



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:06 PM GMT

PDB ID : 4KLR  
Title : E343Q variant of human ferrochelatase  
Authors : Lanzilotta, W.N.; Medlock, A.E.  
Deposited on : 2013-05-07  
Resolution : 2.18 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

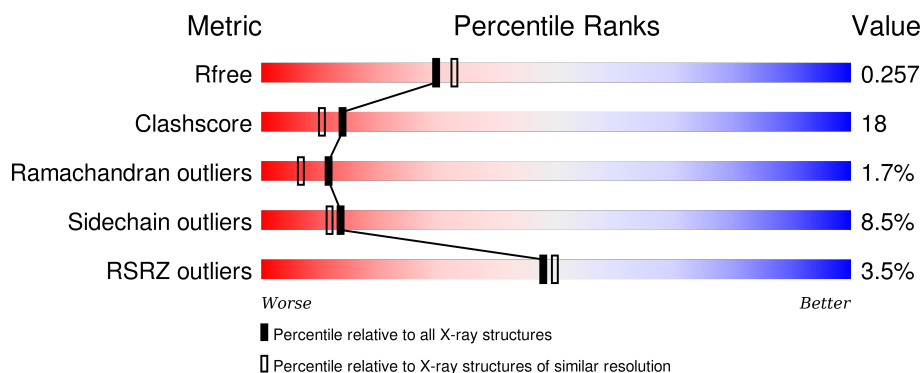
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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	370	<div> <div>2%</div> <div>69%</div> <div>22%</div> <div>5%</div> <div>• •</div> </div>
1	B	370	<div> <div>4%</div> <div>70%</div> <div>21%</div> <div>5%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	503[A]	-	-	-	X
4	GOL	A	503[B]	-	-	-	X
5	CHD	A	504	-	-	-	X
5	CHD	B	504	-	-	-	X
5	CHD	B	505	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6456 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.

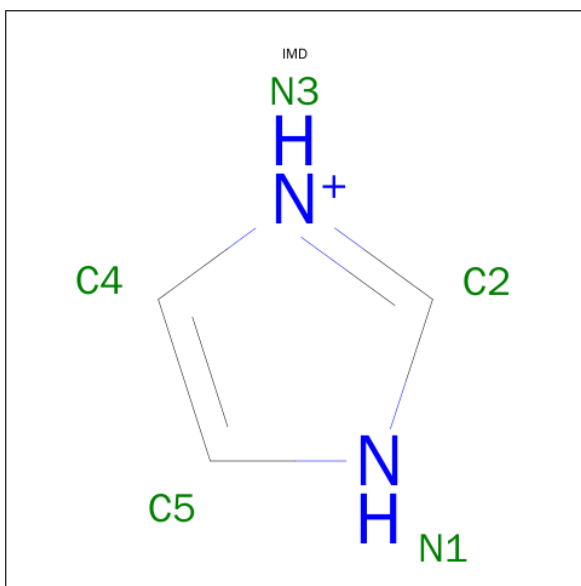
- Molecule 1 is a protein called Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	4	0
			2917	1858	510	531	18			
1	B	359	Total	C	N	O	S	0	6	0
			2928	1864	510	534	20			

There are 24 discrepancies between the modelled and reference sequences:

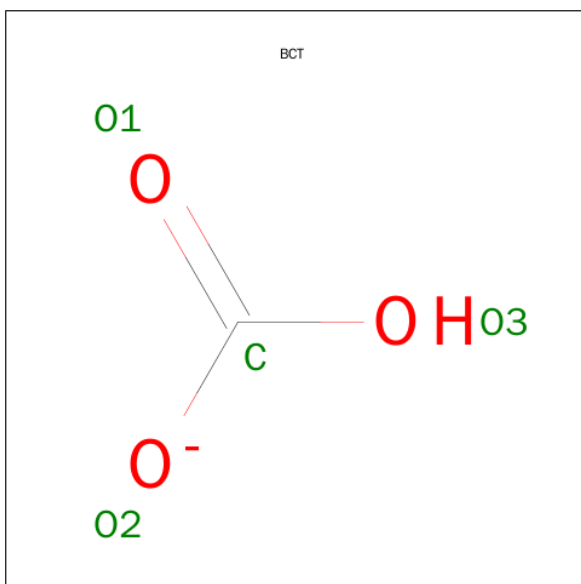
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	MET	-	EXPRESSION TAG	UNP P22830
A	55	GLY	-	EXPRESSION TAG	UNP P22830
A	56	GLY	-	EXPRESSION TAG	UNP P22830
A	57	SER	-	EXPRESSION TAG	UNP P22830
A	58	HIS	-	EXPRESSION TAG	UNP P22830
A	59	HIS	-	EXPRESSION TAG	UNP P22830
A	60	HIS	-	EXPRESSION TAG	UNP P22830
A	61	HIS	-	EXPRESSION TAG	UNP P22830
A	62	HIS	-	EXPRESSION TAG	UNP P22830
A	63	HIS	-	EXPRESSION TAG	UNP P22830
A	64	GLY	-	EXPRESSION TAG	UNP P22830
A	343	GLN	GLU	ENGINEERED MUTATION	UNP P22830
B	54	MET	-	EXPRESSION TAG	UNP P22830
B	55	GLY	-	EXPRESSION TAG	UNP P22830
B	56	GLY	-	EXPRESSION TAG	UNP P22830
B	57	SER	-	EXPRESSION TAG	UNP P22830
B	58	HIS	-	EXPRESSION TAG	UNP P22830
B	59	HIS	-	EXPRESSION TAG	UNP P22830
B	60	HIS	-	EXPRESSION TAG	UNP P22830
B	61	HIS	-	EXPRESSION TAG	UNP P22830
B	62	HIS	-	EXPRESSION TAG	UNP P22830
B	63	HIS	-	EXPRESSION TAG	UNP P22830
B	64	GLY	-	EXPRESSION TAG	UNP P22830
B	343	GLN	GLU	ENGINEERED MUTATION	UNP P22830

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is BICARBONATE ION (three-letter code: BCT) (formula:  $CHO_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		

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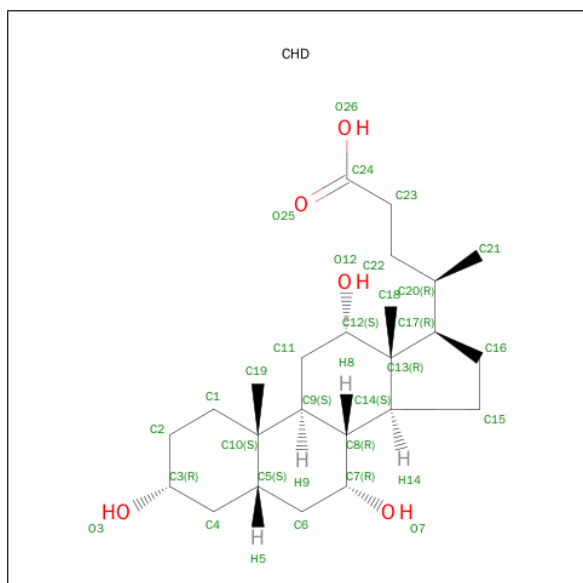
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).

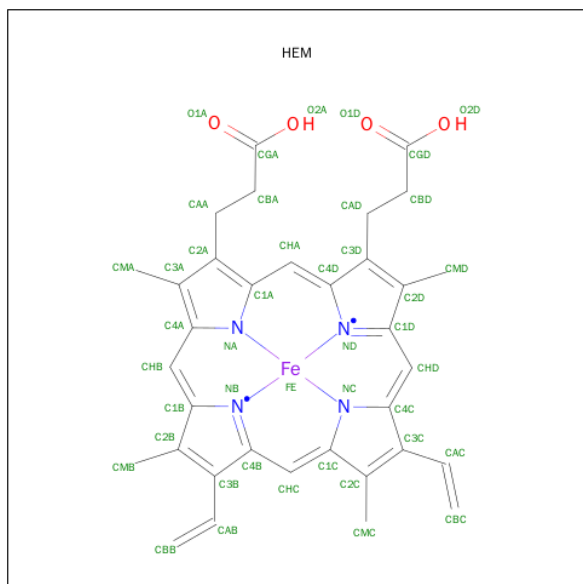


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 29	C 24	O 5	0	0
5	A	1	Total 29	C 24	O 5	0	0
5	B	1	Total 29	C 24	O 5	0	0
5	B	1	Total 29	C 24	O 5	0	0
5	B	1	Total 29	C 24	O 5	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

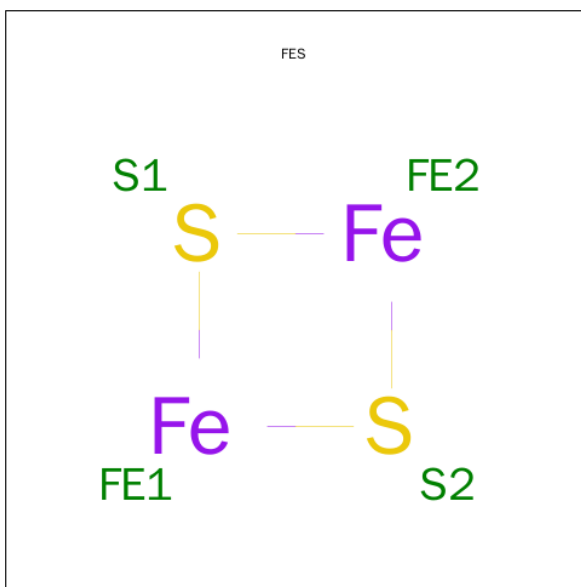
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Fe	S	0	0
			4	2	2		
8	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 9 is water.

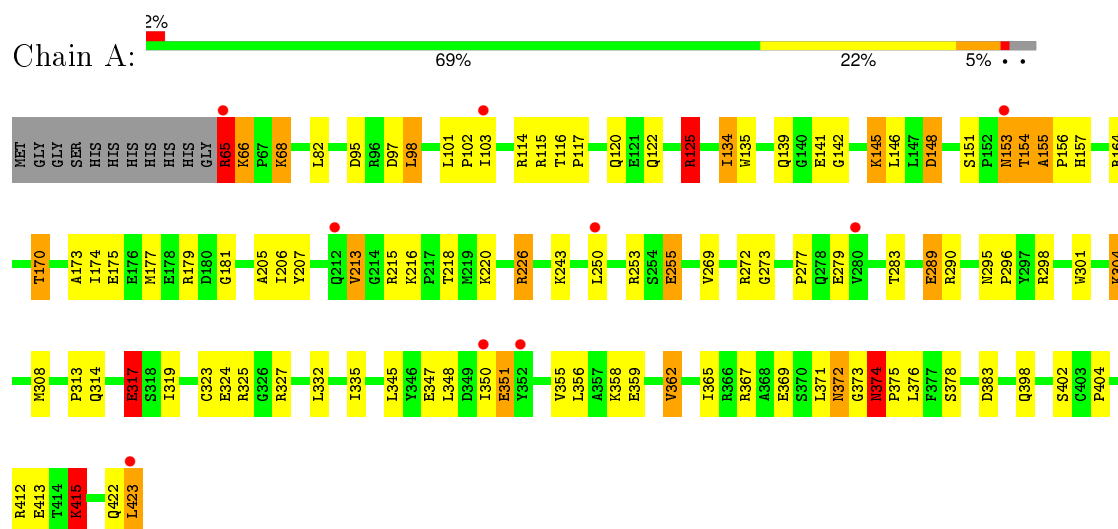
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	170	Total	O	0	0
			170	170		
9	B	171	Total	O	0	0
			171	171		



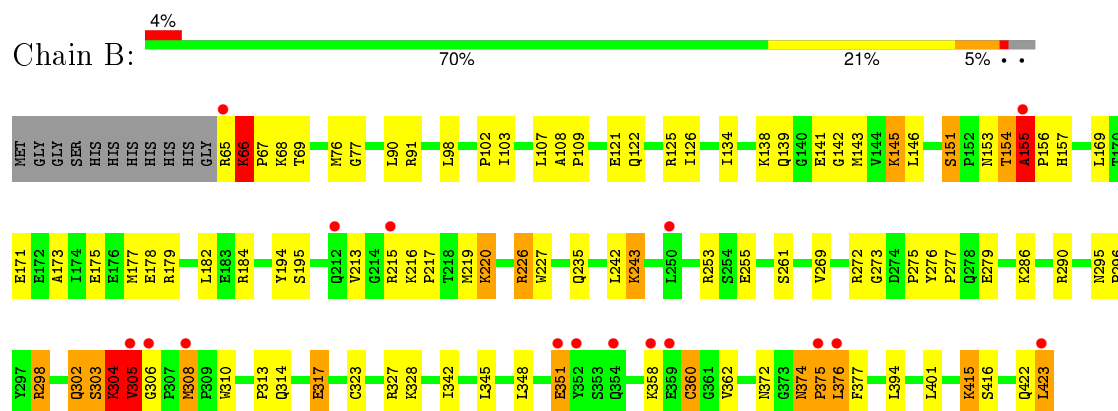
### 3 Residue-property plots [i](#)

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

- Molecule 1: Ferrochelatase, mitochondrial



- Molecule 1: Ferrochelatase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.13 Å 92.56 Å 109.26 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.71 – 2.18 33.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.71-2.18) 99.8 (33.82-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.63 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.200 , 0.258 0.198 , 0.257	Depositor DCC
$R_{free}$ test set	2340 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.822	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 51298 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6456	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.42 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3685e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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, CHD, IMD, CL, FES, BCT, 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	1.08	6/2996 (0.2%)	1.03	8/4056 (0.2%)
1	B	1.09	4/3010 (0.1%)	1.03	7/4076 (0.2%)
All	All	1.09	10/6006 (0.2%)	1.03	15/8132 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	VAL	CB-CG2	6.77	1.67	1.52
1	B	360	CYS	CB-SG	-6.47	1.71	1.82
1	A	317	GLU	CD-OE1	6.33	1.32	1.25
1	A	255	GLU	CB-CG	6.23	1.64	1.52
1	A	255	GLU	CG-CD	5.88	1.60	1.51
1	B	269	VAL	CB-CG2	5.42	1.64	1.52
1	B	305	VAL	CA-CB	5.39	1.66	1.54
1	A	415	LYS	CE-NZ	5.29	1.62	1.49
1	B	317	GLU	CG-CD	5.25	1.59	1.51
1	A	289	GLU	CG-CD	5.24	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ARG	NE-CZ-NH2	-14.15	113.22	120.30
1	A	226	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	B	226	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	A	226	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	A	125[A]	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	A	125[B]	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	A	327	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	383	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	253	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	327	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	298	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	253	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	143	MET	CG-SD-CE	5.31	108.70	100.20
1	B	155	ALA	C-N-CD	5.07	139.05	128.40
1	A	148	ASP	CB-CG-OD1	-5.06	113.74	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	THR	Peptide
1	A	371	LEU	Peptide
1	A	65	ARG	Peptide
1	B	154	THR	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2917	0	2939	107	0
1	B	2928	0	2946	92	1
2	A	5	0	4	0	0
2	B	5	0	4	1	0
3	A	4	0	0	1	0
3	B	4	0	0	0	0
4	A	12	0	16	4	0
5	A	58	0	78	4	0
5	B	87	0	115	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
7	A	43	0	30	0	0
7	B	43	0	30	0	0
8	A	4	0	0	0	0
8	B	4	0	0	0	0
9	A	170	0	0	9	0
9	B	171	0	0	8	1
All	All	6456	0	6162	227	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 18.

All (227) 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:505:CHD:C16	5:B:505:CHD:C15	1.74	1.46
1:A:125[A]:ARG:HB3	1:A:125[A]:ARG:NH1	1.53	1.23
5:B:505:CHD:C21	5:B:505:CHD:H183	1.74	1.15
5:B:504:CHD:H12	5:B:504:CHD:H212	1.17	1.12
5:B:504:CHD:H20	5:B:504:CHD:O26	1.38	1.11
1:A:304:LYS:CE	1:A:314[A]:GLN:HG2	1.79	1.11
5:B:504:CHD:C12	5:B:504:CHD:H212	1.77	1.10
1:A:155:ALA:HB1	1:A:156:PRO:HD2	1.16	1.10
5:B:505:CHD:H212	5:B:505:CHD:C18	1.81	1.07
1:A:125[A]:ARG:CB	1:A:125[A]:ARG:HH11	1.72	1.02
1:A:304:LYS:HE3	1:A:314[A]:GLN:HG2	1.02	1.01
5:B:504:CHD:C12	5:B:504:CHD:C21	2.36	1.01
1:A:125[A]:ARG:HB3	1:A:125[A]:ARG:HH11	1.22	1.01
1:B:328:LYS:HE3	1:B:360:CYS:O	1.63	0.98
1:A:155:ALA:HB1	1:A:156:PRO:CD	1.95	0.96
1:A:170:THR:CG2	9:A:647:HOH:O	2.14	0.95
5:B:505:CHD:H17	5:B:505:CHD:C24	1.96	0.95
5:B:505:CHD:H213	5:B:505:CHD:H12	1.49	0.95
5:B:505:CHD:O26	5:B:505:CHD:H161	1.67	0.94
5:B:504:CHD:H213	5:B:504:CHD:O12	1.67	0.93
1:B:184:ARG:HB3	1:B:220:LYS:HD2	1.50	0.93
5:B:504:CHD:C20	5:B:504:CHD:O26	2.15	0.92
1:A:255:GLU:HB2	9:A:714:HOH:O	1.70	0.91
1:B:374:ASN:CG	1:B:375:PRO:HD2	1.92	0.90
5:B:505:CHD:H212	5:B:505:CHD:H183	0.92	0.88
1:A:125[A]:ARG:CB	1:A:125[A]:ARG:NH1	2.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LYS:H	1:A:304:LYS:CD	1.85	0.88
1:A:142:GLY:O	1:A:146:LEU:CD1	2.21	0.87
1:B:375:PRO:HG2	1:B:376:LEU:H	1.39	0.86
1:B:303[A]:SER:HB2	1:B:314[A]:GLN:NE2	1.92	0.85
1:B:375:PRO:O	1:B:377:PHE:N	2.10	0.84
5:B:505:CHD:H17	5:B:505:CHD:O25	1.78	0.84
1:B:308[A]:MET:HG3	1:B:310:TRP:HE1	1.43	0.83
5:B:505:CHD:C17	5:B:505:CHD:C24	2.56	0.83
1:A:170:THR:HG23	9:A:647:HOH:O	1.77	0.83
1:B:314[B]:GLN:HB3	1:B:317:GLU:HG2	1.61	0.82
1:B:303[A]:SER:OG	1:B:314[A]:GLN:HG3	1.80	0.82
1:A:155:ALA:CB	1:A:156:PRO:HD2	2.05	0.81
1:A:372:ASN:HB3	1:A:373:GLY:CA	2.11	0.80
1:A:173:ALA:O	1:A:177:MET:HG3	1.82	0.80
1:B:328:LYS:CE	1:B:360:CYS:O	2.32	0.78
1:B:155:ALA:HB1	1:B:156:PRO:HD3	1.65	0.77
1:A:314[B]:GLN:HB3	1:A:317:GLU:CG	2.15	0.77
1:A:181:GLY:O	9:A:717:HOH:O	2.02	0.77
5:B:504:CHD:C21	5:B:504:CHD:O12	2.30	0.76
1:A:304:LYS:HE3	1:A:314[A]:GLN:CG	1.99	0.74
1:A:374:ASN:HD22	1:A:376:LEU:H	1.34	0.74
1:A:153:ASN:ND2	1:A:153:ASN:H	1.84	0.73
1:A:142:GLY:O	1:A:146:LEU:HD12	1.89	0.72
1:B:308[A]:MET:HG3	1:B:310:TRP:NE1	2.04	0.72
1:B:235:GLN:HG3	1:B:290:ARG:NH2	2.04	0.72
1:A:304:LYS:HD2	1:A:304:LYS:H	1.56	0.71
1:A:323:CYS:SG	1:A:362:VAL:HG13	2.31	0.70
5:B:505:CHD:C24	5:B:505:CHD:H161	2.21	0.70
1:B:323[B]:CYS:SG	1:B:362:VAL:HG22	2.32	0.70
1:B:68:LYS:HE3	1:B:155:ALA:HB3	1.74	0.69
5:B:505:CHD:C16	5:B:505:CHD:C24	2.71	0.68
1:A:304:LYS:N	1:A:304:LYS:CD	2.57	0.68
1:B:375:PRO:C	1:B:377:PHE:H	1.98	0.67
1:A:314[B]:GLN:HB3	1:A:317:GLU:HG3	1.76	0.67
1:B:122:GLN:HE22	1:B:348:LEU:HD13	1.59	0.67
1:B:142:GLY:O	1:B:146:LEU:CD1	2.42	0.67
1:A:125[A]:ARG:CA	1:A:125[A]:ARG:HH11	2.08	0.66
1:A:373:GLY:O	1:A:374:ASN:O	2.13	0.66
1:A:273:GLY:HA2	1:B:313:PRO:HG3	1.78	0.66
1:A:304:LYS:HD3	1:A:304:LYS:H	1.58	0.66
1:A:304:LYS:HD3	1:A:314[A]:GLN:HE21	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303[A]:SER:OG	1:B:314[A]:GLN:CG	2.43	0.66
1:B:142:GLY:O	1:B:146:LEU:HD12	1.96	0.66
1:A:142:GLY:O	1:A:146:LEU:HD13	1.96	0.65
1:A:289:GLU:OE2	9:A:731:HOH:O	2.14	0.65
1:B:375:PRO:HG2	1:B:376:LEU:N	2.11	0.65
1:A:301:TRP:O	1:A:304:LYS:HE2	1.97	0.64
5:B:505:CHD:C16	5:B:505:CHD:O26	2.44	0.64
1:B:314[B]:GLN:HB3	1:B:317:GLU:CG	2.27	0.64
1:B:155:ALA:CB	1:B:156:PRO:CD	2.74	0.64
1:A:134:ILE:HG13	9:A:696:HOH:O	1.96	0.64
1:A:372:ASN:CB	1:A:373:GLY:CA	2.76	0.64
1:B:351:GLU:N	1:B:351:GLU:OE2	2.30	0.63
1:A:372:ASN:CB	1:A:373:GLY:HA3	2.28	0.63
1:A:95:ASP:O	1:A:97:ASP:O	2.16	0.63
1:A:218:THR:HG22	1:A:218:THR:O	1.99	0.63
1:A:314[B]:GLN:OE1	1:A:317:GLU:HG2	1.98	0.62
5:B:505:CHD:C12	5:B:505:CHD:H213	2.27	0.62
1:B:303[A]:SER:HB2	1:B:314[A]:GLN:CD	2.21	0.61
1:B:304:LYS:HE2	5:B:503:CHD:H211	1.82	0.61
5:B:505:CHD:H12	5:B:505:CHD:C21	2.28	0.61
1:A:374:ASN:ND2	1:A:376:LEU:H	1.97	0.61
1:B:415:LYS:HE3	9:B:750:HOH:O	2.00	0.60
1:B:155:ALA:HB1	1:B:156:PRO:CD	2.31	0.60
1:A:125[A]:ARG:NH1	9:A:738:HOH:O	1.93	0.60
1:A:374:ASN:ND2	1:A:375:PRO:HD2	2.15	0.60
1:B:171:GLU:OE1	1:B:171:GLU:N	2.24	0.60
5:B:504:CHD:H12	5:B:504:CHD:C21	2.03	0.59
1:B:422:GLN:O	1:B:423:LEU:HB2	2.00	0.59
1:B:126:ILE:HB	9:B:749:HOH:O	2.02	0.59
1:A:412:ARG:HA	1:A:415:LYS:HG3	1.84	0.59
1:B:376:LEU:HG	1:B:376:LEU:O	2.02	0.58
1:B:308[A]:MET:CG	1:B:310:TRP:HE1	2.14	0.58
1:B:155:ALA:CB	1:B:156:PRO:HD3	2.31	0.58
1:B:102:PRO:O	1:B:107:LEU:HD12	2.03	0.58
1:A:68:LYS:HB2	1:A:68:LYS:NZ	2.18	0.58
1:A:139:GLN:NE2	1:A:378[A]:SER:OG	2.37	0.58
1:B:66:LYS:HG2	1:B:67:PRO:HD2	1.86	0.58
1:A:304:LYS:HD2	1:A:304:LYS:N	2.18	0.57
5:A:504:CHD:H183	5:A:504:CHD:H212	1.85	0.57
1:B:177:MET:HB3	1:B:182:LEU:HD12	1.86	0.57
1:B:374:ASN:OD1	1:B:375:PRO:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASP:O	1:A:98:LEU:CB	2.52	0.57
1:A:402:SER:OG	1:A:415:LYS:CE	2.53	0.56
1:A:65:ARG:HB3	1:A:65:ARG:NH1	2.19	0.55
1:A:175:GLU:O	1:A:179:ARG:HG3	2.06	0.55
1:A:65:ARG:O	1:A:66:LYS:HB3	2.05	0.55
1:B:175:GLU:HG2	9:B:755:HOH:O	2.05	0.55
1:A:304:LYS:HD3	1:A:314[A]:GLN:NE2	2.23	0.54
1:B:141:GLU:O	1:B:145:LYS:HD2	2.06	0.54
1:A:155:ALA:CB	1:A:156:PRO:CD	2.69	0.54
1:A:298:ARG:NH1	1:B:273:GLY:O	2.40	0.54
1:A:220:LYS:HE2	1:A:423:LEU:HD13	1.90	0.54
1:B:91:ARG:NH1	1:B:169:LEU:HD11	2.23	0.54
5:B:505:CHD:H5	9:B:703:HOH:O	2.08	0.53
1:A:373:GLY:O	1:A:374:ASN:C	2.46	0.53
1:B:66:LYS:O	1:B:156:PRO:HG2	2.09	0.52
1:B:261:SER:OG	1:B:302:GLN:HG2	2.10	0.52
1:B:375:PRO:C	1:B:377:PHE:N	2.62	0.51
1:A:295:ASN:HB3	1:A:296:PRO:HD2	1.92	0.51
1:B:142:GLY:O	1:B:146:LEU:HD13	2.10	0.51
1:B:151:SER:OG	1:B:154:THR:OG1	2.25	0.51
1:A:369:GLU:HG2	9:A:747:HOH:O	2.11	0.51
1:B:215:ARG:NH2	9:B:698:HOH:O	2.44	0.51
1:A:277:PRO:CB	4:A:503[A]:GOL:H2	2.41	0.50
1:B:235:GLN:CG	1:B:290:ARG:NH2	2.74	0.50
1:A:301:TRP:O	1:A:304:LYS:CE	2.59	0.50
1:A:402:SER:OG	1:A:415:LYS:HE3	2.10	0.50
1:B:175:GLU:O	1:B:179:ARG:HG3	2.10	0.50
1:B:226:ARG:HD3	1:B:279:GLU:OE2	2.12	0.50
1:A:314[A]:GLN:HB2	1:A:317:GLU:CG	2.40	0.50
1:A:174:ILE:HD11	1:A:206:ILE:HG12	1.94	0.50
5:B:504:CHD:H213	5:B:504:CHD:HO12	1.76	0.50
1:B:68:LYS:HG2	1:B:156:PRO:HD2	1.94	0.50
1:B:194:TYR:HD2	1:B:275:PRO:HG2	1.77	0.49
1:A:82:LEU:HB3	1:A:120:GLN:HG2	1.94	0.49
1:A:226:ARG:HD3	1:A:279:GLU:OE2	2.13	0.49
1:B:68:LYS:HE3	1:B:155:ALA:CB	2.43	0.48
1:B:323[B]:CYS:SG	1:B:360:CYS:HB2	2.53	0.48
1:A:170:THR:HG22	9:A:647:HOH:O	1.93	0.48
5:B:503:CHD:H162	5:B:503:CHD:H221	1.50	0.48
1:B:122:GLN:HE22	1:B:348:LEU:CD1	2.26	0.48
1:B:178:GLU:HG3	9:B:697:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HB3	1:A:65:ARG:HH11	1.77	0.48
1:A:207:TYR:CZ	1:A:413:GLU:HB3	2.49	0.48
1:A:153:ASN:ND2	1:A:153:ASN:N	2.60	0.47
1:B:134:ILE:HD11	1:B:138:LYS:HE3	1.96	0.47
1:A:125[A]:ARG:HA	1:A:125[A]:ARG:HH11	1.79	0.47
1:A:304:LYS:CE	1:A:314[A]:GLN:CG	2.72	0.47
1:B:125[A]:ARG:HB3	1:B:125[A]:ARG:NH1	2.30	0.47
1:B:76:MET:HG3	1:B:77:GLY:O	2.15	0.47
1:B:103:ILE:O	1:B:103:ILE:HG13	2.15	0.47
1:B:108:ALA:HB3	1:B:109:PRO:HD3	1.98	0.46
1:A:347:GLU:OE1	1:A:367:ARG:HD2	2.16	0.46
1:A:351:GLU:OE2	1:A:351:GLU:N	2.48	0.46
1:A:314[B]:GLN:HB3	1:A:317:GLU:HG2	1.95	0.46
1:B:121:GLU:O	1:B:125[B]:ARG:HG2	2.16	0.46
1:A:148:ASP:OD1	1:A:157:HIS:ND1	2.49	0.46
1:B:195:SER:HB2	1:B:276:TYR:HB2	1.98	0.45
1:B:235:GLN:CG	1:B:290:ARG:HH21	2.30	0.45
1:A:277:PRO:HB3	4:A:503[A]:GOL:H2	1.99	0.45
1:B:122:GLN:HE21	1:B:342:ILE:HG23	1.82	0.45
1:A:308:MET:HG3	5:A:504:CHD:H21	1.98	0.45
1:A:115:ARG:HD2	5:A:504:CHD:H232	1.99	0.45
1:A:402:SER:OG	1:A:415:LYS:HE2	2.17	0.45
1:A:372:ASN:HB3	1:A:373:GLY:HA2	1.97	0.45
5:B:505:CHD:C21	5:B:505:CHD:C18	2.49	0.44
4:A:503[B]:GOL:H12	1:B:277:PRO:HB2	1.99	0.44
1:B:216:LYS:O	1:B:217:PRO:C	2.56	0.44
1:A:324:GLU:HG3	1:A:325:ARG:NH1	2.32	0.44
1:B:242:LEU:HD23	1:B:242:LEU:HA	1.90	0.44
1:A:422:GLN:HG2	1:A:423:LEU:HD12	1.99	0.44
1:A:141:GLU:O	1:A:145:LYS:HD2	2.17	0.44
1:B:305:VAL:HB	9:B:643:HOH:O	2.17	0.44
1:B:173:ALA:O	1:B:177:MET:HG3	2.18	0.44
1:A:273:GLY:HA3	1:A:404:PRO:HD2	2.00	0.43
1:A:65:ARG:O	1:A:66:LYS:CB	2.65	0.43
1:A:68:LYS:NZ	1:A:68:LYS:CB	2.82	0.43
1:A:116:THR:N	1:A:117:PRO:HD2	2.34	0.43
1:B:243:LYS:HE2	1:B:243:LYS:HB3	1.64	0.43
1:B:306:GLY:HA3	1:B:308[A]:MET:HE1	1.99	0.43
1:B:304:LYS:HD2	1:B:308[A]:MET:HE3	2.01	0.43
1:B:69:THR:O	1:B:157:HIS:HA	2.19	0.43
5:B:504:CHD:H111	5:B:504:CHD:H193	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TRP:HA	1:A:135:TRP:CE3	2.53	0.43
1:A:68:LYS:HB2	1:A:68:LYS:HZ2	1.84	0.42
1:A:102:PRO:O	1:A:103:ILE:HG13	2.19	0.42
1:A:98:LEU:HD11	3:A:502:BCT:O1	2.19	0.42
1:A:277:PRO:HB2	4:A:503[A]:GOL:H2	2.01	0.42
1:A:213:VAL:HG21	1:A:215:ARG:HH21	1.83	0.42
1:B:308[B]:MET:HE3	1:B:308[B]:MET:H	1.85	0.42
1:A:68:LYS:HE3	1:A:154:THR:HA	2.00	0.42
1:B:394:LEU:HA	1:B:394:LEU:HD23	1.91	0.42
5:B:504:CHD:H112	5:B:504:CHD:H12A	1.63	0.42
1:A:68:LYS:HB2	1:A:68:LYS:HZ3	1.85	0.42
1:B:304:LYS:HE3	1:B:304:LYS:HB2	1.71	0.42
1:A:313:PRO:HG3	1:B:273:GLY:HA2	2.01	0.41
1:A:319:ILE:HD11	1:A:332:LEU:HD21	2.03	0.41
1:A:122:GLN:HE22	1:A:348:LEU:HD13	1.85	0.41
1:B:69:THR:OG1	1:B:154:THR:HB	2.20	0.41
1:B:303[A]:SER:CB	1:B:314[A]:GLN:CG	2.98	0.41
1:A:283:THR:HG22	1:A:335:ILE:HD11	2.02	0.41
1:A:164:ARG:CZ	1:A:205:ALA:HB2	2.51	0.41
1:A:373:GLY:C	1:A:374:ASN:O	2.59	0.41
1:A:304:LYS:NZ	1:A:314[A]:GLN:HG2	2.31	0.41
1:B:139:GLN:HG3	1:B:372:ASN:OD1	2.21	0.41
5:A:505:CHD:H162	5:A:505:CHD:H221	1.87	0.41
1:B:304:LYS:HB2	1:B:305:VAL:H	1.71	0.41
1:A:213:VAL:HG13	1:A:213:VAL:O	2.21	0.41
1:B:305:VAL:HG13	1:B:306:GLY:N	2.36	0.40
1:A:374:ASN:HD22	1:A:375:PRO:CD	2.34	0.40
1:B:295:ASN:HB3	1:B:296:PRO:HD2	2.03	0.40
1:B:374:ASN:CG	1:B:375:PRO:CD	2.78	0.40
1:B:308[A]:MET:HG3	1:B:310:TRP:CD1	2.56	0.40
2:B:501:IMD:H2	9:B:665:HOH:O	2.20	0.40
1:B:107:LEU:O	1:B:108:ALA:C	2.60	0.40
1:A:355:VAL:O	1:A:359:GLU:HG3	2.21	0.40
1:B:303[B]:SER:OG	1:B:304:LYS:N	2.54	0.40
1:A:398:GLN:OE1	1:A:398:GLN:HA	2.21	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:B:125[A]:ARG:NH1	9:B:741:HOH:O[3_655]	2.02	0.18

## 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	361/370 (98%)	340 (94%)	17 (5%)	4 (1%)	17	13
1	B	363/370 (98%)	343 (94%)	11 (3%)	9 (2%)	7	3
All	All	724/740 (98%)	683 (94%)	28 (4%)	13 (2%)	11	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ALA
1	A	374	ASN
1	B	155	ALA
1	B	375	PRO
1	B	376	LEU
1	B	66	LYS
1	B	304	LYS
1	A	66	LYS
1	B	305	VAL
1	A	372	ASN
1	B	374	ASN
1	B	303[A]	SER
1	B	303[B]	SER

### 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	328/332 (99%)	297 (90%)	31 (10%)	11	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	330/332 (99%)	302 (92%)	28 (8%)	13	11
All	All	658/664 (99%)	599 (91%)	59 (9%)	13	10

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	68	LYS
1	A	98	LEU
1	A	101	LEU
1	A	114	ARG
1	A	125[A]	ARG
1	A	125[B]	ARG
1	A	134	ILE
1	A	145	LYS
1	A	151	SER
1	A	153	ASN
1	A	170	THR
1	A	213	VAL
1	A	216	LYS
1	A	243[A]	LYS
1	A	243[B]	LYS
1	A	250	LEU
1	A	272	ARG
1	A	290	ARG
1	A	304	LYS
1	A	317	GLU
1	A	345	LEU
1	A	350	ILE
1	A	351	GLU
1	A	356	LEU
1	A	358	LYS
1	A	362	VAL
1	A	365	ILE
1	A	374	ASN
1	A	415	LYS
1	A	423	LEU
1	B	65	ARG
1	B	66	LYS
1	B	90	LEU
1	B	98	LEU
1	B	145	LYS

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Mol	Chain	Res	Type
1	B	151	SER
1	B	153	ASN
1	B	213	VAL
1	B	219	MET
1	B	220	LYS
1	B	227	TRP
1	B	243	LYS
1	B	255[A]	GLU
1	B	255[B]	GLU
1	B	272	ARG
1	B	286	LYS
1	B	298	ARG
1	B	302	GLN
1	B	304	LYS
1	B	308[A]	MET
1	B	308[B]	MET
1	B	345	LEU
1	B	351	GLU
1	B	358	LYS
1	B	401	LEU
1	B	415	LYS
1	B	416	SER
1	B	423	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	139	GLN
1	A	153	ASN
1	A	204	ASN
1	A	231	HIS
1	A	235	GLN
1	A	343	GLN
1	A	354	GLN
1	A	364	ASN
1	A	374	ASN
1	A	421	GLN
1	B	122	GLN
1	B	139	GLN
1	B	204	ASN
1	B	231	HIS

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Mol	Chain	Res	Type
1	B	302	GLN
1	B	343	GLN
1	B	354	GLN
1	B	421	GLN

### 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 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	IMD	A	501	7	3,5,5	0.16	0	4,5,5	1.11	0
3	BCT	A	502	7	0,3,3	0.00	-	0,3,3	0.00	-
4	GOL	A	503[A]	-	5,5,5	0.21	0	5,5,5	0.98	0
4	GOL	A	503[B]	-	5,5,5	0.25	0	5,5,5	1.00	0
5	CHD	A	504	-	29,32,32	0.86	0	48,51,51	1.94	14 (29%)
5	CHD	A	505	-	29,32,32	0.70	0	48,51,51	1.69	12 (25%)
7	HEM	A	507	3,2	30,50,50	2.38	7 (23%)	24,82,82	2.40	8 (33%)
8	FES	A	508	1	0,4,4	0.00	-	0,4,4	0.00	-
2	IMD	B	501	7	3,5,5	0.33	0	4,5,5	1.79	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BCT	B	502	7	0,3,3	0.00	-	0,3,3	0.00	-
5	CHD	B	503	-	29,32,32	0.90	1 (3%)	48,51,51	2.32	20 (41%)
5	CHD	B	504	-	29,32,32	1.45	5 (17%)	48,51,51	4.13	30 (62%)
5	CHD	B	505	-	29,32,32	1.58	2 (6%)	48,51,51	2.67	20 (41%)
7	HEM	B	506	3,2	30,50,50	2.30	8 (26%)	24,82,82	2.44	8 (33%)
8	FES	B	507	1	0,4,4	0.00	-	0,4,4	0.00	-

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	IMD	A	501	7	-	0/0/0/0	0/1/1/1
3	BCT	A	502	7	-	0/0/0/0	0/0/0/0
4	GOL	A	503[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	A	503[B]	-	-	0/4/4/4	0/0/0/0
5	CHD	A	504	-	-	0/7/74/74	0/4/4/4
5	CHD	A	505	-	-	0/7/74/74	0/4/4/4
7	HEM	A	507	3,2	-	0/10/54/54	0/0/8/8
8	FES	A	508	1	-	0/0/4/4	0/1/1/1
2	IMD	B	501	7	-	0/0/0/0	0/1/1/1
3	BCT	B	502	7	-	0/0/0/0	0/0/0/0
5	CHD	B	503	-	-	0/7/74/74	0/4/4/4
5	CHD	B	504	-	-	0/7/74/74	0/4/4/4
5	CHD	B	505	-	-	0/7/74/74	0/4/4/4
7	HEM	B	506	3,2	-	0/10/54/54	0/0/8/8
8	FES	B	507	1	-	0/0/4/4	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	507	HEM	C3B-C4B	-7.85	1.44	1.51
7	B	506	HEM	C3D-C4D	-7.23	1.42	1.51
7	A	507	HEM	C3D-C4D	-6.40	1.43	1.51
7	B	506	HEM	C3B-C4B	-6.28	1.46	1.51
7	A	507	HEM	C2C-C1C	-3.98	1.45	1.52
5	B	504	CHD	C10-C9	-3.47	1.49	1.56
5	B	504	CHD	C13-C14	-3.00	1.50	1.55
5	B	504	CHD	C13-C12	-2.88	1.50	1.54
5	B	504	CHD	C13-C17	-2.33	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	506	HEM	C2C-C1C	-2.21	1.48	1.52
5	B	504	CHD	C8-C9	-2.16	1.49	1.53
5	B	505	CHD	C13-C14	-2.14	1.51	1.55
7	B	506	HEM	C2D-C1D	-2.08	1.45	1.51
7	A	507	HEM	C2D-C3D	-2.04	1.48	1.54
7	B	506	HEM	C1C-NC	2.02	1.38	1.36
5	B	503	CHD	C13-C12	2.21	1.58	1.54
7	A	507	HEM	C3C-CAC	2.35	1.55	1.51
7	B	506	HEM	FE-NC	2.72	2.06	1.95
7	A	507	HEM	FE-NC	2.84	2.07	1.95
7	B	506	HEM	C3B-CAB	2.90	1.56	1.51
7	A	507	HEM	CAA-C2A	3.13	1.57	1.52
7	B	506	HEM	C3C-CAC	3.38	1.57	1.51
5	B	505	CHD	C16-C15	7.40	1.74	1.54

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	504	CHD	C14-C8-C9	-10.32	95.43	109.62
5	B	504	CHD	C17-C13-C14	-8.19	91.78	100.05
5	B	504	CHD	C9-C11-C12	-8.05	104.20	114.36
5	B	504	CHD	C1-C10-C9	-7.20	99.84	111.45
5	B	504	CHD	C11-C9-C10	-6.51	107.03	113.79
5	B	505	CHD	C13-C17-C20	-5.83	112.41	119.50
5	B	503	CHD	C13-C17-C20	-5.75	112.50	119.50
5	B	504	CHD	C11-C12-C13	-5.63	105.48	111.20
5	B	504	CHD	C19-C10-C9	-5.45	103.01	111.18
5	B	504	CHD	C14-C8-C7	-5.38	104.29	111.74
5	B	505	CHD	C10-C9-C8	-5.10	106.29	111.88
5	A	504	CHD	C23-C22-C20	-4.77	109.13	114.75
5	B	504	CHD	C21-C20-C17	-4.77	105.01	112.96
5	B	504	CHD	C17-C13-C12	-4.65	113.56	117.68
5	B	504	CHD	C1-C2-C3	-4.56	103.03	110.43
5	B	503	CHD	C11-C12-C13	-4.54	106.58	111.20
5	A	505	CHD	C17-C13-C12	-4.49	113.70	117.68
5	B	504	CHD	C23-C22-C20	-4.47	109.48	114.75
5	B	504	CHD	C5-C4-C3	-4.46	106.28	112.91
5	B	505	CHD	C4-C3-C2	-4.42	104.89	110.52
5	B	505	CHD	C17-C13-C12	-4.37	113.81	117.68
5	B	505	CHD	C5-C4-C3	-4.22	106.64	112.91
5	B	505	CHD	C11-C9-C10	-4.20	109.43	113.79
5	B	504	CHD	C4-C3-C2	-3.96	105.47	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	CHD	C17-C13-C12	-3.78	114.33	117.68
7	A	507	HEM	CAA-C2A-C1A	-3.77	122.91	127.01
5	B	505	CHD	C13-C14-C8	-3.76	109.90	114.75
5	A	504	CHD	C19-C10-C5	-3.47	104.12	110.25
5	B	503	CHD	C13-C14-C8	-3.47	110.27	114.75
7	B	506	HEM	CMA-C3A-C4A	-3.45	122.65	128.36
5	B	503	CHD	C18-C13-C14	-3.43	105.81	111.22
7	A	507	HEM	CMA-C3A-C4A	-3.42	122.70	128.36
5	B	504	CHD	O7-C7-C8	-3.42	101.71	109.26
5	A	504	CHD	C21-C20-C22	-3.39	104.69	110.35
5	A	504	CHD	C1-C10-C9	-3.29	106.14	111.45
5	B	505	CHD	C16-C15-C14	-3.18	98.71	105.12
5	B	504	CHD	C13-C17-C20	-3.00	115.84	119.50
5	B	504	CHD	O12-C12-C13	-2.85	106.50	111.11
7	B	506	HEM	CAA-C2A-C1A	-2.75	124.03	127.01
5	B	503	CHD	C23-C22-C20	-2.68	111.59	114.75
5	B	505	CHD	C19-C10-C9	-2.55	107.36	111.18
5	B	505	CHD	C15-C14-C8	-2.55	114.62	118.32
5	B	503	CHD	C19-C10-C5	-2.41	105.99	110.25
5	B	504	CHD	C15-C16-C17	-2.37	100.36	105.12
5	B	504	CHD	C22-C23-C24	-2.27	103.74	113.02
5	B	503	CHD	C9-C8-C7	-2.27	109.24	111.92
5	B	505	CHD	C23-C22-C20	-2.26	112.08	114.75
5	A	505	CHD	C21-C20-C17	-2.19	109.30	112.96
5	B	504	CHD	C19-C10-C5	-2.18	106.40	110.25
5	B	505	CHD	C9-C8-C7	-2.14	109.40	111.92
5	B	503	CHD	C1-C10-C9	-2.06	108.12	111.45
5	A	505	CHD	C14-C8-C9	-2.06	106.79	109.62
5	B	504	CHD	C9-C8-C7	-2.03	109.53	111.92
5	B	505	CHD	C15-C16-C17	-2.00	101.09	105.12
5	A	504	CHD	C19-C10-C9	2.02	114.21	111.18
7	A	507	HEM	C2C-C1C-CHC	2.03	126.77	123.68
5	B	503	CHD	C17-C13-C14	2.11	102.18	100.05
5	A	504	CHD	C14-C8-C7	2.16	114.74	111.74
5	B	503	CHD	C6-C7-C8	2.20	113.81	111.47
5	A	505	CHD	C18-C13-C12	2.21	111.25	109.09
5	B	503	CHD	C2-C1-C10	2.22	116.80	112.84
5	A	505	CHD	C23-C22-C20	2.31	117.48	114.75
5	A	505	CHD	C21-C20-C22	2.34	114.25	110.35
5	A	505	CHD	C2-C1-C10	2.39	117.11	112.84
7	B	506	HEM	C2C-C1C-CHC	2.41	127.34	123.68
5	B	503	CHD	C18-C13-C12	2.43	111.46	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	CHD	C11-C12-C13	2.44	113.68	111.20
5	B	504	CHD	C10-C9-C8	2.46	114.58	111.88
5	A	504	CHD	C4-C5-C10	2.46	115.37	112.66
5	A	504	CHD	C10-C9-C8	2.49	114.61	111.88
5	A	505	CHD	C14-C13-C12	2.52	109.64	107.39
5	A	505	CHD	C1-C10-C5	2.52	111.95	107.81
5	B	504	CHD	O3-C3-C4	2.64	115.11	109.86
5	A	505	CHD	C6-C7-C8	2.72	114.35	111.47
7	B	506	HEM	CMD-C2D-C3D	2.78	126.63	114.35
5	B	503	CHD	C5-C6-C7	2.83	117.59	114.44
2	B	501	IMD	C4-C5-N1	2.85	112.86	107.74
5	B	504	CHD	C6-C5-C10	2.90	115.85	112.66
5	B	505	CHD	C6-C5-C10	2.91	115.86	112.66
5	A	504	CHD	C21-C20-C17	3.03	118.00	112.96
5	B	505	CHD	C9-C11-C12	3.03	118.19	114.36
7	A	507	HEM	CMD-C2D-C3D	3.09	128.03	114.35
5	A	505	CHD	C10-C9-C8	3.13	115.32	111.88
5	A	504	CHD	C6-C7-C8	3.33	115.00	111.47
5	B	503	CHD	C1-C10-C5	3.33	113.28	107.81
5	B	504	CHD	C6-C7-C8	3.39	115.06	111.47
5	A	504	CHD	C1-C10-C5	3.45	113.48	107.81
5	B	505	CHD	C5-C6-C7	3.57	118.41	114.44
7	A	507	HEM	CMB-C2B-C3B	3.63	125.60	116.53
7	A	507	HEM	C3C-CAC-CBC	3.64	130.04	124.46
5	B	503	CHD	C15-C14-C13	3.71	107.29	103.60
5	B	504	CHD	C18-C13-C17	3.75	117.14	111.22
5	B	505	CHD	C1-C10-C5	3.78	114.02	107.81
7	B	506	HEM	CMB-C2B-C3B	3.86	126.18	116.53
5	B	503	CHD	C14-C13-C12	3.89	110.87	107.39
5	A	504	CHD	C18-C13-C12	3.89	112.88	109.09
5	B	505	CHD	C11-C9-C8	3.96	116.36	110.73
5	B	503	CHD	C9-C11-C12	3.97	119.37	114.36
5	A	505	CHD	C16-C17-C20	3.97	119.14	112.05
5	B	503	CHD	O12-C12-C11	4.08	117.41	109.06
7	B	506	HEM	CAD-C3D-C4D	4.27	127.52	112.47
5	B	504	CHD	C16-C17-C20	4.30	119.72	112.05
7	A	507	HEM	CAD-C3D-C4D	4.34	127.77	112.47
5	B	503	CHD	C16-C17-C13	4.39	107.97	103.60
5	B	505	CHD	C16-C17-C13	4.41	107.98	103.60
5	B	503	CHD	C11-C9-C8	4.43	117.03	110.73
7	B	506	HEM	CAD-C3D-C2D	5.08	127.81	113.22
7	A	507	HEM	CAD-C3D-C2D	5.10	127.89	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	504	CHD	C9-C10-C5	5.23	116.42	108.67
7	B	506	HEM	CMC-C2C-C3C	5.26	129.65	116.53
5	B	504	CHD	C1-C10-C5	6.80	118.99	107.81
5	B	505	CHD	C14-C13-C12	7.13	113.77	107.39
5	B	504	CHD	C14-C13-C12	8.57	115.06	107.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	BCT	1	0
4	A	503[A]	GOL	3	0
4	A	503[B]	GOL	1	0
5	A	504	CHD	3	0
5	A	505	CHD	1	0
2	B	501	IMD	1	0
5	B	503	CHD	2	0
5	B	504	CHD	11	0
5	B	505	CHD	16	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	359/370 (97%)	0.22	9 (2%) 61 62	9, 30, 52, 61	0
1	B	359/370 (97%)	0.21	16 (4%) 37 39	8, 29, 51, 62	0
All	All	718/740 (97%)	0.21	25 (3%) 48 50	8, 30, 51, 62	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	VAL	6.9
1	A	423	LEU	6.0
1	B	423	LEU	5.8
1	B	358	LYS	3.9
1	B	306	GLY	3.5
1	A	153	ASN	3.4
1	B	352	TYR	3.3
1	B	308[A]	MET	3.2
1	A	212	GLN	3.0
1	A	352	TYR	2.9
1	B	250	LEU	2.7
1	B	375	PRO	2.6
1	B	359	GLU	2.6
1	A	250	LEU	2.5
1	B	155	ALA	2.4
1	A	65	ARG	2.3
1	B	212	GLN	2.3
1	B	376	LEU	2.3
1	B	215	ARG	2.2
1	B	354	GLN	2.2
1	A	350	ILE	2.2
1	A	103	ILE	2.2
1	B	65	ARG	2.1
1	A	280	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	351	GLU	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
5	CHD	B	505	29/29	0.01	0.87	14.45	66,68,69,70	29
5	CHD	A	504	29/29	0.76	0.25	3.79	52,58,74,75	0
5	CHD	B	504	29/29	0.68	0.35	3.64	46,47,50,50	29
4	GOL	A	503[B]	6/6	0.95	0.19	2.18	14,16,19,24	6
4	GOL	A	503[A]	6/6	0.95	0.19	2.01	10,12,14,16	6
5	CHD	A	505	29/29	0.83	0.23	1.95	62,64,76,76	0
3	BCT	B	502	4/4	0.88	0.18	1.66	37,38,39,41	0
6	CL	A	506	1/1	0.85	0.34	1.62	77,77,77,77	0
5	CHD	B	503	29/29	0.54	0.32	1.34	69,78,87,88	0
3	BCT	A	502	4/4	0.88	0.15	0.20	36,36,38,40	0
2	IMD	B	501	5/5	0.93	0.16	0.18	21,23,25,25	0
2	IMD	A	501	5/5	0.96	0.14	-0.03	26,26,27,28	0
7	HEM	B	506	43/43	0.98	0.12	-0.20	12,19,28,32	0
7	HEM	A	507	43/43	0.98	0.12	-0.43	9,22,30,35	0
8	FES	A	508	4/4	0.98	0.06	-1.27	26,26,26,28	0
8	FES	B	507	4/4	0.98	0.05	-2.42	25,25,25,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.