



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:37 PM GMT

PDB ID : 4CUN
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with (9aS)-2-amino-9a-methyl-8,9,9a,10-tetrahydrobenzo[g]pteridine-4,6(3H,7H)-dione
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2014-03-20
Resolution : 2.48 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

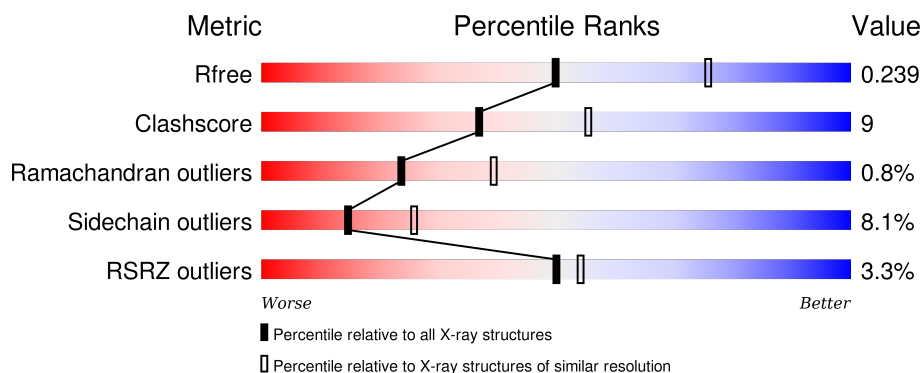
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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	443	 3% 70% 17% • 9%
1	B	443	 3% 68% 21% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	WS6	B	800	-	-	-	X
5	ACT	B	860	-	-	-	X
6	GOL	A	880	-	-	-	X
6	GOL	B	880	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6670 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.

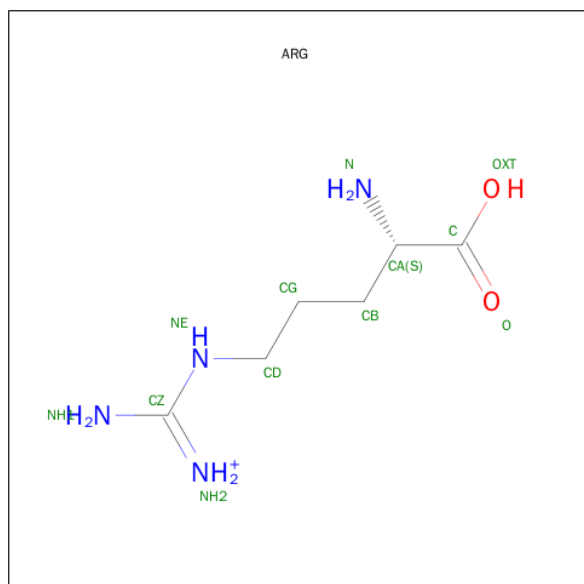
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3223	1	2049	568	589	16			
1	B	405	Total	As	C	N	O	S	0	0	0
			3229	1	2054	569	589	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	CONFLICT	UNP P29473
B	100	ARG	CYS	CONFLICT	UNP P29473

- Molecule 2 is ARGinine (three-letter code: ARG) (formula: C₆H₁₅N₄O₂).



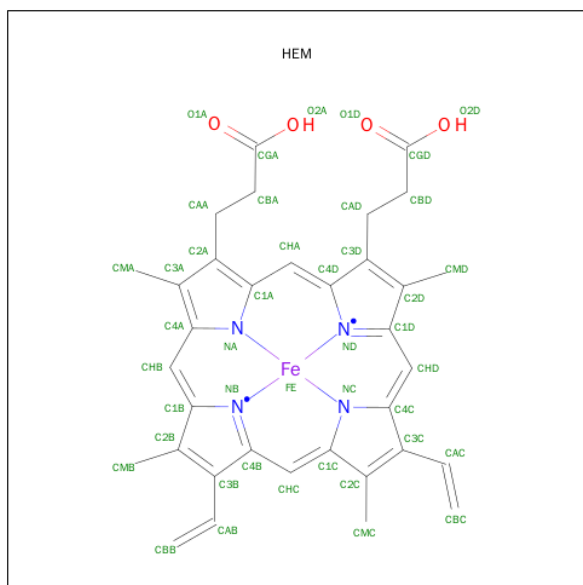
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		

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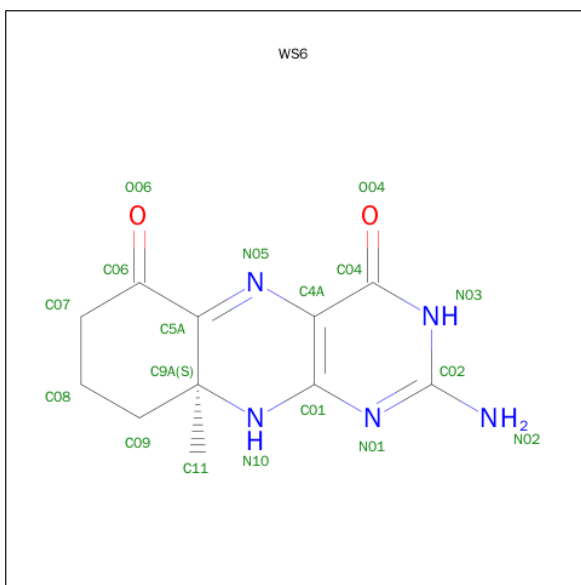
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is (9AS)-2-AMINO-9A-METHYL-8,9,9A,10-TETRAHYDROBENZO[G]PTERIDINE-4,6(3H,7H)-DIONE (three-letter code: WS6) (formula: $C_{11}H_{13}N_5O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	11	5	2		
4	B	1	Total	C	N	O	0	0
			18	11	5	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

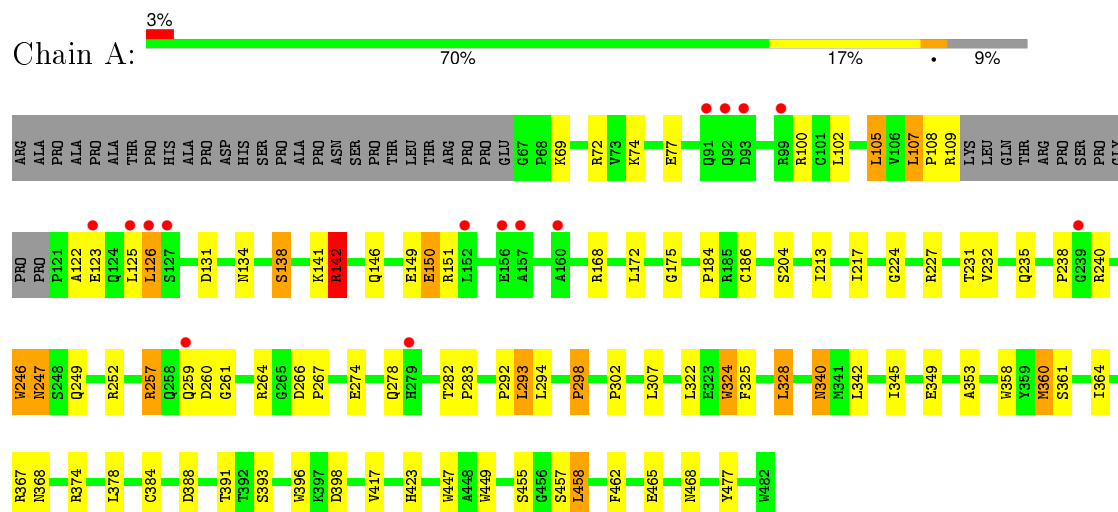
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	36	Total	O	0	0
			36	36		
8	B	15	Total	O	0	0
			15	15		

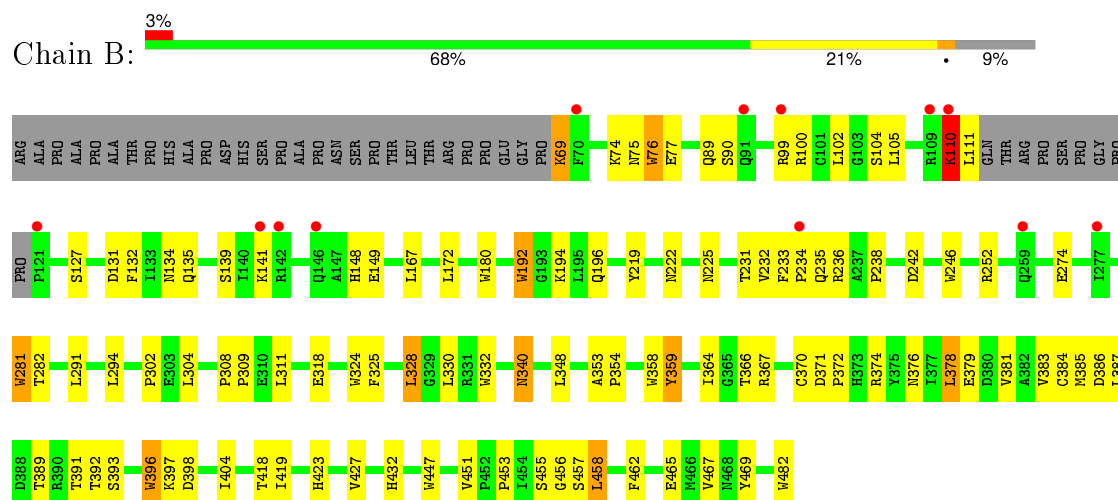
3 Residue-property plots [i](#)

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



• 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	58.87Å 106.18Å 156.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.90 – 2.48 43.03 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.4 (87.90-2.48) 99.5 (43.03-2.48)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.184 , 0.242 0.184 , 0.239	Depositor DCC
R_{free} test set	1761 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	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	0 of 35501 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6670	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: GOL, ZN, CAS, WS6, 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	0.78	4/3303 (0.1%)	0.83	2/4497 (0.0%)
1	B	0.83	9/3308 (0.3%)	0.88	1/4502 (0.0%)
All	All	0.80	13/6611 (0.2%)	0.86	3/8999 (0.0%)

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	B	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	TRP	CD2-CE2	7.20	1.50	1.41
1	A	396	TRP	CD2-CE2	6.36	1.49	1.41
1	B	76	TRP	CD2-CE2	6.17	1.48	1.41
1	B	281	TRP	CD2-CE2	5.76	1.48	1.41
1	A	358	TRP	CD2-CE2	5.71	1.48	1.41
1	B	396	TRP	CD2-CE2	5.69	1.48	1.41
1	A	324	TRP	CD2-CE2	5.53	1.48	1.41
1	B	192	TRP	CD2-CE2	5.49	1.48	1.41
1	B	324	TRP	CD2-CE2	5.41	1.47	1.41
1	B	246	TRP	CD2-CE2	5.28	1.47	1.41
1	B	180	TRP	CD2-CE2	5.28	1.47	1.41
1	B	482	TRP	CD2-CE2	5.22	1.47	1.41
1	A	246	TRP	CD2-CE2	5.17	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	311	LEU	CA-CB-CG	5.27	127.41	115.30
1	A	142	ARG	NE-CZ-NH1	5.17	122.89	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	359	TYR	Peptide

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	3223	0	3127	65	0
1	B	3229	0	3141	60	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	43	0	30	6	0
3	B	43	0	30	4	0
4	A	18	0	13	4	0
4	B	18	0	13	6	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	36	0	0	3	0
8	B	15	0	0	0	0
All	All	6670	0	6400	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ARG:HG2	1:A:142:ARG:HH11	1.14	1.08
1:A:384:CAS:AS	1:A:384:CAS:SG	2.78	1.01
1:B:384:CAS:AS	1:B:384:CAS:SG	2.81	0.97
1:B:69:LYS:HZ2	1:B:69:LYS:N	1.75	0.85
1:B:358:TRP:H	3:B:500:HEM:HAB	1.44	0.82
1:B:366:THR:HG21	1:B:453:PRO:HB2	1.61	0.81
3:B:500:HEM:HBC2	3:B:500:HEM:HMC1	1.66	0.78
1:A:447:TRP:CZ2	4:B:800:WS6:H112	2.19	0.78
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.48	0.77
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.67	0.76
3:B:500:HEM:HBC2	3:B:500:HEM:CMC	2.17	0.75
1:A:142:ARG:HG2	1:A:142:ARG:NH1	1.92	0.74
1:B:379:GLU:O	1:B:383:VAL:HG23	1.86	0.74
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.70	0.73
1:A:109:ARG:HH22	1:B:69:LYS:HG3	1.56	0.71
1:B:385:MET:HE2	1:B:387:LEU:HD11	1.73	0.70
1:A:109:ARG:HH12	1:B:69:LYS:HB3	1.59	0.67
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.25	0.67
1:A:109:ARG:HH22	1:B:69:LYS:CG	2.10	0.65
4:A:800:WS6:H113	1:B:462:PHE:CE1	2.32	0.65
1:B:359:TYR:CD2	1:B:364:ILE:HD11	2.36	0.61
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.83	0.61
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.81	0.60
4:A:800:WS6:H112	1:B:447:TRP:CZ2	2.37	0.60
3:A:500:HEM:HBB2	3:A:500:HEM:HHC	1.84	0.59
1:B:74:LYS:HD3	1:B:76:TRP:CE2	2.36	0.59
1:B:236:ARG:HD3	1:B:242:ASP:OD2	2.04	0.58
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.11	0.58
1:B:252:ARG:HB2	1:B:291:LEU:HD12	1.86	0.57
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.85	0.57
1:B:132:PHE:O	1:B:135:GLN:HB2	2.05	0.56
1:A:292:PRO:HA	8:A:2020:HOH:O	2.06	0.56
1:A:146:GLN:O	1:A:150:GLU:HB2	2.05	0.56
1:B:231:THR:O	1:B:354:PRO:HD2	2.06	0.56
1:A:367:ARG:HH12	4:A:800:WS6:C04	2.19	0.55
1:A:259:GLN:C	1:A:261:GLY:H	2.08	0.55
1:A:213:ILE:O	1:A:217:ILE:HG13	2.07	0.55
1:A:378:LEU:HB2	8:A:2026:HOH:O	2.06	0.55
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.22	0.54
1:A:184:PRO:CB	1:A:468:ASN:HD21	2.21	0.54
1:B:325:PHE:O	1:B:328:LEU:HB2	2.07	0.54
1:B:423:HIS:O	1:B:427:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ASN:HD22	1:B:340:ASN:C	2.12	0.53
1:B:456:GLY:O	1:B:462:PHE:HB2	2.09	0.53
1:A:134:ASN:O	1:A:138:SER:HB2	2.09	0.53
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.90	0.52
1:A:342:LEU:HD11	1:A:349:GLU:HB3	1.89	0.52
1:A:184:PRO:HB3	1:A:468:ASN:HD21	1.75	0.52
1:B:74:LYS:HD3	1:B:76:TRP:CZ2	2.46	0.51
1:A:151:ARG:HD3	1:A:168:ARG:NH1	2.25	0.51
3:A:500:HEM:CBB	3:A:500:HEM:HHC	2.41	0.51
1:A:465:GLU:OE1	1:B:105:LEU:HD13	2.11	0.51
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.52	0.50
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.47	0.50
1:B:131:ASP:O	1:B:135:GLN:HG3	2.12	0.50
1:B:366:THR:O	1:B:370:CYS:HB2	2.12	0.50
1:A:74:LYS:O	1:A:465:GLU:HG3	2.13	0.49
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.94	0.49
1:B:359:TYR:CG	1:B:364:ILE:HD11	2.48	0.49
1:B:134:ASN:HA	1:B:148:HIS:HE2	1.78	0.48
1:A:266:ASP:OD1	1:A:266:ASP:C	2.52	0.48
1:A:325:PHE:HA	1:A:328:LEU:HD22	1.97	0.47
1:A:109:ARG:NH1	1:B:69:LYS:HB3	2.28	0.47
1:A:267:PRO:HD2	1:A:374:ARG:HA	1.96	0.47
1:A:186:CYS:HB2	3:A:500:HEM:ND	2.28	0.47
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.14	0.47
3:B:500:HEM:HMC1	3:B:500:HEM:CBC	2.42	0.47
1:B:467:VAL:HG12	1:B:469:TYR:CD1	2.50	0.47
1:A:264:ARG:HD3	8:A:2017:HOH:O	2.14	0.47
1:B:110:LYS:HD3	1:B:111:LEU:N	2.30	0.47
1:A:259:GLN:C	1:A:261:GLY:N	2.68	0.47
1:A:340:ASN:HD22	1:A:340:ASN:H	1.63	0.47
1:B:457:SER:HA	1:B:462:PHE:CG	2.50	0.46
1:A:224:GLY:O	1:A:417:VAL:HA	2.15	0.46
1:B:104:SER:O	4:B:800:WS6:H081	2.16	0.46
1:A:138:SER:O	1:A:141:LYS:HE3	2.16	0.46
1:A:175:GLY:HA3	1:A:345:ILE:HD13	1.97	0.46
1:B:172:LEU:HD11	1:B:232:VAL:HG11	1.97	0.46
1:A:462:PHE:CE1	4:B:800:WS6:H113	2.51	0.46
1:B:236:ARG:CD	1:B:242:ASP:OD2	2.63	0.46
1:A:423:HIS:HB2	1:B:392:THR:HB	1.98	0.45
1:B:455:SER:O	1:B:458:LEU:HB2	2.16	0.45
1:A:246:TRP:CZ2	1:A:302:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:TRP:CZ2	1:B:397:LYS:HE2	2.52	0.45
1:A:447:TRP:CZ2	4:B:800:WS6:C11	2.96	0.45
1:A:105:LEU:HD23	1:A:105:LEU:N	2.31	0.45
1:A:172:LEU:HD11	1:A:232:VAL:HG11	1.98	0.45
1:B:294:LEU:HD22	1:B:302:PRO:HB2	1.98	0.45
1:A:126:LEU:HA	1:A:126:LEU:HD12	1.72	0.45
1:A:360:MET:HB3	1:A:360:MET:HE3	1.91	0.45
1:A:231:THR:O	1:A:353:ALA:HA	2.16	0.44
1:A:282:THR:HA	1:A:283:PRO:HD2	1.78	0.44
1:B:231:THR:O	1:B:353:ALA:HA	2.19	0.43
1:A:259:GLN:O	1:A:261:GLY:N	2.51	0.43
1:A:457:SER:HB3	1:B:453:PRO:HB3	2.00	0.43
1:A:447:TRP:CH2	4:B:800:WS6:H112	2.54	0.43
1:B:308:PRO:HA	1:B:309:PRO:HD2	1.87	0.43
1:A:384:CAS:SG	1:A:384:CAS:CE1	3.07	0.43
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.99	0.43
1:B:367:ARG:HH12	4:B:800:WS6:C04	2.32	0.42
1:A:364:ILE:HA	1:A:368:ASN:HD22	1.84	0.42
1:A:477:TYR:OH	3:A:500:HEM:O1D	2.20	0.42
1:A:388:ASP:OD2	1:A:391:THR:HG22	2.18	0.42
1:A:449:TRP:CE3	4:A:800:WS6:C02	3.02	0.42
1:A:360:MET:HE2	3:A:500:HEM:HMA1	2.02	0.42
1:B:371:ASP:HB2	1:B:374:ARG:CG	2.50	0.42
1:B:75:ASN:OD1	1:B:77:GLU:N	2.53	0.42
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.55	0.42
1:A:249:GLN:HB2	1:A:252:ARG:HG2	2.02	0.42
1:B:222:ASN:HB3	1:B:225:ASN:O	2.20	0.41
1:B:467:VAL:HG12	1:B:469:TYR:HD1	1.85	0.41
1:B:372:PRO:HA	1:B:376:ASN:ND2	2.35	0.41
1:A:107:LEU:HA	1:A:108:PRO:HD2	1.74	0.41
3:A:500:HEM:HBB2	3:A:500:HEM:CHC	2.45	0.41
1:A:247:ASN:OD1	1:A:247:ASN:N	2.54	0.41
1:A:455:SER:O	1:A:458:LEU:HB2	2.20	0.41
1:A:257:ARG:CG	1:A:257:ARG:HH11	2.24	0.41
1:B:192:TRP:CD1	1:B:432:HIS:HE1	2.39	0.41
1:A:293:LEU:HD21	1:A:307:LEU:HD21	2.03	0.40
1:B:196:GLN:HG2	1:B:219:TYR:CZ	2.56	0.40
1:B:366:THR:CG2	1:B:453:PRO:HB2	2.41	0.40
1:A:151:ARG:HD3	1:A:168:ARG:HH12	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/443 (90%)	381 (95%)	16 (4%)	3 (1%)	24	39
1	B	400/443 (90%)	374 (94%)	23 (6%)	3 (1%)	24	39
All	All	800/886 (90%)	755 (94%)	39 (5%)	6 (1%)	24	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	PRO
1	A	122	ALA
1	A	260	ASP
1	B	110	LYS
1	B	328	LEU
1	A	238	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	343/375 (92%)	314 (92%)	29 (8%)	13	23
1	B	344/375 (92%)	317 (92%)	27 (8%)	16	27
All	All	687/750 (92%)	631 (92%)	56 (8%)	15	25

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	72	ARG
1	A	100	ARG
1	A	102	LEU
1	A	105	LEU
1	A	107	LEU
1	A	123	GLU
1	A	125	LEU
1	A	126	LEU
1	A	131	ASP
1	A	138	SER
1	A	142	ARG
1	A	149	GLU
1	A	150	GLU
1	A	204	SER
1	A	235	GLN
1	A	247	ASN
1	A	257	ARG
1	A	274	GLU
1	A	278	GLN
1	A	293	LEU
1	A	298	PRO
1	A	328	LEU
1	A	340	ASN
1	A	360	MET
1	A	361	SER
1	A	393	SER
1	A	398	ASP
1	A	458	LEU
1	B	69	LYS
1	B	89	GLN
1	B	90	SER
1	B	99	ARG
1	B	100	ARG
1	B	102	LEU
1	B	110	LYS
1	B	127	SER
1	B	139	SER
1	B	141	LYS
1	B	149	GLU
1	B	194	LYS
1	B	235	GLN
1	B	274	GLU

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Mol	Chain	Res	Type
1	B	282	THR
1	B	318	GLU
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	386	ASP
1	B	389	THR
1	B	391	THR
1	B	393	SER
1	B	398	ASP
1	B	418	THR
1	B	419	ILE
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	124	GLN
1	B	191	GLN
1	B	222	ASN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN
1	B	432	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.35	1 (20%)	2,9,11	1.42	0
1	CAS	B	384	1	5,8,9	1.30	0	2,9,11	1.40	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
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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	CAS	AS-CE2	2.12	2.01	1.96

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CAS	2	0
1	B	384	CAS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z > 2$
3	HEM	A	500	1	30,50,50	2.53	14 (46%)	24,82,82	2.96	8 (33%)
2	ARG	A	700	-	5,11,11	0.57	0	3,13,13	1.12	0
4	WS6	A	800	-	16,20,20	1.32	1 (6%)	16,31,31	2.78	8 (50%)
5	ACT	A	860	-	1,3,3	0.54	0	0,3,3	0.00	-
6	GOL	A	880	-	5,5,5	0.30	0	5,5,5	1.20	0
3	HEM	B	500	1	30,50,50	2.57	11 (36%)	24,82,82	3.31	14 (58%)
2	ARG	B	700	-	5,11,11	0.40	0	3,13,13	1.69	1 (33%)
4	WS6	B	800	-	16,20,20	1.31	1 (6%)	16,31,31	2.64	9 (56%)
5	ACT	B	860	-	1,3,3	1.34	0	0,3,3	0.00	-
6	GOL	B	880	-	5,5,5	0.42	0	5,5,5	0.56	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
3	HEM	A	500	1	-	0/10/54/54	0/0/8/8
2	ARG	A	700	-	-	0/5/11/11	0/0/0/0
4	WS6	A	800	-	-	0/0/26/26	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
6	GOL	A	880	-	-	0/4/4/4	0/0/0/0
3	HEM	B	500	1	-	0/10/54/54	0/0/8/8
2	ARG	B	700	-	-	0/5/11/11	0/0/0/0
4	WS6	B	800	-	-	0/0/26/26	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0
6	GOL	B	880	-	-	0/4/4/4	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C3B-C4B	-4.47	1.47	1.51
3	B	500	HEM	C3B-C4B	-3.66	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C3D-C4D	-3.21	1.47	1.51
3	B	500	HEM	C2D-C3D	-3.13	1.45	1.54
3	A	500	HEM	C2D-C3D	-3.04	1.45	1.54
3	A	500	HEM	C3B-CAB	-2.29	1.47	1.51
3	B	500	HEM	CMB-C2B	-2.10	1.48	1.53
3	A	500	HEM	CAD-C3D	-2.07	1.50	1.54
3	A	500	HEM	FE-NB	2.00	2.08	1.97
3	A	500	HEM	C4A-CHB	2.20	1.45	1.39
3	A	500	HEM	CHC-C4B	2.22	1.45	1.38
3	B	500	HEM	FE-ND	2.39	2.10	1.97
3	A	500	HEM	FE-ND	2.41	2.10	1.97
3	B	500	HEM	CHD-C1D	2.45	1.45	1.38
3	B	500	HEM	CHC-C4B	2.50	1.45	1.38
3	A	500	HEM	CHC-C1C	2.97	1.43	1.36
4	B	800	WS6	C5A-N05	2.99	1.34	1.29
4	A	800	WS6	C5A-N05	3.11	1.34	1.29
3	B	500	HEM	C2A-C3A	3.17	1.47	1.37
3	B	500	HEM	CHC-C1C	3.28	1.44	1.36
3	A	500	HEM	C2A-C3A	3.37	1.47	1.37
3	B	500	HEM	CHD-C4C	3.42	1.44	1.36
3	A	500	HEM	CHD-C4C	3.77	1.45	1.36
3	A	500	HEM	C1C-NC	4.86	1.42	1.36
3	B	500	HEM	C4C-NC	6.78	1.44	1.36
3	A	500	HEM	C4C-NC	6.96	1.44	1.36
3	B	500	HEM	C1C-NC	7.02	1.44	1.36

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	HEM	CBA-CAA-C2A	-8.15	97.92	112.53
3	A	500	HEM	CBA-CAA-C2A	-7.23	99.57	112.53
4	A	800	WS6	O06-C06-C5A	-4.84	117.58	121.59
3	B	500	HEM	C3C-CAC-CBC	-4.49	117.56	124.46
4	A	800	WS6	C4A-C04-N03	-4.00	118.11	123.59
4	B	800	WS6	C4A-C04-N03	-3.78	118.42	123.59
3	B	500	HEM	C3B-CAB-CBB	-3.47	119.13	124.46
3	A	500	HEM	C3B-CAB-CBB	-3.46	119.15	124.46
3	B	500	HEM	C3B-C4B-CHC	-3.44	118.32	123.16
3	B	500	HEM	C1D-CHD-C4C	-3.20	120.48	125.82
3	B	500	HEM	CBD-CAD-C3D	-3.11	104.52	113.55
2	B	700	ARG	CG-CD-NE	-2.92	102.24	112.35
4	B	800	WS6	N03-C02-N01	-2.78	120.97	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	WS6	O06-C06-C5A	-2.73	119.33	121.59
4	A	800	WS6	N03-C02-N01	-2.25	121.85	125.53
4	B	800	WS6	N02-C02-N03	2.05	120.60	117.20
3	A	500	HEM	CMA-C3A-C4A	2.38	132.30	128.36
4	A	800	WS6	C4A-N05-C5A	2.38	121.98	117.34
3	B	500	HEM	C2C-C1C-NC	2.50	114.42	110.21
4	B	800	WS6	C4A-N05-C5A	2.53	122.28	117.34
3	B	500	HEM	C3B-C4B-NB	2.57	116.55	111.63
3	B	500	HEM	CAA-CBA-CGA	3.25	118.71	112.75
3	B	500	HEM	CMD-C2D-C3D	3.37	129.28	114.35
4	A	800	WS6	N10-C01-N01	3.47	122.15	116.62
4	A	800	WS6	C02-N01-C01	3.49	122.38	114.54
3	A	500	HEM	CMD-C2D-C3D	3.55	130.06	114.35
4	B	800	WS6	C02-N01-C01	3.60	122.63	114.54
4	B	800	WS6	N10-C01-N01	3.67	122.46	116.62
4	B	800	WS6	C04-C4A-C01	3.77	117.04	114.52
3	B	500	HEM	CAD-C3D-C2D	4.16	125.18	113.22
4	A	800	WS6	C04-C4A-C01	4.31	117.40	114.52
3	B	500	HEM	CMC-C2C-C3C	4.37	127.43	116.53
3	A	500	HEM	CMC-C2C-C3C	4.48	127.70	116.53
4	A	800	WS6	C04-N03-C02	4.61	122.34	115.94
3	A	500	HEM	CAD-C3D-C4D	4.87	129.65	112.47
4	B	800	WS6	C04-N03-C02	4.89	122.72	115.94
3	B	500	HEM	CMB-C2B-C3B	4.93	128.83	116.53
3	B	500	HEM	CAD-C3D-C4D	5.44	131.67	112.47
3	A	500	HEM	CMB-C2B-C3B	5.61	130.53	116.53
3	A	500	HEM	CAD-C3D-C2D	5.72	129.65	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	HEM	6	0
4	A	800	WS6	4	0
3	B	500	HEM	4	0
4	B	800	WS6	6	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	404/443 (91%)	-0.01	15 (3%) 45 50	44, 65, 100, 129	0
1	B	404/443 (91%)	-0.01	12 (2%) 54 58	40, 66, 99, 124	0
All	All	808/886 (91%)	-0.01	27 (3%) 50 54	40, 66, 100, 129	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	4.5
1	A	160	ALA	3.7
1	B	146	GLN	3.6
1	A	239	GLY	3.4
1	A	123	GLU	3.3
1	B	142	ARG	3.3
1	A	156	GLU	3.1
1	B	141	LYS	3.1
1	A	93	ASP	3.0
1	B	121	PRO	2.9
1	A	91	GLN	2.9
1	B	110	LYS	2.8
1	A	92	GLN	2.8
1	B	91	GLN	2.8
1	A	259	GLN	2.8
1	A	152	LEU	2.7
1	B	99	ARG	2.7
1	B	70	PHE	2.6
1	A	126	LEU	2.5
1	A	99	ARG	2.5
1	B	277	ILE	2.2
1	A	157	ALA	2.2
1	A	279	HIS	2.2
1	B	109	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	127	SER	2.1
1	A	125	LEU	2.1
1	B	234	PRO	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, 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
1	CAS	B	384	9/10	0.95	0.15	-	84,91,140,163	0
1	CAS	A	384	9/10	0.95	0.08	-	67,70,90,113	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, 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
6	GOL	A	880	6/6	0.86	0.40	8.29	87,93,104,139	0
6	GOL	B	880	6/6	0.93	0.31	4.71	60,68,79,80	0
5	ACT	B	860	4/4	0.97	0.15	2.97	66,71,75,78	0
4	WS6	B	800	18/18	0.94	0.24	2.04	80,90,102,117	0
2	ARG	A	700	12/12	0.96	0.23	1.45	47,51,65,66	0
3	HEM	B	500	43/43	0.98	0.19	1.02	43,51,58,64	0
3	HEM	A	500	43/43	0.98	0.18	1.02	37,43,64,71	0
4	WS6	A	800	18/18	0.95	0.16	0.62	74,79,89,91	0
5	ACT	A	860	4/4	0.99	0.17	0.44	54,56,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ARG	B	700	12/12	0.96	0.16	-0.12	41,48,63,63	0
7	ZN	A	1483	1/1	1.00	0.08	-0.99	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.