Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:31 pm BST

PDB ID	:	1AJP
Title	:	PENICILLIN ACYLASE COMPLEXED WITH 2,5-DIHYDROXYPHENYL ACETIC ACID
Authors	:	Done, S.H.
Deposited on	:	1997-05-07
Resolution	:	2.31 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
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:

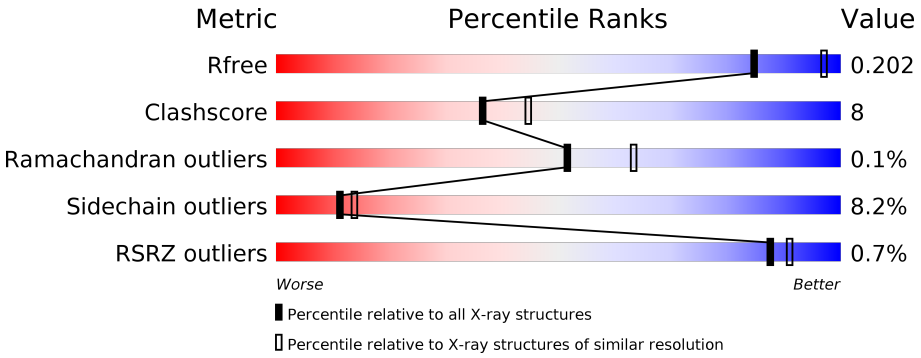
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 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.

Mol	Chain	Length	Quality of chain
1	A	209	% 78% 15%
2	B	557	% 74% 21%

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
3	OMD	A	210	-	-	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
			Total	C	N	O	S			
1	A	206	1678	1073	283	314	8	0	2	0

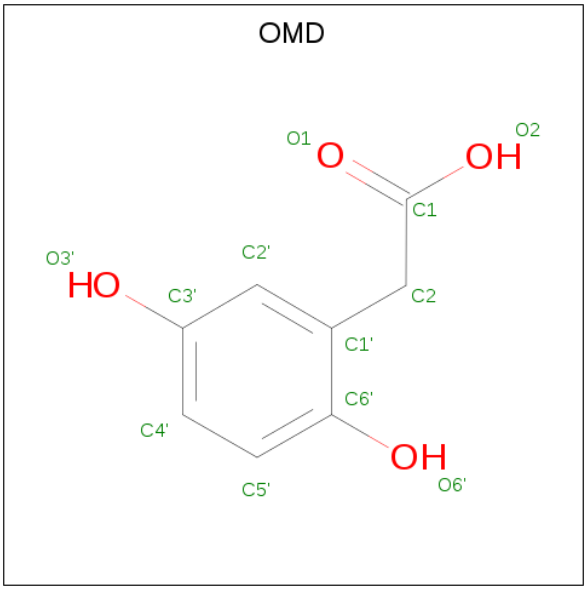
- Molecule 2 is a protein called PENICILLIN AMIDOHYDROLASE.

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 2-(3,6-DIHYDROXYPHENYL)ACETIC ACID (three-letter code: OMD) (formula: $C_8H_8O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 8 4	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

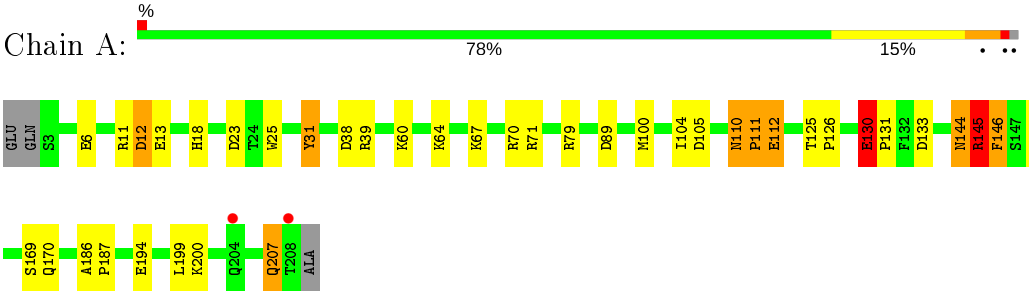
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	183	Total O 183 183	0	0
5	B	479	Total O 479 479	0	0

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 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.

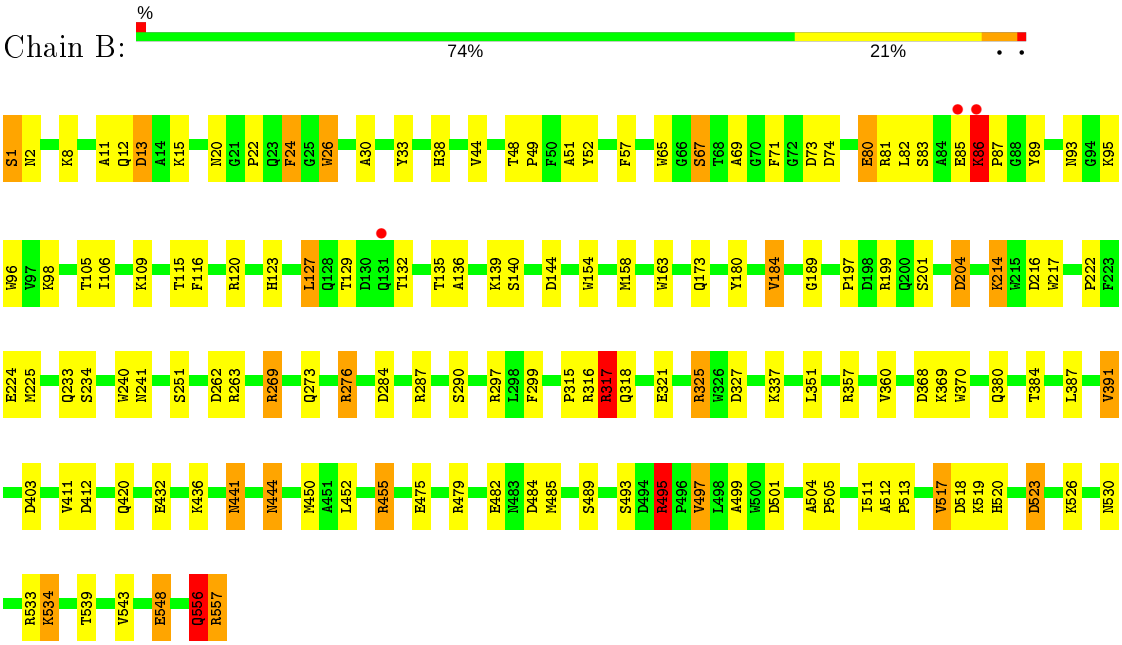
- Molecule 1: PENICILLIN AMIDOHYDROLASE

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)	26.81 – 2.31 28.06 – 2.36	Depositor EDS
% Data completeness (in resolution range)	96.1 (26.81-2.31) 96.3 (28.06-2.36)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.28 (at 2.36Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.146 , 0.225 0.134 , 0.202	Depositor DCC
R_{free} test set	2431 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 87.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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, 0.333 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: CA, OMD

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	0.68	0/1721	1.87	31/2335 (1.3%)
2	B	0.67	1/4541 (0.0%)	1.65	67/6192 (1.1%)
All	All	0.67	1/6262 (0.0%)	1.71	98/8527 (1.1%)

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	3
2	B	0	4
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	132	THR	CB-OG1	6.06	1.55	1.43

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145[A]	ARG	CD-NE-CZ	27.41	161.97	123.60
1	A	145[B]	ARG	CD-NE-CZ	27.41	161.97	123.60
2	B	263	ARG	NE-CZ-NH2	-17.29	111.66	120.30
2	B	263	ARG	NE-CZ-NH1	14.72	127.66	120.30
2	B	269	ARG	NE-CZ-NH1	14.70	127.65	120.30
2	B	479	ARG	NE-CZ-NH1	14.28	127.44	120.30
2	B	73	ASP	CB-CG-OD2	13.63	130.57	118.30
1	A	145[A]	ARG	NE-CZ-NH1	13.37	126.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145[B]	ARG	NE-CZ-NH1	13.37	126.99	120.30
2	B	479	ARG	NE-CZ-NH2	-13.04	113.78	120.30
2	B	287	ARG	NE-CZ-NH1	12.71	126.65	120.30
2	B	269	ARG	CD-NE-CZ	11.51	139.72	123.60
2	B	216	ASP	CB-CG-OD1	11.28	128.45	118.30
1	A	145[A]	ARG	CB-CA-C	11.14	132.68	110.40
1	A	145[B]	ARG	CB-CA-C	11.14	132.68	110.40
2	B	357	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	A	38	ASP	CB-CG-OD2	10.13	127.41	118.30
2	B	199	ARG	NE-CZ-NH2	-9.97	115.31	120.30
1	A	12	ASP	CB-CG-OD2	-9.81	109.47	118.30
2	B	316	ARG	NE-CZ-NH2	9.72	125.16	120.30
2	B	475	GLU	OE1-CD-OE2	-9.63	111.74	123.30
1	A	70	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	A	23	ASP	CB-CG-OD1	9.40	126.76	118.30
1	A	148	ASP	CB-CG-OD1	8.70	126.13	118.30
2	B	144	ASP	CB-CG-OD1	8.66	126.10	118.30
1	A	144	ASN	C-N-CA	-8.61	100.17	121.70
1	A	133	ASP	CB-CG-OD1	8.49	125.94	118.30
1	A	79	ARG	CD-NE-CZ	8.38	135.34	123.60
1	A	145[A]	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	A	145[B]	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	A	70	ARG	NE-CZ-NH1	8.34	124.47	120.30
2	B	317	ARG	CD-NE-CZ	8.33	135.26	123.60
2	B	287	ARG	CD-NE-CZ	8.14	135.00	123.60
2	B	557	ARG	NE-CZ-NH2	-8.00	116.30	120.30
2	B	269	ARG	CA-CB-CG	7.89	130.76	113.40
2	B	287	ARG	NE-CZ-NH2	-7.81	116.39	120.30
2	B	144	ASP	OD1-CG-OD2	-7.75	108.57	123.30
1	A	12	ASP	CB-CG-OD1	7.75	125.27	118.30
2	B	455	ARG	CD-NE-CZ	7.74	134.44	123.60
2	B	533	ARG	NE-CZ-NH2	7.63	124.11	120.30
2	B	144	ASP	CB-CG-OD2	7.60	125.14	118.30
2	B	204	ASP	CB-CG-OD1	7.46	125.01	118.30
2	B	455	ARG	NE-CZ-NH2	-7.22	116.69	120.30
2	B	184	VAL	CB-CA-C	-7.19	97.75	111.40
2	B	391	VAL	CB-CA-C	-7.10	97.92	111.40
2	B	548	GLU	CA-CB-CG	7.02	128.85	113.40
1	A	11	ARG	CD-NE-CZ	6.99	133.38	123.60
1	A	39	ARG	NE-CZ-NH2	-6.98	116.81	120.30
2	B	204	ASP	CB-CG-OD2	-6.95	112.05	118.30
2	B	86	LYS	CA-CB-CG	6.82	128.41	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	ARG	CD-NE-CZ	6.77	133.08	123.60
1	A	71	ARG	NE-CZ-NH1	6.76	123.68	120.30
2	B	73	ASP	OD1-CG-OD2	-6.74	110.50	123.30
2	B	74	ASP	CB-CG-OD2	6.66	124.29	118.30
2	B	120	ARG	NE-CZ-NH2	-6.57	117.02	120.30
2	B	518	ASP	CB-CG-OD2	6.57	124.21	118.30
2	B	57	PHE	CB-CG-CD2	6.39	125.28	120.80
2	B	199	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	B	269	ARG	NH1-CZ-NH2	-6.25	112.52	119.40
1	A	130	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	A	144	ASN	CA-C-O	-6.23	107.02	120.10
2	B	80	GLU	CA-CB-CG	6.18	127.01	113.40
1	A	89	ASP	CB-CG-OD2	6.07	123.76	118.30
2	B	105	THR	O-C-N	6.06	132.39	122.70
2	B	391	VAL	CG1-CB-CG2	6.01	120.52	110.90
2	B	276	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	B	316	ARG	NE-CZ-NH1	-5.87	117.37	120.30
2	B	548	GLU	N-CA-CB	5.84	121.12	110.60
2	B	269	ARG	N-CA-CB	5.83	121.09	110.60
2	B	30	ALA	N-CA-CB	5.70	118.08	110.10
2	B	484	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	146[A]	PHE	N-CA-C	5.62	126.17	111.00
1	A	146[B]	PHE	N-CA-C	5.62	126.17	111.00
1	A	154	ASP	CB-CG-OD1	5.61	123.35	118.30
2	B	290	SER	CB-CA-C	-5.61	99.44	110.10
2	B	325	ARG	CD-NE-CZ	-5.61	115.74	123.60
2	B	33	TYR	CB-CG-CD2	-5.58	117.66	121.00
2	B	57	PHE	CB-CG-CD1	-5.53	116.93	120.80
2	B	30	ALA	O-C-N	5.49	131.48	122.70
2	B	327	ASP	CB-CG-OD1	5.47	123.23	118.30
2	B	276	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	B	132	THR	OG1-CB-CG2	-5.42	97.53	110.00
2	B	71	PHE	CB-CG-CD1	-5.42	117.00	120.80
2	B	497	VAL	CB-CA-C	-5.41	101.11	111.40
2	B	482	GLU	OE1-CD-OE2	-5.38	116.85	123.30
1	A	111	PRO	N-CA-CB	5.37	109.74	103.30
2	B	412	ASP	CB-CG-OD1	5.36	123.12	118.30
2	B	495	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	B	523	ASP	CB-CG-OD1	5.33	123.09	118.30
2	B	325	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	31	TYR	CA-CB-CG	5.20	123.27	113.40
1	A	105	ASP	CB-CG-OD1	5.16	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	184	VAL	N-CA-CB	5.16	122.85	111.50
2	B	13	ASP	CB-CG-OD1	5.15	122.93	118.30
2	B	284	ASP	CB-CG-OD1	-5.12	113.69	118.30
2	B	24	PHE	CB-CG-CD1	-5.10	117.23	120.80
2	B	556	GLN	N-CA-CB	5.08	119.74	110.60
2	B	1	SER	CB-CA-C	-5.04	100.53	110.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ASN	Mainchain
1	A	145[A]	ARG	Mainchain
1	A	145[B]	ARG	Mainchain
2	B	234	SER	Mainchain
2	B	26	TRP	Mainchain
2	B	299	PHE	Mainchain
2	B	370	TRP	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	1678	0	1625	30	0
2	B	4415	0	4244	73	0
3	A	12	0	6	16	0
4	B	1	0	0	0	0
5	A	183	0	0	0	0
5	B	479	0	0	0	0
All	All	6768	0	5875	94	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 8.

All (94) 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:146[B]:PHE:CE1	3:A:210:OMD:H22	1.42	1.52
1:A:146[B]:PHE:CD1	3:A:210:OMD:H21	1.55	1.40
1:A:146[B]:PHE:CZ	3:A:210:OMD:H22	1.61	1.35
1:A:146[B]:PHE:CD1	3:A:210:OMD:C2	2.21	1.18
1:A:207:GLN:HE22	2:B:204:ASP:H	1.14	0.94
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.36	0.88
1:A:146[B]:PHE:CE1	3:A:210:OMD:C1	2.67	0.77
1:A:18:HIS:HD2	2:B:38:HIS:NE2	1.83	0.76
2:B:240:TRP:O	2:B:241:ASN:HB2	1.88	0.72
2:B:86:LYS:N	2:B:87:PRO:HD3	2.06	0.70
2:B:384:THR:HG22	2:B:455:ARG:NH2	2.10	0.67
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.09	0.67
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.77	0.66
2:B:384:THR:HG22	2:B:455:ARG:HH22	1.61	0.66
2:B:315:PRO:HA	2:B:318:GLN:HG3	1.76	0.66
2:B:384:THR:HG22	2:B:455:ARG:NH1	2.11	0.66
2:B:384:THR:HG22	2:B:455:ARG:HH12	1.62	0.65
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.32	0.64
2:B:520:HIS:HE1	2:B:548:GLU:OE2	1.81	0.64
2:B:15:LYS:HG3	2:B:489:SER:HB2	1.81	0.63
1:A:146[B]:PHE:CG	3:A:210:OMD:H21	2.28	0.63
1:A:199:LEU:HG	2:B:225:MET:HE1	1.81	0.62
1:A:207:GLN:NE2	2:B:204:ASP:H	1.91	0.62
2:B:384:THR:HG22	2:B:455:ARG:CZ	2.31	0.61
1:A:12:ASP:O	2:B:548:GLU:HG2	2.01	0.59
2:B:86:LYS:N	2:B:87:PRO:CD	2.65	0.59
2:B:214:LYS:H	2:B:214:LYS:HD2	1.66	0.59
2:B:11:ALA:O	2:B:276:ARG:NH1	2.31	0.58
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.38	0.58
1:A:146[B]:PHE:CG	3:A:210:OMD:O6'	2.58	0.57
2:B:384:THR:CG2	2:B:455:ARG:HH12	2.18	0.57
1:A:25:TRP:CE2	2:B:557:ARG:HG3	2.40	0.56
2:B:512:ALA:HB1	2:B:513:PRO:CD	2.35	0.56
2:B:123:HIS:O	2:B:140:SER:HB2	2.06	0.55
2:B:360:VAL:HG13	2:B:368:ASP:HB2	1.88	0.55
1:A:146[B]:PHE:HE1	3:A:210:OMD:O1	1.90	0.55
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.14	0.54
2:B:129:THR:HG22	2:B:136:ALA:CB	2.37	0.54
1:A:146[B]:PHE:CE2	3:A:210:OMD:H22	2.34	0.53
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.74	0.53
3:A:210:OMD:C2	2:B:69:ALA:HB2	2.38	0.53
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:GLN:OE1	2:B:557:ARG:N	2.39	0.52
1:A:146[B]:PHE:CE1	3:A:210:OMD:O1	2.61	0.52
2:B:495:ARG:HH11	2:B:495:ARG:HG3	1.75	0.52
1:A:146[B]:PHE:CG	3:A:210:OMD:C2	2.89	0.52
1:A:207:GLN:HE21	1:A:207:GLN:H	1.57	0.52
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.93	0.52
2:B:214:LYS:H	2:B:214:LYS:CD	2.23	0.51
3:A:210:OMD:H4'	2:B:67:SER:HB3	1.93	0.51
1:A:67:LYS:HG2	2:B:116:PHE:CE1	2.46	0.50
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.93	0.50
2:B:89:TYR:CZ	2:B:98:LYS:HG3	2.47	0.50
2:B:222:PRO:HD2	2:B:225:MET:HG3	1.94	0.49
1:A:194:GLU:OE2	2:B:233:GLN:HG3	2.12	0.49
2:B:83:SER:HB2	2:B:96:TRP:CZ3	2.48	0.49
2:B:65:TRP:HA	2:B:180:TYR:O	2.12	0.49
2:B:519:LYS:HE3	2:B:548:GLU:OE2	2.13	0.48
3:A:210:OMD:C1'	2:B:69:ALA:HB2	2.43	0.48
1:A:166:TYR:O	1:A:170:GLN:HB3	2.13	0.48
2:B:86:LYS:H	2:B:87:PRO:HD3	1.75	0.48
1:A:18:HIS:CD2	2:B:38:HIS:NE2	2.74	0.47
2:B:539:THR:O	2:B:543:VAL:HG23	2.15	0.46
1:A:100:MET:O	1:A:104:ILE:HG13	2.16	0.46
1:A:145[A]:ARG:HD2	1:A:145[A]:ARG:HA	1.83	0.46
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.51	0.45
2:B:444:ASN:C	2:B:444:ASN:HD22	2.18	0.45
1:A:187:PRO:HG2	2:B:262:ASP:HB3	1.98	0.45
2:B:129:THR:HG22	2:B:136:ALA:HB1	1.97	0.45
2:B:317:ARG:O	2:B:321:GLU:HG3	2.17	0.44
2:B:441:ASN:O	2:B:444:ASN:ND2	2.50	0.44
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.99	0.44
2:B:325:ARG:HH11	2:B:325:ARG:HD2	1.59	0.44
2:B:93:ASN:HD22	2:B:93:ASN:HA	1.68	0.44
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.53	0.44
1:A:110:ASN:ND2	1:A:112:GLU:OE1	2.50	0.44
2:B:80:GLU:O	2:B:135:THR:HA	2.18	0.43
2:B:48:THR:HA	2:B:49:PRO:HD3	1.89	0.43
2:B:450:MET:HB2	2:B:450:MET:HE2	1.79	0.43
1:A:130:GLU:HB2	1:A:131:PRO:HD2	2.01	0.42
2:B:12:GLN:O	2:B:13:ASP:HB2	2.18	0.42
2:B:317:ARG:HH11	2:B:317:ARG:HG3	1.85	0.42
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:210:OMD:H2'	2:B:1:SER:OG	2.20	0.42
1:A:125:THR:HB	1:A:126:PRO:HD2	2.01	0.41
2:B:127:LEU:CD1	2:B:139:LYS:HB2	2.50	0.41
2:B:127:LEU:HD11	2:B:139:LYS:HB2	2.03	0.41
1:A:110:ASN:N	1:A:111:PRO:HD3	2.35	0.41
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.56	0.41
2:B:485:MET:O	2:B:499:ALA:HA	2.20	0.41
3:A:210:OMD:O2	3:A:210:OMD:H2'	2.21	0.41
2:B:51:ALA:O	2:B:52:TYR:C	2.60	0.40
2:B:504:ALA:HA	2:B:505:PRO:C	2.41	0.40
2:B:501:ASP:OD1	2:B:534:LYS:NZ	2.52	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	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
2	B	555/557 (100%)	538 (97%)	16 (3%)	1 (0%)	47	58
All	All	761/766 (99%)	738 (97%)	22 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	180/180 (100%)	167 (93%)	13 (7%)	14 18
2	B	460/460 (100%)	420 (91%)	40 (9%)	10 12
All	All	640/640 (100%)	587 (92%)	53 (8%)	11 13

All (53) 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	60	LYS
1	A	64	LYS
1	A	110	ASN
1	A	112	GLU
1	A	130	GLU
1	A	145[A]	ARG
1	A	145[B]	ARG
1	A	169	SER
1	A	200	LYS
1	A	207	GLN
2	B	2	ASN
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	109	LYS
2	B	115	THR
2	B	127	LEU
2	B	154	TRP
2	B	173	GLN
2	B	184	VAL
2	B	201	SER
2	B	214	LYS
2	B	224	GLU
2	B	273	GLN
2	B	317	ARG
2	B	337	LYS

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Mol	Chain	Res	Type
2	B	351	LEU
2	B	369	LYS
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	441	ASN
2	B	444	ASN
2	B	493	SER
2	B	495	ARG
2	B	497	VAL
2	B	517	VAL
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	110	ASN
1	A	204	GLN
1	A	205	ASN
1	A	207	GLN
2	B	2	ASN
2	B	93	ASN
2	B	241	ASN
2	B	245	GLN
2	B	348	ASN
2	B	441	ASN
2	B	444	ASN
2	B	520	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (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	$\#\|Z\| > 2$
3	OMD	A	210	1	9,12,12	4.39	1 (11%)	13,16,16	1.86	5 (38%)

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
3	OMD	A	210	1	-	2/2/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	210	OMD	O6'-C6'	-13.10	1.09	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	210	OMD	O3'-C3'-C4'	-3.20	110.89	120.02
3	A	210	OMD	C4'-C3'-C2'	3.07	123.53	120.17
3	A	210	OMD	C5'-C4'-C3'	-2.32	117.33	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	210	OMD	O3'-C3'-C2'	2.21	125.58	119.84
3	A	210	OMD	C5'-C6'-C1'	2.05	122.89	120.41

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	210	OMD	C6'-C1'-C2-C1
3	A	210	OMD	C2'-C1'-C2-C1

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	210	OMD	16	0

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

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%)	-0.63	2 (0%)	82	86	13, 24, 55, 69	0
2	B	557/557 (100%)	-0.73	3 (0%)	91	94	8, 23, 56, 100	0
All	All	763/766 (99%)	-0.71	5 (0%)	87	91	8, 24, 55, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	86	LYS	3.3
2	B	85	GLU	3.0
2	B	131	GLN	2.7
1	A	208	THR	2.5
1	A	204	GLN	2.4

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. 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	B-factors(Å^2)	Q<0.9
3	OMD	A	210	12/12	0.75	0.40	20,30,41,43	12
4	CA	B	558	1/1	0.99	0.05	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.