



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 09:31 am BST

PDB ID : 1AI4
Title : PENICILLIN ACYLASE COMPLEXED WITH 3,4-DIHYDROXYPHENYL ACETIC ACID
Authors : Done, S.H.
Deposited on : 1997-05-01
Resolution : 2.35 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

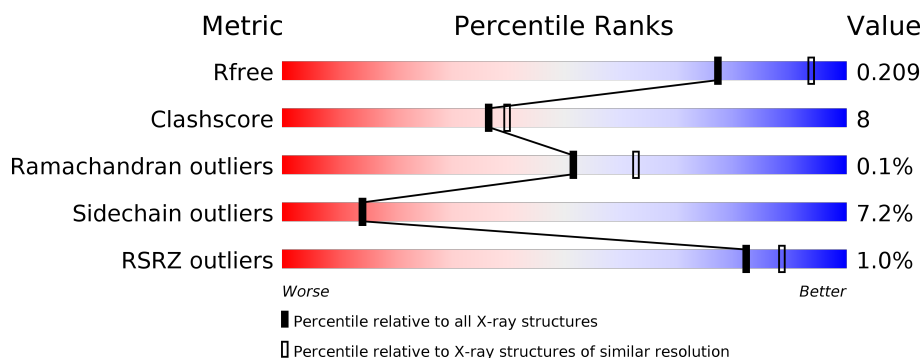
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 $\leq 5\%$. 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>74%</div> <div>22%</div> <div>••</div> </div> </div>
2	B	557	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>•</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6684 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			

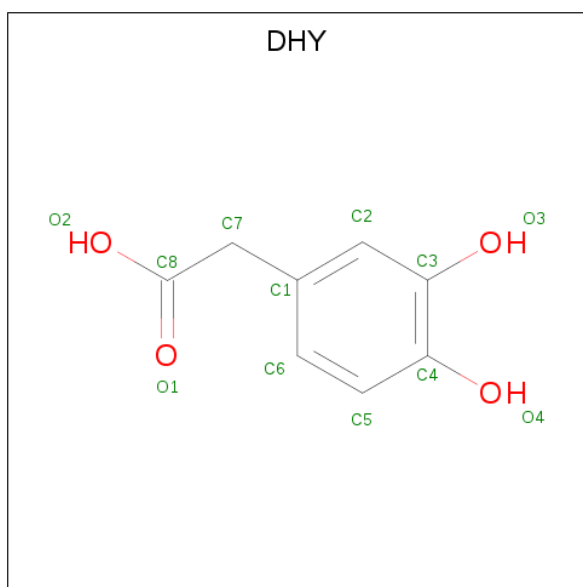
There is a discrepancy between the modelled and reference sequences:

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-(3,4-DIHYDROXYPHENYL)ACETIC ACID (three-letter code: DHY) (formula: C₈H₈O₄).



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

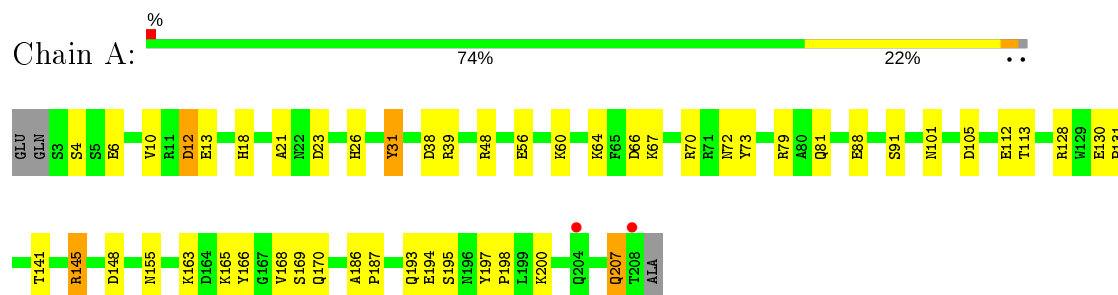
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	153	Total	O	0	0
			153	153		
5	B	447	Total	O	0	0
			447	447		

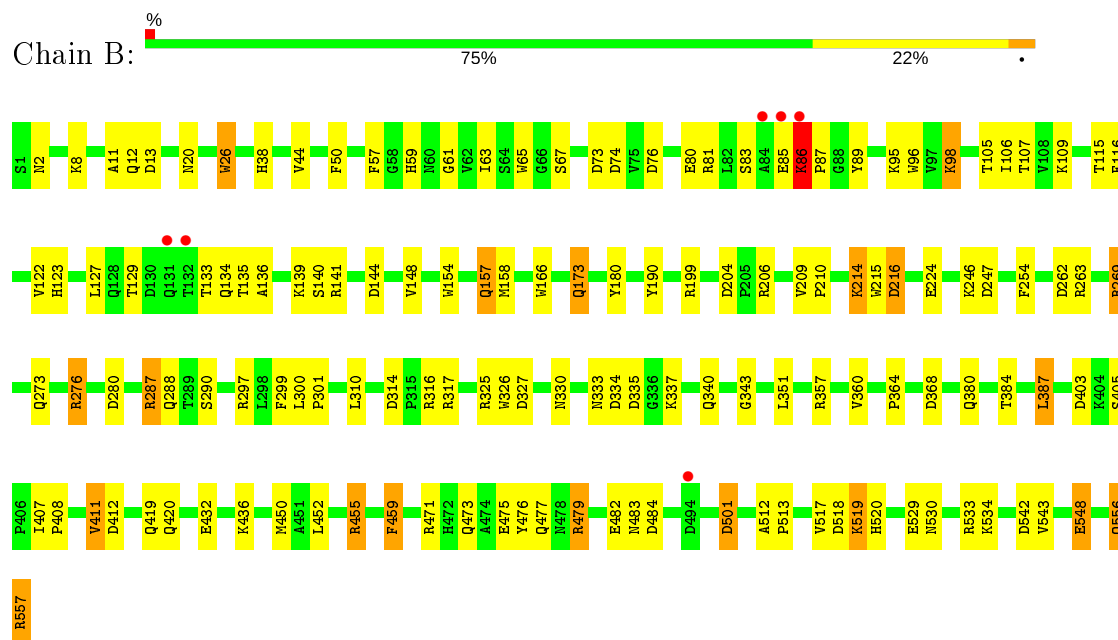
3 Residue-property plots

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, α , β , γ	52.12Å 65.08Å 76.30Å 100.20° 111.44° 105.81°	Depositor
Resolution (Å)	19.85 – 2.35 19.85 – 2.36	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.85-2.35) 95.8 (19.85-2.36)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.93 (at 2.35Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.150 , 0.236 0.138 , 0.209	Depositor DCC
R_{free} test set	2413 reflections (7.16%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6684	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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, 0.333 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, DHY

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	0.64	0/1698	1.46	16/2305 (0.7%)
2	B	0.64	0/4541	1.56	57/6192 (0.9%)
All	All	0.64	0/6239	1.53	73/8497 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	ARG	NE-CZ-NH1	17.53	129.06	120.30
2	B	263	ARG	NE-CZ-NH2	-15.35	112.62	120.30
1	A	79	ARG	CD-NE-CZ	14.45	143.83	123.60
2	B	263	ARG	NE-CZ-NH1	12.82	126.71	120.30
2	B	479	ARG	NE-CZ-NH1	12.74	126.67	120.30
2	B	157	GLN	CG-CD-OE1	12.09	145.77	121.60
2	B	455	ARG	NE-CZ-NH2	-11.67	114.46	120.30
2	B	269	ARG	NE-CZ-NH2	-11.16	114.72	120.30
2	B	157	GLN	CG-CD-NE2	-9.66	93.52	116.70
1	A	145	ARG	NE-CZ-NH1	9.35	124.97	120.30
2	B	144	ASP	CB-CG-OD1	9.35	126.71	118.30
2	B	479	ARG	NE-CZ-NH2	-8.86	115.87	120.30
2	B	287	ARG	NE-CZ-NH1	8.80	124.70	120.30
2	B	357	ARG	NE-CZ-NH1	8.55	124.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ASP	CB-CG-OD1	8.50	125.95	118.30
2	B	557	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	38	ASP	CB-CG-OD2	8.21	125.69	118.30
2	B	73	ASP	CB-CG-OD2	8.11	125.60	118.30
2	B	475	GLU	OE1-CD-OE2	-7.94	113.77	123.30
2	B	216	ASP	CB-CG-OD1	7.74	125.26	118.30
2	B	287	ARG	CD-NE-CZ	7.66	134.32	123.60
1	A	12	ASP	CB-CG-OD2	-7.41	111.63	118.30
2	B	206	ARG	NE-CZ-NH1	-7.39	116.60	120.30
2	B	276	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	79	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	A	23	ASP	CB-CG-OD1	7.11	124.70	118.30
2	B	533	ARG	NE-CZ-NH1	7.07	123.84	120.30
2	B	173	GLN	CG-CD-OE1	6.85	135.30	121.60
1	A	48	ARG	NE-CZ-NH2	6.46	123.53	120.30
2	B	471	ARG	CD-NE-CZ	6.42	132.59	123.60
2	B	157	GLN	CA-CB-CG	6.37	127.42	113.40
2	B	518	ASP	CB-CG-OD2	6.29	123.96	118.30
2	B	74	ASP	CB-CG-OD2	6.26	123.93	118.30
2	B	276	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	B	542	ASP	CB-CG-OD2	6.12	123.81	118.30
2	B	287	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	B	316	ARG	NE-CZ-NH2	6.01	123.31	120.30
2	B	262	ASP	CB-CG-OD2	6.01	123.71	118.30
2	B	351	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	70	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	B	76	ASP	CB-CG-OD1	5.91	123.62	118.30
2	B	455	ARG	NH1-CZ-NH2	5.90	125.89	119.40
1	A	31	TYR	CB-CG-CD1	5.77	124.46	121.00
2	B	57	PHE	CB-CG-CD2	5.77	124.84	120.80
2	B	157	GLN	CB-CG-CD	5.74	126.53	111.60
2	B	412	ASP	O-C-N	-5.73	113.53	122.70
2	B	548	GLU	CA-CB-CG	5.69	125.92	113.40
2	B	455	ARG	CD-NE-CZ	5.66	131.52	123.60
2	B	269	ARG	CD-NE-CZ	5.61	131.46	123.60
2	B	141	ARG	CD-NE-CZ	5.58	131.41	123.60
2	B	334	ASP	CB-CG-OD2	-5.51	113.34	118.30
2	B	73	ASP	OD1-CG-OD2	-5.50	112.85	123.30
1	A	39	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	70	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	B	335	ASP	CB-CG-OD1	5.41	123.17	118.30
2	B	327	ASP	CB-CG-OD2	-5.41	113.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	50	PHE	O-C-N	-5.38	114.10	122.70
2	B	280	ASP	CB-CG-OD1	5.34	123.11	118.30
2	B	86	LYS	CA-CB-CG	5.26	124.97	113.40
1	A	145	ARG	CD-NE-CZ	5.23	130.92	123.60
2	B	215	TRP	CA-CB-CG	-5.17	103.87	113.70
1	A	141	THR	O-C-N	-5.16	114.44	122.70
2	B	190	TYR	CB-CG-CD1	-5.16	117.91	121.00
2	B	297	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	105	ASP	CB-CG-OD1	5.13	122.92	118.30
2	B	484	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	66	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	548	GLU	N-CA-CB	5.08	119.74	110.60
2	B	411	VAL	N-CA-CB	5.07	122.65	111.50
2	B	534	LYS	CD-CE-NZ	-5.07	100.05	111.70
2	B	144	ASP	OD1-CG-OD2	-5.04	113.72	123.30
2	B	330	ASN	CB-CG-ND2	5.02	128.75	116.70
2	B	482	GLU	OE1-CD-OE2	-5.02	117.28	123.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	122	VAL	Mainchain
2	B	26	TRP	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	31	0
2	B	4415	0	4244	79	0
3	B	1	0	0	0	0
4	B	12	0	7	0	0
5	A	153	0	0	0	0
5	B	447	0	0	1	0
All	All	6684	0	5855	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:207:GLN:HE22	2:B:204:ASP:H	1.03	1.01
2:B:59:HIS:HD2	2:B:61:GLY:H	1.23	0.85
2:B:157:GLN:OE1	2:B:166:TRP:NE1	2.12	0.82
2:B:59:HIS:CD2	2:B:61:GLY:H	1.99	0.81
1:A:207:GLN:NE2	2:B:204:ASP:H	1.79	0.80
2:B:556:GLN:NE2	2:B:557:ARG:H	1.85	0.73
2:B:86:LYS:N	2:B:87:PRO:HD3	2.05	0.72
1:A:18:HIS:HD2	2:B:38:HIS:NE2	1.88	0.71
2:B:214:LYS:H	2:B:214:LYS:HD2	1.54	0.70
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.75	0.69
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.29	0.68
2:B:86:LYS:H	2:B:87:PRO:HD3	1.59	0.68
1:A:207:GLN:HE22	2:B:204:ASP:N	1.87	0.68
2:B:479:ARG:HH21	2:B:483:ASN:HD22	1.42	0.68
1:A:72:ASN:HD21	2:B:139:LYS:NZ	1.92	0.67
2:B:479:ARG:HH21	2:B:483:ASN:ND2	1.93	0.65
2:B:556:GLN:NE2	2:B:557:ARG:N	2.43	0.65
2:B:360:VAL:HG13	2:B:368:ASP:HB2	1.79	0.64
2:B:129:THR:HG22	2:B:136:ALA:CB	2.28	0.63
2:B:12:GLN:O	2:B:13:ASP:HB2	1.98	0.63
2:B:384:THR:HG22	2:B:455:ARG:NH1	2.16	0.60
1:A:67:LYS:HG2	2:B:116:PHE:CE1	2.36	0.60
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.37	0.58
2:B:86:LYS:N	2:B:87:PRO:CD	2.66	0.58
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.85	0.57
2:B:317:ARG:HH11	2:B:317:ARG:HG3	1.70	0.57
2:B:519:LYS:HG2	2:B:520:HIS:CD2	2.39	0.57
2:B:129:THR:HG22	2:B:136:ALA:HA	1.88	0.56
2:B:123:HIS:O	2:B:140:SER:HB2	2.06	0.56
2:B:214:LYS:H	2:B:214:LYS:CD	2.18	0.56
2:B:89:TYR:CZ	2:B:98:LYS:HG3	2.42	0.55
2:B:384:THR:HG22	2:B:455:ARG:HH12	1.72	0.55
1:A:165:LYS:HD3	1:A:166:TYR:CE2	2.42	0.54
1:A:56:GLU:O	2:B:109:LYS:HB2	2.08	0.54
2:B:384:THR:HG22	2:B:455:ARG:CZ	2.39	0.53
1:A:155:ASN:ND2	2:B:254:PHE:HB3	2.24	0.53
2:B:512:ALA:HB1	2:B:513:PRO:CD	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HB3	1:A:128:ARG:HH12	1.75	0.52
2:B:333:ASN:ND2	2:B:340:GLN:HG2	2.25	0.52
2:B:11:ALA:O	2:B:276:ARG:NH1	2.34	0.51
1:A:101:ASN:HB3	1:A:128:ARG:NH1	2.25	0.51
1:A:128:ARG:HH11	1:A:128:ARG:HG2	1.75	0.51
1:A:145:ARG:HG3	2:B:459:PHE:HZ	1.74	0.51
1:A:155:ASN:HD21	2:B:254:PHE:HB3	1.74	0.51
2:B:209:VAL:HB	2:B:210:PRO:HD2	1.93	0.51
1:A:21:ALA:HB1	1:A:26:HIS:HB3	1.93	0.51
2:B:65:TRP:HA	2:B:180:TYR:O	2.12	0.50
2:B:556:GLN:HE21	2:B:557:ARG:N	2.10	0.50
2:B:459:PHE:C	2:B:459:PHE:CD1	2.84	0.50
1:A:128:ARG:NH1	1:A:128:ARG:HG2	2.26	0.50
1:A:72:ASN:HD21	2:B:139:LYS:HZ2	1.60	0.49
1:A:81:GLN:NE2	2:B:148:VAL:H	2.11	0.49
1:A:163:LYS:HG2	1:A:168:VAL:HA	1.95	0.49
2:B:288:GLN:HG2	5:B:980:HOH:O	2.13	0.49
1:A:166:TYR:O	1:A:170:GLN:HB3	2.13	0.48
1:A:130:GLU:HB2	1:A:131:PRO:HD2	1.95	0.48
2:B:123:HIS:NE2	2:B:216:ASP:OD1	2.46	0.48
2:B:384:THR:HG22	2:B:455:ARG:NH2	2.29	0.48
2:B:384:THR:CG2	2:B:455:ARG:HH12	2.25	0.48
2:B:59:HIS:HB2	2:B:63:ILE:O	2.14	0.48
1:A:10:VAL:HG11	2:B:543:VAL:HG12	1.94	0.47
2:B:310:LEU:HD13	2:B:314:ASP:OD2	2.14	0.47
2:B:317:ARG:NH1	2:B:317:ARG:HG3	2.29	0.47
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.50	0.47
2:B:473:GLN:HE22	2:B:477:GLN:NE2	2.13	0.47
2:B:325:ARG:HD2	2:B:325:ARG:HH11	1.59	0.47
2:B:246:LYS:O	2:B:247:ASP:HB2	2.14	0.46
1:A:197:TYR:CD1	1:A:198:PRO:HD2	2.50	0.46
2:B:387:LEU:HD22	2:B:476:TYR:CE2	2.50	0.46
2:B:199:ARG:HH11	2:B:199:ARG:HD2	1.63	0.45
2:B:83:SER:HB2	2:B:96:TRP:CZ3	2.51	0.45
2:B:129:THR:HG22	2:B:136:ALA:CA	2.47	0.45
1:A:12:ASP:O	2:B:548:GLU:HG2	2.17	0.45
2:B:80:GLU:O	2:B:135:THR:HA	2.18	0.44
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.83	0.44
2:B:287:ARG:HH11	2:B:287:ARG:HG2	1.83	0.44
2:B:450:MET:HB2	2:B:450:MET:HE2	1.76	0.43
1:A:148:ASP:OD2	2:B:139:LYS:NZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:HB2	1:A:131:PRO:CD	2.49	0.43
1:A:194:GLU:O	1:A:195:SER:HB3	2.18	0.42
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.89	0.42
2:B:407:ILE:HA	2:B:408:PRO:HD3	1.89	0.41
2:B:129:THR:HG22	2:B:136:ALA:HB2	2.02	0.41
1:A:88:GLU:O	1:A:91:SER:HB2	2.20	0.41
2:B:133:THR:O	2:B:134:GLN:HB2	2.19	0.41
2:B:529:GLU:HG2	2:B:530:ASN:OD1	2.20	0.41
1:A:56:GLU:HG2	2:B:107:THR:HB	2.03	0.41
2:B:483:ASN:O	2:B:501:ASP:HA	2.20	0.41
1:A:197:TYR:HA	1:A:198:PRO:HD3	1.92	0.40
2:B:209:VAL:HB	2:B:210:PRO:CD	2.50	0.40
2:B:300:LEU:N	2:B:301:PRO:CD	2.84	0.40
2:B:479:ARG:HE	2:B:483:ASN:ND2	2.19	0.40
2:B:479:ARG:NH2	2:B:483:ASN:HD22	2.15	0.40
2:B:105:THR:HG23	2:B:115:THR:HG22	2.03	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%)	196 (96%)	8 (4%)	0	100	100
2	B	555/557 (100%)	537 (97%)	17 (3%)	1 (0%)	47	56
All	All	759/766 (99%)	733 (97%)	25 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	86	LYS

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%)	165 (93%)	13 (7%)	14	14
2	B	460/460 (100%)	427 (93%)	33 (7%)	14	14
All	All	638/640 (100%)	592 (93%)	46 (7%)	14	14

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	6	GLU
1	A	13	GLU
1	A	31	TYR
1	A	60	LYS
1	A	64	LYS
1	A	73	TYR
1	A	112	GLU
1	A	113	THR
1	A	169	SER
1	A	193	GLN
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	98	LYS
2	B	127	LEU
2	B	154	TRP
2	B	173	GLN
2	B	214	LYS
2	B	224	GLU

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Mol	Chain	Res	Type
2	B	269	ARG
2	B	273	GLN
2	B	290	SER
2	B	337	LYS
2	B	364	PRO
2	B	380	GLN
2	B	387	LEU
2	B	403	ASP
2	B	405	SER
2	B	411	VAL
2	B	419	GLN
2	B	420	GLN
2	B	432	GLU
2	B	436	LYS
2	B	459	PHE
2	B	501	ASP
2	B	517	VAL
2	B	519	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	18	HIS
1	A	72	ASN
1	A	81	GLN
1	A	120	ASN
1	A	155	ASN
1	A	193	GLN
1	A	203	GLN
1	A	207	GLN
2	B	2	ASN
2	B	59	HIS
2	B	110	ASN
2	B	156	HIS
2	B	245	GLN
2	B	304	GLN
2	B	333	ASN
2	B	348	ASN
2	B	477	GLN
2	B	483	ASN
2	B	507	GLN

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Mol	Chain	Res	Type
2	B	556	GLN

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 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	DHY	B	559	-	9,12,12	0.76	0	12,16,16	2.26	5 (41%)

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	DHY	B	559	-	-	0/2/4/4	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	559	DHY	O3-C3-C2	4.08	130.38	119.46
4	B	559	DHY	O4-C4-C5	3.35	128.43	119.33
4	B	559	DHY	O3-C3-C4	-3.08	110.25	118.45
4	B	559	DHY	O4-C4-C3	-2.99	110.49	118.45
4	B	559	DHY	C7-C1-C2	-2.79	115.27	120.69

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%)	-0.55	2 (0%) 82 88	14, 26, 59, 80	0
2	B	557/557 (100%)	-0.68	6 (1%) 80 87	9, 24, 56, 95	0
All	All	763/766 (99%)	-0.64	8 (1%) 82 88	9, 25, 57, 95	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	GLN	4.0
1	A	208	THR	3.9
2	B	85	GLU	3.0
2	B	86	LYS	2.9
2	B	131	GLN	2.6
2	B	84	ALA	2.4
2	B	494	ASP	2.3
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. 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	B-factors(\AA^2)	Q<0.9
4	DHY	B	559	12/12	0.93	0.14	27,34,37,37	0
3	CA	B	558	1/1	1.00	0.04	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.