



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:08 am GMT

PDB ID : 1PNM  
Title : PENICILLIN ACYLASE HAS A SINGLE-AMINO-ACID CATALYTIC CENTRE  
Authors : Duggleby, H.J.; Moody, P.C.E.  
Deposited on : 1995-03-16  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

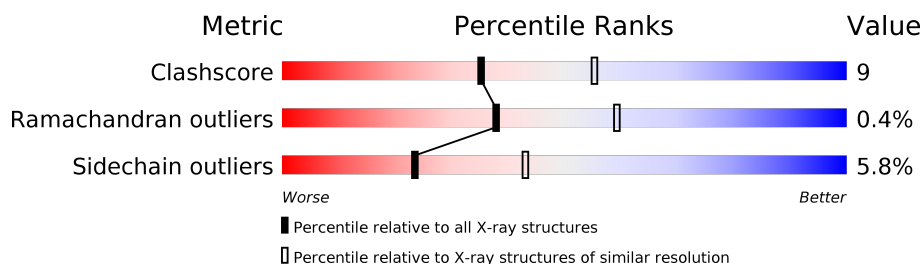
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	
2	B	557	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6440 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	193	Total	C	N	O	S	0	0	0
			1545	989	258	290	8			

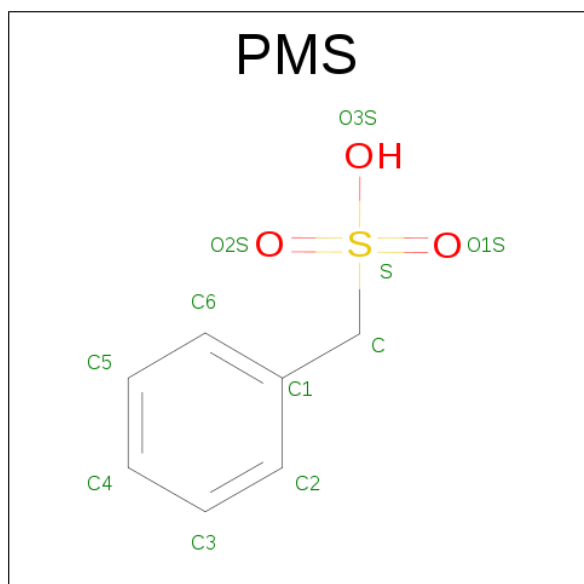
- Molecule 2 is a protein called PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	0	0	0
			4415	2805	766	834	10			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is PHENYLMETHANESULFONIC ACID (three-letter code: PMS) (formula: C<sub>7</sub>H<sub>8</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			10	7	2	1		

- Molecule 5 is water.

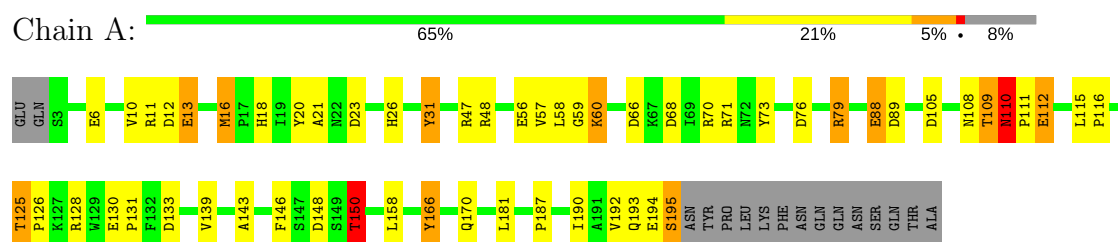
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total	O	0	0
			120	120		
5	B	349	Total	O	0	0
			349	349		

### 3 Residue-property plots [i](#)

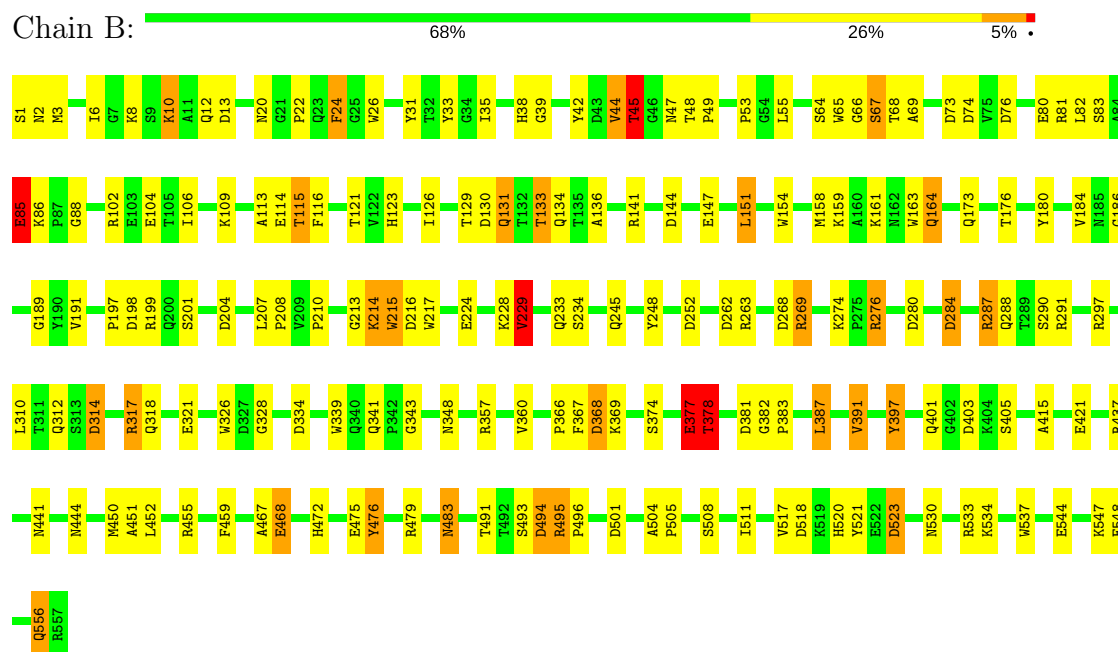
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: PENICILLIN AMIDOHYDROLASE



#### • Molecule 2: PENICILLIN AMIDOHYDROLASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.12Å 65.08Å 76.30Å 100.20° 111.44° 105.81°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.163 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0/1584	1.79	48/2150 (2.2%)
2	B	0.85	0/4541	1.92	119/6192 (1.9%)
All	All	0.85	0/6125	1.89	167/8342 (2.0%)

There are no bond length outliers.

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	437	ARG	NE-CZ-NH1	21.71	131.16	120.30
2	B	317	ARG	NE-CZ-NH1	16.64	128.62	120.30
2	B	269	ARG	NE-CZ-NH1	16.45	128.52	120.30
2	B	276	ARG	NE-CZ-NH1	15.64	128.12	120.30
2	B	479	ARG	NE-CZ-NH1	15.07	127.84	120.30
2	B	357	ARG	NE-CZ-NH1	12.31	126.46	120.30
2	B	144	ASP	CB-CG-OD1	11.52	128.66	118.30
2	B	269	ARG	NH1-CZ-NH2	-11.49	106.76	119.40
2	B	269	ARG	CA-CB-CG	11.19	138.02	113.40
1	A	150	THR	N-CA-CB	11.03	131.26	110.30
2	B	495	ARG	NE-CZ-NH1	10.78	125.69	120.30
2	B	198	ASP	CB-CG-OD2	-10.63	108.73	118.30
2	B	291	ARG	NE-CZ-NH1	10.61	125.61	120.30
2	B	141	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	A	128	ARG	NE-CZ-NH2	10.44	125.52	120.30
2	B	204	ASP	CB-CG-OD1	10.11	127.40	118.30
2	B	269	ARG	CD-NE-CZ	9.99	137.59	123.60
2	B	455	ARG	NE-CZ-NH2	-9.95	115.33	120.30
2	B	76	ASP	CB-CG-OD1	9.85	127.16	118.30
2	B	263	ARG	NE-CZ-NH1	9.71	125.15	120.30
2	B	317	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	A	31	TYR	CB-CG-CD1	9.45	126.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	533	ARG	CD-NE-CZ	9.27	136.58	123.60
2	B	45	THR	OG1-CB-CG2	9.09	130.91	110.00
1	A	48	ARG	NE-CZ-NH2	-8.95	115.83	120.30
2	B	334	ASP	CB-CG-OD2	-8.95	110.25	118.30
2	B	495	ARG	CG-CD-NE	8.64	129.95	111.80
2	B	269	ARG	NE-CZ-NH2	8.64	124.62	120.30
2	B	141	ARG	NE-CZ-NH1	8.64	124.62	120.30
2	B	83	SER	N-CA-CB	8.61	123.41	110.50
2	B	523	ASP	CB-CG-OD1	8.54	125.99	118.30
2	B	24	PHE	CB-CG-CD1	8.44	126.70	120.80
1	A	79	ARG	NE-CZ-NH1	8.34	124.47	120.30
2	B	437	ARG	NE-CZ-NH2	-8.24	116.18	120.30
2	B	81	ARG	NE-CZ-NH1	8.23	124.41	120.30
2	B	130	ASP	CB-CG-OD2	-8.22	110.90	118.30
2	B	229	VAL	N-CA-CB	8.09	129.29	111.50
2	B	287	ARG	NE-CZ-NH1	8.06	124.33	120.30
2	B	24	PHE	CB-CG-CD2	-7.99	115.20	120.80
2	B	533	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	B	233	GLN	CB-CG-CD	7.78	131.83	111.60
2	B	314	ASP	CB-CG-OD2	-7.76	111.31	118.30
2	B	357	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	B	391	VAL	CB-CA-C	-7.60	96.95	111.40
2	B	269	ARG	N-CA-CB	7.57	124.22	110.60
1	A	166	TYR	CB-CG-CD1	-7.53	116.48	121.00
2	B	276	ARG	CD-NE-CZ	7.51	134.12	123.60
2	B	491	THR	C-N-CA	7.45	140.32	121.70
2	B	459	PHE	CB-CG-CD2	-7.42	115.60	120.80
1	A	105	ASP	CB-CG-OD1	7.32	124.89	118.30
2	B	216	ASP	CB-CG-OD1	7.29	124.86	118.30
2	B	479	ARG	NH1-CZ-NH2	-7.29	111.38	119.40
2	B	523	ASP	CB-CG-OD2	-7.14	111.88	118.30
2	B	191	VAL	CA-CB-CG2	7.08	121.52	110.90
2	B	67	SER	N-CA-CB	-7.01	99.99	110.50
2	B	45	THR	N-CA-CB	7.01	123.61	110.30
2	B	455	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	B	45	THR	CA-CB-CG2	-6.86	102.80	112.40
1	A	110	ASN	N-CA-CB	-6.73	98.48	110.60
1	A	23	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	31	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	A	13	GLU	CA-CB-CG	6.67	128.09	113.40
2	B	229	VAL	CB-CA-C	-6.67	98.73	111.40
1	A	71	ARG	CD-NE-CZ	6.64	132.90	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	377	GLU	C-N-CA	6.60	138.21	121.70
2	B	81	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	70	ARG	NE-CZ-NH2	-6.57	117.02	120.30
2	B	437	ARG	CD-NE-CZ	6.56	132.78	123.60
1	A	146	PHE	CB-CG-CD1	-6.50	116.25	120.80
1	A	76	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	105	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	71	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	B	263	ARG	NE-CZ-NH2	-6.43	117.08	120.30
2	B	133	THR	N-CA-CB	6.40	122.46	110.30
2	B	268	ASP	CB-CG-OD2	-6.39	112.55	118.30
2	B	164	GLN	CB-CG-CD	6.38	128.18	111.60
2	B	556	GLN	N-CA-CB	6.38	122.08	110.60
2	B	69	ALA	CB-CA-C	6.37	119.66	110.10
1	A	133	ASP	CB-CG-OD1	6.35	124.02	118.30
2	B	284	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	150	THR	CB-CA-C	-6.33	94.50	111.60
2	B	468	GLU	CG-CD-OE2	-6.33	105.64	118.30
1	A	79	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	68	ASP	CB-CG-OD2	-6.30	112.63	118.30
2	B	176	THR	CA-CB-CG2	6.26	121.17	112.40
2	B	74	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	47	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	B	284	ASP	CA-CB-CG	-6.16	99.85	113.40
2	B	314	ASP	CB-CG-OD1	6.13	123.82	118.30
2	B	437	ARG	NH1-CZ-NH2	-6.13	112.66	119.40
1	A	143	ALA	CB-CA-C	6.12	119.28	110.10
2	B	518	ASP	CB-CG-OD2	6.11	123.80	118.30
2	B	494	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	130	GLU	CA-CB-CG	6.06	126.73	113.40
2	B	397	TYR	CB-CG-CD1	-6.02	117.39	121.00
2	B	321	GLU	OE1-CD-OE2	5.97	130.46	123.30
2	B	1	SER	O-C-N	5.96	132.24	122.70
2	B	191	VAL	CG1-CB-CG2	-5.93	101.42	110.90
1	A	11	ARG	CD-NE-CZ	5.85	131.79	123.60
2	B	224	GLU	CB-CG-CD	5.84	129.97	114.20
2	B	403	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	195	SER	N-CA-CB	5.79	119.18	110.50
2	B	321	GLU	CG-CD-OE2	-5.78	106.74	118.30
2	B	215	TRP	CA-CB-CG	-5.77	102.73	113.70
2	B	317	ARG	CD-NE-CZ	5.77	131.68	123.60
2	B	276	ARG	NH1-CZ-NH2	-5.76	113.07	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	60	LYS	CB-CA-C	-5.71	98.98	110.40
2	B	248	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	A	58	LEU	CA-C-N	5.68	127.56	116.20
2	B	368	ASP	CB-CG-OD1	5.67	123.41	118.30
2	B	544	GLU	OE1-CD-OE2	5.65	130.09	123.30
1	A	131	PRO	O-C-N	-5.63	113.69	122.70
1	A	66	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	13	GLU	CB-CG-CD	5.58	129.25	114.20
1	A	6	GLU	CG-CD-OE1	-5.53	107.25	118.30
2	B	234	SER	CB-CA-C	-5.51	99.63	110.10
2	B	381	ASP	C-N-CA	5.48	133.81	122.30
2	B	483	ASN	N-CA-CB	5.47	120.45	110.60
2	B	415	ALA	N-CA-CB	-5.46	102.45	110.10
2	B	290	SER	CB-CA-C	-5.46	99.72	110.10
1	A	181	LEU	CA-CB-CG	5.46	127.85	115.30
2	B	496	PRO	C-N-CA	5.45	135.32	121.70
1	A	125	THR	CA-CB-CG2	5.45	120.03	112.40
2	B	475	GLU	CG-CD-OE1	5.43	129.17	118.30
2	B	245	GLN	CA-CB-CG	5.41	125.31	113.40
2	B	33	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	A	109	THR	CA-CB-CG2	5.36	119.91	112.40
1	A	112	GLU	CG-CD-OE1	5.36	129.01	118.30
1	A	79	ARG	CD-NE-CZ	5.34	131.08	123.60
2	B	199	ARG	NE-CZ-NH2	-5.33	117.64	120.30
2	B	73	ASP	CB-CG-OD2	5.32	123.08	118.30
2	B	472	HIS	CA-CB-CG	-5.31	104.58	113.60
2	B	161	LYS	CB-CG-CD	5.30	125.39	111.60
2	B	13	ASP	CB-CG-OD1	5.30	123.07	118.30
2	B	403	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	48	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	B	213	GLY	N-CA-C	5.24	126.19	113.10
2	B	391	VAL	N-CA-CB	5.22	122.99	111.50
1	A	66	ASP	CB-CG-OD1	5.21	122.99	118.30
2	B	114	GLU	OE1-CD-OE2	5.21	129.55	123.30
1	A	148	ASP	CB-CG-OD2	5.18	122.97	118.30
2	B	291	ARG	NH1-CZ-NH2	-5.18	113.71	119.40
1	A	59	GLY	C-N-CA	5.17	134.63	121.70
1	A	60	LYS	CA-CB-CG	5.16	124.76	113.40
1	A	16	MET	CG-SD-CE	5.16	108.46	100.20
2	B	44	VAL	CA-CB-CG1	5.15	118.63	110.90
2	B	102	ARG	NE-CZ-NH1	5.15	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	ASN	CB-CA-C	5.14	120.69	110.40
1	A	71	ARG	CB-CA-C	-5.14	100.12	110.40
2	B	1	SER	N-CA-CB	5.13	118.19	110.50
1	A	108	ASN	C-N-CA	5.12	134.51	121.70
2	B	88	GLY	C-N-CA	5.12	134.50	121.70
2	B	328	GLY	CA-C-O	-5.12	111.38	120.60
2	B	421	GLU	OE1-CD-OE2	5.12	129.44	123.30
2	B	467	ALA	C-N-CA	5.10	134.46	121.70
1	A	89	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	64	SER	N-CA-CB	5.09	118.14	110.50
1	A	166	TYR	CB-CG-CD2	5.09	124.05	121.00
2	B	248	TYR	CB-CG-CD2	5.08	124.05	121.00
2	B	85	GLU	OE1-CD-OE2	5.06	129.37	123.30
2	B	68	THR	N-CA-CB	5.05	119.90	110.30
2	B	113	ALA	N-CA-CB	5.05	117.17	110.10
2	B	476	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	B	130	ASP	CB-CG-OD1	5.01	122.81	118.30
2	B	284	ASP	OD1-CG-OD2	5.01	132.81	123.30
2	B	493	SER	CA-C-O	5.00	130.61	120.10

There are no chirality outliers.

There are no planarity outliers.

## 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	1545	0	1501	32	0
2	B	4415	0	4240	95	0
3	B	1	0	0	0	0
4	B	10	0	7	0	0
5	A	120	0	0	5	0
5	B	349	0	0	16	0
All	All	6440	0	5748	109	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 (109) 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:377:GLU:HA	5:B:804:HOH:O	1.42	1.16
1:A:18:HIS:HD2	2:B:38:HIS:NE2	1.66	0.93
2:B:288:GLN:HG2	5:B:757:HOH:O	1.68	0.93
2:B:318:GLN:HG2	5:B:906:HOH:O	1.66	0.92
2:B:534:LYS:HE3	5:B:628:HOH:O	1.68	0.92
1:A:150:THR:HG22	2:B:252:ASP:OD2	1.76	0.85
1:A:190:ILE:HG12	2:B:229:VAL:HG22	1.61	0.81
1:A:16:MET:CE	2:B:45:THR:HG22	2.11	0.79
1:A:16:MET:HE1	2:B:45:THR:HG22	1.62	0.79
1:A:10:VAL:HG13	2:B:547:LYS:HG3	1.64	0.79
2:B:288:GLN:CG	5:B:757:HOH:O	2.30	0.75
2:B:164:GLN:HG3	5:B:904:HOH:O	1.87	0.74
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.53	0.73
2:B:214:LYS:H	2:B:214:LYS:HD2	1.59	0.68
1:A:56:GLU:O	2:B:109:LYS:HB2	1.94	0.67
1:A:150:THR:CG2	2:B:252:ASP:OD2	2.42	0.66
1:A:150:THR:HG22	2:B:252:ASP:CG	2.17	0.65
2:B:378:THR:HG22	2:B:383:PRO:HG3	1.78	0.64
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.61	0.64
1:A:60:LYS:HG3	5:B:709:HOH:O	1.96	0.63
1:A:125:THR:HB	1:A:126:PRO:HD2	1.80	0.63
2:B:378:THR:HG21	2:B:450:MET:HG2	1.82	0.62
2:B:6:ILE:HG23	2:B:10:LYS:HB3	1.81	0.61
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.82	0.61
1:A:18:HIS:CD2	2:B:38:HIS:NE2	2.58	0.61
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.83	0.60
1:A:88:GLU:CG	5:A:294:HOH:O	2.49	0.60
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.38	0.59
1:A:150:THR:HG22	2:B:252:ASP:OD1	2.02	0.58
1:A:166:TYR:O	1:A:170:GLN:HB3	2.04	0.58
2:B:12:GLN:HB2	2:B:276:ARG:HB3	1.88	0.56
2:B:274:LYS:HE2	5:B:704:HOH:O	2.06	0.55
1:A:21:ALA:O	2:B:39:GLY:HA3	2.06	0.55
2:B:312:GLN:HG3	5:B:888:HOH:O	2.07	0.54
2:B:121:THR:HG23	2:B:126:ILE:HD11	1.89	0.54
2:B:129:THR:HA	2:B:136:ALA:HA	1.91	0.53
2:B:501:ASP:OD1	2:B:534:LYS:HE2	2.09	0.53
1:A:26:HIS:HE1	2:B:556:GLN:NE2	2.07	0.52
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.22	0.52
2:B:326:TRP:CD1	2:B:341:GLN:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ARG:NH2	2:B:297:ARG:HB2	2.25	0.51
2:B:3:MET:HE3	2:B:180:TYR:HB2	1.92	0.51
1:A:57:VAL:HG12	5:A:322:HOH:O	2.11	0.51
2:B:214:LYS:N	2:B:214:LYS:HD2	2.24	0.50
1:A:16:MET:HE2	2:B:45:THR:HG22	1.94	0.50
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.76	0.50
2:B:387:LEU:HD21	2:B:450:MET:HE3	1.95	0.49
2:B:397:TYR:O	2:B:401:GLN:HG2	2.11	0.49
2:B:382:GLY:HA3	2:B:451:ALA:O	2.13	0.48
2:B:341:GLN:HG2	5:B:663:HOH:O	2.12	0.48
2:B:104:GLU:O	2:B:115:THR:HA	2.13	0.48
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.48	0.48
1:A:88:GLU:HG2	5:A:294:HOH:O	2.13	0.48
2:B:42:TYR:CZ	2:B:159:LYS:HE3	2.49	0.48
2:B:534:LYS:NZ	5:B:644:HOH:O	2.47	0.48
2:B:378:THR:HG21	2:B:450:MET:SD	2.54	0.48
2:B:520:HIS:HE1	2:B:548:GLU:OE2	1.98	0.47
1:A:166:TYR:HB3	1:A:170:GLN:CG	2.45	0.47
2:B:401:GLN:HB2	2:B:405:SER:HB2	1.96	0.47
2:B:483:ASN:O	2:B:501:ASP:HA	2.15	0.47
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.50	0.47
1:A:88:GLU:HG3	5:A:294:HOH:O	2.13	0.46
2:B:274:LYS:CE	5:B:704:HOH:O	2.61	0.46
1:A:110:ASN:N	1:A:111:PRO:HD3	2.29	0.46
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.98	0.46
2:B:318:GLN:HA	5:B:906:HOH:O	2.15	0.46
1:A:187:PRO:HG2	2:B:262:ASP:HB3	1.98	0.46
1:A:60:LYS:CG	5:B:709:HOH:O	2.59	0.46
1:A:158:LEU:HD13	2:B:367:PHE:HB3	1.97	0.46
2:B:274:LYS:NZ	5:B:704:HOH:O	2.36	0.46
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.51	0.46
2:B:164:GLN:H	2:B:164:GLN:HG3	1.51	0.45
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.51	0.45
1:A:139:VAL:HG22	2:B:147:GLU:HB3	1.98	0.45
2:B:378:THR:HG21	2:B:450:MET:CG	2.47	0.45
1:A:194:GLU:O	1:A:195:SER:HB3	2.16	0.45
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.27	0.45
2:B:210:PRO:HD2	2:B:215:TRP:CD1	2.51	0.45
2:B:280:ASP:O	2:B:284:ASP:HB2	2.17	0.45
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.99	0.45
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:HA	2:B:38:HIS:O	2.17	0.45
2:B:31:TYR:CE2	2:B:49:PRO:HB3	2.53	0.44
2:B:287:ARG:NH1	5:B:757:HOH:O	2.50	0.44
2:B:8:LYS:HG3	2:B:186:GLY:HA3	2.00	0.44
2:B:348:ASN:ND2	2:B:374:SER:OG	2.50	0.44
1:A:166:TYR:HB3	1:A:170:GLN:HG3	2.00	0.44
2:B:494:ASP:OD1	2:B:495:ARG:HG3	2.17	0.44
2:B:504:ALA:HA	2:B:505:PRO:C	2.38	0.44
2:B:131:GLN:HG3	2:B:131:GLN:H	1.64	0.43
2:B:106:ILE:HD11	2:B:116:PHE:CE1	2.49	0.43
2:B:80:GLU:OE2	2:B:123:HIS:ND1	2.51	0.43
2:B:383:PRO:HD2	2:B:476:TYR:CD1	2.53	0.43
2:B:468:GLU:H	2:B:468:GLU:HG3	1.46	0.43
2:B:48:THR:HA	2:B:49:PRO:HD3	1.96	0.43
2:B:129:THR:HG22	2:B:136:ALA:CB	2.48	0.43
1:A:79:ARG:NE	5:A:307:HOH:O	2.47	0.43
2:B:35:ILE:HG23	2:B:55:LEU:HD11	2.00	0.43
2:B:360:VAL:HG13	2:B:368:ASP:HB2	2.02	0.42
2:B:53:PRO:HD2	2:B:151:LEU:HD21	2.01	0.42
2:B:85:GLU:O	2:B:86:LYS:C	2.58	0.42
2:B:495:ARG:HH12	2:B:537:TRP:HZ3	1.68	0.41
2:B:65:TRP:HA	2:B:180:TYR:O	2.20	0.41
2:B:387:LEU:HD22	2:B:476:TYR:CE2	2.55	0.41
2:B:508:SER:O	2:B:521:TYR:HA	2.21	0.41
2:B:284:ASP:OD2	2:B:287:ARG:NH2	2.54	0.41
2:B:310:LEU:HD13	2:B:314:ASP:OD2	2.21	0.40
2:B:207:LEU:HA	2:B:208:PRO:HD3	1.92	0.40
2:B:3:MET:HE1	2:B:66:GLY:HA3	2.03	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	191/209 (91%)	189 (99%)	2 (1%)	0	100	100
2	B	555/557 (100%)	537 (97%)	15 (3%)	3 (0%)	32	53
All	All	746/766 (97%)	726 (97%)	17 (2%)	3 (0%)	38	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	377	GLU
2	B	378	THR
2	B	134	GLN

### 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	165/180 (92%)	155 (94%)	10 (6%)	22	40
2	B	460/460 (100%)	434 (94%)	26 (6%)	24	44
All	All	625/640 (98%)	589 (94%)	36 (6%)	23	43

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	31	TYR
1	A	73	TYR
1	A	88	GLU
1	A	109	THR
1	A	110	ASN
1	A	112	GLU
1	A	150	THR
1	A	192	VAL
1	A	193	GLN
2	B	2	ASN
2	B	10	LYS
2	B	20	ASN

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Mol	Chain	Res	Type
2	B	45	THR
2	B	67	SER
2	B	85	GLU
2	B	115	THR
2	B	131	GLN
2	B	133	THR
2	B	151	LEU
2	B	154	TRP
2	B	173	GLN
2	B	184	VAL
2	B	201	SER
2	B	214	LYS
2	B	228	LYS
2	B	229	VAL
2	B	317	ARG
2	B	366	PRO
2	B	369	LYS
2	B	378	THR
2	B	387	LEU
2	B	391	VAL
2	B	441	ASN
2	B	444	ASN
2	B	530	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	110	ASN
2	B	2	ASN
2	B	93	ASN
2	B	245	GLN
2	B	348	ASN
2	B	441	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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	PMS	B	559	2	7,10,11	0.60	0	11,12,15	2.77	8 (72%)

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	PMS	B	559	2	-	0/4/4/5	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559	PMS	C4-C5-C6	-3.58	115.29	120.21
4	B	559	PMS	O1S-S-C	-3.40	99.88	105.55
4	B	559	PMS	C-C1-C6	-3.34	116.80	120.56
4	B	559	PMS	C3-C2-C1	-2.58	116.71	120.64
4	B	559	PMS	C-C1-C2	-2.13	118.16	120.56
4	B	559	PMS	O2S-S-C	2.78	110.19	105.55
4	B	559	PMS	C5-C4-C3	3.05	124.97	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559	PMS	C2-C1-C6	4.16	124.76	118.16

There are no chirality outliers.

There are no torsion outliers.

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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.