



Full wwPDB X-ray Structure Validation Report

Oct 10, 2014 – 12:57 AM EDT

PDB ID : 4D1N
Title : Structure of human nNOS heme domain with L-Arg bound
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-05-02
Resolution : 2.03 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

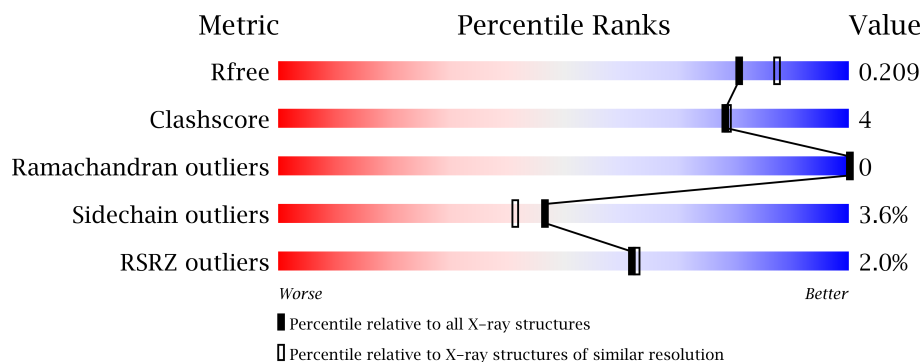
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23828

1 Overall quality at a glance

The reported resolution of this entry is 2.03 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}	66092	6003 (2.04-2.00)
Clashscore	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)
RSRZ outliers	66119	6006 (2.04-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	420	
1	B	420	
1	C	420	
1	D	420	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ARG	C	770	-	X
5	GOL	C	881	-	X
5	GOL	C	882	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14747 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

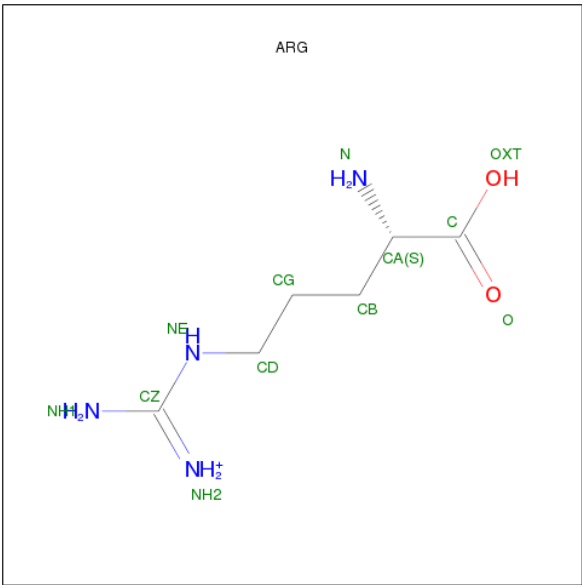
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, BRAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	1	0
			3430	2192	590	626	22			
1	B	411	Total	C	N	O	S	0	1	0
			3351	2147	571	611	22			
1	C	420	Total	C	N	O	S	0	1	0
			3430	2192	589	627	22			
1	D	411	Total	C	N	O	S	0	0	0
			3348	2145	571	610	22			

There are 8 discrepancies between the modelled and reference sequences:

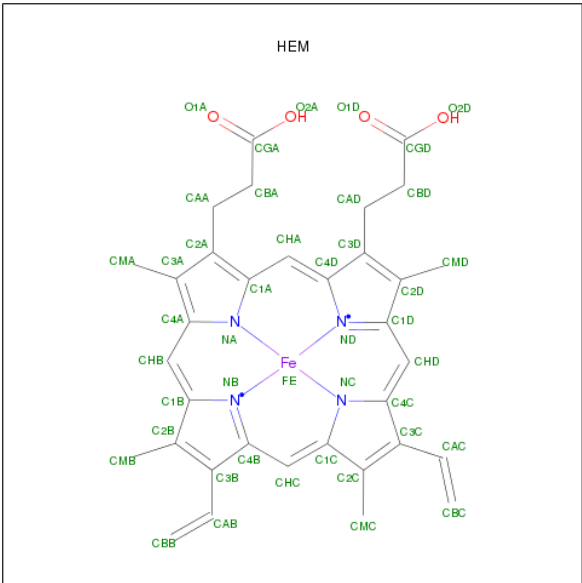
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	ENGINEERED MUTATION	UNP P29475
A	357	ASP	GLY	ENGINEERED MUTATION	UNP P29475
B	354	ALA	ARG	ENGINEERED MUTATION	UNP P29475
B	357	ASP	GLY	ENGINEERED MUTATION	UNP P29475
C	354	ALA	ARG	ENGINEERED MUTATION	UNP P29475
C	357	ASP	GLY	ENGINEERED MUTATION	UNP P29475
D	354	ALA	ARG	ENGINEERED MUTATION	UNP P29475
D	357	ASP	GLY	ENGINEERED MUTATION	UNP P29475

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



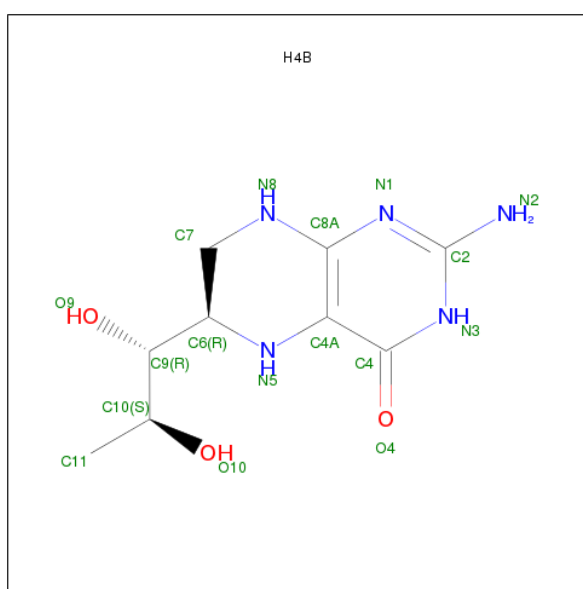
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		
2	B	1	Total	C	N	O	0	0
			12	6	4	2		
2	C	1	Total	C	N	O	0	0
			12	6	4	2		
2	D	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



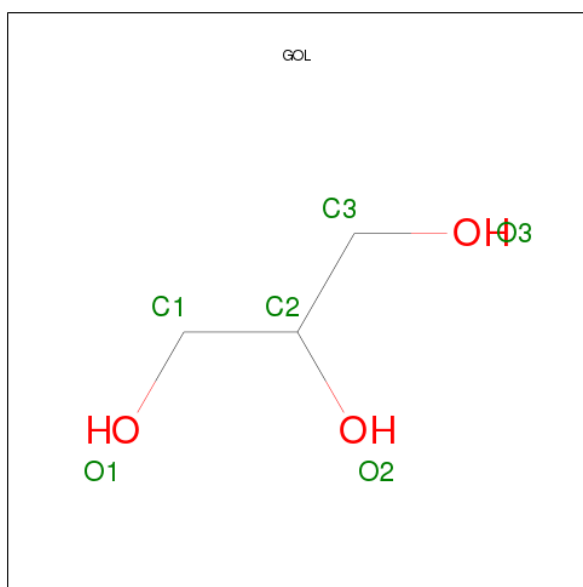
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	C	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

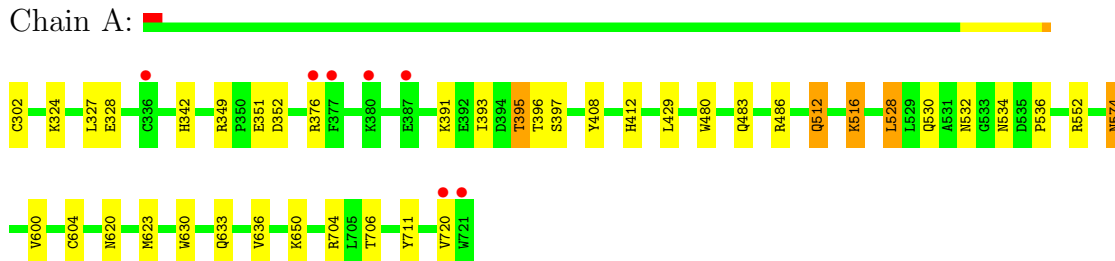
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	214	Total 214	O 214	0	0
7	B	206	Total 206	O 206	0	0
7	C	265	Total 265	O 265	0	0
7	D	171	Total 171	O 171	0	0

3 Residue-property plots

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

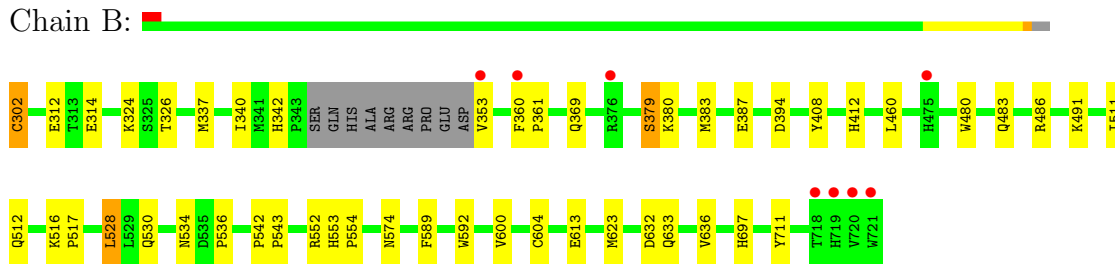
• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain A:



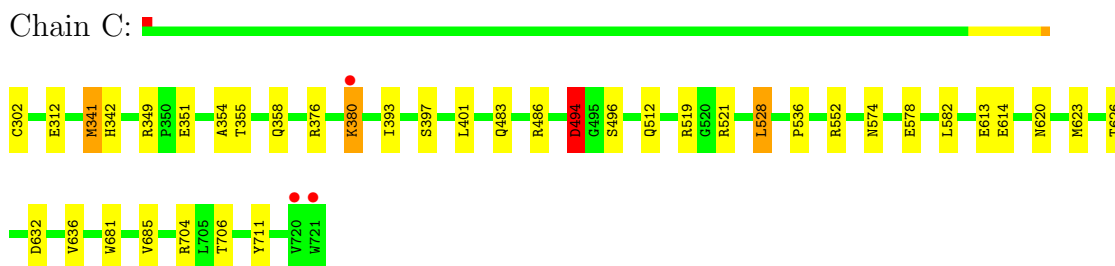
• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain B:



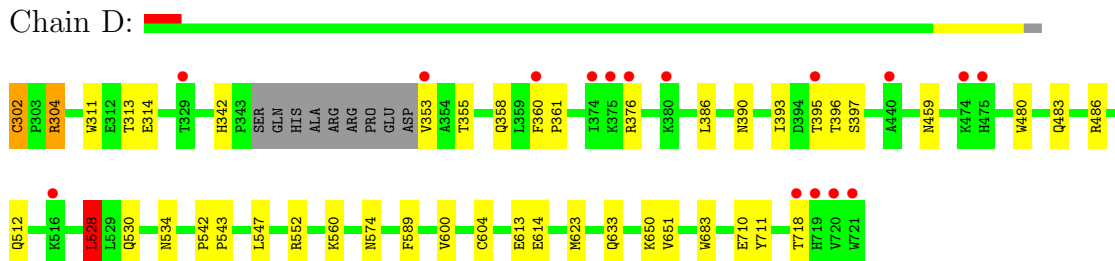
• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain C:



• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.92Å 84.66Å 166.75Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	46.60 – 2.03 46.56 – 2.03	Depositor EDS
% Data completeness (in resolution range)	94.5 (46.60-2.03) 94.6 (46.56-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.177 , 0.209 0.177 , 0.209	Depositor DCC
R_{free} test set	7549 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.6	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 149427 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14747	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.85 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.2984e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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, H4B, 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	0.52	0/3532	0.63	0/4794
1	B	0.55	0/3450	0.65	1/4682 (0.0%)
1	C	0.58	0/3532	0.67	1/4794 (0.0%)
1	D	0.56	0/3444	0.67	2/4674 (0.0%)
All	All	0.55	0/13958	0.65	4/18944 (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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	CYS	CA-CB-SG	-5.85	103.48	114.00
1	D	302	CYS	CA-CB-SG	-5.50	104.09	114.00
1	C	494	ASP	CB-CA-C	-5.18	100.04	110.40
1	D	528	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	379	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3332	26	0
1	B	3351	0	3260	29	0
1	C	3430	0	3330	22	0
1	D	3348	0	3255	25	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	43	0	30	0	0
3	B	43	0	30	2	0
3	C	43	0	30	1	0
3	D	43	0	30	2	0
4	A	17	0	15	0	0
4	B	17	0	15	0	0
4	C	17	0	15	1	0
4	D	17	0	15	1	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	C	18	0	24	0	0
5	D	12	0	16	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	214	0	0	1	0
7	B	206	0	0	0	0
7	C	265	0	0	5	0
7	D	171	0	0	1	0
All	All	14747	0	13461	99	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (99) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:379:SER:HB2	1:B:380:LYS:HB2	1.31	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:519:ARG:HD2	7:C:2167:HOH:O	1.64	0.97
1:D:355:THR:H	1:D:358:GLN:HE21	1.27	0.83
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.64	0.78
1:C:494:ASP:HB3	1:C:496:SER:H	1.52	0.74
1:D:395:THR:HG23	1:D:396:THR:HG23	1.70	0.73
1:B:360:PHE:HB2	1:B:361:PRO:HD3	1.71	0.71
1:C:528:LEU:HD22	1:C:536:PRO:HB2	1.74	0.70
7:A:2166:HOH:O	1:B:312:GLU:OE2	2.11	0.69
1:D:360:PHE:HB2	1:D:361:PRO:HD3	1.74	0.69
3:D:750:HEM:HHC	3:D:750:HEM:HBB2	1.73	0.69
1:A:636:VAL:HG11	1:B:633:GLN:HG2	1.78	0.64
1:D:355:THR:H	1:D:358:GLN:NE2	1.94	0.64
1:C:613:GLU:HG3	1:C:623:MET:HE3	1.82	0.61
1:C:312:GLU:OE2	7:C:2010:HOH:O	2.16	0.61
1:A:342:HIS:HD2	1:A:711:TYR:CD2	2.20	0.60
1:D:342:HIS:HD2	1:D:711:TYR:CD2	2.20	0.59
1:C:342:HIS:HD2	1:C:711:TYR:CD2	2.21	0.59
1:B:324:LYS:HA	1:D:304:ARG:HD3	1.85	0.59
1:B:342:HIS:HD2	1:B:711:TYR:CE2	2.21	0.58
1:C:636:VAL:HG11	1:D:633:GLN:HG2	1.84	0.58
1:D:614:GLU:HG3	7:D:2133:HOH:O	2.03	0.58
1:B:379:SER:O	1:B:383:MET:HG2	2.03	0.58
1:B:312:GLU:HG3	1:B:697:HIS:CG	2.38	0.58
1:A:395:THR:HG23	1:A:396:THR:HG23	1.85	0.57
1:D:483:GLN:HB2	1:D:486:ARG:HG3	1.89	0.54
1:C:521:ARG:NH1	7:C:2171:HOH:O	2.29	0.54
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.90	0.54
1:D:342:HIS:HD2	1:D:711:TYR:CE2	2.26	0.53
1:D:530:GLN:HG3	1:D:534:ASN:O	2.08	0.53
1:A:483:GLN:HB2	1:A:486:ARG:HG3	1.90	0.53
1:B:326:THR:HG22	1:D:304:ARG:HB3	1.91	0.53
1:A:633:GLN:HG2	1:B:636:VAL:HG11	1.90	0.53
1:C:341:MET:HE3	1:D:311:TRP:CE2	2.45	0.52
1:C:483:GLN:HB2	1:C:486:ARG:HG3	1.90	0.52
1:C:380:LYS:N	1:C:380:LYS:HD2	2.25	0.52
1:A:408:TYR:CE2	1:A:412:HIS:CE1	2.98	0.51
1:B:342:HIS:HD2	1:B:711:TYR:CD2	2.28	0.51
1:A:342:HIS:CD2	1:A:711:TYR:CD2	3.00	0.51
1:B:408:TYR:CE2	1:B:412:HIS:CE1	2.99	0.50
1:C:355:THR:H	1:C:358:GLN:NE2	2.09	0.50
1:A:342:HIS:HD2	1:A:711:TYR:CE2	2.29	0.50
1:B:613:GLU:HG3	1:B:623:MET:HE3	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:750:HEM:HHC	3:C:750:HEM:HBB2	1.93	0.50
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.93	0.50
1:C:393:ILE:O	1:C:397:SER:HA	2.12	0.49
1:D:393:ILE:O	1:D:397:SER:HA	2.12	0.49
1:A:574:ASN:HD22	1:A:574:ASN:H	1.59	0.49
1:D:313:THR:O	1:D:314:GLU:HB2	2.12	0.49
1:B:600:VAL:O	1:B:604:CYS:HB2	2.13	0.49
1:B:460:LEU:HD12	1:B:592:TRP:HB3	1.95	0.49
1:B:530:GLN:HG3	1:B:534:ASN:O	2.13	0.49
1:C:613:GLU:HG3	1:C:623:MET:CE	2.42	0.49
1:A:395:THR:CG2	1:A:396:THR:HG23	2.42	0.48
1:B:379:SER:HB2	1:B:380:LYS:CB	2.22	0.48
1:D:480:TRP:HB2	1:D:528:LEU:HB3	1.96	0.48
1:A:351:GLU:CD	1:A:351:GLU:H	2.17	0.47
1:B:483:GLN:HB2	1:B:486:ARG:HG3	1.96	0.47
1:A:391:LYS:O	1:A:395:THR:HB	2.14	0.47
1:A:393:ILE:O	1:A:397:SER:HA	2.15	0.46
1:C:341:MET:HE2	4:C:760:H4B:H9	1.97	0.46
1:B:360:PHE:CB	1:B:361:PRO:HD3	2.43	0.46
1:D:358:GLN:O	1:D:361:PRO:HD2	2.15	0.46
3:B:750:HEM:HHC	3:B:750:HEM:HBB2	1.97	0.46
1:C:349:ARG:HB3	1:C:351:GLU:OE2	2.16	0.46
1:B:511:ILE:HG12	1:B:517:PRO:HG3	1.97	0.46
1:B:623:MET:HB3	1:B:623:MET:HE2	1.78	0.46
1:A:600:VAL:O	1:A:604:CYS:HB2	2.17	0.45
1:D:547:LEU:HD21	1:D:651:VAL:HG22	1.97	0.45
1:A:349:ARG:HB2	1:A:352:ASP:OD2	2.16	0.45
1:B:337:MET:CE	1:B:340:ILE:HG13	2.47	0.45
1:A:349:ARG:HB3	1:A:351:GLU:OE2	2.17	0.45
1:D:600:VAL:O	1:D:604:CYS:HB2	2.17	0.45
1:A:530:GLN:HG3	1:A:534:ASN:O	2.16	0.44
1:B:480:TRP:HB2	1:B:528:LEU:HB3	2.00	0.44
1:A:328:GLU:O	1:A:704:ARG:HD3	2.18	0.43
1:D:589:PHE:CD1	3:D:750:HEM:CAC	3.02	0.43
1:B:589:PHE:CD1	3:B:750:HEM:CAC	3.02	0.43
1:C:354:ALA:HA	1:C:358:GLN:NE2	2.33	0.43
1:D:683:TRP:HA	4:D:760:H4B:N1	2.33	0.43
1:C:401:LEU:HG	1:C:582:LEU:HD12	2.00	0.43
1:A:327:LEU:HD11	1:A:706:THR:CG2	2.48	0.43
1:C:706:THR:HG23	7:C:2038:HOH:O	2.18	0.42
1:B:542:PRO:HA	1:B:543:PRO:HD3	1.92	0.42
1:D:360:PHE:CB	1:D:361:PRO:HD3	2.46	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:613:GLU:HG3	1:D:623:MET:CE	2.50	0.42
1:A:516:LYS:HD2	1:A:516:LYS:N	2.33	0.42
1:A:342:HIS:CD2	1:A:711:TYR:CE2	3.08	0.42
1:B:613:GLU:HG3	1:B:623:MET:CE	2.49	0.42
1:A:512:GLN:HE21	1:A:512:GLN:HB3	1.65	0.42
1:D:542:PRO:HA	1:D:543:PRO:HD3	1.90	0.42
1:B:553:HIS:CG	1:B:554:PRO:HD2	2.54	0.41
1:D:355:THR:N	1:D:358:GLN:HE21	2.05	0.41
1:A:623:MET:HG2	1:A:630:TRP:CD2	2.56	0.41
1:C:380:LYS:HD2	1:C:380:LYS:H	1.85	0.41
1:C:681:TRP:CE2	1:C:685:VAL:HG21	2.55	0.41
1:B:383:MET:O	1:B:387:GLU:HG3	2.21	0.40
1:C:626:THR:HG22	7:C:2163:HOH:O	2.21	0.40
1:A:429:LEU:O	5:A:880:GOL:H32	2.21	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	419/420 (100%)	411 (98%)	8 (2%)	0	100	100
1	B	408/420 (97%)	396 (97%)	12 (3%)	0	100	100
1	C	419/420 (100%)	411 (98%)	8 (2%)	0	100	100
1	D	407/420 (97%)	396 (97%)	11 (3%)	0	100	100
All	All	1653/1680 (98%)	1614 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	376/375 (100%)	363 (96%)	13 (4%)	48	43
1	B	368/375 (98%)	356 (97%)	12 (3%)	50	45
1	C	376/375 (100%)	362 (96%)	14 (4%)	45	40
1	D	367/375 (98%)	352 (96%)	15 (4%)	41	35
All	All	1487/1500 (99%)	1433 (96%)	54 (4%)	47	41

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	CYS
1	A	324	LYS
1	A	376	ARG
1	A	395	THR
1	A	512	GLN
1	A	516	LYS
1	A	528	LEU
1	A	532	ASN
1	A	552	ARG
1	A	574	ASN
1	A	620	ASN
1	A	650	LYS
1	A	720	VAL
1	B	302	CYS
1	B	314	GLU
1	B	353	VAL
1	B	369	GLN
1	B	394	ASP
1	B	491	LYS
1	B	512	GLN
1	B	516	LYS
1	B	528	LEU
1	B	552	ARG
1	B	574	ASN
1	B	632	ASP
1	C	302	CYS

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Mol	Chain	Res	Type
1	C	341	MET
1	C	376	ARG
1	C	380	LYS
1	C	494	ASP
1	C	512	GLN
1	C	528	LEU
1	C	552	ARG
1	C	574	ASN
1	C	578	GLU
1	C	614	GLU
1	C	620	ASN
1	C	632	ASP
1	C	704	ARG
1	D	302	CYS
1	D	304	ARG
1	D	353	VAL
1	D	376	ARG
1	D	386	LEU
1	D	390	ASN
1	D	459	ASN
1	D	512	GLN
1	D	528	LEU
1	D	552	ARG
1	D	560	LYS
1	D	574	ASN
1	D	650	LYS
1	D	710	GLU
1	D	718	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	HIS
1	A	412	HIS
1	A	445	ASN
1	A	459	ASN
1	A	512	GLN
1	A	532	ASN
1	A	574	ASN
1	A	610	ASN
1	A	702	ASN
1	B	342	HIS

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Mol	Chain	Res	Type
1	B	358	GLN
1	B	369	GLN
1	B	459	ASN
1	B	512	GLN
1	B	532	ASN
1	B	574	ASN
1	B	610	ASN
1	B	647	GLN
1	B	702	ASN
1	C	342	HIS
1	C	346	HIS
1	C	358	GLN
1	C	412	HIS
1	C	430	GLN
1	C	441	HIS
1	C	445	ASN
1	C	459	ASN
1	C	513	GLN
1	C	532	ASN
1	C	574	ASN
1	C	610	ASN
1	C	647	GLN
1	C	702	ASN
1	D	342	HIS
1	D	358	GLN
1	D	459	ASN
1	D	512	GLN
1	D	513	GLN
1	D	532	ASN
1	D	574	ASN
1	D	610	ASN
1	D	702	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	750	1	42,50,50	2.55	12 (28%)	27,82,82	1.52	5 (18%)
4	H4B	A	760	-	18,18,18	1.19	2 (11%)	24,26,26	1.79	6 (25%)
2	ARG	A	770	-	11,11,11	0.66	0	13,13,13	0.97	1 (7%)
5	GOL	A	880	-	5,5,5	0.25	0	5,5,5	0.32	0
3	HEM	B	750	1	42,50,50	2.59	12 (28%)	27,82,82	1.38	5 (18%)
4	H4B	B	760	-	18,18,18	1.13	1 (5%)	24,26,26	1.64	5 (20%)
2	ARG	B	770	-	11,11,11	0.79	0	13,13,13	0.99	1 (7%)
5	GOL	B	880	-	5,5,5	0.43	0	5,5,5	0.65	0
3	HEM	C	750	1	42,50,50	2.68	11 (26%)	27,82,82	1.46	3 (11%)
4	H4B	C	760	-	18,18,18	1.16	1 (5%)	24,26,26	1.66	5 (20%)
2	ARG	C	770	-	11,11,11	0.98	0	13,13,13	0.92	0
5	GOL	C	880	-	5,5,5	0.25	0	5,5,5	0.21	0
5	GOL	C	881	-	5,5,5	0.19	0	5,5,5	0.38	0
5	GOL	C	882	-	5,5,5	0.25	0	5,5,5	0.46	0
3	HEM	D	750	1	42,50,50	2.65	14 (33%)	27,82,82	1.38	4 (14%)
4	H4B	D	760	-	18,18,18	1.19	2 (11%)	24,26,26	1.61	6 (25%)
2	ARG	D	770	-	11,11,11	0.85	0	13,13,13	1.06	1 (7%)
5	GOL	D	880	-	5,5,5	0.29	0	5,5,5	0.29	0
5	GOL	D	881	-	5,5,5	0.33	0	5,5,5	0.39	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	750	1	-	0/14/114/114	0/0/8/8
4	H4B	A	760	-	-	0/8/17/17	0/2/2/2
2	ARG	A	770	-	-	0/11/11/11	0/0/0/0
5	GOL	A	880	-	-	0/4/4/4	0/0/0/0
3	HEM	B	750	1	-	0/14/114/114	0/0/8/8
4	H4B	B	760	-	-	0/8/17/17	0/2/2/2
2	ARG	B	770	-	-	0/11/11/11	0/0/0/0
5	GOL	B	880	-	-	0/4/4/4	0/0/0/0
3	HEM	C	750	1	-	0/14/114/114	0/0/8/8
4	H4B	C	760	-	-	0/8/17/17	0/2/2/2
2	ARG	C	770	-	-	0/11/11/11	0/0/0/0
5	GOL	C	880	-	-	0/4/4/4	0/0/0/0
5	GOL	C	881	-	-	0/4/4/4	0/0/0/0
5	GOL	C	882	-	-	0/4/4/4	0/0/0/0
3	HEM	D	750	1	-	0/14/114/114	0/0/8/8
4	H4B	D	760	-	-	0/8/17/17	0/2/2/2
2	ARG	D	770	-	-	0/11/11/11	0/0/0/0
5	GOL	D	880	-	-	0/4/4/4	0/0/0/0
5	GOL	D	881	-	-	0/4/4/4	0/0/0/0

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	750	HEM	C3B-C2B	-8.95	1.36	1.45
3	B	750	HEM	C3B-C2B	-8.72	1.37	1.45
3	A	750	HEM	C3B-C2B	-8.60	1.37	1.45
3	D	750	HEM	C3B-C2B	-8.47	1.37	1.45
3	B	750	HEM	C3C-C2C	-7.78	1.39	1.45
3	D	750	HEM	C3C-C2C	-7.78	1.39	1.45
3	C	750	HEM	C3C-C2C	-7.70	1.39	1.45
3	A	750	HEM	C3C-C2C	-6.48	1.40	1.45
3	A	750	HEM	CMC-C2C	4.66	1.53	1.45
3	C	750	HEM	C1B-C2B	-4.66	1.41	1.45
3	C	750	HEM	CMB-C2B	4.59	1.53	1.45
3	C	750	HEM	CMD-C2D	4.40	1.52	1.45
3	A	750	HEM	FE-NB	4.38	2.11	1.95
3	C	750	HEM	CMC-C2C	4.37	1.52	1.45
3	B	750	HEM	CMD-C2D	4.35	1.52	1.45
3	D	750	HEM	FE-NB	4.24	2.10	1.95
3	D	750	HEM	C3C-C4C	-4.20	1.42	1.45
3	A	750	HEM	CMD-C2D	4.19	1.52	1.45
3	D	750	HEM	CMB-C2B	4.07	1.52	1.45
3	B	750	HEM	CMC-C2C	4.04	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	750	HEM	CMB-C2B	4.02	1.52	1.45
3	D	750	HEM	CMD-C2D	4.02	1.52	1.45
3	D	750	HEM	CMC-C2C	3.95	1.52	1.45
3	B	750	HEM	FE-NB	3.81	2.09	1.95
3	B	750	HEM	CMB-C2B	3.81	1.51	1.45
3	C	750	HEM	C3D-C2D	-3.79	1.33	1.43
3	A	750	HEM	C3D-C2D	-3.63	1.34	1.43
3	C	750	HEM	FE-NB	3.62	2.08	1.95
3	D	750	HEM	C3D-C2D	-3.52	1.34	1.43
3	B	750	HEM	C3D-C2D	-3.50	1.34	1.43
4	C	760	H4B	C7-C6	3.41	1.55	1.52
3	A	750	HEM	FE-NC	3.34	2.09	1.95
3	C	750	HEM	FE-NC	3.12	2.08	1.95
3	B	750	HEM	FE-NC	3.04	2.07	1.95
3	D	750	HEM	FE-NC	2.99	2.07	1.95
4	A	760	H4B	C7-C6	2.91	1.55	1.52
3	A	750	HEM	C3B-CAB	2.86	1.49	1.40
3	D	750	HEM	C1B-C2B	-2.78	1.43	1.45
4	B	760	H4B	C2-N2	2.78	1.36	1.32
3	B	750	HEM	C1B-C2B	-2.73	1.43	1.45
3	A	750	HEM	C3C-CAC	2.55	1.48	1.40
3	D	750	HEM	C3B-CAB	2.54	1.48	1.40
4	D	760	H4B	C7-C6	2.53	1.54	1.52
3	B	750	HEM	C3B-CAB	2.49	1.48	1.40
3	B	750	HEM	C3C-CAC	2.49	1.48	1.40
3	B	750	HEM	C3C-C4C	-2.44	1.43	1.45
3	D	750	HEM	C3C-CAC	2.40	1.48	1.40
4	D	760	H4B	C2-N1	2.35	1.36	1.33
4	A	760	H4B	C2-N1	2.32	1.36	1.33
3	C	750	HEM	C3B-CAB	2.29	1.47	1.40
3	D	750	HEM	C3B-C4B	2.22	1.50	1.45
3	D	750	HEM	C4A-NA	2.20	1.40	1.36
3	C	750	HEM	C3C-CAC	2.08	1.47	1.40
3	A	750	HEM	C3B-C4B	2.06	1.50	1.45
3	A	750	HEM	C1C-NC	2.04	1.38	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	760	H4B	C4-C4A-C8A	4.75	118.86	114.56
4	D	760	H4B	C4-C4A-C8A	4.71	118.83	114.56
4	C	760	H4B	C4-C4A-C8A	4.54	118.67	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	750	HEM	CBA-CAA-C2A	-4.52	105.11	112.63
3	A	750	HEM	CBD-CAD-C3D	-4.43	104.89	114.51
4	B	760	H4B	C4-C4A-C8A	4.35	118.50	114.56
3	D	750	HEM	CBD-CAD-C3D	-3.51	106.90	114.51
4	A	760	H4B	C6-C7-N8	-3.47	107.02	111.56
4	C	760	H4B	C6-C7-N8	-3.40	107.11	111.56
4	A	760	H4B	C4-N3-C2	3.37	122.10	120.20
3	D	750	HEM	CBA-CAA-C2A	-3.33	107.09	112.63
3	B	750	HEM	CBD-CAD-C3D	-3.25	107.46	114.51
3	B	750	HEM	CBA-CAA-C2A	-3.15	107.39	112.63
4	C	760	H4B	C4A-C8A-N8	3.09	122.07	118.43
3	C	750	HEM	CBD-CAD-C3D	-2.97	108.06	114.51
4	B	760	H4B	C4-N3-C2	2.85	121.81	120.20
4	C	760	H4B	C4A-N5-C6	-2.64	113.97	121.16
4	B	760	H4B	N2-C2-N3	2.52	120.52	117.82
4	D	760	H4B	C9-C6-N5	2.49	114.97	111.10
3	A	750	HEM	O2D-CGD-CBD	2.47	122.73	114.19
3	A	750	HEM	CAD-C3D-C4D	2.39	128.97	125.60
3	B	750	HEM	O2A-CGA-O1A	-2.38	117.29	123.31
2	B	770	ARG	CD-NE-CZ	2.37	129.78	124.58
3	B	750	HEM	O2D-CGD-CBD	2.33	122.26	114.19
3	C	750	HEM	O2D-CGD-CBD	2.30	122.13	114.19
4	D	760	H4B	C4A-N5-C6	-2.29	114.92	121.16
4	A	760	H4B	C4A-N5-C6	-2.29	114.94	121.16
4	A	760	H4B	O9-C9-C10	-2.29	104.33	108.99
4	B	760	H4B	O9-C9-C10	-2.27	104.36	108.99
4	D	760	H4B	C6-C7-N8	-2.26	108.60	111.56
3	D	750	HEM	O2D-CGD-CBD	2.20	121.81	114.19
2	A	770	ARG	OXT-C-CA	2.18	121.86	116.90
4	D	760	H4B	N8-C8A-N1	2.17	119.00	115.82
4	A	760	H4B	C7-C6-C9	-2.16	110.11	113.45
3	D	750	HEM	O2D-CGD-O1D	-2.15	117.87	123.31
3	B	750	HEM	O2D-CGD-O1D	-2.14	117.89	123.31
2	D	770	ARG	CB-CG-CD	2.08	117.26	111.96
3	A	750	HEM	O2A-CGA-O1A	-2.06	118.11	123.31
4	B	760	H4B	C4-C4A-N5	2.05	122.00	119.07
4	C	760	H4B	C4-C4A-N5	2.04	122.00	119.07
4	D	760	H4B	C7-C6-C9	-2.03	110.32	113.45
3	A	750	HEM	CBA-CAA-C2A	-2.00	109.30	112.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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, 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	420/420 (100%)	0.20	7 (1%) 67 68	27, 45, 66, 83	0
1	B	411/420 (97%)	0.18	8 (1%) 64 64	26, 42, 68, 87	0
1	C	420/420 (100%)	0.07	3 (0%) 84 86	24, 39, 61, 78	0
1	D	411/420 (97%)	0.24	16 (3%) 37 37	24, 43, 71, 96	0
All	All	1662/1680 (98%)	0.17	34 (2%) 62 63	24, 42, 67, 96	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	720	VAL	8.7
1	D	720	VAL	8.1
1	D	721	TRP	6.1
1	A	720	VAL	5.2
1	B	721	TRP	5.1
1	B	353	VAL	5.0
1	D	474	LYS	3.6
1	D	718	THR	3.6
1	B	718	THR	3.6
1	D	719	HIS	3.4
1	B	376	ARG	3.3
1	D	380	LYS	3.0
1	D	374	ILE	3.0
1	A	377	PHE	3.0
1	A	721	TRP	2.9
1	C	720	VAL	2.8
1	B	719	HIS	2.7
1	A	376	ARG	2.7
1	D	375	LYS	2.6
1	D	376	ARG	2.6
1	D	516	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	380	LYS	2.6
1	D	329	THR	2.5
1	C	380	LYS	2.4
1	D	353	VAL	2.4
1	A	336	CYS	2.2
1	D	395	THR	2.2
1	C	721	TRP	2.1
1	D	440	ALA	2.1
1	B	475	HIS	2.1
1	D	360	PHE	2.1
1	D	475	HIS	2.0
1	B	360	PHE	2.0
1	A	387	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	C	882	6/6	0.16	4.64	43,53,55,57	0
5	GOL	C	881	6/6	0.24	3.39	67,71,73,73	0
2	ARG	C	770	12/12	0.15	2.39	35,39,42,42	0
5	GOL	B	880	6/6	0.16	0.82	53,58,61,62	0
5	GOL	D	881	6/6	0.15	0.75	66,74,74,74	0
2	ARG	D	770	12/12	0.13	0.70	40,43,45,46	0
3	HEM	A	750	43/43	0.15	0.66	33,37,42,46	0
5	GOL	D	880	6/6	0.14	0.57	48,55,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HEM	B	750	43/43	0.13	0.47	32,35,39,44	0
3	HEM	C	750	43/43	0.13	0.44	27,32,36,38	0
2	ARG	A	770	12/12	0.14	0.43	42,45,48,48	0
3	HEM	D	750	43/43	0.12	0.36	31,34,42,45	0
2	ARG	B	770	12/12	0.11	0.02	39,43,48,49	0
5	GOL	C	880	6/6	0.12	-0.02	43,51,54,54	0
4	H4B	A	760	17/17	0.16	-0.15	28,31,32,32	0
4	H4B	C	760	17/17	0.17	-0.25	23,26,30,30	0
5	GOL	A	880	6/6	0.12	-0.53	51,57,60,63	0
4	H4B	D	760	17/17	0.15	-0.62	27,29,31,32	0
4	H4B	B	760	17/17	0.15	-0.70	29,31,32,33	0
6	ZN	A	900	1/1	0.16	-1.71	28,28,28,28	0
6	ZN	C	900	1/1	0.13	-3.27	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.