



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:41 AM GMT

PDB ID : 2BCN  
Title : Solvent isotope effects on interfacial protein electron transfer between cytochrome c and cytochrome c peroxidase  
Authors : Kang, S.A.; Crane, B.R.  
Deposited on : 2005-10-19  
Resolution : 1.70 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

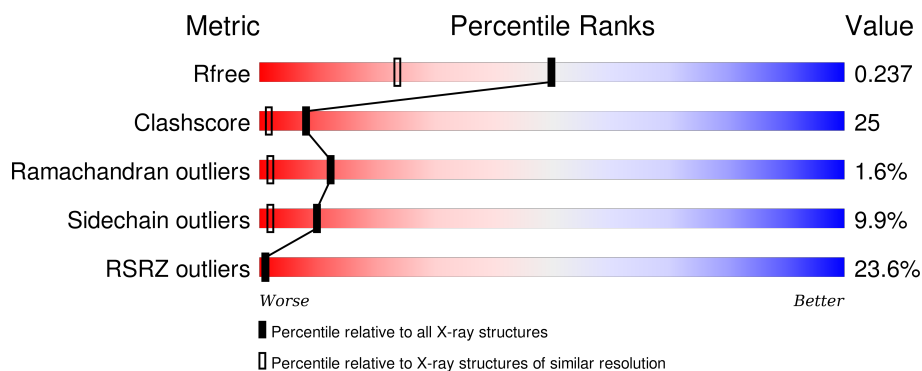
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	296	 10% 67% 20% 8% . .
1	C	296	 14% 68% 21% 8% ..
2	B	108	 84% 36% 32% 27% 5%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6265 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 c peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2371	1514	395	456	6			
1	C	294	Total	C	N	O	S	0	0	0
			2371	1514	395	456	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	CLONING ARTIFACT	GB 171177
A	0	ILE	-	CLONING ARTIFACT	GB 171177
C	-1	MET	-	CLONING ARTIFACT	GB 171177
C	0	ILE	-	CLONING ARTIFACT	GB 171177

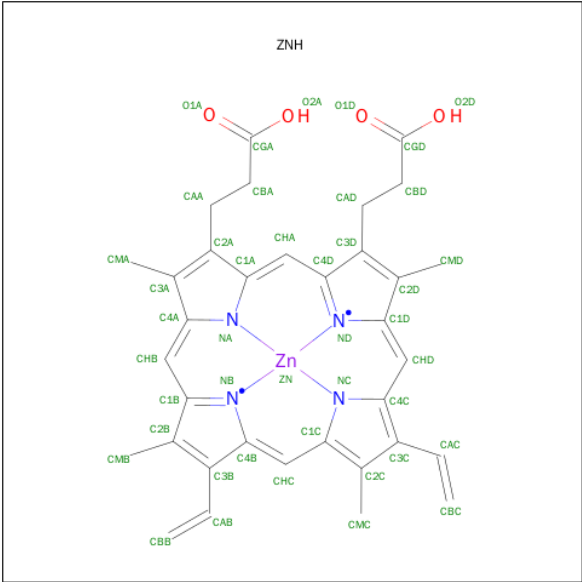
- Molecule 2 is a protein called Cytochrome c iso-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	108	Total	C	N	O	S	0	0	0
			847	534	151	158	4			

There is a discrepancy between the modelled and reference sequences:

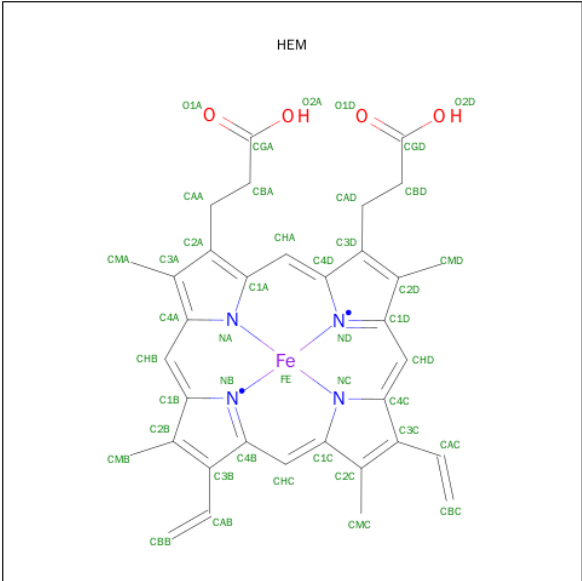
Chain	Residue	Modelled	Actual	Comment	Reference
B	107	SER	CYS	ENGINEERED	UNP P00044

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING ZN (three-letter code: ZNH) (formula: C<sub>34</sub>H<sub>32</sub>N<sub>4</sub>O<sub>4</sub>Zn).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	Zn	0	0
			43	34	4	4	1		
3	C	1	Total	C	N	O	Zn	0	0
			43	34	4	4	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

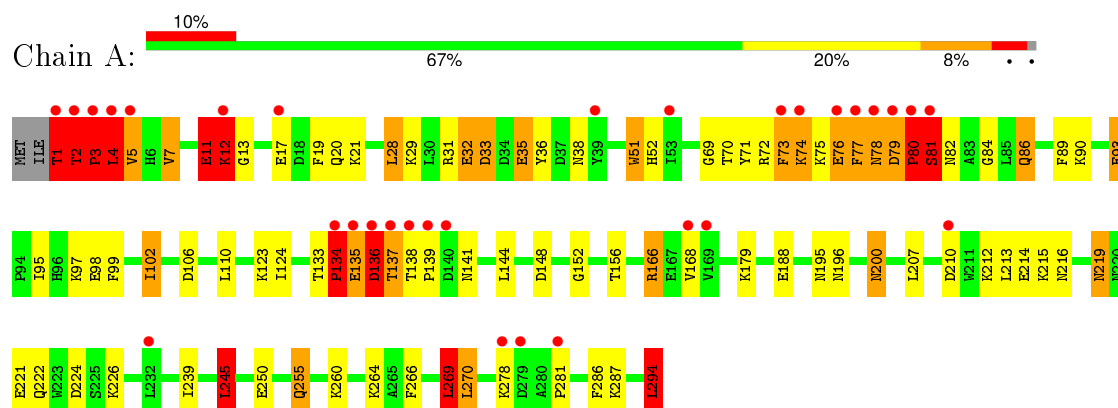
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	286	Total 286	O 286	0	0
5	B	27	Total 27	O 27	0	0
5	C	234	Total 234	O 234	0	0

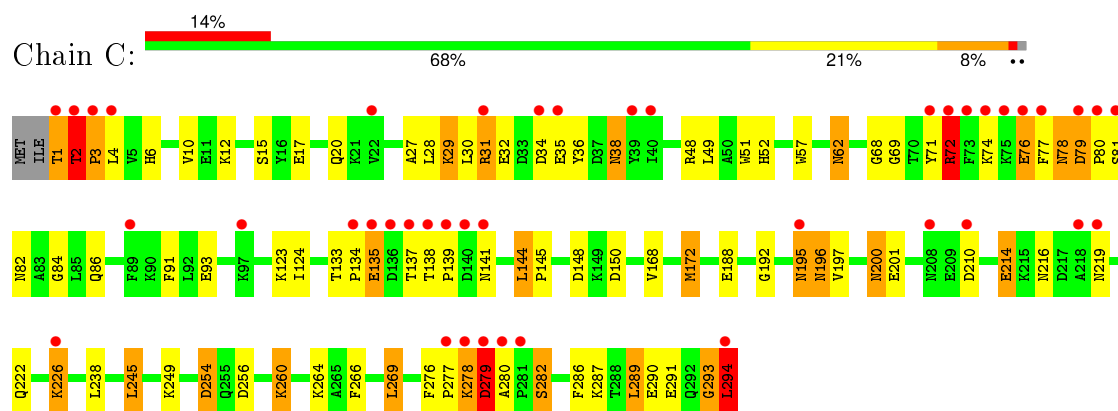
### 3 Residue-property plots

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.

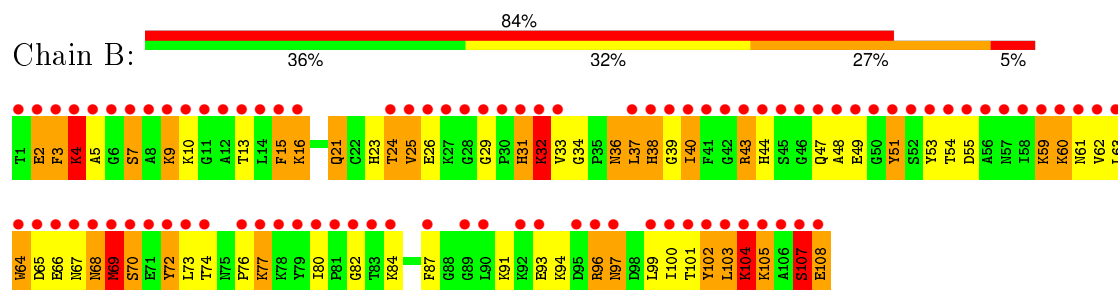
- Molecule 1: cytochrome c peroxidase



- Molecule 1: cytochrome c peroxidase



- Molecule 2: Cytochrome c iso-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.53Å 47.09Å 84.29Å 102.47° 98.74° 102.16°	Depositor
Resolution (Å)	19.61 – 1.70 19.61 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.61-1.70) 86.3 (19.61-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.219 , 0.230 0.225 , 0.237	Depositor DCC
$R_{free}$ test set	3335 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65527 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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

### 5.1 Standard geometry

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

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	1.26	11/2438 (0.5%)	1.15	43/3302 (1.3%)
1	C	0.98	4/2438 (0.2%)	1.38	40/3302 (1.2%)
2	B	0.82	5/865 (0.6%)	1.47	35/1156 (3.0%)
All	All	1.09	20/5741 (0.3%)	1.30	118/7760 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	C	1	6
All	All	1	14

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	THR	C-N	-30.02	0.65	1.34
1	A	79	ASP	C-N	21.35	1.74	1.34
1	A	2	THR	C-N	18.65	1.69	1.34
1	A	11	GLU	C-N	17.40	1.74	1.34
1	C	79	ASP	C-N	16.80	1.66	1.34
1	A	12	LYS	C-N	14.63	1.59	1.33
1	C	277	PRO	C-N	13.86	1.66	1.34
1	A	134	PRO	C-N	12.85	1.63	1.34
1	A	3	PRO	C-N	9.89	1.56	1.34
2	B	26	GLU	C-N	9.11	1.55	1.34
1	A	135	GLU	C-N	-8.48	1.14	1.34
1	A	73	PHE	C-N	-6.58	1.19	1.34
1	C	3	PRO	N-CD	6.45	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	LYS	C-N	-6.10	1.20	1.34
2	B	25	VAL	C-N	5.65	1.47	1.34
2	B	10	LYS	C-N	5.54	1.43	1.33
1	C	2	THR	C-N	5.48	1.44	1.34
1	A	81	SER	C-N	-5.35	1.21	1.34
2	B	108	GLU	C-OXT	5.28	1.33	1.23
1	A	74	LYS	C-N	5.11	1.45	1.34

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	279	ASP	O-C-N	-39.65	59.26	122.70
1	C	294	LEU	CB-CA-C	-19.94	72.31	110.20
1	A	1	THR	O-C-N	-17.22	95.15	122.70
1	C	279	ASP	CB-CA-C	12.24	134.88	110.40
1	A	4	LEU	O-C-N	-11.80	103.82	122.70
1	A	1	THR	C-N-CA	11.15	149.59	121.70
2	B	69	MET	CB-CA-C	10.81	132.02	110.40
2	B	107	SER	CB-CA-C	10.66	130.35	110.10
1	A	81	SER	CB-CA-C	10.44	129.94	110.10
2	B	77	LYS	CB-CA-C	9.82	130.04	110.40
1	C	34	ASP	CB-CA-C	9.76	129.91	110.40
2	B	104	LYS	CB-CA-C	9.75	129.90	110.40
1	A	81	SER	O-C-N	-9.58	107.37	122.70
1	A	219	ASN	CB-CA-C	9.33	129.06	110.40
1	A	12	LYS	C-N-CA	-9.30	102.76	122.30
1	A	79	ASP	C-N-CD	9.16	147.63	128.40
2	B	59	LYS	CB-CA-C	8.48	127.35	110.40
1	A	2	THR	O-C-N	-8.44	105.06	121.10
1	C	150	ASP	CB-CG-OD1	8.43	125.88	118.30
1	C	279	ASP	C-N-CA	7.98	141.65	121.70
1	C	278	LYS	C-N-CA	-7.95	101.83	121.70
1	A	4	LEU	CA-C-N	7.94	134.66	117.20
1	A	134	PRO	C-N-CA	-7.70	102.45	121.70
1	A	1	THR	CA-C-N	7.61	133.95	117.20
1	C	214	GLU	CB-CA-C	-7.33	95.75	110.40
2	B	32	LYS	CB-CA-C	7.16	124.72	110.40
1	C	148	ASP	CB-CG-OD2	7.10	124.69	118.30
1	C	2	THR	N-CA-CB	7.08	123.75	110.30
1	A	79	ASP	CB-CA-C	7.06	124.52	110.40
1	C	79	ASP	C-N-CD	7.05	143.20	128.40
1	C	293	GLY	O-C-N	-7.04	111.43	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	GLU	C-N-CA	-7.03	104.13	121.70
2	B	2	GLU	CB-CA-C	6.92	124.23	110.40
1	C	3	PRO	CA-N-CD	-6.89	101.85	111.50
2	B	9	LYS	CB-CA-C	-6.88	96.63	110.40
1	A	195	ASN	CB-CA-C	-6.85	96.71	110.40
1	A	79	ASP	C-N-CA	-6.83	93.31	122.00
2	B	31	HIS	CB-CA-C	6.83	124.05	110.40
1	C	148	ASP	C-N-CA	6.73	138.53	121.70
2	B	103	LEU	CB-CA-C	-6.56	97.74	110.20
1	A	80	PRO	C-N-CA	-6.56	105.31	121.70
2	B	108	GLU	CB-CA-C	-6.47	97.45	110.40
2	B	43	ARG	CB-CA-C	-6.45	97.51	110.40
1	C	2	THR	C-N-CD	6.43	141.90	128.40
2	B	87	PHE	CB-CA-C	6.42	123.24	110.40
1	C	81	SER	CB-CA-C	6.42	122.29	110.10
1	C	269	LEU	CA-CB-CG	6.39	130.00	115.30
1	C	29	LYS	CB-CA-C	6.38	123.15	110.40
1	A	213	LEU	CB-CA-C	6.37	122.30	110.20
1	A	33	ASP	CB-CA-C	-6.35	97.70	110.40
1	A	76	GLU	CB-CA-C	-6.34	97.72	110.40
1	A	210	ASP	CB-CA-C	6.27	122.95	110.40
2	B	63	LEU	CB-CA-C	6.26	122.10	110.20
2	B	36	ASN	CB-CA-C	6.21	122.82	110.40
1	A	245	LEU	CA-CB-CG	6.19	129.55	115.30
2	B	4	LYS	CB-CA-C	6.19	122.79	110.40
1	A	81	SER	C-N-CA	6.18	137.16	121.70
1	A	294	LEU	CB-CA-C	-6.18	98.47	110.20
2	B	70	SER	CB-CA-C	6.17	121.81	110.10
2	B	21	GLN	CB-CA-C	-6.14	98.12	110.40
1	C	31	ARG	CB-CA-C	-6.11	98.17	110.40
1	C	210	ASP	CB-CA-C	6.11	122.62	110.40
2	B	105	LYS	CB-CA-C	-6.11	98.19	110.40
2	B	7	SER	CB-CA-C	6.08	121.66	110.10
1	A	98	GLU	CB-CA-C	-6.07	98.26	110.40
2	B	51	TYR	CB-CA-C	-6.07	98.26	110.40
2	B	64	TRP	CB-CA-C	-6.07	98.26	110.40
1	C	172	MET	CB-CA-C	-6.05	98.30	110.40
1	A	74	LYS	O-C-N	6.04	132.37	122.70
1	A	38	ASN	CB-CA-C	6.02	122.44	110.40
1	C	2	THR	CA-C-N	-6.00	100.29	117.10
1	C	72	ARG	CB-CA-C	5.99	122.38	110.40
1	A	81	SER	CA-C-N	5.96	130.31	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	TYR	CB-CA-C	5.95	122.29	110.40
1	A	269	LEU	CA-CB-CG	5.91	128.90	115.30
1	A	73	PHE	C-N-CA	5.90	136.45	121.70
1	A	136	ASP	O-C-N	-5.88	113.29	122.70
2	B	68	ASN	CB-CA-C	5.83	122.05	110.40
1	C	282	SER	CB-CA-C	-5.79	99.10	110.10
1	A	13	GLY	O-C-N	5.78	131.95	122.70
1	A	110	LEU	CB-CA-C	5.78	121.17	110.20
1	C	277	PRO	O-C-N	-5.77	113.46	122.70
1	C	135	GLU	CB-CA-C	-5.75	98.91	110.40
1	A	78	ASN	CB-CA-C	5.72	121.85	110.40
1	C	290	GLU	CB-CA-C	5.72	121.84	110.40
2	B	24	THR	CB-CA-C	5.71	127.01	111.60
1	C	74	LYS	CB-CA-C	-5.69	99.01	110.40
1	A	35	GLU	CB-CA-C	-5.69	99.03	110.40
2	B	10	LYS	CB-CA-C	5.67	121.75	110.40
2	B	84	LYS	CB-CA-C	5.62	121.64	110.40
1	A	137	THR	CB-CA-C	-5.62	96.43	111.60
1	C	1	THR	O-C-N	-5.61	113.72	122.70
1	C	78	ASN	CB-CA-C	5.61	121.61	110.40
1	C	2	THR	CA-CB-OG1	5.57	120.70	109.00
2	B	72	TYR	CB-CA-C	5.55	121.49	110.40
1	C	76	GLU	CB-CA-C	5.53	121.47	110.40
1	C	226	LYS	CB-CA-C	5.53	121.45	110.40
1	A	5	VAL	CB-CA-C	5.51	121.87	111.40
2	B	38	HIS	CB-CA-C	5.51	121.42	110.40
1	A	255	GLN	CB-CA-C	5.50	121.41	110.40
1	C	77	PHE	CB-CA-C	5.48	121.36	110.40
1	C	197	VAL	CB-CA-C	-5.45	101.04	111.40
1	A	77	PHE	CB-CA-C	5.41	121.21	110.40
2	B	97	ASN	CB-CA-C	5.39	121.18	110.40
1	C	38	ASN	CB-CA-C	5.32	121.04	110.40
1	C	254	ASP	CB-CG-OD1	5.29	123.06	118.30
2	B	67	ASN	CB-CA-C	5.29	120.98	110.40
2	B	37	LEU	CB-CA-C	5.27	120.22	110.20
1	C	219	ASN	CB-CA-C	5.27	120.94	110.40
2	B	15	PHE	CB-CA-C	5.23	120.87	110.40
1	C	2	THR	CA-CB-CG2	5.13	119.59	112.40
1	C	17	GLU	CB-CA-C	5.13	120.67	110.40
1	A	136	ASP	CB-CA-C	5.13	120.66	110.40
2	B	55	ASP	CB-CA-C	5.12	120.64	110.40
1	A	28	LEU	CB-CA-C	5.10	119.89	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25	VAL	N-CA-C	5.07	124.69	111.00
1	A	7	VAL	CB-CA-C	5.07	121.03	111.40
1	A	73	PHE	O-C-N	-5.03	114.66	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	279	ASP	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	THR	Mainchain,Peptide
1	A	136	ASP	Mainchain
1	A	166	ARG	Sidechain
1	A	3	PRO	Mainchain,Peptide
1	A	80	PRO	Mainchain
1	A	81	SER	Mainchain
1	C	1	THR	Mainchain,Peptide
1	C	2	THR	Mainchain
1	C	279	ASP	Mainchain
1	C	293	GLY	Peptide
1	C	72	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2371	0	2246	118	4
1	C	2371	0	2251	72	4
2	B	847	0	848	89	3
3	A	43	0	30	0	0
3	C	43	0	30	0	0
4	B	43	0	30	3	0
5	A	286	0	0	66	2
5	B	27	0	0	12	1
5	C	234	0	0	37	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6265	0	5435	276	9

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 25.

All (276) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:THR:C	1:A:3:PRO:N	1.69	1.45
1:A:11:GLU:C	1:A:12:LYS:N	1.74	1.39
1:A:79:ASP:C	1:A:80:PRO:N	1.74	1.36
2:B:100:ILE:O	2:B:104:LYS:HG3	1.22	1.34
1:C:76:GLU:HB3	5:C:1082:HOH:O	1.17	1.34
1:A:12:LYS:HE3	5:A:1377:HOH:O	1.16	1.30
1:C:141:ASN:HB2	5:C:1206:HOH:O	1.14	1.28
2:B:60:LYS:HE3	5:B:1525:HOH:O	1.34	1.27
1:A:12:LYS:CE	5:A:1377:HOH:O	1.69	1.22
1:C:260:LYS:HA	1:C:260:LYS:CE	1.69	1.22
2:B:40:ILE:CD1	2:B:40:ILE:H	1.51	1.19
1:C:260:LYS:CA	1:C:260:LYS:HE3	1.70	1.18
1:A:79:ASP:HA	5:A:1409:HOH:O	1.43	1.16
1:A:74:LYS:HE3	5:A:1403:HOH:O	1.47	1.13
1:A:12:LYS:HG2	5:A:1377:HOH:O	1.49	1.12
2:B:40:ILE:HD12	2:B:40:ILE:N	1.55	1.10
1:A:141:ASN:ND2	5:A:1409:HOH:O	1.87	1.07
1:C:278:LYS:O	1:C:279:ASP:C	1.78	1.07
2:B:100:ILE:O	2:B:104:LYS:CG	2.03	1.06
2:B:61:ASN:OD1	5:B:1510:HOH:O	1.71	1.06
1:A:77:PHE:CD2	5:A:1408:HOH:O	2.10	1.05
2:B:4:LYS:HB2	2:B:4:LYS:NZ	1.71	1.04
1:C:139:PRO:HD2	5:C:1529:HOH:O	1.56	1.03
2:B:74:THR:HB	2:B:96:ARG:HE	1.23	1.03
2:B:101:THR:HA	2:B:104:LYS:HD3	1.40	1.01
1:A:77:PHE:CA	5:A:1405:HOH:O	2.10	1.00
1:C:201:GLU:O	5:C:1524:HOH:O	1.78	0.99
1:A:156:THR:HG22	5:A:1085:HOH:O	1.60	0.99
1:C:82:ASN:ND2	5:C:1455:HOH:O	1.95	0.99
2:B:62:VAL:HA	5:B:1535:HOH:O	1.63	0.96
2:B:105:LYS:HE3	2:B:105:LYS:HA	1.45	0.96
2:B:49:GLU:OE2	5:B:1185:HOH:O	1.82	0.96
1:A:77:PHE:HA	5:A:1405:HOH:O	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ASN:CB	5:C:1206:HOH:O	1.82	0.96
1:A:79:ASP:C	1:A:80:PRO:CA	2.35	0.95
2:B:44:HIS:NE2	5:B:1501:HOH:O	1.96	0.94
1:A:139:PRO:HD2	5:A:1108:HOH:O	1.68	0.92
1:A:221:GLU:CD	5:A:1180:HOH:O	2.07	0.91
1:C:69:GLY:HA2	5:C:1457:HOH:O	1.70	0.90
2:B:33:VAL:O	2:B:51:TYR:OH	1.89	0.89
2:B:38:HIS:CD2	2:B:107:SER:HA	2.10	0.87
2:B:4:LYS:CB	2:B:4:LYS:NZ	2.38	0.86
2:B:4:LYS:HB2	2:B:4:LYS:HZ3	1.39	0.86
2:B:40:ILE:HD12	2:B:40:ILE:H	0.69	0.84
1:A:77:PHE:CG	5:A:1408:HOH:O	2.28	0.84
2:B:65:ASP:OD2	5:B:1536:HOH:O	1.96	0.84
1:A:70:THR:O	5:A:1511:HOH:O	1.95	0.83
1:A:75:LYS:O	5:A:1513:HOH:O	1.96	0.82
1:A:78:ASN:N	5:A:1513:HOH:O	2.12	0.81
2:B:105:LYS:HE3	2:B:105:LYS:CA	2.11	0.81
2:B:3:PHE:HE1	2:B:97:ASN:CB	1.95	0.80
1:C:20:GLN:HE22	1:C:287:LYS:H	1.29	0.80
1:C:10:VAL:O	5:C:1445:HOH:O	1.99	0.80
1:A:52:HIS:NE2	5:A:1143:HOH:O	2.14	0.80
1:C:134:PRO:HD2	5:C:1471:HOH:O	1.82	0.79
2:B:64:TRP:CZ2	4:B:109:HEM:HAA1	2.18	0.79
1:A:135:GLU:OE2	5:A:1250:HOH:O	2.01	0.78
2:B:77:LYS:HD2	2:B:82:GLY:H	1.48	0.78
1:A:80:PRO:HB3	5:A:1514:HOH:O	1.82	0.78
1:A:36:TYR:OH	5:A:1241:HOH:O	2.02	0.78
1:A:77:PHE:N	5:A:1405:HOH:O	2.15	0.77
2:B:74:THR:HB	2:B:96:ARG:NE	1.99	0.77
1:A:76:GLU:C	5:A:1513:HOH:O	2.23	0.76
2:B:4:LYS:HB2	2:B:4:LYS:HZ2	1.50	0.76
1:A:11:GLU:C	1:A:12:LYS:CA	2.54	0.75
1:C:38:ASN:OD1	5:C:1506:HOH:O	2.04	0.75
1:A:73:PHE:O	5:A:1511:HOH:O	2.05	0.74
1:A:188:GLU:H	1:A:222:GLN:HE22	1.35	0.74
2:B:96:ARG:HH11	2:B:96:ARG:HG3	1.51	0.74
2:B:96:ARG:NH1	2:B:96:ARG:HG3	2.03	0.74
2:B:3:PHE:CE1	2:B:97:ASN:CB	2.71	0.73
2:B:4:LYS:CB	2:B:4:LYS:HZ3	2.00	0.73
1:C:137:THR:HG23	5:C:1471:HOH:O	1.88	0.73
1:A:71:TYR:CD1	5:A:1405:HOH:O	2.41	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:N	5:A:1417:HOH:O	2.21	0.73
1:A:216:ASN:HD22	1:A:222:GLN:HE21	1.37	0.72
2:B:105:LYS:CE	2:B:105:LYS:HA	2.16	0.72
1:C:144:LEU:HD12	1:C:145:PRO:HD2	1.71	0.72
1:A:264:LYS:CD	5:A:1225:HOH:O	2.38	0.71
1:A:139:PRO:CD	5:A:1108:HOH:O	2.33	0.70
1:A:12:LYS:CG	5:A:1377:HOH:O	2.13	0.69
1:C:27:ALA:HB1	1:C:289:LEU:HD22	1.73	0.69
1:C:134:PRO:CD	5:C:1471:HOH:O	2.37	0.69
1:A:29:LYS:HE2	5:A:1189:HOH:O	1.93	0.68
2:B:96:ARG:CG	2:B:96:ARG:HH11	2.06	0.68
1:C:254:ASP:OD2	5:C:1226:HOH:O	2.11	0.68
2:B:4:LYS:HG2	2:B:5:ALA:H	1.58	0.68
1:A:221:GLU:CG	5:A:1180:HOH:O	2.40	0.67
1:C:4:LEU:O	1:C:62:ASN:OD1	2.12	0.67
1:C:76:GLU:HB2	5:C:1529:HOH:O	1.96	0.66
1:A:281:PRO:CB	5:A:1438:HOH:O	2.42	0.66
1:A:20:GLN:HE22	1:A:287:LYS:H	1.41	0.66
1:A:166:ARG:HH22	1:A:250:GLU:CD	1.98	0.66
1:A:134:PRO:O	5:A:1417:HOH:O	2.14	0.65
1:A:221:GLU:OE2	5:A:1180:HOH:O	2.07	0.65
1:C:52:HIS:NE2	5:C:1454:HOH:O	2.28	0.65
1:A:264:LYS:HD2	5:A:1225:HOH:O	1.97	0.64
1:A:239:ILE:HG22	1:A:245:LEU:HD23	1.79	0.64
1:A:270:LEU:N	1:A:270:LEU:HD23	2.12	0.64
1:A:79:ASP:N	5:A:1513:HOH:O	2.30	0.64
1:A:32:GLU:HB3	5:A:1543:HOH:O	1.96	0.64
1:A:32:GLU:CB	5:A:1543:HOH:O	2.45	0.64
1:C:123:LYS:NZ	1:C:286:PHE:O	2.27	0.63
1:C:260:LYS:HA	1:C:260:LYS:HE3	0.80	0.63
1:A:200:ASN:H	1:A:200:ASN:HD22	1.46	0.63
2:B:62:VAL:HG12	5:B:1535:HOH:O	1.99	0.63
1:A:166:ARG:NH2	1:A:250:GLU:OE1	2.31	0.63
1:A:264:LYS:HD3	5:A:1225:HOH:O	1.99	0.63
1:C:80:PRO:O	5:C:1314:HOH:O	2.16	0.63
2:B:3:PHE:CE1	2:B:97:ASN:HB3	2.34	0.62
2:B:39:GLY:O	2:B:43:ARG:HG3	1.99	0.62
1:C:289:LEU:HG	1:C:294:LEU:HD22	1.80	0.62
1:C:196:ASN:H	1:C:196:ASN:HD22	1.45	0.62
2:B:7:SER:HB3	5:B:1491:HOH:O	1.99	0.62
1:A:21:LYS:HE3	5:A:1382:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:HD22	1:A:222:GLN:NE2	1.98	0.62
1:C:15:SER:HB2	5:C:1161:HOH:O	1.99	0.62
2:B:77:LYS:CD	2:B:82:GLY:H	2.12	0.61
1:C:200:ASN:HD22	1:C:200:ASN:H	1.46	0.61
1:A:5:VAL:HG12	1:A:7:VAL:HG23	1.82	0.61
1:C:138:THR:HG23	5:C:1529:HOH:O	2.00	0.60
2:B:3:PHE:CD1	2:B:97:ASN:HB3	2.36	0.60
1:C:134:PRO:HB2	5:C:1471:HOH:O	2.01	0.60
1:C:188:GLU:H	1:C:222:GLN:HE22	1.48	0.60
1:A:281:PRO:CA	5:A:1438:HOH:O	2.49	0.59
2:B:3:PHE:HE1	2:B:97:ASN:HA	1.67	0.59
1:A:99:PHE:O	1:A:102:ILE:HG22	2.02	0.59
2:B:48:ALA:HB3	2:B:53:TYR:OH	2.02	0.59
1:C:135:GLU:O	1:C:138:THR:HB	2.01	0.59
1:A:138:THR:HG23	5:A:1108:HOH:O	2.03	0.59
1:A:31:ARG:NH2	2:B:91:LYS:HB3	2.18	0.59
1:A:89:PHE:O	1:A:93:GLU:HG2	2.03	0.59
2:B:59:LYS:HG2	1:C:196:ASN:OD1	2.03	0.58
1:A:281:PRO:HA	5:A:1438:HOH:O	2.03	0.58
2:B:16:LYS:NZ	2:B:16:LYS:CB	2.67	0.58
1:A:156:THR:HG21	5:A:1421:HOH:O	2.02	0.58
2:B:93:GLU:HA	2:B:96:ARG:NH1	2.19	0.58
2:B:64:TRP:HZ2	4:B:109:HEM:HAA1	1.68	0.57
2:B:76:PRO:HD2	5:B:1495:HOH:O	2.03	0.57
2:B:3:PHE:HE1	2:B:97:ASN:HB2	1.70	0.57
1:C:144:LEU:HD12	1:C:145:PRO:CD	2.34	0.57
1:C:172:MET:HG2	1:C:238:LEU:HD11	1.87	0.56
1:A:77:PHE:CE2	5:A:1408:HOH:O	2.47	0.56
2:B:40:ILE:CD1	2:B:107:SER:HB2	2.36	0.56
1:A:152:GLY:O	1:A:156:THR:HG23	2.06	0.56
1:A:74:LYS:HD2	5:A:1404:HOH:O	2.05	0.56
1:A:73:PHE:HE2	5:A:1401:HOH:O	1.88	0.56
2:B:51:TYR:HB3	2:B:53:TYR:CE2	2.41	0.56
1:C:76:GLU:CB	5:C:1082:HOH:O	2.02	0.55
1:C:289:LEU:HD12	1:C:294:LEU:HD13	1.87	0.55
2:B:3:PHE:CE1	2:B:97:ASN:HA	2.42	0.55
1:C:216:ASN:HD22	1:C:222:GLN:HE21	1.54	0.55
1:A:69:GLY:HA2	5:A:1391:HOH:O	2.07	0.55
2:B:9:LYS:HE2	2:B:9:LYS:N	2.21	0.55
1:C:57:TRP:HE1	1:C:62:ASN:ND2	2.05	0.55
1:A:69:GLY:O	1:A:72:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:PRO:CB	5:C:1471:HOH:O	2.55	0.54
1:A:74:LYS:CD	5:A:1404:HOH:O	2.54	0.54
1:A:139:PRO:N	5:A:1108:HOH:O	2.40	0.54
1:A:2:THR:O	1:A:3:PRO:N	2.34	0.53
2:B:3:PHE:HE1	2:B:97:ASN:CA	2.22	0.53
1:C:6:HIS:CD2	5:C:1443:HOH:O	2.61	0.53
2:B:72:TYR:CE2	2:B:80:ILE:HD12	2.44	0.53
1:A:134:PRO:HB2	1:A:136:ASP:OD1	2.09	0.53
1:A:216:ASN:HB2	5:A:1142:HOH:O	2.08	0.53
2:B:7:SER:CB	5:B:1491:HOH:O	2.57	0.53
1:C:134:PRO:N	5:C:1471:HOH:O	2.41	0.53
1:A:260:LYS:HG3	5:A:1437:HOH:O	2.09	0.53
2:B:40:ILE:HD11	2:B:107:SER:HB2	1.91	0.53
1:A:221:GLU:HG3	5:A:1180:HOH:O	2.05	0.53
2:B:40:ILE:CD1	2:B:40:ILE:N	2.31	0.52
1:A:214:GLU:OE1	1:A:224:ASP:HB2	2.10	0.52
1:C:57:TRP:HE1	1:C:62:ASN:HD22	1.57	0.52
2:B:37:LEU:HA	2:B:40:ILE:HG13	1.91	0.52
1:C:36:TYR:OH	5:C:1075:HOH:O	2.19	0.52
2:B:3:PHE:CE1	2:B:97:ASN:HB2	2.44	0.51
1:A:269:LEU:HB3	1:A:270:LEU:HD23	1.91	0.51
2:B:93:GLU:HA	2:B:96:ARG:HH12	1.75	0.51
1:A:138:THR:CG2	5:A:1108:HOH:O	2.58	0.51
2:B:65:ASP:CG	5:B:1536:HOH:O	2.43	0.51
1:A:52:HIS:ND1	1:A:144:LEU:HD13	2.25	0.51
1:A:79:ASP:O	1:A:80:PRO:CA	2.59	0.51
1:A:200:ASN:H	1:A:255:GLN:HE21	1.59	0.51
1:A:138:THR:N	5:A:1417:HOH:O	2.44	0.50
1:A:200:ASN:N	1:A:200:ASN:HD22	2.09	0.50
1:C:245:LEU:O	1:C:249:LYS:HG3	2.11	0.50
2:B:37:LEU:HB3	2:B:40:ILE:HG12	1.93	0.49
1:C:276:PHE:O	5:C:1348:HOH:O	2.18	0.49
1:C:200:ASN:HD22	1:C:200:ASN:N	2.08	0.49
1:A:124:ILE:HD13	1:A:266:PHE:HD2	1.76	0.49
1:C:124:ILE:HD13	1:C:266:PHE:HD2	1.76	0.49
2:B:16:LYS:HB3	2:B:16:LYS:NZ	2.27	0.49
1:C:29:LYS:HG2	1:C:91:PHE:CE2	2.47	0.49
2:B:39:GLY:N	2:B:40:ILE:HD12	2.28	0.49
1:A:76:GLU:C	5:A:1405:HOH:O	2.49	0.48
1:C:260:LYS:CA	1:C:260:LYS:CE	2.47	0.48
2:B:16:LYS:HZ3	2:B:16:LYS:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:PHE:HB2	5:A:1511:HOH:O	2.14	0.48
1:C:2:THR:HG22	1:C:3:PRO:HD2	1.94	0.48
1:C:68:GLY:HA2	1:C:133:THR:HG23	1.95	0.48
1:C:192:GLY:O	1:C:195:ASN:ND2	2.47	0.48
2:B:108:GLU:OXT	2:B:108:GLU:CG	2.59	0.48
1:A:2:THR:OG1	1:A:3:PRO:HD2	2.14	0.47
1:A:11:GLU:CA	1:A:12:LYS:N	2.71	0.47
1:A:294:LEU:N	1:A:294:LEU:HD23	2.29	0.47
1:C:245:LEU:HD22	1:C:249:LYS:HE3	1.96	0.47
1:A:12:LYS:NZ	5:A:1378:HOH:O	1.69	0.47
2:B:33:VAL:C	2:B:51:TYR:OH	2.51	0.47
2:B:34:GLY:HA2	2:B:51:TYR:OH	2.14	0.47
2:B:108:GLU:OXT	2:B:108:GLU:HG2	2.15	0.47
1:C:76:GLU:CB	5:C:1529:HOH:O	2.60	0.46
1:A:84:GLY:H	1:A:86:GLN:HE22	1.62	0.46
2:B:73:LEU:HD13	2:B:99:LEU:HD23	1.97	0.46
1:C:80:PRO:HB3	5:C:1314:HOH:O	2.14	0.46
2:B:59:LYS:HB2	5:B:1507:HOH:O	2.15	0.46
1:A:226:LYS:HG2	5:A:1290:HOH:O	2.16	0.46
1:C:86:GLN:H	1:C:86:GLN:CD	2.19	0.46
1:A:77:PHE:N	5:A:1513:HOH:O	2.46	0.46
2:B:69:MET:HG3	2:B:100:ILE:HD13	1.97	0.46
2:B:38:HIS:HA	2:B:107:SER:HB3	1.97	0.46
1:A:52:HIS:ND1	1:A:82:ASN:OD1	2.41	0.46
1:A:270:LEU:N	1:A:270:LEU:CD2	2.76	0.46
1:A:79:ASP:C	1:A:80:PRO:HA	2.30	0.46
1:A:28:LEU:HG	1:A:32:GLU:OE1	2.16	0.45
1:A:19:PHE:HE1	1:A:102:ILE:HD12	1.80	0.45
1:C:71:TYR:N	5:C:1456:HOH:O	2.50	0.45
1:C:260:LYS:HE2	5:C:1031:HOH:O	2.17	0.45
1:A:86:GLN:O	1:A:90:LYS:HG3	2.17	0.45
1:C:79:ASP:HA	1:C:141:ASN:ND2	2.31	0.45
1:C:216:ASN:HD22	1:C:222:GLN:NE2	2.15	0.45
1:A:102:ILE:HD11	1:A:106:ASP:HB3	1.98	0.45
2:B:4:LYS:HG2	2:B:5:ALA:N	2.27	0.45
1:A:51:TRP:CD1	1:A:52:HIS:HD2	2.34	0.44
2:B:29:GLY:HA3	2:B:36:ASN:ND2	2.33	0.44
1:A:148:ASP:O	1:A:148:ASP:OD2	2.36	0.44
2:B:29:GLY:HA3	2:B:36:ASN:HD21	1.83	0.44
1:C:80:PRO:CA	5:C:1314:HOH:O	2.65	0.44
1:A:156:THR:CG2	5:A:1085:HOH:O	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:PRO:CA	5:C:1471:HOH:O	2.65	0.43
1:A:73:PHE:CD1	1:A:135:GLU:HG3	2.54	0.43
2:B:34:GLY:CA	2:B:51:TYR:OH	2.66	0.43
2:B:70:SER:O	2:B:74:THR:HG22	2.18	0.43
1:A:3:PRO:O	1:A:4:LEU:C	2.56	0.43
1:A:29:LYS:NZ	1:A:33:ASP:OD2	2.51	0.43
1:A:80:PRO:O	1:A:81:SER:C	2.57	0.43
2:B:16:LYS:HZ2	2:B:16:LYS:CB	2.31	0.43
1:C:48:ARG:NH2	5:C:1460:HOH:O	2.50	0.43
2:B:77:LYS:HG3	2:B:77:LYS:O	2.19	0.42
1:C:78:ASN:O	5:C:1459:HOH:O	2.21	0.42
2:B:15:PHE:CZ	2:B:25:VAL:HG13	2.54	0.42
1:A:123:LYS:NZ	1:A:286:PHE:O	2.45	0.42
1:A:207:LEU:HD22	5:A:1287:HOH:O	2.18	0.42
2:B:16:LYS:HZ2	2:B:16:LYS:HB2	1.84	0.42
1:A:12:LYS:CE	5:A:1378:HOH:O	2.44	0.42
2:B:13:THR:HA	2:B:16:LYS:HG2	2.01	0.42
1:A:179:LYS:HE3	5:A:1275:HOH:O	2.19	0.42
1:C:137:THR:CG2	5:C:1471:HOH:O	2.59	0.42
1:C:71:TYR:HB2	5:C:1456:HOH:O	2.19	0.42
1:A:31:ARG:CZ	2:B:91:LYS:HB3	2.50	0.42
1:A:124:ILE:HD13	1:A:266:PHE:CD2	2.53	0.42
1:A:11:GLU:C	1:A:12:LYS:C	2.79	0.41
1:A:133:THR:HB	1:A:137:THR:HG21	2.02	0.41
1:A:97:LYS:NZ	5:A:1412:HOH:O	2.36	0.41
2:B:54:THR:HG22	4:B:109:HEM:O2D	2.20	0.41
1:C:138:THR:HA	1:C:139:PRO:HD3	1.78	0.41
2:B:23:HIS:CD2	2:B:37:LEU:HD11	2.56	0.41
1:C:2:THR:HB	1:C:3:PRO:HD2	2.03	0.41
2:B:40:ILE:O	2:B:64:TRP:HB2	2.20	0.41
2:B:31:HIS:HB2	2:B:51:TYR:CD1	2.56	0.41
1:C:6:HIS:HD2	5:C:1443:HOH:O	1.99	0.41
2:B:104:LYS:HB2	2:B:104:LYS:HE2	1.38	0.41
1:A:19:PHE:CE1	1:A:102:ILE:HD12	2.56	0.41
1:C:264:LYS:HE2	5:C:1542:HOH:O	2.21	0.41
1:A:75:LYS:C	5:A:1513:HOH:O	2.52	0.40
2:B:101:THR:CA	2:B:104:LYS:HD3	2.29	0.40
1:A:35:GLU:HB2	5:A:1385:HOH:O	2.20	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:NZ	5:A:1233:HOH:O[1_445]	0.39	1.81
5:C:1321:HOH:O	5:C:1332:HOH:O[1_655]	0.68	1.52
1:A:226:LYS:CE	5:A:1233:HOH:O[1_445]	1.14	1.06
1:A:1:THR:OG1	5:C:1472:HOH:O[1_564]	1.86	0.34
1:A:17:GLU:OE1	2:B:49:GLU:OE1[1_665]	1.87	0.33
1:C:84:GLY:CA	1:C:278:LYS:NZ[1_455]	2.02	0.18
2:B:2:GLU:OE2	1:C:93:GLU:OE1[1_565]	2.05	0.15
1:C:291:GLU:OE1	5:B:1168:HOH:O[1_655]	2.06	0.14
2:B:108:GLU:OE2	1:C:256:ASP:OD1[1_455]	2.18	0.02

## 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	292/296 (99%)	281 (96%)	5 (2%)	6 (2%)	9	1
1	C	292/296 (99%)	284 (97%)	6 (2%)	2 (1%)	26	9
2	B	106/108 (98%)	97 (92%)	6 (6%)	3 (3%)	6	1
All	All	690/700 (99%)	662 (96%)	17 (2%)	11 (2%)	12	2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	C	279	ASP
1	C	280	ALA
1	A	2	THR
2	B	66	GLU
1	A	134	PRO
1	A	136	ASP
2	B	32	LYS
1	A	11	GLU
1	A	12	LYS
2	B	4	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	252/254 (99%)	233 (92%)	19 (8%)	17	4
1	C	252/254 (99%)	229 (91%)	23 (9%)	12	2
2	B	89/89 (100%)	72 (81%)	17 (19%)	2	0
All	All	593/597 (99%)	534 (90%)	59 (10%)	10	2

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

Mol	Chain	Res	Type
1	A	2	THR
1	A	12	LYS
1	A	32	GLU
1	A	51	TRP
1	A	86	GLN
1	A	93	GLU
1	A	95	ILE
1	A	102	ILE
1	A	168	VAL
1	A	196	ASN
1	A	200	ASN
1	A	212	LYS
1	A	215	LYS
1	A	219	ASN
1	A	245	LEU
1	A	269	LEU
1	A	270	LEU
1	A	278	LYS
1	A	294	LEU
2	B	3	PHE
2	B	4	LYS
2	B	16	LYS
2	B	21	GLN
2	B	24	THR
2	B	32	LYS
2	B	40	ILE

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Mol	Chain	Res	Type
2	B	47	GLN
2	B	60	LYS
2	B	68	ASN
2	B	69	MET
2	B	94	LYS
2	B	96	ARG
2	B	102	TYR
2	B	103	LEU
2	B	104	LYS
2	B	107	SER
1	C	12	LYS
1	C	28	LEU
1	C	30	LEU
1	C	31	ARG
1	C	32	GLU
1	C	35	GLU
1	C	49	LEU
1	C	51	TRP
1	C	62	ASN
1	C	72	ARG
1	C	144	LEU
1	C	168	VAL
1	C	195	ASN
1	C	196	ASN
1	C	200	ASN
1	C	214	GLU
1	C	226	LYS
1	C	245	LEU
1	C	260	LYS
1	C	269	LEU
1	C	282	SER
1	C	289	LEU
1	C	294	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	86	GLN
1	A	159	GLN
1	A	181	HIS

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Mol	Chain	Res	Type
1	A	196	ASN
1	A	200	ASN
1	A	208	ASN
1	A	222	GLN
1	A	255	GLN
1	A	292	GLN
2	B	21	GLN
2	B	36	ASN
2	B	38	HIS
2	B	61	ASN
2	B	68	ASN
1	C	6	HIS
1	C	20	GLN
1	C	24	ASN
1	C	62	ASN
1	C	82	ASN
1	C	159	GLN
1	C	184	ASN
1	C	200	ASN
1	C	208	ASN
1	C	222	GLN
1	C	292	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](#)

3 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
3	ZNH	A	295	1	28,50,50	1.08	2 (7%)	17,82,82	2.97	7 (41%)
4	HEM	B	109	2	30,50,50	2.40	9 (30%)	24,82,82	2.36	10 (41%)
3	ZNH	C	295	1	28,50,50	1.55	6 (21%)	17,82,82	1.74	3 (17%)

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
3	ZNH	A	295	1	-	0/6/54/54	0/0/8/8
4	HEM	B	109	2	-	0/10/54/54	0/0/8/8
3	ZNH	C	295	1	-	0/6/54/54	0/0/8/8

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	109	HEM	C3B-CAB	-5.85	1.40	1.51
4	B	109	HEM	C2D-C3D	-5.54	1.37	1.54
4	B	109	HEM	C3C-CAC	-5.10	1.41	1.51
3	C	295	ZNH	C1B-NB	-4.18	1.32	1.37
4	B	109	HEM	C3B-C4B	-4.04	1.48	1.51
4	B	109	HEM	C3D-C4D	-3.63	1.46	1.51
3	C	295	ZNH	C3C-CAC	-2.84	1.41	1.47
4	B	109	HEM	C2C-C1C	-2.83	1.47	1.52
3	C	295	ZNH	C3B-CAB	-2.78	1.41	1.47
3	A	295	ZNH	C3C-CAC	-2.52	1.42	1.47
3	A	295	ZNH	C3B-CAB	-2.21	1.42	1.47
4	B	109	HEM	FE-NB	2.07	2.08	1.97
3	C	295	ZNH	CAD-C3D	2.11	1.56	1.52
3	C	295	ZNH	C4C-NC	2.13	1.39	1.37
4	B	109	HEM	CHD-C4C	2.14	1.41	1.36
4	B	109	HEM	FE-NC	2.77	2.06	1.95
3	C	295	ZNH	CMC-C2C	3.04	1.57	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	295	ZNH	CMC-C2C-C1C	-4.60	120.76	128.36
3	A	295	ZNH	CAD-C3D-C2D	-3.24	119.74	129.00
3	C	295	ZNH	CMC-C2C-C1C	-2.07	124.94	128.36
3	A	295	ZNH	CMB-C2B-C3B	2.05	129.09	125.09
4	B	109	HEM	C1D-CHD-C4C	2.19	129.48	125.82
4	B	109	HEM	C4B-CHC-C1C	2.62	130.21	125.82
4	B	109	HEM	C3C-CAC-CBC	2.78	128.72	124.46
3	C	295	ZNH	CMB-C2B-C3B	2.80	130.57	125.09
4	B	109	HEM	C2D-C3D-C4D	2.86	106.35	101.50
4	B	109	HEM	C3B-C4B-CHC	3.00	127.39	123.16
4	B	109	HEM	CMD-C2D-C3D	3.09	128.02	114.35
3	A	295	ZNH	CMC-C2C-C3C	3.16	131.26	125.09
3	A	295	ZNH	CBA-CAA-C2A	3.61	118.99	112.53
3	C	295	ZNH	CBA-CAA-C2A	4.14	119.94	112.53
4	B	109	HEM	CAD-C3D-C4D	4.27	127.52	112.47
4	B	109	HEM	CMC-C2C-C3C	4.30	127.27	116.53
4	B	109	HEM	CAD-C3D-C2D	4.48	126.09	113.22
4	B	109	HEM	CMB-C2B-C3B	4.73	128.34	116.53
3	A	295	ZNH	CAD-C3D-C4D	5.66	133.16	127.01
3	A	295	ZNH	CBD-CAD-C3D	6.46	124.11	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	109	HEM	3	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	294/296 (99%)	0.88	31 (10%)	8 9	20, 24, 35, 50	0
1	C	294/296 (99%)	0.93	42 (14%)	4 4	18, 24, 39, 49	0
2	B	108/108 (100%)	5.09	91 (84%)	0 0	18, 34, 49, 50	0
All	All	696/700 (99%)	1.56	164 (23%)	1 1	18, 25, 43, 50	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	37	LEU	15.0
2	B	50	GLY	14.5
2	B	1	THR	13.1
2	B	63	LEU	12.8
2	B	3	PHE	12.3
2	B	62	VAL	12.3
2	B	52	SER	12.2
1	A	2	THR	12.1
2	B	55	ASP	11.7
1	A	1	THR	11.5
2	B	58	ILE	11.1
2	B	108	GLU	10.8
1	C	1	THR	10.4
2	B	42	GLY	10.3
2	B	31	HIS	10.2
2	B	41	PHE	9.9
2	B	51	TYR	9.6
2	B	57	ASN	9.4
2	B	2	GLU	9.4
2	B	64	TRP	8.8
2	B	59	LYS	8.8
2	B	49	GLU	8.5
2	B	44	HIS	8.2

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Mol	Chain	Res	Type	RSRZ
2	B	61	ASN	8.1
2	B	56	ALA	7.4
2	B	47	GLN	7.2
2	B	4	LYS	7.2
2	B	8	ALA	7.1
2	B	27	LYS	7.1
2	B	7	SER	7.0
2	B	38	HIS	7.0
2	B	29	GLY	6.8
2	B	53	TYR	6.8
1	C	80	PRO	6.4
2	B	73	LEU	6.3
2	B	6	GLY	6.3
1	A	3	PRO	6.3
1	C	294	LEU	6.2
2	B	28	GLY	5.8
1	C	77	PHE	5.7
2	B	48	ALA	5.7
2	B	90	LEU	5.7
2	B	79	TYR	5.6
2	B	40	ILE	5.6
2	B	100	ILE	5.6
2	B	106	ALA	5.6
2	B	54	THR	5.6
2	B	107	SER	5.3
2	B	103	LEU	5.2
2	B	69	MET	5.0
1	C	81	SER	5.0
2	B	72	TYR	5.0
2	B	60	LYS	4.9
1	C	75	LYS	4.9
2	B	43	ARG	4.8
2	B	101	THR	4.8
2	B	81	PRO	4.7
2	B	46	GLY	4.7
2	B	83	THR	4.7
1	C	2	THR	4.7
2	B	68	ASN	4.6
2	B	33	VAL	4.4
1	C	138	THR	4.4
1	C	39	TYR	4.3
2	B	99	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	278	LYS	4.3
1	C	35	GLU	4.2
1	A	4	LEU	4.2
2	B	102	TYR	4.2
1	C	71	TYR	4.2
1	C	79	ASP	4.2
1	A	12	LYS	4.1
1	C	72	ARG	4.1
1	C	135	GLU	4.1
2	B	93	GLU	4.1
1	A	136	ASP	4.0
2	B	92	LYS	4.0
2	B	30	PRO	4.0
2	B	26	GLU	3.8
2	B	67	ASN	3.8
2	B	24	THR	3.7
2	B	65	ASP	3.7
2	B	9	LYS	3.7
1	A	278	LYS	3.6
1	C	279	ASP	3.6
2	B	39	GLY	3.6
1	C	73	PHE	3.6
2	B	82	GLY	3.6
2	B	45	SER	3.6
1	C	140	ASP	3.5
2	B	105	LYS	3.4
2	B	74	THR	3.4
1	A	210	ASP	3.4
2	B	77	LYS	3.4
2	B	71	GLU	3.3
2	B	97	ASN	3.3
2	B	78	LYS	3.2
1	C	281	PRO	3.2
2	B	80	ILE	3.2
1	C	210	ASP	3.1
1	A	80	PRO	3.1
2	B	25	VAL	3.1
1	A	134	PRO	3.0
1	A	281	PRO	3.0
1	A	137	THR	3.0
1	C	141	ASN	2.9
1	C	139	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	280	ALA	2.9
2	B	14	LEU	2.8
1	A	73	PHE	2.8
2	B	5	ALA	2.8
1	C	4	LEU	2.7
2	B	104	LYS	2.7
2	B	70	SER	2.7
2	B	87	PHE	2.7
1	A	77	PHE	2.6
2	B	66	GLU	2.6
1	A	140	ASP	2.6
2	B	15	PHE	2.6
2	B	12	ALA	2.6
1	A	79	ASP	2.6
1	C	137	THR	2.6
2	B	11	GLY	2.6
2	B	96	ARG	2.6
2	B	32	LYS	2.6
1	C	136	ASP	2.6
2	B	76	PRO	2.5
1	C	208	ASN	2.5
1	C	22	VAL	2.5
1	A	74	LYS	2.4
1	C	134	PRO	2.4
1	A	17	GLU	2.4
2	B	95	ASP	2.4
1	C	219	ASN	2.4
1	A	138	THR	2.4
1	C	3	PRO	2.4
1	A	78	ASN	2.4
1	A	232	LEU	2.4
2	B	89	GLY	2.4
1	C	34	ASP	2.4
1	A	5	VAL	2.3
2	B	16	LYS	2.3
1	A	279	ASP	2.3
1	C	218	ALA	2.3
1	A	169	VAL	2.3
1	A	39	TYR	2.3
1	A	81	SER	2.3
1	C	97	LYS	2.2
2	B	84	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	74	LYS	2.2
1	A	139	PRO	2.2
1	A	135	GLU	2.2
1	C	226	LYS	2.2
1	C	76	GLU	2.1
1	C	40	ILE	2.1
1	C	277	PRO	2.1
1	A	53	ILE	2.1
2	B	13	THR	2.1
1	A	76	GLU	2.1
1	C	195	ASN	2.1
2	B	10	LYS	2.1
1	A	168	VAL	2.1
1	C	89	PHE	2.1
1	C	31	ARG	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
3	ZNH	C	295	43/43	0.97	0.10	-0.75	19,21,23,26	0
4	HEM	B	109	43/43	0.91	0.15	-0.87	17,20,21,23	0
3	ZNH	A	295	43/43	0.98	0.09	-1.09	19,22,26,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.