Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:10 AM GMT

PDB ID	:	1ZZT
Title	:	Bovine eNOS N368D/V106M double mutant with L-N(omega)-Nitroarginine-(4R)-Amino-L-Proline Amide Bound
Authors	:	Li, H.; Flinspach, M.L.; Igarashi, J.; Jamal, J.; Yang, W.; Gomez-Vidal, J.A.; Litzinger, E.A.; Silverman, R.B.; Poulos, T.L.
Deposited on	:	2005-06-14
Resolution	:	2.14 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

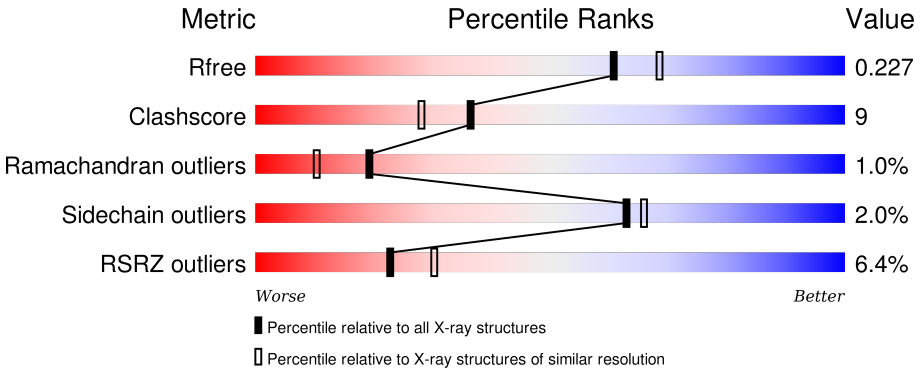
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.14 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	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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	416	8% 76% 19%
1	B	416	5% 81% 15%

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	ACT	A	860	-	-	-	X
2	ACT	B	861	-	-	X	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6994 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.

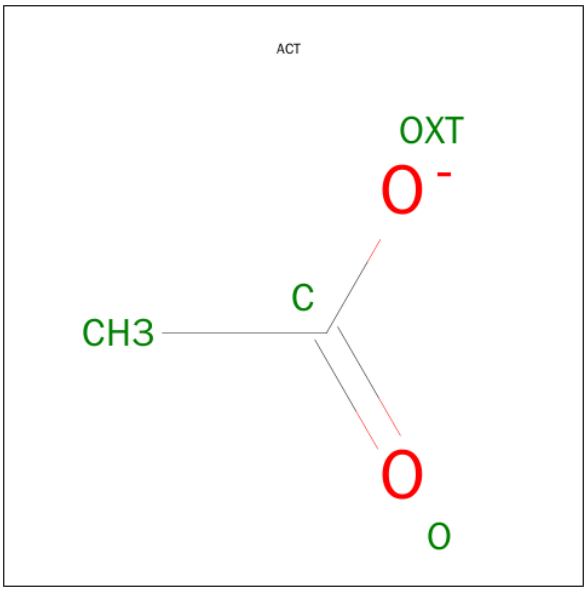
- Molecule 1 is a protein called Nitric-oxide synthase, endothelial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3220	1	2048	564	590	17			
1	B	405	Total	As	C	N	O	S	0	0	0
			3227	1	2052	567	590	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	see remark 999	UNP P29473
A	106	MET	VAL	engineered	UNP P29473
A	368	ASP	ASN	engineered	UNP P29473
A	384	CAS	CYS	modified residue	UNP P29473
B	100	ARG	CYS	see remark 999	UNP P29473
B	106	MET	VAL	engineered	UNP P29473
B	368	ASP	ASN	engineered	UNP P29473
B	384	CAS	CYS	modified residue	UNP P29473

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

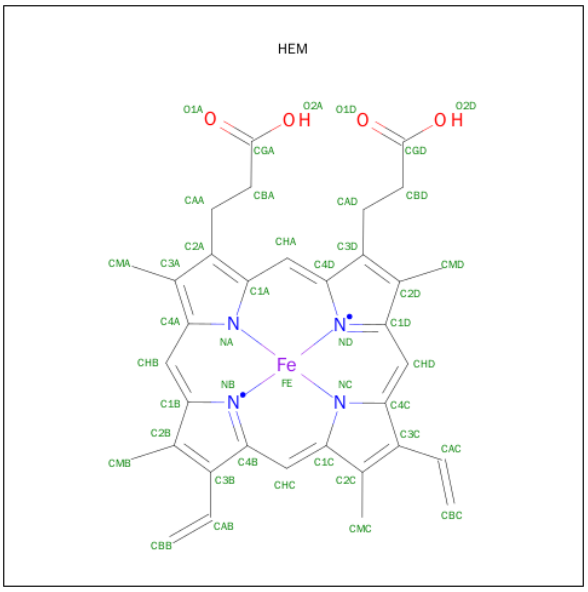


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

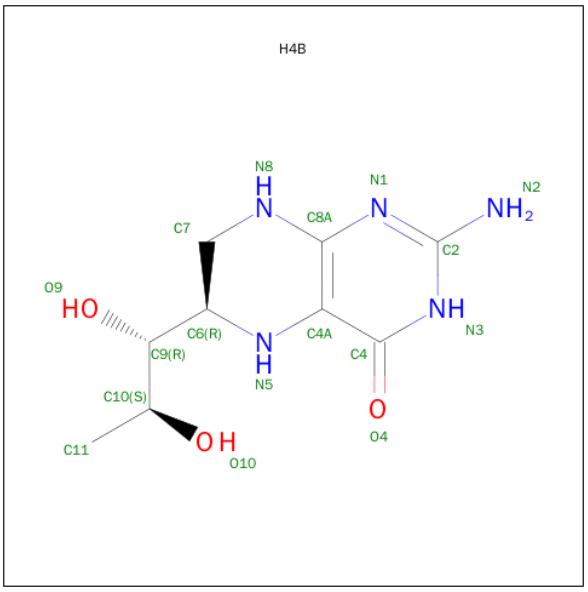
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	9	5	3		

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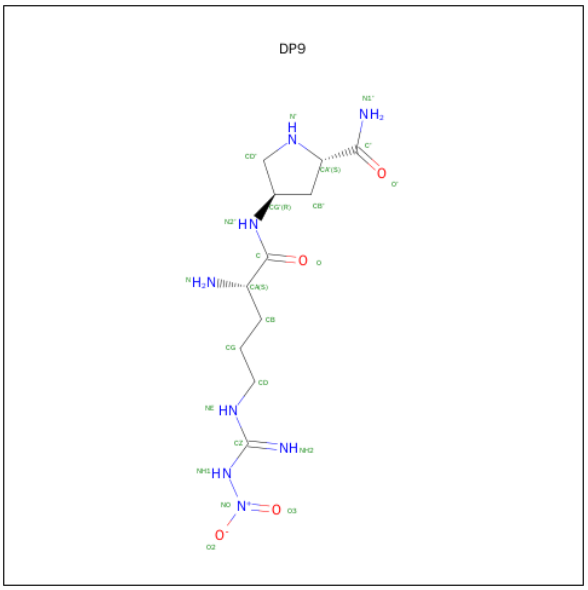
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 17 9 5 3	0	0

- Molecule 6 is L-N(OMEGA)-NITROARGININE-(4R)-AMINO-L-PROLINE AMIDE (three-letter code: DP9) (formula: $C_{11}H_{22}N_8O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 23 11 8 4	0	0
6	B	1	Total C N O 23 11 8 4	0	0

- Molecule 7 is water.

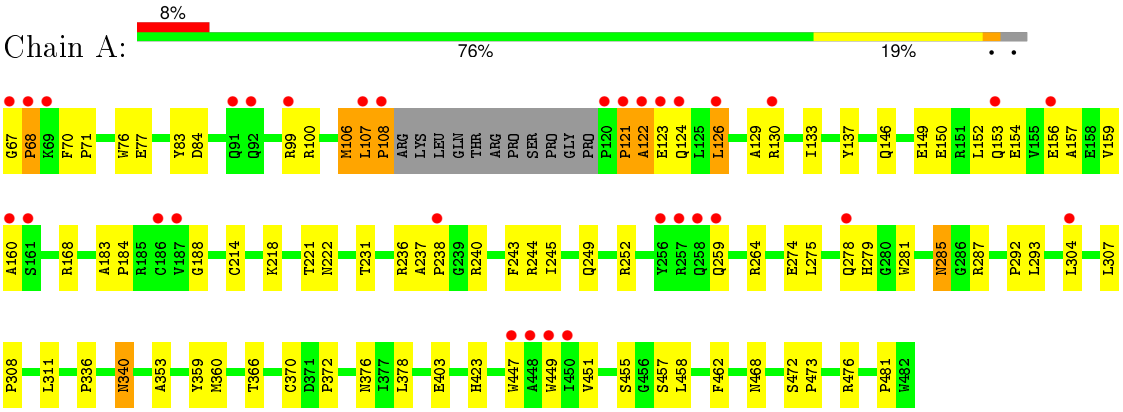
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	189	Total O 189 189	0	0
7	B	183	Total O 183 183	0	0

3 Residue-property plots (i)

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

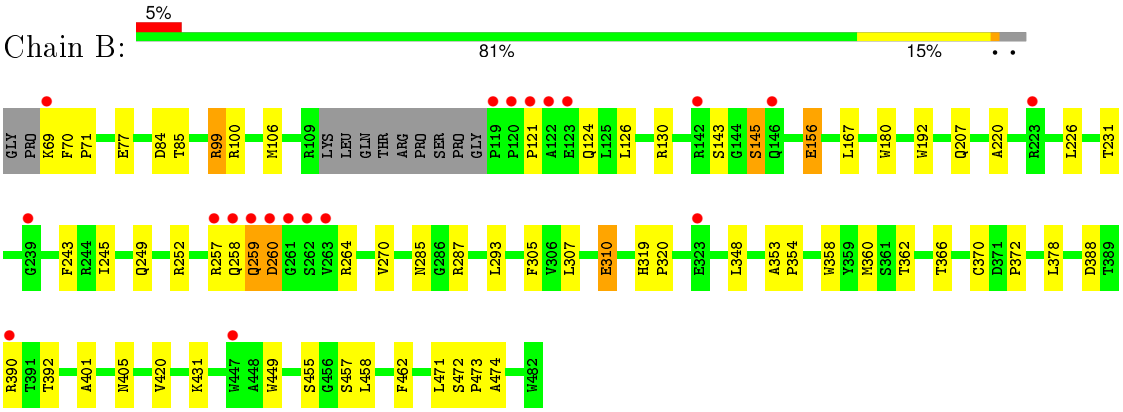
- Molecule 1: Nitric-oxide synthase, endothelial

Chain A:



- Molecule 1: Nitric-oxide synthase, endothelial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.45Å 105.74Å 155.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.43 – 2.14 47.43 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.43-2.14) 95.5 (47.43-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.233 0.185 , 0.227	Depositor DCC
R_{free} test set	2583 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 54769 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6994	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, H4B, CAS, DP9, ACT, HEM

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	0.49	0/3301	0.72	3/4495 (0.1%)
1	B	0.48	0/3308	0.71	3/4504 (0.1%)
All	All	0.48	0/6609	0.71	6/8999 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	360	MET	N-CA-C	-6.09	94.57	111.00
1	A	360	MET	N-CA-C	-5.71	95.58	111.00
1	B	243	PHE	N-CA-C	-5.29	96.72	111.00
1	B	245	ILE	N-CA-C	-5.29	96.73	111.00
1	A	243	PHE	N-CA-C	-5.20	96.97	111.00
1	A	245	ILE	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	TYR	Sidechain

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	3220	0	3119	73	0
1	B	3227	0	3129	55	0
2	A	4	0	3	1	0
2	B	4	0	3	8	0
3	A	1	0	0	0	0
4	A	43	0	30	0	0
4	B	43	0	30	0	0
5	A	17	0	15	3	0
5	B	17	0	15	3	0
6	A	23	0	21	0	0
6	B	23	0	21	0	0
7	A	189	0	0	6	0
7	B	183	0	0	4	0
All	All	6994	0	6386	123	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 9.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:MET:HE2	5:B:761:H4B:H9	1.47	0.97
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.48	0.92
1:B:126:LEU:O	1:B:130:ARG:HG3	1.74	0.88
1:B:358:TRP:HE1	2:B:861:ACT:H2	1.39	0.86
1:B:358:TRP:HE1	2:B:861:ACT:CH3	1.87	0.86
1:A:249:GLN:HB2	1:A:252:ARG:HG3	1.64	0.80
1:B:388:ASP:OD1	1:B:390:ARG:HB2	1.83	0.78
1:A:126:LEU:O	1:A:130:ARG:HG3	1.86	0.75
1:A:126:LEU:HD12	1:A:130:ARG:HE	1.50	0.75
1:A:68:PRO:HD2	1:A:83:TYR:CE2	2.26	0.71
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.31	0.70
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.33	0.68
1:A:293:LEU:HG	1:A:307:LEU:HD21	1.75	0.67
1:A:126:LEU:HD23	1:A:159:VAL:HG11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.78	0.66
1:B:257:ARG:HE	1:B:270:VAL:HG11	1.60	0.65
1:B:358:TRP:NE1	2:B:861:ACT:H2	2.09	0.65
1:B:249:GLN:HB2	1:B:252:ARG:HG2	1.78	0.64
1:A:126:LEU:HD12	1:A:130:ARG:NE	2.13	0.63
1:A:293:LEU:HG	1:A:307:LEU:CD2	2.30	0.62
1:A:146:GLN:HG2	1:A:150:GLU:OE2	2.02	0.60
1:A:106:MET:HE1	5:A:760:H4B:HN5	1.66	0.60
1:B:249:GLN:HB2	1:B:252:ARG:CG	2.32	0.60
1:A:279:HIS:HE1	7:A:1069:HOH:O	1.84	0.59
1:A:274:GLU:O	1:A:278:GLN:HG3	2.01	0.59
1:B:293:LEU:HD11	1:B:307:LEU:HD21	1.85	0.59
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.85	0.59
1:A:152:LEU:O	1:A:156:GLU:HG3	2.02	0.58
1:B:420:VAL:HG11	2:B:861:ACT:H3	1.84	0.58
1:A:107:LEU:HB3	1:A:108:PRO:CD	2.33	0.58
1:B:431:LYS:HE3	7:B:936:HOH:O	2.03	0.57
1:A:372:PRO:HG2	1:B:77:GLU:HG3	1.86	0.56
1:B:378:LEU:HB2	7:B:863:HOH:O	2.05	0.56
1:B:449:TRP:HA	5:B:761:H4B:N1	2.20	0.56
1:A:107:LEU:HB3	1:A:108:PRO:HD2	1.87	0.56
1:A:188:GLY:HA2	2:A:860:ACT:H1	1.89	0.55
1:A:68:PRO:CD	1:A:83:TYR:CZ	2.89	0.55
1:B:71:PRO:HG2	1:B:84:ASP:HB3	1.89	0.55
1:A:149:GLU:O	1:A:153:GLN:HG3	2.07	0.55
1:B:310:GLU:HG2	1:B:310:GLU:O	2.07	0.55
1:A:287:ARG:HD2	7:A:962:HOH:O	2.07	0.54
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.73	0.54
1:A:76:TRP:CD1	1:B:106:MET:HE3	2.43	0.54
1:B:130:ARG:HB3	1:B:130:ARG:HH11	1.71	0.54
1:A:275:LEU:O	1:A:279:HIS:HD2	1.92	0.53
1:A:106:MET:HE1	5:A:760:H4B:N5	2.22	0.53
1:A:423:HIS:HB2	1:B:392:THR:HB	1.92	0.52
1:A:107:LEU:O	1:A:108:PRO:C	2.47	0.52
1:A:237:ALA:HB3	1:A:240:ARG:HB3	1.90	0.52
1:B:106:MET:CE	5:B:761:H4B:H9	2.32	0.52
1:A:146:GLN:O	1:A:150:GLU:HG3	2.11	0.51
1:B:390:ARG:HD2	7:B:972:HOH:O	2.10	0.51
1:A:68:PRO:HG2	1:A:83:TYR:CG	2.44	0.51
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.73	0.51
1:A:279:HIS:CE1	7:A:1069:HOH:O	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:HB3	1:A:84:ASP:O	2.11	0.51
1:A:264:ARG:NE	1:A:285:ASN:O	2.40	0.50
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.26	0.50
1:B:287:ARG:HD3	7:B:974:HOH:O	2.11	0.50
1:B:126:LEU:HD11	1:B:156:GLU:HG2	1.93	0.50
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.76	0.49
1:B:264:ARG:NE	1:B:285:ASN:O	2.44	0.49
1:A:154:GLU:OE1	1:A:168:ARG:NH2	2.46	0.49
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.94	0.49
1:B:420:VAL:CB	2:B:861:ACT:H3	2.43	0.48
1:A:68:PRO:HD3	1:A:83:TYR:CZ	2.48	0.48
1:A:472:SER:HA	1:A:473:PRO:C	2.34	0.48
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.94	0.48
1:A:99:ARG:NH1	1:A:99:ARG:HG3	2.29	0.48
1:B:264:ARG:HG3	1:B:264:ARG:HH11	1.78	0.48
1:A:293:LEU:CG	1:A:307:LEU:HD21	2.43	0.47
1:B:69:LYS:HD2	1:B:70:PHE:CE1	2.49	0.47
1:A:236:ARG:NH1	7:A:1073:HOH:O	2.44	0.47
1:B:130:ARG:HB3	1:B:130:ARG:NH1	2.30	0.47
1:A:336:PRO:HB3	1:A:359:TYR:CZ	2.49	0.47
1:A:378:LEU:HB2	7:A:909:HOH:O	2.14	0.47
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.50	0.47
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.51	0.46
1:A:366:THR:O	1:A:370:CYS:HB2	2.15	0.46
1:B:362:THR:HA	1:B:405:ASN:HD21	1.80	0.46
1:B:362:THR:HA	1:B:405:ASN:ND2	2.29	0.46
1:A:292:PRO:HA	7:A:970:HOH:O	2.15	0.46
1:B:207:GLN:NE2	1:B:305:PHE:HE2	2.13	0.46
1:A:68:PRO:CD	1:A:83:TYR:CE2	2.98	0.45
1:A:121:PRO:O	1:A:124:GLN:N	2.50	0.45
1:A:457:SER:HA	1:A:462:PHE:CG	2.51	0.45
1:A:157:ALA:O	1:A:160:ALA:HB3	2.17	0.45
1:A:449:TRP:HA	5:A:760:H4B:N1	2.32	0.45
1:A:121:PRO:O	1:A:123:GLU:N	2.51	0.44
1:A:403:GLU:HA	1:A:403:GLU:OE1	2.16	0.44
1:B:457:SER:HA	1:B:462:PHE:CG	2.52	0.44
1:B:472:SER:HA	1:B:473:PRO:C	2.38	0.44
1:B:70:PHE:HD2	1:B:85:THR:HA	1.83	0.44
1:B:121:PRO:HG2	1:B:124:GLN:HE21	1.83	0.44
1:A:308:PRO:HD2	1:A:311:LEU:HD12	2.00	0.43
1:A:455:SER:HB3	1:A:458:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ARG:HH11	1:A:476:ARG:HG2	1.82	0.43
1:A:214:CYS:O	1:A:218:LYS:HG3	2.18	0.43
1:A:126:LEU:CD2	1:A:159:VAL:HG11	2.48	0.43
1:B:420:VAL:CG1	2:B:861:ACT:H3	2.46	0.43
1:A:447:TRP:CZ2	1:A:451:VAL:HG21	2.53	0.43
1:B:358:TRP:HE1	2:B:861:ACT:H1	1.77	0.43
1:A:129:ALA:O	1:A:133:ILE:HG12	2.19	0.43
1:B:231:THR:O	1:B:353:ALA:HA	2.18	0.43
1:A:121:PRO:C	1:A:123:GLU:N	2.72	0.43
1:A:476:ARG:NH1	1:A:476:ARG:HG2	2.33	0.42
1:A:231:THR:O	1:A:353:ALA:HA	2.19	0.42
1:A:458:LEU:HD11	1:B:401:ALA:CB	2.50	0.42
1:B:143:SER:C	1:B:145:SER:H	2.23	0.42
1:B:126:LEU:HG	1:B:130:ARG:HD2	2.01	0.42
1:A:67:GLY:HA3	1:A:68:PRO:HD3	1.54	0.42
1:B:471:LEU:O	1:B:474:ALA:HB2	2.19	0.42
1:A:122:ALA:O	1:A:126:LEU:HB2	2.19	0.41
1:A:285:ASN:HD22	1:A:285:ASN:C	2.24	0.41
1:A:71:PRO:HD2	1:A:84:ASP:O	2.20	0.41
1:B:420:VAL:HG21	2:B:861:ACT:H3	2.02	0.41
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.93	0.41
1:A:340:ASN:HD22	1:A:340:ASN:H	1.68	0.41
1:B:366:THR:O	1:B:370:CYS:HB2	2.21	0.41
1:B:258:GLN:O	1:B:259:GLN:C	2.59	0.40
1:A:221:THR:O	1:A:222:ASN:C	2.60	0.40
1:B:231:THR:O	1:B:354:PRO:HD2	2.21	0.40
1:B:220:ALA:O	1:B:226:LEU:HA	2.22	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	400/416 (96%)	380 (95%)	15 (4%)	5 (1%)	15 7
1	B	400/416 (96%)	384 (96%)	13 (3%)	3 (1%)	24 14
All	All	800/832 (96%)	764 (96%)	28 (4%)	8 (1%)	19 10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	PRO
1	B	259	GLN
1	B	145	SER
1	B	260	ASP
1	A	121	PRO
1	A	122	ALA
1	A	238	PRO
1	A	107	LEU

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	343/353 (97%)	334 (97%)	9 (3%)	54 54
1	B	344/353 (98%)	339 (98%)	5 (2%)	72 76
All	All	687/706 (97%)	673 (98%)	14 (2%)	63 66

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

Mol	Chain	Res	Type
1	A	100	ARG
1	A	106	MET
1	A	108	PRO
1	A	126	LEU
1	A	259	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN

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Mol	Chain	Res	Type
1	A	468	ASN
1	B	99	ARG
1	B	100	ARG
1	B	156	GLU
1	B	260	ASP
1	B	310	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	191	GLN
1	A	207	GLN
1	A	279	HIS
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	124	GLN
1	B	146	GLN
1	B	191	GLN
1	B	207	GLN
1	B	215	ASN
1	B	222	ASN
1	B	279	HIS
1	B	405	ASN
1	B	413	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	CAS	A	384	1	5,8,9	2.82	2 (40%)	2,9,11	1.30	0
1	CAS	B	384	1	5,8,9	2.94	2 (40%)	2,9,11	1.99	1 (50%)

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
1	CAS	A	384	1	-	0/0/7/9	0/0/0/0
1	CAS	B	384	1	-	0/0/7/9	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-CE1	-4.61	1.83	1.96
1	B	384	CAS	AS-CE2	-4.57	1.84	1.96
1	A	384	CAS	AS-CE2	-4.45	1.84	1.96
1	A	384	CAS	AS-CE1	-4.40	1.84	1.96

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	384	CAS	CA-CB-SG	2.07	121.51	114.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	HEM	A	700	1	30,50,50	2.82	8 (26%)	24,82,82	2.36	10 (41%)
5	H4B	A	760	-	13,18,18	2.14	3 (23%)	11,26,26	4.13	6 (54%)
6	DP9	A	799	-	17,23,23	0.81	1 (5%)	16,30,30	1.64	4 (25%)
2	ACT	A	860	-	1,3,3	0.35	0	0,3,3	0.00	-
4	HEM	B	700	1	30,50,50	2.66	8 (26%)	24,82,82	2.27	9 (37%)
5	H4B	B	761	-	13,18,18	2.19	4 (30%)	11,26,26	4.06	6 (54%)
6	DP9	B	800	-	17,23,23	0.82	1 (5%)	16,30,30	1.89	4 (25%)
2	ACT	B	861	-	1,3,3	0.71	0	0,3,3	0.00	-

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
4	HEM	A	700	1	-	0/10/54/54	0/0/8/8
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
6	DP9	A	799	-	-	0/17/32/32	0/1/1/1
2	ACT	A	860	-	-	0/0/0/0	0/0/0/0
4	HEM	B	700	1	-	0/10/54/54	0/0/8/8
5	H4B	B	761	-	-	0/8/17/17	0/2/2/2
6	DP9	B	800	-	-	0/17/32/32	0/1/1/1
2	ACT	B	861	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	700	HEM	C3B-C4B	-7.51	1.45	1.51
4	A	700	HEM	C3D-C4D	-6.52	1.43	1.51
4	B	700	HEM	C3D-C4D	-6.15	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	700	HEM	C2D-C3D	-5.96	1.36	1.54
4	A	700	HEM	C2D-C3D	-5.96	1.36	1.54
4	A	700	HEM	C3B-C4B	-5.74	1.46	1.51
4	A	700	HEM	C3B-CAB	-5.70	1.40	1.51
4	A	700	HEM	C3C-CAC	-5.35	1.41	1.51
4	B	700	HEM	C2C-C1C	-4.21	1.44	1.52
4	B	700	HEM	C3C-CAC	-4.12	1.43	1.51
4	B	700	HEM	C3B-CAB	-4.10	1.43	1.51
4	A	700	HEM	C2C-C1C	-4.04	1.44	1.52
4	B	700	HEM	C2B-C1B	-2.61	1.43	1.51
4	B	700	HEM	C2D-C1D	-2.38	1.44	1.51
4	A	700	HEM	C1C-NC	2.39	1.38	1.36
6	A	799	DP9	CG'-N2'	2.42	1.51	1.46
5	B	761	H4B	C8A-N1	2.43	1.39	1.34
6	B	800	DP9	CG'-N2'	2.61	1.51	1.46
5	B	761	H4B	C6-N5	3.47	1.52	1.45
5	A	760	H4B	C4A-N5	3.80	1.46	1.38
5	B	761	H4B	C4A-N5	3.98	1.47	1.38
5	A	760	H4B	C6-N5	4.16	1.54	1.45
5	A	760	H4B	C4-N3	4.63	1.41	1.33
4	A	700	HEM	C4C-NC	4.71	1.41	1.36
5	B	761	H4B	C4-N3	4.92	1.42	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	700	HEM	CBA-CAA-C2A	-5.28	103.07	112.53
4	B	700	HEM	CBA-CAA-C2A	-4.85	103.83	112.53
5	A	760	H4B	N3-C2-N1	-4.83	117.61	125.53
5	B	761	H4B	N3-C2-N1	-4.81	117.65	125.53
6	B	800	DP9	O'-C'-N1'	-4.08	117.03	123.08
6	B	800	DP9	C'-CA'-N'	-3.82	104.63	111.88
6	A	799	DP9	C'-CA'-N'	-3.32	105.58	111.88
6	A	799	DP9	O'-C'-N1'	-3.31	118.17	123.08
4	A	700	HEM	CAA-C2A-C1A	-2.27	124.55	127.01
4	A	700	HEM	CBD-CAD-C3D	-2.13	107.36	113.55
4	B	700	HEM	CBD-CAD-C3D	-2.10	107.45	113.55
6	B	800	DP9	CG'-N2'-C	2.24	126.65	123.18
4	A	700	HEM	CMD-C2D-C3D	2.31	124.58	114.35
4	B	700	HEM	CMD-C2D-C3D	2.37	124.81	114.35
6	A	799	DP9	CG'-N2'-C	2.40	126.91	123.18
6	A	799	DP9	CA'-C'-N1'	2.42	120.50	116.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	700	HEM	C2D-C3D-C4D	2.48	105.70	101.50
4	A	700	HEM	C3C-CAC-CBC	2.67	128.56	124.46
4	B	700	HEM	CMB-C2B-C3B	2.81	123.55	116.53
6	B	800	DP9	CA'-C'-N1'	2.94	121.34	116.60
4	A	700	HEM	CMB-C2B-C3B	2.96	123.92	116.53
5	A	760	H4B	N2-C2-N1	3.27	122.62	117.20
4	A	700	HEM	C2D-C3D-C4D	3.27	107.05	101.50
5	B	761	H4B	N2-C2-N1	3.45	122.91	117.20
5	B	761	H4B	C2-N1-C8A	3.56	122.53	114.54
5	B	761	H4B	C4A-C8A-N8	3.57	122.63	118.43
4	B	700	HEM	CAD-C3D-C4D	3.61	125.19	112.47
4	A	700	HEM	CAD-C3D-C4D	3.62	125.23	112.47
4	B	700	HEM	C3B-CAB-CBB	3.64	130.04	124.46
5	A	760	H4B	C2-N1-C8A	3.65	122.74	114.54
5	A	760	H4B	C4A-C8A-N8	3.92	123.05	118.43
4	B	700	HEM	CMC-C2C-C3C	4.29	127.24	116.53
4	A	700	HEM	CMC-C2C-C3C	4.39	127.48	116.53
4	A	700	HEM	CAD-C3D-C2D	5.00	127.59	113.22
4	B	700	HEM	CAD-C3D-C2D	5.04	127.71	113.22
5	B	761	H4B	C4-N3-C2	6.43	124.86	115.94
5	A	760	H4B	C4-N3-C2	6.60	125.10	115.94
5	A	760	H4B	C4-C4A-C8A	8.70	122.43	114.56
5	B	761	H4B	C4-C4A-C8A	8.70	122.44	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	760	H4B	3	0
2	A	860	ACT	1	0
5	B	761	H4B	3	0
2	B	861	ACT	8	0

5.7 Other polymers (i)

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^{th} 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	404/416 (97%)	0.61	32 (7%)	15	21	27, 37, 63, 85	0
1	B	404/416 (97%)	0.38	20 (4%)	32	42	29, 40, 65, 92	0
All	All	808/832 (97%)	0.49	52 (6%)	23	30	27, 39, 64, 92	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	GLY	14.9
1	B	120	PRO	9.4
1	B	119	PRO	7.6
1	A	120	PRO	7.1
1	B	259	GLN	5.9
1	A	126	LEU	5.4
1	A	122	ALA	5.2
1	A	121	PRO	5.0
1	A	123	GLU	4.6
1	A	160	ALA	4.3
1	A	259	GLN	4.2
1	B	261	GLY	4.0
1	A	161	SER	3.8
1	B	257	ARG	3.8
1	A	108	PRO	3.6
1	A	153	GLN	3.6
1	A	69	LYS	3.5
1	B	121	PRO	3.5
1	A	91	GLN	3.5
1	A	68	PRO	3.4
1	B	258	GLN	3.3
1	A	238	PRO	3.3
1	B	323	GLU	3.2
1	B	123	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	107	LEU	3.0
1	B	69	LYS	3.0
1	B	390	ARG	2.8
1	B	239	GLY	2.8
1	A	448	ALA	2.7
1	A	92	GLN	2.5
1	A	256	TYR	2.5
1	B	122	ALA	2.5
1	B	260	ASP	2.5
1	A	124	GLN	2.5
1	A	257	ARG	2.5
1	A	450	ILE	2.5
1	A	130	ARG	2.5
1	A	278	GLN	2.4
1	A	187	VAL	2.4
1	A	304	LEU	2.3
1	A	258	GLN	2.3
1	A	186	CYS	2.3
1	A	99	ARG	2.2
1	B	223	ARG	2.2
1	A	156	GLU	2.2
1	B	263	VAL	2.2
1	B	142	ARG	2.1
1	A	447	TRP	2.1
1	B	447	TRP	2.1
1	B	262	SER	2.1
1	B	146	GLN	2.0
1	A	449	TRP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CAS	B	384	9/10	0.97	0.10	-	49,51,66,67	0
1	CAS	A	384	9/10	0.99	0.09	-	36,37,52,56	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ACT	B	861	4/4	0.95	0.24	8.17	46,48,51,53	0
2	ACT	A	860	4/4	0.92	0.40	7.04	41,42,42,43	0
6	DP9	B	800	23/23	0.93	0.15	1.28	31,38,51,53	0
4	HEM	A	700	43/43	0.98	0.20	1.06	23,28,34,42	0
5	H4B	B	761	17/17	0.96	0.17	0.55	30,32,36,36	0
5	H4B	A	760	17/17	0.97	0.18	0.33	30,35,38,39	0
4	HEM	B	700	43/43	0.98	0.13	0.16	25,29,37,39	0
6	DP9	A	799	23/23	0.95	0.15	-0.27	33,38,49,52	0
3	ZN	A	900	1/1	1.00	0.08	-1.97	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.