



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:42 AM UTC

PDB ID : 4GYR / pdb_00004gyr
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

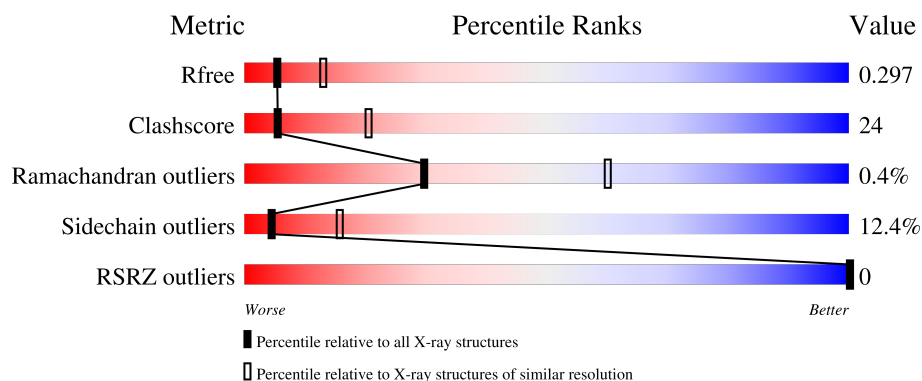
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	 44% 25% 5% 26%
1	B	621	 44% 25% 5% 26%

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

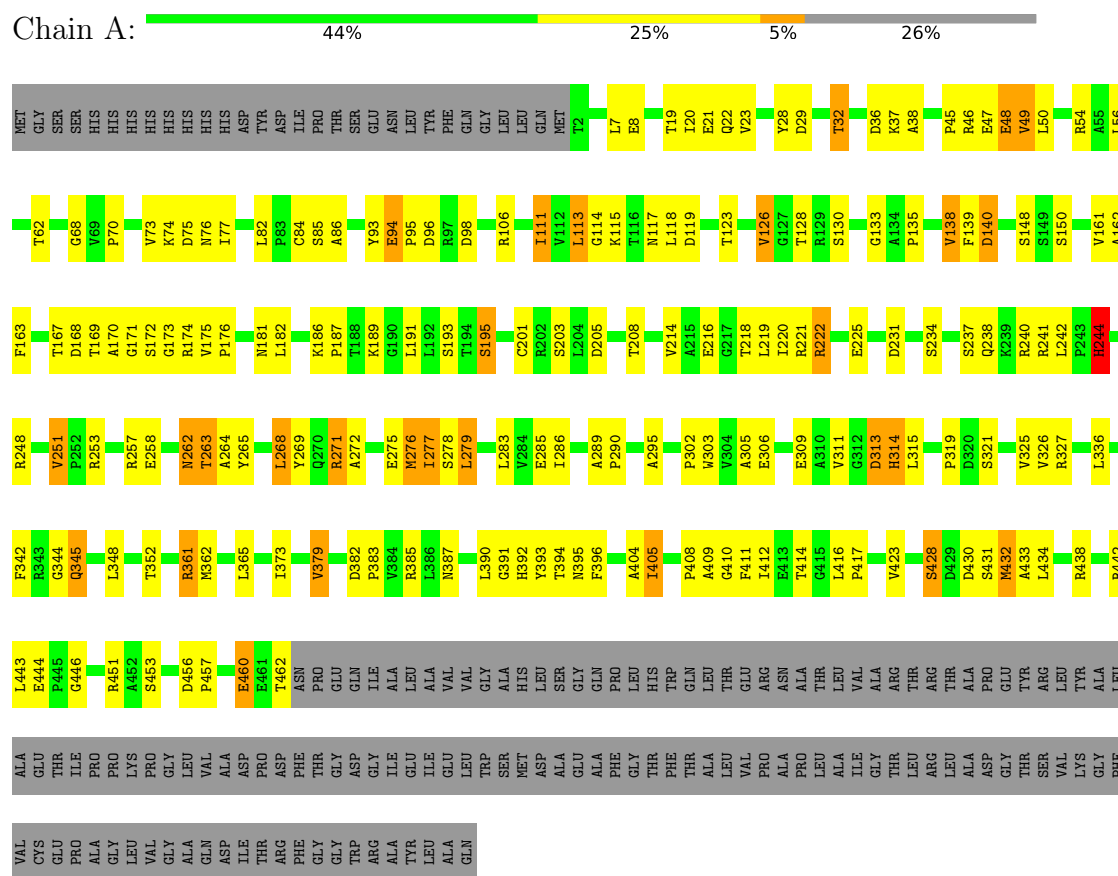
- Molecule 2 is water.

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

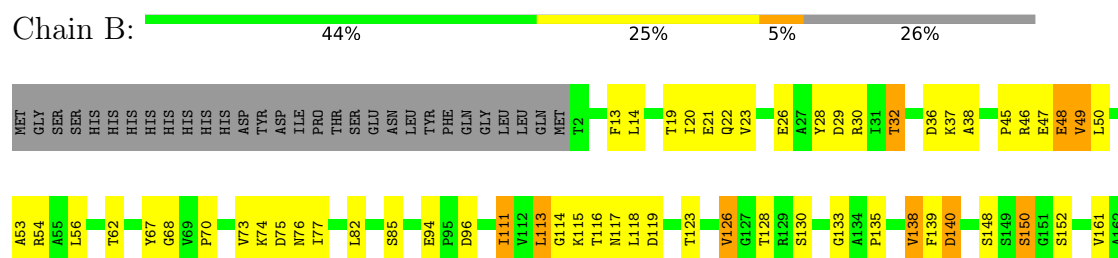
3 Residue-property plots [i](#)

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



• Molecule 1: Allophanate hydrolase



PHE	VAL	CYS	GLU	PRO	ALA	GLY	LEU	VAL	GLN	ASP	ILE	THR	ARG	PHE	GLY	TRP	ARG	TYR	LEU	ALA	GLN
L443	E444	P445	G446	R451	A452	S453	D456	P457	E460	E461	T462	ASN	PRO	THR	GLY	ASP	GLY	ILE	ALA	GLU	LEU
L336	F342	R343	G344	Q345	L351	Q354	R361	M362	L365	I373	V379	D382	V383	R384	R385	L386	N387	L390	G391	H392	Y393
R248	V251	P252	R253	R257	E258	F259	Y260	G261	N262	T263	A264	Y265	L268	R271	A272	E275	M276	I277	S278	L279	D280
F163	T167	D168	T169	A170	G171	S172	G173	R174	V175	P176	A177	A178	F179	N180	N181	L182	K186	P187	L191	L192	S193
L416	P417	V420	V423	S428	D429	D430	S431	M432	A433	L434	R438	P408	A409	G410	F411	I412	L416	P417	V420	V423	S428
E225	D231	S234	S237	Q238	R239	R240	R241	L242	F243	H244	V245	E309	A310	V311	G312	D313	H314	L315	P319	D320	S321
T208	V214	T218	L219	I220	R221	R222	E225	D231	S234	S237	Q238	R239	R240	R241	L242	F243	H244	V245	A289	P290	A295
C201	R202	S203	L204	D205	T208	V214	T218	L219	I220	R221	R222	E225	D231	S234	S237	Q238	R239	R240	R241	L242	F243
A289	P290	A295	P302	W303	V304	A305	E306	E309	A310	V311	G312	D313	H314	L315	P319	D320	S321	V325	V326		

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	14.92 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.256 , 0.307 0.248 , 0.297	Depositor DCC
R_{free} test set	2027 reflections (3.02%)	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 , 18.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.34	0/3478	0.87	3/4752 (0.1%)
1	B	0.34	0/3484	0.87	1/4757 (0.0%)
All	All	0.34	0/6962	0.87	4/9509 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	GLY	N-CA-C	9.28	122.26	110.38
1	A	114	GLY	N-CA-C	8.92	121.80	110.38
1	A	244	HIS	N-CA-C	-5.05	107.09	114.12
1	A	460	GLU	CG-CD-OE1	-5.03	106.84	118.40

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	164	0
1	B	3410	0	3347	158	1
2	A	65	0	0	23	1
2	B	51	0	0	10	0
All	All	6930	0	6680	321	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 24.

All (321) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:410:GLY:C	1:A:411:PHE:CD1	2.87	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:56:LEU:O	1:B:67:TYR:OH	2.15	0.49
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:203:SER:HG	1:A:306:GLU:CD	2.20	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
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:75:ASP:OD2	1:A:85:SER:OG	2.28	0.48
1:A:169:THR:OG1	1:A:205:ASP:OD1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:404:ALA:C	1:B:405:ILE:HG13	2.38	0.48
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:A:303:TRP:C	1:A:305:ALA:H	2.23	0.47
1:B:303:TRP:C	1:B:305:ALA:H	2.21	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:A:139:PHE:O	1:A:140:ASP:HB2	2.14	0.46
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:A:404:ALA:C	1:A:405:ILE:HG13	2.39	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:75:ASP:OD2	1:B:85:SER:OG	2.27	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:277:ILE:C	1:A:279:LEU:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:432:MET:HE3	1:A:432:MET:HB3	1.78	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:B:277:ILE:C	1:B:279:LEU:H	2.25	0.44
1:B:396:PHE:CD1	1:B:396:PHE:C	2.95	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:396:PHE:CD1	1:A:396:PHE:C	2.95	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:A:410:GLY:C	1:A:411:PHE:HD1	2.26	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:303:TRP:C	1:B:305:ALA:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:O	1:A:286:ILE:HG13	2.18	0.43
1:A:348:LEU:O	1:A:352:THR:OG1	2.34	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: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:74:LYS:C	1:A:76:ASN:H	2.27	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:74:LYS:C	1:B:76:ASN:H	2.28	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:B:241:ARG:C	1:B:242:LEU:HD23	2.44	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:B:116:THR:OG1	1:B:152:SER:OG	2.37	0.41
1:A:94:GLU:HA	1:A:95:PRO:HD2	1.85	0.41
1:A:241:ARG:C	1:A:242:LEU:HD23	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:O	1:A:244:HIS:HE1	2.04	0.40
1:B:178:ALA:HA	2:B:617:HOH:O	2.20	0.40
1:B:279:LEU:C	1:B:281:ALA:H	2.29	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:B:117:ASN:ND2	1:B:133:GLY:O	2.54	0.40
1:B:262:ASN:O	1:B:263:THR:C	2.65	0.40
1:B:432:MET:HE3	1:B:432:MET:HB3	1.80	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%)	30	60
1	B	460/621 (74%)	428 (93%)	30 (6%)	2 (0%)	30	60
All	All	920/1242 (74%)	857 (93%)	59 (6%)	4 (0%)	30	60

All (4) Ramachandran outliers are listed below:

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

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

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	340/482 (70%)	299 (88%)	41 (12%)	5	16
1	B	340/482 (70%)	297 (87%)	43 (13%)	4	15
All	All	680/964 (70%)	596 (88%)	84 (12%)	4	16

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	48	GLU
1	A	49	VAL
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	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	248	ARG
1	A	251	VAL
1	A	268	LEU

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Mol	Chain	Res	Type
1	A	271	ARG
1	A	276	MET
1	A	277	ILE
1	A	279	LEU
1	A	283	LEU
1	A	311	VAL
1	A	313	ASP
1	A	314	HIS
1	A	321	SER
1	A	345	GLN
1	A	361	ARG
1	A	373	ILE
1	A	379	VAL
1	A	387	ASN
1	A	405	ILE
1	A	428	SER
1	A	431	SER
1	A	432	MET
1	A	460	GLU
1	A	462	THR
1	B	32	THR
1	B	48	GLU
1	B	49	VAL
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	126	VAL
1	B	138	VAL
1	B	150	SER
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	248	ARG
1	B	251	VAL
1	B	268	LEU

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Mol	Chain	Res	Type
1	B	271	ARG
1	B	276	MET
1	B	277	ILE
1	B	279	LEU
1	B	283	LEU
1	B	311	VAL
1	B	313	ASP
1	B	314	HIS
1	B	321	SER
1	B	345	GLN
1	B	361	ARG
1	B	373	ILE
1	B	379	VAL
1	B	382	ASP
1	B	387	ASN
1	B	405	ILE
1	B	431	SER
1	B	432	MET
1	B	451	ARG
1	B	460	GLU
1	B	462	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
1	A	354	GLN
1	A	389	GLN
1	A	449	GLN
1	B	244	HIS
1	B	354	GLN
1	B	389	GLN
1	B	440	HIS
1	B	449	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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, 95th 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%)	-1.47	0 100 100	25, 40, 59, 73	10 (2%)
1	B	461/621 (74%)	-1.47	0 100 100	25, 40, 58, 74	9 (1%)
All	All	922/1242 (74%)	-1.47	0 100 100	25, 40, 59, 74	19 (2%)

There are no RSRZ outliers to report.

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 oligosaccharides 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.