



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2017 – 04:48 AM EDT

PDB ID : 5O1L  
Title : Structure of Latex Clearing Protein LCP in the open state with bound imidazole  
Authors : Ilcu, L.; Roether, W.; Birke, J.; Brausemann, A.; Einsle, O.; Jendrossek, D.  
Deposited on : unknown  
Resolution : 1.48 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

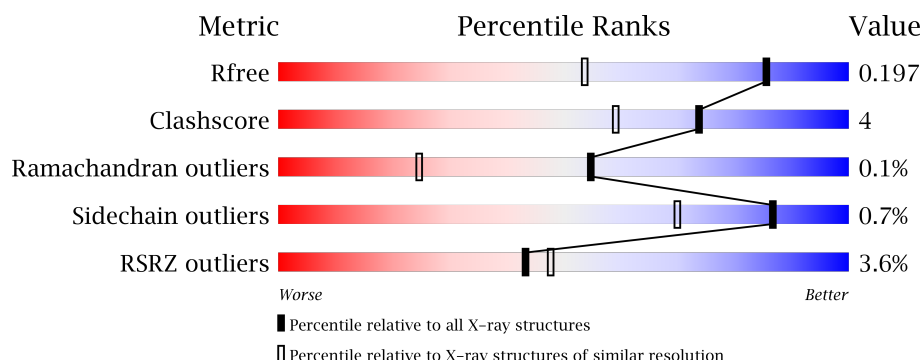
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.48 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	3517 (1.50-1.46)
Clashscore	112137	3795 (1.50-1.46)
Ramachandran outliers	110173	3721 (1.50-1.46)
Sidechain outliers	110143	3719 (1.50-1.46)
RSRZ outliers	101464	3549 (1.50-1.46)

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	407	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>
1	B	407	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</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
3	IMD	A	503	-	-	-	X
3	IMD	B	503	-	-	-	X
4	BU3	A	504	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6352 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 Rubber oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	8	0
			2920	1875	507	526	12			
1	B	373	Total	C	N	O	S	0	9	0
			2922	1872	511	527	12			

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



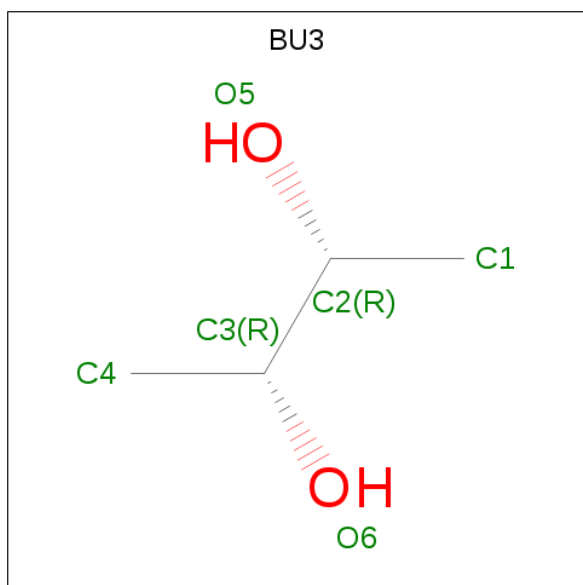
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



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

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

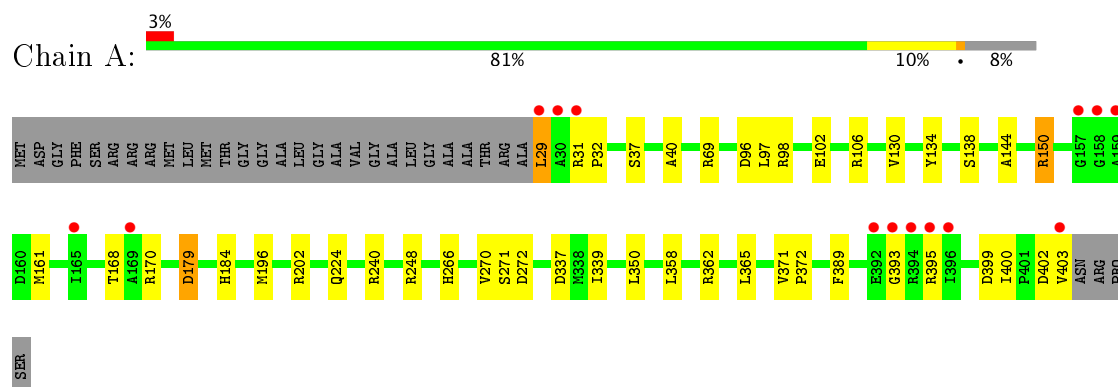
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	186	Total	O	0	0
			186	186		
6	B	198	Total	O	0	0
			198	198		

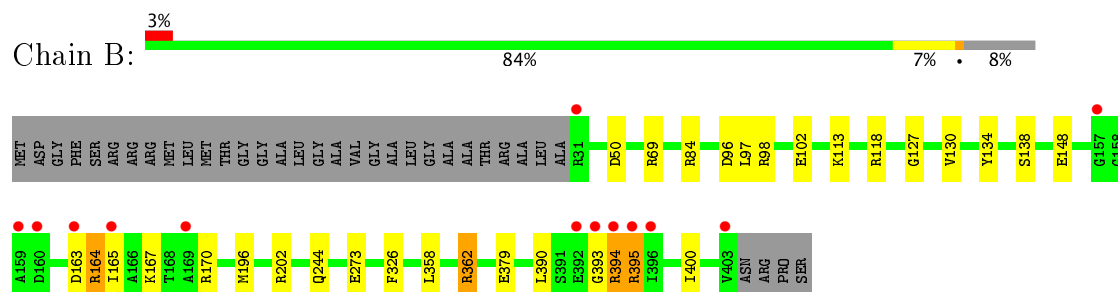
### 3 Residue-property plots [i](#)

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: Rubber oxygenase



- Molecule 1: Rubber oxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.76Å 62.80Å 64.42Å 85.43° 66.06° 74.16°	Depositor
Resolution (Å)	60.37 – 1.48 60.37 – 1.48	Depositor EDS
% Data completeness (in resolution range)	90.0 (60.37-1.48) 89.0 (60.37-1.48)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.166 , 0.189 0.174 , 0.197	Depositor DCC
$R_{free}$ test set	5840 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,-h+l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BU3, EDO, HEM, IMD

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	1.00	3/3015 (0.1%)	1.09	14/4109 (0.3%)
1	B	1.03	2/3011 (0.1%)	1.06	14/4102 (0.3%)
All	All	1.02	5/6026 (0.1%)	1.07	28/8211 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	273	GLU	CB-CG	-5.64	1.41	1.52
1	A	102	GLU	CD-OE2	5.60	1.31	1.25
1	A	134	TYR	CE1-CZ	-5.51	1.31	1.38
1	A	130	VAL	CB-CG1	-5.12	1.42	1.52
1	B	102	GLU	CG-CD	5.08	1.59	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	A	69	ARG	NE-CZ-NH2	8.75	124.67	120.30
1	B	98	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	358	LEU	CB-CG-CD2	-7.04	99.03	111.00
1	A	202	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	A	96	ASP	CB-CG-OD1	6.88	124.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	150	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	362	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	240	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	A	179	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	B	50	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	395	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	B	164	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	362	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	106	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	84	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	A	98	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	69	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	395	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	337	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	326	PHE	CB-CG-CD1	-5.32	117.08	120.80
1	A	98	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	163	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	362	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	399	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	118	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	202	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	395	ARG	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	2920	0	2971	24	0
1	B	2922	0	2961	19	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	9	3	0
3	B	10	0	9	2	0
4	A	6	0	10	0	0
4	B	6	0	10	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	A	186	0	0	5	0
6	B	198	0	0	6	0
All	All	6352	0	6042	46	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 4.

All (46) 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:A:144:ALA:HB2	1:A:339:ILE:HD11	1.38	1.05
1:A:32:PRO:O	6:A:601:HOH:O	1.85	0.93
1:B:362:ARG:HG3	6:B:772:HOH:O	1.84	0.75
1:A:29:LEU:N	6:A:603:HOH:O	2.23	0.70
1:B:362:ARG:HD2	1:B:379:GLU:OE2	1.92	0.68
1:A:196[A]:MET:HE2	1:A:400:ILE:HD11	1.75	0.68
1:A:266:HIS:HD2	1:A:272:ASP:OD1	1.76	0.68
1:B:196[A]:MET:HE2	1:B:400:ILE:HD11	1.76	0.67
1:B:196[A]:MET:CE	1:B:400:ILE:HD11	2.26	0.66
1:A:37:SER:O	6:A:602:HOH:O	2.15	0.64
1:A:196[A]:MET:CE	1:A:400:ILE:HD11	2.29	0.62
1:B:167:LYS:HA	6:B:617:HOH:O	2.00	0.62
1:A:138:SER:HB3	3:A:503:IMD:H4	1.83	0.61
1:A:40:ALA:HB3	6:A:602:HOH:O	2.01	0.60
1:B:362:ARG:CG	6:B:772:HOH:O	2.47	0.59
1:A:402:ASP:O	1:A:403:VAL:HG22	2.02	0.59
1:A:224[A]:GLN:HE22	1:A:270:VAL:HA	1.66	0.59
1:B:170:ARG:NE	1:B:393:GLY:HA3	2.21	0.55
1:A:358:LEU:HD11	1:A:371:VAL:HG21	1.89	0.54
1:B:148:GLU:OE2	3:B:503:IMD:N1	2.38	0.54
1:B:244[B]:GLN:NE2	6:B:601:HOH:O	2.26	0.54
1:B:164:ARG:HD3	2:B:501:HEM:CGD	2.38	0.53
1:A:170[A]:ARG:HG2	1:A:389:PHE:CD2	2.44	0.52
1:A:144:ALA:HB2	1:A:339:ILE:CD1	2.26	0.52
1:B:390:LEU:O	1:B:394[B]:ARG:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:HG3	6:B:608:HOH:O	2.09	0.52
1:A:144:ALA:CB	1:A:339:ILE:HD11	2.27	0.51
1:B:127:GLY:HA2	1:B:130[A]:VAL:HG22	1.93	0.51
1:B:170:ARG:HB3	6:B:617:HOH:O	2.09	0.51
1:B:138:SER:HB3	3:B:503:IMD:H4	1.93	0.51
1:A:248:ARG:HD3	1:A:365:LEU:HD11	1.93	0.48
1:A:350:LEU:HD22	1:A:372:PRO:HG2	1.95	0.48
1:B:394[B]:ARG:HE	1:B:394[B]:ARG:HA	1.79	0.48
1:B:97:LEU:HD11	1:B:196[B]:MET:SD	2.56	0.45
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.99	0.45
2:B:501:HEM:HBB2	2:B:501:HEM:HMB1	1.99	0.44
1:A:170[B]:ARG:CZ	1:A:393:GLY:HA3	2.48	0.44
1:A:224[A]:GLN:HE22	1:A:271:SER:H	1.66	0.44
1:A:168:THR:OG1	3:A:502:IMD:H5	2.18	0.43
1:A:168:THR:O	3:A:503:IMD:H2	2.18	0.43
1:B:130[B]:VAL:HG12	1:B:134:TYR:CE2	2.52	0.43
1:A:97:LEU:HD11	1:A:196[B]:MET:SD	2.58	0.42
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	2.02	0.41
1:A:150:ARG:HD2	6:A:622:HOH:O	2.20	0.41
1:A:179:ASP:OD1	1:A:184:HIS:HE1	2.04	0.41
1:B:390:LEU:O	1:B:394[B]:ARG:CG	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/407 (94%)	371 (97%)	9 (2%)	1 (0%)	44	18
1	B	380/407 (93%)	371 (98%)	9 (2%)	0	100	100
All	All	761/814 (94%)	742 (98%)	18 (2%)	1 (0%)	55	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ARG

### 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	303/315 (96%)	301 (99%)	2 (1%)	87	70
1	B	303/315 (96%)	300 (99%)	3 (1%)	80	57
All	All	606/630 (96%)	601 (99%)	5 (1%)	87	67

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	161	MET
1	B	165	ILE
1	B	394[A]	ARG
1	B	394[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	184	HIS
1	A	203	HIS
1	A	266	HIS
1	B	184	HIS

### 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](#)

10 ligands are modelled in this entry.

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	1,3	28,50,50	1.77	5 (17%)	17,82,82	1.93	6 (35%)
3	IMD	A	502	2	3,5,5	0.45	0	4,5,5	1.13	0
3	IMD	A	503	-	3,5,5	0.52	0	4,5,5	0.87	0
4	BU3	A	504	-	4,5,5	0.30	0	6,6,6	1.03	1 (16%)
5	EDO	A	505	-	3,3,3	0.50	0	2,2,2	0.20	0
2	HEM	B	501	1,3	28,50,50	1.69	3 (10%)	17,82,82	2.55	8 (47%)
3	IMD	B	502	2	3,5,5	0.69	0	4,5,5	0.99	0
3	IMD	B	503	-	3,5,5	0.36	0	4,5,5	1.05	0
4	BU3	B	504	-	4,5,5	0.39	0	6,6,6	0.56	0
5	EDO	B	505	-	3,3,3	0.33	0	2,2,2	0.82	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	1,3	-	0/6/54/54	0/0/8/8
3	IMD	A	502	2	-	0/0/0/0	0/1/1/1
3	IMD	A	503	-	-	0/0/0/0	0/1/1/1
4	BU3	A	504	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	505	-	-	0/1/1/1	0/0/0/0
2	HEM	B	501	1,3	-	0/6/54/54	0/0/8/8
3	IMD	B	502	2	-	0/0/0/0	0/1/1/1
3	IMD	B	503	-	-	0/0/0/0	0/1/1/1
4	BU3	B	504	-	-	0/4/4/4	0/0/0/0
5	EDO	B	505	-	-	0/1/1/1	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C2B	-5.69	1.32	1.40
2	B	501	HEM	C3B-C2B	-5.68	1.32	1.40
2	A	501	HEM	C3C-C2C	-3.22	1.36	1.40
2	B	501	HEM	C4B-NB	-2.67	1.30	1.36
2	A	501	HEM	C4A-CHB	-2.62	1.33	1.40
2	B	501	HEM	C1B-NB	-2.50	1.33	1.36
2	A	501	HEM	C4B-NB	-2.20	1.31	1.36
2	A	501	HEM	CBB-CAB	2.08	1.43	1.28

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CBD-CAD-C3D	-5.29	102.38	112.47
2	B	501	HEM	CAD-CBD-CGD	-4.01	105.80	112.66
2	A	501	HEM	CMD-C2D-C1D	-3.94	122.40	128.46
2	A	501	HEM	CBD-CAD-C3D	-2.77	107.19	112.47
2	A	501	HEM	CAD-CBD-CGD	-2.46	108.47	112.66
2	B	501	HEM	CBA-CAA-C2A	-2.37	107.95	112.48
4	A	504	BU3	O6-C3-C4	-2.22	102.78	109.70
2	B	501	HEM	C4A-C3A-C2A	-2.20	105.46	107.00
2	B	501	HEM	CMD-C2D-C1D	-2.11	125.21	128.46
2	A	501	HEM	C4A-C3A-C2A	2.20	108.53	107.00
2	B	501	HEM	CMB-C2B-C3B	2.24	129.05	124.89
2	A	501	HEM	CMD-C2D-C3D	2.60	129.84	124.94
2	A	501	HEM	CMC-C2C-C3C	2.91	130.28	124.89
2	B	501	HEM	CMC-C2C-C3C	4.24	132.77	124.89
2	B	501	HEM	C4C-C3C-C2C	4.49	110.03	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
3	A	502	IMD	1	0
3	A	503	IMD	2	0
2	B	501	HEM	2	0
3	B	503	IMD	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	375/407 (92%)	-0.10	14 (3%)	42 46	10, 20, 43, 82	0
1	B	373/407 (91%)	-0.07	13 (3%)	44 49	11, 19, 47, 86	0
All	All	748/814 (91%)	-0.08	27 (3%)	43 48	10, 20, 45, 86	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	LEU	7.4
1	B	393	GLY	6.9
1	B	396	ILE	6.6
1	B	403	VAL	6.5
1	A	159	ALA	5.9
1	B	159	ALA	5.9
1	B	394[A]	ARG	5.4
1	A	394	ARG	4.7
1	B	395	ARG	4.7
1	B	169	ALA	3.7
1	A	158	GLY	3.5
1	A	393	GLY	3.5
1	B	160	ASP	3.4
1	B	31	ARG	3.4
1	A	165	ILE	3.4
1	A	392	GLU	3.2
1	A	396	ILE	2.9
1	B	165	ILE	2.8
1	B	392	GLU	2.8
1	B	157	GLY	2.7
1	A	30	ALA	2.7
1	A	169	ALA	2.7
1	A	403	VAL	2.6
1	A	31	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	395	ARG	2.4
1	A	157	GLY	2.4
1	B	163	ASP	2.4

## 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
3	IMD	B	503	5/5	0.84	0.26	5.42	29,31,32,33	0
4	BU3	A	504	6/6	0.87	0.16	3.85	31,33,33,33	0
3	IMD	A	503	5/5	0.93	0.18	2.59	23,23,25,25	0
4	BU3	B	504	6/6	0.83	0.17	0.86	27,29,30,31	0
2	HEM	B	501	43/43	0.99	0.09	-0.16	11,13,31,34	0
3	IMD	B	502	5/5	0.97	0.09	-0.29	16,16,17,18	0
2	HEM	A	501	43/43	0.99	0.08	-0.35	13,15,32,36	0
3	IMD	A	502	5/5	0.98	0.06	-1.17	15,15,16,17	0
5	EDO	A	505	4/4	0.74	0.34	-	47,55,56,60	0
5	EDO	B	505	4/4	0.92	0.16	-	29,38,39,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.