



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2017 – 01:54 AM EDT

PDB ID : 5UOC  
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with (S)-3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-(2-(methylamino)propyl)benzonitrile  
Authors : Chreifi, G.; Li, H.; Poulos, T.L.  
Deposited on : unknown  
Resolution : 2.20 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

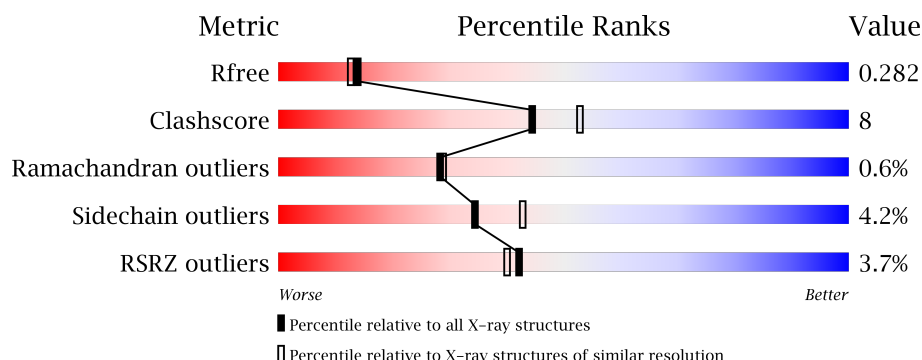
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 8%</div> </div> </div>
1	B	440	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 9%</div> </div> </div>
1	C	440	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>• 9%</div> </div> </div>
1	D	440	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 9%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	H4B	A	502	-	-	-	X
3	H4B	B	502	-	-	-	X
3	H4B	C	502	-	-	-	X
3	H4B	D	502	-	-	-	X
5	BTB	B	505	-	-	-	X
6	ZN	A	511	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13445 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	2	0
			3215	2048	565	586	16			
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:  $C_{34}H_{32}FeN_4O_4$ ).



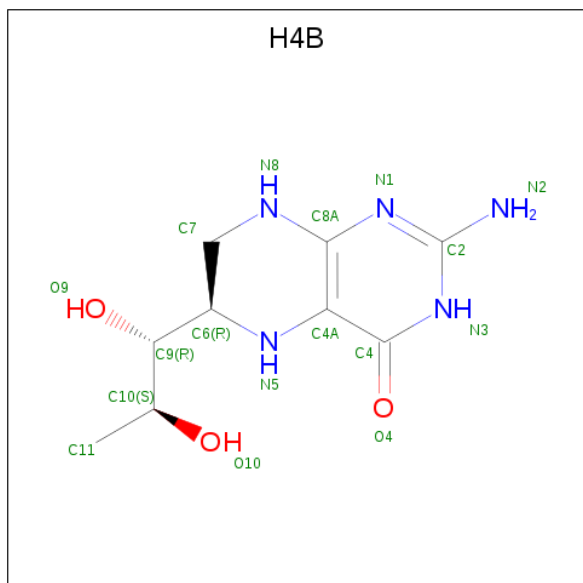
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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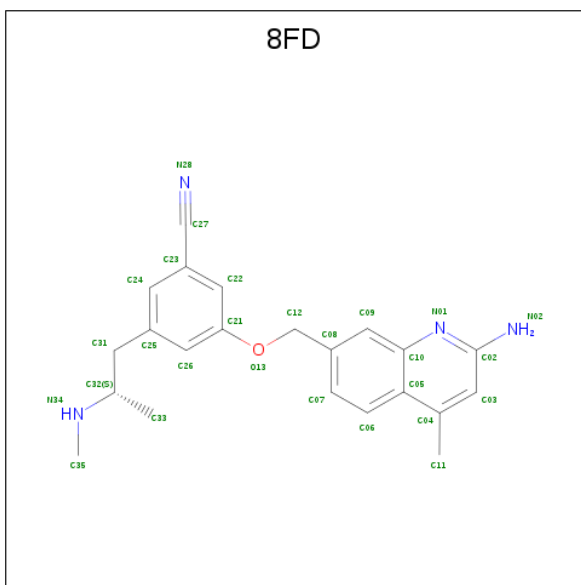
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



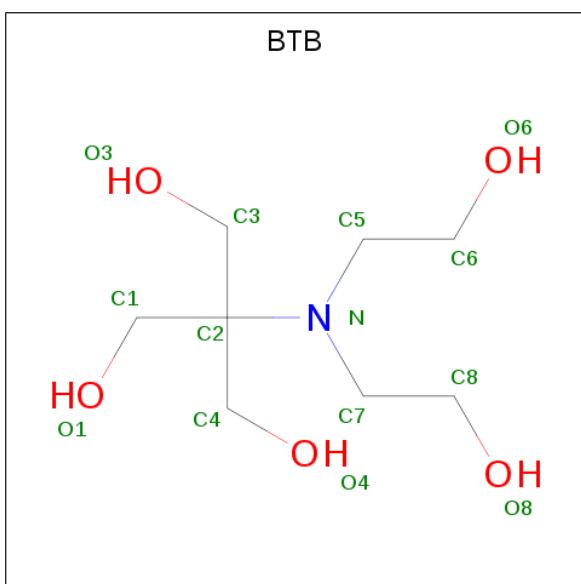
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-[(2S)-2-(methylamino)propyl]benzonitrile (three-letter code: 8FD) (formula:  $C_{22}H_{24}N_4O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	22	4	1		
4	B	1	Total	C	N	O	0	0
			27	22	4	1		
4	C	1	Total	C	N	O	0	0
			27	22	4	1		
4	D	1	Total	C	N	O	0	0
			27	22	4	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Zn	0	0
			2	2		
6	C	2	Total	Zn	0	0
			2	2		

- 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	1	Total	Cl	0	0
			1	1		
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 1	Gd 1	0	0

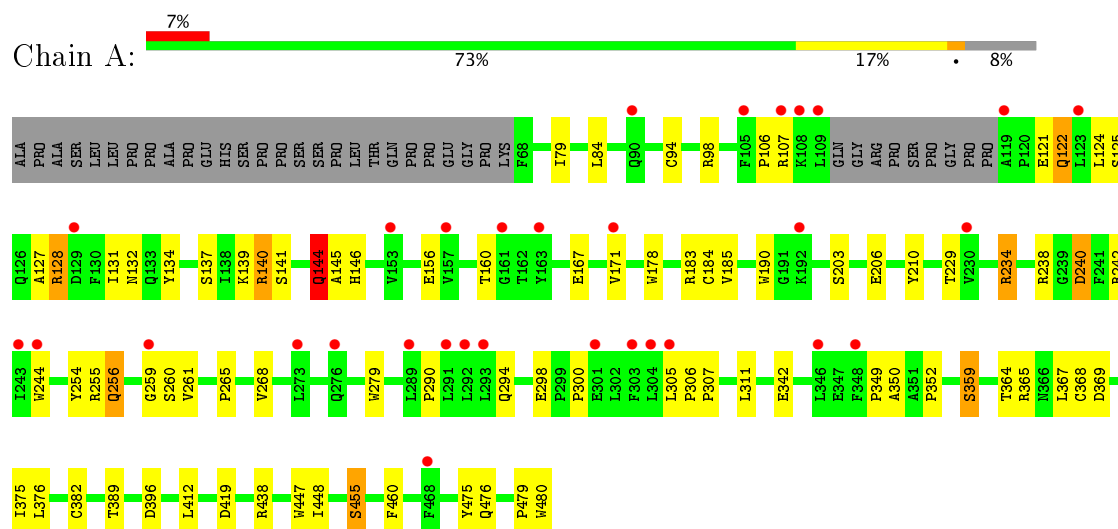
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	10	Total 10	O 10	0	0
10	B	12	Total 12	O 12	0	0
10	C	8	Total 8	O 8	0	0
10	D	7	Total 7	O 7	0	0

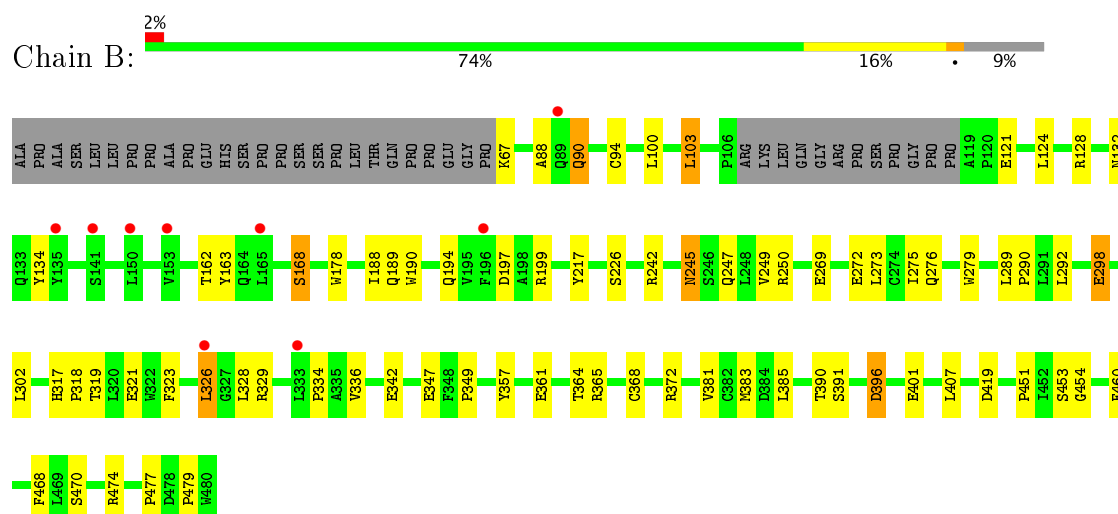
### 3 Residue-property plots [i](#)

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

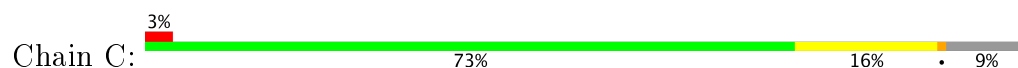
- Molecule 1: Nitric oxide synthase, endothelial

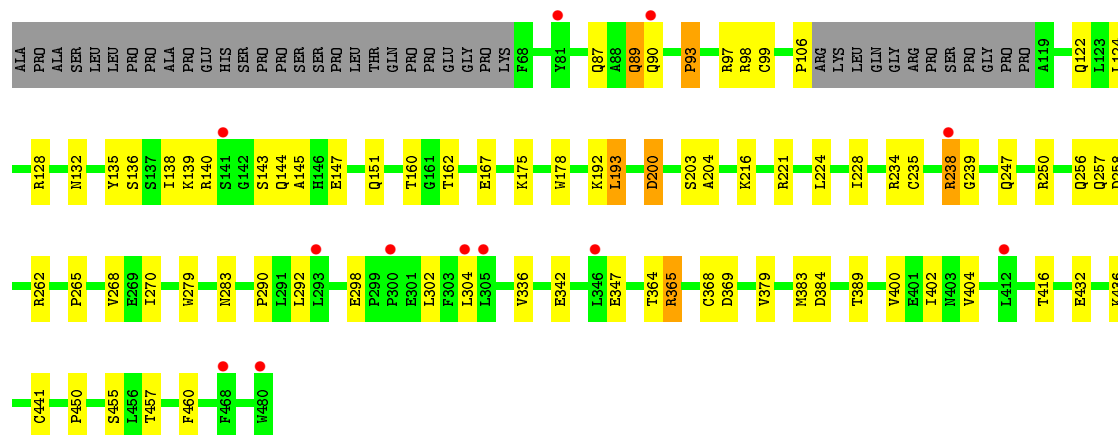


- Molecule 1: Nitric oxide synthase, endothelial

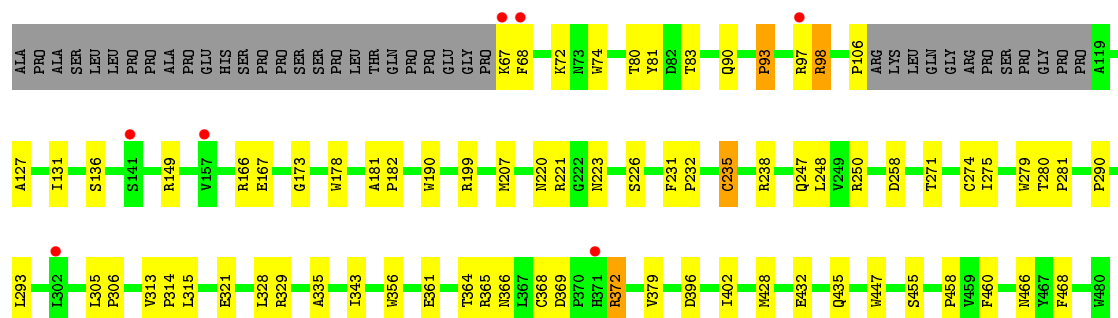
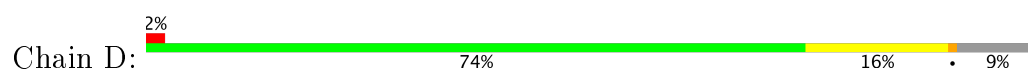


- Molecule 1: Nitric oxide synthase, endothelial





• 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, $\alpha$ , $\beta$ , $\gamma$	58.96 Å   153.50 Å   109.73 Å 90.00°   90.62°   90.00°	Depositor
Resolution (Å)	39.05 – 2.20 39.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.2 (39.05-2.20) 90.4 (39.05-2.20)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.20 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.212 , 0.287 0.206 , 0.282	Depositor DCC
$R_{free}$ test set	4605 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	1.486	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.196 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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, ZN, H4B, CL, 8FD, 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	0.34	0/3335	0.51	0/4543
1	B	0.39	0/3313	0.53	0/4514
1	C	0.36	0/3307	0.51	0/4507
1	D	0.40	0/3319	0.55	0/4523
All	All	0.38	0/13274	0.53	0/18087

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	51	0
1	B	3215	0	3121	43	0
1	C	3209	0	3109	44	0
1	D	3221	0	3126	39	1
2	A	43	0	30	4	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	17	0	15	0	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	0	0
3	D	17	0	15	1	0
4	A	27	0	0	0	0
4	B	27	0	0	2	0
4	C	27	0	0	2	0
4	D	27	0	0	2	0
5	A	42	0	56	3	0
5	B	42	0	54	8	1
5	C	42	0	57	8	0
5	D	28	0	36	6	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
7	A	6	0	8	0	0
7	C	6	0	8	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	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	10	0	0	0	0
10	B	12	0	0	1	0
10	C	8	0	0	1	0
10	D	7	0	0	0	0
All	All	13445	0	12901	198	1

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 (198) 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)
5:B:504:BTB:O4	10:B:601:HOH:O	1.77	1.00
5:B:504:BTB:O3	5:B:504:BTB:O4	1.81	0.89
1:C:235:CYS:HB2	1:C:238:ARG:HD3	1.59	0.83
1:C:365:ARG:NH2	1:C:369:ASP:OD2	2.12	0.83
1:A:365:ARG:NH2	1:A:369:ASP:OD2	2.12	0.81
1:A:144:GLN:HG2	1:A:145:ALA:H	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:GLN:NE2	10:C:601:HOH:O	2.18	0.75
2:A:501:HEM:HHC	2:A:501:HEM:HBB2	1.71	0.73
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.69	0.73
1:C:200:ASP:OD1	1:C:200:ASP:N	2.22	0.70
1:C:175:LYS:HG2	1:C:193:LEU:HD23	1.75	0.68
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.74	0.67
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.77	0.67
1:A:255:ARG:NH1	1:A:259:GLY:O	2.28	0.65
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.33	0.64
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.79	0.64
1:C:298:GLU:OE1	5:C:506:BTB:O8	2.15	0.63
5:D:504:BTB:O6	5:D:504:BTB:H82	1.99	0.63
1:A:242:ARG:NH1	1:A:476:GLN:OE1	2.31	0.63
1:A:294:GLN:HB2	1:A:300:PRO:HB3	1.80	0.61
1:A:455:SER:HB3	1:B:451:PRO:HB2	1.82	0.61
1:D:93:PRO:HG3	1:D:106:PRO:HB3	1.83	0.61
1:B:321:GLU:OE1	5:B:504:BTB:O6	2.19	0.60
1:A:127:ALA:O	1:A:131:ILE:HG12	2.01	0.60
1:D:81:TYR:O	1:D:435:GLN:NE2	2.33	0.59
1:C:93:PRO:HG3	1:C:106:PRO:HB3	1.84	0.59
1:C:128:ARG:O	1:C:132:ASN:ND2	2.36	0.58
1:A:144:GLN:HG2	1:A:145:ALA:N	2.17	0.58
1:B:334:PRO:HB3	1:B:357:TYR:CZ	2.40	0.57
1:C:139:LYS:O	1:C:140:ARG:NE	2.31	0.56
1:C:238:ARG:HG3	1:C:239:GLY:N	2.19	0.56
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.40	0.56
2:C:501:HEM:HHC	2:C:501:HEM:HBB2	1.87	0.56
1:C:203:SER:OG	1:C:204:ALA:N	2.33	0.56
1:D:321:GLU:OE2	5:D:504:BTB:O3	2.23	0.56
1:A:125:SER:HA	1:A:128:ARG:HE	1.70	0.55
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.39	0.55
5:C:506:BTB:O1	5:C:506:BTB:O4	2.25	0.54
1:B:364:THR:O	1:B:368:CYS:HB2	2.07	0.54
1:B:298:GLU:OE2	5:B:505:BTB:N	2.41	0.54
1:A:382:CYS:HA	5:A:504:BTB:H41	1.91	0.53
1:C:262:ARG:NH1	1:C:283:ASN:O	2.42	0.53
1:D:207:MET:HG2	1:D:231:PHE:CE1	2.44	0.52
1:D:93:PRO:O	1:D:98:ARG:NH1	2.42	0.52
1:B:128:ARG:O	1:B:132:ASN:ND2	2.43	0.52
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.90	0.52
1:D:321:GLU:OE1	5:D:504:BTB:O6	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.91	0.52
1:A:234:ARG:HB2	1:A:240:ASP:HB3	1.91	0.52
1:B:275:ILE:HG12	1:B:279:TRP:HE3	1.75	0.52
1:C:364:THR:O	1:C:368:CYS:HB2	2.09	0.52
1:C:400:VAL:O	1:C:404:VAL:HG23	2.09	0.52
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.92	0.52
5:C:504:BTB:O8	5:C:504:BTB:O4	2.26	0.52
1:A:156:GLU:O	1:A:160:THR:OG1	2.23	0.51
1:C:238:ARG:HG3	1:C:239:GLY:O	2.11	0.51
1:B:245:ASN:OD1	1:B:245:ASN:N	2.43	0.51
1:C:193:LEU:HD11	1:C:228:ILE:HG22	1.92	0.51
1:D:220:ASN:HB3	1:D:223:ASN:O	2.11	0.51
1:C:379:VAL:O	1:C:383:MET:HG3	2.12	0.50
1:D:365:ARG:O	1:D:369:ASP:HB2	2.12	0.50
1:A:256:GLN:NE2	1:A:260:SER:OG	2.41	0.50
1:C:432:GLU:HG2	1:C:436:LYS:NZ	2.26	0.50
1:A:279:TRP:CD1	1:A:290:PRO:HG3	2.47	0.50
1:A:242:ARG:HA	1:A:350:ALA:HB2	1.93	0.50
1:A:364:THR:O	1:A:368:CYS:HB2	2.12	0.50
1:D:207:MET:HB3	1:D:293:LEU:HD13	1.94	0.50
1:A:242:ARG:HD3	1:A:479:PRO:HG3	1.94	0.49
1:C:132:ASN:O	1:C:136:SER:OG	2.23	0.49
1:B:121:GLU:O	1:B:124:LEU:HB2	2.12	0.49
1:A:134:TYR:O	1:A:137:SER:OG	2.22	0.49
1:D:447:TRP:CZ2	3:D:502:H4B:H6	2.48	0.48
1:D:231:PHE:HB3	1:D:232:PRO:HD2	1.94	0.48
1:B:317:HIS:NE2	1:B:401:GLU:OE1	2.45	0.48
1:D:149:ARG:HD3	1:D:166:ARG:CZ	2.44	0.48
1:C:87:GLN:O	1:C:89:GLN:NE2	2.46	0.48
1:D:315:LEU:HB2	1:D:328:LEU:HB2	1.96	0.47
1:B:323:PHE:O	1:B:326:LEU:HB2	2.15	0.47
1:C:279:TRP:CG	1:C:290:PRO:HG3	2.50	0.47
5:C:504:BTB:H52	5:C:504:BTB:H31	1.46	0.47
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.49	0.47
1:D:361:GLU:HB3	1:D:365:ARG:HH21	1.80	0.47
1:C:135:TYR:HA	1:C:138:ILE:HG12	1.95	0.47
5:C:506:BTB:H52	5:C:506:BTB:H42	1.69	0.47
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.95	0.47
1:C:93:PRO:HG3	1:C:106:PRO:CB	2.45	0.47
1:D:235[B]:CYS:SG	1:D:238:ARG:HB3	2.54	0.47
3:B:502:H4B:O10	3:B:502:H4B:H71	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:ASP:OD1	5:C:504:BTB:O3	2.31	0.47
1:D:366:ASN:OD1	1:D:372:ARG:NH1	2.46	0.47
1:A:139:LYS:O	1:A:141:SER:N	2.37	0.46
1:B:336:VAL:HG21	4:B:503:8FD:C07	2.45	0.46
1:B:347:GLU:O	1:B:349:PRO:HD3	2.15	0.46
1:B:247:GLN:HB2	1:B:250:ARG:HG2	1.97	0.46
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.31	0.46
1:A:203:SER:HB3	1:A:206:GLU:HB2	1.98	0.46
1:B:90:GLN:HB2	1:B:468:PHE:CD2	2.51	0.46
1:A:367:LEU:HB3	1:A:375:ILE:HD13	1.97	0.46
1:A:185:VAL:HG23	1:A:448:ILE:HG23	1.98	0.46
2:B:501:HEM:HMA2	2:B:501:HEM:HBA1	1.97	0.46
5:D:505:BTB:H61	5:D:505:BTB:H72	1.48	0.46
1:A:412:LEU:HA	1:A:412:LEU:HD12	1.80	0.46
1:D:279:TRP:CD1	1:D:290:PRO:HG3	2.51	0.46
1:B:361:GLU:HB3	1:B:365:ARG:NH2	2.30	0.46
5:B:506:BTB:H52	5:B:506:BTB:H11	1.58	0.46
1:A:144:GLN:CG	1:A:145:ALA:N	2.79	0.45
2:B:501:HEM:HBA2	4:B:503:8FD:C09	2.47	0.45
1:C:379:VAL:HG21	1:C:402:ILE:HD11	1.97	0.45
1:C:160:THR:HG23	1:C:162:THR:H	1.82	0.45
1:A:244:TRP:CH2	1:A:300:PRO:HG3	2.51	0.45
1:B:249:VAL:O	1:B:250:ARG:HG2	2.17	0.45
5:D:505:BTB:H11	5:D:505:BTB:H52	1.83	0.45
1:A:298:GLU:OE1	5:A:506:BTB:O6	2.23	0.45
1:B:162:THR:OG1	1:B:163:TYR:N	2.50	0.45
1:A:359:SER:OG	1:A:419:ASP:HA	2.17	0.45
1:C:455:SER:HA	1:C:460:PHE:CG	2.52	0.45
1:D:199:ARG:O	1:D:232:PRO:HG3	2.16	0.45
1:D:364:THR:O	1:D:368:CYS:HB2	2.16	0.45
1:D:90:GLN:HB3	1:D:468:PHE:HB3	1.98	0.45
1:D:220:ASN:O	1:D:221:ARG:HG2	2.17	0.45
1:C:336:VAL:HG21	4:C:503:8FD:C07	2.47	0.45
1:B:242:ARG:NH2	1:B:477:PRO:O	2.41	0.44
1:A:122:GLN:H	1:A:122:GLN:HG2	1.43	0.44
1:A:240:ASP:HB3	1:A:349:PRO:HG2	1.99	0.44
1:A:396:ASP:OD2	1:B:453:SER:OG	2.25	0.44
1:B:188:ILE:HG23	1:B:189:GLN:HG2	1.99	0.44
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.88	0.44
1:D:313:VAL:HA	1:D:314:PRO:HD2	1.86	0.44
1:D:356:TRP:O	4:D:503:8FD:N02	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:SER:HA	1:D:460:PHE:CG	2.53	0.44
1:A:94:CYS:HB3	1:B:94:CYS:HB3	2.00	0.44
1:B:298:GLU:CD	5:B:505:BTB:H41	2.38	0.44
1:D:173:GLY:HA3	1:D:343:ILE:HD13	1.99	0.44
1:A:254:TYR:O	1:A:261:VAL:HA	2.18	0.44
1:B:134:TYR:OH	1:B:168[A]:SER:HB3	2.17	0.44
2:D:501:HEM:HBA2	4:D:503:8FD:C12	2.47	0.44
1:B:269:GLU:O	1:B:272:GLU:HB2	2.18	0.44
1:A:128:ARG:O	1:A:132:ASN:ND2	2.50	0.44
1:D:428:MET:HG3	1:D:458:PRO:HB2	2.00	0.43
1:C:143:SER:O	1:C:145:ALA:N	2.51	0.43
1:C:147:GLU:O	1:C:151:GLN:HG2	2.18	0.43
1:C:247:GLN:HB2	1:C:250:ARG:HG2	2.00	0.43
1:D:68:PHE:CD2	1:D:83:THR:HA	2.53	0.43
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.53	0.43
1:B:289:LEU:HD23	1:B:290:PRO:HD2	2.01	0.43
5:A:505:BTB:H52	5:A:505:BTB:H31	1.73	0.43
1:B:273:LEU:HA	1:B:276:GLN:HG2	2.01	0.42
1:C:450:PRO:HG3	1:C:457:THR:HG21	2.01	0.42
5:D:504:BTB:H42	5:D:504:BTB:H71	1.70	0.42
1:D:72:LYS:HD3	1:D:74:TRP:CE2	2.53	0.42
1:A:140:ARG:O	1:A:146:HIS:HB2	2.19	0.42
1:A:229:THR:O	1:A:352:PRO:HD2	2.19	0.42
1:A:244:TRP:CZ2	1:A:300:PRO:HG3	2.54	0.42
1:A:455:SER:HA	1:A:460:PHE:CG	2.54	0.42
1:C:99:CYS:HB3	1:D:466:ASN:HB3	2.01	0.42
1:B:383:MET:HB2	1:B:385:LEU:HG	2.01	0.42
5:C:505:BTB:H62	5:C:505:BTB:H72	1.63	0.42
1:D:271:THR:O	1:D:275:ILE:HG12	2.19	0.42
1:B:407:LEU:HD21	1:B:419:ASP:HB3	2.01	0.42
1:D:181:ALA:HA	1:D:182:PRO:HD3	1.89	0.42
5:C:505:BTB:H31	5:C:505:BTB:O6	2.20	0.42
1:C:265:PRO:O	1:C:268:VAL:HG23	2.20	0.42
1:C:178:TRP:HZ3	1:C:193:LEU:HB2	1.85	0.42
1:A:84:LEU:HD22	1:A:438:ARG:HB3	2.00	0.42
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.55	0.42
1:D:247:GLN:HB2	1:D:250:ARG:HG2	2.01	0.42
1:A:419:ASP:OD2	1:B:390:THR:OG1	2.24	0.42
1:A:238:ARG:HD3	1:A:238:ARG:HA	1.86	0.41
1:A:305:LEU:HA	1:A:306:PRO:HD3	1.87	0.41
1:C:432:GLU:HG2	1:C:436:LYS:HZ1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:LEU:HB2	1:D:335:ALA:HB3	2.02	0.41
1:A:124:LEU:O	1:A:128:ARG:HG3	2.19	0.41
1:B:454:GLY:O	1:B:460:PHE:HB2	2.20	0.41
1:B:319:THR:HB	5:B:504:BTB:O4	2.19	0.41
1:C:167:GLU:OE1	7:C:508:GOL:H31	2.20	0.41
1:B:194:GLN:HG2	1:B:217:TYR:CZ	2.56	0.41
1:C:270:ILE:HD11	1:C:292:LEU:HD12	2.03	0.41
1:D:305:LEU:HA	1:D:306:PRO:HD3	1.84	0.41
1:A:184:CYS:HB2	2:A:501:HEM:ND	2.35	0.41
1:A:306:PRO:HA	1:A:307:PRO:HD3	1.78	0.41
5:B:504:BTB:H52	5:B:504:BTB:H31	1.58	0.41
1:A:183:ARG:NH1	1:A:475:TYR:OH	2.53	0.41
1:C:124:LEU:O	1:C:128:ARG:HG3	2.20	0.41
1:D:280:THR:HA	1:D:281:PRO:HD3	1.92	0.41
1:A:131:ILE:O	1:A:134:TYR:HB3	2.21	0.41
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.51	0.41
1:B:197:ASP:OD2	1:B:199:ARG:NH2	2.36	0.41
1:C:97:ARG:HE	1:C:97:ARG:HB3	1.68	0.41
1:C:97:ARG:HH22	1:D:67:LYS:NZ	2.18	0.41
1:D:127:ALA:O	1:D:131:ILE:HG12	2.21	0.41
1:A:167:GLU:O	1:A:171:VAL:HG23	2.21	0.41
1:B:396:ASP:N	1:B:396:ASP:OD1	2.44	0.41
1:D:379:VAL:HG21	1:D:402:ILE:HD11	2.02	0.41
1:A:376:LEU:HD12	1:A:376:LEU:HA	1.94	0.40
1:C:224:LEU:HD12	1:C:416:THR:HB	2.03	0.40
2:C:501:HEM:HBA1	4:C:503:8FD:C09	2.51	0.40
1:C:135:TYR:CD1	1:C:138:ILE:HD11	2.57	0.40
1:B:342:GLU:OE1	1:B:474:ARG:NH1	2.54	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:GLU:OE2	5:B:505:BTB:O6[1_554]	2.14	0.06

## 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	402/440 (91%)	372 (92%)	26 (6%)	4 (1%)	18	16
1	B	400/440 (91%)	387 (97%)	11 (3%)	2 (0%)	32	34
1	C	399/440 (91%)	374 (94%)	23 (6%)	2 (0%)	32	34
1	D	401/440 (91%)	378 (94%)	21 (5%)	2 (0%)	32	34
All	All	1602/1760 (91%)	1511 (94%)	81 (5%)	10 (1%)	28	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	372	ARG
1	A	140	ARG
1	A	144	GLN
1	B	88	ALA
1	B	372	ARG
1	A	106	PRO
1	A	107	ARG
1	C	144	GLN
1	C	93	PRO
1	D	93	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/373 (92%)	329 (95%)	16 (5%)	31	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	343/373 (92%)	329 (96%)	14 (4%)	35	44
1	C	342/373 (92%)	324 (95%)	18 (5%)	26	31
1	D	344/373 (92%)	332 (96%)	12 (4%)	41	51
All	All	1374/1492 (92%)	1314 (96%)	60 (4%)	34	40

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	A	98	ARG
1	A	121	GLU
1	A	122	GLN
1	A	128	ARG
1	A	144	GLN
1	A	210	TYR
1	A	234	ARG
1	A	240	ASP
1	A	256	GLN
1	A	311	LEU
1	A	342	GLU
1	A	359	SER
1	A	389	THR
1	A	455	SER
1	A	480	TRP
1	B	67	LYS
1	B	90	GLN
1	B	103	LEU
1	B	168[A]	SER
1	B	168[B]	SER
1	B	226	SER
1	B	245	ASN
1	B	298	GLU
1	B	326	LEU
1	B	329	ARG
1	B	381	VAL
1	B	391	SER
1	B	396	ASP
1	B	470	SER
1	C	89	GLN
1	C	90	GLN
1	C	98	ARG

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Mol	Chain	Res	Type
1	C	122	GLN
1	C	192	LYS
1	C	193	LEU
1	C	200	ASP
1	C	216	LYS
1	C	221	ARG
1	C	238	ARG
1	C	256	GLN
1	C	258	ASP
1	C	302	LEU
1	C	304	LEU
1	C	342	GLU
1	C	365	ARG
1	C	389	THR
1	C	441	CYS
1	D	80	THR
1	D	97	ARG
1	D	98	ARG
1	D	136	SER
1	D	226	SER
1	D	235[A]	CYS
1	D	235[B]	CYS
1	D	258	ASP
1	D	274	CYS
1	D	329	ARG
1	D	396	ASP
1	D	432	GLU

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

Mol	Chain	Res	Type
1	B	132	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 12 are monoatomic - leaving 25 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	2.21	6 (21%)	17,82,82	1.40	4 (23%)
3	H4B	A	502	-	14,18,18	0.97	0	12,26,26	2.73	6 (50%)
4	8FD	A	503	-	29,29,29	1.51	2 (6%)	37,40,40	1.13	3 (8%)
5	BTB	A	504	9	13,13,13	0.46	0	9,16,16	1.16	1 (11%)
5	BTB	A	505	-	13,13,13	0.56	0	9,16,16	1.11	0
5	BTB	A	506	-	13,13,13	0.34	0	9,16,16	0.62	0
7	GOL	A	508	-	5,5,5	0.30	0	5,5,5	0.32	0
2	HEM	B	501	1	28,50,50	2.23	8 (28%)	17,82,82	1.79	4 (23%)
3	H4B	B	502	-	14,18,18	0.85	0	12,26,26	2.75	6 (50%)
4	8FD	B	503	-	29,29,29	1.54	3 (10%)	37,40,40	1.15	4 (10%)
5	BTB	B	504	9	13,13,13	0.41	0	9,16,16	1.17	1 (11%)
5	BTB	B	505	-	13,13,13	0.39	0	9,16,16	1.14	0
5	BTB	B	506	-	13,13,13	0.45	0	9,16,16	0.60	0
2	HEM	C	501	1	28,50,50	2.18	6 (21%)	17,82,82	1.56	3 (17%)
3	H4B	C	502	-	14,18,18	0.92	0	12,26,26	2.44	5 (41%)
4	8FD	C	503	-	29,29,29	1.52	2 (6%)	37,40,40	1.04	3 (8%)
5	BTB	C	504	9	13,13,13	0.35	0	9,16,16	0.51	0
5	BTB	C	505	-	13,13,13	0.65	0	9,16,16	0.92	0
5	BTB	C	506	-	13,13,13	0.35	0	9,16,16	0.65	0
7	GOL	C	508	-	5,5,5	0.38	0	5,5,5	0.54	0
2	HEM	D	501	1	28,50,50	2.18	7 (25%)	17,82,82	2.10	7 (41%)
3	H4B	D	502	-	14,18,18	0.92	0	12,26,26	2.58	5 (41%)
4	8FD	D	503	-	29,29,29	1.50	2 (6%)	37,40,40	1.06	2 (5%)
5	BTB	D	504	9	13,13,13	0.60	0	9,16,16	1.26	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BTB	D	505	-	13,13,13	0.39	0	9,16,16	1.22	1 (11%)

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
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
4	8FD	A	503	-	-	0/13/13/13	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
5	BTB	A	506	-	-	0/21/21/21	0/0/0/0
7	GOL	A	508	-	-	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	8FD	B	503	-	-	0/13/13/13	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
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	8FD	C	503	-	-	0/13/13/13	0/3/3/3
5	BTB	C	504	9	-	0/21/21/21	0/0/0/0
5	BTB	C	505	-	-	0/21/21/21	0/0/0/0
5	BTB	C	506	-	-	0/21/21/21	0/0/0/0
7	GOL	C	508	-	-	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	8FD	D	503	-	-	0/13/13/13	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

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	8FD	C23-C27	-6.48	1.28	1.44
4	B	503	8FD	C23-C27	-6.38	1.29	1.44
4	A	503	8FD	C23-C27	-6.37	1.29	1.44
4	D	503	8FD	C23-C27	-6.22	1.29	1.44
2	D	501	HEM	C3B-C2B	-5.20	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C2B	-4.59	1.34	1.40
2	B	501	HEM	C3B-C2B	-4.54	1.34	1.40
2	C	501	HEM	C3B-C2B	-4.50	1.34	1.40
2	D	501	HEM	C3C-C2C	-4.14	1.34	1.40
2	A	501	HEM	C3C-C2C	-3.85	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.39	1.35	1.40
2	B	501	HEM	C3C-C2C	-3.24	1.36	1.40
4	A	503	8FD	C05-C10	-2.14	1.39	1.42
4	B	503	8FD	C05-C10	-2.09	1.39	1.42
4	B	503	8FD	C09-C10	-2.06	1.38	1.41
4	D	503	8FD	C09-C10	-2.02	1.38	1.41
2	B	501	HEM	C1D-ND	2.04	1.40	1.36
2	D	501	HEM	C1D-ND	2.07	1.40	1.36
4	C	503	8FD	C02-N01	2.40	1.35	1.33
2	D	501	HEM	C4D-ND	2.52	1.39	1.36
2	C	501	HEM	C4D-ND	2.67	1.39	1.36
2	B	501	HEM	C4D-ND	2.74	1.40	1.36
2	A	501	HEM	C4D-ND	2.79	1.40	1.36
2	B	501	HEM	C1B-NB	2.97	1.40	1.36
2	D	501	HEM	C3B-CAB	3.76	1.55	1.47
2	B	501	HEM	C3B-CAB	3.77	1.55	1.47
2	A	501	HEM	C3C-CAC	3.87	1.55	1.47
2	D	501	HEM	C3C-CAC	3.90	1.55	1.47
2	A	501	HEM	C3B-CAB	3.96	1.55	1.47
2	C	501	HEM	C3C-CAC	3.97	1.55	1.47
2	C	501	HEM	C3B-CAB	4.20	1.56	1.47
2	B	501	HEM	C3C-CAC	4.77	1.57	1.47
2	D	501	HEM	C3D-C2D	5.01	1.52	1.37
2	B	501	HEM	C3D-C2D	5.09	1.52	1.37
2	A	501	HEM	C3D-C2D	5.28	1.53	1.37
2	C	501	HEM	C3D-C2D	5.37	1.53	1.37

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CAD-CBD-CGD	-3.98	105.87	112.66
3	B	502	H4B	C6-C7-N8	-3.74	105.08	111.01
2	B	501	HEM	CBA-CAA-C2A	-3.73	105.35	112.48
5	D	504	BTB	O3-C3-C2	-3.60	101.24	111.37
3	A	502	H4B	C6-C7-N8	-3.57	105.34	111.01
2	B	501	HEM	CAD-CBD-CGD	-3.56	106.58	112.66
3	B	502	H4B	N3-C2-N1	-3.44	119.87	125.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CMA-C3A-C4A	-3.36	123.30	128.46
3	C	502	H4B	N3-C2-N1	-3.32	120.06	125.45
3	D	502	H4B	N3-C2-N1	-3.13	120.38	125.45
3	A	502	H4B	N3-C2-N1	-3.09	120.45	125.45
2	C	501	HEM	CAD-CBD-CGD	-3.08	107.39	112.66
2	D	501	HEM	CBA-CAA-C2A	-3.07	106.61	112.48
4	C	503	8FD	C25-C31-C32	-3.06	107.71	113.42
5	B	504	BTB	O3-C3-C2	-3.03	102.85	111.37
3	B	502	H4B	C4A-N5-C6	-2.68	113.87	121.16
2	C	501	HEM	C1D-C2D-C3D	-2.66	105.14	107.00
4	C	503	8FD	C05-C10-N01	-2.56	120.19	122.84
4	A	503	8FD	C25-C31-C32	-2.56	108.64	113.42
3	D	502	H4B	C6-C7-N8	-2.55	106.97	111.01
3	C	502	H4B	C6-C7-N8	-2.47	107.09	111.01
2	D	501	HEM	C1D-C2D-C3D	-2.46	105.29	107.00
2	B	501	HEM	CMA-C3A-C4A	-2.45	124.70	128.46
2	D	501	HEM	CAA-CBA-CGA	-2.43	108.51	112.66
3	A	502	H4B	C4A-N5-C6	-2.43	114.55	121.16
4	B	503	8FD	C05-C10-N01	-2.43	120.33	122.84
5	D	505	BTB	C5-N-C2	-2.42	106.55	113.70
5	A	504	BTB	O3-C3-C2	-2.39	104.65	111.37
2	A	501	HEM	CAD-CBD-CGD	-2.32	108.69	112.66
4	A	503	8FD	C05-C10-N01	-2.14	120.63	122.84
4	D	503	8FD	C05-C10-N01	-2.13	120.64	122.84
2	C	501	HEM	CBA-CAA-C2A	-2.08	108.51	112.48
2	A	501	HEM	CMA-C3A-C4A	-2.04	125.33	128.46
2	B	501	HEM	CMC-C2C-C3C	2.01	128.63	124.89
4	B	503	8FD	C04-C05-C10	2.04	119.14	117.99
4	B	503	8FD	C12-O13-C21	2.09	122.83	117.61
2	A	501	HEM	CMC-C2C-C3C	2.13	128.85	124.89
2	D	501	HEM	CMC-C2C-C3C	2.32	129.20	124.89
2	D	501	HEM	C4A-C3A-C2A	2.48	108.72	107.00
2	A	501	HEM	C4A-C3A-C2A	2.52	108.75	107.00
4	B	503	8FD	N02-C02-N01	2.66	119.70	118.06
3	A	502	H4B	C2-N1-C8A	2.80	120.81	114.51
4	D	503	8FD	C04-C05-C10	2.80	119.57	117.99
3	D	502	H4B	C2-N1-C8A	2.82	120.86	114.51
3	C	502	H4B	C2-N1-C8A	2.86	120.94	114.51
3	B	502	H4B	C2-N1-C8A	2.88	120.99	114.51
4	C	503	8FD	C04-C05-C10	2.93	119.65	117.99
4	A	503	8FD	N02-C02-N01	3.07	119.96	118.06
3	A	502	H4B	C4-N3-C2	3.18	120.63	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	H4B	C4-N3-C2	3.25	120.74	116.06
3	D	502	H4B	C4-N3-C2	3.28	120.78	116.06
3	B	502	H4B	C4-N3-C2	3.79	121.51	116.06
3	C	502	H4B	C4-C4A-C8A	4.92	119.02	114.56
3	B	502	H4B	C4-C4A-C8A	5.04	119.12	114.56
3	D	502	H4B	C4-C4A-C8A	5.60	119.63	114.56
3	A	502	H4B	C4-C4A-C8A	5.89	119.89	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	4	0
5	A	504	BTB	1	0
5	A	505	BTB	1	0
5	A	506	BTB	1	0
2	B	501	HEM	3	0
3	B	502	H4B	1	0
4	B	503	8FD	2	0
5	B	504	BTB	5	0
5	B	505	BTB	2	1
5	B	506	BTB	1	0
2	C	501	HEM	2	0
4	C	503	8FD	2	0
5	C	504	BTB	3	0
5	C	505	BTB	2	0
5	C	506	BTB	3	0
7	C	508	GOL	1	0
2	D	501	HEM	3	0
3	D	502	H4B	1	0
4	D	503	8FD	2	0
5	D	504	BTB	4	0
5	D	505	BTB	2	0

## 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	404/440 (91%)	0.50	31 (7%) 14 13	42, 86, 146, 177	0
1	B	402/440 (91%)	0.18	9 (2%) 62 60	44, 69, 112, 140	0
1	C	401/440 (91%)	0.31	12 (2%) 51 48	45, 77, 127, 170	0
1	D	402/440 (91%)	0.18	7 (1%) 70 68	42, 67, 111, 155	0
All	All	1609/1760 (91%)	0.29	59 (3%) 42 40	42, 74, 129, 177	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	ALA	6.2
1	C	304	LEU	5.7
1	A	305	LEU	5.5
1	D	141[A]	SER	4.9
1	A	109	LEU	4.8
1	A	153	VAL	4.7
1	C	141	SER	4.5
1	A	293	LEU	4.4
1	A	163	TYR	4.2
1	A	108	LYS	4.2
1	A	273	LEU	4.0
1	C	238	ARG	3.9
1	A	244	TRP	3.8
1	C	346	LEU	3.4
1	A	107	ARG	3.4
1	A	346	LEU	3.3
1	C	305	LEU	3.3
1	A	292	LEU	3.2
1	C	90	GLN	3.1
1	A	161	GLY	3.1
1	B	333	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	171	VAL	3.0
1	A	304	LEU	3.0
1	B	89	GLN	2.9
1	A	129	ASP	2.9
1	A	303	PHE	2.9
1	A	259	GLY	2.8
1	D	68	PHE	2.7
1	B	141[A]	SER	2.7
1	C	300	PRO	2.7
1	D	157	VAL	2.7
1	D	371	HIS	2.7
1	A	157	VAL	2.7
1	D	67	LYS	2.6
1	B	135	TYR	2.6
1	A	243	ILE	2.6
1	B	153	VAL	2.6
1	B	150	LEU	2.5
1	C	81	TYR	2.5
1	A	291	LEU	2.5
1	A	105	PHE	2.5
1	A	289	LEU	2.5
1	C	468	PHE	2.4
1	A	348	PHE	2.4
1	A	276	GLN	2.3
1	B	165	LEU	2.3
1	D	302	LEU	2.3
1	A	123	LEU	2.2
1	C	293	LEU	2.2
1	C	412	LEU	2.2
1	A	192	LYS	2.2
1	A	90	GLN	2.1
1	B	326	LEU	2.1
1	A	301	GLU	2.1
1	A	468	PHE	2.1
1	D	97	ARG	2.1
1	C	480	TRP	2.1
1	B	196	PHE	2.1
1	A	230	VAL	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	H4B	C	502	17/17	0.89	0.27	5.46	70,89,113,113	0
3	H4B	B	502	17/17	0.82	0.21	3.84	51,77,126,134	0
5	BTB	B	505	14/14	0.85	0.30	3.45	33,85,99,99	0
6	ZN	A	511	1/1	0.95	0.16	2.90	57,57,57,57	1
3	H4B	D	502	17/17	0.86	0.22	2.75	36,61,120,128	0
3	H4B	A	502	17/17	0.86	0.22	2.19	59,82,98,99	0
6	ZN	A	507	1/1	0.99	0.18	1.95	67,67,67,67	0
4	8FD	D	503	27/27	0.91	0.19	1.82	43,77,119,120	0
4	8FD	B	503	27/27	0.91	0.18	1.78	47,89,112,117	0
4	8FD	A	503	27/27	0.87	0.20	1.43	63,101,131,135	0
4	8FD	C	503	27/27	0.86	0.18	1.24	50,98,115,116	0
5	BTB	A	504	14/14	0.96	0.17	1.02	33,95,103,107	0
6	ZN	C	507	1/1	1.00	0.16	0.79	61,61,61,61	0
2	HEM	A	501	43/43	0.98	0.18	0.75	58,75,102,108	0
2	HEM	B	501	43/43	0.98	0.15	0.74	39,56,84,111	0
2	HEM	D	501	43/43	0.98	0.16	0.71	40,57,77,84	0
5	BTB	A	505	14/14	0.93	0.15	0.51	74,92,103,108	0
5	BTB	B	504	14/14	0.95	0.16	0.23	35,75,93,103	0
2	HEM	C	501	43/43	0.97	0.16	0.19	46,74,100,118	0
6	ZN	C	511	1/1	0.95	0.15	-0.16	52,52,52,52	1
5	BTB	C	504	14/14	0.93	0.13	-0.57	61,111,121,123	0
5	BTB	D	504	14/14	0.95	0.12	-0.91	48,67,86,88	0
8	CL	C	509	1/1	0.93	0.10	-1.91	87,87,87,87	0
8	CL	D	507	1/1	0.96	0.08	-2.24	56,56,56,56	0
8	CL	B	507	1/1	0.98	0.08	-3.29	62,62,62,62	0
8	CL	A	509	1/1	0.89	0.05	-4.18	81,81,81,81	0
5	BTB	A	506	14/14	0.86	0.10	-	85,104,109,113	0
5	BTB	D	505	14/14	0.94	0.29	-	66,87,92,98	0
7	GOL	A	508	6/6	0.84	0.29	-	53,66,78,79	0
5	BTB	C	506	14/14	0.88	0.18	-	87,102,110,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BTB	C	505	14/14	0.94	0.23	-	62,78,106,111	0
9	GD	B	508	1/1	0.98	0.23	-	69,69,69,69	0
9	GD	C	510	1/1	0.98	0.17	-	143,143,143,143	0
9	GD	A	510	1/1	0.89	0.15	-	175,175,175,175	0
5	BTB	B	506	14/14	0.79	0.14	-	87,106,109,110	0
7	GOL	C	508	6/6	0.97	0.27	-	46,50,54,59	0
9	GD	D	506	1/1	0.99	0.24	-	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.