



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:34 PM GMT

PDB ID : 1PNL  
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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

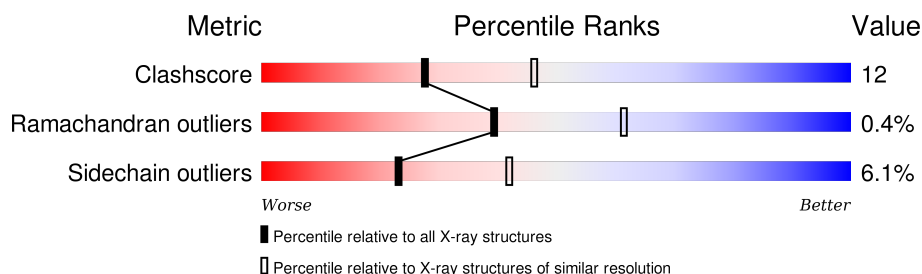
# 1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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	

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
4	PAC	B	559	-	-	X	-

## 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			

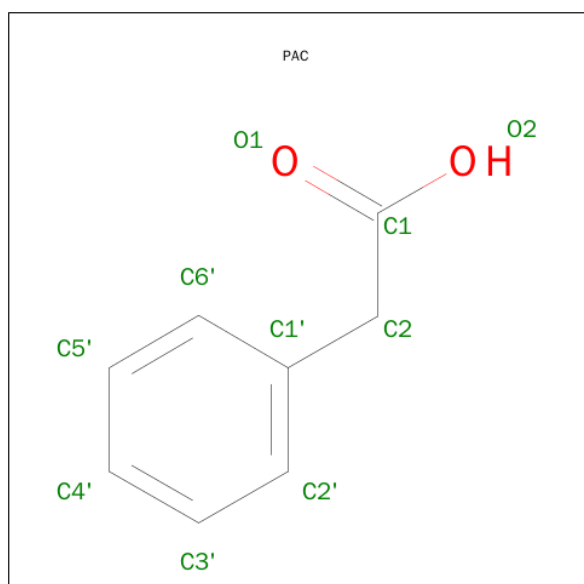
- Molecule 2 is a protein called PENICILLIN AMIDOHYDROLASE.

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 2-PHENYLACETIC ACID (three-letter code: PAC) (formula: C<sub>8</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	8	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		
5	B	348	Total	O	0	0
			348	348		



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.152 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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, PAC

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	1.04	0/1584	2.00	52/2150 (2.4%)
2	B	1.01	1/4541 (0.0%)	1.94	113/6192 (1.8%)
All	All	1.02	1/6125 (0.0%)	1.95	165/8342 (2.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	34	GLY	CA-C	5.27	1.60	1.51

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	437	ARG	NE-CZ-NH1	22.20	131.40	120.30
2	B	479	ARG	NE-CZ-NH1	16.65	128.63	120.30
1	A	79	ARG	NE-CZ-NH1	15.65	128.13	120.30
2	B	317	ARG	NE-CZ-NH1	15.56	128.08	120.30
2	B	269	ARG	NE-CZ-NH1	15.39	128.00	120.30
2	B	357	ARG	NE-CZ-NH1	14.14	127.37	120.30
2	B	198	ASP	CB-CG-OD2	-13.06	106.54	118.30
1	A	71	ARG	NE-CZ-NH1	12.94	126.77	120.30
1	A	79	ARG	NE-CZ-NH2	-12.92	113.84	120.30
2	B	269	ARG	CD-NE-CZ	12.63	141.28	123.60
2	B	81	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	A	23	ASP	CB-CG-OD1	12.07	129.17	118.30
1	A	150	THR	N-CA-CB	12.06	133.22	110.30
2	B	276	ARG	NE-CZ-NH1	11.98	126.29	120.30
2	B	216	ASP	CB-CG-OD1	11.55	128.69	118.30
2	B	269	ARG	NH1-CZ-NH2	-11.49	106.76	119.40
1	A	47	ARG	NE-CZ-NH1	11.40	126.00	120.30
2	B	455	ARG	NE-CZ-NH2	-11.29	114.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	437	ARG	NE-CZ-NH2	-10.92	114.84	120.30
2	B	76	ASP	CB-CG-OD1	10.83	128.04	118.30
2	B	518	ASP	CB-CG-OD2	10.73	127.96	118.30
2	B	317	ARG	NE-CZ-NH2	-10.60	115.00	120.30
2	B	269	ARG	CA-CB-CG	10.60	136.72	113.40
2	B	263	ARG	NE-CZ-NH1	10.51	125.55	120.30
1	A	31	TYR	CB-CG-CD2	-10.33	114.80	121.00
2	B	33	TYR	CB-CG-CD1	-10.20	114.88	121.00
2	B	130	ASP	CB-CG-OD2	-10.17	109.15	118.30
2	B	495	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	A	128	ARG	NE-CZ-NH2	9.86	125.23	120.30
2	B	269	ARG	NE-CZ-NH2	9.84	125.22	120.30
1	A	48	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	A	12	ASP	CB-CG-OD2	-9.48	109.77	118.30
2	B	45	THR	OG1-CB-CG2	9.32	131.43	110.00
2	B	533	ARG	CD-NE-CZ	9.28	136.59	123.60
2	B	495	ARG	CG-CD-NE	9.15	131.03	111.80
2	B	314	ASP	CB-CG-OD2	-9.13	110.09	118.30
1	A	48	ARG	NE-CZ-NH2	-9.01	115.80	120.30
2	B	141	ARG	NE-CZ-NH2	-8.93	115.83	120.30
2	B	397	TYR	CB-CG-CD1	-8.93	115.64	121.00
1	A	105	ASP	CB-CG-OD2	-8.80	110.38	118.30
2	B	144	ASP	CB-CG-OD1	8.77	126.19	118.30
1	A	31	TYR	CB-CG-CD1	8.73	126.24	121.00
2	B	73	ASP	CB-CG-OD2	8.68	126.11	118.30
2	B	357	ARG	NE-CZ-NH2	-8.60	116.00	120.30
2	B	284	ASP	CB-CG-OD1	-8.54	110.61	118.30
2	B	81	ARG	NE-CZ-NH2	-8.38	116.11	120.30
2	B	391	VAL	CB-CA-C	-8.30	95.62	111.40
1	A	133	ASP	CB-CG-OD1	8.29	125.77	118.30
2	B	455	ARG	NE-CZ-NH1	8.29	124.44	120.30
2	B	291	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	A	71	ARG	CD-NE-CZ	7.99	134.79	123.60
2	B	204	ASP	CB-CG-OD1	7.92	125.43	118.30
2	B	314	ASP	CB-CG-OD1	7.82	125.34	118.30
1	A	47	ARG	NE-CZ-NH2	-7.79	116.41	120.30
2	B	321	GLU	OE1-CD-OE2	7.77	132.62	123.30
2	B	45	THR	N-CA-CB	7.74	125.00	110.30
2	B	321	GLU	CG-CD-OE2	-7.67	102.97	118.30
1	A	110	ASN	N-CA-CB	-7.61	96.90	110.60
2	B	437	ARG	CD-NE-CZ	7.61	134.25	123.60
1	A	70	ARG	NE-CZ-NH2	-7.58	116.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	459	PHE	CB-CG-CD2	-7.50	115.55	120.80
2	B	83	SER	N-CA-CB	7.49	121.73	110.50
2	B	229	VAL	N-CA-CB	7.38	127.75	111.50
1	A	68	ASP	CB-CG-OD2	-7.34	111.70	118.30
2	B	50	PHE	CB-CG-CD2	-7.26	115.72	120.80
1	A	145	ARG	CD-NE-CZ	7.25	133.75	123.60
1	A	145	ARG	NE-CZ-NH1	-7.25	116.67	120.30
2	B	469	GLU	OE1-CD-OE2	7.24	131.99	123.30
2	B	518	ASP	CB-CG-OD1	-7.17	111.85	118.30
2	B	325	ARG	CD-NE-CZ	-7.11	113.64	123.60
2	B	334	ASP	CB-CG-OD2	-7.08	111.92	118.30
2	B	284	ASP	OD1-CG-OD2	7.06	136.71	123.30
1	A	150	THR	CB-CA-C	-7.06	92.55	111.60
2	B	284	ASP	CA-CB-CG	-7.05	97.90	113.40
2	B	85	GLU	OE1-CD-OE2	7.00	131.70	123.30
2	B	233	GLN	CB-CG-CD	6.97	129.73	111.60
2	B	50	PHE	CB-CG-CD1	6.94	125.66	120.80
1	A	76	ASP	CB-CG-OD2	-6.86	112.13	118.30
2	B	276	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	B	248	TYR	CB-CG-CD1	-6.71	116.97	121.00
2	B	141	ARG	NE-CZ-NH1	6.69	123.64	120.30
2	B	215	TRP	CA-CB-CG	-6.61	101.15	113.70
2	B	284	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	105	ASP	CB-CG-OD1	6.56	124.21	118.30
2	B	248	TYR	CB-CG-CD2	6.53	124.92	121.00
2	B	415	ALA	N-CA-CB	-6.52	100.97	110.10
1	A	76	ASP	CB-CG-OD1	6.51	124.16	118.30
2	B	133	THR	N-CA-CB	6.47	122.59	110.30
2	B	397	TYR	CB-CG-CD2	6.41	124.84	121.00
1	A	11	ARG	CD-NE-CZ	6.40	132.56	123.60
1	A	71	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	B	468	GLU	CG-CD-OE2	-6.38	105.54	118.30
2	B	472	HIS	CA-CB-CG	-6.36	102.79	113.60
1	A	148	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	112	GLU	CG-CD-OE1	6.33	130.96	118.30
2	B	475	GLU	CG-CD-OE1	6.24	130.78	118.30
2	B	476	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	166	TYR	CB-CG-CD1	-6.19	117.29	121.00
1	A	66	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	6	GLU	CG-CD-OE1	-6.18	105.93	118.30
2	B	556	GLN	N-CA-CB	6.14	121.66	110.60
2	B	199	ARG	NE-CZ-NH2	-6.13	117.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	GLU	CA-CB-CG	6.11	126.85	113.40
2	B	64	SER	N-CA-CB	6.02	119.53	110.50
2	B	229	VAL	CB-CA-C	-6.02	99.95	111.40
2	B	459	PHE	CB-CG-CD1	6.02	125.02	120.80
1	A	13	GLU	CB-CG-CD	5.87	130.06	114.20
1	A	109	THR	CA-CB-CG2	5.87	120.62	112.40
2	B	164	GLN	CB-CG-CD	5.87	126.86	111.60
2	B	548	GLU	CA-CB-CG	5.86	126.29	113.40
2	B	269	ARG	N-CA-CB	5.84	121.11	110.60
1	A	130	GLU	CA-CB-CG	5.83	126.24	113.40
2	B	328	GLY	CA-C-O	-5.80	110.16	120.60
2	B	557	ARG	NE-CZ-NH1	-5.80	117.40	120.30
2	B	290	SER	CB-CA-C	-5.77	99.13	110.10
2	B	130	ASP	CB-CG-OD1	5.71	123.44	118.30
2	B	403	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	33	TYR	CB-CG-CD2	-5.70	117.58	121.00
2	B	272	GLU	CG-CD-OE2	-5.69	106.93	118.30
2	B	378	THR	CA-C-O	5.60	131.86	120.10
1	A	60	LYS	CA-CB-CG	5.57	125.66	113.40
1	A	181	LEU	CA-CB-CG	5.54	128.05	115.30
2	B	327	ASP	CB-CG-OD2	-5.52	113.33	118.30
2	B	335	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	94	GLN	CB-CG-CD	5.51	125.94	111.60
2	B	483	ASN	N-CA-CB	5.50	120.51	110.60
2	B	316	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	145	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	A	71	ARG	CB-CA-C	-5.47	99.46	110.40
1	A	180	TRP	CA-CB-CG	5.46	124.07	113.70
2	B	181	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	144	ASN	C-N-CA	-5.42	108.14	121.70
1	A	151	SER	N-CA-CB	5.42	118.63	110.50
2	B	45	THR	CB-CA-C	-5.39	97.04	111.60
2	B	83	SER	CA-CB-OG	5.37	125.71	111.20
2	B	297	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	B	377	GLU	C-N-CA	5.35	135.08	121.70
2	B	213	GLY	N-CA-C	5.31	126.38	113.10
2	B	272	GLU	CG-CD-OE1	5.31	128.93	118.30
2	B	479	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
2	B	491	THR	C-N-CA	5.30	134.95	121.70
2	B	27	TYR	CB-CG-CD2	-5.28	117.83	121.00
2	B	55	LEU	O-C-N	5.27	131.14	122.70
1	A	154	ASP	CB-CG-OD1	5.26	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	471	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	B	335	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	B	493	SER	CA-CB-OG	5.19	125.22	111.20
1	A	166	TYR	CB-CG-CD2	5.18	124.11	121.00
1	A	43	MET	CA-CB-CG	-5.17	104.51	113.30
1	A	96	TYR	CB-CG-CD2	-5.16	117.90	121.00
2	B	398	GLU	OE1-CD-OE2	-5.16	117.11	123.30
2	B	437	ARG	NH1-CZ-NH2	-5.13	113.76	119.40
2	B	143	TRP	CB-CG-CD2	5.12	133.25	126.60
2	B	391	VAL	CG1-CB-CG2	5.11	119.07	110.90
2	B	494	ASP	CB-CG-OD1	5.09	122.88	118.30
2	B	234	SER	CB-CA-C	-5.09	100.43	110.10
2	B	429	ASP	O-C-N	5.06	130.80	122.70
2	B	146	LYS	O-C-N	5.06	130.79	122.70
1	A	181	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	A	193	GLN	CB-CA-C	-5.04	100.31	110.40
2	B	233	GLN	CA-CB-CG	5.04	124.50	113.40
2	B	380	GLN	CB-CG-CD	5.04	124.71	111.60
1	A	143	ALA	CB-CA-C	5.03	117.64	110.10
2	B	378	THR	CA-C-N	-5.03	106.14	117.20
2	B	47	ASN	CB-CA-C	5.02	120.43	110.40

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	43	0
2	B	4415	0	4242	114	0
3	B	1	0	0	0	0
4	B	10	0	7	6	0
5	A	121	0	0	10	0
5	B	348	0	0	16	0
All	All	6440	0	5750	138	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 12.

All (138) 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:18:HIS:HD2	2:B:38:HIS:NE2	1.66	0.93
2:B:377:GLU:HA	5:B:803:HOH:O	1.67	0.93
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.37	0.89
2:B:288:GLN:HG2	5:B:756:HOH:O	1.77	0.84
2:B:214:LYS:H	2:B:214:LYS:HD2	1.40	0.84
2:B:318:GLN:HG2	5:B:905:HOH:O	1.79	0.81
2:B:164:GLN:HG3	5:B:903:HOH:O	1.77	0.81
1:A:190:ILE:HG12	2:B:229:VAL:HG22	1.60	0.81
1:A:16:MET:HE1	2:B:45:THR:HG22	1.63	0.81
1:A:10:VAL:HG13	2:B:547:LYS:HG3	1.64	0.80
1:A:150:THR:HG22	2:B:252:ASP:OD2	1.81	0.80
5:A:235:HOH:O	2:B:534:LYS:HE3	1.82	0.79
2:B:214:LYS:N	2:B:214:LYS:HD2	2.00	0.77
2:B:6:ILE:HG23	2:B:10:LYS:HB3	1.65	0.77
1:A:60:LYS:HG3	5:B:708:HOH:O	1.85	0.76
1:A:16:MET:CE	2:B:45:THR:HG22	2.18	0.74
2:B:378:THR:HG21	2:B:450:MET:HG2	1.71	0.73
2:B:378:THR:HG22	2:B:383:PRO:HG3	1.72	0.72
2:B:501:ASP:OD1	2:B:534:LYS:HE2	1.90	0.71
1:A:166:TYR:O	1:A:170:GLN:HB3	1.91	0.70
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.54	0.70
2:B:12:GLN:HB2	2:B:276:ARG:HB3	1.74	0.70
2:B:288:GLN:CG	5:B:756:HOH:O	2.38	0.68
2:B:104:GLU:O	2:B:115:THR:HA	1.94	0.68
1:A:56:GLU:O	2:B:109:LYS:HB2	1.93	0.68
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.06	0.67
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.32	0.65
2:B:269:ARG:NH2	2:B:297:ARG:HB2	2.14	0.63
2:B:69:ALA:HB2	4:B:559:PAC:C1	2.29	0.62
1:A:18:HIS:CD2	2:B:38:HIS:NE2	2.58	0.61
1:A:150:THR:HG22	2:B:252:ASP:CG	2.21	0.61
2:B:397:TYR:O	2:B:401:GLN:HG2	2.00	0.61
1:A:194:GLU:O	1:A:195:SER:HB3	2.02	0.60
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.11	0.60
1:A:150:THR:CG2	2:B:252:ASP:OD2	2.48	0.60
2:B:121:THR:HG23	2:B:126:ILE:HD11	1.84	0.59
2:B:214:LYS:H	2:B:214:LYS:CD	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:HIS:HE1	2:B:548:GLU:OE2	1.86	0.59
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.83	0.59
1:A:166:TYR:HB3	1:A:170:GLN:CG	2.33	0.59
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.69	0.58
1:A:110:ASN:N	1:A:111:PRO:HD3	2.20	0.56
2:B:80:GLU:OE2	2:B:123:HIS:ND1	2.39	0.56
2:B:129:THR:HA	2:B:136:ALA:HA	1.88	0.56
1:A:166:TYR:HB3	1:A:170:GLN:HG3	1.88	0.56
1:A:57:VAL:HG12	5:A:323:HOH:O	2.06	0.55
2:B:534:LYS:NZ	5:B:642:HOH:O	2.39	0.55
1:A:88:GLU:CG	5:A:295:HOH:O	2.54	0.55
2:B:274:LYS:NZ	5:B:702:HOH:O	2.33	0.55
1:A:187:PRO:HG2	2:B:262:ASP:HB3	1.89	0.55
1:A:21:ALA:O	2:B:39:GLY:HA3	2.07	0.55
2:B:326:TRP:CD1	2:B:341:GLN:HG3	2.42	0.55
2:B:382:GLY:HA3	2:B:451:ALA:O	2.07	0.55
1:A:125:THR:HB	1:A:126:PRO:HD2	1.88	0.54
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.90	0.54
1:A:26:HIS:HE1	2:B:556:GLN:NE2	2.06	0.53
2:B:11:ALA:O	2:B:276:ARG:NH1	2.39	0.53
2:B:42:TYR:CZ	2:B:159:LYS:HE3	2.44	0.53
2:B:67:SER:HB3	4:B:559:PAC:H3'	1.90	0.53
2:B:129:THR:HG22	2:B:136:ALA:CB	2.38	0.53
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.43	0.52
2:B:378:THR:HG21	2:B:450:MET:CG	2.40	0.52
2:B:210:PRO:HD2	2:B:215:TRP:CD1	2.45	0.51
2:B:383:PRO:HD2	2:B:476:TYR:CD1	2.46	0.51
1:A:145:ARG:CA	5:A:327:HOH:O	2.59	0.51
1:A:115:LEU:O	2:B:513:PRO:HG3	2.11	0.50
2:B:106:ILE:HD11	2:B:116:PHE:CE1	2.41	0.50
1:A:145:ARG:HA	5:A:327:HOH:O	2.10	0.50
2:B:318:GLN:HA	5:B:905:HOH:O	2.11	0.50
2:B:8:LYS:HG3	2:B:186:GLY:HA3	1.94	0.50
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.94	0.50
1:A:150:THR:HG22	2:B:252:ASP:OD1	2.10	0.49
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.94	0.49
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.48	0.49
2:B:339:TRP:CH2	2:B:450:MET:HE2	2.48	0.49
1:A:88:GLU:HG3	5:A:295:HOH:O	2.12	0.48
2:B:280:ASP:O	2:B:284:ASP:HB2	2.13	0.48
2:B:488:PHE:CD1	2:B:497:VAL:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:TRP:HA	2:B:180:TYR:O	2.14	0.47
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.50	0.47
2:B:274:LYS:HE2	5:B:702:HOH:O	2.13	0.47
2:B:1:SER:OG	4:B:559:PAC:H22	2.14	0.47
1:A:60:LYS:CG	5:B:708:HOH:O	2.55	0.47
1:A:20:TYR:HA	2:B:38:HIS:O	2.15	0.46
2:B:3:MET:HE3	2:B:180:TYR:HB2	1.97	0.46
1:A:130:GLU:HB2	1:A:131:PRO:CD	2.46	0.46
1:A:150:THR:HG22	1:A:152:GLU:HG3	1.96	0.45
2:B:274:LYS:CE	5:B:702:HOH:O	2.64	0.45
2:B:495:ARG:HH12	2:B:537:TRP:HZ3	1.65	0.44
2:B:360:VAL:HG13	2:B:368:ASP:HB2	2.00	0.44
1:A:32:GLY:O	1:A:100:MET:HG2	2.18	0.44
2:B:287:ARG:NH1	5:B:756:HOH:O	2.51	0.44
2:B:284:ASP:OD2	2:B:287:ARG:NH2	2.51	0.44
2:B:312:GLN:HG3	5:B:887:HOH:O	2.16	0.44
2:B:269:ARG:HH21	2:B:297:ARG:HB2	1.82	0.43
2:B:348:ASN:ND2	2:B:374:SER:OG	2.50	0.43
2:B:483:ASN:O	2:B:501:ASP:HA	2.19	0.43
2:B:69:ALA:CB	4:B:559:PAC:O2	2.66	0.43
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.92	0.43
2:B:378:THR:HG21	2:B:450:MET:SD	2.59	0.43
1:A:79:ARG:NE	5:A:307:HOH:O	2.46	0.43
2:B:164:GLN:H	2:B:164:GLN:HG3	1.43	0.43
2:B:494:ASP:OD1	2:B:495:ARG:HG3	2.18	0.42
2:B:133:THR:HB	2:B:135:THR:OG1	2.19	0.42
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.54	0.42
2:B:105:THR:HG23	2:B:115:THR:HG22	2.00	0.42
1:A:145:ARG:HD2	2:B:459:PHE:CZ	2.53	0.42
2:B:164:GLN:CG	5:B:903:HOH:O	2.53	0.42
2:B:48:THR:HB	2:B:55:LEU:HA	2.01	0.42
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.96	0.42
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.85	0.42
2:B:129:THR:HG22	2:B:136:ALA:HB2	2.02	0.42
2:B:488:PHE:CE1	2:B:497:VAL:HG22	2.55	0.42
1:A:47:ARG:NE	5:A:317:HOH:O	2.52	0.42
2:B:69:ALA:CB	4:B:559:PAC:C1	2.98	0.42
2:B:85:GLU:O	2:B:86:LYS:C	2.58	0.42
1:A:139:VAL:HG22	2:B:147:GLU:HB3	2.01	0.41
2:B:556:GLN:OE1	2:B:557:ARG:N	2.48	0.41
1:A:130:GLU:HB2	1:A:131:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:GLN:HG2	5:B:661:HOH:O	2.20	0.41
2:B:246:LYS:O	2:B:247:ASP:HB2	2.20	0.41
1:A:144:ASN:C	5:A:327:HOH:O	2.59	0.41
2:B:53:PRO:HD2	2:B:151:LEU:HD21	2.02	0.41
2:B:131:GLN:H	2:B:131:GLN:HG3	1.52	0.41
2:B:90:TYR:CZ	2:B:121:THR:HB	2.55	0.41
2:B:35:ILE:HG23	2:B:55:LEU:HD11	2.03	0.41
2:B:363:VAL:HA	2:B:364:PRO:HD3	1.87	0.41
2:B:504:ALA:HA	2:B:505:PRO:C	2.40	0.41
2:B:83:SER:HB3	2:B:96:TRP:CH2	2.56	0.41
1:A:158:LEU:HD13	2:B:367:PHE:HB3	2.02	0.41
2:B:369:LYS:HA	2:B:369:LYS:HD2	1.87	0.41
2:B:1:SER:OG	4:B:559:PAC:C1	2.69	0.40
2:B:210:PRO:O	2:B:215:TRP:HB2	2.21	0.40
2:B:45:THR:HG21	2:B:537:TRP:O	2.21	0.40
2:B:243:SER:HA	2:B:244:PRO:HD3	1.91	0.40
2:B:401:GLN:HB2	2:B:405:SER:HB2	2.03	0.40
1:A:88:GLU:HG2	5:A:295:HOH:O	2.20	0.40
2:B:432:GLU:O	2:B:436:LYS:HB2	2.21	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	191/209 (91%)	188 (98%)	3 (2%)	0	100	100
2	B	555/557 (100%)	536 (97%)	16 (3%)	3 (0%)	34	55
All	All	746/766 (97%)	724 (97%)	19 (2%)	3 (0%)	39	61

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 ⓘ

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%)	156 (94%)	9 (6%)	27	48
2	B	460/460 (100%)	431 (94%)	29 (6%)	22	40
All	All	625/640 (98%)	587 (94%)	38 (6%)	23	42

All (38) 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	193	GLN
2	B	2	ASN
2	B	10	LYS
2	B	20	ASN
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	161	LYS

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Mol	Chain	Res	Type
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	337	LYS
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	468	GLU
2	B	519	LYS
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 ⓘ

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PAC	B	559	-	7,10,10	0.42	0	9,12,12	2.40	6 (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	PAC	B	559	-	-	0/2/4/4	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559	PAC	C4'-C3'-C2'	-3.98	114.36	120.19
4	B	559	PAC	C2-C1'-C6'	-2.42	113.48	120.90
4	B	559	PAC	C5'-C6'-C1'	-2.38	116.86	120.65
4	B	559	PAC	C1-C2-C1'	-2.03	108.70	112.73
4	B	559	PAC	C6'-C1'-C2'	2.71	122.47	118.13
4	B	559	PAC	C5'-C4'-C3'	3.33	125.77	119.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	559	PAC	6	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.