



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 10:41 AM UTC

PDB ID : 1AJN / pdb_00001ajn
Title : PENICILLIN ACYLASE COMPLEXED WITH P-NITROPHENYLACETIC ACID
Authors : Done, S.H.
Deposited on : 1997-05-07
Resolution : 2.36 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

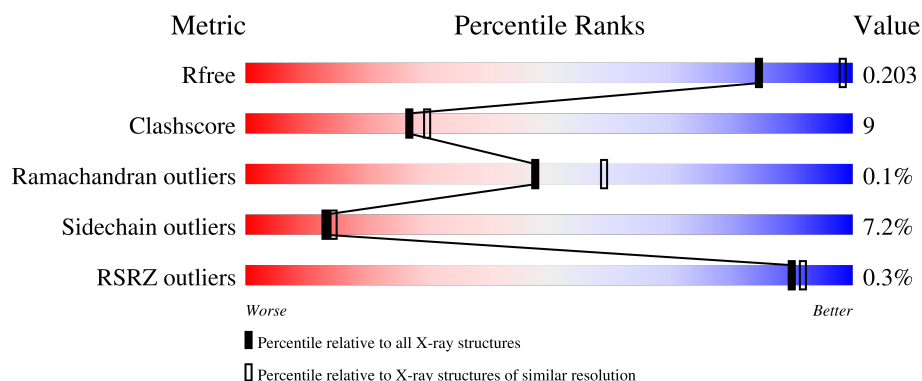
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	209	
2	B	557	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6754 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 PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1656	1058	278	312	8			

- Molecule 2 is a protein called PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	0	0	0
			4415	2805	767	833	10			

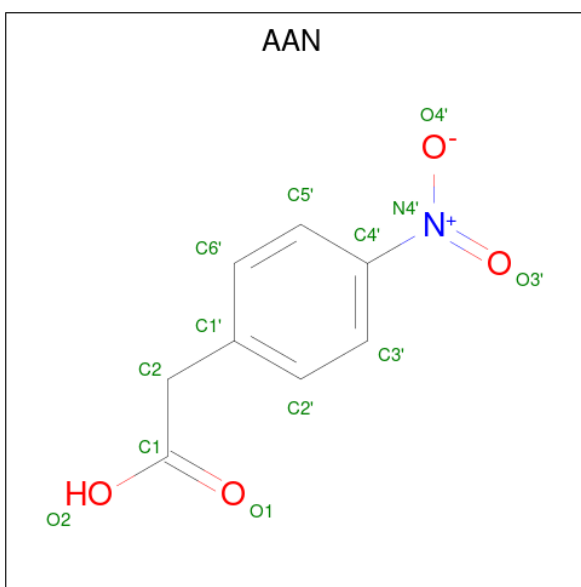
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	165	GLN	GLU	conflict	UNP P06875

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-(4-NITROPHENYL)ACETIC ACID (CCD ID: AAN) (formula: C₈H₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			13	8	1	4		

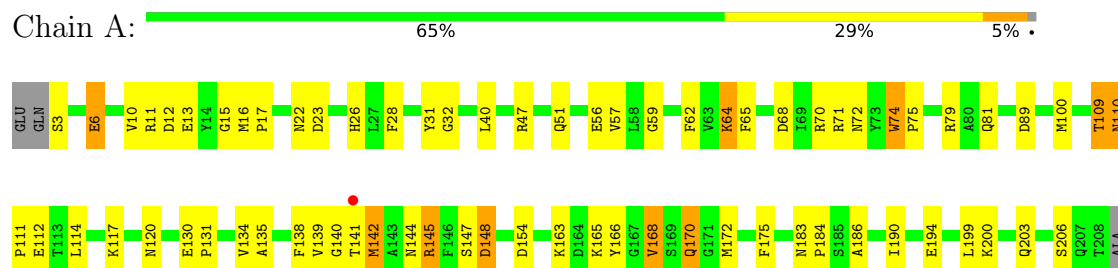
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	0
			172	172		
5	B	497	Total	O	0	0
			497	497		

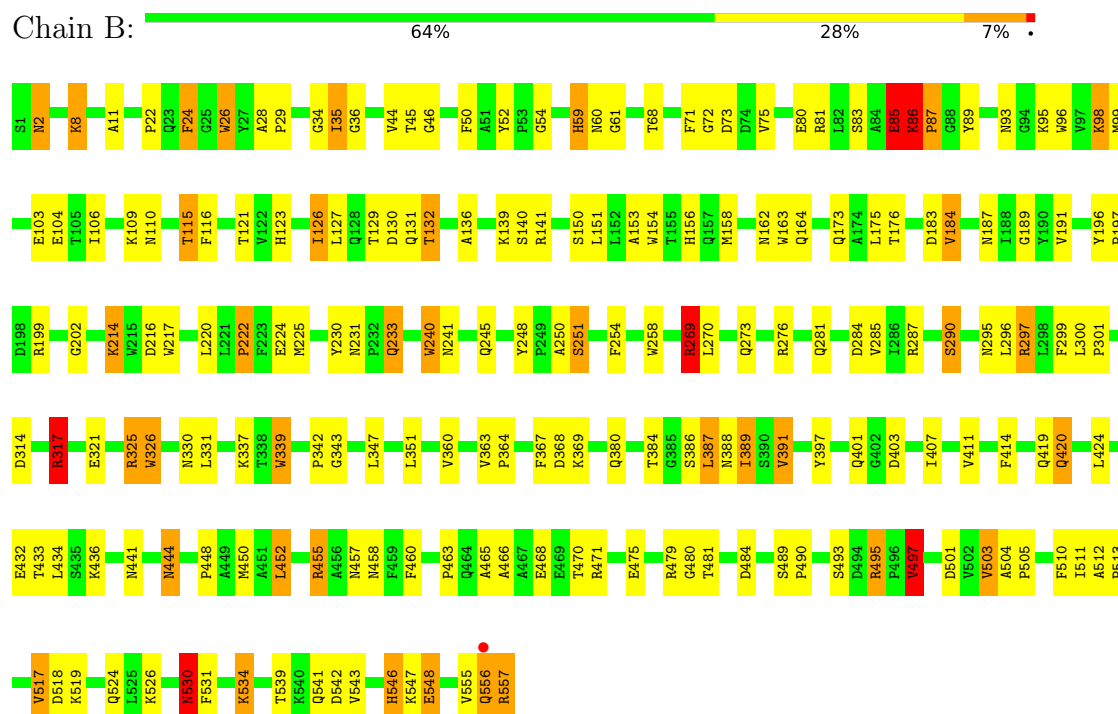
3 Residue-property plots

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: PENICILLIN AMIDOHYDROLASE



• Molecule 2: PENICILLIN AMIDOHYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.12Å 65.08Å 76.30Å 100.20° 111.44° 105.81°	Depositor
Resolution (Å)	26.12 – 2.36 26.12 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.5 (26.12-2.36) 97.4 (26.12-2.36)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.36Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.152 , 0.218 0.138 , 0.203	Depositor DCC
R_{free} test set	2438 reflections (7.16%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 98.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6754	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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

Bond lengths and bond angles in the following residue types are not validated in this section: AAN, CA

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	0.83	1/1698 (0.1%)	2.07	64/2305 (2.8%)
2	B	0.84	1/4541 (0.0%)	1.94	141/6192 (2.3%)
All	All	0.84	2/6239 (0.0%)	1.98	205/8497 (2.4%)

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
2	B	0	4
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	MET	SD-CE	-6.38	1.63	1.79
2	B	132	THR	CB-OG1	5.16	1.52	1.43

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLY	CA-C-O	-12.82	107.54	120.75
2	B	269	ARG	CD-NE-CZ	12.70	142.19	124.40
2	B	363	VAL	CA-C-O	12.65	127.98	119.38
2	B	541	GLN	CG-CD-NE2	-12.12	98.22	116.40
1	A	144	ASN	CA-CB-CG	-11.84	100.76	112.60
2	B	391	VAL	CB-CA-C	-10.76	98.11	111.88
2	B	441	ASN	CB-CG-ND2	-10.46	100.70	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	29	PRO	CA-C-N	10.37	135.52	120.90
2	B	29	PRO	C-N-CA	10.37	135.52	120.90
1	A	170	GLN	CG-CD-NE2	-10.36	100.86	116.40
2	B	530	ASN	CA-CB-CG	10.22	122.83	112.60
2	B	131	GLN	CG-CD-NE2	9.91	131.27	116.40
2	B	162	ASN	CB-CG-ND2	-9.73	101.81	116.40
2	B	465	ALA	CA-C-O	-9.68	110.92	121.28
2	B	407	ILE	CA-C-O	9.64	124.52	119.12
2	B	231	ASN	CA-C-O	9.54	127.83	120.48
1	A	139	VAL	O-C-N	9.24	130.96	121.91
1	A	28	PHE	CA-CB-CG	-9.11	104.69	113.80
2	B	389	ILE	CA-C-O	-9.11	110.00	120.65
2	B	541	GLN	CG-CD-OE1	8.75	138.30	120.80
2	B	548	GLU	N-CA-CB	8.63	122.67	110.67
2	B	455	ARG	CD-NE-CZ	8.55	136.37	124.40
2	B	240	TRP	N-CA-C	-8.51	100.37	110.41
2	B	269	ARG	N-CA-CB	8.32	122.07	110.01
2	B	131	GLN	CA-CB-CG	-8.19	97.73	114.10
1	A	109	THR	CA-C-N	8.12	130.56	122.28
1	A	109	THR	C-N-CA	8.12	130.56	122.28
2	B	131	GLN	CG-CD-OE1	-8.04	104.72	120.80
1	A	168	VAL	CA-C-O	-8.03	113.06	121.41
1	A	135	ALA	CA-C-O	-7.95	112.12	120.55
1	A	168	VAL	N-CA-C	7.87	118.42	110.23
1	A	110	ASN	O-C-N	-7.83	114.16	121.05
2	B	284	ASP	CA-CB-CG	-7.69	104.91	112.60
2	B	480	GLY	CA-C-N	7.68	130.90	120.38
2	B	480	GLY	C-N-CA	7.68	130.90	120.38
2	B	441	ASN	CB-CG-OD1	7.67	136.13	120.80
2	B	367	PHE	CA-CB-CG	-7.60	106.20	113.80
1	A	62	PHE	CA-CB-CG	-7.46	106.34	113.80
1	A	170	GLN	CG-CD-OE1	7.38	135.57	120.80
2	B	287	ARG	CD-NE-CZ	7.34	134.68	124.40
2	B	86	LYS	CA-CB-CG	7.32	128.74	114.10
2	B	248	TYR	CA-C-O	7.24	126.21	119.76
2	B	444	ASN	CB-CG-ND2	7.24	127.26	116.40
1	A	139	VAL	CA-CB-CG1	7.22	122.67	110.40
1	A	71	ARG	CD-NE-CZ	7.21	134.49	124.40
2	B	224	GLU	CB-CG-CD	7.14	124.73	112.60
2	B	71	PHE	CA-CB-CG	-7.13	106.67	113.80
2	B	269	ARG	CA-CB-CG	7.13	128.36	114.10
1	A	139	VAL	CA-C-O	-7.09	113.66	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	GLY	CA-C-N	7.08	130.47	120.28
1	A	59	GLY	C-N-CA	7.08	130.47	120.28
1	A	79	ARG	CD-NE-CZ	7.00	134.20	124.40
2	B	162	ASN	CB-CG-OD1	6.99	134.78	120.80
2	B	326	TRP	CA-C-O	-6.98	112.89	120.92
2	B	164	GLN	CB-CG-CD	6.95	124.42	112.60
2	B	325	ARG	CD-NE-CZ	-6.93	114.69	124.40
1	A	72	ASN	CB-CG-ND2	-6.91	106.04	116.40
1	A	165	LYS	CA-C-O	-6.86	113.63	120.70
2	B	363	VAL	O-C-N	-6.82	115.27	121.41
2	B	391	VAL	CA-C-N	6.81	127.50	119.94
2	B	391	VAL	C-N-CA	6.81	127.50	119.94
1	A	56	GLU	N-CA-CB	6.79	120.11	110.12
2	B	34	GLY	CA-C-O	-6.79	115.40	121.64
1	A	111	PRO	N-CA-CB	6.77	110.01	103.51
2	B	330	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	A	148	ASP	CA-CB-CG	-6.73	105.87	112.60
2	B	317	ARG	CD-NE-CZ	6.72	133.81	124.40
2	B	330	ASN	CB-CG-ND2	6.72	126.48	116.40
2	B	183	ASP	CA-CB-CG	6.72	119.32	112.60
2	B	342	PRO	CA-C-N	6.69	127.55	119.99
2	B	342	PRO	C-N-CA	6.69	127.55	119.99
2	B	479	ARG	CA-C-N	-6.68	113.99	120.34
2	B	479	ARG	C-N-CA	-6.68	113.99	120.34
1	A	100	MET	CA-C-O	6.56	127.38	120.42
2	B	495	ARG	CA-C-N	6.55	126.18	119.56
2	B	495	ARG	C-N-CA	6.55	126.18	119.56
2	B	241	ASN	CA-CB-CG	6.54	119.14	112.60
2	B	391	VAL	N-CA-CB	6.53	117.76	110.51
2	B	28	ALA	CA-C-O	-6.45	114.56	119.59
1	A	32	GLY	CA-C-O	6.42	127.67	121.05
2	B	233	GLN	CB-CG-CD	6.41	123.49	112.60
2	B	297	ARG	CA-C-N	6.40	129.38	120.29
2	B	297	ARG	C-N-CA	6.40	129.38	120.29
1	A	134	VAL	O-C-N	6.40	128.42	121.83
1	A	70	ARG	NE-CZ-NH2	-6.38	113.45	119.20
2	B	131	GLN	CB-CG-CD	6.38	123.44	112.60
2	B	46	GLY	CA-C-O	-6.36	116.52	120.91
2	B	99	MET	CA-C-O	-6.35	114.17	121.47
2	B	68	THR	CA-C-O	-6.34	114.24	121.40
2	B	199	ARG	CD-NE-CZ	-6.22	115.70	124.40
1	A	22	ASN	CB-CG-ND2	6.21	125.71	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	230	TYR	CA-C-N	-6.20	116.14	122.83
2	B	230	TYR	C-N-CA	-6.20	116.14	122.83
2	B	191	VAL	N-CA-CB	6.14	121.53	111.58
1	A	11	ARG	CD-NE-CZ	6.14	132.99	124.40
2	B	546	HIS	CB-CG-CD2	-6.13	123.22	131.20
2	B	281	GLN	CA-C-O	-6.13	113.92	120.42
1	A	135	ALA	O-C-N	6.10	128.59	122.12
2	B	300	LEU	CA-C-N	6.10	126.27	119.32
2	B	300	LEU	C-N-CA	6.10	126.27	119.32
2	B	285	VAL	CA-C-O	-6.09	114.06	120.57
2	B	444	ASN	CB-CG-OD1	-6.08	108.64	120.80
2	B	245	GLN	N-CA-CB	-6.08	102.14	111.56
2	B	471	ARG	CA-C-N	6.08	131.39	123.00
2	B	471	ARG	C-N-CA	6.08	131.39	123.00
2	B	475	GLU	N-CA-C	6.05	118.15	108.41
1	A	31	TYR	CA-C-N	5.98	126.74	119.99
1	A	31	TYR	C-N-CA	5.98	126.74	119.99
2	B	296	LEU	CA-C-N	5.98	128.61	120.54
2	B	296	LEU	C-N-CA	5.98	128.61	120.54
1	A	16	MET	CA-C-N	5.97	126.44	119.99
1	A	16	MET	C-N-CA	5.97	126.44	119.99
1	A	141	THR	O-C-N	5.96	129.96	122.22
2	B	463	PRO	N-CA-CB	5.96	108.63	103.27
1	A	175	PHE	CA-C-O	-5.95	114.53	120.90
1	A	40	LEU	CA-C-O	-5.93	114.59	120.82
1	A	154	ASP	CA-C-O	-5.92	114.14	120.42
1	A	74	TRP	CA-C-N	5.90	126.05	119.32
1	A	74	TRP	C-N-CA	5.90	126.05	119.32
2	B	269	ARG	NE-CZ-NH1	5.89	127.39	121.50
2	B	548	GLU	CA-CB-CG	5.89	125.87	114.10
2	B	52	TYR	O-C-N	-5.87	114.57	121.32
2	B	54	GLY	O-C-N	-5.86	117.49	123.35
1	A	120	ASN	CA-CB-CG	-5.85	106.75	112.60
2	B	220	LEU	CA-C-O	-5.85	114.27	121.11
2	B	530	ASN	CB-CG-ND2	5.84	125.16	116.40
2	B	50	PHE	CA-CB-CG	5.84	119.64	113.80
2	B	466	ALA	CA-C-O	-5.82	114.94	121.81
1	A	47	ARG	CA-C-O	-5.82	114.71	120.82
2	B	364	PRO	N-CA-CB	5.80	108.47	103.31
1	A	117	LYS	N-CA-C	5.80	118.34	111.33
2	B	222	PRO	CA-C-N	5.76	128.58	120.28
2	B	222	PRO	C-N-CA	5.76	128.58	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	24	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	72	ASN	N-CA-CB	-5.74	102.65	110.56
2	B	248	TYR	O-C-N	-5.71	115.36	121.42
1	A	134	VAL	CA-C-O	-5.71	114.80	120.85
1	A	147	SER	N-CA-C	-5.70	104.54	112.30
2	B	434	LEU	CA-C-O	-5.69	114.39	120.42
2	B	301	PRO	CA-C-N	5.68	128.35	120.29
2	B	301	PRO	C-N-CA	5.68	128.35	120.29
1	A	57	VAL	CA-C-O	-5.67	113.58	118.96
2	B	270	LEU	CA-C-O	-5.65	114.43	120.42
2	B	87	PRO	N-CA-CB	5.63	108.54	103.19
1	A	51	GLN	N-CA-C	-5.61	106.32	114.12
2	B	290	SER	CB-CA-C	-5.61	101.15	110.68
2	B	141	ARG	NE-CZ-NH2	5.60	124.24	119.20
2	B	433	THR	O-C-N	-5.59	116.31	122.07
2	B	287	ARG	CA-C-O	-5.59	114.95	120.70
2	B	72	GLY	N-CA-C	-5.58	104.07	112.89
2	B	503	VAL	N-CA-CB	-5.49	107.16	112.65
2	B	269	ARG	NH1-CZ-NH2	-5.49	112.17	119.30
2	B	59	HIS	CA-CB-CG	-5.47	108.33	113.80
2	B	176	THR	O-C-N	-5.47	115.23	122.57
2	B	490	PRO	N-CA-CB	5.47	108.19	103.27
2	B	196	TYR	CA-C-N	5.46	125.40	119.78
2	B	196	TYR	C-N-CA	5.46	125.40	119.78
2	B	557	ARG	CD-NE-CZ	-5.43	116.80	124.40
2	B	153	ALA	O-C-N	-5.41	115.62	122.27
2	B	75	VAL	CA-C-O	-5.40	114.82	120.27
2	B	85	GLU	CA-C-O	-5.39	114.82	120.80
2	B	497	VAL	CB-CA-C	-5.39	101.07	110.71
2	B	452	LEU	O-C-N	-5.38	117.02	123.31
1	A	81	GLN	CA-C-O	5.37	126.14	119.97
1	A	15	GLY	N-CA-C	-5.36	107.92	115.32
2	B	484	ASP	CA-C-O	-5.36	114.17	120.60
2	B	295	ASN	CB-CG-ND2	5.35	124.43	116.40
2	B	184	VAL	CB-CA-C	-5.34	101.58	111.79
2	B	187	ASN	OD1-CG-ND2	5.34	127.94	122.60
2	B	386	SER	O-C-N	-5.34	116.56	122.86
2	B	231	ASN	N-CA-CB	-5.33	103.90	111.51
2	B	448	PRO	N-CA-CB	5.31	108.03	103.36
2	B	420	GLN	CG-CD-NE2	-5.31	108.44	116.40
2	B	363	VAL	N-CA-C	5.30	113.67	107.89
2	B	510	PHE	CA-C-O	5.29	126.73	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	530	ASN	CB-CG-OD1	-5.29	110.22	120.80
2	B	470	THR	CA-C-O	-5.27	115.39	121.19
1	A	140	GLY	O-C-N	5.25	127.23	122.19
1	A	22	ASN	CB-CG-OD1	-5.22	110.36	120.80
2	B	73	ASP	CB-CG-OD2	5.22	130.41	118.40
1	A	190	ILE	O-C-N	-5.22	116.08	122.97
1	A	183	ASN	CA-C-N	5.21	124.82	119.56
1	A	183	ASN	C-N-CA	5.21	124.82	119.56
1	A	186	ALA	CA-C-N	5.20	125.45	119.83
1	A	186	ALA	C-N-CA	5.20	125.45	119.83
2	B	110	ASN	CA-CB-CG	-5.19	107.41	112.60
1	A	184	PRO	CA-C-O	-5.18	111.75	119.00
1	A	144	ASN	CA-C-N	-5.17	113.26	122.42
1	A	144	ASN	C-N-CA	-5.17	113.26	122.42
2	B	489	SER	CB-CA-C	-5.17	107.53	111.20
1	A	17	PRO	N-CA-CB	5.16	108.09	103.19
1	A	89	ASP	CA-CB-CG	-5.16	107.44	112.60
2	B	481	THR	CA-C-O	-5.16	115.06	120.63
2	B	339	TRP	CA-C-N	5.11	128.08	120.31
2	B	339	TRP	C-N-CA	5.11	128.08	120.31
2	B	386	SER	CA-C-O	5.09	127.11	121.56
2	B	424	LEU	CA-C-N	-5.09	113.46	120.28
2	B	424	LEU	C-N-CA	-5.09	113.46	120.28
2	B	314	ASP	CA-C-N	5.08	125.11	119.32
2	B	314	ASP	C-N-CA	5.08	125.11	119.32
2	B	126	ILE	CA-C-N	5.07	127.53	120.63
2	B	126	ILE	C-N-CA	5.07	127.53	120.63
2	B	156	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	184	PRO	N-CA-CB	5.05	108.36	103.51
2	B	331	LEU	CA-C-O	-5.02	114.11	120.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Mainchain
2	B	26	TRP	Mainchain
2	B	299	PHE	Mainchain
2	B	325	ARG	Mainchain
2	B	518	ASP	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	1656	0	1604	27	0
2	B	4415	0	4244	93	0
3	B	1	0	0	0	0
4	B	13	0	6	0	0
5	A	172	0	0	1	0
5	B	497	0	0	0	0
All	All	6754	0	5854	110	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 9.

All (110) 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)
2:B:214:LYS:H	2:B:214:LYS:HD2	1.22	1.03
2:B:80:GLU:OE2	2:B:123:HIS:HD2	1.41	1.00
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.43	0.82
2:B:387:LEU:HD21	2:B:450:MET:HE1	1.66	0.77
2:B:80:GLU:OE2	2:B:123:HIS:CD2	2.32	0.76
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.49	0.76
2:B:59:HIS:HD2	2:B:61:GLY:H	1.35	0.75
2:B:86:LYS:N	2:B:87:PRO:HD3	2.01	0.75
1:A:26:HIS:HE1	2:B:555:VAL:O	1.70	0.73
2:B:123:HIS:HE1	2:B:216:ASP:OD1	1.72	0.73
2:B:388:ASN:ND2	2:B:389:ILE:H	1.89	0.71
2:B:384:THR:HG22	2:B:455:ARG:HH12	1.56	0.70
2:B:59:HIS:CD2	2:B:61:GLY:H	2.10	0.68
2:B:384:THR:HG22	2:B:455:ARG:NH1	2.09	0.67
1:A:199:LEU:HD21	2:B:225:MET:HE1	1.76	0.67
2:B:173:GLN:HE22	2:B:175:LEU:H	1.41	0.66
2:B:173:GLN:NE2	2:B:175:LEU:H	1.96	0.64
2:B:556:GLN:OE1	2:B:557:ARG:N	2.31	0.64
2:B:388:ASN:HD22	2:B:389:ILE:H	1.44	0.63
2:B:317:ARG:HG3	2:B:317:ARG:HH11	1.61	0.63
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:503:VAL:H	2:B:524:GLN:NE2	1.96	0.63
2:B:150:SER:HB3	2:B:173:GLN:HE21	1.64	0.61
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.35	0.61
2:B:86:LYS:H	2:B:87:PRO:HD3	1.65	0.60
2:B:384:THR:CG2	2:B:455:ARG:HH12	2.14	0.60
2:B:214:LYS:HD2	2:B:214:LYS:N	2.04	0.59
1:A:170:GLN:NE2	1:A:170:GLN:HA	2.18	0.59
2:B:458:ASN:OD1	2:B:458:ASN:C	2.46	0.58
2:B:89:TYR:CZ	2:B:98:LYS:HG3	2.39	0.57
2:B:214:LYS:H	2:B:214:LYS:CD	2.05	0.57
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.87	0.56
1:A:3:SER:HB3	1:A:6:GLU:HB3	1.89	0.55
2:B:339:TRP:CH2	2:B:450:MET:HE2	2.38	0.55
2:B:384:THR:HG22	2:B:455:ARG:CZ	2.37	0.55
2:B:86:LYS:N	2:B:87:PRO:CD	2.71	0.54
1:A:64:LYS:HE3	1:A:68:ASP:OD2	2.07	0.54
2:B:414:PHE:CZ	2:B:419:GLN:HG2	2.41	0.54
2:B:151:LEU:HD23	2:B:151:LEU:C	2.33	0.54
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.16	0.53
2:B:384:THR:HG22	2:B:455:ARG:NH2	2.24	0.52
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.45	0.52
2:B:388:ASN:HD22	2:B:389:ILE:N	2.06	0.51
2:B:123:HIS:O	2:B:140:SER:HB2	2.10	0.51
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.76	0.51
1:A:170:GLN:CA	1:A:170:GLN:HE21	2.06	0.51
2:B:317:ARG:O	2:B:321:GLU:HG3	2.11	0.51
1:A:130:GLU:HB2	1:A:131:PRO:HD2	1.92	0.51
2:B:384:THR:HG22	2:B:455:ARG:HH22	1.76	0.50
2:B:129:THR:HG22	2:B:136:ALA:CB	2.41	0.50
2:B:512:ALA:HB1	2:B:513:PRO:CD	2.42	0.50
1:A:12:ASP:O	2:B:548:GLU:HG2	2.12	0.49
1:A:199:LEU:CD2	2:B:225:MET:HE1	2.41	0.49
2:B:360:VAL:HG13	2:B:368:ASP:HB2	1.95	0.49
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.94	0.49
1:A:138:PHE:O	1:A:142:MET:HB3	2.11	0.49
2:B:317:ARG:HG3	2:B:317:ARG:NH1	2.25	0.48
2:B:397:TYR:O	2:B:401:GLN:HG2	2.12	0.48
2:B:457:ASN:HD22	2:B:457:ASN:N	2.05	0.48
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.48	0.48
2:B:542:ASP:O	2:B:546:HIS:HD2	1.97	0.48
1:A:110:ASN:HB3	1:A:114:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:THR:HG23	2:B:126:ILE:HD11	1.97	0.47
1:A:26:HIS:CE1	2:B:555:VAL:O	2.60	0.47
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.96	0.47
1:A:23:ASP:OD1	1:A:26:HIS:HD2	1.98	0.47
2:B:11:ALA:O	2:B:276:ARG:NH1	2.45	0.47
1:A:172:MET:HE2	1:A:203:GLN:O	2.15	0.46
2:B:60:ASN:C	2:B:60:ASN:OD1	2.59	0.46
2:B:530:ASN:O	2:B:531:PHE:HB2	2.15	0.46
1:A:194:GLU:OE2	2:B:233:GLN:HG3	2.16	0.46
2:B:501:ASP:OD1	2:B:534:LYS:HE2	2.15	0.46
1:A:130:GLU:HB2	1:A:131:PRO:CD	2.46	0.45
1:A:206:SER:HB2	2:B:202:GLY:O	2.17	0.45
2:B:504:ALA:HA	2:B:505:PRO:C	2.41	0.45
2:B:129:THR:HA	2:B:136:ALA:HA	1.98	0.45
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.52	0.45
2:B:8:LYS:HE2	2:B:8:LYS:HB2	1.76	0.45
1:A:163:LYS:HG2	1:A:168:VAL:HA	1.98	0.45
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.52	0.44
1:A:170:GLN:HA	1:A:170:GLN:HE21	1.76	0.44
2:B:45:THR:CG2	2:B:59:HIS:CE1	3.00	0.44
1:A:166:TYR:O	1:A:170:GLN:HB3	2.17	0.44
2:B:104:GLU:O	2:B:115:THR:HA	2.18	0.44
1:A:10:VAL:HG13	2:B:547:LYS:HD3	1.99	0.44
2:B:35:ILE:HG13	2:B:36:GLY:N	2.33	0.44
1:A:148:ASP:OD2	2:B:139:LYS:NZ	2.48	0.43
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.53	0.43
2:B:93:ASN:HD22	2:B:93:ASN:HA	1.69	0.43
2:B:59:HIS:HD2	2:B:61:GLY:N	2.11	0.43
2:B:539:THR:O	2:B:543:VAL:HG23	2.18	0.43
1:A:110:ASN:HB2	5:A:373:HOH:O	2.17	0.43
2:B:85:GLU:O	2:B:86:LYS:HG2	2.18	0.43
1:A:145:ARG:HD3	1:A:145:ARG:HA	1.67	0.42
2:B:173:GLN:HE22	2:B:175:LEU:HG	1.85	0.42
2:B:61:GLY:HA2	2:B:497:VAL:HG21	2.00	0.42
2:B:2:ASN:HB3	2:B:240:TRP:CG	2.55	0.42
2:B:388:ASN:ND2	2:B:389:ILE:N	2.63	0.42
2:B:222:PRO:HD2	2:B:225:MET:HG3	2.01	0.42
2:B:2:ASN:C	2:B:2:ASN:HD22	2.27	0.42
1:A:65:PHE:CE1	2:B:460:PHE:HB3	2.55	0.42
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.54	0.42
2:B:347:LEU:O	2:B:351:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ASP:OD1	2:B:132:THR:OG1	2.30	0.41
1:A:166:TYR:HB3	1:A:170:GLN:CG	2.50	0.41
2:B:457:ASN:N	2:B:457:ASN:ND2	2.67	0.41
2:B:59:HIS:CD2	2:B:61:GLY:N	2.86	0.41
1:A:74:TRP:HA	1:A:75:PRO:HD2	1.89	0.41
2:B:250:ALA:O	2:B:251:SER:C	2.64	0.41
2:B:254:PHE:CD1	2:B:254:PHE:C	2.98	0.40

There are no symmetry-related clashes.

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	204/209 (98%)	201 (98%)	3 (2%)	0	100	100
2	B	555/557 (100%)	538 (97%)	16 (3%)	1 (0%)	43	52
All	All	759/766 (99%)	739 (97%)	19 (2%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/180 (99%)	172 (97%)	6 (3%)	32	43
2	B	460/460 (100%)	420 (91%)	40 (9%)	9	10
All	All	638/640 (100%)	592 (93%)	46 (7%)	13	14

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	13	GLU
1	A	64	LYS
1	A	109	THR
1	A	112	GLU
1	A	200	LYS
2	B	2	ASN
2	B	8	LYS
2	B	35	ILE
2	B	81	ARG
2	B	85	GLU
2	B	86	LYS
2	B	95	LYS
2	B	98	LYS
2	B	103	GLU
2	B	109	LYS
2	B	115	THR
2	B	127	LEU
2	B	154	TRP
2	B	184	VAL
2	B	214	LYS
2	B	269	ARG
2	B	273	GLN
2	B	290	SER
2	B	317	ARG
2	B	337	LYS
2	B	369	LYS
2	B	380	GLN
2	B	387	LEU
2	B	391	VAL
2	B	403	ASP
2	B	411	VAL
2	B	420	GLN
2	B	432	GLU
2	B	436	LYS

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Mol	Chain	Res	Type
2	B	444	ASN
2	B	468	GLU
2	B	493	SER
2	B	495	ARG
2	B	497	VAL
2	B	517	VAL
2	B	519	LYS
2	B	526	LYS
2	B	530	ASN
2	B	534	LYS
2	B	556	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	108	ASN
1	A	110	ASN
1	A	144	ASN
1	A	170	GLN
1	A	193	GLN
1	A	196	ASN
1	A	204	GLN
1	A	205	ASN
2	B	2	ASN
2	B	59	HIS
2	B	93	ASN
2	B	123	HIS
2	B	168	GLN
2	B	169	GLN
2	B	173	GLN
2	B	245	GLN
2	B	388	ASN
2	B	420	GLN
2	B	440	ASN
2	B	441	ASN
2	B	457	ASN
2	B	507	GLN
2	B	524	GLN
2	B	541	GLN
2	B	546	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	AAN	B	559	-	13,13,13	5.32	3 (23%)	15,17,17	3.21	8 (53%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AAN	B	559	-	-	2/6/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	559	AAN	C4'-N4'	-15.14	1.09	1.45
4	B	559	AAN	O3'-N4'	11.37	1.42	1.22
4	B	559	AAN	O2-C1	-2.04	1.24	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559	AAN	O3'-N4'-C4'	-6.97	109.22	118.82
4	B	559	AAN	C6'-C5'-C4'	-5.28	113.08	120.08
4	B	559	AAN	O2-C1-O1	-4.00	113.05	123.33
4	B	559	AAN	C3'-C2'-C1'	-3.92	115.85	121.00
4	B	559	AAN	C5'-C4'-N4'	-3.89	115.94	119.34
4	B	559	AAN	O2-C1-C2	3.26	126.41	113.98
4	B	559	AAN	C5'-C4'-C3'	2.92	124.57	119.88
4	B	559	AAN	C6'-C1'-C2'	2.37	121.75	118.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	559	AAN	O1-C1-C2-C1'
4	B	559	AAN	O2-C1-C2-C1'

There are no ring outliers.

No monomer is involved in short contacts.

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	206/209 (98%)	-0.54	1 (0%) 87 90	16, 28, 55, 73	0
2	B	557/557 (100%)	-0.66	1 (0%) 91 92	10, 26, 56, 104	0
All	All	763/766 (99%)	-0.63	2 (0%) 90 92	10, 26, 56, 104	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	THR	2.7
2	B	556	GLN	2.5

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AAN	B	559	13/13	0.93	0.07	18,34,44,46	0
3	CA	B	558	1/1	1.00	0.01	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.