



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:15 AM GMT

PDB ID : 3LG1
Title : Structure of the Thioalkalivibrio nitratreducens cytochrome c nitrite reductase reduced by sodium borohydride (in complex with sulfite)
Authors : Trofimov, A.A.; Polyakov, K.M.; Boyko, K.M.; Filimonenkov, A.A.; Dorovatsky, P.V.; Tikhonova, T.V.; Popov, V.O.
Deposited on : 2010-01-19
Resolution : 1.95 Å(reported)

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

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

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

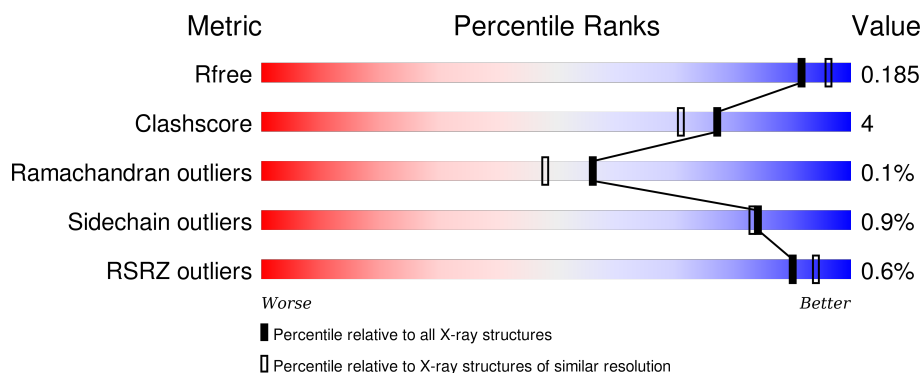
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	525	<div> <div></div> <div>94%</div> <div>5% .</div> </div>
1	B	525	<div> <div></div> <div>93%</div> <div>5% ..</div> </div>

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[A]	-	-	-	X
2	HEC	B	1007[A]	-	-	-	X
3	SO3	A	526	-	-	-	X
3	SO3	B	526	-	-	-	X
6	PG6	A	532	-	-	-	X
6	PG6	A	539	-	-	-	X
6	PG6	A	542	-	-	-	X
6	PG6	A	543	-	-	-	X
6	PG6	B	531	-	-	-	X
6	PG6	B	534	-	-	-	X
6	PG6	B	538[A]	-	-	-	X
6	PG6	B	541	-	-	-	X
6	PG6	B	542	-	-	-	X
7	PG4	A	545	-	-	-	X

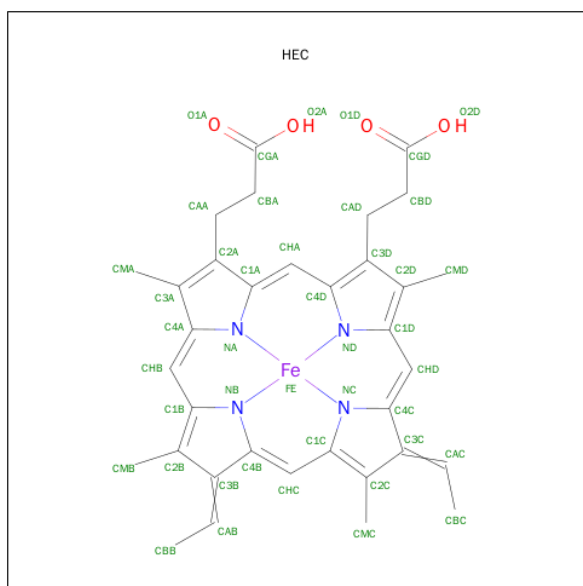
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In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues 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 4127	C 2565	N 745	O 780	S 37	0	10	1
1	B	519	Total 4159	C 2579	N 758	O 784	S 38	0	12	0

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



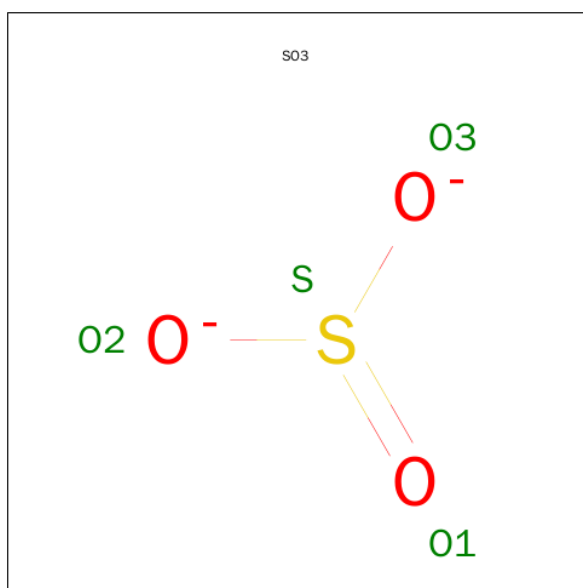
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	1

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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	1
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	1
			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
			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
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 4 3 1	0	0
3	A	1	Total O S 4 3 1	0	0
3	B	1	Total O S 4 3 1	0	0
3	B	1	Total O S 4 3 1	0	0
3	B	1	Total O S 4 3 1	0	0

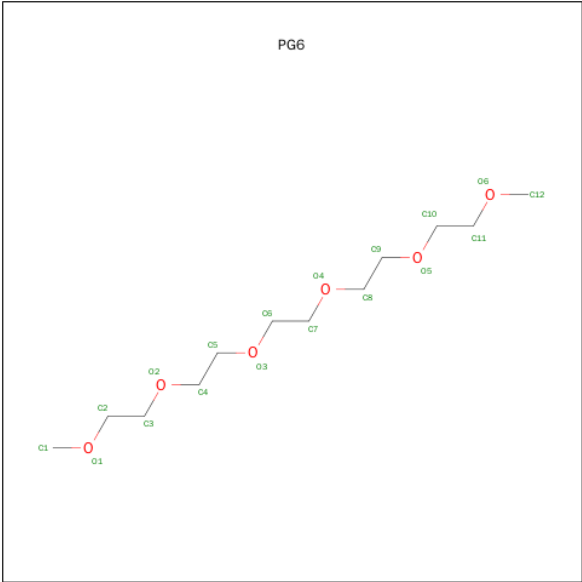
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

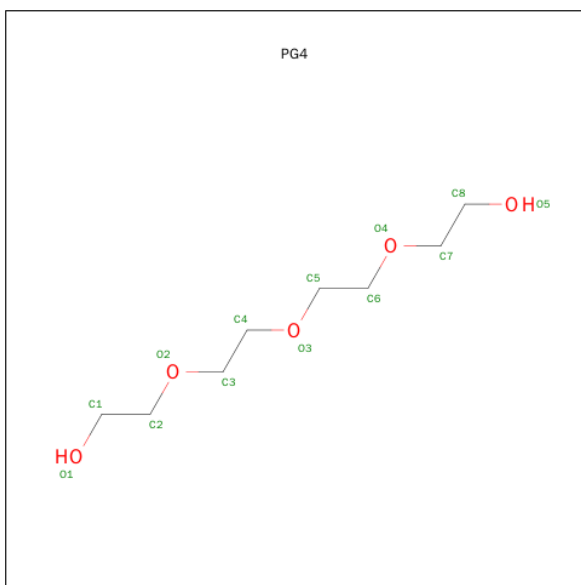
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total Na 3 3	0	0
5	A	5	Total Na 5 5	0	0

- Molecule 6 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (three-letter code: PG6) (formula: C₁₂H₂₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			17	11	6		
6	A	1	Total	C	O	0	0
			8	5	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			16	10	6		
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			17	11	6		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	1
			10	6	4		
6	B	1	Total	C	O	0	0
			8	5	3		
6	B	1	Total	C	O	0	0
			14	9	5		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

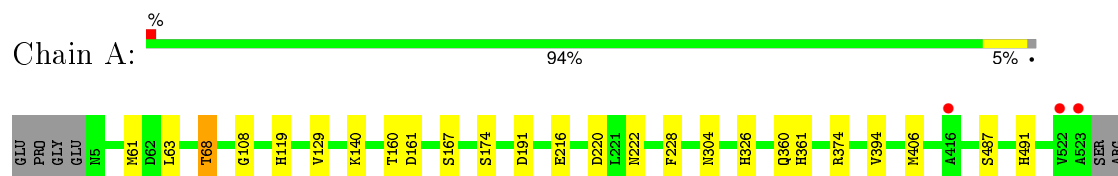
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	503	Total	O	0	0
			503	503		
8	B	471	Total	O	0	0
			471	471		

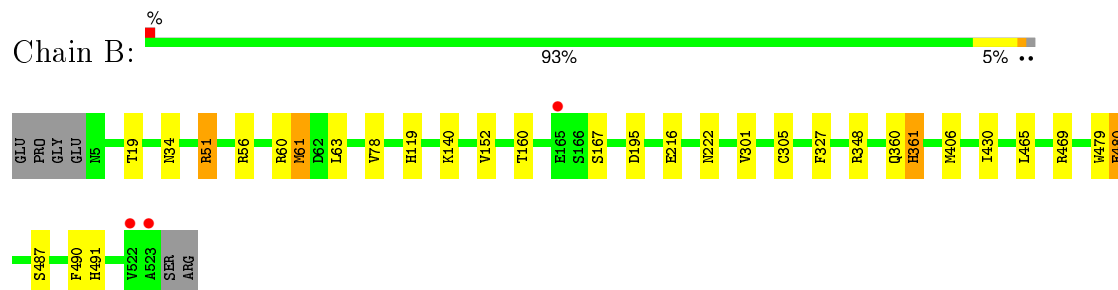
3 Residue-property plots [i](#)

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

- Molecule 1: 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, α , β , γ	192.62Å 192.62Å 192.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 1.95 19.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.90-1.95) 99.5 (19.97-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.161 , 0.183 0.164 , 0.185	Depositor DCC
R_{free} test set	8614 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.6	EDS
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 184703 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10172	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, SO3, PG6, 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	0.75	0/4294	0.70	1/5825 (0.0%)
1	B	0.76	0/4340	0.71	0/5883
All	All	0.76	0/8634	0.71	1/11708 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ASP	CB-CG-OD1	5.50	123.25	118.30

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	4127	0	3834	17	0
1	B	4159	0	3875	21	0
2	A	344	0	160	5	0
2	B	344	0	188	9	0
3	A	8	0	0	1	0
3	B	12	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
5	B	3	0	0	0	0
6	A	62	0	73	1	0
6	B	69	0	71	5	0
7	A	37	0	38	3	0
7	B	24	0	24	5	0
8	A	503	0	0	6	0
8	B	471	0	0	6	0
All	All	10172	0	8263	59	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 4.

All (59) 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:222[B]:ASN:ND2	8:A:876:HOH:O	1.85	1.08
1:B:222[A]:ASN:ND2	8:B:892:HOH:O	1.91	1.02
7:B:537:PG4:C1	7:B:537:PG4:C4	2.49	0.91
1:B:51[A]:ARG:HH11	1:B:51[A]:ARG:HG3	1.38	0.85
7:B:532:PG4:C4	8:B:704:HOH:O	2.31	0.78
7:B:537:PG4:H11	7:B:537:PG4:C4	2.14	0.77
2:A:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.68	0.75
7:B:532:PG4:H42	8:B:704:HOH:O	1.87	0.73
2:B:1002:HEC:HBC3	2:B:1002:HEC:HMC1	1.73	0.70
1:B:51[A]:ARG:NH1	1:B:51[A]:ARG:HG3	2.05	0.66
7:B:537:PG4:C4	7:B:537:PG4:H12	2.28	0.63
1:B:167:SER:HB2	1:B:216:GLU:HG2	1.83	0.59
2:A:1008:HEC:HMB1	2:A:1008:HEC:HBB3	1.86	0.58
2:B:1008:HEC:HMB1	2:B:1008:HEC:HBB3	1.86	0.57
1:B:60:ARG:HH22	6:B:539:PG6:H31	1.68	0.57
2:B:1008:HEC:HBC3	2:B:1008:HEC:HMC1	1.86	0.57
1:A:108:GLY:HA3	6:A:544:PG6:H31	1.86	0.57
6:B:531:PG6:H111	8:B:896:HOH:O	2.05	0.56
1:A:167:SER:HB2	1:A:216:GLU:HG2	1.88	0.55
1:A:68:THR:HG23	8:A:816:HOH:O	2.07	0.55
1:B:51[A]:ARG:CG	1:B:51[A]:ARG:NH1	2.73	0.51
1:B:56[A]:ARG:NH2	1:B:195:ASP:OD1	2.36	0.51
1:A:394[B]:VAL:HG12	8:A:1036:HOH:O	2.10	0.51
1:A:61[A]:MET:SD	1:A:191:ASP:O	2.70	0.50
6:B:534:PG6:O4	6:B:534:PG6:C5	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1004:HEC:HBB3	2:A:1004:HEC:HMB1	1.93	0.49
1:A:360:GLN:HB3	1:A:361:HIS:CE1	2.47	0.49
3:A:537:SO3:O2	8:A:938:HOH:O	0.48	0.48
1:A:487:SER:HB3	1:A:491:HIS:CE1	2.50	0.47
1:B:61[C]:MET:SD	8:B:748:HOH:O	2.61	0.47
1:A:216:GLU:HG3	8:A:968:HOH:O	2.15	0.46
2:B:1001:HEC:HBC3	2:B:1001:HEC:HMC1	1.96	0.46
6:B:534:PG6:O4	6:B:534:PG6:H52	2.15	0.46
1:A:174:SER:HA	7:A:538:PG4:H11	1.98	0.46
7:A:546:PG4:H32	7:A:546:PG4:H12	1.39	0.46
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.52	0.44
1:B:360:GLN:HB3	1:B:361:HIS:CE1	2.53	0.43
1:B:140:LYS:HG2	1:B:160:THR:HG23	1.99	0.43
1:B:430:ILE:HG21	1:B:490:PHE:HA	1.99	0.43
1:B:34:ASN:HA	6:B:534:PG6:H21	2.01	0.42
1:A:119:HIS:CD2	2:A:1006:HEC:ND	2.88	0.42
1:B:301:VAL:HG21	1:B:327:PHE:CE2	2.55	0.42
1:A:63:LEU:HD12	1:A:63:LEU:N	2.35	0.42
1:B:78:VAL:HG12	1:B:152:VAL:HG21	2.02	0.42
7:A:533:PG4:C4	8:A:687:HOH:O	2.69	0.41
1:B:479:TRP:CZ3	1:B:480:GLU:HG3	2.55	0.41
2:B:1002:HEC:HBD2	2:B:1002:HEC:HHA	2.03	0.41
1:A:304:ASN:HB2	1:A:326:HIS:HB3	2.01	0.41
1:B:119:HIS:CD2	2:B:1006:HEC:ND	2.89	0.41
2:B:1006:HEC:HMA3	2:B:1007[A]:HEC:HBA2	2.02	0.41
1:A:61[A]:MET:HG2	1:A:228:PHE:CZ	2.56	0.41
1:B:63:LEU:HD12	1:B:63:LEU:N	2.36	0.41
2:B:1001:HEC:HBB3	2:B:1001:HEC:HMB1	2.02	0.40
1:B:305:CYS:CB	2:B:1004:HEC:HMC2	2.52	0.40
1:A:140:LYS:HG2	1:A:160:THR:HG23	2.02	0.40
1:B:465:LEU:O	1:B:469:ARG:HG3	2.21	0.40
1:A:129:VAL:HG11	2:A:1004:HEC:HMA1	2.03	0.40
1:B:348[A]:ARG:NH1	8:B:807:HOH:O	2.45	0.40
1:A:374:ARG:NE	1:A:374:ARG:HA	2.37	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	528/525 (101%)	503 (95%)	25 (5%)	0	100	100
1	B	530/525 (101%)	503 (95%)	26 (5%)	1 (0%)	52	43
All	All	1058/1050 (101%)	1006 (95%)	51 (5%)	1 (0%)	56	48

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	442/443 (100%)	438 (99%)	4 (1%)	84	83
1	B	449/443 (101%)	439 (98%)	10 (2%)	60	51
All	All	891/886 (101%)	877 (98%)	14 (2%)	84	66

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	THR
1	A	220	ASP
1	A	406[A]	MET
1	A	406[B]	MET
1	B	19[A]	THR

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Mol	Chain	Res	Type
1	B	19[B]	THR
1	B	51[A]	ARG
1	B	51[B]	ARG
1	B	61[A]	MET
1	B	61[B]	MET
1	B	61[C]	MET
1	B	406[A]	MET
1	B	406[B]	MET
1	B	480	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	GLN

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 55 ligands modelled in this entry, 12 are monoatomic - leaving 43 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	1001[A]	-	24,50,50	2.24	6 (25%)	19,82,82	3.23	8 (42%)
2	HEC	A	1002	1	24,50,50	2.26	8 (33%)	19,82,82	3.00	6 (31%)
2	HEC	A	1003[A]	-	24,50,50	2.36	9 (37%)	19,82,82	2.63	9 (47%)
2	HEC	A	1004	1,8,3	24,50,50	2.05	5 (20%)	19,82,82	2.85	6 (31%)
2	HEC	A	1005	1	24,50,50	2.44	9 (37%)	19,82,82	3.07	7 (36%)
2	HEC	A	1006	1,4	24,50,50	2.16	9 (37%)	19,82,82	3.42	8 (42%)
2	HEC	A	1007[A]	-	24,50,50	2.32	7 (29%)	19,82,82	3.14	7 (36%)
2	HEC	A	1008	1	24,50,50	2.32	5 (20%)	19,82,82	3.27	7 (36%)
3	SO3	A	526	2	1,3,3	0.37	0	0,3,3	0.00	-
6	PG6	A	532	5,7	16,16,17	0.84	0	15,15,16	1.13	2 (13%)
7	PG4	A	533	6	3,3,12	0.64	0	2,2,11	0.40	0
6	PG6	A	534	-	7,7,17	0.60	0	6,6,16	0.24	0
3	SO3	A	537	-	1,3,3	0.38	0	0,3,3	0.00	-
7	PG4	A	538	-	5,5,12	0.49	0	4,4,11	0.29	0
6	PG6	A	539	-	6,6,17	0.27	0	5,5,16	0.63	0
7	PG4	A	540	-	8,8,12	0.50	0	7,7,11	0.13	0
7	PG4	A	541	-	4,4,12	0.38	0	3,3,11	0.52	0
6	PG6	A	542	-	15,15,17	0.53	0	14,14,16	0.28	0
6	PG6	A	543	-	9,9,17	0.51	0	8,8,16	0.32	0
6	PG6	A	544	-	3,3,17	0.36	0	2,2,16	0.23	0
7	PG4	A	545	-	6,6,12	0.50	0	5,5,11	0.35	0
7	PG4	A	546	-	5,5,12	0.48	0	4,4,11	0.16	0
2	HEC	B	1001	1	24,50,50	2.03	4 (16%)	19,82,82	2.95	7 (36%)
2	HEC	B	1002	1	24,50,50	2.09	6 (25%)	19,82,82	3.13	6 (31%)
2	HEC	B	1003[A]	-	24,50,50	2.41	9 (37%)	19,82,82	2.97	8 (42%)
2	HEC	B	1004	1,8,3	24,50,50	2.00	6 (25%)	19,82,82	2.72	6 (31%)
2	HEC	B	1005	1	24,50,50	2.37	9 (37%)	19,82,82	2.94	6 (31%)
2	HEC	B	1006	1,4	24,50,50	2.37	7 (29%)	19,82,82	3.18	7 (36%)
2	HEC	B	1007[A]	-	24,50,50	2.27	5 (20%)	19,82,82	3.26	6 (31%)
2	HEC	B	1008	1	24,50,50	2.35	5 (20%)	19,82,82	3.08	6 (31%)
3	SO3	B	526	2	1,3,3	0.38	0	0,3,3	0.00	-
6	PG6	B	531	5,7	16,16,17	0.91	0	15,15,16	1.09	1 (6%)
7	PG4	B	532	6	4,4,12	0.45	0	3,3,11	0.23	0
3	SO3	B	533	-	1,3,3	0.70	0	0,3,3	0.00	-
6	PG6	B	534	-	9,9,17	0.44	0	8,8,16	0.44	0
3	SO3	B	536	-	1,3,3	0.57	0	0,3,3	0.00	-
7	PG4	B	537	-	5,5,12	0.46	0	4,4,11	0.39	0
6	PG6	B	538[A]	-	9,9,17	0.36	0	8,8,16	0.62	0
6	PG6	B	539	-	7,7,17	0.58	0	6,6,16	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PG4	B	540	-	7,7,12	0.65	0	6,6,11	0.36	0
6	PG6	B	541	-	13,13,17	0.62	0	12,12,16	0.39	0
6	PG6	B	542	-	9,9,17	0.45	0	8,8,16	0.35	0
7	PG4	B	543	-	4,4,12	0.46	0	3,3,11	0.30	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	1001[A]	-	-	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[A]	-	-	0/6/54/54	0/0/8/8
2	HEC	A	1004	1,8,3	-	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	1,4	-	0/6/54/54	0/0/8/8
2	HEC	A	1007[A]	-	-	0/6/54/54	0/0/8/8
2	HEC	A	1008	1	-	0/6/54/54	0/0/8/8
3	SO3	A	526	2	-	0/0/0/0	0/0/0/0
6	PG6	A	532	5,7	-	0/14/14/15	0/0/0/0
7	PG4	A	533	6	-	0/0/1/10	0/0/0/0
6	PG6	A	534	-	-	0/5/5/15	0/0/0/0
3	SO3	A	537	-	-	0/0/0/0	0/0/0/0
7	PG4	A	538	-	-	0/3/3/10	0/0/0/0
6	PG6	A	539	-	-	0/4/4/15	0/0/0/0
7	PG4	A	540	-	-	0/6/6/10	0/0/0/0
7	PG4	A	541	-	-	0/2/2/10	0/0/0/0
6	PG6	A	542	-	-	0/13/13/15	0/0/0/0
6	PG6	A	543	-	-	0/7/7/15	0/0/0/0
6	PG6	A	544	-	-	0/1/1/15	0/0/0/0
7	PG4	A	545	-	-	0/4/4/10	0/0/0/0
7	PG4	A	546	-	-	0/3/3/10	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[A]	-	-	0/6/54/54	0/0/8/8
2	HEC	B	1004	1,8,3	-	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	1,4	-	0/6/54/54	0/0/8/8
2	HEC	B	1007[A]	-	-	0/6/54/54	0/0/8/8
2	HEC	B	1008	1	-	0/6/54/54	0/0/8/8
3	SO3	B	526	2	-	0/0/0/0	0/0/0/0
6	PG6	B	531	5,7	-	0/14/14/15	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	B	532	6	-	0/2/2/10	0/0/0/0
3	SO3	B	533	-	-	0/0/0/0	0/0/0/0
6	PG6	B	534	-	-	0/7/7/15	0/0/0/0
3	SO3	B	536	-	-	0/0/0/0	0/0/0/0
7	PG4	B	537	-	-	0/3/3/10	0/0/0/0
6	PG6	B	538[A]	-	-	0/7/7/15	0/0/0/0
6	PG6	B	539	-	-	0/5/5/15	0/0/0/0
7	PG4	B	540	-	-	0/5/5/10	0/0/0/0
6	PG6	B	541	-	-	0/11/11/15	0/0/0/0
6	PG6	B	542	-	-	0/7/7/15	0/0/0/0
7	PG4	B	543	-	-	0/2/2/10	0/0/0/0

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1005	HEC	C3B-C2B	-6.59	1.33	1.40
2	B	1007[A]	HEC	C3C-C2C	-6.56	1.33	1.40
2	A	1008	HEC	C3B-C2B	-6.49	1.34	1.40
2	A	1007[A]	HEC	C3C-C2C	-6.30	1.34	1.40
2	B	1003[A]	HEC	C3B-C2B	-6.30	1.34	1.40
2	B	1008	HEC	C3B-C2B	-6.27	1.34	1.40
2	B	1006	HEC	C3B-C2B	-6.26	1.34	1.40
2	A	1005	HEC	C3B-C2B	-6.12	1.34	1.40
2	B	1003[A]	HEC	C3C-C2C	-5.97	1.34	1.40
2	A	1001[A]	HEC	C3B-C2B	-5.88	1.34	1.40
2	B	1006	HEC	C3C-C2C	-5.58	1.34	1.40
2	A	1003[A]	HEC	C3C-C2C	-5.52	1.35	1.40
2	A	1002	HEC	C3B-C2B	-5.52	1.35	1.40
2	A	1007[A]	HEC	C3B-C2B	-5.37	1.35	1.40
2	B	1008	HEC	C3C-C2C	-5.32	1.35	1.40
2	A	1003[A]	HEC	C3B-C2B	-5.26	1.35	1.40
2	A	1005	HEC	C3C-C2C	-5.14	1.35	1.40
2	A	1004	HEC	C3B-C2B	-5.11	1.35	1.40
2	B	1007[A]	HEC	C3B-C2B	-5.10	1.35	1.40
2	A	1006	HEC	C3B-C2B	-4.86	1.35	1.40
2	B	1005	HEC	C3C-C2C	-4.78	1.35	1.40
2	B	1002	HEC	C3B-C2B	-4.70	1.35	1.40
2	B	1001	HEC	C3B-C2B	-4.37	1.36	1.40
2	B	1001	HEC	C3C-C2C	-4.32	1.36	1.40
2	A	1008	HEC	C3C-C2C	-4.31	1.36	1.40
2	B	1004	HEC	C3C-C2C	-4.31	1.36	1.40
2	A	1002	HEC	C3C-C2C	-4.15	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1004	HEC	C3C-C2C	-4.12	1.36	1.40
2	B	1002	HEC	C3C-C2C	-3.90	1.36	1.40
2	A	1006	HEC	C3C-C2C	-3.85	1.36	1.40
2	A	1001[A]	HEC	C3C-C2C	-3.79	1.36	1.40
2	B	1004	HEC	C3B-C2B	-3.02	1.37	1.40
2	B	1003[A]	HEC	C4C-NC	2.00	1.39	1.36
2	B	1002	HEC	CAD-C3D	2.00	1.55	1.52
2	A	1005	HEC	CMB-C2B	2.00	1.56	1.51
2	A	1007[A]	HEC	CAA-C2A	2.01	1.56	1.52
2	A	1004	HEC	C4C-NC	2.01	1.39	1.36
2	A	1006	HEC	CMA-C3A	2.02	1.56	1.51
2	B	1005	HEC	CMD-C2D	2.03	1.55	1.51
2	B	1003[A]	HEC	CAD-C3D	2.05	1.55	1.52
2	A	1006	HEC	CMC-C2C	2.05	1.56	1.51
2	B	1003[A]	HEC	CMD-C2D	2.05	1.55	1.51
2	A	1008	HEC	C3C-C4C	2.07	1.47	1.42
2	A	1003[A]	HEC	CAD-C3D	2.07	1.55	1.52
2	A	1001[A]	HEC	CAD-C3D	2.08	1.55	1.52
2	B	1007[A]	HEC	C4C-NC	2.08	1.39	1.36
2	A	1001[A]	HEC	CMB-C2B	2.08	1.56	1.51
2	B	1003[A]	HEC	CAA-C2A	2.09	1.56	1.52
2	A	1002	HEC	CMA-C3A	2.11	1.56	1.51
2	B	1002	HEC	C3C-C4C	2.11	1.47	1.42
2	B	1005	HEC	C1A-NA	2.17	1.39	1.36
2	B	1005	HEC	C4A-NA	2.18	1.39	1.36
2	A	1003[A]	HEC	CMA-C3A	2.19	1.56	1.51
2	B	1001	HEC	C3C-C4C	2.19	1.47	1.42
2	A	1005	HEC	CBB-CAB	2.21	1.58	1.49
2	B	1005	HEC	CMB-C2B	2.21	1.56	1.51
2	B	1006	HEC	CMB-C2B	2.21	1.56	1.51
2	B	1006	HEC	C3C-C4C	2.22	1.47	1.42
2	A	1006	HEC	CMB-C2B	2.23	1.56	1.51
2	B	1003[A]	HEC	CMA-C3A	2.24	1.56	1.51
2	A	1002	HEC	C3B-C4B	2.26	1.47	1.42
2	A	1004	HEC	CMD-C2D	2.26	1.56	1.51
2	B	1003[A]	HEC	CMB-C2B	2.29	1.56	1.51
2	B	1005	HEC	C4C-NC	2.32	1.39	1.36
2	B	1006	HEC	C4B-NB	2.33	1.39	1.36
2	B	1008	HEC	CMD-C2D	2.36	1.56	1.51
2	B	1002	HEC	C4B-NB	2.40	1.39	1.36
2	B	1006	HEC	CMC-C2C	2.40	1.56	1.51
2	A	1002	HEC	CMB-C2B	2.41	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1007[A]	HEC	C4C-NC	2.42	1.39	1.36
2	A	1002	HEC	C3C-C4C	2.43	1.48	1.42
2	A	1008	HEC	CMC-C2C	2.47	1.57	1.51
2	A	1002	HEC	C4A-NA	2.47	1.40	1.36
2	B	1004	HEC	CMC-C2C	2.48	1.57	1.51
2	B	1004	HEC	CAD-C3D	2.50	1.56	1.52
2	A	1006	HEC	CAD-C3D	2.52	1.56	1.52
2	A	1007[A]	HEC	C4A-NA	2.54	1.40	1.36
2	A	1006	HEC	C3C-C4C	2.59	1.48	1.42
2	B	1004	HEC	C4B-NB	2.60	1.40	1.36
2	A	1005	HEC	CMA-C3A	2.63	1.57	1.51
2	A	1005	HEC	CAA-C2A	2.63	1.57	1.52
2	B	1008	HEC	CMC-C2C	2.64	1.57	1.51
2	B	1007[A]	HEC	C1A-NA	2.65	1.40	1.36
2	A	1001[A]	HEC	C3C-C4C	2.65	1.48	1.42
2	A	1005	HEC	C4A-NA	2.70	1.40	1.36
2	A	1003[A]	HEC	CMB-C2B	2.72	1.57	1.51
2	A	1007[A]	HEC	C1A-NA	2.75	1.40	1.36
2	B	1005	HEC	CMA-C3A	2.77	1.57	1.51
2	A	1003[A]	HEC	C4C-NC	2.81	1.40	1.36
2	A	1003[A]	HEC	C4A-NA	3.00	1.40	1.36
2	A	1003[A]	HEC	C4B-NB	3.03	1.40	1.36
2	A	1005	HEC	C4B-NB	3.05	1.40	1.36
2	A	1006	HEC	C4B-NB	3.07	1.40	1.36
2	A	1003[A]	HEC	C3D-C2D	3.76	1.48	1.37
2	B	1007[A]	HEC	C3D-C2D	3.95	1.49	1.37
2	B	1003[A]	HEC	C3D-C2D	4.06	1.49	1.37
2	A	1004	HEC	C3D-C2D	4.21	1.50	1.37
2	B	1005	HEC	C3D-C2D	4.22	1.50	1.37
2	A	1007[A]	HEC	C3D-C2D	4.31	1.50	1.37
2	A	1006	HEC	C3D-C2D	4.36	1.50	1.37
2	A	1005	HEC	C3D-C2D	4.52	1.51	1.37
2	B	1004	HEC	C3D-C2D	4.54	1.51	1.37
2	B	1006	HEC	C3D-C2D	4.69	1.51	1.37
2	B	1008	HEC	C3D-C2D	5.01	1.52	1.37
2	B	1001	HEC	C3D-C2D	5.04	1.52	1.37
2	A	1002	HEC	C3D-C2D	5.06	1.52	1.37
2	B	1002	HEC	C3D-C2D	5.07	1.52	1.37
2	A	1001[A]	HEC	C3D-C2D	5.23	1.53	1.37
2	A	1008	HEC	C3D-C2D	5.23	1.53	1.37

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1008	HEC	CBB-CAB-C3B	-10.50	104.01	127.35
2	A	1006	HEC	CBB-CAB-C3B	-9.99	105.15	127.35
2	B	1008	HEC	CBB-CAB-C3B	-9.85	105.45	127.35
2	B	1006	HEC	CBB-CAB-C3B	-9.52	106.19	127.35
2	A	1005	HEC	CBB-CAB-C3B	-9.30	106.69	127.35
2	B	1007[A]	HEC	CBB-CAB-C3B	-9.29	106.70	127.35
2	B	1005	HEC	CBB-CAB-C3B	-8.89	107.61	127.35
2	A	1007[A]	HEC	CBB-CAB-C3B	-8.37	108.75	127.35
2	A	1004	HEC	CBB-CAB-C3B	-8.23	109.06	127.35
2	A	1002	HEC	CBB-CAB-C3B	-8.20	109.12	127.35
2	B	1004	HEC	CBB-CAB-C3B	-8.02	109.53	127.35
2	A	1003[A]	HEC	CBB-CAB-C3B	-7.94	109.70	127.35
2	B	1003[A]	HEC	CBB-CAB-C3B	-7.79	110.05	127.35
2	B	1002	HEC	CBB-CAB-C3B	-7.40	110.90	127.35
2	A	1001[A]	HEC	CBB-CAB-C3B	-7.24	111.27	127.35
2	B	1001	HEC	CBB-CAB-C3B	-7.11	111.55	127.35
2	B	1006	HEC	CBC-CAC-C3C	-6.45	113.02	127.35
2	A	1007[A]	HEC	CBC-CAC-C3C	-6.28	113.39	127.35
2	B	1002	HEC	CBC-CAC-C3C	-6.25	113.46	127.35
2	A	1006	HEC	CBC-CAC-C3C	-6.03	113.95	127.35
2	A	1001[A]	HEC	CBD-CAD-C3D	-5.97	101.84	112.53
2	A	1001[A]	HEC	CBC-CAC-C3C	-5.96	114.10	127.35
2	B	1007[A]	HEC	CBD-CAD-C3D	-5.67	102.36	112.53
2	B	1002	HEC	CMC-C2C-C1C	-5.67	118.98	128.36
2	B	1003[A]	HEC	CBA-CAA-C2A	-5.62	102.46	112.53
2	B	1001	HEC	CBC-CAC-C3C	-5.43	115.29	127.35
2	A	1002	HEC	CBC-CAC-C3C	-5.41	115.33	127.35
2	A	1001[A]	HEC	CMC-C2C-C1C	-5.36	119.50	128.36
2	B	1003[A]	HEC	CMC-C2C-C1C	-5.05	120.00	128.36
2	B	1007[A]	HEC	CMB-C2B-C1B	-4.95	120.17	128.36
2	B	1001	HEC	CBD-CAD-C3D	-4.93	103.69	112.53
2	A	1004	HEC	CMB-C2B-C1B	-4.86	120.33	128.36
2	B	1002	HEC	CAA-CBA-CGA	-4.80	103.95	112.75
2	B	1008	HEC	CBC-CAC-C3C	-4.71	116.88	127.35
2	A	1007[A]	HEC	CBD-CAD-C3D	-4.69	104.12	112.53
2	A	1004	HEC	CBC-CAC-C3C	-4.69	116.93	127.35
2	A	1007[A]	HEC	CMB-C2B-C1B	-4.69	120.61	128.36
2	B	1008	HEC	CBD-CAD-C3D	-4.65	104.20	112.53
2	A	1006	HEC	CMC-C2C-C1C	-4.59	120.77	128.36
2	B	1007[A]	HEC	CBC-CAC-C3C	-4.59	117.16	127.35
2	B	1005	HEC	CBC-CAC-C3C	-4.53	117.29	127.35
2	A	1005	HEC	CBC-CAC-C3C	-4.52	117.30	127.35
2	B	1007[A]	HEC	CBA-CAA-C2A	-4.51	104.45	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	HEC	CMC-C2C-C1C	-4.47	120.96	128.36
2	B	1004	HEC	CBC-CAC-C3C	-4.45	117.47	127.35
2	A	1002	HEC	CAA-CBA-CGA	-4.37	104.73	112.75
2	B	1004	HEC	CMC-C2C-C1C	-4.34	121.18	128.36
2	B	1006	HEC	CMC-C2C-C1C	-4.31	121.24	128.36
2	B	1001	HEC	CBA-CAA-C2A	-4.31	104.81	112.53
2	B	1004	HEC	CMB-C2B-C1B	-4.27	121.30	128.36
2	A	1006	HEC	CAA-C2A-C1A	-4.24	122.40	127.01
2	B	1001	HEC	CAA-C2A-C1A	-4.23	122.41	127.01
2	A	1005	HEC	CMC-C2C-C1C	-4.20	121.41	128.36
2	A	1008	HEC	CMC-C2C-C1C	-4.20	121.42	128.36
2	A	1003[A]	HEC	CMC-C2C-C1C	-4.20	121.42	128.36
2	B	1005	HEC	CMC-C2C-C1C	-4.14	121.51	128.36
2	A	1008	HEC	CBC-CAC-C3C	-4.12	118.21	127.35
2	A	1008	HEC	CBD-CAD-C3D	-4.06	105.25	112.53
2	B	1002	HEC	CAA-C2A-C1A	-4.06	122.61	127.01
2	A	1004	HEC	CMC-C2C-C1C	-3.92	121.87	128.36
2	A	1005	HEC	CAA-C2A-C1A	-3.90	122.78	127.01
2	A	1008	HEC	CAA-C2A-C1A	-3.84	122.84	127.01
2	B	1005	HEC	CMB-C2B-C1B	-3.81	122.05	128.36
2	B	1001	HEC	CMC-C2C-C1C	-3.75	122.16	128.36
2	A	1001[A]	HEC	CBA-CAA-C2A	-3.71	105.88	112.53
2	A	1005	HEC	CMB-C2B-C1B	-3.66	122.30	128.36
2	A	1001[A]	HEC	CAA-C2A-C1A	-3.66	123.04	127.01
2	A	1008	HEC	CMB-C2B-C1B	-3.48	122.61	128.36
2	A	1006	HEC	CBD-CAD-C3D	-3.47	106.30	112.53
2	B	1003[A]	HEC	CAA-C2A-C1A	-3.45	123.26	127.01
2	B	1008	HEC	CMC-C2C-C1C	-3.40	122.74	128.36
2	A	1005	HEC	CBD-CAD-C3D	-3.37	106.49	112.53
2	A	1007[A]	HEC	CBA-CAA-C2A	-3.36	106.52	112.53
2	B	1005	HEC	CBD-CAD-C3D	-3.33	106.57	112.53
2	A	1002	HEC	CAA-C2A-C1A	-3.30	123.42	127.01
2	A	1006	HEC	CBA-CAA-C2A	-3.29	106.62	112.53
2	B	1008	HEC	CMB-C2B-C1B	-3.23	123.01	128.36
2	A	1006	HEC	CMB-C2B-C1B	-3.17	123.11	128.36
2	A	1007[A]	HEC	CMC-C2C-C1C	-3.12	123.20	128.36
2	B	1006	HEC	CMB-C2B-C1B	-2.95	123.49	128.36
2	B	1006	HEC	CBD-CAD-C3D	-2.93	107.28	112.53
2	B	1002	HEC	CMB-C2B-C1B	-2.91	123.54	128.36
2	A	1003[A]	HEC	CMB-C2B-C1B	-2.89	123.59	128.36
2	A	1002	HEC	CMB-C2B-C1B	-2.69	123.91	128.36
2	A	1003[A]	HEC	CBC-CAC-C3C	-2.68	121.39	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1005	HEC	CAA-C2A-C1A	-2.66	124.12	127.01
2	B	1003[A]	HEC	CBC-CAC-C3C	-2.65	121.46	127.35
2	B	1008	HEC	CBA-CAA-C2A	-2.61	107.85	112.53
2	A	1001[A]	HEC	CMB-C2B-C1B	-2.57	124.11	128.36
2	B	1003[A]	HEC	CMB-C2B-C1B	-2.55	124.15	128.36
2	A	1008	HEC	CBA-CAA-C2A	-2.54	107.97	112.53
2	A	1003[A]	HEC	CBD-CAD-C3D	-2.51	108.03	112.53
2	A	1005	HEC	CAD-CBD-CGD	-2.46	108.25	112.75
2	B	1003[A]	HEC	CAD-CBD-CGD	-2.45	108.25	112.75
2	A	1001[A]	HEC	CAA-CBA-CGA	-2.40	108.35	112.75
2	B	1007[A]	HEC	CMC-C2C-C1C	-2.32	124.52	128.36
2	B	1006	HEC	CBA-CAA-C2A	-2.30	108.41	112.53
2	A	1007[A]	HEC	CAA-C2A-C1A	-2.27	124.54	127.01
2	B	1001	HEC	CMB-C2B-C1B	-2.22	124.69	128.36
2	A	1003[A]	HEC	CAA-C2A-C3A	-2.21	122.70	129.00
2	B	1004	HEC	CAA-C2A-C1A	-2.15	124.67	127.01
2	A	1003[A]	HEC	CBA-CAA-C2A	-2.06	108.84	112.53
2	A	1004	HEC	CBA-CAA-C2A	-2.03	108.88	112.53
2	B	1006	HEC	CAA-C2A-C1A	-2.02	124.81	127.01
6	A	532	PG6	C8-O4-C7	2.10	122.34	113.31
2	A	1006	HEC	CMA-C3A-C2A	2.10	129.63	125.24
2	A	1003[A]	HEC	CAD-C3D-C4D	2.10	129.29	127.01
6	B	531	PG6	C8-O4-C7	2.14	122.53	113.31
6	A	532	PG6	C6-O3-C5	2.43	123.77	113.31
2	B	1004	HEC	CAD-C3D-C4D	2.49	129.71	127.01
2	A	1004	HEC	CAD-C3D-C4D	2.65	129.88	127.01
2	A	1003[A]	HEC	CAA-C2A-C1A	3.05	130.32	127.01
2	B	1003[A]	HEC	CAA-CBA-CGA	3.20	118.61	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	HEC	1	0
2	A	1004	HEC	2	0
2	A	1006	HEC	1	0
2	A	1008	HEC	1	0
7	A	533	PG4	1	0
3	A	537	SO3	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	538	PG4	1	0
6	A	544	PG6	1	0
7	A	546	PG4	1	0
2	B	1001	HEC	2	0
2	B	1002	HEC	2	0
2	B	1004	HEC	1	0
2	B	1006	HEC	2	0
2	B	1007[A]	HEC	1	0
2	B	1008	HEC	2	0
6	B	531	PG6	1	0
7	B	532	PG4	2	0
6	B	534	PG6	3	0
7	B	537	PG4	3	0
6	B	539	PG6	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	519/525 (98%)	-0.56	3 (0%)	90 94	13, 19, 31, 49	0
1	B	519/525 (98%)	-0.53	3 (0%)	90 94	13, 19, 32, 49	1 (0%)
All	All	1038/1050 (98%)	-0.55	6 (0%)	90 94	13, 19, 31, 49	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	523	ALA	4.8
1	A	522	VAL	3.9
1	A	523	ALA	3.2
1	B	522	VAL	2.7
1	A	416	ALA	2.4
1	B	165	GLU	2.1

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(\AA^2)	Q<0.9
6	PG6	B	531	17/18	0.78	0.17	10.06	31,39,45,46	0
6	PG6	B	534	10/18	0.80	0.42	8.96	17,20,32,33	10
7	PG4	A	545	7/13	0.80	0.28	8.33	32,33,34,35	7
6	PG6	A	532	17/18	0.87	0.14	7.68	24,34,44,45	2
6	PG6	A	543	10/18	0.67	0.30	6.49	31,32,35,37	10
3	SO3	B	526	4/4	0.98	0.16	5.30	12,12,14,14	4
6	PG6	B	538[A]	10/18	0.88	0.14	5.15	29,40,47,47	1
6	PG6	B	541	14/18	0.80	0.27	4.11	54,61,63,63	0
3	SO3	A	526	4/4	0.99	0.10	3.37	13,16,16,18	4
6	PG6	B	542	10/18	0.83	0.21	3.35	27,29,31,32	10
6	PG6	A	542	16/18	0.75	0.24	3.15	28,35,37,38	16
6	PG6	A	539	7/18	0.94	0.12	3.04	28,31,40,43	0
2	HEC	A	1007[A]	43/43	0.97	0.10	2.11	11,14,16,17	3
2	HEC	B	1007[A]	43/43	0.97	0.10	2.05	10,13,15,16	4
2	HEC	A	1008	43/43	0.97	0.09	1.68	15,19,28,36	0
2	HEC	A	1003[A]	43/43	0.98	0.10	1.05	11,14,25,34	4
6	PG6	A	534	8/18	0.91	0.12	0.96	33,40,50,50	0
2	HEC	B	1003[A]	43/43	0.97	0.10	0.96	12,16,29,35	4
2	HEC	B	1005	43/43	0.98	0.08	0.89	12,14,20,24	0
2	HEC	B	1008	43/43	0.97	0.09	0.88	14,18,29,38	0
2	HEC	B	1002	43/43	0.98	0.10	0.76	16,19,22,23	0
2	HEC	A	1002	43/43	0.99	0.09	0.50	15,17,19,22	0
2	HEC	A	1001[A]	43/43	0.98	0.09	0.42	16,19,21,24	4
2	HEC	B	1006	43/43	0.99	0.07	0.36	10,14,15,18	0
2	HEC	A	1005	43/43	0.98	0.07	0.35	12,13,20,22	0
2	HEC	A	1006	43/43	0.99	0.07	0.29	11,13,15,15	0
2	HEC	A	1004	43/43	0.99	0.06	-0.09	11,15,17,17	0
2	HEC	B	1004	43/43	0.99	0.06	-0.19	11,14,17,19	0
2	HEC	B	1001	43/43	0.97	0.10	-0.43	19,23,29,31	0
4	CA	B	527	1/1	0.99	0.03	-3.42	18,18,18,18	0
4	CA	A	527	1/1	0.99	0.03	-3.69	19,19,19,19	0
6	PG6	B	539	8/18	0.75	0.21	-	51,53,55,56	0
7	PG4	B	540	8/13	0.66	0.25	-	49,54,59,59	0
3	SO3	B	536	4/4	0.96	0.06	-	37,37,37,37	4
4	CA	A	528	1/1	0.98	0.06	-	16,16,16,16	1
3	SO3	B	533	4/4	0.93	0.12	-	44,44,44,45	4
7	PG4	A	538	6/13	0.89	0.14	-	51,53,53,55	0
5	NA	B	530	1/1	0.95	0.06	-	40,40,40,40	1
7	PG4	B	532	5/13	0.85	0.23	-	31,31,32,33	5
4	CA	B	528	1/1	0.99	0.04	-	16,16,16,16	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	PG6	A	544	4/18	0.94	0.14	-	20,21,23,23	4
7	PG4	A	540	9/13	0.88	0.21	-	26,28,33,33	9
7	PG4	B	537	6/13	0.86	0.24	-	29,30,31,32	6
3	SO3	A	537	4/4	0.96	0.09	-	38,38,38,38	4
7	PG4	B	543	5/13	0.79	0.17	-	58,60,61,62	0
7	PG4	A	541	5/13	0.90	0.15	-	46,47,48,50	0
7	PG4	A	533	4/13	0.88	0.20	-	25,27,27,28	4
5	NA	B	535	1/1	0.97	0.18	-	17,17,17,17	1
5	NA	A	536	1/1	0.94	0.19	-	38,38,38,38	0
5	NA	A	529	1/1	0.84	0.17	-	28,28,28,28	1
5	NA	A	535	1/1	0.96	0.17	-	13,13,13,13	1
7	PG4	A	546	6/13	0.81	0.29	-	36,37,37,37	6
5	NA	B	529	1/1	0.98	0.17	-	29,29,29,29	0
5	NA	A	530	1/1	0.95	0.24	-	29,29,29,29	0
5	NA	A	531	1/1	0.99	0.14	-	43,43,43,43	1

6.5 Other polymers [i](#)

There are no such residues in this entry.