



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:10 PM UTC

PDB ID : 2ZC7 / pdb_00002zc7
Title : Crystal Structure of Class C beta-Lactamase ACT-1
Authors : Shimizu-Ibuka, A.; Sakai, H.; Galleni, M.
Deposited on : 2007-11-02
Resolution : 2.40 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

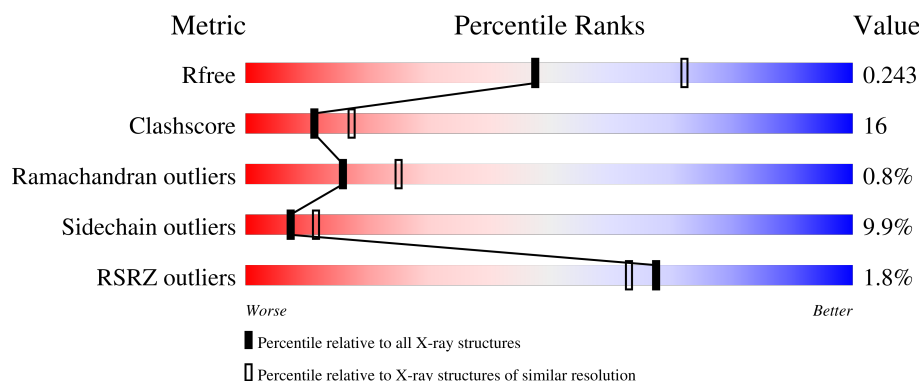
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

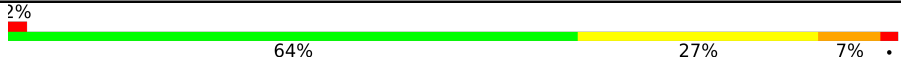
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	359	 2% 64% 27% 7%
1	B	359	 3% 64% 29% 7%
1	C	359	 2% 66% 26% 6%
1	D	359	 % 60% 33% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11444 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 Beta-lactamase ACT-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	8	0	0
			2772	1782	471	507	12			
1	B	359	Total	C	N	O	S	14	0	0
			2772	1782	471	507	12			
1	C	359	Total	C	N	O	S	19	0	0
			2772	1782	471	507	12			
1	D	359	Total	C	N	O	S	25	0	0
			2772	1782	471	507	12			

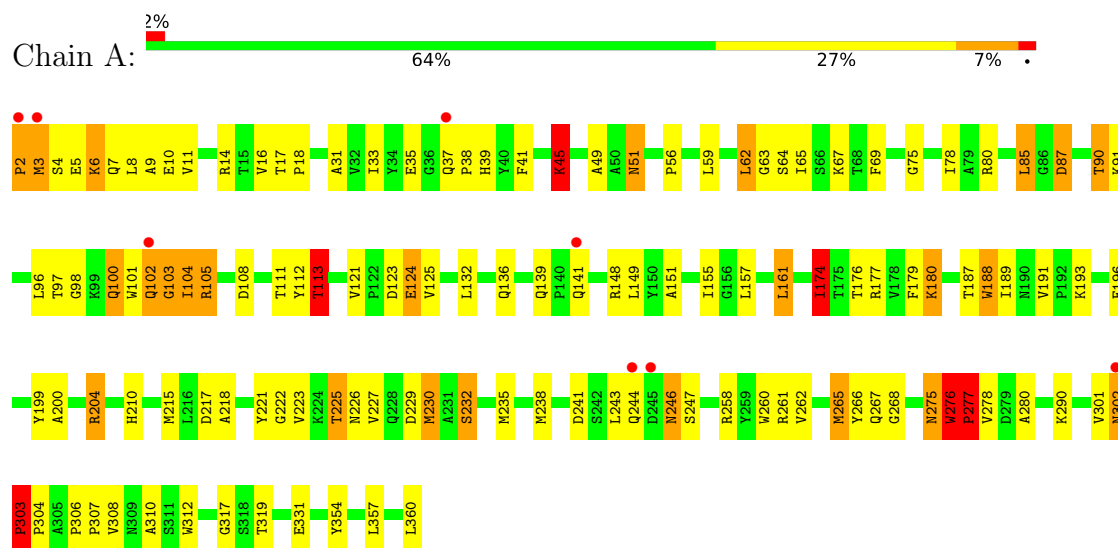
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	105	Total	O	0	0
			105	105		
2	B	97	Total	O	0	0
			97	97		
2	C	83	Total	O	0	0
			83	83		
2	D	71	Total	O	0	0
			71	71		

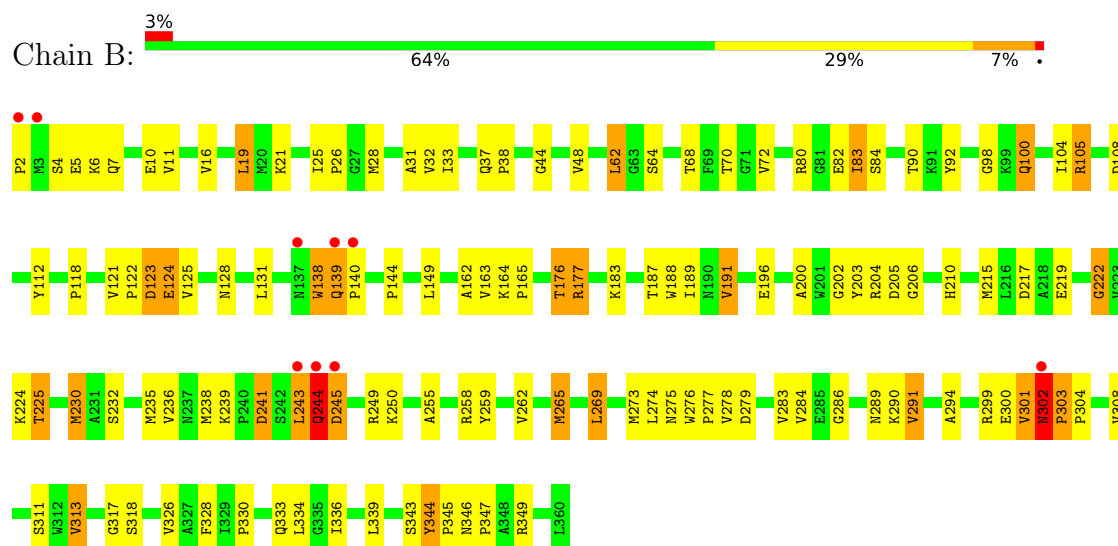
3 Residue-property plots

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: Beta-lactamase ACT-1

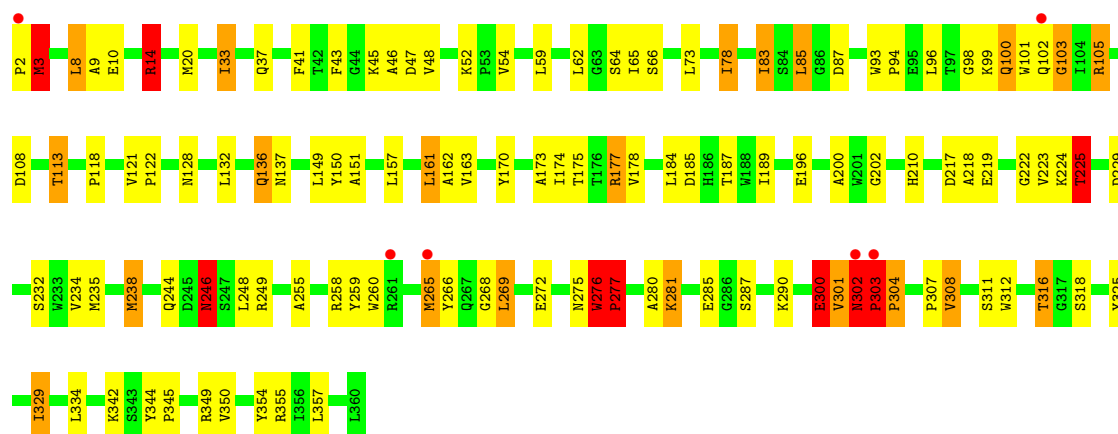


• Molecule 1: Beta-lactamase ACT-1

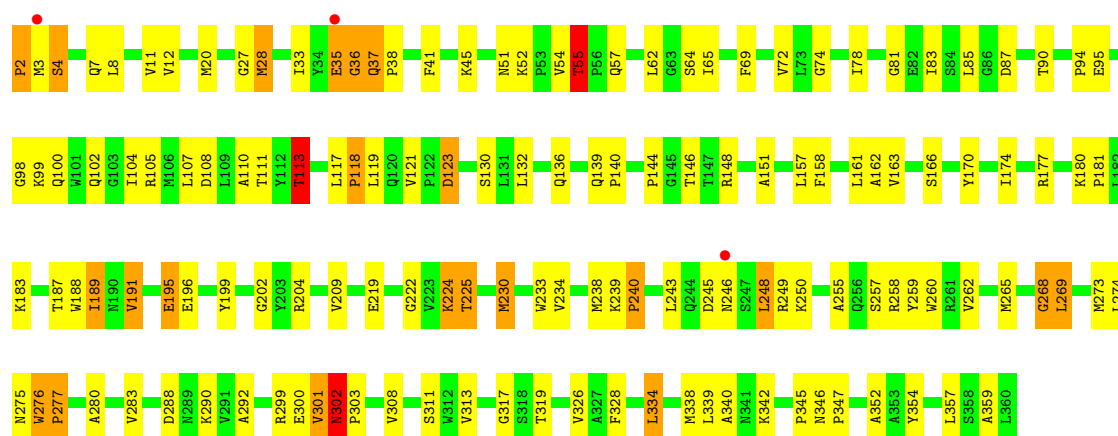


• Molecule 1: Beta-lactamase ACT-1





● Molecule 1: Beta-lactamase ACT-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.05Å 80.52Å 86.88Å 76.23° 68.88° 63.46°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.40) 98.3 (20.00-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.247 0.236 , 0.243	Depositor DCC
R_{free} test set	8681 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11444	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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	1.14	13/2849 (0.5%)	1.48	35/3883 (0.9%)
1	B	1.04	4/2849 (0.1%)	1.59	38/3883 (1.0%)
1	C	1.14	12/2849 (0.4%)	1.44	49/3883 (1.3%)
1	D	1.07	6/2849 (0.2%)	1.46	44/3883 (1.1%)
All	All	1.10	35/11396 (0.3%)	1.49	166/15532 (1.1%)

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	2
1	B	0	1
1	C	0	2
All	All	0	5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	PRO	CA-C	-9.32	1.43	1.52
1	A	302	ASN	N-CA	8.75	1.60	1.46
1	C	301	VAL	CA-C	-8.41	1.43	1.53
1	C	277	PRO	CA-CB	7.57	1.67	1.53
1	C	121	VAL	CA-C	7.24	1.60	1.53
1	D	276	TRP	C-N	7.19	1.48	1.34
1	C	302	ASN	N-CA	-6.95	1.36	1.46
1	C	277	PRO	N-CD	-6.75	1.38	1.47
1	B	302	ASN	C-N	6.51	1.41	1.33
1	C	276	TRP	C-N	6.37	1.46	1.34
1	D	301	VAL	CA-CB	5.99	1.60	1.53
1	A	246	ASN	N-CA	-5.99	1.38	1.46
1	C	303	PRO	CA-C	5.99	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	ASN	C-O	-5.98	1.16	1.23
1	A	304	PRO	CA-C	5.91	1.59	1.52
1	C	54	VAL	CA-C	5.63	1.58	1.52
1	A	301	VAL	CA-C	5.55	1.59	1.52
1	C	128	ASN	CA-C	5.50	1.59	1.52
1	D	117	LEU	CA-C	5.47	1.58	1.53
1	C	54	VAL	CA-CB	5.42	1.60	1.54
1	B	191	VAL	CA-CB	5.41	1.61	1.54
1	D	196	GLU	CA-C	-5.39	1.45	1.52
1	A	121	VAL	CA-C	5.34	1.58	1.53
1	B	284	VAL	CA-CB	5.30	1.60	1.54
1	A	306	PRO	CA-C	5.29	1.57	1.52
1	C	276	TRP	CA-C	5.26	1.60	1.52
1	D	245	ASP	CA-C	5.25	1.59	1.52
1	A	104	ILE	CA-CB	5.21	1.59	1.53
1	A	111	THR	CA-CB	5.09	1.60	1.53
1	A	49	ALA	CA-CB	5.08	1.61	1.53
1	C	102	GLN	CA-C	-5.08	1.46	1.53
1	D	55	THR	CA-C	5.03	1.57	1.52
1	B	11	VAL	CA-CB	5.02	1.60	1.54
1	A	174	ILE	CA-CB	5.02	1.60	1.54
1	A	277	PRO	C-O	-5.02	1.13	1.23

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	ASN	CA-C-N	-26.18	93.42	120.38
1	B	302	ASN	C-N-CA	-26.18	93.42	120.38
1	A	303	PRO	CA-N-CD	-18.99	85.41	112.00
1	D	302	ASN	CA-C-N	-15.11	108.78	119.66
1	D	302	ASN	C-N-CA	-15.11	108.78	119.66
1	B	303	PRO	N-CA-C	-13.87	93.77	110.70
1	A	103	GLY	N-CA-C	-12.58	100.11	115.08
1	A	101	TRP	CA-C-N	-12.02	101.87	122.67
1	A	101	TRP	C-N-CA	-12.02	101.87	122.67
1	D	303	PRO	N-CA-C	-10.66	99.18	110.58
1	B	245	ASP	N-CA-C	-10.07	89.36	110.80
1	B	244	GLN	CA-C-N	9.68	140.02	121.54
1	B	244	GLN	C-N-CA	9.68	140.02	121.54
1	A	303	PRO	N-CA-C	-8.26	100.62	110.70
1	D	189	ILE	N-CA-C	-7.96	103.14	111.58
1	D	276	TRP	CA-C-O	-7.87	111.00	120.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	189	ILE	N-CA-C	-7.74	103.37	111.58
1	D	121	VAL	N-CA-C	-7.68	102.02	108.63
1	D	276	TRP	CB-CA-C	-7.61	98.34	108.76
1	B	189	ILE	N-CA-C	-7.49	103.64	111.58
1	C	3	MET	N-CA-C	7.49	126.75	110.80
1	A	204	ARG	CA-C-N	-7.40	112.99	123.20
1	A	204	ARG	C-N-CA	-7.40	112.99	123.20
1	A	244	GLN	N-CA-C	7.37	121.98	112.41
1	A	303	PRO	N-CA-CB	7.31	110.17	103.08
1	C	357	LEU	N-CA-C	7.30	120.29	111.82
1	B	206	GLY	N-CA-C	-7.18	105.93	115.40
1	D	204	ARG	CA-C-N	-7.17	109.85	122.62
1	D	204	ARG	C-N-CA	-7.17	109.85	122.62
1	C	302	ASN	CA-CB-CG	-7.14	105.46	112.60
1	A	189	ILE	N-CA-C	-7.14	104.02	111.58
1	D	239	LYS	CA-C-N	7.04	126.67	119.56
1	D	239	LYS	C-N-CA	7.04	126.67	119.56
1	A	276	TRP	C-N-CD	-6.91	105.40	120.60
1	C	65	ILE	N-CA-C	-6.88	104.05	113.00
1	D	4	SER	N-CA-C	6.87	120.19	110.50
1	B	38	PRO	N-CA-C	6.86	121.74	110.55
1	A	87	ASP	N-CA-C	6.81	119.31	109.84
1	D	319	THR	N-CA-C	-6.80	99.27	108.86
1	C	303	PRO	N-CA-C	-6.77	102.44	110.70
1	D	346	ASN	CA-C-N	6.76	127.03	119.32
1	D	346	ASN	C-N-CA	6.76	127.03	119.32
1	A	139	GLN	CA-C-N	6.76	126.72	119.76
1	A	139	GLN	C-N-CA	6.76	126.72	119.76
1	A	312	TRP	N-CA-C	-6.74	96.67	108.20
1	C	276	TRP	C-N-CD	-6.69	105.88	120.60
1	B	202	GLY	N-CA-C	-6.65	102.45	113.02
1	B	303	PRO	CA-N-CD	-6.62	102.73	112.00
1	D	292	ALA	N-CA-C	6.57	119.27	111.71
1	C	196	GLU	N-CA-C	6.55	118.97	111.11
1	C	303	PRO	CB-CA-C	6.53	118.89	110.92
1	D	118	PRO	N-CA-C	6.53	121.20	111.41
1	D	188	TRP	N-CA-C	6.50	119.77	109.50
1	D	202	GLY	N-CA-C	-6.48	102.72	113.02
1	B	70	THR	N-CA-C	-6.46	104.23	111.28
1	D	209	VAL	N-CA-C	6.46	117.66	108.42
1	C	103	GLY	N-CA-C	-6.45	97.89	113.18
1	A	301	VAL	CA-C-N	6.43	129.28	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	VAL	C-N-CA	6.43	129.28	120.67
1	D	113	THR	N-CA-C	6.40	121.13	112.88
1	D	37	GLN	CA-C-N	6.39	127.35	120.13
1	D	37	GLN	C-N-CA	6.39	127.35	120.13
1	B	7	GLN	N-CA-C	-6.37	104.42	111.36
1	C	14	ARG	CG-CD-NE	6.29	125.84	112.00
1	A	45	LYS	N-CA-C	6.28	119.70	109.59
1	B	245	ASP	N-CA-CB	6.28	121.11	110.49
1	D	196	GLU	N-CA-C	6.27	118.11	111.28
1	B	241	ASP	N-CA-C	6.22	119.96	112.38
1	C	128	ASN	CB-CA-C	6.21	120.52	110.96
1	A	357	LEU	N-CA-C	6.17	118.00	111.28
1	B	222	GLY	N-CA-C	6.14	125.47	115.46
1	B	239	LYS	CA-C-N	6.08	125.77	119.56
1	B	239	LYS	C-N-CA	6.08	125.77	119.56
1	C	2	PRO	CA-C-N	6.08	133.15	121.54
1	C	2	PRO	C-N-CA	6.08	133.15	121.54
1	D	345	PRO	N-CA-C	6.08	120.75	111.15
1	C	277	PRO	CA-N-CD	6.07	119.99	111.50
1	D	54	VAL	N-CA-C	-6.06	100.97	109.21
1	C	277	PRO	N-CA-CB	-6.05	95.94	102.60
1	C	246	ASN	N-CA-C	6.04	116.26	108.34
1	B	345	PRO	N-CA-C	6.04	120.69	111.15
1	C	121	VAL	N-CA-C	-6.03	103.04	108.95
1	D	250	LYS	N-CA-C	-6.01	104.81	111.36
1	D	38	PRO	N-CA-C	6.00	120.32	110.55
1	A	151	ALA	N-CA-C	5.99	118.15	108.32
1	C	316	THR	N-CA-C	-5.99	100.53	110.17
1	A	276	TRP	CA-C-O	5.98	125.21	120.19
1	B	118	PRO	N-CA-C	5.98	120.37	111.41
1	A	113	THR	N-CA-CB	-5.95	101.50	110.73
1	D	268	GLY	N-CA-C	-5.90	102.16	112.55
1	C	276	TRP	CB-CA-C	-5.83	100.77	108.76
1	B	291	VAL	N-CA-CB	-5.83	103.92	111.90
1	B	344	TYR	CA-C-N	-5.82	113.97	119.90
1	B	344	TYR	C-N-CA	-5.82	113.97	119.90
1	B	286	GLY	N-CA-C	-5.82	108.27	114.67
1	A	111	THR	N-CA-C	5.81	119.96	112.41
1	C	301	VAL	CB-CA-C	5.80	117.49	111.23
1	C	312	TRP	N-CA-C	-5.79	98.30	108.20
1	D	277	PRO	CA-C-N	-5.78	113.91	122.23
1	D	277	PRO	C-N-CA	-5.78	113.91	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	VAL	CA-C-N	-5.76	107.73	121.80
1	C	301	VAL	C-N-CA	-5.76	107.73	121.80
1	C	300	GLU	CA-C-N	-5.74	113.86	122.01
1	C	300	GLU	C-N-CA	-5.74	113.86	122.01
1	A	176	THR	N-CA-C	5.71	117.58	111.36
1	A	193	LYS	N-CA-C	-5.70	105.14	111.36
1	C	268	GLY	N-CA-C	-5.70	104.46	112.60
1	C	137	ASN	N-CA-C	5.68	120.36	113.38
1	D	240	PRO	N-CA-C	5.68	120.95	113.86
1	D	195	GLU	N-CA-C	5.64	120.28	113.17
1	A	277	PRO	CA-C-N	-5.64	114.58	122.71
1	A	277	PRO	C-N-CA	-5.64	114.58	122.71
1	C	99	LYS	N-CA-C	5.58	119.70	113.01
1	C	225	THR	CB-CA-C	-5.58	100.43	111.91
1	A	319	THR	N-CA-C	-5.57	101.27	109.18
1	B	219	GLU	N-CA-C	5.57	117.35	111.28
1	C	78	ILE	CB-CA-C	-5.51	104.92	111.97
1	A	222	GLY	N-CA-C	5.50	125.19	115.61
1	B	188	TRP	N-CA-C	5.50	117.62	108.99
1	B	138	TRP	N-CA-C	-5.49	103.29	110.53
1	B	265	MET	N-CA-C	5.48	118.67	109.95
1	C	175	THR	CA-C-N	5.48	128.07	120.29
1	C	175	THR	C-N-CA	5.48	128.07	120.29
1	D	219	GLU	N-CA-C	5.46	117.24	111.28
1	A	307	PRO	N-CA-C	5.45	119.42	111.03
1	D	87	ASP	CA-C-N	-5.43	114.99	120.31
1	D	87	ASP	C-N-CA	-5.43	114.99	120.31
1	B	196	GLU	N-CA-C	5.41	118.98	112.38
1	C	48	VAL	N-CA-C	5.41	115.61	110.42
1	D	98	GLY	CA-C-N	5.39	127.94	120.29
1	D	98	GLY	C-N-CA	5.39	127.94	120.29
1	C	238	MET	N-CA-C	-5.37	105.43	111.28
1	A	268	GLY	N-CA-C	-5.34	104.97	112.60
1	D	99	LYS	N-CA-C	5.34	117.18	111.36
1	C	307	PRO	CA-C-N	-5.33	116.58	123.19
1	C	307	PRO	C-N-CA	-5.33	116.58	123.19
1	B	128	ASN	N-CA-C	5.32	116.77	111.07
1	C	277	PRO	O-C-N	5.25	131.07	121.10
1	A	124	GLU	N-CA-C	-5.24	105.75	111.82
1	B	32	VAL	N-CA-C	-5.23	100.85	108.17
1	B	16	VAL	N-CA-C	5.23	116.00	110.72
1	A	16	VAL	N-CA-C	5.22	115.43	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	LEU	N-CA-C	5.21	117.40	109.63
1	C	277	PRO	N-CA-C	-5.20	98.59	112.10
1	B	294	ALA	N-CA-C	5.19	116.37	109.93
1	B	2	PRO	CA-N-CD	-5.16	104.77	112.00
1	C	45	LYS	N-CA-C	5.16	117.90	109.59
1	B	44	GLY	N-CA-C	5.15	121.18	111.80
1	D	35	GLU	N-CA-C	-5.15	99.83	110.80
1	D	74	GLY	N-CA-C	-5.15	106.26	112.49
1	C	345	PRO	N-CA-C	5.14	119.28	111.15
1	C	185	ASP	N-CA-C	5.14	119.42	113.20
1	C	46	ALA	N-CA-C	-5.13	106.17	112.90
1	C	87	ASP	N-CA-C	5.13	116.16	109.64
1	C	202	GLY	N-CA-C	-5.13	104.86	113.02
1	D	117	LEU	CA-C-N	-5.12	114.97	120.03
1	D	117	LEU	C-N-CA	-5.12	114.97	120.03
1	B	300	GLU	CA-C-N	-5.11	115.99	122.43
1	B	300	GLU	C-N-CA	-5.11	115.99	122.43
1	C	184	LEU	N-CA-C	-5.11	101.27	109.39
1	C	151	ALA	N-CA-C	5.08	116.65	108.32
1	C	303	PRO	CA-N-CD	-5.04	104.94	112.00
1	A	188	TRP	N-CA-C	5.04	116.85	109.24
1	B	48	VAL	N-CA-C	5.04	115.26	110.53
1	D	111	THR	N-CA-C	5.03	118.96	111.87
1	C	329	ILE	N-CA-C	-5.03	103.17	108.15

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	TRP	Mainchain
1	A	277	PRO	Mainchain
1	B	302	ASN	Mainchain
1	C	276	TRP	Mainchain
1	C	277	PRO	Mainchain

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	2772	0	2765	83	2
1	B	2772	0	2765	82	1
1	C	2772	0	2765	94	1
1	D	2772	0	2765	98	0
2	A	105	0	0	0	0
2	B	97	0	0	1	0
2	C	83	0	0	1	0
2	D	71	0	0	0	0
All	All	11444	0	11060	355	2

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 16.

All (355) 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:D:273:MET:HG3	1:D:313:VAL:HG22	1.26	1.15
1:C:302:ASN:HB3	1:C:303:PRO:HD2	1.25	1.13
1:B:138:TRP:CD2	1:B:140:PRO:HD3	1.92	1.04
1:C:108:ASP:HA	1:C:113:THR:HG22	1.42	1.01
1:A:108:ASP:HA	1:A:113:THR:HG22	1.45	0.98
1:B:138:TRP:CE2	1:B:140:PRO:HD3	1.97	0.98
1:D:28:MET:HA	1:D:339:LEU:O	1.63	0.98
1:C:302:ASN:HB3	1:C:303:PRO:CD	2.01	0.90
1:D:108:ASP:HA	1:D:113:THR:HG22	1.52	0.90
1:B:258:ARG:HH12	1:B:275:ASN:HD21	1.16	0.89
1:D:55:THR:HG22	1:D:57:GLN:H	1.37	0.89
1:C:301:VAL:O	1:C:302:ASN:O	1.91	0.88
1:D:273:MET:CG	1:D:313:VAL:HG22	2.04	0.87
1:D:258:ARG:HH12	1:D:275:ASN:HD21	1.20	0.87
1:C:302:ASN:O	1:C:304:PRO:N	2.07	0.86
1:B:138:TRP:CD1	1:B:139:GLN:H	1.94	0.85
1:D:28:MET:CA	1:D:339:LEU:O	2.25	0.84
1:B:98:GLY:HA3	1:B:100:GLN:HE22	1.43	0.84
1:B:262:VAL:HB	1:B:265:MET:HE3	1.59	0.84
1:D:45:LYS:HE2	1:D:51:ASN:ND2	1.95	0.80
1:C:10:GLU:O	1:C:14:ARG:HG3	1.83	0.80
1:C:232:SER:HA	1:C:235:MET:HE3	1.64	0.80
1:A:258:ARG:HH12	1:A:275:ASN:HD21	1.27	0.79
1:A:124:GLU:N	1:A:124:GLU:OE1	2.15	0.78
1:B:122:PRO:C	1:B:124:GLU:H	1.92	0.78
1:A:102:GLN:HG2	1:A:103:GLY:H	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:PRO:O	1:D:151:ALA:HB1	1.85	0.75
1:D:113:THR:HG21	1:D:260:TRP:CZ2	2.21	0.75
1:A:4:SER:HB3	1:A:7:GLN:HG3	1.69	0.75
1:A:276:TRP:CE3	1:A:278:VAL:HG12	2.22	0.75
1:C:280:ALA:HB2	1:C:354:TYR:CE2	2.20	0.75
1:C:281:LYS:O	1:C:285:GLU:HG3	1.88	0.74
1:D:28:MET:CE	1:D:338:MET:HB3	2.16	0.74
1:D:222:GLY:O	1:D:224:LYS:HE3	1.88	0.74
1:B:187:THR:OG1	1:B:225:THR:CG2	2.36	0.73
1:C:302:ASN:CB	1:C:303:PRO:HD2	2.12	0.73
1:A:187:THR:OG1	1:A:225:THR:HG23	1.88	0.73
1:C:246:ASN:HD22	1:C:246:ASN:C	1.97	0.73
1:A:4:SER:H	1:A:7:GLN:HE21	1.36	0.73
1:B:125:VAL:HG12	1:B:215:MET:HG3	1.69	0.73
1:A:191:VAL:HG11	1:A:199:TYR:CD2	2.23	0.73
1:A:113:THR:HG21	1:A:260:TRP:CZ2	2.23	0.72
1:C:255:ALA:HA	1:C:269:LEU:HB2	1.69	0.72
1:A:276:TRP:CZ3	1:A:278:VAL:HG12	2.26	0.71
1:B:262:VAL:HB	1:B:265:MET:CE	2.20	0.71
1:D:276:TRP:CD2	1:D:277:PRO:HA	2.26	0.70
1:B:274:LEU:HD22	1:B:283:VAL:HG12	1.72	0.70
1:A:276:TRP:CD2	1:A:277:PRO:HA	2.27	0.69
1:B:230:MET:CE	1:B:326:VAL:HG11	2.22	0.69
1:D:35:GLU:O	1:D:37:GLN:N	2.25	0.69
1:B:230:MET:HE3	1:B:326:VAL:HG11	1.73	0.69
1:C:258:ARG:HH12	1:C:275:ASN:HD21	1.41	0.69
1:A:69:PHE:HB3	1:A:174:ILE:HD11	1.73	0.68
1:B:105:ARG:HD3	1:B:108:ASP:OD2	1.92	0.68
1:B:98:GLY:HA3	1:B:100:GLN:NE2	2.07	0.68
1:B:187:THR:OG1	1:B:225:THR:HG22	1.93	0.67
1:B:100:GLN:H	1:B:100:GLN:HE21	1.41	0.67
1:A:105:ARG:HD3	1:A:108:ASP:OD2	1.94	0.67
1:B:131:LEU:HD22	1:B:215:MET:HE2	1.77	0.67
1:C:10:GLU:O	1:C:14:ARG:CG	2.42	0.67
1:B:163:VAL:HG12	1:B:163:VAL:O	1.92	0.67
1:C:234:VAL:HG12	1:C:238:MET:CE	2.24	0.67
1:D:2:PRO:HB3	1:D:7:GLN:HB3	1.77	0.66
1:B:138:TRP:CD1	1:B:139:GLN:N	2.62	0.66
1:D:28:MET:CB	1:D:339:LEU:O	2.44	0.65
1:C:3:MET:HE2	1:C:8:LEU:HD13	1.78	0.65
1:A:45:LYS:HE2	1:A:51:ASN:HD21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:TYR:CZ	1:C:349:ARG:HG2	2.32	0.64
1:C:47:ASP:OD2	1:C:52:LYS:HE3	1.97	0.64
1:C:265:MET:HE3	1:C:272:GLU:HB3	1.78	0.63
1:D:123:ASP:OD1	1:D:123:ASP:N	2.24	0.63
1:D:301:VAL:O	1:D:302:ASN:O	2.16	0.63
1:C:259:TYR:CE1	1:C:269:LEU:HD13	2.32	0.63
1:C:285:GLU:OE1	1:D:299:ARG:HD3	1.99	0.63
1:B:232:SER:HA	1:B:235:MET:HE3	1.81	0.62
1:C:187:THR:OG1	1:C:225:THR:HG23	1.98	0.62
1:C:265:MET:HE1	1:C:272:GLU:CG	2.29	0.62
1:C:316:THR:HG22	1:C:325:TYR:CD1	2.33	0.62
1:B:138:TRP:CG	1:B:139:GLN:N	2.68	0.62
1:A:157:LEU:HG	1:A:161:LEU:HD22	1.80	0.62
1:C:265:MET:HE1	1:C:272:GLU:CD	2.25	0.62
1:D:258:ARG:HH12	1:D:275:ASN:ND2	1.95	0.62
1:D:240:PRO:O	1:D:249:ARG:HG3	2.01	0.61
1:C:302:ASN:O	1:C:303:PRO:C	2.44	0.60
1:B:238:MET:HG2	1:B:333:GLN:NE2	2.17	0.60
1:C:93:TRP:CZ2	1:C:132:LEU:HD13	2.35	0.60
1:D:55:THR:HG21	1:D:57:GLN:NE2	2.17	0.60
1:D:95:GLU:OE1	1:D:95:GLU:N	2.29	0.60
1:C:20:MET:HE1	1:C:43:PHE:HB3	1.84	0.60
1:D:274:LEU:HD22	1:D:283:VAL:HG12	1.83	0.60
1:C:246:ASN:ND2	1:C:249:ARG:H	1.99	0.60
1:B:255:ALA:HA	1:B:269:LEU:HB2	1.84	0.59
1:C:98:GLY:HA3	1:C:100:GLN:HE22	1.67	0.59
1:C:105:ARG:HD3	1:C:108:ASP:OD2	2.02	0.59
1:A:225:THR:HG22	1:A:229:ASP:HB2	1.83	0.59
1:B:258:ARG:HH12	1:B:275:ASN:ND2	1.94	0.59
1:D:105:ARG:NH2	1:D:300:GLU:OE2	2.35	0.58
1:C:265:MET:CE	1:C:272:GLU:HG2	2.33	0.58
1:A:262:VAL:HB	1:A:265:MET:HE2	1.85	0.58
1:C:234:VAL:HG12	1:C:238:MET:HE2	1.86	0.58
1:D:55:THR:CG2	1:D:57:GLN:HE21	2.16	0.58
1:A:191:VAL:HG11	1:A:199:TYR:CE2	2.39	0.58
1:C:78:ILE:HD11	1:C:85:LEU:HD13	1.85	0.58
1:C:47:ASP:HB3	1:C:52:LYS:HB2	1.85	0.58
1:D:28:MET:HE1	1:D:338:MET:HB3	1.85	0.58
1:C:259:TYR:O	1:C:301:VAL:N	2.30	0.57
1:B:238:MET:HG2	1:B:333:GLN:HE22	1.69	0.57
1:D:45:LYS:HE2	1:D:51:ASN:HD21	1.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:H	1:A:136:GLN:HE22	1.51	0.56
1:D:20:MET:HE3	1:D:27:GLY:HA2	1.85	0.56
1:A:225:THR:CG2	1:A:229:ASP:HB2	2.35	0.56
1:D:28:MET:HE2	1:D:338:MET:HB3	1.87	0.56
1:D:187:THR:OG1	1:D:225:THR:CG2	2.53	0.56
1:D:255:ALA:HA	1:D:269:LEU:HB2	1.88	0.56
1:D:2:PRO:HB3	1:D:7:GLN:CB	2.36	0.56
1:D:55:THR:CG2	1:D:57:GLN:NE2	2.69	0.56
1:A:4:SER:HB3	1:A:7:GLN:HE21	1.71	0.55
1:C:93:TRP:CZ2	1:C:132:LEU:CD1	2.89	0.55
1:B:112:TYR:HB3	1:B:149:LEU:O	2.07	0.55
1:C:290:LYS:HB3	1:D:146:THR:HG22	1.87	0.55
1:A:265:MET:HE1	1:A:267:GLN:HB2	1.87	0.55
1:B:33:ILE:HG21	1:B:238:MET:HE1	1.89	0.55
1:B:200:ALA:O	1:B:210:HIS:HE1	1.89	0.55
1:C:108:ASP:CA	1:C:113:THR:HG22	2.25	0.55
1:C:37:GLN:HA	1:C:37:GLN:OE1	2.07	0.55
1:C:93:TRP:CE2	1:C:132:LEU:HD13	2.41	0.55
1:D:94:PRO:HG2	1:D:95:GLU:OE1	2.07	0.55
1:D:243:LEU:HD11	1:D:248:LEU:HD12	1.88	0.55
1:C:265:MET:HG3	1:C:266:TYR:N	2.22	0.55
1:D:20:MET:CE	1:D:27:GLY:HA2	2.37	0.55
1:D:187:THR:OG1	1:D:225:THR:HG23	2.07	0.55
1:A:187:THR:OG1	1:A:225:THR:CG2	2.53	0.55
1:B:259:TYR:CE1	1:B:269:LEU:HD13	2.41	0.55
1:D:246:ASN:OD1	1:D:246:ASN:C	2.50	0.55
1:C:265:MET:HE1	1:C:272:GLU:HG2	1.87	0.55
1:B:274:LEU:HD22	1:B:283:VAL:CG1	2.36	0.54
1:B:313:VAL:CG1	1:B:328:PHE:CE1	2.90	0.54
1:D:2:PRO:HG2	1:D:11:VAL:HG21	1.88	0.54
1:A:112:TYR:HB3	1:A:149:LEU:O	2.07	0.54
1:B:28:MET:HA	1:B:339:LEU:O	2.08	0.54
1:A:302:ASN:O	1:A:303:PRO:O	2.25	0.54
1:B:138:TRP:CE3	1:B:140:PRO:HD3	2.41	0.54
1:B:163:VAL:O	1:B:163:VAL:CG1	2.55	0.54
1:D:27:GLY:O	1:D:340:ALA:HA	2.08	0.54
1:A:261:ARG:HD2	1:A:266:TYR:CE1	2.42	0.54
1:B:244:GLN:HA	1:B:244:GLN:NE2	2.18	0.53
1:B:344:TYR:CZ	1:B:349:ARG:HG2	2.43	0.53
1:B:122:PRO:O	1:B:124:GLU:N	2.39	0.53
1:A:200:ALA:O	1:A:210:HIS:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:MET:HE1	1:D:338:MET:HE2	1.90	0.53
1:D:108:ASP:OD1	1:D:113:THR:HG23	2.09	0.53
1:C:265:MET:CE	1:C:272:GLU:CG	2.87	0.53
1:D:69:PHE:HB3	1:D:174:ILE:HD11	1.91	0.53
1:D:191:VAL:HG11	1:D:199:TYR:CD2	2.43	0.53
1:A:2:PRO:HD2	1:A:360:LEU:HD23	1.91	0.53
1:C:98:GLY:HA3	1:C:100:GLN:NE2	2.24	0.52
1:B:122:PRO:C	1:B:124:GLU:N	2.61	0.52
1:C:260:TRP:CZ3	1:C:300:GLU:HB2	2.43	0.52
1:B:313:VAL:HG13	1:B:328:PHE:CE1	2.45	0.52
1:C:258:ARG:CZ	1:C:308:VAL:HG13	2.40	0.52
1:D:64:SER:HB2	1:D:317:GLY:HA2	1.92	0.52
1:A:310:ALA:HB2	1:A:331:GLU:OE1	2.10	0.52
1:C:83:ILE:HD11	1:C:162:ALA:O	2.11	0.51
1:A:108:ASP:CA	1:A:113:THR:HG22	2.31	0.51
1:A:302:ASN:O	1:A:303:PRO:HB2	2.10	0.51
1:C:265:MET:CE	1:C:272:GLU:HB3	2.41	0.51
1:A:302:ASN:C	1:A:303:PRO:O	2.53	0.51
1:B:104:ILE:HG12	1:B:144:PRO:HB3	1.93	0.51
1:C:83:ILE:CD1	1:C:162:ALA:O	2.58	0.51
1:D:262:VAL:HB	1:D:265:MET:HE3	1.92	0.51
1:D:338:MET:HE1	1:D:352:ALA:HB3	1.91	0.51
1:D:180:LYS:HB2	1:D:181:PRO:HD3	1.92	0.51
1:D:2:PRO:HD2	1:D:359:ALA:O	2.10	0.51
1:A:56:PRO:HA	1:A:227:VAL:HG12	1.94	0.50
1:B:344:TYR:CE2	1:B:349:ARG:HG2	2.46	0.50
1:C:108:ASP:OD1	1:C:113:THR:HG23	2.12	0.50
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.47	0.50
1:C:33:ILE:HD12	1:C:33:ILE:N	2.26	0.50
1:C:187:THR:OG1	1:C:225:THR:CG2	2.60	0.50
1:D:110:ALA:HB2	1:D:158:PHE:CD1	2.46	0.50
1:A:4:SER:HB3	1:A:7:GLN:CG	2.38	0.50
1:A:37:GLN:HG3	1:A:39:HIS:CE1	2.47	0.50
1:A:174:ILE:HG12	1:A:179:PHE:CZ	2.47	0.50
1:A:204:ARG:HG3	1:A:204:ARG:HH11	1.77	0.50
1:B:19:LEU:HD11	1:B:344:TYR:CE2	2.47	0.50
1:D:248:LEU:HD13	1:D:248:LEU:O	2.12	0.50
1:A:258:ARG:HH22	1:A:275:ASN:HD22	1.60	0.49
1:B:4:SER:C	1:B:6:LYS:H	2.20	0.49
1:B:278:VAL:HG22	1:B:279:ASP:N	2.27	0.49
1:D:301:VAL:O	1:D:302:ASN:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:HB3	1:A:7:GLN:NE2	2.28	0.49
1:C:113:THR:HG21	1:C:260:TRP:CZ2	2.48	0.49
1:D:90:THR:HG22	1:D:90:THR:O	2.13	0.49
1:C:302:ASN:CB	1:C:303:PRO:CD	2.75	0.49
1:D:33:ILE:HG21	1:D:238:MET:HE1	1.94	0.49
1:A:4:SER:H	1:A:7:GLN:NE2	2.08	0.49
1:D:136:GLN:HA	1:D:136:GLN:OE1	2.13	0.49
1:D:276:TRP:CE3	1:D:277:PRO:HA	2.47	0.49
1:A:2:PRO:HG2	1:A:11:VAL:HG21	1.94	0.48
1:A:64:SER:HB2	1:A:317:GLY:HA2	1.94	0.48
1:A:302:ASN:O	1:A:303:PRO:CB	2.60	0.48
1:C:258:ARG:HG2	1:C:266:TYR:HB3	1.95	0.48
1:D:230:MET:HE3	1:D:326:VAL:HG21	1.96	0.48
1:D:45:LYS:HE2	1:D:51:ASN:HD22	1.75	0.48
1:D:33:ILE:HG22	1:D:36:GLY:HA2	1.96	0.48
1:B:176:THR:HG22	1:B:177:ARG:HG2	1.95	0.48
1:B:273:MET:HG3	1:B:313:VAL:HB	1.94	0.48
1:C:136:GLN:OE1	1:C:136:GLN:HA	2.13	0.48
1:A:9:ALA:HA	1:A:41:PHE:CE1	2.49	0.48
1:C:108:ASP:HA	1:C:113:THR:CG2	2.30	0.48
1:D:262:VAL:HB	1:D:265:MET:CE	2.44	0.48
1:A:80:ARG:HG3	1:A:247:SER:OG	2.14	0.48
1:B:64:SER:HB2	1:B:317:GLY:HA2	1.96	0.48
1:A:102:GLN:HG2	1:A:103:GLY:N	2.24	0.48
1:A:280:ALA:HB2	1:A:354:TYR:CE1	2.48	0.48
1:C:258:ARG:HG2	1:C:266:TYR:CB	2.44	0.48
1:A:102:GLN:C	1:A:104:ILE:H	2.22	0.47
1:A:258:ARG:HH22	1:A:275:ASN:ND2	2.12	0.47
1:B:138:TRP:CD2	1:B:140:PRO:CD	2.83	0.47
1:D:238:MET:HG3	1:D:328:PHE:CD2	2.49	0.47
1:A:67:LYS:HE3	1:A:155:ILE:CG2	2.45	0.47
1:B:121:VAL:O	1:B:122:PRO:C	2.57	0.47
1:C:93:TRP:CE2	1:C:132:LEU:CD1	2.98	0.47
1:B:62:LEU:HD13	1:B:225:THR:OG1	2.15	0.47
1:D:105:ARG:NH2	1:D:107:LEU:HD23	2.30	0.47
1:B:26:PRO:HG2	1:B:203:TYR:CD2	2.50	0.47
1:A:2:PRO:O	1:A:3:MET:C	2.56	0.47
1:C:173:ALA:O	1:C:177:ARG:CG	2.62	0.47
1:B:80:ARG:NH2	1:B:177:ARG:HD2	2.29	0.46
1:B:232:SER:O	1:B:236:VAL:HG23	2.15	0.46
1:A:141:GLN:OE1	1:A:141:GLN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LEU:HD13	1:B:25:ILE:HD12	1.97	0.46
1:B:313:VAL:HG11	1:B:328:PHE:CE1	2.50	0.46
1:C:200:ALA:O	1:C:210:HIS:HE1	1.97	0.46
1:C:173:ALA:O	1:C:177:ARG:HG3	2.15	0.46
1:C:260:TRP:CE3	1:C:300:GLU:HA	2.50	0.46
1:C:96:LEU:HD11	1:C:101:TRP:NE1	2.31	0.46
1:C:217:ASP:OD1	1:C:218:ALA:N	2.48	0.46
1:C:280:ALA:HB2	1:C:354:TYR:CZ	2.50	0.46
1:C:287:SER:CB	1:C:350:VAL:HG21	2.45	0.46
1:D:65:ILE:HG21	1:D:230:MET:CE	2.46	0.46
1:A:98:GLY:HA3	1:A:100:GLN:NE2	2.30	0.46
1:C:258:ARG:CZ	1:C:308:VAL:CG1	2.93	0.46
1:B:204:ARG:HG3	1:B:204:ARG:HH11	1.81	0.46
1:C:174:ILE:HD12	1:C:178:VAL:CG2	2.46	0.45
1:B:238:MET:HG3	1:B:330:PRO:HA	1.98	0.45
1:C:73:LEU:HB2	1:C:174:ILE:HD13	1.97	0.45
1:A:67:LYS:HE3	1:A:155:ILE:HG21	1.98	0.45
1:B:68:THR:O	1:B:72:VAL:HG23	2.16	0.45
1:A:5:GLU:OE1	1:A:6:LYS:HD3	2.17	0.45
1:A:276:TRP:CE2	1:A:277:PRO:HA	2.52	0.45
1:D:148:ARG:HD2	1:D:262:VAL:HG21	1.98	0.45
1:C:108:ASP:OD1	1:C:113:THR:CG2	2.65	0.45
1:A:87:ASP:CG	1:A:91:LYS:HE3	2.42	0.45
1:A:33:ILE:HG21	1:A:238:MET:HE1	1.99	0.45
1:A:33:ILE:HG12	1:A:235:MET:HG3	1.99	0.45
1:B:83:ILE:HG13	1:B:92:TYR:CE1	2.52	0.45
1:D:78:ILE:O	1:D:81:GLY:N	2.47	0.45
1:D:85:LEU:HB3	1:D:107:LEU:HB2	1.99	0.45
1:D:139:GLN:HA	1:D:140:PRO:HD2	1.80	0.45
1:D:28:MET:HB3	1:D:339:LEU:O	2.15	0.44
1:D:191:VAL:HG23	1:D:195:GLU:HB2	1.99	0.44
1:D:334:LEU:HD22	1:D:357:LEU:HD22	1.99	0.44
1:B:19:LEU:HD13	1:B:25:ILE:CD1	2.47	0.44
1:C:301:VAL:O	1:C:302:ASN:C	2.43	0.44
1:A:75:GLY:HA2	1:A:78:ILE:HD12	1.99	0.44
1:A:125:VAL:HG12	1:A:215:MET:HG3	2.00	0.44
1:A:62:LEU:HD22	1:A:223:VAL:HG12	1.98	0.44
1:D:280:ALA:HB2	1:D:354:TYR:CE1	2.52	0.44
1:B:303:PRO:O	1:B:304:PRO:C	2.59	0.44
1:C:311:SER:O	1:C:329:ILE:HA	2.18	0.44
1:D:243:LEU:CD1	1:D:248:LEU:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:GLY:O	1:C:224:LYS:HE3	2.17	0.44
1:C:66:SER:HB3	1:C:223:VAL:HG23	2.00	0.43
1:C:149:LEU:O	1:C:150:TYR:C	2.61	0.43
1:C:316:THR:HG22	1:C:325:TYR:HD1	1.82	0.43
1:D:8:LEU:O	1:D:12:VAL:HG23	2.18	0.43
1:A:59:LEU:HA	1:A:225:THR:O	2.17	0.43
1:B:82:GLU:OE1	1:B:177:ARG:NH2	2.51	0.43
1:C:64:SER:HB3	1:C:150:TYR:HH	1.83	0.43
1:B:37:GLN:OE1	1:B:37:GLN:HA	2.18	0.43
1:D:37:GLN:OE1	1:D:37:GLN:HA	2.19	0.43
1:C:170:TYR:CD1	1:C:219:GLU:HG3	2.54	0.43
1:C:225:THR:HG22	1:C:229:ASP:HB2	2.00	0.43
1:D:257:SER:O	1:D:268:GLY:HA2	2.19	0.43
1:B:302:ASN:HD22	1:B:302:ASN:HA	1.62	0.43
1:D:104:ILE:HD13	1:D:144:PRO:HG3	1.99	0.43
1:D:108:ASP:HA	1:D:113:THR:CG2	2.37	0.43
1:D:108:ASP:OD1	1:D:113:THR:CG2	2.65	0.43
1:B:217:ASP:O	1:B:222:GLY:N	2.52	0.43
1:B:258:ARG:NH2	1:B:311:SER:OG	2.51	0.43
1:B:313:VAL:HG13	1:B:328:PHE:CD1	2.54	0.43
1:C:59:LEU:HA	1:C:225:THR:O	2.18	0.43
1:A:65:ILE:HG21	1:A:230:MET:HE2	2.00	0.43
1:B:83:ILE:CG2	1:B:84:SER:N	2.80	0.43
1:C:157:LEU:HG	1:C:161:LEU:HD22	1.99	0.43
1:A:232:SER:HA	1:A:235:MET:HE3	2.01	0.43
1:D:288:ASP:OD1	1:D:290:LYS:HB2	2.19	0.43
1:A:31:ALA:HB2	1:A:227:VAL:HG22	2.01	0.43
1:A:63:GLY:O	1:A:221:TYR:HA	2.19	0.43
1:D:72:VAL:HG21	1:D:233:TRP:CH2	2.54	0.43
1:C:94:PRO:C	1:C:96:LEU:H	2.27	0.42
1:D:170:TYR:O	1:D:174:ILE:HG22	2.19	0.42
1:C:100:GLN:H	1:C:100:GLN:HE21	1.66	0.42
1:A:148:ARG:HD2	1:A:262:VAL:HG21	2.00	0.42
1:A:180:LYS:HA	1:A:180:LYS:HD2	1.79	0.42
1:B:83:ILE:CD1	1:B:162:ALA:O	2.68	0.42
1:B:138:TRP:CZ2	1:B:140:PRO:HD3	2.52	0.42
1:D:259:TYR:CE1	1:D:269:LEU:HD13	2.54	0.42
1:C:276:TRP:HA	1:C:277:PRO:C	2.44	0.42
1:C:258:ARG:HH12	1:C:275:ASN:ND2	2.14	0.42
1:B:28:MET:HG3	1:B:339:LEU:O	2.20	0.42
1:D:28:MET:HB3	1:D:340:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:THR:HG22	1:A:226:ASN:H	1.85	0.42
1:B:31:ALA:O	1:B:336:ILE:HA	2.18	0.42
1:B:164:LYS:N	1:B:165:PRO:CD	2.82	0.42
1:C:98:GLY:C	1:C:100:GLN:NE2	2.78	0.42
1:D:258:ARG:NH2	1:D:311:SER:OG	2.53	0.42
1:B:122:PRO:CB	1:B:124:GLU:HG3	2.49	0.42
1:D:78:ILE:HG13	1:D:83:ILE:HD11	2.02	0.42
1:D:104:ILE:HD13	1:D:144:PRO:HB3	2.01	0.42
1:D:234:VAL:HG12	1:D:238:MET:HE2	2.01	0.42
1:A:2:PRO:HD2	1:A:360:LEU:HA	2.01	0.41
1:A:65:ILE:HG13	1:A:317:GLY:HA3	2.02	0.41
1:B:243:LEU:HB3	1:B:244:GLN:H	1.66	0.41
1:D:83:ILE:HG21	1:D:162:ALA:HA	2.02	0.41
1:D:157:LEU:O	1:D:161:LEU:HG	2.20	0.41
1:A:4:SER:CB	1:A:7:GLN:HE21	2.33	0.41
1:A:96:LEU:HD12	1:A:96:LEU:HA	1.95	0.41
1:A:38:PRO:HD3	1:A:235:MET:SD	2.61	0.41
1:D:12:VAL:HG21	1:D:41:PHE:CE1	2.55	0.41
1:B:259:TYR:C	1:B:301:VAL:HG13	2.46	0.41
1:C:105:ARG:NH1	1:C:108:ASP:OD1	2.54	0.41
1:A:78:ILE:HD13	1:A:85:LEU:HD22	2.01	0.41
1:B:90:THR:HG23	2:B:406:HOH:O	2.20	0.41
1:B:278:VAL:CG2	1:B:279:ASP:N	2.84	0.41
1:B:346:ASN:N	1:B:347:PRO:CD	2.83	0.41
1:C:9:ALA:HA	1:C:41:PHE:CE2	2.55	0.41
1:C:244:GLN:O	1:C:249:ARG:HD3	2.20	0.41
1:D:35:GLU:O	1:D:36:GLY:C	2.63	0.41
1:A:2:PRO:HB3	1:A:7:GLN:HB3	2.02	0.41
1:A:10:GLU:O	1:A:14:ARG:HG2	2.21	0.41
1:A:217:ASP:OD1	1:A:218:ALA:N	2.54	0.41
1:C:98:GLY:C	1:C:100:GLN:HE21	2.29	0.41
1:C:244:GLN:HG2	2:C:441:HOH:O	2.20	0.41
1:D:35:GLU:C	1:D:37:GLN:N	2.78	0.41
1:D:187:THR:CB	1:D:225:THR:HG23	2.51	0.41
1:D:119:LEU:HA	1:D:151:ALA:HA	2.03	0.40
1:C:105:ARG:NH2	1:C:300:GLU:OE1	2.46	0.40
1:A:8:LEU:HD12	1:A:8:LEU:HA	1.88	0.40
1:D:187:THR:HA	1:D:225:THR:HG23	2.04	0.40
1:B:289:ASN:C	1:B:291:VAL:N	2.80	0.40
1:D:55:THR:HG22	1:D:57:GLN:N	2.18	0.40
1:A:17:THR:HB	1:A:18:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LYS:O	1:B:299:ARG:NH2[1_544]	2.10	0.10
1:A:196:GLU:OE2	1:C:355:ARG:NH2[1_455]	2.15	0.05

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	357/359 (99%)	344 (96%)	11 (3%)	2 (1%)	21	32
1	B	357/359 (99%)	337 (94%)	17 (5%)	3 (1%)	16	25
1	C	357/359 (99%)	337 (94%)	15 (4%)	5 (1%)	9	13
1	D	357/359 (99%)	341 (96%)	14 (4%)	2 (1%)	21	32
All	All	1428/1436 (99%)	1359 (95%)	57 (4%)	12 (1%)	16	25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	PRO
1	B	123	ASP
1	B	245	ASP
1	C	3	MET
1	C	302	ASN
1	D	36	GLY
1	D	302	ASN
1	A	90	THR

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Mol	Chain	Res	Type
1	C	303	PRO
1	B	290	LYS
1	C	304	PRO
1	C	103	GLY

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	289/289 (100%)	261 (90%)	28 (10%)	8	12
1	B	289/289 (100%)	258 (89%)	31 (11%)	6	10
1	C	289/289 (100%)	262 (91%)	27 (9%)	8	14
1	D	289/289 (100%)	261 (90%)	28 (10%)	8	12
All	All	1156/1156 (100%)	1042 (90%)	114 (10%)	7	11

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	3	MET
1	A	6	LYS
1	A	35	GLU
1	A	45	LYS
1	A	51	ASN
1	A	62	LEU
1	A	85	LEU
1	A	90	THR
1	A	100	GLN
1	A	102	GLN
1	A	105	ARG
1	A	113	THR
1	A	123	ASP
1	A	132	LEU
1	A	161	LEU
1	A	174	ILE

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Mol	Chain	Res	Type
1	A	177	ARG
1	A	180	LYS
1	A	188	TRP
1	A	225	THR
1	A	230	MET
1	A	232	SER
1	A	241	ASP
1	A	246	ASN
1	A	265	MET
1	A	303	PRO
1	A	308	VAL
1	B	5	GLU
1	B	10	GLU
1	B	19	LEU
1	B	21	LYS
1	B	62	LEU
1	B	83	ILE
1	B	100	GLN
1	B	105	ARG
1	B	123	ASP
1	B	124	GLU
1	B	139	GLN
1	B	176	THR
1	B	177	ARG
1	B	183	LYS
1	B	191	VAL
1	B	205	ASP
1	B	224	LYS
1	B	225	THR
1	B	230	MET
1	B	241	ASP
1	B	243	LEU
1	B	244	GLN
1	B	249	ARG
1	B	250	LYS
1	B	269	LEU
1	B	301	VAL
1	B	308	VAL
1	B	313	VAL
1	B	318	SER
1	B	334	LEU
1	B	343	SER

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Mol	Chain	Res	Type
1	C	3	MET
1	C	8	LEU
1	C	14	ARG
1	C	33	ILE
1	C	62	LEU
1	C	83	ILE
1	C	85	LEU
1	C	100	GLN
1	C	105	ARG
1	C	113	THR
1	C	118	PRO
1	C	122	PRO
1	C	136	GLN
1	C	161	LEU
1	C	163	VAL
1	C	177	ARG
1	C	225	THR
1	C	246	ASN
1	C	248	LEU
1	C	265	MET
1	C	269	LEU
1	C	281	LYS
1	C	300	GLU
1	C	308	VAL
1	C	318	SER
1	C	334	LEU
1	C	342	LYS
1	D	2	PRO
1	D	3	MET
1	D	4	SER
1	D	28	MET
1	D	52	LYS
1	D	55	THR
1	D	62	LEU
1	D	100	GLN
1	D	102	GLN
1	D	113	THR
1	D	123	ASP
1	D	130	SER
1	D	132	LEU
1	D	163	VAL
1	D	166	SER

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Mol	Chain	Res	Type
1	D	177	ARG
1	D	183	LYS
1	D	189	ILE
1	D	191	VAL
1	D	224	LYS
1	D	225	THR
1	D	230	MET
1	D	248	LEU
1	D	269	LEU
1	D	308	VAL
1	D	334	LEU
1	D	342	LYS
1	D	347	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	39	HIS
1	A	51	ASN
1	A	100	GLN
1	A	190	ASN
1	A	210	HIS
1	A	246	ASN
1	A	275	ASN
1	A	333	GLN
1	B	7	GLN
1	B	23	GLN
1	B	100	GLN
1	B	190	ASN
1	B	210	HIS
1	B	228	GLN
1	B	244	GLN
1	B	256	GLN
1	B	275	ASN
1	B	302	ASN
1	B	333	GLN
1	C	39	HIS
1	C	51	ASN
1	C	100	GLN
1	C	172	GLN
1	C	190	ASN

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Mol	Chain	Res	Type
1	C	210	HIS
1	C	246	ASN
1	C	256	GLN
1	C	275	ASN
1	D	23	GLN
1	D	39	HIS
1	D	51	ASN
1	D	57	GLN
1	D	100	GLN
1	D	190	ASN
1	D	210	HIS
1	D	228	GLN
1	D	275	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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	359/359 (100%)	0.16	8 (2%) 62 58	13, 22, 39, 51	2 (0%)
1	B	359/359 (100%)	0.29	9 (2%) 58 54	16, 24, 42, 66	4 (1%)
1	C	359/359 (100%)	0.00	6 (1%) 69 65	15, 25, 45, 57	5 (1%)
1	D	359/359 (100%)	0.29	3 (0%) 82 80	17, 31, 48, 58	6 (1%)
All	All	1436/1436 (100%)	0.19	26 (1%) 67 63	13, 25, 45, 66	17 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	ASN	4.7
1	C	102	GLN	4.4
1	C	302	ASN	4.2
1	B	139	GLN	3.7
1	B	2	PRO	3.5
1	A	244	GLN	3.5
1	B	302	ASN	3.4
1	B	244	GLN	3.3
1	B	140	PRO	3.1
1	B	3	MET	3.1
1	D	246	ASN	3.1
1	C	2	PRO	3.0
1	A	302	ASN	2.7
1	D	35	GLU	2.6
1	C	303	PRO	2.5
1	A	245	ASP	2.4
1	A	141	GLN	2.3
1	A	102	GLN	2.3
1	B	243	LEU	2.3
1	D	3	MET	2.2
1	A	37	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	265	MET	2.1
1	C	261	ARG	2.1
1	B	245	ASP	2.1
1	A	2	PRO	2.1
1	A	3	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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.