



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 AM GMT

PDB ID : 2F9I  
Title : Crystal Structure of the carboxyltransferase subunit of ACC from Staphylococcus aureus  
Authors : Bilder, P.W.  
Deposited on : 2005-12-05  
Resolution : 1.98 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

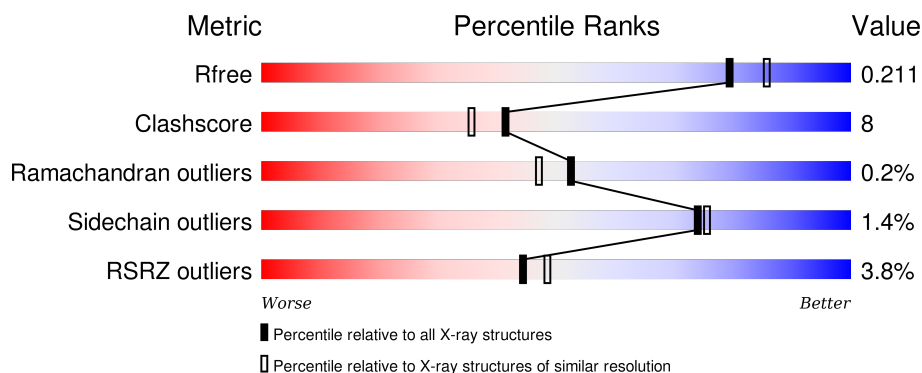
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	327	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>•• 6%</div> </div> </div>
1	C	327	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•• 9%</div> </div> </div>
2	B	285	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>• 9%</div> </div> </div>
2	D	285	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>• 11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9270 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 acetyl-coenzyme A carboxylase carboxyl transferase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	45	0	0
			2407	1523	417	459	8			
1	C	297	Total	C	N	O	S	48	0	0
			2289	1447	396	438	8			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	CLONING ARTIFACT	GB 49244968
A	-11	HIS	-	EXPRESSION TAG	GB 49244968
A	-10	HIS	-	EXPRESSION TAG	GB 49244968
A	-9	HIS	-	EXPRESSION TAG	GB 49244968
A	-8	HIS	-	EXPRESSION TAG	GB 49244968
A	-7	HIS	-	EXPRESSION TAG	GB 49244968
A	-6	HIS	-	EXPRESSION TAG	GB 49244968
A	-5	LEU	-	CLONING ARTIFACT	GB 49244968
A	-4	VAL	-	CLONING ARTIFACT	GB 49244968
A	-3	PRO	-	CLONING ARTIFACT	GB 49244968
A	-2	ARG	-	CLONING ARTIFACT	GB 49244968
A	-1	GLY	-	CLONING ARTIFACT	GB 49244968
A	0	SER	-	CLONING ARTIFACT	GB 49244968
C	-12	MET	-	CLONING ARTIFACT	GB 49244968
C	-11	HIS	-	EXPRESSION TAG	GB 49244968
C	-10	HIS	-	EXPRESSION TAG	GB 49244968
C	-9	HIS	-	EXPRESSION TAG	GB 49244968
C	-8	HIS	-	EXPRESSION TAG	GB 49244968
C	-7	HIS	-	EXPRESSION TAG	GB 49244968
C	-6	HIS	-	EXPRESSION TAG	GB 49244968
C	-5	LEU	-	CLONING ARTIFACT	GB 49244968
C	-4	VAL	-	CLONING ARTIFACT	GB 49244968
C	-3	PRO	-	CLONING ARTIFACT	GB 49244968
C	-2	ARG	-	CLONING ARTIFACT	GB 49244968

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	CLONING ARTIFACT	GB 49244968
C	0	SER	-	CLONING ARTIFACT	GB 49244968

- Molecule 2 is a protein called acetyl-coenzyme A carboxylase carboxyl transferase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	20	0	0
			2009	1263	344	385	17			
2	D	255	Total	C	N	O	S	26	0	0
			1980	1246	339	378	17			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

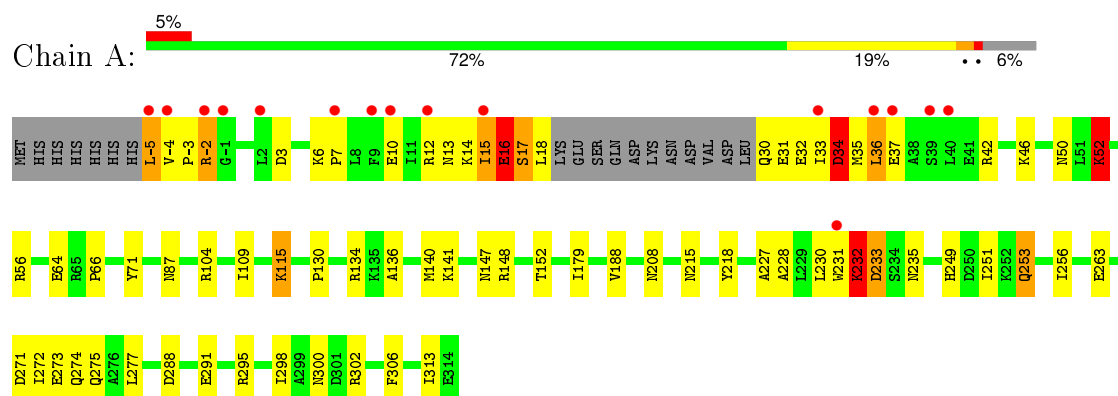
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	155	Total	O	0	0
			155	155		
4	C	163	Total	O	0	0
			163	163		
4	D	132	Total	O	0	0
			132	132		

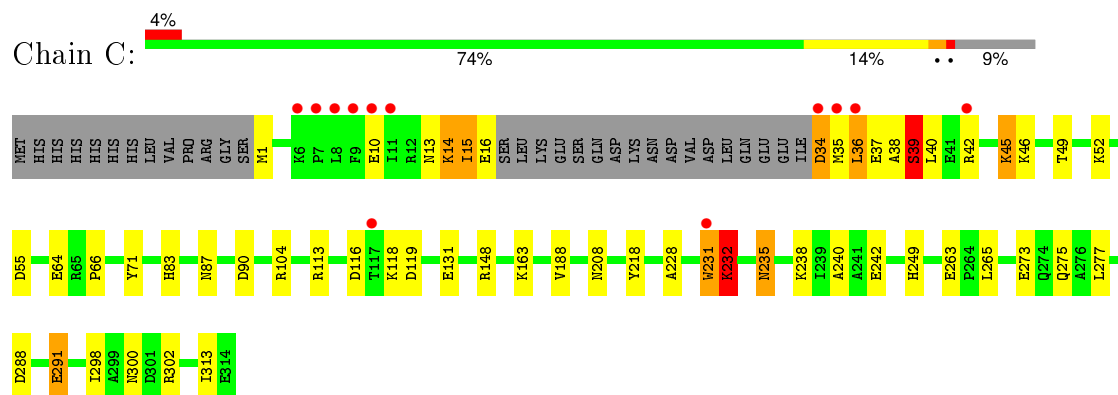
### 3 Residue-property plots

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.

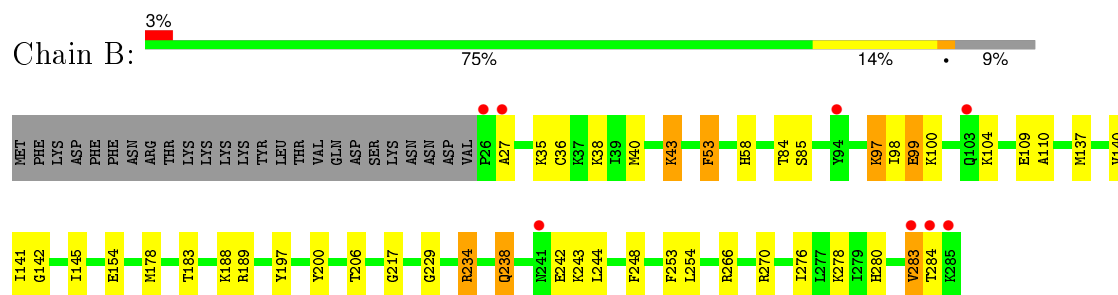
- Molecule 1: acetyl-coenzyme A carboxylase carboxyl transferase subunit alpha



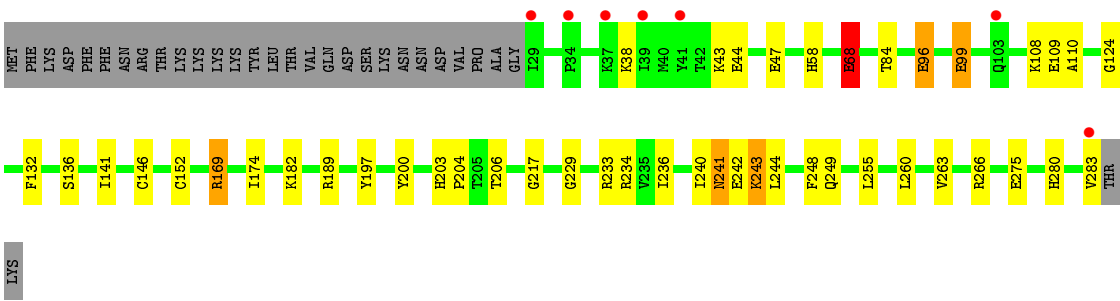
- Molecule 1: acetyl-coenzyme A carboxylase carboxyl transferase subunit alpha



- Molecule 2: acetyl-coenzyme A carboxylase carboxyl transferase subunit beta



- Molecule 2: acetyl-coenzyme A carboxylase carboxyl transferase subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.98Å 50.86Å 149.64Å 90.00° 113.51° 90.00°	Depositor
Resolution (Å)	50.00 – 1.98 49.43 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-1.98) 97.5 (49.43-1.98)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.186 , 0.213 0.185 , 0.211	Depositor DCC
$R_{free}$ test set	9030 reflections (11.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 90018 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9270	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	2.10	29/2446 (1.2%)	1.34	33/3292 (1.0%)
1	C	1.79	30/2326 (1.3%)	1.66	49/3134 (1.6%)
2	B	1.17	12/2041 (0.6%)	1.03	13/2741 (0.5%)
2	D	1.14	11/2011 (0.5%)	1.02	19/2701 (0.7%)
All	All	1.64	82/8824 (0.9%)	1.31	114/11868 (1.0%)

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	4
1	C	1	7
2	B	0	3
2	D	0	2
All	All	1	16

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	GLU	CD-OE2	-52.02	0.68	1.25
1	A	232	LYS	CE-NZ	-33.86	0.64	1.49
1	A	-4	VAL	CB-CG2	32.45	2.21	1.52
1	A	-4	VAL	CB-CG1	26.37	2.08	1.52
1	C	291	GLU	CD-OE2	23.22	1.51	1.25
1	C	36	LEU	CB-CG	22.84	2.18	1.52
1	C	232	LYS	CD-CE	22.56	2.07	1.51
1	C	232	LYS	CE-NZ	22.47	2.05	1.49
1	A	-2	ARG	CB-CG	22.10	2.12	1.52
1	C	52	LYS	CD-CE	-21.43	0.97	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	243	LYS	CD-CE	19.43	1.99	1.51
2	B	99	GLU	CG-CD	19.33	1.80	1.51
1	C	36	LEU	CA-CB	19.02	1.97	1.53
1	C	45	LYS	CD-CE	17.40	1.94	1.51
2	B	97	LYS	CD-CE	16.80	1.93	1.51
2	B	242	GLU	CB-CG	-16.72	1.20	1.52
1	C	118	LYS	CE-NZ	16.59	1.90	1.49
2	D	68	GLU	CG-CD	16.25	1.76	1.51
1	A	17	SER	N-CA	16.18	1.78	1.46
1	A	18	LEU	CA-C	15.61	1.93	1.52
1	C	37	GLU	CD-OE2	-15.54	1.08	1.25
1	A	233	ASP	CB-CG	15.31	1.83	1.51
1	A	-5	LEU	CA-CB	15.26	1.88	1.53
1	A	12	ARG	CB-CG	15.21	1.93	1.52
1	A	233	ASP	CG-OD1	-15.15	0.90	1.25
1	A	253	GLN	CG-CD	14.60	1.84	1.51
1	A	16	GLU	C-O	-14.57	0.95	1.23
1	C	231	TRP	CD1-NE1	13.96	1.61	1.38
1	C	45	LYS	CE-NZ	-13.92	1.14	1.49
1	C	52	LYS	CE-NZ	-13.77	1.14	1.49
1	C	232	LYS	CG-CD	13.62	1.98	1.52
1	A	16	GLU	C-N	13.43	1.65	1.34
1	C	14	LYS	C-O	12.91	1.47	1.23
2	D	99	GLU	CB-CG	12.67	1.76	1.52
2	D	243	LYS	CB-CG	12.57	1.86	1.52
1	C	291	GLU	CG-CD	12.53	1.70	1.51
1	A	15	ILE	CA-C	12.49	1.85	1.52
1	C	36	LEU	CG-CD1	12.43	1.97	1.51
2	B	238	GLN	CG-CD	12.23	1.79	1.51
2	D	234	ARG	CZ-NH1	11.39	1.47	1.33
1	A	46	LYS	CE-NZ	10.33	1.74	1.49
2	B	242	GLU	CG-CD	10.32	1.67	1.51
2	B	154	GLU	CD-OE1	10.13	1.36	1.25
2	D	283	VAL	C-O	10.11	1.42	1.23
1	C	46	LYS	CE-NZ	-9.90	1.24	1.49
1	A	115	LYS	CD-CE	9.34	1.74	1.51
1	A	42	ARG	CZ-NH1	9.31	1.45	1.33
1	A	34	ASP	CB-CG	9.11	1.70	1.51
1	C	14	LYS	C-N	8.94	1.54	1.34
1	C	15	ILE	CA-C	8.82	1.75	1.52
1	A	64	GLU	CD-OE2	-8.71	1.16	1.25
1	A	52	LYS	CE-NZ	-8.69	1.27	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	291	GLU	CD-OE1	8.54	1.35	1.25
1	A	52	LYS	CD-CE	8.47	1.72	1.51
2	D	96	GLU	CG-CD	8.36	1.64	1.51
2	B	43	LYS	CD-CE	8.31	1.72	1.51
1	C	34	ASP	CA-C	8.29	1.74	1.52
2	B	100	LYS	CD-CE	8.12	1.71	1.51
1	C	231	TRP	CZ3-CH2	8.02	1.52	1.40
1	C	42	ARG	CZ-NH1	7.77	1.43	1.33
2	D	243	LYS	CA-CB	-7.52	1.37	1.53
2	B	283	VAL	N-CA	7.40	1.61	1.46
2	B	234	ARG	CB-CG	7.01	1.71	1.52
1	A	235	ASN	CG-OD1	-6.89	1.08	1.24
1	C	235	ASN	CB-CG	6.72	1.66	1.51
1	A	-2	ARG	CA-CB	-6.67	1.39	1.53
1	C	36	LEU	CG-CD2	6.61	1.76	1.51
1	A	42	ARG	NE-CZ	6.23	1.41	1.33
1	C	116	ASP	CG-OD1	-6.18	1.11	1.25
2	D	68	GLU	CD-OE1	5.98	1.32	1.25
1	C	1	MET	CA-CB	-5.94	1.40	1.53
1	A	13	ASN	C-O	-5.88	1.12	1.23
1	C	15	ILE	C-N	5.80	1.47	1.34
2	D	44	GLU	CD-OE2	-5.74	1.19	1.25
1	C	10	GLU	CA-CB	-5.67	1.41	1.53
1	A	50	ASN	CG-ND2	-5.66	1.18	1.32
2	B	284	THR	CA-C	5.49	1.67	1.52
2	D	68	GLU	CB-CG	-5.35	1.42	1.52
1	C	163	LYS	CD-CE	-5.34	1.38	1.51
1	A	233	ASP	CA-CB	5.23	1.65	1.53
1	A	14	LYS	C-O	-5.04	1.13	1.23
2	B	234	ARG	CZ-NH2	5.01	1.39	1.33

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASP	CB-CG-OD2	-32.68	88.89	118.30
1	C	36	LEU	CB-CG-CD1	-30.23	59.61	111.00
1	C	116	ASP	CB-CG-OD1	27.09	142.68	118.30
2	B	234	ARG	NE-CZ-NH2	-21.89	109.36	120.30
1	C	291	GLU	CG-CD-OE2	-21.06	76.18	118.30
1	C	232	LYS	CD-CE-NZ	-20.40	64.78	111.70
1	A	34	ASP	CB-CG-OD2	-20.24	100.08	118.30
1	C	104	ARG	NE-CZ-NH1	17.03	128.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASP	OD1-CG-OD2	15.33	152.43	123.30
2	B	99	GLU	CG-CD-OE1	-15.31	87.69	118.30
1	C	14	LYS	O-C-N	-15.12	98.52	122.70
1	C	36	LEU	CA-CB-CG	-14.94	80.95	115.30
1	C	291	GLU	CG-CD-OE1	14.25	146.80	118.30
1	C	116	ASP	OD1-CG-OD2	-14.12	96.47	123.30
1	C	15	ILE	O-C-N	-13.64	100.88	122.70
1	C	16	GLU	CA-C-O	-13.62	91.50	120.10
1	A	34	ASP	CB-CG-OD1	13.35	130.31	118.30
1	A	50	ASN	OD1-CG-ND2	-12.90	92.23	121.90
1	A	17	SER	N-CA-CB	-12.62	91.57	110.50
1	A	50	ASN	CB-CG-ND2	12.58	146.88	116.70
1	C	1	MET	N-CA-CB	12.35	132.84	110.60
1	C	52	LYS	CD-CE-NZ	12.22	139.81	111.70
2	B	238	GLN	CG-CD-OE1	-12.17	97.26	121.60
2	D	68	GLU	CG-CD-OE2	-12.06	94.18	118.30
2	D	44	GLU	OE1-CD-OE2	-11.89	109.03	123.30
2	B	154	GLU	OE1-CD-OE2	-11.79	109.15	123.30
1	C	231	TRP	CG-CD1-NE1	-11.76	98.34	110.10
1	C	36	LEU	CB-CG-CD2	-11.49	91.46	111.00
1	C	38	ALA	N-CA-CB	-11.39	94.16	110.10
1	C	39	SER	O-C-N	-10.87	105.30	122.70
2	B	234	ARG	NE-CZ-NH1	-10.57	115.02	120.30
2	D	234	ARG	NE-CZ-NH1	-10.25	115.17	120.30
2	D	38	LYS	CD-CE-NZ	-10.14	88.38	111.70
1	C	231	TRP	CD1-CG-CD2	10.12	114.40	106.30
1	A	15	ILE	CB-CA-C	-9.66	92.27	111.60
1	C	104	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	A	16	GLU	CA-C-N	-9.55	96.18	117.20
1	C	55	ASP	CB-CG-OD2	-9.45	109.79	118.30
1	C	64	GLU	OE1-CD-OE2	-9.29	112.15	123.30
2	D	169	ARG	NE-CZ-NH2	-9.26	115.67	120.30
2	B	99	GLU	CG-CD-OE2	-9.23	99.85	118.30
1	A	232	LYS	CD-CE-NZ	-8.94	91.13	111.70
1	A	-4	VAL	CA-CB-CG2	8.94	124.31	110.90
1	A	253	GLN	CG-CD-OE1	-8.89	103.82	121.60
1	A	46	LYS	CD-CE-NZ	-8.88	91.28	111.70
2	D	243	LYS	CD-CE-NZ	-8.85	91.34	111.70
1	C	15	ILE	N-CA-C	-8.82	87.19	111.00
1	C	14	LYS	CA-C-O	-8.76	101.70	120.10
1	C	34	ASP	CB-CA-C	-8.71	92.98	110.40
2	D	68	GLU	CG-CD-OE1	-8.71	100.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	169	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	C	39	SER	CA-C-O	8.47	137.89	120.10
1	C	15	ILE	CA-C-N	8.42	135.72	117.20
1	A	288	ASP	CB-CG-OD2	8.31	125.78	118.30
1	A	36	LEU	CB-CG-CD1	-8.28	96.92	111.00
1	C	15	ILE	C-N-CA	8.12	142.00	121.70
1	C	231	TRP	CB-CG-CD1	-8.02	116.58	127.00
1	C	288	ASP	CB-CG-OD2	7.96	125.46	118.30
2	D	283	VAL	CA-C-O	7.93	136.76	120.10
2	D	242	GLU	CB-CA-C	7.82	126.03	110.40
1	C	49	THR	CA-CB-CG2	7.72	123.21	112.40
1	C	36	LEU	CD1-CG-CD2	-7.68	87.46	110.50
1	A	104	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	D	68	GLU	OE1-CD-OE2	-7.56	114.22	123.30
1	A	16	GLU	CA-C-O	7.53	135.90	120.10
2	D	243	LYS	CB-CG-CD	-7.42	92.31	111.60
1	C	42	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	C	291	GLU	CB-CG-CD	7.32	133.95	114.20
2	D	242	GLU	CG-CD-OE2	-7.28	103.75	118.30
1	C	42	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	A	-5	LEU	CB-CA-C	-7.06	96.79	110.20
1	C	36	LEU	CB-CA-C	-6.87	97.15	110.20
2	B	238	GLN	CG-CD-NE2	-6.72	100.57	116.70
1	A	291	GLU	OE1-CD-OE2	6.62	131.25	123.30
1	A	34	ASP	CB-CA-C	-6.62	97.17	110.40
2	D	242	GLU	CG-CD-OE1	6.49	131.28	118.30
2	B	242	GLU	CA-CB-CG	6.48	127.65	113.40
2	B	154	GLU	CG-CD-OE1	6.44	131.19	118.30
1	A	104	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	D	44	GLU	CG-CD-OE2	6.43	131.17	118.30
1	C	34	ASP	CA-C-O	6.37	133.47	120.10
1	C	232	LYS	CG-CD-CE	6.34	130.91	111.90
1	C	14	LYS	CA-C-N	-6.32	103.29	117.20
2	B	97	LYS	CD-CE-NZ	-6.23	97.38	111.70
1	A	18	LEU	N-CA-C	-6.22	94.21	111.00
1	A	18	LEU	CB-CA-C	-6.21	98.41	110.20
1	A	64	GLU	OE1-CD-OE2	-6.16	115.91	123.30
1	A	-5	LEU	CB-CG-CD1	6.12	121.41	111.00
1	C	42	ARG	NH1-CZ-NH2	6.08	126.09	119.40
1	A	-5	LEU	CB-CG-CD2	6.07	121.31	111.00
1	C	40	LEU	CB-CG-CD1	5.94	121.10	111.00
2	D	234	ARG	NH1-CZ-NH2	5.90	125.89	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	ARG	C-N-CA	-5.88	109.95	122.30
1	A	-3	PRO	N-CA-CB	-5.83	96.19	102.60
1	C	291	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	C	38	ALA	CB-CA-C	-5.76	101.46	110.10
2	D	108	LYS	CD-CE-NZ	-5.72	98.55	111.70
1	C	298	ILE	CG1-CB-CG2	-5.68	98.91	111.40
1	A	16	GLU	C-N-CA	-5.62	107.66	121.70
2	D	38	LYS	CA-CB-CG	-5.58	101.12	113.40
2	B	284	THR	N-CA-C	5.52	125.91	111.00
1	A	17	SER	N-CA-C	-5.47	96.23	111.00
1	C	265	LEU	CB-CG-CD2	-5.45	101.74	111.00
1	A	291	GLU	CG-CD-OE2	-5.33	107.65	118.30
1	C	235	ASN	CB-CG-OD1	-5.31	110.98	121.60
2	B	284	THR	CB-CA-C	-5.30	97.30	111.60
1	C	14	LYS	C-N-CA	-5.26	108.55	121.70
2	B	238	GLN	CB-CG-CD	5.26	125.28	111.60
1	A	230	LEU	CB-CG-CD1	5.25	119.92	111.00
1	A	-3	PRO	CA-CB-CG	5.22	114.73	104.80
1	A	15	ILE	C-N-CA	5.16	134.59	121.70
2	D	243	LYS	CG-CD-CE	-5.15	96.44	111.90
1	C	118	LYS	N-CA-CB	5.12	119.82	110.60
1	C	232	LYS	CB-CG-CD	-5.02	98.55	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	1	MET	CA

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ILE	Mainchain
1	A	16	GLU	Mainchain
1	A	253	GLN	Sidechain
1	A	34	ASP	Sidechain
2	B	234	ARG	Sidechain
2	B	238	GLN	Sidechain
2	B	99	GLU	Sidechain
1	C	13	ASN	Mainchain
1	C	131	GLU	Sidechain
1	C	14	LYS	Mainchain
1	C	15	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	C	235	ASN	Sidechain
1	C	291	GLU	Sidechain
1	C	39	SER	Mainchain
2	D	68	GLU	Sidechain
2	D	96	GLU	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	2407	0	2419	53	0
1	C	2289	0	2273	34	0
2	B	2009	0	2017	43	0
2	D	1980	0	1992	33	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	133	0	0	5	0
4	B	155	0	0	8	0
4	C	163	0	0	6	0
4	D	132	0	0	6	0
All	All	9270	0	8701	144	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 8.

All (144) 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:C:36:LEU:CG	1:C:36:LEU:CD2	1.76	1.56
1:C:34:ASP:CA	1:C:34:ASP:C	1.74	1.53
1:C:36:LEU:CD1	1:C:36:LEU:CG	1.97	1.38
1:C:232:LYS:NZ	1:C:232:LYS:CE	2.05	1.19
1:A:274:GLN:HG2	4:A:413:HOH:O	1.66	0.96
1:C:34:ASP:C	1:C:34:ASP:CB	2.37	0.93
2:B:58:HIS:HE1	2:B:266:ARG:H	1.25	0.84
2:D:58:HIS:HE1	2:D:266:ARG:H	1.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:CD1	1:C:36:LEU:CD2	2.58	0.80
4:C:345:HOH:O	2:D:84:THR:HG22	1.81	0.79
1:A:263:GLU:HG2	1:A:275:GLN:NE2	2.00	0.77
1:C:188:VAL:H	1:C:208:ASN:HD22	1.30	0.76
1:C:34:ASP:CA	1:C:35:MET:N	2.49	0.75
2:B:110:ALA:HB3	2:B:141:ILE:HD11	1.68	0.75
1:A:300:ASN:HD22	2:B:189:ARG:HH22	1.33	0.75
1:C:300:ASN:HD22	2:D:189:ARG:HH22	1.32	0.74
1:C:231:TRP:HZ3	1:C:240:ALA:HB2	1.52	0.74
1:A:188:VAL:H	1:A:208:ASN:HD22	1.36	0.73
1:A:263:GLU:HG2	1:A:275:GLN:HE22	1.53	0.73
1:C:263:GLU:HG2	1:C:275:GLN:HE22	1.55	0.71
1:A:52:LYS:HD2	1:A:52:LYS:N	2.06	0.71
2:D:99:GLU:CG	2:D:99:GLU:CA	2.69	0.70
2:D:243:LYS:CA	2:D:243:LYS:CG	2.68	0.70
2:D:110:ALA:HB3	2:D:141:ILE:HD11	1.73	0.69
1:C:36:LEU:CA	1:C:36:LEU:CG	2.70	0.69
2:D:243:LYS:CE	2:D:243:LYS:CG	2.70	0.69
1:A:208:ASN:HD21	1:A:302:ARG:HH21	1.40	0.68
2:D:109:GLU:OE1	2:D:169:ARG:NH2	2.24	0.67
1:C:119:ASP:OD2	4:C:473:HOH:O	2.13	0.66
1:A:3:ASP:HA	1:A:6:LYS:HE2	1.77	0.66
1:C:36:LEU:CD1	1:C:36:LEU:HD22	2.26	0.65
1:A:87:ASN:HD21	1:C:87:ASN:ND2	1.94	0.65
2:B:43:LYS:HB3	2:B:43:LYS:NZ	2.13	0.64
1:C:34:ASP:HB3	1:C:34:ASP:C	2.16	0.64
1:C:263:GLU:HG2	1:C:275:GLN:NE2	2.13	0.63
1:A:30:GLN:HA	1:A:33:ILE:HD12	1.80	0.62
1:A:295:ARG:O	1:A:298:ILE:HG22	2.00	0.62
1:A:115:LYS:CE	1:A:115:LYS:CG	2.78	0.61
1:A:272:ILE:HD11	4:A:408:HOH:O	2.00	0.61
1:C:188:VAL:H	1:C:208:ASN:ND2	2.01	0.59
2:B:84:THR:HG22	4:B:727:HOH:O	2.03	0.58
1:A:52:LYS:CD	1:A:52:LYS:N	2.68	0.57
2:B:276:ILE:O	2:B:280:HIS:HD2	1.88	0.57
2:D:233:ARG:NH2	2:D:244:LEU:O	2.38	0.57
1:A:233:ASP:CA	1:A:233:ASP:CG	2.73	0.57
2:D:58:HIS:CE1	2:D:266:ARG:H	2.16	0.56
1:A:3:ASP:O	1:A:6:LYS:HG2	2.06	0.56
2:B:36:CYS:SG	2:B:38:LYS:HB2	2.45	0.56
1:C:313:ILE:HB	2:D:84:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASN:HD21	1:C:302:ARG:HH21	1.55	0.55
2:B:43:LYS:HB3	2:B:43:LYS:HZ3	1.72	0.55
1:A:300:ASN:ND2	2:B:189:ARG:HH22	2.04	0.55
1:C:36:LEU:HD13	1:C:36:LEU:HD22	1.88	0.55
2:B:270:ARG:NH2	4:B:752:HOH:O	2.33	0.55
2:D:275:GLU:HB3	4:D:714:HOH:O	2.07	0.54
2:D:206:THR:HB	4:D:730:HOH:O	2.07	0.54
1:A:16:GLU:C	1:A:17:SER:CA	2.77	0.54
1:A:263:GLU:HA	1:A:275:GLN:HE22	1.72	0.53
2:B:243:LYS:HD3	4:B:737:HOH:O	2.07	0.53
2:B:85:SER:HB2	2:B:98:ILE:HD13	1.91	0.53
2:D:263:VAL:HG23	4:D:734:HOH:O	2.08	0.53
1:A:87:ASN:HD21	1:C:87:ASN:HD21	1.55	0.53
1:A:-5:LEU:CA	1:A:-5:LEU:CG	2.86	0.52
1:A:87:ASN:ND2	1:C:87:ASN:HD21	2.07	0.52
2:D:68:GLU:CB	2:D:68:GLU:CD	2.78	0.52
2:B:244:LEU:HD13	2:B:248:PHE:CD2	2.44	0.52
1:A:313:ILE:HB	2:B:84:THR:CG2	2.40	0.51
1:A:306:PHE:CE1	2:B:178:MET:HE1	2.45	0.51
2:B:137:MET:HE2	2:B:141:ILE:HG22	1.91	0.51
2:B:270:ARG:NE	4:B:752:HOH:O	2.33	0.51
1:A:249:HIS:HB3	4:A:411:HOH:O	2.10	0.51
2:B:137:MET:HE3	2:B:145:ILE:HD12	1.92	0.51
1:A:306:PHE:HE1	2:B:178:MET:HE1	1.76	0.51
2:B:278:LYS:HE2	4:B:742:HOH:O	2.11	0.51
2:B:283:VAL:N	4:B:723:HOH:O	2.41	0.50
2:B:58:HIS:CE1	2:B:266:ARG:H	2.16	0.50
1:A:227:ALA:HA	1:A:231:TRP:HE3	1.76	0.50
1:A:32:GLU:O	1:A:35:MET:HB3	2.11	0.50
1:C:263:GLU:HA	1:C:275:GLN:HE22	1.77	0.49
2:B:197:TYR:CD2	2:B:217:GLY:HA2	2.47	0.49
1:A:179:ILE:O	2:B:188:LYS:HG2	2.13	0.49
2:D:197:TYR:CD2	2:D:217:GLY:HA2	2.48	0.49
2:B:35:LYS:NZ	4:B:647:HOH:O	2.43	0.49
1:A:228:ALA:O	1:A:232:LYS:HA	2.13	0.49
2:B:97:LYS:CE	2:B:97:LYS:CG	2.91	0.49
2:D:43:LYS:O	2:D:47:GLU:HG3	2.13	0.48
4:A:333:HOH:O	2:B:178:MET:HE1	2.12	0.48
2:D:206:THR:HA	2:D:229:GLY:O	2.14	0.48
1:A:306:PHE:CE1	2:B:178:MET:CE	2.97	0.48
1:C:83:HIS:HD2	1:C:90:ASP:OD2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:MET:HE1	2:B:183:THR:HG21	1.95	0.47
2:D:260:LEU:HB2	4:D:734:HOH:O	2.14	0.47
2:B:109:GLU:HG3	2:B:140:VAL:HG11	1.96	0.47
1:A:34:ASP:HA	1:A:37:GLU:HB2	1.96	0.46
2:D:110:ALA:HB2	2:D:132:PHE:HB3	1.95	0.46
1:A:87:ASN:CG	1:C:87:ASN:HD21	2.18	0.46
2:B:280:HIS:HE1	4:C:330:HOH:O	1.99	0.46
2:D:248:PHE:CD2	2:D:249:GLN:HG3	2.51	0.45
1:C:249:HIS:CD2	4:C:340:HOH:O	2.69	0.45
1:A:66:PRO:HB2	1:A:71:TYR:CZ	2.52	0.45
1:A:300:ASN:HD22	2:B:189:ARG:NH2	2.07	0.45
1:A:263:GLU:CG	1:A:275:GLN:HE22	2.26	0.45
1:C:66:PRO:HB2	1:C:71:TYR:CZ	2.51	0.44
1:A:251:ILE:HG22	1:A:256:ILE:HB	2.00	0.44
2:B:137:MET:HE1	2:B:142:GLY:HA2	1.99	0.44
1:C:45:LYS:CG	1:C:45:LYS:CE	2.96	0.44
1:A:313:ILE:HB	2:B:84:THR:HG22	2.00	0.44
2:B:104:LYS:HE2	4:B:684:HOH:O	2.17	0.44
1:A:273:GLU:O	1:A:277:LEU:HG	2.17	0.44
2:B:206:THR:HA	2:B:229:GLY:O	2.18	0.44
4:C:451:HOH:O	2:D:174:ILE:HG22	2.18	0.44
1:C:228:ALA:O	1:C:232:LYS:HA	2.18	0.43
2:D:136:SER:OG	2:D:169:ARG:HD3	2.18	0.43
2:B:280:HIS:CE1	1:C:148:ARG:HH12	2.37	0.43
1:A:56:ARG:HH11	1:A:215:ASN:ND2	2.17	0.43
1:A:32:GLU:O	1:A:36:LEU:HD12	2.19	0.43
2:D:124:GLY:HA3	2:D:152:CYS:SG	2.58	0.43
1:A:208:ASN:HD21	1:A:302:ARG:NH2	2.13	0.43
1:C:238:LYS:O	1:C:242:GLU:HG3	2.19	0.43
1:A:148:ARG:HH12	2:D:280:HIS:CE1	2.37	0.42
2:D:203:HIS:HA	2:D:204:PRO:HA	1.90	0.42
1:A:271:ASP:CG	1:A:274:GLN:HB3	2.39	0.42
1:A:306:PHE:HE1	2:B:178:MET:CE	2.33	0.42
1:A:109:ILE:O	1:A:152:THR:HA	2.19	0.42
2:B:137:MET:CE	2:B:141:ILE:HG22	2.49	0.42
1:A:6:LYS:O	1:A:10:GLU:HG3	2.20	0.42
2:D:146:CYS:SG	2:D:182:LYS:HG2	2.60	0.41
2:D:244:LEU:HD13	2:D:248:PHE:CD2	2.55	0.41
1:A:6:LYS:HB2	1:A:7:PRO:HD3	2.01	0.41
1:A:136:ALA:O	1:A:140:MET:HG3	2.21	0.41
2:B:40:MET:HG2	2:B:53:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:255:LEU:HB2	4:D:734:HOH:O	2.19	0.41
2:D:255:LEU:HD12	4:D:734:HOH:O	2.21	0.41
1:A:141:LYS:HD3	1:A:141:LYS:HA	1.82	0.41
2:B:244:LEU:HD13	2:B:248:PHE:CE2	2.56	0.41
2:D:241:ASN:HD22	2:D:241:ASN:HA	1.71	0.41
1:C:242:GLU:OE1	4:C:437:HOH:O	2.22	0.41
2:B:253:PHE:HD2	2:B:254:LEU:HD12	1.86	0.41
1:A:313:ILE:HB	2:B:84:THR:HG23	2.03	0.40
4:A:330:HOH:O	2:D:280:HIS:HE1	2.04	0.40
2:D:236:ILE:O	2:D:240:ILE:HG12	2.21	0.40
1:C:273:GLU:O	1:C:277:LEU:HG	2.22	0.40
1:A:30:GLN:O	1:A:34:ASP:OD1	2.40	0.40
1:A:130:PRO:O	1:A:134:ARG:HG3	2.22	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	305/327 (93%)	290 (95%)	14 (5%)	1 (0%)	46	39
1	C	293/327 (90%)	278 (95%)	15 (5%)	0	100	100
2	B	258/285 (90%)	252 (98%)	5 (2%)	1 (0%)	39	31
2	D	253/285 (89%)	248 (98%)	5 (2%)	0	100	100
All	All	1109/1224 (91%)	1068 (96%)	39 (4%)	2 (0%)	52	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	27	ALA
1	A	31	GLU

### 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	252/274 (92%)	246 (98%)	6 (2%)	57	55
1	C	235/274 (86%)	232 (99%)	3 (1%)	76	77
2	B	221/247 (90%)	219 (99%)	2 (1%)	84	86
2	D	219/247 (89%)	217 (99%)	2 (1%)	84	86
All	All	927/1042 (89%)	914 (99%)	13 (1%)	74	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	ARG
1	A	34	ASP
1	A	52	LYS
1	A	147	ASN
1	A	218	TYR
1	A	232	LYS
2	B	53	PHE
2	B	200	TYR
1	C	39	SER
1	C	218	TYR
1	C	232	LYS
2	D	200	TYR
2	D	241	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	124	ASN
1	A	147	ASN
1	A	208	ASN
1	A	215	ASN
1	A	275	GLN

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Mol	Chain	Res	Type
1	A	300	ASN
2	B	48	ASN
2	B	50	ASN
2	B	58	HIS
2	B	241	ASN
2	B	280	HIS
1	C	83	HIS
1	C	87	ASN
1	C	124	ASN
1	C	147	ASN
1	C	208	ASN
1	C	275	GLN
1	C	300	ASN
1	C	308	ASN
2	D	48	ASN
2	D	50	ASN
2	D	58	HIS
2	D	155	ASN
2	D	241	ASN
2	D	280	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	309/327 (94%)	0.23	16 (5%) 31 35	23, 35, 72, 90	29 (9%)
1	C	297/327 (90%)	0.25	12 (4%) 42 46	23, 34, 79, 94	30 (10%)
2	B	260/285 (91%)	0.04	8 (3%) 52 56	24, 35, 55, 71	12 (4%)
2	D	255/285 (89%)	-0.04	7 (2%) 58 61	25, 35, 53, 63	17 (6%)
All	All	1121/1224 (91%)	0.13	43 (3%) 44 48	23, 35, 65, 94	88 (7%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	PHE	8.2
2	D	29	ILE	6.8
1	C	11	ILE	6.8
2	D	283	VAL	6.5
1	A	9	PHE	5.3
1	C	36	LEU	5.2
1	C	35	MET	5.2
2	B	283	VAL	5.0
1	A	231	TRP	5.0
1	A	15	ILE	4.5
1	A	33	ILE	4.5
1	C	10	GLU	4.3
2	B	27	ALA	4.2
2	B	285	LYS	4.1
1	C	6	LYS	3.7
2	B	284	THR	3.6
2	B	103	GLN	3.2
1	A	-1	GLY	3.2
2	B	26	PRO	3.1
1	A	40	LEU	3.0
2	D	34	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	8	LEU	3.0
1	A	36	LEU	2.9
2	D	103	GLN	2.8
1	A	-4	VAL	2.7
1	A	-5	LEU	2.7
1	A	10	GLU	2.7
1	C	7	PRO	2.7
1	C	34	ASP	2.6
1	A	7	PRO	2.5
1	C	42	ARG	2.5
1	A	2	LEU	2.5
2	D	39	ILE	2.4
2	D	41	TYR	2.4
2	B	241	ASN	2.3
1	A	-2	ARG	2.3
1	A	39	SER	2.2
1	C	231	TRP	2.2
2	B	94	TYR	2.2
2	D	37	LYS	2.1
1	A	37	GLU	2.1
1	A	12	ARG	2.1
1	C	117	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	601	1/1	1.00	0.09	-0.83	35,35,35,35	0
3	ZN	D	602	1/1	0.98	0.07	-1.03	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.