



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:37 AM UTC

PDB ID : 1AI6 / pdb_00001ai6
Title : PENICILLIN ACYLASE WITH P-HYDROXYPHENYLACETIC ACID
Authors : Done, S.H.
Deposited on : 1997-05-01
Resolution : 2.55 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

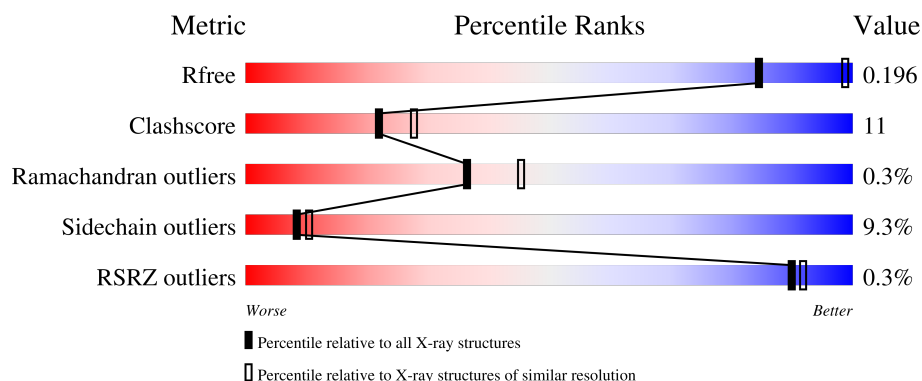
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	% 68% 19% 6% 7%
2	B	557	63% 29% 6% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6598 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	195	Total	C	N	O	S	0	0	0
			1565	1002	261	294	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			

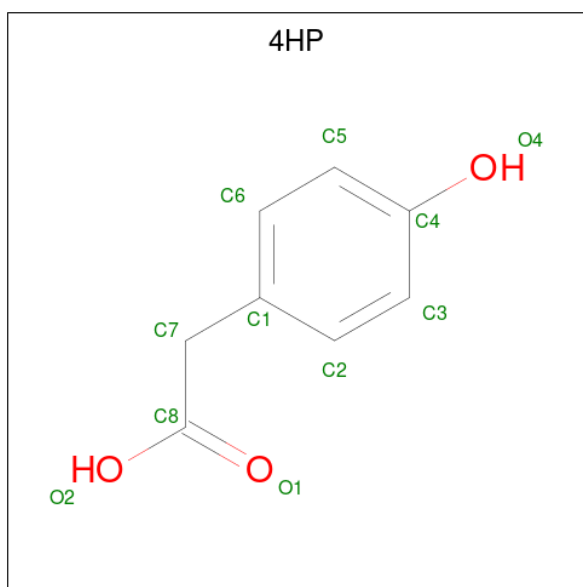
There is a discrepancy between the modelled and reference sequences:

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 4-HYDROXYPHENYLACETATE (CCD ID: 4HP) (formula: C₈H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	8	3		

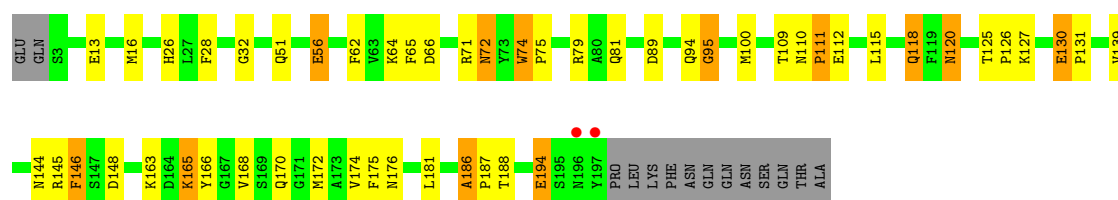
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	148	Total	O	0	0
			148	148		
5	B	458	Total	O	0	0
			458	458		

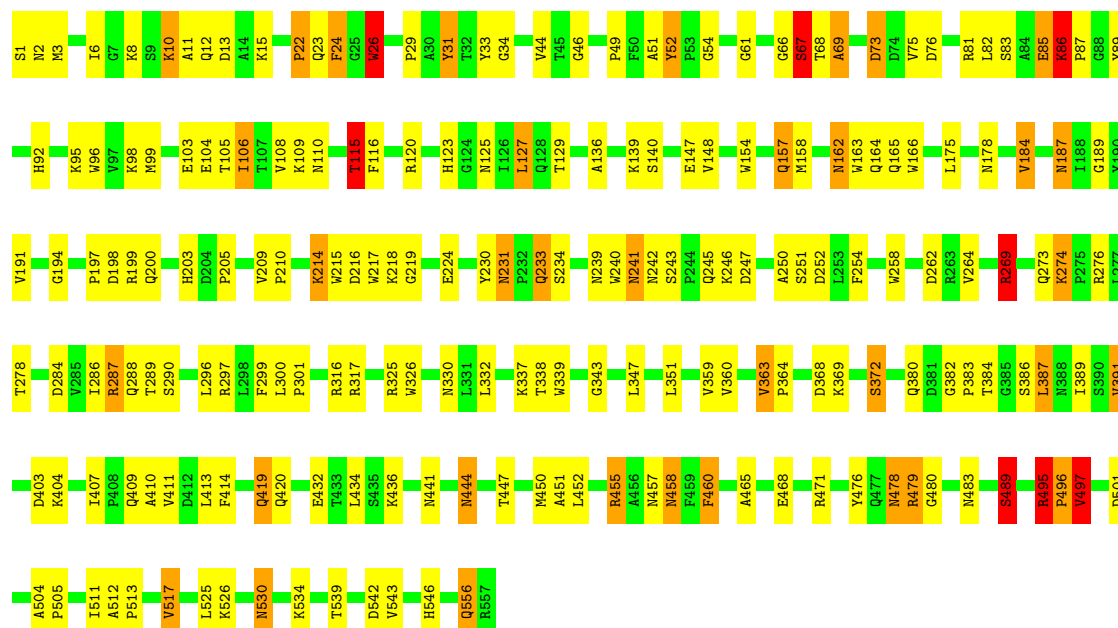
3 Residue-property plots

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)	28.06 – 2.55 28.06 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.6 (28.06-2.55) 94.1 (28.06-2.55)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.54 (at 2.57Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.137 , 0.220 0.128 , 0.196	Depositor DCC
R_{free} test set	1887 reflections (7.23%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 85.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6598	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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: 4HP, 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	0.81	2/1605 (0.1%)	1.84	31/2179 (1.4%)
2	B	0.87	5/4541 (0.1%)	1.98	109/6192 (1.8%)
All	All	0.85	7/6146 (0.1%)	1.94	140/8371 (1.7%)

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	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	241	ASN	C-N	-20.60	1.04	1.33
2	B	69	ALA	C-N	-19.57	1.04	1.33
1	A	146	PHE	C-N	-14.62	1.08	1.34
2	B	240	TRP	C-N	-11.62	1.18	1.33
2	B	68	THR	C-N	-9.78	1.20	1.33
1	A	144	ASN	C-N	-9.05	1.21	1.33
2	B	68	THR	CA-C	5.74	1.59	1.52

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	69	ALA	CA-C-N	25.82	172.03	121.41
2	B	69	ALA	C-N-CA	25.82	172.03	121.41
2	B	241	ASN	O-C-N	-22.08	94.40	122.00
2	B	241	ASN	CA-C-N	21.27	162.16	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	ASN	C-N-CA	21.27	162.16	121.54
2	B	69	ALA	O-C-N	-19.81	98.39	122.95
2	B	240	TRP	CA-C-O	-17.41	103.09	121.20
2	B	68	THR	CA-C-O	-13.08	105.89	121.06
2	B	75	VAL	CA-C-O	-11.72	107.94	120.36
2	B	76	ASP	CA-CB-CG	11.39	123.99	112.60
2	B	407	ILE	CA-C-O	10.08	124.77	119.12
2	B	391	VAL	CB-CA-C	-9.81	99.42	111.97
2	B	240	TRP	O-C-N	9.35	133.58	121.99
2	B	530	ASN	CA-CB-CG	9.26	121.86	112.60
2	B	391	VAL	N-CA-CB	8.99	121.07	110.55
2	B	269	ARG	CD-NE-CZ	8.90	136.86	124.40
1	A	79	ARG	CD-NE-CZ	8.81	136.74	124.40
2	B	489	SER	CA-C-O	8.13	126.74	120.48
2	B	242	ASN	N-CA-CB	7.95	123.92	110.49
2	B	67	SER	N-CA-CB	-7.88	97.98	111.69
2	B	46	GLY	CA-C-O	-7.84	115.50	120.91
2	B	525	LEU	N-CA-C	7.82	119.80	111.28
2	B	269	ARG	N-CA-CB	7.75	121.68	110.06
2	B	419	GLN	OE1-CD-NE2	7.64	130.24	122.60
2	B	240	TRP	N-CA-C	-7.59	101.12	110.61
1	A	62	PHE	CA-CB-CG	-7.50	106.30	113.80
1	A	146	PHE	CA-C-N	7.49	135.00	121.15
1	A	146	PHE	C-N-CA	7.49	135.00	121.15
2	B	465	ALA	CA-C-O	-7.39	113.37	121.28
2	B	219	GLY	CA-C-O	-7.34	114.48	120.79
2	B	288	GLN	OE1-CD-NE2	-7.25	115.35	122.60
1	A	168	VAL	N-CA-C	7.18	117.70	110.23
2	B	495	ARG	CA-C-N	7.04	126.67	119.56
2	B	495	ARG	C-N-CA	7.04	126.67	119.56
1	A	89	ASP	CA-CB-CG	-6.97	105.63	112.60
2	B	296	LEU	CA-C-N	6.97	129.93	120.38
2	B	296	LEU	C-N-CA	6.97	129.93	120.38
2	B	76	ASP	OD1-CG-OD2	-6.84	106.49	122.90
2	B	231	ASN	CA-C-N	6.72	126.70	119.78
2	B	231	ASN	C-N-CA	6.72	126.70	119.78
1	A	100	MET	CA-C-O	6.70	127.60	120.70
1	A	186	ALA	CA-C-O	6.70	125.33	119.71
2	B	241	ASN	CA-CB-CG	6.64	119.24	112.60
2	B	479	ARG	NE-CZ-NH2	-6.63	113.23	119.20
2	B	407	ILE	N-CA-C	6.57	113.53	107.56
2	B	460	PHE	CA-CB-CG	6.54	120.34	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	ASP	CB-CG-OD1	6.52	133.40	118.40
1	A	146	PHE	O-C-N	-6.52	114.51	122.20
2	B	458	ASN	CA-CB-CG	6.47	119.07	112.60
2	B	288	GLN	CB-CG-CD	6.40	123.48	112.60
2	B	245	GLN	N-CA-CB	-6.39	101.66	111.56
2	B	54	GLY	O-C-N	-6.38	116.84	123.48
2	B	33	TYR	CA-C-O	-6.28	113.58	120.24
2	B	194	GLY	CA-C-N	6.27	130.77	122.30
2	B	194	GLY	C-N-CA	6.27	130.77	122.30
1	A	26	HIS	CA-CB-CG	-6.25	107.55	113.80
2	B	269	ARG	CA-CB-CG	6.25	126.59	114.10
1	A	72	ASN	N-CA-C	6.20	119.87	112.93
2	B	29	PRO	CA-C-N	6.17	129.59	120.90
2	B	29	PRO	C-N-CA	6.17	129.59	120.90
1	A	111	PRO	N-CA-CB	6.16	109.43	103.51
2	B	241	ASN	CA-C-O	6.16	127.65	119.59
2	B	284	ASP	CA-CB-CG	-6.11	106.49	112.60
2	B	24	PHE	CA-CB-CG	6.07	119.87	113.80
2	B	290	SER	CB-CA-C	-6.07	100.72	110.79
1	A	144	ASN	CA-C-O	-6.06	112.64	119.79
2	B	471	ARG	O-C-N	-6.02	115.36	123.19
2	B	22	PRO	CA-C-O	-5.99	114.20	121.03
2	B	34	GLY	CA-C-O	-5.98	116.14	121.64
2	B	455	ARG	CD-NE-CZ	5.97	132.76	124.40
2	B	86	LYS	CA-CB-CG	5.97	126.03	114.10
2	B	434	LEU	CA-C-O	-5.91	114.62	120.70
2	B	175	LEU	CA-C-O	-5.90	114.69	121.47
2	B	389	ILE	CA-C-O	-5.89	114.05	120.71
2	B	363	VAL	CA-C-O	5.89	123.38	119.38
2	B	187	ASN	OD1-CG-ND2	5.83	128.43	122.60
2	B	497	VAL	CB-CA-C	-5.80	100.50	110.30
2	B	239	ASN	OD1-CG-ND2	-5.79	116.81	122.60
2	B	287	ARG	CD-NE-CZ	5.79	132.51	124.40
1	A	56	GLU	N-CA-CB	5.71	118.51	110.12
2	B	278	THR	CA-C-N	5.69	127.83	120.44
2	B	278	THR	C-N-CA	5.69	127.83	120.44
2	B	556	GLN	N-CA-CB	5.68	120.72	110.83
1	A	120	ASN	CA-CB-CG	-5.67	106.93	112.60
2	B	252	ASP	OD1-CG-OD2	-5.65	109.34	122.90
2	B	478	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	120	ASN	CA-C-O	-5.61	114.93	120.70
2	B	73	ASP	CA-CB-CG	-5.57	107.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ASP	N-CA-CB	5.56	118.07	110.01
1	A	115	LEU	CA-C-O	5.49	123.69	119.46
2	B	316	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	B	205	PRO	O-C-N	-5.48	112.24	122.33
2	B	480	GLY	CA-C-N	5.44	127.57	120.28
2	B	480	GLY	C-N-CA	5.44	127.57	120.28
2	B	108	VAL	N-CA-C	5.44	115.93	107.28
1	A	51	GLN	N-CA-C	-5.42	106.58	114.12
2	B	233	GLN	CA-C-N	5.41	128.07	120.28
2	B	233	GLN	C-N-CA	5.41	128.07	120.28
2	B	330	ASN	CB-CG-OD1	5.40	131.61	120.80
1	A	95	GLY	CA-C-N	5.40	127.83	120.54
1	A	95	GLY	C-N-CA	5.40	127.83	120.54
1	A	28	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	56	GLU	CB-CA-C	-5.38	101.86	110.79
2	B	286	ILE	N-CA-CB	5.36	116.82	110.55
1	A	175	PHE	CA-C-O	-5.33	115.19	120.90
2	B	52	TYR	CA-C-N	5.33	125.40	119.32
2	B	52	TYR	C-N-CA	5.33	125.40	119.32
2	B	457	ASN	CA-C-O	-5.27	114.86	120.92
2	B	332	LEU	CA-C-O	-5.27	115.81	121.56
2	B	330	ASN	OD1-CG-ND2	-5.27	117.33	122.60
2	B	54	GLY	CA-C-O	5.25	125.70	120.92
2	B	199	ARG	CA-C-N	5.25	128.16	120.71
2	B	199	ARG	C-N-CA	5.25	128.16	120.71
2	B	115	THR	N-CA-CB	5.24	120.49	111.00
2	B	269	ARG	CA-C-O	-5.24	114.97	120.63
1	A	174	VAL	CA-C-N	5.23	127.60	120.54
1	A	174	VAL	C-N-CA	5.23	127.60	120.54
2	B	240	TRP	CB-CA-C	5.22	120.33	111.35
2	B	289	THR	CA-C-N	5.22	127.27	120.28
2	B	289	THR	C-N-CA	5.22	127.27	120.28
2	B	234	SER	N-CA-C	5.22	117.71	111.71
2	B	200	GLN	CA-CB-CG	5.21	124.52	114.10
2	B	339	TRP	CA-C-N	5.16	128.15	120.31
2	B	339	TRP	C-N-CA	5.16	128.15	120.31
2	B	359	VAL	CB-CA-C	-5.16	105.37	111.97
2	B	359	VAL	N-CA-C	5.16	115.37	110.42
2	B	495	ARG	CD-NE-CZ	5.14	131.60	124.40
2	B	31	TYR	CA-C-O	-5.14	114.97	120.42
2	B	184	VAL	CB-CA-C	-5.14	101.98	111.79
2	B	191	VAL	N-CA-CB	5.13	119.90	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	TRP	CA-C-N	5.10	125.14	119.32
1	A	74	TRP	C-N-CA	5.10	125.14	119.32
1	A	32	GLY	O-C-N	-5.08	117.31	122.19
1	A	16	MET	CA-C-N	5.08	124.84	119.76
1	A	16	MET	C-N-CA	5.08	124.84	119.76
2	B	496	PRO	N-CA-CB	5.08	108.39	103.51
2	B	26	TRP	O-C-N	-5.07	117.34	123.27
2	B	465	ALA	O-C-N	5.05	128.34	123.29
2	B	106	ILE	CA-C-O	-5.04	114.90	120.74
2	B	245	GLN	N-CA-C	5.00	116.44	108.79

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	198	ASP	Mainchain
2	B	241	ASN	Mainchain,Peptide
2	B	26	TRP	Mainchain
2	B	299	PHE	Mainchain
2	B	372	SER	Mainchain
2	B	69	ALA	Peptide

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	1565	0	1515	24	0
2	B	4415	0	4242	111	0
3	B	1	0	0	0	0
4	B	11	0	7	1	0
5	A	148	0	0	1	0
5	B	458	0	0	2	0
All	All	6598	0	5764	126	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 11.

All (126) 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:387:LEU:HD21	2:B:450:MET:HE1	1.47	0.95
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.42	0.84
2:B:162:ASN:HD22	2:B:165:GLN:H	1.28	0.81
2:B:162:ASN:ND2	2:B:165:GLN:H	1.80	0.80
2:B:187:ASN:HD22	2:B:231:ASN:HD21	1.26	0.79
2:B:15:LYS:HG3	2:B:489:SER:HB2	1.62	0.79
2:B:120:ARG:HH11	2:B:125:ASN:ND2	1.82	0.78
2:B:479:ARG:HH21	2:B:483:ASN:HD22	1.37	0.70
2:B:384:THR:HG22	2:B:455:ARG:HH22	1.58	0.68
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.76	0.67
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.77	0.66
1:A:194:GLU:OE2	2:B:233:GLN:HG3	1.96	0.66
2:B:384:THR:HG22	2:B:455:ARG:NH2	2.10	0.65
1:A:118:GLN:NE2	1:A:118:GLN:H	1.93	0.65
2:B:187:ASN:ND2	2:B:231:ASN:HD21	1.96	0.64
1:A:72:ASN:HD21	2:B:139:LYS:NZ	1.96	0.64
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.33	0.64
2:B:384:THR:HG22	2:B:455:ARG:HH12	1.62	0.64
2:B:384:THR:HG22	2:B:455:ARG:NH1	2.13	0.63
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.14	0.63
2:B:86:LYS:N	2:B:87:PRO:HD3	2.14	0.62
2:B:105:THR:HG23	2:B:115:THR:HG22	1.80	0.62
2:B:214:LYS:H	2:B:214:LYS:HD2	1.65	0.62
2:B:387:LEU:HD22	2:B:476:TYR:CE2	2.34	0.62
2:B:539:THR:O	2:B:543:VAL:HG23	2.01	0.61
1:A:166:TYR:O	1:A:170:GLN:HB3	2.00	0.60
2:B:384:THR:HG22	2:B:455:ARG:CZ	2.31	0.60
2:B:512:ALA:HB1	2:B:513:PRO:CD	2.32	0.60
2:B:129:THR:HG22	2:B:136:ALA:CB	2.31	0.60
2:B:86:LYS:H	2:B:87:PRO:HD3	1.68	0.59
2:B:1:SER:HB3	2:B:22:PRO:HA	1.85	0.58
1:A:118:GLN:H	1:A:118:GLN:HE21	1.50	0.58
2:B:92:HIS:HE1	2:B:216:ASP:OD2	1.87	0.58
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.40	0.56
2:B:479:ARG:HH21	2:B:483:ASN:ND2	2.03	0.56
1:A:72:ASN:HD21	2:B:139:LYS:HZ3	1.52	0.56
2:B:89:TYR:CZ	2:B:98:LYS:HG3	2.41	0.56
2:B:86:LYS:N	2:B:87:PRO:CD	2.69	0.55
2:B:243:SER:HB2	2:B:258:TRP:CE3	2.41	0.55
2:B:123:HIS:O	2:B:140:SER:HB2	2.07	0.55
2:B:6:ILE:HG23	2:B:10:LYS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:ASN:HD21	2:B:165:GLN:HG3	1.73	0.54
2:B:387:LEU:HD22	2:B:476:TYR:HE2	1.74	0.53
2:B:109:LYS:HD2	2:B:110:ASN:ND2	2.24	0.53
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.44	0.53
2:B:129:THR:HG22	2:B:136:ALA:HB2	1.91	0.53
1:A:148:ASP:OD2	2:B:139:LYS:NZ	2.42	0.52
2:B:384:THR:CG2	2:B:455:ARG:HH12	2.22	0.52
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.19	0.51
2:B:413:LEU:HD12	5:B:730:HOH:O	2.10	0.51
2:B:413:LEU:CD1	5:B:730:HOH:O	2.58	0.51
2:B:243:SER:HB2	2:B:258:TRP:CD2	2.46	0.50
5:A:219:HOH:O	2:B:203:HIS:HE1	1.95	0.50
2:B:338:THR:HB	2:B:447:THR:O	2.11	0.50
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.77	0.50
2:B:209:VAL:HB	2:B:210:PRO:HD2	1.96	0.48
1:A:81:GLN:NE2	2:B:148:VAL:H	2.11	0.48
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.48	0.48
2:B:441:ASN:O	2:B:444:ASN:ND2	2.46	0.48
2:B:1:SER:HA	2:B:23:GLN:HG3	1.94	0.48
2:B:73:ASP:OD1	2:B:73:ASP:C	2.55	0.48
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.96	0.47
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.97	0.47
1:A:56:GLU:O	2:B:109:LYS:HB2	2.15	0.47
2:B:262:ASP:OD1	2:B:264:VAL:HG12	2.14	0.47
1:A:130:GLU:HB2	1:A:131:PRO:HD2	1.98	0.46
2:B:501:ASP:OD1	2:B:534:LYS:HE2	2.15	0.46
2:B:1:SER:OG	4:B:559:4HP:O2	2.29	0.46
2:B:504:ALA:HA	2:B:505:PRO:C	2.41	0.46
1:A:172:MET:HE3	1:A:176:ASN:OD1	2.16	0.45
2:B:31:TYR:CE2	2:B:49:PRO:HB3	2.51	0.45
2:B:3:MET:HE1	2:B:66:GLY:HA3	1.98	0.45
1:A:125:THR:HB	1:A:126:PRO:HD2	1.97	0.45
2:B:386:SER:HB2	2:B:478:ASN:HD21	1.80	0.45
2:B:127:LEU:CD1	2:B:139:LYS:HB2	2.47	0.45
2:B:300:LEU:N	2:B:301:PRO:CD	2.79	0.45
2:B:347:LEU:O	2:B:351:LEU:HB2	2.16	0.45
1:A:120:ASN:HD22	1:A:120:ASN:HA	1.59	0.45
2:B:157:GLN:NE2	2:B:166:TRP:HE1	2.14	0.44
2:B:214:LYS:H	2:B:214:LYS:CD	2.28	0.44
2:B:15:LYS:HG3	2:B:489:SER:CB	2.42	0.44
2:B:287:ARG:HG2	2:B:287:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:LYS:NZ	2:B:274:LYS:O	2.50	0.44
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.84	0.44
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.53	0.44
2:B:542:ASP:O	2:B:546:HIS:HD2	2.00	0.44
1:A:110:ASN:N	1:A:111:PRO:HD3	2.32	0.43
2:B:129:THR:HA	2:B:136:ALA:HA	2.00	0.43
2:B:86:LYS:HE2	2:B:96:TRP:CG	2.53	0.43
2:B:127:LEU:HD12	2:B:139:LYS:HB2	2.00	0.43
2:B:12:GLN:O	2:B:13:ASP:HB2	2.18	0.43
2:B:104:GLU:O	2:B:115:THR:HA	2.19	0.43
2:B:11:ALA:O	2:B:276:ARG:NH1	2.44	0.43
2:B:86:LYS:HE2	2:B:96:TRP:CB	2.49	0.43
2:B:61:GLY:HA2	2:B:497:VAL:HG21	2.01	0.43
2:B:85:GLU:H	2:B:85:GLU:HG3	1.61	0.43
2:B:495:ARG:HA	2:B:496:PRO:HD3	1.93	0.42
2:B:51:ALA:O	2:B:52:TYR:C	2.62	0.42
2:B:67:SER:HA	2:B:178:ASN:O	2.19	0.42
1:A:139:VAL:HG22	2:B:147:GLU:HB3	2.01	0.42
2:B:325:ARG:HH11	2:B:325:ARG:HD2	1.63	0.42
2:B:230:TYR:O	2:B:231:ASN:C	2.63	0.42
2:B:444:ASN:C	2:B:444:ASN:HD22	2.27	0.42
1:A:145:ARG:HD3	1:A:146:PHE:CE2	2.54	0.42
1:A:186:ALA:O	1:A:188:THR:HG23	2.20	0.42
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.55	0.42
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.55	0.42
2:B:414:PHE:CZ	2:B:419:GLN:HG2	2.55	0.42
1:A:65:PHE:CE1	2:B:460:PHE:HB3	2.54	0.42
2:B:246:LYS:O	2:B:247:ASP:HB2	2.19	0.42
2:B:409:GLN:O	2:B:410:ALA:C	2.63	0.41
1:A:74:TRP:HA	1:A:75:PRO:HD2	1.91	0.41
1:A:165:LYS:HG2	1:A:166:TYR:CE2	2.55	0.41
2:B:360:VAL:HG13	2:B:368:ASP:HB2	2.02	0.41
2:B:86:LYS:H	2:B:87:PRO:CD	2.33	0.41
1:A:81:GLN:HE22	2:B:148:VAL:H	1.67	0.41
2:B:120:ARG:HH11	2:B:125:ASN:HD21	1.62	0.41
2:B:363:VAL:HA	2:B:364:PRO:HD3	1.83	0.41
1:A:94:GLN:O	1:A:95:GLY:C	2.62	0.41
2:B:382:GLY:HA3	2:B:451:ALA:O	2.21	0.41
2:B:383:PRO:HG2	2:B:476:TYR:CE1	2.55	0.41
2:B:123:HIS:NE2	2:B:216:ASP:OD1	2.54	0.41
2:B:210:PRO:HG2	2:B:215:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:PHE:CD1	2:B:254:PHE:C	2.99	0.40
1:A:166:TYR:HB3	1:A:170:GLN:CG	2.51	0.40
2:B:89:TYR:CE1	2:B:98:LYS:HG3	2.57	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	193/209 (92%)	189 (98%)	4 (2%)	0	100	100
2	B	555/557 (100%)	539 (97%)	14 (2%)	2 (0%)	30	39
All	All	748/766 (98%)	728 (97%)	18 (2%)	2 (0%)	36	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	SER
2	B	86	LYS

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	167/180 (93%)	155 (93%)	12 (7%)	13	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	460/460 (100%)	414 (90%)	46 (10%)	7 9
All	All	627/640 (98%)	569 (91%)	58 (9%)	8 10

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	64	LYS
1	A	71	ARG
1	A	109	THR
1	A	112	GLU
1	A	118	GLN
1	A	127	LYS
1	A	130	GLU
1	A	163	LYS
1	A	165	LYS
1	A	181	LEU
1	A	194	GLU
2	B	2	ASN
2	B	8	LYS
2	B	10	LYS
2	B	67	SER
2	B	81	ARG
2	B	85	GLU
2	B	86	LYS
2	B	95	LYS
2	B	99	MET
2	B	103	GLU
2	B	115	THR
2	B	127	LEU
2	B	154	TRP
2	B	157	GLN
2	B	162	ASN
2	B	164	GLN
2	B	184	VAL
2	B	214	LYS
2	B	218	LYS
2	B	224	GLU
2	B	269	ARG
2	B	273	GLN
2	B	274	LYS
2	B	317	ARG

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Mol	Chain	Res	Type
2	B	337	LYS
2	B	369	LYS
2	B	372	SER
2	B	380	GLN
2	B	387	LEU
2	B	391	VAL
2	B	403	ASP
2	B	404	LYS
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	489	SER
2	B	495	ARG
2	B	497	VAL
2	B	517	VAL
2	B	526	LYS
2	B	530	ASN
2	B	556	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	72	ASN
1	A	81	GLN
1	A	118	GLN
1	A	120	ASN
1	A	170	GLN
2	B	2	ASN
2	B	20	ASN
2	B	92	HIS
2	B	93	ASN
2	B	125	ASN
2	B	131	GLN
2	B	157	GLN
2	B	162	ASN
2	B	164	GLN
2	B	169	GLN

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Mol	Chain	Res	Type
2	B	187	ASN
2	B	200	GLN
2	B	203	HIS
2	B	245	GLN
2	B	340	GLN
2	B	348	ASN
2	B	401	GLN
2	B	440	ASN
2	B	444	ASN
2	B	458	ASN
2	B	464	GLN
2	B	477	GLN
2	B	478	ASN
2	B	483	ASN
2	B	507	GLN
2	B	546	HIS
2	B	550	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	4HP	B	559	-	11,11,11	0.87	0	14,14,14	1.80	3 (21%)

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	4HP	B	559	-	-	0/4/4/4	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559	4HP	C7-C1-C6	-3.92	115.13	120.89
4	B	559	4HP	C6-C1-C2	2.73	122.29	118.23
4	B	559	4HP	C6-C5-C4	-2.35	117.39	119.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	4
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	68:THR	C	69:ALA	N	1.20
1	B	240:TRP	C	241:ASN	N	1.18
1	A	146:PHE	C	147:SER	N	1.08
1	B	69:ALA	C	70:GLY	N	1.04
1	B	241:ASN	C	242:ASN	N	1.04

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	195/209 (93%)	-0.81	2 (1%) 79 80	23, 35, 62, 77	0
2	B	557/557 (100%)	-0.84	0 100 100	18, 35, 70, 116	0
All	All	752/766 (98%)	-0.83	2 (0%) 90 92	18, 35, 67, 116	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	TYR	3.1
1	A	196	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	4HP	B	559	11/11	0.97	0.10	17,21,29,30	0
3	CA	B	558	1/1	0.99	0.06	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.