



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:57 AM GMT

PDB ID : 2J7A
Title : CRYSTAL STRUCTURE OF CYTOCHROME C NITRITE REDUCTASE
NRFHA COMPLEX FROM DESULFOVIBRIO VULGARIS
Authors : Rodrigues, M.L.; Oliveira, T.F.; Pereira, I.A.C.; Archer, M.
Deposited on : 2006-10-06
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

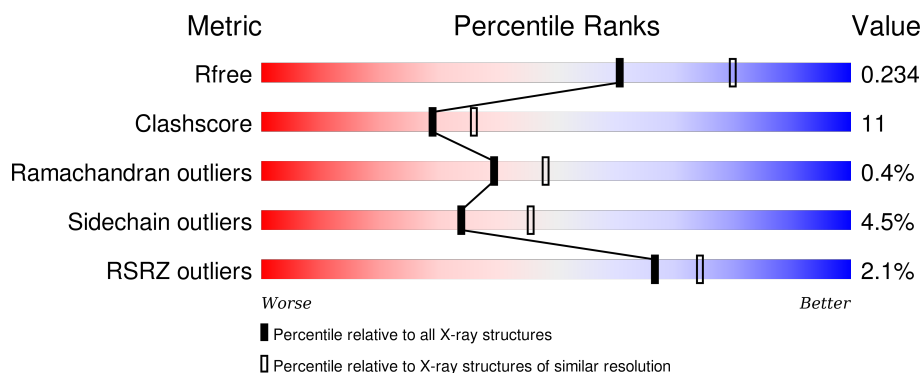
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



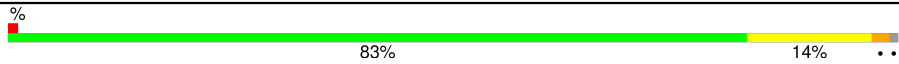


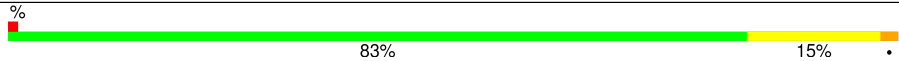
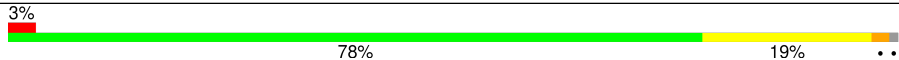
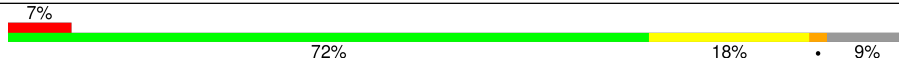
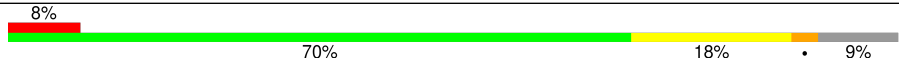


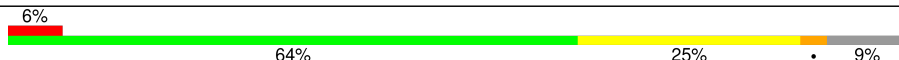
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	<div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	B	500	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	D	500	<div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	E	500	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	G	500	<div> <div>85%</div> <div>13%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	H	500		..
1	J	500		..
1	K	500		..
1	M	500		..
1	N	500		.
1	P	500		..
1	Q	500		..
2	C	159		. 9%
2	F	159		. 9%
2	I	159		. 9%
2	L	159		. 9%
2	O	159		. 9%
2	R	159		. 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CA	J	1006	-	-	-	X
5	LMT	I	1005	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 60930 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 NRFA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	2	0
			4022	2556	695	742	29			
1	B	498	Total	C	N	O	S	0	1	0
			4032	2560	697	746	29			
1	D	494	Total	C	N	O	S	0	1	0
			4009	2546	693	741	29			
1	E	494	Total	C	N	O	S	0	1	0
			4009	2546	693	741	29			
1	G	494	Total	C	N	O	S	0	1	0
			4008	2545	691	743	29			
1	H	497	Total	C	N	O	S	0	3	0
			4037	2563	694	751	29			
1	J	494	Total	C	N	O	S	0	3	0
			4021	2554	693	745	29			
1	K	496	Total	C	N	O	S	0	0	0
			4014	2549	693	743	29			
1	M	494	Total	C	N	O	S	0	2	0
			4014	2549	693	743	29			
1	N	498	Total	C	N	O	S	0	1	0
			4032	2560	697	746	29			
1	P	494	Total	C	N	O	S	0	1	0
			4007	2544	691	743	29			
1	Q	495	Total	C	N	O	S	0	1	0
			4016	2551	694	742	29			

- Molecule 2 is a protein called CYTOCHROME C QUINOL DEHYDROGENASE NRFH.

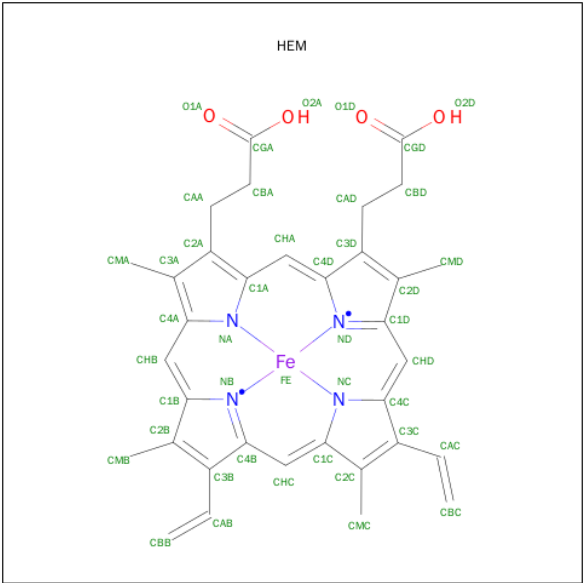
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	145	Total	C	N	O	S	0	1	0
			1094	680	201	197	16			
2	F	145	Total	C	N	O	S	0	1	0
			1093	679	199	199	16			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	145	Total	C	N	O	S	0	0	0
			1087	675	199	197	16			
2	L	145	Total	C	N	O	S	0	0	0
			1087	675	199	197	16			
2	O	144	Total	C	N	O	S	0	0	0
			1078	669	197	196	16			
2	R	145	Total	C	N	O	S	0	0	0
			1087	675	199	197	16			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

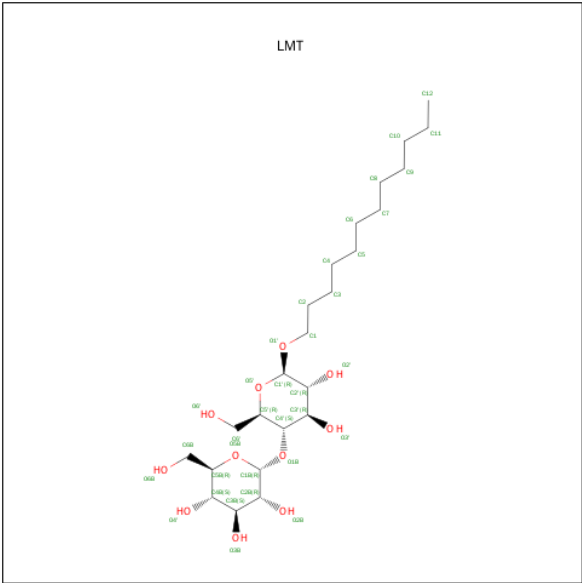
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	2	Total 2	Ca 2	0	0
4	G	2	Total 2	Ca 2	0	0
4	J	2	Total 2	Ca 2	0	0
4	Q	2	Total 2	Ca 2	0	0
4	D	2	Total 2	Ca 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	2	Total	Ca	0	0
			2	2		
4	E	2	Total	Ca	0	0
			2	2		
4	H	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		
4	A	2	Total	Ca	0	0
			2	2		
4	N	2	Total	Ca	0	0
			2	2		
4	M	2	Total	Ca	0	0
			2	2		

- Molecule 5 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



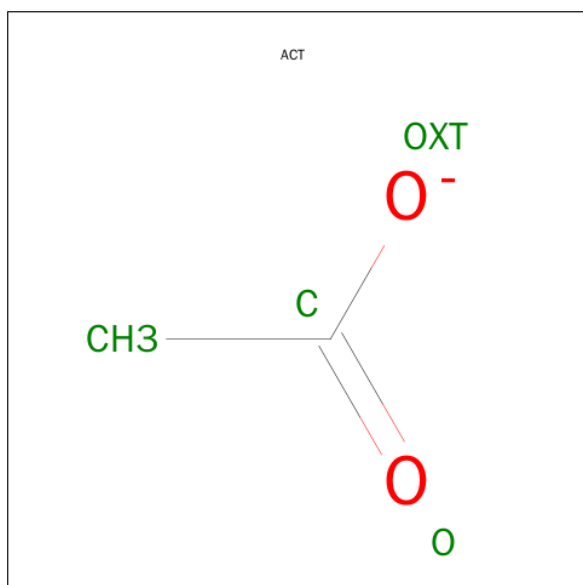
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			35	24	11		
5	F	1	Total	C	O	0	0
			35	24	11		
5	I	1	Total	C	O	0	0
			35	24	11		
5	L	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	O	1	Total	C	O	0	0
			35	24	11		
5	R	1	Total	C	O	0	0
			35	24	11		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		
6	O	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	201	Total	O	0	0
			201	201		
7	B	188	Total	O	0	0
			188	188		
7	C	50	Total	O	0	0
			50	50		
7	D	170	Total	O	0	0
			170	170		

Continued on next page...

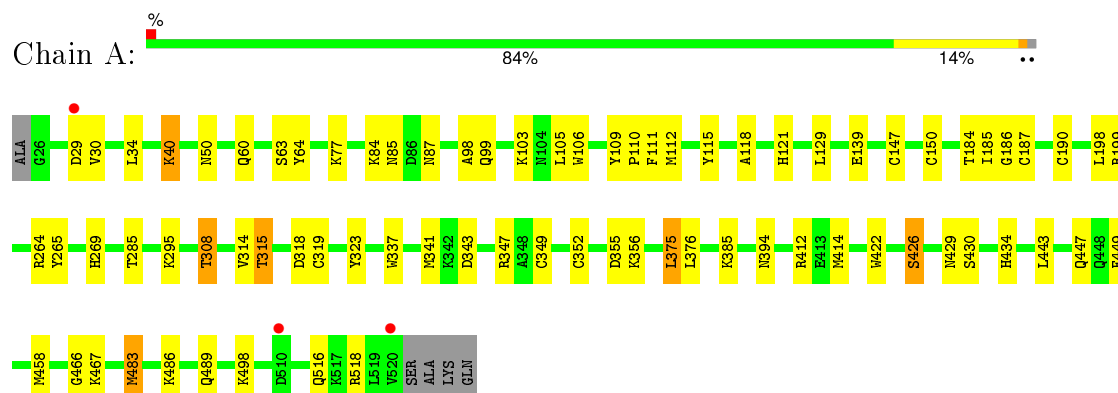
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	155	Total 155	O 155	0	0
7	F	42	Total 42	O 42	0	0
7	G	160	Total 160	O 160	0	0
7	H	194	Total 194	O 194	0	0
7	I	40	Total 40	O 40	0	0
7	J	168	Total 168	O 168	0	0
7	K	106	Total 106	O 106	0	0
7	L	43	Total 43	O 43	0	0
7	M	203	Total 203	O 203	0	0
7	N	206	Total 206	O 206	0	0
7	O	50	Total 50	O 50	0	0
7	P	173	Total 173	O 173	0	0
7	Q	132	Total 132	O 132	0	0
7	R	44	Total 44	O 44	0	0

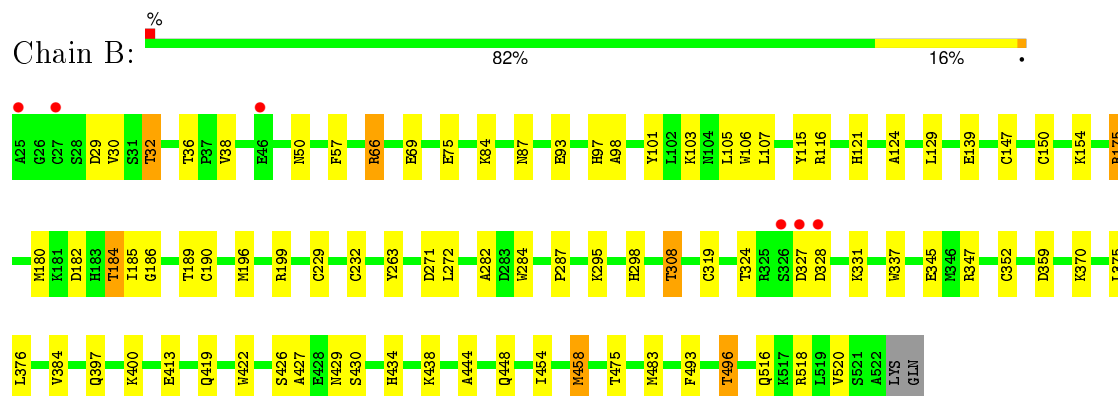
3 Residue-property plots [i](#)

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.

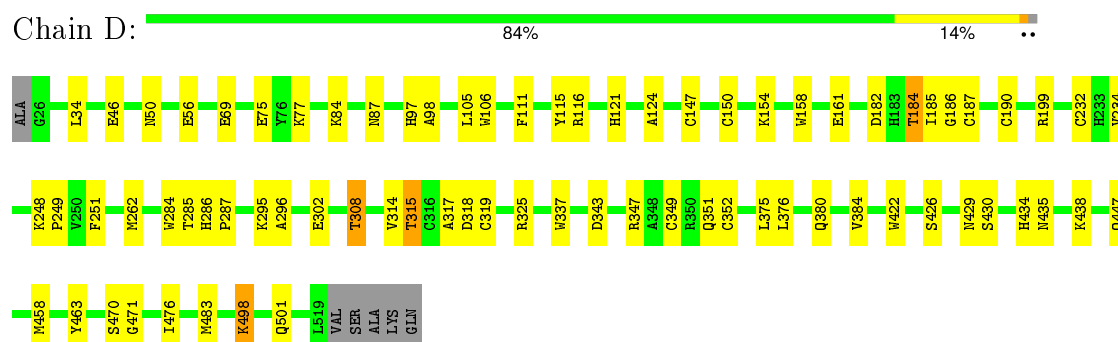
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA



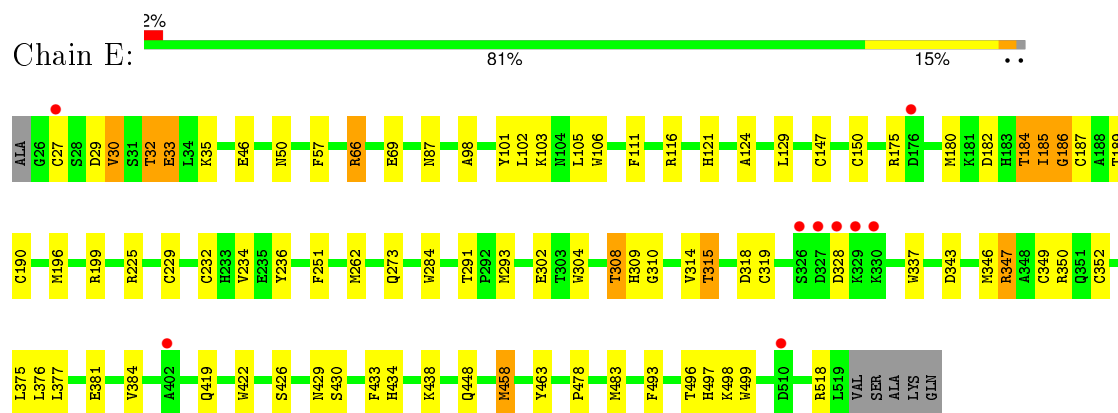
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA



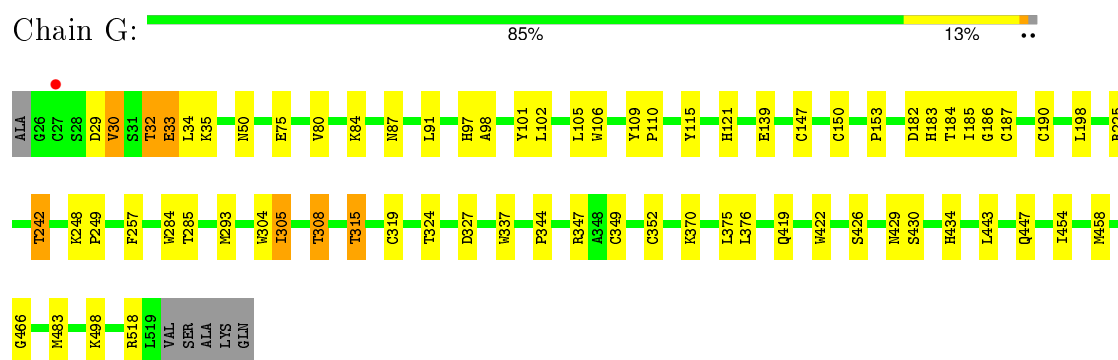
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA



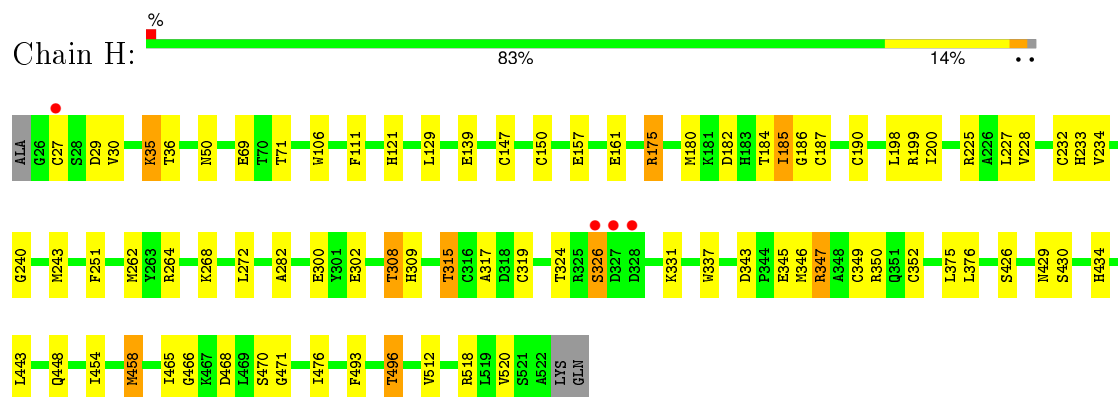
- Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA



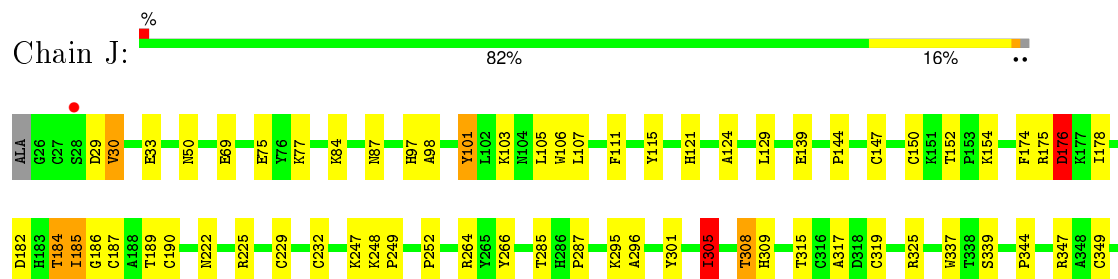
- Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA



- Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

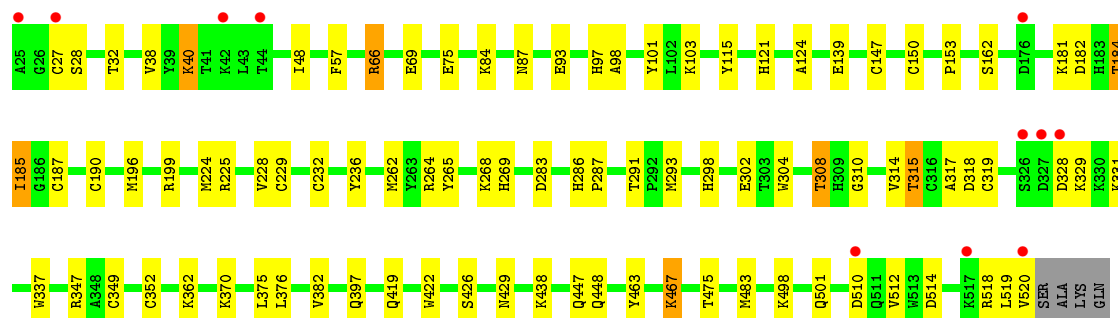
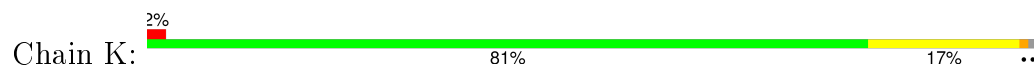


- Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

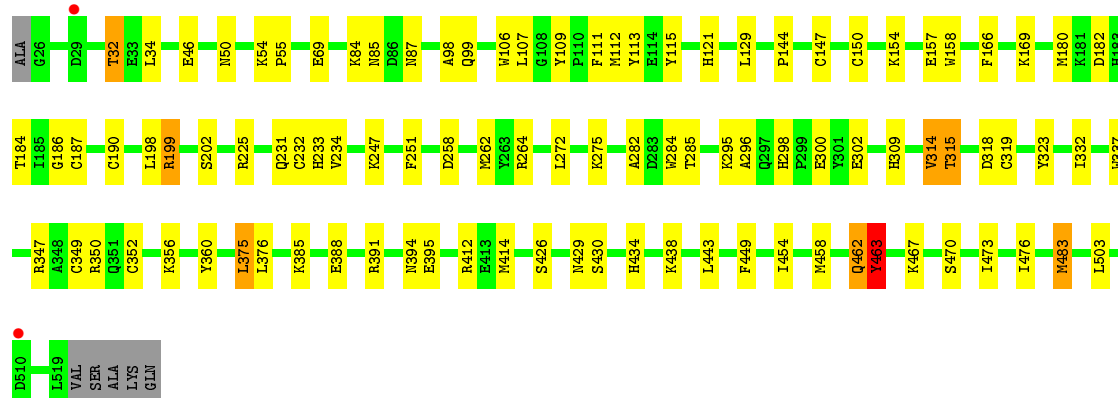
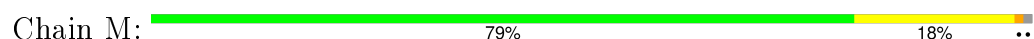




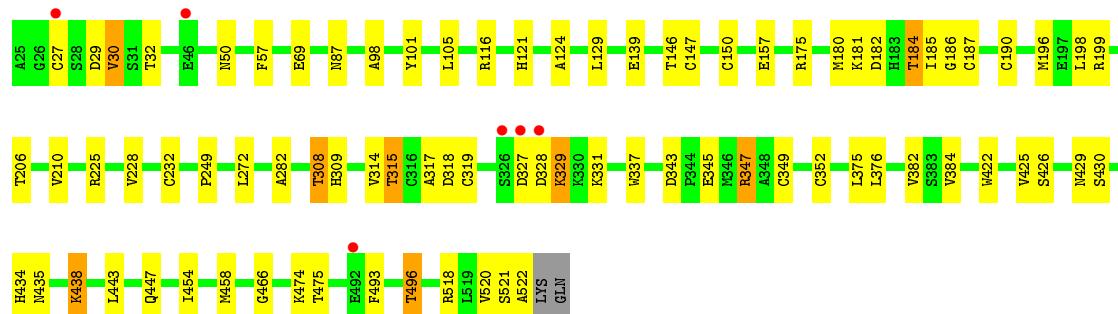
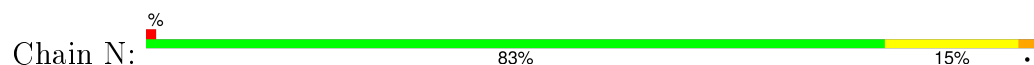
● Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA



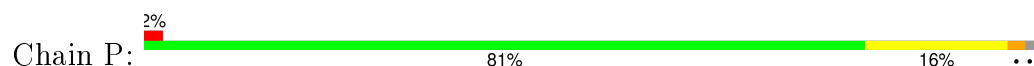
● Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

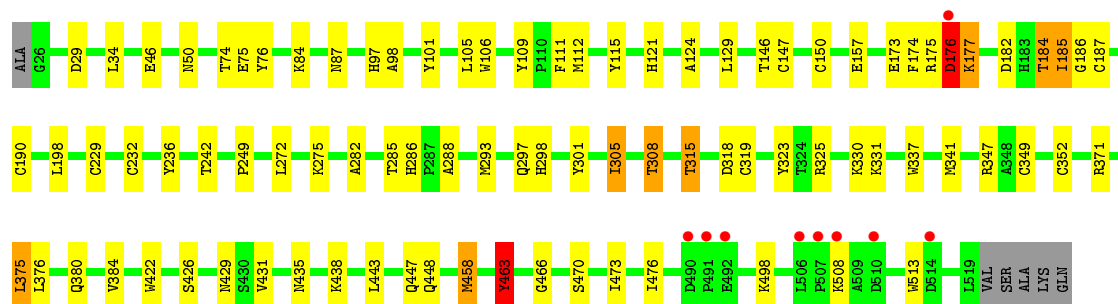


● Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

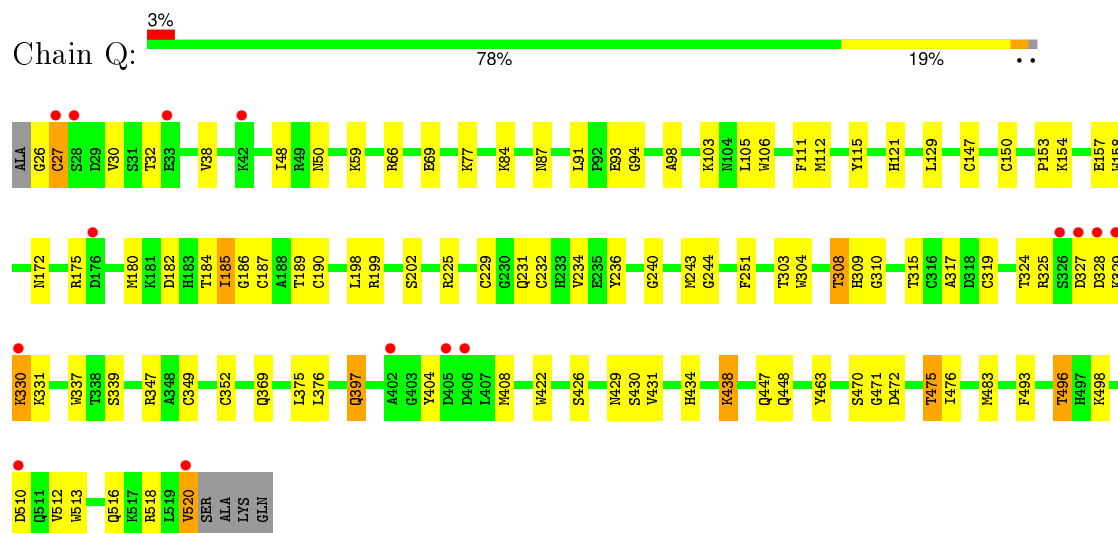


● Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

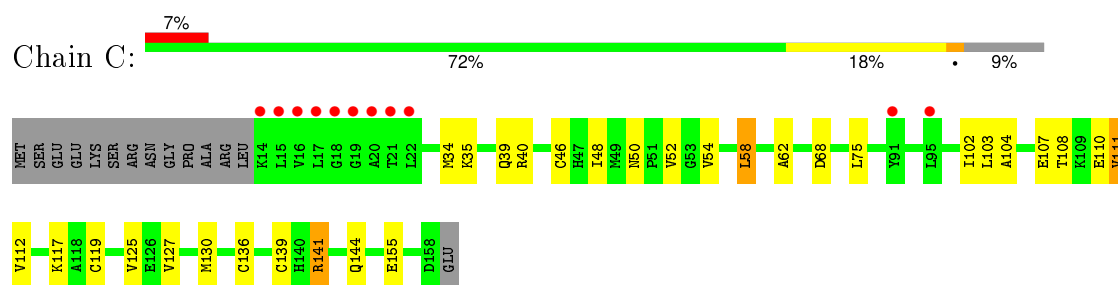




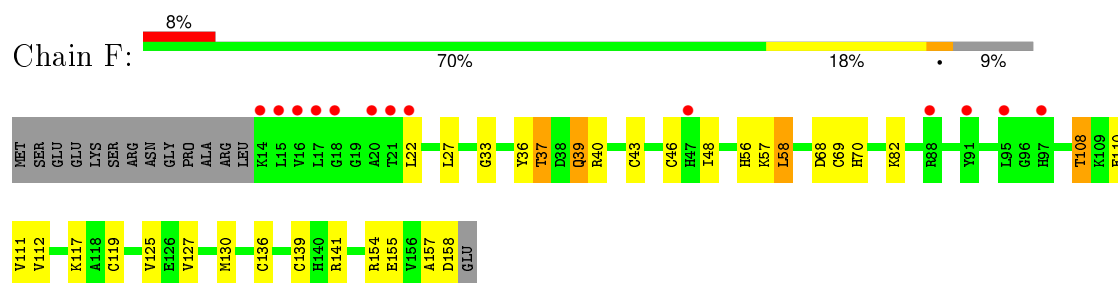
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA



• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH

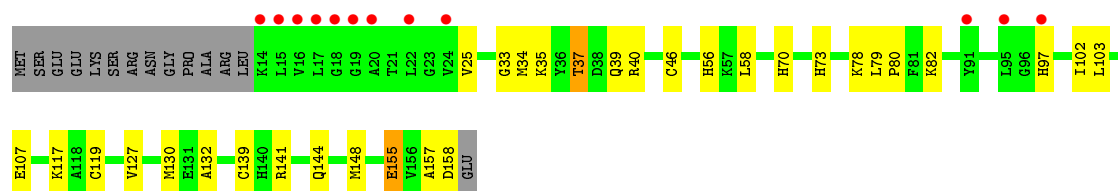


• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH

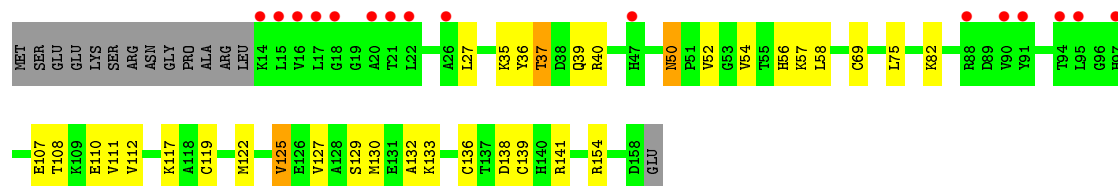


• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH

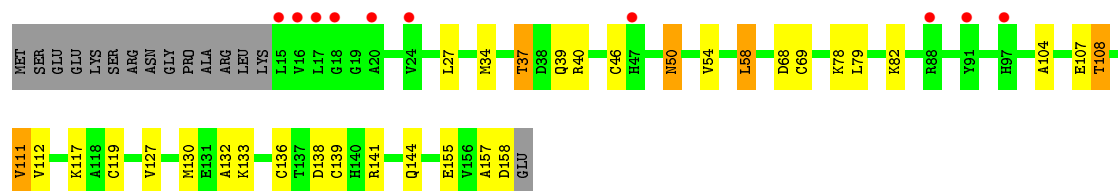




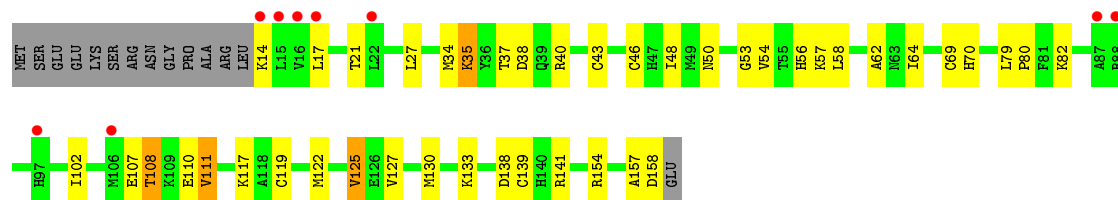
• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH



• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH



• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.66Å 258.12Å 580.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	288.67 – 2.30 53.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	83.7 (288.67-2.30) 83.7 (53.69-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.240 0.197 , 0.234	Depositor DCC
R_{free} test set	22270 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 443579 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	60930	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.56	0/4143	0.65	0/5605
1	B	0.56	0/4150	0.67	1/5616 (0.0%)
1	D	0.55	0/4127	0.65	0/5584
1	E	0.55	0/4127	0.65	0/5584
1	G	0.57	0/4125	0.68	0/5581
1	H	0.55	0/4160	0.66	1/5629 (0.0%)
1	J	0.58	0/4145	0.66	1/5608 (0.0%)
1	K	0.56	0/4128	0.65	0/5586
1	M	0.62	2/4135 (0.0%)	0.68	1/5595 (0.0%)
1	N	0.57	0/4150	0.66	1/5616 (0.0%)
1	P	0.58	0/4124	0.68	2/5580 (0.0%)
1	Q	0.55	0/4134	0.67	1/5594 (0.0%)
2	C	0.51	0/1118	0.73	1/1513 (0.1%)
2	F	0.52	0/1116	0.72	0/1509
2	I	0.50	0/1107	0.68	0/1497
2	L	0.51	0/1107	0.77	0/1497
2	O	0.53	0/1098	0.74	0/1486
2	R	0.47	0/1107	0.69	0/1497
All	All	0.56	2/56301 (0.0%)	0.67	9/76177 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	M	0	3
1	Q	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	462	GLN	C-N	-12.07	1.06	1.34
1	M	463	TYR	C-N	-10.40	1.14	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	463	TYR	O-C-N	5.94	133.30	123.20
1	Q	27	CYS	N-CA-C	5.67	126.31	111.00
1	M	463	TYR	CA-C-N	-5.66	104.89	116.20
1	J	305	ILE	CB-CA-C	-5.65	100.30	111.60
1	B	175	ARG	NE-CZ-NH2	-5.49	117.56	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	314	VAL	Peptide
1	G	327	ASP	Peptide
1	M	314	VAL	Peptide
1	M	462	GLN	Mainchain
1	M	463	TYR	Mainchain

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	4022	0	3896	80	0
1	B	4032	0	3896	77	0
1	D	4009	0	3874	70	0
1	E	4009	0	3875	92	0
1	G	4008	0	3874	80	0
1	H	4037	0	3903	93	0
1	J	4021	0	3886	78	0
1	K	4014	0	3882	83	0
1	M	4014	0	3877	79	0
1	N	4032	0	3899	81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	4007	0	3870	95	0
1	Q	4016	0	3884	123	0
2	C	1094	0	1095	34	0
2	F	1093	0	1096	46	0
2	I	1087	0	1089	35	0
2	L	1087	0	1090	44	0
2	O	1078	0	1077	48	0
2	R	1087	0	1090	55	0
3	A	215	0	150	32	0
3	B	215	0	150	33	0
3	C	172	0	120	23	0
3	D	215	0	150	37	0
3	E	215	0	150	40	0
3	F	172	0	120	27	0
3	G	215	0	150	41	0
3	H	215	0	150	39	0
3	I	172	0	120	11	0
3	J	215	0	150	37	0
3	K	215	0	150	37	0
3	L	172	0	120	20	0
3	M	215	0	150	35	0
3	N	215	0	150	37	0
3	O	172	0	120	24	0
3	P	215	0	150	45	0
3	Q	215	0	150	46	0
3	R	172	0	120	25	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	P	2	0	0	0	0
4	Q	2	0	0	0	0
5	C	35	0	46	2	0
5	F	35	0	46	0	0
5	I	35	0	46	3	0
5	L	35	0	46	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	35	0	46	0	0
5	R	35	0	46	0	0
6	C	4	0	3	0	0
6	I	4	0	3	0	0
6	O	4	0	3	0	0
7	A	201	0	0	7	0
7	B	188	0	0	6	0
7	C	50	0	0	0	0
7	D	170	0	0	3	0
7	E	155	0	0	2	0
7	F	42	0	0	1	0
7	G	160	0	0	7	0
7	H	194	0	0	4	0
7	I	40	0	0	1	0
7	J	168	0	0	2	0
7	K	106	0	0	5	0
7	L	43	0	0	5	0
7	M	203	0	0	6	0
7	N	206	0	0	4	0
7	O	50	0	0	3	0
7	P	173	0	0	7	0
7	Q	132	0	0	3	0
7	R	44	0	0	4	0
All	All	60930	0	55958	1257	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 11.

The worst 5 of 1257 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:O:46:CYS:SG	3:O:1001:HEM:HAC	1.22	1.73
1:M:150:CYS:SG	3:M:1001:HEM:HAC	1.28	1.73
1:K:319:CYS:SG	3:K:1004:HEM:HAC	1.30	1.72
2:F:43:CYS:SG	3:F:1001:HEM:HAB	1.26	1.72
1:N:187:CYS:SG	3:N:1002:HEM:HAB	1.21	1.71

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/500 (99%)	481 (97%)	13 (3%)	1 (0%)	52	64
1	B	497/500 (99%)	482 (97%)	14 (3%)	1 (0%)	52	64
1	D	493/500 (99%)	478 (97%)	13 (3%)	2 (0%)	39	48
1	E	493/500 (99%)	474 (96%)	17 (3%)	2 (0%)	39	48
1	G	493/500 (99%)	479 (97%)	12 (2%)	2 (0%)	39	48
1	H	498/500 (100%)	483 (97%)	13 (3%)	2 (0%)	39	48
1	J	495/500 (99%)	477 (96%)	16 (3%)	2 (0%)	39	48
1	K	494/500 (99%)	473 (96%)	19 (4%)	2 (0%)	39	48
1	M	494/500 (99%)	477 (97%)	15 (3%)	2 (0%)	39	48
1	N	497/500 (99%)	476 (96%)	19 (4%)	2 (0%)	39	48
1	P	493/500 (99%)	474 (96%)	15 (3%)	4 (1%)	24	27
1	Q	494/500 (99%)	473 (96%)	19 (4%)	2 (0%)	39	48
2	C	144/159 (91%)	139 (96%)	5 (4%)	0	100	100
2	F	144/159 (91%)	138 (96%)	5 (4%)	1 (1%)	26	31
2	I	143/159 (90%)	142 (99%)	1 (1%)	0	100	100
2	L	143/159 (90%)	136 (95%)	7 (5%)	0	100	100
2	O	142/159 (89%)	139 (98%)	3 (2%)	0	100	100
2	R	143/159 (90%)	139 (97%)	4 (3%)	0	100	100
All	All	6795/6954 (98%)	6560 (96%)	210 (3%)	25 (0%)	39	48

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	185	ILE
1	E	186	GLY
1	N	329	LYS
1	J	176	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	463	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/432 (100%)	417 (97%)	14 (3%)	46	62
1	B	431/432 (100%)	408 (95%)	23 (5%)	28	37
1	D	429/432 (99%)	413 (96%)	16 (4%)	41	55
1	E	429/432 (99%)	409 (95%)	20 (5%)	32	43
1	G	429/432 (99%)	413 (96%)	16 (4%)	41	55
1	H	433/432 (100%)	419 (97%)	14 (3%)	46	62
1	J	431/432 (100%)	418 (97%)	13 (3%)	48	65
1	K	429/432 (99%)	408 (95%)	21 (5%)	31	41
1	M	430/432 (100%)	412 (96%)	18 (4%)	36	49
1	N	431/432 (100%)	415 (96%)	16 (4%)	41	55
1	P	429/432 (99%)	413 (96%)	16 (4%)	41	55
1	Q	430/432 (100%)	408 (95%)	22 (5%)	29	39
2	C	120/131 (92%)	113 (94%)	7 (6%)	25	33
2	F	120/131 (92%)	109 (91%)	11 (9%)	11	13
2	I	119/131 (91%)	112 (94%)	7 (6%)	24	32
2	L	119/131 (91%)	108 (91%)	11 (9%)	11	13
2	O	118/131 (90%)	111 (94%)	7 (6%)	24	32
2	R	119/131 (91%)	107 (90%)	12 (10%)	9	11
All	All	5877/5970 (98%)	5613 (96%)	264 (4%)	34	46

5 of 264 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	470	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	101	TYR
1	Q	375	LEU
2	I	35	LYS
1	J	184	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	447	GLN
1	J	394	ASN
1	Q	397	GLN
1	H	298	HIS
2	I	73	HIS

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 117 ligands modelled in this entry, 24 are monoatomic - leaving 93 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	1001	1,7	30,50,50	2.27	10 (33%)	24,82,82	2.43	11 (45%)
3	HEM	A	1002	1	30,50,50	2.44	11 (36%)	24,82,82	2.53	10 (41%)
3	HEM	A	1003	1,4	30,50,50	2.37	10 (33%)	24,82,82	2.50	10 (41%)
3	HEM	A	1004	1,4	30,50,50	2.38	11 (36%)	24,82,82	2.37	11 (45%)
3	HEM	A	1005	1	30,50,50	2.16	10 (33%)	24,82,82	2.69	11 (45%)
3	HEM	B	1001	1,7	30,50,50	2.42	11 (36%)	24,82,82	2.35	10 (41%)
3	HEM	B	1002	1	30,50,50	2.46	10 (33%)	24,82,82	2.52	11 (45%)
3	HEM	B	1003	1,4	30,50,50	2.43	11 (36%)	24,82,82	2.41	10 (41%)
3	HEM	B	1004	1,4	30,50,50	2.40	9 (30%)	24,82,82	2.63	10 (41%)
3	HEM	B	1005	1	30,50,50	2.18	9 (30%)	24,82,82	2.31	9 (37%)
3	HEM	C	1001	2	30,50,50	2.32	10 (33%)	24,82,82	2.45	11 (45%)
3	HEM	C	1002	2	30,50,50	2.24	8 (26%)	24,82,82	2.73	13 (54%)
3	HEM	C	1003	2	30,50,50	2.38	9 (30%)	24,82,82	2.47	13 (54%)
3	HEM	C	1004	1,2	30,50,50	2.44	9 (30%)	24,82,82	2.61	10 (41%)
5	LMT	C	1005	-	36,36,36	0.55	0	47,47,47	0.83	1 (2%)
6	ACT	C	1006	-	1,3,3	0.37	0	0,3,3	0.00	-
3	HEM	D	1001	1	30,50,50	2.31	12 (40%)	24,82,82	2.42	12 (50%)
3	HEM	D	1002	1	30,50,50	2.32	9 (30%)	24,82,82	2.36	9 (37%)
3	HEM	D	1003	1,4	30,50,50	2.34	9 (30%)	24,82,82	2.32	9 (37%)
3	HEM	D	1004	1,4	30,50,50	2.46	11 (36%)	24,82,82	2.81	13 (54%)
3	HEM	D	1005	1	30,50,50	2.24	9 (30%)	24,82,82	2.35	11 (45%)
3	HEM	E	1001	1,7	30,50,50	2.55	9 (30%)	24,82,82	2.33	9 (37%)
3	HEM	E	1002	1	30,50,50	2.38	11 (36%)	24,82,82	2.47	10 (41%)
3	HEM	E	1003	1,4	30,50,50	2.30	11 (36%)	24,82,82	2.42	11 (45%)
3	HEM	E	1004	1,4	30,50,50	2.13	10 (33%)	24,82,82	2.55	14 (58%)
3	HEM	E	1005	1	30,50,50	2.24	11 (36%)	24,82,82	2.56	11 (45%)
3	HEM	F	1001	2	30,50,50	2.34	9 (30%)	24,82,82	2.34	10 (41%)
3	HEM	F	1002	2	30,50,50	2.30	10 (33%)	24,82,82	2.62	13 (54%)
3	HEM	F	1003	2	30,50,50	2.14	8 (26%)	24,82,82	2.40	11 (45%)
3	HEM	F	1004	1,2	30,50,50	2.31	7 (23%)	24,82,82	2.79	10 (41%)
5	LMT	F	1005	-	36,36,36	0.61	0	47,47,47	0.96	2 (4%)
3	HEM	G	1001	1,7	30,50,50	2.28	9 (30%)	24,82,82	2.38	11 (45%)
3	HEM	G	1002	1	30,50,50	2.16	8 (26%)	24,82,82	2.37	8 (33%)
3	HEM	G	1003	1,4	30,50,50	2.47	8 (26%)	24,82,82	2.49	10 (41%)
3	HEM	G	1004	1,4	30,50,50	2.31	10 (33%)	24,82,82	2.74	12 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	G	1005	1	30,50,50	2.51	10 (33%)	24,82,82	2.55	11 (45%)
3	HEM	H	1001	1,7	30,50,50	2.38	11 (36%)	24,82,82	2.29	9 (37%)
3	HEM	H	1002	1	30,50,50	2.12	8 (26%)	24,82,82	2.40	10 (41%)
3	HEM	H	1003	1,4	30,50,50	2.38	7 (23%)	24,82,82	2.53	12 (50%)
3	HEM	H	1004	1,4	30,50,50	2.39	11 (36%)	24,82,82	2.49	12 (50%)
3	HEM	H	1005	1	30,50,50	2.18	10 (33%)	24,82,82	2.48	10 (41%)
3	HEM	I	1001	2	30,50,50	2.23	10 (33%)	24,82,82	2.53	14 (58%)
3	HEM	I	1002	2	30,50,50	2.28	10 (33%)	24,82,82	2.80	13 (54%)
3	HEM	I	1003	2	30,50,50	2.13	11 (36%)	24,82,82	2.61	11 (45%)
3	HEM	I	1004	1,2	30,50,50	2.38	9 (30%)	24,82,82	2.67	11 (45%)
5	LMT	I	1005	-	36,36,36	0.57	0	47,47,47	0.97	2 (4%)
6	ACT	I	1006	-	1,3,3	1.13	0	0,3,3	0.00	-
3	HEM	J	1001	1,7	30,50,50	2.26	9 (30%)	24,82,82	2.43	11 (45%)
3	HEM	J	1002	1	30,50,50	2.33	8 (26%)	24,82,82	2.43	10 (41%)
3	HEM	J	1003	1,4	30,50,50	2.09	6 (20%)	24,82,82	2.47	10 (41%)
3	HEM	J	1004	1,4	30,50,50	2.35	10 (33%)	24,82,82	2.71	14 (58%)
3	HEM	J	1005	1	30,50,50	2.27	11 (36%)	24,82,82	2.34	10 (41%)
3	HEM	K	1001	1	30,50,50	2.31	8 (26%)	24,82,82	2.29	9 (37%)
3	HEM	K	1002	1	30,50,50	2.39	12 (40%)	24,82,82	2.34	10 (41%)
3	HEM	K	1003	1,4	30,50,50	2.24	9 (30%)	24,82,82	2.39	12 (50%)
3	HEM	K	1004	1,4	30,50,50	2.18	9 (30%)	24,82,82	2.66	14 (58%)
3	HEM	K	1005	1	30,50,50	2.34	8 (26%)	24,82,82	2.33	9 (37%)
3	HEM	L	1002	2	30,50,50	2.07	8 (26%)	24,82,82	2.72	12 (50%)
3	HEM	L	1003	2	30,50,50	2.19	8 (26%)	24,82,82	2.57	11 (45%)
3	HEM	L	1004	1,2	30,50,50	2.29	8 (26%)	24,82,82	2.65	9 (37%)
5	LMT	L	1005	-	36,36,36	0.57	0	47,47,47	0.68	1 (2%)
3	HEM	L	1101	2	30,50,50	2.33	12 (40%)	24,82,82	2.51	11 (45%)
3	HEM	M	1001	1	30,50,50	2.30	8 (26%)	24,82,82	2.36	8 (33%)
3	HEM	M	1002	1	30,50,50	2.44	8 (26%)	24,82,82	2.42	10 (41%)
3	HEM	M	1003	1,4	30,50,50	2.22	8 (26%)	24,82,82	2.85	16 (66%)
3	HEM	M	1004	1,4	30,50,50	2.34	8 (26%)	24,82,82	2.82	13 (54%)
3	HEM	M	1005	1	30,50,50	2.29	9 (30%)	24,82,82	2.34	10 (41%)
3	HEM	N	1001	1,7	30,50,50	2.44	8 (26%)	24,82,82	2.48	12 (50%)
3	HEM	N	1002	1	30,50,50	2.11	10 (33%)	24,82,82	2.54	13 (54%)
3	HEM	N	1003	1,4	30,50,50	2.23	11 (36%)	24,82,82	2.46	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	N	1004	1,4	30,50,50	2.34	10 (33%)	24,82,82	2.62	11 (45%)
3	HEM	N	1005	1	30,50,50	2.29	6 (20%)	24,82,82	2.47	10 (41%)
3	HEM	O	1001	2	30,50,50	2.28	10 (33%)	24,82,82	2.45	13 (54%)
3	HEM	O	1002	2	30,50,50	2.44	10 (33%)	24,82,82	2.57	12 (50%)
3	HEM	O	1003	2	30,50,50	2.37	8 (26%)	24,82,82	2.50	10 (41%)
3	HEM	O	1004	1,2	30,50,50	2.33	10 (33%)	24,82,82	2.84	10 (41%)
5	LMT	O	1005	-	36,36,36	0.63	1 (2%)	47,47,47	0.81	1 (2%)
6	ACT	O	1006	-	1,3,3	1.14	0	0,3,3	0.00	-
3	HEM	P	1001	1,7	30,50,50	2.46	12 (40%)	24,82,82	2.16	7 (29%)
3	HEM	P	1002	1	30,50,50	2.02	8 (26%)	24,82,82	2.39	11 (45%)
3	HEM	P	1003	1,4	30,50,50	2.28	9 (30%)	24,82,82	2.50	13 (54%)
3	HEM	P	1004	1,4	30,50,50	2.39	10 (33%)	24,82,82	2.60	13 (54%)
3	HEM	P	1005	1	30,50,50	2.14	10 (33%)	24,82,82	2.34	12 (50%)
3	HEM	Q	1001	1,7	30,50,50	2.42	8 (26%)	24,82,82	2.22	7 (29%)
3	HEM	Q	1002	1	30,50,50	2.38	12 (40%)	24,82,82	2.39	10 (41%)
3	HEM	Q	1003	1,4	30,50,50	2.18	10 (33%)	24,82,82	2.44	10 (41%)
3	HEM	Q	1004	1,4	30,50,50	2.20	8 (26%)	24,82,82	2.73	11 (45%)
3	HEM	Q	1005	1	30,50,50	2.31	10 (33%)	24,82,82	2.56	11 (45%)
3	HEM	R	1001	2	30,50,50	2.27	10 (33%)	24,82,82	2.51	14 (58%)
3	HEM	R	1002	2	30,50,50	2.35	8 (26%)	24,82,82	2.51	10 (41%)
3	HEM	R	1003	2	30,50,50	2.22	7 (23%)	24,82,82	2.51	11 (45%)
3	HEM	R	1004	1,2	30,50,50	2.18	9 (30%)	24,82,82	2.79	10 (41%)
5	LMT	R	1005	-	36,36,36	0.56	0	47,47,47	1.06	3 (6%)

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	1001	1,7	-	0/10/54/54	0/0/8/8
3	HEM	A	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	A	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	A	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	A	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	B	1001	1,7	-	0/10/54/54	0/0/8/8
3	HEM	B	1002	1	-	0/10/54/54	0/0/8/8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	B	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	B	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	C	1001	2	-	0/10/54/54	0/0/8/8
3	HEM	C	1002	2	-	0/10/54/54	0/0/8/8
3	HEM	C	1003	2	-	0/10/54/54	0/0/8/8
3	HEM	C	1004	1,2	-	0/10/54/54	0/0/8/8
5	LMT	C	1005	-	-	0/21/61/61	0/2/2/2
6	ACT	C	1006	-	-	0/0/0/0	0/0/0/0
3	HEM	D	1001	1	-	0/10/54/54	0/0/8/8
3	HEM	D	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	D	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	D	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	D	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	E	1001	1,7	-	0/10/54/54	0/0/8/8
3	HEM	E	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	E	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	E	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	E	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	F	1001	2	-	0/10/54/54	0/0/8/8
3	HEM	F	1002	2	-	0/10/54/54	0/0/8/8
3	HEM	F	1003	2	-	0/10/54/54	0/0/8/8
3	HEM	F	1004	1,2	-	0/10/54/54	0/0/8/8
5	LMT	F	1005	-	-	0/21/61/61	0/2/2/2
3	HEM	G	1001	1,7	-	0/10/54/54	0/0/8/8
3	HEM	G	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	G	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	G	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	G	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	H	1001	1,7	-	0/10/54/54	0/0/8/8
3	HEM	H	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	H	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	H	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	H	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	I	1001	2	-	0/10/54/54	0/0/8/8
3	HEM	I	1002	2	-	0/10/54/54	0/0/8/8
3	HEM	I	1003	2	-	0/10/54/54	0/0/8/8
3	HEM	I	1004	1,2	-	0/10/54/54	0/0/8/8
5	LMT	I	1005	-	-	0/21/61/61	0/2/2/2
6	ACT	I	1006	-	-	0/0/0/0	0/0/0/0
3	HEM	J	1001	1,7	-	0/10/54/54	0/0/8/8
3	HEM	J	1002	1	-	0/10/54/54	0/0/8/8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	J	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	J	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	J	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	K	1001	1	-	0/10/54/54	0/0/8/8
3	HEM	K	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	K	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	K	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	K	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	L	1002	2	-	0/10/54/54	0/0/8/8
3	HEM	L	1003	2	-	0/10/54/54	0/0/8/8
3	HEM	L	1004	1,2	-	0/10/54/54	0/0/8/8
5	LMT	L	1005	-	-	0/21/61/61	0/2/2/2
3	HEM	L	1101	2	-	0/10/54/54	0/0/8/8
3	HEM	M	1001	1	-	0/10/54/54	0/0/8/8
3	HEM	M	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	M	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	M	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	M	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	N	1001	1,7	-	0/10/54/54	0/0/8/8
3	HEM	N	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	N	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	N	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	N	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	O	1001	2	-	0/10/54/54	0/0/8/8
3	HEM	O	1002	2	-	0/10/54/54	0/0/8/8
3	HEM	O	1003	2	-	0/10/54/54	0/0/8/8
3	HEM	O	1004	1,2	-	0/10/54/54	0/0/8/8
5	LMT	O	1005	-	-	0/21/61/61	0/2/2/2
6	ACT	O	1006	-	-	0/0/0/0	0/0/0/0
3	HEM	P	1001	1,7	-	0/10/54/54	0/0/8/8
3	HEM	P	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	P	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	P	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	P	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	Q	1001	1,7	-	0/10/54/54	0/0/8/8
3	HEM	Q	1002	1	-	0/10/54/54	0/0/8/8
3	HEM	Q	1003	1,4	-	0/10/54/54	0/0/8/8
3	HEM	Q	1004	1,4	-	0/10/54/54	0/0/8/8
3	HEM	Q	1005	1	-	0/10/54/54	0/0/8/8
3	HEM	R	1001	2	-	0/10/54/54	0/0/8/8
3	HEM	R	1002	2	-	0/10/54/54	0/0/8/8
3	HEM	R	1003	2	-	0/10/54/54	0/0/8/8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	R	1004	1,2	-	0/10/54/54	0/0/8/8
5	LMT	R	1005	-	-	0/21/61/61	0/2/2/2

The worst 5 of 788 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1003	HEM	C3B-C4B	-9.46	1.43	1.51
3	G	1003	HEM	C3B-C4B	-9.44	1.43	1.51
3	N	1001	HEM	C3B-C4B	-9.25	1.43	1.51
3	P	1001	HEM	C3B-C4B	-9.17	1.43	1.51
3	Q	1001	HEM	C3B-C4B	-9.02	1.43	1.51

The worst 5 of 927 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	1004	HEM	CBA-CAA-C2A	-6.88	100.20	112.53
3	O	1004	HEM	CBA-CAA-C2A	-6.80	100.33	112.53
3	L	1004	HEM	CBA-CAA-C2A	-6.71	100.50	112.53
3	Q	1004	HEM	CAA-C2A-C1A	-6.43	120.03	127.01
3	F	1004	HEM	CBA-CAA-C2A	-6.16	101.50	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

85 monomers are involved in 596 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	HEM	6	0
3	A	1002	HEM	11	0
3	A	1004	HEM	7	0
3	A	1005	HEM	8	0
3	B	1001	HEM	5	0
3	B	1002	HEM	7	0
3	B	1003	HEM	11	0
3	B	1004	HEM	7	0
3	B	1005	HEM	4	0
3	C	1001	HEM	5	0
3	C	1002	HEM	3	0
3	C	1003	HEM	5	0
3	C	1004	HEM	10	0
5	C	1005	LMT	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1001	HEM	6	0
3	D	1002	HEM	10	0
3	D	1003	HEM	4	0
3	D	1004	HEM	7	0
3	D	1005	HEM	11	0
3	E	1001	HEM	9	0
3	E	1002	HEM	10	0
3	E	1003	HEM	8	0
3	E	1004	HEM	5	0
3	E	1005	HEM	9	0
3	F	1001	HEM	7	0
3	F	1002	HEM	9	0
3	F	1003	HEM	4	0
3	F	1004	HEM	7	0
3	G	1001	HEM	10	0
3	G	1002	HEM	11	0
3	G	1003	HEM	1	0
3	G	1004	HEM	9	0
3	G	1005	HEM	11	0
3	H	1001	HEM	9	0
3	H	1002	HEM	9	0
3	H	1003	HEM	5	0
3	H	1004	HEM	9	0
3	H	1005	HEM	8	0
3	I	1001	HEM	2	0
3	I	1002	HEM	2	0
3	I	1003	HEM	3	0
3	I	1004	HEM	4	0
5	I	1005	LMT	3	0
3	J	1001	HEM	5	0
3	J	1002	HEM	8	0
3	J	1003	HEM	10	0
3	J	1004	HEM	7	0
3	J	1005	HEM	8	0
3	K	1001	HEM	10	0
3	K	1002	HEM	9	0
3	K	1003	HEM	8	0
3	K	1004	HEM	6	0
3	K	1005	HEM	6	0
3	L	1002	HEM	7	0
3	L	1003	HEM	6	0
3	L	1004	HEM	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1005	LMT	3	0
3	M	1001	HEM	5	0
3	M	1002	HEM	9	0
3	M	1003	HEM	5	0
3	M	1004	HEM	8	0
3	M	1005	HEM	9	0
3	N	1001	HEM	8	0
3	N	1002	HEM	8	0
3	N	1003	HEM	4	0
3	N	1004	HEM	8	0
3	N	1005	HEM	10	0
3	O	1001	HEM	3	0
3	O	1002	HEM	8	0
3	O	1003	HEM	5	0
3	O	1004	HEM	8	0
3	P	1001	HEM	9	0
3	P	1002	HEM	12	0
3	P	1003	HEM	8	0
3	P	1004	HEM	7	0
3	P	1005	HEM	9	0
3	Q	1001	HEM	9	0
3	Q	1002	HEM	11	0
3	Q	1003	HEM	8	0
3	Q	1004	HEM	9	0
3	Q	1005	HEM	10	0
3	R	1001	HEM	6	0
3	R	1002	HEM	10	0
3	R	1003	HEM	5	0
3	R	1004	HEM	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	495/500 (99%)	-0.33	3 (0%) 90 93	5, 17, 32, 50	0
1	B	498/500 (99%)	-0.29	6 (1%) 81 85	5, 16, 33, 52	0
1	D	494/500 (98%)	-0.36	0 100 100	6, 18, 34, 50	0
1	E	494/500 (98%)	-0.19	9 (1%) 71 78	8, 21, 37, 53	0
1	G	494/500 (98%)	-0.33	1 (0%) 95 97	6, 17, 32, 50	0
1	H	497/500 (99%)	-0.33	4 (0%) 87 90	5, 17, 33, 51	0
1	J	494/500 (98%)	-0.33	4 (0%) 87 90	7, 18, 34, 50	0
1	K	496/500 (99%)	-0.15	11 (2%) 65 73	9, 21, 38, 53	0
1	M	494/500 (98%)	-0.34	2 (0%) 93 95	5, 17, 32, 50	0
1	N	498/500 (99%)	-0.32	6 (1%) 81 85	6, 16, 33, 51	0
1	P	494/500 (98%)	-0.28	9 (1%) 71 78	8, 19, 34, 49	0
1	Q	495/500 (99%)	-0.14	15 (3%) 54 63	9, 21, 37, 53	0
2	C	145/159 (91%)	0.16	11 (7%) 17 24	8, 21, 80, 97	0
2	F	145/159 (91%)	0.34	13 (8%) 12 17	8, 26, 80, 96	0
2	I	145/159 (91%)	0.14	12 (8%) 14 20	8, 22, 80, 96	0
2	L	145/159 (91%)	0.25	16 (11%) 7 11	11, 27, 81, 96	0
2	O	144/159 (90%)	0.11	10 (6%) 20 27	9, 21, 76, 96	0
2	R	145/159 (91%)	0.18	9 (6%) 24 32	10, 27, 80, 96	0
All	All	6812/6954 (97%)	-0.22	141 (2%) 67 74	5, 19, 38, 97	0

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	15	LEU	9.4
2	C	16	VAL	7.9
2	R	15	LEU	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	17	LEU	6.8
2	L	16	VAL	6.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CA	J	1006	1/1	0.99	0.11	2.50	13,13,13,13	0
5	LMT	I	1005	35/35	0.90	0.29	2.41	36,41,72,73	0
5	LMT	F	1005	35/35	0.89	0.21	1.80	37,44,70,71	0
5	LMT	O	1005	35/35	0.85	0.27	1.71	38,45,74,75	0
5	LMT	C	1005	35/35	0.91	0.25	1.69	36,41,72,73	0
5	LMT	L	1005	35/35	0.88	0.24	1.57	40,46,66,67	0
3	HEM	J	1004	43/43	0.98	0.13	1.43	3,6,13,21	0
5	LMT	R	1005	35/35	0.84	0.28	1.43	41,49,75,75	0
3	HEM	P	1004	43/43	0.98	0.13	1.11	5,8,13,18	0
4	CA	K	1007	1/1	0.99	0.11	1.09	17,17,17,17	0
3	HEM	P	1001	43/43	0.98	0.12	1.00	12,16,21,24	0
3	HEM	G	1003	43/43	0.98	0.12	0.98	4,7,11,13	0
3	HEM	R	1003	43/43	0.98	0.13	0.97	7,11,17,21	0
3	HEM	D	1004	43/43	0.99	0.13	0.82	2,5,10,16	0
3	HEM	Q	1003	43/43	0.97	0.11	0.76	14,17,20,23	0
3	HEM	K	1005	43/43	0.97	0.14	0.75	9,15,23,26	0
3	HEM	E	1003	43/43	0.98	0.12	0.70	12,14,16,18	0
3	HEM	K	1003	43/43	0.98	0.11	0.69	9,15,17,18	0
3	HEM	I	1002	43/43	0.97	0.12	0.69	11,15,26,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	G	1007	1/1	0.99	0.11	0.69	16,16,16,16	0
3	HEM	P	1005	43/43	0.98	0.14	0.65	8,13,18,22	0
3	HEM	C	1002	43/43	0.98	0.12	0.64	8,13,27,29	0
3	HEM	D	1005	43/43	0.98	0.15	0.60	6,12,18,19	0
3	HEM	E	1005	43/43	0.98	0.14	0.53	11,14,20,24	0
3	HEM	H	1004	43/43	0.99	0.13	0.50	3,6,8,12	0
3	HEM	G	1004	43/43	0.99	0.13	0.49	2,5,12,14	0
3	HEM	H	1005	43/43	0.98	0.15	0.49	5,8,18,22	0
3	HEM	A	1004	43/43	0.99	0.13	0.44	2,5,11,14	0
3	HEM	K	1001	43/43	0.97	0.12	0.40	15,19,23,25	0
3	HEM	L	1002	43/43	0.97	0.12	0.40	16,18,26,29	0
3	HEM	G	1005	43/43	0.98	0.15	0.40	5,8,12,16	0
4	CA	Q	1006	1/1	0.99	0.10	0.40	17,17,17,17	0
3	HEM	R	1001	43/43	0.95	0.14	0.39	22,26,37,42	0
3	HEM	Q	1004	43/43	0.98	0.12	0.39	7,11,18,19	0
3	HEM	Q	1005	43/43	0.98	0.14	0.38	12,15,20,29	0
3	HEM	M	1004	43/43	0.99	0.12	0.37	2,5,14,16	0
3	HEM	B	1003	43/43	0.99	0.11	0.36	5,7,9,13	0
3	HEM	D	1001	43/43	0.98	0.11	0.35	6,12,16,19	0
3	HEM	N	1005	43/43	0.98	0.14	0.33	3,8,21,24	0
3	HEM	D	1003	43/43	0.99	0.10	0.33	2,5,8,11	0
3	HEM	Q	1001	43/43	0.97	0.11	0.29	13,18,20,22	0
3	HEM	H	1001	43/43	0.98	0.11	0.28	5,11,13,14	0
3	HEM	C	1004	43/43	0.98	0.14	0.28	3,8,17,22	0
3	HEM	C	1001	43/43	0.96	0.13	0.27	17,20,29,34	0
3	HEM	K	1004	43/43	0.98	0.12	0.26	7,13,21,25	0
3	HEM	A	1003	43/43	0.99	0.11	0.26	2,6,9,12	0
4	CA	H	1006	1/1	1.00	0.10	0.26	11,11,11,11	0
3	HEM	F	1003	43/43	0.98	0.13	0.25	7,10,18,24	0
3	HEM	J	1005	43/43	0.99	0.13	0.25	10,13,19,22	0
3	HEM	B	1004	43/43	0.99	0.13	0.22	2,5,7,12	0
3	HEM	P	1003	43/43	0.98	0.10	0.22	6,9,12,14	0
3	HEM	A	1005	43/43	0.99	0.15	0.22	2,7,16,22	0
3	HEM	J	1001	43/43	0.98	0.11	0.21	8,12,16,16	0
3	HEM	E	1001	43/43	0.97	0.11	0.20	14,16,18,20	0
3	HEM	J	1003	43/43	0.98	0.11	0.20	5,8,12,16	0
3	HEM	G	1001	43/43	0.98	0.10	0.19	3,8,11,13	0
3	HEM	I	1004	43/43	0.98	0.12	0.18	3,6,16,20	0
3	HEM	B	1001	43/43	0.98	0.11	0.17	5,10,13,16	0
3	HEM	R	1002	43/43	0.97	0.12	0.16	17,20,28,32	0
3	HEM	O	1004	43/43	0.98	0.13	0.14	5,8,20,23	0
3	HEM	I	1001	43/43	0.97	0.12	0.13	18,21,29,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HEM	B	1005	43/43	0.98	0.14	0.11	4,8,18,21	0
3	HEM	N	1004	43/43	0.99	0.12	0.09	2,5,8,13	0
3	HEM	G	1002	43/43	0.98	0.11	0.09	7,9,14,19	0
3	HEM	F	1002	43/43	0.98	0.12	0.08	14,17,27,30	0
3	HEM	J	1002	43/43	0.98	0.10	0.07	9,11,16,21	0
3	HEM	M	1001	43/43	0.98	0.10	0.07	3,9,11,12	0
3	HEM	E	1004	43/43	0.98	0.12	0.07	7,11,14,21	0
3	HEM	N	1003	43/43	0.99	0.11	0.06	3,7,8,11	0
3	HEM	Q	1002	43/43	0.98	0.11	0.05	19,21,22,23	0
4	CA	E	1007	1/1	0.99	0.09	0.04	18,18,18,18	0
3	HEM	O	1002	43/43	0.98	0.12	0.04	12,14,23,29	0
3	HEM	M	1005	43/43	0.99	0.14	0.04	4,7,16,21	0
3	HEM	L	1003	43/43	0.98	0.12	0.02	8,11,16,21	0
3	HEM	L	1004	43/43	0.98	0.12	0.01	7,10,19,21	0
3	HEM	C	1003	43/43	0.98	0.12	-0.00	8,11,15,23	0
3	HEM	I	1003	43/43	0.98	0.12	-0.01	7,12,19,24	0
3	HEM	M	1002	43/43	0.98	0.10	-0.02	6,11,13,17	0
3	HEM	H	1003	43/43	0.99	0.10	-0.04	3,8,10,13	0
3	HEM	O	1003	43/43	0.98	0.12	-0.07	8,12,17,20	0
3	HEM	L	1101	43/43	0.95	0.14	-0.07	23,27,33,36	0
3	HEM	M	1003	43/43	0.98	0.10	-0.08	3,7,12,14	0
4	CA	P	1007	1/1	0.99	0.09	-0.09	15,15,15,15	0
3	HEM	N	1001	43/43	0.98	0.10	-0.11	6,9,12,13	0
3	HEM	K	1002	43/43	0.97	0.11	-0.11	18,21,23,24	0
3	HEM	D	1002	43/43	0.99	0.10	-0.13	4,7,13,19	0
3	HEM	A	1002	43/43	0.98	0.10	-0.14	5,9,14,18	0
3	HEM	P	1002	43/43	0.98	0.11	-0.16	6,9,17,24	0
3	HEM	F	1001	43/43	0.97	0.13	-0.20	20,24,27,31	0
4	CA	N	1006	1/1	1.00	0.10	-0.25	10,10,10,10	0
4	CA	A	1007	1/1	1.00	0.09	-0.27	11,11,11,11	0
3	HEM	A	1001	43/43	0.99	0.10	-0.27	2,7,12,15	0
3	HEM	E	1002	43/43	0.98	0.11	-0.30	13,16,19,21	0
3	HEM	H	1002	43/43	0.98	0.10	-0.35	6,9,14,21	0
3	HEM	R	1004	43/43	0.99	0.11	-0.35	3,8,16,21	0
3	HEM	B	1002	43/43	0.98	0.10	-0.37	6,10,15,17	0
3	HEM	F	1004	43/43	0.98	0.12	-0.41	3,6,16,24	0
4	CA	A	1006	1/1	1.00	0.09	-0.48	13,13,13,13	0
3	HEM	N	1002	43/43	0.98	0.10	-0.57	6,10,12,14	0
4	CA	K	1006	1/1	0.98	0.10	-0.60	16,16,16,16	0
4	CA	J	1007	1/1	0.99	0.09	-0.62	11,11,11,11	0
3	HEM	O	1001	43/43	0.98	0.10	-0.69	17,20,28,34	0
4	CA	H	1007	1/1	0.98	0.09	-1.04	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	B	1006	1/1	1.00	0.09	-1.08	11,11,11,11	0
4	CA	M	1006	1/1	0.99	0.08	-1.23	12,12,12,12	0
4	CA	D	1007	1/1	0.99	0.08	-1.35	11,11,11,11	0
4	CA	B	1007	1/1	0.99	0.09	-1.35	13,13,13,13	0
4	CA	G	1006	1/1	1.00	0.08	-1.42	13,13,13,13	0
4	CA	E	1006	1/1	0.99	0.09	-1.62	17,17,17,17	0
4	CA	D	1006	1/1	0.99	0.09	-1.66	16,16,16,16	0
4	CA	M	1007	1/1	1.00	0.08	-1.68	14,14,14,14	0
4	CA	P	1006	1/1	0.99	0.07	-2.01	16,16,16,16	0
4	CA	N	1007	1/1	0.99	0.08	-2.49	11,11,11,11	0
4	CA	Q	1007	1/1	0.98	0.06	-2.91	20,20,20,20	0
6	ACT	C	1006	4/4	0.94	0.22	-	34,34,34,34	0
6	ACT	O	1006	4/4	0.93	0.20	-	32,32,33,33	0
6	ACT	I	1006	4/4	0.95	0.24	-	38,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.