



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:18 PM UTC

PDB ID : 1AJP / pdb_00001ajp
Title : PENICILLIN ACYLASE COMPLEXED WITH 2,5-DIHYDROXYPHENYL ACETIC ACID
Authors : Done, S.H.
Deposited on : 1997-05-07
Resolution : 2.31 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

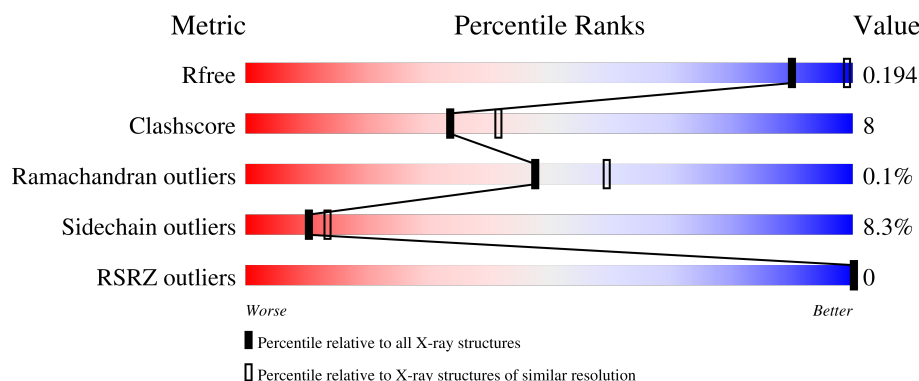
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OMD	A	210	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6768 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	2	0
			1678	1073	283	314	8			

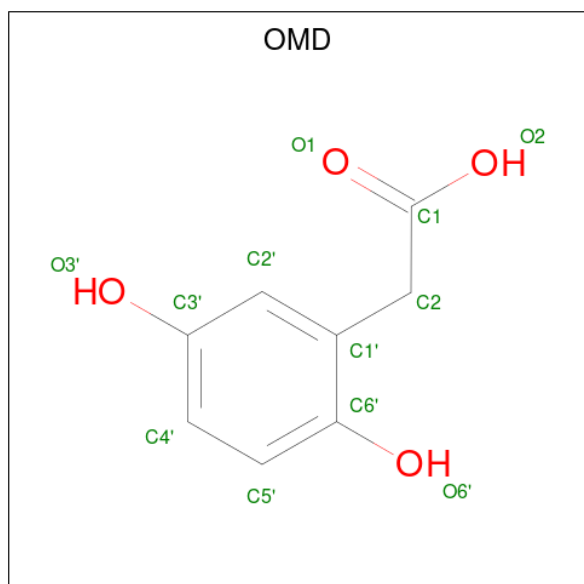
- Molecule 2 is a protein called PENICILLIN AMIDOHYDROLASE.

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 2-(3,6-DIHYDROXYPHENYL)ACETIC ACID (CCD ID: OMD) (formula: $C_8H_8O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is water.

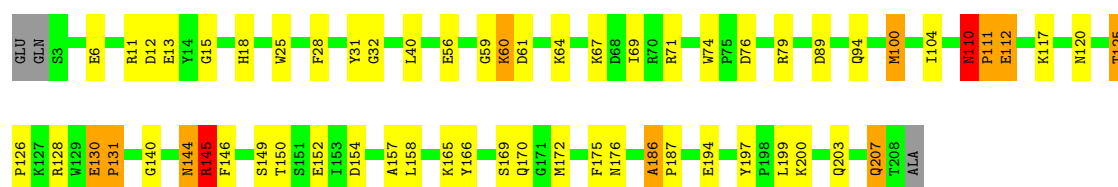
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total	O	0	0
			183	183		
5	B	479	Total	O	0	0
			479	479		

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.

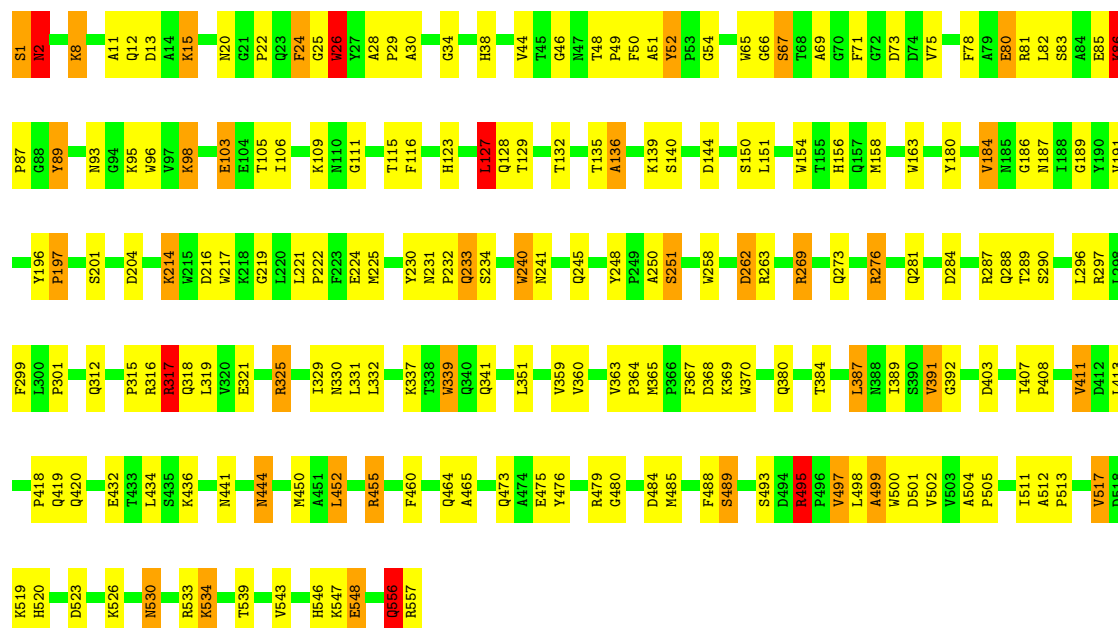
• Molecule 1: PENICILLIN AMIDOHYDROLASE

Chain A: 



• Molecule 2: PENICILLIN AMIDOHYDROLASE

Chain B: 



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)	26.81 – 2.31 26.81 – 2.36	Depositor EDS
% Data completeness (in resolution range)	96.1 (26.81-2.31) 96.2 (26.81-2.36)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.28 (at 2.36Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.146 , 0.225 (Not available) , 0.194	Depositor DCC
R_{free} test set	2431 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.2	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	6768	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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, OMD

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	0.85	1/1721 (0.1%)	2.04	57/2335 (2.4%)
2	B	0.85	1/4541 (0.0%)	2.00	156/6192 (2.5%)
All	All	0.85	2/6262 (0.0%)	2.01	213/8527 (2.5%)

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	3
2	B	0	4
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	132	THR	CB-OG1	7.26	1.55	1.43
1	A	125	THR	N-CA	6.35	1.51	1.45

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	363	VAL	CA-C-O	12.82	127.53	119.19
1	A	144	ASN	CA-C-N	12.61	144.22	122.79
1	A	144	ASN	C-N-CA	12.61	144.22	122.79
1	A	145[A]	ARG	CD-NE-CZ	11.08	139.91	124.40
1	A	145[B]	ARG	CD-NE-CZ	11.08	139.91	124.40
2	B	391	VAL	CB-CA-C	-10.98	97.92	111.97
2	B	269	ARG	CD-NE-CZ	10.94	139.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145[A]	ARG	CB-CA-C	-10.39	93.76	110.08
1	A	145[B]	ARG	CB-CA-C	-10.39	93.76	110.08
1	A	144	ASN	CA-C-O	-10.17	107.02	119.82
2	B	530	ASN	CA-CB-CG	9.53	122.13	112.60
2	B	184	VAL	CB-CA-C	-9.30	97.75	112.16
2	B	419	GLN	OE1-CD-NE2	9.17	131.77	122.60
2	B	407	ILE	CA-C-O	9.13	124.53	119.15
2	B	312	GLN	OE1-CD-NE2	8.76	131.36	122.60
2	B	219	GLY	CA-C-O	-8.52	113.47	120.79
2	B	547	LYS	CA-C-O	-8.45	111.29	120.92
2	B	389	ILE	CA-C-O	-8.44	111.23	120.85
2	B	263	ARG	NE-CZ-NH2	-8.38	111.66	119.20
2	B	269	ARG	CA-CB-CG	8.33	130.76	114.10
2	B	71	PHE	CA-CB-CG	-8.26	105.54	113.80
2	B	105	THR	CA-C-O	-8.16	111.54	120.36
2	B	248	TYR	CA-C-O	8.04	125.65	119.46
2	B	391	VAL	N-CA-CB	7.98	119.89	110.55
2	B	465	ALA	CA-C-O	-7.88	112.84	121.28
1	A	79	ARG	CD-NE-CZ	7.81	135.34	124.40
2	B	136	ALA	CA-C-O	-7.76	111.74	120.66
2	B	317	ARG	CD-NE-CZ	7.76	135.26	124.40
2	B	330	ASN	CB-CG-ND2	7.71	127.96	116.40
2	B	460	PHE	CA-CB-CG	7.70	121.50	113.80
2	B	367	PHE	CA-CB-CG	-7.69	106.11	113.80
2	B	105	THR	O-C-N	7.64	132.39	123.30
2	B	287	ARG	CD-NE-CZ	7.57	135.00	124.40
2	B	500	TRP	CA-C-O	-7.56	113.36	121.45
2	B	29	PRO	CA-C-N	7.49	132.06	120.75
2	B	29	PRO	C-N-CA	7.49	132.06	120.75
2	B	269	ARG	N-CA-CB	7.42	121.09	109.82
2	B	46	GLY	CA-C-O	-7.39	115.20	121.04
2	B	548	GLU	CA-CB-CG	7.38	128.85	114.10
2	B	50	PHE	CA-CB-CG	7.29	121.09	113.80
2	B	548	GLU	N-CA-CB	7.20	121.12	110.53
2	B	455	ARG	CD-NE-CZ	7.17	134.44	124.40
1	A	28	PHE	CA-CB-CG	-7.16	106.64	113.80
2	B	86	LYS	CA-CB-CG	7.16	128.41	114.10
2	B	331	LEU	CA-C-O	-7.16	112.01	120.60
2	B	341	GLN	CA-C-N	7.15	128.13	120.83
2	B	341	GLN	C-N-CA	7.15	128.13	120.83
2	B	184	VAL	N-CA-CB	7.13	122.85	110.65
2	B	363	VAL	O-C-N	-7.12	115.14	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	30	ALA	O-C-N	7.05	131.48	122.81
2	B	248	TYR	O-C-N	-7.04	115.32	121.31
1	A	100	MET	CA-C-O	7.04	127.89	120.42
1	A	117	LYS	N-CA-C	6.96	119.75	111.33
2	B	66	GLY	CA-C-O	-6.82	114.99	121.60
2	B	24	PHE	CA-CB-CG	6.79	120.59	113.80
2	B	103	GLU	CA-C-O	-6.77	113.54	120.71
2	B	34	GLY	CA-C-O	-6.71	115.47	121.64
1	A	149	SER	CA-C-O	-6.62	113.05	120.54
2	B	316	ARG	NE-CZ-NH2	6.62	125.16	119.20
2	B	290	SER	CB-CA-C	-6.61	99.44	110.68
2	B	284	ASP	CA-CB-CG	-6.55	106.05	112.60
1	A	165	LYS	CA-C-O	-6.53	113.97	120.82
2	B	319	LEU	CA-C-O	-6.51	113.93	120.90
1	A	111	PRO	N-CA-CB	6.49	109.74	103.51
2	B	80	GLU	CA-CB-CG	6.45	127.01	114.10
1	A	110	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	140	GLY	CA-C-O	-6.42	111.92	119.50
1	A	11	ARG	CD-NE-CZ	6.42	133.38	124.40
2	B	54	GLY	O-C-N	-6.33	117.02	123.35
2	B	276	ARG	CA-C-O	-6.30	113.73	121.11
2	B	231	ASN	CA-C-O	6.29	125.33	120.48
1	A	56	GLU	N-CA-CB	6.29	119.36	110.12
1	A	186	ALA	CA-C-N	6.27	126.60	119.83
1	A	186	ALA	C-N-CA	6.27	126.60	119.83
2	B	187	ASN	CA-C-O	-6.24	114.29	121.47
2	B	245	GLN	N-CA-CB	-6.23	101.91	111.56
1	A	71	ARG	CD-NE-CZ	6.20	133.08	124.40
2	B	325	ARG	CD-NE-CZ	-6.18	115.74	124.40
2	B	263	ARG	NE-CZ-NH1	6.16	127.66	121.50
2	B	473	GLN	OE1-CD-NE2	-6.16	116.44	122.60
2	B	156	HIS	CA-CB-CG	-6.15	107.65	113.80
2	B	269	ARG	NE-CZ-NH1	6.15	127.65	121.50
1	A	32	GLY	O-C-N	-6.13	116.31	122.19
1	A	32	GLY	CA-C-N	6.12	128.76	120.44
1	A	32	GLY	C-N-CA	6.12	128.76	120.44
1	A	150	THR	CA-C-O	-6.11	114.73	121.33
1	A	117	LYS	O-C-N	-6.09	115.66	122.12
2	B	479	ARG	NE-CZ-NH2	-6.02	113.78	119.20
2	B	339	TRP	CA-C-N	6.00	129.42	120.31
2	B	339	TRP	C-N-CA	6.00	129.42	120.31
1	A	60	LYS	CA-C-O	-6.00	113.33	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	144	ASP	OD1-CG-OD2	-5.97	108.57	122.90
1	A	120	ASN	CA-CB-CG	-5.96	106.64	112.60
1	A	186	ALA	CA-C-O	5.94	125.33	119.75
2	B	479	ARG	NE-CZ-NH1	5.94	127.44	121.50
2	B	132	THR	OG1-CB-CG2	-5.89	97.53	109.30
2	B	216	ASP	CA-CB-CG	5.87	118.47	112.60
2	B	233	GLN	O-C-N	-5.86	115.91	122.12
2	B	301	PRO	CA-C-N	5.86	128.13	120.28
2	B	301	PRO	C-N-CA	5.86	128.13	120.28
2	B	233	GLN	CB-CG-CD	5.85	122.55	112.60
2	B	418	PRO	N-CA-CB	5.84	108.51	103.31
2	B	546	HIS	CA-CB-CG	-5.84	107.96	113.80
2	B	489	SER	CB-CA-C	-5.84	107.05	111.20
1	A	175	PHE	CA-C-O	-5.82	114.67	120.90
2	B	364	PRO	N-CA-CB	5.80	108.74	103.34
2	B	89	TYR	CA-C-O	-5.77	114.71	121.46
2	B	15	LYS	CA-C-O	-5.77	112.80	118.97
2	B	2	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	61	ASP	CA-CB-CG	5.75	118.35	112.60
2	B	75	VAL	CA-C-O	-5.75	114.46	120.27
2	B	29	PRO	N-CA-CB	5.73	108.91	102.60
2	B	52	TYR	CA-C-N	5.71	125.18	119.24
2	B	52	TYR	C-N-CA	5.71	125.18	119.24
2	B	408	PRO	N-CA-CB	5.71	108.25	103.17
2	B	407	ILE	N-CA-C	5.66	113.47	107.76
2	B	240	TRP	N-CA-C	-5.64	103.75	110.41
2	B	498	LEU	CA-C-O	-5.62	113.85	120.60
1	A	176	ASN	OD1-CG-ND2	-5.62	116.98	122.60
2	B	28	ALA	CA-C-O	-5.61	115.21	119.59
1	A	146[A]	PHE	CA-C-N	5.60	131.52	121.15
1	A	146[A]	PHE	C-N-CA	5.60	131.52	121.15
1	A	146[B]	PHE	CA-C-N	5.60	131.52	121.15
1	A	146[B]	PHE	C-N-CA	5.60	131.52	121.15
2	B	296	LEU	CA-C-N	5.60	127.78	120.28
2	B	296	LEU	C-N-CA	5.60	127.78	120.28
2	B	480	GLY	CA-C-N	5.59	127.77	120.28
2	B	480	GLY	C-N-CA	5.59	127.77	120.28
1	A	15	GLY	N-CA-C	-5.58	107.61	115.32
2	B	86	LYS	CA-C-N	5.58	126.02	119.99
2	B	86	LYS	C-N-CA	5.58	126.02	119.99
2	B	8	LYS	CB-CA-C	-5.58	101.58	110.84
2	B	391	VAL	CA-C-N	5.57	126.28	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391	VAL	C-N-CA	5.57	126.28	119.99
2	B	127	LEU	CA-C-O	5.56	126.43	120.70
1	A	56	GLU	CA-C-O	-5.54	114.67	120.55
2	B	150	SER	CA-C-N	5.53	128.00	120.54
2	B	150	SER	C-N-CA	5.53	128.00	120.54
2	B	25	GLY	N-CA-C	-5.52	104.44	112.17
2	B	191	VAL	N-CA-CB	5.52	120.52	111.58
1	A	157	ALA	CA-C-O	-5.51	113.63	119.97
2	B	281	GLN	CA-C-O	-5.51	114.58	120.42
1	A	152	GLU	N-CA-CB	5.49	118.19	110.12
1	A	144	ASN	O-C-N	-5.49	115.13	122.43
2	B	301	PRO	O-C-N	-5.48	115.94	122.24
2	B	30	ALA	N-CA-CB	5.47	118.08	110.04
2	B	533	ARG	NE-CZ-NH2	5.46	124.11	119.20
2	B	488	PHE	CA-C-O	5.44	126.84	120.80
2	B	15	LYS	O-C-N	5.44	129.06	122.48
1	A	76	ASP	CB-CA-C	-5.41	100.63	110.63
2	B	363	VAL	CA-C-N	5.37	125.13	119.76
2	B	363	VAL	C-N-CA	5.37	125.13	119.76
1	A	186	ALA	O-C-N	-5.37	116.53	121.30
2	B	497	VAL	CB-CA-C	-5.36	101.11	110.71
2	B	262	ASP	CA-CB-CG	-5.35	107.25	112.60
2	B	248	TYR	CA-C-N	5.35	125.11	119.76
2	B	248	TYR	C-N-CA	5.35	125.11	119.76
1	A	128	ARG	CA-C-O	-5.34	115.33	121.47
2	B	452	LEU	O-C-N	-5.34	117.03	123.27
2	B	196	TYR	CA-C-N	5.33	125.27	119.78
2	B	196	TYR	C-N-CA	5.33	125.27	119.78
1	A	40	LEU	N-CA-C	5.32	116.76	111.07
1	A	74	TRP	CA-C-N	5.31	125.37	119.32
1	A	74	TRP	C-N-CA	5.31	125.37	119.32
1	A	158	LEU	CA-C-N	5.31	127.39	120.28
1	A	158	LEU	C-N-CA	5.31	127.39	120.28
2	B	359	VAL	CA-C-O	5.31	126.80	121.17
2	B	73	ASP	CB-CG-OD2	5.29	130.57	118.40
2	B	20	ASN	CA-C-O	-5.29	114.45	120.32
2	B	495	ARG	CA-C-N	5.29	124.90	119.56
2	B	495	ARG	C-N-CA	5.29	124.90	119.56
1	A	154	ASP	CA-C-O	-5.28	114.82	120.42
2	B	341	GLN	CA-C-O	-5.28	113.85	120.23
2	B	434	LEU	CA-C-O	-5.27	114.83	120.42
2	B	392	GLY	CA-C-O	-5.25	115.65	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	ARG	NH1-CZ-NH2	-5.22	112.52	119.30
1	A	31	TYR	CA-CB-CG	5.21	123.27	113.90
2	B	499	ALA	CA-C-O	-5.20	115.17	120.99
2	B	484	ASP	CA-C-O	-5.20	115.17	120.99
2	B	128	GLN	CA-C-O	5.19	126.78	121.23
1	A	197	TYR	O-C-N	5.18	127.23	121.43
2	B	289	THR	CA-C-O	-5.18	115.06	120.55
2	B	78	PHE	CA-CB-CG	5.18	118.98	113.80
2	B	230	TYR	CA-C-N	-5.18	117.24	122.83
2	B	230	TYR	C-N-CA	-5.18	117.24	122.83
2	B	464	GLN	CG-CD-NE2	5.18	124.17	116.40
1	A	59	GLY	CA-C-N	5.17	127.73	120.28
1	A	59	GLY	C-N-CA	5.17	127.73	120.28
2	B	556	GLN	N-CA-CB	5.17	119.74	110.80
2	B	73	ASP	OD1-CG-OD2	-5.17	110.50	122.90
2	B	287	ARG	NE-CZ-NH1	5.15	126.65	121.50
2	B	186	GLY	CA-C-O	-5.11	113.18	119.06
1	A	69	ILE	O-C-N	-5.11	116.83	121.94
2	B	411	VAL	N-CA-CB	5.09	120.24	111.39
2	B	464	GLN	OE1-CD-NE2	-5.09	117.51	122.60
2	B	413	LEU	O-C-N	-5.08	115.62	122.43
2	B	329	ILE	CA-C-O	-5.08	114.75	120.74
2	B	187	ASN	OD1-CG-ND2	5.07	127.67	122.60
2	B	475	GLU	N-CA-C	5.07	117.03	108.96
1	A	94	GLN	CG-CD-NE2	5.05	123.98	116.40
2	B	232	PRO	O-C-N	-5.05	116.92	123.03
2	B	288	GLN	N-CA-C	5.05	117.18	111.02
2	B	132	THR	N-CA-CB	5.04	117.32	110.01
2	B	197	PRO	N-CA-CB	5.04	107.73	103.35
2	B	1	SER	CB-CA-C	-5.04	100.53	110.10
2	B	111	GLY	O-C-N	-5.04	116.15	122.70
1	A	89	ASP	CA-CB-CG	-5.03	107.57	112.60
2	B	325	ARG	N-CA-CB	-5.03	102.56	110.46
2	B	452	LEU	CA-C-O	5.03	125.57	120.24
2	B	476	TYR	N-CA-CB	5.03	117.39	109.69
2	B	258	TRP	N-CA-CB	5.03	118.59	110.65
2	B	26	TRP	CA-C-O	-5.02	114.92	120.24
2	B	332	LEU	CA-C-O	-5.01	115.71	121.47

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ASN	Mainchain
1	A	145[A]	ARG	Mainchain
1	A	145[B]	ARG	Mainchain
2	B	234	SER	Mainchain
2	B	26	TRP	Mainchain
2	B	299	PHE	Mainchain
2	B	370	TRP	Mainchain

5.2 Too-close contacts [i](#)

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	1678	0	1625	22	0
2	B	4415	0	4244	81	0
3	A	12	0	6	4	0
4	B	1	0	0	0	0
5	A	183	0	0	0	0
5	B	479	0	0	0	0
All	All	6768	0	5875	92	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 8.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLN:HE22	2:B:204:ASP:H	1.14	0.94
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.36	0.88
1:A:18:HIS:HD2	2:B:38:HIS:NE2	1.83	0.76
2:B:86:LYS:N	2:B:87:PRO:HD3	2.06	0.70
2:B:240:TRP:O	2:B:241:ASN:HB2	1.88	0.70
2:B:387:LEU:HD21	2:B:450:MET:HE1	1.73	0.70
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.57	0.69
2:B:384:THR:HG22	2:B:455:ARG:NH2	2.10	0.67
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.09	0.67
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.77	0.66
2:B:384:THR:HG22	2:B:455:ARG:HH22	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:PRO:HA	2:B:318:GLN:HG3	1.76	0.66
2:B:384:THR:HG22	2:B:455:ARG:NH1	2.11	0.66
2:B:384:THR:HG22	2:B:455:ARG:HH12	1.62	0.65
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.32	0.64
2:B:520:HIS:HE1	2:B:548:GLU:OE2	1.81	0.64
2:B:15:LYS:HG3	2:B:489:SER:HB2	1.81	0.63
1:A:207:GLN:NE2	2:B:204:ASP:H	1.91	0.62
2:B:384:THR:HG22	2:B:455:ARG:CZ	2.31	0.61
1:A:12:ASP:O	2:B:548:GLU:HG2	2.01	0.59
2:B:86:LYS:N	2:B:87:PRO:CD	2.65	0.59
2:B:214:LYS:H	2:B:214:LYS:HD2	1.66	0.59
2:B:11:ALA:O	2:B:276:ARG:NH1	2.31	0.58
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.38	0.58
2:B:384:THR:CG2	2:B:455:ARG:HH12	2.18	0.57
1:A:25:TRP:CE2	2:B:557:ARG:HG3	2.40	0.56
2:B:512:ALA:HB1	2:B:513:PRO:CD	2.35	0.56
2:B:123:HIS:O	2:B:140:SER:HB2	2.06	0.55
2:B:360:VAL:HG13	2:B:368:ASP:HB2	1.88	0.55
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.14	0.54
2:B:129:THR:HG22	2:B:136:ALA:CB	2.37	0.54
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.74	0.53
3:A:210:OMD:C2	2:B:69:ALA:HB2	2.38	0.53
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.91	0.52
2:B:556:GLN:OE1	2:B:557:ARG:N	2.39	0.52
2:B:495:ARG:HH11	2:B:495:ARG:HG3	1.75	0.52
1:A:207:GLN:H	1:A:207:GLN:HE21	1.57	0.52
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.93	0.52
2:B:214:LYS:H	2:B:214:LYS:CD	2.23	0.51
3:A:210:OMD:H4'	2:B:67:SER:HB3	1.93	0.51
2:B:444:ASN:C	2:B:444:ASN:HD22	2.18	0.50
1:A:67:LYS:HG2	2:B:116:PHE:CE1	2.46	0.50
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.93	0.50
2:B:89:TYR:CZ	2:B:98:LYS:HG3	2.47	0.50
2:B:222:PRO:HD2	2:B:225:MET:HG3	1.94	0.49
1:A:194:GLU:OE2	2:B:233:GLN:HG3	2.12	0.49
2:B:83:SER:HB2	2:B:96:TRP:CZ3	2.48	0.49
2:B:65:TRP:HA	2:B:180:TYR:O	2.12	0.49
3:A:210:OMD:C1'	2:B:69:ALA:HB2	2.43	0.48
2:B:519:LYS:HE3	2:B:548:GLU:OE2	2.13	0.48
1:A:199:LEU:HD21	2:B:225:MET:HE1	1.95	0.48
1:A:166:TYR:O	1:A:170:GLN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:LYS:H	2:B:87:PRO:HD3	1.75	0.48
1:A:18:HIS:CD2	2:B:38:HIS:NE2	2.74	0.47
2:B:339:TRP:CH2	2:B:450:MET:HE2	2.43	0.47
1:A:172:MET:HE2	1:A:203:GLN:O	2.16	0.46
2:B:539:THR:O	2:B:543:VAL:HG23	2.15	0.46
1:A:100:MET:O	1:A:104:ILE:HG13	2.16	0.46
1:A:145[A]:ARG:HD2	1:A:145[A]:ARG:HA	1.83	0.46
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.51	0.45
1:A:187:PRO:HG2	2:B:262:ASP:HB3	1.98	0.45
2:B:51:ALA:O	2:B:52:TYR:C	2.60	0.45
2:B:129:THR:HG22	2:B:136:ALA:HB1	1.97	0.45
2:B:504:ALA:HA	2:B:505:PRO:C	2.41	0.45
2:B:317:ARG:O	2:B:321:GLU:HG3	2.17	0.44
2:B:441:ASN:O	2:B:444:ASN:ND2	2.50	0.44
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.99	0.44
2:B:325:ARG:HH11	2:B:325:ARG:HD2	1.59	0.44
2:B:93:ASN:HD22	2:B:93:ASN:HA	1.68	0.44
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.53	0.44
1:A:110:ASN:ND2	1:A:112:GLU:OE1	2.50	0.44
2:B:80:GLU:O	2:B:135:THR:HA	2.18	0.43
2:B:250:ALA:O	2:B:251:SER:C	2.61	0.43
2:B:2:ASN:C	2:B:2:ASN:HD22	2.26	0.43
2:B:48:THR:HA	2:B:49:PRO:HD3	1.89	0.43
2:B:221:LEU:HD22	2:B:225:MET:HE2	2.00	0.43
1:A:100:MET:HE2	1:A:100:MET:HB3	1.90	0.42
1:A:130:GLU:HB2	1:A:131:PRO:HD2	2.01	0.42
2:B:12:GLN:O	2:B:13:ASP:HB2	2.18	0.42
2:B:317:ARG:HG3	2:B:317:ARG:HH11	1.85	0.42
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.88	0.42
3:A:210:OMD:H2'	2:B:1:SER:OG	2.20	0.42
1:A:125:THR:HB	1:A:126:PRO:HD2	2.01	0.41
2:B:127:LEU:CD1	2:B:139:LYS:HB2	2.50	0.41
2:B:127:LEU:HD11	2:B:139:LYS:HB2	2.03	0.41
1:A:110:ASN:N	1:A:111:PRO:HD3	2.35	0.41
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.56	0.41
2:B:485:MET:O	2:B:499:ALA:HA	2.20	0.41
1:A:199:LEU:CD2	2:B:225:MET:HE1	2.51	0.40
2:B:151:LEU:HD23	2:B:151:LEU:C	2.47	0.40
2:B:501:ASP:OD1	2:B:534:LYS:NZ	2.52	0.40
2:B:1:SER:H3	2:B:241:ASN:HD21	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
2	B	555/557 (100%)	538 (97%)	16 (3%)	1 (0%)	43	53
All	All	761/766 (99%)	738 (97%)	22 (3%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	SER

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	180/180 (100%)	167 (93%)	13 (7%)	13	17
2	B	460/460 (100%)	419 (91%)	41 (9%)	9	11
All	All	640/640 (100%)	586 (92%)	54 (8%)	10	13

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	13	GLU
1	A	60	LYS
1	A	64	LYS
1	A	110	ASN

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Mol	Chain	Res	Type
1	A	112	GLU
1	A	130	GLU
1	A	131	PRO
1	A	145[A]	ARG
1	A	145[B]	ARG
1	A	169	SER
1	A	200	LYS
1	A	207	GLN
2	B	2	ASN
2	B	8	LYS
2	B	67	SER
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	201	SER
2	B	214	LYS
2	B	224	GLU
2	B	273	GLN
2	B	317	ARG
2	B	337	LYS
2	B	351	LEU
2	B	365	MET
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	493	SER
2	B	495	ARG

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Mol	Chain	Res	Type
2	B	497	VAL
2	B	502	VAL
2	B	517	VAL
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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	94	GLN
1	A	110	ASN
1	A	204	GLN
1	A	207	GLN
2	B	2	ASN
2	B	93	ASN
2	B	233	GLN
2	B	241	ASN
2	B	245	GLN
2	B	288	GLN
2	B	348	ASN
2	B	440	ASN
2	B	444	ASN
2	B	520	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$
3	OMD	A	210	-	12,12,12	3.92	2 (16%)	16,16,16	1.91	8 (50%)

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
3	OMD	A	210	-	-	4/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	210	OMD	O6'-C6'	-13.24	1.09	1.36
3	A	210	OMD	O2-C1	-2.13	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	210	OMD	O3'-C3'-C4'	-3.27	110.89	120.00
3	A	210	OMD	C4'-C3'-C2'	3.05	123.53	120.19
3	A	210	OMD	C5'-C4'-C3'	-2.41	117.33	119.88
3	A	210	OMD	O3'-C3'-C2'	2.19	125.58	119.85
3	A	210	OMD	C5'-C6'-C1'	2.16	122.89	120.43
3	A	210	OMD	O2-C1-O1	-2.09	117.95	123.33
3	A	210	OMD	O2-C1-C2	2.08	121.91	113.98
3	A	210	OMD	O6'-C6'-C5'	-2.02	113.94	119.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	210	OMD	C6'-C1'-C2-C1
3	A	210	OMD	C2'-C1'-C2-C1
3	A	210	OMD	O1-C1-C2-C1'
3	A	210	OMD	O2-C1-C2-C1'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	210	OMD	4	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%)	-0.58	0 100 100	11, 24, 55, 69	2 (0%)
2	B	557/557 (100%)	-0.68	0 100 100	8, 23, 56, 100	0
All	All	763/766 (99%)	-0.65	0 100 100	8, 24, 55, 100	2 (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
3	OMD	A	210	12/12	0.79	0.23	20,30,41,43	12
4	CA	B	558	1/1	1.00	0.01	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.