



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:01 PM GMT

PDB ID : 1RS8
Title : Bovine endothelial NOS heme domain with D-lysine-D-nitroarginine amide bound
Authors : Flinspach, M.; Li, H.; Jamal, J.; Yang, W.; Huang, H.; Silverman, R.B.; Poulos, T.L.
Deposited on : 2003-12-09
Resolution : 2.30 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

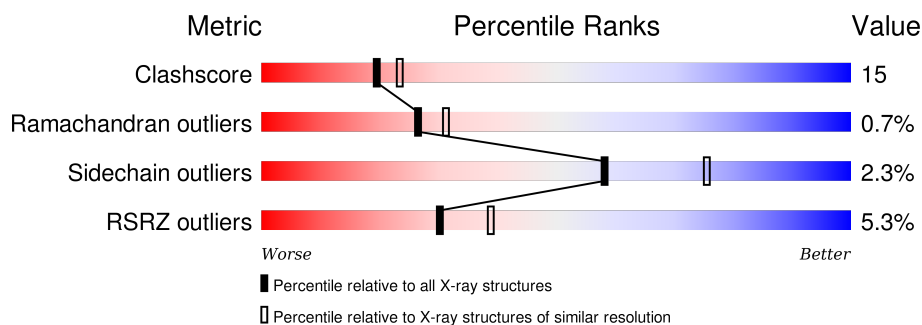
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	416	<div> <div>5%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>
1	B	416	<div> <div>6%</div> <div>67%</div> <div>30%</div> <div>.</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
3	ACT	B	861	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7079 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.

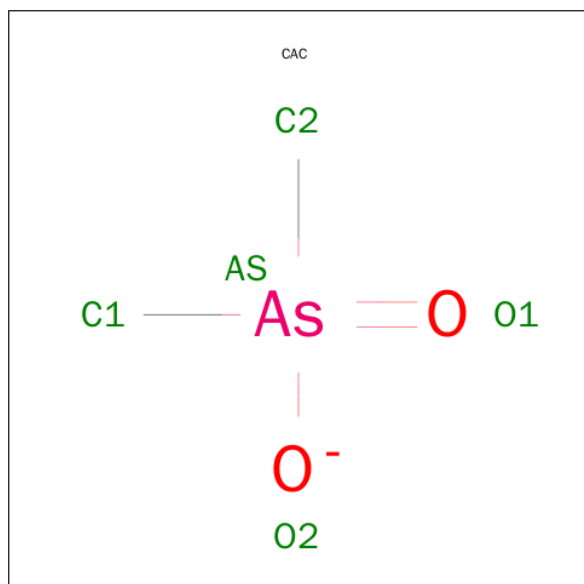
- Molecule 1 is a protein called Nitric-oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3227	2052	569	590	16			
1	B	404	Total	C	N	O	S	0	0	0
			3216	2045	567	588	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	As C	0	0
			3	1 2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

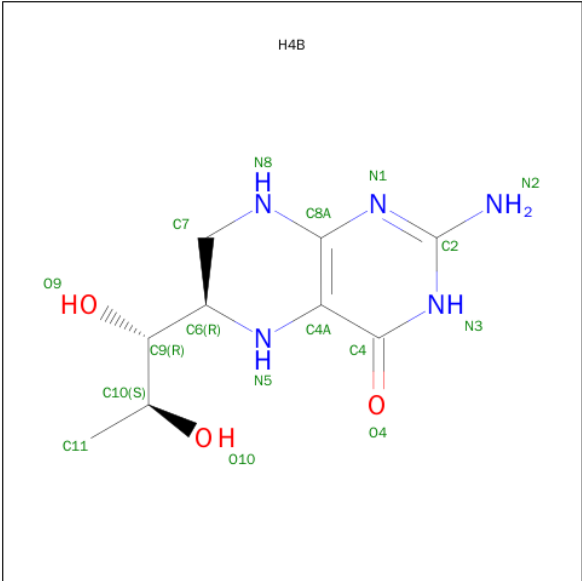
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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



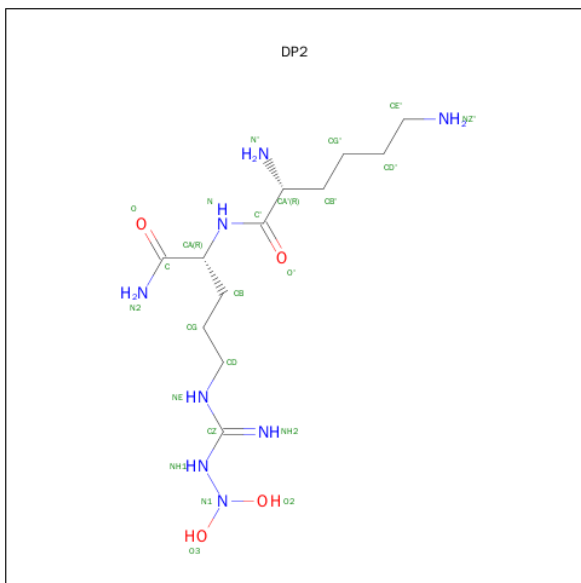
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			17	9	5	3		

Continued on next page...

Continued from previous page...

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

- Molecule 7 is L-LYSYL-N 5 -[(Z)-(2,2-DIHYDROXYHYDRAZINO)(IMINO)METHYL]-L-ORNITHINAMIDE (three-letter code: DP2) (formula: $C_{12}H_{28}N_8O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 24	C 12	N 8	O 4	0	0
7	B	1	Total 24	C 12	N 8	O 4	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

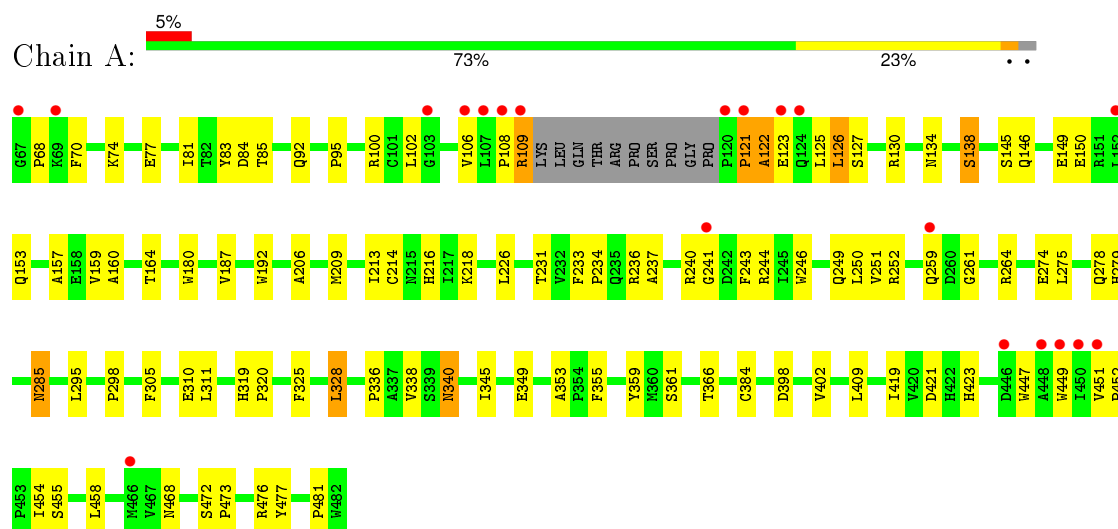
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	231	Total	O	0	0
			231	231		
9	B	210	Total	O	0	0
			210	210		

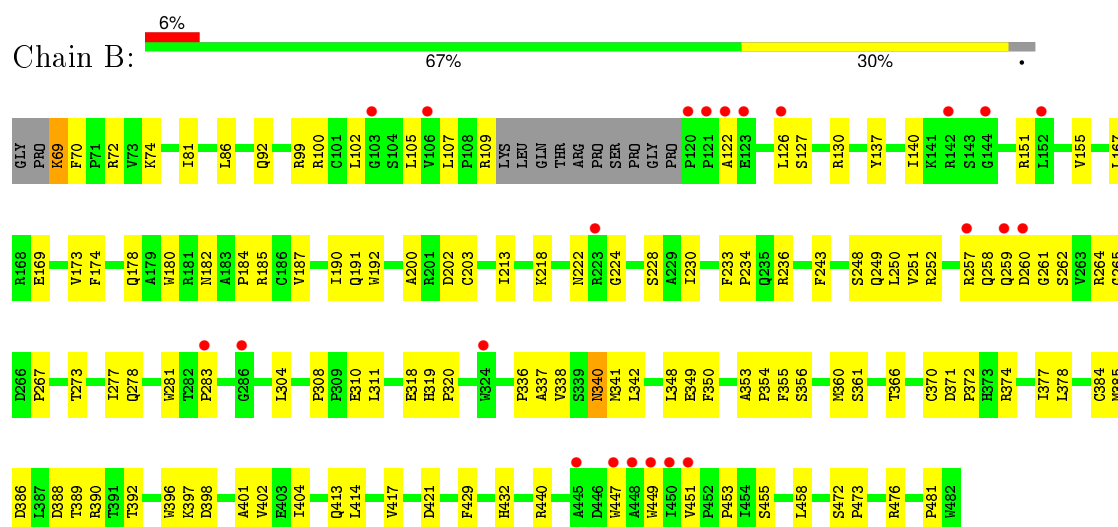
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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



- Molecule 1: Nitric-oxide synthase, endothelial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.01Å 106.22Å 156.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.83 – 2.30 46.83 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.83-2.30) 82.2 (46.83-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.276 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 48100 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7079	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, ACT, CAC, HEM, DP2

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	0.42	0/3318	0.65	0/4520
1	B	0.40	0/3306	0.65	1/4503 (0.0%)
All	All	0.41	0/6624	0.65	1/9023 (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	B	360	MET	N-CA-C	-5.46	96.25	111.00

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	3227	0	3135	93	0
1	B	3216	0	3125	103	0
2	A	3	0	0	3	0
2	B	3	0	0	1	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	1	0	0	0	0
5	A	43	0	30	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	43	0	30	2	0
6	A	17	0	15	1	0
6	B	17	0	15	1	0
7	A	24	0	27	1	0
7	B	24	0	27	2	0
8	A	6	0	8	0	0
8	B	6	0	8	2	0
9	A	231	0	0	5	0
9	B	210	0	0	14	0
All	All	7079	0	6426	196	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 15.

All (196) 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:384:CYS:SG	2:A:850:CAC:AS	2.84	0.95
1:B:350:PHE:HB3	9:B:1071:HOH:O	1.76	0.85
1:B:249:GLN:HB2	1:B:252:ARG:HD2	1.60	0.84
1:B:388:ASP:OD1	1:B:390:ARG:HB3	1.79	0.82
1:A:149:GLU:O	1:A:153:GLN:HG2	1.79	0.81
1:B:384:CYS:SG	2:B:852:CAC:AS	3.01	0.79
1:B:259:GLN:HG2	1:B:260:ASP:H	1.47	0.79
1:B:277:ILE:HG12	1:B:283:PRO:HG3	1.66	0.77
1:B:190:ILE:HB	9:B:1059:HOH:O	1.84	0.77
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.50	0.76
1:A:146:GLN:O	1:A:150:GLU:HG3	1.85	0.75
1:A:108:PRO:HD3	9:A:1118:HOH:O	1.86	0.74
1:B:259:GLN:HG2	1:B:260:ASP:N	2.03	0.73
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.71	0.72
1:B:432:HIS:HB2	9:B:1059:HOH:O	1.89	0.71
1:A:274:GLU:O	1:A:278:GLN:HG3	1.91	0.71
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.73	0.70
1:B:429:PHE:HA	9:B:1059:HOH:O	1.91	0.70
1:B:248:SER:HA	1:B:340:ASN:HB3	1.73	0.70
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.06	0.69
1:A:122:ALA:O	1:A:126:LEU:HB2	1.95	0.67
1:B:69:LYS:HE2	1:B:70:PHE:H	1.60	0.66
1:B:281:TRP:O	1:B:283:PRO:HD3	1.97	0.65
1:B:398:ASP:O	1:B:402:VAL:HG23	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLY:O	1:B:267:PRO:HD3	1.96	0.64
1:B:260:ASP:C	1:B:262:SER:H	2.01	0.64
1:B:340:ASN:HD22	1:B:340:ASN:H	1.44	0.64
1:A:127:SER:HB3	9:A:1106:HOH:O	1.97	0.64
1:B:258:GLN:NE2	1:B:264:ARG:HB2	2.12	0.64
1:A:134:ASN:O	1:A:138:SER:HB2	1.98	0.64
1:B:178:GLN:HB3	9:B:1078:HOH:O	1.97	0.63
1:A:92:GLN:HE22	1:A:476:ARG:HH22	1.46	0.63
1:B:182:ASN:O	1:B:184:PRO:HD3	1.98	0.63
1:A:126:LEU:O	1:A:130:ARG:HG3	1.98	0.62
1:A:285:ASN:HD22	1:A:285:ASN:H	1.46	0.62
1:A:366:THR:HG21	1:A:454:ILE:HG23	1.81	0.62
1:A:237:ALA:HB3	1:A:240:ARG:HB3	1.82	0.62
1:A:285:ASN:N	1:A:285:ASN:HD22	1.98	0.62
1:B:249:GLN:HB2	1:B:252:ARG:CD	2.30	0.61
1:B:361:SER:OG	1:B:421:ASP:HA	2.03	0.59
1:B:251:VAL:O	1:B:252:ARG:HG2	2.02	0.59
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.38	0.58
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.85	0.58
1:B:378:LEU:HB2	9:B:887:HOH:O	2.03	0.58
1:A:145:SER:O	1:A:149:GLU:HG2	2.03	0.58
1:B:224:GLY:O	1:B:417:VAL:HA	2.04	0.57
1:B:69:LYS:HE2	1:B:70:PHE:N	2.20	0.57
1:A:121:PRO:O	1:A:123:GLU:N	2.38	0.57
1:A:74:LYS:HB2	1:A:81:ILE:HD13	1.86	0.57
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.20	0.57
1:A:214:CYS:O	1:A:218:LYS:HG3	2.05	0.57
1:B:257:ARG:HG3	1:B:257:ARG:HH11	1.69	0.56
1:B:250:LEU:N	9:B:1070:HOH:O	2.39	0.55
1:B:371:ASP:HB2	1:B:374:ARG:HG2	1.89	0.55
1:B:340:ASN:N	1:B:340:ASN:HD22	2.03	0.54
1:B:338:VAL:HB	1:B:355:PHE:CZ	2.42	0.54
1:B:371:ASP:HB2	1:B:374:ARG:CG	2.37	0.53
1:B:218:LYS:CG	1:B:311:LEU:HD11	2.38	0.53
1:B:258:GLN:HE22	1:B:264:ARG:HD2	1.74	0.52
1:B:102:LEU:HB3	1:B:105:LEU:HD22	1.92	0.52
1:B:388:ASP:C	1:B:390:ARG:H	2.12	0.52
1:B:257:ARG:HG3	1:B:257:ARG:NH1	2.25	0.52
1:A:340:ASN:HD22	1:A:340:ASN:H	1.57	0.52
1:A:249:GLN:HB2	1:A:252:ARG:CG	2.38	0.52
1:B:260:ASP:O	1:B:262:SER:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:SER:CB	1:A:421:ASP:HA	2.41	0.51
1:B:310:GLU:N	1:B:310:GLU:OE2	2.32	0.51
1:A:361:SER:OG	1:A:409:LEU:HG	2.10	0.51
1:B:337:ALA:HA	1:B:355:PHE:O	2.10	0.51
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.93	0.51
1:A:70:PHE:CD1	1:A:85:THR:HG22	2.46	0.51
1:B:151:ARG:O	1:B:155:VAL:HG23	2.11	0.51
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.93	0.50
1:B:353:ALA:HB2	9:B:1071:HOH:O	2.10	0.50
1:B:228:SER:HA	1:B:356:SER:O	2.11	0.50
1:A:213:ILE:HG23	1:A:250:LEU:HD13	1.94	0.50
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.94	0.49
1:B:366:THR:O	1:B:370:CYS:HB2	2.13	0.49
1:A:476:ARG:HH11	1:A:476:ARG:HG2	1.77	0.49
1:B:218:LYS:HG2	1:B:311:LEU:HD11	1.93	0.49
1:B:107:LEU:HD21	7:B:793:DP2:HE'1	1.94	0.49
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.41	0.49
1:B:273:THR:O	1:B:277:ILE:HG13	2.12	0.49
1:B:340:ASN:H	1:B:340:ASN:ND2	2.09	0.49
1:A:384:CYS:CB	2:A:850:CAC:AS	3.21	0.49
1:A:236:ARG:HG3	1:A:349:GLU:O	2.13	0.49
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.48	0.49
1:A:449:TRP:HA	6:A:760:H4B:N1	2.28	0.49
1:A:92:GLN:HE22	1:A:476:ARG:NH2	2.09	0.48
1:A:409:LEU:HD11	1:A:421:ASP:HB3	1.95	0.48
1:B:260:ASP:C	1:B:262:SER:N	2.64	0.48
1:A:240:ARG:HD2	1:A:241:GLY:O	2.14	0.48
1:A:361:SER:HB2	1:A:421:ASP:HA	1.96	0.48
1:A:398:ASP:O	1:A:402:VAL:HG23	2.13	0.48
1:B:72:ARG:HH21	1:B:74:LYS:HD2	1.78	0.48
1:B:191:GLN:HB3	9:B:892:HOH:O	2.13	0.48
1:A:423:HIS:HB2	1:B:392:THR:HB	1.96	0.47
1:B:126:LEU:O	1:B:130:ARG:HG3	2.13	0.47
1:A:476:ARG:NH1	1:A:476:ARG:HG2	2.29	0.47
1:A:340:ASN:N	1:A:340:ASN:HD22	2.12	0.47
1:A:95:PRO:O	1:A:102:LEU:HD12	2.15	0.47
1:A:251:VAL:O	1:A:252:ARG:HG2	2.15	0.47
1:A:275:LEU:O	1:A:279:HIS:HD2	1.97	0.47
1:B:200:ALA:O	1:B:203:CYS:HB2	2.15	0.47
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.45	0.47
1:A:231:THR:O	1:A:353:ALA:HA	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.50	0.47
1:B:234:PRO:HB2	1:B:243:PHE:CE1	2.50	0.47
1:B:137:TYR:HA	1:B:140:ILE:HG12	1.96	0.46
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.96	0.46
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.81	0.46
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.50	0.46
1:A:472:SER:HA	1:A:473:PRO:C	2.36	0.46
1:A:246:TRP:CD1	1:A:481:PRO:HG3	2.50	0.46
1:A:106:VAL:HG11	9:A:931:HOH:O	2.16	0.46
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.96	0.46
1:A:226:LEU:CD1	1:A:226:LEU:N	2.78	0.46
1:A:240:ARG:NH2	9:A:955:HOH:O	2.48	0.46
1:B:236:ARG:HG3	1:B:349:GLU:O	2.15	0.45
1:A:477:TYR:CE1	7:A:792:DP2:HG'1	2.52	0.45
1:B:213:ILE:HG23	1:B:250:LEU:HD13	1.97	0.45
1:A:249:GLN:HB3	9:A:934:HOH:O	2.15	0.45
1:A:421:ASP:OD2	1:A:423:HIS:HB2	2.17	0.45
1:A:338:VAL:HB	1:A:355:PHE:CZ	2.52	0.45
1:B:258:GLN:HE21	1:B:264:ARG:HB2	1.81	0.45
1:A:366:THR:CG2	1:A:454:ILE:HG23	2.44	0.45
1:B:185:ARG:HB3	1:B:449:TRP:CE3	2.51	0.45
1:B:169:GLU:O	1:B:173:VAL:HG23	2.16	0.45
1:B:122:ALA:O	1:B:126:LEU:HB2	2.17	0.45
1:B:81:ILE:HD11	9:B:954:HOH:O	2.17	0.45
1:B:69:LYS:CE	1:B:70:PHE:H	2.28	0.44
1:A:361:SER:HA	1:A:419:ILE:HD11	1.99	0.44
5:B:500:HEM:HBA2	7:B:793:DP2:HD1	1.99	0.44
1:B:342:LEU:HD23	1:B:342:LEU:C	2.37	0.44
8:B:882:GOL:H32	9:B:1046:HOH:O	2.16	0.44
1:A:384:CYS:HB3	2:A:850:CAC:AS	2.77	0.44
1:A:325:PHE:O	1:A:328:LEU:HB2	2.17	0.44
1:A:150:GLU:O	1:A:153:GLN:HB2	2.18	0.44
1:B:218:LYS:HG2	1:B:311:LEU:CD1	2.48	0.44
1:A:187:VAL:O	1:A:187:VAL:HG22	2.17	0.44
1:A:295:LEU:HD12	1:A:305:PHE:CD1	2.53	0.44
1:A:244:ARG:CZ	1:A:481:PRO:HD3	2.46	0.44
1:B:174:PHE:O	1:B:178:GLN:HG2	2.17	0.44
1:A:159:VAL:HA	1:A:164:THR:O	2.17	0.44
1:B:385:MET:O	1:B:386:ASP:HB3	2.17	0.44
1:A:70:PHE:HB3	1:A:84:ASP:O	2.18	0.43
8:B:882:GOL:C3	9:B:1046:HOH:O	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:O	1:A:122:ALA:C	2.56	0.43
1:A:157:ALA:O	1:A:160:ALA:HB3	2.19	0.43
1:B:69:LYS:N	1:B:69:LYS:HZ3	2.17	0.43
1:B:472:SER:HA	1:B:473:PRO:C	2.39	0.43
1:B:366:THR:HG21	1:B:453:PRO:HB2	2.00	0.43
1:A:206:ALA:O	1:A:209:MET:HB2	2.19	0.43
1:B:230:ILE:HG13	1:B:354:PRO:O	2.18	0.43
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.54	0.43
1:A:310:GLU:N	1:A:310:GLU:OE1	2.47	0.43
5:B:500:HEM:HBB2	5:B:500:HEM:HHC	2.01	0.42
1:B:318:GLU:OE1	1:B:414:LEU:HD22	2.18	0.42
1:B:86:LEU:HD13	1:B:440:ARG:HB3	2.01	0.42
1:B:476:ARG:HD2	9:B:898:HOH:O	2.18	0.42
1:A:458:LEU:HD22	1:B:378:LEU:HD21	2.01	0.42
1:A:340:ASN:ND2	1:A:340:ASN:H	2.17	0.42
1:B:99:ARG:HD3	9:B:1061:HOH:O	2.18	0.42
1:A:125:LEU:HD12	1:A:125:LEU:O	2.18	0.42
1:A:216:HIS:CD2	1:A:216:HIS:C	2.93	0.42
1:B:167:LEU:HG	1:B:348:LEU:HD12	2.02	0.42
1:A:74:LYS:HD2	1:A:81:ILE:HD11	2.02	0.42
1:A:458:LEU:HD11	1:B:401:ALA:CB	2.50	0.42
1:B:377:ILE:HD11	1:B:404:ILE:HD13	2.00	0.42
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.87	0.41
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.55	0.41
1:B:449:TRP:HA	6:B:761:H4B:N1	2.35	0.41
1:B:385:MET:O	1:B:386:ASP:CB	2.68	0.41
1:B:202:ASP:CG	1:B:202:ASP:O	2.59	0.41
1:B:234:PRO:HB2	1:B:243:PHE:CD1	2.55	0.41
1:B:396:TRP:CH2	1:B:397:LYS:HG2	2.55	0.41
1:B:109:ARG:HH11	1:B:109:ARG:HG2	1.86	0.41
1:B:137:TYR:CD2	1:B:140:ILE:HD11	2.56	0.41
1:B:182:ASN:O	1:B:184:PRO:CD	2.68	0.41
1:A:285:ASN:N	1:A:285:ASN:ND2	2.65	0.41
1:B:187:VAL:O	1:B:187:VAL:HG22	2.21	0.41
1:A:259:GLN:C	1:A:261:GLY:H	2.24	0.41
1:A:345:ILE:HG12	1:A:473:PRO:HB3	2.03	0.41
1:A:447:TRP:CZ2	1:A:451:VAL:HG21	2.56	0.41
1:B:258:GLN:HE21	1:B:264:ARG:CB	2.34	0.40
1:A:361:SER:HB3	1:A:421:ASP:HA	2.03	0.40
1:A:259:GLN:CD	1:A:259:GLN:H	2.25	0.40
1:B:249:GLN:HB2	1:B:252:ARG:CG	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:N	1:A:340:ASN:ND2	2.68	0.40
1:B:388:ASP:O	1:B:390:ARG:N	2.53	0.40
1:B:396:TRP:CZ3	1:B:397:LYS:HG2	2.55	0.40
1:B:340:ASN:ND2	1:B:341:MET:HG3	2.36	0.40
1:B:308:PRO:HB2	1:B:311:LEU:HB2	2.03	0.40
1:A:68:PRO:HB2	1:A:83:TYR:CD2	2.57	0.40
1:A:233:PHE:HB3	1:A:234:PRO:HD2	2.03	0.40
1:A:336:PRO:HB3	1:A:359:TYR:CZ	2.57	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	402/416 (97%)	375 (93%)	25 (6%)	2 (0%)	34	41
1	B	400/416 (96%)	367 (92%)	29 (7%)	4 (1%)	19	21
All	All	802/832 (96%)	742 (92%)	54 (7%)	6 (1%)	26	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA
1	B	261	GLY
1	B	389	THR
1	A	121	PRO
1	B	336	PRO
1	B	481	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/354 (98%)	337 (98%)	8 (2%)	58	75
1	B	344/354 (97%)	336 (98%)	8 (2%)	58	75
All	All	689/708 (97%)	673 (98%)	16 (2%)	58	75

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	109	ARG
1	A	126	LEU
1	A	138	SER
1	A	285	ASN
1	A	328	LEU
1	A	340	ASN
1	A	468	ASN
1	B	69	LYS
1	B	92	GLN
1	B	100	ARG
1	B	127	SER
1	B	222	ASN
1	B	278	GLN
1	B	340	ASN
1	B	413	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	124	GLN
1	A	191	GLN
1	A	278	GLN
1	A	279	HIS
1	A	285	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	178	GLN
1	B	222	ASN
1	B	225	ASN
1	B	258	GLN
1	B	278	GLN
1	B	340	ASN
1	B	405	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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$
5	HEM	A	500	1	30,50,50	2.81	9 (30%)	24,82,82	2.42	10 (41%)
6	H4B	A	760	-	13,18,18	2.29	4 (30%)	11,26,26	4.25	6 (54%)
7	DP2	A	792	-	17,23,23	0.84	0	19,28,28	1.32	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CAC	A	850	-	0,2,4	0.00	-	0,1,6	0.00	-
3	ACT	A	860	-	1,3,3	3.80	1 (100%)	0,3,3	0.00	-
8	GOL	A	880	-	5,5,5	0.08	0	5,5,5	0.22	0
5	HEM	B	500	1	30,50,50	2.47	11 (36%)	24,82,82	2.40	8 (33%)
6	H4B	B	761	-	13,18,18	1.99	4 (30%)	11,26,26	4.13	6 (54%)
7	DP2	B	793	-	17,23,23	0.73	0	19,28,28	1.27	2 (10%)
2	CAC	B	852	-	0,2,4	0.00	-	0,1,6	0.00	-
3	ACT	B	861	-	1,3,3	4.40	1 (100%)	0,3,3	0.00	-
8	GOL	B	882	-	5,5,5	0.17	0	5,5,5	0.13	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
5	HEM	A	500	1	-	0/10/54/54	0/0/8/8
6	H4B	A	760	-	-	0/8/17/17	0/2/2/2
7	DP2	A	792	-	-	0/22/28/28	0/0/0/0
2	CAC	A	850	-	-	0/0/0/0	0/0/0/0
3	ACT	A	860	-	-	0/0/0/0	0/0/0/0
8	GOL	A	880	-	-	0/4/4/4	0/0/0/0
5	HEM	B	500	1	-	0/10/54/54	0/0/8/8
6	H4B	B	761	-	-	0/8/17/17	0/2/2/2
7	DP2	B	793	-	-	0/22/28/28	0/0/0/0
2	CAC	B	852	-	-	0/0/0/0	0/0/0/0
3	ACT	B	861	-	-	0/0/0/0	0/0/0/0
8	GOL	B	882	-	-	0/4/4/4	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	HEM	C2D-C3D	-6.44	1.35	1.54
5	A	500	HEM	C3B-CAB	-5.90	1.40	1.51
5	A	500	HEM	C3D-C4D	-5.83	1.44	1.51
5	B	500	HEM	C3B-C4B	-5.57	1.46	1.51
5	B	500	HEM	C2D-C3D	-5.35	1.38	1.54
5	B	500	HEM	C3B-CAB	-5.25	1.41	1.51
5	A	500	HEM	C3B-C4B	-4.92	1.47	1.51
5	A	500	HEM	C3C-CAC	-4.88	1.42	1.51
5	B	500	HEM	C3C-CAC	-4.71	1.42	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	HEM	C3D-C4D	-3.30	1.47	1.51
5	B	500	HEM	C2C-C1C	-3.21	1.46	1.52
5	B	500	HEM	C2B-C1B	-2.32	1.44	1.51
5	A	500	HEM	C2C-C1C	-2.27	1.48	1.52
5	B	500	HEM	C2D-C1D	-2.15	1.44	1.51
5	A	500	HEM	C2B-C1B	-2.05	1.45	1.51
5	B	500	HEM	CHD-C4C	2.26	1.41	1.36
6	B	761	H4B	C8A-N1	2.51	1.39	1.34
6	A	760	H4B	C8A-N1	2.53	1.39	1.34
5	B	500	HEM	C4C-NC	3.34	1.40	1.36
5	B	500	HEM	C1C-NC	3.35	1.40	1.36
6	B	761	H4B	C6-N5	3.38	1.52	1.45
6	B	761	H4B	C4A-N5	3.53	1.46	1.38
6	A	760	H4B	C4A-N5	3.57	1.46	1.38
3	A	860	ACT	CH3-C	3.80	1.54	1.48
6	B	761	H4B	C4-N3	4.08	1.40	1.33
6	A	760	H4B	C6-N5	4.34	1.54	1.45
3	B	861	ACT	CH3-C	4.40	1.54	1.48
5	A	500	HEM	C1C-NC	4.79	1.41	1.36
5	A	500	HEM	C4C-NC	4.85	1.42	1.36
6	A	760	H4B	C4-N3	5.08	1.42	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	760	H4B	N3-C2-N1	-5.04	117.28	125.53
5	B	500	HEM	CBA-CAA-C2A	-4.93	103.69	112.53
6	B	761	H4B	N3-C2-N1	-4.58	118.02	125.53
7	A	792	DP2	O-C-N2	-4.00	117.14	123.08
7	B	793	DP2	O-C-N2	-3.73	117.54	123.08
5	A	500	HEM	CBD-CAD-C3D	-2.97	104.91	113.55
5	A	500	HEM	CAA-C2A-C1A	-2.31	124.50	127.01
5	A	500	HEM	C4B-CHC-C1C	-2.01	122.45	125.82
5	A	500	HEM	CMD-C2D-C3D	2.19	124.02	114.35
5	B	500	HEM	C3C-CAC-CBC	2.23	127.87	124.46
7	B	793	DP2	CA-C-N2	2.66	120.89	116.60
5	B	500	HEM	CMD-C2D-C3D	2.72	126.36	114.35
7	A	792	DP2	CA-C-N2	2.78	121.08	116.60
5	A	500	HEM	C2D-C3D-C4D	2.99	106.57	101.50
6	B	761	H4B	C2-N1-C8A	3.16	121.64	114.54
6	A	760	H4B	C4A-C8A-N8	3.27	122.29	118.43
5	A	500	HEM	CMC-C2C-C3C	3.36	124.91	116.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	761	H4B	C4A-C8A-N8	3.45	122.49	118.43
6	A	760	H4B	C2-N1-C8A	3.47	122.33	114.54
6	B	761	H4B	N2-C2-N1	3.47	122.95	117.20
5	B	500	HEM	C3B-CAB-CBB	3.64	130.04	124.46
6	A	760	H4B	N2-C2-N1	3.64	123.23	117.20
5	B	500	HEM	CMB-C2B-C3B	3.96	126.40	116.53
5	B	500	HEM	CMC-C2C-C3C	4.01	126.55	116.53
5	A	500	HEM	CAD-C3D-C4D	4.11	126.96	112.47
5	B	500	HEM	CAD-C3D-C4D	4.28	127.58	112.47
5	A	500	HEM	CAD-C3D-C2D	4.59	126.41	113.22
5	A	500	HEM	CMB-C2B-C3B	4.81	128.53	116.53
5	B	500	HEM	CAD-C3D-C2D	5.14	127.99	113.22
5	A	500	HEM	C3C-CAC-CBC	5.25	132.50	124.46
6	B	761	H4B	C4-N3-C2	6.50	124.97	115.94
6	A	760	H4B	C4-N3-C2	6.93	125.56	115.94
6	A	760	H4B	C4-C4A-C8A	9.20	122.89	114.56
6	B	761	H4B	C4-C4A-C8A	9.29	122.97	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	760	H4B	1	0
7	A	792	DP2	1	0
2	A	850	CAC	3	0
5	B	500	HEM	2	0
6	B	761	H4B	1	0
7	B	793	DP2	2	0
2	B	852	CAC	1	0
8	B	882	GOL	2	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 ⓘ

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, 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	406/416 (97%)	0.36	20 (4%) 33 42	29, 46, 71, 104	0
1	B	404/416 (97%)	0.37	23 (5%) 27 36	30, 48, 74, 102	0
All	All	810/832 (97%)	0.36	43 (5%) 30 39	29, 47, 74, 104	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	PRO	7.1
1	A	67	GLY	6.1
1	B	120	PRO	4.7
1	A	123	GLU	4.2
1	A	121	PRO	3.5
1	B	122	ALA	3.5
1	A	259	GLN	3.5
1	A	69	LYS	3.5
1	B	259	GLN	3.4
1	A	109	ARG	3.3
1	B	121	PRO	3.3
1	A	448	ALA	3.0
1	B	448	ALA	3.0
1	B	106	VAL	3.0
1	B	324	TRP	3.0
1	B	142	ARG	2.8
1	B	286	GLY	2.6
1	A	449	TRP	2.6
1	B	447	TRP	2.5
1	A	450	ILE	2.5
1	B	144	GLY	2.5
1	B	451	VAL	2.4
1	B	126	LEU	2.4
1	B	152	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	106	VAL	2.4
1	A	451	VAL	2.3
1	B	103	GLY	2.3
1	B	123	GLU	2.3
1	A	103	GLY	2.3
1	B	223	ARG	2.3
1	B	260	ASP	2.2
1	B	449	TRP	2.2
1	A	107	LEU	2.2
1	B	445	ALA	2.2
1	B	283	PRO	2.1
1	A	152	LEU	2.1
1	A	108	PRO	2.1
1	A	446	ASP	2.1
1	A	466	MET	2.1
1	A	241	GLY	2.1
1	A	124	GLN	2.1
1	B	257	ARG	2.1
1	B	450	ILE	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(Å ²)	Q<0.9
3	ACT	B	861	4/4	0.85	0.20	4.26	49,50,56,57	0
7	DP2	B	793	24/24	0.91	0.21	1.17	40,55,63,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ACT	A	860	4/4	0.87	0.19	0.98	49,51,51,53	0
8	GOL	A	880	6/6	0.84	0.21	0.78	45,47,50,51	0
5	HEM	A	500	43/43	0.96	0.18	0.39	25,34,41,45	0
8	GOL	B	882	6/6	0.91	0.20	0.25	35,40,44,50	0
5	HEM	B	500	43/43	0.96	0.17	0.17	28,34,39,44	0
7	DP2	A	792	24/24	0.90	0.17	0.13	37,45,56,60	0
6	H4B	B	761	17/17	0.93	0.22	0.02	31,34,40,42	0
6	H4B	A	760	17/17	0.92	0.21	0.00	29,38,41,45	0
2	CAC	A	850	3/5	0.98	0.10	-1.01	76,76,77,78	0
4	ZN	A	900	1/1	0.99	0.11	-1.37	46,46,46,46	0
2	CAC	B	852	3/5	0.97	0.16	-	86,86,88,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.