



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:38 AM GMT

PDB ID : 3BGT  
Title : Structural Studies of Acetoacetate Decarboxylase  
Authors : Ho, M.; Allen, K.N.  
Deposited on : 2007-11-27  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

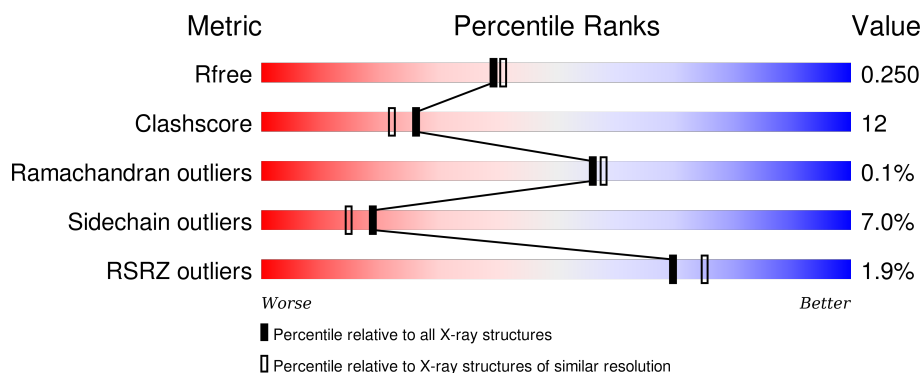
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	246	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	246	<div> <div></div> <div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>
1	C	246	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	D	246	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8082 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 Probable acetoacetate decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	Se	0	2	0
			1924	1241	327	346	2	8			
1	B	244	Total	C	N	O	S	Se	0	1	0
			1913	1235	323	345	2	8			
1	C	244	Total	C	N	O	S	Se	0	1	0
			1913	1235	323	345	2	8			
1	D	245	Total	C	N	O	S	Se	0	1	0
			1924	1241	327	346	2	8			

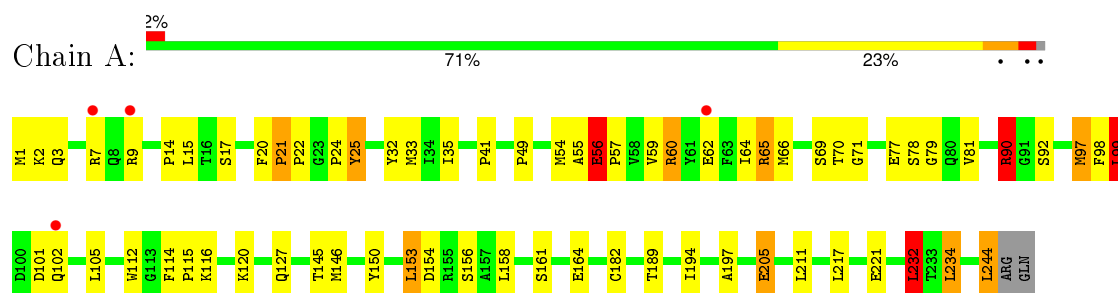
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		
2	B	122	Total	O	0	0
			122	122		
2	C	86	Total	O	0	0
			86	86		
2	D	86	Total	O	0	0
			86	86		

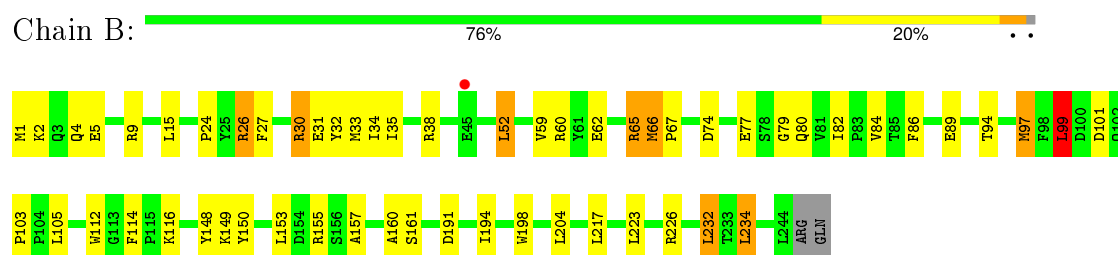
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

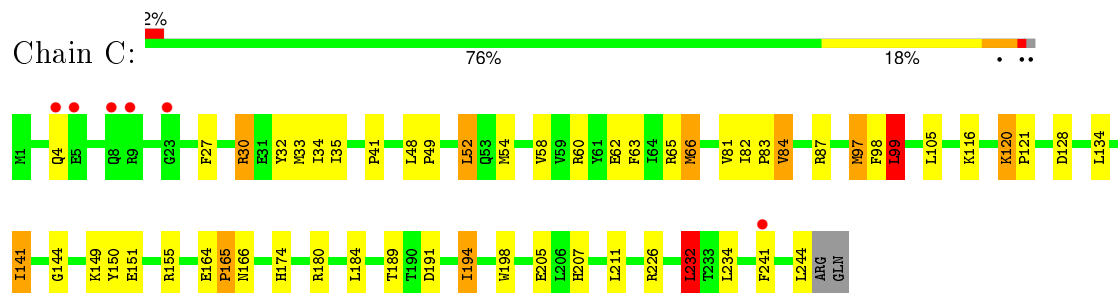
#### • Molecule 1: Probable acetoacetate decarboxylase



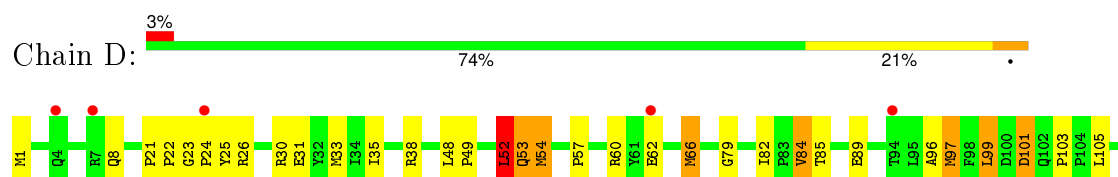
#### • Molecule 1: Probable acetoacetate decarboxylase

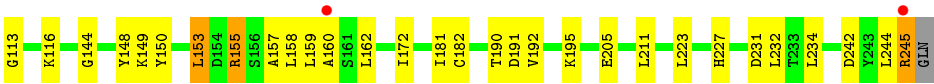


#### • Molecule 1: Probable acetoacetate decarboxylase



#### • Molecule 1: Probable acetoacetate decarboxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.45Å 105.45Å 252.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.30 – 2.10 30.28 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.30-2.10) 93.1 (30.28-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.201 , 0.245 0.206 , 0.250	Depositor DCC
$R_{free}$ test set	5815 reflections (9.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.7	EDS
Estimated twinning fraction	0.009 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.009 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.004 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.002 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.005 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.003 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.020 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 133725 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8082	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

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	1.59	46/1972 (2.3%)	1.05	11/2677 (0.4%)
1	B	1.01	12/1961 (0.6%)	0.89	7/2663 (0.3%)
1	C	1.10	23/1961 (1.2%)	0.88	8/2663 (0.3%)
1	D	1.31	38/1972 (1.9%)	1.00	12/2677 (0.4%)
All	All	1.27	119/7866 (1.5%)	0.96	38/10680 (0.4%)

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	1	0

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ARG	CB-CG	-16.57	1.07	1.52
1	B	89	GLU	CB-CG	-13.94	1.25	1.52
1	B	31	GLU	CD-OE1	-13.66	1.10	1.25
1	A	205	GLU	CB-CG	-12.84	1.27	1.52
1	B	31	GLU	CD-OE2	-12.84	1.11	1.25
1	A	205	GLU	CD-OE2	-11.76	1.12	1.25
1	A	62	GLU	CB-CG	-11.53	1.30	1.52
1	D	205	GLU	CD-OE1	-11.38	1.13	1.25
1	D	205	GLU	CD-OE2	-11.21	1.13	1.25
1	A	20	PHE	CE2-CZ	-10.00	1.18	1.37
1	A	24	PRO	CG-CD	-9.96	1.17	1.50
1	A	20	PHE	C-O	-9.85	1.04	1.23
1	A	25	TYR	CD1-CE1	-9.80	1.24	1.39
1	C	205	GLU	CD-OE1	-9.77	1.15	1.25
1	D	62	GLU	C-O	-9.53	1.05	1.23
1	C	98	PHE	CE2-CZ	-9.30	1.19	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	53	GLN	CB-CG	-9.29	1.27	1.52
1	A	62	GLU	CD-OE2	-9.27	1.15	1.25
1	A	71	GLY	C-O	-9.25	1.08	1.23
1	A	69	SER	CB-OG	-9.13	1.30	1.42
1	A	90	ARG	CG-CD	-9.10	1.29	1.51
1	C	191	ASP	C-O	-9.09	1.06	1.23
1	D	22	PRO	CA-C	-8.98	1.34	1.52
1	A	70	THR	C-O	-8.78	1.06	1.23
1	A	20	PHE	CG-CD1	-8.77	1.25	1.38
1	D	54	MSE	CG-SE	8.64	2.24	1.95
1	D	53	GLN	C-O	-8.53	1.07	1.23
1	C	98	PHE	CG-CD2	-8.51	1.25	1.38
1	A	221	GLU	C-O	-8.42	1.07	1.23
1	D	22	PRO	CA-CB	-8.39	1.36	1.53
1	D	155	ARG	CZ-NH2	-8.36	1.22	1.33
1	A	127	GLN	C-O	-8.33	1.07	1.23
1	A	56	GLU	CD-OE1	-8.28	1.16	1.25
1	D	22	PRO	CG-CD	-8.27	1.23	1.50
1	A	3	GLN	C-O	-8.13	1.07	1.23
1	D	25	TYR	CE1-CZ	-7.97	1.28	1.38
1	C	205	GLU	CD-OE2	-7.94	1.17	1.25
1	A	90	ARG	CA-CB	-7.90	1.36	1.53
1	C	98	PHE	C-O	-7.90	1.08	1.23
1	D	23	GLY	C-O	-7.86	1.11	1.23
1	D	62	GLU	CB-CG	-7.85	1.37	1.52
1	C	98	PHE	CD2-CE2	-7.75	1.23	1.39
1	C	97[A]	MSE	N-CA	-7.67	1.31	1.46
1	C	97[B]	MSE	N-CA	-7.67	1.31	1.46
1	D	53	GLN	CG-CD	-7.67	1.33	1.51
1	D	54	MSE	CA-CB	-7.63	1.37	1.53
1	B	31	GLU	C-O	-7.59	1.08	1.23
1	D	54	MSE	CB-CG	-7.46	1.30	1.52
1	C	97[A]	MSE	C-O	-7.42	1.09	1.23
1	C	97[B]	MSE	C-O	-7.42	1.09	1.23
1	B	89	GLU	CG-CD	-7.42	1.40	1.51
1	A	102	GLN	CD-OE1	-7.37	1.07	1.24
1	A	22	PRO	CB-CG	-7.33	1.13	1.50
1	C	166	ASN	CG-ND2	-7.28	1.14	1.32
1	B	31	GLU	CG-CD	-7.22	1.41	1.51
1	A	62	GLU	CG-CD	7.20	1.62	1.51
1	C	98	PHE	CG-CD1	-7.20	1.27	1.38
1	D	52	LEU	CG-CD1	-7.17	1.25	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	22	PRO	C-O	-7.16	1.08	1.23
1	A	21	PRO	C-O	-7.02	1.09	1.23
1	C	205	GLU	C-O	-6.99	1.10	1.23
1	C	166	ASN	CG-OD1	-6.96	1.08	1.24
1	C	87	ARG	C-O	-6.94	1.10	1.23
1	A	25	TYR	CG-CD1	-6.91	1.30	1.39
1	D	52	LEU	C-O	-6.87	1.10	1.23
1	D	62	GLU	CD-OE1	-6.86	1.18	1.25
1	C	150	TYR	CD1-CE1	-6.85	1.29	1.39
1	A	24	PRO	C-O	-6.79	1.09	1.23
1	D	25	TYR	C-O	-6.78	1.10	1.23
1	A	56	GLU	C-O	-6.69	1.10	1.23
1	A	22	PRO	CG-CD	-6.69	1.28	1.50
1	D	52	LEU	CG-CD2	-6.60	1.27	1.51
1	D	62	GLU	CD-OE2	-6.60	1.18	1.25
1	D	155	ARG	N-CA	-6.54	1.33	1.46
1	D	116	LYS	CG-CD	-6.50	1.30	1.52
1	C	165	PRO	C-O	-6.44	1.10	1.23
1	D	25	TYR	CZ-OH	-6.41	1.26	1.37
1	A	22	PRO	C-O	-6.40	1.10	1.23
1	D	54	MSE	N-CA	-6.34	1.33	1.46
1	A	25	TYR	CD2-CE2	-6.30	1.29	1.39
1	D	52	LEU	CA-C	-6.16	1.36	1.52
1	D	25	TYR	CD1-CE1	-6.12	1.30	1.39
1	B	150	TYR	CD1-CE1	-6.07	1.30	1.39
1	A	60[A]	ARG	C-O	-6.07	1.11	1.23
1	A	60[B]	ARG	C-O	-6.07	1.11	1.23
1	A	102	GLN	CD-NE2	-6.07	1.17	1.32
1	D	150	TYR	CD1-CE1	-6.04	1.30	1.39
1	D	24	PRO	C-O	-6.01	1.11	1.23
1	A	90	ARG	C-O	-6.00	1.11	1.23
1	A	205	GLU	CD-OE1	-5.96	1.19	1.25
1	C	98	PHE	CE1-CZ	-5.94	1.26	1.37
1	A	21	PRO	CA-CB	-5.81	1.42	1.53
1	A	57	PRO	C-O	-5.75	1.11	1.23
1	D	97[A]	MSE	C-O	-5.74	1.12	1.23
1	D	97[B]	MSE	C-O	-5.74	1.12	1.23
1	A	70	THR	CB-CG2	-5.71	1.33	1.52
1	D	21	PRO	C-O	-5.71	1.11	1.23
1	B	97[A]	MSE	C-N	-5.67	1.21	1.34
1	B	97[B]	MSE	C-N	-5.67	1.21	1.34
1	B	150	TYR	CE2-CZ	-5.66	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	ASN	C-O	-5.63	1.12	1.23
1	A	102	GLN	N-CA	-5.56	1.35	1.46
1	A	21	PRO	CG-CD	-5.52	1.32	1.50
1	A	62	GLU	C-O	-5.52	1.12	1.23
1	C	165	PRO	CG-CD	-5.44	1.32	1.50
1	D	54	MSE	C-O	-5.43	1.13	1.23
1	A	221	GLU	CD-OE1	-5.38	1.19	1.25
1	D	23	GLY	N-CA	-5.36	1.38	1.46
1	A	24	PRO	CA-CB	-5.29	1.43	1.53
1	C	150	TYR	CE2-CZ	-5.28	1.31	1.38
1	A	22	PRO	N-CD	-5.22	1.40	1.47
1	D	205	GLU	CB-CG	-5.16	1.42	1.52
1	C	150	TYR	CD2-CE2	-5.09	1.31	1.39
1	A	205	GLU	C-O	-5.08	1.13	1.23
1	B	89	GLU	CD-OE1	-5.06	1.20	1.25
1	D	155	ARG	CB-CG	-5.05	1.39	1.52
1	B	150	TYR	CD2-CE2	-5.05	1.31	1.39
1	A	60[A]	ARG	CZ-NH2	-5.03	1.26	1.33
1	A	60[B]	ARG	CZ-NH2	-5.03	1.26	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	155	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	D	155	ARG	NE-CZ-NH2	-11.43	114.59	120.30
1	C	191	ASP	CB-CG-OD1	10.64	127.87	118.30
1	A	90	ARG	NE-CZ-NH1	-9.59	115.51	120.30
1	B	31	GLU	OE1-CD-OE2	-8.30	113.34	123.30
1	D	97[A]	MSE	CA-CB-CG	8.17	127.19	113.30
1	D	97[B]	MSE	CA-CB-CG	8.17	127.19	113.30
1	B	232	LEU	CA-CB-CG	7.68	132.96	115.30
1	A	56	GLU	OE1-CD-OE2	-7.19	114.68	123.30
1	A	90	ARG	NE-CZ-NH2	6.89	123.74	120.30
1	C	191	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	99	LEU	CA-CB-CG	6.58	130.43	115.30
1	A	232	LEU	CA-CB-CG	6.47	130.19	115.30
1	B	101	ASP	CB-CG-OD1	6.34	124.01	118.30
1	B	97[A]	MSE	O-C-N	6.16	132.56	122.70
1	B	97[B]	MSE	O-C-N	6.16	132.56	122.70
1	B	99	LEU	CA-CB-CG	6.12	129.37	115.30
1	D	232	LEU	CA-CB-CG	6.09	129.31	115.30
1	C	232	LEU	CA-CB-CG	5.95	128.99	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	MSE	CG-SE-CE	-5.68	86.40	98.90
1	C	232	LEU	CB-CG-CD2	5.50	120.34	111.00
1	A	65	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	D	62	GLU	CG-CD-OE2	5.40	129.10	118.30
1	D	53	GLN	CB-CA-C	-5.35	99.70	110.40
1	A	90	ARG	N-CA-C	5.30	125.32	111.00
1	A	97[A]	MSE	O-C-N	5.27	131.13	122.70
1	A	97[B]	MSE	O-C-N	5.27	131.13	122.70
1	D	53	GLN	N-CA-C	5.25	125.17	111.00
1	D	116	LYS	CD-CE-NZ	5.24	123.75	111.70
1	C	97[A]	MSE	CA-CB-CG	5.23	122.19	113.30
1	C	97[B]	MSE	CA-CB-CG	5.23	122.19	113.30
1	C	66	MSE	CG-SE-CE	-5.22	87.41	98.90
1	C	99	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	101	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	52	LEU	CB-CG-CD2	5.18	119.80	111.00
1	D	62	GLU	N-CA-C	5.14	124.89	111.00
1	A	101	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	25	TYR	CD1-CE1-CZ	5.06	124.36	119.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	90	ARG	CA

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1924	0	1923	57	3
1	B	1913	0	1911	54	0
1	C	1913	0	1911	42	0
1	D	1924	0	1924	39	0
2	A	114	0	0	3	0
2	B	122	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	86	0	0	2	3
2	D	86	0	0	5	0
All	All	8082	0	7669	189	3

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 12.

All (189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLU:HG2	1:B:97[B]:MSE:CE	1.51	1.38
1:D:54:MSE:CG	1:D:54:MSE:SE	2.24	1.36
1:A:77:GLU:HG2	1:A:97[B]:MSE:CE	1.56	1.35
1:D:54:MSE:CE	1:D:54:MSE:SE	2.24	1.35
1:A:77:GLU:CG	1:A:97[B]:MSE:HE3	1.66	1.24
1:A:97[A]:MSE:HE1	1:A:114:PHE:CD1	1.80	1.17
1:A:33:MSE:HE2	1:A:35:ILE:HD11	1.32	1.10
1:A:79:GLY:HA3	1:A:97[B]:MSE:SE	2.00	1.10
1:A:77:GLU:CG	1:A:97[B]:MSE:CE	2.27	1.10
1:C:226:ARG:NH1	2:C:331:HOH:O	1.84	1.08
1:A:205:GLU:OE1	2:A:331:HOH:O	1.72	1.05
1:A:33:MSE:HE3	1:A:146:MSE:HG3	1.38	1.05
1:B:77:GLU:HG2	1:B:97[B]:MSE:HE3	1.10	1.05
1:B:77:GLU:CG	1:B:97[B]:MSE:CE	2.35	1.05
1:B:77:GLU:HG2	1:B:97[B]:MSE:HE2	1.37	1.04
1:B:94:THR:HG21	1:B:97[A]:MSE:HE3	1.41	1.02
1:B:1:MSE:HE3	1:B:15:LEU:HD23	1.41	1.02
1:A:77:GLU:HG2	1:A:97[B]:MSE:HE3	1.29	0.99
1:B:34:ILE:HD12	1:B:62:GLU:HG2	1.41	0.99
1:A:77:GLU:HG2	1:A:97[B]:MSE:HE1	1.44	0.99
1:B:153:LEU:HD21	1:B:226:ARG:HD2	1.43	0.97
1:B:77:GLU:CG	1:B:97[B]:MSE:HE3	1.94	0.95
1:C:33:MSE:HE3	1:C:35:ILE:CD1	1.98	0.94
1:B:1:MSE:HE3	1:B:15:LEU:CD2	1.97	0.94
1:B:77:GLU:CG	1:B:97[B]:MSE:HE2	1.98	0.93
1:C:33:MSE:HE2	1:C:63:PHE:HD2	1.33	0.92
1:C:33:MSE:HE3	1:C:35:ILE:HD12	1.50	0.92
1:D:48:LEU:HD13	1:D:82:ILE:HD11	1.50	0.91
1:C:33:MSE:HE2	1:C:63:PHE:CD2	2.05	0.90
1:A:56:GLU:OE1	1:A:90:ARG:NH2	2.07	0.87
1:A:33:MSE:CE	1:A:35:ILE:HD11	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:HG3	1:A:97[B]:MSE:HE3	1.58	0.83
1:A:97[A]:MSE:CE	1:A:114:PHE:HB3	2.08	0.83
1:A:97[A]:MSE:HE1	1:A:114:PHE:CG	2.13	0.82
1:A:153:LEU:HD22	1:A:197:ALA:HB1	1.59	0.82
1:D:113:GLY:O	2:D:254:HOH:O	1.99	0.79
1:B:1:MSE:CE	1:B:15:LEU:HD23	2.12	0.79
1:A:33:MSE:HE2	1:A:35:ILE:CD1	2.12	0.78
1:D:96:ALA:O	1:D:97[A]:MSE:HE2	1.82	0.78
1:A:154:ASP:OD2	2:A:294:HOH:O	2.03	0.77
1:B:77:GLU:CD	1:B:97[B]:MSE:HE2	2.05	0.76
1:D:8:GLN:O	2:D:322:HOH:O	2.04	0.76
1:A:97[A]:MSE:CE	1:A:114:PHE:CD1	2.65	0.75
1:B:34:ILE:CD1	1:B:62:GLU:HG2	2.16	0.75
1:D:79:GLY:HA3	1:D:97[A]:MSE:HE2	1.68	0.74
1:B:77:GLU:OE2	1:B:97[B]:MSE:HE2	1.87	0.74
1:D:26:ARG:HH12	1:D:191:ASP:HB3	1.54	0.72
1:D:79:GLY:HA3	1:D:97[A]:MSE:CE	2.20	0.71
1:A:97[A]:MSE:HE1	1:A:114:PHE:HB3	1.72	0.71
1:C:33:MSE:CE	1:C:35:ILE:HD12	2.20	0.71
1:A:153:LEU:HD22	1:A:197:ALA:CB	2.20	0.70
1:A:32:TYR:CD2	1:A:64:ILE:HD12	2.27	0.69
1:C:33:MSE:CE	1:C:63:PHE:CD2	2.74	0.69
1:A:97[A]:MSE:HE1	1:A:114:PHE:HD1	1.49	0.69
1:B:38:ARG:HB2	1:B:223:LEU:HD11	1.73	0.69
1:B:79:GLY:HA3	1:B:97[B]:MSE:SE	2.43	0.68
1:A:158:LEU:HD23	1:A:194:ILE:HD13	1.76	0.67
1:D:33:MSE:HE3	1:D:35:ILE:HD11	1.77	0.67
1:D:99:LEU:CD1	1:D:105:LEU:HG	2.25	0.67
1:C:34:ILE:HD12	1:C:62:GLU:HG2	1.78	0.66
1:A:97[A]:MSE:CE	1:A:114:PHE:HD1	2.07	0.66
1:B:60:ARG:HD2	2:B:299:HOH:O	1.96	0.66
1:A:97[A]:MSE:HE1	1:A:114:PHE:CB	2.27	0.65
1:A:153:LEU:CD2	1:A:197:ALA:HB1	2.26	0.65
1:B:157:ALA:O	1:B:160:ALA:HB3	1.97	0.65
1:B:26:ARG:NH2	1:B:191:ASP:O	2.30	0.64
1:C:33:MSE:CE	1:C:35:ILE:CD1	2.77	0.62
1:A:97[A]:MSE:HE2	1:A:115:PRO:HD2	1.82	0.62
1:C:27:PHE:HB3	1:C:30:ARG:HD3	1.82	0.62
1:B:1:MSE:HA	1:B:5:GLU:OE2	2.00	0.62
1:D:60:ARG:NH2	2:D:327:HOH:O	2.33	0.61
1:B:94:THR:CG2	1:B:97[A]:MSE:HE3	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PRO:HA	1:B:1:MSE:HG2	1.81	0.61
1:B:99:LEU:HD11	1:B:116:LYS:HG2	1.81	0.61
1:C:149:LYS:HD3	1:C:198:TRP:CE2	2.37	0.60
1:A:97[A]:MSE:HE3	1:A:114:PHE:HB3	1.82	0.59
1:A:77:GLU:CD	1:A:97[B]:MSE:CE	2.70	0.59
1:A:97[A]:MSE:HE3	1:A:116:LYS:HG3	1.85	0.59
1:B:99:LEU:HD13	1:B:105:LEU:HG	1.83	0.59
1:C:99:LEU:HD13	1:C:105:LEU:HG	1.85	0.59
1:C:33:MSE:HE1	1:C:144:GLY:HA3	1.85	0.58
1:C:32:TYR:HD2	1:C:34:ILE:HD11	1.69	0.58
1:C:120:LYS:HG3	1:C:120:LYS:O	2.03	0.58
1:B:155:ARG:HG2	1:B:194:ILE:HG21	1.84	0.58
1:D:33:MSE:HE1	1:D:144:GLY:C	2.24	0.57
1:C:49:PRO:O	1:C:52:LEU:HB2	2.03	0.57
1:D:242:ASP:O	1:D:245:ARG:HG3	2.05	0.57
1:D:182:CYS:HB3	1:D:244:LEU:HD13	1.86	0.56
1:B:59:VAL:HG11	1:B:80:GLN:HG2	1.87	0.55
1:C:134:LEU:HG	1:C:141:ILE:HD11	1.88	0.55
1:D:38:ARG:HB2	1:D:223:LEU:HD11	1.87	0.54
1:C:65:ARG:HD3	2:C:258:HOH:O	2.07	0.54
1:A:189:THR:HB	1:A:232:LEU:HG	1.90	0.54
1:B:33:MSE:O	1:B:34:ILE:HD13	2.08	0.53
1:A:1:MSE:HE1	1:A:15:LEU:HD21	1.91	0.53
1:C:33:MSE:HE3	1:C:35:ILE:HD11	1.87	0.53
1:D:99:LEU:HD11	1:D:105:LEU:HG	1.91	0.53
1:B:148:TYR:CE2	1:B:149:LYS:HD2	2.43	0.53
1:C:27:PHE:CB	1:C:30:ARG:HD3	2.39	0.52
1:A:99:LEU:HD13	1:A:105:LEU:HG	1.91	0.52
1:B:65:ARG:HB3	1:B:65:ARG:HH11	1.73	0.52
1:C:155:ARG:NE	1:C:194:ILE:HD11	2.25	0.52
1:C:60:ARG:HH21	1:C:83:PRO:HB3	1.75	0.51
1:B:153:LEU:CD2	1:B:226:ARG:HD2	2.30	0.51
1:A:41:PRO:HB3	1:A:54:MSE:HE1	1.93	0.50
1:B:34:ILE:HD12	1:B:62:GLU:CG	2.29	0.50
1:B:99:LEU:HD11	1:B:116:LYS:CG	2.40	0.50
1:C:164:GLU:HB3	1:C:165:PRO:HD2	1.93	0.50
1:D:148:TYR:CE2	1:D:149:LYS:HD2	2.47	0.49
1:A:77:GLU:CD	1:A:97[B]:MSE:HE2	2.33	0.49
1:C:27:PHE:HB2	1:C:232:LEU:HD22	1.94	0.49
1:B:35:ILE:HG21	1:B:204:LEU:HB2	1.93	0.49
1:C:33:MSE:HE1	1:C:63:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:CD2	1:A:197:ALA:CB	2.87	0.49
1:A:33:MSE:HE1	1:A:145:THR:N	2.28	0.48
1:B:112:TRP:CZ2	1:B:234:LEU:HD13	2.47	0.48
1:C:164:GLU:HB3	1:C:165:PRO:CD	2.42	0.48
1:A:182:CYS:HB3	1:A:244:LEU:HD13	1.95	0.48
1:B:59:VAL:CG1	1:B:80:GLN:HG2	2.44	0.47
1:D:54:MSE:HE1	1:D:57:PRO:HB3	1.97	0.47
1:C:62:GLU:OE1	1:C:97[B]:MSE:HE1	2.14	0.47
1:D:99:LEU:H	1:D:99:LEU:HD12	1.80	0.47
1:B:52:LEU:HD12	1:B:86:PHE:HB2	1.97	0.47
1:B:82:ILE:HD11	1:B:217:LEU:HD21	1.98	0.46
1:D:97[B]:MSE:CE	2:D:332:HOH:O	2.64	0.46
1:A:33:MSE:HE2	1:A:35:ILE:CG1	2.45	0.46
1:A:54:MSE:HG2	1:A:55:ALA:O	2.16	0.46
1:B:74:ASP:OD1	1:B:74:ASP:C	2.54	0.45
1:B:149:LYS:HG2	1:B:198:TRP:CD2	2.51	0.45
1:D:153:LEU:HD12	1:D:153:LEU:HA	1.50	0.45
1:A:161:SER:O	1:A:164:GLU:HG2	2.16	0.45
1:D:195:LYS:HE3	1:D:231:ASP:OD1	2.16	0.45
1:C:99:LEU:HD11	1:C:116:LYS:HD3	1.98	0.45
1:B:60:ARG:NH2	2:B:345:HOH:O	2.15	0.45
1:C:174:HIS:HB2	1:C:180:ARG:HB2	1.99	0.44
1:A:81:VAL:CG1	1:A:92:SER:HB2	2.46	0.44
1:A:99:LEU:HD11	1:A:116:LYS:HD3	1.99	0.44
1:D:85:THR:HA	1:D:89:GLU:O	2.17	0.44
1:C:120:LYS:HE2	1:C:121:PRO:O	2.18	0.44
1:C:189:THR:HB	1:C:232:LEU:HG	2.00	0.44
1:C:141:ILE:HA	1:C:207:HIS:HB2	2.00	0.44
1:B:65:ARG:HH12	1:B:67:PRO:N	2.15	0.44
1:C:58:VAL:HG22	1:C:83:PRO:HG3	2.01	0.43
1:D:49:PRO:O	1:D:52:LEU:HB2	2.18	0.43
1:A:59:VAL:HG21	1:A:217:LEU:HD23	2.00	0.43
1:D:48:LEU:CD1	1:D:82:ILE:HD11	2.35	0.43
1:D:79:GLY:CA	1:D:97[A]:MSE:CE	2.93	0.43
1:D:31:GLU:OE2	1:D:227:HIS:NE2	2.36	0.43
1:C:184:LEU:HB2	1:C:241:PHE:HB3	2.01	0.43
1:B:26:ARG:NH2	1:B:191:ASP:HB3	2.34	0.43
1:D:48:LEU:HD21	1:D:84:VAL:HG23	2.00	0.43
1:D:97[B]:MSE:HE1	2:D:332:HOH:O	2.17	0.43
1:D:99:LEU:N	1:D:99:LEU:HD12	2.34	0.43
1:C:99:LEU:HD11	1:C:116:LYS:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:PRO:HA	1:C:54:MSE:HE1	2.01	0.43
1:A:49:PRO:HD3	1:B:1:MSE:HE2	2.01	0.42
1:C:33:MSE:CE	1:C:63:PHE:CE2	3.02	0.42
1:B:26:ARG:HH21	1:B:191:ASP:HB3	1.84	0.42
1:D:26:ARG:NH1	1:D:191:ASP:HB3	2.29	0.42
1:B:82:ILE:HD11	1:B:217:LEU:CD2	2.49	0.42
1:A:77:GLU:OE2	1:A:99:LEU:HG	2.19	0.42
1:B:33:MSE:C	1:B:34:ILE:HD13	2.40	0.42
1:A:56:GLU:HG3	1:A:56:GLU:H	1.42	0.42
1:A:112:TRP:CZ2	1:A:234:LEU:HD13	2.54	0.42
1:A:14:PRO:HD2	1:A:17:SER:O	2.20	0.42
1:B:1:MSE:HA	1:B:5:GLU:CD	2.40	0.42
1:B:97[A]:MSE:HE1	1:B:114:PHE:CE1	2.55	0.42
1:D:99:LEU:HD13	1:D:105:LEU:HG	2.01	0.42
1:C:164:GLU:CB	1:C:165:PRO:CD	2.95	0.42
1:C:48:LEU:HD11	1:C:84:VAL:HG23	2.02	0.42
1:A:156:SER:HB2	2:A:294:HOH:O	2.19	0.41
1:B:27:PHE:CB	1:B:30:ARG:HD3	2.51	0.41
1:A:97[B]:MSE:C	1:A:98:PHE:CD2	2.94	0.41
1:D:162:LEU:HD12	1:D:192:VAL:HG11	2.01	0.41
1:D:172:ILE:HG13	1:D:181:ILE:HD12	2.02	0.41
1:A:97[A]:MSE:C	1:A:98:PHE:CD2	2.94	0.41
1:B:103:PRO:HG2	1:C:128:ASP:CB	2.51	0.41
1:D:30:ARG:NH1	1:D:66:MSE:HE3	2.36	0.41
1:B:2:LYS:O	1:B:5:GLU:HB3	2.21	0.41
1:D:190:THR:O	1:D:191:ASP:HB2	2.21	0.41
1:A:33:MSE:HE3	1:A:146:MSE:CG	2.29	0.41
1:B:32:TYR:HD2	1:B:34:ILE:HD11	1.86	0.41
1:D:157:ALA:O	1:D:160:ALA:HB3	2.21	0.41
1:B:24:PRO:HA	2:B:254:HOH:O	2.20	0.41
1:A:78:SER:O	1:A:97[B]:MSE:HA	2.21	0.41
1:C:155:ARG:HD2	1:C:194:ILE:HG12	2.03	0.41
1:C:164:GLU:HA	1:C:165:PRO:HD3	1.71	0.41
1:A:79:GLY:CA	1:A:97[B]:MSE:SE	2.94	0.40
1:D:101:ASP:OD1	1:D:103:PRO:HD2	2.22	0.40

All (3) 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:150:TYR:OH	2:C:301:HOH:O[2_765]	0.18	2.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TYR:CZ	2:C:301:HOH:O[2_765]	1.17	1.03
1:A:150:TYR:CE2	2:C:301:HOH:O[2_765]	2.14	0.06

## 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	244/246 (99%)	236 (97%)	8 (3%)	0	100	100
1	B	243/246 (99%)	233 (96%)	10 (4%)	0	100	100
1	C	243/246 (99%)	233 (96%)	10 (4%)	0	100	100
1	D	244/246 (99%)	233 (96%)	10 (4%)	1 (0%)	39	37
All	All	974/984 (99%)	935 (96%)	38 (4%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	159	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/198 (104%)	187 (91%)	18 (9%)	12	8
1	B	204/198 (103%)	192 (94%)	12 (6%)	24	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	204/198 (103%)	188 (92%)	16 (8%)	16	11
1	D	205/198 (104%)	193 (94%)	12 (6%)	24	20
All	All	818/792 (103%)	760 (93%)	58 (7%)	19	14

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	7	ARG
1	A	9	ARG
1	A	21	PRO
1	A	25	TYR
1	A	56	GLU
1	A	60[A]	ARG
1	A	60[B]	ARG
1	A	65	ARG
1	A	66	MSE
1	A	90	ARG
1	A	99	LEU
1	A	120	LYS
1	A	153	LEU
1	A	211	LEU
1	A	232	LEU
1	A	234	LEU
1	A	244	LEU
1	B	4	GLN
1	B	9	ARG
1	B	26	ARG
1	B	30	ARG
1	B	52	LEU
1	B	65	ARG
1	B	66	MSE
1	B	84	VAL
1	B	99	LEU
1	B	161	SER
1	B	232	LEU
1	B	234	LEU
1	C	4	GLN
1	C	30	ARG
1	C	52	LEU
1	C	66	MSE

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Mol	Chain	Res	Type
1	C	81	VAL
1	C	82	ILE
1	C	84	VAL
1	C	99	LEU
1	C	120	LYS
1	C	141	ILE
1	C	151	GLU
1	C	194	ILE
1	C	211	LEU
1	C	232	LEU
1	C	234	LEU
1	C	244	LEU
1	D	1	MSE
1	D	52	LEU
1	D	53	GLN
1	D	66	MSE
1	D	84	VAL
1	D	99	LEU
1	D	153	LEU
1	D	155	ARG
1	D	158	LEU
1	D	211	LEU
1	D	234	LEU
1	D	245	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	B	102	GLN
1	D	166	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	237/246 (96%)	-0.20	4 (1%) 73 78	19, 31, 48, 71	3 (1%)
1	B	237/246 (96%)	-0.28	1 (0%) 93 94	18, 29, 54, 68	3 (1%)
1	C	237/246 (96%)	-0.02	6 (2%) 61 67	25, 37, 57, 79	2 (0%)
1	D	238/246 (96%)	0.00	7 (2%) 55 63	25, 39, 63, 80	2 (0%)
All	All	949/984 (96%)	-0.12	18 (1%) 70 75	18, 34, 57, 80	10 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	GLU	2.9
1	C	8	GLN	2.9
1	D	4	GLN	2.7
1	D	62	GLU	2.6
1	D	245	ARG	2.6
1	C	241	PHE	2.5
1	D	24	PRO	2.5
1	A	102	GLN	2.5
1	C	4	GLN	2.3
1	A	9	ARG	2.3
1	D	160	ALA	2.3
1	D	7	ARG	2.2
1	B	45	GLU	2.2
1	C	9	ARG	2.1
1	C	5	GLU	2.1
1	A	7	ARG	2.0
1	C	23	GLY	2.0
1	D	94	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.