:76:LYS:HZ2	1.02	1.11
2:B:76:LYS:HA	2:B:76:LYS:HZ2	1.11	1.02
2:D:142:ALA:O	2:D:144:LYS:N	2.06	0.89
2:H:142:ALA:O	2:H:144:LYS:N	2.07	0.88
2:F:142:ALA:O	2:F:144:LYS:N	2.06	0.88
2:B:142:ALA:O	2:B:144:LYS:N	2.08	0.87
1:C:140:TYR:C	1:C:141:ARG:HH11	1.81	0.84
1:G:141:ARG:HB2	1:G:141:ARG:NH1	1.93	0.84
2:D:82:LYS:HD3	2:D:83:ASN:N	1.95	0.82
1:A:141:ARG:HB2	1:A:141:ARG:NH1	1.95	0.81
1:G:140:TYR:C	1:G:141:ARG:HH11	1.82	0.81
2:H:82:LYS:HD3	2:H:83:ASN:N	1.94	0.81
1:C:141:ARG:NH1	1:C:141:ARG:HB2	1.95	0.81
2:F:82:LYS:HD3	2:F:83:ASN:N	1.96	0.81
2:B:82:LYS:HD3	2:B:83:ASN:N	1.96	0.81
1:E:141:ARG:HB2	1:E:141:ARG:NH1	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:TYR:C	1:A:141:ARG:HH11	1.84	0.80
1:E:140:TYR:C	1:E:141:ARG:HH11	1.85	0.80
2:F:76:LYS:NZ	2:F:76:LYS:CA	2.46	0.78
1:G:141:ARG:HH11	1:G:141:ARG:N	1.82	0.78
1:G:39:THR:HG22	1:G:97:ASN:ND2	1.97	0.78
1:C:141:ARG:N	1:C:141:ARG:HH11	1.80	0.77
1:A:39:THR:HG22	1:A:97:ASN:ND2	1.99	0.77
1:A:141:ARG:N	1:A:141:ARG:HH11	1.82	0.77
2:B:52:THR:HA	2:B:55:LEU:HD23	1.67	0.77
1:E:39:THR:HG22	1:E:97:ASN:ND2	1.99	0.77
2:F:52:THR:HA	2:F:55:LEU:HD23	1.67	0.76
2:H:57:ASN:ND2	2:H:59:MET:H	1.83	0.76
1:G:38:GLN:H	1:G:38:GLN:HE21	1.32	0.76
1:E:1:VAL:HG22	1:G:141:ARG:OXT	1.86	0.76
1:C:38:GLN:HE21	1:C:38:GLN:H	1.34	0.75
2:D:57:ASN:ND2	2:D:59:MET:H	1.83	0.75
2:D:133:LEU:O	2:D:137:VAL:HG23	1.86	0.75
2:D:52:THR:HA	2:D:55:LEU:HD23	1.67	0.75
1:C:39:THR:HG22	1:C:97:ASN:ND2	2.02	0.75
1:G:99:LYS:HD3	2:H:104:ARG:HH22	1.50	0.75
2:D:76:LYS:NZ	2:D:76:LYS:CA	2.47	0.75
1:G:38:GLN:H	1:G:38:GLN:NE2	1.84	0.75
1:C:134:THR:O	1:C:138:ALA:HB2	1.87	0.74
2:F:144:LYS:HA	2:F:144:LYS:HE2	1.69	0.74
2:B:144:LYS:HA	2:B:144:LYS:HE2	1.69	0.74
1:E:141:ARG:HH11	1:E:141:ARG:N	1.83	0.74
2:H:52:THR:HA	2:H:55:LEU:HD23	1.67	0.74
2:B:76:LYS:CA	2:B:76:LYS:NZ	2.47	0.74
2:H:144:LYS:HA	2:H:144:LYS:HE2	1.69	0.74
1:A:99:LYS:HD3	2:B:104:ARG:HH22	1.52	0.73
1:C:38:GLN:NE2	1:C:38:GLN:H	1.86	0.73
2:B:57:ASN:ND2	2:B:59:MET:H	1.86	0.73
1:E:38:GLN:HE21	1:E:38:GLN:H	1.36	0.73
2:H:133:LEU:O	2:H:137:VAL:HG23	1.88	0.73
2:D:144:LYS:HA	2:D:144:LYS:HE2	1.69	0.73
2:D:91:LEU:HD12	2:D:92:HIS:N	2.03	0.73
1:C:99:LYS:HD3	2:D:104:ARG:HH22	1.52	0.73
1:E:99:LYS:HD3	2:F:104:ARG:HH22	1.53	0.73
2:H:91:LEU:HD12	2:H:92:HIS:N	2.03	0.72
2:B:91:LEU:HD12	2:B:92:HIS:N	2.05	0.72
1:E:38:GLN:NE2	1:E:38:GLN:H	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:ILE:HG22	1:E:112:HIS:HD2	1.53	0.72
2:F:133:LEU:O	2:F:137:VAL:HG23	1.89	0.72
1:A:138:ALA:HA	1:A:141:ARG:NH1	2.05	0.72
1:C:138:ALA:HA	1:C:141:ARG:HH12	1.55	0.71
1:A:138:ALA:O	1:A:141:ARG:N	2.22	0.71
1:E:138:ALA:HA	1:E:141:ARG:HH12	1.55	0.71
2:H:76:LYS:NZ	2:H:76:LYS:CA	2.47	0.71
1:C:138:ALA:HA	1:C:141:ARG:NH1	2.05	0.71
1:A:138:ALA:HA	1:A:141:ARG:HH12	1.55	0.71
1:E:138:ALA:HA	1:E:141:ARG:NH1	2.04	0.71
1:A:1:VAL:HG22	1:C:141:ARG:OXT	1.91	0.71
2:F:91:LEU:HD12	2:F:92:HIS:N	2.06	0.71
1:G:138:ALA:HA	1:G:141:ARG:NH1	2.06	0.70
1:G:134:THR:O	1:G:138:ALA:HB2	1.92	0.70
2:F:57:ASN:ND2	2:F:59:MET:H	1.88	0.70
1:C:138:ALA:O	1:C:141:ARG:N	2.24	0.70
1:C:111:ILE:HG22	1:C:112:HIS:HD2	1.57	0.70
2:B:133:LEU:O	2:B:137:VAL:HG23	1.92	0.70
1:A:38:GLN:H	1:A:38:GLN:HE21	1.38	0.70
1:A:38:GLN:H	1:A:38:GLN:NE2	1.88	0.69
1:G:111:ILE:HG22	1:G:112:HIS:HD2	1.55	0.69
1:A:111:ILE:HG22	1:A:112:HIS:HD2	1.56	0.69
1:E:138:ALA:O	1:E:141:ARG:N	2.25	0.69
1:G:138:ALA:HA	1:G:141:ARG:HH12	1.57	0.69
1:A:134:THR:O	1:A:138:ALA:HB2	1.92	0.69
1:G:138:ALA:O	1:G:141:ARG:N	2.26	0.68
2:H:87:GLN:CD	2:H:87:GLN:H	1.94	0.68
1:E:134:THR:O	1:E:138:ALA:HB2	1.93	0.67
2:H:57:ASN:HD22	2:H:57:ASN:C	1.98	0.67
2:D:87:GLN:CD	2:D:87:GLN:H	1.98	0.67
1:G:140:TYR:C	1:G:141:ARG:NH1	2.47	0.67
1:A:39:THR:HG22	1:A:97:ASN:HD22	1.58	0.67
1:C:140:TYR:C	1:C:141:ARG:NH1	2.46	0.67
2:D:57:ASN:C	2:D:57:ASN:HD22	1.96	0.67
2:F:87:GLN:CD	2:F:87:GLN:H	1.97	0.66
1:A:140:TYR:C	1:A:141:ARG:NH1	2.49	0.66
1:G:39:THR:HG22	1:G:97:ASN:HD22	1.60	0.66
2:B:87:GLN:H	2:B:87:GLN:CD	1.98	0.66
1:A:134:THR:O	1:A:138:ALA:N	2.30	0.65
1:E:39:THR:HG22	1:E:97:ASN:HD22	1.59	0.65
2:B:82:LYS:HG2	2:B:143:ARG:HH12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:ASN:HD22	2:F:57:ASN:C	2.00	0.65
1:C:39:THR:HG22	1:C:97:ASN:HD22	1.62	0.65
2:B:143:ARG:HG3	2:B:144:LYS:N	2.12	0.64
2:F:59:MET:CE	2:F:59:MET:HA	2.27	0.64
2:D:143:ARG:HG3	2:D:144:LYS:N	2.11	0.64
1:E:134:THR:O	1:E:138:ALA:N	2.29	0.64
2:B:59:MET:CE	2:B:59:MET:HA	2.28	0.64
1:C:24:TYR:O	1:C:28:THR:HG23	1.96	0.64
1:C:3:SER:O	1:C:7:LYS:HG3	1.97	0.64
2:B:57:ASN:HD22	2:B:57:ASN:C	1.99	0.64
2:B:76:LYS:HA	2:B:76:LYS:HZ3	1.57	0.64
1:G:134:THR:O	1:G:138:ALA:N	2.31	0.64
1:E:140:TYR:C	1:E:141:ARG:NH1	2.51	0.64
2:H:143:ARG:HG3	2:H:144:LYS:N	2.12	0.64
1:C:134:THR:O	1:C:138:ALA:N	2.31	0.64
1:E:3:SER:O	1:E:7:LYS:HG3	1.98	0.64
1:A:141:ARG:OXT	1:C:1:VAL:HG22	1.97	0.63
2:F:82:LYS:HG2	2:F:143:ARG:HH12	1.62	0.63
1:G:138:ALA:HA	1:G:141:ARG:NH2	2.14	0.63
2:D:82:LYS:HG2	2:D:143:ARG:HH12	1.64	0.62
1:G:24:TYR:O	1:G:28:THR:HG23	1.99	0.62
2:D:1:VAL:HG12	2:D:2:HIS:N	2.15	0.62
2:D:80:ASN:O	2:D:84:THR:HG23	2.00	0.62
2:H:57:ASN:HD22	2:H:58:PRO:N	1.98	0.62
1:A:3:SER:O	1:A:7:LYS:HG3	2.00	0.62
2:F:89:SER:HB2	2:F:141:LEU:O	2.00	0.62
2:B:89:SER:HB2	2:B:141:LEU:O	1.99	0.62
1:C:138:ALA:HA	1:C:141:ARG:NH2	2.15	0.62
1:G:3:SER:O	1:G:7:LYS:HG3	1.99	0.62
2:F:59:MET:HA	2:F:59:MET:HE3	1.81	0.61
2:H:34:VAL:O	2:H:36:PRO:HD3	2.00	0.61
2:H:82:LYS:HG2	2:H:143:ARG:HH12	1.64	0.61
1:E:141:ARG:OXT	1:G:1:VAL:HG22	2.00	0.61
2:D:57:ASN:HD22	2:D:58:PRO:N	1.99	0.61
2:F:143:ARG:HG3	2:F:144:LYS:N	2.15	0.61
1:G:135:VAL:HA	1:G:138:ALA:HB3	1.83	0.61
2:F:80:ASN:O	2:F:84:THR:HG23	2.01	0.61
1:C:135:VAL:HA	1:C:138:ALA:HB3	1.82	0.60
1:A:135:VAL:HA	1:A:138:ALA:HB3	1.83	0.60
2:D:57:ASN:HD21	2:D:59:MET:HB2	1.66	0.60
2:H:59:MET:CE	2:H:59:MET:HA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:VAL:HG12	2:H:2:HIS:N	2.16	0.60
2:H:104:ARG:HD3	2:H:104:ARG:C	2.22	0.60
2:D:34:VAL:O	2:D:36:PRO:HD3	2.01	0.60
2:B:104:ARG:HD3	2:B:104:ARG:C	2.22	0.60
1:E:24:TYR:O	1:E:28:THR:HG23	2.02	0.60
2:F:57:ASN:HD22	2:F:58:PRO:N	2.00	0.60
2:H:80:ASN:O	2:H:84:THR:HG23	2.01	0.60
2:B:57:ASN:HD21	2:B:59:MET:HB2	1.66	0.60
1:C:47:ASP:OD1	1:C:49:GLN:HG2	2.01	0.60
2:D:59:MET:HA	2:D:59:MET:CE	2.31	0.60
1:A:24:TYR:O	1:A:28:THR:HG23	2.02	0.60
1:E:138:ALA:HA	1:E:141:ARG:NH2	2.17	0.60
2:D:104:ARG:C	2:D:104:ARG:HD3	2.22	0.60
2:B:1:VAL:HG12	2:B:2:HIS:N	2.17	0.60
1:A:138:ALA:HA	1:A:141:ARG:NH2	2.17	0.59
2:B:80:ASN:O	2:B:84:THR:HG23	2.02	0.59
2:H:57:ASN:HD21	2:H:59:MET:HB2	1.67	0.59
2:B:37:TRP:HE1	2:B:102:ASN:HD21	1.50	0.59
1:G:47:ASP:OD1	1:G:49:GLN:HG2	2.03	0.59
1:C:141:ARG:NH1	1:C:141:ARG:N	2.50	0.59
1:E:135:VAL:HA	1:E:138:ALA:HB3	1.82	0.59
2:F:104:ARG:HD3	2:F:104:ARG:C	2.22	0.59
2:B:34:VAL:O	2:B:36:PRO:HD3	2.01	0.59
2:F:37:TRP:HE1	2:F:102:ASN:HD21	1.50	0.59
2:H:76:LYS:HA	2:H:76:LYS:HZ3	1.64	0.59
1:A:138:ALA:O	1:A:139:LYS:C	2.41	0.59
2:B:57:ASN:HD22	2:B:58:PRO:N	1.99	0.59
1:E:91:LEU:O	2:H:40:ARG:HD2	2.03	0.59
1:C:138:ALA:HA	1:C:141:ARG:HH22	1.68	0.59
1:A:141:ARG:N	1:A:141:ARG:NH1	2.51	0.59
1:A:91:LEU:O	2:D:40:ARG:HD2	2.03	0.58
2:F:34:VAL:O	2:F:36:PRO:HD3	2.03	0.58
2:F:1:VAL:HG12	2:F:2:HIS:N	2.18	0.58
2:H:37:TRP:HE1	2:H:102:ASN:HD21	1.49	0.58
1:G:138:ALA:HA	1:G:141:ARG:HH22	1.68	0.58
2:D:37:TRP:HE1	2:D:102:ASN:HD21	1.50	0.58
1:E:47:ASP:OD1	1:E:52:SER:HB2	2.04	0.58
1:C:132:VAL:O	1:C:136:LEU:HD23	2.03	0.58
2:F:57:ASN:HD21	2:F:59:MET:HB2	1.68	0.58
1:G:132:VAL:O	1:G:136:LEU:HD23	2.04	0.58
2:H:87:GLN:N	2:H:87:GLN:CD	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82:LYS:HZ1	2:H:143:ARG:HH22	1.53	0.57
1:A:138:ALA:C	1:A:140:TYR:N	2.56	0.57
2:D:14:LEU:O	2:D:18:VAL:HG23	2.05	0.57
2:B:76:LYS:CA	2:B:76:LYS:HZ3	2.15	0.57
2:D:93:CYS:SG	2:D:145:TYR:CG	2.93	0.57
1:A:132:VAL:O	1:A:136:LEU:HD23	2.04	0.57
2:F:87:GLN:CD	2:F:87:GLN:N	2.58	0.57
2:B:6:GLU:CD	2:B:6:GLU:H	2.07	0.57
2:F:6:GLU:H	2:F:6:GLU:CD	2.07	0.57
2:H:91:LEU:O	2:H:95:LYS:HB3	2.05	0.57
1:E:111:ILE:HG22	1:E:112:HIS:CD2	2.39	0.57
1:A:47:ASP:OD1	1:A:52:SER:HB2	2.05	0.57
1:E:47:ASP:OD1	1:E:49:GLN:HG2	2.04	0.56
1:G:141:ARG:NH1	1:G:141:ARG:N	2.51	0.56
1:A:138:ALA:HA	1:A:141:ARG:HH22	1.71	0.56
1:E:138:ALA:O	1:E:139:LYS:C	2.42	0.56
2:B:87:GLN:CD	2:B:87:GLN:N	2.59	0.56
1:G:138:ALA:O	1:G:139:LYS:C	2.44	0.56
2:F:93:CYS:SG	2:F:145:TYR:CG	2.95	0.56
2:H:87:GLN:H	2:H:87:GLN:NE2	2.04	0.56
1:C:138:ALA:O	1:C:139:LYS:C	2.42	0.56
1:G:138:ALA:HA	1:G:141:ARG:CZ	2.35	0.56
2:H:14:LEU:O	2:H:18:VAL:HG23	2.06	0.56
1:A:24:TYR:CE2	1:A:112:HIS:ND1	2.72	0.56
1:C:82:LYS:HD3	1:C:82:LYS:O	2.06	0.56
1:G:9:ASN:HD22	1:G:9:ASN:N	2.03	0.56
2:D:89:SER:HB2	2:D:141:LEU:O	2.06	0.56
2:H:93:CYS:SG	2:H:145:TYR:CG	2.95	0.56
1:E:138:ALA:HA	1:E:141:ARG:CZ	2.36	0.56
1:G:47:ASP:OD1	1:G:52:SER:HB2	2.05	0.56
1:E:135:VAL:HA	1:E:138:ALA:CB	2.36	0.55
1:E:138:ALA:C	1:E:140:TYR:N	2.57	0.55
1:A:138:ALA:O	1:A:140:TYR:N	2.39	0.55
1:G:141:ARG:CZ	1:G:141:ARG:HB2	2.35	0.55
1:E:138:ALA:HA	1:E:141:ARG:HH22	1.71	0.55
1:A:141:ARG:HB2	1:A:141:ARG:HH11	1.71	0.55
1:A:47:ASP:OD1	1:A:49:GLN:HG2	2.05	0.55
1:C:138:ALA:O	1:C:140:TYR:N	2.40	0.55
1:A:138:ALA:HA	1:A:141:ARG:CZ	2.36	0.55
2:D:87:GLN:N	2:D:87:GLN:CD	2.58	0.55
2:D:91:LEU:O	2:D:95:LYS:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:TYR:O	1:C:141:ARG:HD3	2.07	0.55
1:C:138:ALA:C	1:C:140:TYR:N	2.56	0.55
1:E:28:THR:HG22	1:E:108:VAL:HG21	1.88	0.55
1:C:135:VAL:HA	1:C:138:ALA:CB	2.36	0.55
1:G:138:ALA:C	1:G:140:TYR:N	2.57	0.55
2:H:6:GLU:O	2:H:10:LEU:HD23	2.07	0.55
1:C:134:THR:O	1:C:138:ALA:CB	2.54	0.54
1:E:141:ARG:HH11	1:E:141:ARG:HB2	1.71	0.54
1:C:9:ASN:HD22	1:C:9:ASN:N	2.04	0.54
2:D:6:GLU:O	2:D:10:LEU:HD23	2.06	0.54
2:H:89:SER:HB2	2:H:141:LEU:O	2.07	0.54
1:C:138:ALA:HA	1:C:141:ARG:CZ	2.36	0.54
1:E:141:ARG:NH1	1:E:141:ARG:N	2.53	0.54
1:E:140:TYR:O	1:G:127:LYS:HD3	2.07	0.54
1:G:135:VAL:HA	1:G:138:ALA:CB	2.37	0.54
1:A:135:VAL:HA	1:A:138:ALA:CB	2.37	0.54
1:A:24:TYR:OH	1:A:113:HIS:HE1	1.89	0.54
1:G:137:THR:HB	1:G:140:TYR:CE1	2.43	0.54
1:C:111:ILE:HG22	1:C:112:HIS:CD2	2.42	0.54
2:B:14:LEU:O	2:B:18:VAL:HG23	2.07	0.54
1:A:6:ASP:O	1:A:10:VAL:HG23	2.06	0.54
1:C:137:THR:HB	1:C:140:TYR:CE1	2.43	0.54
1:A:141:ARG:HB2	1:A:141:ARG:CZ	2.37	0.54
1:E:141:ARG:CZ	1:E:141:ARG:HB2	2.38	0.54
1:A:28:THR:HG22	1:A:108:VAL:HG21	1.89	0.54
1:E:132:VAL:O	1:E:136:LEU:HD23	2.07	0.54
1:G:141:ARG:HH11	1:G:141:ARG:HB2	1.68	0.54
1:A:111:ILE:HG22	1:A:112:HIS:CD2	2.42	0.54
2:F:14:LEU:O	2:F:18:VAL:HG23	2.07	0.54
1:E:138:ALA:O	1:E:140:TYR:N	2.41	0.54
2:H:47:ASN:ND2	2:H:53:ALA:HB1	2.23	0.54
1:G:76:ILE:O	1:G:80:LEU:HD12	2.08	0.54
2:H:6:GLU:CD	2:H:6:GLU:H	2.11	0.54
1:E:82:LYS:O	1:E:82:LYS:HD3	2.08	0.54
1:G:7:LYS:HD3	1:G:73:ILE:HG23	1.90	0.53
1:C:47:ASP:OD1	1:C:52:SER:HB2	2.08	0.53
2:B:93:CYS:SG	2:B:145:TYR:CG	2.95	0.53
1:C:24:TYR:CE2	1:C:112:HIS:ND1	2.76	0.53
1:G:138:ALA:O	1:G:140:TYR:N	2.42	0.53
1:G:111:ILE:HG22	1:G:112:HIS:CD2	2.40	0.53
1:C:141:ARG:HB2	1:C:141:ARG:CZ	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:TYR:O	1:G:141:ARG:HD3	2.09	0.53
1:G:1:VAL:HG23	1:G:2:LEU:N	2.23	0.53
1:G:82:LYS:O	1:G:82:LYS:HD3	2.08	0.53
1:E:9:ASN:HD22	1:E:9:ASN:N	2.05	0.53
1:C:76:ILE:O	1:C:80:LEU:HD12	2.08	0.53
1:C:80:LEU:HD23	1:C:83:LEU:HD12	1.91	0.53
2:D:82:LYS:HZ1	2:D:143:ARG:HH22	1.57	0.53
2:F:91:LEU:O	2:F:95:LYS:HB3	2.09	0.53
1:G:111:ILE:HG12	2:H:115:ALA:O	2.08	0.53
2:D:47:ASN:ND2	2:D:53:ALA:HB1	2.24	0.53
2:D:57:ASN:HD22	2:D:59:MET:H	1.57	0.53
1:E:24:TYR:CE2	1:E:112:HIS:ND1	2.75	0.53
2:B:47:ASN:ND2	2:B:53:ALA:HB1	2.24	0.53
1:A:82:LYS:HD3	1:A:82:LYS:O	2.09	0.53
1:A:137:THR:HB	1:A:140:TYR:CE1	2.44	0.52
1:C:1:VAL:HG23	1:C:2:LEU:N	2.24	0.52
1:E:137:THR:HB	1:E:140:TYR:CE1	2.44	0.52
1:C:111:ILE:HG12	2:D:115:ALA:O	2.09	0.52
1:E:1:VAL:HG23	1:E:2:LEU:N	2.24	0.52
1:G:134:THR:O	1:G:138:ALA:CB	2.58	0.52
2:D:133:LEU:O	2:D:136:VAL:HG12	2.09	0.52
2:D:87:GLN:NE2	2:D:87:GLN:H	2.07	0.52
2:B:133:LEU:O	2:B:136:VAL:HG12	2.10	0.52
2:F:87:GLN:H	2:F:87:GLN:NE2	2.07	0.52
1:C:141:ARG:HB2	1:C:141:ARG:HH11	1.71	0.52
1:A:140:TYR:O	1:C:127:LYS:HD3	2.09	0.52
2:F:6:GLU:N	2:F:6:GLU:CD	2.63	0.52
1:G:1:VAL:CG2	1:G:2:LEU:N	2.73	0.52
1:E:6:ASP:O	1:E:10:VAL:HG23	2.09	0.52
1:A:1:VAL:HG23	1:A:2:LEU:N	2.25	0.52
1:A:134:THR:O	1:A:138:ALA:CB	2.57	0.52
1:E:134:THR:O	1:E:138:ALA:CB	2.57	0.52
2:D:59:MET:HE3	2:D:59:MET:HA	1.92	0.52
2:B:84:THR:C	2:B:87:GLN:HE22	2.13	0.52
2:F:47:ASN:ND2	2:F:53:ALA:HB1	2.25	0.52
2:B:6:GLU:CD	2:B:6:GLU:N	2.63	0.51
2:D:93:CYS:SG	2:D:145:TYR:CD2	3.02	0.51
1:G:141:ARG:HH11	1:G:141:ARG:CB	2.23	0.51
1:G:24:TYR:CE2	1:G:112:HIS:ND1	2.77	0.51
1:E:7:LYS:HD3	1:E:73:ILE:HG23	1.91	0.51
2:B:91:LEU:O	2:B:95:LYS:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:VAL:HG12	2:D:2:HIS:H	1.73	0.51
2:B:141:LEU:CD1	3:B:152:HEM:HBB2	2.41	0.51
1:A:80:LEU:HD23	1:A:83:LEU:HD12	1.93	0.51
1:A:9:ASN:N	1:A:9:ASN:HD22	2.08	0.51
1:E:1:VAL:CG2	1:E:2:LEU:N	2.73	0.51
1:A:138:ALA:CA	1:A:141:ARG:HH12	2.23	0.51
1:C:1:VAL:CG2	1:C:2:LEU:N	2.73	0.51
1:E:24:TYR:OH	1:E:113:HIS:HE1	1.93	0.51
1:C:138:ALA:CA	1:C:141:ARG:HH12	2.23	0.51
1:A:7:LYS:HD3	1:A:73:ILE:HG23	1.93	0.51
1:C:134:THR:C	1:C:138:ALA:HB2	2.30	0.51
1:A:134:THR:C	1:A:138:ALA:HB2	2.31	0.51
2:H:1:VAL:HG12	2:H:2:HIS:H	1.75	0.51
1:E:63:VAL:O	1:E:67:VAL:HG23	2.11	0.51
2:D:76:LYS:HA	2:D:76:LYS:HZ3	1.68	0.51
1:G:138:ALA:CA	1:G:141:ARG:HH12	2.24	0.51
1:C:7:LYS:HD3	1:C:73:ILE:HG23	1.92	0.51
1:E:134:THR:C	1:E:138:ALA:HB2	2.31	0.50
2:B:57:ASN:HD22	2:B:59:MET:H	1.57	0.50
1:G:49:GLN:CD	1:G:49:GLN:H	2.14	0.50
1:E:76:ILE:O	1:E:80:LEU:HD12	2.11	0.50
2:F:142:ALA:HA	2:F:145:TYR:CE2	2.46	0.50
1:G:80:LEU:HD23	1:G:83:LEU:HD12	1.94	0.50
1:A:63:VAL:O	1:A:67:VAL:HG23	2.12	0.50
2:F:135:ARG:NH2	2:H:146:HIS:NE2	2.59	0.50
1:C:141:ARG:CB	1:C:141:ARG:HH11	2.25	0.50
1:G:22:GLU:OE2	1:G:56:LYS:HB3	2.12	0.50
1:A:1:VAL:CG2	1:A:2:LEU:N	2.74	0.50
1:G:134:THR:C	1:G:138:ALA:HB2	2.31	0.50
2:D:6:GLU:CD	2:D:6:GLU:H	2.13	0.50
1:A:141:ARG:CB	1:A:141:ARG:HH11	2.25	0.50
1:E:138:ALA:CA	1:E:141:ARG:HH12	2.23	0.50
2:H:59:MET:HE2	2:H:59:MET:HA	1.94	0.50
1:C:22:GLU:OE2	1:C:56:LYS:HB3	2.12	0.50
2:B:87:GLN:H	2:B:87:GLN:NE2	2.09	0.49
2:B:1:VAL:HG12	2:B:2:HIS:H	1.77	0.49
1:G:24:TYR:OH	1:G:113:HIS:HE1	1.95	0.49
1:A:22:GLU:OE2	1:A:56:LYS:HB3	2.12	0.49
1:A:76:ILE:O	1:A:80:LEU:HD12	2.12	0.49
1:C:6:ASP:O	1:C:10:VAL:HG23	2.12	0.49
2:D:57:ASN:C	2:D:57:ASN:ND2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:141:LEU:CD1	3:F:156:HEM:HBB2	2.42	0.49
2:H:34:VAL:C	2:H:36:PRO:HD3	2.33	0.49
2:H:133:LEU:O	2:H:136:VAL:HG12	2.12	0.49
1:A:43:PHE:HB3	1:A:46:PHE:HB2	1.93	0.49
2:H:57:ASN:C	2:H:57:ASN:ND2	2.66	0.49
2:D:84:THR:C	2:D:87:GLN:HE22	2.16	0.49
1:E:80:LEU:HD23	1:E:83:LEU:HD12	1.94	0.49
1:C:7:LYS:HD3	1:C:73:ILE:CG2	2.43	0.49
2:H:6:GLU:N	2:H:6:GLU:CD	2.65	0.49
2:B:6:GLU:O	2:B:10:LEU:HD23	2.13	0.49
2:B:93:CYS:SG	2:B:145:TYR:CD2	3.05	0.49
2:F:133:LEU:O	2:F:136:VAL:HG12	2.13	0.49
1:C:24:TYR:OH	1:C:113:HIS:HE1	1.96	0.49
1:E:22:GLU:OE2	1:E:56:LYS:HB3	2.13	0.49
2:H:142:ALA:HA	2:H:145:TYR:CE2	2.47	0.48
1:C:28:THR:HG22	1:C:108:VAL:HG21	1.94	0.48
2:F:84:THR:C	2:F:87:GLN:HE22	2.15	0.48
1:E:111:ILE:HG12	2:F:115:ALA:O	2.13	0.48
1:G:28:THR:HG22	1:G:108:VAL:HG21	1.95	0.48
1:C:49:GLN:CD	1:C:49:GLN:H	2.15	0.48
1:C:141:ARG:CB	1:C:141:ARG:NH1	2.74	0.48
1:E:43:PHE:HB3	1:E:46:PHE:HB2	1.95	0.48
2:B:59:MET:HE2	2:B:59:MET:HA	1.93	0.48
1:E:49:GLN:H	1:E:49:GLN:CD	2.16	0.48
2:D:6:GLU:CD	2:D:6:GLU:N	2.67	0.48
2:F:57:ASN:HD22	2:F:58:PRO:CD	2.27	0.48
1:A:111:ILE:HG12	2:B:115:ALA:O	2.13	0.48
1:G:6:ASP:O	1:G:10:VAL:HG23	2.12	0.48
2:B:142:ALA:HA	2:B:145:TYR:CE2	2.48	0.48
1:E:141:ARG:HH11	1:E:141:ARG:CB	2.26	0.48
1:G:7:LYS:HD3	1:G:73:ILE:CG2	2.43	0.48
1:A:49:GLN:H	1:A:49:GLN:CD	2.17	0.48
2:H:84:THR:C	2:H:87:GLN:HE22	2.16	0.48
2:B:34:VAL:C	2:B:36:PRO:HD3	2.34	0.48
2:F:77:ASN:O	2:F:79:ASP:N	2.47	0.48
2:B:135:ARG:NH2	2:D:146:HIS:NE2	2.61	0.48
2:F:96:LEU:H	2:F:96:LEU:HD22	1.79	0.48
2:F:34:VAL:C	2:F:36:PRO:HD3	2.34	0.47
2:B:131:GLN:HE21	2:B:131:GLN:CA	2.27	0.47
2:B:146:HIS:NE2	2:D:135:ARG:NH2	2.62	0.47
2:H:76:LYS:CA	2:H:76:LYS:HZ3	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1:VAL:HG12	2:F:2:HIS:H	1.79	0.47
2:F:6:GLU:O	2:F:10:LEU:HD23	2.14	0.47
2:D:34:VAL:C	2:D:36:PRO:HD3	2.34	0.47
2:H:50:SER:O	2:H:54:ILE:HG13	2.14	0.47
2:H:93:CYS:SG	2:H:145:TYR:CD2	3.06	0.47
2:B:85:PHE:N	2:B:87:GLN:HE22	2.13	0.47
2:F:93:CYS:SG	2:F:145:TYR:CD2	3.08	0.47
2:B:93:CYS:SG	2:B:145:TYR:CD1	3.03	0.47
2:F:57:ASN:HD22	2:F:59:MET:H	1.59	0.47
2:F:85:PHE:N	2:F:87:GLN:HE22	2.14	0.46
2:D:131:GLN:HE21	2:D:131:GLN:CA	2.28	0.46
2:F:146:HIS:NE2	2:H:135:ARG:NH2	2.63	0.46
1:A:140:TYR:O	1:A:141:ARG:HD3	2.15	0.46
2:H:57:ASN:HD22	2:H:59:MET:H	1.57	0.46
1:A:72:HIS:C	1:A:74:ASP:H	2.19	0.46
2:D:50:SER:O	2:D:54:ILE:HG13	2.15	0.46
1:C:138:ALA:C	1:C:141:ARG:HH12	2.18	0.46
1:G:110:ALA:HB1	2:H:116:ALA:HB2	1.98	0.46
2:B:77:ASN:O	2:B:79:ASP:N	2.48	0.46
1:G:43:PHE:HB3	1:G:46:PHE:HB2	1.98	0.46
2:D:142:ALA:HA	2:D:145:TYR:CE2	2.51	0.46
2:D:93:CYS:SG	2:D:145:TYR:CD1	3.03	0.46
1:E:7:LYS:HD3	1:E:73:ILE:CG2	2.46	0.46
2:H:131:GLN:CA	2:H:131:GLN:HE21	2.27	0.46
1:E:127:LYS:HD3	1:G:140:TYR:O	2.15	0.46
2:F:82:LYS:HZ1	2:F:143:ARG:HH22	1.64	0.46
2:H:57:ASN:HD22	2:H:58:PRO:CD	2.27	0.46
2:F:88:LEU:HA	2:F:88:LEU:HD13	1.85	0.46
2:H:96:LEU:H	2:H:96:LEU:HD22	1.81	0.46
1:C:72:HIS:C	1:C:74:ASP:H	2.20	0.46
1:C:137:THR:HB	1:C:140:TYR:HE1	1.81	0.45
1:E:140:TYR:O	1:E:141:ARG:HD3	2.16	0.45
2:B:57:ASN:ND2	2:B:57:ASN:C	2.68	0.45
2:F:57:ASN:ND2	2:F:57:ASN:C	2.69	0.45
1:G:63:VAL:O	1:G:67:VAL:HG23	2.16	0.45
2:D:57:ASN:HD22	2:D:58:PRO:CD	2.29	0.45
1:E:141:ARG:NH1	1:E:141:ARG:CB	2.75	0.45
2:B:57:ASN:HD22	2:B:58:PRO:CD	2.30	0.45
1:A:47:ASP:N	1:A:54:GLN:OE1	2.48	0.45
1:A:119:ALA:HA	2:B:30:ARG:NH1	2.31	0.45
1:C:43:PHE:HB3	1:C:46:PHE:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:CYS:SG	2:H:145:TYR:CD1	3.03	0.45
1:A:137:THR:HB	1:A:140:TYR:HE1	1.81	0.45
2:D:85:PHE:N	2:D:87:GLN:HE22	2.15	0.45
2:F:93:CYS:SG	2:F:145:TYR:CD1	3.01	0.45
2:H:85:PHE:N	2:H:87:GLN:HE22	2.15	0.45
2:F:131:GLN:CA	2:F:131:GLN:HE21	2.28	0.45
2:H:52:THR:HA	2:H:55:LEU:CD2	2.43	0.45
1:A:52:SER:O	1:A:56:LYS:HG3	2.17	0.45
1:C:110:ALA:HB1	2:D:116:ALA:HB2	1.98	0.45
1:A:24:TYR:HE2	1:A:112:HIS:HD1	1.56	0.45
1:A:92:ARG:O	2:D:40:ARG:HD3	2.16	0.45
2:D:96:LEU:H	2:D:96:LEU:HD22	1.80	0.45
1:G:138:ALA:C	1:G:141:ARG:HH12	2.20	0.44
1:G:137:THR:O	1:G:139:LYS:N	2.50	0.44
1:G:72:HIS:C	1:G:74:ASP:H	2.19	0.44
1:E:72:HIS:C	1:E:74:ASP:H	2.20	0.44
2:B:73:ASP:HA	2:B:76:LYS:HB2	2.00	0.44
1:A:138:ALA:C	1:A:141:ARG:HH12	2.20	0.44
1:E:24:TYR:HE2	1:E:112:HIS:HD1	1.60	0.44
1:A:7:LYS:HD3	1:A:73:ILE:CG2	2.47	0.44
1:C:63:VAL:O	1:C:67:VAL:HG23	2.17	0.44
2:F:65:LYS:HG3	2:F:66:LYS:N	2.31	0.44
2:D:145:TYR:CD2	2:D:145:TYR:N	2.85	0.44
1:C:137:THR:O	1:C:139:LYS:N	2.51	0.44
2:D:1:VAL:CG1	2:D:2:HIS:N	2.80	0.44
1:G:119:ALA:HA	2:H:30:ARG:NH1	2.33	0.44
2:F:73:ASP:HA	2:F:76:LYS:HB2	1.99	0.44
1:G:97:ASN:HA	1:G:100:PHE:CD1	2.53	0.44
2:D:88:LEU:HD13	2:D:88:LEU:HA	1.83	0.44
2:D:77:ASN:O	2:D:79:ASP:N	2.51	0.44
1:A:127:LYS:HD3	1:C:140:TYR:O	2.18	0.44
1:E:97:ASN:HA	1:E:100:PHE:CD1	2.53	0.44
1:E:52:SER:O	1:E:56:LYS:HG3	2.17	0.44
2:F:77:ASN:C	2:F:79:ASP:H	2.21	0.44
2:B:82:LYS:HZ1	2:B:143:ARG:HH22	1.65	0.44
1:E:119:ALA:HA	2:F:30:ARG:NH1	2.33	0.44
2:H:73:ASP:HA	2:H:76:LYS:HB2	1.99	0.43
1:G:137:THR:HB	1:G:140:TYR:HE1	1.81	0.43
2:F:52:THR:HA	2:F:55:LEU:CD2	2.43	0.43
2:D:82:LYS:HD3	2:D:83:ASN:CG	2.38	0.43
2:H:145:TYR:N	2:H:145:TYR:CD2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:GLN:HA	2:F:131:GLN:NE2	2.33	0.43
2:B:20:VAL:HA	2:B:68:LEU:HD23	1.99	0.43
1:G:141:ARG:CB	1:G:141:ARG:NH1	2.72	0.43
2:B:95:LYS:HE2	2:B:95:LYS:O	2.18	0.43
2:H:131:GLN:NE2	2:H:131:GLN:HA	2.34	0.43
2:H:65:LYS:HG3	2:H:66:LYS:N	2.32	0.43
2:H:14:LEU:HD11	2:H:118:PHE:CD2	2.53	0.43
2:D:73:ASP:HA	2:D:76:LYS:HB2	1.99	0.43
1:E:137:THR:HB	1:E:140:TYR:HE1	1.82	0.43
2:H:1:VAL:CG1	2:H:2:HIS:N	2.82	0.43
2:B:77:ASN:C	2:B:79:ASP:H	2.21	0.43
1:E:138:ALA:C	1:E:141:ARG:HH12	2.21	0.43
2:B:131:GLN:HA	2:B:131:GLN:NE2	2.33	0.43
1:E:20:HIS:O	1:E:21:ALA:C	2.57	0.43
2:B:51:PRO:O	2:B:55:LEU:HD22	2.18	0.43
2:B:96:LEU:H	2:B:96:LEU:HD22	1.82	0.43
1:G:38:GLN:N	1:G:38:GLN:HE21	2.08	0.43
1:G:66:LEU:O	1:G:70:VAL:HG23	2.19	0.43
2:H:141:LEU:CD1	3:H:158:HEM:HBB2	2.49	0.43
2:B:141:LEU:HD12	3:B:152:HEM:HBB2	2.01	0.43
1:A:20:HIS:O	1:A:21:ALA:C	2.57	0.43
2:F:141:LEU:O	2:F:142:ALA:O	2.37	0.42
2:H:95:LYS:HE2	2:H:95:LYS:O	2.19	0.42
2:B:85:PHE:CA	2:B:87:GLN:HE22	2.32	0.42
1:G:52:SER:O	1:G:56:LYS:HG3	2.18	0.42
2:H:82:LYS:HD3	2:H:83:ASN:CG	2.39	0.42
1:A:137:THR:O	1:A:139:LYS:N	2.53	0.42
2:D:52:THR:HA	2:D:55:LEU:CD2	2.44	0.42
2:D:131:GLN:HA	2:D:131:GLN:NE2	2.34	0.42
2:B:145:TYR:CD2	2:B:145:TYR:N	2.87	0.42
2:H:85:PHE:CA	2:H:87:GLN:HE22	2.33	0.42
1:C:119:ALA:HA	2:D:30:ARG:NH1	2.33	0.42
1:E:137:THR:O	1:E:139:LYS:N	2.52	0.42
2:D:51:PRO:O	2:D:55:LEU:HD22	2.20	0.42
2:F:95:LYS:O	2:F:95:LYS:HE2	2.19	0.42
2:D:94:ASP:N	2:D:94:ASP:OD2	2.53	0.42
2:F:85:PHE:CA	2:F:87:GLN:HE22	2.31	0.42
2:B:65:LYS:HG3	2:B:66:LYS:N	2.33	0.42
1:C:97:ASN:HA	1:C:100:PHE:CD1	2.54	0.42
2:H:51:PRO:O	2:H:55:LEU:HD22	2.19	0.42
2:B:141:LEU:O	2:B:142:ALA:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:SER:O	2:B:54:ILE:HG13	2.20	0.42
2:D:65:LYS:HG3	2:D:66:LYS:N	2.35	0.42
2:H:77:ASN:O	2:H:79:ASP:N	2.52	0.42
1:A:97:ASN:HA	1:A:100:PHE:CD1	2.55	0.42
1:C:52:SER:O	1:C:56:LYS:HG3	2.20	0.42
2:F:1:VAL:CG1	2:F:2:HIS:N	2.83	0.42
1:C:86:LEU:O	1:C:90:LYS:HB3	2.20	0.42
2:D:76:LYS:HZ3	2:D:76:LYS:CA	2.30	0.42
2:B:14:LEU:HD11	2:B:118:PHE:CD2	2.54	0.42
2:D:14:LEU:HD11	2:D:118:PHE:CD2	2.55	0.41
1:C:66:LEU:O	1:C:70:VAL:HG23	2.20	0.41
2:F:40:ARG:HD2	1:G:91:LEU:O	2.20	0.41
2:H:87:GLN:OE1	2:H:88:LEU:N	2.53	0.41
2:F:14:LEU:HD11	2:F:118:PHE:CD2	2.55	0.41
2:B:50:SER:OG	2:B:53:ALA:HB2	2.20	0.41
2:F:141:LEU:HD12	3:F:156:HEM:HBB2	2.02	0.41
2:D:85:PHE:CA	2:D:87:GLN:HE22	2.34	0.41
1:E:92:ARG:O	2:H:40:ARG:HD3	2.20	0.41
1:C:89:GLN:OE1	1:C:139:LYS:HG2	2.21	0.41
2:H:144:LYS:CA	2:H:144:LYS:HE2	2.47	0.41
1:E:1:VAL:O	1:E:2:LEU:HB2	2.21	0.41
2:D:95:LYS:O	2:D:95:LYS:HE2	2.20	0.41
2:B:87:GLN:OE1	2:B:88:LEU:N	2.54	0.41
2:F:20:VAL:HA	2:F:68:LEU:HD23	2.02	0.41
1:E:110:ALA:HB1	2:F:116:ALA:HB2	2.01	0.41
2:D:141:LEU:CD1	3:D:154:HEM:HBB2	2.49	0.41
2:F:145:TYR:N	2:F:145:TYR:CD2	2.88	0.41
1:G:89:GLN:OE1	1:G:139:LYS:HG2	2.20	0.41
2:B:59:MET:HE3	2:B:59:MET:HA	2.02	0.41
2:B:47:ASN:OD1	2:B:49:SER:HB2	2.20	0.41
2:B:50:SER:H	2:B:53:ALA:HB3	1.86	0.41
2:D:77:ASN:C	2:D:79:ASP:H	2.24	0.41
1:G:20:HIS:O	1:G:21:ALA:C	2.58	0.41
1:C:84:SER:O	1:C:88:ALA:HB3	2.21	0.41
2:B:82:LYS:HD3	2:B:83:ASN:CG	2.40	0.41
2:D:57:ASN:HA	2:D:58:PRO:HD2	1.84	0.41
2:F:50:SER:OG	2:F:53:ALA:HB2	2.20	0.41
1:E:47:ASP:N	1:E:54:GLN:OE1	2.50	0.40
1:C:63:VAL:HA	1:C:66:LEU:HD12	2.03	0.40
2:H:77:ASN:C	2:H:79:ASP:H	2.24	0.40
1:E:89:GLN:OE1	1:E:139:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:GLN:OE1	2:F:88:LEU:N	2.54	0.40
2:F:47:ASN:OD1	2:F:49:SER:HB2	2.21	0.40
1:G:86:LEU:O	1:G:90:LYS:HB3	2.21	0.40
2:D:141:LEU:O	2:D:142:ALA:O	2.39	0.40
2:F:82:LYS:HD3	2:F:83:ASN:CG	2.42	0.40
2:D:87:GLN:OE1	2:D:88:LEU:N	2.54	0.40
2:H:101:GLU:O	2:H:105:LEU:HG	2.21	0.40
2:H:20:VAL:HA	2:H:68:LEU:HD23	2.02	0.40
2:F:106:LEU:HD23	3:F:156:HEM:HAB	2.03	0.40
2:H:141:LEU:O	2:H:142:ALA:O	2.39	0.40
2:F:6:GLU:O	2:F:7:GLU:C	2.59	0.40
1:C:20:HIS:O	1:C:21:ALA:C	2.60	0.40
2:B:40:ARG:HD2	1:C:91:LEU:O	2.21	0.40

There are no symmetry-related clashes.

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	139/141 (99%)	123 (88%)	13 (9%)	3 (2%)	8	28
1	C	139/141 (99%)	123 (88%)	13 (9%)	3 (2%)	8	28
1	E	139/141 (99%)	123 (88%)	13 (9%)	3 (2%)	8	28
1	G	139/141 (99%)	124 (89%)	12 (9%)	3 (2%)	8	28
2	B	144/146 (99%)	132 (92%)	7 (5%)	5 (4%)	4	15
2	D	144/146 (99%)	132 (92%)	7 (5%)	5 (4%)	4	15
2	F	144/146 (99%)	132 (92%)	7 (5%)	5 (4%)	4	15
2	H	144/146 (99%)	131 (91%)	8 (6%)	5 (4%)	4	15
All	All	1132/1148 (99%)	1020 (90%)	80 (7%)	32 (3%)	6	21

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	142	ALA
2	B	143	ARG
2	D	142	ALA
2	D	143	ARG
2	F	142	ALA
2	F	143	ARG
1	G	138	ALA
2	H	142	ALA
2	H	143	ARG
1	A	41	THR
1	A	138	ALA
1	C	41	THR
1	C	138	ALA
2	D	78	LEU
1	E	41	THR
1	E	138	ALA
2	F	78	LEU
1	G	41	THR
2	H	78	LEU
2	B	78	LEU
2	B	144	LYS
2	D	144	LYS
2	F	144	LYS
2	B	80	ASN
2	D	80	ASN
2	H	80	ASN
2	H	144	LYS
1	A	73	ILE
2	F	80	ASN
1	C	73	ILE
1	E	73	ILE
1	G	73	ILE

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	114/114 (100%)	104 (91%)	10 (9%)	12 35
1	C	114/114 (100%)	104 (91%)	10 (9%)	12 35
1	E	114/114 (100%)	103 (90%)	11 (10%)	10 29
1	G	114/114 (100%)	104 (91%)	10 (9%)	12 35
2	B	121/121 (100%)	108 (89%)	13 (11%)	8 24
2	D	121/121 (100%)	108 (89%)	13 (11%)	8 24
2	F	121/121 (100%)	106 (88%)	15 (12%)	6 17
2	H	121/121 (100%)	108 (89%)	13 (11%)	8 24
All	All	940/940 (100%)	845 (90%)	95 (10%)	9 27

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	38	GLN
1	A	49	GLN
1	A	63	VAL
1	A	80	LEU
1	A	82	LYS
1	A	86	LEU
1	A	130	CYS
1	A	140	TYR
1	A	141	ARG
2	B	57	ASN
2	B	59	MET
2	B	76	LYS
2	B	87	GLN
2	B	88	LEU
2	B	95	LYS
2	B	101	GLU
2	B	104	ARG
2	B	131	GLN
2	B	136	VAL
2	B	143	ARG
2	B	144	LYS
2	B	146	HIS
1	C	28	THR
1	C	38	GLN
1	C	49	GLN
1	C	50	HIS

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Mol	Chain	Res	Type
1	C	63	VAL
1	C	82	LYS
1	C	86	LEU
1	C	130	CYS
1	C	140	TYR
1	C	141	ARG
2	D	57	ASN
2	D	59	MET
2	D	76	LYS
2	D	87	GLN
2	D	88	LEU
2	D	95	LYS
2	D	101	GLU
2	D	104	ARG
2	D	131	GLN
2	D	134	VAL
2	D	143	ARG
2	D	144	LYS
2	D	146	HIS
1	E	28	THR
1	E	38	GLN
1	E	49	GLN
1	E	50	HIS
1	E	63	VAL
1	E	80	LEU
1	E	82	LYS
1	E	86	LEU
1	E	130	CYS
1	E	140	TYR
1	E	141	ARG
2	F	57	ASN
2	F	59	MET
2	F	76	LYS
2	F	87	GLN
2	F	88	LEU
2	F	95	LYS
2	F	100	PRO
2	F	101	GLU
2	F	104	ARG
2	F	131	GLN
2	F	134	VAL
2	F	136	VAL

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Mol	Chain	Res	Type
2	F	143	ARG
2	F	144	LYS
2	F	146	HIS
1	G	28	THR
1	G	38	GLN
1	G	49	GLN
1	G	50	HIS
1	G	63	VAL
1	G	82	LYS
1	G	86	LEU
1	G	130	CYS
1	G	140	TYR
1	G	141	ARG
2	H	57	ASN
2	H	59	MET
2	H	76	LYS
2	H	87	GLN
2	H	88	LEU
2	H	95	LYS
2	H	101	GLU
2	H	104	ARG
2	H	131	GLN
2	H	134	VAL
2	H	143	ARG
2	H	144	LYS
2	H	146	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	38	GLN
1	A	97	ASN
1	A	113	HIS
2	B	57	ASN
2	B	102	ASN
1	C	9	ASN
1	C	38	GLN
1	C	97	ASN
1	C	113	HIS
2	D	57	ASN
2	D	77	ASN

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Mol	Chain	Res	Type
2	D	102	ASN
1	E	9	ASN
1	E	38	GLN
1	E	97	ASN
1	E	113	HIS
2	F	57	ASN
2	F	102	ASN
1	G	9	ASN
1	G	38	GLN
1	G	97	ASN
1	G	113	HIS
2	H	57	ASN
2	H	77	ASN
2	H	102	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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEM	A	151	1	30,50,50	3.12	14 (46%)	24,82,82	3.03	13 (54%)
3	HEM	B	152	2	30,50,50	3.10	12 (40%)	24,82,82	3.14	11 (45%)
3	HEM	C	153	1	30,50,50	3.14	11 (36%)	24,82,82	2.98	13 (54%)
3	HEM	D	154	2	30,50,50	2.96	12 (40%)	24,82,82	3.08	11 (45%)
3	HEM	E	155	1	30,50,50	3.25	13 (43%)	24,82,82	3.12	13 (54%)
3	HEM	F	156	2	30,50,50	2.99	12 (40%)	24,82,82	3.13	11 (45%)
3	HEM	G	157	1	30,50,50	2.96	12 (40%)	24,82,82	2.92	12 (50%)
3	HEM	H	158	2	30,50,50	2.97	13 (43%)	24,82,82	3.08	11 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	151	1	-	0/10/54/54	0/0/8/8
3	HEM	B	152	2	-	1/10/54/54	0/0/8/8
3	HEM	C	153	1	-	0/10/54/54	0/0/8/8
3	HEM	D	154	2	-	1/10/54/54	0/0/8/8
3	HEM	E	155	1	-	0/10/54/54	0/0/8/8
3	HEM	F	156	2	-	1/10/54/54	0/0/8/8
3	HEM	G	157	1	-	0/10/54/54	0/0/8/8
3	HEM	H	158	2	-	1/10/54/54	0/0/8/8

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	155	HEM	C3B-C4B	-9.94	1.43	1.51
3	C	153	HEM	C3B-C4B	-9.22	1.43	1.51
3	B	152	HEM	C3B-C4B	-8.83	1.44	1.51
3	A	151	HEM	C3B-C4B	-8.42	1.44	1.51
3	G	157	HEM	C3B-C4B	-8.00	1.44	1.51
3	F	156	HEM	C3B-C4B	-7.76	1.44	1.51
3	C	153	HEM	C3B-CAB	-7.17	1.37	1.51
3	A	151	HEM	C3B-CAB	-7.15	1.37	1.51
3	E	155	HEM	C3B-CAB	-6.95	1.38	1.51
3	B	152	HEM	C3B-CAB	-6.93	1.38	1.51
3	F	156	HEM	C3B-CAB	-6.93	1.38	1.51
3	H	158	HEM	C3B-C4B	-6.69	1.45	1.51
3	H	158	HEM	C2D-C3D	-6.66	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	157	HEM	C3B-CAB	-6.61	1.38	1.51
3	F	156	HEM	C2D-C3D	-6.59	1.34	1.54
3	D	154	HEM	C2D-C3D	-6.50	1.35	1.54
3	D	154	HEM	C3C-CAC	-6.44	1.39	1.51
3	D	154	HEM	C3B-C4B	-6.36	1.46	1.51
3	A	151	HEM	C2D-C3D	-6.31	1.35	1.54
3	G	157	HEM	C2D-C3D	-6.26	1.35	1.54
3	B	152	HEM	C2D-C3D	-6.24	1.35	1.54
3	B	152	HEM	C3C-CAC	-6.17	1.39	1.51
3	E	155	HEM	C2D-C3D	-6.13	1.36	1.54
3	C	153	HEM	C2D-C3D	-6.11	1.36	1.54
3	D	154	HEM	C3B-CAB	-6.06	1.40	1.51
3	H	158	HEM	C3B-CAB	-6.05	1.40	1.51
3	H	158	HEM	C3C-CAC	-6.04	1.40	1.51
3	F	156	HEM	C3C-CAC	-5.76	1.40	1.51
3	G	157	HEM	C3C-CAC	-5.27	1.41	1.51
3	E	155	HEM	C3C-CAC	-5.26	1.41	1.51
3	A	151	HEM	C3C-CAC	-5.04	1.41	1.51
3	C	153	HEM	C3C-CAC	-5.03	1.41	1.51
3	A	151	HEM	C3D-C4D	-4.60	1.45	1.51
3	D	154	HEM	C3D-C4D	-4.57	1.45	1.51
3	C	153	HEM	C3D-C4D	-4.57	1.45	1.51
3	E	155	HEM	C3D-C4D	-4.41	1.45	1.51
3	H	158	HEM	C3D-C4D	-4.24	1.46	1.51
3	G	157	HEM	C2C-C1C	-4.04	1.44	1.52
3	C	153	HEM	C2C-C1C	-4.03	1.44	1.52
3	B	152	HEM	C2C-C1C	-4.01	1.45	1.52
3	G	157	HEM	C2B-C1B	-4.00	1.38	1.51
3	A	151	HEM	C2B-C1B	-3.97	1.38	1.51
3	C	153	HEM	C2B-C1B	-3.96	1.38	1.51
3	B	152	HEM	C3D-C4D	-3.91	1.46	1.51
3	E	155	HEM	C2B-C1B	-3.75	1.39	1.51
3	D	154	HEM	C2C-C1C	-3.65	1.45	1.52
3	G	157	HEM	C3D-C4D	-3.49	1.47	1.51
3	H	158	HEM	C2C-C1C	-3.47	1.46	1.52
3	F	156	HEM	C2C-C1C	-3.44	1.46	1.52
3	F	156	HEM	C3D-C4D	-3.43	1.47	1.51
3	C	153	HEM	C2D-C1D	-2.94	1.42	1.51
3	E	155	HEM	C2C-C1C	-2.82	1.47	1.52
3	F	156	HEM	C2D-C1D	-2.73	1.42	1.51
3	B	152	HEM	C2D-C1D	-2.71	1.43	1.51
3	E	155	HEM	C2D-C1D	-2.69	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	156	HEM	C2B-C1B	-2.69	1.43	1.51
3	A	151	HEM	C2D-C1D	-2.66	1.43	1.51
3	A	151	HEM	FE-NC	-2.61	1.85	1.95
3	A	151	HEM	C2C-C1C	-2.59	1.47	1.52
3	D	154	HEM	C2D-C1D	-2.58	1.43	1.51
3	G	157	HEM	C2D-C1D	-2.57	1.43	1.51
3	H	158	HEM	C2D-C1D	-2.54	1.43	1.51
3	B	152	HEM	C2B-C1B	-2.48	1.43	1.51
3	D	154	HEM	C2B-C1B	-2.32	1.44	1.51
3	E	155	HEM	FE-NC	-2.20	1.87	1.95
3	H	158	HEM	C2B-C1B	-2.20	1.44	1.51
3	F	156	HEM	CBB-CAB	2.03	1.41	1.29
3	B	152	HEM	CBB-CAB	2.08	1.41	1.29
3	B	152	HEM	CAA-C2A	2.09	1.55	1.52
3	A	151	HEM	C4C-NC	2.15	1.38	1.36
3	G	157	HEM	CBC-CAC	2.15	1.41	1.29
3	H	158	HEM	CBB-CAB	2.25	1.42	1.29
3	D	154	HEM	C1C-NC	2.28	1.38	1.36
3	H	158	HEM	CAA-C2A	2.30	1.55	1.52
3	H	158	HEM	C1C-NC	2.32	1.38	1.36
3	D	154	HEM	CBB-CAB	2.35	1.42	1.29
3	A	151	HEM	FE-NB	2.44	2.10	1.97
3	C	153	HEM	C4C-NC	2.53	1.39	1.36
3	G	157	HEM	C4C-NC	2.57	1.39	1.36
3	C	153	HEM	CBC-CAC	2.70	1.44	1.29
3	D	154	HEM	CBC-CAC	2.78	1.45	1.29
3	A	151	HEM	CBC-CAC	2.79	1.45	1.29
3	B	152	HEM	CBC-CAC	2.82	1.45	1.29
3	A	151	HEM	CBB-CAB	2.83	1.45	1.29
3	G	157	HEM	CBB-CAB	2.85	1.45	1.29
3	F	156	HEM	CBC-CAC	2.85	1.45	1.29
3	G	157	HEM	C1C-NC	2.85	1.39	1.36
3	H	158	HEM	CBC-CAC	2.88	1.45	1.29
3	E	155	HEM	CBC-CAC	2.88	1.46	1.29
3	C	153	HEM	CBB-CAB	2.90	1.46	1.29
3	E	155	HEM	CBB-CAB	2.92	1.46	1.29
3	E	155	HEM	C1C-NC	3.00	1.39	1.36
3	B	152	HEM	FE-NC	3.08	2.08	1.95
3	A	151	HEM	C1C-NC	3.31	1.40	1.36
3	E	155	HEM	C4C-NC	3.32	1.40	1.36
3	F	156	HEM	C4C-NC	3.42	1.40	1.36
3	F	156	HEM	FE-NC	3.55	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	154	HEM	FE-NC	4.87	2.15	1.95
3	H	158	HEM	FE-NC	5.51	2.17	1.95

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	153	HEM	C3B-CAB-CBB	-4.06	118.23	124.46
3	G	157	HEM	C3B-CAB-CBB	-3.66	118.84	124.46
3	E	155	HEM	CAA-C2A-C3A	-3.65	118.57	129.00
3	G	157	HEM	CAA-C2A-C3A	-3.54	118.88	129.00
3	A	151	HEM	C3B-CAB-CBB	-3.43	119.20	124.46
3	F	156	HEM	CMA-C3A-C4A	-3.42	122.71	128.36
3	A	151	HEM	CAA-C2A-C3A	-3.40	119.31	129.00
3	E	155	HEM	C3B-CAB-CBB	-3.34	119.33	124.46
3	C	153	HEM	CAA-C2A-C3A	-3.32	119.52	129.00
3	B	152	HEM	C3B-CAB-CBB	-3.15	119.63	124.46
3	B	152	HEM	CMA-C3A-C4A	-3.14	123.17	128.36
3	B	152	HEM	CAA-C2A-C3A	-3.12	120.09	129.00
3	F	156	HEM	C3B-CAB-CBB	-3.12	119.67	124.46
3	H	158	HEM	C3B-CAB-CBB	-3.09	119.71	124.46
3	F	156	HEM	CAA-C2A-C3A	-3.09	120.18	129.00
3	D	154	HEM	C3B-CAB-CBB	-2.99	119.88	124.46
3	D	154	HEM	CAA-C2A-C3A	-2.97	120.52	129.00
3	H	158	HEM	CAA-C2A-C3A	-2.97	120.53	129.00
3	H	158	HEM	CMA-C3A-C4A	-2.81	123.72	128.36
3	D	154	HEM	CMA-C3A-C4A	-2.80	123.73	128.36
3	C	153	HEM	C2D-C3D-C4D	2.11	105.07	101.50
3	A	151	HEM	C2D-C3D-C4D	2.24	105.30	101.50
3	E	155	HEM	C2D-C3D-C4D	2.27	105.34	101.50
3	A	151	HEM	CAD-C3D-C2D	2.42	120.17	113.22
3	C	153	HEM	CAD-C3D-C2D	2.43	120.20	113.22
3	E	155	HEM	CAD-C3D-C2D	2.43	120.21	113.22
3	G	157	HEM	CMD-C2D-C3D	2.57	125.72	114.35
3	C	153	HEM	CMD-C2D-C3D	2.64	126.03	114.35
3	H	158	HEM	CMD-C2D-C3D	2.65	126.06	114.35
3	B	152	HEM	CMD-C2D-C3D	2.65	126.08	114.35
3	G	157	HEM	CAD-C3D-C2D	2.67	120.90	113.22
3	D	154	HEM	CMD-C2D-C3D	2.68	126.21	114.35
3	G	157	HEM	C3B-C4B-CHC	2.72	126.99	123.16
3	F	156	HEM	CMD-C2D-C3D	2.75	126.53	114.35
3	E	155	HEM	CMD-C2D-C3D	2.83	126.89	114.35
3	A	151	HEM	CMD-C2D-C3D	2.92	127.27	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	151	HEM	C3B-C4B-CHC	2.95	127.32	123.16
3	E	155	HEM	C3B-C4B-CHC	3.13	127.57	123.16
3	C	153	HEM	C3B-C4B-CHC	3.27	127.76	123.16
3	F	156	HEM	CAD-C3D-C2D	3.32	122.77	113.22
3	B	152	HEM	CAD-C3D-C2D	3.36	122.86	113.22
3	H	158	HEM	CAD-C3D-C2D	3.39	122.95	113.22
3	D	154	HEM	CAD-C3D-C2D	3.41	123.01	113.22
3	F	156	HEM	CMB-C2B-C3B	3.52	125.31	116.53
3	H	158	HEM	CMB-C2B-C3B	3.58	125.47	116.53
3	D	154	HEM	CMB-C2B-C3B	3.60	125.52	116.53
3	B	152	HEM	CMB-C2B-C3B	3.61	125.55	116.53
3	C	153	HEM	CBD-CAD-C3D	3.66	124.21	113.55
3	G	157	HEM	CBD-CAD-C3D	3.80	124.61	113.55
3	G	157	HEM	CMC-C2C-C3C	3.81	126.04	116.53
3	G	157	HEM	CAA-C2A-C1A	3.87	131.21	127.01
3	A	151	HEM	CBD-CAD-C3D	3.97	125.09	113.55
3	C	153	HEM	CMC-C2C-C3C	3.97	126.43	116.53
3	F	156	HEM	CMC-C2C-C3C	3.97	126.43	116.53
3	C	153	HEM	CAA-C2A-C1A	4.06	131.41	127.01
3	A	151	HEM	CAA-C2A-C1A	4.08	131.43	127.01
3	F	156	HEM	C2D-C3D-C4D	4.09	108.44	101.50
3	C	153	HEM	C3C-CAC-CBC	4.12	130.78	124.46
3	B	152	HEM	C2D-C3D-C4D	4.12	108.49	101.50
3	A	151	HEM	C3C-CAC-CBC	4.14	130.80	124.46
3	B	152	HEM	CMC-C2C-C3C	4.14	126.88	116.53
3	E	155	HEM	CBD-CAD-C3D	4.16	125.65	113.55
3	A	151	HEM	CMC-C2C-C3C	4.26	127.17	116.53
3	D	154	HEM	CMC-C2C-C3C	4.28	127.21	116.53
3	H	158	HEM	CMC-C2C-C3C	4.30	127.26	116.53
3	D	154	HEM	CAD-C3D-C4D	4.31	127.67	112.47
3	H	158	HEM	CAD-C3D-C4D	4.36	127.83	112.47
3	E	155	HEM	CMC-C2C-C3C	4.41	127.55	116.53
3	E	155	HEM	CAA-C2A-C1A	4.43	131.82	127.01
3	H	158	HEM	C2D-C3D-C4D	4.46	109.06	101.50
3	B	152	HEM	CAD-C3D-C4D	4.54	128.49	112.47
3	D	154	HEM	C2D-C3D-C4D	4.54	109.20	101.50
3	F	156	HEM	CAD-C3D-C4D	4.57	128.59	112.47
3	G	157	HEM	C3C-CAC-CBC	4.61	131.52	124.46
3	E	155	HEM	C3C-CAC-CBC	4.66	131.61	124.46
3	G	157	HEM	CBA-CAA-C2A	4.88	121.28	112.53
3	C	153	HEM	CBA-CAA-C2A	5.03	121.54	112.53
3	E	155	HEM	CBA-CAA-C2A	5.05	121.58	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	157	HEM	CMB-C2B-C3B	5.26	129.66	116.53
3	A	151	HEM	CBA-CAA-C2A	5.34	122.10	112.53
3	C	153	HEM	CMB-C2B-C3B	5.46	130.17	116.53
3	G	157	HEM	CAD-C3D-C4D	5.71	132.60	112.47
3	E	155	HEM	CAD-C3D-C4D	5.77	132.80	112.47
3	A	151	HEM	CAD-C3D-C4D	5.81	132.95	112.47
3	A	151	HEM	CMB-C2B-C3B	5.81	131.04	116.53
3	C	153	HEM	CAD-C3D-C4D	5.87	133.17	112.47
3	E	155	HEM	CMB-C2B-C3B	5.97	131.44	116.53
3	H	158	HEM	CAA-C2A-C1A	6.93	134.53	127.01
3	D	154	HEM	CAA-C2A-C1A	7.09	134.71	127.01
3	F	156	HEM	CAA-C2A-C1A	7.31	134.94	127.01
3	B	152	HEM	CBA-CAA-C2A	7.43	125.84	112.53
3	D	154	HEM	CBA-CAA-C2A	7.49	125.95	112.53
3	H	158	HEM	CBA-CAA-C2A	7.51	125.99	112.53
3	B	152	HEM	CAA-C2A-C1A	7.54	135.19	127.01
3	F	156	HEM	CBA-CAA-C2A	7.58	126.11	112.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	156	HEM	C3A-C2A-CAA-CBA
3	B	152	HEM	C3A-C2A-CAA-CBA
3	D	154	HEM	C3A-C2A-CAA-CBA
3	H	158	HEM	C3A-C2A-CAA-CBA

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	152	HEM	2	0
3	D	154	HEM	1	0
3	F	156	HEM	3	0
3	H	158	HEM	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	141/141 (100%)	-0.75	1 (0%) 89 84	7, 25, 50, 65	0
1	C	141/141 (100%)	-0.79	2 (1%) 78 69	5, 21, 43, 66	0
1	E	141/141 (100%)	-0.76	2 (1%) 78 69	8, 25, 49, 66	0
1	G	141/141 (100%)	-0.81	2 (1%) 78 69	4, 21, 46, 67	0
2	B	146/146 (100%)	-0.72	1 (0%) 89 84	6, 27, 53, 63	0
2	D	146/146 (100%)	-0.70	0 100 100	5, 29, 52, 68	0
2	F	146/146 (100%)	-0.72	1 (0%) 89 84	4, 26, 53, 62	0
2	H	146/146 (100%)	-0.73	1 (0%) 89 84	6, 27, 50, 66	0
All	All	1148/1148 (100%)	-0.75	10 (0%) 85 79	4, 25, 52, 68	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	140	TYR	6.2
1	C	140	TYR	5.9
1	A	140	TYR	4.4
1	E	140	TYR	3.9
2	B	144	LYS	2.9
1	C	139	LYS	2.7
1	G	139	LYS	2.7
2	H	144	LYS	2.4
1	E	139	LYS	2.2
2	F	144	LYS	2.0

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

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

6.3 Carbohydrates (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, 95^{th} 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
3	HEM	F	156	43/43	0.96	0.16	0.70	15,29,54,64	0
3	HEM	H	158	43/43	0.94	0.16	0.51	19,40,55,63	0
3	HEM	D	154	43/43	0.93	0.16	0.38	23,40,54,64	0
3	HEM	C	153	43/43	0.97	0.14	0.37	3,17,32,36	0
3	HEM	B	152	43/43	0.96	0.14	0.12	19,29,52,64	0
3	HEM	E	155	43/43	0.96	0.14	0.11	3,24,44,50	0
3	HEM	A	151	43/43	0.97	0.13	0.01	10,23,42,52	0
3	HEM	G	157	43/43	0.97	0.12	-0.44	3,16,33,42	0

6.5 Other polymers (i)

There are no such residues in this entry.