Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 09:43 AM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

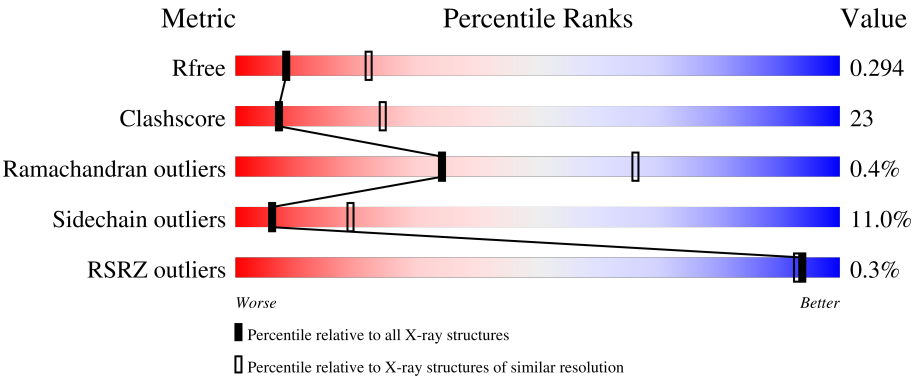
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	46% 24% · 26%
1	B	621	46% 24% · 26%

2 Entry composition (i)

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.

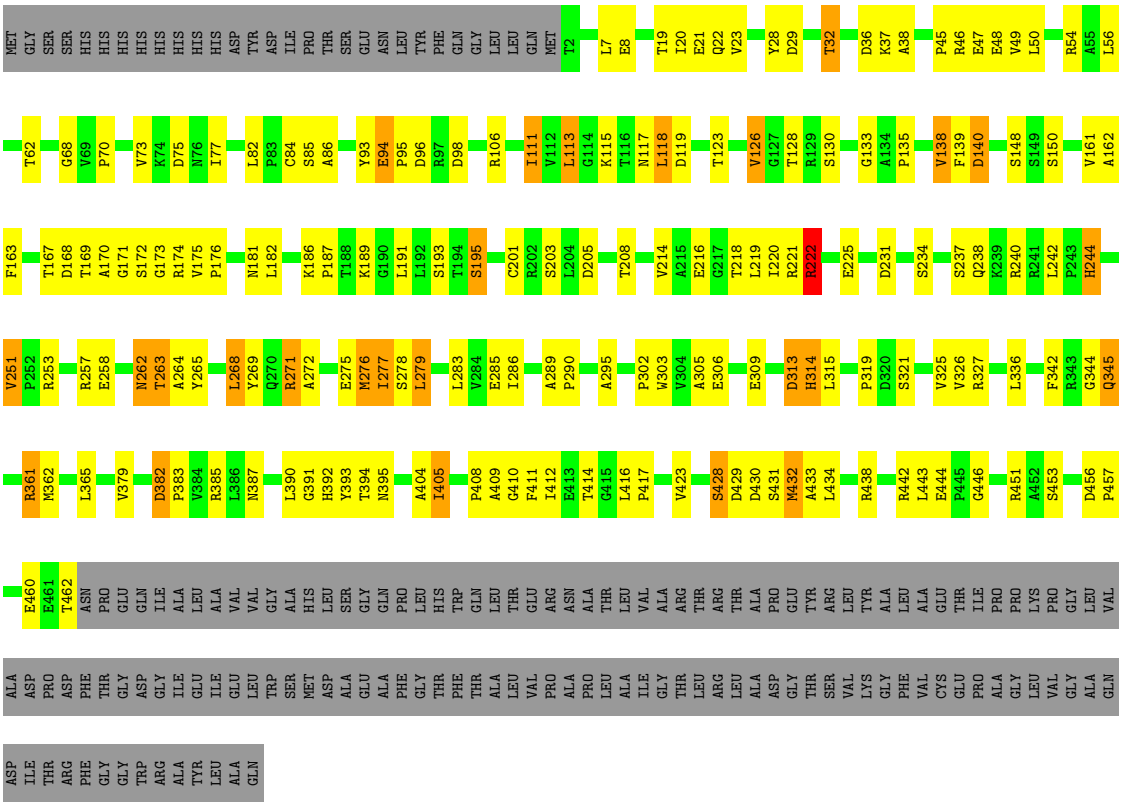
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	65	Total O 65 65	0	0
2	B	51	Total O 51 51	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

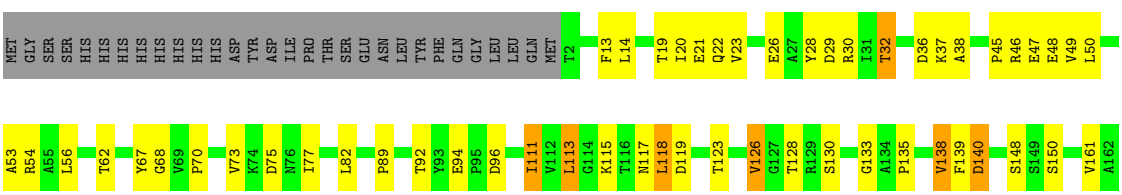
• Molecule 1: Allophanate hydrolase

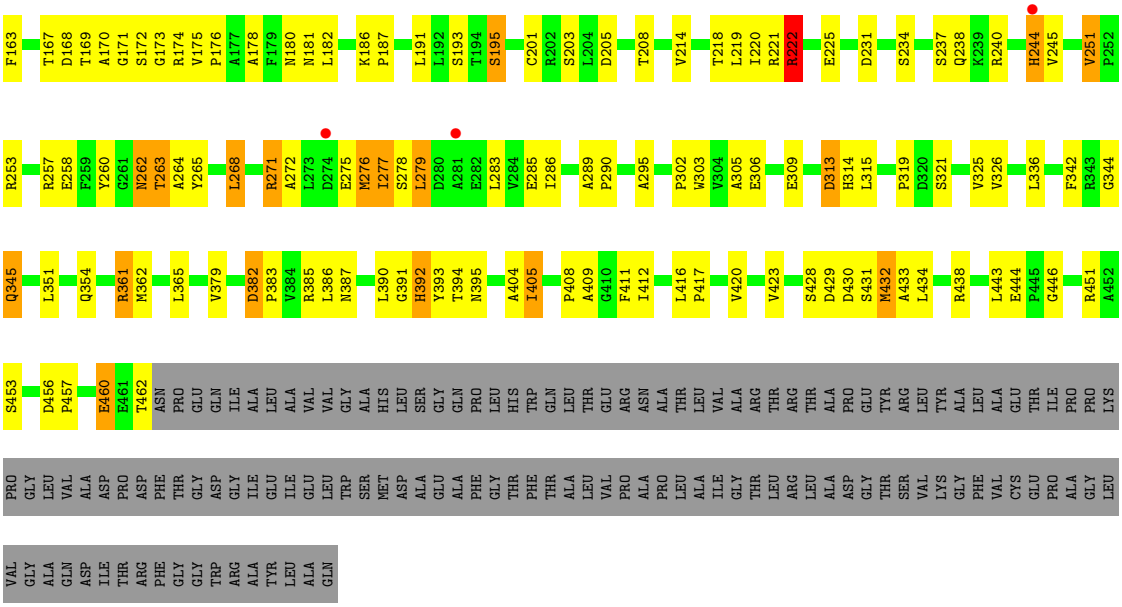
Chain A:



• Molecule 1: Allophanate hydrolase

Chain B:




F163 T167 D168 T169 A170 G171 S172 G173 R174 V175 P176 A177 A178 F179 N180 N181 L182 K186 P187 L191 L192 S193 T194 S195 C201 R202 S203 L204 D205 T208 V214 T218 L219 I220 R221 R222 E225 D231 S234 S237 Q238 K239 R240 H244 V245 V251 P252
R253 R257 E258 P259 Y260 G261 N262 T263 A264 Y265 L268 R271 A272 L273 D274 E275 M276 I277 S278 L279 D280 A281 E282 L283 V284 E285 I286 A289 P290 A295 P302 W303 V304 A305 E306 E309 D313 H314 L315 P319 D320 S321 V325 V326 L336 F342 R343 G344
Q345 L351 Q354 R361 M362 L365 V379 D382 P383 V384 R385 L386 N387 L390 G391 H392 Y393 T394 N395 A404 I405 P408 A409 G410 F411 I412 L416 P417 V420 V423 S428 D429 D430 S431 M432 A433 L434 R438 L443 E444 P445 G446 R451 A452
S453 D456 P457 E460 E461 T462 ASN PRO GLU GLN ILE ALA LEU ALA VAL VAL GLY ALA HIS LEU SER GLY GLN PRO LEU HIS TRP GLN LEU THR GLU ARG ASN ALA THR LEU VAL ALA ARG THR ARG THR ALA PRO GLU TYR ARG LEU TYR ALA LEU ALA GLU THR ILE PRO PRO LYS
PRO GLY LEU VAL ALA ASP PRO ASP PHE THR GLY ASP GLY ILE GLU ILE GLU LEU TRP SER MET ASP ALA GLU ALA PHE GLY THR PHE THR ALA LEU VAL PRO ALA PRO LEU ALA ILE GLY THR LEU ARG LEU ALA ASP GLY THR SER VAL LYS GLY PHE VAL CYS GLU PRO ALA GLY LEU
VAL GLY ALA GLN ASP ILE THR ARG PHE GLY GLY TRP ARG ALA TYR LEU ALA GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	78.09Å 78.09Å 397.54Å 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
$< I/\sigma(I) >$ [1]	14.92 (at 2.81Å)	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^2)	40.3	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 17.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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 (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	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:OD1	1:A:313:ASP:N	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:HH11	1:B:222:ARG:CG	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:A:279:LEU:HG	1:B:37:LYS:CD	2.34	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: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:A:70:PRO:HB2	1:A:113:LEU:HD21	1.87	0.56
1:B:148:SER:H	1:B:172:SER:CB	2.18	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:86:ALA:N	2:A:619:HOH:O	2.23	0.55
1:A:262:ASN:ND2	1:A:265:TYR:H	2.04	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:123:THR:HB	1:B:326:VAL:HG22	1.88	0.54
1:B:272:ALA:O	1:B:276:MET:HB2	2.07	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:28:TYR:O	1:A:32:THR:OG1	2.22	0.53
1:A:163:PHE:CG	1:A:220:ILE:HD13	2.44	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:45:PRO:O	1:A:49:VAL:HG23	2.11	0.52
1:A:412:ILE:HG12	1:A:416:LEU:O	2.10	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:45:PRO:O	1:B:49:VAL:HG23	2.11	0.51
1:B:263:THR:OG1	1:B:264:ALA:N	2.44	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:73:VAL:HG13	1:A:77:ILE:HB	1.93	0.50
1:A:263:THR:OG1	1:A:264:ALA:N	2.43	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:OE1	1:A:47:GLU:HA	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:37:LYS:O	2:A:615:HOH:O	2.21	0.46
1:A:168:ASP:HB2	1:A:208:THR:CG2	2.44	0.46
1:B:49:VAL:HG11	1:B:113:LEU:CD1	2.45	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: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:8:GLU:HG2	2:A:604:HOH:O	2.15	0.46
1:A:271:ARG:O	1:A:275:GLU:HG2	2.16	0.46
1:B:222:ARG:NH1	1:B:222:ARG:HG3	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:19:THR:O	1:A:23:VAL:HG23	2.17	0.45
1:A:171:GLY:HA2	1:A:174:ARG:NH2	2.32	0.45
1:A:113:LEU:HD23	1:A:161:VAL:HG12	1.98	0.45
1:A:222:ARG:NH1	1:A:222:ARG:HG3	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:N	1:B:113:LEU:HD13	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:O	1:A:442:ARG:NH1	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:7:LEU:N	2:A:603:HOH:O	2.49	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: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:214:VAL:HG11	1:B:433:ALA:O	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: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:HE	1:A:271:ARG:HB3	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:98:ASP:OD1	1:A:106:ARG:NH1	2.52	0.42
1:A:118:LEU:O	1:A:130:SER:HB2	2.20	0.42
1:B:19:THR:O	1:B:23:VAL:HG23	2.20	0.42
1:B:182:LEU:O	1:B:408:PRO:HD3	2.19	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:262:ASN:HD22	1:A:265:TYR:CB	2.33	0.41
1:A:428:SER:O	1:A:432:MET:HB2	2.20	0.41
1:B:30:ARG:O	2:B:644:HOH:O	2.22	0.41
1:B:118:LEU:O	1:B:130:SER:HB2	2.21	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:84:CYS:HB3	1:A:93:TYR:CE1	2.57	0.40
1:A:432:MET:HE3	1:A:432:MET:HB3	1.94	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

Sometimes 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

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} 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^2)	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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.