



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:31 pm BST

PDB ID : 4GYR  
Title : Granulibacter bethesdensis allophanate hydrolase apo  
Authors : Lin, Y.; St Maurice, M.  
Deposited on : 2012-09-05  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

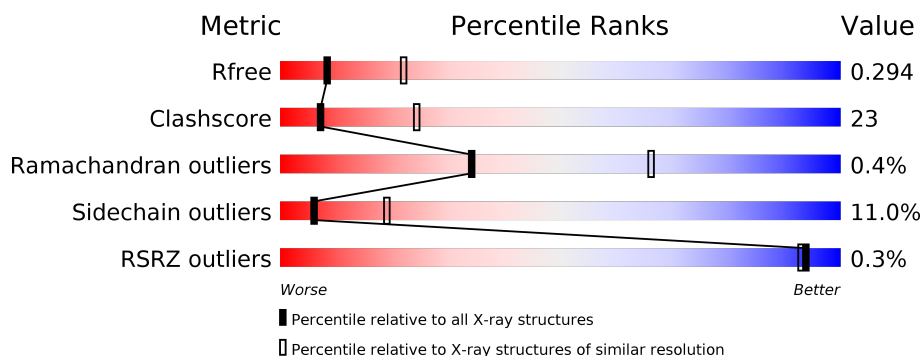
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	621	
1	B	621	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6930 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 Allophanate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	11	1	0
			3404	2159	583	651	11			
1	B	461	Total	C	N	O	S	9	1	0
			3410	2165	586	648	11			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	EXPRESSION TAG	UNP Q0BRB0
A	-27	GLY	-	EXPRESSION TAG	UNP Q0BRB0
A	-26	SER	-	EXPRESSION TAG	UNP Q0BRB0
A	-25	SER	-	EXPRESSION TAG	UNP Q0BRB0
A	-24	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-23	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-22	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-21	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-20	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-19	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-18	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-17	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-16	ASP	-	EXPRESSION TAG	UNP Q0BRB0
A	-15	TYR	-	EXPRESSION TAG	UNP Q0BRB0
A	-14	ASP	-	EXPRESSION TAG	UNP Q0BRB0
A	-13	ILE	-	EXPRESSION TAG	UNP Q0BRB0
A	-12	PRO	-	EXPRESSION TAG	UNP Q0BRB0
A	-11	THR	-	EXPRESSION TAG	UNP Q0BRB0
A	-10	SER	-	EXPRESSION TAG	UNP Q0BRB0
A	-9	GLU	-	EXPRESSION TAG	UNP Q0BRB0
A	-8	ASN	-	EXPRESSION TAG	UNP Q0BRB0
A	-7	LEU	-	EXPRESSION TAG	UNP Q0BRB0
A	-6	TYR	-	EXPRESSION TAG	UNP Q0BRB0
A	-5	PHE	-	EXPRESSION TAG	UNP Q0BRB0
A	-4	GLN	-	EXPRESSION TAG	UNP Q0BRB0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q0BRB0
A	-2	LEU	-	EXPRESSION TAG	UNP Q0BRB0
A	-1	LEU	-	EXPRESSION TAG	UNP Q0BRB0
A	0	GLN	-	EXPRESSION TAG	UNP Q0BRB0
B	-28	MET	-	EXPRESSION TAG	UNP Q0BRB0
B	-27	GLY	-	EXPRESSION TAG	UNP Q0BRB0
B	-26	SER	-	EXPRESSION TAG	UNP Q0BRB0
B	-25	SER	-	EXPRESSION TAG	UNP Q0BRB0
B	-24	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-23	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-22	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-21	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-20	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-19	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-18	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-17	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-16	ASP	-	EXPRESSION TAG	UNP Q0BRB0
B	-15	TYR	-	EXPRESSION TAG	UNP Q0BRB0
B	-14	ASP	-	EXPRESSION TAG	UNP Q0BRB0
B	-13	ILE	-	EXPRESSION TAG	UNP Q0BRB0
B	-12	PRO	-	EXPRESSION TAG	UNP Q0BRB0
B	-11	THR	-	EXPRESSION TAG	UNP Q0BRB0
B	-10	SER	-	EXPRESSION TAG	UNP Q0BRB0
B	-9	GLU	-	EXPRESSION TAG	UNP Q0BRB0
B	-8	ASN	-	EXPRESSION TAG	UNP Q0BRB0
B	-7	LEU	-	EXPRESSION TAG	UNP Q0BRB0
B	-6	TYR	-	EXPRESSION TAG	UNP Q0BRB0
B	-5	PHE	-	EXPRESSION TAG	UNP Q0BRB0
B	-4	GLN	-	EXPRESSION TAG	UNP Q0BRB0
B	-3	GLY	-	EXPRESSION TAG	UNP Q0BRB0
B	-2	LEU	-	EXPRESSION TAG	UNP Q0BRB0
B	-1	LEU	-	EXPRESSION TAG	UNP Q0BRB0
B	0	GLN	-	EXPRESSION TAG	UNP Q0BRB0

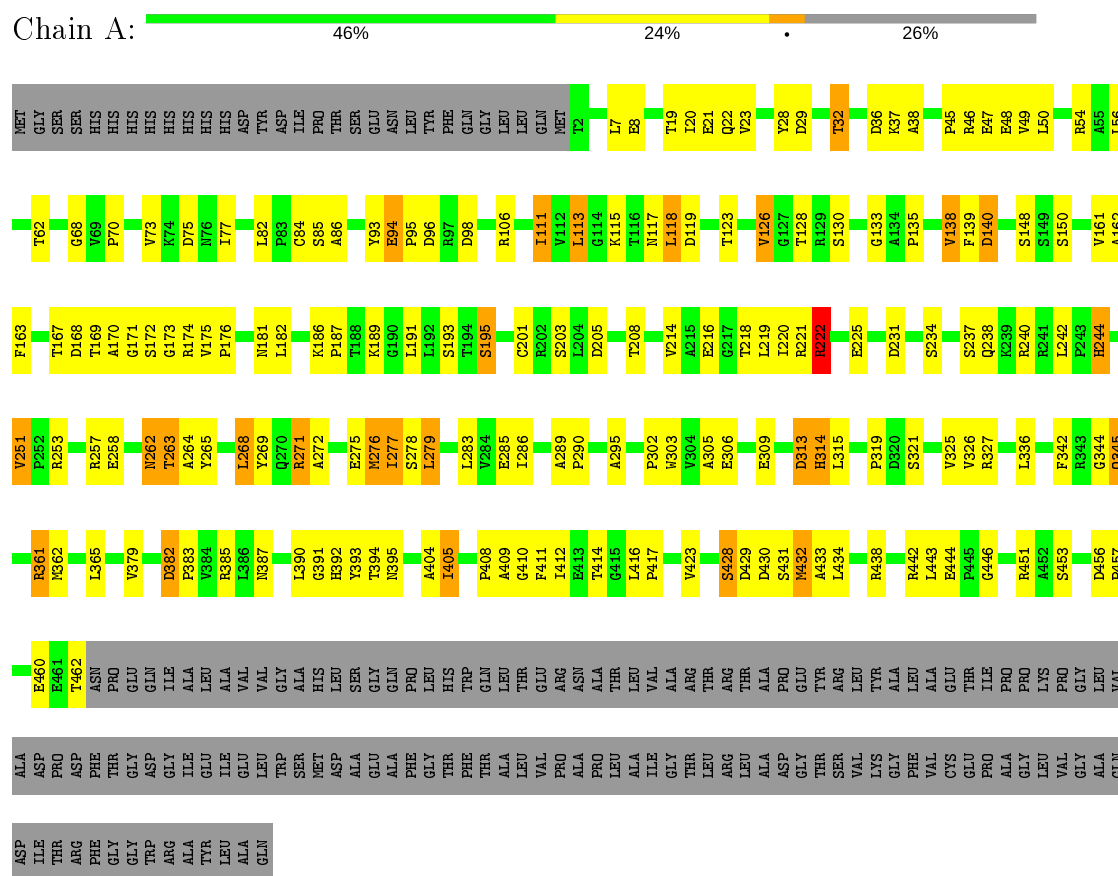
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	65	Total O 65 65	0	0
2	B	51	Total O 51 51	0	0

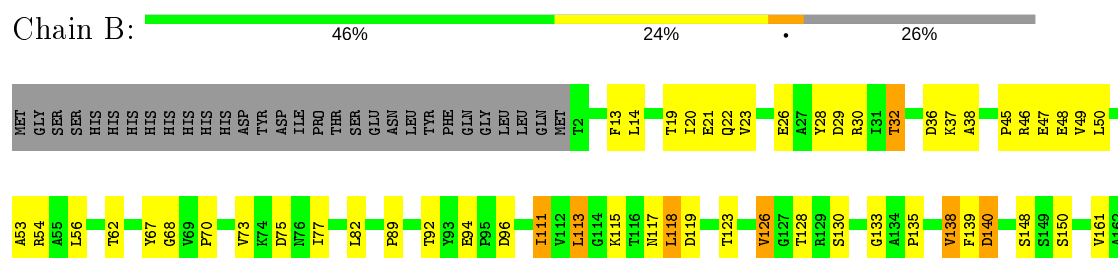
### 3 Residue-property plots

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

- Molecule 1: Allophanate hydrolase



- Molecule 1: Allophanate hydrolase



VAL	PRO	S453	Q345	R253	F163
GLY	GLY	D456	L351	R257	T167
ALA	LEU	P457	E258	D168	D168
GLN	VAL		F259	T169	A170
ASP	ALA		Q354	Y260	G171
ILE	ASP	E460	R361	G261	S172
THR	PRO	E461	R362	N262	G173
ARG	ASP	T462	T263	A264	R174
PHE	THR	ASN	L365	Y265	V175
GLY	PRO	GLU	V379		P176
LEU	GLY	GLN		L268	A177
TRP	ASP	ILE	D882		A178
ARG	GLY	ALA	P383	R271	F179
ALA	ILE	ALA	V384	A272	N180
ALA	ILE	ALA	R385	L273	N181
LEU	GLU	VAL	R386	D274	L182
GLN	LEU	VAL	L387	E275	
	TRP	GLY		H276	K186
	SER	ALA	L390	I277	P187
	MET	HIS	G391	S278	
	ASP	LEU	H392	L279	L191
	ALA	SER	Y393	D280	L192
	GLU	GLY	T394	A281	S193
	ALA	GLN	H395	E282	T194
	PHE	PRO		L283	S195
	GLY	LEU	A404	V284	
	THR	HIS	I405	E285	C201
	PHE	TRP		I286	R202
	THR	GLN	P408		S203
	ALA	LEU	A409	A288	L204
	LEU	THR	G410	F290	D205
	LEU	GLU	F411	A295	
	VAL	ARG	I412		T208
	PRO	ALA			
	PRO	ALA	L416	P302	V214
	LEU	THR	P417	H303	
	ALA	LEU		V304	T218
	ILE	VAL	V420	A305	L219
	GLY	ALA		E306	I220
	THR	ARG	V423		R221
	LEU	THR		E309	R222
	ARG	ARG	S428		
	LEU	THR	D429	D813	E225
	ALA	ALA	D430	H314	
	ASP	PRO	S431	L315	D231
	GLY	GLU	H432		
	THR	TYR	A433	P319	S234
	SER	ARG	L434	D320	
	VAL	LEU		S321	S237
	LYS	TYR	R438		Q238
	GLY	ALA		V325	R239
	PHE	LEU	L443	V326	R240
	VAL	ALA	P444		
	CYS	GLU	P445	L336	S237
	GLU	THR	G446		Q238
	PRO	ILE			R240
	ALA	PRO	R451	F342	H244
	GLY	PRO	J452	R343	V245
	LEU	LYS		G344	V251
					P252

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.09 Å 78.09 Å 397.54 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.05 – 2.80 40.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.05-2.80) 99.9 (40.05-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	14.92 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.256 , 0.307 0.246 , 0.294	Depositor DCC
$R_{free}$ test set	2027 reflections (6.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 17.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	6930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.32	1/3478 (0.0%)	0.52	3/4752 (0.1%)
1	B	0.31	1/3484 (0.0%)	0.52	2/4757 (0.0%)
All	All	0.32	2/6962 (0.0%)	0.52	5/9509 (0.1%)

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	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	GLU	CD-OE1	-8.74	1.16	1.25
1	A	460	GLU	CD-OE1	-8.44	1.16	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	A	222	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	460	GLU	CG-CD-OE1	-5.73	106.84	118.30
1	B	460	GLU	CG-CD-OE1	-5.68	106.94	118.30
1	A	460	GLU	CG-CD-OE2	5.02	128.33	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	262	ASN	Peptide
1	B	262	ASN	Peptide

## 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	3404	0	3333	157	0
1	B	3410	0	3347	149	1
2	A	65	0	0	23	1
2	B	51	0	0	10	0
All	All	6930	0	6680	305	1

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 23.

All (305) 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:411:PHE:CE1	1:B:417:PRO:HB3	1.64	1.32
1:B:411:PHE:CE2	1:B:451:ARG:HD2	1.73	1.24
1:A:411:PHE:CE2	1:A:451:ARG:HD2	1.74	1.21
1:B:411:PHE:HE2	1:B:451:ARG:CD	1.54	1.20
1:A:218:THR:CG2	1:A:222:ARG:HH12	1.57	1.17
1:B:218:THR:CG2	1:B:222:ARG:HH12	1.57	1.16
1:A:218:THR:HG22	1:A:222:ARG:NH1	1.63	1.14
1:B:411:PHE:HD1	1:B:417:PRO:HA	1.17	1.09
1:A:411:PHE:CE1	1:A:417:PRO:HB3	1.87	1.09
1:B:411:PHE:HE2	1:B:451:ARG:HD2	0.92	1.08
1:B:218:THR:HG22	1:B:222:ARG:NH1	1.69	1.05
1:B:411:PHE:HE1	1:B:417:PRO:CB	1.69	1.03
1:A:218:THR:HG22	1:A:222:ARG:HH12	1.15	0.98
1:A:411:PHE:HE2	1:A:451:ARG:HD2	1.17	0.98
1:A:75:ASP:O	2:A:619:HOH:O	1.84	0.94
1:B:411:PHE:CD1	1:B:417:PRO:HA	2.01	0.94
1:B:218:THR:HG22	1:B:222:ARG:HH12	1.25	0.93
1:B:244:HIS:CD2	1:B:434:LEU:HD23	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:O	2:A:646:HOH:O	1.88	0.90
1:A:327:ARG:NE	2:A:663:HOH:O	2.06	0.89
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.39	0.88
1:B:411:PHE:CE1	1:B:417:PRO:CB	2.50	0.87
1:A:382:ASP:OD2	1:A:385:ARG:NH1	2.07	0.87
1:A:244:HIS:CD2	1:A:434:LEU:HD23	2.10	0.87
1:B:411:PHE:CE2	1:B:451:ARG:CD	2.46	0.86
1:B:244:HIS:HD2	1:B:434:LEU:HD23	1.42	0.84
1:B:382:ASP:OD2	1:B:385:ARG:NH1	2.11	0.84
1:B:218:THR:CG2	1:B:222:ARG:NH1	2.31	0.84
1:A:410:GLY:O	1:A:411:PHE:HD1	1.63	0.82
1:A:138:VAL:HG23	1:A:139:PHE:CE2	2.15	0.82
1:A:390:LEU:O	2:A:625:HOH:O	1.97	0.82
1:B:411:PHE:HE1	1:B:417:PRO:HB3	0.75	0.81
1:A:138:VAL:HG23	1:A:139:PHE:CD2	2.16	0.80
1:B:169:THR:HG21	1:B:201:CYS:HB2	1.62	0.80
1:A:169:THR:HG21	1:A:201:CYS:HB2	1.62	0.80
1:B:411:PHE:HD2	1:B:451:ARG:CZ	1.94	0.80
1:A:411:PHE:CE2	1:A:451:ARG:CD	2.63	0.79
1:A:140:ASP:OD2	2:A:611:HOH:O	1.99	0.79
1:A:85:SER:N	2:A:619:HOH:O	2.16	0.79
1:A:216:GLU:OE2	2:A:603:HOH:O	1.99	0.78
1:B:138:VAL:HG23	1:B:139:PHE:CE2	2.18	0.78
1:A:218:THR:CG2	1:A:222:ARG:NH1	2.31	0.78
1:B:138:VAL:HG23	1:B:139:PHE:CD2	2.19	0.78
1:A:411:PHE:CD1	1:A:417:PRO:HA	2.19	0.77
1:B:390:LEU:O	2:B:616:HOH:O	2.03	0.77
1:A:313:ASP:N	1:A:313:ASP:OD1	2.17	0.76
1:A:221:ARG:NH1	1:A:225:GLU:OE1	2.18	0.76
1:B:221:ARG:NH1	1:B:225:GLU:OE1	2.19	0.76
1:B:411:PHE:CD2	1:B:451:ARG:CZ	2.69	0.76
1:A:244:HIS:HD2	1:A:434:LEU:HD23	1.51	0.76
1:B:47:GLU:OE2	1:B:54:ARG:NH2	2.18	0.75
1:B:222:ARG:HG3	1:B:222:ARG:HH11	1.50	0.75
1:B:313:ASP:N	1:B:313:ASP:OD1	2.17	0.74
1:A:29:ASP:OD1	1:A:46:ARG:NH2	2.21	0.73
1:A:411:PHE:HE1	1:A:417:PRO:HB3	1.52	0.73
1:A:117:ASN:O	2:A:635:HOH:O	2.07	0.72
1:B:29:ASP:OD1	1:B:46:ARG:NH2	2.21	0.72
1:B:411:PHE:CD1	1:B:417:PRO:CA	2.71	0.72
1:A:244:HIS:HD2	1:A:434:LEU:CD2	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:NH2	1:A:409:ALA:O	2.23	0.71
1:A:47:GLU:HG3	2:A:616:HOH:O	1.90	0.71
1:A:410:GLY:O	1:A:411:PHE:CD1	2.43	0.71
1:B:271:ARG:NH2	1:B:409:ALA:O	2.24	0.70
1:B:148:SER:H	1:B:172:SER:HB3	1.57	0.70
1:A:411:PHE:CE1	1:A:417:PRO:CB	2.70	0.70
1:B:222:ARG:CG	1:B:222:ARG:HH11	2.06	0.69
1:A:148:SER:H	1:A:172:SER:HB3	1.56	0.69
1:B:244:HIS:HD2	1:B:434:LEU:CD2	2.06	0.69
1:A:20:ILE:HG12	1:A:68:GLY:HA3	1.75	0.68
1:A:36:ASP:OD2	2:A:608:HOH:O	2.11	0.68
1:B:20:ILE:HG12	1:B:68:GLY:HA3	1.75	0.67
1:B:262:ASN:ND2	1:B:265:TYR:CG	2.63	0.67
1:A:168:ASP:HB2	1:A:208:THR:HG21	1.77	0.67
1:A:262:ASN:ND2	1:A:265:TYR:CG	2.63	0.66
1:A:411:PHE:HD2	1:A:451:ARG:NH1	1.93	0.66
1:A:309:GLU:OE1	2:A:622:HOH:O	2.14	0.66
1:A:222:ARG:HH11	1:A:222:ARG:CG	2.07	0.66
1:A:218:THR:HG21	1:A:222:ARG:HH12	1.59	0.65
1:B:117:ASN:O	2:B:602:HOH:O	2.14	0.65
1:A:231:ASP:OD2	2:A:631:HOH:O	2.15	0.65
1:A:453:SER:OG	2:A:660:HOH:O	2.13	0.64
1:A:126:VAL:HG11	1:A:379:VAL:HG11	1.80	0.64
1:B:168:ASP:HB2	1:B:208:THR:HG21	1.79	0.64
1:A:411:PHE:CD2	1:A:451:ARG:NH1	2.66	0.63
1:B:411:PHE:CE2	1:B:451:ARG:NE	2.66	0.62
1:A:314:HIS:ND1	2:A:662:HOH:O	2.31	0.62
1:B:126:VAL:HG11	1:B:379:VAL:HG11	1.80	0.62
1:A:244:HIS:CD2	1:A:434:LEU:CD2	2.81	0.62
1:B:13:PHE:HD2	1:B:14:LEU:HD23	1.64	0.62
1:B:218:THR:HG21	1:B:222:ARG:HH12	1.60	0.61
1:B:135:PRO:HG2	1:B:150:SER:HB2	1.82	0.61
1:B:411:PHE:HE2	1:B:451:ARG:NE	1.97	0.61
1:A:411:PHE:HD1	1:A:417:PRO:HA	1.64	0.60
1:B:309:GLU:OE1	2:B:628:HOH:O	2.16	0.60
1:A:56:LEU:HD12	1:A:111:ILE:HD11	1.83	0.60
1:B:56:LEU:HD12	1:B:111:ILE:HD11	1.84	0.60
1:A:135:PRO:HG2	1:A:150:SER:HB2	1.84	0.60
1:B:203:SER:OG	1:B:306:GLU:OE1	2.19	0.59
1:B:444:GLU:OE2	1:B:451:ARG:NE	2.32	0.59
1:A:203:SER:OG	1:A:306:GLU:OE1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:OE2	1:A:54:ARG:NH1	2.35	0.59
1:A:442:ARG:NE	2:A:646:HOH:O	2.13	0.59
1:A:162:ALA:O	2:A:602:HOH:O	2.17	0.59
1:B:231:ASP:OD2	2:B:621:HOH:O	2.17	0.58
1:B:21:GLU:OE2	1:B:54:ARG:NH1	2.36	0.58
1:B:36:ASP:OD2	2:B:608:HOH:O	2.17	0.58
1:B:221:ARG:NH2	1:B:430:ASP:OD1	2.36	0.58
1:B:342:PHE:HA	1:B:345:GLN:HG3	1.85	0.58
1:A:119:ASP:HB2	1:A:148:SER:HB2	1.84	0.58
1:B:351:LEU:HA	1:B:354:GLN:HE21	1.69	0.58
1:A:45:PRO:HB2	1:A:48:GLU:HB2	1.86	0.58
1:A:444:GLU:OE2	1:A:451:ARG:NE	2.32	0.57
1:B:181:ASN:OD1	1:B:408:PRO:HB3	2.05	0.57
1:A:221:ARG:NH2	1:A:430:ASP:OD1	2.38	0.57
1:B:45:PRO:HB2	1:B:48:GLU:HB2	1.85	0.57
1:A:244:HIS:ND1	1:A:244:HIS:N	2.53	0.57
1:B:119:ASP:HB2	1:B:148:SER:HB2	1.85	0.57
1:B:19:THR:N	1:B:22:GLN:OE1	2.38	0.57
1:B:277:ILE:HG12	1:B:278:SER:N	2.20	0.57
1:A:279:LEU:HG	1:B:37:LYS:CD	2.34	0.57
1:A:148:SER:H	1:A:172:SER:CB	2.18	0.57
1:A:123:THR:HB	1:A:326:VAL:HG22	1.87	0.56
1:A:181:ASN:OD1	1:A:408:PRO:HB3	2.05	0.56
1:B:148:SER:H	1:B:172:SER:CB	2.18	0.56
1:A:70:PRO:HB2	1:A:113:LEU:HD21	1.87	0.56
1:B:70:PRO:HB2	1:B:113:LEU:HD21	1.87	0.56
1:A:342:PHE:HA	1:A:345:GLN:HG3	1.86	0.56
1:A:411:PHE:CD2	1:A:451:ARG:CZ	2.89	0.56
1:B:244:HIS:CD2	1:B:434:LEU:CD2	2.83	0.56
1:B:28:TYR:O	1:B:32:THR:OG1	2.23	0.55
1:B:231:ASP:HB3	1:B:234:SER:HB2	1.88	0.55
1:A:272:ALA:O	1:A:276:MET:HB2	2.07	0.55
1:B:56:LEU:O	1:B:67:TYR:OH	2.15	0.55
1:A:231:ASP:HB3	1:A:234:SER:HB2	1.87	0.55
1:A:262:ASN:ND2	1:A:265:TYR:H	2.04	0.55
1:A:86:ALA:N	2:A:619:HOH:O	2.23	0.55
1:B:262:ASN:ND2	1:B:265:TYR:H	2.04	0.55
1:B:392:HIS:O	1:B:392:HIS:ND1	2.39	0.55
1:B:26:GLU:OE2	2:B:603:HOH:O	2.18	0.54
1:A:277:ILE:HG12	1:A:278:SER:N	2.21	0.54
1:B:411:PHE:CD2	1:B:451:ARG:NH1	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ALA:O	1:B:276:MET:HB2	2.07	0.54
1:B:123:THR:HB	1:B:326:VAL:HG22	1.88	0.54
1:A:19:THR:N	1:A:22:GLN:OE1	2.38	0.54
1:B:89:PRO:O	1:B:92:THR:OG1	2.18	0.54
1:B:351:LEU:HD23	1:B:354:GLN:NE2	2.23	0.54
1:A:49:VAL:HG11	1:A:113:LEU:HD12	1.90	0.53
1:A:75:ASP:HA	1:A:115:LYS:HE2	1.91	0.53
1:B:49:VAL:HG11	1:B:113:LEU:HD12	1.91	0.53
1:B:262:ASN:ND2	1:B:265:TYR:CD1	2.77	0.53
1:B:75:ASP:HA	1:B:115:LYS:HE2	1.91	0.53
1:B:285:GLU:O	1:B:361:ARG:NH2	2.41	0.53
1:A:285:GLU:O	1:A:361:ARG:NH2	2.41	0.53
1:B:126:VAL:HB	1:B:128:THR:HG23	1.89	0.53
1:A:126:VAL:HB	1:A:128:THR:HG23	1.91	0.53
1:A:163:PHE:CG	1:A:220:ILE:HD13	2.44	0.53
1:A:28:TYR:O	1:A:32:THR:OG1	2.22	0.53
1:A:325:VAL:HG21	1:A:383:PRO:HB2	1.90	0.52
1:A:262:ASN:ND2	1:A:265:TYR:CD1	2.77	0.52
1:B:163:PHE:CG	1:B:220:ILE:HD13	2.44	0.52
1:A:412:ILE:HG12	1:A:416:LEU:O	2.10	0.52
1:A:45:PRO:O	1:A:49:VAL:HG23	2.11	0.52
1:B:244:HIS:ND1	1:B:244:HIS:N	2.58	0.51
1:B:240:ARG:O	1:B:428:SER:HA	2.11	0.51
1:A:302:PRO:HA	1:A:336:LEU:HD13	1.93	0.51
1:B:263:THR:OG1	1:B:264:ALA:N	2.44	0.51
1:B:45:PRO:O	1:B:49:VAL:HG23	2.11	0.51
1:B:302:PRO:HA	1:B:336:LEU:HD13	1.93	0.51
1:A:20:ILE:HD13	1:A:56:LEU:HB3	1.92	0.50
1:B:412:ILE:HG12	1:B:416:LEU:O	2.11	0.50
1:A:263:THR:OG1	1:A:264:ALA:N	2.43	0.50
1:A:73:VAL:HG13	1:A:77:ILE:HB	1.93	0.50
1:B:169:THR:OG1	1:B:205:ASP:OD1	2.29	0.50
1:B:20:ILE:HD13	1:B:56:LEU:HB3	1.92	0.50
1:B:411:PHE:HD2	1:B:451:ARG:NH1	2.09	0.50
1:B:119:ASP:HB2	1:B:148:SER:CB	2.42	0.49
1:A:119:ASP:HB2	1:A:148:SER:CB	2.42	0.49
1:A:414:THR:HG22	2:A:611:HOH:O	2.11	0.49
1:A:47:GLU:HA	1:A:47:GLU:OE1	2.11	0.49
1:B:289:ALA:N	1:B:290:PRO:HD2	2.27	0.49
1:A:289:ALA:N	1:A:290:PRO:HD2	2.27	0.49
1:B:73:VAL:HG13	1:B:77:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:PHE:CE1	1:B:417:PRO:CA	2.94	0.48
1:B:258:GLU:N	1:B:393:TYR:OH	2.47	0.48
1:A:169:THR:OG1	1:A:205:ASP:OD1	2.29	0.48
1:A:139:PHE:O	1:A:140:ASP:HB2	2.14	0.48
1:A:258:GLU:N	1:A:393:TYR:OH	2.47	0.48
1:B:325:VAL:HG21	1:B:383:PRO:HB2	1.95	0.48
1:A:38:ALA:O	1:A:135:PRO:HG3	2.14	0.48
1:A:73:VAL:CG1	1:A:77:ILE:HB	2.44	0.48
1:A:410:GLY:C	1:A:411:PHE:CD1	2.87	0.47
1:B:38:ALA:O	1:B:135:PRO:HG3	2.15	0.47
1:B:73:VAL:CG1	1:B:77:ILE:HB	2.44	0.47
1:B:170:ALA:O	1:B:174:ARG:NH2	2.47	0.47
1:B:444:GLU:O	1:B:446:GLY:N	2.41	0.47
1:A:391:GLY:HA2	1:A:394:THR:OG1	2.14	0.47
1:A:170:ALA:O	1:A:174:ARG:NH2	2.48	0.47
1:B:139:PHE:O	1:B:140:ASP:HB2	2.13	0.46
1:A:49:VAL:HG11	1:A:113:LEU:CD1	2.45	0.46
1:A:168:ASP:HB2	1:A:208:THR:CG2	2.44	0.46
1:A:37:LYS:O	2:A:615:HOH:O	2.21	0.46
1:B:193:SER:OG	1:B:195:SER:HB2	2.16	0.46
1:B:391:GLY:HA2	1:B:394:THR:OG1	2.15	0.46
1:B:49:VAL:HG11	1:B:113:LEU:CD1	2.45	0.46
1:A:258:GLU:HB3	1:A:392:HIS:NE2	2.31	0.46
1:B:271:ARG:O	1:B:275:GLU:HG2	2.16	0.46
1:A:271:ARG:O	1:A:275:GLU:HG2	2.16	0.46
1:A:8:GLU:HG2	2:A:604:HOH:O	2.15	0.46
1:B:222:ARG:HG3	1:B:222:ARG:NH1	2.23	0.46
1:A:411:PHE:CD1	1:A:417:PRO:CA	2.94	0.46
1:B:175:VAL:HB	1:B:176:PRO:HD3	1.98	0.46
1:A:193:SER:OG	1:A:195:SER:HB2	2.15	0.45
1:B:167:THR:O	1:B:172:SER:HB2	2.15	0.45
1:B:113:LEU:HD23	1:B:161:VAL:HG12	1.97	0.45
1:A:113:LEU:N	1:A:113:LEU:HD13	2.32	0.45
1:A:138:VAL:CG2	1:A:139:PHE:CE2	2.95	0.45
1:A:167:THR:O	1:A:172:SER:HB2	2.15	0.45
1:A:242:LEU:O	1:A:244:HIS:CE1	2.69	0.45
1:A:171:GLY:HA2	1:A:174:ARG:NH2	2.32	0.45
1:A:19:THR:O	1:A:23:VAL:HG23	2.17	0.45
1:A:113:LEU:HD23	1:A:161:VAL:HG12	1.98	0.45
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.18	0.45
1:A:315:LEU:O	1:A:319:PRO:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LYS:HE3	1:B:187:PRO:O	2.16	0.45
1:B:434:LEU:HD11	1:B:438:ARG:HE	1.82	0.45
1:A:175:VAL:HB	1:A:176:PRO:HD3	1.99	0.45
1:B:113:LEU:HD13	1:B:113:LEU:N	2.32	0.45
1:B:262:ASN:ND2	1:B:265:TYR:CB	2.80	0.45
1:A:214:VAL:HG11	1:A:433:ALA:O	2.17	0.45
1:A:442:ARG:NH1	1:A:442:ARG:O	2.49	0.45
1:B:171:GLY:HA2	1:B:174:ARG:NH2	2.32	0.45
1:A:434:LEU:HD11	1:A:438:ARG:HE	1.82	0.44
1:A:262:ASN:ND2	1:A:265:TYR:CB	2.81	0.44
1:A:186:LYS:HE3	1:A:187:PRO:O	2.17	0.44
1:A:444:GLU:O	1:A:446:GLY:N	2.40	0.44
1:A:7:LEU:N	2:A:603:HOH:O	2.49	0.44
1:B:201:CYS:HA	1:B:306:GLU:HB2	1.99	0.44
1:A:201:CYS:HA	1:A:306:GLU:HB2	1.99	0.44
1:A:456:ASP:HB3	1:A:457:PRO:HA	1.99	0.44
1:B:268:LEU:HA	1:B:268:LEU:HD22	1.66	0.44
1:A:362:MET:SD	1:A:365:LEU:HD13	2.58	0.44
1:A:365:LEU:HB3	1:A:423:VAL:HB	2.00	0.44
1:B:365:LEU:HB3	1:B:423:VAL:HB	2.00	0.44
1:A:189:LYS:HG2	2:A:633:HOH:O	2.18	0.44
1:A:240:ARG:O	1:A:428:SER:HA	2.17	0.44
1:A:409:ALA:HB1	1:A:443:LEU:HD23	2.00	0.44
1:B:302:PRO:HG3	1:B:344:GLY:HA3	2.00	0.44
1:B:456:ASP:HB3	1:B:457:PRO:HA	1.99	0.43
1:B:258:GLU:CG	1:B:260:TYR:CE2	3.01	0.43
1:A:8:GLU:N	2:A:603:HOH:O	2.09	0.43
1:B:303:TRP:C	1:B:305:ALA:H	2.21	0.43
1:B:453:SER:OG	2:B:651:HOH:O	2.21	0.43
1:B:168:ASP:HB2	1:B:208:THR:CG2	2.46	0.43
1:B:362:MET:SD	1:B:365:LEU:HD13	2.58	0.43
1:A:168:ASP:OD2	1:A:173:GLY:N	2.49	0.43
1:B:409:ALA:HB1	1:B:443:LEU:HD23	2.01	0.43
1:A:82:LEU:HD13	1:A:115:LYS:HG2	2.01	0.43
1:A:251:VAL:O	1:A:286:ILE:HG13	2.18	0.43
1:B:258:GLU:HG3	1:B:260:TYR:CE2	2.54	0.43
1:B:428:SER:O	1:B:432:MET:HB2	2.19	0.43
1:B:214:VAL:HG11	1:B:433:ALA:O	2.18	0.43
1:A:303:TRP:C	1:A:305:ALA:H	2.23	0.42
1:B:404:ALA:C	1:B:405:ILE:HG13	2.38	0.42
1:A:404:ALA:C	1:A:405:ILE:HG13	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:O	1:B:286:ILE:HG13	2.19	0.42
1:B:315:LEU:O	1:B:319:PRO:HB3	2.20	0.42
1:A:302:PRO:HG3	1:A:344:GLY:HA3	2.00	0.42
1:A:271:ARG:HB3	1:A:271:ARG:HE	1.39	0.42
1:B:168:ASP:OD2	1:B:173:GLY:N	2.48	0.42
1:A:251:VAL:HG12	1:A:269:TYR:OH	2.19	0.42
1:B:253:ARG:O	1:B:257:ARG:HG3	2.20	0.42
1:B:262:ASN:HD22	1:B:265:TYR:CB	2.33	0.42
1:A:118:LEU:O	1:A:130:SER:HB2	2.20	0.42
1:A:98:ASP:OD1	1:A:106:ARG:NH1	2.52	0.42
1:B:182:LEU:O	1:B:408:PRO:HD3	2.19	0.42
1:B:19:THR:O	1:B:23:VAL:HG23	2.20	0.42
1:A:268:LEU:HD22	1:A:268:LEU:HA	1.70	0.42
1:B:258:GLU:HG3	1:B:260:TYR:CD2	2.54	0.42
1:A:182:LEU:O	1:A:408:PRO:HD3	2.19	0.42
1:A:295:ALA:HB1	1:A:395:ASN:HB2	2.02	0.41
1:B:82:LEU:HD13	1:B:115:LYS:HG2	2.02	0.41
1:B:138:VAL:HG22	1:B:180:ASN:OD1	2.20	0.41
1:B:295:ALA:HB1	1:B:395:ASN:HB2	2.02	0.41
1:A:253:ARG:O	1:A:257:ARG:HG3	2.21	0.41
1:B:20:ILE:HG22	1:B:53:ALA:HB1	2.03	0.41
1:A:94:GLU:HA	1:A:95:PRO:HD2	1.85	0.41
1:B:258:GLU:HB3	1:B:392:HIS:NE2	2.35	0.41
1:B:411:PHE:CE2	1:B:451:ARG:CZ	3.01	0.41
1:A:428:SER:O	1:A:432:MET:HB2	2.20	0.41
1:B:118:LEU:O	1:B:130:SER:HB2	2.21	0.41
1:B:30:ARG:O	2:B:644:HOH:O	2.22	0.41
1:A:262:ASN:HD22	1:A:265:TYR:CB	2.33	0.41
1:B:262:ASN:HD22	1:B:265:TYR:HB2	1.86	0.41
1:B:409:ALA:HB2	1:B:420:VAL:HG22	2.02	0.41
1:A:411:PHE:HE1	1:A:417:PRO:CB	2.25	0.40
1:A:242:LEU:O	1:A:244:HIS:HE1	2.04	0.40
1:A:277:ILE:C	1:A:279:LEU:H	2.25	0.40
1:B:178:ALA:HA	2:B:617:HOH:O	2.20	0.40
1:A:117:ASN:ND2	1:A:133:GLY:O	2.54	0.40
1:A:262:ASN:HD22	1:A:265:TYR:HB2	1.87	0.40
1:B:245:VAL:O	2:B:645:HOH:O	2.22	0.40
1:B:386:LEU:HD12	1:B:386:LEU:HA	1.81	0.40
1:A:432:MET:HE3	1:A:432:MET:HB3	1.94	0.40
1:A:84:CYS:HB3	1:A:93:TYR:CE1	2.57	0.40
1:B:117:ASN:ND2	1:B:133:GLY:O	2.54	0.40



All (1) 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:B:279:LEU:O	2:A:661:HOH:O[1_565]	2.03	0.17

## 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	460/621 (74%)	429 (93%)	29 (6%)	2 (0%)	34 66
1	B	460/621 (74%)	428 (93%)	30 (6%)	2 (0%)	34 66
All	All	920/1242 (74%)	857 (93%)	59 (6%)	4 (0%)	34 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	THR
1	B	263	THR
1	A	140	ASP
1	B	140	ASP

### 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	340/482 (70%)	303 (89%)	37 (11%)	6 19
1	B	340/482 (70%)	302 (89%)	38 (11%)	6 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	680/964 (70%)	605 (89%)	75 (11%)	6 19

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	50	LEU
1	A	62	THR
1	A	94	GLU
1	A	96	ASP
1	A	111	ILE
1	A	113	LEU
1	A	118	LEU
1	A	126	VAL
1	A	138	VAL
1	A	191	LEU
1	A	195	SER
1	A	219	LEU
1	A	222	ARG
1	A	237	SER
1	A	238	GLN
1	A	244	HIS
1	A	251	VAL
1	A	268	LEU
1	A	271	ARG
1	A	276	MET
1	A	277	ILE
1	A	279	LEU
1	A	283	LEU
1	A	313	ASP
1	A	314	HIS
1	A	321	SER
1	A	345	GLN
1	A	361	ARG
1	A	382	ASP
1	A	387	ASN
1	A	405	ILE
1	A	428	SER
1	A	429	ASP
1	A	431	SER
1	A	432	MET
1	A	462	THR

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Mol	Chain	Res	Type
1	B	32	THR
1	B	50	LEU
1	B	62	THR
1	B	94	GLU
1	B	96	ASP
1	B	111	ILE
1	B	113	LEU
1	B	118	LEU
1	B	126	VAL
1	B	138	VAL
1	B	191	LEU
1	B	195	SER
1	B	219	LEU
1	B	222	ARG
1	B	237	SER
1	B	238	GLN
1	B	244	HIS
1	B	251	VAL
1	B	268	LEU
1	B	271	ARG
1	B	276	MET
1	B	277	ILE
1	B	279	LEU
1	B	283	LEU
1	B	313	ASP
1	B	314	HIS
1	B	321	SER
1	B	345	GLN
1	B	361	ARG
1	B	382	ASP
1	B	387	ASN
1	B	392	HIS
1	B	405	ILE
1	B	429	ASP
1	B	431	SER
1	B	432	MET
1	B	460	GLU
1	B	462	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
1	A	354	GLN
1	B	244	HIS
1	B	354	GLN
1	B	440	HIS

### 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](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	461/621 (74%)	-0.32	0 100 100	25, 40, 59, 73	9 (1%)
1	B	461/621 (74%)	-0.33	3 (0%) 87 84	25, 41, 59, 74	8 (1%)
All	All	922/1242 (74%)	-0.32	3 (0%) 94 93	25, 40, 59, 74	17 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	HIS	2.8
1	B	274	ASP	2.8
1	B	281	ALA	2.3

### 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.