



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:38 AM GMT

PDB ID : 3UU9  
Title : Structure of the free TvNiRb form of Thioalkalivibrio nitratreducens cytochrome c nitrite reductase  
Authors : Trofimov, A.A.; Polyakov, K.M.; Tikhonova, T.V.; Tikhonov, A.V.; Dorovatovskii, P.V.; Popov, V.O.  
Deposited on : 2011-11-28  
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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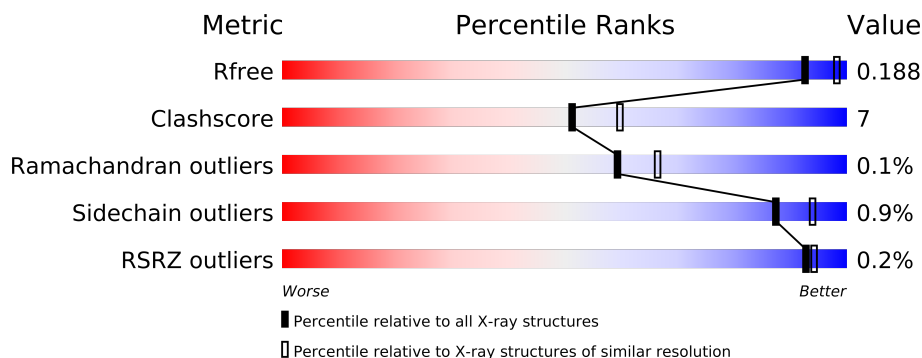
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	520	
1	B	520	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	HEC	A	605	-	X
3	CA	A	610	-	X
4	PG4	A	611	-	X
4	PG4	A	612	-	X
4	PG4	A	613	-	X
4	PG4	B	611	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	PG4	B	613	-	X
4	PG4	B	615	-	X
4	PG4	B	616	-	X
4	PG4	B	617	-	X
4	PG4	B	618	-	X
4	PG4	B	619	-	X
4	PG4	B	620	-	X

## 2 Entry composition i

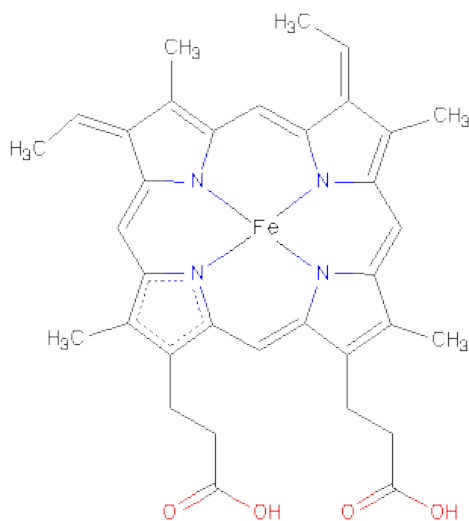
There are 6 unique types of molecules in this entry. The entry contains 10001 atoms, of which 0 are hydrogen and 0 are deuterium.

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	519	Total	C	N	O	S	0	12	0
			4147	2574	757	779	37			
1	B	520	Total	C	N	O	S	0	12	0
			4157	2579	757	785	36			

- 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		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	1
			46	35	1	4	6		

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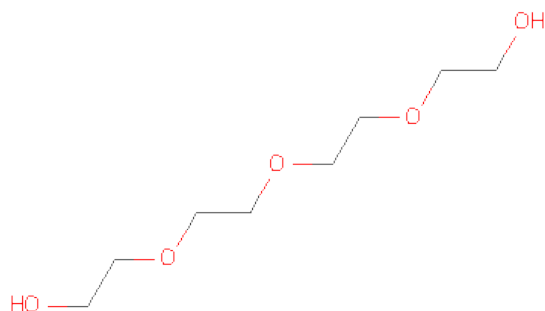
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	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 46	C 35	Fe 1	N 4	O 6	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 47	C 36	Fe 1	N 4	O 6	0	1
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			8	5	3		
4	A	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			9	6	3		
4	B	1	Total	C	O	0	0
			8	5	3		
4	B	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Na 1	0	0

- Molecule 6 is water.

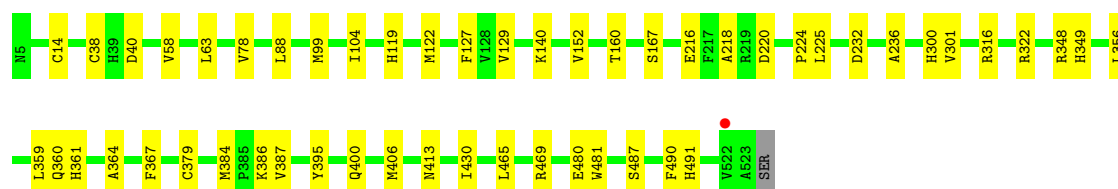
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	442	Total 442	O 442	0	0
6	B	458	Total 458	O 458	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

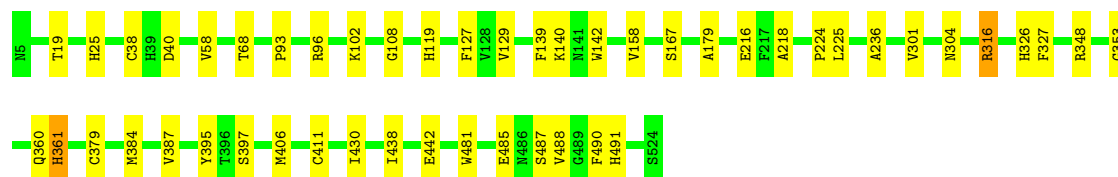
- Molecule 1: Eight-heme nitrite reductase

Chain A: 



- Molecule 1: Eight-heme nitrite reductase

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.39Å 191.39Å 191.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.20 46.42 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (100.00-2.20) 99.6 (46.42-1.95)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.157 , 0.184 0.163 , 0.188	Depositor DCC
$R_{free}$ test set	5897 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.4	EDS
Estimated twinning fraction	0.064 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 168139 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, PG4, 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	0.74	0/4321	0.74	0/5858
1	B	0.75	1/4333 (0.0%)	0.75	0/5874
All	All	0.75	1/8654 (0.0%)	0.75	0/11732

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	CYS	CB-SG	-5.07	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4147	0	3860	52	0
1	B	4157	0	3862	46	0
2	A	347	0	214	15	0
2	B	351	0	192	19	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	26	0	29	18	0
4	B	68	0	77	22	0
5	B	1	0	0	0	0
6	A	442	0	0	4	0
6	B	458	0	0	6	0
All	All	10001	0	8234	122	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (122) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:348[B]:ARG:NH2	4:A:612:PG4:H21	1.37	1.33
1:A:348[B]:ARG:NH2	4:A:612:PG4:C2	2.09	1.16
4:A:611:PG4:O3	4:A:612:PG4:C3	2.04	1.06
1:A:348[B]:ARG:HH22	4:A:612:PG4:C2	1.72	1.02
1:B:348[B]:ARG:NH2	4:B:611:PG4:O4	1.99	0.95
1:A:348[B]:ARG:HH21	4:A:612:PG4:H21	1.21	0.92
2:B:605:HEC:HMC1	2:B:605:HEC:HBC3	1.55	0.88
1:B:108:GLY:HA3	4:B:619:PG4:H32	1.57	0.86
1:A:348[B]:ARG:HH22	4:A:612:PG4:C1	1.89	0.84
1:B:348[B]:ARG:HH21	4:B:612:PG4:C4	1.93	0.80
1:B:348[B]:ARG:NH2	4:B:611:PG4:O5	2.15	0.78
1:A:348[B]:ARG:NH2	4:A:612:PG4:O1	2.20	0.74
1:A:384:MET:HG3	1:A:400:GLN:HG3	1.76	0.66
1:A:348[A]:ARG:NE	4:A:611:PG4:H52	2.11	0.65
1:B:348[B]:ARG:NH2	4:B:612:PG4:C4	2.58	0.65
1:A:348[B]:ARG:HH21	4:A:612:PG4:C3	2.09	0.65
1:A:348[A]:ARG:HE	4:A:611:PG4:H52	1.62	0.65
2:B:606:HEC:HMC1	2:B:606:HEC:HBC3	1.78	0.65
1:B:348[A]:ARG:HH21	4:B:612:PG4:C4	2.10	0.65
1:B:179:ALA:HB2	4:B:619:PG4:H31	1.79	0.65
1:B:167:SER:HB2	1:B:216:GLU:HG2	1.79	0.64
2:A:605:HEC:HBC3	2:A:605:HEC:HMC1	1.81	0.62
1:B:316[A]:ARG:NH1	6:B:706:HOH:O	2.32	0.62
2:B:605:HEC:HMB1	2:B:605:HEC:HBB3	1.79	0.62
2:A:606:HEC:HBC3	2:A:606:HEC:HMC1	1.81	0.61
2:B:605:HEC:HMC1	2:B:605:HEC:CBC	2.30	0.61
1:B:348[B]:ARG:HE	4:B:612:PG4:H21	1.65	0.61
1:A:348[A]:ARG:CZ	4:A:611:PG4:H52	2.27	0.60
1:A:167:SER:HB2	1:A:216[A]:GLU:HG2	1.84	0.59
1:B:139:PHE:HB2	4:B:613:PG4:H12	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:348[A]:ARG:HH11	1:B:348[A]:ARG:HG3	1.68	0.58
1:B:179:ALA:CB	4:B:619:PG4:H31	2.33	0.58
1:A:465:LEU:O	1:A:469:ARG:HG3	2.05	0.57
1:B:348[B]:ARG:HH22	4:B:611:PG4:C8	2.17	0.57
1:A:348[B]:ARG:HE	4:A:611:PG4:H52	1.70	0.57
2:B:607[B]:HEC:O1A	6:B:1114:HOH:O	2.16	0.56
1:A:348[B]:ARG:NH2	4:A:612:PG4:C3	2.69	0.56
2:A:608:HEC:HMC1	2:A:608:HEC:HBC3	1.87	0.55
1:A:360:GLN:HB3	1:A:361:HIS:CE1	2.41	0.55
2:B:608:HEC:HMB1	2:B:608:HEC:HBB3	1.89	0.54
1:B:360:GLN:HB3	1:B:361:HIS:CE1	2.42	0.54
1:A:316[B]:ARG:HH11	1:A:316[B]:ARG:CG	2.20	0.54
1:B:316[A]:ARG:HG2	6:B:1123:HOH:O	2.09	0.52
1:A:348[B]:ARG:HH21	4:A:612:PG4:C2	2.01	0.52
4:B:619:PG4:H22	6:B:1073:HOH:O	2.08	0.52
2:B:606:HEC:HBD2	2:B:606:HEC:HHA	1.91	0.51
1:A:40:ASP:HB3	1:A:58:VAL:HB	1.93	0.51
1:B:40:ASP:HB3	1:B:58:VAL:HB	1.92	0.51
1:A:122:MET:HB2	2:A:603:HEC:HMD2	1.92	0.51
2:B:605:HEC:HBC1	4:B:616:PG4:H52	1.93	0.51
1:B:430:ILE:HG21	1:B:490:PHE:HA	1.92	0.51
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.46	0.50
1:B:348[B]:ARG:NH1	4:B:611:PG4:O5	2.42	0.50
2:A:607:HEC:HBB3	2:A:607:HEC:HMB1	1.94	0.49
2:B:605:HEC:CBC	4:B:616:PG4:H52	2.41	0.49
2:B:605:HEC:HBC1	4:B:616:PG4:H42	1.95	0.49
1:B:140:LYS:HG3	1:B:158:VAL:O	2.14	0.48
1:A:384:MET:CG	1:A:400:GLN:HG3	2.44	0.48
1:B:348[B]:ARG:HH22	4:B:611:PG4:C7	2.27	0.48
2:A:605:HEC:CBC	2:A:605:HEC:HMC1	2.44	0.48
1:A:413:ASN:HB2	6:A:1005:HOH:O	2.14	0.48
1:A:387:VAL:HG21	1:A:395:TYR:CE1	2.47	0.48
1:A:487:SER:HB3	1:A:491:HIS:CE1	2.49	0.48
1:B:304:ASN:HB2	1:B:326:HIS:HB3	1.95	0.47
1:B:384:MET:HB2	1:B:397:SER:O	2.15	0.47
1:A:348[B]:ARG:NH1	4:A:612:PG4:O1	2.48	0.47
1:A:119:HIS:CD2	2:A:603:HEC:ND	2.83	0.46
1:A:99[B]:MET:CE	6:A:1023:HOH:O	2.63	0.46
1:A:359:LEU:HD22	1:A:359:LEU:N	2.31	0.46
1:B:301:VAL:HG21	1:B:327:PHE:CE2	2.50	0.46
2:B:602:HEC:HMB1	2:B:602:HEC:HBB3	1.98	0.46
1:A:348[B]:ARG:NH2	4:A:612:PG4:C1	2.63	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:25:HIS:CD2	2:B:606:HEC:HBB2	2.51	0.46
1:A:301:VAL:HG12	1:A:364:ALA:HB3	1.97	0.46
1:A:386:LYS:NZ	6:A:742:HOH:O	2.48	0.46
1:B:348[B]:ARG:CZ	4:B:611:PG4:O5	2.64	0.45
1:B:142:TRP:CZ2	4:B:613:PG4:H22	2.52	0.45
1:A:14:CYS:HA	2:A:608:HEC:CHC	2.46	0.45
1:A:63:LEU:N	1:A:63:LEU:HD12	2.32	0.45
1:A:224:PRO:O	1:A:225:LEU:C	2.55	0.45
1:A:316[B]:ARG:CG	1:A:316[B]:ARG:NH1	2.79	0.45
1:A:300:HIS:CE1	2:A:601:HEC:HMD1	2.52	0.45
1:B:119:HIS:CD2	2:B:603:HEC:ND	2.86	0.44
1:B:348[A]:ARG:NH1	1:B:348[A]:ARG:HG3	2.32	0.44
2:A:603:HEC:HMA3	2:A:604[B]:HEC:HBA2	2.00	0.44
1:B:348[B]:ARG:HG2	1:B:353:GLY:O	2.17	0.44
1:A:140:LYS:HG2	1:A:160:THR:HG23	1.98	0.44
1:B:96:ARG:CZ	1:B:488:VAL:HG22	2.47	0.44
1:B:129:VAL:HG11	2:B:601:HEC:HMA1	1.99	0.44
2:A:602:HEC:HBC3	2:A:602:HEC:HMC1	2.00	0.44
1:A:99[B]:MET:HE3	6:A:1023:HOH:O	2.18	0.43
1:B:38:CYS:HB2	2:B:606:HEC:C4C	2.48	0.43
2:A:608:HEC:HMB1	2:A:608:HEC:HBB3	2.00	0.43
1:B:225:LEU:HD13	2:B:603:HEC:HBC3	2.00	0.43
1:B:127:PHE:CE1	1:B:218:ALA:HB1	2.54	0.43
1:A:430:ILE:HG21	1:A:490:PHE:HA	2.01	0.42
2:A:607:HEC:HMC1	2:A:607:HEC:HBC3	2.01	0.42
1:A:38:CYS:HB2	2:A:606:HEC:C4C	2.49	0.42
1:B:102[A]:LYS:NZ	6:B:1057:HOH:O	2.51	0.42
1:A:348[A]:ARG:CZ	4:A:611:PG4:C5	2.94	0.41
1:A:348[B]:ARG:CZ	4:A:612:PG4:O1	2.68	0.41
1:B:142:TRP:CE2	4:B:613:PG4:H22	2.56	0.41
1:A:129:VAL:HG11	2:A:601:HEC:HMA1	2.03	0.41
1:A:349:HIS:HB2	1:A:356:LEU:HD11	2.01	0.41
2:B:605:HEC:CBC	4:B:616:PG4:H42	2.51	0.41
1:B:93:PRO:HD2	6:B:1064:HOH:O	2.20	0.41
1:B:438:ILE:O	1:B:442:GLU:HG3	2.20	0.41
1:B:224:PRO:O	1:B:225:LEU:C	2.59	0.41
1:A:480:GLU:O	1:A:481:TRP:C	2.59	0.41
1:A:104:ILE:HA	1:A:104:ILE:HD12	1.92	0.41
1:B:236:ALA:HB1	2:B:607[B]:HEC:HBA1	2.03	0.40
1:A:360:GLN:O	1:A:361:HIS:C	2.58	0.40
1:B:348[A]:ARG:HE	4:B:612:PG4:H21	1.52	0.40
1:A:78[A]:VAL:HG23	1:A:152:VAL:HG21	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:232:ASP:O	1:A:236:ALA:HA	2.20	0.40
1:B:387:VAL:HG21	1:B:395:TYR:CE1	2.57	0.40
1:B:481:TRP:O	1:B:485:GLU:HB2	2.22	0.40
1:A:127:PHE:CE1	1:A:218:ALA:HB1	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	529/520 (102%)	504 (95%)	25 (5%)	0	100	100
1	B	530/520 (102%)	509 (96%)	20 (4%)	1 (0%)	56	62
All	All	1059/1040 (102%)	1013 (96%)	45 (4%)	1 (0%)	59	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	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	445/439 (101%)	440 (99%)	5 (1%)	84	92
1	B	447/439 (102%)	440 (98%)	7 (2%)	75	85
All	All	892/878 (102%)	880 (99%)	12 (1%)	87	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	220	ASP
1	A	322	ARG
1	A	406[A]	MET
1	A	406[B]	MET
1	B	19[A]	THR
1	B	19[B]	THR
1	B	68	THR
1	B	316[A]	ARG
1	B	316[B]	ARG
1	B	406[A]	MET
1	B	406[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 38 ligands modelled in this entry, 5 are monoatomic - leaving 33 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
2	HEC	A	601	1,6	50,50,50	2.84	12 (24%)	56,82,82	1.81	10 (17%)
2	HEC	A	602	1	50,50,50	2.73	12 (24%)	56,82,82	2.00	13 (23%)
2	HEC	A	603	1,3	50,50,50	2.70	13 (26%)	56,82,82	2.28	16 (28%)
2	HEC	A	604[A]	-	2,2,50	0.51	0	1,1,82	0.64	0
2	HEC	A	604[B]	3	2,2,50	0.62	0	1,1,82	0.77	0
2	HEC	A	605	1	50,50,50	2.76	13 (26%)	56,82,82	2.24	13 (23%)
2	HEC	A	606	1	50,50,50	2.75	13 (26%)	56,82,82	2.00	14 (25%)
2	HEC	A	607	1	50,50,50	2.72	11 (22%)	56,82,82	2.00	14 (25%)
2	HEC	A	608	1	50,50,50	2.78	14 (28%)	56,82,82	2.17	16 (28%)
4	PG4	A	611	-	6,6,12	0.76	0	5,5,11	0.35	0
4	PG4	A	612	-	3,4,12	0.66	0	2,3,11	0.62	0
4	PG4	A	613	-	6,7,12	0.84	0	5,6,11	0.48	0
4	PG4	A	614	-	5,5,12	1.19	1 (20%)	3,4,11	0.70	0
2	HEC	B	601	1,6	50,50,50	2.95	13 (26%)	56,82,82	1.90	11 (19%)
2	HEC	B	602	1	50,50,50	2.85	11 (22%)	56,82,82	2.01	11 (19%)
2	HEC	B	603	1,3,5	50,50,50	2.72	12 (24%)	56,82,82	2.05	15 (26%)
2	HEC	B	604[A]	3,5	2,2,50	0.63	0	1,1,82	0.97	0
2	HEC	B	604[B]	5	2,2,50	0.54	0	1,1,82	0.64	0
2	HEC	B	605	1	50,50,50	2.84	13 (26%)	56,82,82	2.21	15 (26%)
2	HEC	B	606	1	50,50,50	2.86	13 (26%)	56,82,82	2.18	16 (28%)
2	HEC	B	607[A]	-	2,3,50	1.59	1 (50%)	1,3,82	0.28	0
2	HEC	B	607[B]	-	2,3,50	2.09	1 (50%)	1,3,82	0.16	0
2	HEC	B	608	1	50,50,50	2.82	15 (30%)	56,82,82	2.08	15 (26%)
4	PG4	B	611	-	5,5,12	2.94	1 (20%)	3,4,11	0.24	0
4	PG4	B	612	-	5,5,12	3.18	1 (20%)	3,4,11	0.59	0
4	PG4	B	613	-	3,4,12	0.83	0	2,3,11	1.32	0
4	PG4	B	614	-	3,4,12	0.60	0	2,3,11	0.59	0
4	PG4	B	615	-	9,9,12	0.67	0	8,8,11	0.60	0
4	PG4	B	616	-	8,8,12	1.81	1 (12%)	6,7,11	0.33	0
4	PG4	B	617	-	6,7,12	0.55	0	5,6,11	0.06	0
4	PG4	B	618	-	3,4,12	1.04	0	2,3,11	0.74	0
4	PG4	B	619	-	6,6,12	1.00	0	5,5,11	0.79	0
4	PG4	B	620	-	6,6,12	0.71	0	5,5,11	0.82	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
2	HEC	A	601	1,6	-	0/10/54/54	0/0/8/8
2	HEC	A	602	1	-	0/10/54/54	0/0/8/8
2	HEC	A	603	1,3	-	0/10/54/54	0/0/8/8
2	HEC	A	604[A]	-	-	0/0/0/54	0/0/0/8
2	HEC	A	604[B]	3	-	0/0/0/54	0/0/0/8
2	HEC	A	605	1	-	0/10/54/54	0/0/8/8
2	HEC	A	606	1	-	0/10/54/54	0/0/8/8
2	HEC	A	607	1	-	0/10/54/54	0/0/8/8
2	HEC	A	608	1	-	0/10/54/54	0/0/8/8
4	PG4	A	611	-	-	0/4/4/10	0/0/0/0
4	PG4	A	612	-	-	0/2/2/10	0/0/0/0
4	PG4	A	613	-	-	0/5/5/10	0/0/0/0
4	PG4	A	614	-	-	0/3/3/10	0/0/0/0
2	HEC	B	601	1,6	-	0/10/54/54	0/0/8/8
2	HEC	B	602	1	-	0/10/54/54	0/0/8/8
2	HEC	B	603	1,3,5	-	0/10/54/54	0/0/8/8
2	HEC	B	604[A]	3,5	-	0/0/0/54	0/0/0/8
2	HEC	B	604[B]	5	-	0/0/0/54	0/0/0/8
2	HEC	B	605	1	-	0/10/54/54	0/0/8/8
2	HEC	B	606	1	-	0/10/54/54	0/0/8/8
2	HEC	B	607[A]	-	-	0/0/0/54	0/0/0/8
2	HEC	B	607[B]	-	-	0/0/0/54	0/0/0/8
2	HEC	B	608	1	-	0/10/54/54	0/0/8/8
4	PG4	B	611	-	-	0/3/3/10	0/0/0/0
4	PG4	B	612	-	-	0/3/3/10	0/0/0/0
4	PG4	B	613	-	-	0/2/2/10	0/0/0/0
4	PG4	B	614	-	-	0/2/2/10	0/0/0/0
4	PG4	B	615	-	-	0/7/7/10	0/0/0/0
4	PG4	B	616	-	-	0/6/6/10	0/0/0/0
4	PG4	B	617	-	-	0/5/5/10	0/0/0/0
4	PG4	B	618	-	-	0/2/2/10	0/0/0/0
4	PG4	B	619	-	-	0/4/4/10	0/0/0/0
4	PG4	B	620	-	-	0/4/4/10	0/0/0/0

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEC	C3B-CAB	11.14	1.58	1.35
2	B	605	HEC	C3C-CAC	11.09	1.58	1.35
2	B	601	HEC	C3B-CAB	11.00	1.58	1.35
2	B	601	HEC	C3C-CAC	10.70	1.57	1.35
2	A	605	HEC	C3C-CAC	10.70	1.57	1.35
2	B	602	HEC	C3C-CAC	10.69	1.57	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	608	HEC	C3C-CAC	10.64	1.57	1.35
2	B	608	HEC	C3C-CAC	10.62	1.57	1.35
2	A	602	HEC	C3C-CAC	10.45	1.56	1.35
2	B	606	HEC	C3B-CAB	10.37	1.56	1.35
2	A	606	HEC	C3B-CAB	10.25	1.56	1.35
2	B	603	HEC	C3C-CAC	10.24	1.56	1.35
2	A	608	HEC	C3B-CAB	10.20	1.56	1.35
2	B	606	HEC	C3C-CAC	10.17	1.56	1.35
2	A	603	HEC	C3B-CAB	10.14	1.56	1.35
2	B	602	HEC	C3B-CAB	10.01	1.56	1.35
2	A	607	HEC	C3B-CAB	10.01	1.56	1.35
2	A	607	HEC	C3C-CAC	9.90	1.55	1.35
2	A	606	HEC	C3C-CAC	9.84	1.55	1.35
2	B	603	HEC	C3B-CAB	9.71	1.55	1.35
2	A	601	HEC	C3C-CAC	9.60	1.55	1.35
2	A	602	HEC	C3B-CAB	9.52	1.55	1.35
2	A	603	HEC	C3C-CAC	9.50	1.55	1.35
2	B	605	HEC	C3B-CAB	9.40	1.54	1.35
2	B	608	HEC	C3B-CAB	9.29	1.54	1.35
2	A	605	HEC	C3B-CAB	9.21	1.54	1.35
4	B	612	PG4	C4-C3	-7.06	1.52	1.55
4	B	611	PG4	C5-C6	-6.50	1.52	1.55
2	B	602	HEC	C1B-C2B	5.76	1.47	1.40
2	A	607	HEC	C1C-C2C	5.35	1.46	1.40
2	B	605	HEC	C3C-C4C	5.21	1.48	1.41
2	B	606	HEC	C3D-C2D	5.21	1.53	1.37
2	A	601	HEC	C1B-C2B	5.14	1.46	1.40
2	A	602	HEC	C1C-C2C	5.12	1.46	1.40
2	A	606	HEC	C3D-C2D	5.08	1.52	1.37
2	A	605	HEC	C3D-C2D	5.04	1.52	1.37
2	B	601	HEC	C3D-C2D	5.03	1.52	1.37
4	B	616	PG4	C6-C5	-4.98	1.53	1.55
2	B	608	HEC	C3D-C2D	4.93	1.52	1.37
2	B	605	HEC	C3D-C2D	4.85	1.52	1.37
2	B	601	HEC	C1C-C2C	4.84	1.46	1.40
2	B	606	HEC	FE-ND	4.80	2.13	1.92
2	B	601	HEC	C1B-C2B	4.75	1.46	1.40
2	B	603	HEC	C3D-C2D	4.71	1.51	1.37
2	A	602	HEC	C1B-C2B	4.67	1.46	1.40
2	A	603	HEC	C3D-C2D	4.67	1.51	1.37
2	A	601	HEC	C1C-C2C	4.65	1.46	1.40
2	B	602	HEC	C1C-C2C	4.65	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	HEC	C3C-C4C	4.65	1.47	1.41
2	B	605	HEC	C1C-C2C	4.63	1.45	1.40
2	B	608	HEC	FE-NC	4.54	2.12	1.92
2	A	608	HEC	C3D-C2D	4.53	1.51	1.37
2	A	601	HEC	C3D-C2D	4.52	1.51	1.37
2	A	601	HEC	C3B-C4B	4.45	1.47	1.41
2	A	602	HEC	C3B-C4B	4.41	1.47	1.41
2	A	605	HEC	C1C-C2C	4.39	1.45	1.40
2	A	607	HEC	C3D-C2D	4.38	1.50	1.37
2	A	603	HEC	C1B-C2B	4.36	1.45	1.40
2	B	606	HEC	C3C-C4C	4.35	1.47	1.41
2	B	603	HEC	C1D-C2D	4.34	1.45	1.40
2	A	603	HEC	C3C-C4C	4.34	1.47	1.41
2	A	603	HEC	C1C-C2C	4.34	1.45	1.40
2	A	605	HEC	C1D-C2D	4.30	1.45	1.40
2	A	602	HEC	C3D-C2D	4.29	1.50	1.37
2	A	601	HEC	FE-ND	4.26	2.10	1.92
2	B	608	HEC	C1C-C2C	4.24	1.45	1.40
2	B	608	HEC	C1B-C2B	4.23	1.45	1.40
2	B	601	HEC	C3C-C4C	4.22	1.46	1.41
2	B	602	HEC	C3D-C2D	4.19	1.50	1.37
2	B	605	HEC	C3B-C2B	-4.16	1.32	1.41
2	B	608	HEC	C1D-C2D	4.16	1.45	1.40
2	B	603	HEC	C3C-C4C	4.15	1.46	1.41
2	B	608	HEC	C3B-C4B	4.12	1.46	1.41
2	A	608	HEC	FE-NC	4.11	2.10	1.92
2	A	607	HEC	C3C-C4C	4.10	1.46	1.41
2	B	605	HEC	C1D-C2D	4.06	1.45	1.40
2	A	608	HEC	C1D-C2D	4.06	1.45	1.40
2	A	606	HEC	C1B-C2B	4.05	1.45	1.40
2	B	608	HEC	C3C-C4C	4.01	1.46	1.41
2	A	605	HEC	C3B-C2B	-3.95	1.33	1.41
2	A	606	HEC	C3C-C4C	3.95	1.46	1.41
2	B	606	HEC	C1C-C2C	3.90	1.45	1.40
2	A	605	HEC	FE-NC	3.87	2.09	1.92
2	A	608	HEC	FE-NB	3.87	2.09	1.92
2	B	606	HEC	C3B-C4B	3.84	1.46	1.41
2	B	603	HEC	C3B-C4B	3.81	1.46	1.41
2	A	607	HEC	C1D-C2D	3.81	1.44	1.40
2	B	601	HEC	C3B-C4B	3.78	1.46	1.41
2	A	605	HEC	C3C-C4C	3.70	1.46	1.41
2	B	606	HEC	FE-NA	3.66	2.08	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEC	C3C-C2C	-3.65	1.33	1.41
2	B	602	HEC	C3B-C2B	-3.64	1.33	1.41
2	B	605	HEC	FE-NA	3.64	2.08	1.92
2	A	603	HEC	FE-NC	3.63	2.08	1.92
2	A	606	HEC	FE-ND	3.62	2.08	1.92
2	A	606	HEC	C3B-C2B	-3.60	1.33	1.41
2	A	608	HEC	C1C-C2C	3.57	1.44	1.40
2	A	606	HEC	C3B-C4B	3.57	1.46	1.41
2	A	605	HEC	C1B-C2B	3.57	1.44	1.40
2	A	602	HEC	C3B-C2B	-3.55	1.34	1.41
2	A	601	HEC	C3B-C2B	-3.54	1.34	1.41
2	A	602	HEC	C3C-C4C	3.53	1.46	1.41
2	B	606	HEC	C1B-C2B	3.52	1.44	1.40
2	B	602	HEC	C3B-C4B	3.51	1.46	1.41
2	A	607	HEC	C1B-C2B	3.51	1.44	1.40
2	B	605	HEC	C3C-C2C	-3.51	1.34	1.41
2	B	606	HEC	C1D-C2D	3.47	1.44	1.40
2	B	601	HEC	FE-ND	3.47	2.07	1.92
2	A	606	HEC	FE-NC	3.46	2.07	1.92
2	A	602	HEC	C3C-C2C	-3.45	1.34	1.41
2	B	601	HEC	C1D-C2D	3.43	1.44	1.40
2	A	607	HEC	C3C-C2C	-3.42	1.34	1.41
2	B	608	HEC	FE-NA	3.42	2.07	1.92
2	B	603	HEC	C1C-C2C	3.40	1.44	1.40
2	A	601	HEC	C1D-C2D	3.39	1.44	1.40
2	A	606	HEC	C1C-C2C	3.39	1.44	1.40
2	B	603	HEC	C3B-C2B	-3.38	1.34	1.41
2	A	608	HEC	C3B-C2B	-3.38	1.34	1.41
2	A	603	HEC	C3B-C4B	3.36	1.45	1.41
2	B	605	HEC	FE-NC	3.31	2.06	1.92
2	A	608	HEC	FE-NA	3.27	2.06	1.92
2	A	608	HEC	C3C-C4C	3.24	1.45	1.41
2	A	606	HEC	C1D-C2D	3.22	1.44	1.40
2	B	602	HEC	C3C-C2C	-3.21	1.34	1.41
2	A	608	HEC	C3C-C2C	-3.20	1.34	1.41
2	A	607	HEC	C3B-C4B	3.18	1.45	1.41
2	B	606	HEC	FE-NC	3.16	2.06	1.92
2	A	602	HEC	FE-ND	3.13	2.05	1.92
2	A	605	HEC	FE-ND	3.11	2.05	1.92
2	A	601	HEC	C3C-C2C	-3.09	1.35	1.41
2	B	603	HEC	FE-NC	3.07	2.05	1.92
2	A	608	HEC	C3B-C4B	3.06	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEC	FE-NA	3.04	2.05	1.92
2	A	603	HEC	C1D-C2D	3.02	1.43	1.40
2	B	606	HEC	C3C-C2C	-3.01	1.35	1.41
2	A	603	HEC	C3B-C2B	-3.01	1.35	1.41
2	B	603	HEC	C1B-C2B	2.97	1.43	1.40
2	B	603	HEC	C3C-C2C	-2.96	1.35	1.41
2	A	605	HEC	C3C-C2C	-2.92	1.35	1.41
2	B	606	HEC	C3B-C2B	-2.91	1.35	1.41
2	A	607	HEC	C3B-C2B	-2.91	1.35	1.41
2	A	601	HEC	FE-NC	2.82	2.04	1.92
2	B	608	HEC	FE-NB	2.79	2.04	1.92
2	B	605	HEC	C1B-C2B	2.77	1.43	1.40
2	A	603	HEC	C4B-NB	2.73	1.40	1.37
2	B	605	HEC	FE-ND	2.72	2.04	1.92
2	B	607[B]	HEC	O1A-CGA	2.71	1.28	1.22
2	B	608	HEC	FE-ND	2.71	2.04	1.92
2	B	601	HEC	CAD-C3D	2.69	1.56	1.52
2	A	608	HEC	C1B-C2B	2.68	1.43	1.40
2	A	608	HEC	FE-ND	2.65	2.03	1.92
2	A	603	HEC	C3C-C2C	-2.57	1.36	1.41
2	B	608	HEC	C3B-C2B	-2.56	1.36	1.41
2	B	601	HEC	C3B-C2B	-2.55	1.36	1.41
2	B	608	HEC	C3C-C2C	-2.52	1.36	1.41
2	A	606	HEC	C3C-C2C	-2.50	1.36	1.41
2	B	603	HEC	FE-NA	2.45	2.02	1.92
4	A	614	PG4	C4-C3	-2.43	1.54	1.55
2	B	605	HEC	CMD-C2D	2.38	1.56	1.51
2	A	601	HEC	C3C-C4C	2.36	1.44	1.41
2	B	601	HEC	FE-NB	2.35	2.02	1.92
2	A	606	HEC	FE-NA	2.34	2.02	1.92
2	A	602	HEC	CAA-C2A	2.29	1.57	1.52
2	A	602	HEC	C1D-C2D	2.23	1.42	1.40
2	B	607[A]	HEC	O1A-CGA	2.20	1.27	1.22
2	B	602	HEC	FE-NB	2.15	2.01	1.92
2	A	607	HEC	FE-NC	2.15	2.01	1.92
2	B	608	HEC	C1D-ND	2.10	1.40	1.36
2	A	605	HEC	CMD-C2D	2.10	1.56	1.51
2	A	603	HEC	CBB-CAB	2.05	1.58	1.49
2	B	602	HEC	C1D-ND	2.03	1.40	1.36

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEC	CBB-CAB-C3B	-8.88	103.44	128.44
2	A	603	HEC	CBB-CAB-C3B	-8.40	104.79	128.44
2	B	602	HEC	CBB-CAB-C3B	-7.94	106.07	128.44
2	A	607	HEC	CBB-CAB-C3B	-7.80	106.49	128.44
2	B	605	HEC	CBB-CAB-C3B	-7.45	107.46	128.44
2	B	606	HEC	CBB-CAB-C3B	-7.30	107.89	128.44
2	B	608	HEC	CBB-CAB-C3B	-7.20	108.18	128.44
2	B	603	HEC	CBB-CAB-C3B	-7.18	108.23	128.44
2	A	602	HEC	CBB-CAB-C3B	-7.05	108.60	128.44
2	A	606	HEC	CBB-CAB-C3B	-6.57	109.95	128.44
2	A	608	HEC	CBB-CAB-C3B	-6.55	110.00	128.44
2	B	601	HEC	CBB-CAB-C3B	-6.47	110.21	128.44
2	A	608	HEC	CMC-C2C-C1C	-6.01	119.38	128.62
2	B	601	HEC	CMC-C2C-C1C	-5.55	120.08	128.62
2	B	608	HEC	CBC-CAC-C3C	-5.41	113.19	128.44
2	B	606	HEC	CMC-C2C-C1C	-5.34	120.40	128.62
2	B	603	HEC	CBC-CAC-C3C	-5.30	113.51	128.44
2	B	602	HEC	CBC-CAC-C3C	-5.28	113.57	128.44
2	A	602	HEC	C1D-C2D-C3D	-5.26	103.34	107.00
2	A	603	HEC	CBC-CAC-C3C	-5.21	113.78	128.44
2	B	608	HEC	CMC-C2C-C1C	-5.08	120.81	128.62
2	A	601	HEC	CBC-CAC-C3C	-5.01	114.34	128.44
2	A	606	HEC	CMC-C2C-C1C	-4.78	121.27	128.62
2	B	605	HEC	CBD-CAD-C3D	-4.72	104.37	112.69
2	A	601	HEC	CBB-CAB-C3B	-4.70	115.21	128.44
2	A	608	HEC	CBC-CAC-C3C	-4.70	115.21	128.44
2	A	603	HEC	CMC-C2C-C1C	-4.67	121.43	128.62
2	A	605	HEC	CMC-C2C-C1C	-4.63	121.50	128.62
2	A	602	HEC	CBC-CAC-C3C	-4.59	115.52	128.44
2	A	601	HEC	CMB-C2B-C1B	-4.57	121.59	128.62
2	B	606	HEC	CBC-CAC-C3C	-4.55	115.64	128.44
2	A	606	HEC	CBC-CAC-C3C	-4.50	115.76	128.44
2	B	605	HEC	CBA-CAA-C2A	-4.48	103.97	112.35
2	A	605	HEC	C2A-C1A-NA	-4.48	106.27	109.64
2	B	603	HEC	CBD-CAD-C3D	-4.48	104.80	112.69
2	B	605	HEC	CBC-CAC-C3C	-4.47	115.85	128.44
2	B	605	HEC	CMB-C2B-C1B	-4.42	121.82	128.62
2	A	603	HEC	CMC-C2C-C3C	4.33	130.50	125.72
2	B	602	HEC	CMB-C2B-C1B	-4.32	121.98	128.62
2	B	605	HEC	CMC-C2C-C1C	-4.29	122.02	128.62
2	B	606	HEC	CAA-CBA-CGA	-4.29	99.69	113.47
2	A	608	HEC	CMB-C2B-C1B	-4.27	122.06	128.62
2	B	608	HEC	CBA-CAA-C2A	-4.24	104.43	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	607	HEC	CBA-CAA-C2A	-4.23	104.45	112.35
2	A	607	HEC	CMB-C2B-C1B	-4.22	122.13	128.62
2	B	601	HEC	CBC-CAC-C3C	-4.13	116.81	128.44
2	B	606	HEC	C3B-C2B-C1B	4.05	109.76	107.07
2	B	606	HEC	CMB-C2B-C1B	-4.05	122.39	128.62
2	A	601	HEC	CMC-C2C-C1C	-4.02	122.44	128.62
2	B	601	HEC	CMB-C2B-C1B	-4.01	122.45	128.62
2	B	605	HEC	C4D-ND-C1D	3.99	112.03	106.76
2	A	608	HEC	CAD-CBD-CGD	-3.93	100.83	113.47
2	A	608	HEC	C4D-ND-C1D	3.93	111.94	106.76
2	A	603	HEC	CBA-CAA-C2A	-3.89	105.08	112.35
2	A	605	HEC	CBC-CAC-C3C	-3.87	117.55	128.44
2	A	603	HEC	CBD-CAD-C3D	-3.85	105.91	112.69
2	B	603	HEC	CMC-C2C-C1C	-3.84	122.72	128.62
2	B	602	HEC	CBD-CAD-C3D	-3.84	105.93	112.69
2	A	605	HEC	C4D-ND-C1D	3.78	111.74	106.76
2	B	608	HEC	CBD-CAD-C3D	-3.78	106.04	112.69
2	A	606	HEC	CMB-C2B-C1B	-3.72	122.90	128.62
2	A	606	HEC	CMC-C2C-C3C	3.71	129.81	125.72
2	A	601	HEC	C1D-C2D-C3D	-3.66	104.45	107.00
2	A	602	HEC	CMB-C2B-C1B	-3.65	123.00	128.62
2	B	603	HEC	CMB-C2B-C1B	-3.62	123.05	128.62
2	A	602	HEC	CBD-CAD-C3D	-3.62	106.32	112.69
2	A	605	HEC	CBA-CAA-C2A	-3.58	105.66	112.35
2	B	606	HEC	CBD-CAD-C3D	-3.57	106.41	112.69
2	A	601	HEC	CBA-CAA-C2A	-3.56	105.70	112.35
2	A	608	HEC	C3B-C2B-C1B	3.53	109.42	107.07
2	B	602	HEC	C1D-C2D-C3D	-3.52	104.55	107.00
2	B	605	HEC	C1D-C2D-C3D	-3.50	104.56	107.00
2	A	605	HEC	CBD-CAD-C3D	-3.45	106.62	112.69
2	A	606	HEC	CBA-CAA-C2A	-3.40	105.99	112.35
2	A	602	HEC	C4C-C3C-C2C	-3.40	104.50	106.68
2	A	601	HEC	CMB-C2B-C3B	3.38	129.46	125.72
2	B	602	HEC	CMC-C2C-C1C	-3.37	123.44	128.62
2	A	606	HEC	C4D-ND-C1D	3.32	111.14	106.76
2	A	605	HEC	C1A-C2A-C3A	3.31	109.29	106.69
2	A	605	HEC	C1D-C2D-C3D	-3.29	104.70	107.00
2	A	602	HEC	CMB-C2B-C3B	3.29	129.35	125.72
2	A	607	HEC	CMC-C2C-C1C	-3.26	123.60	128.62
2	B	606	HEC	C4D-ND-C1D	3.26	111.06	106.76
2	A	607	HEC	CAD-CBD-CGD	-3.23	103.07	113.47
2	A	607	HEC	C4B-CHC-C1C	-3.22	123.24	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	608	HEC	C4D-ND-C1D	3.15	110.92	106.76
2	A	605	HEC	CMB-C2B-C1B	-3.10	123.85	128.62
2	B	601	HEC	C4D-C3D-C2D	-3.10	103.71	106.92
2	B	605	HEC	C3B-C2B-C1B	3.09	109.12	107.07
2	A	607	HEC	CBC-CAC-C3C	-3.08	119.78	128.44
2	A	607	HEC	C1D-C2D-C3D	-3.07	104.86	107.00
2	A	603	HEC	C3B-C2B-C1B	3.06	109.10	107.07
2	B	602	HEC	CMB-C2B-C3B	3.03	129.07	125.72
2	A	602	HEC	C4A-CHB-C1B	-3.03	123.49	127.47
2	A	603	HEC	CMB-C2B-C1B	-3.01	123.99	128.62
2	B	601	HEC	CBA-CAA-C2A	-3.00	106.75	112.35
2	A	606	HEC	C1D-C2D-C3D	-2.96	104.94	107.00
2	A	601	HEC	C4D-ND-C1D	2.95	110.65	106.76
2	B	603	HEC	CBA-CAA-C2A	-2.92	106.89	112.35
2	A	603	HEC	C2A-C1A-NA	-2.91	107.45	109.64
2	B	608	HEC	C3A-C4A-NA	-2.89	107.23	109.41
2	A	602	HEC	C3C-C2C-C1C	2.88	108.98	107.07
2	A	603	HEC	CMA-C3A-C2A	2.81	130.24	124.94
2	A	607	HEC	CMC-C2C-C3C	2.81	128.82	125.72
2	B	603	HEC	C4A-CHB-C1B	-2.80	123.78	127.47
2	B	602	HEC	CMC-C2C-C3C	2.80	128.81	125.72
2	A	607	HEC	CBD-CAD-C3D	-2.79	107.78	112.69
2	B	605	HEC	C2B-C1B-NB	-2.77	107.32	109.41
2	A	603	HEC	C1A-C2A-C3A	2.75	108.86	106.69
2	B	608	HEC	C2A-C1A-NA	-2.74	107.58	109.64
2	B	605	HEC	C1A-C2A-C3A	2.73	108.84	106.69
2	A	605	HEC	CMC-C2C-C3C	2.69	128.69	125.72
2	B	601	HEC	C3B-C2B-C1B	2.67	108.84	107.07
2	B	605	HEC	C2A-C1A-NA	-2.65	107.64	109.64
2	A	607	HEC	CMB-C2B-C3B	2.64	128.64	125.72
2	A	606	HEC	C3B-C2B-C1B	2.63	108.82	107.07
2	A	606	HEC	CAA-CBA-CGA	-2.61	105.08	113.47
2	B	606	HEC	C3A-C4A-NA	-2.60	107.45	109.41
2	B	608	HEC	CMB-C2B-C1B	-2.56	124.69	128.62
2	B	606	HEC	CMC-C2C-C3C	2.55	128.54	125.72
2	B	606	HEC	C2A-C1A-NA	-2.55	107.72	109.64
2	A	608	HEC	CBD-CAD-C3D	-2.55	108.20	112.69
2	A	603	HEC	C4A-CHB-C1B	-2.55	124.12	127.47
2	A	602	HEC	CAD-CBD-CGD	-2.51	105.39	113.47
2	B	602	HEC	CAD-CBD-CGD	-2.51	105.42	113.47
2	A	606	HEC	C1A-C2A-C3A	2.50	108.66	106.69
2	B	603	HEC	CMC-C2C-C3C	2.50	128.48	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	HEC	C1A-CHA-C4D	-2.50	124.18	127.47
2	A	605	HEC	C4A-NA-C1A	2.50	109.33	105.58
2	B	602	HEC	C4D-ND-C1D	2.50	110.05	106.76
2	A	608	HEC	C2B-C1B-NB	-2.49	107.53	109.41
2	A	602	HEC	CMC-C2C-C1C	-2.49	124.79	128.62
2	B	603	HEC	CMB-C2B-C3B	2.47	128.45	125.72
2	B	608	HEC	C3C-C4C-NC	-2.47	107.95	111.52
2	B	608	HEC	C4A-NA-C1A	2.44	109.24	105.58
2	B	606	HEC	C2B-C1B-NB	-2.43	107.57	109.41
2	A	605	HEC	O1A-CGA-CBA	-2.42	114.70	123.03
2	A	608	HEC	C3C-C4C-NC	-2.41	108.04	111.52
2	A	601	HEC	C4A-CHB-C1B	-2.40	124.31	127.47
2	A	601	HEC	C4A-C3A-C2A	2.40	108.42	106.89
2	B	603	HEC	C3C-C2C-C1C	2.38	108.65	107.07
2	B	605	HEC	C4A-CHB-C1B	-2.37	124.35	127.47
2	A	608	HEC	C3A-C4A-NA	-2.34	107.64	109.41
2	A	608	HEC	CBA-CAA-C2A	-2.34	107.97	112.35
2	B	606	HEC	C1A-C2A-C3A	2.31	108.51	106.69
2	A	607	HEC	C1A-C2A-C3A	2.30	108.50	106.69
2	A	607	HEC	C1A-CHA-C4D	-2.30	124.45	127.47
2	A	606	HEC	C2A-C1A-NA	-2.29	107.92	109.64
2	B	606	HEC	C3C-C4C-NC	-2.24	108.28	111.52
2	B	601	HEC	CMB-C2B-C3B	2.23	128.19	125.72
2	A	608	HEC	C4B-CHC-C1C	-2.23	124.54	127.47
2	B	602	HEC	C4A-CHB-C1B	-2.21	124.56	127.47
2	A	603	HEC	C4D-C3D-C2D	-2.21	104.63	106.92
2	B	608	HEC	CMC-C2C-C3C	2.21	128.16	125.72
2	B	601	HEC	C4C-CHD-C1D	-2.19	124.58	127.47
2	A	603	HEC	C4B-CHC-C1C	-2.18	124.60	127.47
2	A	608	HEC	C3B-C4B-NB	-2.18	108.38	111.52
2	A	603	HEC	C1D-C2D-C3D	-2.18	105.48	107.00
2	B	603	HEC	C4D-C3D-C2D	-2.17	104.67	106.92
2	B	601	HEC	C4D-ND-C1D	2.17	109.61	106.76
2	B	603	HEC	C1A-CHA-C4D	-2.15	124.64	127.47
2	B	606	HEC	C4A-NA-C1A	2.15	108.81	105.58
2	B	608	HEC	O1D-CGD-CBD	-2.15	115.64	123.03
2	B	605	HEC	CHB-C1B-NB	2.11	128.09	124.58
2	B	603	HEC	C3C-C4C-NC	-2.10	108.49	111.52
2	B	605	HEC	C3C-C4C-NC	-2.08	108.51	111.52
2	A	602	HEC	CMD-C2D-C3D	2.08	128.87	124.94
2	B	606	HEC	CHB-C1B-NB	2.08	128.05	124.58
2	A	608	HEC	C1D-C2D-C3D	-2.08	105.55	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	606	HEC	CBD-CAD-C3D	-2.07	109.05	112.69
2	A	607	HEC	CHB-C1B-NB	2.07	128.03	124.58
2	B	603	HEC	C2D-C1D-CHD	-2.06	122.09	126.00
2	B	601	HEC	C4C-C3C-C2C	-2.06	105.36	106.68
2	A	606	HEC	CMB-C2B-C3B	2.05	127.98	125.72
2	B	608	HEC	C3B-C4B-NB	-2.02	108.60	111.52
2	B	603	HEC	CMA-C3A-C2A	2.02	128.74	124.94
2	B	608	HEC	C4D-C3D-C2D	-2.01	104.84	106.92
2	A	602	HEC	C4C-CHD-C1D	-2.01	124.83	127.47
2	A	608	HEC	C4A-NA-C1A	2.00	108.58	105.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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	519/520 (99%)	-0.85	1 (0%) 93 94	28, 34, 47, 63	0
1	B	520/520 (100%)	-0.88	0 100 100	27, 32, 46, 63	1 (0%)
All	All	1039/1040 (99%)	-0.86	1 (0%) 93 95	27, 33, 46, 63	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	522	VAL	2.6

### 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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PG4	B	615	10/13	1.06	34.92	39,42,44,46	10
4	PG4	B	620	7/13	0.28	18.98	54,55,55,55	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PG4	B	617	8/13	0.39	10.24	44,49,52,52	8
4	PG4	B	619	7/13	0.22	9.19	55,56,61,61	0
4	PG4	A	613	8/13	0.18	6.72	48,61,72,74	0
4	PG4	B	613	5/13	0.13	5.07	42,47,50,53	0
4	PG4	A	611	7/13	0.21	4.79	54,56,57,57	7
4	PG4	B	616	9/13	0.22	4.09	42,44,48,48	9
4	PG4	B	618	5/13	0.13	3.61	42,42,43,45	5
2	HEC	A	605	43/43	0.13	3.57	32,36,52,61	0
4	PG4	B	611	6/13	0.17	3.11	33,35,37,38	6
3	CA	A	610	1/1	0.18	3.06	47,47,47,47	1
4	PG4	A	612	5/13	0.17	2.21	39,40,41,42	5
2	HEC	B	607[B]	4/43	0.08	1.72	26,30,30,30	4
4	PG4	B	614	5/13	0.12	1.07	65,65,68,69	0
4	PG4	A	614	6/13	0.11	0.94	69,70,73,74	0
2	HEC	B	605	43/43	0.10	0.78	29,34,49,57	0
2	HEC	A	607	43/43	0.08	0.61	24,28,43,54	0
4	PG4	B	612	6/13	0.11	0.61	37,42,43,44	6
2	HEC	A	604[A]	3/43	0.08	0.56	26,26,27,28	3
2	HEC	A	604[B]	3/43	0.08	0.56	31,31,31,32	3
2	HEC	B	607[A]	4/43	0.08	0.54	34,36,36,38	4
2	HEC	B	601	43/43	0.11	0.47	24,28,31,31	0
2	HEC	A	601	43/43	0.11	0.38	26,30,32,35	0
2	HEC	A	603	43/43	0.09	0.36	25,28,31,31	0
2	HEC	B	604[A]	3/43	0.08	0.32	30,30,31,32	3
2	HEC	B	604[B]	3/43	0.08	0.32	27,27,28,29	3
2	HEC	B	602	43/43	0.08	0.27	24,28,39,45	0
2	HEC	B	603	43/43	0.09	0.13	23,27,29,30	0
2	HEC	A	602	43/43	0.07	-0.00	24,27,36,46	0
2	HEC	A	608	43/43	0.07	-0.07	27,34,40,47	0
2	HEC	B	608	43/43	0.08	-0.29	29,38,41,41	0
2	HEC	A	606	43/43	0.06	-0.46	27,31,33,34	0
2	HEC	B	606	43/43	0.06	-0.64	27,32,35,36	0
3	CA	B	610	1/1	0.09	-0.74	42,42,42,42	1
3	CA	A	609	1/1	0.04	-1.36	36,36,36,36	0
3	CA	B	609	1/1	0.05	-1.49	34,34,34,34	0
5	NA	B	621	1/1	0.04	-1.98	36,36,36,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.