



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:14 PM GMT

PDB ID : 1VAF  
Title : Inducible nitric oxide synthase oxygenase domain complexed with the inhibitor AR-R17477  
Authors : Fedorov, R.; Vasan, R.; Ghosh, D.K.; Schlichting, I.  
Deposited on : 2004-02-16  
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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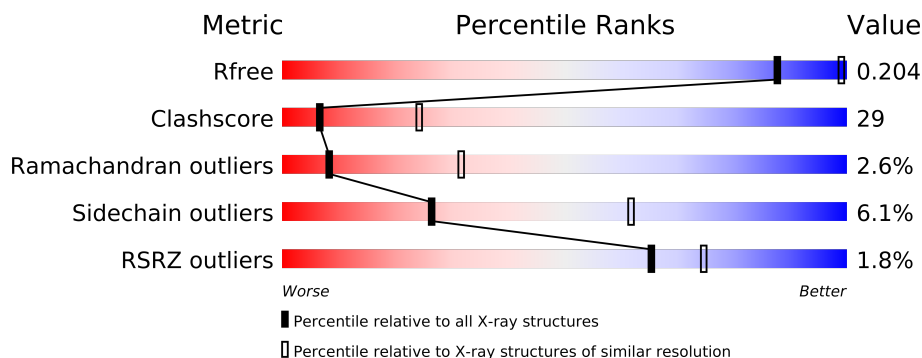
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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  $\geq 3$ , 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	419	
1	B	419	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	ARR	A	902[A]	-	X
5	ARR	A	902[B]	-	X
5	ARR	B	903[A]	-	X
5	ARR	B	903[B]	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7233 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.

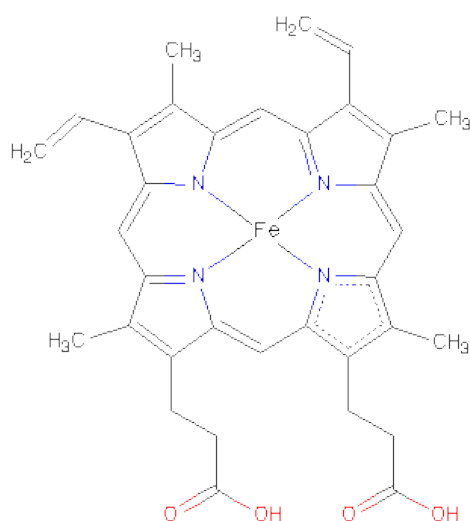
- Molecule 1 is a protein called Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3415	2189	588	617	21			
1	B	419	Total	C	N	O	S	0	0	0
			3415	2189	588	617	21			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

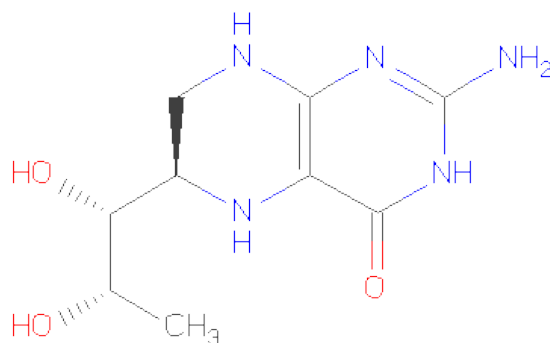
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

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



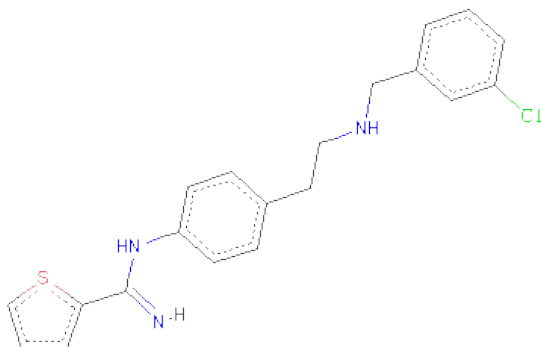
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	0	0
			17	9	5	3		
4	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is N-(4-{2-[(3-CHLOROBENZYL)AMINO]ETHYL}PHENYL)THIOPHENE-2-CARBOXIMIDAMIDE (three-letter code: ARR) (formula:  $C_{20}H_{20}ClN_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	S	0	1
			50	40	2	6	2		
5	B	1	Total	C	Cl	N	S	0	1
			50	40	2	6	2		

- Molecule 6 is water.

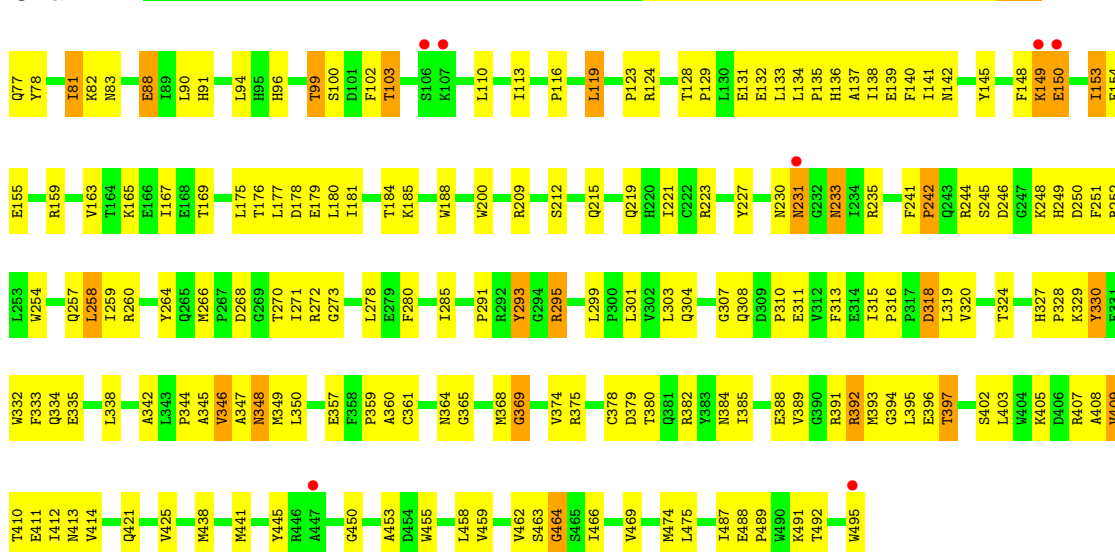
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total	O	0	0
			89	89		
6	B	92	Total	O	0	0
			92	92		

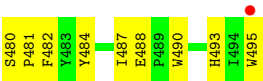
### 3 Residue-property plots

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, inducible

Chain A:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	216.34Å 216.34Å 117.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.90 19.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.90) 98.1 (19.95-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.71Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207 , 0.262 0.213 , 0.204	Depositor DCC
$R_{free}$ test set	1790 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43964 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: HEM, ARR, ZN, H4B

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	0.43	0/3515	0.66	1/4778 (0.0%)
1	B	0.42	0/3515	0.63	1/4778 (0.0%)
All	All	0.43	0/7030	0.65	2/9556 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLY	N-CA-C	-6.26	97.44	113.10
1	B	365	GLY	N-CA-C	-5.29	99.87	113.10

There are no chirality outliers.

There are no planarity outliers.

### 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	3415	0	3312	175	0
1	B	3415	0	3312	207	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	43	0	30	1	0
4	A	17	0	15	0	0
4	B	17	0	15	0	0
5	A	50	0	38	13	3
5	B	50	0	38	20	0
6	A	89	0	0	4	3
6	B	92	0	0	3	0
All	All	7233	0	6790	406	3

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 29.

All (406) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:254:TRP:HE1	1:B:304:GLN:NE2	1.49	1.09
1:B:153:ILE:H	1:B:153:ILE:HD12	1.20	1.06
1:A:271:ILE:HD13	1:A:278:LEU:HD11	1.37	1.05
1:A:153:ILE:HD12	1:A:153:ILE:H	1.18	1.05
5:B:903[A]:ARR:C10	5:B:903[A]:ARR:H3	1.86	1.05
5:B:903[B]:ARR:H3	5:B:903[B]:ARR:C10	1.86	1.05
5:A:902[B]:ARR:H3	5:A:902[B]:ARR:C10	1.86	1.04
5:A:902[A]:ARR:H3	5:A:902[A]:ARR:C10	1.86	1.04
5:A:902[B]:ARR:H141	6:A:994:HOH:O	1.57	1.00
1:B:77:GLN:HG3	1:B:78:TYR:H	1.27	0.96
1:B:124:ARG:HH12	1:B:128:THR:HB	1.32	0.95
1:B:83:ASN:ND2	1:B:86:SER:H	1.67	0.93
1:B:254:TRP:HE1	1:B:304:GLN:HE21	1.15	0.90
1:B:330:TYR:HB3	1:B:332:TRP:NE1	1.86	0.90
1:A:154:GLU:HG2	1:A:155:GLU:H	1.35	0.90
1:A:273:GLY:HA2	1:A:295:ARG:HA	1.56	0.88
1:B:124:ARG:NH1	1:B:128:THR:HB	1.90	0.87
1:A:230:ASN:HD22	1:A:235:ARG:CZ	1.88	0.86
5:A:902[A]:ARR:C3	5:A:902[A]:ARR:H10	2.06	0.86
5:A:902[B]:ARR:C3	5:A:902[B]:ARR:H10	2.06	0.86
5:B:903[A]:ARR:C3	5:B:903[A]:ARR:H10	2.05	0.86
5:B:903[B]:ARR:H10	5:B:903[B]:ARR:C3	2.05	0.86
1:A:342:ALA:HB1	1:A:425:VAL:HG11	1.60	0.82
5:A:902[A]:ARR:C3	5:A:902[A]:ARR:C10	2.58	0.81
5:A:902[B]:ARR:C3	5:A:902[B]:ARR:C10	2.58	0.81
1:B:230:ASN:HD22	1:B:233:ASN:HB3	1.44	0.81
5:B:903[A]:ARR:C3	5:B:903[A]:ARR:C10	2.58	0.81
5:B:903[B]:ARR:C10	5:B:903[B]:ARR:C3	2.58	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:289:TRP:HZ2	1:B:292:ARG:HH21	1.27	0.81
1:A:149:LYS:O	1:A:150:GLU:HG2	1.82	0.79
1:A:330:TYR:HB3	1:A:332:TRP:NE1	1.97	0.79
5:B:903[A]:ARR:H10	5:B:903[A]:ARR:H3	1.63	0.79
5:B:903[B]:ARR:H3	5:B:903[B]:ARR:H10	1.63	0.79
5:A:902[A]:ARR:H3	5:A:902[A]:ARR:H10	1.63	0.79
5:A:902[B]:ARR:H3	5:A:902[B]:ARR:H10	1.63	0.79
1:B:330:TYR:HD1	1:B:330:TYR:H	1.29	0.78
1:A:153:ILE:HD12	1:A:153:ILE:N	1.98	0.77
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.51	0.75
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.87	0.75
1:B:272:ARG:HH11	1:B:272:ARG:HB2	1.53	0.74
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.22	0.74
1:A:488:GLU:HG3	1:A:491:LYS:NZ	2.02	0.74
1:A:246:ASP:OD2	1:A:248:LYS:HB2	1.88	0.73
1:B:311:GLU:HB2	1:B:313:PHE:HE1	1.54	0.72
1:B:153:ILE:N	1:B:153:ILE:HD12	2.00	0.71
1:A:153:ILE:H	1:A:153:ILE:CD1	1.95	0.71
1:B:148:PHE:HD1	1:B:148:PHE:H	1.38	0.70
1:A:154:GLU:HG2	1:A:155:GLU:N	2.06	0.70
1:B:230:ASN:ND2	1:B:233:ASN:HB3	2.06	0.70
1:A:230:ASN:HD22	1:A:235:ARG:NE	1.89	0.70
1:B:252:ARG:HD3	1:B:359:PRO:HB2	1.72	0.70
1:B:213:THR:OG1	1:B:216:GLU:HG3	1.91	0.69
1:B:107:LYS:HB3	1:B:107:LYS:NZ	2.08	0.69
1:B:77:GLN:HG3	1:B:78:TYR:N	2.06	0.69
1:A:330:TYR:HD1	1:A:332:TRP:CZ2	2.09	0.69
1:A:230:ASN:ND2	1:A:235:ARG:CZ	2.55	0.69
1:A:149:LYS:NZ	1:A:150:GLU:HB3	2.08	0.69
1:B:81:ILE:HD11	1:B:475:LEU:HD13	1.74	0.68
1:B:77:GLN:CG	1:B:78:TYR:H	2.05	0.68
1:A:266:MET:HB2	1:A:270:THR:HB	1.76	0.67
1:A:285:ILE:HD11	1:A:291:PRO:HB3	1.77	0.67
1:B:114:MET:HE3	5:B:903[B]:ARR:H16	1.77	0.67
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.76	0.67
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.10	0.67
1:A:266:MET:CE	1:A:272:ARG:HH11	2.08	0.67
1:B:342:ALA:HB1	1:B:425:VAL:HG11	1.76	0.67
1:B:410:THR:O	1:B:414:VAL:HG23	1.95	0.66
1:A:209:ARG:O	1:A:242:PRO:HG3	1.97	0.65
1:B:330:TYR:N	1:B:330:TYR:CD1	2.65	0.65
1:B:82:LYS:O	1:B:473:GLU:HG3	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:407:ARG:HG3	1:A:407:ARG:HH11	1.61	0.65
1:B:254:TRP:NE1	1:B:304:GLN:NE2	2.35	0.65
1:B:176:THR:OG1	1:B:179:GLU:HG3	1.97	0.64
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.79	0.64
1:B:292:ARG:HG2	1:B:292:ARG:HH11	1.62	0.64
1:A:259:ILE:HD13	1:A:320:VAL:HG13	1.80	0.64
1:A:488:GLU:HG3	1:A:491:LYS:HZ3	1.60	0.63
1:A:132:GLU:C	1:A:135:PRO:HD2	2.19	0.63
1:A:441:MET:O	1:A:445:TYR:HD1	1.82	0.63
1:A:438:MET:HE3	1:A:469:VAL:HA	1.80	0.62
1:B:271:ILE:HD13	6:B:1938:HOH:O	1.98	0.62
1:B:83:ASN:HD22	1:B:86:SER:H	1.47	0.62
1:B:300:PRO:HB2	1:B:312:VAL:HG13	1.81	0.62
1:A:81:ILE:HG22	1:A:90:LEU:HB2	1.82	0.62
1:A:271:ILE:HD13	1:A:278:LEU:CD1	2.24	0.61
1:A:134:LEU:O	1:A:138:ILE:HG12	1.99	0.61
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.81	0.61
1:B:198:ILE:HB	1:B:440:HIS:HB2	1.82	0.61
1:B:374:VAL:O	1:B:378:CYS:HB2	2.01	0.60
1:A:382:ARG:HH11	1:A:382:ARG:HG3	1.66	0.60
1:B:321:LEU:HD12	1:B:322:GLU:N	2.17	0.60
1:A:330:TYR:CD2	1:A:330:TYR:N	2.70	0.60
1:A:176:THR:HG23	1:A:179:GLU:OE1	2.02	0.60
1:A:304:GLN:HG3	1:A:308:GLN:O	2.02	0.60
1:A:330:TYR:HD2	1:A:330:TYR:N	1.99	0.59
1:A:223:ARG:HG2	1:A:223:ARG:HH11	1.67	0.59
1:A:393:MET:HE3	1:A:411:GLU:HG3	1.84	0.59
1:A:405:LYS:O	1:A:409:VAL:HG12	2.02	0.59
1:A:244:ARG:HG3	1:A:250:ASP:OD1	2.02	0.59
1:A:163:VAL:O	1:A:167:ILE:HG13	2.02	0.59
1:A:82:LYS:HG2	1:A:83:ASN:N	2.18	0.58
1:A:129:PRO:HB2	1:A:132:GLU:HG2	1.84	0.58
1:B:259:ILE:HD13	1:B:320:VAL:HG13	1.85	0.58
1:B:252:ARG:CD	1:B:359:PRO:HB2	2.34	0.58
1:A:410:THR:O	1:A:414:VAL:HG23	2.04	0.58
1:A:348:ASN:HD22	1:A:348:ASN:H	1.52	0.57
1:A:154:GLU:H	1:A:154:GLU:CD	2.07	0.57
1:A:110:LEU:HD12	1:A:110:LEU:N	2.19	0.57
1:A:260:ARG:HG2	1:A:260:ARG:HH11	1.68	0.57
1:B:254:TRP:CZ3	1:B:490:TRP:HB3	2.39	0.57
1:B:152:LYS:HE2	1:B:155:GLU:CD	2.25	0.57
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.40	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:114:MET:CE	5:B:903[B]:ARR:C17	2.83	0.57
1:A:316:PRO:HD2	1:A:319:LEU:HD12	1.85	0.57
1:B:114:MET:HE1	5:B:903[B]:ARR:C17	2.34	0.57
1:A:389:VAL:O	1:A:393:MET:HG3	2.05	0.56
5:B:903[B]:ARR:H141	6:B:1929:HOH:O	2.04	0.56
1:B:330:TYR:HD2	1:B:332:TRP:HE1	1.52	0.56
1:A:438:MET:HE2	1:A:469:VAL:HG22	1.87	0.56
1:B:248:LYS:NZ	1:B:248:LYS:HB3	2.20	0.56
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.87	0.56
1:A:251:PHE:O	1:A:360:ALA:HB2	2.05	0.56
1:A:94:LEU:HB3	1:A:450:GLY:HA3	1.88	0.56
1:B:252:ARG:HH11	1:B:252:ARG:HG3	1.71	0.56
1:A:330:TYR:HB3	1:A:332:TRP:CD1	2.40	0.56
1:A:285:ILE:CD1	1:A:291:PRO:HB3	2.36	0.56
1:B:102:PHE:CG	1:B:103:THR:N	2.74	0.56
1:B:120:THR:HG22	1:B:121:ARG:N	2.20	0.56
1:B:166:GLU:OE2	1:B:173:TYR:HA	2.06	0.55
1:A:264:TYR:CE2	1:A:293:TYR:HA	2.42	0.55
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.88	0.55
1:A:466:ILE:O	1:A:466:ILE:HG22	2.05	0.55
1:B:124:ARG:NH1	1:B:128:THR:CB	2.67	0.55
1:A:348:ASN:ND2	1:A:348:ASN:H	2.03	0.55
1:B:480:SER:HA	1:B:481:PRO:C	2.26	0.55
1:B:268:ASP:OD1	1:B:270:THR:HG23	2.05	0.55
1:A:330:TYR:HD1	1:A:332:TRP:HZ2	1.54	0.55
1:A:374:VAL:O	1:A:378:CYS:HB2	2.05	0.55
1:B:126:LYS:NZ	1:B:126:LYS:HB3	2.21	0.55
1:B:249:HIS:HA	1:B:307:GLY:HA3	1.87	0.55
1:B:165:LYS:O	1:B:169:THR:HG23	2.07	0.55
1:B:345:ALA:HB2	1:B:364:ASN:HB3	1.89	0.55
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.42	0.55
1:B:77:GLN:O	1:B:96:HIS:HE1	1.91	0.55
1:A:77:GLN:O	1:A:96:HIS:CE1	2.60	0.55
1:B:253:LEU:HD22	1:B:347:ALA:HB1	1.88	0.54
1:A:233:ASN:C	1:A:233:ASN:HD22	2.11	0.54
1:B:164:THR:O	1:B:168:GLU:HG3	2.07	0.54
1:A:385:ILE:O	1:A:389:VAL:HG23	2.08	0.54
1:B:153:ILE:H	1:B:153:ILE:CD1	1.93	0.53
1:A:395:LEU:O	1:A:397:THR:N	2.35	0.53
1:A:230:ASN:HB3	1:A:233:ASN:O	2.08	0.53
1:B:350:LEU:HD23	1:B:350:LEU:C	2.29	0.53
1:B:137:ALA:O	1:B:141:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:283:LEU:C	1:B:283:LEU:HD23	2.29	0.53
1:A:266:MET:HE2	1:A:272:ARG:HH11	1.73	0.53
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.90	0.53
1:B:407:ARG:HH11	1:B:407:ARG:HG3	1.72	0.53
1:A:310:PRO:HD2	1:A:495:TRP:CZ3	2.43	0.53
1:A:149:LYS:HZ1	1:A:150:GLU:HB3	1.74	0.53
1:B:273:GLY:HA2	1:B:295:ARG:HG3	1.90	0.53
1:B:152:LYS:HE2	1:B:155:GLU:OE2	2.09	0.53
1:B:114:MET:CE	5:B:903[B]:ARR:H17	2.38	0.53
1:A:88:GLU:OE1	6:A:957:HOH:O	2.19	0.53
1:B:453:ALA:HB1	1:B:458:LEU:CD1	2.40	0.52
1:A:380:THR:HA	1:A:384:ASN:HB2	1.90	0.52
1:B:190:ASN:O	1:B:192:PRO:HD3	2.09	0.52
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.91	0.52
1:A:215:GLN:HG3	1:A:219:GLN:NE2	2.24	0.52
1:A:270:THR:HG22	1:A:271:ILE:N	2.24	0.52
1:B:104:CYS:HA	1:B:110:LEU:CD1	2.38	0.52
1:A:138:ILE:O	1:A:142:ASN:ND2	2.43	0.52
1:B:215:GLN:HG3	1:B:219:GLN:HE21	1.73	0.52
1:A:165:LYS:O	1:A:169:THR:HG23	2.10	0.52
1:B:244:ARG:HG3	1:B:250:ASP:OD1	2.09	0.52
1:B:114:MET:CE	5:B:903[B]:ARR:C16	2.87	0.52
1:B:159:ARG:O	1:B:163:VAL:HG23	2.10	0.52
1:A:254:TRP:CE2	1:A:489:PRO:HB2	2.45	0.52
1:A:295:ARG:NH2	1:A:338:LEU:HD23	2.25	0.52
1:A:78:TYR:CG	1:A:91:HIS:HB3	2.44	0.52
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.44	0.52
1:B:300:PRO:HB2	1:B:312:VAL:CG1	2.39	0.52
1:A:145:TYR:HA	1:A:148:PHE:CD2	2.45	0.52
1:B:134:LEU:O	1:B:138:ILE:HG13	2.10	0.52
1:B:230:ASN:HB3	1:B:233:ASN:O	2.09	0.52
1:B:163:VAL:O	1:B:167:ILE:HG13	2.10	0.51
1:B:381:GLN:O	1:B:382:ARG:HD2	2.10	0.51
5:A:902[B]:ARR:H20	5:A:902[B]:ARR:H132	1.92	0.51
1:B:78:TYR:CE1	1:B:91:HIS:HD2	2.29	0.51
1:A:159:ARG:O	1:A:163:VAL:HG23	2.10	0.51
1:A:264:TYR:CD2	1:A:293:TYR:HA	2.45	0.51
1:A:258:LEU:HD13	1:A:347:ALA:HB2	1.92	0.51
1:B:114:MET:HE3	5:B:903[B]:ARR:C16	2.40	0.51
1:A:327:HIS:HB2	1:A:333:PHE:CD1	2.45	0.51
1:B:428:MET:CE	1:B:432:THR:HG22	2.41	0.51
1:B:329:LYS:HB2	1:B:330:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:389:VAL:HG21	1:A:412:ILE:HD11	1.92	0.51
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.41	0.51
1:A:382:ARG:HG3	1:A:382:ARG:NH1	2.26	0.51
1:B:245:SER:OG	1:B:246:ASP:N	2.42	0.51
5:B:903[B]:ARR:H132	5:B:903[B]:ARR:H20	1.92	0.51
1:B:254:TRP:HE1	1:B:304:GLN:HE22	1.51	0.50
1:B:254:TRP:HZ3	1:B:283:LEU:HD11	1.74	0.50
1:B:148:PHE:N	1:B:148:PHE:CD1	2.79	0.50
1:B:197:ARG:C	1:B:199:GLN:H	2.13	0.50
1:B:77:GLN:HA	1:B:77:GLN:OE1	2.12	0.50
1:B:434:SER:OG	1:B:467:THR:HB	2.11	0.50
1:B:292:ARG:HG2	1:B:292:ARG:NH1	2.26	0.50
1:A:129:PRO:HB3	1:A:131:GLU:CD	2.32	0.50
1:B:154:GLU:OE2	1:B:155:GLU:HG3	2.12	0.50
1:A:397:THR:O	1:A:397:THR:HG22	2.11	0.50
1:A:455:TRP:O	1:A:459:VAL:HG23	2.11	0.50
1:A:462:VAL:O	1:A:463:SER:HB2	2.10	0.50
1:A:332:TRP:CE3	1:A:392:ARG:HD3	2.46	0.50
1:A:249:HIS:HA	1:A:307:GLY:HA3	1.93	0.50
1:B:149:LYS:HD2	1:B:149:LYS:O	2.11	0.50
1:B:438:MET:HE3	1:B:469:VAL:HA	1.94	0.49
1:B:130:LEU:C	1:B:130:LEU:HD23	2.32	0.49
1:B:412:ILE:O	1:B:416:VAL:HG23	2.11	0.49
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.48	0.49
1:A:334:GLN:H	1:A:334:GLN:NE2	2.10	0.49
1:B:126:LYS:HG3	1:B:127:PRO:O	2.12	0.49
1:B:330:TYR:HD2	1:B:332:TRP:NE1	2.10	0.49
1:A:378:CYS:O	1:A:379:ASP:C	2.51	0.49
1:A:453:ALA:HB1	1:A:458:LEU:CD1	2.42	0.49
1:A:252:ARG:CD	1:A:359:PRO:HB2	2.42	0.49
1:B:383:TYR:O	1:B:385:ILE:N	2.45	0.49
1:B:385:ILE:HD11	1:B:412:ILE:HD13	1.94	0.49
1:A:81:ILE:CD1	1:A:475:LEU:HD13	2.43	0.48
1:B:252:ARG:HB2	1:B:304:GLN:NE2	2.29	0.48
1:B:445:TYR:CE2	1:B:450:GLY:HA2	2.48	0.48
1:B:475:LEU:HB3	1:B:477:TYR:CE1	2.48	0.48
1:A:397:THR:CG2	1:A:397:THR:O	2.61	0.48
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.96	0.48
1:B:378:CYS:SG	1:B:386:LEU:HD23	2.53	0.48
1:A:124:ARG:HB3	1:A:244:ARG:HD3	1.95	0.48
1:A:348:ASN:HD22	1:A:348:ASN:N	2.09	0.48
1:A:338:LEU:HD11	1:A:385:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:466:ILE:O	1:B:466:ILE:HG22	2.14	0.48
1:B:177:LEU:O	1:B:181:ILE:HG13	2.14	0.48
1:B:221:ILE:O	1:B:225:ILE:HG13	2.13	0.47
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.44	0.47
1:B:366:TRP:CZ2	3:B:900:HEM:HBB1	2.49	0.47
1:A:181:ILE:HG22	1:A:185:LYS:HE3	1.96	0.47
1:B:311:GLU:HB2	1:B:313:PHE:CE1	2.44	0.47
1:B:475:LEU:HB3	1:B:477:TYR:HE1	1.78	0.47
1:A:223:ARG:CG	1:A:223:ARG:HH11	2.27	0.47
1:B:248:LYS:HB3	1:B:248:LYS:HZ3	1.79	0.47
1:A:330:TYR:O	1:A:333:PHE:HB2	2.14	0.47
1:B:387:GLU:OE1	1:B:397:THR:HG21	2.14	0.47
1:B:342:ALA:CB	1:B:425:VAL:HG11	2.42	0.47
1:B:138:ILE:O	1:B:142:ASN:ND2	2.48	0.47
1:B:83:ASN:C	1:B:85:GLY:H	2.18	0.47
1:B:289:TRP:HZ2	1:B:292:ARG:NH2	2.05	0.47
1:B:211:CYS:SG	1:B:216:GLU:HB2	2.54	0.47
1:B:379:ASP:CB	1:B:382:ARG:HG2	2.45	0.47
1:B:271:ILE:N	1:B:271:ILE:HD12	2.30	0.47
1:A:301:LEU:CD1	1:A:315:ILE:HD11	2.45	0.47
1:B:215:GLN:HG3	1:B:219:GLN:NE2	2.30	0.47
1:B:461:PRO:HD3	6:B:1932:HOH:O	2.14	0.47
1:A:318:ASP:OD2	1:A:318:ASP:N	2.47	0.47
1:B:254:TRP:CZ3	1:B:283:LEU:HD11	2.49	0.47
1:B:285:ILE:HG12	1:B:291:PRO:HD3	1.96	0.47
1:B:445:TYR:HA	1:B:450:GLY:H	1.80	0.46
1:A:311:GLU:HB2	1:A:313:PHE:HE1	1.80	0.46
1:A:180:LEU:O	1:A:184:THR:HG23	2.15	0.46
1:B:332:TRP:CZ3	1:B:392:ARG:HB2	2.49	0.46
1:A:233:ASN:ND2	1:A:233:ASN:C	2.65	0.46
1:B:120:THR:CG2	1:B:121:ARG:N	2.78	0.46
1:B:134:LEU:HD12	1:B:134:LEU:O	2.15	0.46
1:B:145:TYR:HA	1:B:148:PHE:CE1	2.50	0.46
1:A:375:ARG:O	1:A:379:ASP:HB2	2.16	0.46
1:A:258:LEU:HD22	1:A:345:ALA:CB	2.45	0.46
1:A:176:THR:HG23	1:A:179:GLU:CD	2.35	0.46
1:B:227:TYR:C	1:B:227:TYR:CD1	2.89	0.46
1:A:230:ASN:OD1	1:A:230:ASN:O	2.33	0.46
1:B:382:ARG:HG3	1:B:382:ARG:HH11	1.81	0.46
1:A:177:LEU:O	1:A:181:ILE:HG13	2.16	0.46
1:A:295:ARG:NH2	1:A:338:LEU:CD2	2.78	0.46
1:B:379:ASP:HB2	1:B:382:ARG:CG	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:197:ARG:C	1:B:199:GLN:N	2.69	0.46
1:B:107:LYS:HZ3	1:B:107:LYS:HB3	1.80	0.46
1:B:247:GLY:HA2	1:B:250:ASP:OD1	2.15	0.45
1:B:429:ASP:OD2	1:B:432:THR:HB	2.15	0.45
1:B:115:ASN:OD1	5:B:903[A]:ARR:H17	2.16	0.45
1:B:437:PHE:O	1:B:440:HIS:HB3	2.15	0.45
1:A:244:ARG:NH1	1:A:357:GLU:OE2	2.49	0.45
1:A:227:TYR:CD1	1:A:227:TYR:C	2.88	0.45
1:A:342:ALA:CB	1:A:425:VAL:HG11	2.38	0.45
1:B:272:ARG:CB	1:B:272:ARG:HH11	2.26	0.45
1:B:151:ALA:O	1:B:152:LYS:HG3	2.17	0.45
1:A:140:PHE:HE2	1:A:175:LEU:HD22	1.82	0.45
1:A:369:GLY:HA3	6:A:1035:HOH:O	2.15	0.45
1:A:332:TRP:CE3	1:A:392:ARG:HB3	2.51	0.45
1:A:134:LEU:N	1:A:135:PRO:CD	2.79	0.45
1:A:327:HIS:C	1:A:329:LYS:H	2.19	0.45
1:A:215:GLN:HG3	1:A:219:GLN:HE22	1.81	0.45
1:B:252:ARG:NH1	1:B:252:ARG:HG3	2.32	0.45
1:A:303:LEU:O	1:A:310:PRO:HA	2.17	0.45
1:A:348:ASN:N	1:A:348:ASN:ND2	2.63	0.45
1:B:427:ILE:HG12	1:B:428:MET:N	2.32	0.45
1:A:280:PHE:HD2	1:A:299:LEU:HD13	1.82	0.45
1:B:78:TYR:CZ	1:B:91:HIS:HD2	2.34	0.44
1:A:257:GLN:HA	1:A:345:ALA:O	2.17	0.44
1:B:309:ASP:OD1	1:B:493:HIS:NE2	2.49	0.44
5:B:903[A]:ARR:C6	5:B:903[A]:ARR:H3	2.45	0.44
5:B:903[B]:ARR:H3	5:B:903[B]:ARR:C6	2.45	0.44
1:B:330:TYR:CD2	1:B:332:TRP:NE1	2.85	0.44
1:A:463:SER:O	1:A:464:GLY:C	2.54	0.44
1:B:329:LYS:HB2	1:B:330:TYR:HD1	1.82	0.44
1:B:430:HIS:O	1:B:434:SER:HB2	2.18	0.44
1:B:149:LYS:HE3	1:B:150:GLU:HB3	2.00	0.44
1:B:239:THR:O	1:B:361:CYS:HA	2.18	0.44
1:A:133:LEU:O	1:A:133:LEU:HD23	2.17	0.44
1:A:391:ARG:C	1:A:393:MET:H	2.21	0.44
1:B:438:MET:HE2	1:B:469:VAL:HG12	1.99	0.44
1:B:373:GLY:HA2	1:B:416:VAL:HG21	1.99	0.44
1:A:181:ILE:CG2	1:A:185:LYS:HE3	2.48	0.44
1:B:78:TYR:CD1	1:B:78:TYR:C	2.90	0.44
1:A:231:ASN:HB3	6:A:1025:HOH:O	2.18	0.44
5:A:902[A]:ARR:H3	5:A:902[A]:ARR:C6	2.45	0.44
5:A:902[B]:ARR:H3	5:A:902[B]:ARR:C6	2.45	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:487:ILE:O	1:A:488:GLU:C	2.56	0.44
1:A:402:SER:O	1:A:403:LEU:HB2	2.17	0.44
1:B:348:ASN:C	1:B:348:ASN:HD22	2.20	0.44
1:B:330:TYR:HB3	1:B:332:TRP:CD1	2.53	0.43
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.52	0.43
1:B:332:TRP:CE3	1:B:392:ARG:HD2	2.53	0.43
1:B:397:THR:HA	1:B:404:TRP:CE2	2.53	0.43
1:B:493:HIS:HD2	1:B:495:TRP:CE2	2.36	0.43
1:B:342:ALA:HB1	1:B:425:VAL:CG1	2.45	0.43
1:A:453:ALA:HB3	1:A:474:MET:HB3	1.99	0.43
1:B:380:THR:HA	1:B:384:ASN:ND2	2.33	0.43
1:A:438:MET:CE	1:A:469:VAL:HG22	2.48	0.43
1:B:110:LEU:O	1:B:113:ILE:HG12	2.19	0.43
1:B:330:TYR:CD2	1:B:332:TRP:CZ2	3.07	0.43
1:B:107:LYS:HB3	1:B:107:LYS:HZ2	1.81	0.43
1:B:83:ASN:ND2	1:B:86:SER:N	2.50	0.43
1:B:80:ARG:CZ	1:B:89:ILE:HG21	2.48	0.43
1:B:132:GLU:C	1:B:135:PRO:HD2	2.39	0.43
1:B:487:ILE:O	1:B:488:GLU:C	2.56	0.43
1:B:97:LYS:HD2	1:B:97:LYS:N	2.34	0.43
1:A:332:TRP:HA	1:A:335:GLU:OE2	2.19	0.43
1:A:131:GLU:HG2	1:A:132:GLU:N	2.34	0.43
1:B:465:SER:HA	1:B:470:PHE:CD1	2.53	0.43
1:B:379:ASP:HB2	1:B:382:ARG:HG2	2.00	0.43
1:A:99:THR:HG22	1:A:100:SER:N	2.33	0.43
1:B:163:VAL:HG13	1:B:173:TYR:CD2	2.54	0.42
1:B:352:GLU:O	1:B:481:PRO:HA	2.19	0.42
1:B:368:MET:O	1:B:369:GLY:C	2.57	0.42
1:A:270:THR:CG2	1:A:271:ILE:N	2.81	0.42
1:B:459:VAL:HA	1:B:460:PRO:HD3	1.90	0.42
1:A:82:LYS:CG	1:A:83:ASN:N	2.82	0.42
1:B:428:MET:HE2	1:B:432:THR:HG22	2.00	0.42
1:A:136:HIS:O	1:A:139:GLU:HB3	2.19	0.42
1:A:145:TYR:HA	1:A:148:PHE:HD2	1.84	0.42
1:A:350:LEU:HD23	1:A:350:LEU:C	2.39	0.42
1:B:83:ASN:O	1:B:87:GLY:N	2.50	0.42
1:A:123:PRO:HG2	1:A:492:THR:HG21	2.02	0.42
1:A:393:MET:CE	1:A:411:GLU:HG3	2.50	0.42
1:A:132:GLU:O	1:A:135:PRO:HD2	2.18	0.42
1:B:264:TYR:CE2	1:B:293:TYR:HA	2.54	0.42
1:B:469:VAL:HG23	1:B:470:PHE:N	2.35	0.42
1:A:102:PHE:CD2	1:A:103:THR:N	2.78	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:99:THR:OG1	1:B:100:SER:N	2.52	0.42
1:B:282:GLN:O	1:B:285:ILE:HB	2.20	0.42
1:A:149:LYS:HZ2	1:A:150:GLU:HB3	1.85	0.42
1:B:104:CYS:HA	1:B:110:LEU:HD12	2.01	0.42
1:A:368:MET:O	1:A:369:GLY:C	2.56	0.42
1:A:102:PHE:CG	1:A:103:THR:N	2.88	0.41
1:B:322:GLU:OE2	1:B:339:LYS:HE2	2.20	0.41
1:B:395:LEU:O	1:B:397:THR:N	2.46	0.41
1:A:349:MET:HE2	1:A:349:MET:HB3	1.96	0.41
1:B:114:MET:HE1	5:B:903[B]:ARR:C16	2.50	0.41
1:A:245:SER:OG	1:A:246:ASP:N	2.51	0.41
1:A:258:LEU:CD1	1:A:347:ALA:HB2	2.49	0.41
1:B:180:LEU:HD11	1:B:240:VAL:HG21	2.02	0.41
1:B:77:GLN:O	1:B:96:HIS:CE1	2.73	0.41
1:B:130:LEU:O	1:B:130:LEU:HD23	2.21	0.41
1:A:311:GLU:HB2	1:A:313:PHE:CE1	2.56	0.41
1:A:421:GLN:HB2	1:A:421:GLN:HE21	1.62	0.41
1:B:482:PHE:HB3	1:B:484:TYR:CE2	2.55	0.41
1:A:266:MET:CE	1:A:272:ARG:HD3	2.51	0.41
1:B:151:ALA:C	1:B:152:LYS:HG3	2.40	0.41
1:B:251:PHE:CE1	1:B:306:ASP:N	2.88	0.41
1:A:223:ARG:NH1	1:A:223:ARG:CG	2.83	0.41
1:B:97:LYS:HD2	1:B:97:LYS:H	1.85	0.41
1:A:391:ARG:O	1:A:394:GLY:N	2.40	0.41
1:A:330:TYR:CE1	1:A:393:MET:HE3	2.56	0.41
1:A:342:ALA:HB1	1:A:425:VAL:CG1	2.42	0.41
1:B:301:LEU:HD12	1:B:301:LEU:HA	1.90	0.41
1:B:390:GLY:HA2	1:B:395:LEU:HD12	2.02	0.41
1:A:137:ALA:O	1:A:141:ILE:HG12	2.21	0.41
1:B:269:GLY:O	1:B:271:ILE:HD12	2.21	0.41
1:B:228:ALA:O	1:B:234:ILE:HA	2.21	0.41
1:B:377:PHE:HA	1:B:383:TYR:HB2	2.03	0.40
1:A:361:CYS:O	1:A:361:CYS:SG	2.79	0.40
1:B:107:LYS:CB	1:B:107:LYS:NZ	2.83	0.40
1:B:327:HIS:ND1	1:B:329:LYS:N	2.70	0.40
1:B:327:HIS:CE1	1:B:329:LYS:HB2	2.57	0.40
1:B:198:ILE:HG21	1:B:436:SER:HB3	2.03	0.40
1:A:110:LEU:HB3	1:A:113:ILE:CG1	2.51	0.40
1:A:345:ALA:HB2	1:A:364:ASN:HB3	2.02	0.40
1:A:346:VAL:HG23	5:A:902[B]:ARR:H2	2.03	0.40
1:A:374:VAL:CG2	1:A:413:ASN:HD21	2.34	0.40
1:B:138:ILE:HG22	1:B:142:ASN:HD21	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:902[B]:ARR:C17	6:A:1002:HOH:O[10_665]	0.71	1.49
5:A:902[B]:ARR:C18	6:A:1002:HOH:O[10_665]	1.34	0.86
5:A:902[B]:ARR:C16	6:A:1002:HOH:O[10_665]	2.04	0.16

## 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	417/419 (100%)	359 (86%)	43 (10%)	15 (4%)	5	22
1	B	417/419 (100%)	366 (88%)	44 (11%)	7 (2%)	14	45
All	All	834/838 (100%)	725 (87%)	87 (10%)	22 (3%)	8	32

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	THR
1	B	99	THR
1	B	330	TYR
1	B	384	ASN
1	A	295	ARG
1	A	396	GLU
1	A	397	THR
1	A	464	GLY
1	B	151	ALA
1	A	150	GLU
1	A	268	ASP
1	B	396	GLU
1	A	293	TYR
1	A	392	ARG
1	A	408	ALA
1	B	397	THR
1	B	401	ALA
1	A	242	PRO

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Mol	Chain	Res	Type
1	A	369	GLY
1	A	328	PRO
1	A	409	VAL
1	A	344	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	367/367 (100%)	349 (95%)	18 (5%)	35	73
1	B	367/367 (100%)	340 (93%)	27 (7%)	20	50
All	All	734/734 (100%)	689 (94%)	45 (6%)	26	62

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ILE
1	A	88	GLU
1	A	103	THR
1	A	119	LEU
1	A	128	THR
1	A	149	LYS
1	A	153	ILE
1	A	178	ASP
1	A	212	SER
1	A	231	ASN
1	A	233	ASN
1	A	258	LEU
1	A	318	ASP
1	A	324	THR
1	A	330	TYR
1	A	346	VAL
1	A	348	ASN
1	A	388	GLU
1	B	97	LYS
1	B	107	LYS
1	B	110	LEU

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Mol	Chain	Res	Type
1	B	126	LYS
1	B	128	THR
1	B	139	GLU
1	B	148	PHE
1	B	149	LYS
1	B	150	GLU
1	B	153	ILE
1	B	154	GLU
1	B	165	LYS
1	B	173	TYR
1	B	223	ARG
1	B	258	LEU
1	B	265	GLN
1	B	272	ARG
1	B	292	ARG
1	B	324	THR
1	B	330	TYR
1	B	348	ASN
1	B	353	VAL
1	B	368	MET
1	B	386	LEU
1	B	406	ASP
1	B	442	GLN
1	B	446	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	174	GLN
1	A	202	ASN
1	A	215	GLN
1	A	219	GLN
1	A	230	ASN
1	A	231	ASN
1	A	233	ASN
1	A	249	HIS
1	A	257	GLN
1	A	334	GLN
1	A	348	ASN
1	A	421	GLN
1	B	83	ASN

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Mol	Chain	Res	Type
1	B	91	HIS
1	B	96	HIS
1	B	142	ASN
1	B	174	GLN
1	B	215	GLN
1	B	219	GLN
1	B	230	ASN
1	B	231	ASN
1	B	282	GLN
1	B	304	GLN
1	B	334	GLN
1	B	348	ASN
1	B	384	ASN
1	B	413	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 10 ligands modelled in this entry, 2 are 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
3	HEM	A	900	1	49,50,50	3.19	9 (18%)	46,82,82	1.69	10 (21%)
4	H4B	A	901	-	18,18,18	1.51	4 (22%)	24,26,26	2.38	7 (29%)
5	ARR	A	902[A]	-	27,27,27	4.30	11 (40%)	35,35,35	2.60	2 (5%)
5	ARR	A	902[B]	-	27,27,27	4.30	11 (40%)	35,35,35	2.60	2 (5%)
4	H4B	B	1901	-	18,18,18	1.43	4 (22%)	24,26,26	2.40	7 (29%)
3	HEM	B	900	1	49,50,50	2.43	8 (16%)	46,82,82	1.34	6 (13%)
5	ARR	B	903[A]	-	27,27,27	4.31	10 (37%)	35,35,35	2.60	2 (5%)
5	ARR	B	903[B]	-	27,27,27	4.31	10 (37%)	35,35,35	2.60	2 (5%)

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	900	1	-	0/14/114/114	0/0/8/8
4	H4B	A	901	-	-	0/8/17/17	0/0/2/2
5	ARR	A	902[A]	-	-	0/11/15/15	0/3/3/3
5	ARR	A	902[B]	-	-	0/11/15/15	0/3/3/3
4	H4B	B	1901	-	-	0/8/17/17	0/0/2/2
3	HEM	B	900	1	-	0/14/114/114	0/0/8/8
5	ARR	B	903[A]	-	-	0/11/15/15	0/3/3/3
5	ARR	B	903[B]	-	-	0/11/15/15	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	903[B]	ARR	C4-S	-19.40	1.47	1.72
5	B	903[A]	ARR	C4-S	-19.40	1.47	1.72
5	A	902[B]	ARR	C4-S	-19.36	1.47	1.72
5	A	902[A]	ARR	C4-S	-19.36	1.47	1.72
3	A	900	HEM	C2D-C1D	13.02	1.47	1.44
3	A	900	HEM	C3D-C4D	12.59	1.47	1.44
3	B	900	HEM	C3D-C4D	9.80	1.47	1.44
3	B	900	HEM	C2D-C1D	7.01	1.46	1.44
3	A	900	HEM	C3D-C2D	-5.53	1.34	1.43
3	B	900	HEM	C3B-C2B	-5.46	1.34	1.43
3	A	900	HEM	C3B-C2B	-5.39	1.34	1.43
5	A	902[B]	ARR	C4-C5	-5.29	1.39	1.45
5	A	902[A]	ARR	C4-C5	-5.29	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	903[B]	ARR	C4-C5	-5.28	1.39	1.45
5	B	903[A]	ARR	C4-C5	-5.28	1.39	1.45
3	B	900	HEM	C3D-C2D	-5.17	1.34	1.43
5	A	902[B]	ARR	C1-S	-4.72	1.47	1.70
5	A	902[A]	ARR	C1-S	-4.72	1.47	1.70
5	B	903[B]	ARR	C1-S	-4.71	1.47	1.70
5	B	903[A]	ARR	C1-S	-4.71	1.47	1.70
3	B	900	HEM	C4A-C3A	4.69	1.46	1.40
3	A	900	HEM	C3C-C2C	-4.21	1.36	1.43
3	B	900	HEM	C3C-C2C	-4.17	1.36	1.43
3	A	900	HEM	C2B-C1B	-3.93	1.43	1.44
3	A	900	HEM	CHA-C4D	3.81	1.41	1.35
5	A	902[B]	ARR	C10-C6	3.72	1.45	1.39
5	A	902[A]	ARR	C10-C6	3.72	1.45	1.39
5	B	903[B]	ARR	C10-C6	3.70	1.45	1.39
5	B	903[A]	ARR	C10-C6	3.70	1.45	1.39
3	A	900	HEM	C4A-C3A	3.34	1.44	1.40
4	A	901	H4B	C6-N5	3.34	1.53	1.46
3	A	900	HEM	FE-NA	3.21	2.06	1.92
4	B	1901	H4B	C4-N3	3.19	1.42	1.37
4	B	1901	H4B	C6-N5	3.01	1.52	1.46
4	A	901	H4B	C4-N3	2.89	1.42	1.37
5	A	902[B]	ARR	C20-C19	2.78	1.43	1.38
5	B	903[B]	ARR	C20-C19	2.76	1.43	1.38
5	A	902[A]	ARR	C20-C15	2.75	1.44	1.39
5	B	903[A]	ARR	C20-C19	2.73	1.43	1.38
5	A	902[A]	ARR	C20-C19	2.72	1.43	1.38
4	A	901	H4B	C4A-N5	2.71	1.47	1.38
5	B	903[A]	ARR	C20-C15	2.71	1.44	1.39
5	B	903[B]	ARR	C20-C15	2.70	1.44	1.39
5	A	902[B]	ARR	C20-C15	2.70	1.44	1.39
5	A	902[B]	ARR	C18-C19	2.61	1.43	1.38
5	B	903[A]	ARR	C18-C19	2.60	1.43	1.38
5	A	902[A]	ARR	C18-C19	2.59	1.43	1.38
5	B	903[B]	ARR	C18-C19	2.57	1.43	1.38
3	B	900	HEM	FE-NA	2.51	2.03	1.92
4	B	1901	H4B	C4A-N5	2.43	1.46	1.38
5	B	903[B]	ARR	C7-C6	2.38	1.43	1.39
5	B	903[A]	ARR	C7-C6	2.38	1.43	1.39
5	A	902[B]	ARR	C7-C6	2.34	1.43	1.39
5	A	902[A]	ARR	C7-C6	2.34	1.43	1.39
5	B	903[A]	ARR	C16-C15	2.13	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	902[A]	ARR	C16-C15	2.13	1.43	1.38
5	B	903[B]	ARR	C2-C3	-2.12	1.32	1.39
5	B	903[A]	ARR	C2-C3	-2.12	1.32	1.39
5	B	903[B]	ARR	C16-C15	2.12	1.43	1.38
5	A	902[B]	ARR	C2-C3	-2.10	1.33	1.39
5	A	902[A]	ARR	C2-C3	-2.10	1.33	1.39
5	A	902[B]	ARR	C16-C15	2.09	1.43	1.38
4	B	1901	H4B	C8A-N1	2.08	1.38	1.34
3	B	900	HEM	CMC-C2C	2.06	1.53	1.47
4	A	901	H4B	C8A-N1	2.02	1.38	1.34
5	A	902[B]	ARR	C7-C8	2.00	1.42	1.38
5	A	902[A]	ARR	C7-C8	2.00	1.42	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	903[B]	ARR	C1-S-C4	14.49	98.29	91.91
5	B	903[A]	ARR	C1-S-C4	14.49	98.29	91.91
5	A	902[B]	ARR	C1-S-C4	14.47	98.28	91.91
5	A	902[A]	ARR	C1-S-C4	14.47	98.28	91.91
4	B	1901	H4B	C4-C4A-C8A	8.01	121.98	114.56
4	A	901	H4B	C4-C4A-C8A	7.99	121.96	114.56
3	A	900	HEM	C3B-C4B-NB	-4.86	110.52	114.00
3	A	900	HEM	CBA-CAA-C2A	3.96	119.67	112.69
3	B	900	HEM	C3B-C4B-NB	-3.84	111.25	114.00
4	B	1901	H4B	C4-N3-C2	3.52	125.66	119.51
4	A	901	H4B	C4-N3-C2	3.45	125.54	119.51
4	B	1901	H4B	C2-N1-C8A	3.41	122.45	117.61
4	B	1901	H4B	C4A-N5-C6	-3.40	111.92	121.16
3	A	900	HEM	CHD-C1D-ND	-3.38	121.78	124.58
4	A	901	H4B	C2-N1-C8A	3.36	122.39	117.61
4	A	901	H4B	C4A-N5-C6	-3.21	112.41	121.16
3	A	900	HEM	C3A-C4A-NA	3.16	111.80	109.41
3	A	900	HEM	C4A-CHB-C1B	-3.13	123.36	127.47
4	B	1901	H4B	N3-C2-N1	-3.05	117.51	121.78
3	B	900	HEM	CBA-CAA-C2A	3.00	117.98	112.69
3	B	900	HEM	CAD-C3D-C4D	2.98	129.89	124.53
4	A	901	H4B	N3-C2-N1	-2.94	117.66	121.78
5	B	903[B]	ARR	N1-C5-N3	-2.76	116.09	121.43
5	B	903[A]	ARR	N1-C5-N3	-2.76	116.09	121.43
5	A	902[B]	ARR	N1-C5-N3	-2.76	116.10	121.43
5	A	902[A]	ARR	N1-C5-N3	-2.76	116.10	121.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	HEM	C4A-NA-C1A	-2.45	103.54	106.76
3	A	900	HEM	CAA-C2A-C3A	-2.42	122.10	129.00
4	B	1901	H4B	C4A-C8A-N8	2.30	122.39	119.23
3	A	900	HEM	CAA-C2A-C1A	2.18	132.09	125.50
4	A	901	H4B	N8-C8A-N1	2.18	119.02	115.82
4	B	1901	H4B	N2-C2-N3	2.15	120.22	117.86
3	B	900	HEM	C4A-NA-C1A	-2.14	103.95	106.76
4	A	901	H4B	C4A-C8A-N8	2.10	122.12	119.23
3	B	900	HEM	CBD-CAD-C3D	-2.07	109.86	114.37
3	A	900	HEM	CAD-C3D-C4D	2.02	128.17	124.53
3	A	900	HEM	C4C-NC-C1C	-2.02	103.44	105.53
3	B	900	HEM	CHD-C1D-ND	-2.01	122.91	124.58

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	419/419 (100%)	-0.30	7 (1%) 67 76	42, 59, 78, 93	0
1	B	419/419 (100%)	-0.28	8 (1%) 64 72	48, 62, 82, 95	0
All	All	838/838 (100%)	-0.29	15 (1%) 65 74	42, 60, 80, 95	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	SER	7.1
1	B	101	ASP	4.2
1	A	106	SER	3.7
1	B	149	LYS	3.3
1	A	150	GLU	3.1
1	A	231	ASN	3.0
1	A	149	LYS	2.5
1	A	107	LYS	2.4
1	A	495	TRP	2.3
1	B	495	TRP	2.3
1	B	77	GLN	2.2
1	B	446	ARG	2.2
1	B	102	PHE	2.2
1	A	447	ALA	2.1
1	B	154	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	ARR	B	903[A]	25/25	0.41	10.07	41,56,59,59	25
5	ARR	B	903[B]	25/25	0.41	9.90	40,55,58,59	25
5	ARR	A	902[A]	25/25	0.40	7.76	40,48,58,59	25
5	ARR	A	902[B]	25/25	0.40	7.69	40,48,57,59	25
3	HEM	B	900	43/43	0.16	0.24	48,51,52,53	0
3	HEM	A	900	43/43	0.12	-0.87	42,45,48,50	0
4	H4B	B	1901	17/17	0.12	-1.01	51,52,55,57	0
4	H4B	A	901	17/17	0.11	-1.05	48,49,51,54	0
2	ZN	A	950	1/1	0.04	-2.12	55,55,55,55	1
2	ZN	B	950	1/1	0.04	-11.20	53,53,53,53	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.