



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:37 am GMT

PDB ID : 4EGO  
Title : The X-ray crystal structure of CYP199A4 in complex with indole-6-carboxylic acid  
Authors : Zhou, W.; Bell, S.G.; Yang, W.; Zhou, R.M.; Tan, A.B.H.; Wong, L.-L.  
Deposited on : 2012-03-31  
Resolution : 1.76 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 : trunk28620  
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) : recalc28949

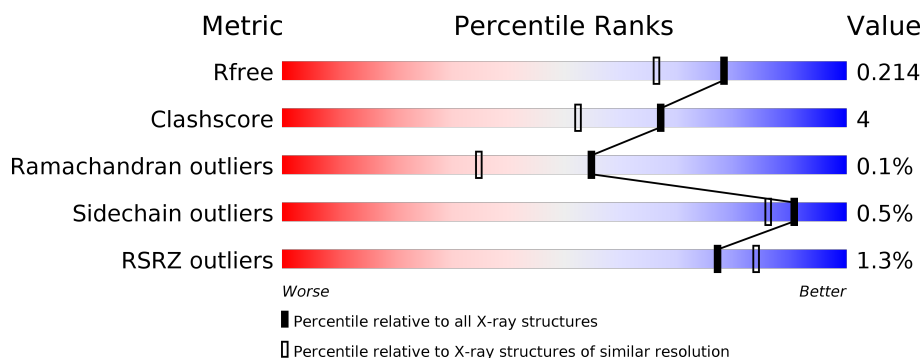
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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	410	
1	B	410	
1	C	410	
1	D	410	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1F1	A	503	-	-	-	X
3	1F1	A	504	-	-	-	X
3	1F1	B	503	-	-	-	X
3	1F1	C	503	-	-	-	X
3	1F1	D	501	-	-	-	X
4	SO4	A	506	-	-	-	X
4	SO4	C	506	-	-	-	X
4	SO4	D	505	-	-	-	X
5	GOL	B	506	-	-	-	X

2 Entry composition ⓘ

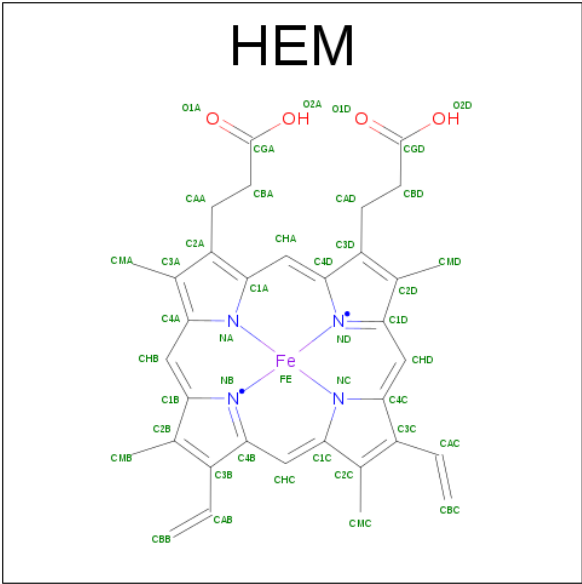
There are 7 unique types of molecules in this entry. The entry contains 13688 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	3	0
			3035	1922	535	566	12			
1	B	393	Total	C	N	O	S	0	1	0
			3027	1916	534	566	11			
1	C	393	Total	C	N	O	S	0	0	0
			3021	1912	534	564	11			
1	D	393	Total	C	N	O	S	0	0	0
			3021	1912	534	564	11			

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



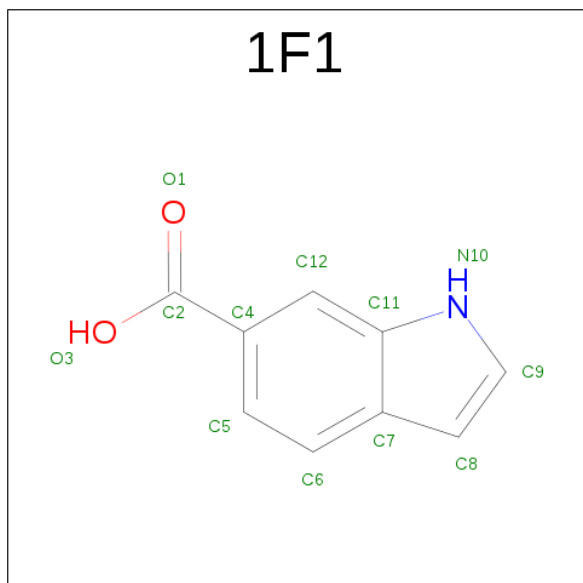
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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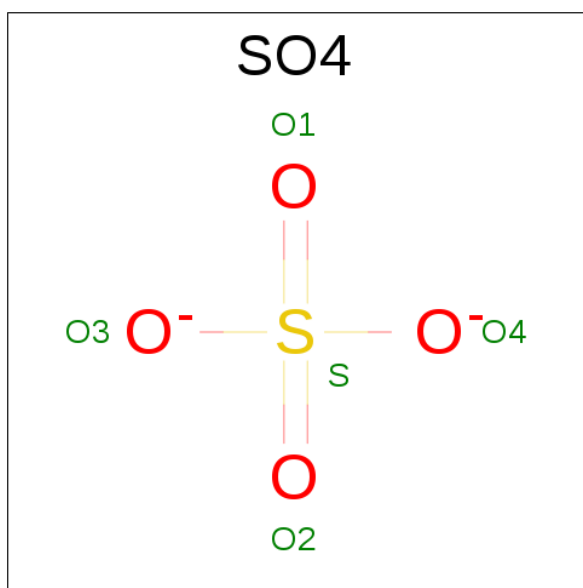
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 1H-INDOLE-6-CARBOXYLIC ACID (three-letter code: 1F1) (formula:  $C_9H_7NO_2$ ).



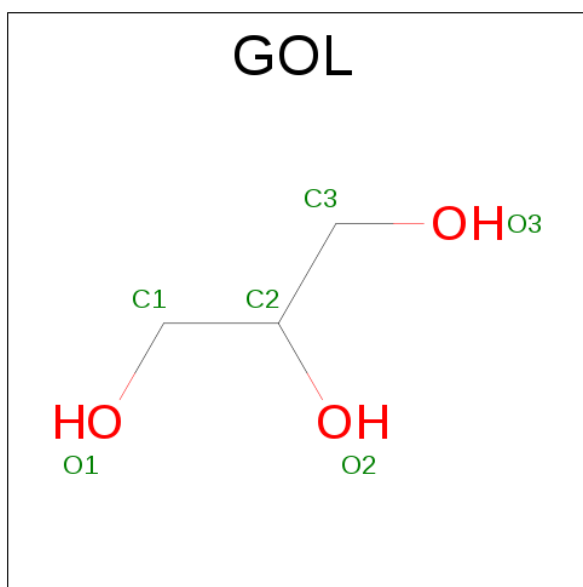
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	B	1	Total	C	N	O	0	0
			12	9	1	2		
3	B	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		
3	D	1	Total	C	N	O	0	0
			12	9	1	2		
3	D	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

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

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

- Molecule 7 is water.

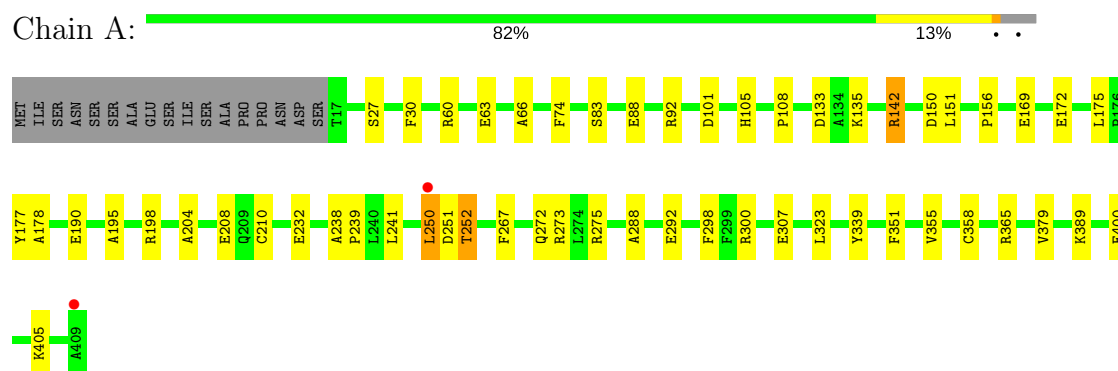
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	347	Total 347	O 347	0	0
7	B	332	Total 332	O 332	0	0
7	C	314	Total 314	O 314	0	0
7	D	225	Total 225	O 225	0	0



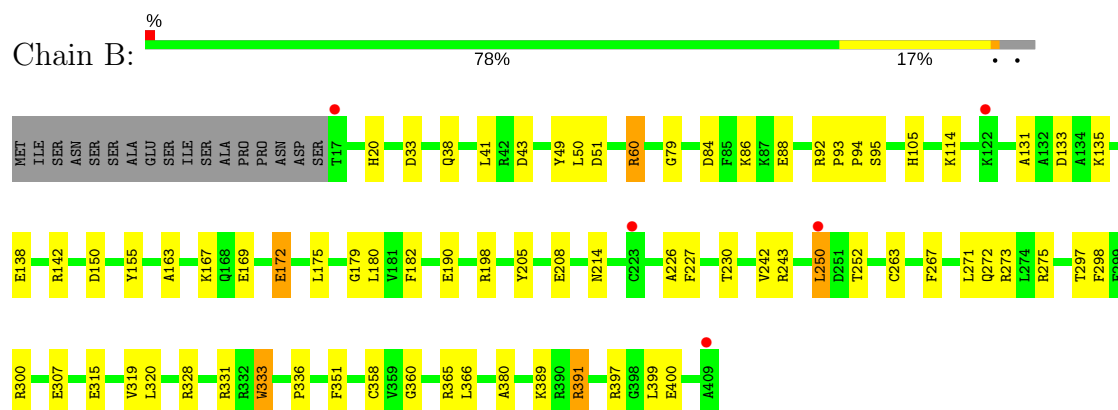
### 3 Residue-property plots [i](#)

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

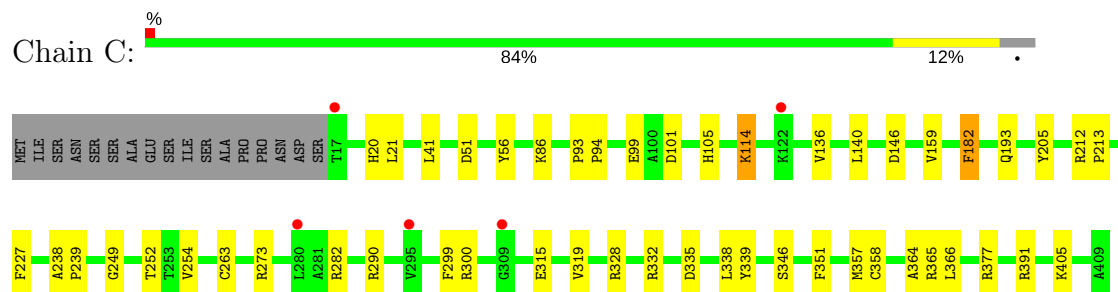
#### • Molecule 1: Cytochrome P450



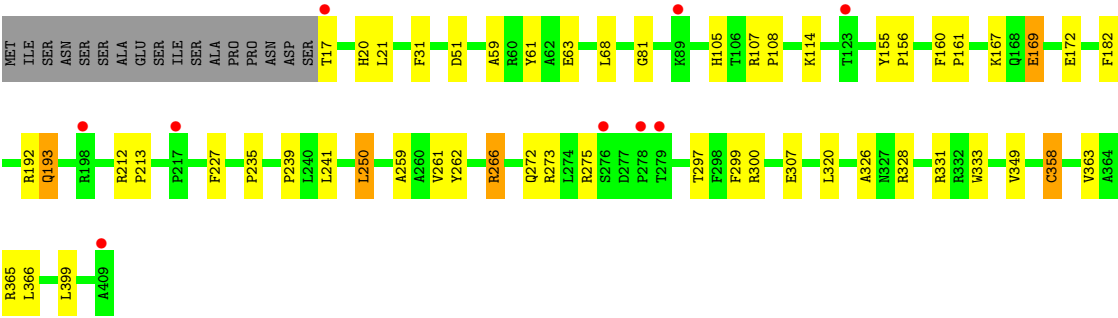
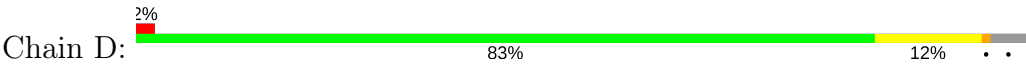
#### • Molecule 1: Cytochrome P450



#### • Molecule 1: Cytochrome P450



#### • Molecule 1: Cytochrome P450



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.86Å 143.67Å 172.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 1.76 39.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	90.0 (39.00-1.76) 90.0 (39.00-1.76)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.182 , 0.214 0.183 , 0.214	Depositor DCC
$R_{free}$ test set	11782 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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 49.59 % 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 7.2997e-05. 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, 0.333 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: GOL, SO4, 1F1, HEM, CL

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	1.57	28/3116 (0.9%)	1.22	16/4239 (0.4%)
1	B	1.58	25/3102 (0.8%)	1.34	26/4221 (0.6%)
1	C	1.49	20/3093 (0.6%)	1.19	14/4209 (0.3%)
1	D	1.41	15/3093 (0.5%)	1.18	13/4209 (0.3%)
All	All	1.52	88/12404 (0.7%)	1.23	69/16878 (0.4%)

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	GLU	CD-OE2	11.59	1.38	1.25
1	B	169	GLU	CG-CD	11.59	1.69	1.51
1	A	210	CYS	CB-SG	8.82	1.97	1.82
1	A	172	GLU	CG-CD	8.73	1.65	1.51
1	A	307	GLU	CG-CD	8.17	1.64	1.51
1	C	193	GLN	CG-CD	8.15	1.69	1.51
1	A	74	PHE	CD2-CE2	8.14	1.55	1.39
1	B	172	GLU	CD-OE1	8.01	1.34	1.25
1	A	88	GLU	CB-CG	7.82	1.67	1.52
1	C	56	TYR	CD1-CE1	7.62	1.50	1.39
1	A	169	GLU	CG-CD	7.60	1.63	1.51
1	D	169	GLU	CG-CD	7.46	1.63	1.51
1	A	208	GLU	CG-CD	7.23	1.62	1.51
1	D	193	GLN	CB-CG	7.20	1.72	1.52
1	D	193	GLN	CG-CD	7.12	1.67	1.51
1	B	169	GLU	CD-OE1	7.06	1.33	1.25
1	A	190	GLU	CG-CD	7.05	1.62	1.51
1	A	88	GLU	CG-CD	6.94	1.62	1.51
1	C	351	PHE	CE1-CZ	6.87	1.50	1.37
1	B	315	GLU	CG-CD	6.69	1.61	1.51
1	B	88	GLU	CG-CD	6.67	1.61	1.51
1	C	315	GLU	CG-CD	6.66	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	PHE	CE1-CZ	6.50	1.49	1.37
1	B	267	PHE	CE1-CZ	6.48	1.49	1.37
1	D	61	TYR	CD1-CE1	6.46	1.49	1.39
1	B	49	TYR	CD1-CE1	6.39	1.49	1.39
1	A	177	TYR	CG-CD2	6.31	1.47	1.39
1	A	172	GLU	CD-OE1	6.25	1.32	1.25
1	D	259	ALA	CA-CB	6.21	1.65	1.52
1	D	363	VAL	CB-CG2	6.13	1.65	1.52
1	B	333	TRP	CG-CD1	6.01	1.45	1.36
1	A	63	GLU	CG-CD	5.98	1.60	1.51
1	B	79	GLY	N-CA	5.97	1.55	1.46
1	A	298	PHE	CD2-CE2	5.95	1.51	1.39
1	D	326	ALA	CA-CB	5.92	1.64	1.52
1	A	27	SER	CA-CB	5.89	1.61	1.52
1	B	380	ALA	CA-CB	5.89	1.64	1.52
1	C	339	TYR	CG-CD1	5.87	1.46	1.39
1	B	138	GLU	CG-CD	5.86	1.60	1.51
1	B	319	VAL	CB-CG2	5.84	1.65	1.52
1	B	131	ALA	CA-CB	5.83	1.64	1.52
1	D	31	PHE	CE1-CZ	5.79	1.48	1.37
1	B	250	LEU	CG-CD1	-5.78	1.30	1.51
1	C	136	VAL	CB-CG2	5.76	1.65	1.52
1	A	292	GLU	CD-OE2	5.73	1.31	1.25
1	A	379	VAL	CB-CG2	5.72	1.64	1.52
1	C	319	VAL	CB-CG1	5.71	1.64	1.52
1	D	333	TRP	CE3-CZ3	5.69	1.48	1.38
1	C	263	CYS	CB-SG	5.64	1.91	1.82
1	A	288	ALA	CA-CB	5.61	1.64	1.52
1	A	232	GLU	CB-CG	5.57	1.62	1.52
1	C	299	PHE	CD1-CE1	5.53	1.50	1.39
1	B	397	ARG	CZ-NH1	5.53	1.40	1.33
1	D	59	ALA	CA-CB	5.49	1.64	1.52
1	A	204	ALA	CA-CB	5.49	1.64	1.52
1	B	190	GLU	CG-CD	5.45	1.60	1.51
1	B	163	ALA	CA-CB	5.43	1.63	1.52
1	B	190	GLU	CD-OE1	5.40	1.31	1.25
1	A	30	PHE	CE2-CZ	5.38	1.47	1.37
1	D	349	VAL	CB-CG2	5.37	1.64	1.52
1	A	66	ALA	CA-CB	5.35	1.63	1.52
1	C	182	PHE	CD1-CE1	5.32	1.49	1.39
1	D	261	VAL	CB-CG1	5.27	1.64	1.52
1	B	351	PHE	CE2-CZ	5.25	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	227	PHE	CE2-CZ	5.24	1.47	1.37
1	D	81	GLY	N-CA	5.23	1.53	1.46
1	C	290	ARG	CB-CG	5.22	1.66	1.52
1	B	155	TYR	CD1-CE1	5.22	1.47	1.39
1	D	63	GLU	CD-OE1	-5.19	1.20	1.25
1	C	193	GLN	CB-CG	5.19	1.66	1.52
1	A	351	PHE	CE1-CZ	5.18	1.47	1.37
1	C	159	VAL	CB-CG2	5.17	1.63	1.52
1	A	355	VAL	CB-CG2	-5.17	1.42	1.52
1	C	99	GLU	CB-CG	5.15	1.61	1.52
1	C	299	PHE	CE1-CZ	5.14	1.47	1.37
1	B	227	PHE	CE2-CZ	5.12	1.47	1.37
1	B	226	ALA	N-CA	5.12	1.56	1.46
1	C	205	TYR	CD1-CE1	5.11	1.47	1.39
1	B	263	CYS	CB-SG	5.10	1.91	1.82
1	C	346	SER	CB-OG	-5.09	1.35	1.42
1	A	339	TYR	CG-CD2	5.08	1.45	1.39
1	A	195	ALA	CA-CB	5.08	1.63	1.52
1	D	172	GLU	CG-CD	5.08	1.59	1.51
1	C	364	ALA	CA-CB	5.06	1.63	1.52
1	B	242	VAL	CB-CG1	5.05	1.63	1.52
1	A	83	SER	CB-OG	5.04	1.48	1.42
1	C	254	VAL	CB-CG1	5.03	1.63	1.52
1	B	95	SER	CB-OG	5.00	1.48	1.42

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	397	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	B	391	ARG	NE-CZ-NH1	-11.94	114.33	120.30
1	D	273	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	D	328	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	D	273	ARG	NE-CZ-NH1	10.75	125.68	120.30
1	B	142	ARG	NE-CZ-NH1	-10.36	115.12	120.30
1	A	273	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	B	142	ARG	NE-CZ-NH2	9.65	125.13	120.30
1	D	328	ARG	NE-CZ-NH2	-9.41	115.60	120.30
1	B	198	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	A	142	ARG	NE-CZ-NH2	9.23	124.92	120.30
1	A	273	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	C	273	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	B	273	ARG	NE-CZ-NH1	8.66	124.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	B	243	ARG	NE-CZ-NH1	-8.39	116.11	120.30
1	C	273	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	300	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	B	133	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	397	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	A	198	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	D	300	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	D	266	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	273	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	D	107	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	377	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	B	243	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	C	101	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	C	365	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	B	92	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	B	328	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	C	328	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	C	282	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	331	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	C	114	LYS	CD-CE-NZ	-6.30	97.22	111.70
1	C	300	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	D	365	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	60	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	B	328	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	D	266	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	D	331	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	198	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	60	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	B	180	LEU	CB-CG-CD2	-6.03	100.76	111.00
1	D	21	LEU	CB-CG-CD1	-5.97	100.84	111.00
1	A	133	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	198	ARG	CB-CG-CD	5.90	126.94	111.60
1	A	142	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	A	101	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	B	84	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	299	PHE	CB-CG-CD1	-5.73	116.79	120.80
1	C	332	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	365	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	298	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	B	86	LYS	CD-CE-NZ	-5.51	99.02	111.70
1	B	365	ARG	NE-CZ-NH1	5.45	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	391	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	198	ARG	CB-CG-CD	5.27	125.29	111.60
1	A	198	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	101	ASP	OD1-CG-OD2	5.20	133.18	123.30
1	B	300	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	266	ARG	CG-CD-NE	5.18	122.68	111.80
1	A	92	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	43	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	391	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	252	THR	CA-CB-CG2	-5.09	105.28	112.40
1	B	33	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	C	146	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	299	PHE	CB-CG-CD2	-5.03	117.28	120.80

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	3035	0	3015	25	0
1	B	3027	0	2999	38	0
1	C	3021	0	2993	20	0
1	D	3021	0	2993	24	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
2	C	43	0	30	5	0
2	D	43	0	30	3	0
3	A	36	0	18	0	0
3	B	24	0	12	3	0
3	C	24	0	12	3	0
3	D	24	0	12	2	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	15	0	0	0	0
4	D	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	16	0	0
5	B	18	0	24	2	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	347	0	0	3	0
7	B	332	0	0	5	0
7	C	314	0	0	5	0
7	D	225	0	0	5	0
All	All	13688	0	12230	111	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 (111) 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:B:60:ARG:HH12	5:B:506:GOL:H32	1.09	1.10
1:D:272:GLN:HE22	1:D:275:ARG:HH11	1.14	0.91
1:A:272:GLN:HE22	1:A:275:ARG:HH11	1.21	0.86
1:B:307:GLU:HG2	7:B:670:HOH:O	1.75	0.84
1:B:135:LYS:CE	1:B:150:ASP:O	2.27	0.82
1:B:272:GLN:HE22	1:B:275:ARG:HH11	1.27	0.82
1:B:60:ARG:NH1	5:B:506:GOL:H32	1.93	0.79
1:D:307:GLU:HG2	7:D:717:HOH:O	1.85	0.75
1:D:105:HIS:HD2	7:D:613:HOH:O	1.70	0.73
2:D:502:HEM:HBC2	2:D:502:HEM:HMC1	1.70	0.73
1:D:262:TYR:CE2	1:D:266:ARG:HD3	2.24	0.72
1:D:105:HIS:HE1	2:D:502:HEM:O1D	1.73	0.71
1:C:105:HIS:HD2	7:C:607:HOH:O	1.74	0.70
1:D:262:TYR:CZ	1:D:266:ARG:HD3	2.27	0.69
1:A:105:HIS:HD2	7:A:626:HOH:O	1.75	0.69
1:B:208[B]:GLU:HG2	7:B:826:HOH:O	1.92	0.68
1:B:250:LEU:C	1:B:250:LEU:HD13	2.15	0.67
1:B:135:LYS:HE3	1:B:150:ASP:O	1.95	0.66
1:B:105:HIS:HE1	2:B:501:HEM:O1D	1.79	0.64
1:A:135:LYS:CE	1:A:150:ASP:O	2.46	0.64
1:B:114:LYS:HE3	7:B:804:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LEU:HD12	1:A:323:LEU:N	2.12	0.63
1:A:135:LYS:HE3	1:A:150:ASP:O	1.97	0.63
1:C:105:HIS:HE1	2:C:501:HEM:O1D	1.81	0.62
1:B:135:LYS:NZ	1:B:150:ASP:O	2.32	0.62
1:B:272:GLN:HE22	1:B:275:ARG:NH1	1.97	0.62
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.83	0.61
1:D:167:LYS:HE3	1:D:169:GLU:HG2	1.81	0.61
1:A:105:HIS:HE1	2:A:501:HEM:O1D	1.83	0.61
1:A:323:LEU:H	1:A:323:LEU:HD12	1.67	0.60
1:B:167:LYS:NZ	1:B:214:ASN:ND2	2.49	0.60
3:C:503:1F1:H6	7:C:734:HOH:O	2.01	0.60
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	1.83	0.59
1:C:114:LYS:NZ	7:C:727:HOH:O	2.35	0.59
1:A:405:LYS:HE3	7:A:779:HOH:O	2.01	0.59
1:C:405:LYS:HE3	7:D:749:HOH:O	2.01	0.59
1:D:20:HIS:HD2	1:D:51:ASP:OD1	1.86	0.58
1:D:17:THR:O	1:D:17:THR:OG1	2.21	0.58
1:B:167:LYS:HZ2	1:B:214:ASN:ND2	2.02	0.57
1:D:272:GLN:HE22	1:D:275:ARG:NH1	1.95	0.56
1:D:114:LYS:HD3	1:D:227:PHE:CZ	2.43	0.53
1:D:114:LYS:HD3	1:D:227:PHE:HZ	1.73	0.53
1:B:179:GLY:HA3	3:B:503:1F1:C2	2.38	0.53
1:B:230:THR:O	1:B:230:THR:HG22	2.10	0.52
1:B:389:LYS:HE3	1:B:400:GLU:OE2	2.09	0.52
1:C:20:HIS:HD2	1:C:51:ASP:OD1	1.91	0.52
1:A:142:ARG:HD3	1:B:205:TYR:HA	1.92	0.51
1:B:358:CYS:HA	2:B:501:HEM:CHA	2.41	0.51
1:C:21:LEU:HD12	1:C:41:LEU:HD23	1.93	0.51
1:D:250:LEU:HD12	1:D:250:LEU:O	2.12	0.50
1:C:335:ASP:HB3	1:C:338:LEU:HD22	1.94	0.49
1:B:172:GLU:HG2	7:B:747:HOH:O	2.12	0.49
1:B:230:THR:O	1:B:230:THR:CG2	2.60	0.49
1:C:252:THR:HB	2:C:501:HEM:C3B	2.48	0.49
1:A:272:GLN:HE22	1:A:275:ARG:NH1	2.01	0.48
1:A:358:CYS:HA	2:A:501:HEM:CHA	2.44	0.48
3:D:501:1F1:H6	7:D:713:HOH:O	2.14	0.48
1:C:358:CYS:HA	2:C:501:HEM:CHA	2.43	0.48
1:B:20:HIS:HD2	1:B:51:ASP:OD1	1.97	0.47
1:B:297:THR:HB	1:B:320:LEU:HD11	1.97	0.47
1:C:182:PHE:CE2	3:C:502:1F1:H8	2.50	0.47
1:A:175:LEU:HD23	1:A:251[B]:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:LEU:HD12	7:D:694:HOH:O	2.16	0.46
1:D:235:PRO:O	1:D:239:PRO:HD3	2.16	0.46
1:B:271:LEU:O	1:B:275:ARG:HG3	2.16	0.46
1:A:156:PRO:HB2	1:A:250:LEU:HD11	1.96	0.46
1:B:182:PHE:CZ	3:B:502:1F1:H8	2.51	0.46
1:D:108:PRO:HB3	1:D:241:LEU:HD21	1.99	0.45
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.99	0.44
1:A:108:PRO:HB3	1:A:241:LEU:HD21	1.98	0.44
1:A:323:LEU:CD1	1:A:323:LEU:H	2.29	0.44
1:A:405:LYS:CE	7:A:779:HOH:O	2.63	0.44
1:D:297:THR:HB	1:D:320:LEU:HD11	1.99	0.44
1:B:167:LYS:NZ	1:B:214:ASN:HD22	2.14	0.44
1:A:252:THR:HB	2:A:501:HEM:C3B	2.52	0.44
1:D:358:CYS:HA	2:D:502:HEM:CHA	2.47	0.44
1:B:175:LEU:HB3	3:B:503:1F1:C8	2.48	0.44
1:B:399:LEU:HD12	7:B:885:HOH:O	2.18	0.43
1:C:140:LEU:HA	1:C:140:LEU:HD23	1.87	0.43
1:A:272:GLN:HE22	1:A:275:ARG:HD3	1.83	0.43
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.90	0.43
1:C:238:ALA:HB3	1:C:239:PRO:HD3	1.99	0.43
1:A:272:GLN:NE2	1:A:275:ARG:HD3	2.33	0.43
1:C:182:PHE:CZ	3:C:502:1F1:H8	2.54	0.43
1:C:114:LYS:CE	7:C:727:HOH:O	2.66	0.43
1:A:323:LEU:CD1	1:A:323:LEU:N	2.82	0.42
1:B:391:ARG:HH11	1:B:391:ARG:HD2	1.48	0.42
1:B:360:GLY:HA3	2:B:501:HEM:C3C	2.54	0.42
1:D:192:ARG:HH21	1:D:193:GLN:HE22	1.68	0.42
2:C:501:HEM:CMC	2:C:501:HEM:HBC2	2.50	0.42
1:D:68:LEU:HA	1:D:68:LEU:HD23	1.92	0.42
1:C:249:GLY:HA2	2:C:501:HEM:C2C	2.54	0.42
1:C:93:PRO:HA	1:C:94:PRO:HD3	1.81	0.42
1:C:357:MET:O	1:C:358:CYS:C	2.58	0.42
1:B:333:TRP:O	1:B:336:PRO:HD3	2.19	0.42
1:C:212:ARG:N	1:C:213:PRO:CD	2.83	0.42
1:A:178:ALA:HB3	1:A:251[B]:ASP:CG	2.40	0.41
1:B:38:GLN:HA	1:B:41:LEU:HD12	2.02	0.41
1:D:155:TYR:HB3	1:D:156:PRO:HD3	2.02	0.41
1:B:252:THR:HB	2:B:501:HEM:C3B	2.55	0.41
1:A:142:ARG:HG3	1:B:208[A]:GLU:OE1	2.21	0.41
1:A:151:LEU:C	1:A:151:LEU:HD23	2.41	0.41
1:A:238:ALA:HB3	1:A:239:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HA	1:B:50:LEU:HD23	1.86	0.41
1:A:389:LYS:NZ	1:A:400:GLU:OE2	2.53	0.41
1:B:167:LYS:HZ1	1:B:214:ASN:HD22	1.69	0.40
1:C:20:HIS:CD2	1:C:51:ASP:OD1	2.73	0.40
1:B:175:LEU:HD23	1:B:250:LEU:HD12	2.02	0.40
1:C:86:LYS:NZ	7:C:767:HOH:O	2.34	0.40
1:D:212:ARG:N	1:D:213:PRO:CD	2.84	0.40
1:D:182:PHE:CE2	3:D:503:1F1:H8	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/410 (96%)	386 (98%)	8 (2%)	0	100	100
1	B	392/410 (96%)	384 (98%)	8 (2%)	0	100	100
1	C	391/410 (95%)	383 (98%)	8 (2%)	0	100	100
1	D	391/410 (95%)	384 (98%)	6 (2%)	1 (0%)	44	24
All	All	1568/1640 (96%)	1537 (98%)	30 (2%)	1 (0%)	55	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	358	CYS

### 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	322/334 (96%)	321 (100%)	1 (0%)	94	91
1	B	320/334 (96%)	318 (99%)	2 (1%)	89	82
1	C	319/334 (96%)	318 (100%)	1 (0%)	94	91
1	D	319/334 (96%)	317 (99%)	2 (1%)	89	82
All	All	1280/1336 (96%)	1274 (100%)	6 (0%)	91	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	LEU
1	B	298	PHE
1	B	366	LEU
1	C	366	LEU
1	D	250	LEU
1	D	366	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	209	GLN
1	A	211	GLN
1	A	214	ASN
1	A	272	GLN
1	A	283	ASN
1	A	296	GLN
1	B	20	HIS
1	B	105	HIS
1	B	207	ASN
1	B	211	GLN
1	B	214	ASN
1	B	255	ASN
1	B	272	GLN
1	B	283	ASN
1	B	296	GLN
1	C	20	HIS
1	C	105	HIS
1	C	211	GLN

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Mol	Chain	Res	Type
1	C	214	ASN
1	C	283	ASN
1	C	296	GLN
1	D	20	HIS
1	D	105	HIS
1	D	168	GLN
1	D	193	GLN
1	D	211	GLN
1	D	214	ASN
1	D	272	GLN
1	D	283	ASN
1	D	296	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 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	HEM	A	501	1	28,50,50	2.34	11 (39%)	17,82,82	2.68	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1F1	A	502	-	8,13,13	2.77	4 (50%)	10,18,18	2.84	5 (50%)
3	1F1	A	503	-	8,13,13	1.62	2 (25%)	10,18,18	3.40	6 (60%)
3	1F1	A	504	-	8,13,13	1.26	0	10,18,18	2.35	5 (50%)
4	SO4	A	505	-	4,4,4	0.41	0	6,6,6	1.32	1 (16%)
4	SO4	A	506	-	4,4,4	0.64	0	6,6,6	0.50	0
5	GOL	A	507	-	5,5,5	0.30	0	5,5,5	1.26	0
5	GOL	A	508	-	5,5,5	0.43	0	5,5,5	1.60	0
2	HEM	B	501	1	28,50,50	2.25	11 (39%)	17,82,82	2.36	7 (41%)
3	1F1	B	502	-	8,13,13	2.54	4 (50%)	10,18,18	2.15	6 (60%)
3	1F1	B	503	-	8,13,13	1.76	3 (37%)	10,18,18	3.07	5 (50%)
4	SO4	B	504	-	4,4,4	0.44	0	6,6,6	0.75	0
5	GOL	B	505	-	5,5,5	0.66	0	5,5,5	1.14	0
5	GOL	B	506	-	5,5,5	0.80	0	5,5,5	3.74	3 (60%)
5	GOL	B	507	-	5,5,5	0.50	0	5,5,5	1.01	0
2	HEM	C	501	1	28,50,50	1.83	8 (28%)	17,82,82	2.44	5 (29%)
3	1F1	C	502	-	8,13,13	1.78	2 (25%)	10,18,18	2.96	7 (70%)
3	1F1	C	503	-	8,13,13	1.68	1 (12%)	10,18,18	2.54	4 (40%)
4	SO4	C	504	-	4,4,4	0.46	0	6,6,6	0.78	0
4	SO4	C	505	-	4,4,4	0.23	0	6,6,6	0.81	0
4	SO4	C	506	-	4,4,4	0.39	0	6,6,6	0.50	0
5	GOL	C	507	-	5,5,5	0.48	0	5,5,5	0.95	0
3	1F1	D	501	-	8,13,13	1.88	3 (37%)	10,18,18	3.04	3 (30%)
2	HEM	D	502	1	28,50,50	2.24	9 (32%)	17,82,82	2.66	6 (35%)
3	1F1	D	503	-	8,13,13	1.87	4 (50%)	10,18,18	1.78	3 (30%)
4	SO4	D	504	-	4,4,4	0.47	0	6,6,6	0.48	0
4	SO4	D	505	-	4,4,4	0.49	0	6,6,6	1.32	1 (16%)
5	GOL	D	506	-	5,5,5	0.32	0	5,5,5	1.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	501	1	-	0/6/54/54	0/0/8/8
3	1F1	A	502	-	-	0/0/4/4	0/2/2/2
3	1F1	A	503	-	-	0/0/4/4	0/2/2/2
3	1F1	A	504	-	-	0/0/4/4	0/2/2/2
4	SO4	A	505	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	506	-	-	0/0/0/0	0/0/0/0
5	GOL	A	507	-	-	0/4/4/4	0/0/0/0
5	GOL	A	508	-	-	0/4/4/4	0/0/0/0
2	HEM	B	501	1	-	0/6/54/54	0/0/8/8
3	1F1	B	502	-	-	0/0/4/4	0/2/2/2
3	1F1	B	503	-	-	0/0/4/4	0/2/2/2
4	SO4	B	504	-	-	0/0/0/0	0/0/0/0
5	GOL	B	505	-	-	0/4/4/4	0/0/0/0
5	GOL	B	506	-	-	0/4/4/4	0/0/0/0
5	GOL	B	507	-	-	0/4/4/4	0/0/0/0
2	HEM	C	501	1	-	0/6/54/54	0/0/8/8
3	1F1	C	502	-	-	0/0/4/4	0/2/2/2
3	1F1	C	503	-	-	0/0/4/4	0/2/2/2
4	SO4	C	504	-	-	0/0/0/0	0/0/0/0
4	SO4	C	505	-	-	0/0/0/0	0/0/0/0
4	SO4	C	506	-	-	0/0/0/0	0/0/0/0
5	GOL	C	507	-	-	0/4/4/4	0/0/0/0
3	1F1	D	501	-	-	0/0/4/4	0/2/2/2
2	HEM	D	502	1	-	0/6/54/54	0/0/8/8
3	1F1	D	503	-	-	0/0/4/4	0/2/2/2
4	SO4	D	504	-	-	0/0/0/0	0/0/0/0
4	SO4	D	505	-	-	0/0/0/0	0/0/0/0
5	GOL	D	506	-	-	0/4/4/4	0/0/0/0

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	1F1	C12-C11	-5.25	1.34	1.41
3	A	502	1F1	C12-C11	-4.96	1.34	1.41
2	A	501	HEM	C3B-C2B	-4.78	1.34	1.40
2	A	501	HEM	C3C-C2C	-4.53	1.34	1.40
2	C	501	HEM	C3C-C2C	-3.99	1.35	1.40
2	D	502	HEM	C3C-C2C	-3.67	1.35	1.40
2	B	501	HEM	C3C-C2C	-3.60	1.35	1.40
2	C	501	HEM	C3B-C2B	-3.46	1.35	1.40
3	C	502	1F1	C12-C11	-3.15	1.37	1.41
3	A	503	1F1	C12-C11	-3.03	1.37	1.41
3	B	502	1F1	C11-N10	-2.78	1.30	1.38
3	A	502	1F1	C6-C7	-2.43	1.36	1.41
2	B	501	HEM	C4C-NC	-2.27	1.34	1.36
2	D	502	HEM	C3B-C2B	-2.19	1.37	1.40
3	D	503	1F1	C12-C11	-2.08	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	1F1	C6-C5	2.01	1.40	1.36
3	A	503	1F1	C9-N10	2.05	1.46	1.37
2	A	501	HEM	C1D-ND	2.07	1.40	1.36
2	C	501	HEM	C1A-NA	2.08	1.40	1.36
3	B	502	1F1	C6-C5	2.09	1.41	1.36
2	A	501	HEM	C4D-ND	2.10	1.39	1.36
2	C	501	HEM	C1B-NB	2.15	1.39	1.36
3	D	503	1F1	C12-C4	2.17	1.43	1.38
2	D	502	HEM	CMD-C2D	2.19	1.56	1.51
3	B	503	1F1	C12-C4	2.26	1.43	1.38
2	C	501	HEM	CMB-C2B	2.27	1.56	1.51
2	C	501	HEM	C3D-C2D	2.30	1.44	1.37
3	A	502	1F1	C12-C4	2.41	1.44	1.38
2	A	501	HEM	C3C-CAC	2.44	1.52	1.47
2	A	501	HEM	CAA-C2A	2.46	1.56	1.52
3	D	501	1F1	C6-C5	2.50	1.41	1.36
3	D	503	1F1	C6-C5	2.50	1.41	1.36
3	C	502	1F1	C5-C4	2.52	1.44	1.39
2	B	501	HEM	CMC-C2C	2.55	1.57	1.51
3	D	501	1F1	C9-N10	2.55	1.49	1.37
3	B	503	1F1	C9-N10	2.56	1.49	1.37
2	A	501	HEM	CMD-C2D	2.57	1.56	1.51
3	B	502	1F1	C5-C4	2.60	1.44	1.39
3	D	503	1F1	C5-C4	2.69	1.45	1.39
2	C	501	HEM	C3C-CAC	2.74	1.53	1.47
2	D	502	HEM	CMA-C3A	2.75	1.57	1.51
3	D	501	1F1	C12-C4	2.79	1.44	1.38
2	B	501	HEM	CAD-C3D	2.92	1.57	1.52
2	B	501	HEM	CAA-C2A	2.94	1.57	1.52
2	B	501	HEM	C3D-C2D	3.01	1.46	1.37
2	A	501	HEM	C1B-NB	3.05	1.40	1.36
2	D	502	HEM	CAA-C2A	3.30	1.57	1.52
2	A	501	HEM	C3D-C2D	3.47	1.48	1.37
2	B	501	HEM	C1C-NC	3.48	1.40	1.36
2	B	501	HEM	C3B-CAB	3.49	1.54	1.47
2	B	501	HEM	C3C-CAC	3.50	1.54	1.47
2	C	501	HEM	C3B-CAB	3.51	1.54	1.47
3	C	503	1F1	C9-N10	3.55	1.53	1.37
2	D	502	HEM	C3D-C2D	3.76	1.48	1.37
2	D	502	HEM	C4C-NC	3.86	1.41	1.36
2	B	501	HEM	C1D-ND	4.09	1.44	1.36
2	A	501	HEM	CMC-C2C	4.16	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	1F1	C5-C4	4.30	1.48	1.39
2	D	502	HEM	C3B-CAB	4.37	1.56	1.47
2	D	502	HEM	C3C-CAC	4.80	1.57	1.47
2	B	501	HEM	C4D-ND	5.03	1.42	1.36
2	A	501	HEM	C3B-CAB	5.08	1.58	1.47

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	506	GOL	C3-C2-C1	-7.02	83.61	111.52
2	C	501	HEM	CBD-CAD-C3D	-6.28	100.48	112.47
2	D	502	HEM	CMA-C3A-C4A	-5.86	119.45	128.46
3	A	503	1F1	C5-C6-C7	-5.71	111.98	120.83
2	C	501	HEM	CAD-CBD-CGD	-4.68	104.67	112.66
2	D	502	HEM	CBD-CAD-C3D	-4.61	103.67	112.47
2	B	501	HEM	CBD-CAD-C3D	-4.52	103.84	112.47
3	C	502	1F1	C5-C6-C7	-4.48	113.89	120.83
2	A	501	HEM	CBD-CAD-C3D	-4.22	104.41	112.47
3	A	502	1F1	C8-C7-C6	-4.07	122.46	136.68
2	B	501	HEM	CMA-C3A-C4A	-3.96	122.38	128.46
2	A	501	HEM	CMA-C3A-C4A	-3.94	122.41	128.46
2	B	501	HEM	C1D-C2D-C3D	-3.85	104.32	107.00
2	A	501	HEM	C1D-C2D-C3D	-3.83	104.33	107.00
3	B	503	1F1	C5-C6-C7	-3.78	114.97	120.83
3	A	503	1F1	C8-C7-C6	-3.74	123.61	136.68
3	B	503	1F1	C8-C7-C6	-3.73	123.65	136.68
2	A	501	HEM	CAD-CBD-CGD	-3.53	106.63	112.66
3	D	501	1F1	C5-C4-C2	-3.34	115.97	120.45
2	B	501	HEM	CAA-CBA-CGA	-3.16	107.25	112.66
2	D	502	HEM	C3B-C4B-NB	-3.07	105.24	109.21
3	C	503	1F1	C8-C7-C6	-3.02	126.11	136.68
3	C	502	1F1	C8-C7-C6	-3.02	126.12	136.68
3	A	502	1F1	C5-C6-C7	-2.85	116.40	120.83
3	B	502	1F1	C5-C6-C7	-2.80	116.49	120.83
3	D	501	1F1	C8-C7-C6	-2.74	127.10	136.68
3	A	504	1F1	C8-C7-C6	-2.72	127.19	136.68
3	A	504	1F1	C5-C4-C2	-2.67	116.86	120.45
3	D	503	1F1	C8-C7-C6	-2.65	127.43	136.68
2	D	502	HEM	CAD-CBD-CGD	-2.60	108.21	112.66
5	B	506	GOL	O1-C1-C2	-2.50	97.48	110.07
3	C	502	1F1	C5-C4-C2	-2.43	117.19	120.45
3	B	502	1F1	C8-C7-C6	-2.37	128.38	136.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	1F1	C6-C5-C4	-2.34	117.27	121.13
2	A	501	HEM	C3C-C4C-NC	-2.31	106.59	110.94
4	D	505	SO4	O4-S-O3	-2.30	98.59	108.96
3	C	503	1F1	C5-C6-C7	-2.13	117.53	120.83
3	A	504	1F1	C5-C6-C7	-2.12	117.54	120.83
3	A	503	1F1	C12-C11-N10	-2.05	125.24	130.81
3	B	502	1F1	C12-C11-N10	-2.03	125.28	130.81
3	B	502	1F1	C5-C4-C2	-2.02	117.74	120.45
2	C	501	HEM	CMB-C2B-C3B	2.04	128.68	124.89
3	C	503	1F1	C5-C4-C12	2.09	121.33	118.19
3	C	502	1F1	C6-C7-C11	2.21	123.09	119.91
3	D	503	1F1	C8-C7-C11	2.24	108.12	106.20
3	B	502	1F1	C5-C4-C12	2.29	121.63	118.19
2	B	501	HEM	C3B-C4B-NB	2.32	112.20	109.21
3	B	503	1F1	C5-C4-C12	2.47	121.90	118.19
4	A	505	SO4	O2-S-O1	2.49	127.06	109.64
2	D	502	HEM	CMA-C3A-C2A	2.54	129.73	124.94
3	A	504	1F1	C5-C4-C12	2.63	122.14	118.19
3	C	502	1F1	C12-C11-C7	2.75	124.65	121.14
3	C	502	1F1	C5-C4-C12	2.82	122.43	118.19
3	D	503	1F1	C6-C7-C11	2.87	124.04	119.91
2	B	501	HEM	CMA-C3A-C2A	2.92	130.45	124.94
2	C	501	HEM	C4C-C3C-C2C	3.01	109.00	106.90
2	B	501	HEM	C4C-C3C-C2C	3.08	109.05	106.90
5	B	506	GOL	O2-C2-C3	3.27	124.27	108.84
3	B	503	1F1	C6-C7-C11	3.31	124.68	119.91
3	B	502	1F1	C8-C7-C11	3.38	109.09	106.20
2	C	501	HEM	C4A-C3A-C2A	3.49	109.42	107.00
2	A	501	HEM	CMC-C2C-C3C	3.57	131.51	124.89
2	A	501	HEM	C3B-C4B-NB	4.11	114.52	109.21
2	A	501	HEM	C4A-C3A-C2A	4.25	109.95	107.00
3	A	503	1F1	C8-C7-C11	4.30	109.88	106.20
3	A	502	1F1	C8-C7-C11	4.47	110.02	106.20
3	A	503	1F1	C6-C7-C11	4.53	126.44	119.91
3	A	503	1F1	C5-C4-C12	4.60	125.10	118.19
3	A	504	1F1	C8-C7-C11	4.87	110.36	106.20
3	A	502	1F1	C6-C7-C11	5.13	127.30	119.91
3	C	502	1F1	C8-C7-C11	5.30	110.73	106.20
2	D	502	HEM	C4A-C3A-C2A	5.47	110.81	107.00
3	C	503	1F1	C8-C7-C11	6.19	111.49	106.20
3	B	503	1F1	C8-C7-C11	6.40	111.67	106.20
3	D	501	1F1	C8-C7-C11	7.96	113.00	106.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	4	0
2	B	501	HEM	5	0
3	B	502	1F1	1	0
3	B	503	1F1	2	0
5	B	506	GOL	2	0
2	C	501	HEM	5	0
3	C	502	1F1	2	0
3	C	503	1F1	1	0
3	D	501	1F1	1	0
2	D	502	HEM	3	0
3	D	503	1F1	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	393/410 (95%)	-0.19	2 (0%) 90 93	12, 18, 30, 38	0
1	B	393/410 (95%)	-0.12	5 (1%) 77 84	11, 19, 31, 42	0
1	C	393/410 (95%)	-0.10	5 (1%) 77 84	14, 21, 33, 41	0
1	D	393/410 (95%)	0.14	9 (2%) 61 68	15, 25, 39, 54	0
All	All	1572/1640 (95%)	-0.07	21 (1%) 77 84	11, 21, 35, 54	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	409	ALA	4.6
1	C	295	VAL	3.6
1	D	17	THR	3.4
1	D	279	THR	3.2
1	A	409	ALA	3.0
1	D	89	LYS	3.0
1	B	17	THR	2.7
1	C	17	THR	2.6
1	B	250	LEU	2.6
1	A	250	LEU	2.5
1	D	217	PRO	2.3
1	C	309	GLY	2.3
1	D	276	SER	2.3
1	D	123	THR	2.1
1	B	409	ALA	2.1
1	D	198	ARG	2.1
1	C	122	LYS	2.1
1	C	280	LEU	2.1
1	B	223	CYS	2.0
1	B	122	LYS	2.0
1	D	278	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	C	506	5/5	0.86	0.45	46.49	30,30,30,30	0
4	SO4	A	506	5/5	0.90	0.28	8.52	30,30,30,30	0
5	GOL	B	506	6/6	0.83	0.16	8.45	32,35,38,40	0
3	1F1	C	503	12/12	0.68	0.26	6.40	74,77,78,79	0
3	1F1	B	503	12/12	0.68	0.26	5.93	38,43,52,57	0
3	1F1	A	504	12/12	0.92	0.13	3.79	23,31,46,49	0
3	1F1	A	503	12/12	0.82	0.22	3.35	40,45,58,59	0
3	1F1	D	501	12/12	0.78	0.15	2.84	48,50,53,56	0
4	SO4	D	505	5/5	0.93	0.12	2.13	46,52,54,58	0
4	SO4	C	505	5/5	0.98	0.07	1.83	36,39,45,47	0
3	1F1	D	503	12/12	0.96	0.12	1.16	16,21,22,24	0
2	HEM	C	501	43/43	0.99	0.14	0.90	12,16,18,21	0
2	HEM	D	502	43/43	0.98	0.12	0.87	12,18,22,24	0
2	HEM	B	501	43/43	0.99	0.10	0.24	10,13,15,19	0
2	HEM	A	501	43/43	0.99	0.10	0.21	10,13,15,17	0
3	1F1	C	502	12/12	0.98	0.10	0.17	15,17,19,20	0
5	GOL	B	505	6/6	0.96	0.07	-0.29	18,21,24,34	0
3	1F1	B	502	12/12	0.98	0.08	-0.45	11,13,15,15	0
5	GOL	C	507	6/6	0.97	0.07	-0.47	22,25,29,35	0
5	GOL	D	506	6/6	0.94	0.08	-0.50	21,33,36,37	0
5	GOL	A	507	6/6	0.96	0.07	-0.50	20,23,28,32	0
3	1F1	A	502	12/12	0.99	0.08	-1.50	10,14,15,17	0
6	CL	D	507	1/1	0.97	0.06	-	32,32,32,32	0
4	SO4	B	504	5/5	0.99	0.05	-	22,23,27,27	0
4	SO4	D	504	5/5	0.98	0.09	-	33,37,40,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CL	C	508	1/1	0.99	0.04	-	27,27,27,27	0
6	CL	B	508	1/1	0.98	0.07	-	18,18,18,18	0
4	SO4	C	504	5/5	0.99	0.06	-	24,24,26,27	0
4	SO4	A	505	5/5	0.97	0.07	-	24,32,37,38	0
5	GOL	B	507	6/6	0.90	0.23	-	31,45,52,55	0
5	GOL	A	508	6/6	0.88	0.26	-	38,52,54,58	0
6	CL	A	509	1/1	0.99	0.07	-	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.