



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:21 AM UTC

PDB ID : 2BLS / pdb_00002bls
Title : AMPC BETA-LACTAMASE FROM ESCHERICHIA COLI
Authors : Usher, K.C.; Wery, J.-P.; Blaszczyk, L.C.; Remington, S.J.
Deposited on : 1998-06-03
Resolution : 2.00 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

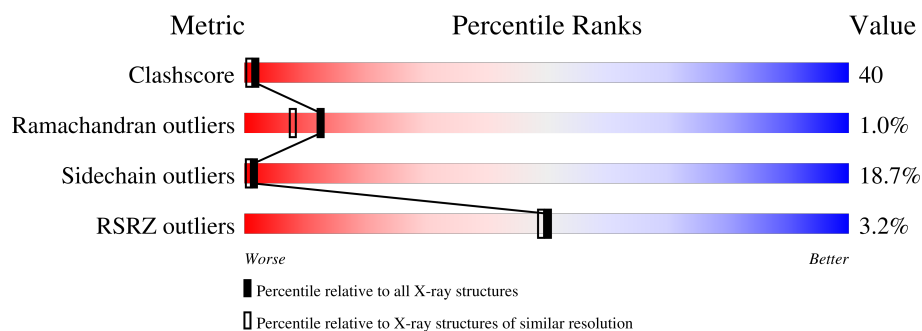
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	358	3% 31% 48% 15% 5%
1	B	358	4% 34% 47% 16% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5662 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 AMPC BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	4	0	0
			2790	1799	474	511	6			
1	B	357	Total	C	N	O	S	4	0	0
			2790	1799	474	511	6			

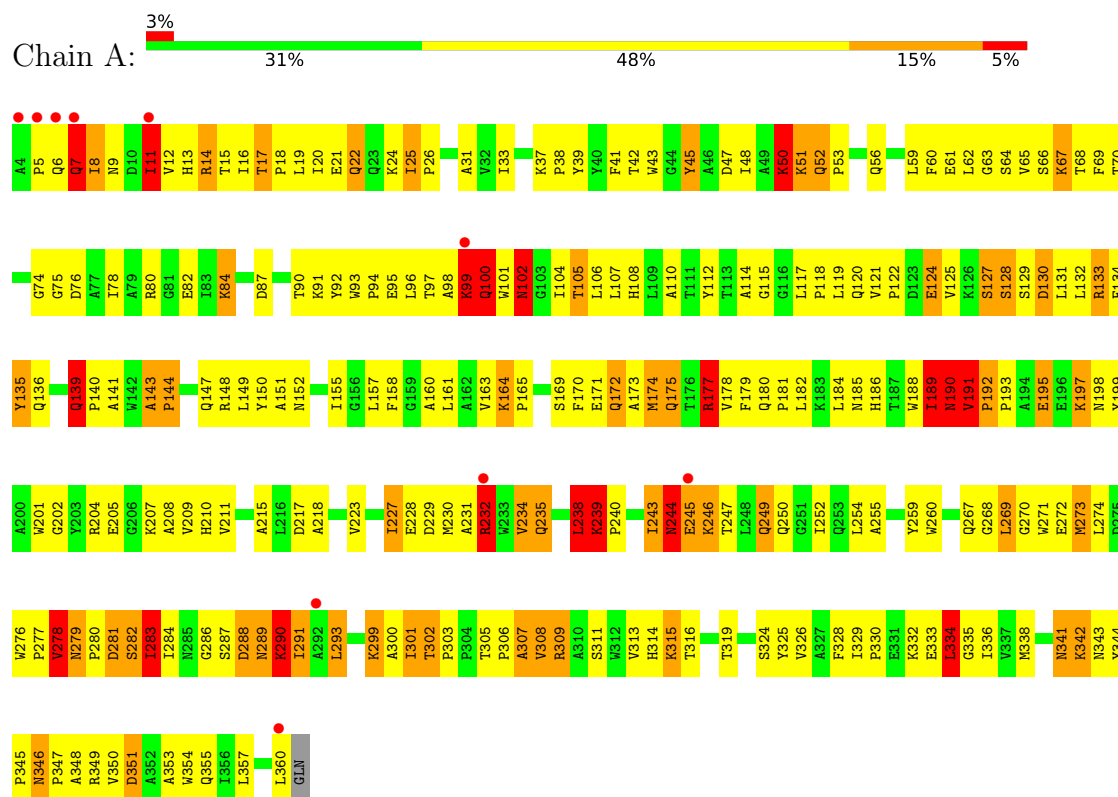
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	42	Total	O	0	0
			42	42		

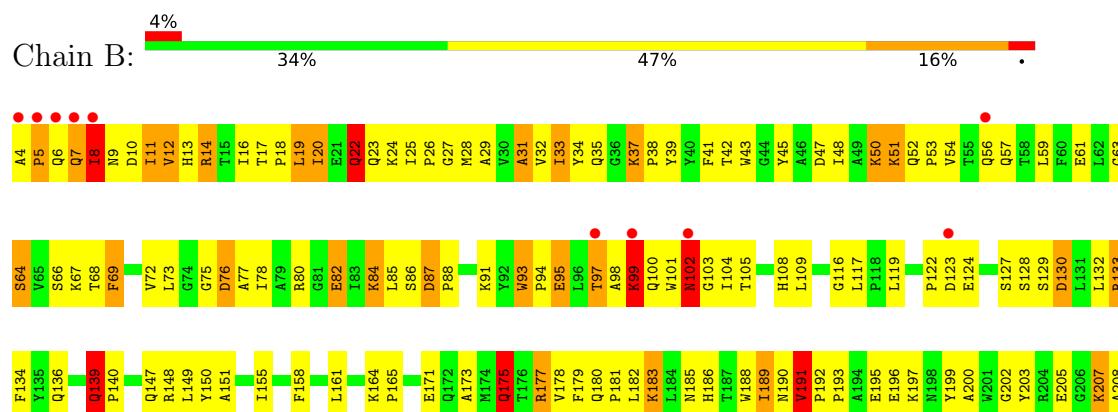
3 Residue-property plots

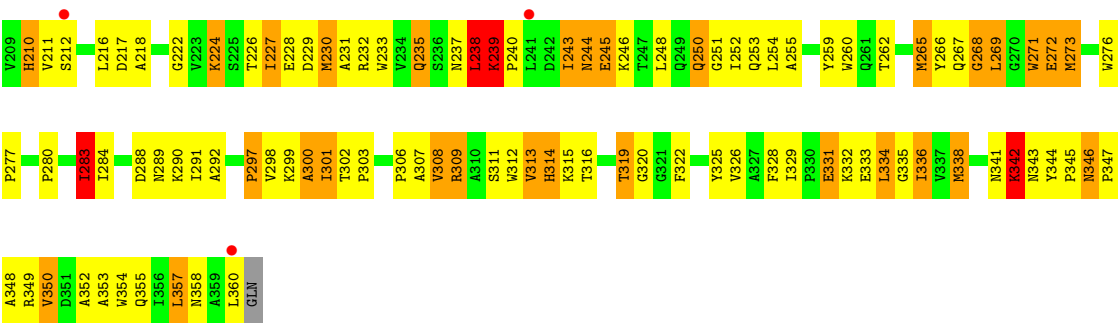
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: AMPC BETA-LACTAMASE



• Molecule 1: AMPC BETA-LACTAMASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.73Å 77.35Å 97.59Å 90.00° 116.45° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	77.4 (25.00-2.00) 77.0 (25.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.90Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.216 , (Not available) 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 114.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5662	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.34% 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	1.53	5/2870 (0.2%)	2.02	102/3921 (2.6%)
1	B	1.52	8/2870 (0.3%)	1.95	72/3921 (1.8%)
All	All	1.53	13/5740 (0.2%)	1.98	174/7842 (2.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	THR	C-N	-7.65	1.24	1.34
1	B	87	ASP	CG-OD1	6.27	1.37	1.25
1	A	229	ASP	CG-OD1	5.79	1.36	1.25
1	B	271	TRP	C-N	5.74	1.42	1.33
1	A	70	THR	C-O	-5.69	1.17	1.24
1	B	252	ILE	CA-C	-5.58	1.46	1.52
1	B	69	PHE	CA-C	-5.51	1.45	1.52
1	B	312	TRP	CA-CB	5.25	1.60	1.53
1	A	195	GLU	CD-OE2	5.14	1.35	1.25
1	B	54	VAL	CA-C	-5.12	1.47	1.52
1	A	22	GLN	N-CA	5.09	1.52	1.46
1	B	133	ARG	N-CA	5.06	1.52	1.46
1	B	272	GLU	CA-C	-5.05	1.46	1.52

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	PRO	O-C-N	15.31	128.35	121.15
1	B	189	ILE	N-CA-C	-15.03	98.63	111.56
1	A	189	ILE	N-CA-C	-14.30	100.31	111.90
1	A	244	ASN	CA-CB-CG	-10.94	101.66	112.60
1	A	99	LYS	CB-CA-C	-10.29	91.60	110.63
1	B	82	GLU	N-CA-CB	-9.69	95.25	110.28
1	A	139	GLN	CA-C-N	9.27	129.21	119.85
1	A	139	GLN	C-N-CA	9.27	129.21	119.85
1	A	239	LYS	O-C-N	9.18	128.28	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	VAL	N-CA-C	8.92	116.77	107.76
1	A	190	ASN	CA-C-N	-8.91	113.75	123.02
1	A	190	ASN	C-N-CA	-8.91	113.75	123.02
1	A	11	ILE	CA-C-N	-8.56	110.28	120.72
1	A	11	ILE	C-N-CA	-8.56	110.28	120.72
1	B	191	VAL	N-CA-CB	8.14	121.34	111.08
1	A	191	VAL	CA-C-O	8.03	125.06	119.20
1	A	238	LEU	CA-C-N	-7.98	115.26	122.28
1	A	238	LEU	C-N-CA	-7.98	115.26	122.28
1	A	100	GLN	CB-CG-CD	-7.93	99.12	112.60
1	A	53	PRO	CB-CA-C	-7.90	99.69	110.60
1	A	147	GLN	N-CA-CB	-7.72	97.32	111.13
1	A	122	PRO	N-CA-CB	7.56	109.90	103.25
1	B	93	TRP	CA-C-N	7.36	128.01	119.47
1	B	93	TRP	C-N-CA	7.36	128.01	119.47
1	A	144	PRO	N-CA-CB	7.31	110.26	103.39
1	A	17	THR	CA-C-O	7.21	125.80	118.73
1	A	283	ILE	N-CA-C	7.19	117.91	110.36
1	A	278	VAL	CB-CA-C	-7.18	99.51	111.29
1	A	45	TYR	N-CA-C	7.16	120.60	109.07
1	A	13	HIS	CA-CB-CG	-7.14	106.66	113.80
1	A	14	ARG	CB-CA-C	-7.10	99.73	110.88
1	A	239	LYS	CA-C-N	7.08	126.91	119.05
1	A	239	LYS	C-N-CA	7.08	126.91	119.05
1	A	234	VAL	N-CA-C	6.93	117.07	110.42
1	B	268	GLY	N-CA-C	-6.87	103.33	112.81
1	B	238	LEU	CA-C-N	-6.83	115.33	122.85
1	B	238	LEU	C-N-CA	-6.83	115.33	122.85
1	B	69	PHE	CA-CB-CG	-6.83	106.97	113.80
1	A	52	GLN	CA-C-O	6.83	125.26	119.66
1	A	189	ILE	CA-C-O	6.83	126.72	120.30
1	B	248	LEU	N-CA-C	-6.75	103.85	111.14
1	A	192	PRO	CA-C-N	6.74	127.00	119.32
1	A	192	PRO	C-N-CA	6.74	127.00	119.32
1	B	13	HIS	CA-CB-CG	-6.72	107.08	113.80
1	B	99	LYS	CB-CA-C	-6.66	99.35	110.68
1	B	212	SER	CA-C-O	6.60	127.43	120.64
1	A	185	ASN	CA-CB-CG	-6.56	106.04	112.60
1	A	130	ASP	N-CA-C	-6.46	104.24	111.28
1	B	239	LYS	O-C-N	6.46	126.46	121.23
1	B	5	PRO	N-CA-CB	6.41	108.89	103.25
1	B	341	ASN	CA-CB-CG	-6.38	106.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ASN	CA-C-O	6.37	125.45	119.59
1	A	141	ALA	N-CA-C	-6.37	105.64	113.41
1	A	186	HIS	CA-CB-CG	-6.33	107.47	113.80
1	A	43	TRP	CB-CA-C	-6.29	98.64	110.16
1	B	140	PRO	CB-CA-C	-6.29	103.18	111.23
1	B	210	HIS	CA-CB-CG	-6.29	107.51	113.80
1	B	12	VAL	N-CA-CB	6.28	117.46	110.62
1	B	283	ILE	N-CA-CB	6.27	119.99	110.58
1	A	68	THR	N-CA-C	-6.24	104.36	112.23
1	A	302	THR	N-CA-CB	-6.24	99.44	110.05
1	B	229	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	127	SER	N-CA-C	6.18	118.01	110.41
1	B	130	ASP	N-CA-C	-6.18	104.46	111.07
1	A	289	ASN	CA-CB-CG	-6.16	106.44	112.60
1	A	319	THR	N-CA-C	-6.12	100.49	109.18
1	A	299	LYS	CA-C-N	-6.10	113.06	122.09
1	A	299	LYS	C-N-CA	-6.10	113.06	122.09
1	A	191	VAL	N-CA-C	6.09	114.59	107.77
1	A	191	VAL	N-CA-CB	6.09	118.72	111.23
1	B	272	GLU	N-CA-CB	6.07	122.41	111.37
1	A	133	ARG	CB-CA-C	-6.01	101.44	110.88
1	B	99	LYS	N-CA-C	6.00	118.58	111.33
1	B	358	ASN	CA-CB-CG	-5.97	106.63	112.60
1	A	191	VAL	CA-C-N	5.96	123.95	119.66
1	A	191	VAL	C-N-CA	5.96	123.95	119.66
1	B	350	VAL	N-CA-C	5.95	116.69	110.62
1	A	115	GLY	CA-C-N	-5.95	114.29	122.26
1	A	115	GLY	C-N-CA	-5.95	114.29	122.26
1	A	351	ASP	CA-CB-CG	-5.94	106.66	112.60
1	B	124	GLU	N-CA-C	-5.94	106.00	113.18
1	A	282	SER	CA-C-N	-5.93	112.95	120.60
1	A	282	SER	C-N-CA	-5.93	112.95	120.60
1	A	313	VAL	CA-C-N	-5.93	111.90	122.45
1	A	313	VAL	C-N-CA	-5.93	111.90	122.45
1	A	288	ASP	N-CA-CB	5.91	118.74	109.69
1	B	341	ASN	N-CA-CB	5.91	119.86	110.22
1	B	191	VAL	CB-CA-C	5.90	117.02	110.71
1	A	117	LEU	CA-C-N	5.90	125.92	119.90
1	A	117	LEU	C-N-CA	5.90	125.92	119.90
1	B	53	PRO	CB-CA-C	-5.89	103.26	110.98
1	B	76	ASP	CA-C-N	5.86	128.41	120.38
1	B	76	ASP	C-N-CA	5.86	128.41	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	THR	CB-CA-C	5.84	116.86	110.15
1	B	8	ILE	CB-CA-C	5.82	120.84	111.29
1	B	319	THR	N-CA-C	-5.82	100.65	108.86
1	A	60	PHE	CA-CB-CG	5.81	119.61	113.80
1	A	191	VAL	O-C-N	5.78	125.97	121.46
1	A	143	ALA	CA-C-N	-5.73	113.79	119.92
1	A	143	ALA	C-N-CA	-5.73	113.79	119.92
1	B	244	ASN	OD1-CG-ND2	5.73	128.33	122.60
1	B	175	GLN	CA-C-O	5.72	127.36	121.07
1	A	25	ILE	CA-C-N	5.71	125.07	118.85
1	A	25	ILE	C-N-CA	5.71	125.07	118.85
1	B	139	GLN	CB-CA-C	-5.67	102.78	109.47
1	A	283	ILE	N-CA-CB	5.66	116.79	110.51
1	A	341	ASN	N-CA-CB	5.61	119.10	110.79
1	A	31	ALA	CA-C-N	-5.61	115.64	123.10
1	A	31	ALA	C-N-CA	-5.61	115.64	123.10
1	B	329	ILE	CA-C-N	5.60	126.84	119.84
1	B	329	ILE	C-N-CA	5.60	126.84	119.84
1	B	133	ARG	CB-CA-C	-5.59	101.86	110.81
1	B	185	ASN	N-CA-C	5.59	119.72	113.01
1	B	297	PRO	CB-CA-C	-5.55	104.74	111.46
1	B	230	MET	CA-C-O	5.54	126.36	120.10
1	B	329	ILE	O-C-N	5.53	127.40	121.10
1	B	300	ALA	CB-CA-C	5.51	118.83	109.84
1	B	243	ILE	CA-C-N	5.46	128.37	120.79
1	B	243	ILE	C-N-CA	5.46	128.37	120.79
1	A	135	TYR	N-CA-C	5.45	117.22	111.28
1	A	75	GLY	N-CA-C	-5.43	105.71	113.86
1	A	281	ASP	O-C-N	5.40	127.65	122.03
1	A	19	LEU	CA-C-O	5.40	126.49	120.82
1	B	346	ASN	CA-C-O	5.39	123.57	118.34
1	A	291	ILE	CB-CA-C	5.37	118.14	111.80
1	B	25	ILE	N-CA-CB	-5.36	103.71	111.21
1	B	252	ILE	N-CA-CB	5.36	116.24	110.62
1	B	320	GLY	N-CA-C	5.35	119.15	112.73
1	B	313	VAL	CB-CA-C	-5.35	102.86	110.83
1	B	128	SER	CA-C-O	5.34	125.95	119.38
1	A	105	THR	N-CA-C	5.32	118.61	110.36
1	A	50	LYS	N-CA-C	-5.31	106.57	113.16
1	A	67	LYS	N-CA-C	5.31	118.86	112.38
1	A	5	PRO	N-CA-CB	5.31	108.03	103.31
1	A	139	GLN	CA-C-O	5.29	126.14	120.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	GLN	CB-CG-CD	5.28	121.57	112.60
1	B	191	VAL	O-C-N	5.27	126.15	121.57
1	A	223	VAL	N-CA-C	5.23	116.82	108.87
1	A	15	THR	N-CA-C	5.23	117.78	111.40
1	B	322	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	208	ALA	CA-C-N	-5.20	114.88	122.58
1	A	208	ALA	C-N-CA	-5.20	114.88	122.58
1	A	290	LYS	N-CA-C	-5.19	106.21	112.54
1	A	141	ALA	CA-C-N	-5.19	113.75	123.03
1	A	141	ALA	C-N-CA	-5.19	113.75	123.03
1	A	192	PRO	CA-C-O	-5.18	116.64	120.73
1	B	338	MET	CG-SD-CE	-5.17	89.52	100.90
1	B	185	ASN	CA-CB-CG	-5.17	107.43	112.60
1	B	331	GLU	CB-CA-C	5.17	120.60	110.67
1	B	8	ILE	N-CA-CB	5.17	119.75	111.23
1	B	128	SER	N-CA-C	-5.16	106.24	112.54
1	B	297	PRO	N-CA-CB	5.16	107.90	103.36
1	B	31	ALA	CA-C-N	-5.16	116.38	123.14
1	B	31	ALA	C-N-CA	-5.16	116.38	123.14
1	A	50	LYS	CG-CD-CE	5.16	123.17	111.30
1	A	68	THR	CA-C-O	5.14	125.86	119.79
1	A	128	SER	CA-C-O	5.12	125.68	119.49
1	B	314	HIS	N-CA-C	5.10	115.27	108.38
1	B	22	GLN	N-CA-C	5.10	117.22	111.11
1	B	312	TRP	N-CA-C	-5.09	98.99	107.99
1	A	334	LEU	N-CA-CB	-5.08	102.03	111.13
1	A	346	ASN	CA-C-O	5.08	123.22	118.44
1	A	177	ARG	N-CA-C	5.07	119.55	112.90
1	B	97	THR	N-CA-C	5.07	118.62	112.23
1	A	59	LEU	CB-CA-C	-5.06	101.41	109.75
1	B	342	LYS	CB-CA-C	5.06	118.96	109.86
1	A	324	SER	N-CA-C	5.06	117.36	109.52
1	B	268	GLY	CA-C-O	-5.05	115.72	122.23
1	A	232	ARG	CA-C-N	5.04	127.35	120.54
1	A	232	ARG	C-N-CA	5.04	127.35	120.54
1	B	87	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	100	GLN	O-C-N	5.03	127.46	122.12
1	B	69	PHE	N-CA-C	-5.03	105.70	111.14
1	A	174	MET	CG-SD-CE	-5.01	89.87	100.90

There are no chirality outliers.

There are no planarity outliers.

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	2790	0	2770	235	0
1	B	2790	0	2770	216	0
2	A	40	0	0	1	0
2	B	42	0	0	1	0
All	All	5662	0	5540	445	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (445) 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:A:26:PRO:HB3	1:A:48:ILE:HD11	1.37	1.04
1:A:244:ASN:H	1:A:244:ASN:ND2	1.54	1.01
1:B:8:ILE:HA	1:B:11:ILE:HD11	1.46	0.95
1:A:67:LYS:HD3	1:A:155:ILE:HG21	1.49	0.92
1:B:67:LYS:HD3	1:B:155:ILE:HG21	1.51	0.91
1:B:8:ILE:HD12	1:B:41:PHE:HZ	1.38	0.88
1:A:98:ALA:HB3	1:A:101:TRP:HD1	1.39	0.87
1:A:334:LEU:HD12	1:A:335:GLY:N	1.88	0.87
1:A:260:TRP:CZ3	1:A:300:ALA:HB2	2.13	0.84
1:B:17:THR:HB	1:B:18:PRO:HD3	1.61	0.83
1:B:11:ILE:HD13	1:B:11:ILE:H	1.43	0.82
1:A:119:LEU:HA	1:A:151:ALA:HA	1.62	0.82
1:A:316:THR:HG22	1:A:325:TYR:HD1	1.45	0.82
1:B:316:THR:HG22	1:B:325:TYR:CD1	2.15	0.81
1:B:336:ILE:HD13	1:B:338:MET:HE3	1.61	0.81
1:A:232:ARG:HA	1:A:235:GLN:NE2	1.96	0.80
1:B:260:TRP:CZ3	1:B:300:ALA:HB2	2.16	0.80
1:B:334:LEU:HD13	1:B:357:LEU:HG	1.64	0.79
1:A:56:GLN:CB	1:A:227:ILE:HD11	2.12	0.79
1:A:244:ASN:ND2	1:A:244:ASN:N	2.29	0.78
1:B:316:THR:HG22	1:B:325:TYR:HD1	1.47	0.78
1:B:164:LYS:HB2	1:B:165:PRO:HD3	1.65	0.78
1:A:336:ILE:HD13	1:A:338:MET:HE2	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:TYR:CZ	1:A:349:ARG:HG2	2.18	0.78
1:A:357:LEU:O	1:A:360:LEU:HD12	1.84	0.78
1:A:316:THR:HG22	1:A:325:TYR:CD1	2.18	0.77
1:B:56:GLN:HA	1:B:227:ILE:HD11	1.66	0.77
1:A:272:GLU:N	1:A:273:MET:HE3	1.99	0.77
1:A:17:THR:O	1:A:21:GLU:HG2	1.84	0.77
1:A:118:PRO:O	1:A:151:ALA:HB1	1.85	0.76
1:B:77:ALA:O	1:B:82:GLU:HB2	1.85	0.76
1:B:101:TRP:HA	1:B:104:ILE:HD12	1.67	0.76
1:A:107:LEU:HD22	1:B:303:PRO:HD3	1.67	0.76
1:A:255:ALA:HA	1:A:269:LEU:HB2	1.66	0.76
1:B:10:ASP:HB3	1:B:14:ARG:HH21	1.50	0.76
1:B:171:GLU:HG2	1:B:175:GLN:HE22	1.50	0.76
1:B:67:LYS:HE2	1:B:150:TYR:OH	1.86	0.74
1:B:334:LEU:CD1	1:B:357:LEU:HG	2.17	0.74
1:B:8:ILE:HD12	1:B:41:PHE:CZ	2.23	0.73
1:B:259:TYR:CE2	1:B:269:LEU:HD13	2.23	0.73
1:A:7:GLN:O	1:A:11:ILE:HG23	1.88	0.73
1:B:80:ARG:HB3	1:B:82:GLU:HG3	1.71	0.73
1:A:130:ASP:HA	1:A:133:ARG:HH11	1.53	0.73
1:B:8:ILE:O	1:B:12:VAL:HG23	1.89	0.72
1:A:56:GLN:HA	1:A:227:ILE:HD11	1.70	0.72
1:B:47:ASP:OD2	1:B:50:LYS:HD2	1.90	0.72
1:A:260:TRP:HZ3	1:A:300:ALA:HB2	1.55	0.72
1:B:357:LEU:O	1:B:360:LEU:HD12	1.90	0.71
1:B:344:TYR:CZ	1:B:349:ARG:HG2	2.25	0.71
1:A:336:ILE:HD13	1:A:338:MET:CE	2.20	0.71
1:A:98:ALA:HB3	1:A:101:TRP:CD1	2.24	0.71
1:B:161:LEU:HA	1:B:164:LYS:HG2	1.71	0.71
1:B:181:PRO:HB3	1:B:245:GLU:OE2	1.90	0.70
1:B:26:PRO:HB3	1:B:48:ILE:HD11	1.74	0.70
1:A:7:GLN:O	1:A:11:ILE:HD13	1.92	0.70
1:B:11:ILE:HD13	1:B:11:ILE:N	2.03	0.69
1:A:336:ILE:CD1	1:A:338:MET:HE2	2.22	0.69
1:B:336:ILE:HD13	1:B:338:MET:CE	2.22	0.69
1:A:47:ASP:OD2	1:A:50:LYS:HD2	1.92	0.69
1:A:56:GLN:CA	1:A:227:ILE:HD11	2.22	0.69
1:A:7:GLN:O	1:A:7:GLN:HG3	1.91	0.68
1:A:67:LYS:HE2	1:A:150:TYR:OH	1.94	0.68
1:B:56:GLN:CB	1:B:227:ILE:HD11	2.23	0.68
1:B:173:ALA:O	1:B:177:ARG:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ARG:HA	1:B:235:GLN:HE21	1.59	0.67
1:B:95:GLU:OE1	1:B:95:GLU:N	2.28	0.67
1:A:280:PRO:O	1:A:284:ILE:HG13	1.95	0.66
1:B:80:ARG:HD2	1:B:177:ARG:NH2	2.10	0.66
1:A:8:ILE:O	1:A:12:VAL:HG23	1.95	0.66
1:B:29:ALA:HB1	1:B:227:ILE:HG12	1.77	0.66
1:B:4:ALA:HB3	1:B:9:ASN:HD21	1.59	0.66
1:B:192:PRO:HG2	1:B:195:GLU:HG3	1.77	0.66
1:A:8:ILE:HA	1:A:11:ILE:HD13	1.78	0.66
1:A:66:SER:O	1:A:69:PHE:HB2	1.94	0.66
1:A:238:LEU:HD13	1:A:328:PHE:CD2	2.31	0.66
1:A:16:ILE:O	1:A:20:ILE:HG13	1.95	0.65
1:A:197:LYS:HD3	1:A:198:ASN:OD1	1.96	0.65
1:B:8:ILE:CA	1:B:11:ILE:HD11	2.24	0.65
1:B:238:LEU:HD11	1:B:328:PHE:HB2	1.77	0.65
1:B:37:LYS:HG3	1:B:38:PRO:N	2.11	0.65
1:A:8:ILE:HA	1:A:11:ILE:CD1	2.26	0.65
1:A:105:THR:H	1:A:108:HIS:CD2	2.15	0.65
1:A:173:ALA:O	1:A:177:ARG:HB2	1.96	0.65
1:A:37:LYS:HG2	1:A:39:TYR:CZ	2.32	0.65
1:B:268:GLY:HA3	1:B:273:MET:HE1	1.78	0.65
1:B:183:LYS:O	1:B:232:ARG:NH1	2.30	0.65
1:A:217:ASP:OD1	1:A:218:ALA:N	2.29	0.64
1:A:276:TRP:CZ3	1:A:278:VAL:HG22	2.32	0.64
1:B:10:ASP:CB	1:B:14:ARG:HH21	2.10	0.64
1:A:8:ILE:HD11	1:A:41:PHE:CE1	2.32	0.64
1:A:148:ARG:NH1	1:A:267:GLN:OE1	2.29	0.64
1:A:50:LYS:O	1:A:52:GLN:NE2	2.28	0.64
1:A:130:ASP:HA	1:A:133:ARG:NH1	2.12	0.64
1:B:288:ASP:OD2	1:B:290:LYS:HD2	1.98	0.63
1:A:74:GLY:O	1:A:78:ILE:HG13	1.97	0.63
1:B:308:VAL:HG22	1:B:311:SER:OG	1.98	0.63
1:B:228:GLU:O	1:B:231:ALA:HB3	1.98	0.63
1:B:232:ARG:HA	1:B:235:GLN:NE2	2.14	0.62
1:A:338:MET:HE1	1:A:353:ALA:CA	2.30	0.62
1:B:129:SER:OG	1:B:133:ARG:NH1	2.32	0.62
1:B:11:ILE:HG12	1:B:12:VAL:N	2.14	0.62
1:B:355:GLN:NE2	1:B:355:GLN:HA	2.14	0.62
1:B:240:PRO:HA	1:B:243:ILE:CD1	2.30	0.62
1:B:68:THR:HG21	1:B:271:TRP:CZ3	2.35	0.61
1:B:203:TYR:HA	1:B:207:LYS:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HG12	1:A:12:VAL:N	2.15	0.61
1:A:217:ASP:O	1:A:218:ALA:C	2.40	0.61
1:A:243:ILE:HD11	1:A:249:GLN:HA	1.81	0.61
1:B:171:GLU:HG2	1:B:175:GLN:NE2	2.16	0.61
1:B:338:MET:HE1	1:B:353:ALA:HA	1.81	0.61
1:A:351:ASP:OD1	1:A:355:GLN:NE2	2.34	0.61
1:B:72:VAL:HG21	1:B:233:TRP:CH2	2.36	0.61
1:A:303:PRO:CG	1:B:85:LEU:HB2	2.30	0.61
1:B:260:TRP:HZ3	1:B:300:ALA:HB2	1.66	0.61
1:A:276:TRP:CE3	1:A:278:VAL:HG22	2.35	0.60
1:B:127:SER:OG	1:B:130:ASP:N	2.28	0.60
1:B:271:TRP:HB3	1:B:273:MET:HE2	1.82	0.60
1:B:344:TYR:CE1	1:B:349:ARG:HG2	2.36	0.60
1:A:308:VAL:HG22	1:A:311:SER:OG	2.02	0.60
1:B:148:ARG:HB2	1:B:298:VAL:CG1	2.32	0.60
1:B:193:PRO:O	1:B:196:GLU:HB2	2.01	0.60
1:A:232:ARG:HA	1:A:235:GLN:HE21	1.67	0.60
1:B:127:SER:OG	1:B:129:SER:HB3	2.01	0.60
1:B:240:PRO:O	1:B:243:ILE:HD12	2.01	0.60
1:B:56:GLN:CA	1:B:227:ILE:HD11	2.30	0.59
1:A:93:TRP:CE3	1:A:96:LEU:HD13	2.38	0.59
1:A:272:GLU:CA	1:A:273:MET:HE3	2.33	0.59
1:A:99:LYS:NZ	1:A:99:LYS:HB3	2.06	0.58
1:A:99:LYS:O	1:A:102:ASN:HB2	2.03	0.58
1:A:345:PRO:O	1:A:348:ALA:HB3	2.03	0.58
1:B:5:PRO:O	1:B:8:ILE:HG13	2.03	0.58
1:B:10:ASP:CG	1:B:14:ARG:HH21	2.11	0.58
1:B:59:LEU:HD21	1:B:186:HIS:O	2.03	0.58
1:A:100:GLN:NE2	1:A:136:GLN:O	2.36	0.58
1:A:243:ILE:HD11	1:A:249:GLN:CA	2.33	0.58
1:A:56:GLN:HB3	1:A:228:GLU:HG3	1.85	0.57
1:A:8:ILE:HD11	1:A:41:PHE:CZ	2.40	0.57
1:B:200:ALA:O	1:B:210:HIS:NE2	2.30	0.57
1:A:338:MET:HE1	1:A:353:ALA:HB2	1.86	0.57
1:A:33:ILE:HD12	1:A:33:ILE:N	2.20	0.56
1:A:188:TRP:CZ3	1:A:192:PRO:HG3	2.40	0.56
1:B:148:ARG:NH1	1:B:267:GLN:OE1	2.37	0.56
1:B:271:TRP:C	1:B:273:MET:HE3	2.30	0.56
1:A:303:PRO:HD2	1:B:86:SER:N	2.20	0.56
1:B:16:ILE:O	1:B:20:ILE:HG13	2.05	0.56
1:A:120:GLN:OE1	1:A:152:ASN:ND2	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD12	1:A:330:PRO:HA	1.88	0.56
1:A:228:GLU:O	1:A:231:ALA:HB3	2.06	0.56
1:B:33:ILE:N	1:B:33:ILE:HD12	2.21	0.56
1:B:105:THR:H	1:B:108:HIS:CD2	2.24	0.56
1:B:32:VAL:C	1:B:33:ILE:HD12	2.32	0.55
1:B:61:GLU:CD	1:B:211:VAL:H	2.14	0.55
1:B:37:LYS:HG2	1:B:39:TYR:CZ	2.41	0.55
1:B:28:MET:CE	1:B:338:MET:HB3	2.37	0.55
1:A:62:LEU:HB3	1:A:65:VAL:HB	1.87	0.55
1:A:104:ILE:HA	1:A:108:HIS:HD2	1.72	0.55
1:B:338:MET:HE1	1:B:353:ALA:CA	2.36	0.54
1:B:240:PRO:HA	1:B:243:ILE:HD11	1.89	0.54
1:B:6:GLN:C	1:B:8:ILE:H	2.16	0.54
1:A:56:GLN:HB3	1:A:228:GLU:CG	2.38	0.54
1:A:139:GLN:HE21	1:A:139:GLN:CA	2.20	0.54
1:A:334:LEU:HD12	1:A:334:LEU:C	2.32	0.54
1:B:119:LEU:HA	1:B:151:ALA:HA	1.89	0.54
1:A:56:GLN:HB3	1:A:227:ILE:HD11	1.87	0.54
1:B:66:SER:O	1:B:69:PHE:HB2	2.08	0.54
1:A:234:VAL:HG12	1:A:238:LEU:HD22	1.89	0.54
1:A:119:LEU:HA	1:A:151:ALA:CA	2.37	0.53
1:A:56:GLN:CG	1:A:227:ILE:HD11	2.38	0.53
1:A:164:LYS:HB2	1:A:165:PRO:HD3	1.90	0.53
1:A:286:GLY:O	1:A:291:ILE:HG23	2.08	0.53
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.43	0.53
1:A:311:SER:O	1:A:330:PRO:HD2	2.08	0.53
1:A:150:TYR:OH	1:A:315:LYS:NZ	2.42	0.53
1:A:230:MET:O	1:A:234:VAL:HG23	2.07	0.53
1:B:276:TRP:HA	1:B:277:PRO:C	2.34	0.53
1:A:51:LYS:N	1:A:51:LYS:HD3	2.24	0.53
1:A:139:GLN:H	1:A:139:GLN:NE2	2.06	0.53
1:A:346:ASN:HB2	1:A:347:PRO:HD3	1.89	0.53
1:B:148:ARG:HB2	1:B:298:VAL:HG11	1.91	0.53
1:A:180:GLN:O	1:A:181:PRO:C	2.47	0.53
1:A:201:TRP:O	1:A:341:ASN:HB2	2.07	0.53
1:A:314:HIS:HB2	1:A:326:VAL:O	2.09	0.53
1:B:8:ILE:CD1	1:B:41:PHE:HZ	2.18	0.53
1:B:227:ILE:HG13	2:B:385:HOH:O	2.09	0.53
1:A:124:GLU:H	1:A:124:GLU:CD	2.17	0.52
1:B:28:MET:HE3	1:B:338:MET:HB3	1.91	0.52
1:B:80:ARG:CB	1:B:82:GLU:HG3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:PRO:O	1:B:307:ALA:C	2.53	0.52
1:A:92:TYR:CE1	1:A:106:LEU:HD11	2.44	0.52
1:B:265:MET:HE3	1:B:272:GLU:HB3	1.91	0.52
1:B:271:TRP:CB	1:B:273:MET:HE2	2.39	0.52
1:A:114:ALA:HB3	2:A:380:HOH:O	2.09	0.52
1:A:306:PRO:O	1:A:307:ALA:C	2.52	0.52
1:B:34:TYR:O	1:B:35:GLN:C	2.50	0.52
1:A:6:GLN:O	1:A:8:ILE:N	2.43	0.52
1:A:101:TRP:CZ2	1:A:135:TYR:HB3	2.45	0.52
1:A:303:PRO:HG2	1:B:85:LEU:HB2	1.91	0.52
1:B:147:GLN:NE2	1:B:297:PRO:HA	2.24	0.52
1:A:20:ILE:HG23	1:A:25:ILE:HB	1.92	0.51
1:A:127:SER:OG	1:A:129:SER:HB3	2.10	0.51
1:A:355:GLN:OE1	1:A:355:GLN:HA	2.11	0.51
1:B:222:GLY:O	1:B:224:LYS:HE3	2.10	0.51
1:A:67:LYS:NZ	1:A:152:ASN:OD1	2.43	0.51
1:A:110:ALA:O	1:A:155:ILE:HD12	2.10	0.51
1:A:182:LEU:HB2	1:A:184:LEU:HG	1.93	0.51
1:A:332:LYS:O	1:A:333:GLU:HB2	2.11	0.51
1:B:238:LEU:CD1	1:B:328:PHE:CD2	2.94	0.51
1:A:6:GLN:O	1:A:9:ASN:N	2.43	0.51
1:B:19:LEU:O	1:B:19:LEU:HD12	2.11	0.51
1:B:199:TYR:CZ	1:B:210:HIS:CD2	2.99	0.51
1:B:314:HIS:N	1:B:314:HIS:CD2	2.79	0.51
1:A:280:PRO:HG3	1:A:354:TRP:CZ2	2.46	0.51
1:B:280:PRO:HG3	1:B:354:TRP:CZ2	2.45	0.51
1:A:47:ASP:CG	1:A:50:LYS:HD2	2.36	0.51
1:A:118:PRO:HG2	1:A:134:PHE:HZ	1.76	0.51
1:B:164:LYS:HB2	1:B:165:PRO:CD	2.37	0.51
1:B:265:MET:HG2	1:B:266:TYR:N	2.25	0.51
1:B:16:ILE:HG21	1:B:43:TRP:CH2	2.46	0.51
1:B:59:LEU:HB2	1:B:199:TYR:HA	1.93	0.51
1:A:112:TYR:CE2	1:A:148:ARG:NH1	2.79	0.50
1:A:288:ASP:OD1	1:A:290:LYS:HD3	2.09	0.50
1:B:19:LEU:HD12	1:B:19:LEU:C	2.37	0.50
1:A:289:ASN:CG	1:A:293:LEU:HD22	2.36	0.50
1:B:149:LEU:O	1:B:150:TYR:C	2.54	0.50
1:A:56:GLN:HG2	1:A:227:ILE:HD11	1.94	0.50
1:A:99:LYS:HB3	1:A:99:LYS:HZ1	1.77	0.50
1:A:80:ARG:HH21	1:A:177:ARG:HG2	1.77	0.50
1:B:105:THR:H	1:B:108:HIS:HD2	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:TRP:CD2	1:B:192:PRO:HD3	2.47	0.49
1:A:268:GLY:HA3	1:A:273:MET:HE1	1.93	0.49
1:B:8:ILE:HA	1:B:11:ILE:CD1	2.32	0.49
1:A:243:ILE:CD1	1:A:249:GLN:HA	2.42	0.49
1:B:272:GLU:N	1:B:273:MET:HE3	2.27	0.49
1:A:98:ALA:HB1	1:A:100:GLN:NE2	2.28	0.49
1:A:271:TRP:C	1:A:273:MET:HE3	2.37	0.49
1:B:47:ASP:O	1:B:52:GLN:N	2.35	0.49
1:B:26:PRO:HG2	1:B:203:TYR:CD2	2.47	0.49
1:A:45:TYR:N	1:A:45:TYR:CD1	2.80	0.49
1:A:344:TYR:CE2	1:A:349:ARG:HG2	2.48	0.49
1:B:12:VAL:HG21	1:B:41:PHE:CZ	2.47	0.49
1:B:164:LYS:CB	1:B:165:PRO:HD3	2.39	0.49
1:A:17:THR:N	1:A:18:PRO:CD	2.76	0.49
1:B:202:GLY:O	1:B:208:ALA:HA	2.13	0.49
1:B:332:LYS:O	1:B:333:GLU:C	2.53	0.49
1:B:23:GLN:O	1:B:24:LYS:HB2	2.12	0.49
1:A:124:GLU:N	1:A:124:GLU:OE1	2.46	0.49
1:B:4:ALA:CB	1:B:9:ASN:HD21	2.25	0.49
1:B:17:THR:HB	1:B:18:PRO:CD	2.39	0.49
1:A:338:MET:HE1	1:A:353:ALA:CB	2.43	0.48
1:A:160:ALA:O	1:A:163:VAL:HG22	2.14	0.48
1:A:202:GLY:O	1:A:209:VAL:N	2.37	0.48
1:A:139:GLN:CA	1:A:139:GLN:NE2	2.74	0.48
1:A:169:SER:OG	1:A:172:GLN:HB2	2.13	0.48
1:A:192:PRO:HG2	1:A:195:GLU:HG3	1.95	0.48
1:A:157:LEU:O	1:A:158:PHE:C	2.54	0.48
1:A:94:PRO:HG2	1:A:95:GLU:OE1	2.13	0.48
1:A:259:TYR:C	1:A:301:ILE:HG13	2.38	0.48
1:A:338:MET:CE	1:A:353:ALA:HB2	2.43	0.48
1:B:23:GLN:HA	1:B:23:GLN:NE2	2.28	0.48
1:B:217:ASP:OD1	1:B:218:ALA:N	2.47	0.48
1:A:174:MET:HG3	1:A:179:PHE:CZ	2.48	0.48
1:B:18:PRO:O	1:B:22:GLN:HB2	2.14	0.48
1:A:234:VAL:HG12	1:A:238:LEU:CD2	2.44	0.48
1:A:288:ASP:O	1:A:291:ILE:HG22	2.14	0.48
1:A:338:MET:HE1	1:A:353:ALA:HA	1.95	0.48
1:B:32:VAL:HG22	1:B:336:ILE:HG13	1.94	0.48
1:B:188:TRP:CZ2	1:B:192:PRO:HG3	2.48	0.48
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.47	0.48
1:B:240:PRO:HA	1:B:243:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ILE:O	1:A:330:PRO:C	2.56	0.48
1:B:72:VAL:HG21	1:B:233:TRP:HH2	1.79	0.48
1:B:289:ASN:HA	1:B:292:ALA:HB3	1.96	0.48
1:A:273:MET:C	1:A:274:LEU:HD12	2.38	0.48
1:A:182:LEU:O	1:A:232:ARG:HD3	2.14	0.47
1:A:287:SER:HB2	1:A:346:ASN:HB3	1.96	0.47
1:A:287:SER:HB3	1:A:350:VAL:HG21	1.96	0.47
1:A:6:GLN:O	1:A:7:GLN:C	2.55	0.47
1:A:8:ILE:CD1	1:A:41:PHE:CE1	2.98	0.47
1:B:175:GLN:HE21	1:B:175:GLN:HB2	1.28	0.47
1:B:33:ILE:N	1:B:33:ILE:CD1	2.77	0.47
1:A:121:VAL:HG11	1:A:215:ALA:HB3	1.96	0.47
1:A:342:LYS:HG2	1:A:343:ASN:N	2.30	0.47
1:A:130:ASP:CA	1:A:133:ARG:NH1	2.77	0.47
1:A:302:THR:O	1:B:86:SER:HA	2.15	0.47
1:A:246:LYS:HG2	1:A:247:THR:N	2.29	0.47
1:A:80:ARG:CD	1:A:177:ARG:NH2	2.79	0.46
1:A:181:PRO:HB3	1:A:245:GLU:OE2	2.16	0.46
1:B:47:ASP:CG	1:B:50:LYS:HD2	2.40	0.46
1:A:100:GLN:H	1:A:100:GLN:HG3	1.23	0.46
1:B:12:VAL:HG21	1:B:41:PHE:CE1	2.50	0.46
1:A:169:SER:O	1:A:170:PHE:C	2.58	0.46
1:A:188:TRP:CE3	1:A:192:PRO:HG3	2.50	0.46
1:A:271:TRP:HB3	1:A:273:MET:CE	2.45	0.46
1:A:281:ASP:O	1:A:282:SER:C	2.58	0.46
1:A:301:ILE:O	1:A:303:PRO:C	2.58	0.46
1:A:309:ARG:O	1:A:330:PRO:HG2	2.16	0.46
1:B:182:LEU:O	1:B:183:LYS:HB2	2.15	0.46
1:B:273:MET:HG3	1:B:313:VAL:HG13	1.97	0.46
1:A:179:PHE:O	1:A:180:GLN:C	2.57	0.46
1:A:274:LEU:HD22	1:A:283:ILE:CG2	2.45	0.46
1:B:272:GLU:CA	1:B:273:MET:HE3	2.46	0.46
1:A:67:LYS:O	1:A:270:GLY:HA3	2.15	0.46
1:B:31:ALA:HA	1:B:39:TYR:O	2.16	0.46
1:B:99:LYS:O	1:B:102:ASN:HB2	2.16	0.46
1:A:61:GLU:CD	1:A:211:VAL:H	2.23	0.46
1:A:139:GLN:NE2	1:A:139:GLN:N	2.64	0.46
1:B:6:GLN:O	1:B:8:ILE:N	2.49	0.46
1:A:171:GLU:HG3	1:A:189:ILE:HB	1.98	0.46
1:A:289:ASN:OD1	1:A:293:LEU:HD22	2.17	0.45
1:B:61:GLU:OE2	1:B:199:TYR:OH	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:THR:O	1:B:230:MET:HG2	2.17	0.45
1:A:139:GLN:CB	1:A:140:PRO:HD2	2.43	0.45
1:B:27:GLY:HA3	1:B:45:TYR:O	2.16	0.45
1:B:109:LEU:HB3	1:B:158:PHE:HB2	1.98	0.45
1:A:112:TYR:HB3	1:A:149:LEU:O	2.16	0.45
1:A:188:TRP:HB3	1:A:190:ASN:O	2.17	0.45
1:B:346:ASN:N	1:B:347:PRO:CD	2.80	0.45
1:A:315:LYS:HG3	1:A:316:THR:N	2.32	0.45
1:B:80:ARG:CD	1:B:177:ARG:NH2	2.79	0.45
1:A:37:LYS:HG2	1:A:39:TYR:CE2	2.52	0.45
1:A:280:PRO:HA	1:A:283:ILE:HD11	1.99	0.45
1:A:346:ASN:N	1:A:347:PRO:CD	2.79	0.45
1:B:191:VAL:HG23	1:B:195:GLU:HB2	1.99	0.45
1:A:238:LEU:CD1	1:A:328:PHE:CD2	2.99	0.45
1:A:271:TRP:HB3	1:A:273:MET:HE2	1.99	0.45
1:A:276:TRP:CD2	1:A:277:PRO:HA	2.52	0.45
1:A:119:LEU:O	1:A:152:ASN:HB2	2.17	0.45
1:A:179:PHE:N	1:A:179:PHE:CD1	2.82	0.45
1:A:118:PRO:C	1:A:151:ALA:HB1	2.42	0.45
1:A:178:VAL:O	1:A:179:PHE:C	2.56	0.44
1:B:237:ASN:HB3	1:B:328:PHE:CZ	2.52	0.44
1:A:33:ILE:HA	1:A:37:LYS:O	2.17	0.44
1:A:139:GLN:HB3	1:A:140:PRO:HD2	1.99	0.44
1:B:280:PRO:O	1:B:284:ILE:HD12	2.17	0.44
1:A:125:VAL:O	1:A:125:VAL:HG12	2.16	0.44
1:A:243:ILE:HD11	1:A:249:GLN:N	2.32	0.44
1:A:276:TRP:CZ3	1:A:278:VAL:CG2	2.99	0.44
1:B:227:ILE:HG13	1:B:227:ILE:H	1.59	0.44
1:A:178:VAL:C	1:A:181:PRO:HD2	2.42	0.44
1:A:199:TYR:CZ	1:A:210:HIS:CD2	3.06	0.44
1:A:271:TRP:CB	1:A:273:MET:CE	2.95	0.44
1:A:62:LEU:O	1:A:63:GLY:C	2.58	0.44
1:B:259:TYR:CE2	1:B:269:LEU:CD1	2.97	0.44
1:A:336:ILE:HB	1:A:357:LEU:HD11	2.00	0.44
1:B:26:PRO:CB	1:B:48:ILE:HD11	2.45	0.44
1:B:179:PHE:N	1:B:179:PHE:CD1	2.85	0.44
1:A:99:LYS:HB3	1:A:99:LYS:HE3	1.66	0.43
1:A:240:PRO:HB3	1:A:252:ILE:HG21	1.99	0.43
1:A:245:GLU:N	1:A:245:GLU:OE1	2.51	0.43
1:B:175:GLN:O	1:B:180:GLN:HB2	2.18	0.43
1:A:191:VAL:HA	1:A:192:PRO:HD3	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:HG23	1:A:243:ILE:HD13	1.57	0.43
1:A:334:LEU:HD12	1:A:335:GLY:H	1.75	0.43
1:B:253:GLN:H	1:B:253:GLN:HG3	1.62	0.43
1:B:265:MET:CE	1:B:272:GLU:HB3	2.48	0.43
1:A:8:ILE:HD11	1:A:41:PHE:HE1	1.78	0.43
1:B:217:ASP:O	1:B:218:ALA:C	2.59	0.43
1:B:342:LYS:HG2	1:B:343:ASN:N	2.33	0.43
1:B:50:LYS:O	1:B:51:LYS:HB2	2.18	0.43
1:B:109:LEU:HA	1:B:109:LEU:HD23	1.70	0.43
1:A:8:ILE:HA	1:A:11:ILE:HD11	2.00	0.43
1:A:84:LYS:HE3	1:A:84:LYS:HB2	1.41	0.43
1:A:82:GLU:CD	1:A:177:ARG:HH22	2.27	0.43
1:A:192:PRO:HA	1:A:193:PRO:HD3	1.88	0.43
1:B:271:TRP:HB3	1:B:273:MET:CE	2.48	0.43
1:A:287:SER:OG	1:A:347:PRO:HA	2.18	0.43
1:B:84:LYS:HB2	1:B:84:LYS:HE3	1.55	0.43
1:A:99:LYS:NZ	1:A:99:LYS:CB	2.78	0.43
1:B:239:LYS:HA	1:B:240:PRO:HD2	1.86	0.43
1:B:99:LYS:HB3	1:B:99:LYS:HE3	1.14	0.43
1:B:164:LYS:CB	1:B:165:PRO:CD	2.96	0.43
1:B:101:TRP:O	1:B:102:ASN:C	2.61	0.43
1:B:116:GLY:O	1:B:117:LEU:C	2.58	0.43
1:A:56:GLN:HG2	1:A:227:ILE:CD1	2.48	0.42
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.79	0.42
1:A:334:LEU:HD11	1:A:357:LEU:HG	2.02	0.42
1:B:16:ILE:O	1:B:19:LEU:HB3	2.20	0.42
1:A:76:ASP:O	1:A:80:ARG:N	2.47	0.42
1:B:61:GLU:HA	1:B:224:LYS:HG3	2.02	0.42
1:B:139:GLN:CA	1:B:139:GLN:HE21	2.23	0.42
1:B:328:PHE:HA	1:B:335:GLY:HA2	2.01	0.42
1:B:255:ALA:HA	1:B:269:LEU:HB2	2.00	0.42
1:B:259:TYR:C	1:B:301:ILE:HG13	2.44	0.42
1:B:283:ILE:HG13	1:B:350:VAL:CG1	2.50	0.42
1:A:8:ILE:CD1	1:A:41:PHE:CZ	3.02	0.42
1:B:271:TRP:CB	1:B:273:MET:CE	2.97	0.42
1:A:87:ASP:OD2	1:A:92:TYR:OH	2.30	0.42
1:A:101:TRP:O	1:A:102:ASN:C	2.62	0.42
1:B:75:GLY:HA2	1:B:78:ILE:HD12	2.01	0.42
1:B:276:TRP:CG	1:B:277:PRO:HA	2.55	0.42
1:A:97:THR:O	1:A:98:ALA:C	2.63	0.42
1:B:97:THR:O	1:B:98:ALA:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:SER:C	1:B:133:ARG:NH1	2.78	0.42
1:B:161:LEU:N	1:B:161:LEU:CD1	2.82	0.42
1:A:143:ALA:O	1:A:144:PRO:C	2.56	0.42
1:B:122:PRO:HD2	1:B:134:PHE:CE1	2.55	0.42
1:B:265:MET:HE3	1:B:272:GLU:CB	2.50	0.42
1:A:37:LYS:HG3	1:A:38:PRO:N	2.35	0.42
1:A:243:ILE:HG21	1:A:243:ILE:HD12	1.58	0.42
1:B:4:ALA:O	1:B:9:ASN:ND2	2.52	0.42
1:B:345:PRO:O	1:B:348:ALA:HB3	2.20	0.42
1:A:239:LYS:HE3	1:A:239:LYS:HB2	1.50	0.41
1:B:127:SER:HG	1:B:129:SER:HB3	1.85	0.41
1:A:119:LEU:HA	1:A:151:ALA:CB	2.50	0.41
1:A:227:ILE:HD12	1:A:228:GLU:N	2.35	0.41
1:A:279:ASN:O	1:A:282:SER:OG	2.34	0.41
1:A:282:SER:O	1:A:283:ILE:C	2.62	0.41
1:A:344:TYR:O	1:A:345:PRO:C	2.61	0.41
1:B:8:ILE:CA	1:B:11:ILE:CD1	2.96	0.41
1:B:100:GLN:NE2	1:B:136:GLN:O	2.52	0.41
1:B:283:ILE:HD12	1:B:283:ILE:HG21	1.78	0.41
1:B:302:THR:HA	1:B:303:PRO:HA	1.82	0.41
1:B:63:GLY:CA	1:B:319:THR:HG23	2.50	0.41
1:A:129:SER:C	1:A:133:ARG:NH1	2.78	0.41
1:B:139:GLN:HE21	1:B:139:GLN:HA	1.84	0.41
1:A:94:PRO:C	1:A:96:LEU:H	2.28	0.41
1:A:260:TRP:N	1:A:301:ILE:HG13	2.36	0.41
1:B:66:SER:O	1:B:69:PHE:N	2.50	0.41
1:A:175:GLN:HG2	1:A:180:GLN:HE21	1.85	0.41
1:B:10:ASP:HB3	1:B:14:ARG:NH2	2.27	0.41
1:B:314:HIS:HB2	1:B:326:VAL:O	2.21	0.41
1:A:80:ARG:HD2	1:A:177:ARG:NH2	2.36	0.41
1:B:102:ASN:HB3	1:B:103:GLY:H	1.43	0.41
1:A:128:SER:O	1:A:131:LEU:HB3	2.21	0.41
1:A:139:GLN:HE21	1:A:139:GLN:C	2.29	0.41
1:A:246:LYS:NZ	1:B:309:ARG:HD3	2.35	0.41
1:B:178:VAL:O	1:B:179:PHE:C	2.64	0.41
1:A:329:ILE:HA	1:A:330:PRO:HD2	1.64	0.41
1:B:50:LYS:C	1:B:51:LYS:HE2	2.46	0.41
1:B:250:GLN:O	1:B:254:LEU:HG	2.20	0.41
1:B:289:ASN:HA	1:B:289:ASN:HD22	1.47	0.41
1:B:291:ILE:HD13	1:B:291:ILE:HG21	1.75	0.41
1:A:139:GLN:N	1:A:139:GLN:CD	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASP:HB3	1:B:88:PRO:HD2	2.03	0.40
1:B:93:TRP:N	1:B:94:PRO:HD3	2.35	0.40
1:B:250:GLN:O	1:B:251:GLY:C	2.65	0.40
1:A:90:THR:HG22	1:A:96:LEU:HB3	2.04	0.40
1:A:124:GLU:CD	1:A:124:GLU:N	2.80	0.40
1:B:271:TRP:C	1:B:273:MET:CE	2.93	0.40
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.84	0.40
1:A:93:TRP:O	1:A:96:LEU:HB2	2.20	0.40
1:B:5:PRO:HD2	1:B:8:ILE:HG12	2.01	0.40
1:B:73:LEU:O	1:B:76:ASP:HB3	2.22	0.40
1:B:182:LEU:O	1:B:232:ARG:HD2	2.22	0.40
1:B:352:ALA:O	1:B:355:GLN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	355/358 (99%)	328 (92%)	23 (6%)	4 (1%)	11	7
1	B	355/358 (99%)	326 (92%)	26 (7%)	3 (1%)	16	11
All	All	710/716 (99%)	654 (92%)	49 (7%)	7 (1%)	12	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	B	102	ASN
1	A	7	GLN
1	B	64	SER
1	A	175	GLN
1	A	307	ALA

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Mol	Chain	Res	Type
1	B	7	GLN

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	291/292 (100%)	237 (81%)	54 (19%)	1	1
1	B	291/292 (100%)	236 (81%)	55 (19%)	1	1
All	All	582/584 (100%)	473 (81%)	109 (19%)	1	1

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	8	ILE
1	A	11	ILE
1	A	14	ARG
1	A	22	GLN
1	A	24	LYS
1	A	42	THR
1	A	50	LYS
1	A	51	LYS
1	A	64	SER
1	A	84	LYS
1	A	91	LYS
1	A	99	LYS
1	A	100	GLN
1	A	102	ASN
1	A	124	GLU
1	A	132	LEU
1	A	139	GLN
1	A	161	LEU
1	A	164	LYS
1	A	172	GLN
1	A	177	ARG

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Mol	Chain	Res	Type
1	A	189	ILE
1	A	190	ASN
1	A	191	VAL
1	A	197	LYS
1	A	204	ARG
1	A	205	GLU
1	A	207	LYS
1	A	227	ILE
1	A	232	ARG
1	A	235	GLN
1	A	238	LEU
1	A	239	LYS
1	A	243	ILE
1	A	244	ASN
1	A	245	GLU
1	A	246	LYS
1	A	249	GLN
1	A	250	GLN
1	A	254	LEU
1	A	269	LEU
1	A	273	MET
1	A	278	VAL
1	A	283	ILE
1	A	290	LYS
1	A	293	LEU
1	A	299	LYS
1	A	301	ILE
1	A	308	VAL
1	A	309	ARG
1	A	315	LYS
1	A	334	LEU
1	A	342	LYS
1	B	7	GLN
1	B	8	ILE
1	B	11	ILE
1	B	14	ARG
1	B	19	LEU
1	B	20	ILE
1	B	22	GLN
1	B	33	ILE
1	B	37	LYS
1	B	42	THR

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Mol	Chain	Res	Type
1	B	50	LYS
1	B	51	LYS
1	B	57	GLN
1	B	64	SER
1	B	84	LYS
1	B	91	LYS
1	B	95	GLU
1	B	99	LYS
1	B	102	ASN
1	B	123	ASP
1	B	132	LEU
1	B	139	GLN
1	B	175	GLN
1	B	177	ARG
1	B	183	LYS
1	B	189	ILE
1	B	190	ASN
1	B	191	VAL
1	B	197	LYS
1	B	205	GLU
1	B	207	LYS
1	B	224	LYS
1	B	227	ILE
1	B	235	GLN
1	B	238	LEU
1	B	239	LYS
1	B	244	ASN
1	B	245	GLU
1	B	246	LYS
1	B	250	GLN
1	B	262	THR
1	B	265	MET
1	B	269	LEU
1	B	273	MET
1	B	283	ILE
1	B	299	LYS
1	B	301	ILE
1	B	308	VAL
1	B	309	ARG
1	B	315	LYS
1	B	331	GLU
1	B	334	LEU

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Mol	Chain	Res	Type
1	B	336	ILE
1	B	342	LYS
1	B	357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	102	ASN
1	A	108	HIS
1	A	139	GLN
1	A	235	GLN
1	A	244	ASN
1	A	249	GLN
1	A	253	GLN
1	A	285	ASN
1	A	358	ASN
1	B	9	ASN
1	B	23	GLN
1	B	56	GLN
1	B	102	ASN
1	B	108	HIS
1	B	137	ASN
1	B	139	GLN
1	B	147	GLN
1	B	175	GLN
1	B	235	GLN
1	B	249	GLN
1	B	250	GLN
1	B	285	ASN
1	B	289	ASN
1	B	355	GLN

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 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 ⓘ

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, 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	357/358 (99%)	0.10	10 (2%) 55 54	19, 34, 63, 97	1 (0%)
1	B	357/358 (99%)	0.10	13 (3%) 46 45	21, 34, 63, 97	1 (0%)
All	All	714/716 (99%)	0.10	23 (3%) 50 49	19, 34, 63, 97	2 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ALA	3.8
1	B	6	GLN	3.2
1	A	6	GLN	3.1
1	B	7	GLN	3.1
1	A	5	PRO	3.0
1	A	360	LEU	3.0
1	B	360	LEU	2.8
1	B	56	GLN	2.7
1	A	7	GLN	2.6
1	A	292	ALA	2.6
1	B	5	PRO	2.6
1	A	11	ILE	2.5
1	B	102	ASN	2.4
1	B	99	LYS	2.4
1	B	212	SER	2.4
1	B	97	THR	2.3
1	B	241	LEU	2.3
1	A	99	LYS	2.2
1	B	4	ALA	2.2
1	A	232	ARG	2.2
1	A	245	GLU	2.1
1	B	123	ASP	2.1
1	B	8	ILE	2.1

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.