



# Full wwPDB X-ray Structure Validation Report i

Jan 27, 2024 – 09:53 AM EST

PDB ID : 1AI6  
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](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

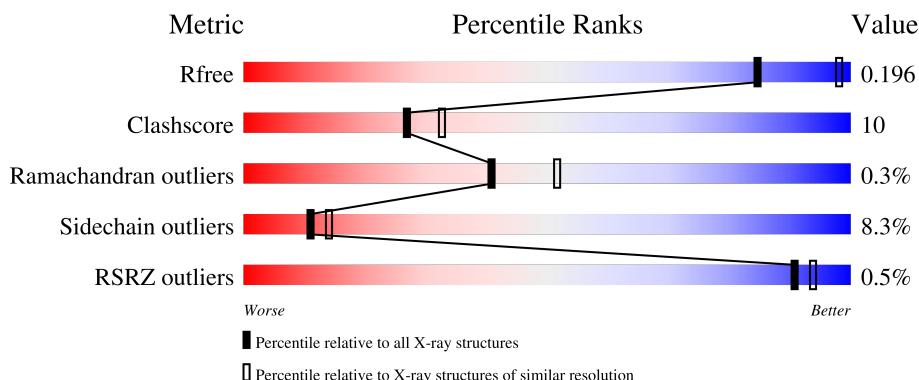
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

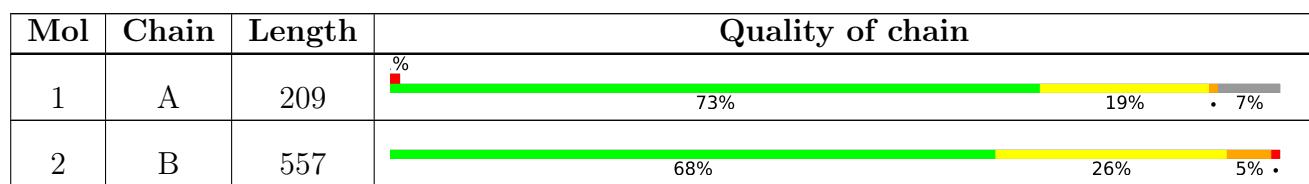
The reported resolution of this entry is 2.55 Å.

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))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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.



## 2 Entry composition i

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
			Total	C	N	O	S			
1	A	195	1565	1002	261	294	8	0	0	0

- Molecule 2 is a protein called PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	557	4415	2805	767	833	10	0	0	0

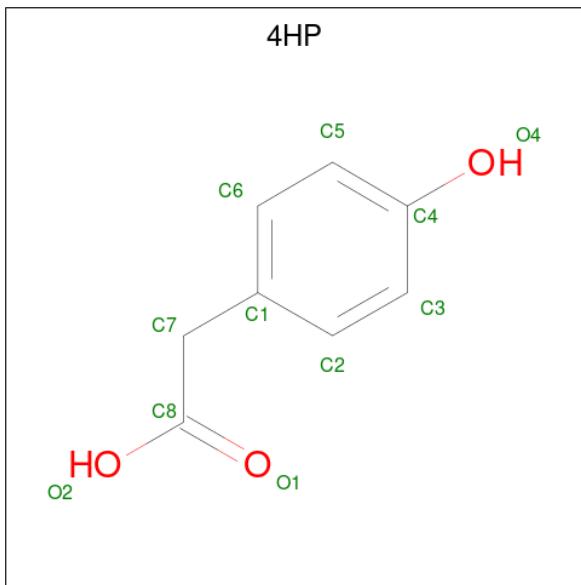
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	165	GLN	GLU	conflict	UNP P06875

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

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

- Molecule 4 is 4-HYDROXYPHENYLACETATE (three-letter code: 4HP) (formula: C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>).



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

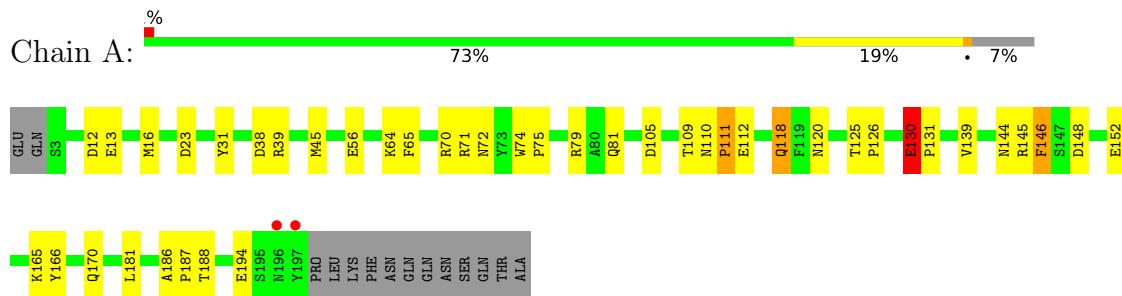
- Molecule 5 is water.

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

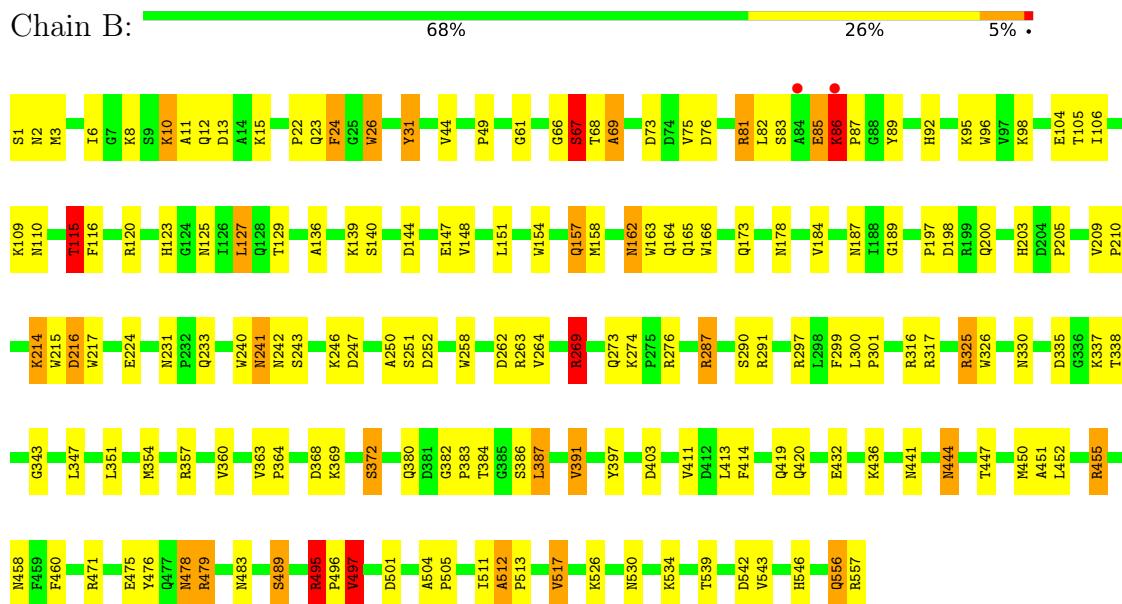
### 3 Residue-property plots [\(i\)](#)

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 (i)

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)	28.06 – 2.55 28.06 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.6 (28.06-2.55) 94.2 (28.06-2.55)	Depositor EDS
$R_{merge}$	0.38	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	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 <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 84.5	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50$ , $< L^2 > = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 4HP

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	0.62	2/1605 (0.1%)	1.43	16/2179 (0.7%)
2	B	0.65	4/4541 (0.1%)	1.54	61/6192 (1.0%)
All	All	0.64	6/6146 (0.1%)	1.51	77/8371 (0.9%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	ALA	C-N	-15.62	1.04	1.33
2	B	241	ASN	C-N	-12.69	1.04	1.34
1	A	146	PHE	C-N	-10.95	1.08	1.34
2	B	240	TRP	C-N	-6.95	1.18	1.34
2	B	68	THR	C-N	-6.00	1.20	1.34
1	A	144	ASN	C-N	-5.70	1.21	1.34

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	69	ALA	C-N-CA	23.68	172.03	122.30
2	B	241	ASN	O-C-N	-17.69	94.40	122.70
2	B	76	ASP	CB-CG-OD1	16.78	133.40	118.30
2	B	241	ASN	C-N-CA	16.19	162.16	121.70
2	B	69	ALA	O-C-N	-14.60	98.39	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	479	ARG	NE-CZ-NH2	-14.14	113.23	120.30
2	B	269	ARG	NE-CZ-NH1	12.28	126.44	120.30
2	B	69	ALA	CA-C-N	12.16	140.52	116.20
2	B	252	ASP	CB-CG-OD2	10.61	127.85	118.30
1	A	12	ASP	CB-CG-OD1	10.25	127.53	118.30
1	A	12	ASP	CB-CG-OD2	-9.64	109.62	118.30
2	B	269	ARG	CD-NE-CZ	9.47	136.86	123.60
2	B	357	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	79	ARG	CD-NE-CZ	9.39	136.74	123.60
2	B	76	ASP	OD1-CG-OD2	-8.85	106.49	123.30
2	B	241	ASN	CA-C-N	8.73	136.42	117.20
2	B	67	SER	N-CA-CB	-8.35	97.98	110.50
2	B	455	ARG	NE-CZ-NH2	-8.26	116.17	120.30
2	B	240	TRP	CA-C-O	-8.10	103.09	120.10
2	B	471	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	A	38	ASP	CB-CG-OD2	7.96	125.47	118.30
2	B	291	ARG	NE-CZ-NH1	7.77	124.18	120.30
2	B	316	ARG	NE-CZ-NH2	7.68	124.14	120.30
2	B	31	TYR	CB-CG-CD1	-7.48	116.51	121.00
2	B	242	ASN	N-CA-CB	7.40	123.92	110.60
2	B	479	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	23	ASP	CB-CG-OD1	7.36	124.93	118.30
2	B	252	ASP	OD1-CG-OD2	-7.35	109.34	123.30
2	B	287	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	152	GLU	OE1-CD-OE2	-7.25	114.60	123.30
2	B	475	GLU	OE1-CD-OE2	-7.25	114.59	123.30
1	A	70	ARG	NE-CZ-NH1	7.03	123.81	120.30
2	B	325	ARG	NE-CZ-NH2	-7.01	116.79	120.30
2	B	495	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	B	287	ARG	NE-CZ-NH1	6.84	123.72	120.30
2	B	263	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	B	240	TRP	O-C-N	6.80	133.58	122.70
1	A	16	MET	CG-SD-CE	6.78	111.05	100.20
2	B	68	THR	CA-C-O	-6.77	105.89	120.10
2	B	31	TYR	CB-CG-CD2	6.72	125.03	121.00
2	B	455	ARG	CD-NE-CZ	6.54	132.76	123.60
2	B	205	PRO	O-C-N	-6.54	112.24	122.70
2	B	287	ARG	CD-NE-CZ	6.36	132.51	123.60
2	B	391	VAL	CB-CA-C	-6.31	99.42	111.40
1	A	130	GLU	OE1-CD-OE2	-6.25	115.81	123.30
2	B	144	ASP	CB-CG-OD1	6.18	123.87	118.30
2	B	216	ASP	CB-CG-OD1	6.17	123.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	ARG	N-CA-CB	6.16	121.68	110.60
2	B	263	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	B	557	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	B	269	ARG	CA-CB-CG	6.00	126.59	113.40
1	A	45	MET	CG-SD-CE	5.98	109.77	100.20
2	B	75	VAL	CA-C-O	-5.79	107.94	120.10
2	B	81	ARG	NE-CZ-NH1	5.77	123.18	120.30
2	B	86	LYS	CA-CB-CG	5.74	126.03	113.40
2	B	497	VAL	CB-CA-C	-5.74	100.50	111.40
2	B	495	ARG	CD-NE-CZ	5.71	131.60	123.60
2	B	335	ASP	CB-CG-OD1	5.66	123.39	118.30
2	B	556	GLN	N-CA-CB	5.62	120.72	110.60
2	B	357	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	B	151	LEU	CA-CB-CG	5.46	127.85	115.30
2	B	479	ARG	CD-NE-CZ	5.39	131.15	123.60
2	B	115	THR	N-CA-CB	5.36	120.49	110.30
1	A	105	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	146	PHE	C-N-CA	5.32	135.00	121.70
2	B	354	MET	CA-CB-CG	5.23	122.20	113.30
1	A	70	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	B	24	PHE	CB-CG-CD2	5.16	124.41	120.80
2	B	397	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	146	PHE	O-C-N	-5.12	114.51	122.70
1	A	39	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	A	111	PRO	N-CA-CB	5.11	109.43	103.30
2	B	144	ASP	OD1-CG-OD2	-5.10	113.60	123.30
2	B	200	GLN	CA-CB-CG	5.05	124.52	113.40
2	B	455	ARG	NH1-CZ-NH2	5.05	124.95	119.40
2	B	330	ASN	CB-CG-OD1	5.00	131.61	121.60
2	B	512	ALA	N-CA-CB	5.00	117.10	110.10

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 [\(i\)](#)

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	1565	0	1515	22	0
2	B	4415	0	4240	107	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	5762	120	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 10.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:387:LEU:HD21	2:B:450:MET:CE	2.43	0.49
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:TYR:CE2	2:B:49:PRO:HB3	2.51	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
2:B:10:LYS:NZ	2:B:274:LYS:O	2.50	0.44
1:A:72:ASN:HD21	2:B:139:LYS:HZ3	1.65	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:73:ASP:OD1	2:B:73:ASP:C	2.55	0.43
2:B:387:LEU:HD21	2:B:450:MET:HE1	2.01	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:1:SER:OG	4:B:559:4HP:O2	2.29	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:3:MET:HE1	2:B:66:GLY:HA3	2.01	0.42
2:B:495:ARG:HA	2:B:496:PRO:HD3	1.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:504:ALA:HA	2:B:505:PRO:C	2.41	0.41
2:B:363:VAL:HA	2:B:364:PRO:HD3	1.83	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
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%)	34   46
All	All	748/766 (98%)	728 (97%)	18 (2%)	2 (0%)	41   51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	SER

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Mol	Chain	Res	Type
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%)	158 (95%)	9 (5%)	22 29
2	B	460/460 (100%)	417 (91%)	43 (9%)	9 10
All	All	627/640 (98%)	575 (92%)	52 (8%)	11 14

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	31	TYR
1	A	64	LYS
1	A	71	ARG
1	A	109	THR
1	A	112	GLU
1	A	118	GLN
1	A	130	GLU
1	A	181	LEU
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	115	THR
2	B	127	LEU
2	B	154	TRP
2	B	157	GLN
2	B	162	ASN

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Mol	Chain	Res	Type
2	B	164	GLN
2	B	173	GLN
2	B	184	VAL
2	B	214	LYS
2	B	224	GLU
2	B	269	ARG
2	B	273	GLN
2	B	290	SER
2	B	317	ARG
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	411	VAL
2	B	420	GLN
2	B	432	GLU
2	B	436	LYS
2	B	444	ASN
2	B	458	ASN
2	B	478	ASN
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	72	ASN
1	A	81	GLN
1	A	118	GLN
1	A	120	ASN
1	A	170	GLN
2	B	2	ASN
2	B	12	GLN
2	B	20	ASN

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Mol	Chain	Res	Type
2	B	92	HIS
2	B	93	ASN
2	B	110	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
2	B	187	ASN
2	B	203	HIS
2	B	245	GLN
2	B	292	GLN
2	B	304	GLN
2	B	330	ASN
2	B	340	GLN
2	B	348	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

### 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 monosaccharides 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	0.85	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	-4.03	115.13	120.89
4	B	559	4HP	C6-C1-C2	2.63	122.29	118.17
4	B	559	4HP	C6-C5-C4	-2.26	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	195/209 (93%)	-0.78	2 (1%) 82 86	23, 35, 62, 77	0
2	B	557/557 (100%)	-0.75	2 (0%) 92 96	18, 35, 70, 116	0
All	All	752/766 (98%)	-0.76	4 (0%) 91 94	18, 35, 67, 116	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	TYR	3.6
2	B	86	LYS	3.1
1	A	196	ASN	3.1
2	B	84	ALA	2.2

### 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	4HP	B	559	11/11	0.98	0.09	17,21,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	B	558	1/1	0.99	0.14	31,31,31,31	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.