



# Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 06:49 PM GMT

PDB ID : 1CF9  
Title : Structure of the mutant VAL169CYS of catalase HP11 from Escherichia coli  
Authors : Mate, M.J.; Loewen, P.C.; Fita, I.  
Deposited on : 1999-03-24  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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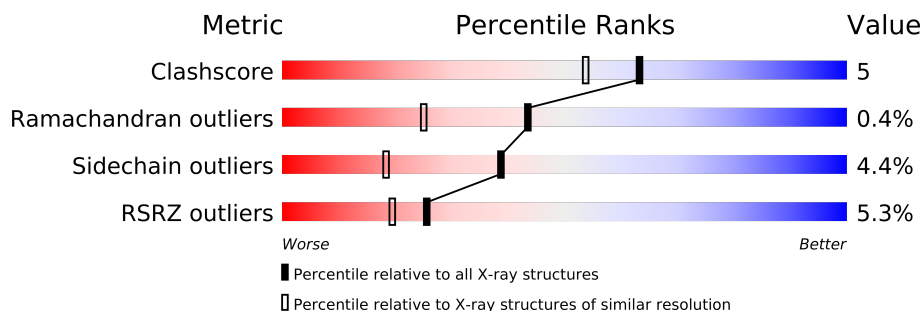
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : trunk22714  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk22714

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	753	
1	B	753	
1	C	753	
1	D	753	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25850 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (CATALASE HP11).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	1	0
			5748	3649	1005	1081	13			
1	B	727	Total	C	N	O	S	0	1	0
			5748	3649	1005	1081	13			
1	C	727	Total	C	N	O	S	0	1	0
			5748	3649	1005	1081	13			
1	D	727	Total	C	N	O	S	0	1	0
			5748	3649	1005	1081	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	CYS	VAL	MUTATION	UNP P21179
B	169	CYS	VAL	MUTATION	UNP P21179
C	169	CYS	VAL	MUTATION	UNP P21179
D	169	CYS	VAL	MUTATION	UNP P21179

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
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 water.

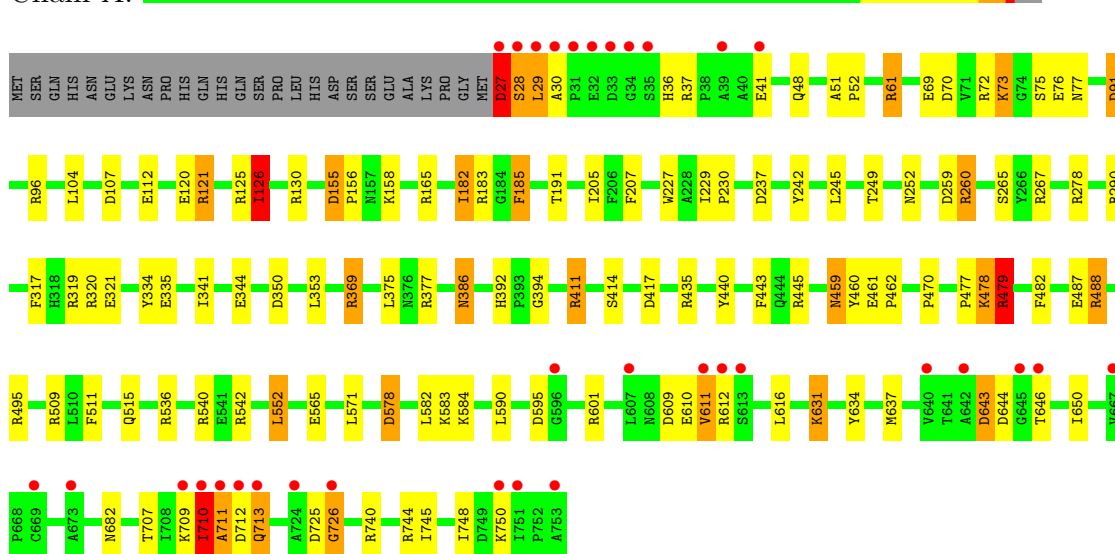
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	727	Total	O	0	0
			727	727		
3	B	616	Total	O	0	0
			616	616		
3	C	638	Total	O	0	0
			638	638		
3	D	705	Total	O	0	0
			705	705		

### 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 ( $RSRZ > 2$ ). 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.

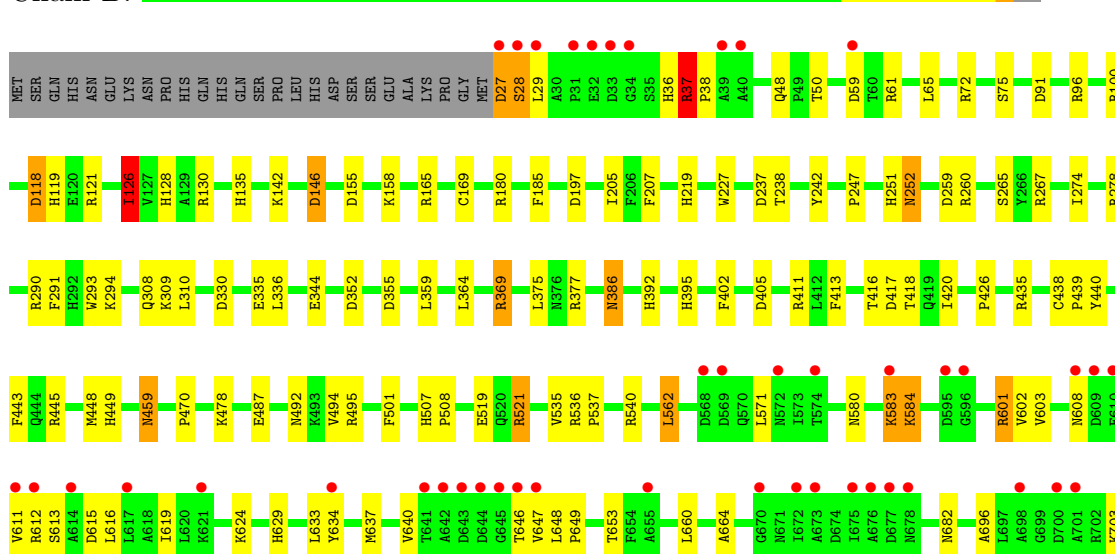
#### • Molecule 1: PROTEIN (CATALASE HP1I)

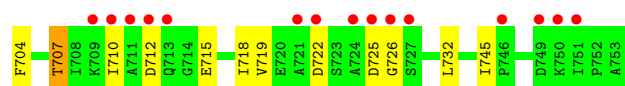
Chain A:



#### • Molecule 1: PROTEIN (CATALASE HP1I)

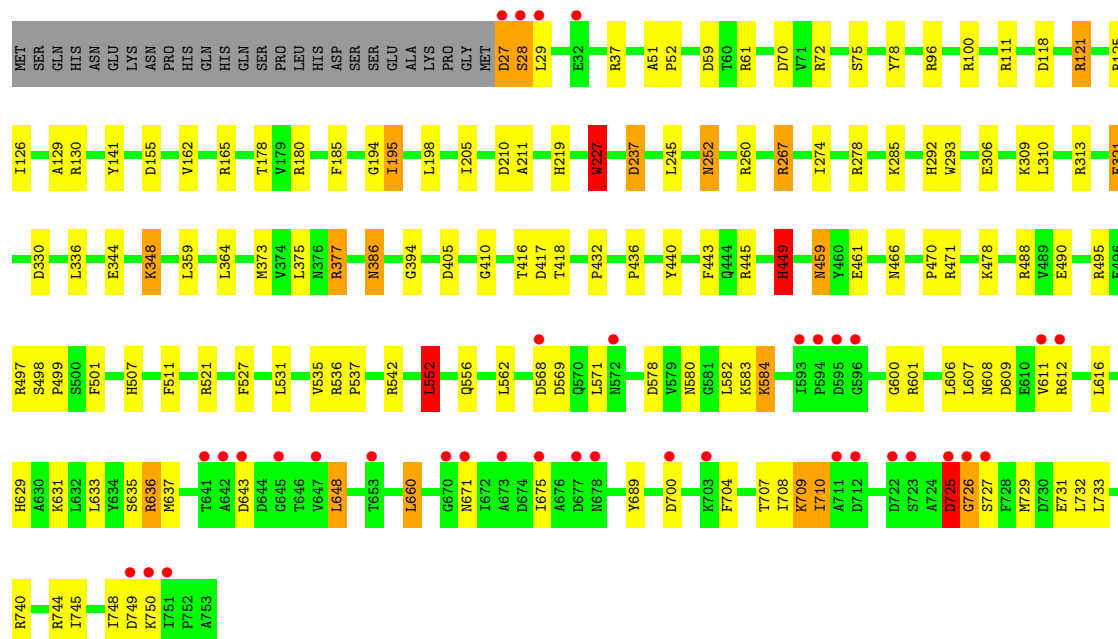
Chain B:





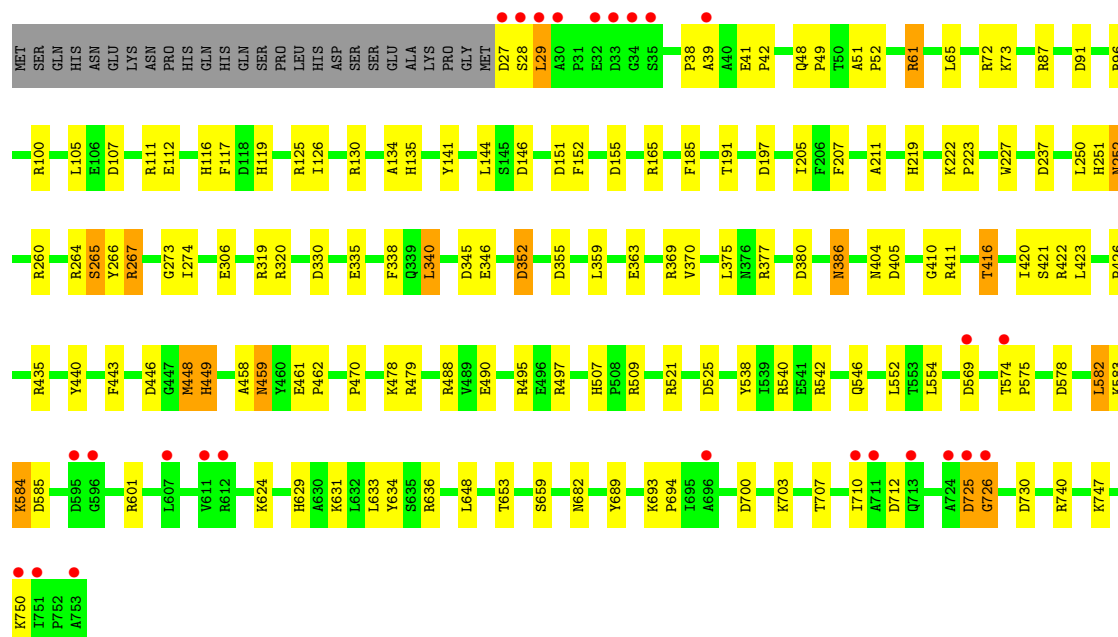
• Molecule 1: PROTEIN (CATALASE HP1I)

Chain C:



• Molecule 1: PROTEIN (CATALASE HP1I)

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.47Å 133.04Å 122.22Å 90.00° 109.64° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.76 – 1.77	Depositor EDS
% Data completeness (in resolution range)	88.3 (20.00-1.80) 83.6 (19.76-1.77)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	9.00	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 1.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.181 , 0.237 0.182 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.5	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 228159 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	25850	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.75	1/5908 (0.0%)	1.69	91/8033 (1.1%)
1	B	0.72	0/5908	1.49	61/8033 (0.8%)
1	C	0.74	0/5908	1.51	68/8033 (0.8%)
1	D	0.71	0/5908	1.50	74/8033 (0.9%)
All	All	0.73	1/23632 (0.0%)	1.55	294/32132 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	4
1	C	1	2
1	D	0	2
All	All	3	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	SER	N-CA	-5.46	1.35	1.46

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	ARG	NE-CZ-NH2	-50.60	95.00	120.30
1	A	479	ARG	NE-CZ-NH1	35.58	138.09	120.30
1	B	377	ARG	CD-NE-CZ	22.63	155.28	123.60
1	A	61	ARG	NE-CZ-NH1	-19.53	110.53	120.30
1	C	180	ARG	NE-CZ-NH1	16.75	128.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	377	ARG	NE-CZ-NH2	-16.30	112.15	120.30
1	C	725	ASP	N-CA-CB	15.90	139.23	110.60
1	C	445	ARG	NE-CZ-NH1	15.59	128.10	120.30
1	B	61	ARG	CD-NE-CZ	15.26	144.97	123.60
1	A	27	ASP	O-C-N	-15.16	98.44	122.70
1	B	495	ARG	NE-CZ-NH1	14.13	127.37	120.30
1	D	61	ARG	CD-NE-CZ	13.80	142.92	123.60
1	D	495	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	D	497	ARG	NE-CZ-NH1	13.62	127.11	120.30
1	D	725	ASP	CA-CB-CG	13.60	143.32	113.40
1	D	740	ARG	NE-CZ-NH1	13.45	127.03	120.30
1	A	710	ILE	CB-CA-C	13.40	138.40	111.60
1	C	72	ARG	NE-CZ-NH2	-13.19	113.70	120.30
1	D	260	ARG	NE-CZ-NH2	-13.17	113.72	120.30
1	B	61	ARG	NE-CZ-NH1	12.97	126.78	120.30
1	C	636	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	B	61	ARG	NE-CZ-NH2	-12.09	114.26	120.30
1	D	740	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	B	445	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	D	112	GLU	OE1-CD-OE2	11.40	136.98	123.30
1	A	740	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	D	636	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	C	521	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	D	100	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	B	290	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	A	27	ASP	CA-C-N	10.31	139.89	117.20
1	D	497	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	D	320	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	C	536	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	B	435	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	C	471	ARG	NE-CZ-NH2	9.79	125.20	120.30
1	C	96	ARG	NE-CZ-NH2	-9.79	115.40	120.30
1	C	377	ARG	NE-CZ-NH1	-9.78	115.41	120.30
1	A	319	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	C	636	ARG	CD-NE-CZ	9.68	137.15	123.60
1	D	96	ARG	NE-CZ-NH1	9.55	125.07	120.30
1	A	27	ASP	CA-CB-CG	9.43	134.14	113.40
1	A	344	GLU	CA-CB-CG	9.42	134.12	113.40
1	D	107	ASP	CB-CG-OD2	9.39	126.75	118.30
1	B	72	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	A	130	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	B	417	ASP	CB-CG-OD2	-9.07	110.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	PHE	CB-CG-CD2	-9.00	114.50	120.80
1	B	411	ARG	NE-CZ-NH2	8.97	124.78	120.30
1	D	377	ARG	NH1-CZ-NH2	8.97	129.27	119.40
1	A	712	ASP	CB-CA-C	8.94	128.28	110.40
1	C	180	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	C	141	TYR	CB-CG-CD2	-8.77	115.74	121.00
1	C	130	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	A	495	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	D	320	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	536	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	740	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	C	278	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	28	SER	C-N-CA	-8.39	100.71	121.70
1	A	350	ASP	CB-CG-OD1	-8.39	110.75	118.30
1	A	61	ARG	CD-NE-CZ	-8.38	111.87	123.60
1	A	29	LEU	N-CA-C	8.36	133.58	111.00
1	D	146	ASP	CB-CG-OD1	8.30	125.77	118.30
1	D	155	ASP	CB-CG-OD1	8.28	125.75	118.30
1	C	490	GLU	OE1-CD-OE2	-8.25	113.39	123.30
1	D	542	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	435	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	A	609	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	A	411	ARG	NE-CZ-NH2	8.05	124.32	120.30
1	D	601	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	C	471	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	A	265	SER	N-CA-CB	-7.92	98.62	110.50
1	C	636	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	C	100	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	712	ASP	N-CA-CB	-7.85	96.47	110.60
1	A	744	ARG	NE-CZ-NH1	-7.85	116.38	120.30
1	A	260	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	C	700	ASP	CB-CG-OD1	7.75	125.27	118.30
1	A	601	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	C	740	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	C	449	HIS	CA-CB-CG	-7.64	100.61	113.60
1	A	267	ARG	CD-NE-CZ	7.62	134.27	123.60
1	C	278	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	417	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	D	411	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	C	121	ARG	CD-NE-CZ	7.55	134.17	123.60
1	B	521	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	C	405	ASP	CB-CG-OD2	7.53	125.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	B	180	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	369	ARG	CD-NE-CZ	7.47	134.05	123.60
1	A	112	GLU	OE1-CD-OE2	7.30	132.06	123.30
1	A	445	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	D	265	SER	N-CA-CB	-7.28	99.58	110.50
1	A	290	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	D	319	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	185	PHE	CB-CG-CD1	7.22	125.86	120.80
1	B	37	ARG	CD-NE-CZ	7.20	133.68	123.60
1	A	445	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	118	ASP	CB-CG-OD1	7.14	124.72	118.30
1	B	242	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	B	377	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	350	ASP	CB-CA-C	7.06	124.52	110.40
1	D	497	ARG	CD-NE-CZ	7.05	133.48	123.60
1	C	155	ASP	CB-CG-OD1	7.03	124.63	118.30
1	A	725	ASP	CB-CG-OD1	6.95	124.55	118.30
1	B	501	PHE	CB-CG-CD2	-6.93	115.95	120.80
1	C	601	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	643	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	121	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	C	542	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	C	495	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	449	HIS	CA-CB-CG	6.86	125.25	113.60
1	D	130	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	96	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	B	96	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	479	ARG	NH1-CZ-NH2	6.78	126.86	119.40
1	A	61	ARG	NH1-CZ-NH2	6.78	126.86	119.40
1	C	725	ASP	CA-C-O	-6.78	105.87	120.10
1	D	585	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	488	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	445	ARG	NH1-CZ-NH2	-6.76	111.97	119.40
1	A	183	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	D	72	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	A	344	GLU	OE1-CD-OE2	-6.67	115.30	123.30
1	C	377	ARG	NH1-CZ-NH2	6.62	126.69	119.40
1	A	259	ASP	CB-CG-OD1	6.62	124.26	118.30
1	B	352	ASP	CB-CG-OD1	6.62	124.26	118.30
1	C	744	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	C	141	TYR	CB-CG-CD1	6.59	124.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	488	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	D	152	PHE	CB-CG-CD2	-6.54	116.22	120.80
1	B	130	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	D	540	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	D	306	GLU	OE1-CD-OE2	-6.50	115.50	123.30
1	A	488	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	C	306	GLU	CA-CB-CG	6.46	127.62	113.40
1	A	713	GLN	N-CA-CB	-6.44	99.00	110.60
1	D	352	ASP	CB-CG-OD1	6.41	124.07	118.30
1	D	264	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	709	LYS	C-N-CA	-6.38	105.75	121.70
1	A	377	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	612	ARG	CB-CA-C	6.35	123.10	110.40
1	C	609	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	69	GLU	OE1-CD-OE2	-6.33	115.71	123.30
1	D	509	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	72	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	207	PHE	CB-CG-CD2	-6.28	116.40	120.80
1	B	72	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	369	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	578	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	405	ASP	CB-CG-OD2	6.25	123.92	118.30
1	D	197	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	259	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	644	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	501	PHE	CB-CG-CD1	6.23	125.16	120.80
1	D	435	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	D	448	MET	CG-SD-CE	6.16	110.05	100.20
1	D	96	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	D	446	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	182	ILE	CA-CB-CG1	-6.14	99.34	111.00
1	B	59	ASP	CB-CA-C	-6.13	98.14	110.40
1	B	146	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	121	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	291	PHE	CB-CG-CD2	6.10	125.07	120.80
1	B	369	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	D	458	ALA	CB-CA-C	-6.10	100.95	110.10
1	D	380	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	320	ARG	CD-NE-CZ	6.06	132.09	123.60
1	A	612	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	D	61	ARG	CB-CG-CD	6.00	127.21	111.60
1	A	637	MET	CG-SD-CE	5.99	109.79	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	ARG	CB-CA-C	-5.96	98.49	110.40
1	A	107	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	611	VAL	CB-CA-C	-5.92	100.16	111.40
1	C	260	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	D	525	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	130	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	521	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	59	ASP	N-CA-CB	5.86	121.16	110.60
1	C	267	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	D	416	THR	CA-CB-CG2	5.84	120.58	112.40
1	A	320	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	538	TYR	CB-CG-CD1	-5.81	117.51	121.00
1	C	497	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	B	100	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	100	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	355	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	29	LEU	CB-CA-C	5.73	121.09	110.20
1	D	631	LYS	CA-CB-CG	5.70	125.94	113.40
1	A	509	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	C	631	LYS	N-CA-CB	5.64	120.76	110.60
1	C	37	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	521	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	B	487	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	C	70	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	178	THR	CA-CB-CG2	-5.60	104.56	112.40
1	C	511	PHE	CB-CG-CD1	-5.59	116.88	120.80
1	B	601	ARG	CA-CB-CG	5.59	125.69	113.40
1	D	111	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	C	495	ARG	CD-NE-CZ	5.57	131.39	123.60
1	B	602	VAL	CB-CA-C	-5.57	100.82	111.40
1	C	59	ASP	CB-CG-OD1	5.56	123.31	118.30
1	D	479	ARG	CD-NE-CZ	5.55	131.37	123.60
1	A	495	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	490	GLU	OE1-CD-OE2	-5.53	116.66	123.30
1	D	134	ALA	CB-CA-C	-5.53	101.80	110.10
1	C	78	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	A	72	ARG	N-CA-CB	5.53	120.55	110.60
1	C	260	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	B	725	ASP	N-CA-CB	-5.50	100.69	110.60
1	B	725	ASP	CB-CA-C	-5.50	99.40	110.40
1	A	540	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	155	ASP	CB-CG-OD2	-5.49	113.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	PHE	CB-CG-CD1	5.49	124.64	120.80
1	C	501	PHE	CB-CG-CD2	-5.49	116.96	120.80
1	D	141	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	A	28	SER	CA-C-N	-5.48	105.14	117.20
1	C	648	LEU	CA-CB-CG	5.47	127.89	115.30
1	D	100	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
1	C	194	GLY	CA-C-O	5.47	130.44	120.60
1	A	377	ARG	CA-CB-CG	-5.46	101.40	113.40
1	A	48	GLN	CA-CB-CG	5.45	125.39	113.40
1	B	72	ARG	CD-NE-CZ	5.45	131.23	123.60
1	D	125	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	210	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	126[A]	ILE	CB-CA-C	5.42	122.45	111.60
1	A	126[B]	ILE	CB-CA-C	5.42	122.45	111.60
1	C	542	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
1	D	91	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	260	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	C	59	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	D	422	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	C	111	ARG	CD-NE-CZ	5.37	131.11	123.60
1	A	414	SER	N-CA-CB	-5.37	102.45	110.50
1	B	207	PHE	O-C-N	-5.37	114.12	122.70
1	C	643	ASP	CB-CG-OD1	5.36	123.13	118.30
1	D	355	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	100	ARG	CD-NE-CZ	5.33	131.06	123.60
1	B	519	GLU	OE1-CD-OE2	-5.32	116.92	123.30
1	C	710	ILE	CB-CA-C	-5.31	100.98	111.60
1	D	346	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	A	542	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	130	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	479	ARG	CG-CD-NE	-5.28	100.72	111.80
1	A	61	ARG	CB-CG-CD	-5.26	97.91	111.60
1	D	151	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	644	ASP	OD1-CG-OD2	-5.26	113.31	123.30
1	A	536	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	C	552	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	121	ARG	CD-NE-CZ	5.23	130.92	123.60
1	B	640	VAL	N-CA-CB	5.23	123.00	111.50
1	D	345	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	237	ASP	CB-CG-OD1	-5.22	113.61	118.30
1	B	290	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	C	501	PHE	CB-CG-CD1	5.21	124.45	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	659	SER	N-CA-CB	5.21	118.31	110.50
1	B	259	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	435	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	707	THR	N-CA-CB	5.19	120.16	110.30
1	A	41	GLU	CA-CB-CG	5.19	124.81	113.40
1	D	266	TYR	CB-CG-CD2	-5.17	117.89	121.00
1	D	421	SER	N-CA-CB	5.17	118.25	110.50
1	B	704	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	A	125	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	411	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	402	PHE	CB-CG-CD1	-5.15	117.19	120.80
1	D	725	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	479	ARG	CA-CB-CG	5.14	124.70	113.40
1	B	494	VAL	CB-CA-C	-5.12	101.68	111.40
1	A	646	THR	N-CA-CB	5.12	120.02	110.30
1	B	27	ASP	CA-C-N	-5.11	105.96	117.20
1	C	601	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	87	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	A	488	ARG	CD-NE-CZ	-5.10	116.45	123.60
1	A	595	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	207	PHE	O-C-N	-5.09	114.55	122.70
1	B	126[A]	ILE	CB-CA-C	5.08	121.77	111.60
1	B	126[B]	ILE	CB-CA-C	5.08	121.77	111.60
1	A	91	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	B	242	TYR	CD1-CE1-CZ	-5.08	115.23	119.80
1	B	495	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
1	C	292	HIS	CB-CA-C	-5.08	100.24	110.40
1	C	445	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
1	A	711	ALA	CA-C-O	5.08	130.76	120.10
1	A	28	SER	N-CA-CB	5.07	118.11	110.50
1	B	601	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	C	227	TRP	CA-CB-CG	5.06	123.32	113.70
1	D	267	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	A	242	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	B	100	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	334	TYR	CG-CD2-CE2	-5.02	117.28	121.30
1	B	540	ARG	NE-CZ-NH1	-5.00	117.80	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	28	SER	CA

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Mol	Chain	Res	Type	Atom
1	A	29	LEU	CA
1	C	725	ASP	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	ASP	Mainchain,Peptide
1	A	394	GLY	Mainchain
1	A	710	ILE	Mainchain
1	C	394	GLY	Mainchain
1	C	725	ASP	Mainchain
1	D	273	GLY	Mainchain
1	D	423	LEU	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5748	0	5580	62	5
1	B	5748	0	5580	92	1
1	C	5748	0	5580	65	0
1	D	5748	0	5580	65	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	727	0	0	10	0
3	B	616	0	0	17	5
3	C	638	0	0	6	1
3	D	705	0	0	9	0
All	All	25850	0	22440	250	6

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (250) close contacts within the same asymmetric unit are listed below.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:126[B]:ILE:HD12	2:B:754:HEM:HMD1	1.43	0.99
1:C:126[B]:ILE:HD12	2:C:754:HEM:HMD1	1.48	0.96
1:D:39:ALA:H	1:D:48:GLN:HE21	1.16	0.93
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.59	0.84
1:A:28:SER:O	1:A:29:LEU:HG	1.77	0.84
1:D:39:ALA:H	1:D:48:GLN:NE2	1.77	0.81
1:B:583:LYS:HE2	1:B:583:LYS:H	1.45	0.81
1:C:27:ASP:O	1:C:28:SER:HB2	1.80	0.81
1:D:267:ARG:HG3	3:D:1243:HOH:O	1.83	0.79
1:B:309:LYS:HG3	3:B:1353:HOH:O	1.83	0.78
1:C:310:LEU:HD13	1:C:660:LEU:HB3	1.65	0.77
1:A:126[A]:ILE:HD12	1:D:117:PHE:CZ	2.20	0.76
1:B:126[A]:ILE:HD13	1:C:121:ARG:NH2	2.00	0.75
1:C:267:ARG:HH12	1:C:600:GLY:HA3	1.51	0.75
1:C:527:PHE:O	1:C:531:LEU:HD13	1.87	0.74
1:B:267:ARG:HG3	3:B:1361:HOH:O	1.87	0.74
1:B:310:LEU:HD13	1:B:660:LEU:HB3	1.70	0.74
1:B:603:VAL:HG22	1:B:664:ALA:HB3	1.69	0.74
1:A:479:ARG:NH1	1:A:479:ARG:HG2	2.05	0.71
1:A:488:ARG:HH11	1:B:492:ASN:ND2	1.88	0.71
1:A:29:LEU:HD23	1:A:30:ALA:O	1.91	0.71
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.71	0.70
1:C:267:ARG:HD2	3:C:998:HOH:O	1.89	0.70
1:D:386:ASN:C	1:D:386:ASN:HD22	1.95	0.69
1:A:611:VAL:HG23	3:A:1053:HOH:O	1.92	0.69
1:D:725:ASP:O	3:D:1208:HOH:O	2.11	0.69
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.76	0.68
1:A:726:GLY:HA3	3:A:1399:HOH:O	1.94	0.68
1:B:386:ASN:C	1:B:386:ASN:HD22	1.98	0.67
1:B:449:HIS:ND1	3:B:1357:HOH:O	2.26	0.67
1:B:309:LYS:HG2	1:B:660:LEU:HD11	1.76	0.66
1:C:309:LYS:HE2	3:C:1387:HOH:O	1.97	0.65
1:A:245:LEU:HD22	1:D:29:LEU:HD13	1.79	0.65
1:D:448:MET:HG2	3:D:1457:HOH:O	1.97	0.65
1:B:37:ARG:HD2	3:B:1367:HOH:O	1.99	0.63
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.80	0.63
1:D:126[A]:ILE:HG22	2:D:754:HEM:HMD1	1.81	0.62
1:C:607:LEU:HD22	1:C:611:VAL:HG21	1.82	0.62
1:B:583:LYS:CE	1:B:583:LYS:H	2.13	0.62
1:A:488:ARG:HH11	1:B:492:ASN:HD21	1.46	0.62
1:B:710:ILE:HG23	1:B:715:GLU:HG2	1.82	0.61
1:C:386:ASN:HD22	1:C:386:ASN:C	2.04	0.61
1:B:449:HIS:NE2	3:B:1356:HOH:O	2.31	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:126[A]:ILE:CG2	2:D:754:HEM:HMD1	2.31	0.61
1:D:375:LEU:N	1:D:375:LEU:HD12	2.15	0.60
1:B:29:LEU:HD13	1:C:245:LEU:HD22	1.82	0.60
1:A:126[B]:ILE:HD11	3:D:1453:HOH:O	2.01	0.60
1:C:704:PHE:O	1:C:707:THR:HG22	2.02	0.60
1:B:448:MET:HE3	3:B:1358:HOH:O	2.02	0.60
1:B:126[B]:ILE:CD1	2:B:754:HEM:HMD1	2.26	0.59
1:C:578:ASP:HB2	1:C:582:LEU:O	2.01	0.59
1:B:583:LYS:O	1:B:584:LYS:HB3	2.02	0.59
1:A:317:PHE:O	1:A:321:GLU:HB2	2.04	0.57
1:A:121:ARG:HG2	1:D:126[B]:ILE:HD13	1.87	0.57
1:A:488:ARG:NH1	1:B:492:ASN:ND2	2.53	0.57
1:B:75:SER:HA	3:B:1368:HOH:O	2.04	0.56
1:B:344:GLU:H	1:B:344:GLU:CD	2.08	0.56
1:A:488:ARG:NH1	1:B:492:ASN:HD21	2.04	0.56
1:D:726:GLY:O	1:D:730:ASP:OD1	2.24	0.56
1:A:28:SER:CB	3:A:1359:HOH:O	2.54	0.56
1:A:182:ILE:HD12	1:A:207:PHE:CE2	2.40	0.56
1:A:27:ASP:HB3	1:A:28:SER:OG	2.07	0.55
1:A:73:LYS:HE2	3:C:951:HOH:O	2.05	0.55
1:B:126[B]:ILE:CD1	1:C:118:ASP:HA	2.37	0.55
1:A:386:ASN:C	1:A:386:ASN:HD22	2.09	0.55
1:D:420:ILE:HD12	1:D:426:PRO:HA	1.89	0.54
1:B:126[B]:ILE:HD11	1:B:418:THR:OG1	2.08	0.54
1:A:461:GLU:HA	1:A:462:PRO:C	2.28	0.54
1:B:330:ASP:OD2	1:B:629:HIS:HE1	1.91	0.54
1:D:39:ALA:N	1:D:48:GLN:HE21	1.96	0.54
1:B:449:HIS:CE1	3:B:1356:HOH:O	2.61	0.53
1:C:359:LEU:H	1:C:507:HIS:HD2	1.56	0.53
3:A:1474:HOH:O	1:D:126[B]:ILE:HD11	2.08	0.53
1:B:646:THR:HA	3:B:1145:HOH:O	2.08	0.53
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.44	0.53
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.44	0.53
1:A:278:ARG:HH22	1:A:487:GLU:CD	2.12	0.52
1:C:165:ARG:HE	1:C:386:ASN:HD21	1.57	0.52
1:A:583:LYS:O	1:A:584:LYS:HB3	2.08	0.52
1:A:552:LEU:HD21	1:A:571:LEU:O	2.10	0.52
1:D:578:ASP:HB3	1:D:582:LEU:O	2.09	0.52
1:D:416:THR:HG23	3:D:1355:HOH:O	2.08	0.52
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.44	0.52
1:C:583:LYS:O	1:C:584:LYS:HB3	2.09	0.52
1:B:165:ARG:HE	1:B:386:ASN:HD21	1.57	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.25	0.52
1:A:707:THR:HG23	3:A:1402:HOH:O	2.09	0.52
1:B:155:ASP:HB3	1:B:158:LYS:HG3	1.92	0.52
1:B:126[B]:ILE:HD13	1:C:118:ASP:HA	1.90	0.52
1:B:38:PRO:HA	1:B:48:GLN:OE1	2.10	0.52
1:B:562:LEU:HA	1:C:637:MET:HB2	1.91	0.52
1:B:624:LYS:HB2	3:B:1060:HOH:O	2.09	0.52
1:B:126[B]:ILE:HD12	2:B:754:HEM:CMD	2.30	0.51
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.93	0.51
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.92	0.51
1:A:28:SER:HB2	3:A:1359:HOH:O	2.08	0.51
1:D:700:ASP:O	1:D:703:LYS:HG3	2.10	0.51
1:D:359:LEU:H	1:D:507:HIS:HD2	1.58	0.51
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.91	0.51
3:B:1357:HOH:O	1:D:449:HIS:CE1	2.63	0.51
1:D:689:TYR:CE1	1:D:710:ILE:HD11	2.46	0.51
1:D:634:TYR:O	1:D:653:THR:HA	2.11	0.51
1:C:416:THR:HA	3:C:1381:HOH:O	2.11	0.51
1:C:126[B]:ILE:HD11	1:C:418:THR:OG1	2.11	0.51
1:A:165:ARG:HE	1:A:386:ASN:HD21	1.58	0.51
1:B:637:MET:HB2	1:C:562:LEU:HA	1.93	0.51
1:B:118:ASP:HA	1:C:126[B]:ILE:CD1	2.42	0.50
1:A:70:ASP:OD2	3:A:1479:HOH:O	2.19	0.50
1:C:725:ASP:O	1:C:726:GLY:C	2.49	0.50
1:B:682:ASN:OD1	1:B:707:THR:HG21	2.12	0.50
1:D:165:ARG:HE	1:D:386:ASN:HD21	1.59	0.49
1:B:274:ILE:HD12	2:B:754:HEM:HMB1	1.94	0.49
1:A:120:GLU:HB2	1:D:126[A]:ILE:CD1	2.41	0.49
1:D:363:GLU:HB2	1:D:582:LEU:HD21	1.94	0.49
1:B:521:ARG:HE	1:B:745:ILE:HG21	1.78	0.49
3:B:924:HOH:O	1:D:52:PRO:HG3	2.11	0.49
1:A:28:SER:O	1:A:29:LEU:CG	2.55	0.49
1:A:36:HIS:CD2	1:A:36:HIS:H	2.31	0.49
1:B:413:PHE:HB2	1:D:105:LEU:HD11	1.94	0.48
1:D:750:LYS:HG3	1:D:750:LYS:O	2.14	0.48
1:A:411:ARG:HG2	2:A:754:HEM:C2C	2.49	0.48
1:A:745:ILE:O	1:A:748:ILE:HG12	2.14	0.48
1:B:416:THR:HA	3:B:1370:HOH:O	2.13	0.48
1:B:308:GLN:OE1	1:C:313:ARG:NH1	2.43	0.48
1:B:267:ARG:HD2	3:B:976:HOH:O	2.13	0.48
1:B:583:LYS:CD	1:B:583:LYS:H	2.26	0.48
1:C:729:MET:O	1:C:733:LEU:HD13	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:479:ARG:HH11	1:A:479:ARG:HG2	1.79	0.47
1:B:27:ASP:O	1:B:28:SER:HB2	2.14	0.47
1:D:330:ASP:OD2	1:D:629:HIS:HE1	1.97	0.47
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.36	0.47
1:B:126[A]:ILE:HD13	1:C:121:ARG:CZ	2.44	0.47
1:B:29:LEU:HD13	1:C:245:LEU:HD13	1.96	0.47
1:B:634:TYR:O	1:B:653:THR:HA	2.15	0.47
1:B:293:TRP:CZ3	1:B:336:LEU:HB2	2.50	0.47
1:C:745:ILE:O	1:C:748:ILE:HG12	2.15	0.47
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.45	0.47
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.97	0.46
1:B:50:THR:HG21	1:C:227:TRP:CZ3	2.50	0.46
1:B:395:HIS:HE1	3:D:1445:HOH:O	1.97	0.46
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.30	0.46
1:A:51:ALA:HB1	1:A:52:PRO:CD	2.44	0.46
1:C:364:LEU:HD11	1:C:580:ASN:HB2	1.97	0.46
1:C:330:ASP:OD2	1:C:629:HIS:HE1	1.99	0.46
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.51	0.46
1:C:727:SER:O	1:C:731:GLU:HG3	2.15	0.46
1:B:535:VAL:O	1:B:537:PRO:HD3	2.15	0.46
1:B:36:HIS:CD2	1:B:37:ARG:HE	2.34	0.46
1:D:725:ASP:O	1:D:726:GLY:C	2.54	0.46
1:B:359:LEU:H	1:B:507:HIS:HD2	1.63	0.46
1:A:126[A]:ILE:HG22	2:A:754:HEM:HMD1	1.97	0.45
1:D:629:HIS:HD2	3:D:1068:HOH:O	1.99	0.45
1:B:165:ARG:HE	1:B:386:ASN:ND2	2.14	0.45
1:A:335:GLU:OE1	1:A:369:ARG:HG3	2.17	0.45
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.98	0.45
1:B:420:ILE:HG21	1:D:119:HIS:CE1	2.51	0.45
1:B:448:MET:HG2	3:B:1358:HOH:O	2.17	0.45
1:B:521:ARG:NE	1:B:745:ILE:HG21	2.32	0.45
1:C:732:LEU:C	1:C:732:LEU:HD13	2.37	0.45
1:D:747:LYS:NZ	3:D:1349:HOH:O	2.47	0.45
1:C:321:GLU:HG2	3:C:1201:HOH:O	2.17	0.45
1:B:197:ASP:OD2	1:B:395:HIS:HD2	2.00	0.44
1:B:252:ASN:HA	1:B:252:ASN:HD22	1.61	0.44
1:A:477:PRO:HB2	1:A:478:LYS:HD2	1.99	0.44
1:D:703:LYS:HD2	3:D:1409:HOH:O	2.17	0.44
1:D:583:LYS:O	1:D:584:LYS:HB3	2.17	0.44
1:B:118:ASP:HA	1:C:126[B]:ILE:HD13	1.99	0.44
1:D:274:ILE:HD12	2:D:754:HEM:HMB1	1.99	0.44
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:369:ARG:HG2	3:B:1110:HOH:O	2.18	0.44
1:A:634:TYR:HB3	1:A:650:ILE:HD13	2.00	0.44
1:A:120:GLU:HB2	1:D:126[A]:ILE:HD11	2.00	0.43
1:C:274:ILE:HD12	2:C:754:HEM:HMB1	2.00	0.43
1:B:426:PRO:HB2	1:D:116:HIS:CD2	2.53	0.43
1:C:359:LEU:C	1:C:359:LEU:HD12	2.39	0.43
1:A:341:ILE:HD12	1:A:353:LEU:HD21	2.00	0.43
1:B:615:ASP:O	1:B:619:ILE:HG13	2.17	0.43
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.54	0.43
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.63	0.43
1:D:41:GLU:CD	1:D:42:PRO:HD2	2.38	0.43
1:C:165:ARG:HE	1:C:386:ASN:ND2	2.16	0.43
1:D:682:ASN:HB3	1:D:707:THR:HG21	2.00	0.43
1:D:38:PRO:HB3	1:D:49:PRO:HD2	2.00	0.43
1:D:404:ASN:O	1:D:405:ASP:C	2.56	0.43
1:C:162:VAL:HG21	1:C:373:MET:SD	2.59	0.43
1:A:260:ARG:HD3	1:A:590:LEU:HD21	2.01	0.43
1:D:461:GLU:HA	1:D:462:PRO:C	2.38	0.43
1:D:222:LYS:HB3	1:D:223:PRO:HD2	2.00	0.43
1:B:36:HIS:HD1	1:B:36:HIS:H	1.66	0.43
1:A:37:ARG:NH2	1:C:466:ASN:HA	2.34	0.43
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.54	0.42
1:C:535:VAL:O	1:C:537:PRO:HD3	2.19	0.42
1:A:76:GLU:O	1:A:77:ASN:HB2	2.19	0.42
1:A:91:ASP:OD2	1:C:461:GLU:OE2	2.36	0.42
1:B:251:HIS:HA	1:B:508:PRO:HG3	2.02	0.42
1:C:749:ASP:HB3	1:C:750:LYS:NZ	2.34	0.42
1:A:165:ARG:HE	1:A:386:ASN:ND2	2.17	0.42
1:A:37:ARG:HH21	1:C:466:ASN:HA	1.84	0.42
1:C:293:TRP:CZ3	1:C:336:LEU:HB2	2.54	0.42
1:B:696:ALA:CB	1:B:719:VAL:HB	2.49	0.42
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.35	0.42
1:B:65:LEU:HD21	1:B:135:HIS:CG	2.55	0.42
1:A:207:PHE:O	1:A:249:THR:HA	2.19	0.42
1:D:335:GLU:OE1	1:D:369:ARG:HG2	2.20	0.42
1:B:507:HIS:N	1:B:508:PRO:CD	2.82	0.42
1:C:51:ALA:HB1	1:C:52:PRO:HD2	2.02	0.42
1:C:125:ARG:HB2	1:C:129:ALA:HA	2.02	0.42
1:D:51:ALA:HB1	1:D:52:PRO:HD2	2.02	0.42
1:D:250:LEU:HD11	1:D:546:GLN:HE21	1.85	0.42
1:A:511:PHE:O	1:A:515:GLN:HG2	2.19	0.42
1:D:375:LEU:N	1:D:375:LEU:CD1	2.82	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:689:TYR:CE1	1:C:710:ILE:HD11	2.55	0.41
1:B:128:HIS:ND1	1:B:169:CYS:HA	2.34	0.41
1:B:91:ASP:OD2	1:D:461:GLU:OE2	2.38	0.41
1:C:195:ILE:HD11	1:C:436:PRO:HA	2.02	0.41
1:A:610:GLU:OE2	1:A:643:ASP:HA	2.19	0.41
1:A:478:LYS:HE2	1:A:478:LYS:HB3	1.79	0.41
1:C:449:HIS:CE1	3:C:1369:HOH:O	2.74	0.41
1:B:118:ASP:OD2	1:C:417:ASP:OD2	2.38	0.41
1:A:104:LEU:HB3	3:A:901:HOH:O	2.20	0.41
1:A:578:ASP:HB3	1:A:582:LEU:O	2.20	0.41
1:B:294:LYS:HG3	3:B:1286:HOH:O	2.20	0.41
1:A:158:LYS:HB3	3:A:1097:HOH:O	2.19	0.41
1:A:631:LYS:HD3	3:A:1188:HOH:O	2.20	0.41
1:D:386:ASN:C	1:D:386:ASN:ND2	2.68	0.41
1:B:459:ASN:H	1:B:459:ASN:HD22	1.68	0.41
1:A:155:ASP:OD1	1:A:156:PRO:HD2	2.21	0.41
1:B:682:ASN:CG	1:B:707:THR:HG21	2.41	0.41
1:D:222:LYS:HB3	1:D:223:PRO:CD	2.51	0.41
1:C:709:LYS:HD2	1:C:709:LYS:N	2.36	0.41
1:C:583:LYS:O	1:C:584:LYS:CB	2.68	0.41
1:C:344:GLU:O	1:C:348:LYS:NZ	2.50	0.41
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.66	0.41
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.56	0.41
1:B:608:ASN:O	1:B:611:VAL:HG23	2.21	0.41
1:B:616:LEU:HA	1:B:616:LEU:HD23	1.93	0.41
1:B:732:LEU:HD13	1:B:732:LEU:C	2.40	0.41
1:C:608:ASN:OD1	1:C:671:ASN:N	2.54	0.41
1:B:392:HIS:HB3	1:B:395:HIS:CD2	2.56	0.40
1:A:460:TYR:CE1	1:B:238:THR:HB	2.56	0.40
1:B:335:GLU:OE1	1:B:369:ARG:HD2	2.21	0.40
1:C:675:ILE:HG13	1:C:704:PHE:HZ	1.86	0.40
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.56	0.40
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.51	0.40
1:D:574:THR:OG1	1:D:575:PRO:HD2	2.21	0.40
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.97	0.40
1:B:648:LEU:HA	1:B:649:PRO:HD3	1.91	0.40
1:C:498:SER:HA	1:C:499:PRO:HD3	1.98	0.40
1:A:126[A]:ILE:CG2	2:A:754:HEM:HMD1	2.51	0.40
1:A:229:ILE:HA	1:A:230:PRO:HA	1.88	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:479:ARG:NH2	3:B:1105:HOH:O[2_545]	1.88	0.32
1:A:479:ARG:NH2	3:B:1315:HOH:O[2_545]	1.91	0.29
1:A:61:ARG:NH1	3:B:881:HOH:O[2_545]	2.03	0.17
1:A:479:ARG:NH1	3:B:1315:HOH:O[2_545]	2.16	0.04
1:B:146:ASP:OD1	3:C:1114:HOH:O[2_555]	2.17	0.03
1:A:479:ARG:CZ	3:B:1315:HOH:O[2_545]	2.19	0.01

## 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	726/753 (96%)	706 (97%)	17 (2%)	3 (0%)	43	25
1	B	726/753 (96%)	707 (97%)	16 (2%)	3 (0%)	43	25
1	C	726/753 (96%)	707 (97%)	16 (2%)	3 (0%)	43	25
1	D	726/753 (96%)	707 (97%)	16 (2%)	3 (0%)	43	25
All	All	2904/3012 (96%)	2827 (97%)	65 (2%)	12 (0%)	43	25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	28	SER
1	C	28	SER
1	D	28	SER
1	A	726	GLY
1	B	726	GLY
1	C	726	GLY
1	D	726	GLY
1	B	584	LYS
1	A	75	SER
1	C	75	SER
1	D	584	LYS



### 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	613/636 (96%)	590 (96%)	23 (4%)	44	24
1	B	613/636 (96%)	587 (96%)	26 (4%)	40	20
1	C	613/636 (96%)	577 (94%)	36 (6%)	28	10
1	D	613/636 (96%)	588 (96%)	25 (4%)	41	21
All	All	2452/2544 (96%)	2342 (96%)	110 (4%)	39	17

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	126[A]	ILE
1	A	126[B]	ILE
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN
1	A	375	LEU
1	A	386	ASN
1	A	392	HIS
1	A	440	TYR
1	A	459	ASN
1	A	478	LYS
1	A	479	ARG
1	A	552	LEU
1	A	565	GLU
1	A	616	LEU
1	A	631	LYS
1	A	710	ILE
1	A	713	GLN
1	A	750	LYS
1	B	37	ARG
1	B	126[A]	ILE
1	B	126[B]	ILE

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Mol	Chain	Res	Type
1	B	142	LYS
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	247	PRO
1	B	252	ASN
1	B	265	SER
1	B	375	LEU
1	B	386	ASN
1	B	440	TYR
1	B	459	ASN
1	B	478	LYS
1	B	562	LEU
1	B	571	LEU
1	B	583	LYS
1	B	601	ARG
1	B	613	SER
1	B	633	LEU
1	B	647	VAL
1	B	703	LYS
1	B	712	ASP
1	B	722	ASP
1	C	27	ASP
1	C	29	LEU
1	C	61	ARG
1	C	185	PHE
1	C	195	ILE
1	C	198	LEU
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	285	LYS
1	C	321	GLU
1	C	348	LYS
1	C	375	LEU
1	C	377	ARG
1	C	386	ASN
1	C	432	PRO
1	C	440	TYR
1	C	449	HIS

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Mol	Chain	Res	Type
1	C	459	ASN
1	C	478	LYS
1	C	552	LEU
1	C	568	ASP
1	C	569	ASP
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	635	SER
1	C	636	ARG
1	C	648	LEU
1	C	660	LEU
1	C	709	LYS
1	C	725	ASP
1	D	27	ASP
1	D	61	ARG
1	D	73	LYS
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	265	SER
1	D	340	LEU
1	D	352	ASP
1	D	386	ASN
1	D	440	TYR
1	D	459	ASN
1	D	478	LYS
1	D	488	ARG
1	D	552	LEU
1	D	554	LEU
1	D	569	ASP
1	D	582	LEU
1	D	624	LYS
1	D	633	LEU
1	D	648	LEU
1	D	712	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	128	HIS
1	A	368	GLN
1	A	386	ASN
1	A	449	HIS
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	128	HIS
1	B	157	ASN
1	B	252	ASN
1	B	386	ASN
1	B	395	HIS
1	B	459	ASN
1	B	492	ASN
1	B	507	HIS
1	B	629	HIS
1	C	128	HIS
1	C	252	ASN
1	C	368	GLN
1	C	386	ASN
1	C	459	ASN
1	C	507	HIS
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	128	HIS
1	D	252	ASN
1	D	386	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN
1	D	713	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	754	1	50,50,50	2.96	15 (30%)	46,82,82	1.81	10 (21%)
2	HEM	B	754	1	50,50,50	3.00	18 (36%)	46,82,82	1.75	6 (13%)
2	HEM	C	754	1	50,50,50	2.65	13 (26%)	46,82,82	1.40	7 (15%)
2	HEM	D	754	1	50,50,50	2.81	14 (28%)	46,82,82	1.53	7 (15%)

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	754	1	-	0/14/114/114	0/0/8/8
2	HEM	B	754	1	-	0/14/114/114	0/0/8/8
2	HEM	C	754	1	-	0/14/114/114	0/0/8/8
2	HEM	D	754	1	-	0/14/114/114	0/0/8/8

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	754	HEM	C3D-C2D	-11.81	1.31	1.44
2	A	754	HEM	C3D-C2D	-11.42	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	754	HEM	C3C-C2C	-10.26	1.32	1.45
2	D	754	HEM	C3D-C2D	-10.05	1.33	1.44
2	C	754	HEM	C3D-C2D	-9.97	1.33	1.44
2	B	754	HEM	C3B-C2B	-9.63	1.33	1.45
2	D	754	HEM	C3C-C2C	-8.97	1.34	1.45
2	B	754	HEM	C3C-C2C	-8.70	1.34	1.45
2	C	754	HEM	C3B-C2B	-8.59	1.34	1.45
2	D	754	HEM	C3B-C2B	-8.42	1.34	1.45
2	A	754	HEM	C3B-C2B	-7.90	1.35	1.45
2	C	754	HEM	C3C-C2C	-7.87	1.35	1.45
2	D	754	HEM	C3B-CAB	4.57	1.55	1.40
2	C	754	HEM	C3B-CAB	4.46	1.54	1.40
2	A	754	HEM	C3C-CAC	4.37	1.54	1.40
2	D	754	HEM	C3C-CAC	4.37	1.54	1.40
2	B	754	HEM	C3B-CAB	4.35	1.54	1.40
2	B	754	HEM	C3C-CAC	4.12	1.53	1.40
2	C	754	HEM	C3C-CAC	3.87	1.53	1.40
2	A	754	HEM	C3B-CAB	3.78	1.52	1.40
2	B	754	HEM	C3D-C4D	3.36	1.48	1.45
2	A	754	HEM	CHB-C1B	3.11	1.40	1.35
2	D	754	HEM	CHB-C1B	2.83	1.39	1.35
2	A	754	HEM	CHC-C1C	2.82	1.40	1.36
2	A	754	HEM	CMC-C2C	2.79	1.56	1.47
2	B	754	HEM	C1A-C2A	2.69	1.48	1.43
2	D	754	HEM	CMC-C2C	2.68	1.56	1.47
2	D	754	HEM	CMD-C2D	2.67	1.56	1.47
2	A	754	HEM	CAA-C2A	2.66	1.56	1.52
2	B	754	HEM	CHB-C1B	2.64	1.39	1.35
2	B	754	HEM	CAA-C2A	2.60	1.56	1.52
2	C	754	HEM	FE-NC	2.54	2.05	1.95
2	C	754	HEM	CHA-C4D	2.54	1.39	1.35
2	A	754	HEM	CHD-C4C	2.51	1.40	1.36
2	A	754	HEM	CMD-C2D	2.51	1.55	1.47
2	A	754	HEM	C3D-C4D	-2.47	1.43	1.45
2	C	754	HEM	CMA-C3A	2.42	1.56	1.51
2	B	754	HEM	CHC-C1C	2.41	1.39	1.36
2	C	754	HEM	CAA-C2A	2.36	1.56	1.52
2	D	754	HEM	C1A-C2A	2.34	1.47	1.43
2	D	754	HEM	CAD-CBD	2.30	1.58	1.52
2	B	754	HEM	CMD-C2D	2.30	1.54	1.47
2	B	754	HEM	CMB-C2B	2.29	1.54	1.47
2	D	754	HEM	C2B-C1B	2.24	1.47	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	754	HEM	CMC-C2C	2.24	1.54	1.47
2	D	754	HEM	CMA-C3A	2.23	1.56	1.51
2	C	754	HEM	FE-ND	2.22	2.05	1.96
2	B	754	HEM	CHA-C4D	2.19	1.38	1.35
2	A	754	HEM	CBA-CGA	2.18	1.55	1.50
2	A	754	HEM	CAD-CBD	2.15	1.58	1.52
2	C	754	HEM	CMD-C2D	2.10	1.54	1.47
2	B	754	HEM	FE-ND	2.09	2.04	1.96
2	B	754	HEM	CMA-C3A	2.05	1.55	1.51
2	C	754	HEM	C2B-C1B	2.03	1.47	1.45
2	B	754	HEM	CMC-C2C	2.03	1.53	1.47
2	B	754	HEM	FE-NB	2.02	2.04	1.96
2	A	754	HEM	C4A-NA	2.02	1.39	1.36
2	D	754	HEM	C3D-C4D	-2.02	1.43	1.45
2	D	754	HEM	CHA-C4D	2.02	1.38	1.35
2	B	754	HEM	FE-NC	2.01	2.03	1.95

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	754	HEM	C3B-C4B-NB	-7.11	108.91	114.00
2	D	754	HEM	C3B-C4B-NB	-5.28	110.22	114.00
2	A	754	HEM	C3B-C4B-NB	-5.20	110.28	114.00
2	A	754	HEM	CBD-CAD-C3D	-4.49	104.58	114.37
2	D	754	HEM	CBD-CAD-C3D	-3.99	105.67	114.37
2	C	754	HEM	C3B-C4B-NB	-3.97	111.16	114.00
2	A	754	HEM	O2A-CGA-O1A	3.86	133.07	123.31
2	A	754	HEM	O1A-CGA-CBA	-3.86	110.02	123.06
2	B	754	HEM	C1A-CHA-C4D	-3.53	122.83	127.47
2	B	754	HEM	CMA-C3A-C4A	-3.44	123.18	128.46
2	C	754	HEM	C4A-CHB-C1B	-3.24	123.20	127.47
2	A	754	HEM	C4A-CHB-C1B	-3.24	123.21	127.47
2	C	754	HEM	C2D-C1D-ND	-3.13	109.24	112.93
2	D	754	HEM	C2D-C1D-ND	-2.86	109.56	112.93
2	D	754	HEM	O1A-CGA-CBA	-2.77	113.70	123.06
2	D	754	HEM	CMA-C3A-C4A	-2.76	124.22	128.46
2	C	754	HEM	CBD-CAD-C3D	-2.75	108.37	114.37
2	C	754	HEM	O2A-CGA-O1A	2.69	130.10	123.31
2	C	754	HEM	O1A-CGA-CBA	-2.54	114.47	123.06
2	A	754	HEM	CMA-C3A-C4A	-2.51	124.61	128.46
2	B	754	HEM	C2D-C1D-ND	-2.44	110.05	112.93
2	A	754	HEM	CAA-CBA-CGA	-2.42	105.77	113.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	754	HEM	C4A-CHB-C1B	-2.43	124.28	127.47
2	A	754	HEM	C2D-C1D-ND	-2.37	110.13	112.93
2	B	754	HEM	O1A-CGA-CBA	-2.32	115.20	123.06
2	A	754	HEM	CHD-C4C-NC	2.28	126.98	124.38
2	B	754	HEM	CAA-CBA-CGA	-2.25	106.34	113.66
2	A	754	HEM	O2D-CGD-O1D	-2.15	117.88	123.31
2	D	754	HEM	O2A-CGA-O1A	2.10	128.62	123.31
2	C	754	HEM	CAD-C3D-C4D	-2.09	121.08	124.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	727/753 (96%)	-0.29	33 (4%) 32 25	8, 16, 52, 85	0
1	B	727/753 (96%)	-0.16	59 (8%) 12 8	9, 17, 52, 85	0
1	C	727/753 (96%)	-0.27	36 (4%) 28 22	9, 17, 52, 85	0
1	D	727/753 (96%)	-0.30	26 (3%) 41 33	8, 16, 51, 85	0
All	All	2908/3012 (96%)	-0.26	154 (5%) 25 19	8, 17, 52, 85	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	27	ASP	11.0
1	B	27	ASP	7.6
1	A	27	ASP	7.4
1	A	29	LEU	6.8
1	B	726	GLY	6.7
1	B	614	ALA	6.3
1	A	28	SER	6.2
1	A	32	GLU	6.1
1	C	726	GLY	5.8
1	C	28	SER	5.7
1	C	725	ASP	5.7
1	A	712	ASP	5.6
1	C	27	ASP	5.5
1	B	641	THR	5.5
1	C	750	LYS	5.5
1	B	29	LEU	5.5
1	B	750	LYS	5.4
1	D	750	LYS	5.3
1	C	677	ASP	5.3
1	D	32	GLU	5.1
1	B	34	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	612	ARG	5.0
1	B	645	GLY	4.8
1	B	677	ASP	4.7
1	A	750	LYS	4.6
1	C	645	GLY	4.5
1	B	647	VAL	4.4
1	D	29	LEU	4.4
1	A	711	ALA	4.4
1	A	612	ARG	4.3
1	A	35	SER	4.3
1	B	32	GLU	4.3
1	D	711	ALA	4.2
1	C	675	ILE	4.1
1	D	33	ASP	4.1
1	C	642	ALA	4.1
1	B	673	ALA	4.0
1	B	642	ALA	4.0
1	C	751	ILE	4.0
1	D	726	GLY	4.0
1	D	595	ASP	4.0
1	A	710	ILE	3.9
1	D	28	SER	3.9
1	A	34	GLY	3.9
1	A	713	GLN	3.8
1	C	594	PRO	3.7
1	C	647	VAL	3.7
1	C	711	ALA	3.7
1	B	33	ASP	3.6
1	B	676	ALA	3.6
1	B	568	ASP	3.6
1	B	712	ASP	3.6
1	B	610	GLU	3.4
1	A	642	ALA	3.4
1	B	721	ALA	3.4
1	B	670	GLY	3.4
1	A	611	VAL	3.3
1	C	595	ASP	3.3
1	B	646	THR	3.3
1	B	644	ASP	3.3
1	B	612	ARG	3.3
1	C	641	THR	3.3
1	D	35	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	643	ASP	3.2
1	C	596	GLY	3.2
1	C	712	ASP	3.1
1	B	713	GLN	3.1
1	D	34	GLY	3.1
1	D	612	ARG	3.1
1	A	753	ALA	3.1
1	B	701	ALA	3.1
1	B	595	ASP	3.1
1	D	710	ILE	2.9
1	A	709	LYS	2.9
1	B	711	ALA	2.9
1	B	617	LEU	2.9
1	C	700	ASP	2.9
1	B	749	ASP	2.9
1	B	596	GLY	2.8
1	A	751	ILE	2.8
1	B	39	ALA	2.8
1	B	727	SER	2.7
1	A	33	ASP	2.7
1	D	569	ASP	2.7
1	C	727	SER	2.7
1	D	30	ALA	2.7
1	C	29	LEU	2.7
1	C	611	VAL	2.7
1	C	722	ASP	2.6
1	B	643	ASP	2.6
1	A	39	ALA	2.6
1	B	609	ASP	2.6
1	C	572	ASN	2.6
1	C	653	THR	2.6
1	A	726	GLY	2.6
1	A	31	PRO	2.6
1	D	725	ASP	2.5
1	B	28	SER	2.5
1	B	59	ASP	2.5
1	A	596	GLY	2.5
1	C	678	ASN	2.5
1	B	672	ILE	2.5
1	B	710	ILE	2.5
1	C	32	GLU	2.5
1	B	725	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	671	ASN	2.5
1	B	611	VAL	2.5
1	B	572	ASN	2.4
1	D	713	GLN	2.4
1	B	722	ASP	2.4
1	D	596	GLY	2.4
1	A	645	GLY	2.4
1	D	39	ALA	2.4
1	C	723	SER	2.3
1	C	749	ASP	2.3
1	A	607	LEU	2.3
1	B	746	PRO	2.3
1	A	30	ALA	2.3
1	B	698	ALA	2.3
1	D	696	ALA	2.3
1	B	608	ASN	2.3
1	B	700	ASP	2.3
1	B	678	ASN	2.2
1	B	709	LYS	2.3
1	A	646	THR	2.2
1	B	621	LYS	2.2
1	C	703	LYS	2.2
1	A	673	ALA	2.2
1	B	634	TYR	2.2
1	C	670	GLY	2.2
1	C	568	ASP	2.2
1	B	31	PRO	2.2
1	D	724	ALA	2.1
1	B	569	ASP	2.1
1	A	669	CYS	2.1
1	C	593	ILE	2.1
1	C	673	ALA	2.1
1	D	751	ILE	2.1
1	A	640	VAL	2.1
1	A	724	ALA	2.1
1	D	574	THR	2.1
1	D	607	LEU	2.1
1	B	655	ALA	2.1
1	D	753	ALA	2.1
1	A	667	VAL	2.1
1	D	611	VAL	2.1
1	B	40	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	675	ILE	2.0
1	A	41	GLU	2.0
1	A	613	SER	2.0
1	B	583	LYS	2.0
1	B	751	ILE	2.0
1	B	574	THR	2.0
1	B	724	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	HEM	C	754	43/43	0.07	0.46	8,12,16,22	0
2	HEM	A	754	43/43	0.07	0.36	7,12,16,22	0
2	HEM	D	754	43/43	0.06	-0.09	7,12,16,22	0
2	HEM	B	754	43/43	0.06	-0.11	8,12,16,22	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.