Full wwPDB X-ray Structure Validation Report (i)

May 4, 2016 – 10:26 AM EDT

PDB ID	:	1AJQ
Title	:	PENICILLIN ACYLASE COMPLEXED WITH THIOPHENEACETIC ACID
Authors	:	Done, S.H.
Deposited on	:	1997-05-07
Resolution	:	2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

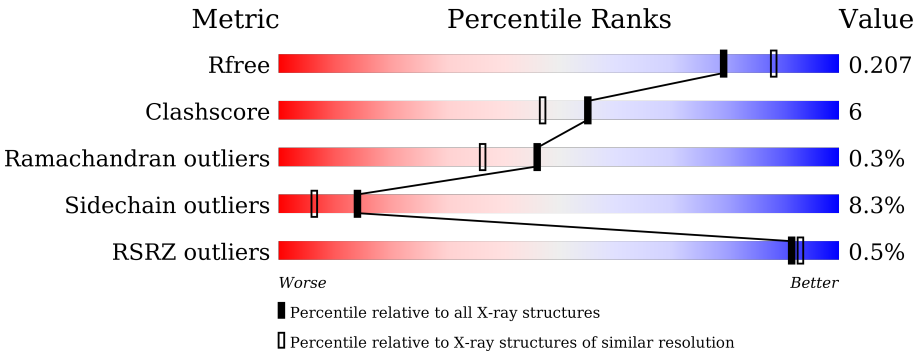
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

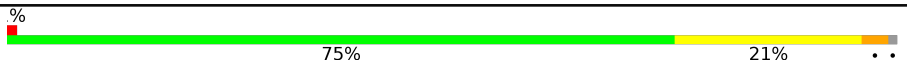
The reported resolution of this entry is 2.05 Å.

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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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 >=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 <=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	
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	SPA	B	559[A]	-	-	-	X
4	SPA	B	559[B]	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6768 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	3	0
			4438	2818	773	837	10			

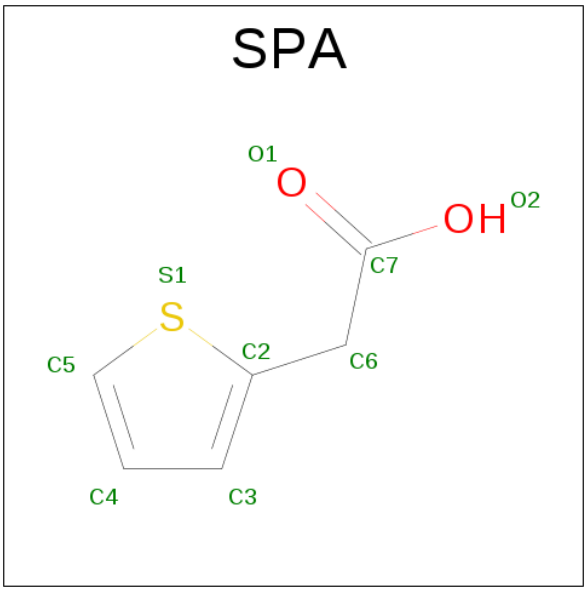
There is a discrepancy between the modelled and reference sequences:

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 THIOPHENEACETIC ACID (three-letter code: SPA) (formula: $C_6H_6O_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O S 13 9 2 2	0	1

- Molecule 5 is water.

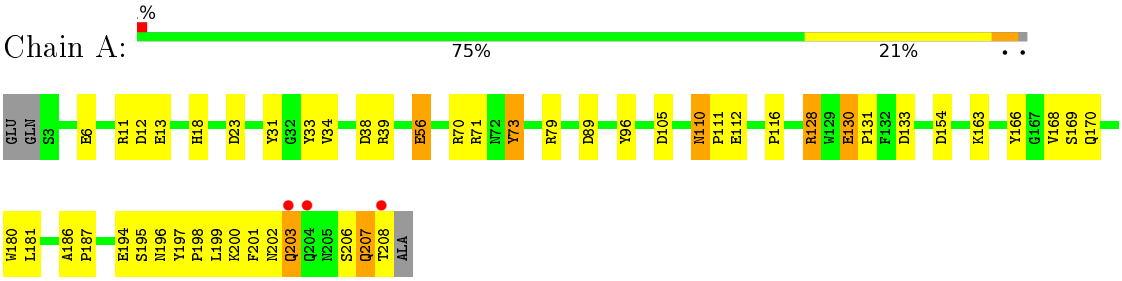
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	168	Total O 168 168	0	0
5	B	492	Total O 492 492	0	0

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 errors 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.

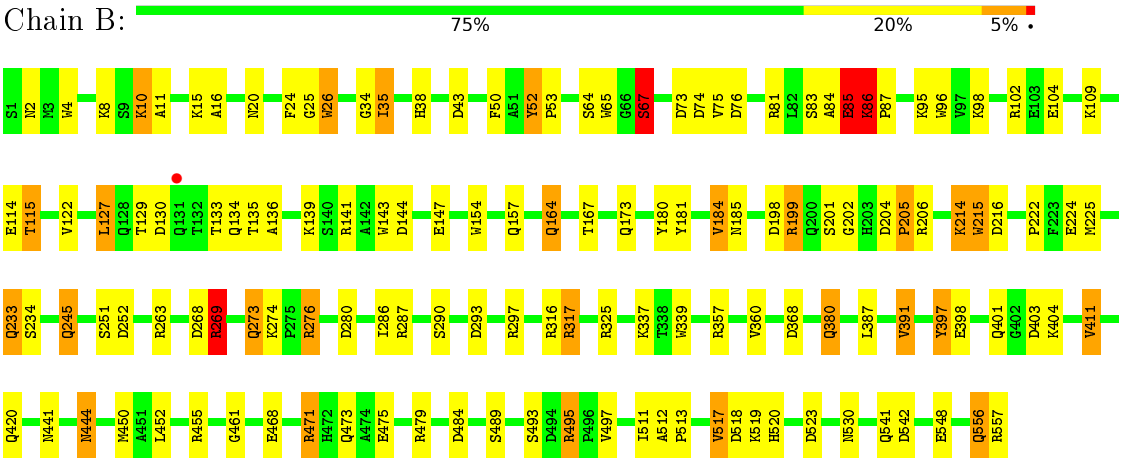
- Molecule 1: PENICILLIN AMIDOHYDROLASE

Chain A:



- Molecule 2: PENICILLIN AMIDOHYDROLASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	52.12Å 65.08Å 76.30Å 100.20° 111.44° 105.81°	Depositor
Resolution (Å)	19.85 – 2.05 14.93 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.85-2.05) 86.4 (14.93-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.03Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.233 0.148 , 0.207	Depositor DCC
R_{free} test set	3707 reflections (7.57%)	DCC
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6768	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SPA, 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	0.85	0/1698	1.75	29/2305 (1.3%)
2	B	0.89	3/4569 (0.1%)	1.74	75/6230 (1.2%)
All	All	0.88	3/6267 (0.0%)	1.75	104/8535 (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	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	143	TRP	CG-CD1	5.46	1.44	1.36
2	B	34	GLY	CA-C	5.43	1.60	1.51
2	B	25	GLY	N-CA	5.38	1.54	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	455	ARG	NE-CZ-NH1	21.36	130.98	120.30
2	B	263	ARG	NE-CZ-NH1	19.67	130.13	120.30
1	A	79	ARG	CD-NE-CZ	16.57	146.80	123.60
2	B	263	ARG	NE-CZ-NH2	-15.62	112.49	120.30
2	B	495	ARG	NE-CZ-NH1	15.51	128.06	120.30
1	A	70	ARG	NE-CZ-NH2	-14.67	112.97	120.30
2	B	471	ARG	CD-NE-CZ	14.64	144.10	123.60
2	B	455	ARG	NE-CZ-NH2	-13.81	113.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	TYR	CB-CG-CD1	13.07	128.84	121.00
2	B	557	ARG	NE-CZ-NH2	-12.74	113.93	120.30
2	B	287	ARG	NE-CZ-NH1	12.51	126.55	120.30
2	B	269	ARG	NE-CZ-NH1	12.12	126.36	120.30
2	B	471	ARG	NE-CZ-NH1	11.93	126.26	120.30
2	B	252	ASP	CB-CG-OD1	11.85	128.97	118.30
2	B	495	ARG	CD-NE-CZ	11.72	140.01	123.60
2	B	269	ARG	CD-NE-CZ	11.27	139.38	123.60
2	B	144	ASP	CB-CG-OD1	11.23	128.41	118.30
2	B	557	ARG	NE-CZ-NH1	11.15	125.88	120.30
1	A	73	TYR	CB-CG-CD2	-10.90	114.46	121.00
2	B	287	ARG	CD-NE-CZ	10.82	138.74	123.60
1	A	23	ASP	CB-CG-OD1	10.66	127.90	118.30
2	B	479	ARG	NE-CZ-NH2	-10.43	115.08	120.30
1	A	70	ARG	NE-CZ-NH1	9.89	125.24	120.30
2	B	76	ASP	CB-CG-OD1	9.80	127.12	118.30
2	B	495	ARG	NE-CZ-NH2	-9.74	115.43	120.30
2	B	455	ARG	CD-NE-CZ	9.57	137.00	123.60
2	B	475	GLU	OE1-CD-OE2	-9.22	112.24	123.30
1	A	154	ASP	CB-CG-OD1	9.12	126.51	118.30
1	A	79	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	A	38	ASP	CB-CG-OD2	9.02	126.42	118.30
2	B	199	ARG	CD-NE-CZ	-9.02	110.97	123.60
2	B	357	ARG	NE-CZ-NH1	8.95	124.78	120.30
2	B	297	ARG	NE-CZ-NH2	8.91	124.76	120.30
2	B	102	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	A	89	ASP	CB-CG-OD2	8.86	126.28	118.30
2	B	391	VAL	CG1-CB-CG2	8.58	124.63	110.90
2	B	518	ASP	CB-CG-OD2	8.58	126.02	118.30
1	A	133	ASP	CB-CG-OD2	-8.45	110.70	118.30
2	B	391	VAL	CB-CA-C	-8.20	95.82	111.40
2	B	76	ASP	OD1-CG-OD2	-7.86	108.37	123.30
2	B	397	TYR	CB-CG-CD2	7.72	125.63	121.00
1	A	128	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	A	39	ARG	NE-CZ-NH2	-7.43	116.59	120.30
2	B	206	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	A	11	ARG	CD-NE-CZ	7.30	133.82	123.60
2	B	316	ARG	NE-CZ-NH2	7.29	123.95	120.30
2	B	397	TYR	CB-CG-CD1	-7.13	116.72	121.00
2	B	216	ASP	CB-CG-OD1	7.06	124.65	118.30
2	B	67	SER	N-CA-CB	-7.00	100.00	110.50
1	A	130	GLU	OE1-CD-OE2	-6.99	114.91	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	52	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	A	71	ARG	CD-NE-CZ	6.95	133.33	123.60
2	B	76	ASP	CB-CG-OD2	6.89	124.50	118.30
2	B	206	ARG	NE-CZ-NH1	-6.85	116.88	120.30
2	B	471	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	B	102	ARG	NE-CZ-NH2	-6.79	116.91	120.30
2	B	471	ARG	CG-CD-NE	6.76	126.01	111.80
2	B	290	SER	CB-CA-C	-6.72	97.33	110.10
2	B	497	VAL	CB-CA-C	-6.71	98.65	111.40
2	B	479	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	B	398	GLU	OE1-CD-OE2	-6.40	115.62	123.30
1	A	11	ARG	NE-CZ-NH1	-6.37	117.11	120.30
2	B	269	ARG	CA-CB-CG	6.36	127.39	113.40
1	A	33	TYR	CB-CG-CD1	6.31	124.79	121.00
1	A	12	ASP	CB-CG-OD2	-6.23	112.69	118.30
2	B	287	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	B	86	LYS	CA-CB-CG	6.14	126.91	113.40
2	B	184	VAL	CB-CA-C	-6.14	99.73	111.40
2	B	269	ARG	NH1-CZ-NH2	-6.11	112.67	119.40
2	B	143	TRP	CB-CG-CD2	6.10	134.53	126.60
2	B	199	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	B	268	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	133	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	33	TYR	CB-CG-CD2	-5.90	117.46	121.00
2	B	74	ASP	CB-CG-OD1	5.85	123.56	118.30
2	B	411	VAL	CB-CA-C	-5.82	100.35	111.40
2	B	205	PRO	O-C-N	-5.68	113.61	122.70
2	B	233	GLN	CB-CG-CD	5.66	126.31	111.60
2	B	114	GLU	OE1-CD-OE2	5.64	130.07	123.30
2	B	50	PHE	CB-CG-CD2	-5.59	116.88	120.80
2	B	53	PRO	N-CA-CB	5.57	109.98	103.30
2	B	24	PHE	N-CA-CB	-5.56	100.59	110.60
2	B	325	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	96	TYR	O-C-N	-5.52	113.87	122.70
2	B	276	ARG	NE-CZ-NH2	5.51	123.05	120.30
2	B	280	ASP	CB-CG-OD1	5.50	123.25	118.30
2	B	198	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	12	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	96	TYR	CB-CG-CD2	-5.42	117.75	121.00
2	B	411	VAL	N-CA-CB	5.38	123.33	111.50
2	B	76	ASP	N-CA-CB	5.31	120.15	110.60
1	A	71	ARG	NE-CZ-NH1	5.30	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	293	ASP	CB-CG-OD1	-5.29	113.53	118.30
2	B	75	VAL	CA-C-O	-5.26	109.05	120.10
2	B	215	TRP	CA-CB-CG	-5.24	103.75	113.70
2	B	245	GLN	N-CA-CB	-5.18	101.28	110.60
1	A	56	GLU	N-CA-CB	5.17	119.90	110.60
1	A	71	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	180	TRP	CA-CB-CG	5.16	123.51	113.70
1	A	34	VAL	CA-CB-CG1	-5.11	103.23	110.90
2	B	252	ASP	OD1-CG-OD2	-5.06	113.69	123.30
2	B	16	ALA	N-CA-CB	5.06	117.18	110.10
2	B	484	ASP	CB-CG-OD1	5.05	122.84	118.30
2	B	64	SER	N-CA-CB	5.02	118.04	110.50

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	122	VAL	Mainchain
2	B	141	ARG	Mainchain
2	B	147	GLU	Mainchain
2	B	167	THR	Mainchain
2	B	181	TYR	Mainchain
2	B	185	ASN	Mainchain
2	B	205	PRO	Mainchain
2	B	222	PRO	Mainchain
2	B	234	SER	Mainchain
2	B	26	TRP	Mainchain
2	B	286	ILE	Mainchain
2	B	35	ILE	Mainchain
2	B	380	GLN	Mainchain
2	B	43	ASP	Mainchain
2	B	461	GLY	Mainchain
2	B	52	TYR	Mainchain
2	B	85[B]	GLU	Mainchain

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	1656	0	1604	23	0
2	B	4438	0	4265	65	0
3	B	1	0	0	0	0
4	B	13	0	6	1	0
5	A	168	0	0	0	0
5	B	492	0	0	0	0
All	All	6768	0	5875	76	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 6.

All (76) 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:207:GLN:HE22	2:B:204:ASP:H	1.10	0.99
2:B:85[A]:GLU:OE1	2:B:85[A]:GLU:HA	1.63	0.95
2:B:269:ARG:HH21	2:B:273:GLN:HE22	1.16	0.88
2:B:85[B]:GLU:O	2:B:86:LYS:HB3	1.76	0.85
2:B:85[A]:GLU:O	2:B:86:LYS:HB3	1.75	0.85
1:A:18:HIS:HD2	2:B:38:HIS:NE2	1.81	0.78
2:B:15:LYS:HG3	2:B:489:SER:HB2	1.64	0.77
2:B:269:ARG:HH21	2:B:273:GLN:NE2	1.81	0.77
2:B:214:LYS:H	2:B:214:LYS:HD2	1.56	0.70
2:B:444:ASN:C	2:B:444:ASN:HD22	1.95	0.69
2:B:269:ARG:NH2	2:B:273:GLN:HE22	1.91	0.67
1:A:207:GLN:NE2	2:B:204:ASP:H	1.88	0.65
1:A:194:GLU:OE2	2:B:233:GLN:HG3	1.95	0.65
2:B:11:ALA:O	2:B:276:ARG:NH1	2.29	0.65
1:A:207:GLN:HE21	1:A:207:GLN:H	1.44	0.64
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.33	0.64
2:B:86:LYS:O	2:B:86:LYS:HG2	1.95	0.64
2:B:85[A]:GLU:OE1	2:B:85[A]:GLU:CA	2.40	0.62
2:B:317:ARG:HH11	2:B:317:ARG:HG3	1.66	0.61
2:B:520:HIS:HE1	2:B:548:GLU:OE1	1.85	0.59
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.84	0.59
2:B:85[B]:GLU:HG3	2:B:85[B]:GLU:O	2.03	0.58
2:B:67:SER:HB3	4:B:559[B]:SPA:H5	1.86	0.57
2:B:214:LYS:H	2:B:214:LYS:CD	2.18	0.57
2:B:85[A]:GLU:O	2:B:86:LYS:CB	2.52	0.56
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.89	0.55
2:B:84:ALA:HB2	2:B:134:GLN:NE2	2.21	0.55
1:A:206:SER:HB2	2:B:202:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ASP:CG	2:B:133:THR:HG22	2.30	0.52
1:A:197:TYR:CD1	1:A:198:PRO:HD2	2.45	0.52
1:A:18:HIS:CD2	2:B:38:HIS:NE2	2.72	0.51
2:B:133:THR:HG23	2:B:135:THR:HB	1.93	0.50
2:B:556:GLN:HA	2:B:556:GLN:OE1	2.11	0.50
1:A:199:LEU:HG	2:B:225:MET:HE1	1.95	0.49
1:A:199:LEU:HG	2:B:225:MET:CE	2.43	0.48
2:B:495:ARG:NH2	2:B:542:ASP:OD1	2.45	0.48
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.50	0.47
1:A:105:ASP:OD1	1:A:128:ARG:NH1	2.48	0.47
1:A:56:GLU:O	2:B:109:LYS:HB2	2.14	0.47
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.80	0.47
1:A:163:LYS:HG2	1:A:168:VAL:HA	1.96	0.47
1:A:195:SER:OG	2:B:245:GLN:NE2	2.48	0.46
2:B:317:ARG:NH1	2:B:317:ARG:HG3	2.30	0.46
2:B:65:TRP:HA	2:B:180:TYR:O	2.16	0.46
2:B:127:LEU:HD11	2:B:139:LYS:HB2	1.97	0.46
2:B:133:THR:HG23	2:B:135:THR:CB	2.46	0.45
2:B:397:TYR:O	2:B:401:GLN:HG2	2.16	0.45
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.99	0.45
1:A:130:GLU:HB2	1:A:131:PRO:CD	2.47	0.44
1:A:166:TYR:O	1:A:170:GLN:HB3	2.17	0.44
2:B:360:VAL:HG13	2:B:368:ASP:HB2	2.00	0.44
1:A:181:LEU:HD21	1:A:201:PHE:HB2	1.98	0.44
2:B:164:GLN:H	2:B:164:GLN:NE2	2.15	0.44
1:A:130:GLU:HB2	1:A:131:PRO:HD2	1.99	0.44
2:B:511:ILE:HG12	2:B:517:VAL:CG2	2.48	0.43
2:B:339:TRP:CH2	2:B:450:MET:HE2	2.54	0.43
2:B:84:ALA:HB2	2:B:134:GLN:HE21	1.84	0.43
2:B:468:GLU:H	2:B:468:GLU:CD	2.23	0.42
1:A:203:GLN:HB2	1:A:203:GLN:HE21	1.50	0.42
2:B:452:LEU:HD23	2:B:473:GLN:NE2	2.35	0.42
2:B:129:THR:HG22	2:B:136:ALA:CB	2.50	0.42
2:B:85[B]:GLU:O	2:B:86:LYS:CB	2.56	0.42
1:A:202:ASN:HB2	2:B:202:GLY:HA2	2.02	0.41
2:B:471:ARG:HA	2:B:471:ARG:HD3	1.73	0.41
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.86	0.41
2:B:127:LEU:CD1	2:B:139:LYS:HB2	2.50	0.41
2:B:199:ARG:HH11	2:B:199:ARG:HD2	1.47	0.41
2:B:73:ASP:C	2:B:73:ASP:OD1	2.59	0.41
1:A:110:ASN:N	1:A:111:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:LYS:NZ	2:B:274:LYS:O	2.54	0.40
2:B:104:GLU:O	2:B:115:THR:HA	2.20	0.40
1:A:207:GLN:HA	2:B:215:TRP:CZ2	2.56	0.40
2:B:224:GLU:HG2	2:B:224:GLU:O	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	204/209 (98%)	200 (98%)	4 (2%)	0	100	100
2	B	558/557 (100%)	542 (97%)	14 (2%)	2 (0%)	39	28
All	All	762/766 (100%)	742 (97%)	18 (2%)	2 (0%)	46	36

All (2) Ramachandran outliers are listed below:

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

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	178/180 (99%)	165 (93%)	13 (7%)	17 8
2	B	463/460 (101%)	420 (91%)	43 (9%)	11 4
All	All	641/640 (100%)	585 (91%)	56 (9%)	14 5

All (56) 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	73	TYR
1	A	110	ASN
1	A	112	GLU
1	A	116	PRO
1	A	169	SER
1	A	196	ASN
1	A	200	LYS
1	A	203	GLN
1	A	207	GLN
1	A	208	THR
2	B	2	ASN
2	B	4	TRP
2	B	8	LYS
2	B	10	LYS
2	B	20	ASN
2	B	35	ILE
2	B	67	SER
2	B	81[A]	ARG
2	B	81[B]	ARG
2	B	85[A]	GLU
2	B	85[B]	GLU
2	B	86	LYS
2	B	95	LYS
2	B	98	LYS
2	B	115	THR
2	B	127	LEU
2	B	154	TRP
2	B	157	GLN
2	B	164	GLN

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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	269	ARG
2	B	273	GLN
2	B	317	ARG
2	B	337	LYS
2	B	380	GLN
2	B	387	LEU
2	B	391	VAL
2	B	403	ASP
2	B	404	LYS
2	B	411	VAL
2	B	420	GLN
2	B	441	ASN
2	B	444	ASN
2	B	493	SER
2	B	517	VAL
2	B	519	LYS
2	B	530	ASN
2	B	541[A]	GLN
2	B	541[B]	GLN
2	B	556	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	94	GLN
1	A	110	ASN
1	A	196	ASN
1	A	203	GLN
1	A	204	GLN
1	A	207	GLN
2	B	2	ASN
2	B	93	ASN
2	B	110	ASN
2	B	131	GLN
2	B	164	GLN
2	B	245	GLN
2	B	273	GLN

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Mol	Chain	Res	Type
2	B	341	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	SPA	B	559[A]	-	5,9,9	0.54	0	3,11,11	0.42	0
4	SPA	B	559[B]	-	5,9,9	0.52	0	3,11,11	0.57	0

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	SPA	B	559[A]	-	-	0/0/4/4	0/1/1/1
4	SPA	B	559[B]	-	-	0/0/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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[B]	SPA	1	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

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	206/209 (98%)	-0.77	3 (1%)	76	81	12, 23, 57, 87	0
2	B	557/557 (100%)	-0.90	1 (0%)	95	96	9, 21, 50, 97	0
All	All	763/766 (99%)	-0.87	4 (0%)	91	93	9, 22, 52, 97	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	THR	3.8
1	A	204	GLN	3.1
2	B	131	GLN	2.6
1	A	203	GLN	2.5

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	SPA	B	559[A]	9/9	0.98	0.08	3.79	14,15,18,19	4
4	SPA	B	559[B]	9/9	0.98	0.08	3.53	14,17,18,19	4
3	CA	B	558	1/1	1.00	0.05	-0.62	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.