Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:44 PM GMT

PDB ID	:	3UU9
Title	:	Structure of the free TvNiRb form of Thioalkalivibrio nitratireducens 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)

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

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	Percentile Ranks	Value
Rfree		0.187
Clashscore		7
Ramachandran outliers		0.1%
Sidechain outliers		0.9%
RSRZ outliers		0.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
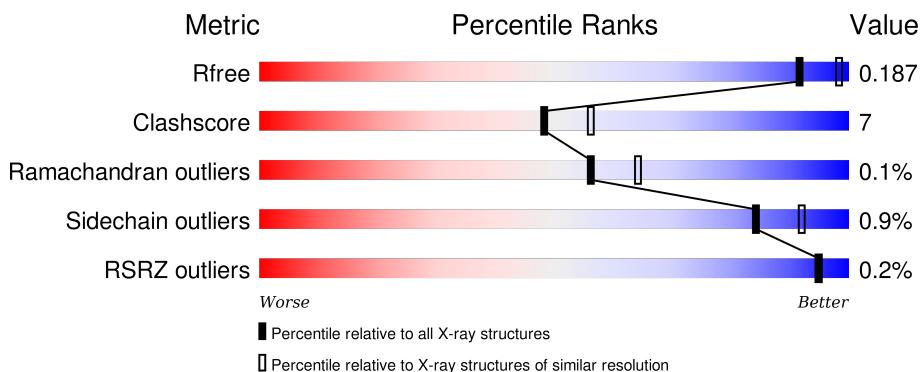
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	520	90% 10%
1	B	520	91% 9%
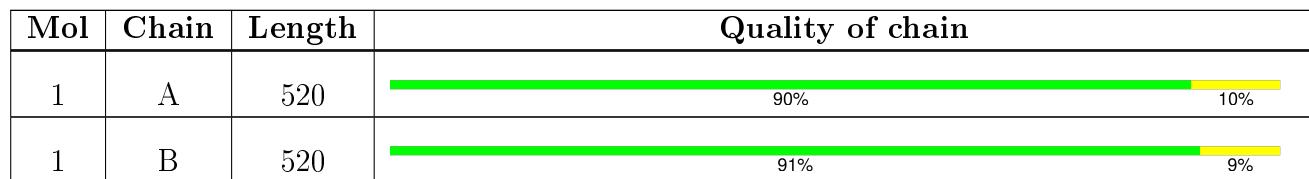
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	605	-	-	-	X
4	PG4	A	611	-	-	-	X
4	PG4	A	612	-	-	X	X
4	PG4	A	613	-	-	-	X
4	PG4	B	611	-	-	-	X
4	PG4	B	613	-	-	-	X
4	PG4	B	615	-	-	-	X
4	PG4	B	616	-	-	-	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 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	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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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	0
			43	34	1	4	4			
2	B	1	Total	C	Fe	N	O		0	0
			43	34	1	4	4			
2	B	1	Total	C	Fe	N	O		0	0
			43	34	1	4	4			
2	B	1	Total	C	Fe	N	O		0	0
			43	34	1	4	4			
2	B	1	Total	C	Fe	N	O		0	1
			46	35	1	4	6			
2	B	1	Total	C	Fe	N	O		0	0
			43	34	1	4	4			
2	B	1	Total	C	Fe	N	O		0	0
			43	34	1	4	4			
2	B	1	Total	C	Fe	N	O		0	1
			47	36	1	4	6			
2	B	1	Total	C	Fe	N	O		0	0
			43	34	1	4	4			

- 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: $C_8H_{18}O_5$).

PG4
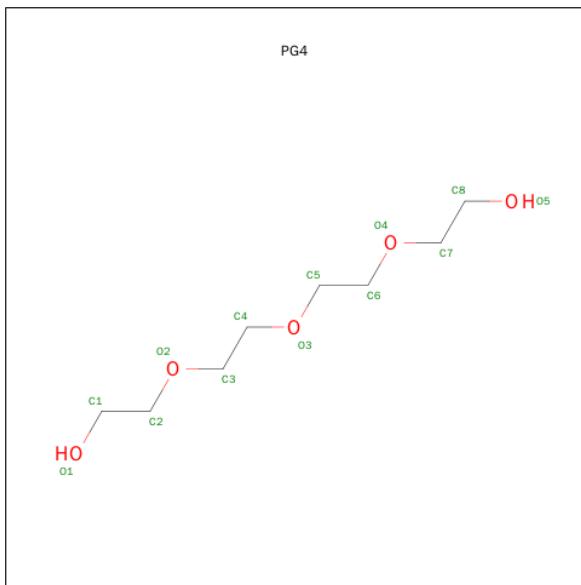
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	C 4	O 3	0	0
4	A	1	Total 5	C 3	O 2	0	0
4	A	1	Total 8	C 5	O 3	0	0
4	A	1	Total 6	C 4	O 2	0	0
4	B	1	Total 6	C 4	O 2	0	0
4	B	1	Total 6	C 4	O 2	0	0
4	B	1	Total 5	C 3	O 2	0	0
4	B	1	Total 5	C 3	O 2	0	0
4	B	1	Total 10	C 6	O 4	0	0
4	B	1	Total 9	C 6	O 3	0	0
4	B	1	Total 8	C 5	O 3	0	0
4	B	1	Total 5	C 3	O 2	0	0
4	B	1	Total 7	C 4	O 3	0	0
4	B	1	Total 7	C 4	O 3	0	0

- 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
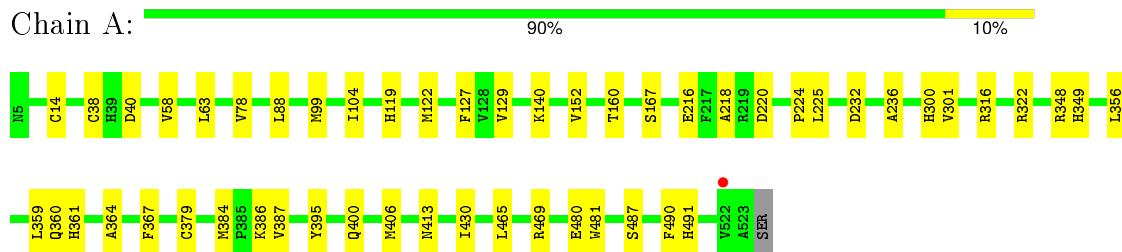
• Molecule 1: Eight-heme nitrite reductase
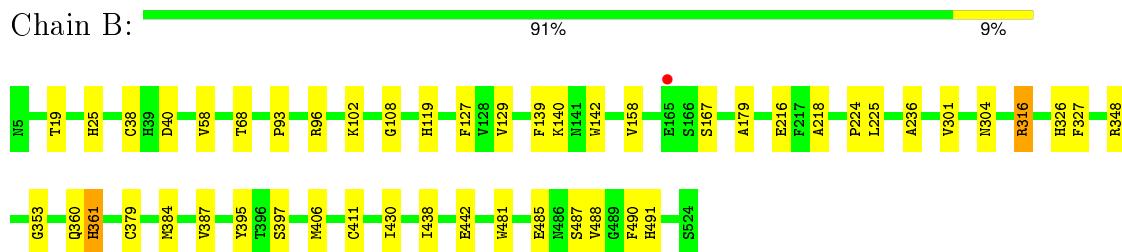
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.22 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.157　,　0.184 0.159　,　0.187	Depositor DCC
R_{free} test set	5897 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.6	EDS
Estimated twinning fraction	0.064 for l,-k,h	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	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^2)	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.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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 Too-close contacts (i)

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	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
4	A	26	0	29	18	0
4	B	68	0	77	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 7.

All (122) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348[B]:ARG:NH2	4:A:612:PG4:C1	2.63	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	529/520 (102%)	504 (95%)	25 (5%)	0	100	100
1	B	530/520 (102%)	509 (96%)	20 (4%)	1 (0%)	52	59
All	All	1059/1040 (102%)	1013 (96%)	45 (4%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	361	HIS

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/439 (101%)	440 (99%)	5 (1%)	80	89
1	B	447/439 (102%)	440 (98%)	7 (2%)	70	82
All	All	892/878 (102%)	880 (99%)	12 (1%)	84	87

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 (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 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	24,50,50	2.29	5 (20%)	19,82,82	2.56	5 (26%)
2	HEC	A	602	1	24,50,50	2.37	4 (16%)	19,82,82	2.89	6 (31%)
2	HEC	A	603	1,3	24,50,50	2.12	6 (25%)	19,82,82	3.51	9 (47%)
2	HEC	A	604[A]	-	24,50,50	2.37	4 (16%)	19,82,82	3.27	7 (36%)
2	HEC	A	604[B]	3	24,50,50	2.37	4 (16%)	19,82,82	3.26	7 (36%)
2	HEC	A	605	1	24,50,50	2.35	5 (20%)	19,82,82	3.26	7 (36%)
2	HEC	A	606	1	24,50,50	2.19	4 (16%)	19,82,82	3.04	7 (36%)
2	HEC	A	607	1	24,50,50	2.27	6 (25%)	19,82,82	3.16	8 (42%)
2	HEC	A	608	1	24,50,50	2.17	3 (12%)	19,82,82	3.34	8 (42%)
4	PG4	A	611	-	6,6,12	0.54	0	5,5,11	0.06	0
4	PG4	A	612	-	4,4,12	0.53	0	3,3,11	0.26	0
4	PG4	A	613	-	7,7,12	0.88	0	6,6,11	0.48	0
4	PG4	A	614	-	5,5,12	0.64	0	4,4,11	0.48	0
2	HEC	B	601	1,6	24,50,50	2.34	4 (16%)	19,82,82	2.80	6 (31%)
2	HEC	B	602	1	24,50,50	2.45	7 (29%)	19,82,82	3.18	6 (31%)
2	HEC	B	603	1,3,5	24,50,50	2.26	4 (16%)	19,82,82	3.15	8 (42%)
2	HEC	B	604[A]	3,5	24,50,50	2.27	4 (16%)	19,82,82	3.42	7 (36%)
2	HEC	B	604[B]	5	24,50,50	2.27	4 (16%)	19,82,82	3.40	7 (36%)
2	HEC	B	605	1	24,50,50	2.55	5 (20%)	19,82,82	3.25	7 (36%)
2	HEC	B	606	1	24,50,50	2.14	3 (12%)	19,82,82	3.42	7 (36%)
2	HEC	B	607[A]	-	24,50,50	2.55	3 (12%)	19,82,82	3.47	8 (42%)
2	HEC	B	607[B]	-	24,50,50	2.55	3 (12%)	19,82,82	3.55	8 (42%)
2	HEC	B	608	1	24,50,50	1.91	3 (12%)	19,82,82	3.25	8 (42%)
4	PG4	B	611	-	5,5,12	0.53	0	4,4,11	0.31	0
4	PG4	B	612	-	5,5,12	0.53	0	4,4,11	0.44	0
4	PG4	B	613	-	4,4,12	0.71	0	3,3,11	0.50	0
4	PG4	B	614	-	4,4,12	0.47	0	3,3,11	0.15	0
4	PG4	B	615	-	9,9,12	0.45	0	8,8,11	0.28	0
4	PG4	B	616	-	8,8,12	0.49	0	7,7,11	0.31	0
4	PG4	B	617	-	7,7,12	0.55	0	6,6,11	0.08	0
4	PG4	B	618	-	4,4,12	0.48	0	3,3,11	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	PG4	B	619	-	6,6,12	0.68	0	5,5,11	0.71	0
4	PG4	B	620	-	6,6,12	0.47	0	5,5,11	0.41	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	-	0/6/54/54	0/0/8/8
2	HEC	A	602	1	-	0/6/54/54	0/0/8/8
2	HEC	A	603	1,3	-	0/6/54/54	0/0/8/8
2	HEC	A	604[A]	-	-	0/6/54/54	0/0/8/8
2	HEC	A	604[B]	3	-	0/6/54/54	0/0/8/8
2	HEC	A	605	1	-	0/6/54/54	0/0/8/8
2	HEC	A	606	1	-	0/6/54/54	0/0/8/8
2	HEC	A	607	1	-	0/6/54/54	0/0/8/8
2	HEC	A	608	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
2	HEC	B	602	1	-	0/6/54/54	0/0/8/8
2	HEC	B	603	1,3,5	-	0/6/54/54	0/0/8/8
2	HEC	B	604[A]	3,5	-	0/6/54/54	0/0/8/8
2	HEC	B	604[B]	5	-	0/6/54/54	0/0/8/8
2	HEC	B	605	1	-	0/6/54/54	0/0/8/8
2	HEC	B	606	1	-	0/6/54/54	0/0/8/8
2	HEC	B	607[A]	-	-	0/6/54/54	0/0/8/8
2	HEC	B	607[B]	-	-	0/6/54/54	0/0/8/8
2	HEC	B	608	1	-	0/6/54/54	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 (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	607[B]	HEC	C3C-C2C	-7.91	1.32	1.40
2	B	607[A]	HEC	C3C-C2C	-7.91	1.32	1.40
2	B	605	HEC	C3B-C2B	-7.81	1.32	1.40
2	A	605	HEC	C3B-C2B	-7.36	1.33	1.40
2	A	604[A]	HEC	C3B-C2B	-6.91	1.33	1.40
2	A	604[B]	HEC	C3B-C2B	-6.91	1.33	1.40
2	B	607[B]	HEC	C3B-C2B	-6.75	1.33	1.40
2	B	607[A]	HEC	C3B-C2B	-6.75	1.33	1.40
2	B	601	HEC	C3C-C2C	-6.73	1.33	1.40
2	B	602	HEC	C3B-C2B	-6.70	1.33	1.40
2	A	606	HEC	C3B-C2B	-6.61	1.33	1.40
2	A	602	HEC	C3B-C2B	-6.50	1.34	1.40
2	A	601	HEC	C3B-C2B	-6.49	1.34	1.40
2	B	605	HEC	C3C-C2C	-6.42	1.34	1.40
2	A	604[A]	HEC	C3C-C2C	-6.33	1.34	1.40
2	A	604[B]	HEC	C3C-C2C	-6.33	1.34	1.40
2	B	604[A]	HEC	C3B-C2B	-6.30	1.34	1.40
2	B	604[B]	HEC	C3B-C2B	-6.30	1.34	1.40
2	A	602	HEC	C3C-C2C	-6.29	1.34	1.40
2	A	607	HEC	C3C-C2C	-6.24	1.34	1.40
2	B	603	HEC	C3B-C2B	-6.14	1.34	1.40
2	A	608	HEC	C3B-C2B	-6.13	1.34	1.40
2	B	602	HEC	C3C-C2C	-5.77	1.34	1.40
2	B	604[A]	HEC	C3C-C2C	-5.77	1.34	1.40
2	B	604[B]	HEC	C3C-C2C	-5.77	1.34	1.40
2	A	608	HEC	C3C-C2C	-5.75	1.34	1.40
2	A	601	HEC	C3C-C2C	-5.53	1.35	1.40
2	B	606	HEC	C3C-C2C	-5.35	1.35	1.40
2	A	603	HEC	C3B-C2B	-5.34	1.35	1.40
2	B	603	HEC	C3C-C2C	-5.24	1.35	1.40
2	A	605	HEC	C3C-C2C	-5.16	1.35	1.40
2	B	606	HEC	C3B-C2B	-5.14	1.35	1.40
2	A	607	HEC	C3B-C2B	-5.13	1.35	1.40
2	A	603	HEC	C3C-C2C	-4.42	1.36	1.40
2	B	608	HEC	C3B-C2B	-4.39	1.36	1.40
2	B	601	HEC	C3B-C2B	-4.38	1.36	1.40
2	B	608	HEC	C3C-C2C	-4.31	1.36	1.40
2	A	606	HEC	C3C-C2C	-4.27	1.36	1.40
2	A	607	HEC	CMB-C2B	2.02	1.56	1.51
2	A	606	HEC	CMA-C3A	2.02	1.56	1.51
2	A	604[A]	HEC	C4C-NC	2.03	1.39	1.36
2	A	604[B]	HEC	C4C-NC	2.03	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	HEC	C3C-C4C	2.03	1.47	1.42
2	A	603	HEC	CAD-C3D	2.05	1.55	1.52
2	B	604[A]	HEC	CMB-C2B	2.07	1.56	1.51
2	B	604[B]	HEC	CMB-C2B	2.07	1.56	1.51
2	A	601	HEC	C1A-NA	2.08	1.39	1.36
2	B	602	HEC	C1A-NA	2.12	1.39	1.36
2	A	605	HEC	CMA-C3A	2.13	1.56	1.51
2	A	605	HEC	CMD-C2D	2.13	1.56	1.51
2	A	607	HEC	C1A-NA	2.14	1.39	1.36
2	A	603	HEC	CBB-CAB	2.17	1.58	1.49
2	B	603	HEC	CMB-C2B	2.17	1.56	1.51
2	B	602	HEC	CMB-C2B	2.17	1.56	1.51
2	A	607	HEC	CMC-C2C	2.23	1.56	1.51
2	A	601	HEC	CMC-C2C	2.26	1.56	1.51
2	B	605	HEC	C3C-C4C	2.34	1.48	1.42
2	B	605	HEC	CMD-C2D	2.43	1.56	1.51
2	B	602	HEC	CMA-C3A	2.50	1.57	1.51
2	A	602	HEC	CAA-C2A	2.50	1.57	1.52
2	B	601	HEC	CAD-C3D	2.77	1.56	1.52
2	A	603	HEC	C4B-NB	3.16	1.40	1.36
2	B	607[B]	HEC	C3D-C2D	3.94	1.49	1.37
2	B	607[A]	HEC	C3D-C2D	3.94	1.49	1.37
2	A	604[A]	HEC	C3D-C2D	4.19	1.50	1.37
2	A	604[B]	HEC	C3D-C2D	4.19	1.50	1.37
2	B	602	HEC	C3D-C2D	4.19	1.50	1.37
2	A	602	HEC	C3D-C2D	4.29	1.50	1.37
2	A	607	HEC	C3D-C2D	4.38	1.50	1.37
2	B	604[A]	HEC	C3D-C2D	4.49	1.51	1.37
2	B	604[B]	HEC	C3D-C2D	4.49	1.51	1.37
2	A	601	HEC	C3D-C2D	4.52	1.51	1.37
2	A	608	HEC	C3D-C2D	4.53	1.51	1.37
2	A	603	HEC	C3D-C2D	4.67	1.51	1.37
2	B	603	HEC	C3D-C2D	4.71	1.51	1.37
2	B	605	HEC	C3D-C2D	4.85	1.52	1.37
2	B	608	HEC	C3D-C2D	4.93	1.52	1.37
2	B	601	HEC	C3D-C2D	5.03	1.52	1.37
2	A	605	HEC	C3D-C2D	5.04	1.52	1.37
2	A	606	HEC	C3D-C2D	5.08	1.52	1.37
2	B	606	HEC	C3D-C2D	5.21	1.53	1.37

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	605	HEC	CBB-CAB-C3B	-10.76	103.44	127.35
2	B	604[A]	HEC	CBB-CAB-C3B	-10.36	104.34	127.35
2	B	604[B]	HEC	CBB-CAB-C3B	-10.36	104.34	127.35
2	A	603	HEC	CBB-CAB-C3B	-10.15	104.79	127.35
2	B	602	HEC	CBB-CAB-C3B	-9.57	106.07	127.35
2	A	607	HEC	CBB-CAB-C3B	-9.39	106.49	127.35
2	B	607[B]	HEC	CBB-CAB-C3B	-9.35	106.58	127.35
2	B	607[A]	HEC	CBB-CAB-C3B	-9.35	106.58	127.35
2	B	605	HEC	CBB-CAB-C3B	-8.95	107.46	127.35
2	B	606	HEC	CBB-CAB-C3B	-8.76	107.89	127.35
2	B	608	HEC	CBB-CAB-C3B	-8.63	108.18	127.35
2	B	603	HEC	CBB-CAB-C3B	-8.60	108.23	127.35
2	A	604[A]	HEC	CBB-CAB-C3B	-8.50	108.46	127.35
2	A	604[B]	HEC	CBB-CAB-C3B	-8.50	108.46	127.35
2	A	602	HEC	CBB-CAB-C3B	-8.44	108.60	127.35
2	A	606	HEC	CBB-CAB-C3B	-7.83	109.95	127.35
2	A	608	HEC	CBB-CAB-C3B	-7.81	110.00	127.35
2	B	601	HEC	CBB-CAB-C3B	-7.71	110.21	127.35
2	B	606	HEC	CAA-CBA-CGA	-7.13	99.69	112.75
2	A	604[A]	HEC	CBD-CAD-C3D	-6.77	100.40	112.53
2	A	604[B]	HEC	CBD-CAD-C3D	-6.77	100.40	112.53
2	A	608	HEC	CAD-CBD-CGD	-6.50	100.83	112.75
2	B	607[B]	HEC	CAA-C2A-C1A	-6.39	120.07	127.01
2	B	607[A]	HEC	CAA-C2A-C1A	-6.39	120.07	127.01
2	B	608	HEC	CBC-CAC-C3C	-6.37	113.19	127.35
2	B	603	HEC	CBC-CAC-C3C	-6.23	113.51	127.35
2	B	602	HEC	CBC-CAC-C3C	-6.20	113.57	127.35
2	A	603	HEC	CBC-CAC-C3C	-6.11	113.78	127.35
2	B	604[A]	HEC	CBD-CAD-C3D	-5.94	101.89	112.53
2	B	604[B]	HEC	CBD-CAD-C3D	-5.94	101.89	112.53
2	A	601	HEC	CBC-CAC-C3C	-5.86	114.34	127.35
2	A	601	HEC	CBB-CAB-C3B	-5.47	115.21	127.35
2	A	608	HEC	CBC-CAC-C3C	-5.46	115.21	127.35
2	A	604[A]	HEC	CMB-C2B-C1B	-5.46	119.34	128.36
2	A	604[B]	HEC	CMB-C2B-C1B	-5.46	119.34	128.36
2	A	608	HEC	CMC-C2C-C1C	-5.43	119.38	128.36
2	A	602	HEC	CBC-CAC-C3C	-5.33	115.52	127.35
2	A	607	HEC	CAD-CBD-CGD	-5.28	103.07	112.75
2	B	606	HEC	CBC-CAC-C3C	-5.27	115.64	127.35
2	A	606	HEC	CBC-CAC-C3C	-5.22	115.76	127.35
2	B	605	HEC	CBC-CAC-C3C	-5.18	115.85	127.35
2	B	601	HEC	CMC-C2C-C1C	-5.00	120.08	128.36
2	B	607[B]	HEC	CMC-C2C-C1C	-4.91	120.23	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	607[A]	HEC	CMC-C2C-C1C	-4.91	120.23	128.36
2	B	606	HEC	CMC-C2C-C1C	-4.81	120.40	128.36
2	B	605	HEC	CBA-CAA-C2A	-4.77	103.97	112.53
2	B	601	HEC	CBC-CAC-C3C	-4.74	116.81	127.35
2	B	604[A]	HEC	CBC-CAC-C3C	-4.74	116.82	127.35
2	B	604[B]	HEC	CBC-CAC-C3C	-4.74	116.82	127.35
2	A	603	HEC	CAA-C2A-C1A	-4.62	122.00	127.01
2	B	607[B]	HEC	CBA-CAA-C2A	-4.60	104.28	112.53
2	B	608	HEC	CMC-C2C-C1C	-4.57	120.81	128.36
2	B	605	HEC	CBD-CAD-C3D	-4.55	104.37	112.53
2	B	608	HEC	CBA-CAA-C2A	-4.52	104.43	112.53
2	A	607	HEC	CBA-CAA-C2A	-4.51	104.45	112.53
2	A	605	HEC	CBC-CAC-C3C	-4.41	117.55	127.35
2	B	607[B]	HEC	CBC-CAC-C3C	-4.35	117.69	127.35
2	B	607[A]	HEC	CBC-CAC-C3C	-4.35	117.69	127.35
2	B	603	HEC	CBD-CAD-C3D	-4.31	104.80	112.53
2	A	606	HEC	CMC-C2C-C1C	-4.29	121.27	128.36
2	B	604[A]	HEC	CMB-C2B-C1B	-4.25	121.34	128.36
2	B	604[B]	HEC	CMB-C2B-C1B	-4.25	121.34	128.36
2	B	607[B]	HEC	CAD-CBD-CGD	-4.21	105.03	112.75
2	B	607[A]	HEC	CAD-CBD-CGD	-4.21	105.03	112.75
2	B	607[B]	HEC	CMB-C2B-C1B	-4.20	121.41	128.36
2	B	607[A]	HEC	CMB-C2B-C1B	-4.20	121.41	128.36
2	A	603	HEC	CMC-C2C-C1C	-4.19	121.43	128.36
2	A	606	HEC	CAA-CBA-CGA	-4.19	105.08	112.75
2	A	603	HEC	CBA-CAA-C2A	-4.16	105.08	112.53
2	A	605	HEC	CMC-C2C-C1C	-4.15	121.50	128.36
2	A	601	HEC	CMB-C2B-C1B	-4.09	121.59	128.36
2	A	604[A]	HEC	CMC-C2C-C1C	-4.04	121.68	128.36
2	A	604[B]	HEC	CMC-C2C-C1C	-4.04	121.68	128.36
2	A	602	HEC	CAD-CBD-CGD	-4.01	105.39	112.75
2	B	602	HEC	CAD-CBD-CGD	-4.00	105.42	112.75
2	B	605	HEC	CMB-C2B-C1B	-3.96	121.82	128.36
2	B	602	HEC	CMB-C2B-C1B	-3.86	121.98	128.36
2	B	605	HEC	CMC-C2C-C1C	-3.84	122.02	128.36
2	A	605	HEC	CBA-CAA-C2A	-3.83	105.66	112.53
2	A	608	HEC	CMB-C2B-C1B	-3.81	122.06	128.36
2	A	601	HEC	CBA-CAA-C2A	-3.81	105.70	112.53
2	B	604[A]	HEC	CBA-CAA-C2A	-3.78	105.75	112.53
2	B	604[B]	HEC	CBA-CAA-C2A	-3.78	105.75	112.53
2	A	607	HEC	CMB-C2B-C1B	-3.77	122.13	128.36
2	A	603	HEC	CBD-CAD-C3D	-3.69	105.91	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602	HEC	CBD-CAD-C3D	-3.68	105.93	112.53
2	A	604[A]	HEC	CBC-CAC-C3C	-3.65	119.23	127.35
2	A	604[B]	HEC	CBC-CAC-C3C	-3.65	119.23	127.35
2	A	606	HEC	CBA-CAA-C2A	-3.65	105.99	112.53
2	A	606	HEC	CAA-C2A-C1A	-3.64	123.05	127.01
2	B	608	HEC	CBD-CAD-C3D	-3.62	106.04	112.53
2	B	606	HEC	CMB-C2B-C1B	-3.61	122.39	128.36
2	B	608	HEC	CAA-C2A-C1A	-3.60	123.10	127.01
2	A	601	HEC	CMC-C2C-C1C	-3.58	122.44	128.36
2	B	601	HEC	CMB-C2B-C1B	-3.57	122.45	128.36
2	A	602	HEC	CBD-CAD-C3D	-3.46	106.32	112.53
2	B	606	HEC	CBD-CAD-C3D	-3.42	106.41	112.53
2	B	603	HEC	CMC-C2C-C1C	-3.41	122.72	128.36
2	A	607	HEC	CBC-CAC-C3C	-3.41	119.78	127.35
2	A	604[A]	HEC	CBA-CAA-C2A	-3.34	106.55	112.53
2	A	604[B]	HEC	CBA-CAA-C2A	-3.34	106.55	112.53
2	A	606	HEC	CMB-C2B-C1B	-3.30	122.90	128.36
2	A	605	HEC	CBD-CAD-C3D	-3.30	106.62	112.53
2	A	602	HEC	CMB-C2B-C1B	-3.24	123.00	128.36
2	B	601	HEC	CBA-CAA-C2A	-3.22	106.75	112.53
2	B	603	HEC	CMB-C2B-C1B	-3.21	123.05	128.36
2	B	603	HEC	CBA-CAA-C2A	-3.15	106.89	112.53
2	B	604[A]	HEC	CMC-C2C-C1C	-3.11	123.22	128.36
2	B	604[B]	HEC	CMC-C2C-C1C	-3.11	123.22	128.36
2	A	608	HEC	CAA-C2A-C1A	-3.02	123.73	127.01
2	B	602	HEC	CMC-C2C-C1C	-2.97	123.44	128.36
2	B	607[A]	HEC	CAA-CBA-CGA	-2.93	107.37	112.75
2	A	607	HEC	CMC-C2C-C1C	-2.88	123.60	128.36
2	A	604[A]	HEC	CAA-C2A-C1A	-2.74	124.04	127.01
2	A	604[B]	HEC	CAA-C2A-C1A	-2.74	124.04	127.01
2	A	605	HEC	CMB-C2B-C1B	-2.73	123.85	128.36
2	A	607	HEC	CBD-CAD-C3D	-2.65	107.78	112.53
2	A	603	HEC	CMB-C2B-C1B	-2.65	123.99	128.36
2	B	601	HEC	CAA-C2A-C1A	-2.59	124.20	127.01
2	B	606	HEC	CAA-C2A-C1A	-2.58	124.21	127.01
2	A	608	HEC	CBA-CAA-C2A	-2.54	107.97	112.53
2	B	603	HEC	CAA-CBA-CGA	-2.44	108.28	112.75
2	A	608	HEC	CBD-CAD-C3D	-2.41	108.20	112.53
2	B	603	HEC	CAA-C2A-C1A	-2.41	124.39	127.01
2	A	607	HEC	CAA-C2A-C1A	-2.40	124.41	127.01
2	B	604[A]	HEC	CAA-C2A-C1A	-2.31	124.50	127.01
2	B	604[B]	HEC	CAA-C2A-C1A	-2.31	124.50	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	608	HEC	CMB-C2B-C1B	-2.22	124.69	128.36
2	A	603	HEC	CAA-CBA-CGA	-2.19	108.74	112.75
2	A	602	HEC	CMC-C2C-C1C	-2.16	124.79	128.36
2	B	605	HEC	CAD-CBD-CGD	-2.10	108.90	112.75
2	A	605	HEC	CAA-CBA-CGA	-2.07	108.96	112.75
2	B	608	HEC	CAD-CBD-CGD	-2.01	109.06	112.75
2	B	607[B]	HEC	CAA-CBA-CGA	2.01	116.44	112.75
2	A	603	HEC	CMA-C3A-C2A	2.39	130.24	125.24
2	B	607[A]	HEC	CBA-CAA-C2A	2.56	117.12	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEC	2	0
2	A	602	HEC	1	0
2	A	603	HEC	3	0
2	A	604[B]	HEC	1	0
2	A	605	HEC	2	0
2	A	606	HEC	2	0
2	A	607	HEC	2	0
2	A	608	HEC	3	0
4	A	611	PG4	6	0
4	A	612	PG4	13	0
2	B	601	HEC	1	0
2	B	602	HEC	1	0
2	B	603	HEC	2	0
2	B	605	HEC	7	0
2	B	606	HEC	4	0
2	B	607[A]	HEC	1	0
2	B	607[B]	HEC	2	0
2	B	608	HEC	1	0
4	B	611	PG4	6	0
4	B	612	PG4	5	0
4	B	613	PG4	3	0
4	B	616	PG4	4	0
4	B	619	PG4	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	519/520 (99%)	-0.71	1 (0%)	95	95	28, 34, 47, 63	0
1	B	520/520 (100%)	-0.72	1 (0%)	95	95	27, 32, 46, 63	1 (0%)
All	All	1039/1040 (99%)	-0.72	2 (0%)	95	95	27, 33, 46, 63	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	522	VAL	3.4
1	B	165	GLU	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, 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(Å²)	Q<0.9
4	PG4	B	615	10/13	0.80	1.20	41.13	39,42,44,46	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
4	PG4	B	620	7/13	0.72	0.31	22.72	54,55,55,55	7
4	PG4	A	613	8/13	0.70	0.20	5.67	48,61,72,74	0
4	PG4	B	619	7/13	0.80	0.20	4.70	55,56,61,61	0
4	PG4	B	616	9/13	0.69	0.24	4.29	42,44,48,48	9
4	PG4	B	613	5/13	0.85	0.14	3.74	42,47,50,53	0
4	PG4	A	611	7/13	0.81	0.24	3.57	54,56,57,57	7
2	HEC	A	605	43/43	0.96	0.15	3.24	32,36,52,61	0
4	PG4	A	612	5/13	0.86	0.23	2.54	39,40,41,42	5
4	PG4	B	611	6/13	0.89	0.17	2.33	33,35,37,38	6
4	PG4	B	612	6/13	0.86	0.15	1.45	37,42,43,44	6
2	HEC	B	605	43/43	0.97	0.12	0.86	29,34,49,57	0
2	HEC	B	607[B]	43/43	0.97	0.09	0.81	22,27,39,50	4
2	HEC	B	607[A]	43/43	0.97	0.09	0.81	22,27,39,50	4
2	HEC	A	604[A]	43/43	0.97	0.09	0.67	22,28,33,34	3
2	HEC	A	604[B]	43/43	0.97	0.09	0.67	22,29,33,34	3
2	HEC	A	603	43/43	0.98	0.10	0.36	25,28,31,31	0
2	HEC	B	604[B]	43/43	0.98	0.09	0.35	23,27,29,30	3
2	HEC	B	604[A]	43/43	0.98	0.09	0.35	23,27,30,32	3
2	HEC	B	608	43/43	0.96	0.11	0.23	29,38,41,41	0
2	HEC	A	601	43/43	0.98	0.11	0.15	26,30,32,35	0
2	HEC	B	601	43/43	0.98	0.12	0.11	24,28,31,31	0
2	HEC	A	608	43/43	0.98	0.08	0.05	27,34,40,47	0
2	HEC	B	603	43/43	0.98	0.10	0.01	23,27,29,30	0
2	HEC	B	602	43/43	0.98	0.08	-0.09	24,28,39,45	0
2	HEC	A	607	43/43	0.98	0.08	-0.15	24,28,43,54	0
2	HEC	A	602	43/43	0.98	0.07	-0.21	24,27,36,46	0
2	HEC	B	606	43/43	0.97	0.08	-0.30	27,32,35,36	0
2	HEC	A	606	43/43	0.98	0.07	-0.33	27,31,33,34	0
3	CA	B	609	1/1	1.00	0.06	-1.33	34,34,34,34	0
3	CA	A	609	1/1	0.99	0.05	-1.39	36,36,36,36	0
5	NA	B	621	1/1	0.99	0.09	-	36,36,36,36	0
4	PG4	B	617	8/13	0.80	0.45	-	44,49,52,52	8
4	PG4	A	614	6/13	0.86	0.10	-	69,70,73,74	0
3	CA	A	610	1/1	0.92	0.21	-	47,47,47,47	1
4	PG4	B	614	5/13	0.82	0.13	-	65,65,68,69	0
4	PG4	B	618	5/13	0.88	0.11	-	42,42,43,45	5
3	CA	B	610	1/1	0.95	0.11	-	42,42,42,42	1

6.5 Other polymers (i)

There are no such residues in this entry.