



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:10 am BST

PDB ID : 1AI7  
Title : PENICILLIN ACYLASE COMPLEXED WITH PHENOL  
Authors : Done, S.H.  
Deposited on : 1997-05-01  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

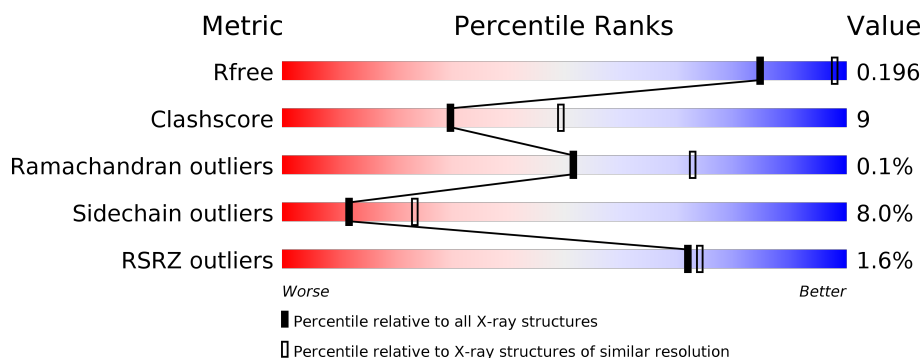
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>...</div> </div> </div>
2	B	557	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>5%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6715 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1656	1058	278	312	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			

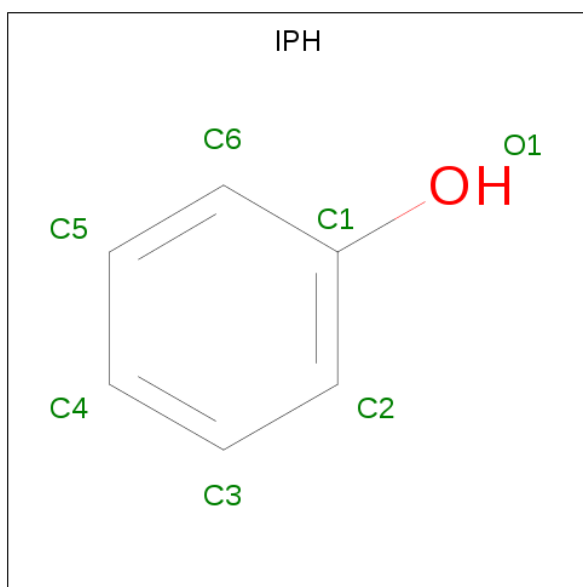
There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 4 is PHENOL (three-letter code: IPH) (formula: C<sub>6</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	6	1		

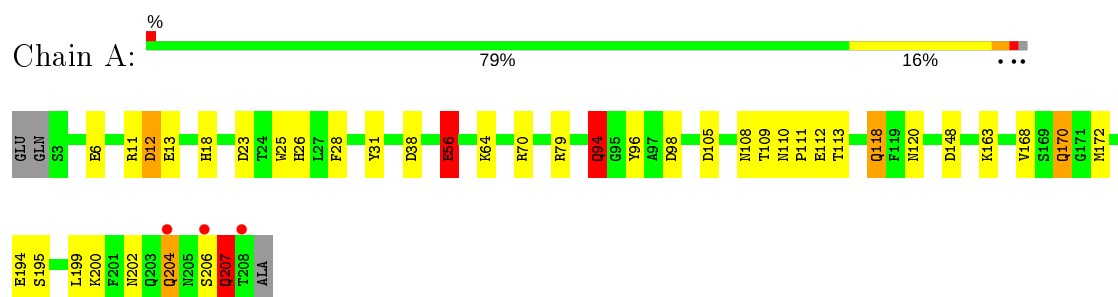
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	0
			172	172		
5	B	464	Total	O	0	0
			464	464		

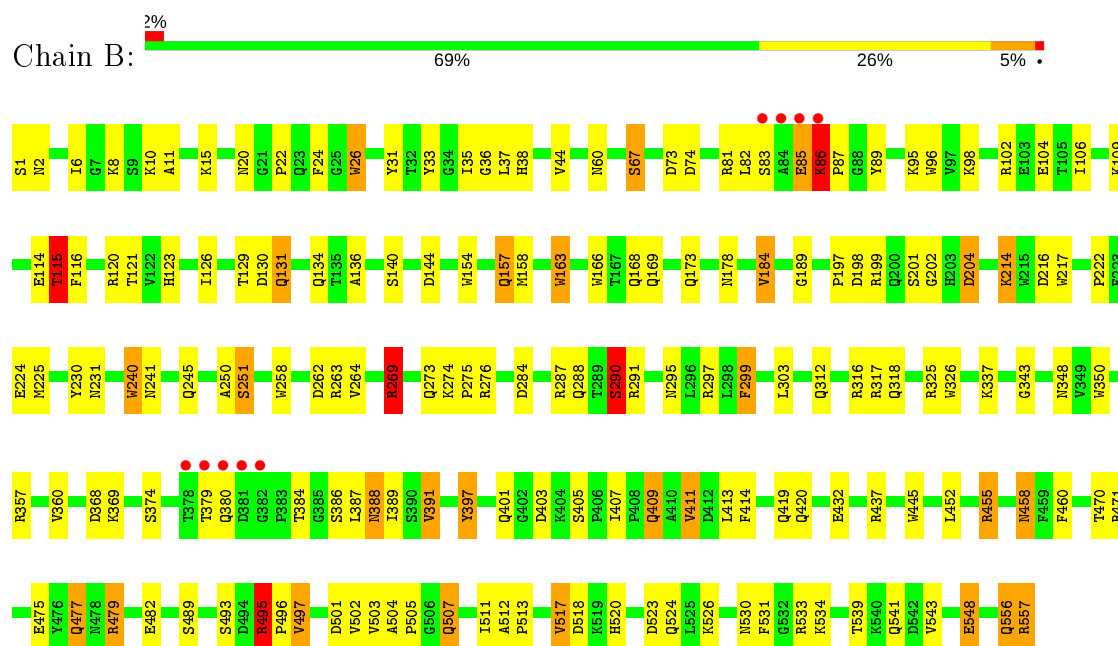
### 3 Residue-property plots

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.

#### • 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, $\alpha$ , $\beta$ , $\gamma$	52.12Å 65.08Å 76.30Å 100.20° 111.44° 105.81°	Depositor
Resolution (Å)	24.97 – 2.50 24.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (24.97-2.50) 94.8 (24.97-2.50)	Depositor EDS
$R_{merge}$	0.42	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.24 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.139 , 0.217 0.138 , 0.196	Depositor DCC
$R_{free}$ test set	2023 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 77.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: IPH, 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	0.71	1/1698 (0.1%)	1.51	22/2305 (1.0%)
2	B	0.71	3/4541 (0.1%)	1.62	82/6192 (1.3%)
All	All	0.71	4/6239 (0.1%)	1.59	104/8497 (1.2%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	445	TRP	NE1-CE2	8.80	1.49	1.37
2	B	240	TRP	NE1-CE2	8.68	1.48	1.37
2	B	163	TRP	NE1-CE2	8.41	1.48	1.37
1	A	25	TRP	NE1-CE2	8.35	1.48	1.37

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	ARG	CD-NE-CZ	16.91	147.27	123.60
2	B	269	ARG	NE-CZ-NH1	16.01	128.31	120.30
2	B	144	ASP	CB-CG-OD1	15.65	132.38	118.30
2	B	287	ARG	NE-CZ-NH1	14.61	127.60	120.30
1	A	70	ARG	NE-CZ-NH2	-13.22	113.69	120.30
2	B	73	ASP	CB-CG-OD2	13.01	130.01	118.30
2	B	287	ARG	CD-NE-CZ	12.77	141.47	123.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	287	ARG	NE-CZ-NH2	-12.63	113.98	120.30
2	B	455	ARG	CD-NE-CZ	11.85	140.19	123.60
2	B	475	GLU	OE1-CD-OE2	-11.79	109.15	123.30
1	A	79	ARG	CD-NE-CZ	11.49	139.68	123.60
1	A	12	ASP	CB-CG-OD2	-10.87	108.52	118.30
2	B	357	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	A	70	ARG	NE-CZ-NH1	9.93	125.26	120.30
2	B	495	ARG	NE-CZ-NH1	9.64	125.12	120.30
2	B	557	ARG	NE-CZ-NH2	-9.31	115.65	120.30
2	B	357	ARG	NE-CZ-NH1	9.09	124.84	120.30
2	B	409	GLN	CG-CD-OE1	8.56	138.73	121.60
2	B	479	ARG	NE-CZ-NH2	-8.53	116.03	120.30
2	B	263	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	170	GLN	CG-CD-OE1	8.36	138.32	121.60
1	A	94	GLN	CG-CD-OE1	8.35	138.29	121.60
2	B	541	GLN	CG-CD-OE1	8.33	138.25	121.60
2	B	2	ASN	CB-CG-OD1	8.16	137.91	121.60
2	B	420	GLN	CG-CD-OE1	8.12	137.83	121.60
2	B	556	GLN	CA-CB-CG	-8.11	95.57	113.40
2	B	541	GLN	CG-CD-NE2	-8.10	97.27	116.70
1	A	94	GLN	CG-CD-NE2	-8.09	97.28	116.70
2	B	495	ARG	NE-CZ-NH2	-8.09	116.26	120.30
2	B	409	GLN	CG-CD-NE2	-7.94	97.65	116.70
2	B	269	ARG	CA-CB-CG	7.91	130.81	113.40
1	A	170	GLN	CG-CD-NE2	-7.71	98.19	116.70
2	B	102	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	204	GLN	CG-CD-OE1	-7.59	106.43	121.60
2	B	168	GLN	CG-CD-OE1	7.47	136.55	121.60
2	B	316	ARG	NE-CZ-NH2	7.42	124.01	120.30
2	B	420	GLN	CG-CD-NE2	-7.41	98.92	116.70
2	B	2	ASN	CB-CG-ND2	-7.39	98.97	116.70
2	B	102	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	11	ARG	CD-NE-CZ	7.32	133.85	123.60
2	B	73	ASP	OD1-CG-OD2	-7.07	109.86	123.30
2	B	420	GLN	CA-CB-CG	7.06	128.93	113.40
2	B	391	VAL	CB-CA-C	-6.96	98.18	111.40
2	B	131	GLN	CG-CD-OE1	6.92	135.43	121.60
2	B	168	GLN	CG-CD-NE2	-6.89	100.17	116.70
2	B	120	ARG	NE-CZ-NH1	-6.78	116.91	120.30
2	B	295	ASN	CB-CG-OD1	6.77	135.15	121.60
2	B	397	TYR	CB-CG-CD1	-6.72	116.97	121.00
2	B	397	TYR	CB-CG-CD2	6.70	125.02	121.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	437	ARG	NE-CZ-NH2	-6.60	117.00	120.30
2	B	482	GLU	OE1-CD-OE2	-6.58	115.40	123.30
2	B	269	ARG	NH1-CZ-NH2	-6.45	112.31	119.40
2	B	131	GLN	CG-CD-NE2	-6.44	101.24	116.70
2	B	86	LYS	CA-CB-CG	6.37	127.41	113.40
2	B	295	ASN	CB-CG-ND2	-6.36	101.43	116.70
2	B	556	GLN	CG-CD-OE1	-6.29	109.01	121.60
2	B	409	GLN	CA-CB-CG	-6.26	99.64	113.40
2	B	284	ASP	CB-CG-OD1	-6.23	112.70	118.30
2	B	144	ASP	OD1-CG-OD2	-6.22	111.48	123.30
1	A	38	ASP	CB-CG-OD2	6.21	123.89	118.30
2	B	74	ASP	CB-CG-OD2	6.19	123.87	118.30
2	B	541	GLN	CA-CB-CG	6.14	126.90	113.40
2	B	1	SER	N-CA-CB	-6.13	101.30	110.50
2	B	184	VAL	CB-CA-C	-6.10	99.81	111.40
1	A	12	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	204	GLN	CB-CG-CD	-6.00	96.01	111.60
1	A	170	GLN	CB-CG-CD	5.99	127.18	111.60
1	A	98	ASP	CB-CG-OD2	5.96	123.66	118.30
2	B	479	ARG	NE-CZ-NH1	5.89	123.24	120.30
2	B	312	GLN	CA-CB-CG	5.83	126.23	113.40
2	B	114	GLU	OE1-CD-OE2	5.82	130.29	123.30
2	B	216	ASP	CB-CG-OD1	5.82	123.54	118.30
2	B	477	GLN	CA-CB-CG	5.82	126.20	113.40
1	A	148	ASP	CB-CG-OD1	5.81	123.53	118.30
2	B	299	PHE	CB-CG-CD1	-5.77	116.76	120.80
2	B	533	ARG	NE-CZ-NH1	-5.72	117.44	120.30
2	B	204	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	105	ASP	CB-CG-OD1	5.66	123.39	118.30
2	B	497	VAL	CB-CA-C	-5.65	100.67	111.40
2	B	316	ARG	NE-CZ-NH1	-5.63	117.48	120.30
2	B	284	ASP	CB-CG-OD2	5.63	123.36	118.30
2	B	477	GLN	CB-CG-CD	5.52	125.96	111.60
1	A	111	PRO	N-CA-CB	5.51	109.92	103.30
1	A	118	GLN	CB-CG-CD	5.48	125.84	111.60
2	B	199	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	B	269	ARG	N-CA-CB	5.44	120.40	110.60
2	B	269	ARG	CG-CD-NE	5.44	123.22	111.80
2	B	291	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	B	548	GLU	CA-CB-CG	5.33	125.13	113.40
2	B	386	SER	O-C-N	-5.30	114.23	122.70
2	B	245	GLN	N-CA-CB	-5.28	101.10	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	518	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	204	GLN	CG-CD-NE2	5.22	129.22	116.70
2	B	460	PHE	CB-CG-CD2	-5.20	117.16	120.80
2	B	460	PHE	CB-CG-CD1	5.15	124.41	120.80
1	A	56	GLU	N-CA-CB	5.14	119.85	110.60
1	A	207	GLN	O-C-N	-5.14	114.48	122.70
2	B	290	SER	CB-CA-C	-5.10	100.41	110.10
2	B	31	TYR	CB-CG-CD1	-5.09	117.95	121.00
2	B	455	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	B	33	TYR	CB-CG-CD2	-5.04	117.98	121.00
2	B	411	VAL	N-CA-CB	5.04	122.58	111.50
2	B	131	GLN	CB-CG-CD	5.03	124.68	111.60
2	B	115	THR	N-CA-CB	5.02	119.84	110.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	169	GLN	Mainchain
2	B	198	ASP	Mainchain
2	B	222	PRO	Mainchain
2	B	251	SER	Mainchain
2	B	26	TRP	Mainchain
2	B	290	SER	Mainchain
2	B	299	PHE	Mainchain

## 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	1656	0	1604	19	0
2	B	4415	0	4244	101	0
3	B	1	0	0	0	0
4	B	7	0	6	0	0
5	A	172	0	0	2	0
5	B	464	0	0	4	0
All	All	6715	0	5854	112	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 (112) 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:318:GLN:HG2	5:B:847:HOH:O	1.54	1.06
1:A:207:GLN:HE22	2:B:204:ASP:H	1.06	0.99
2:B:397:TYR:O	2:B:401:GLN:HG2	1.64	0.96
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.31	0.94
2:B:458:ASN:C	2:B:458:ASN:HD22	1.68	0.93
2:B:317:ARG:HH11	2:B:317:ARG:HG3	1.29	0.92
2:B:318:GLN:CG	5:B:847:HOH:O	2.14	0.86
2:B:157:GLN:HE22	2:B:166:TRP:HE1	1.21	0.85
1:A:18:HIS:HD2	2:B:38:HIS:NE2	1.74	0.85
2:B:317:ARG:NH1	2:B:317:ARG:HG3	1.89	0.84
2:B:157:GLN:NE2	2:B:166:TRP:HE1	1.79	0.80
2:B:384:THR:HG22	2:B:455:ARG:HH12	1.48	0.77
2:B:556:GLN:HG3	2:B:557:ARG:N	1.99	0.76
2:B:157:GLN:NE2	2:B:166:TRP:NE1	2.34	0.74
2:B:503:VAL:H	2:B:524:GLN:NE2	1.84	0.73
2:B:502:VAL:HA	2:B:524:GLN:HE22	1.55	0.71
1:A:172:MET:HG2	1:A:204:GLN:OE1	1.93	0.69
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.07	0.69
1:A:118:GLN:OE1	5:A:229:HOH:O	2.10	0.69
2:B:503:VAL:H	2:B:524:GLN:HE22	1.39	0.69
2:B:520:HIS:HE1	2:B:548:GLU:OE2	1.76	0.68
2:B:86:LYS:N	2:B:87:PRO:HD3	2.09	0.68
2:B:214:LYS:H	2:B:214:LYS:HD2	1.59	0.68
2:B:407:ILE:O	2:B:409:GLN:NE2	2.28	0.67
2:B:240:TRP:O	2:B:241:ASN:HB2	1.96	0.65
1:A:207:GLN:NE2	2:B:204:ASP:H	1.87	0.65
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.04	0.65
2:B:458:ASN:C	2:B:458:ASN:ND2	2.41	0.65
2:B:15:LYS:HG3	2:B:489:SER:HB2	1.77	0.64
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.33	0.63
2:B:556:GLN:CG	2:B:557:ARG:N	2.64	0.60
2:B:388:ASN:HD22	2:B:389:ILE:H	1.51	0.59
2:B:89:TYR:CZ	2:B:98:LYS:HG3	2.38	0.58
2:B:288:GLN:HG2	5:B:727:HOH:O	2.02	0.58
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.40	0.57
2:B:501:ASP:OD1	2:B:534:LYS:HE2	2.05	0.57
2:B:129:THR:HG22	2:B:136:ALA:CB	2.36	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:CG	1:A:26:HIS:HD1	2.07	0.56
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.89	0.56
2:B:86:LYS:N	2:B:87:PRO:CD	2.69	0.55
2:B:384:THR:HG22	2:B:455:ARG:NH1	2.20	0.55
2:B:384:THR:CG2	2:B:455:ARG:HH12	2.17	0.55
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.88	0.54
2:B:214:LYS:H	2:B:214:LYS:CD	2.21	0.54
2:B:157:GLN:NE2	2:B:166:TRP:CD1	2.76	0.54
2:B:503:VAL:N	2:B:524:GLN:HE22	2.05	0.54
2:B:317:ARG:CG	2:B:317:ARG:HH11	2.04	0.53
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.74	0.53
1:A:18:HIS:CD2	2:B:38:HIS:NE2	2.65	0.53
1:A:12:ASP:O	2:B:548:GLU:HG2	2.09	0.53
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.92	0.52
2:B:86:LYS:H	2:B:87:PRO:HD3	1.76	0.51
2:B:11:ALA:O	2:B:276:ARG:NH1	2.42	0.51
2:B:37:LEU:HB2	2:B:44:VAL:HG22	1.92	0.51
2:B:348:ASN:ND2	2:B:374:SER:OG	2.43	0.51
2:B:414:PHE:CZ	2:B:419:GLN:HG2	2.45	0.50
2:B:502:VAL:CA	2:B:524:GLN:HE22	2.23	0.50
2:B:388:ASN:ND2	2:B:389:ILE:H	2.08	0.50
2:B:530:ASN:O	2:B:531:PHE:HB2	2.11	0.50
2:B:121:THR:HG23	2:B:126:ILE:HD11	1.93	0.50
2:B:502:VAL:HA	2:B:524:GLN:NE2	2.23	0.50
1:A:23:ASP:OD1	1:A:26:HIS:ND1	2.41	0.50
1:A:202:ASN:ND2	1:A:206:SER:OG	2.45	0.49
2:B:318:GLN:HG3	5:B:847:HOH:O	1.97	0.48
1:A:194:GLU:O	1:A:195:SER:HB3	2.14	0.48
1:A:23:ASP:C	1:A:23:ASP:OD1	2.51	0.47
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.95	0.47
2:B:502:VAL:HG23	2:B:524:GLN:HE21	1.80	0.47
2:B:539:THR:O	2:B:543:VAL:HG23	2.15	0.47
2:B:317:ARG:CG	2:B:317:ARG:NH1	2.61	0.46
2:B:129:THR:HA	2:B:136:ALA:HA	1.97	0.46
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.96	0.46
2:B:130:ASP:O	2:B:134:GLN:N	2.48	0.46
2:B:262:ASP:OD1	2:B:264:VAL:HG12	2.15	0.46
2:B:470:THR:O	2:B:471:ARG:HD3	2.15	0.46
2:B:477:GLN:HE21	2:B:479:ARG:HD3	1.80	0.46
1:A:163:LYS:HG2	1:A:168:VAL:HA	1.98	0.45
1:A:206:SER:HB2	2:B:202:GLY:O	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:VAL:HG13	2:B:368:ASP:HB2	1.98	0.45
2:B:556:GLN:CD	2:B:557:ARG:H	2.20	0.45
2:B:129:THR:HG22	2:B:136:ALA:HB2	1.99	0.45
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.51	0.45
2:B:157:GLN:HE21	2:B:157:GLN:HB2	1.47	0.45
2:B:60:ASN:C	2:B:60:ASN:OD1	2.56	0.44
2:B:495:ARG:HA	2:B:496:PRO:HD3	1.91	0.44
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.52	0.44
1:A:56:GLU:O	2:B:109:LYS:HB2	2.18	0.44
1:A:199:LEU:HG	2:B:225:MET:HE1	2.00	0.44
2:B:35:ILE:HG13	2:B:36:GLY:N	2.33	0.44
2:B:471:ARG:HH11	2:B:471:ARG:HD3	1.61	0.43
2:B:556:GLN:HA	2:B:556:GLN:OE1	2.12	0.42
2:B:384:THR:HG22	2:B:455:ARG:HH22	1.84	0.42
2:B:507:GLN:HE21	2:B:507:GLN:HB2	1.63	0.42
2:B:504:ALA:HA	2:B:505:PRO:C	2.40	0.42
2:B:104:GLU:O	2:B:115:THR:HA	2.20	0.42
2:B:85:GLU:O	2:B:86:LYS:HG2	2.19	0.42
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.55	0.42
2:B:67:SER:HA	2:B:178:ASN:O	2.20	0.42
2:B:6:ILE:HG23	2:B:10:LYS:HB3	2.02	0.42
2:B:123:HIS:O	2:B:140:SER:HB2	2.20	0.42
2:B:274:LYS:HA	2:B:275:PRO:HD3	1.93	0.42
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.55	0.41
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.56	0.41
2:B:230:TYR:O	2:B:231:ASN:C	2.59	0.41
1:A:120:ASN:HD22	1:A:120:ASN:HA	1.65	0.41
2:B:503:VAL:N	2:B:524:GLN:NE2	2.60	0.41
1:A:94:GLN:NE2	5:A:321:HOH:O	2.54	0.40
2:B:413:LEU:HD23	2:B:413:LEU:HA	1.93	0.40
2:B:303:LEU:HD21	2:B:350:TRP:CE2	2.56	0.40
2:B:325:ARG:HD2	2:B:325:ARG:HH11	1.58	0.40
1:A:28:PHE:O	1:A:96:TYR:HA	2.22	0.40
2:B:388:ASN:HD22	2:B:389:ILE:N	2.16	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	204/209 (98%)	200 (98%)	4 (2%)	0	100	100
2	B	555/557 (100%)	541 (98%)	13 (2%)	1 (0%)	47	68
All	All	759/766 (99%)	741 (98%)	17 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	SER

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/180 (99%)	164 (92%)	14 (8%)	12	24
2	B	460/460 (100%)	423 (92%)	37 (8%)	12	23
All	All	638/640 (100%)	587 (92%)	51 (8%)	12	23

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	13	GLU
1	A	31	TYR
1	A	56	GLU
1	A	64	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	94	GLN
1	A	108	ASN
1	A	109	THR
1	A	110	ASN
1	A	112	GLU
1	A	113	THR
1	A	170	GLN
1	A	200	LYS
1	A	207	GLN
2	B	8	LYS
2	B	20	ASN
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	131	GLN
2	B	154	TRP
2	B	157	GLN
2	B	173	GLN
2	B	184	VAL
2	B	201	SER
2	B	214	LYS
2	B	224	GLU
2	B	269	ARG
2	B	273	GLN
2	B	290	SER
2	B	337	LYS
2	B	369	LYS
2	B	379	THR
2	B	380	GLN
2	B	387	LEU
2	B	388	ASN
2	B	391	VAL
2	B	403	ASP
2	B	405	SER
2	B	411	VAL
2	B	432	GLU
2	B	458	ASN
2	B	493	SER
2	B	495	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	497	VAL
2	B	507	GLN
2	B	517	VAL
2	B	526	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	108	ASN
1	A	120	ASN
1	A	155	ASN
1	A	170	GLN
1	A	207	GLN
2	B	93	ASN
2	B	110	ASN
2	B	157	GLN
2	B	168	GLN
2	B	233	GLN
2	B	241	ASN
2	B	245	GLN
2	B	288	GLN
2	B	348	ASN
2	B	388	ASN
2	B	401	GLN
2	B	441	ASN
2	B	458	ASN
2	B	473	GLN
2	B	477	GLN
2	B	507	GLN
2	B	520	HIS
2	B	524	GLN
2	B	546	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	IPH	B	559	-	7,7,7	0.49	0	8,8,8	2.18	3 (37%)

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	IPH	B	559	-	-	-	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	IPH	C6-C1-C2	3.66	125.94	119.77
4	B	559	IPH	C3-C2-C1	-3.58	114.26	119.31
4	B	559	IPH	C5-C6-C1	-2.52	115.75	119.31

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	206/209 (98%)	-0.48	3 (1%) 73 75	22, 35, 67, 81	0
2	B	557/557 (100%)	-0.60	9 (1%) 72 74	19, 34, 66, 112	0
All	All	763/766 (99%)	-0.57	12 (1%) 72 74	19, 34, 66, 112	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	380	GLN	4.5
2	B	382	GLY	4.4
1	A	208	THR	4.1
2	B	379	THR	3.9
1	A	204	GLN	3.6
2	B	381	ASP	3.2
2	B	86	LYS	3.1
2	B	378	THR	2.9
1	A	206	SER	2.4
2	B	84	ALA	2.4
2	B	83	SER	2.2
2	B	85	GLU	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 carbohydrates 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	IPH	B	559	7/7	0.97	0.13	26,30,36,43	0
3	CA	B	558	1/1	1.00	0.08	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.