



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:23 pm GMT

PDB ID : 3RKH  
Title : Structure of the Thioalkalivibrio nitratreducens cytochrome c nitrite reductase in a complex with nitrite (full occupancy)  
Authors : Trofimov, A.A.; Polyakov, K.M.; Tikhonova, T.V.; Tikhonov, A.V.; Dorovatskii, P.V.; Popov, V.O.  
Deposited on : 2011-04-18  
Resolution : 1.83 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

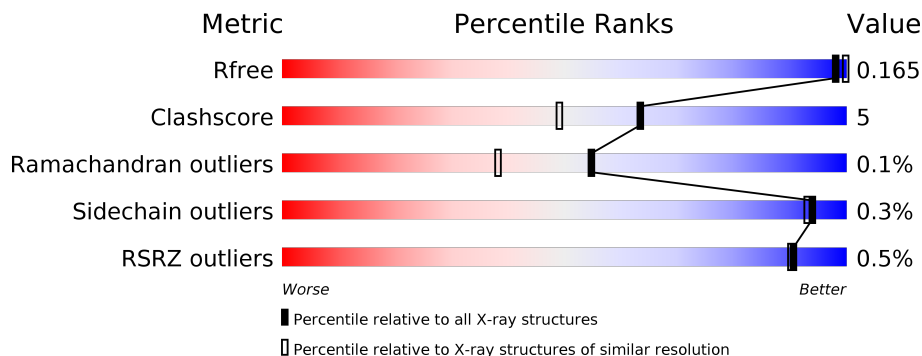
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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))
$R_{free}$	100719	2964 (1.86-1.82)
Clashscore	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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  $\geq 3$ , 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	520	
1	B	520	

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
2	HEC	A	1007[B]	-	-	-	X
2	HEC	A	1008[B]	-	-	-	X
2	HEC	B	1008[B]	-	-	-	X
5	MRD	A	3	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10375 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.

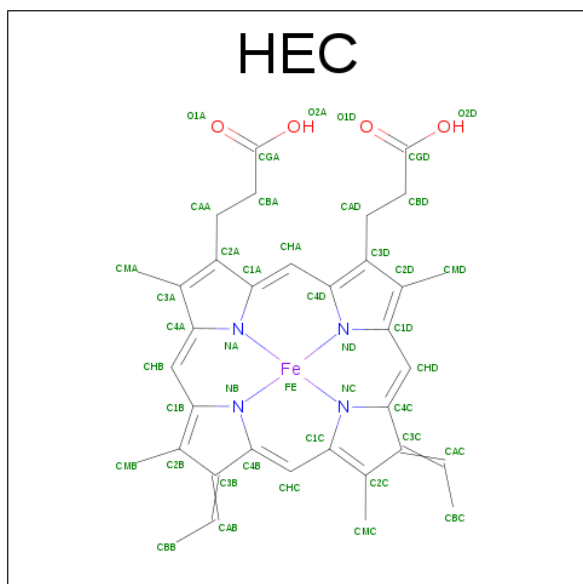
- Molecule 1 is a protein called Eight-heme nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	17	0
			4166	2585	755	790	36			
1	B	520	Total	C	N	O	S	0	16	0
			4170	2589	757	789	35			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	VAL	-	EXPRESSION TAG	UNP Q5F2I3
B	524	VAL	-	EXPRESSION TAG	UNP Q5F2I3

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



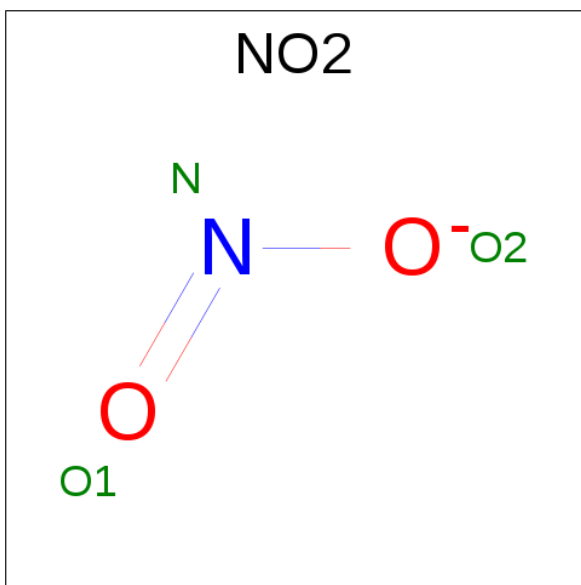
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO<sub>2</sub>).

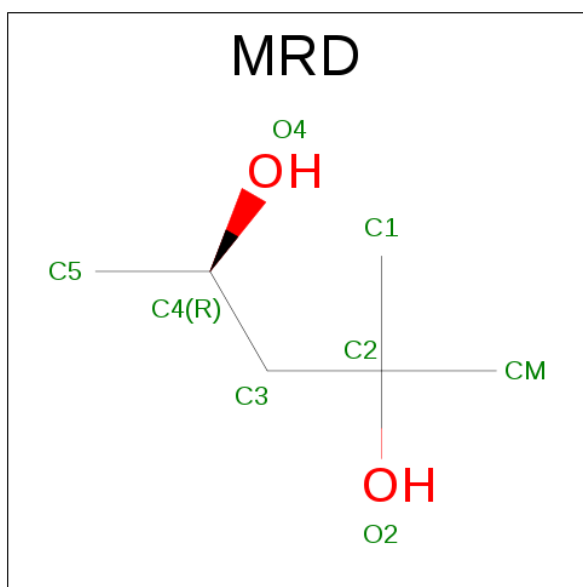


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			3	1	2		
3	B	1	Total	N	O	0	0
			3	1	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

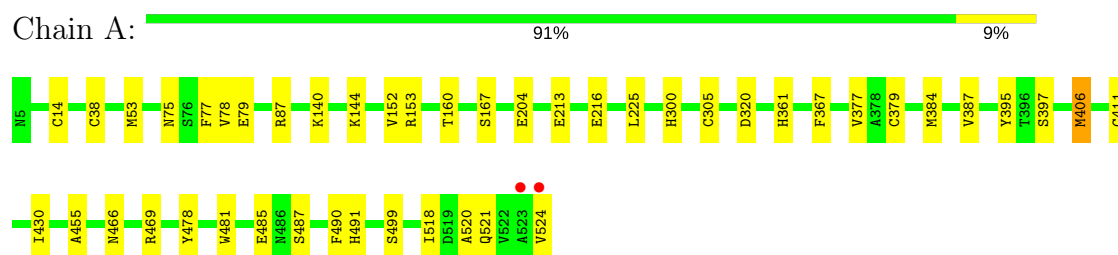
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	665	Total	O	0	0
			665	665		
6	B	662	Total	O	0	0
			662	662		

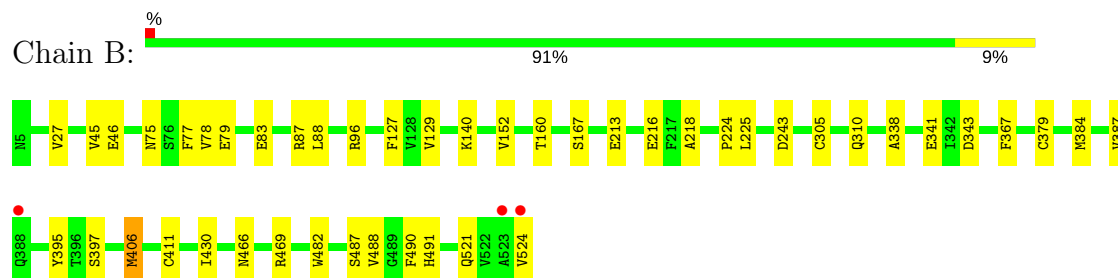
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Eight-heme nitrite reductase



- Molecule 1: Eight-heme nitrite reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.80Å 192.80Å 192.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 1.83 19.68 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (100.00-1.83) 99.9 (19.68-1.83)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.141 , 0.162 0.144 , 0.165	Depositor DCC
$R_{free}$ test set	10471 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MRD, CA, NO2, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.76	2/4370 (0.0%)	0.80	3/5924 (0.1%)
1	B	0.79	2/4368 (0.0%)	0.83	3/5922 (0.1%)
All	All	0.78	4/8738 (0.0%)	0.81	6/11846 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	CYS	CB-SG	-5.74	1.72	1.81
1	A	411	CYS	CB-SG	-5.43	1.73	1.81
1	B	83	GLU	CD-OE1	5.35	1.31	1.25
1	A	204	GLU	CG-CD	5.19	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ASP	CB-CG-OD1	6.48	124.14	118.30
1	B	243	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	153	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	87	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	482	TRP	CA-CB-CG	-5.47	103.30	113.70
1	A	153	ARG	NE-CZ-NH2	-5.35	117.63	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4166	0	3867	35	0
1	B	4170	0	3878	32	0
2	A	344	0	186	13	0
2	B	344	0	186	7	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	8	0	14	5	0
5	B	8	0	14	0	0
6	A	665	0	0	5	0
6	B	662	0	0	5	0
All	All	10375	0	8145	81	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 5.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27[A]:VAL:CG1	6:B:1058:HOH:O	2.14	0.94
5:A:3:MRD:H5C2	6:A:625:HOH:O	1.70	0.92
1:A:521:GLN:O	1:A:524:VAL:HG22	1.82	0.79
1:A:87:ARG:HH12	5:A:3:MRD:H5C1	1.47	0.78
2:B:1002:HEC:HBC3	2:B:1002:HEC:HMC1	1.71	0.72
2:A:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.72	0.72
1:A:87:ARG:HH12	5:A:3:MRD:C5	2.04	0.71
1:B:27[A]:VAL:HG13	6:B:1058:HOH:O	1.83	0.70
1:B:213[B]:GLU:OE1	1:B:216[B]:GLU:CD	2.35	0.65
1:A:79[A]:GLU:HG2	6:A:631:HOH:O	1.96	0.64
1:B:521:GLN:O	1:B:524:VAL:HG22	2.00	0.62
2:A:1008[B]:HEC:O1A	6:A:581:HOH:O	2.16	0.60
1:B:79[B]:GLU:HG2	6:B:659:HOH:O	2.00	0.60
1:A:213[A]:GLU:OE1	1:A:216[A]:GLU:OE2	2.20	0.60
1:A:140:LYS:HG2	1:A:160[B]:THR:HG23	1.84	0.59
1:A:520:ALA:O	1:A:524:VAL:HG13	2.03	0.59
2:A:1003:HEC:HBC3	2:A:1003:HEC:HMC1	1.85	0.58
1:A:384:MET:HB2	1:A:397:SER:O	2.05	0.56
1:A:213[A]:GLU:OE1	1:A:216[A]:GLU:CD	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ASN:ND2	1:A:469:ARG:HH11	2.05	0.55
1:B:140:LYS:HG2	1:B:160:THR:HG23	1.90	0.54
2:B:1006:HEC:HMA3	2:B:1007[B]:HEC:HBA2	1.89	0.54
1:A:167:SER:HB2	1:A:216[B]:GLU:HG2	1.90	0.53
1:B:384:MET:HB2	1:B:397:SER:O	2.08	0.53
1:B:466:ASN:ND2	1:B:469:ARG:HH11	2.07	0.52
1:B:167:SER:HB2	1:B:216[A]:GLU:HG2	1.92	0.52
2:A:1001:HEC:HMB1	2:A:1001:HEC:HBB3	1.93	0.51
2:B:1004:HEC:HMB1	2:B:1004:HEC:HBB3	1.93	0.51
1:A:430:ILE:HG21	1:A:490:PHE:HA	1.93	0.50
2:B:1003:HEC:HMC1	2:B:1003:HEC:HBC3	1.94	0.49
1:B:96[B]:ARG:NH1	6:B:656:HOH:O	0.65	0.49
2:A:1006:HEC:HMA3	2:A:1007[B]:HEC:HBA2	1.93	0.49
2:A:1004:HEC:HBB3	2:A:1004:HEC:HMB1	1.94	0.49
1:A:77:PHE:HE1	1:A:225:LEU:HD23	1.77	0.49
1:A:78[A]:VAL:HG12	1:A:152:VAL:HG21	1.95	0.49
1:B:430:ILE:HG21	1:B:490:PHE:HA	1.94	0.49
1:B:78[A]:VAL:HG12	1:B:152:VAL:HG21	1.96	0.48
1:B:45:VAL:CG2	2:B:1001:HEC:HBB2	2.44	0.48
1:A:53[B]:MET:HE2	6:A:614:HOH:O	2.13	0.48
5:A:3:MRD:H5C3	5:A:3:MRD:O2	2.15	0.47
2:A:1001:HEC:HBC3	2:A:1001:HEC:HMC1	1.97	0.46
1:A:87:ARG:NH1	5:A:3:MRD:H5C1	2.24	0.46
1:A:305:CYS:CB	2:A:1004:HEC:HMC2	2.46	0.46
1:B:140:LYS:HG2	1:B:160:THR:CG2	2.46	0.45
1:B:406:MET:HG2	1:B:406:MET:O	2.16	0.45
1:A:466:ASN:HD22	1:A:469:ARG:HD2	1.81	0.45
1:B:387[A]:VAL:HG21	1:B:395:TYR:CE1	2.52	0.45
1:B:305:CYS:CB	2:B:1004:HEC:HMC2	2.47	0.45
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.51	0.45
1:A:455:ALA:HA	1:A:518:ILE:HG12	1.99	0.44
1:A:487:SER:HB3	1:A:491:HIS:CE1	2.52	0.44
1:B:96[B]:ARG:CZ	1:B:488:VAL:HG22	2.48	0.44
1:B:466:ASN:HD22	1:B:469:ARG:HD2	1.82	0.44
1:A:387[A]:VAL:HG21	1:A:395:TYR:CE1	2.52	0.44
2:A:1002:HEC:HBD2	2:A:1002:HEC:HHA	2.00	0.43
1:B:338:ALA:O	1:B:341:GLU:HG2	2.19	0.42
1:B:127:PHE:CE1	1:B:218:ALA:HB1	2.55	0.42
1:A:144:LYS:CD	6:A:608:HOH:O	2.68	0.42
1:B:310:GLN:HA	1:B:343:ASP:O	2.18	0.42
1:B:75:ASN:O	1:B:79[B]:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TYR:HB3	1:A:499:SER:O	2.21	0.41
1:B:77:PHE:HE1	1:B:225:LEU:HD23	1.85	0.41
1:A:77:PHE:CE1	1:A:225:LEU:HD23	2.55	0.41
1:B:129:VAL:HG11	2:B:1004:HEC:HMA1	2.03	0.41
1:A:38:CYS:HB2	2:A:1002:HEC:C4C	2.51	0.41
1:A:14:CYS:HA	2:A:1001:HEC:CHC	2.51	0.41
1:A:481:TRP:O	1:A:485:GLU:HB2	2.20	0.41
1:A:75:ASN:O	1:A:79[A]:GLU:HG3	2.21	0.41
1:B:213[B]:GLU:OE1	1:B:216[B]:GLU:OE2	2.39	0.40
1:A:300:HIS:CE1	2:A:1004:HEC:HMD1	2.56	0.40
1:A:406:MET:HG2	1:A:406:MET:O	2.20	0.40
1:A:305:CYS:HB3	2:A:1004:HEC:HMC2	2.03	0.40
1:B:224:PRO:O	1:B:225:LEU:C	2.60	0.40
1:B:46:GLU:HG3	6:B:863:HOH:O	2.20	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	535/520 (103%)	511 (96%)	23 (4%)	1 (0%)	51	34
1	B	534/520 (103%)	512 (96%)	22 (4%)	0	100	100
All	All	1069/1040 (103%)	1023 (96%)	45 (4%)	1 (0%)	55	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	HIS

### 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	453/439 (103%)	452 (100%)	1 (0%)	94	94
1	B	452/439 (103%)	449 (99%)	3 (1%)	87	82
All	All	905/878 (103%)	901 (100%)	4 (0%)	94	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	MET
1	B	88[A]	LEU
1	B	88[B]	LEU
1	B	406	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	190	GLN
1	A	466	ASN
1	B	138	GLN
1	B	388	GLN
1	B	413	ASN
1	B	466	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NO2	A	1	2	1,2,2	3.55	1 (100%)	0,1,1	0.00	-
2	HEC	A	1001	1	28,50,50	2.13	7 (25%)	16,82,82	2.87	5 (31%)
2	HEC	A	1002	1	28,50,50	2.09	7 (25%)	16,82,82	2.41	4 (25%)
2	HEC	A	1003	1	28,50,50	2.36	6 (21%)	16,82,82	2.19	5 (31%)
2	HEC	A	1004	1,3	28,50,50	1.96	7 (25%)	16,82,82	2.15	3 (18%)
2	HEC	A	1005	1	28,50,50	2.57	7 (25%)	16,82,82	2.59	6 (37%)
2	HEC	A	1006	1	28,50,50	1.77	5 (17%)	16,82,82	2.80	8 (50%)
2	HEC	A	1007[B]	-	28,50,50	2.23	6 (21%)	16,82,82	2.81	4 (25%)
2	HEC	A	1008[B]	-	28,50,50	2.28	7 (25%)	16,82,82	4.06	8 (50%)
5	MRD	A	3	-	7,7,7	0.39	0	9,10,10	0.56	0
3	NO2	B	1	2	1,2,2	3.24	1 (100%)	0,1,1	0.00	-
2	HEC	B	1001	1	28,50,50	1.91	5 (17%)	16,82,82	2.54	5 (31%)
2	HEC	B	1002	1	28,50,50	2.05	7 (25%)	16,82,82	2.54	5 (31%)
2	HEC	B	1003	1	28,50,50	2.24	5 (17%)	16,82,82	2.17	6 (37%)
2	HEC	B	1004	1,3	28,50,50	1.85	6 (21%)	16,82,82	1.75	2 (12%)
2	HEC	B	1005	1	28,50,50	2.12	6 (21%)	16,82,82	2.37	5 (31%)
2	HEC	B	1006	1	28,50,50	1.86	5 (17%)	16,82,82	2.69	7 (43%)
2	HEC	B	1007[B]	-	28,50,50	2.36	7 (25%)	16,82,82	2.58	4 (25%)
2	HEC	B	1008[B]	-	28,50,50	2.24	6 (21%)	16,82,82	2.61	6 (37%)
5	MRD	B	3	-	7,7,7	0.22	0	9,10,10	0.77	0

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	NO2	A	1	2	-	0/0/0/0	0/0/0/0
2	HEC	A	1001	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1002	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1003	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1004	1,3	-	0/6/54/54	0/0/8/8
2	HEC	A	1005	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1006	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1007[B]	-	-	0/6/54/54	0/0/8/8
2	HEC	A	1008[B]	-	-	0/6/54/54	0/0/8/8
5	MRD	A	3	-	-	0/5/5/5	0/0/0/0
3	NO2	B	1	2	-	0/0/0/0	0/0/0/0
2	HEC	B	1001	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1002	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1003	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1004	1,3	-	0/6/54/54	0/0/8/8
2	HEC	B	1005	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1006	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1007[B]	-	-	0/6/54/54	0/0/8/8
2	HEC	B	1008[B]	-	-	0/6/54/54	0/0/8/8
5	MRD	B	3	-	-	0/5/5/5	0/0/0/0

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	HEC	C3B-C2B	-9.32	1.30	1.40
2	A	1003	HEC	C3B-C2B	-7.65	1.32	1.40
2	B	1008[B]	HEC	C3B-C2B	-7.31	1.33	1.40
2	A	1007[B]	HEC	C3C-C2C	-7.07	1.33	1.40
2	B	1003	HEC	C3B-C2B	-7.05	1.33	1.40
2	B	1005	HEC	C3B-C2B	-7.03	1.33	1.40
2	B	1007[B]	HEC	C3B-C2B	-6.85	1.33	1.40
2	B	1007[B]	HEC	C3C-C2C	-6.61	1.33	1.40
2	A	1001	HEC	C3B-C2B	-6.29	1.34	1.40
2	B	1003	HEC	C3C-C2C	-6.22	1.34	1.40
2	A	1008[B]	HEC	C3C-C2C	-6.15	1.34	1.40
2	A	1005	HEC	C3C-C2C	-5.98	1.34	1.40
2	A	1003	HEC	C3C-C2C	-5.90	1.34	1.40
2	A	1004	HEC	C3B-C2B	-5.88	1.34	1.40
2	A	1007[B]	HEC	C3B-C2B	-5.85	1.34	1.40
2	A	1008[B]	HEC	C3B-C2B	-5.84	1.34	1.40
2	A	1002	HEC	C3B-C2B	-5.69	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	HEC	C3B-C2B	-5.29	1.35	1.40
2	B	1002	HEC	C3C-C2C	-4.98	1.35	1.40
2	B	1006	HEC	C3B-C2B	-4.98	1.35	1.40
2	A	1001	HEC	C3C-C2C	-4.90	1.35	1.40
2	B	1008[B]	HEC	C3C-C2C	-4.70	1.35	1.40
2	B	1001	HEC	C3B-C2B	-4.67	1.35	1.40
2	A	1006	HEC	C3B-C2B	-4.61	1.35	1.40
2	B	1004	HEC	C3B-C2B	-4.60	1.35	1.40
2	B	1005	HEC	C3C-C2C	-4.39	1.36	1.40
2	A	1002	HEC	C3C-C2C	-4.33	1.36	1.40
2	A	1004	HEC	C3C-C2C	-4.02	1.36	1.40
2	A	1006	HEC	C3C-C2C	-3.84	1.36	1.40
2	B	1001	HEC	C3C-C2C	-3.62	1.36	1.40
2	B	1004	HEC	C3C-C2C	-3.50	1.37	1.40
2	B	1006	HEC	C3C-C2C	-3.41	1.37	1.40
2	A	1002	HEC	C1D-CHD	-2.30	1.34	1.40
2	B	1008[B]	HEC	CAA-C2A	2.00	1.56	1.52
2	B	1008[B]	HEC	CMB-C2B	2.01	1.55	1.51
2	B	1002	HEC	CMD-C2D	2.02	1.55	1.51
2	A	1001	HEC	C1D-ND	2.03	1.40	1.36
2	A	1002	HEC	C1B-NB	2.07	1.40	1.36
2	A	1004	HEC	CAD-C3D	2.09	1.55	1.52
2	B	1003	HEC	C4B-NB	2.12	1.39	1.36
2	A	1006	HEC	C4B-NB	2.12	1.39	1.36
2	B	1002	HEC	C1D-ND	2.13	1.40	1.36
2	B	1001	HEC	C1B-NB	2.13	1.40	1.36
2	A	1004	HEC	C1A-NA	2.14	1.39	1.36
2	B	1005	HEC	CMB-C2B	2.15	1.56	1.51
2	A	1002	HEC	CMB-C2B	2.18	1.56	1.51
2	A	1008[B]	HEC	CAA-C2A	2.18	1.56	1.52
2	B	1002	HEC	C3C-C4C	2.22	1.47	1.43
2	A	1008[B]	HEC	CMA-C3A	2.24	1.56	1.51
2	B	1007[B]	HEC	CMB-C2B	2.27	1.56	1.51
2	B	1005	HEC	CBB-CAB	2.29	1.58	1.49
2	B	1004	HEC	C1A-NA	2.30	1.39	1.36
2	A	1004	HEC	CMC-C2C	2.30	1.56	1.51
2	A	1001	HEC	CBB-CAB	2.31	1.58	1.49
2	A	1003	HEC	CMB-C2B	2.32	1.56	1.51
2	B	1004	HEC	CMB-C2B	2.32	1.56	1.51
2	B	1002	HEC	CMA-C3A	2.32	1.56	1.51
2	A	1006	HEC	CMC-C2C	2.33	1.56	1.51
2	B	1007[B]	HEC	C4C-NC	2.33	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	HEC	C4C-NC	2.36	1.39	1.36
2	A	1003	HEC	C1D-ND	2.36	1.41	1.36
2	A	1008[B]	HEC	CMD-C2D	2.36	1.56	1.51
2	B	1001	HEC	C4B-NB	2.37	1.39	1.36
2	B	1008[B]	HEC	C4A-NA	2.37	1.39	1.36
2	A	1007[B]	HEC	C4C-NC	2.39	1.39	1.36
2	B	1004	HEC	CMC-C2C	2.39	1.56	1.51
2	A	1005	HEC	CMD-C2D	2.49	1.56	1.51
2	A	1007[B]	HEC	C4A-NA	2.50	1.39	1.36
2	A	1005	HEC	CMB-C2B	2.52	1.57	1.51
2	A	1005	HEC	C1A-NA	2.53	1.39	1.36
2	A	1008[B]	HEC	C1A-NA	2.54	1.39	1.36
2	B	1006	HEC	C4D-ND	2.55	1.41	1.36
2	A	1001	HEC	CMB-C2B	2.55	1.57	1.51
2	A	1001	HEC	C3C-C4C	2.65	1.48	1.43
2	A	1004	HEC	C3C-C4C	2.67	1.48	1.43
2	B	1005	HEC	C4A-NA	2.77	1.40	1.36
2	A	1005	HEC	C4A-NA	2.84	1.40	1.36
2	B	1003	HEC	CMB-C2B	2.95	1.57	1.51
2	B	1003	HEC	C3D-C2D	2.99	1.46	1.37
2	A	1007[B]	HEC	C3D-C2D	3.14	1.47	1.37
2	B	1007[B]	HEC	C1A-NA	3.21	1.40	1.36
2	B	1005	HEC	C3D-C2D	3.21	1.47	1.37
3	B	1	NO2	O1-N	3.24	1.37	1.21
2	B	1004	HEC	C3D-C2D	3.25	1.47	1.37
2	A	1004	HEC	C3D-C2D	3.35	1.47	1.37
2	A	1005	HEC	C3D-C2D	3.36	1.47	1.37
2	B	1007[B]	HEC	C4A-NA	3.44	1.40	1.36
2	B	1006	HEC	C4B-NB	3.46	1.40	1.36
2	A	1007[B]	HEC	C1A-NA	3.48	1.40	1.36
2	B	1007[B]	HEC	C3D-C2D	3.50	1.48	1.37
3	A	1	NO2	O1-N	3.55	1.38	1.21
2	B	1006	HEC	C3D-C2D	3.56	1.48	1.37
2	A	1003	HEC	C3D-C2D	3.62	1.48	1.37
2	A	1001	HEC	C3D-C2D	3.75	1.48	1.37
2	A	1002	HEC	C3D-C2D	3.82	1.49	1.37
2	B	1002	HEC	C3D-C2D	3.82	1.49	1.37
2	A	1006	HEC	C3D-C2D	3.98	1.49	1.37
2	A	1002	HEC	C4A-NA	4.08	1.41	1.36
2	B	1001	HEC	C3D-C2D	4.31	1.50	1.37
2	B	1008[B]	HEC	C3D-C2D	4.53	1.51	1.37
2	A	1008[B]	HEC	C3D-C2D	4.66	1.51	1.37

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1008[B]	HEC	CBA-CAA-C2A	-8.69	95.89	112.47
2	A	1007[B]	HEC	CBD-CAD-C3D	-7.04	99.03	112.48
2	B	1001	HEC	CMC-C2C-C1C	-6.70	118.16	128.46
2	A	1001	HEC	CMC-C2C-C1C	-6.65	118.25	128.46
2	A	1001	HEC	CAD-CBD-CGD	-6.39	101.73	112.66
2	B	1007[B]	HEC	CMB-C2B-C1B	-6.39	118.65	128.46
2	A	1007[B]	HEC	CMB-C2B-C1B	-6.37	118.68	128.46
2	B	1008[B]	HEC	CMB-C2B-C1B	-6.09	119.10	128.46
2	B	1002	HEC	CAA-CBA-CGA	-6.05	102.32	112.66
2	A	1002	HEC	CMC-C2C-C1C	-6.04	119.19	128.46
2	B	1002	HEC	CMC-C2C-C1C	-6.04	119.19	128.46
2	A	1002	HEC	CAA-CBA-CGA	-5.49	103.27	112.66
2	A	1008[B]	HEC	CMB-C2B-C1B	-5.37	120.21	128.46
2	A	1004	HEC	CMB-C2B-C1B	-5.32	120.28	128.46
2	A	1005	HEC	CMB-C2B-C1B	-5.31	120.30	128.46
2	A	1006	HEC	CMC-C2C-C1C	-5.31	120.30	128.46
2	B	1005	HEC	CMC-C2C-C1C	-5.17	120.52	128.46
2	B	1007[B]	HEC	CBD-CAD-C3D	-5.07	102.79	112.48
2	A	1004	HEC	CMC-C2C-C1C	-4.95	120.86	128.46
2	A	1003	HEC	CAD-CBD-CGD	-4.93	104.23	112.66
2	A	1005	HEC	C1D-C2D-C3D	-4.93	103.57	107.00
2	B	1006	HEC	CBD-CAD-C3D	-4.77	103.36	112.48
2	B	1003	HEC	CMC-C2C-C1C	-4.74	121.18	128.46
2	A	1008[B]	HEC	CBD-CAD-C3D	-4.71	103.48	112.48
2	A	1008[B]	HEC	CMC-C2C-C1C	-4.69	121.25	128.46
2	B	1005	HEC	CMB-C2B-C1B	-4.67	121.29	128.46
2	B	1008[B]	HEC	CMC-C2C-C1C	-4.62	121.37	128.46
2	B	1006	HEC	CMC-C2C-C1C	-4.50	121.54	128.46
2	B	1007[B]	HEC	CBA-CAA-C2A	-4.48	103.92	112.47
2	B	1008[B]	HEC	CBD-CAD-C3D	-4.47	103.93	112.48
2	A	1006	HEC	CBA-CAA-C2A	-4.46	103.96	112.47
2	B	1001	HEC	CBA-CAA-C2A	-4.28	104.31	112.47
2	A	1003	HEC	CBA-CAA-C2A	-4.24	104.39	112.47
2	A	1005	HEC	CMC-C2C-C1C	-4.23	121.96	128.46
2	A	1006	HEC	CMB-C2B-C1B	-4.23	121.96	128.46
2	A	1007[B]	HEC	CBA-CAA-C2A	-4.13	104.59	112.47
2	A	1006	HEC	CBD-CAD-C3D	-4.13	104.59	112.48
2	B	1004	HEC	CMB-C2B-C1B	-4.09	122.17	128.46
2	B	1006	HEC	CMB-C2B-C1B	-4.07	122.21	128.46
2	B	1001	HEC	CBD-CAD-C3D	-4.02	104.80	112.48
2	B	1004	HEC	CMC-C2C-C1C	-3.96	122.37	128.46
2	A	1008[B]	HEC	C1D-C2D-C3D	-3.95	104.25	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1006	HEC	CBA-CAA-C2A	-3.92	104.99	112.47
2	B	1005	HEC	CBD-CAD-C3D	-3.86	105.10	112.48
2	A	1001	HEC	CBD-CAD-C3D	-3.84	105.15	112.48
2	B	1003	HEC	CBA-CAA-C2A	-3.81	105.20	112.47
2	A	1003	HEC	CMB-C2B-C1B	-3.80	122.62	128.46
2	A	1001	HEC	CMB-C2B-C1B	-3.66	122.84	128.46
2	B	1005	HEC	CAD-CBD-CGD	-3.60	106.51	112.66
2	A	1005	HEC	CAD-CBD-CGD	-3.48	106.72	112.66
2	B	1008[B]	HEC	C1D-C2D-C3D	-3.37	104.65	107.00
2	B	1003	HEC	C1D-C2D-C3D	-3.34	104.67	107.00
2	B	1002	HEC	CMB-C2B-C1B	-3.32	123.36	128.46
2	A	1005	HEC	CBD-CAD-C3D	-3.30	106.18	112.48
2	B	1007[B]	HEC	CMC-C2C-C1C	-3.12	123.67	128.46
2	A	1006	HEC	C1D-C2D-C3D	-3.07	104.86	107.00
2	A	1006	HEC	CAA-CBA-CGA	-3.02	107.50	112.66
2	B	1003	HEC	CMB-C2B-C1B	-3.00	123.85	128.46
2	A	1003	HEC	CMC-C2C-C1C	-2.98	123.88	128.46
2	B	1002	HEC	C1D-C2D-C3D	-2.98	104.92	107.00
2	B	1006	HEC	CAA-CBA-CGA	-2.78	107.91	112.66
2	A	1002	HEC	CMB-C2B-C1B	-2.67	124.36	128.46
2	A	1002	HEC	C1D-C2D-C3D	-2.67	105.14	107.00
2	A	1005	HEC	CAA-CBA-CGA	-2.63	108.17	112.66
2	B	1001	HEC	CMB-C2B-C1B	-2.53	124.58	128.46
2	B	1003	HEC	CAD-CBD-CGD	-2.51	108.37	112.66
2	A	1001	HEC	CAA-CBA-CGA	-2.47	108.44	112.66
2	B	1001	HEC	C1D-C2D-C3D	-2.44	105.30	107.00
2	A	1007[B]	HEC	CMC-C2C-C1C	-2.44	124.71	128.46
2	B	1003	HEC	CBD-CAD-C3D	-2.40	107.89	112.48
2	B	1008[B]	HEC	CAD-CBD-CGD	-2.36	108.63	112.66
2	B	1005	HEC	C1D-C2D-C3D	-2.30	105.40	107.00
2	A	1004	HEC	CBA-CAA-C2A	-2.29	108.11	112.47
2	A	1003	HEC	CBD-CAD-C3D	-2.28	108.13	112.48
2	B	1002	HEC	CBA-CAA-C2A	-2.22	108.23	112.47
2	B	1006	HEC	C3C-C4C-NC	-2.11	106.97	110.94
2	A	1006	HEC	CAD-CBD-CGD	-2.04	109.17	112.66
2	B	1008[B]	HEC	CBA-CAA-C2A	-2.02	108.61	112.47
2	A	1008[B]	HEC	CMA-C3A-C2A	2.12	128.94	124.94
2	A	1008[B]	HEC	CMD-C2D-C3D	2.81	130.24	124.94
2	B	1006	HEC	CMA-C3A-C2A	3.04	130.67	124.94
2	A	1006	HEC	CMA-C3A-C2A	3.17	130.93	124.94
2	A	1008[B]	HEC	CAA-CBA-CGA	8.85	127.79	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	HEC	3	0
2	A	1002	HEC	3	0
2	A	1003	HEC	1	0
2	A	1004	HEC	4	0
2	A	1006	HEC	1	0
2	A	1007[B]	HEC	1	0
2	A	1008[B]	HEC	1	0
5	A	3	MRD	5	0
2	B	1001	HEC	1	0
2	B	1002	HEC	1	0
2	B	1003	HEC	1	0
2	B	1004	HEC	3	0
2	B	1006	HEC	1	0
2	B	1007[B]	HEC	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	520/520 (100%)	-0.66	2 (0%) 92 91	14, 19, 29, 49	0
1	B	520/520 (100%)	-0.64	3 (0%) 89 89	13, 18, 30, 50	0
All	All	1040/1040 (100%)	-0.65	5 (0%) 90 90	13, 18, 30, 50	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	524	VAL	4.4
1	B	523	ALA	3.5
1	A	524	VAL	3.2
1	A	523	ALA	2.4
1	B	388	GLN	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	MRD	A	3	8/8	0.94	0.11	2.98	16,20,24,29	0
2	HEC	B	1008[B]	43/43	0.96	0.11	2.87	13,18,36,49	4
2	HEC	A	1008[B]	43/43	0.95	0.13	2.17	14,20,39,48	4
2	HEC	A	1007[B]	43/43	0.98	0.09	2.16	10,14,16,26	3
2	HEC	B	1007[B]	43/43	0.98	0.09	1.65	8,13,15,22	3
5	MRD	B	3	8/8	0.96	0.09	0.80	19,24,26,27	0
3	NO2	B	1	3/3	0.99	0.07	0.80	15,15,16,16	0
2	HEC	A	1003	43/43	0.98	0.09	0.76	12,15,29,40	0
2	HEC	B	1003	43/43	0.98	0.08	0.53	11,14,30,42	0
2	HEC	B	1005	43/43	0.99	0.07	0.42	12,13,18,28	0
2	HEC	A	1004	43/43	0.99	0.06	0.35	11,15,16,17	0
2	HEC	B	1002	43/43	0.99	0.08	0.32	13,16,19,21	0
2	HEC	B	1006	43/43	0.99	0.06	0.31	11,13,14,15	0
2	HEC	A	1005	43/43	0.99	0.07	0.21	12,14,16,28	0
2	HEC	B	1004	43/43	0.99	0.06	0.17	10,14,16,17	0
2	HEC	A	1002	43/43	0.99	0.08	0.15	12,16,18,20	0
2	HEC	A	1006	43/43	0.99	0.06	0.02	11,13,15,15	0
2	HEC	A	1001	43/43	0.98	0.09	-0.04	15,18,30,38	0
3	NO2	A	1	3/3	0.99	0.06	-0.37	15,15,16,18	0
2	HEC	B	1001	43/43	0.98	0.09	-0.62	14,21,26,34	0
4	CA	B	2	1/1	1.00	0.05	-2.02	18,18,18,18	0
4	CA	A	2	1/1	0.99	0.04	-3.67	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.