



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2017 – 09:39 AM EDT

PDB ID : 5UO9  
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 7-[(3-Ethyl-5-((methylamino)methyl)phenoxy)methyl]quinolin-2-amine  
Authors : Chreifi, G.; Li, H.; Poulos, T.L.  
Deposited on : unknown  
Resolution : 2.19 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](mailto: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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

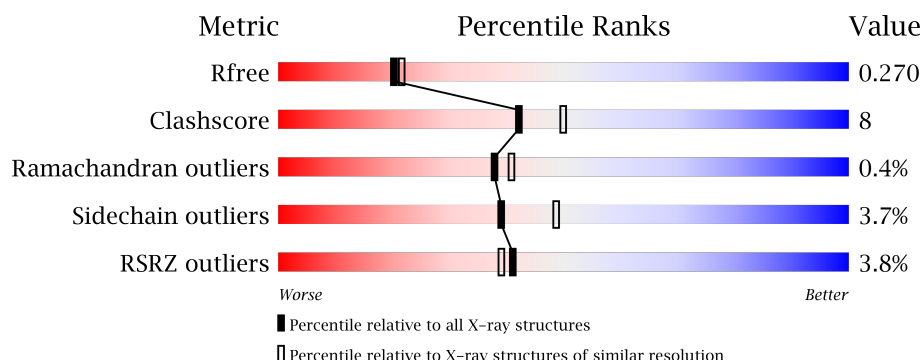
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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. 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	440	
1	B	440	
1	C	440	
1	D	440	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	H4B	C	502	-	-	-	X
4	8J4	A	503	-	-	-	X
4	8J4	B	503	-	-	-	X
4	8J4	C	503	-	-	-	X
4	8J4	D	503	-	-	-	X
5	BTB	A	504	-	-	-	X
5	BTB	D	504	-	-	-	X
6	ZN	A	506	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 13803 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	404	Total	C	N	O	S	0	2	0
			3237	2062	570	589	16			
1	B	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			
1	C	401	Total	C	N	O	S	0	2	0
			3209	2044	563	586	16			
1	D	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



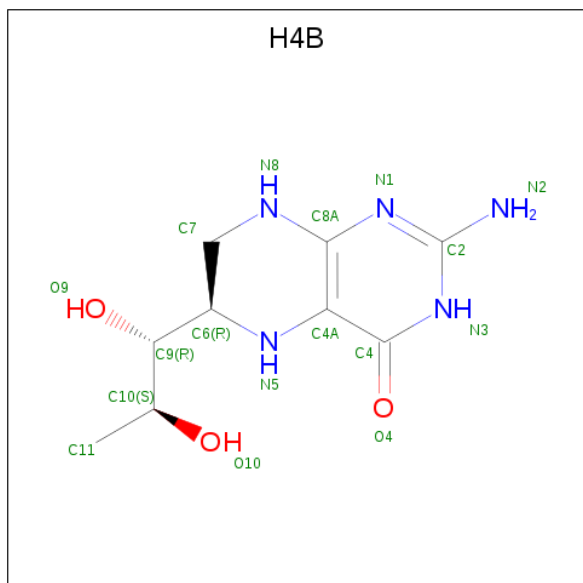
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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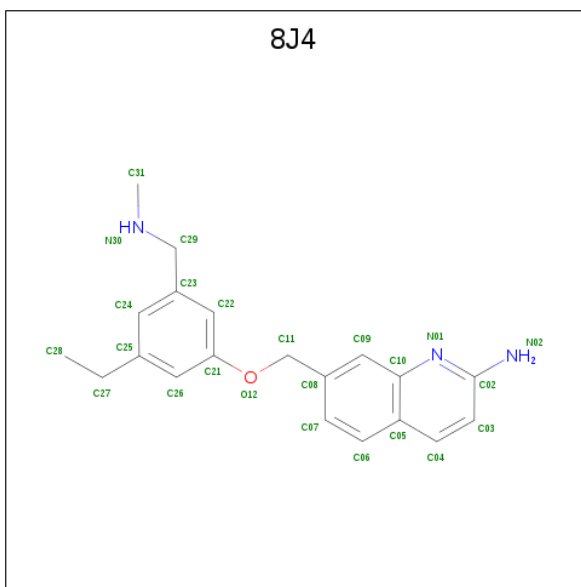
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



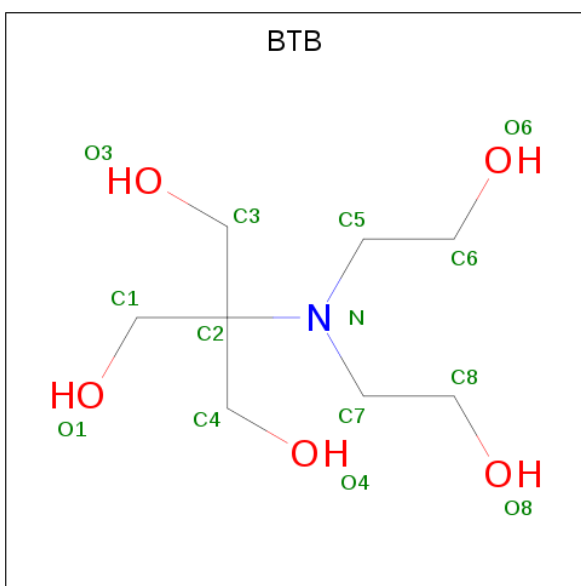
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-({3-ethyl-5-[(methylamino)methyl]phenoxy}methyl)quinolin-2-amine (three-letter code: 8J4) (formula:  $C_{20}H_{23}N_3O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	20	3	1		
4	B	1	Total	C	N	O	0	0
			24	20	3	1		
4	C	1	Total	C	N	O	0	0
			24	20	3	1		
4	D	1	Total	C	N	O	0	0
			24	20	3	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula:  $C_8H_{19}NO_5$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	A	1	Total	Cl	0	0
			1	1		
8	D	2	Total	Cl	0	0
			2	2		
8	C	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Gd	0	0
			1	1		
9	A	1	Total	Gd	0	0
			1	1		
9	D	1	Total	Gd	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Gd	0	0
			1	1		

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Ca	0	0
			1	1		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Mg	0	0
			1	1		

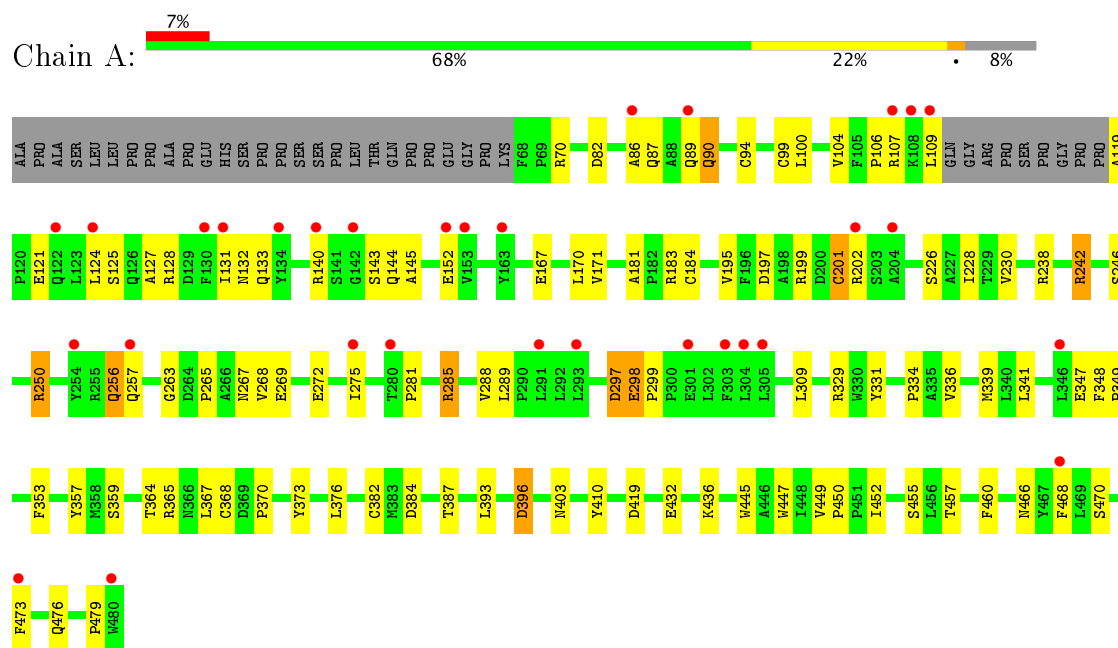
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	78	Total	O	0	0
			78	78		
12	B	118	Total	O	0	0
			118	118		
12	C	76	Total	O	0	0
			76	76		
12	D	114	Total	O	0	0
			114	114		

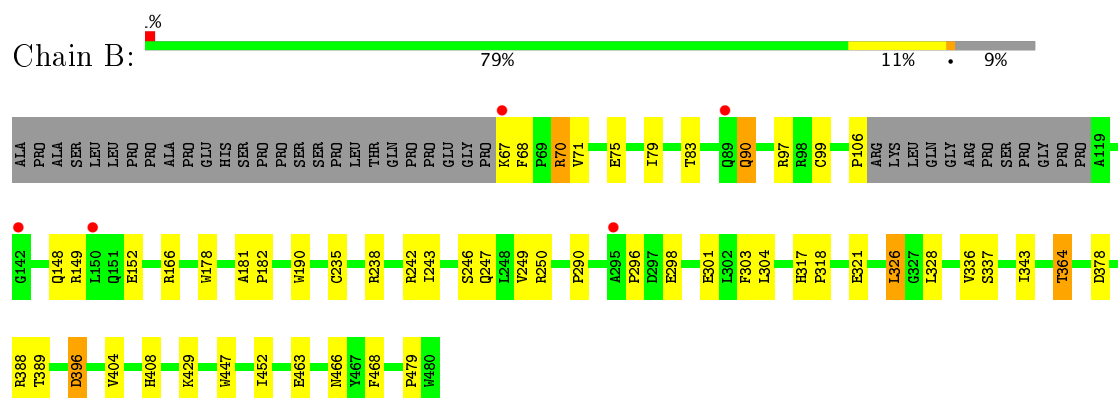
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

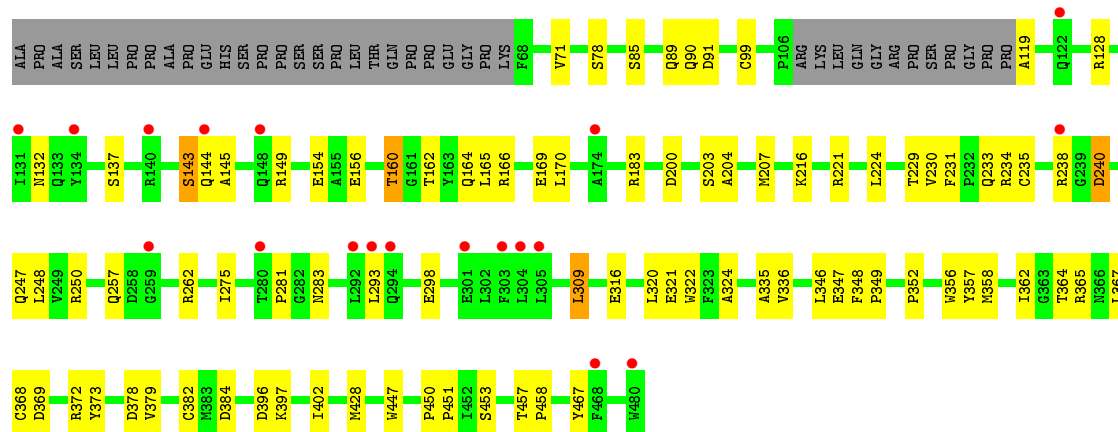


- Molecule 1: Nitric oxide synthase, endothelial

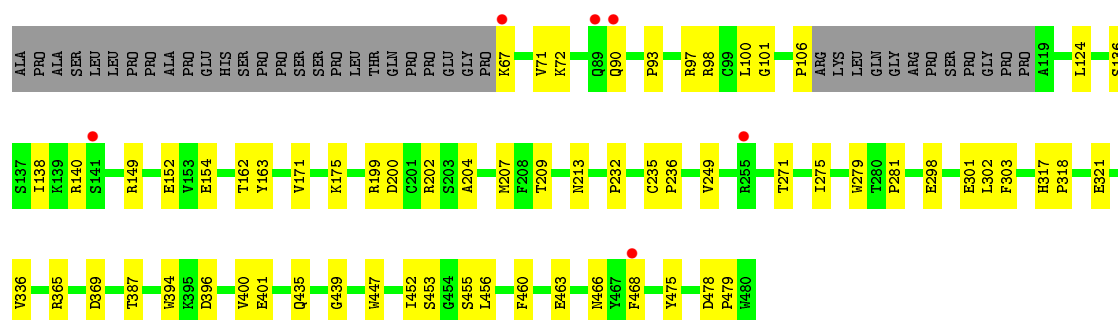
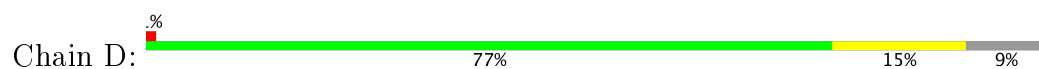


- Molecule 1: Nitric oxide synthase, endothelial





- Molecule 1: Nitric oxide synthase, endothelial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.38 Å 152.09 Å 108.22 Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	38.87 – 2.19 38.86 – 2.19	Depositor EDS
% Data completeness (in resolution range)	94.0 (38.87-2.19) 92.3 (38.86-2.19)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.20 Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.212 , 0.276 0.206 , 0.270	Depositor DCC
$R_{free}$ test set	4649 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.177 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13803	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, H4B, CL, CA, ZN, 8J4, GD, BTB, 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	0.37	0/3335	0.55	0/4543
1	B	0.43	0/3319	0.56	0/4523
1	C	0.38	0/3307	0.55	0/4507
1	D	0.44	0/3319	0.57	0/4523
All	All	0.40	0/13280	0.56	0/18096

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3237	0	3146	59	0
1	B	3221	0	3126	35	0
1	C	3209	0	3109	53	0
1	D	3221	0	3126	41	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	17	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	24	0	0	1	0
4	B	24	0	0	1	0
4	C	24	0	0	1	0
4	D	24	0	0	1	0
5	A	28	0	38	5	0
5	B	84	0	111	12	0
5	C	14	0	19	4	0
5	D	42	0	54	10	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	1	0
7	C	6	0	8	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	2	0	0	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	1	0	0	0	0
11	D	1	0	0	0	0
12	A	78	0	0	11	0
12	B	118	0	0	6	0
12	C	76	0	0	6	0
12	D	114	0	0	4	0
All	All	13803	0	12925	207	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 8.

All (207) 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:C:347:GLU:OE2	12:C:601:HOH:O	2.03	0.76
1:A:144:GLN:O	12:A:601:HOH:O	2.03	0.75
1:C:235:CYS:H	1:C:238:ARG:HD3	1.51	0.75
1:D:93:PRO:HG3	1:D:106:PRO:HB3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HEM:HHC	2:A:501:HEM:HBB2	1.70	0.72
1:A:201:CYS:SG	12:A:639:HOH:O	2.47	0.72
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.70	0.71
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.74	0.70
5:A:505:BTB:O1	5:A:505:BTB:O4	2.04	0.69
1:C:378:ASP:OD1	12:C:602:HOH:O	2.09	0.69
1:B:408:HIS:ND1	12:B:604:HOH:O	2.26	0.69
1:A:298:GLU:HG3	1:A:299:PRO:HD2	1.75	0.69
1:B:70:ARG:HE	1:B:79:ILE:HD13	1.58	0.68
1:B:149:ARG:NH1	1:B:152:GLU:OE1	2.26	0.68
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.13	0.67
1:B:326:LEU:HD12	5:B:510:BTB:H72	1.77	0.67
1:A:201:CYS:O	1:A:202:ARG:NH1	2.24	0.67
2:C:501:HEM:HHC	2:C:501:HEM:HBB2	1.75	0.67
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.77	0.67
1:A:432:GLU:HG2	1:A:436:LYS:HE3	1.78	0.66
1:A:70:ARG:NH1	12:A:609:HOH:O	2.27	0.66
1:A:125:SER:HA	1:A:128:ARG:HE	1.60	0.66
1:D:209:THR:O	1:D:213:ASN:ND2	2.28	0.66
1:A:331:TYR:O	1:A:410:TYR:OH	2.14	0.65
1:A:89:GLN:O	12:A:602:HOH:O	2.15	0.65
1:C:262:ARG:NH1	1:C:283:ASN:O	2.31	0.64
1:A:167:GLU:OE2	7:A:507:GOL:O1	2.15	0.63
1:A:256:GLN:O	12:A:603:HOH:O	2.15	0.63
1:A:87:GLN:O	1:A:89:GLN:NE2	2.31	0.63
2:B:501:HEM:HMC2	2:B:501:HEM:HBC2	1.80	0.63
1:D:101:GLY:N	12:D:604:HOH:O	2.30	0.62
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.82	0.62
1:D:321:GLU:OE2	5:D:504:BTB:O3	2.17	0.62
5:B:510:BTB:O3	1:C:384:ASP:OD2	2.18	0.62
5:B:511:BTB:HO3	5:B:511:BTB:HO1	1.37	0.62
1:D:336:VAL:HG21	4:D:503:8J4:C07	2.31	0.60
1:A:476:GLN:OE1	12:A:604:HOH:O	2.16	0.59
1:A:119:ALA:N	12:A:611:HOH:O	2.34	0.58
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.85	0.57
1:C:336:VAL:HG21	4:C:503:8J4:C07	2.35	0.57
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.20	0.56
1:A:197:ASP:OD2	1:A:199:ARG:NH2	2.33	0.55
1:A:86:ALA:O	1:B:97:ARG:NH2	2.39	0.55
1:C:200:ASP:OD1	1:C:200:ASP:N	2.37	0.55
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ARG:NH1	1:D:152:GLU:OE1	2.39	0.55
1:C:128:ARG:O	1:C:132:ASN:ND2	2.40	0.55
1:C:143:SER:O	1:C:145:ALA:N	2.40	0.55
1:C:170:LEU:HD11	1:C:230:VAL:HG21	1.88	0.55
1:D:124:LEU:HD21	1:D:154:GLU:HG2	1.87	0.55
1:A:339:MET:HE2	1:A:473:PHE:HB3	1.89	0.55
1:D:447:TRP:HA	3:D:502:H4B:N1	2.22	0.54
1:D:67:LYS:O	12:D:601:HOH:O	2.18	0.54
1:C:379:VAL:HG21	1:C:402:ILE:HD11	1.89	0.54
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.90	0.54
1:C:149:ARG:NE	1:C:169:GLU:OE2	2.38	0.53
5:A:504:BTB:O8	5:A:504:BTB:H42	2.09	0.53
1:C:364:THR:O	1:C:368:CYS:HB2	2.09	0.53
1:A:171:VAL:HA	1:A:195:VAL:HG21	1.91	0.53
1:C:320:LEU:HD13	1:C:322:TRP:CZ2	2.44	0.53
1:C:451:PRO:HB2	1:D:455:SER:OG	2.09	0.52
5:D:504:BTB:O4	5:D:504:BTB:O3	2.28	0.52
1:C:78:SER:OG	12:C:603:HOH:O	2.19	0.52
1:A:263:GLY:HA2	1:A:285:ARG:HA	1.92	0.52
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.45	0.52
1:A:455:SER:HA	1:A:460:PHE:CG	2.45	0.52
1:A:450:PRO:HG3	1:A:457:THR:HG21	1.90	0.52
5:A:505:BTB:O4	12:A:605:HOH:O	2.19	0.52
1:A:143:SER:OG	1:A:144:GLN:N	2.44	0.51
5:D:504:BTB:O8	8:D:510:CL:CL	2.64	0.51
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.91	0.51
1:A:170:LEU:HD11	1:A:230:VAL:HG11	1.93	0.51
1:C:166:ARG:N	1:C:169:GLU:OE1	2.44	0.51
1:D:100:LEU:N	12:D:604:HOH:O	2.43	0.51
1:D:455:SER:HA	1:D:460:PHE:CG	2.46	0.51
1:A:387:THR:O	5:A:505:BTB:H61	2.10	0.50
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.46	0.50
1:C:450:PRO:HG3	1:C:457:THR:HG21	1.93	0.50
1:C:156:GLU:OE2	1:C:164:GLN:N	2.43	0.50
1:A:367:LEU:HA	1:A:373:TYR:HB2	1.94	0.50
1:B:378:ASP:OD1	5:B:507:BTB:H71	2.12	0.50
1:B:106:PRO:HB3	12:B:668:HOH:O	2.11	0.49
1:C:453:SER:HA	1:D:452:ILE:HG22	1.94	0.49
1:A:341:LEU:HB3	1:A:348:PHE:HB2	1.95	0.49
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.94	0.49
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.94	0.48
1:D:271:THR:O	1:D:275:ILE:HG12	2.12	0.48
5:C:504:BTB:O8	5:C:504:BTB:O6	2.20	0.48
1:B:336:VAL:HG21	4:B:503:8J4:C07	2.44	0.48
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.47	0.48
1:C:240:ASP:OD1	1:C:349:PRO:HG2	2.14	0.48
1:C:229:THR:O	1:C:352:PRO:HD2	2.14	0.48
1:A:250:ARG:NH1	1:A:267:ASN:OD1	2.46	0.48
1:B:68:PHE:CD2	1:B:83:THR:HG22	2.49	0.47
1:C:367:LEU:HA	1:C:373:TYR:HB2	1.95	0.47
1:D:138:ILE:HD12	1:D:140:ARG:HD3	1.95	0.47
1:A:347:GLU:O	1:A:349:PRO:HD3	2.15	0.47
1:D:365:ARG:NH2	1:D:369:ASP:OD2	2.44	0.47
1:B:243:ILE:HG21	1:B:337:SER:HB2	1.97	0.47
1:C:119:ALA:N	12:C:611:HOH:O	2.47	0.47
1:C:247:GLN:HB2	1:C:250:ARG:HG2	1.97	0.47
5:B:511:BTB:H71	5:B:511:BTB:H32	1.50	0.47
1:C:316[B]:GLU:OE1	12:C:605:HOH:O	2.20	0.47
1:C:428:MET:HG3	1:C:458:PRO:HB2	1.95	0.47
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.50	0.47
1:B:90:GLN:HB2	1:B:468:PHE:CD1	2.50	0.46
5:D:505:BTB:H71	5:D:505:BTB:H42	1.51	0.46
1:B:447:TRP:HA	3:B:502:H4B:N1	2.30	0.46
1:C:238:ARG:HE	1:C:240:ASP:CG	2.18	0.46
1:C:160:THR:HG23	1:C:162:THR:HG22	1.98	0.46
5:C:504:BTB:H52	5:C:504:BTB:H42	1.59	0.46
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.51	0.46
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.81	0.46
1:C:316[B]:GLU:HG2	1:C:324:ALA:HB2	1.97	0.46
1:D:171:VAL:HG12	1:D:175:LYS:HE3	1.98	0.46
5:B:505:BTB:H72	12:B:602:HOH:O	2.16	0.45
1:C:203:SER:OG	1:C:204:ALA:N	2.47	0.45
1:A:99:CYS:HB3	1:B:466:ASN:HB3	1.98	0.45
1:C:248:LEU:HD12	1:C:335:ALA:HB1	1.99	0.45
1:C:99:CYS:HB3	1:D:466:ASN:HB3	1.97	0.45
5:B:506:BTB:H32	5:B:506:BTB:H52	1.51	0.45
1:C:309:LEU:HD12	1:C:309:LEU:HA	1.72	0.45
1:C:85:SER:HB3	1:C:467:TYR:CE2	2.52	0.45
1:C:298:GLU:OE1	5:C:504:BTB:N	2.50	0.45
1:D:298:GLU:OE1	5:D:505:BTB:N	2.50	0.45
5:D:505:BTB:H11	5:D:505:BTB:H51	1.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:505:BTB:H61	5:D:505:BTB:H72	1.46	0.45
1:C:91:ASP:OD1	12:C:604:HOH:O	2.20	0.44
5:B:507:BTB:O8	12:B:602:HOH:O	2.21	0.44
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.57	0.44
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.98	0.44
1:A:275:ILE:HG12	1:A:281:PRO:HG3	1.98	0.44
5:D:504:BTB:H42	5:D:504:BTB:H71	1.53	0.44
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.99	0.44
1:A:336:VAL:HG21	4:A:503:8J4:C07	2.47	0.44
1:A:396:ASP:N	1:A:396:ASP:OD1	2.49	0.44
1:B:247:GLN:HB2	1:B:250:ARG:HG2	2.00	0.44
1:D:200:ASP:O	1:D:202:ARG:HG2	2.17	0.44
1:A:144:GLN:CG	1:A:145:ALA:H	2.30	0.43
1:B:326:LEU:HB3	1:B:328:LEU:HG	2.00	0.43
1:C:451:PRO:HB2	1:D:455:SER:HG	1.82	0.43
1:A:70:ARG:NH2	12:A:614:HOH:O	2.43	0.43
1:B:106:PRO:O	12:B:603:HOH:O	2.21	0.43
1:A:334:PRO:HB3	1:A:357:TYR:CZ	2.53	0.43
1:A:127:ALA:O	1:A:131:ILE:HG12	2.19	0.43
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.31	0.43
1:A:90:GLN:HB2	1:A:468:PHE:CD1	2.53	0.43
1:B:149:ARG:HD3	1:B:166:ARG:CZ	2.48	0.43
1:B:321:GLU:OE1	5:B:504:BTB:H62	2.18	0.43
1:B:388:ARG:HB2	1:B:388:ARG:HE	1.44	0.43
1:B:71:VAL:HG13	1:B:463:GLU:HB2	2.00	0.43
1:A:94:CYS:SG	1:A:100:LEU:N	2.70	0.43
5:B:505:BTB:H52	5:B:505:BTB:H32	1.50	0.43
5:D:506:BTB:H11	5:D:506:BTB:H71	1.76	0.43
1:A:269:GLU:O	1:A:272:GLU:HB3	2.19	0.43
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.54	0.43
1:A:445:TRP:CZ2	1:A:449:VAL:HG21	2.53	0.43
1:B:67:LYS:N	12:B:622:HOH:O	2.52	0.43
1:D:453:SER:HB3	1:D:456:LEU:HD12	2.00	0.43
1:A:242:ARG:NE	1:A:479:PRO:HD3	2.33	0.42
5:B:507:BTB:H52	5:B:507:BTB:H11	1.50	0.42
1:C:396:ASP:OD2	1:D:453:SER:OG	2.18	0.42
1:A:246:SER:OG	1:A:250:ARG:HD2	2.19	0.42
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.54	0.42
1:D:199:ARG:O	1:D:232:PRO:HG3	2.19	0.42
1:C:397:LYS:HG3	1:D:400:VAL:HG11	2.02	0.42
1:C:358:MET:HB3	1:C:358:MET:HE2	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:VAL:O	1:B:250:ARG:HG2	2.18	0.42
1:D:204:ALA:O	1:D:207:MET:HB2	2.20	0.42
1:D:478:ASP:HA	1:D:479:PRO:HD3	1.81	0.42
1:D:90:GLN:HB3	1:D:468:PHE:CD1	2.55	0.42
1:A:228:ILE:HG13	1:A:353:PHE:HB3	2.00	0.42
1:A:359:SER:OG	1:A:419:ASP:HA	2.20	0.42
1:C:369:ASP:HB2	1:C:372:ARG:HG2	2.02	0.42
1:A:298:GLU:OE2	12:A:606:HOH:O	2.22	0.41
1:A:382:CYS:HA	5:A:504:BTB:H11	2.02	0.41
1:C:224:LEU:HD12	1:C:356:TRP:HB3	2.02	0.41
1:D:72:LYS:H	1:D:463:GLU:HB2	1.86	0.41
5:D:506:BTB:H32	5:D:506:BTB:H52	1.59	0.41
1:B:301:GLU:HB3	1:B:303:PHE:HE1	1.85	0.41
1:B:396:ASP:N	1:B:396:ASP:OD1	2.47	0.41
1:D:213:ASN:N	1:D:213:ASN:HD22	2.19	0.41
5:C:504:BTB:H71	5:C:504:BTB:H32	1.77	0.41
1:D:249:VAL:HA	12:D:611:HOH:O	2.21	0.41
1:D:301:GLU:HB3	1:D:303:PHE:HE1	1.86	0.41
1:A:128:ARG:O	1:A:132:ASN:ND2	2.53	0.41
1:A:364:THR:HG21	1:A:452:ILE:HG23	2.03	0.41
5:B:510:BTB:H32	1:C:382:CYS:HA	2.01	0.41
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.33	0.41
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.48	0.41
1:A:370:PRO:HB2	1:B:75:GLU:HG3	2.03	0.41
1:D:235[B]:CYS:HA	1:D:236:PRO:HD3	1.93	0.41
1:A:384:ASP:HB3	12:A:656:HOH:O	2.21	0.41
1:D:435:GLN:O	1:D:439:GLY:HA2	2.21	0.41
1:A:393:LEU:HD12	1:B:404:VAL:HG23	2.03	0.40
1:A:104:VAL:O	1:A:106:PRO:HD3	2.21	0.40
1:A:288:VAL:HG12	1:A:289:LEU:O	2.21	0.40
1:C:238:ARG:NH2	1:C:240:ASP:OD2	2.50	0.40
1:D:387:THR:HA	1:D:394:TRP:CD1	2.56	0.40
1:A:184:CYS:HB2	2:A:501:HEM:ND	2.35	0.40
1:A:466:ASN:HB3	1:B:99:CYS:HB3	2.03	0.40
1:B:429:LYS:HA	1:B:429:LYS:HD2	1.89	0.40
1:C:207:MET:HE2	1:C:293:LEU:HB3	2.03	0.40
1:D:162:THR:OG1	1:D:163:TYR:N	2.54	0.40
1:C:165:LEU:HG	1:C:346:LEU:HD12	2.04	0.40
1:B:364:THR:HG21	1:B:452:ILE:HG23	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/440 (91%)	369 (92%)	29 (7%)	4 (1%)	18	16
1	B	401/440 (91%)	387 (96%)	14 (4%)	0	100	100
1	C	399/440 (91%)	380 (95%)	16 (4%)	3 (1%)	22	21
1	D	401/440 (91%)	388 (97%)	13 (3%)	0	100	100
All	All	1603/1760 (91%)	1524 (95%)	72 (4%)	7 (0%)	38	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	144	GLN
1	A	90	GLN
1	C	89	GLN
1	C	143	SER
1	A	297	ASP
1	A	107	ARG
1	A	181	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/373 (92%)	323 (94%)	22 (6%)	20	23
1	B	344/373 (92%)	332 (96%)	12 (4%)	41	51
1	C	342/373 (92%)	330 (96%)	12 (4%)	41	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	344/373 (92%)	339 (98%)	5 (2%)	70	82
All	All	1375/1492 (92%)	1324 (96%)	51 (4%)	39	49

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	109	LEU
1	A	121	GLU
1	A	124	LEU
1	A	133	GLN
1	A	140	ARG
1	A	152	GLU
1	A	201	CYS
1	A	226	SER
1	A	238	ARG
1	A	242	ARG
1	A	250	ARG
1	A	256	GLN
1	A	257	GLN
1	A	285	ARG
1	A	297	ASP
1	A	298	GLU
1	A	309	LEU
1	A	329	ARG
1	A	396	ASP
1	A	403	ASN
1	A	470	SER
1	B	70	ARG
1	B	90	GLN
1	B	148	GLN
1	B	235[A]	CYS
1	B	235[B]	CYS
1	B	246	SER
1	B	298	GLU
1	B	326	LEU
1	B	343	ILE
1	B	364	THR
1	B	389	THR
1	B	396	ASP
1	C	71	VAL
1	C	90	GLN

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Mol	Chain	Res	Type
1	C	137	SER
1	C	154	GLU
1	C	160	THR
1	C	216	LYS
1	C	221	ARG
1	C	234	ARG
1	C	240	ASP
1	C	257	GLN
1	C	309	LEU
1	C	321	GLU
1	D	71	VAL
1	D	97	ARG
1	D	98	ARG
1	D	136	SER
1	D	396	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	213	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 13 are monoatomic - leaving 26 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
2	HEM	A	501	1	28,50,50	2.13	7 (25%)	17,82,82	1.49	3 (17%)
3	H4B	A	502	-	14,18,18	0.87	0	12,26,26	2.45	5 (41%)
4	8J4	A	503	-	25,26,26	2.95	5 (20%)	33,35,35	2.46	9 (27%)
5	BTB	A	504	9	13,13,13	0.36	0	9,16,16	0.69	0
5	BTB	A	505	-	13,13,13	0.36	0	9,16,16	0.65	0
7	GOL	A	507	-	5,5,5	0.44	0	5,5,5	0.26	0
2	HEM	B	501	1	28,50,50	2.18	7 (25%)	17,82,82	2.18	4 (23%)
3	H4B	B	502	-	14,18,18	0.86	0	12,26,26	2.54	5 (41%)
4	8J4	B	503	-	25,26,26	3.06	5 (20%)	33,35,35	2.49	9 (27%)
5	BTB	B	504	9	13,13,13	0.41	0	9,16,16	0.50	0
5	BTB	B	505	-	13,13,13	0.36	0	9,16,16	0.57	0
5	BTB	B	506	-	13,13,13	0.72	0	9,16,16	1.00	1 (11%)
5	BTB	B	507	-	13,13,13	0.39	0	9,16,16	0.77	0
5	BTB	B	510	9	13,13,13	0.46	0	9,16,16	0.78	0
5	BTB	B	511	-	13,13,13	0.61	0	9,16,16	0.87	0
2	HEM	C	501	1	28,50,50	2.25	6 (21%)	17,82,82	1.52	4 (23%)
3	H4B	C	502	-	14,18,18	0.88	0	12,26,26	2.42	5 (41%)
4	8J4	C	503	-	25,26,26	2.90	5 (20%)	33,35,35	2.52	9 (27%)
5	BTB	C	504	-	13,13,13	0.33	0	9,16,16	0.70	0
7	GOL	C	506	-	5,5,5	0.41	0	5,5,5	0.43	0
2	HEM	D	501	1	28,50,50	2.10	6 (21%)	17,82,82	2.17	5 (29%)
3	H4B	D	502	-	14,18,18	0.88	0	12,26,26	2.70	5 (41%)
4	8J4	D	503	-	25,26,26	3.03	5 (20%)	33,35,35	2.41	9 (27%)
5	BTB	D	504	9	13,13,13	0.47	0	9,16,16	0.46	0
5	BTB	D	505	-	13,13,13	0.40	0	9,16,16	0.76	0
5	BTB	D	506	-	13,13,13	0.43	0	9,16,16	0.91	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
2	HEM	A	501	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
4	8J4	A	503	-	-	0/9/19/19	0/3/3/3
5	BTB	A	504	9	-	0/21/21/21	0/0/0/0
5	BTB	A	505	-	-	0/21/21/21	0/0/0/0
7	GOL	A	507	-	-	0/4/4/4	0/0/0/0
2	HEM	B	501	1	-	0/6/54/54	0/0/8/8
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	8J4	B	503	-	-	0/9/19/19	0/3/3/3
5	BTB	B	504	9	-	0/21/21/21	0/0/0/0
5	BTB	B	505	-	-	0/21/21/21	0/0/0/0
5	BTB	B	506	-	-	0/21/21/21	0/0/0/0
5	BTB	B	507	-	-	0/21/21/21	0/0/0/0
5	BTB	B	510	9	-	0/21/21/21	0/0/0/0
5	BTB	B	511	-	-	0/21/21/21	0/0/0/0
2	HEM	C	501	1	-	0/6/54/54	0/0/8/8
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
4	8J4	C	503	-	-	0/9/19/19	0/3/3/3
5	BTB	C	504	-	-	0/21/21/21	0/0/0/0
7	GOL	C	506	-	-	0/4/4/4	0/0/0/0
2	HEM	D	501	1	-	0/6/54/54	0/0/8/8
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
4	8J4	D	503	-	-	0/9/19/19	0/3/3/3
5	BTB	D	504	9	-	0/21/21/21	0/0/0/0
5	BTB	D	505	-	-	0/21/21/21	0/0/0/0
5	BTB	D	506	-	-	0/21/21/21	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	8J4	C09-C10	-10.41	1.38	1.51
4	A	503	8J4	C09-C10	-9.94	1.39	1.51
4	D	503	8J4	C09-C10	-9.64	1.39	1.51
4	C	503	8J4	C09-C10	-9.25	1.40	1.51
4	D	503	8J4	C06-C05	-7.22	1.39	1.51
4	B	503	8J4	C06-C05	-6.86	1.39	1.51
4	C	503	8J4	C06-C05	-6.78	1.40	1.51
4	A	503	8J4	C06-C05	-6.41	1.40	1.51
4	D	503	8J4	C07-C06	-6.25	1.39	1.52
4	C	503	8J4	C07-C06	-5.98	1.40	1.52
4	A	503	8J4	C07-C06	-5.91	1.40	1.52
4	B	503	8J4	C07-C06	-5.89	1.40	1.52
2	B	501	HEM	C3B-C2B	-5.01	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3B-C2B	-4.92	1.33	1.40
4	D	503	8J4	C09-C08	-4.59	1.38	1.52
2	D	501	HEM	C3B-C2B	-4.57	1.34	1.40
4	A	503	8J4	C07-C08	-4.55	1.39	1.52
4	C	503	8J4	C07-C08	-4.52	1.39	1.52
4	B	503	8J4	C07-C08	-4.50	1.39	1.52
4	D	503	8J4	C07-C08	-4.40	1.40	1.52
4	B	503	8J4	C09-C08	-4.39	1.39	1.52
2	A	501	HEM	C3B-C2B	-4.29	1.34	1.40
4	A	503	8J4	C09-C08	-4.29	1.39	1.52
4	C	503	8J4	C09-C08	-4.15	1.40	1.52
2	B	501	HEM	C3C-C2C	-3.82	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.77	1.35	1.40
2	D	501	HEM	C3C-C2C	-3.72	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.64	1.35	1.40
2	D	501	HEM	C4D-ND	2.09	1.39	1.36
2	A	501	HEM	CMC-C2C	2.14	1.56	1.51
2	B	501	HEM	C4C-NC	2.15	1.39	1.36
2	B	501	HEM	C4D-ND	2.35	1.39	1.36
2	C	501	HEM	C4D-ND	2.58	1.39	1.36
2	A	501	HEM	C4D-ND	2.69	1.39	1.36
2	B	501	HEM	C3C-CAC	3.68	1.55	1.47
2	A	501	HEM	C3B-CAB	3.73	1.55	1.47
2	D	501	HEM	C3B-CAB	3.79	1.55	1.47
2	C	501	HEM	C3B-CAB	3.88	1.55	1.47
2	C	501	HEM	C3C-CAC	3.90	1.55	1.47
2	D	501	HEM	C3C-CAC	3.90	1.55	1.47
2	A	501	HEM	C3C-CAC	3.94	1.55	1.47
2	B	501	HEM	C3B-CAB	4.26	1.56	1.47
2	A	501	HEM	C3D-C2D	4.94	1.52	1.37
2	D	501	HEM	C3D-C2D	5.06	1.52	1.37
2	B	501	HEM	C3D-C2D	5.08	1.52	1.37
2	C	501	HEM	C3D-C2D	5.50	1.54	1.37

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBD-CAD-C3D	-6.22	100.61	112.47
2	B	501	HEM	CBA-CAA-C2A	-5.16	102.61	112.48
2	B	501	HEM	CBD-CAD-C3D	-4.82	103.27	112.47
4	C	503	8J4	C05-C10-N01	-3.88	119.92	122.82
3	B	502	H4B	N3-C2-N1	-3.60	119.61	125.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBD-CAD-C3D	-3.54	105.71	112.47
3	C	502	H4B	N3-C2-N1	-3.21	120.24	125.45
2	B	501	HEM	CAD-CBD-CGD	-3.18	107.22	112.66
3	A	502	H4B	N3-C2-N1	-3.14	120.37	125.45
2	D	501	HEM	C1D-C2D-C3D	-3.13	104.82	107.00
3	D	502	H4B	N3-C2-N1	-3.09	120.44	125.45
4	C	503	8J4	C23-C29-N30	-3.06	104.94	112.69
2	D	501	HEM	CBA-CAA-C2A	-3.02	106.72	112.48
4	A	503	8J4	C05-C10-N01	-2.90	120.65	122.82
3	D	502	H4B	C6-C7-N8	-2.71	106.72	111.01
3	B	502	H4B	C6-C7-N8	-2.57	106.94	111.01
4	D	503	8J4	C05-C10-N01	-2.44	121.00	122.82
4	D	503	8J4	C03-C04-C05	-2.40	118.21	121.40
2	C	501	HEM	C1D-C2D-C3D	-2.30	105.39	107.00
5	B	506	BTB	C5-N-C2	-2.19	107.22	113.70
4	B	503	8J4	C03-C02-N01	-2.18	119.08	121.68
2	C	501	HEM	CBD-CAD-C3D	-2.14	108.38	112.47
4	A	503	8J4	C11-O12-C21	-2.12	113.27	117.89
4	B	503	8J4	C05-C10-N01	-2.10	121.25	122.82
2	A	501	HEM	CMC-C2C-C3C	2.06	128.72	124.89
2	D	501	HEM	CMC-C2C-C3C	2.12	128.83	124.89
2	B	501	HEM	CMC-C2C-C3C	2.12	128.83	124.89
2	C	501	HEM	CMC-C2C-C3C	2.15	128.89	124.89
2	A	501	HEM	C4A-C3A-C2A	2.17	108.50	107.00
4	B	503	8J4	C04-C05-C10	2.39	118.57	117.41
3	A	502	H4B	N2-C2-N3	2.41	121.09	117.24
3	C	502	H4B	N2-C2-N3	2.56	121.33	117.24
4	D	503	8J4	O12-C11-C08	2.64	113.84	107.81
4	A	503	8J4	C06-C07-C08	2.66	119.07	112.81
2	C	501	HEM	C4A-C3A-C2A	2.78	108.93	107.00
2	D	501	HEM	C4A-C3A-C2A	2.78	108.93	107.00
3	A	502	H4B	C2-N1-C8A	2.79	120.81	114.51
4	B	503	8J4	C06-C07-C08	2.81	119.43	112.81
3	D	502	H4B	C2-N1-C8A	2.85	120.93	114.51
4	A	503	8J4	C04-C05-C10	2.89	118.81	117.41
3	C	502	H4B	C2-N1-C8A	2.92	121.08	114.51
4	C	503	8J4	C06-C07-C08	3.03	119.94	112.81
3	B	502	H4B	C2-N1-C8A	3.11	121.51	114.51
4	A	503	8J4	O12-C11-C08	3.13	114.98	107.81
3	C	502	H4B	C4-N3-C2	3.16	120.60	116.06
4	D	503	8J4	C10-C09-C08	3.22	120.14	112.63
3	D	502	H4B	C4-N3-C2	3.35	120.88	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	8J4	C06-C07-C08	3.38	120.78	112.81
3	A	502	H4B	C4-N3-C2	3.40	120.95	116.06
4	A	503	8J4	C10-C09-C08	3.42	120.62	112.63
3	B	502	H4B	C4-N3-C2	3.48	121.07	116.06
4	C	503	8J4	C10-C09-C08	3.49	120.78	112.63
4	D	503	8J4	C07-C06-C05	3.50	119.37	112.86
4	C	503	8J4	O12-C11-C08	3.51	115.85	107.81
4	B	503	8J4	C10-C09-C08	3.65	121.14	112.63
4	C	503	8J4	C04-C05-C10	3.99	119.35	117.41
4	B	503	8J4	C07-C06-C05	4.05	120.39	112.86
4	B	503	8J4	O12-C11-C08	4.08	117.15	107.81
4	D	503	8J4	C04-C05-C10	4.15	119.42	117.41
4	A	503	8J4	C07-C06-C05	4.16	120.60	112.86
4	C	503	8J4	C07-C06-C05	4.18	120.63	112.86
4	C	503	8J4	C07-C08-C11	4.39	120.47	111.42
3	B	502	H4B	C4-C4A-C8A	4.83	118.93	114.56
4	D	503	8J4	C07-C08-C11	5.08	121.90	111.42
3	A	502	H4B	C4-C4A-C8A	5.15	119.22	114.56
3	C	502	H4B	C4-C4A-C8A	5.17	119.24	114.56
4	A	503	8J4	C07-C08-C11	5.17	122.09	111.42
4	B	503	8J4	C07-C08-C11	5.87	123.52	111.42
3	D	502	H4B	C4-C4A-C8A	5.98	119.97	114.56
4	C	503	8J4	C07-C08-C09	8.45	119.31	108.97
4	D	503	8J4	C07-C08-C09	8.55	119.44	108.97
4	B	503	8J4	C07-C08-C09	8.66	119.56	108.97
4	A	503	8J4	C07-C08-C09	9.26	120.30	108.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	4	0
3	A	502	H4B	1	0
4	A	503	8J4	1	0
5	A	504	BTB	2	0
5	A	505	BTB	3	0
7	A	507	GOL	1	0
2	B	501	HEM	2	0
3	B	502	H4B	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	8J4	1	0
5	B	504	BTB	1	0
5	B	505	BTB	2	0
5	B	506	BTB	1	0
5	B	507	BTB	3	0
5	B	510	BTB	3	0
5	B	511	BTB	2	0
2	C	501	HEM	2	0
3	C	502	H4B	1	0
4	C	503	8J4	1	0
5	C	504	BTB	4	0
2	D	501	HEM	3	0
3	D	502	H4B	1	0
4	D	503	8J4	1	0
5	D	504	BTB	4	0
5	D	505	BTB	4	0
5	D	506	BTB	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	404/440 (91%)	0.53	31 (7%) 14 13	31, 60, 107, 126	0
1	B	402/440 (91%)	0.10	5 (1%) 79 77	29, 44, 77, 108	0
1	C	401/440 (91%)	0.28	19 (4%) 32 31	32, 55, 95, 118	0
1	D	402/440 (91%)	0.04	6 (1%) 74 72	28, 43, 71, 117	0
All	All	1609/1760 (91%)	0.24	61 (3%) 41 39	28, 50, 93, 126	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	480	TRP	6.8
1	A	109	LEU	6.2
1	A	107	ARG	6.1
1	A	142	GLY	5.2
1	D	67	LYS	4.9
1	C	301	GLU	4.0
1	D	89	GLN	3.9
1	A	301	GLU	3.9
1	A	346	LEU	3.9
1	B	89	GLN	3.6
1	A	89	GLN	3.6
1	C	480	TRP	3.4
1	C	292	LEU	3.4
1	A	163	TYR	3.3
1	C	305	LEU	3.1
1	A	153	VAL	3.1
1	A	152	GLU	2.9
1	A	202	ARG	2.9
1	A	254	TYR	2.9
1	A	140	ARG	2.9
1	A	257	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	304	LEU	2.8
1	A	305	LEU	2.7
1	A	134	TYR	2.7
1	B	150	LEU	2.7
1	C	148	GLN	2.7
1	C	238	ARG	2.7
1	A	468	PHE	2.6
1	A	86	ALA	2.5
1	C	280	THR	2.5
1	C	140	ARG	2.4
1	A	204	ALA	2.4
1	A	124	LEU	2.4
1	A	275	ILE	2.4
1	D	90	GLN	2.4
1	A	108	LYS	2.4
1	A	291	LEU	2.3
1	A	303	PHE	2.3
1	C	294	GLN	2.3
1	C	303	PHE	2.3
1	A	280	THR	2.3
1	A	473	PHE	2.3
1	B	67	LYS	2.3
1	D	141[A]	SER	2.3
1	C	293	LEU	2.3
1	C	468	PHE	2.3
1	A	122	GLN	2.3
1	C	174	ALA	2.2
1	C	144	GLN	2.1
1	C	122	GLN	2.1
1	A	304	LEU	2.1
1	B	142	GLY	2.1
1	D	468	PHE	2.1
1	A	131	ILE	2.1
1	C	131	ILE	2.1
1	D	255	ARG	2.1
1	C	134	TYR	2.1
1	A	130	PHE	2.0
1	B	295	ALA	2.0
1	A	293	LEU	2.0
1	C	259	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	8J4	A	503	24/24	0.72	0.29	8.05	79,97,117,122	0
4	8J4	B	503	24/24	0.84	0.26	7.40	50,66,103,106	0
4	8J4	C	503	24/24	0.73	0.23	5.24	67,76,92,96	0
4	8J4	D	503	24/24	0.87	0.23	4.78	48,61,96,108	0
3	H4B	C	502	17/17	0.86	0.20	3.85	55,66,78,80	0
5	BTB	A	504	14/14	0.92	0.19	2.84	75,85,93,96	0
6	ZN	A	506	1/1	0.99	0.13	2.44	46,46,46,46	0
5	BTB	D	504	14/14	0.76	0.21	2.33	46,65,77,81	0
5	BTB	B	510	14/14	0.89	0.18	1.76	39,68,83,83	0
2	HEM	D	501	43/43	0.96	0.15	1.45	31,41,68,71	0
2	HEM	B	501	43/43	0.96	0.14	0.95	30,38,61,67	0
3	H4B	A	502	17/17	0.89	0.14	0.88	48,60,66,69	0
5	BTB	D	505	14/14	0.92	0.24	0.75	65,74,78,79	0
2	HEM	A	501	43/43	0.95	0.15	0.60	39,50,73,80	0
3	H4B	D	502	17/17	0.90	0.13	0.47	27,46,52,52	0
2	HEM	C	501	43/43	0.95	0.15	0.46	35,54,73,86	0
6	ZN	C	505	1/1	0.98	0.13	0.42	45,45,45,45	0
5	BTB	B	504	14/14	0.82	0.15	0.39	35,55,72,73	0
3	H4B	B	502	17/17	0.92	0.11	-0.08	34,46,54,61	0
8	CL	A	508	1/1	0.97	0.09	-1.19	67,67,67,67	0
8	CL	C	507	1/1	0.95	0.09	-1.25	71,71,71,71	0
8	CL	D	508	1/1	0.98	0.06	-2.66	47,47,47,47	0
8	CL	B	508	1/1	0.96	0.07	-3.14	50,50,50,50	0
5	BTB	A	505	14/14	0.86	0.16	-	72,84,90,90	0
9	GD	B	509	1/1	0.99	0.18	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CL	D	510	1/1	0.96	0.19	-	79,79,79,79	0
7	GOL	C	506	6/6	0.86	0.21	-	57,65,71,71	0
7	GOL	A	507	6/6	0.93	0.20	-	64,72,77,80	0
11	MG	D	509	1/1	0.98	0.20	-	35,35,35,35	0
9	GD	A	509	1/1	0.68	0.10	-	129,129,129,129	1
5	BTB	B	505	14/14	0.77	0.16	-	82,95,103,105	0
5	BTB	B	506	14/14	0.72	0.25	-	74,83,88,90	0
5	BTB	D	506	14/14	0.83	0.17	-	95,101,106,106	0
5	BTB	B	507	14/14	0.66	0.17	-	77,82,89,90	0
10	CA	A	510	1/1	0.99	0.22	-	37,37,37,37	0
5	BTB	B	511	14/14	0.83	0.23	-	59,63,87,90	0
5	BTB	C	504	14/14	0.79	0.16	-	75,87,92,94	0
9	GD	C	508	1/1	0.88	0.11	-	111,111,111,111	1
9	GD	D	507	1/1	1.00	0.15	-	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.