



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:43 PM GMT

PDB ID : 1Q90  
Title : Structure of the cytochrome b6f (plastohydroquinone : plastocyanin oxidoreductase) from Chlamydomonas reinhardtii  
Authors : Stroebel, D.; Choquet, Y.; Popot, J.-L.; Picot, D.  
Deposited on : 2003-08-22  
Resolution : 3.10 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

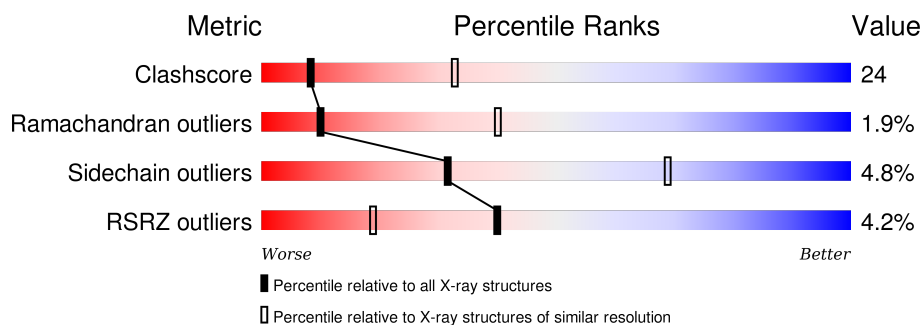
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	292	<div> <div></div> <div>59% 37% .</div> </div>
2	B	215	<div> <div></div> <div>57% 40% ..</div> </div>
3	C	127	<div> <div>24%</div> <div>42% 53% 5% .</div> </div>
4	D	159	<div> <div></div> <div>48% 45% 6% .</div> </div>
5	R	49	<div> <div>6%</div> <div>57% 16% 6% 20%</div> </div>
6	G	37	<div> <div></div> <div>65% 16% 19%</div> </div>
7	L	32	<div> <div></div> <div>53% 34% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
8	M	39	
9	N	31	

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
12	CLA	D	910	X	-	-	-
13	BCR	B	904	-	-	-	X
14	TDS	D	920	-	-	-	X
16	LFA	B	960	-	-	-	X
17	LMG	D	953	-	-	-	X

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 7778 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 Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2266	1457	387	417	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	HIS	-	EXPRESSION TAG	UNP P23577
A	288	HIS	-	EXPRESSION TAG	UNP P23577
A	289	HIS	-	EXPRESSION TAG	UNP P23577
A	290	HIS	-	EXPRESSION TAG	UNP P23577
A	291	HIS	-	EXPRESSION TAG	UNP P23577
A	292	HIS	-	EXPRESSION TAG	UNP P23577

- Molecule 2 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1681	1117	270	281	13			

- Molecule 3 is a protein called Cytochrome B6-F complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	126	Total	C	N	O	S	0	0	0
			955	606	163	181	5			

- Molecule 4 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	156	Total	C	N	O	S	0	0	0
			1201	807	185	204	5			

- Molecule 5 is a protein called Cytochrome B6-F complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	39	Total	C	N	O	S	0	0	0
			283	184	46	51	2			

- Molecule 6 is a protein called Cytochrome b6f complex subunit petG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	30	Total	C	N	O	S	0	0	0
			224	154	31	37	2			

- Molecule 7 is a protein called Cytochrome b6f complex subunit petL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	32	Total	C	N	O	S	0	0	0
			242	168	34	39	1			

- Molecule 8 is a protein called Cytochrome b6f complex subunit PETM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	34	Total	C	N	O	S	0	0	0
			247	162	37	46	2			

- Molecule 9 is a protein called Cytochrome b6f complex subunit PETN.

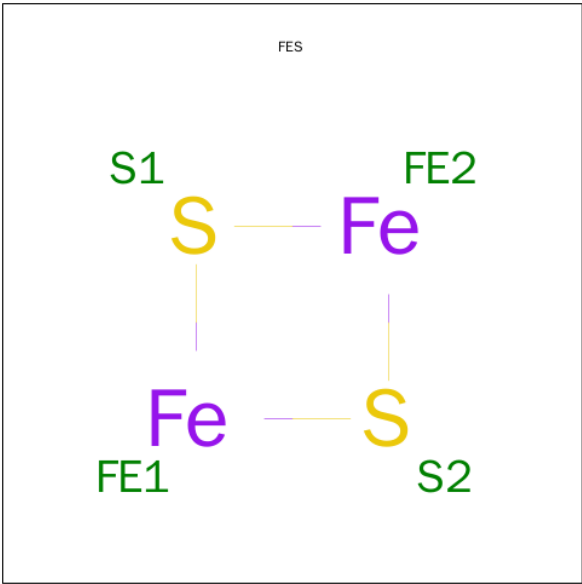
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	31	Total	C	N	O	S	0	0	0
			231	152	37	40	2			

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



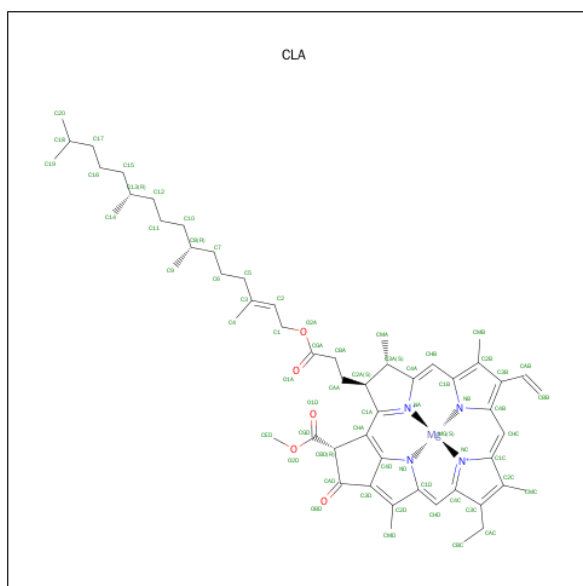
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



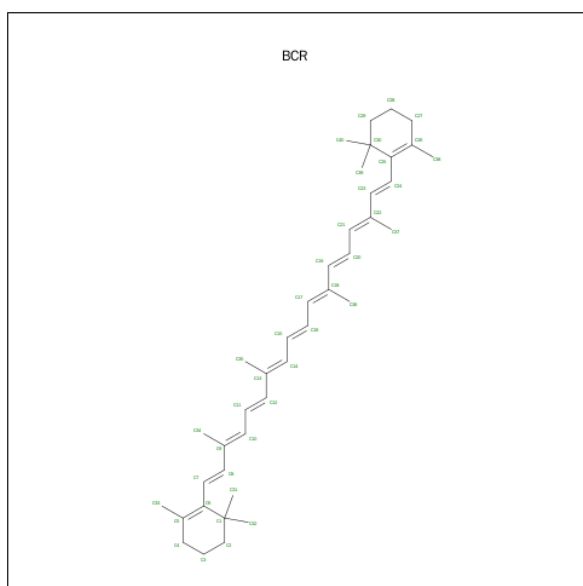
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



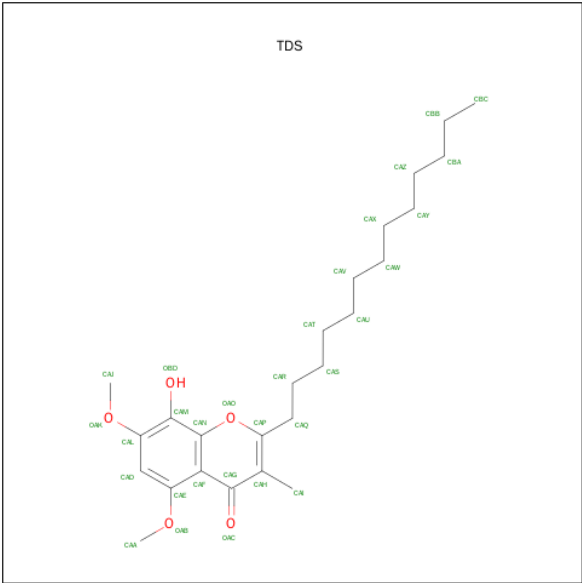
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 13 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



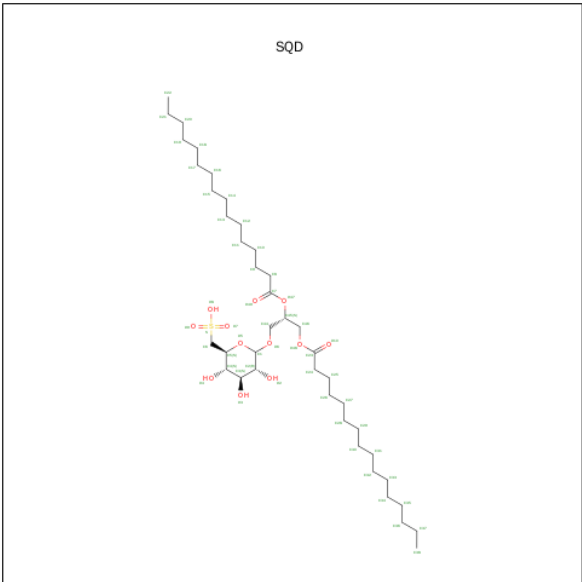
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	C	0	0
			27	27		

- Molecule 14 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROME N-4-ONE (three-letter code: TDS) (formula: C<sub>25</sub>H<sub>38</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	C	O	0	0
			30	25	5		

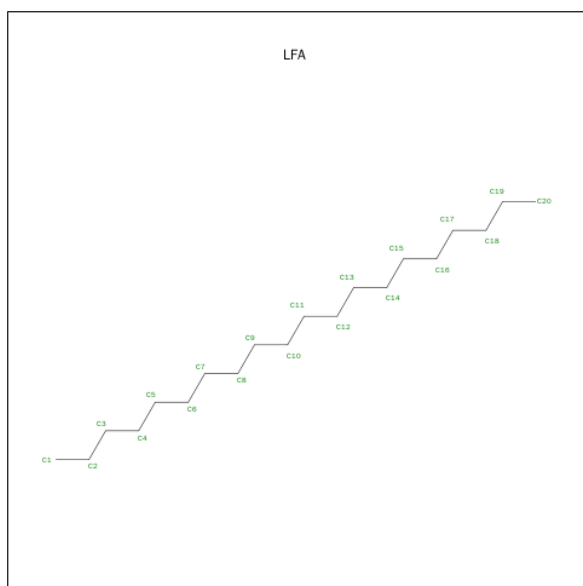
- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).





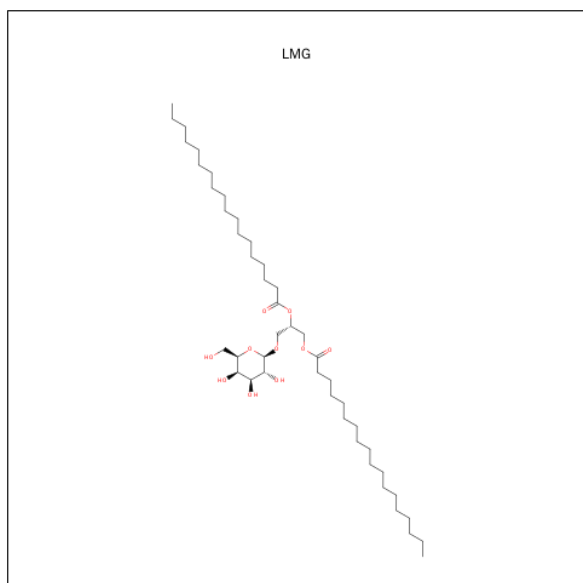
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	R	1	Total	C	O	S	0	0
			33	20	12	1		

- Molecule 16 is EICOSANE (three-letter code: LFA) (formula:  $C_{20}H_{42}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	B	1	Total	C	0	0
			20	20		

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	L	1	Total	C	O	0	0
			42	32	10		
17	D	1	Total	C	O	0	0
			53	43	10		

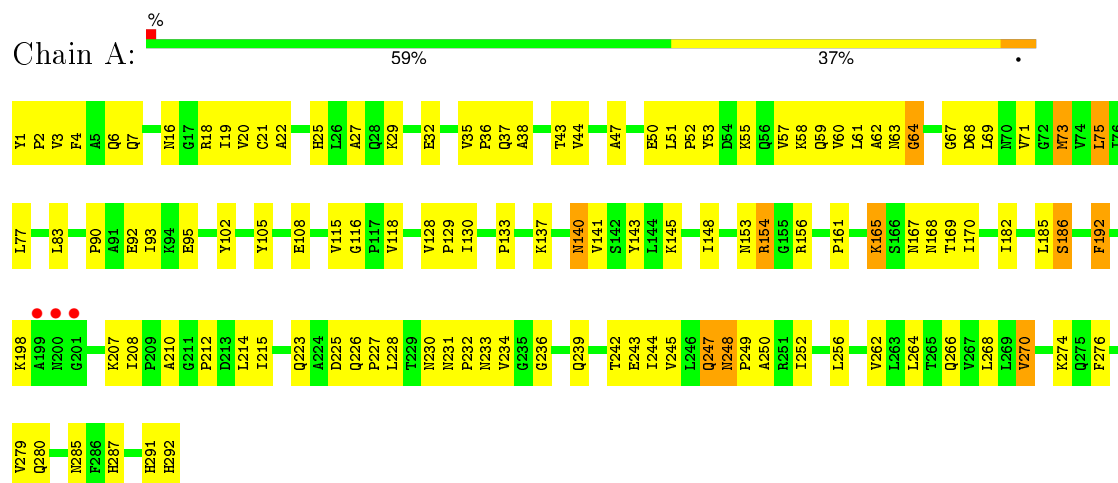
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	B	2	Total	O	0	0
			2	2		

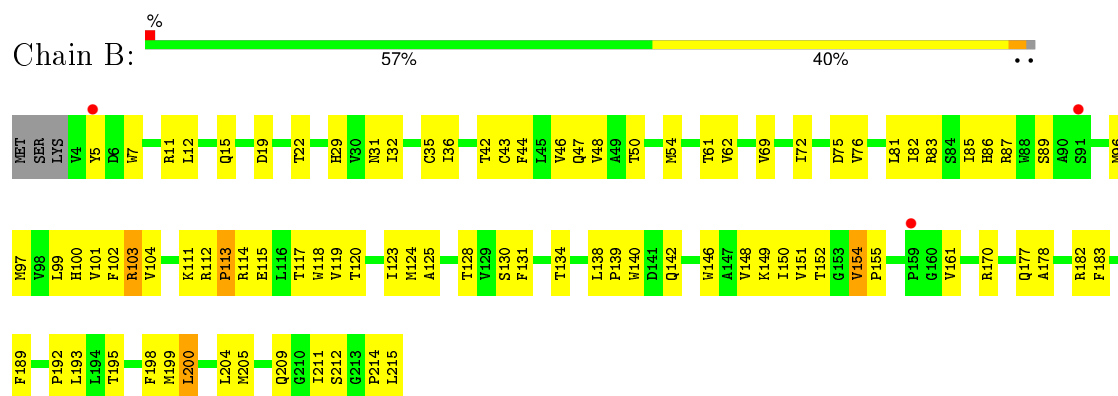
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

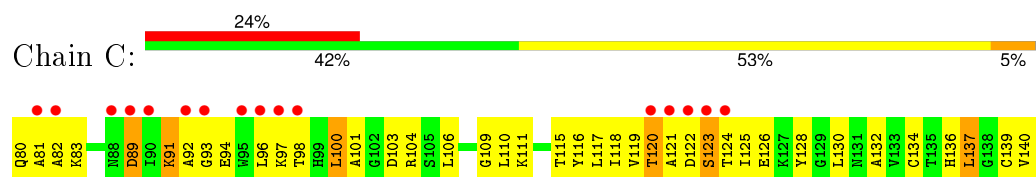
#### • Molecule 1: Apocytochrome f

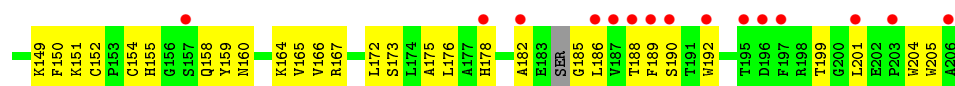


#### • Molecule 2: Cytochrome b6



#### • Molecule 3: Cytochrome B6-F complex iron-sulfur subunit

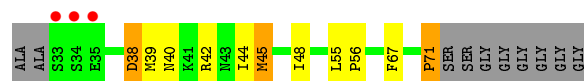




- Molecule 4: Cytochrome b6-f complex subunit 4



- Molecule 5: Cytochrome B6-F complex iron-sulfur subunit



- Molecule 6: Cytochrome b6f complex subunit petG



- Molecule 7: Cytochrome b6f complex subunit petL



- Molecule 8: Cytochrome b6f complex subunit PETM



- Molecule 9: Cytochrome b6f complex subunit PETN



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.45Å 171.21Å 351.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.42 – 3.10 35.14 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.42-3.10) 92.7 (35.14-2.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.29 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.261 0.219 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 77.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	4 of 59045 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.375 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: LFA, CLA, FES, TDS, HEM, LMG, BCR, SQD

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	0.36	0/2318	0.64	0/3148
2	B	0.48	0/1732	0.64	0/2360
3	C	0.29	0/979	0.55	0/1333
4	D	0.38	0/1238	0.62	0/1698
5	R	0.46	0/289	0.94	1/393 (0.3%)
6	G	0.42	0/228	0.60	0/313
7	L	0.39	0/244	0.61	0/329
8	M	0.42	0/248	0.64	0/335
9	N	0.56	0/237	0.57	0/321
All	All	0.40	0/7513	0.63	1/10230 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	71	PRO	CA-N-CD	-13.91	92.03	111.50

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	2266	0	2301	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1681	0	1692	103	0
3	C	955	0	922	67	0
4	D	1201	0	1256	87	0
5	R	283	0	291	13	0
6	G	224	0	248	9	0
7	L	242	0	286	12	0
8	M	247	0	263	19	0
9	N	231	0	230	19	0
10	A	43	0	30	2	0
10	B	129	0	90	5	0
11	C	4	0	0	1	0
12	D	65	0	72	5	0
13	B	27	0	35	3	0
14	D	30	0	38	2	0
15	R	33	0	29	1	0
16	B	20	0	42	2	0
17	D	53	0	79	3	0
17	L	42	0	54	4	0
18	B	2	0	0	0	0
All	All	7778	0	7958	381	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 24.

All (381) 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)
2:B:31:ASN:HA	9:N:98:LEU:HD22	1.24	1.18
3:C:178:HIS:HB2	3:C:190:SER:HB2	1.34	1.10
2:B:50:THR:HG23	2:B:86:HIS:HD1	1.07	1.07
1:A:59:GLN:HE22	1:A:156:ARG:HG3	1.27	1.00
2:B:142:GLN:NE2	4:D:67:ASN:H	1.63	0.96
2:B:50:THR:CG2	2:B:86:HIS:HD1	1.82	0.93
4:D:118:ASN:ND2	4:D:120:PHE:H	1.67	0.93
3:C:92:ALA:H	3:C:185:GLY:HA2	1.33	0.92
3:C:158:GLN:HB2	3:C:167:ARG:HB3	1.49	0.92
2:B:61:THR:HA	2:B:177:GLN:HE22	1.36	0.91
1:A:247:GLN:HE21	1:A:248:ASN:H	1.20	0.89
1:A:116:GLY:HA2	1:A:118:VAL:HG13	1.55	0.88
2:B:47:GLN:NE2	2:B:89:SER:HB3	1.91	0.86
2:B:124:MET:HE2	10:B:901:HEM:HBB2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:THR:HG23	2:B:86:HIS:ND1	1.90	0.85
1:A:92:GLU:CD	1:A:92:GLU:H	1.83	0.82
4:D:118:ASN:HD22	4:D:119:LYS:N	1.77	0.82
1:A:248:ASN:C	1:A:248:ASN:HD22	1.83	0.82
2:B:152:THR:HG23	2:B:170:ARG:HE	1.43	0.81
2:B:124:MET:HE1	2:B:199:MET:HG3	1.61	0.81
4:D:117:ILE:HD12	4:D:118:ASN:H	1.47	0.80
4:D:117:ILE:HD12	4:D:118:ASN:N	1.97	0.79
2:B:31:ASN:HA	9:N:98:LEU:CD2	2.09	0.77
1:A:247:GLN:HE21	1:A:248:ASN:N	1.84	0.76
3:C:143:TRP:HE1	3:C:145:ALA:HB2	1.50	0.76
2:B:214:PRO:O	2:B:215:LEU:HB2	1.86	0.75
1:A:59:GLN:OE1	1:A:69:LEU:HG	1.87	0.75
2:B:32:ILE:N	9:N:98:LEU:HD13	2.01	0.75
2:B:119:VAL:HG13	4:D:109:ILE:HD11	1.69	0.75
1:A:73:MET:HG3	1:A:115:VAL:HG12	1.69	0.74
1:A:280:GLN:HE22	4:D:34:ASN:HD21	1.36	0.74
2:B:215:LEU:CD1	4:D:122:ASN:HD22	2.01	0.73
4:D:106:ALA:O	4:D:109:ILE:HG22	1.89	0.73
3:C:106:LEU:HD12	3:C:106:LEU:H	1.54	0.73
1:A:90:PRO:HD2	1:A:93:ILE:HD12	1.71	0.73
1:A:247:GLN:NE2	1:A:248:ASN:H	1.89	0.71
8:M:92:SER:O	8:M:95:GLU:HB3	1.91	0.70
2:B:31:ASN:CA	9:N:98:LEU:HD22	2.14	0.70
1:A:3:VAL:O	1:A:7:GLN:HG3	1.90	0.69
3:C:182:ALA:O	3:C:186:LEU:HD12	1.93	0.69
4:D:81:PHE:HE2	12:D:910:CLA:H52	1.57	0.69
3:C:134:CYS:HB2	3:C:141:VAL:HG23	1.74	0.69
4:D:4:THR:HG22	4:D:5:LYS:H	1.56	0.69
2:B:47:GLN:HE21	2:B:89:SER:HB3	1.56	0.68
4:D:118:ASN:HD22	4:D:118:ASN:C	1.95	0.68
3:C:92:ALA:N	3:C:185:GLY:HA2	2.09	0.68
1:A:143:TYR:CE2	1:A:248:ASN:HB2	2.28	0.68
4:D:137:THR:HA	17:D:953:LMG:H242	1.76	0.68
1:A:60:VAL:HG12	1:A:167:ASN:ND2	2.10	0.68
2:B:152:THR:CG2	2:B:170:ARG:HE	2.07	0.68
1:A:59:GLN:HE22	1:A:156:ARG:CG	2.05	0.67
2:B:124:MET:CE	2:B:199:MET:HG3	2.23	0.67
2:B:113:PRO:HB2	2:B:209:GLN:HE22	1.59	0.67
2:B:215:LEU:HD12	4:D:122:ASN:HD22	1.59	0.67
7:L:21:ILE:O	7:L:25:LEU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:LEU:HG	4:D:125:ARG:HH12	1.60	0.66
1:A:27:ALA:HB3	1:A:236:GLY:HA2	1.76	0.66
1:A:53:TYR:HB3	1:A:154:ARG:HD2	1.77	0.66
1:A:27:ALA:HB2	1:A:233:ASN:ND2	2.10	0.66
2:B:154:VAL:HB	2:B:155:PRO:HD3	1.77	0.65
3:C:118:ILE:HD12	3:C:118:ILE:H	1.61	0.65
4:D:30:PRO:HG2	4:D:34:ASN:ND2	2.12	0.64
2:B:81:LEU:O	2:B:85:ILE:HG13	1.97	0.64
7:L:4:ILE:O	7:L:4:ILE:HD13	1.96	0.64
3:C:143:TRP:NE1	3:C:145:ALA:HB2	2.13	0.64
2:B:113:PRO:HB2	2:B:209:GLN:NE2	2.13	0.64
1:A:266:GLN:O	1:A:270:VAL:HG12	1.98	0.63
3:C:104:ARG:HD2	3:C:143:TRP:CE2	2.34	0.63
5:R:44:ILE:CG2	7:L:31:LEU:HD21	2.28	0.63
1:A:27:ALA:HB2	1:A:233:ASN:HD21	1.63	0.63
1:A:71:VAL:HG12	1:A:154:ARG:HB3	1.80	0.63
4:D:104:VAL:HB	4:D:105:PRO:CD	2.30	0.62
1:A:71:VAL:HG12	1:A:154:ARG:CB	2.29	0.62
3:C:104:ARG:HD2	3:C:143:TRP:CD2	2.35	0.61
3:C:103:ASP:HB3	3:C:119:VAL:CG2	2.30	0.61
4:D:85:PHE:HD2	4:D:147:SER:HB2	1.66	0.60
4:D:4:THR:HG22	4:D:5:LYS:N	2.15	0.60
4:D:95:LEU:HG	4:D:99:LEU:CD2	2.31	0.60
4:D:95:LEU:HG	4:D:99:LEU:HD23	1.84	0.60
2:B:36:ILE:HG22	2:B:100:HIS:HB2	1.84	0.60
3:C:172:LEU:HD13	3:C:204:TRP:CG	2.36	0.60
9:N:72:ILE:HG23	9:N:73:VAL:N	2.17	0.60
4:D:128:ILE:O	4:D:132:LEU:HD23	2.01	0.59
3:C:141:VAL:HG22	3:C:152:CYS:HB2	1.83	0.59
2:B:215:LEU:CG	4:D:125:ARG:HH12	2.15	0.59
3:C:83:LYS:HA	3:C:89:ASP:HA	1.85	0.59
1:A:36:PRO:O	1:A:244:ILE:HD12	2.02	0.59
1:A:143:TYR:CD2	1:A:248:ASN:HB2	2.37	0.59
8:M:89:ARG:HH21	8:M:93:LEU:HD21	1.68	0.59
1:A:60:VAL:HG12	1:A:167:ASN:HD22	1.66	0.59
2:B:151:VAL:HG13	14:D:920:TDS:HAT1	1.84	0.58
3:C:116:TYR:OH	3:C:142:PRO:HA	2.03	0.58
1:A:248:ASN:C	1:A:248:ASN:ND2	2.53	0.58
4:D:158:GLY:O	4:D:159:LEU:HD23	2.04	0.58
4:D:12:PRO:HA	4:D:15:LYS:HE3	1.85	0.58
2:B:150:ILE:HD11	3:C:139:CYS:SG	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:951:LMG:H112	8:M:69:THR:HG23	1.85	0.58
4:D:150:PRO:HD2	4:D:153:ILE:HD11	1.85	0.57
2:B:11:ARG:O	2:B:12:LEU:HD23	2.04	0.57
2:B:154:VAL:HA	3:C:137:LEU:HD11	1.85	0.57
4:D:88:LEU:HD22	14:D:920:TDS:HAI1	1.85	0.57
4:D:4:THR:HA	4:D:29:GLU:OE2	2.03	0.57
1:A:92:GLU:O	1:A:95:GLU:HB2	2.05	0.57
3:C:110:LEU:O	3:C:111:LYS:HB2	2.04	0.57
3:C:93:GLY:O	3:C:97:LYS:HG3	2.05	0.57
3:C:109:GLY:HA3	3:C:115:THR:OG1	2.05	0.57
1:A:145:LYS:HD2	4:D:61:ALA:HB2	1.85	0.57
17:D:953:LMG:H292	8:M:66:ILE:HD11	1.87	0.57
1:A:285:ASN:OD1	1:A:287:HIS:HB2	2.04	0.57
2:B:15:GLN:HA	2:B:15:GLN:OE1	2.05	0.56
2:B:102:PHE:HE1	6:G:14:VAL:HG13	1.70	0.56
2:B:47:GLN:HE21	2:B:89:SER:CB	2.17	0.56
3:C:136:HIS:NE2	3:C:137:LEU:HD22	2.20	0.56
2:B:120:THR:HG21	2:B:205:MET:CE	2.35	0.56
3:C:92:ALA:H	3:C:185:GLY:CA	2.13	0.55
3:C:100:LEU:O	3:C:119:VAL:HG11	2.06	0.55
4:D:108:LEU:O	4:D:111:VAL:HG23	2.07	0.55
2:B:103:ARG:HA	6:G:21:LEU:HD11	1.88	0.55
4:D:93:ASN:HB2	4:D:96:LEU:HB3	1.87	0.55
4:D:16:ALA:O	4:D:19:ALA:HB3	2.07	0.55
2:B:32:ILE:CA	9:N:98:LEU:HD13	2.36	0.54
2:B:152:THR:HG23	2:B:170:ARG:NE	2.17	0.54
3:C:120:THR:HG22	3:C:121:ALA:N	2.23	0.54
2:B:142:GLN:HE21	4:D:66:ALA:HA	1.73	0.54
6:G:13:LEU:HA	6:G:16:VAL:HG12	1.88	0.54
1:A:2:PRO:HG3	10:A:900:HEM:CMB	2.37	0.54
1:A:63:ASN:OD1	1:A:64:GLY:N	2.39	0.54
2:B:211:ILE:HG23	2:B:212:SER:O	2.07	0.53
3:C:118:ILE:HD12	3:C:118:ILE:N	2.22	0.53
1:A:291:HIS:O	1:A:292:HIS:HB2	2.08	0.53
4:D:91:VAL:HG11	4:D:96:LEU:HD12	1.90	0.53
9:N:95:ARG:HE	9:N:98:LEU:HD11	1.72	0.53
2:B:5:TYR:OH	2:B:15:GLN:HG2	2.08	0.53
3:C:82:ALA:HB2	3:C:189:PHE:CD2	2.43	0.53
1:A:16:ASN:HD22	4:D:73:LEU:HD21	1.73	0.53
5:R:40:ASN:O	5:R:44:ILE:HG12	2.09	0.53
2:B:47:GLN:NE2	2:B:89:SER:CB	2.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:SER:O	3:C:204:TRP:HZ2	1.91	0.53
3:C:106:LEU:HD12	3:C:106:LEU:N	2.22	0.53
1:A:1:TYR:H3	1:A:4:PHE:HD2	1.57	0.53
2:B:72:ILE:HA	2:B:76:VAL:CG2	2.39	0.53
1:A:61:LEU:HD11	1:A:67:GLY:HA3	1.90	0.53
2:B:214:PRO:HD2	4:D:24:HIS:CE1	2.43	0.53
1:A:192:PHE:CD1	1:A:192:PHE:N	2.76	0.53
4:D:100:LEU:O	4:D:103:ALA:HB3	2.09	0.53
1:A:248:ASN:HD22	1:A:249:PRO:N	2.07	0.52
2:B:104:VAL:HG11	10:B:901:HEM:HMD2	1.91	0.52
3:C:172:LEU:HD13	3:C:204:TRP:CD2	2.43	0.52
5:R:45:MET:HE2	5:R:45:MET:HA	1.91	0.52
1:A:59:GLN:NE2	1:A:156:ARG:HG3	2.09	0.52
1:A:268:LEU:HD13	5:R:48:ILE:HG22	1.90	0.52
1:A:248:ASN:ND2	1:A:250:ALA:H	2.08	0.52
3:C:143:TRP:HB2	3:C:150:PHE:CE1	2.45	0.52
4:D:108:LEU:C	4:D:110:THR:H	2.12	0.52
4:D:124:TYR:HE1	6:G:26:TYR:CA	2.23	0.52
1:A:44:VAL:HA	1:A:130:ILE:O	2.09	0.52
2:B:215:LEU:HD13	4:D:122:ASN:HD22	1.74	0.52
4:D:11:ASP:OD1	4:D:13:VAL:N	2.43	0.52
2:B:42:THR:O	2:B:46:VAL:HG23	2.09	0.52
8:M:73:MET:HA	8:M:76:MET:HE3	1.92	0.52
3:C:101:ALA:HA	3:C:119:VAL:CG1	2.40	0.51
3:C:103:ASP:O	3:C:118:ILE:HA	2.10	0.51
1:A:32:GLU:HB2	1:A:50:GLU:HB2	1.92	0.51
4:D:85:PHE:CD2	4:D:147:SER:HB2	2.44	0.51
8:M:86:VAL:O	8:M:90:VAL:HG23	2.11	0.51
7:L:24:GLY:O	7:L:28:VAL:HB	2.08	0.51
2:B:31:ASN:C	9:N:98:LEU:HD13	2.30	0.51
4:D:118:ASN:HD21	4:D:120:PHE:HD1	1.57	0.51
3:C:192:TRP:HB3	3:C:205:TRP:HE1	1.75	0.51
5:R:45:MET:CE	5:R:45:MET:HA	2.40	0.50
1:A:51:LEU:HD12	1:A:51:LEU:N	2.26	0.50
2:B:130:SER:HA	12:D:910:CLA:H143	1.92	0.50
4:D:75:ILE:HG23	4:D:75:ILE:O	2.12	0.50
5:R:55:LEU:HB2	5:R:56:PRO:CD	2.42	0.50
2:B:44:PHE:O	2:B:48:VAL:HG23	2.12	0.50
3:C:116:TYR:HH	3:C:142:PRO:HA	1.76	0.50
4:D:110:THR:HG22	4:D:114:ILE:HG12	1.93	0.50
2:B:149:LYS:O	2:B:152:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:GLU:HG3	3:C:128:TYR:H	1.77	0.50
1:A:182:ILE:HG21	1:A:214:LEU:HD13	1.92	0.49
1:A:223:GLN:O	1:A:226:GLN:HB2	2.12	0.49
1:A:21:CYS:O	1:A:25:HIS:HB2	2.13	0.49
3:C:155:HIS:HB2	11:C:210:FES:S1	2.52	0.49
2:B:72:ILE:HA	2:B:76:VAL:HG23	1.92	0.49
8:M:90:VAL:O	8:M:94:VAL:HG23	2.12	0.49
8:M:94:VAL:O	8:M:94:VAL:HG12	2.11	0.49
2:B:142:GLN:NE2	4:D:67:ASN:N	2.46	0.49
8:M:93:LEU:C	8:M:95:GLU:H	2.14	0.49
12:D:910:CLA:HBB1	12:D:910:CLA:HHC	1.93	0.49
2:B:103:ARG:NH1	10:B:901:HEM:O1A	2.46	0.49
1:A:37:GLN:HB2	17:L:951:LMG:HC4	1.94	0.49
4:D:118:ASN:ND2	4:D:118:ASN:C	2.63	0.49
2:B:142:GLN:HE21	4:D:67:ASN:H	1.57	0.49
4:D:137:THR:HA	17:D:953:LMG:C24	2.43	0.49
1:A:108:GLU:N	1:A:108:GLU:OE2	2.45	0.49
2:B:215:LEU:CD1	4:D:125:ARG:HH12	2.26	0.48
4:D:107:GLY:O	4:D:110:THR:HB	2.12	0.48
2:B:120:THR:HG21	2:B:205:MET:HE2	1.93	0.48
4:D:124:TYR:CE1	6:G:26:TYR:HA	2.48	0.48
4:D:81:PHE:CE2	12:D:910:CLA:H52	2.43	0.48
3:C:96:LEU:HD11	3:C:124:THR:HA	1.96	0.48
1:A:274:LYS:HE3	9:N:93:TRP:NE1	2.29	0.48
3:C:81:ALA:HA	3:C:188:THR:HG22	1.95	0.48
3:C:199:THR:C	3:C:201:LEU:H	2.17	0.48
2:B:61:THR:HA	2:B:177:GLN:NE2	2.17	0.48
3:C:160:ASN:HD21	3:C:164:LYS:HB3	1.79	0.48
2:B:7:TRP:CZ2	2:B:11:ARG:NH1	2.81	0.48
1:A:16:ASN:HD22	4:D:73:LEU:CD2	2.27	0.48
8:M:73:MET:SD	8:M:76:MET:HE1	2.53	0.48
3:C:175:ALA:HA	3:C:205:TRP:CE3	2.48	0.48
2:B:112:ARG:HA	2:B:115:GLU:OE2	2.14	0.48
1:A:2:PRO:HG3	10:A:900:HEM:HMB2	1.95	0.48
1:A:226:GLN:CG	1:A:227:PRO:HD2	2.44	0.48
13:B:904:BCR:H15C	8:M:81:LEU:HD11	1.96	0.47
2:B:103:ARG:HA	6:G:21:LEU:CD1	2.44	0.47
1:A:208:ILE:HD12	1:A:214:LEU:HD21	1.96	0.47
2:B:113:PRO:HA	2:B:115:GLU:OE2	2.14	0.47
1:A:53:TYR:CZ	1:A:55:LYS:HG2	2.49	0.47
2:B:62:VAL:HG13	2:B:140:TRP:NE1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:89:ARG:NH2	8:M:93:LEU:HD21	2.29	0.47
1:A:153:ASN:CG	1:A:154:ARG:N	2.66	0.47
7:L:1:MET:O	7:L:4:ILE:HG22	2.15	0.47
8:M:93:LEU:C	8:M:95:GLU:N	2.67	0.47
2:B:47:GLN:HA	2:B:50:THR:HG22	1.97	0.47
8:M:92:SER:O	8:M:95:GLU:CB	2.61	0.47
1:A:18:ARG:HB2	4:D:73:LEU:HD11	1.96	0.47
1:A:102:TYR:CZ	1:A:128:VAL:HG22	2.50	0.47
2:B:47:GLN:HE22	2:B:89:SER:HB3	1.75	0.46
1:A:133:PRO:CG	1:A:141:VAL:HG11	2.46	0.46
1:A:170:ILE:HD11	1:A:231:ASN:HB2	1.98	0.46
1:A:1:TYR:O	1:A:4:PHE:HB2	2.15	0.46
2:B:54:MET:CE	2:B:83:ARG:HB2	2.46	0.46
3:C:151:LYS:HG2	3:C:158:GLN:HG2	1.97	0.46
1:A:83:LEU:HD12	1:A:129:PRO:O	2.15	0.46
9:N:69:GLU:N	9:N:69:GLU:OE1	2.42	0.46
1:A:262:VAL:HG13	4:D:45:LEU:HB3	1.97	0.46
2:B:82:ILE:HG13	5:R:67:PHE:CD1	2.50	0.46
1:A:83:LEU:HD22	1:A:102:TYR:HB2	1.97	0.46
3:C:122:ASP:O	3:C:123:SER:C	2.52	0.46
2:B:142:GLN:HA	2:B:142:GLN:HE21	1.80	0.46
1:A:52:PRO:O	1:A:154:ARG:NH1	2.48	0.46
2:B:150:ILE:HD11	3:C:154:CYS:SG	2.56	0.46
6:G:14:VAL:HB	6:G:15:PRO:CD	2.46	0.46
3:C:103:ASP:H	3:C:119:VAL:HB	1.81	0.46
8:M:62:GLU:O	8:M:65:PHE:HB3	2.16	0.46
3:C:125:ILE:HD12	3:C:125:ILE:N	2.31	0.46
2:B:114:ARG:CZ	2:B:212:SER:HA	2.46	0.46
3:C:141:VAL:CG1	3:C:150:PHE:HB3	2.46	0.45
1:A:16:ASN:ND2	4:D:73:LEU:HD21	2.32	0.45
1:A:57:VAL:HG12	1:A:58:LYS:N	2.31	0.45
8:M:93:LEU:O	8:M:95:GLU:N	2.49	0.45
5:R:45:MET:HE3	5:R:48:ILE:HD12	1.99	0.45
1:A:60:VAL:CG1	1:A:167:ASN:HD22	2.27	0.45
4:D:14:LEU:CD1	4:D:18:LEU:HD13	2.47	0.45
1:A:279:VAL:HG21	5:R:42:ARG:HD3	1.98	0.45
9:N:72:ILE:CG2	9:N:73:VAL:N	2.79	0.45
1:A:170:ILE:HG12	1:A:230:ASN:O	2.16	0.45
2:B:200:LEU:HD22	2:B:204:LEU:HG	1.99	0.45
4:D:40:PHE:HB2	4:D:41:PRO:HD3	1.99	0.45
2:B:123:ILE:HD13	2:B:198:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:MET:SD	17:L:951:LMG:H232	2.56	0.45
1:A:226:GLN:HG3	1:A:227:PRO:HD2	1.99	0.45
2:B:142:GLN:HA	2:B:142:GLN:NE2	2.32	0.45
1:A:77:LEU:HD23	1:A:148:ILE:HG23	1.99	0.45
7:L:26:LEU:O	7:L:30:LYS:HA	2.17	0.45
3:C:91:LYS:HB2	3:C:94:GLU:HB2	1.99	0.45
2:B:29:HIS:CG	2:B:214:PRO:HA	2.52	0.45
8:M:72:THR:HG22	8:M:76:MET:HE2	1.99	0.45
3:C:164:LYS:O	3:C:166:VAL:HG23	2.17	0.45
7:L:29:VAL:HG12	7:L:29:VAL:O	2.17	0.45
2:B:69:VAL:HG21	2:B:139:PRO:HB3	1.99	0.45
4:D:84:VAL:HG11	4:D:101:MET:SD	2.57	0.45
4:D:82:TYR:HB2	4:D:83:PRO:HD3	1.99	0.45
1:A:156:ARG:HH12	1:A:167:ASN:ND2	2.15	0.44
1:A:29:LYS:HG3	1:A:236:GLY:HA3	1.99	0.44
1:A:274:LYS:HE3	9:N:93:TRP:CE2	2.52	0.44
2:B:148:VAL:O	2:B:152:THR:HG22	2.17	0.44
8:M:89:ARG:O	8:M:92:SER:HB3	2.18	0.44
2:B:81:LEU:CD2	16:B:960:LFA:H121	2.48	0.44
16:B:960:LFA:H101	4:D:52:ILE:HD13	1.99	0.44
2:B:54:MET:HE1	2:B:83:ARG:HB2	1.99	0.44
1:A:6:GLN:HE21	1:A:105:TYR:HA	1.82	0.44
6:G:13:LEU:HA	6:G:16:VAL:CG1	2.47	0.44
1:A:20:VAL:C	1:A:22:ALA:N	2.70	0.44
3:C:141:VAL:HG22	3:C:152:CYS:CB	2.46	0.44
5:R:45:MET:HE2	5:R:48:ILE:HB	1.99	0.44
1:A:232:PRO:O	1:A:234:VAL:HG13	2.18	0.44
5:R:39:MET:O	5:R:42:ARG:HB2	2.17	0.44
4:D:38:TYR:O	4:D:41:PRO:HD2	2.18	0.44
13:B:904:BCR:HC41	4:D:43:VAL:HG13	2.00	0.43
2:B:102:PHE:CE1	6:G:14:VAL:HG13	2.53	0.43
1:A:247:GLN:HE21	1:A:247:GLN:CA	2.30	0.43
2:B:97:MET:SD	2:B:125:ALA:HA	2.58	0.43
3:C:130:LEU:HD23	3:C:176:LEU:HD23	2.00	0.43
7:L:1:MET:O	7:L:2:LEU:C	2.57	0.43
1:A:133:PRO:HG2	1:A:141:VAL:HG11	2.00	0.43
4:D:118:ASN:ND2	4:D:120:PHE:CD1	2.82	0.43
4:D:104:VAL:HG11	12:D:910:CLA:H42	2.01	0.43
1:A:287:HIS:ND1	1:A:292:HIS:CD2	2.87	0.43
1:A:210:ALA:O	1:A:212:PRO:HD2	2.19	0.43
3:C:119:VAL:HA	3:C:124:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:LYS:HB2	3:C:159:TYR:O	2.19	0.42
1:A:145:LYS:HD3	1:A:243:GLU:CD	2.40	0.42
2:B:118:TRP:HZ2	4:D:108:LEU:HD22	1.83	0.42
2:B:178:ALA:O	2:B:182:ARG:HG3	2.18	0.42
1:A:19:ILE:N	1:A:239:GLN:OE1	2.35	0.42
4:D:118:ASN:HD22	4:D:120:PHE:H	1.58	0.42
4:D:87:ILE:O	4:D:90:VAL:HG12	2.19	0.42
4:D:25:ASN:HD22	4:D:25:ASN:N	2.17	0.42
2:B:101:VAL:HG22	10:B:901:HEM:HBC2	2.01	0.42
2:B:152:THR:CG2	2:B:170:ARG:NE	2.79	0.42
4:D:104:VAL:CB	4:D:105:PRO:CD	2.97	0.42
2:B:152:THR:HG23	2:B:170:ARG:HH21	1.85	0.42
2:B:118:TRP:CZ2	4:D:108:LEU:HD22	2.55	0.42
7:L:3:THR:HG22	9:N:74:GLN:NE2	2.34	0.42
2:B:32:ILE:HD11	13:B:904:BCR:H333	2.00	0.42
9:N:97:GLY:O	9:N:98:LEU:HB2	2.20	0.42
3:C:134:CYS:HB2	3:C:141:VAL:CG2	2.48	0.42
2:B:215:LEU:HD12	4:D:125:ARG:NH1	2.34	0.42
3:C:91:LYS:N	3:C:91:LYS:HD2	2.35	0.42
2:B:211:ILE:HG13	2:B:212:SER:N	2.35	0.42
4:D:8:ASP:C	4:D:10:SER:H	2.23	0.42
1:A:256:LEU:HA	1:A:256:LEU:HD23	1.89	0.42
4:D:96:LEU:HD13	4:D:96:LEU:C	2.40	0.42
1:A:4:PHE:CD1	1:A:161:PRO:HG2	2.55	0.42
3:C:141:VAL:HG12	3:C:150:PHE:HB3	2.01	0.42
3:C:117:LEU:HD13	3:C:189:PHE:HZ	1.84	0.42
1:A:215:ILE:HG13	1:A:228:LEU:O	2.20	0.42
1:A:35:VAL:HG12	1:A:47:ALA:HA	2.02	0.42
2:B:138:LEU:HA	2:B:138:LEU:HD23	1.81	0.42
2:B:195:THR:O	2:B:199:MET:HB2	2.19	0.41
3:C:80:GLN:O	3:C:188:THR:HB	2.19	0.41
1:A:210:ALA:C	1:A:212:PRO:HD2	2.39	0.41
7:L:11:LEU:HD13	8:M:83:ILE:HD11	2.02	0.41
1:A:38:ALA:HB2	1:A:245:VAL:HB	2.02	0.41
3:C:132:ALA:HB1	3:C:140:VAL:HG13	2.02	0.41
1:A:62:ALA:HA	1:A:156:ARG:NH2	2.35	0.41
4:D:24:HIS:HA	4:D:27:TYR:CE2	2.55	0.41
3:C:136:HIS:HE1	3:C:155:HIS:CG	2.37	0.41
3:C:103:ASP:HB3	3:C:119:VAL:HG23	2.01	0.41
2:B:120:THR:HG21	2:B:205:MET:HE1	2.02	0.41
2:B:146:TRP:HH2	3:C:140:VAL:HG23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:86:PHE:O	9:N:89:SER:HB2	2.19	0.41
1:A:43:THR:HG22	1:A:44:VAL:N	2.36	0.41
1:A:276:PHE:HE1	5:R:42:ARG:NH1	2.17	0.41
1:A:75:LEU:HD21	1:A:148:ILE:CG2	2.51	0.41
1:A:148:ILE:HB	1:A:242:THR:HG23	2.02	0.41
9:N:97:GLY:O	9:N:98:LEU:CB	2.68	0.41
4:D:11:ASP:OD1	4:D:13:VAL:HG23	2.21	0.41
2:B:43:CYS:O	2:B:47:GLN:HG2	2.21	0.41
1:A:215:ILE:HD11	1:A:227:PRO:O	2.21	0.41
3:C:165:VAL:O	3:C:165:VAL:HG13	2.21	0.41
2:B:134:THR:HG22	2:B:183:PHE:CD2	2.56	0.41
4:D:126:ARG:N	4:D:127:PRO:HD3	2.36	0.41
1:A:185:LEU:O	1:A:186:SER:C	2.59	0.41
4:D:135:LEU:O	4:D:139:VAL:HG23	2.21	0.41
3:C:106:LEU:H	3:C:106:LEU:CD1	2.30	0.41
4:D:25:ASN:ND2	4:D:25:ASN:H	2.18	0.41
4:D:37:LEU:HD11	15:R:950:SQD:H261	2.03	0.41
3:C:178:HIS:CB	3:C:190:SER:HB2	2.25	0.41
1:A:61:LEU:O	1:A:167:ASN:ND2	2.54	0.41
2:B:111:LYS:O	2:B:113:PRO:O	2.38	0.41
2:B:114:ARG:O	2:B:117:THR:HB	2.21	0.41
4:D:91:VAL:CG1	4:D:96:LEU:HD12	2.51	0.41
1:A:223:GLN:O	1:A:226:GLN:CB	2.68	0.41
9:N:69:GLU:HB3	9:N:70:PRO:HD2	2.02	0.41
4:D:90:VAL:HG21	4:D:155:LEU:HG	2.02	0.41
7:L:18:THR:HG1	9:N:86:PHE:HZ	1.64	0.41
2:B:35:CYS:HA	10:B:903:HEM:C3B	2.56	0.41
2:B:128:THR:O	2:B:131:PHE:HB2	2.21	0.41
2:B:113:PRO:HB2	2:B:114:ARG:H	1.68	0.41
5:R:38:ASP:O	5:R:39:MET:C	2.59	0.41
4:D:4:THR:CG2	4:D:5:LYS:N	2.83	0.40
4:D:47:THR:HG23	17:L:951:LMG:C25	2.50	0.40
2:B:99:LEU:O	2:B:102:PHE:HB2	2.21	0.40
4:D:98:VAL:O	4:D:101:MET:HB3	2.21	0.40
7:L:32:ILE:O	7:L:32:ILE:HG22	2.20	0.40
1:A:165:LYS:HB3	1:A:169:THR:HG21	2.04	0.40
4:D:89:ARG:NH2	4:D:151:ILE:HG12	2.35	0.40
1:A:252:ILE:HD13	9:N:73:VAL:HA	2.02	0.40
2:B:189:PHE:C	2:B:192:PRO:HD2	2.42	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	290/292 (99%)	263 (91%)	21 (7%)	6 (2%)	9	37
2	B	210/215 (98%)	179 (85%)	29 (14%)	2 (1%)	19	58
3	C	122/127 (96%)	96 (79%)	22 (18%)	4 (3%)	5	26
4	D	154/159 (97%)	134 (87%)	15 (10%)	5 (3%)	5	26
5	R	37/49 (76%)	32 (86%)	5 (14%)	0	100	100
6	G	28/37 (76%)	24 (86%)	4 (14%)	0	100	100
7	L	30/32 (94%)	25 (83%)	5 (17%)	0	100	100
8	M	32/39 (82%)	31 (97%)	0	1 (3%)	5	27
9	N	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	932/981 (95%)	811 (87%)	103 (11%)	18 (2%)	10	40

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	89	ASP
1	A	140	ASN
1	A	165	LYS
1	A	198	LYS
3	C	100	LEU
4	D	104	VAL
1	A	186	SER
2	B	113	PRO
3	C	120	THR
4	D	109	ILE
4	D	114	ILE
1	A	137	LYS
2	B	154	VAL
3	C	123	SER
1	A	64	GLY
4	D	92	PRO

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Mol	Chain	Res	Type
8	M	94	VAL
4	D	151	ILE

### 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	246/246 (100%)	233 (95%)	13 (5%)	28	64
2	B	179/182 (98%)	171 (96%)	8 (4%)	34	70
3	C	99/100 (99%)	96 (97%)	3 (3%)	48	81
4	D	131/134 (98%)	126 (96%)	5 (4%)	40	76
5	R	30/32 (94%)	27 (90%)	3 (10%)	9	34
6	G	25/30 (83%)	25 (100%)	0	100	100
7	L	27/27 (100%)	23 (85%)	4 (15%)	4	16
8	M	26/29 (90%)	24 (92%)	2 (8%)	16	50
9	N	24/24 (100%)	24 (100%)	0	100	100
All	All	787/804 (98%)	749 (95%)	38 (5%)	31	69

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	73	MET
1	A	75	LEU
1	A	140	ASN
1	A	154	ARG
1	A	168	ASN
1	A	192	PHE
1	A	207	LYS
1	A	225	ASP
1	A	247	GLN
1	A	248	ASN
1	A	264	LEU

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Mol	Chain	Res	Type
1	A	270	VAL
2	B	19	ASP
2	B	22	THR
2	B	75	ASP
2	B	87	ARG
2	B	103	ARG
2	B	161	VAL
2	B	193	LEU
2	B	200	LEU
3	C	91	LYS
3	C	98	THR
3	C	137	LEU
4	D	18	LEU
4	D	25	ASN
4	D	90	VAL
4	D	108	LEU
4	D	118	ASN
5	R	38	ASP
5	R	45	MET
5	R	71	PRO
7	L	2	LEU
7	L	3	THR
7	L	4	ILE
7	L	11	LEU
8	M	62	GLU
8	M	66	ILE

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	23	ASN
1	A	28	GLN
1	A	59	GLN
1	A	70	ASN
1	A	168	ASN
1	A	247	GLN
1	A	248	ASN
2	B	31	ASN
2	B	47	GLN
2	B	142	GLN
2	B	209	GLN
3	C	80	GLN

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Mol	Chain	Res	Type
3	C	148	ASN
4	D	25	ASN
4	D	34	ASN
4	D	118	ASN
4	D	121	GLN
5	R	43	ASN
9	N	74	GLN

### 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 ⓘ

12 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	$\# Z  > 2$
10	HEM	A	900	1	30,50,50	2.52	9 (30%)	24,82,82	2.93	9 (37%)
10	HEM	B	901	2	30,50,50	2.14	6 (20%)	24,82,82	2.53	9 (37%)
10	HEM	B	902	2	30,50,50	1.93	5 (16%)	24,82,82	2.52	10 (41%)
10	HEM	B	903	18,2	30,50,50	2.37	10 (33%)	24,82,82	3.15	12 (50%)
13	BCR	B	904	-	27,27,41	1.54	4 (14%)	35,35,56	1.98	11 (31%)
16	LFA	B	960	-	19,19,19	0.42	0	18,18,18	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	FES	C	210	3	0,4,4	0.00	-	0,4,4	0.00	-
12	CLA	D	910	-	55,73,73	1.28	6 (10%)	61,113,113	1.56	9 (14%)
14	TDS	D	920	-	29,31,31	3.05	13 (44%)	29,40,40	2.37	8 (27%)
17	LMG	D	953	-	53,53,55	1.37	8 (15%)	61,61,63	1.42	6 (9%)
17	LMG	L	951	-	42,42,55	1.32	6 (14%)	50,50,63	1.45	5 (10%)
15	SQD	R	950	-	32,33,54	2.09	10 (31%)	40,44,65	3.30	12 (30%)

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
10	HEM	A	900	1	-	0/10/54/54	0/0/8/8
10	HEM	B	901	2	-	0/10/54/54	0/0/8/8
10	HEM	B	902	2	-	0/10/54/54	0/0/8/8
10	HEM	B	903	18,2	-	0/10/54/54	0/0/8/8
13	BCR	B	904	-	-	0/21/38/63	0/1/1/2
16	LFA	B	960	-	-	0/17/17/17	0/0/0/0
11	FES	C	210	3	-	0/0/4/4	0/1/1/1
12	CLA	D	910	-	4/4/20/25	0/37/135/135	0/0/9/9
14	TDS	D	920	-	-	1/16/17/17	0/2/2/2
17	LMG	D	953	-	-	0/48/68/70	0/1/1/1
17	LMG	L	951	-	-	0/37/57/70	0/1/1/1
15	SQD	R	950	-	-	0/28/48/69	0/1/1/1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	903	HEM	C2D-C3D	-6.84	1.34	1.54
10	A	900	HEM	C2D-C3D	-6.83	1.34	1.54
10	B	901	HEM	C3B-C4B	-6.61	1.46	1.51
10	B	902	HEM	C3B-C4B	-5.95	1.46	1.51
10	A	900	HEM	C3B-C4B	-5.50	1.47	1.51
10	B	901	HEM	C2D-C3D	-5.13	1.39	1.54
10	A	900	HEM	C2C-C1C	-5.11	1.42	1.52
10	B	902	HEM	C2D-C3D	-4.77	1.40	1.54
10	B	901	HEM	C3D-C4D	-4.69	1.45	1.51
10	B	903	HEM	C2C-C1C	-4.40	1.44	1.52
10	B	902	HEM	C3D-C4D	-4.03	1.46	1.51
17	L	951	LMG	O1-C7	-3.96	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	951	LMG	O7-C8	-3.58	1.37	1.46
10	B	902	HEM	C2C-C1C	-3.11	1.46	1.52
10	B	901	HEM	C2C-C1C	-3.01	1.46	1.52
10	B	903	HEM	C2B-C1B	-2.93	1.42	1.51
15	R	950	SQD	O6-C44	-2.75	1.38	1.43
10	B	903	HEM	C3B-C4B	-2.67	1.49	1.51
10	A	900	HEM	CAD-C3D	-2.66	1.48	1.54
10	A	900	HEM	C2B-C1B	-2.52	1.43	1.51
10	B	903	HEM	CAD-C3D	-2.11	1.49	1.54
10	B	901	HEM	C3B-CAB	-2.01	1.47	1.51
10	B	903	HEM	C3B-CAB	2.00	1.55	1.51
10	B	903	HEM	CHC-C1C	2.01	1.41	1.36
12	D	910	CLA	CHC-C1C	2.02	1.41	1.35
10	B	903	HEM	FE-NC	2.07	2.04	1.95
17	D	953	LMG	C4-C3	2.11	1.57	1.52
15	R	950	SQD	C6-S	2.16	1.81	1.77
17	L	951	LMG	O7-C10	2.23	1.40	1.34
10	A	900	HEM	C3B-CAB	2.28	1.55	1.51
10	A	900	HEM	CAA-C2A	2.31	1.56	1.52
15	R	950	SQD	O3-C3	2.40	1.48	1.43
17	L	951	LMG	C4-C3	2.42	1.58	1.52
15	R	950	SQD	C1-C2	2.43	1.59	1.52
13	B	904	BCR	C14-C13	2.46	1.39	1.35
17	D	953	LMG	C9-C8	2.47	1.57	1.50
12	D	910	CLA	O1D-CGD	2.51	1.27	1.21
14	D	920	TDS	CAD-CAE	2.64	1.46	1.37
10	B	902	HEM	FE-NC	2.65	2.06	1.95
12	D	910	CLA	O2A-CGA	2.67	1.41	1.33
17	D	953	LMG	O6-C5	2.68	1.51	1.44
17	L	951	LMG	O6-C1	2.68	1.48	1.41
14	D	920	TDS	CAE-CAF	2.69	1.48	1.42
15	R	950	SQD	O5-C5	2.79	1.51	1.44
17	D	953	LMG	C3-C2	2.83	1.59	1.52
15	R	950	SQD	O48-C23	2.85	1.41	1.33
17	L	951	LMG	O8-C28	2.91	1.42	1.33
17	D	953	LMG	O7-C10	2.93	1.43	1.34
15	R	950	SQD	O47-C7	3.04	1.43	1.34
14	D	920	TDS	CAF-CAN	3.11	1.45	1.41
13	B	904	BCR	C5-C6	3.15	1.39	1.34
14	D	920	TDS	CAL-CAM	3.17	1.44	1.40
13	B	904	BCR	C2-C1	3.18	1.61	1.54
12	D	910	CLA	CMC-C2C	3.23	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	953	LMG	O6-C1	3.26	1.50	1.41
10	B	901	HEM	FE-NC	3.26	2.08	1.95
14	D	920	TDS	CAG-CAH	3.46	1.51	1.41
12	D	910	CLA	C2-C3	3.51	1.39	1.33
15	R	950	SQD	O8-S	3.61	1.55	1.46
17	D	953	LMG	O8-C28	3.69	1.44	1.33
17	D	953	LMG	C4-C5	3.75	1.61	1.53
15	R	950	SQD	O7-S	3.79	1.57	1.45
14	D	920	TDS	OA0-CAN	3.80	1.43	1.36
14	D	920	TDS	OAB-CAE	3.99	1.44	1.36
12	D	910	CLA	O2D-CGD	4.22	1.44	1.33
14	D	920	TDS	OAK-CAL	4.28	1.44	1.37
10	B	903	HEM	CBC-CAC	4.29	1.54	1.29
13	B	904	BCR	C1-C6	4.31	1.59	1.53
14	D	920	TDS	CAD-CAL	4.42	1.47	1.38
10	A	900	HEM	CBC-CAC	4.49	1.55	1.29
14	D	920	TDS	CAH-CAP	4.64	1.44	1.39
10	B	903	HEM	CBB-CAB	5.09	1.58	1.29
10	A	900	HEM	CBB-CAB	5.09	1.58	1.29
14	D	920	TDS	OA0-CAP	5.90	1.42	1.35
14	D	920	TDS	CAQ-CAP	6.27	1.59	1.50
15	R	950	SQD	C4-C3	6.58	1.69	1.52
14	D	920	TDS	CAG-CAF	7.48	1.51	1.41

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	903	HEM	C3B-CAB-CBB	-6.99	113.73	124.46
10	A	900	HEM	C3B-CAB-CBB	-6.52	114.46	124.46
10	A	900	HEM	C3C-CAC-CBC	-5.96	115.32	124.46
10	B	903	HEM	C3C-CAC-CBC	-5.67	115.76	124.46
10	B	903	HEM	CBA-CAA-C2A	-4.12	105.15	112.53
13	B	904	BCR	C33-C5-C4	-3.73	106.36	113.43
15	R	950	SQD	O3-C3-C2	-3.54	102.37	110.34
17	L	951	LMG	C12-C11-C10	-3.50	99.83	113.59
12	D	910	CLA	OBD-CAD-CBD	-3.01	121.40	125.94
13	B	904	BCR	C1-C6-C5	-2.96	118.31	122.66
12	D	910	CLA	CMB-C2B-C1B	-2.92	123.53	128.36
12	D	910	CLA	O1D-CGD-CBD	-2.90	120.47	124.62
15	R	950	SQD	O9-S-C6	-2.79	104.59	106.94
10	B	903	HEM	CMA-C3A-C4A	-2.66	123.96	128.36
10	A	900	HEM	CMA-C3A-C4A	-2.59	124.09	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	910	CLA	O2A-CGA-O1A	-2.31	117.53	123.49
17	L	951	LMG	C21-C20-C19	-2.26	102.86	114.53
14	D	920	TDS	CAD-CAL-CAM	-2.24	118.32	120.56
10	B	901	HEM	CAA-C2A-C1A	-2.22	124.60	127.01
12	D	910	CLA	C2C-C1C-NC	-2.10	108.68	110.24
10	B	902	HEM	CMA-C3A-C4A	-2.09	124.91	128.36
17	D	953	LMG	C12-C11-C10	-2.05	105.54	113.59
15	R	950	SQD	O6-C44-C45	-2.04	106.14	110.99
17	L	951	LMG	C14-C13-C12	-2.03	104.05	114.53
17	D	953	LMG	C14-C13-C12	-2.00	104.18	114.53
15	R	950	SQD	C3-C4-C5	-2.00	106.70	110.20
14	D	920	TDS	CBC-CBB-CBA	2.00	129.16	113.44
13	B	904	BCR	C7-C8-C9	2.01	129.27	126.22
13	B	904	BCR	C36-C18-C19	2.05	121.51	118.10
13	B	904	BCR	C1-C6-C7	2.05	121.57	115.82
10	B	903	HEM	CMA-C3A-C2A	2.05	129.53	125.24
10	B	903	HEM	C3B-C4B-CHC	2.10	126.12	123.16
10	A	900	HEM	CMA-C3A-C2A	2.11	129.65	125.24
10	B	901	HEM	C3B-CAB-CBB	2.12	127.71	124.46
13	B	904	BCR	C11-C10-C9	2.14	130.29	127.20
13	B	904	BCR	C16-C17-C18	2.27	130.48	127.20
14	D	920	TDS	CAW-CAX-CAY	2.29	126.37	114.53
12	D	910	CLA	C1D-CHD-C4C	2.29	126.07	122.60
10	B	902	HEM	CAA-CBA-CGA	2.35	117.05	112.75
10	B	902	HEM	C3C-CAC-CBC	2.41	128.15	124.46
14	D	920	TDS	CAJ-OAK-CAL	2.41	121.20	117.54
15	R	950	SQD	O4-C4-C5	2.43	115.69	109.24
14	D	920	TDS	CAV-CAW-CAX	2.47	127.31	114.53
13	B	904	BCR	C32-C1-C6	2.60	114.38	110.30
14	D	920	TDS	CAI-CAH-CAP	2.68	126.39	122.06
14	D	920	TDS	CAY-CAZ-CBA	2.74	128.70	114.53
10	B	902	HEM	C2D-C3D-C4D	2.78	106.22	101.50
15	R	950	SQD	O5-C5-C4	2.78	114.91	109.68
13	B	904	BCR	C8-C7-C6	2.81	135.74	127.32
17	L	951	LMG	O8-C28-C29	2.85	120.58	111.90
17	D	953	LMG	O7-C10-C11	2.89	117.81	111.53
10	B	901	HEM	C2D-C3D-C4D	2.89	106.41	101.50
15	R	950	SQD	C44-O6-C1	2.90	119.91	113.82
10	B	901	HEM	CMD-C2D-C3D	3.04	127.80	114.35
10	B	903	HEM	CAA-CBA-CGA	3.23	118.66	112.75
10	B	902	HEM	CMD-C2D-C3D	3.24	128.68	114.35
10	A	900	HEM	CMD-C2D-C3D	3.24	128.69	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	953	LMG	O8-C28-C29	3.31	122.00	111.90
10	B	903	HEM	CMD-C2D-C3D	3.32	129.01	114.35
13	B	904	BCR	C2-C1-C6	3.43	115.79	110.36
10	B	902	HEM	C3B-CAB-CBB	3.48	129.79	124.46
15	R	950	SQD	O48-C23-C24	3.59	122.82	111.90
12	D	910	CLA	O2A-CGA-CBA	3.72	123.24	111.90
10	B	902	HEM	CAD-C3D-C4D	3.79	125.85	112.47
10	B	901	HEM	CAD-C3D-C4D	3.92	126.31	112.47
17	D	953	LMG	C7-O1-C1	4.15	122.54	113.82
10	B	903	HEM	CAD-C3D-C4D	4.50	128.35	112.47
12	D	910	CLA	C4A-NA-C1A	4.59	112.29	106.36
10	A	900	HEM	CAD-C3D-C4D	4.61	128.72	112.47
10	A	900	HEM	CAD-C3D-C2D	4.66	126.61	113.22
12	D	910	CLA	O2D-CGD-CBD	4.78	117.86	111.30
10	B	901	HEM	CMB-C2B-C3B	4.78	128.47	116.53
10	B	903	HEM	CAD-C3D-C2D	4.81	127.04	113.22
10	B	903	HEM	CMC-C2C-C3C	4.86	128.65	116.53
10	B	901	HEM	CAD-C3D-C2D	4.89	127.29	113.22
10	B	901	HEM	CAA-CBA-CGA	4.90	121.72	112.75
10	B	903	HEM	CMB-C2B-C3B	4.98	128.96	116.53
10	A	900	HEM	CMB-C2B-C3B	5.00	129.01	116.53
10	B	902	HEM	CMB-C2B-C3B	5.07	129.19	116.53
10	A	900	HEM	CMC-C2C-C3C	5.08	129.20	116.53
10	B	902	HEM	CAD-C3D-C2D	5.12	127.93	113.22
10	B	901	HEM	CMC-C2C-C3C	5.18	129.45	116.53
10	B	902	HEM	CMC-C2C-C3C	5.30	129.76	116.53
15	R	950	SQD	C25-C24-C23	5.62	135.70	113.59
17	D	953	LMG	C30-C29-C28	5.80	136.41	113.59
17	L	951	LMG	C30-C29-C28	6.11	137.60	113.59
13	B	904	BCR	C33-C5-C6	6.13	130.62	124.61
15	R	950	SQD	O5-C1-O6	8.49	130.49	110.05
15	R	950	SQD	O6-C1-C2	9.20	119.65	108.04
14	D	920	TDS	CAQ-CAP-CAH	9.85	133.55	120.56
15	R	950	SQD	O7-S-C6	12.56	117.53	106.94

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	D	910	CLA	C8
12	D	910	CLA	NC
12	D	910	CLA	ND
12	D	910	CLA	NA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	D	920	TDS	CAH-CAP-CAQ-CAR

There are no ring outliers.

11 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	900	HEM	2	0
10	B	901	HEM	4	0
10	B	903	HEM	1	0
13	B	904	BCR	3	0
16	B	960	LFA	2	0
11	C	210	FES	1	0
12	D	910	CLA	5	0
14	D	920	TDS	2	0
17	D	953	LMG	3	0
17	L	951	LMG	4	0
15	R	950	SQD	1	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	292/292 (100%)	-0.14	3 (1%) 84 69	42, 66, 102, 131	3 (1%)
2	B	212/215 (98%)	-0.08	3 (1%) 78 60	29, 47, 76, 114	0
3	C	126/127 (99%)	1.04	31 (24%) 1 0	70, 121, 159, 180	0
4	D	156/159 (98%)	-0.18	0 100 100	37, 62, 96, 131	0
5	R	39/49 (79%)	-0.08	3 (7%) 16 5	37, 51, 135, 159	0
6	G	30/37 (81%)	-0.19	0 100 100	41, 54, 77, 97	0
7	L	32/32 (100%)	-0.30	0 100 100	46, 65, 86, 126	0
8	M	34/39 (87%)	-0.39	0 100 100	41, 57, 83, 130	0
9	N	31/31 (100%)	-0.34	0 100 100	36, 50, 68, 91	0
All	All	952/981 (97%)	0.00	40 (4%) 40 19	29, 62, 135, 180	3 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	33	SER	4.2
3	C	186	LEU	3.9
3	C	93	GLY	3.6
3	C	196	ASP	3.6
3	C	81	ALA	3.4
3	C	97	LYS	3.4
3	C	89	ASP	3.3
3	C	98	THR	3.3
1	A	200	ASN	3.1
3	C	157	SER	3.0
2	B	5	TYR	3.0
3	C	206	ALA	2.9
3	C	120	THR	2.8
3	C	203	PRO	2.8
3	C	123	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	192	TRP	2.7
3	C	197	PHE	2.7
3	C	190	SER	2.7
3	C	88	ASN	2.7
3	C	187	VAL	2.6
3	C	195	THR	2.5
3	C	182	ALA	2.5
3	C	82	ALA	2.5
3	C	95	TRP	2.5
3	C	122	ASP	2.4
3	C	96	LEU	2.4
5	R	34	SER	2.4
3	C	189	PHE	2.4
3	C	124	THR	2.3
3	C	201	LEU	2.3
3	C	188	THR	2.2
3	C	90	ILE	2.2
3	C	121	ALA	2.2
1	A	199	ALA	2.2
3	C	92	ALA	2.2
2	B	91	SER	2.1
5	R	35	GLU	2.1
2	B	159	PRO	2.1
3	C	178	HIS	2.0
1	A	201	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	LMG	D	953	53/55	0.63	0.43	3.62	88,88,107,107	0
14	TDS	D	920	30/30	0.87	0.30	3.01	87,89,89,89	0
16	LFA	B	960	20/20	0.91	0.29	2.89	59,59,59,59	0
13	BCR	B	904	27/40	0.85	0.40	2.42	49,49,64,64	0
17	LMG	L	951	42/55	0.77	0.33	1.52	78,85,85,85	0
12	CLA	D	910	65/65	0.88	0.28	1.19	63,70,92,94	0
15	SQD	R	950	33/54	0.93	0.19	0.14	62,62,111,111	0
10	HEM	A	900	43/43	0.95	0.22	-0.15	63,67,77,80	0
10	HEM	B	901	43/43	0.97	0.21	-0.37	30,37,45,50	0
10	HEM	B	902	43/43	0.97	0.19	-0.46	35,43,48,50	0
10	HEM	B	903	43/43	0.95	0.21	-0.63	53,53,53,53	0
11	FES	C	210	4/4	0.99	0.09	-1.62	62,62,63,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.