



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:07 PM UTC

PDB ID : 1AI5 / pdb_00001ai5
Title : PENICILLIN ACYLASE COMPLEXED WITH M-NITROPHENYLACETIC ACID
Authors : Done, S.H.
Deposited on : 1997-05-01
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

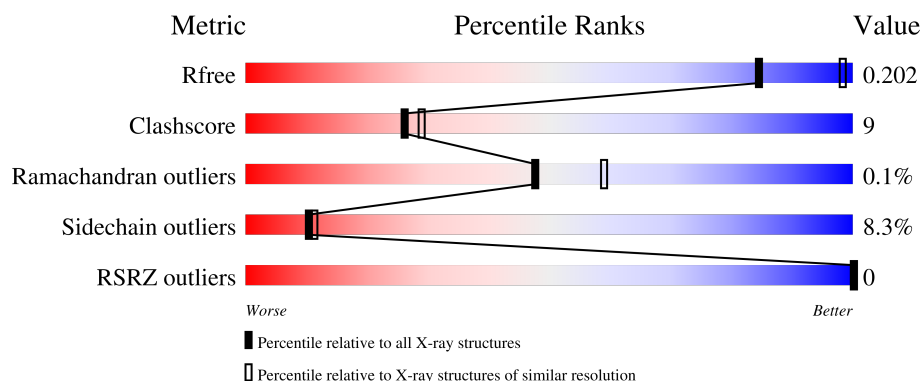
1 Overall quality at a glance

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	 67% 28% . .
2	B	557	 65% 27% 6% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6748 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			

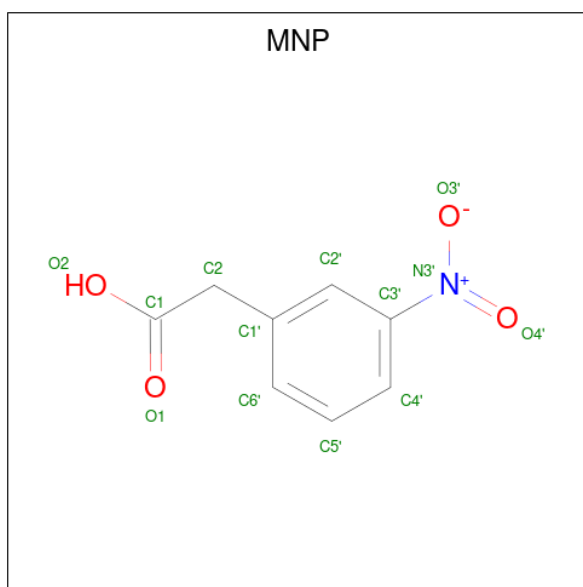
There is a discrepancy between the modelled and reference sequences:

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-(3-NITROPHENYL)ACETIC ACID (CCD ID: MNP) (formula: C₈H₇NO₄).



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

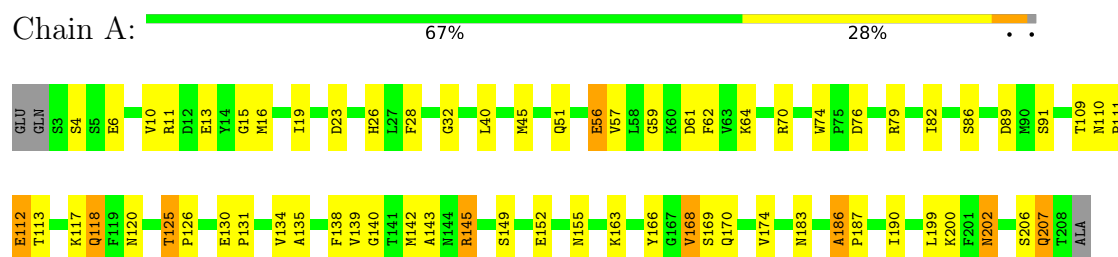
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		
5	B	490	Total	O	0	0
			490	490		

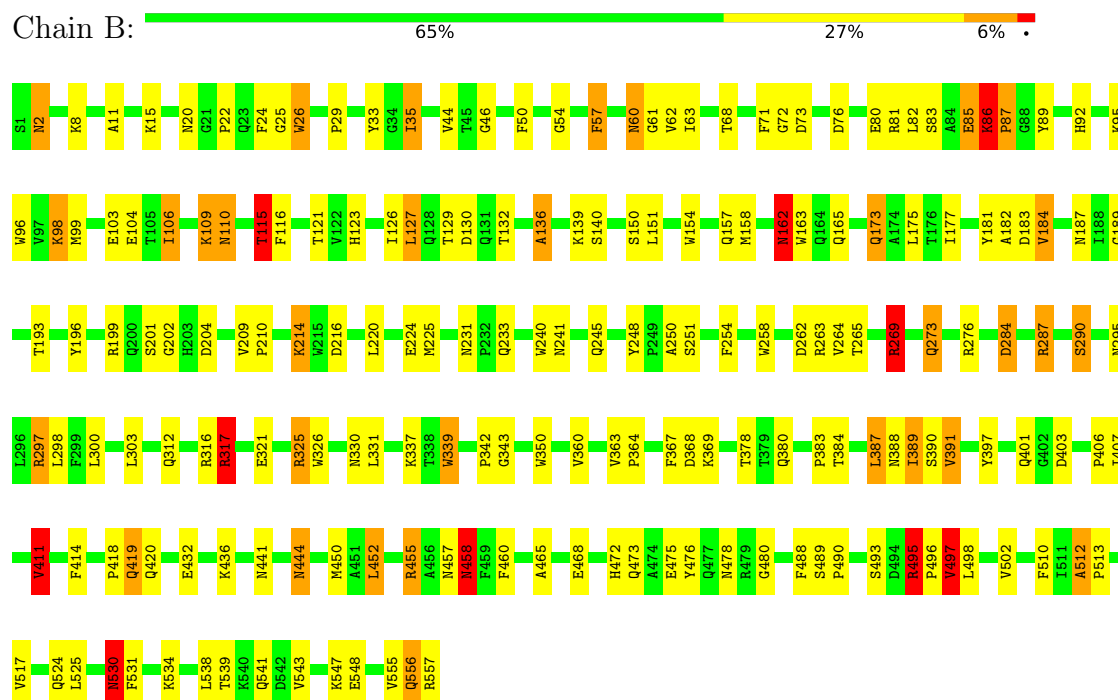
3 Residue-property plots

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)	97.4 (26.12-2.36) 97.3 (26.12-2.36)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.36Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.149 , 0.222 0.137 , 0.202	Depositor DCC
R_{free} test set	2451 reflections (7.16%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.6	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	6748	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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: CA, MNP

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	0.84	1/1698 (0.1%)	2.03	58/2305 (2.5%)
2	B	0.82	1/4541 (0.0%)	1.91	132/6192 (2.1%)
All	All	0.83	2/6239 (0.0%)	1.94	190/8497 (2.2%)

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
2	B	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	132	THR	CB-OG1	5.55	1.52	1.43
1	A	125	THR	N-CA	5.47	1.50	1.45

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	ARG	CD-NE-CZ	10.89	139.65	124.40
2	B	391	VAL	CB-CA-C	-10.87	97.96	111.88
2	B	389	ILE	CA-C-O	-9.93	109.03	120.65
2	B	363	VAL	CA-C-O	9.88	126.10	119.38
1	A	135	ALA	CA-C-O	-9.77	110.19	120.55
2	B	269	ARG	CA-CB-CG	9.68	133.47	114.10
1	A	28	PHE	CA-CB-CG	-9.19	104.61	113.80
2	B	241	ASN	CA-CB-CG	8.94	121.54	112.60
2	B	530	ASN	CA-CB-CG	8.87	121.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	50	PHE	CA-CB-CG	8.84	122.64	113.80
2	B	287	ARG	CD-NE-CZ	8.83	136.76	124.40
2	B	455	ARG	CD-NE-CZ	8.74	136.64	124.40
2	B	465	ALA	CA-C-O	-8.56	112.12	121.28
2	B	269	ARG	N-CA-CB	8.40	122.47	110.12
2	B	284	ASP	CA-CB-CG	-8.27	104.33	112.60
2	B	342	PRO	CA-C-N	8.21	129.22	120.03
2	B	342	PRO	C-N-CA	8.21	129.22	120.03
2	B	220	LEU	CA-C-O	-8.12	111.93	121.11
2	B	297	ARG	CA-C-N	7.83	131.08	120.44
2	B	297	ARG	C-N-CA	7.83	131.08	120.44
1	A	168	VAL	N-CA-C	7.71	118.45	110.36
2	B	46	GLY	CA-C-O	-7.70	115.60	120.91
1	A	139	VAL	O-C-N	7.56	129.61	121.83
1	A	145	ARG	CB-CG-CD	-7.55	93.94	111.30
2	B	495	ARG	CA-C-N	7.55	127.18	119.56
2	B	495	ARG	C-N-CA	7.55	127.18	119.56
1	A	61	ASP	CA-CB-CG	7.42	120.02	112.60
2	B	407	ILE	CA-C-O	7.41	123.27	119.12
2	B	316	ARG	NE-CZ-NH2	7.38	125.84	119.20
2	B	162	ASN	OD1-CG-ND2	-7.37	115.23	122.60
2	B	224	GLU	CB-CG-CD	7.33	125.07	112.60
2	B	472	HIS	CA-CB-CG	-7.31	106.49	113.80
1	A	79	ARG	CD-NE-CZ	7.22	134.51	124.40
2	B	290	SER	CB-CA-C	-7.03	98.73	110.68
1	A	32	GLY	O-C-N	-7.02	115.18	122.13
2	B	419	GLN	OE1-CD-NE2	7.01	129.61	122.60
2	B	181	TYR	CA-C-O	-7.00	112.61	120.66
2	B	312	GLN	OE1-CD-NE2	6.98	129.58	122.60
1	A	51	GLN	OE1-CD-NE2	-6.94	115.66	122.60
2	B	263	ARG	NE-CZ-NH2	-6.88	113.01	119.20
2	B	317	ARG	CD-NE-CZ	6.87	134.02	124.40
1	A	140	GLY	CA-C-N	-6.81	111.69	122.79
1	A	140	GLY	C-N-CA	-6.81	111.69	122.79
1	A	139	VAL	CA-C-O	-6.81	113.63	120.85
2	B	541	GLN	CB-CG-CD	6.80	124.17	112.60
2	B	157	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	A	111	PRO	N-CA-CB	6.73	109.97	103.51
2	B	326	TRP	CA-C-O	-6.69	113.33	121.36
2	B	391	VAL	N-CA-CB	6.61	117.84	110.51
2	B	245	GLN	N-CA-CB	-6.60	101.33	111.56
2	B	54	GLY	CA-C-O	6.59	126.92	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ILE	CA-C-N	6.58	130.68	120.75
1	A	190	ILE	C-N-CA	6.58	130.68	120.75
2	B	182	ALA	CA-C-O	-6.57	113.97	121.40
2	B	86	LYS	CA-CB-CG	6.54	127.18	114.10
1	A	62	PHE	CA-CB-CG	-6.50	107.30	113.80
2	B	29	PRO	CA-C-N	6.42	129.94	120.90
2	B	29	PRO	C-N-CA	6.42	129.94	120.90
2	B	183	ASP	CA-CB-CG	6.41	119.01	112.60
2	B	325	ARG	CD-NE-CZ	-6.41	115.42	124.40
1	A	120	ASN	CA-CB-CG	-6.41	106.19	112.60
2	B	367	PHE	CA-CB-CG	-6.41	107.39	113.80
1	A	70	ARG	NE-CZ-NH2	-6.36	113.47	119.20
2	B	33	TYR	CA-C-O	-6.35	113.51	120.24
2	B	54	GLY	O-C-N	-6.30	116.93	123.48
2	B	233	GLN	CA-CB-CG	6.24	126.57	114.10
1	A	40	LEU	CA-C-O	-6.18	113.86	120.42
2	B	199	ARG	CD-NE-CZ	-6.17	115.76	124.40
1	A	59	GLY	CA-C-N	6.17	129.39	120.38
1	A	59	GLY	C-N-CA	6.17	129.39	120.38
2	B	72	GLY	N-CA-C	-6.11	103.23	112.89
2	B	187	ASN	OD1-CG-ND2	6.11	128.71	122.60
2	B	71	PHE	CA-CB-CG	-6.10	107.70	113.80
1	A	56	GLU	N-CA-CB	6.09	119.72	110.28
2	B	330	ASN	CB-CG-ND2	6.07	125.50	116.40
1	A	57	VAL	CA-C-O	-6.07	113.56	118.90
1	A	64	LYS	CA-C-O	6.07	126.98	120.55
2	B	538	LEU	CA-C-O	-6.06	112.72	119.81
2	B	488	PHE	CA-C-N	6.05	129.36	122.83
2	B	488	PHE	C-N-CA	6.05	129.36	122.83
1	A	168	VAL	CA-C-O	-6.04	114.99	121.27
2	B	458	ASN	CA-C-O	6.04	128.70	121.88
2	B	184	VAL	CB-CA-C	-6.01	100.31	111.79
2	B	297	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	A	145	ARG	CA-C-O	-6.00	112.91	119.08
2	B	68	THR	CA-C-O	-5.99	114.64	121.40
1	A	143	ALA	CA-C-O	5.98	127.80	120.56
2	B	473	GLN	OE1-CD-NE2	-5.95	116.65	122.60
2	B	480	GLY	CA-C-N	5.95	128.52	120.38
2	B	480	GLY	C-N-CA	5.95	128.52	120.38
1	A	139	VAL	CA-CB-CG1	5.91	120.45	110.40
2	B	331	LEU	CA-C-O	-5.91	113.51	120.60
1	A	145	ARG	CB-CA-C	-5.88	99.88	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	136	ALA	CA-C-O	-5.88	113.89	120.66
2	B	231	ASN	CA-C-O	5.87	125.00	120.48
1	A	15	GLY	N-CA-C	-5.85	107.18	115.43
1	A	135	ALA	O-C-N	5.84	128.31	122.12
2	B	452	LEU	O-C-N	-5.83	115.82	123.28
2	B	498	LEU	CA-C-O	-5.81	113.63	120.60
2	B	460	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	19	ILE	CB-CG1-CD1	5.78	125.94	113.80
2	B	524	GLN	O-C-N	-5.78	115.39	122.20
1	A	139	VAL	N-CA-C	5.76	116.54	110.72
2	B	57	PHE	CA-C-O	-5.76	114.11	120.33
2	B	298	LEU	CA-C-O	-5.75	114.78	120.70
2	B	269	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	A	45	MET	CA-C-O	5.70	126.52	119.79
2	B	273	GLN	OE1-CD-NE2	5.67	128.27	122.60
2	B	110	ASN	CA-CB-CG	-5.66	106.94	112.60
1	A	202	ASN	CA-C-O	-5.64	114.84	121.16
2	B	233	GLN	O-C-N	-5.64	116.14	122.12
2	B	548	GLU	N-CA-CB	5.60	118.45	110.67
2	B	29	PRO	N-CA-CB	5.58	108.73	102.60
2	B	130	ASP	CA-CB-CG	5.57	118.17	112.60
2	B	25	GLY	N-CA-C	-5.55	104.59	111.70
2	B	86	LYS	CA-C-O	5.55	127.77	120.16
1	A	32	GLY	CA-C-O	5.55	126.77	121.05
1	A	190	ILE	O-C-N	-5.54	115.66	122.97
2	B	458	ASN	O-C-N	-5.53	114.87	122.23
1	A	134	VAL	CA-C-O	-5.51	115.01	120.85
2	B	73	ASP	CB-CG-OD2	5.50	131.05	118.40
2	B	196	TYR	CA-C-N	5.49	125.40	119.85
2	B	196	TYR	C-N-CA	5.49	125.40	119.85
2	B	524	GLN	CA-C-N	5.48	128.07	120.29
2	B	524	GLN	C-N-CA	5.48	128.07	120.29
2	B	490	PRO	CA-C-O	-5.46	115.39	121.23
2	B	455	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	A	117	LYS	N-CA-C	5.46	117.93	111.33
2	B	162	ASN	CB-CG-ND2	5.45	124.58	116.40
2	B	233	GLN	CB-CG-CD	5.45	121.86	112.60
2	B	478	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	A	186	ALA	CA-C-N	5.43	125.70	119.83
1	A	186	ALA	C-N-CA	5.43	125.70	119.83
2	B	497	VAL	CB-CA-C	-5.43	101.00	110.71
2	B	455	ARG	NH1-CZ-NH2	5.42	126.34	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	VAL	CB-CA-C	-5.41	102.56	110.62
1	A	134	VAL	O-C-N	5.41	127.40	121.83
1	A	140	GLY	O-C-N	5.40	128.78	122.68
2	B	177	ILE	CB-CG1-CD1	5.38	125.11	113.80
1	A	86	SER	CA-CB-OG	-5.38	100.34	111.10
1	A	149	SER	CA-C-O	-5.37	114.41	120.43
2	B	173	GLN	CG-CD-NE2	5.37	124.45	116.40
2	B	339	TRP	CA-C-N	5.37	127.47	120.28
2	B	339	TRP	C-N-CA	5.37	127.47	120.28
2	B	343	GLY	N-CA-C	5.37	119.38	112.83
2	B	300	LEU	CA-C-N	5.33	125.40	119.32
2	B	300	LEU	C-N-CA	5.33	125.40	119.32
2	B	419	GLN	CA-C-N	5.28	127.62	120.38
2	B	419	GLN	C-N-CA	5.28	127.62	120.38
1	A	11	ARG	CD-NE-CZ	5.28	131.79	124.40
2	B	364	PRO	N-CA-CB	5.28	107.94	103.35
2	B	510	PHE	CA-C-N	5.26	130.44	122.98
2	B	510	PHE	C-N-CA	5.26	130.44	122.98
2	B	240	TRP	N-CA-C	-5.25	104.05	110.61
1	A	138	PHE	CA-C-O	-5.25	114.86	120.42
2	B	363	VAL	O-C-N	-5.24	116.69	121.41
1	A	82	ILE	CA-C-O	-5.22	115.31	120.85
1	A	139	VAL	CB-CA-C	-5.21	105.02	112.22
2	B	295	ASN	CA-CB-CG	-5.21	107.39	112.60
2	B	441	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	89	ASP	CA-CB-CG	-5.18	107.42	112.60
2	B	406	PRO	O-C-N	-5.16	115.30	122.37
2	B	525	LEU	O-C-N	-5.14	116.30	122.15
2	B	86	LYS	CA-C-N	5.13	125.53	119.99
2	B	86	LYS	C-N-CA	5.13	125.53	119.99
2	B	106	ILE	CA-C-O	-5.13	115.00	120.59
2	B	475	GLU	OE1-CD-OE2	-5.13	110.59	122.90
2	B	99	MET	CA-C-O	-5.13	115.57	121.47
2	B	330	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	183	ASN	CA-C-N	5.09	124.75	119.56
1	A	183	ASN	C-N-CA	5.09	124.75	119.56
2	B	390	SER	N-CA-C	5.08	117.09	110.43
2	B	248	TYR	CA-C-O	5.08	124.28	119.76
2	B	457	ASN	N-CA-CB	5.07	118.67	110.41
2	B	512	ALA	N-CA-CB	5.07	116.78	110.04
2	B	265	THR	CA-C-N	5.06	127.57	120.28
2	B	265	THR	C-N-CA	5.06	127.57	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	TRP	CA-C-N	5.06	125.09	119.32
1	A	74	TRP	C-N-CA	5.06	125.09	119.32
1	A	117	LYS	O-C-N	-5.05	116.77	122.12
2	B	411	VAL	N-CA-CB	5.05	120.17	111.39
1	A	76	ASP	CB-CA-C	-5.03	102.43	110.79
1	A	186	ALA	O-C-N	-5.03	116.82	121.30
2	B	193	THR	CA-C-N	5.02	129.36	122.63
2	B	193	THR	C-N-CA	5.02	129.36	122.63
2	B	87	PRO	N-CA-CB	5.02	107.96	103.19
2	B	418	PRO	N-CA-CB	5.02	107.78	103.31
1	A	91	SER	CA-C-O	-5.02	115.21	120.63
2	B	406	PRO	CA-C-O	5.01	125.22	118.90
2	B	115	THR	N-CA-CB	5.01	119.54	110.83

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	110	ASN	Mainchain
2	B	26	TRP	Mainchain
2	B	290	SER	Mainchain
2	B	325	ARG	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	25	0
2	B	4415	0	4244	99	0
3	B	1	0	0	0	0
4	B	13	0	6	1	0
5	A	173	0	0	0	0
5	B	490	0	0	0	0
All	All	6748	0	5854	112	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 (112) 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:269:ARG:HH21	2:B:297:ARG:HD3	1.35	0.92
1:A:207:GLN:HE22	2:B:204:ASP:H	1.20	0.87
2:B:86:LYS:N	2:B:87:PRO:HD3	1.93	0.82
2:B:162:ASN:ND2	2:B:165:GLN:H	1.77	0.81
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.46	0.80
2:B:388:ASN:HD22	2:B:389:ILE:H	1.31	0.79
2:B:86:LYS:H	2:B:87:PRO:HD3	1.50	0.76
2:B:80:GLU:OE2	2:B:123:HIS:HD2	1.71	0.73
2:B:15:LYS:HG3	2:B:489:SER:HB2	1.71	0.71
1:A:118:GLN:NE2	1:A:118:GLN:H	1.87	0.70
2:B:162:ASN:HD22	2:B:165:GLN:H	1.37	0.70
2:B:384:THR:HG22	2:B:455:ARG:NH1	2.07	0.70
2:B:387:LEU:HD21	2:B:450:MET:HE1	1.72	0.70
2:B:173:GLN:HE22	2:B:175:LEU:H	1.40	0.68
2:B:60:ASN:HD21	2:B:63:ILE:H	1.40	0.68
2:B:384:THR:HG22	2:B:455:ARG:HH12	1.59	0.68
1:A:207:GLN:NE2	2:B:204:ASP:H	1.93	0.67
2:B:60:ASN:ND2	2:B:62:VAL:H	1.95	0.65
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.31	0.65
2:B:80:GLU:OE2	2:B:123:HIS:CD2	2.50	0.65
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.79	0.65
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.32	0.64
2:B:214:LYS:H	2:B:214:LYS:HD2	1.62	0.64
2:B:11:ALA:O	2:B:276:ARG:NH1	2.31	0.63
2:B:150:SER:HB3	2:B:173:GLN:HE21	1.64	0.63
1:A:199:LEU:HD21	2:B:225:MET:HE1	1.80	0.63
2:B:388:ASN:ND2	2:B:389:ILE:H	1.96	0.62
2:B:444:ASN:C	2:B:444:ASN:HD22	2.08	0.62
1:A:118:GLN:H	1:A:118:GLN:HE21	1.46	0.62
1:A:26:HIS:HE1	2:B:555:VAL:O	1.83	0.61
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.08	0.61
2:B:123:HIS:O	2:B:140:SER:HB2	2.00	0.61
2:B:173:GLN:NE2	2:B:175:LEU:H	1.99	0.60
2:B:89:TYR:CZ	2:B:98:LYS:HG3	2.38	0.59
2:B:129:THR:HG22	2:B:136:ALA:CB	2.32	0.59
2:B:384:THR:HG22	2:B:455:ARG:CZ	2.33	0.58
2:B:539:THR:O	2:B:543:VAL:HG23	2.04	0.58
2:B:60:ASN:HD22	2:B:62:VAL:H	1.51	0.58
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.11	0.58
2:B:60:ASN:HD22	2:B:60:ASN:C	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.83	0.58
2:B:339:TRP:CH2	2:B:450:MET:HE2	2.33	0.58
2:B:458:ASN:C	2:B:458:ASN:HD22	2.11	0.58
2:B:60:ASN:ND2	2:B:63:ILE:H	2.02	0.58
1:A:23:ASP:OD1	1:A:26:HIS:HD2	1.88	0.57
1:A:166:TYR:O	1:A:170:GLN:HB3	2.06	0.55
1:A:207:GLN:H	1:A:207:GLN:HE21	1.54	0.55
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.89	0.55
2:B:123:HIS:HE1	2:B:216:ASP:OD1	1.90	0.55
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.73	0.54
2:B:86:LYS:N	2:B:87:PRO:CD	2.67	0.54
2:B:384:THR:CG2	2:B:455:ARG:HH12	2.20	0.54
2:B:387:LEU:HD22	2:B:476:TYR:CE2	2.43	0.53
1:A:110:ASN:ND2	1:A:112:GLU:OE1	2.42	0.53
1:A:163:LYS:HG2	1:A:168:VAL:HA	1.91	0.52
2:B:89:TYR:CE1	2:B:98:LYS:HG3	2.45	0.52
1:A:206:SER:HB2	2:B:202:GLY:O	2.10	0.51
2:B:388:ASN:HD22	2:B:389:ILE:N	2.03	0.51
2:B:397:TYR:O	2:B:401:GLN:HG2	2.09	0.51
2:B:512:ALA:HB1	2:B:513:PRO:CD	2.38	0.51
2:B:121:THR:HG23	2:B:126:ILE:HD11	1.91	0.50
2:B:556:GLN:OE1	2:B:557:ARG:N	2.45	0.50
2:B:129:THR:HG22	2:B:136:ALA:HB2	1.93	0.50
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.47	0.50
1:A:130:GLU:HB2	1:A:131:PRO:HD2	1.94	0.49
2:B:61:GLY:HA2	2:B:497:VAL:HG21	1.95	0.49
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.47	0.49
2:B:151:LEU:HD23	2:B:151:LEU:C	2.38	0.48
1:A:155:ASN:ND2	2:B:254:PHE:HB3	2.29	0.48
2:B:384:THR:HG22	2:B:455:ARG:NH2	2.28	0.48
1:A:199:LEU:CD2	2:B:225:MET:HE1	2.44	0.48
2:B:262:ASP:OD1	2:B:264:VAL:HG12	2.14	0.48
2:B:317:ARG:O	2:B:321:GLU:HG3	2.14	0.47
2:B:20:ASN:ND2	2:B:57:PHE:HD1	2.12	0.47
2:B:495:ARG:HH11	2:B:495:ARG:HG3	1.78	0.47
2:B:317:ARG:HG3	2:B:317:ARG:HH11	1.80	0.47
2:B:129:THR:HA	2:B:136:ALA:HA	1.96	0.47
2:B:303:LEU:HD21	2:B:350:TRP:CE2	2.50	0.46
2:B:360:VAL:HG13	2:B:368:ASP:HB2	1.98	0.46
2:B:214:LYS:H	2:B:214:LYS:CD	2.26	0.45
2:B:387:LEU:HD22	2:B:476:TYR:HE2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:GLN:HE22	2:B:175:LEU:HG	1.82	0.44
2:B:60:ASN:ND2	2:B:60:ASN:C	2.74	0.44
2:B:20:ASN:ND2	2:B:57:PHE:CD1	2.85	0.44
2:B:92:HIS:HE1	2:B:216:ASP:OD2	1.99	0.44
2:B:250:ALA:O	2:B:251:SER:C	2.61	0.44
2:B:495:ARG:HA	2:B:496:PRO:HD3	1.92	0.43
1:A:152:GLU:OE2	2:B:76:ASP:HA	2.19	0.43
1:A:202:ASN:ND2	1:A:206:SER:OG	2.52	0.43
1:A:23:ASP:OD1	1:A:26:HIS:CD2	2.69	0.43
2:B:530:ASN:O	2:B:531:PHE:HB2	2.18	0.43
2:B:104:GLU:O	2:B:115:THR:HA	2.19	0.42
1:A:174:VAL:HG22	2:B:411:VAL:HG22	2.00	0.42
2:B:383:PRO:HG2	2:B:476:TYR:CE1	2.54	0.42
2:B:22:PRO:HB3	4:B:559:MNP:O4'	2.20	0.42
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.87	0.42
2:B:85:GLU:O	2:B:86:LYS:HG2	2.19	0.42
2:B:86:LYS:HE2	2:B:96:TRP:CB	2.50	0.42
2:B:86:LYS:HE2	2:B:96:TRP:CG	2.55	0.42
1:A:16:MET:HE3	2:B:35:ILE:N	2.35	0.42
1:A:56:GLU:O	2:B:109:LYS:HB2	2.21	0.41
1:A:130:GLU:HB2	1:A:131:PRO:CD	2.50	0.41
2:B:209:VAL:HB	2:B:210:PRO:HD2	2.02	0.41
2:B:284:ASP:OD1	2:B:287:ARG:NH2	2.53	0.41
2:B:378:THR:HG21	2:B:383:PRO:HD3	2.03	0.41
1:A:10:VAL:HG13	2:B:547:LYS:HD3	2.02	0.41
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.55	0.41
2:B:414:PHE:CZ	2:B:419:GLN:HG2	2.56	0.41
1:A:125:THR:HB	1:A:126:PRO:HD2	2.02	0.40
2:B:85:GLU:H	2:B:85:GLU:HG3	1.67	0.40
2:B:127:LEU:CD1	2:B:139:LYS:HB2	2.51	0.40
2:B:2:ASN:HD22	2:B:2:ASN:C	2.29	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%)	199 (98%)	4 (2%)	1 (0%)	24	27
2	B	555/557 (100%)	540 (97%)	15 (3%)	0	100	100
All	All	759/766 (99%)	739 (97%)	19 (2%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	MET

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	178/180 (99%)	167 (94%)	11 (6%)	16	19
2	B	460/460 (100%)	418 (91%)	42 (9%)	9	9
All	All	638/640 (100%)	585 (92%)	53 (8%)	10	11

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	6	GLU
1	A	13	GLU
1	A	109	THR
1	A	112	GLU
1	A	113	THR
1	A	118	GLN
1	A	145	ARG
1	A	169	SER
1	A	200	LYS
1	A	207	GLN
2	B	2	ASN

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Mol	Chain	Res	Type
2	B	8	LYS
2	B	35	ILE
2	B	60	ASN
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	162	ASN
2	B	184	VAL
2	B	201	SER
2	B	214	LYS
2	B	269	ARG
2	B	273	GLN
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
2	B	444	ASN
2	B	458	ASN
2	B	468	GLU
2	B	493	SER
2	B	495	ARG
2	B	497	VAL
2	B	502	VAL
2	B	517	VAL
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 (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	26	HIS
1	A	81	GLN
1	A	118	GLN
1	A	155	ASN
1	A	193	GLN
1	A	205	ASN
1	A	207	GLN
2	B	2	ASN
2	B	20	ASN
2	B	60	ASN
2	B	92	HIS
2	B	93	ASN
2	B	123	HIS
2	B	162	ASN
2	B	173	GLN
2	B	304	GLN
2	B	348	ASN
2	B	388	ASN
2	B	440	ASN
2	B	444	ASN
2	B	458	ASN
2	B	473	GLN

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](#)

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	MNP	B	559	-	13,13,13	2.92	2 (15%)	15,17,17	4.41	10 (66%)

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	MNP	B	559	-	-	1/6/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	559	MNP	O4'-N3'	9.52	1.39	1.22
4	B	559	MNP	O2-C1	-2.95	1.21	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559	MNP	C3'-C2'-C1'	-8.42	115.33	121.11
4	B	559	MNP	O4'-N3'-C3'	7.77	129.51	118.82
4	B	559	MNP	C4'-C3'-N3'	-7.41	112.87	119.34
4	B	559	MNP	C4'-C3'-C2'	5.80	127.57	120.11
4	B	559	MNP	O2-C1-C2	4.53	131.24	113.98
4	B	559	MNP	O2-C1-O1	-4.09	112.82	123.33
4	B	559	MNP	C2-C1'-C2'	-3.42	115.20	120.38
4	B	559	MNP	C2-C1'-C6'	2.70	124.86	120.89
4	B	559	MNP	C5'-C4'-C3'	-2.55	115.96	119.40
4	B	559	MNP	O1-C1-C2	-2.37	115.78	122.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	559	MNP	1	0

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%)	-0.64	0 100 100	15, 27, 55, 70	0
2	B	557/557 (100%)	-0.76	0 100 100	10, 24, 55, 101	0
All	All	763/766 (99%)	-0.72	0 100 100	10, 25, 55, 101	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	MNP	B	559	13/13	0.95	0.07	11,23,37,50	0
3	CA	B	558	1/1	0.99	0.02	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.