



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AJN
Title : PENICILLIN ACYLASE COMPLEXED WITH P-NITROPHENYLACETIC ACID
Authors : Done, S.H.
Deposited on : 1997-05-07
Resolution : 2.36 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 ⓘ symbol.

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) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

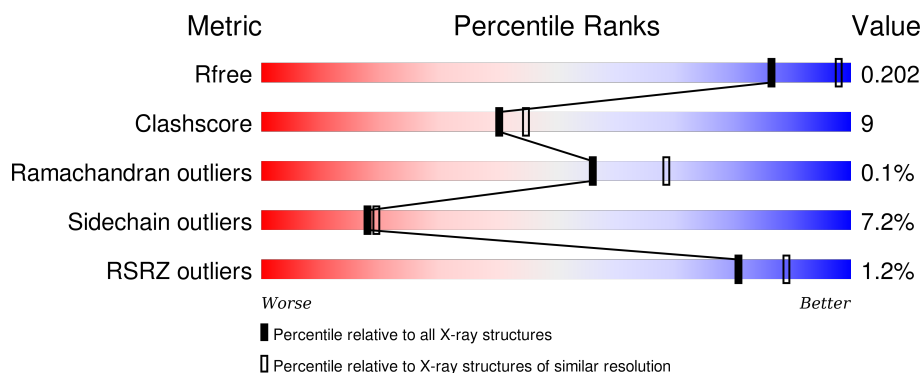
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 $\leq 5\%$. 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>76%</div> <div>19%</div> <div>...</div> </div>
2	B	557	<div> <div></div> <div>72%</div> <div>23%</div> <div>..</div> </div>

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	AAN	B	559	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6754 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			

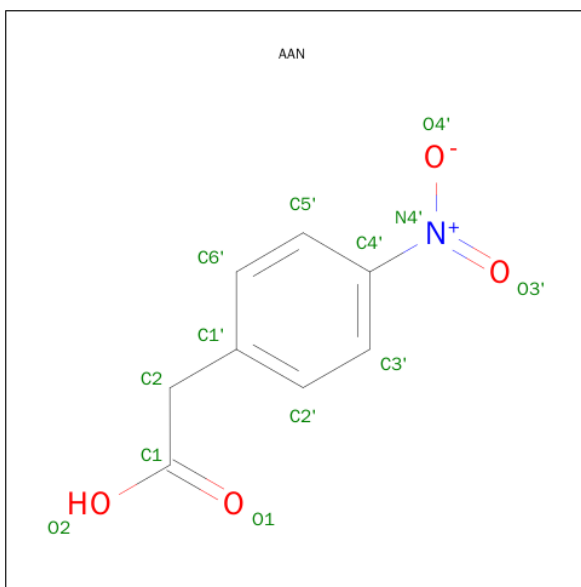
There is a discrepancy between the modelled and reference sequences:

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 2-(4-NITROPHENYL)ACETIC ACID (three-letter code: AAN) (formula: C₈H₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			13	8	1	4		

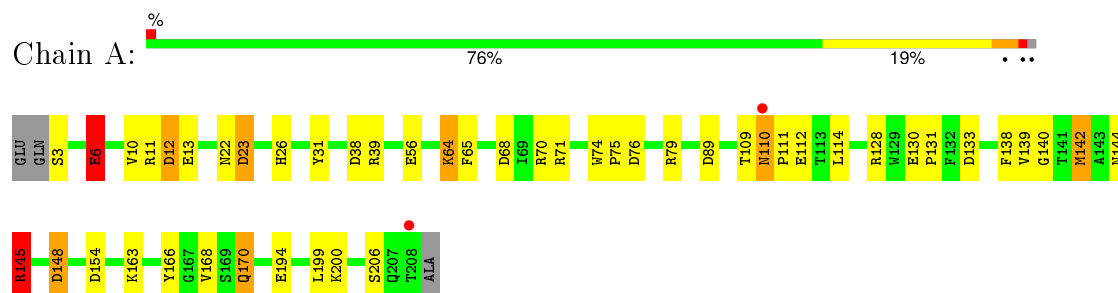
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	0
			172	172		
5	B	497	Total	O	0	0
			497	497		

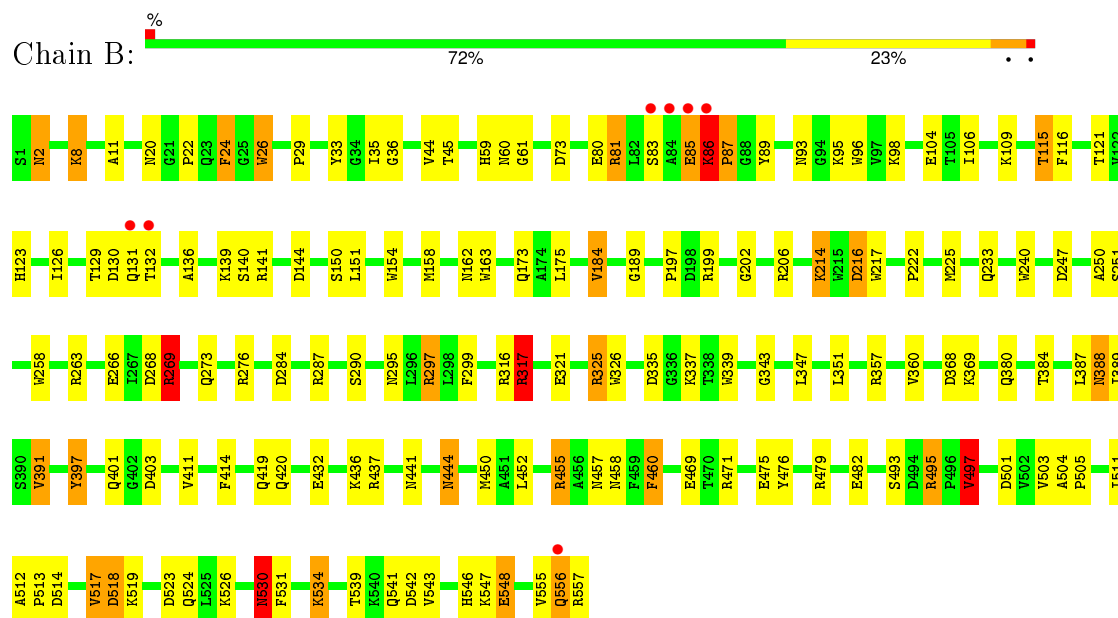
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



• Molecule 2: PENICILLIN AMIDOHYDROLASE



4 Data and refinement statistics

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)	26.12 – 2.36 26.12 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.5 (26.12-2.36) 87.8 (26.12-2.36)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.36Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.152 , 0.218 0.138 , 0.202	Depositor DCC
R_{free} test set	2438 reflections (7.72%)	DCC
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 90.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 34038 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6754	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CA, AAN

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	0.63	0/1698	1.68	32/2305 (1.4%)
2	B	0.65	0/4541	1.57	78/6192 (1.3%)
All	All	0.64	0/6239	1.60	110/8497 (1.3%)

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
1	A	0	1
2	B	0	4
All	All	0	5

There are no bond length outliers.

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	ARG	NE-CZ-NH1	14.19	127.39	120.30
1	A	70	ARG	NE-CZ-NH2	-13.69	113.45	120.30
2	B	73	ASP	CB-CG-OD2	13.45	130.41	118.30
2	B	269	ARG	CD-NE-CZ	13.28	142.19	123.60
1	A	148	ASP	CB-CG-OD1	12.48	129.53	118.30
2	B	357	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	A	38	ASP	CB-CG-OD2	10.45	127.71	118.30
2	B	144	ASP	CB-CG-OD1	10.39	127.65	118.30
1	A	12	ASP	CB-CG-OD2	-10.17	109.14	118.30
2	B	475	GLU	OE1-CD-OE2	-9.96	111.35	123.30
1	A	70	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	145	ARG	NE-CZ-NH1	9.45	125.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ASP	CB-CG-OD2	9.45	126.80	118.30
1	A	133	ASP	CB-CG-OD1	9.44	126.79	118.30
2	B	455	ARG	CD-NE-CZ	9.12	136.37	123.60
2	B	479	ARG	NE-CZ-NH2	-9.03	115.79	120.30
2	B	437	ARG	NE-CZ-NH1	9.03	124.81	120.30
2	B	495	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	A	89	ASP	CB-CG-OD2	8.85	126.26	118.30
1	A	154	ASP	CB-CG-OD1	8.69	126.12	118.30
2	B	325	ARG	NE-CZ-NH2	-8.62	115.99	120.30
2	B	263	ARG	NE-CZ-NH2	-8.58	116.01	120.30
2	B	287	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	B	131	GLN	CG-CD-OE1	-8.44	104.72	121.60
2	B	541	GLN	CG-CD-OE1	8.35	138.30	121.60
1	A	71	ARG	NE-CZ-NH1	8.01	124.30	120.30
2	B	287	ARG	CD-NE-CZ	7.92	134.68	123.60
2	B	141	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	A	139	VAL	CA-CB-CG1	7.85	122.67	110.90
1	A	71	ARG	CD-NE-CZ	7.78	134.49	123.60
2	B	455	ARG	NE-CZ-NH2	-7.70	116.45	120.30
2	B	541	GLN	CG-CD-NE2	-7.70	98.22	116.70
1	A	79	ARG	CD-NE-CZ	7.57	134.20	123.60
2	B	476	TYR	CB-CG-CD2	7.56	125.54	121.00
1	A	23	ASP	CB-CG-OD1	7.53	125.08	118.30
2	B	317	ARG	CD-NE-CZ	7.29	133.81	123.60
2	B	441	ASN	CB-CG-OD1	7.27	136.13	121.60
1	A	140	GLY	CA-C-O	-7.25	107.54	120.60
2	B	199	ARG	NE-CZ-NH1	7.25	123.92	120.30
2	B	437	ARG	NE-CZ-NH2	-7.16	116.72	120.30
2	B	287	ARG	NE-CZ-NH2	-7.16	116.72	120.30
2	B	131	GLN	CA-CB-CG	-7.12	97.73	113.40
2	B	518	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	39	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	12	ASP	CB-CG-OD1	7.05	124.64	118.30
2	B	268	ASP	CB-CG-OD1	7.00	124.60	118.30
2	B	391	VAL	CB-CA-C	-6.99	98.11	111.40
1	A	170	GLN	CG-CD-OE1	6.98	135.57	121.60
2	B	86	LYS	CA-CB-CG	6.97	128.74	113.40
2	B	479	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	B	357	ARG	NE-CZ-NH2	-6.82	116.89	120.30
2	B	216	ASP	CB-CG-OD1	6.81	124.43	118.30
2	B	269	ARG	CA-CB-CG	6.80	128.36	113.40
1	A	11	ARG	CD-NE-CZ	6.71	132.99	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	548	GLU	N-CA-CB	6.71	122.67	110.60
2	B	263	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	B	316	ARG	NE-CZ-NH2	6.69	123.64	120.30
2	B	441	ASN	CB-CG-ND2	-6.67	100.70	116.70
1	A	170	GLN	CG-CD-NE2	-6.60	100.86	116.70
2	B	162	ASN	CB-CG-OD1	6.59	134.78	121.60
2	B	268	ASP	CB-CG-OD2	-6.59	112.37	118.30
2	B	269	ARG	NH1-CZ-NH2	-6.57	112.17	119.40
2	B	469	GLU	OE1-CD-OE2	6.56	131.17	123.30
2	B	444	ASN	CB-CG-OD1	-6.48	108.64	121.60
2	B	266	GLU	OE1-CD-OE2	-6.48	115.53	123.30
2	B	523	ASP	CB-CG-OD2	6.43	124.09	118.30
2	B	471	ARG	NE-CZ-NH1	6.41	123.51	120.30
2	B	269	ARG	N-CA-CB	6.37	122.07	110.60
2	B	325	ARG	CD-NE-CZ	-6.36	114.69	123.60
2	B	24	PHE	CB-CG-CD1	-6.27	116.41	120.80
2	B	162	ASN	CB-CG-ND2	-6.20	101.81	116.70
2	B	284	ASP	CB-CG-OD1	-6.18	112.73	118.30
2	B	141	ARG	NE-CZ-NH1	-6.16	117.22	120.30
2	B	460	PHE	CB-CG-CD1	6.11	125.08	120.80
2	B	73	ASP	OD1-CG-OD2	-6.09	111.73	123.30
2	B	131	GLN	CG-CD-NE2	6.07	131.27	116.70
2	B	495	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	133	ASP	CB-CG-OD2	-5.96	112.94	118.30
2	B	335	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	144	ASN	CA-CB-CG	-5.75	100.76	113.40
1	A	142	MET	CG-SD-CE	5.72	109.35	100.20
2	B	206	ARG	NE-CZ-NH1	-5.70	117.45	120.30
2	B	530	ASN	CB-CG-OD1	-5.69	110.22	121.60
2	B	548	GLU	CA-CB-CG	5.67	125.87	113.40
2	B	247	ASP	CB-CG-OD1	5.65	123.38	118.30
2	B	199	ARG	CD-NE-CZ	-5.64	115.70	123.60
1	A	22	ASN	CB-CG-OD1	-5.62	110.36	121.60
2	B	297	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	111	PRO	N-CA-CB	5.59	110.01	103.30
2	B	397	TYR	CB-CG-CD1	-5.59	117.65	121.00
2	B	476	TYR	CB-CG-CD1	-5.58	117.65	121.00
2	B	199	ARG	NE-CZ-NH2	-5.57	117.51	120.30
2	B	29	PRO	C-N-CA	5.53	135.52	121.70
2	B	397	TYR	CB-CG-CD2	5.46	124.28	121.00
2	B	24	PHE	CB-CG-CD2	5.44	124.61	120.80
2	B	497	VAL	CB-CA-C	-5.44	101.07	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ARG	NE-CZ-NH1	-5.37	117.61	120.30
2	B	284	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	56	GLU	N-CA-CB	5.28	120.11	110.60
2	B	144	ASP	OD1-CG-OD2	-5.25	113.33	123.30
2	B	514	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	81	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	B	184	VAL	CB-CA-C	-5.17	101.58	111.40
2	B	482	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	A	139	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	A	70	ARG	CD-NE-CZ	5.09	130.73	123.60
1	A	6	GLU	OE1-CD-OE2	5.08	129.39	123.30
1	A	89	ASP	OD1-CG-OD2	-5.05	113.70	123.30
2	B	295	ASN	CB-CG-OD1	-5.05	111.51	121.60
2	B	33	TYR	CB-CG-CD2	-5.04	117.98	121.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Mainchain
2	B	26	TRP	Mainchain
2	B	299	PHE	Mainchain
2	B	325	ARG	Mainchain
2	B	518	ASP	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	26	0
2	B	4415	0	4244	88	0
3	B	1	0	0	0	0
4	B	13	0	6	0	0
5	A	172	0	0	1	0
5	B	497	0	0	0	0
All	All	6754	0	5854	104	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 (104) 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:214:LYS:H	2:B:214:LYS:HD2	1.22	1.03
2:B:80:GLU:OE2	2:B:123:HIS:HD2	1.41	1.00
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.43	0.82
2:B:80:GLU:OE2	2:B:123:HIS:CD2	2.32	0.76
2:B:86:LYS:N	2:B:87:PRO:HD3	2.01	0.75
2:B:59:HIS:HD2	2:B:61:GLY:H	1.35	0.75
1:A:26:HIS:HE1	2:B:555:VAL:O	1.70	0.73
2:B:123:HIS:HE1	2:B:216:ASP:OD1	1.72	0.73
2:B:388:ASN:ND2	2:B:389:ILE:H	1.89	0.71
2:B:384:THR:HG22	2:B:455:ARG:HH12	1.56	0.70
2:B:59:HIS:CD2	2:B:61:GLY:H	2.10	0.68
2:B:384:THR:HG22	2:B:455:ARG:NH1	2.09	0.67
2:B:173:GLN:HE22	2:B:175:LEU:H	1.41	0.66
2:B:173:GLN:NE2	2:B:175:LEU:H	1.96	0.64
2:B:556:GLN:OE1	2:B:557:ARG:N	2.31	0.64
2:B:388:ASN:HD22	2:B:389:ILE:H	1.44	0.63
2:B:317:ARG:HH11	2:B:317:ARG:HG3	1.61	0.63
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.13	0.63
2:B:503:VAL:H	2:B:524:GLN:NE2	1.96	0.63
1:A:199:LEU:HD21	2:B:225:MET:HE1	1.81	0.62
2:B:150:SER:HB3	2:B:173:GLN:HE21	1.64	0.61
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.35	0.61
2:B:86:LYS:H	2:B:87:PRO:HD3	1.65	0.60
2:B:384:THR:CG2	2:B:455:ARG:HH12	2.14	0.60
2:B:214:LYS:HD2	2:B:214:LYS:N	2.04	0.59
1:A:170:GLN:NE2	1:A:170:GLN:HA	2.18	0.59
2:B:89:TYR:CZ	2:B:98:LYS:HG3	2.39	0.57
2:B:214:LYS:H	2:B:214:LYS:CD	2.05	0.57
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.87	0.56
1:A:3:SER:HB3	1:A:6:GLU:HB3	1.89	0.55
2:B:384:THR:HG22	2:B:455:ARG:CZ	2.37	0.55
2:B:86:LYS:N	2:B:87:PRO:CD	2.71	0.54
2:B:414:PHE:CZ	2:B:419:GLN:HG2	2.41	0.54
1:A:64:LYS:HE3	1:A:68:ASP:OD2	2.07	0.54
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.16	0.53
2:B:458:ASN:C	2:B:458:ASN:OD1	2.46	0.53
2:B:384:THR:HG22	2:B:455:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.45	0.52
2:B:388:ASN:HD22	2:B:389:ILE:N	2.06	0.51
2:B:123:HIS:O	2:B:140:SER:HB2	2.10	0.51
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.76	0.51
1:A:170:GLN:CA	1:A:170:GLN:HE21	2.06	0.51
2:B:317:ARG:O	2:B:321:GLU:HG3	2.11	0.51
1:A:130:GLU:HB2	1:A:131:PRO:HD2	1.92	0.51
2:B:384:THR:HG22	2:B:455:ARG:HH22	1.76	0.50
2:B:129:THR:HG22	2:B:136:ALA:CB	2.41	0.50
2:B:512:ALA:HB1	2:B:513:PRO:CD	2.42	0.50
1:A:12:ASP:O	2:B:548:GLU:HG2	2.12	0.49
2:B:151:LEU:HD23	2:B:151:LEU:C	2.33	0.49
2:B:360:VAL:HG13	2:B:368:ASP:HB2	1.95	0.49
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.94	0.49
1:A:138:PHE:O	1:A:142:MET:HB3	2.11	0.49
2:B:317:ARG:NH1	2:B:317:ARG:HG3	2.25	0.48
1:A:199:LEU:CD2	2:B:225:MET:HE1	2.42	0.48
2:B:397:TYR:O	2:B:401:GLN:HG2	2.12	0.48
2:B:457:ASN:N	2:B:457:ASN:HD22	2.05	0.48
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.48	0.48
2:B:542:ASP:O	2:B:546:HIS:HD2	1.97	0.48
1:A:110:ASN:HB3	1:A:114:LEU:HD12	1.96	0.48
2:B:121:THR:HG23	2:B:126:ILE:HD11	1.97	0.47
1:A:26:HIS:CE1	2:B:555:VAL:O	2.60	0.47
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.96	0.47
1:A:23:ASP:OD1	1:A:26:HIS:HD2	1.98	0.47
2:B:11:ALA:O	2:B:276:ARG:NH1	2.45	0.47
2:B:530:ASN:O	2:B:531:PHE:HB2	2.15	0.46
1:A:194:GLU:OE2	2:B:233:GLN:HG3	2.16	0.46
2:B:501:ASP:OD1	2:B:534:LYS:HE2	2.15	0.46
1:A:130:GLU:HB2	1:A:131:PRO:CD	2.46	0.45
1:A:206:SER:HB2	2:B:202:GLY:O	2.17	0.45
2:B:129:THR:HA	2:B:136:ALA:HA	1.98	0.45
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.52	0.45
2:B:8:LYS:HB2	2:B:8:LYS:HE2	1.76	0.45
1:A:163:LYS:HG2	1:A:168:VAL:HA	1.98	0.45
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.52	0.44
2:B:45:THR:CG2	2:B:59:HIS:CE1	3.00	0.44
1:A:170:GLN:HA	1:A:170:GLN:HE21	1.76	0.44
1:A:166:TYR:O	1:A:170:GLN:HB3	2.17	0.44
2:B:104:GLU:O	2:B:115:THR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG13	2:B:547:LYS:HD3	1.99	0.44
2:B:35:ILE:HG13	2:B:36:GLY:N	2.33	0.44
1:A:148:ASP:OD2	2:B:139:LYS:NZ	2.48	0.43
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.53	0.43
2:B:93:ASN:HD22	2:B:93:ASN:HA	1.69	0.43
2:B:59:HIS:HD2	2:B:61:GLY:N	2.11	0.43
2:B:539:THR:O	2:B:543:VAL:HG23	2.18	0.43
2:B:85:GLU:O	2:B:86:LYS:HG2	2.18	0.43
1:A:110:ASN:HB2	5:A:373:HOH:O	2.17	0.43
2:B:173:GLN:HE22	2:B:175:LEU:HG	1.85	0.42
1:A:145:ARG:HA	1:A:145:ARG:HD3	1.67	0.42
2:B:61:GLY:HA2	2:B:497:VAL:HG21	2.00	0.42
2:B:2:ASN:HB3	2:B:240:TRP:CG	2.55	0.42
2:B:388:ASN:ND2	2:B:389:ILE:N	2.63	0.42
2:B:222:PRO:HD2	2:B:225:MET:HG3	2.01	0.42
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.85	0.42
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.54	0.42
2:B:347:LEU:O	2:B:351:LEU:HB2	2.20	0.42
1:A:65:PHE:CE1	2:B:460:PHE:HB3	2.55	0.42
2:B:130:ASP:OD1	2:B:132:THR:OG1	2.30	0.41
2:B:60:ASN:C	2:B:60:ASN:OD1	2.59	0.41
1:A:166:TYR:HB3	1:A:170:GLN:CG	2.50	0.41
2:B:457:ASN:N	2:B:457:ASN:ND2	2.67	0.41
2:B:59:HIS:CD2	2:B:61:GLY:N	2.86	0.41
1:A:74:TRP:HA	1:A:75:PRO:HD2	1.89	0.41
2:B:504:ALA:HA	2:B:505:PRO:C	2.41	0.41

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%)	201 (98%)	3 (2%)	0	100	100
2	B	555/557 (100%)	538 (97%)	16 (3%)	1 (0%)	52	63
All	All	759/766 (99%)	739 (97%)	19 (2%)	1 (0%)	56	69

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%)	170 (96%)	8 (4%)	34	43
2	B	460/460 (100%)	422 (92%)	38 (8%)	14	15
All	All	638/640 (100%)	592 (93%)	46 (7%)	18	19

All (46) 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	64	LYS
1	A	109	THR
1	A	110	ASN
1	A	112	GLU
1	A	200	LYS
2	B	2	ASN
2	B	8	LYS
2	B	20	ASN
2	B	81	ARG
2	B	85	GLU
2	B	86	LYS
2	B	87	PRO

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Mol	Chain	Res	Type
2	B	95	LYS
2	B	109	LYS
2	B	115	THR
2	B	154	TRP
2	B	184	VAL
2	B	214	LYS
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	380	GLN
2	B	387	LEU
2	B	388	ASN
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	493	SER
2	B	495	ARG
2	B	497	VAL
2	B	517	VAL
2	B	519	LYS
2	B	526	LYS
2	B	530	ASN
2	B	534	LYS
2	B	556	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	144	ASN
1	A	170	GLN
1	A	193	GLN
1	A	204	GLN
1	A	205	ASN
2	B	2	ASN

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Mol	Chain	Res	Type
2	B	59	HIS
2	B	93	ASN
2	B	123	HIS
2	B	173	GLN
2	B	245	GLN
2	B	388	ASN
2	B	420	GLN
2	B	444	ASN
2	B	457	ASN
2	B	507	GLN
2	B	524	GLN
2	B	541	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 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	AAN	B	559	-	8,13,13	3.52	1 (12%)	12,17,17	2.95	6 (50%)

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	AAN	B	559	-	-	0/6/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	559	AAN	O3'-N4'	9.90	1.42	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559	AAN	O3'-N4'-C4'	-5.38	109.22	118.89
4	B	559	AAN	C6'-C5'-C4'	-5.04	113.08	120.15
4	B	559	AAN	C5'-C4'-N4'	-4.39	115.94	119.48
4	B	559	AAN	C3'-C2'-C1'	-3.79	115.85	121.04
4	B	559	AAN	C6'-C1'-C2'	2.26	121.75	118.13
4	B	559	AAN	C5'-C4'-C3'	2.74	124.57	119.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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%)	-0.43	2 (0%) 84 92	16, 28, 55, 73	0
2	B	557/557 (100%)	-0.49	7 (1%) 79 87	10, 26, 56, 104	0
All	All	763/766 (99%)	-0.47	9 (1%) 81 89	10, 26, 56, 104	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	84	ALA	3.7
2	B	86	LYS	3.6
2	B	85	GLU	2.9
2	B	83	SER	2.9
2	B	131	GLN	2.9
2	B	556	GLN	2.8
1	A	208	THR	2.4
1	A	110	ASN	2.2
2	B	132	THR	2.0

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. 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, 95th 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	AAN	B	559	13/13	0.97	0.14	2.02	18,34,44,46	0
3	CA	B	558	1/1	1.00	0.09	-1.23	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.