



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:38 PM GMT

PDB ID : 3UDX
Title : Crystal structure of *Acinetobacter baumannii* PBP1a in complex with Imipenem
Authors : Han, S.
Deposited on : 2011-10-28
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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

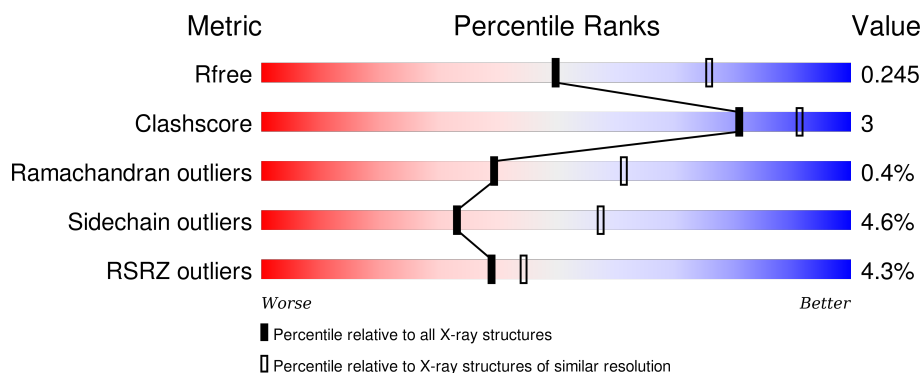
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	731	<div> <div>4%</div> <div>70%</div> <div>11%</div> <div>•</div> <div>18%</div> </div>
1	B	731	<div> <div>3%</div> <div>73%</div> <div>9%</div> <div>19%</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
2	IM2	A	998	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9771 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-binding protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4715	3006	832	861	16			
1	B	595	Total	C	N	O	S	0	1	0
			4691	2990	829	856	16			

There are 32 discrepancies between the modelled and reference sequences:

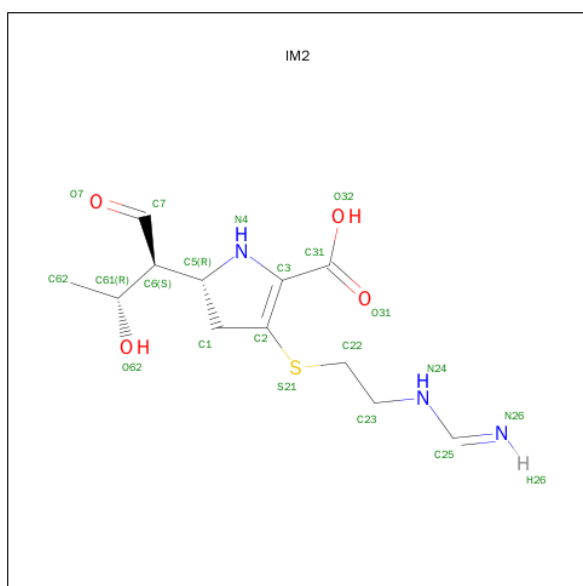
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	EXPRESSION TAG	UNP G1C794
A	10	HIS	-	EXPRESSION TAG	UNP G1C794
A	11	HIS	-	EXPRESSION TAG	UNP G1C794
A	12	HIS	-	EXPRESSION TAG	UNP G1C794
A	13	HIS	-	EXPRESSION TAG	UNP G1C794
A	14	HIS	-	EXPRESSION TAG	UNP G1C794
A	15	HIS	-	EXPRESSION TAG	UNP G1C794
A	16	GLU	-	EXPRESSION TAG	UNP G1C794
A	17	ASN	-	EXPRESSION TAG	UNP G1C794
A	18	LEU	-	EXPRESSION TAG	UNP G1C794
A	19	TYR	-	EXPRESSION TAG	UNP G1C794
A	20	PHE	-	EXPRESSION TAG	UNP G1C794
A	21	GLN	-	EXPRESSION TAG	UNP G1C794
A	22	SER	-	EXPRESSION TAG	UNP G1C794
A	23	HIS	-	EXPRESSION TAG	UNP G1C794
A	24	MET	-	EXPRESSION TAG	UNP G1C794
B	9	MET	-	EXPRESSION TAG	UNP G1C794
B	10	HIS	-	EXPRESSION TAG	UNP G1C794
B	11	HIS	-	EXPRESSION TAG	UNP G1C794
B	12	HIS	-	EXPRESSION TAG	UNP G1C794
B	13	HIS	-	EXPRESSION TAG	UNP G1C794
B	14	HIS	-	EXPRESSION TAG	UNP G1C794
B	15	HIS	-	EXPRESSION TAG	UNP G1C794
B	16	GLU	-	EXPRESSION TAG	UNP G1C794
B	17	ASN	-	EXPRESSION TAG	UNP G1C794

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Chain	Residue	Modelled	Actual	Comment	Reference
B	18	LEU	-	EXPRESSION TAG	UNP G1C794
B	19	TYR	-	EXPRESSION TAG	UNP G1C794
B	20	PHE	-	EXPRESSION TAG	UNP G1C794
B	21	GLN	-	EXPRESSION TAG	UNP G1C794
B	22	SER	-	EXPRESSION TAG	UNP G1C794
B	23	HIS	-	EXPRESSION TAG	UNP G1C794
B	24	MET	-	EXPRESSION TAG	UNP G1C794

- Molecule 2 is (5R)-5-[(1S,2R)-1-FORMYL-2-HYDROXYPROPYL]-3-[(2-[(E)-IMINOMETHYL]AMINO)ETHYL)SULFANYL]-4,5-DIHYDRO-1H-PYRROLE-2-CARBOXYLIC ACID (three-letter code: IM2) (formula: C₁₂H₁₉N₃O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	12	3	4	1		
2	B	1	Total	C	N	O	S	0	0
			20	12	3	4	1		

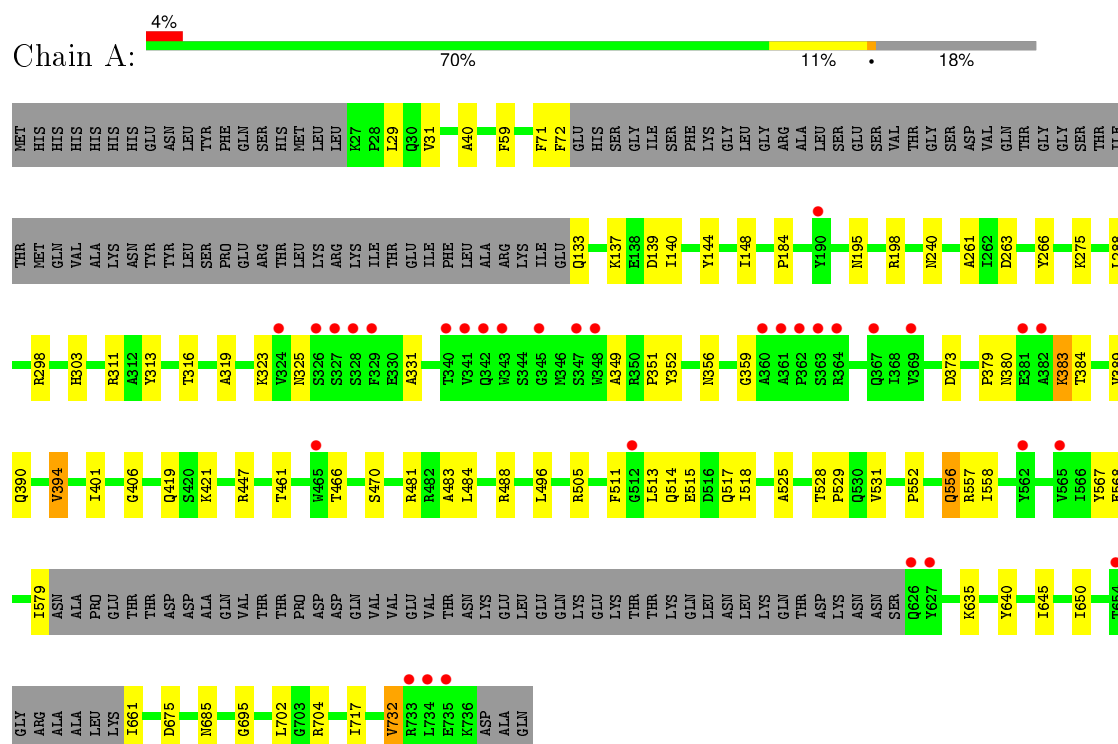
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		
3	B	192	Total	O	0	0
			192	192		

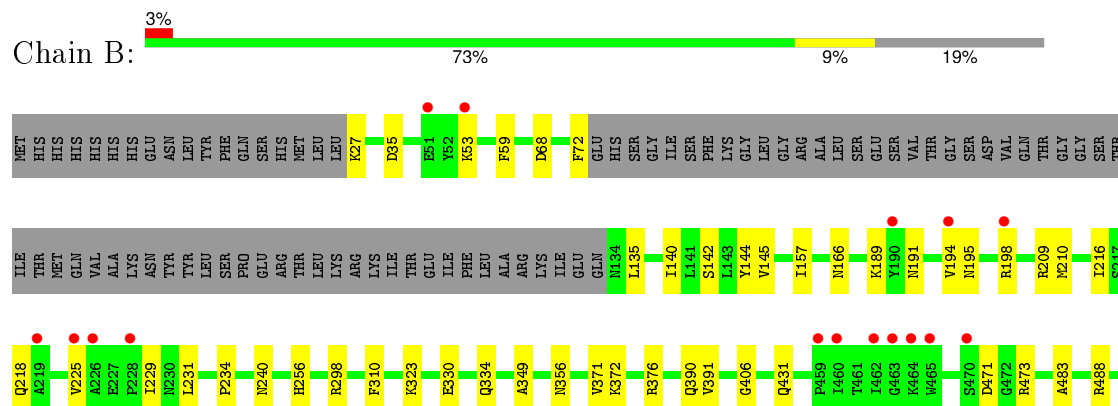
3 Residue-property plots

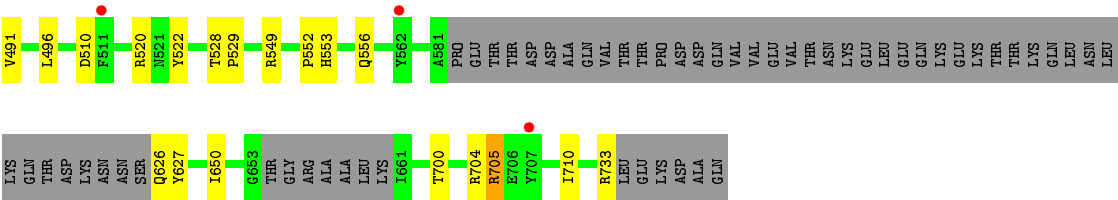
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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-binding protein 1a



• Molecule 1: Penicillin-binding protein 1a





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.27 Å 242.93 Å 49.12 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 2.50 48.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.1 (48.02-2.50) 93.6 (48.02-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.51 Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.187 , 0.238 0.188 , 0.245	Depositor DCC
R_{free} test set	2376 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 47096 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9771	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: IM2

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	0.49	0/4824	0.70	0/6541
1	B	0.53	0/4803	0.73	0/6514
All	All	0.51	0/9627	0.71	0/13055

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4715	0	4701	35	0
1	B	4691	0	4673	31	0
2	A	20	0	16	0	0
2	B	20	0	16	0	0
3	A	133	0	0	0	0
3	B	192	0	0	0	0
All	All	9771	0	9406	63	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 3.

All (63) 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:B:298:ARG:H	1:B:390:GLN:HE22	1.17	0.88
1:A:298:ARG:H	1:A:390:GLN:HE22	1.23	0.83
1:B:356:ASN:HD21	1:B:704:ARG:H	1.38	0.71
1:A:323:LYS:HE3	1:A:325:ASN:HD21	1.58	0.68
1:A:505:ARG:HH22	1:A:515:GLU:HG3	1.58	0.68
1:A:513:LEU:HB3	1:A:518:ILE:HD11	1.79	0.65
1:B:406:GLY:O	1:B:552:PRO:HA	1.97	0.64
1:B:704:ARG:O	1:B:705:ARG:HB2	1.96	0.64
1:B:528:THR:N	1:B:529:PRO:HD2	2.13	0.63
1:B:356:ASN:ND2	1:B:704:ARG:HG2	2.18	0.59
1:A:288:LEU:HD22	1:A:394:VAL:HG13	1.85	0.59
1:A:556:GLN:HE21	1:A:557:ARG:HH11	1.50	0.58
1:B:376:ARG:HD2	1:B:391:VAL:HG23	1.86	0.57
1:B:471:ASP:HB2	1:B:473:ARG:HH11	1.71	0.56
1:A:496:LEU:HD22	1:A:525:ALA:HB2	1.87	0.56
1:A:71:PHE:O	1:B:553:HIS:HA	2.08	0.54
1:A:695:GLY:HA2	1:A:702:LEU:HD21	1.90	0.53
1:A:661:ILE:HD11	1:A:717:ILE:HA	1.92	0.52
1:A:351:PRO:HG2	1:A:359:GLY:HA3	1.92	0.52
1:B:431:GLN:HG2	1:B:528:THR:O	2.10	0.51
1:A:31:VAL:HB	1:A:40:ALA:HB3	1.93	0.51
1:A:261:ALA:HA	1:B:144:TYR:CE1	2.45	0.50
1:A:528:THR:N	1:A:529:PRO:HD2	2.26	0.50
1:B:528:THR:H	1:B:529:PRO:HD2	1.75	0.49
1:A:513:LEU:HD21	1:A:531:VAL:HG12	1.93	0.49
1:A:461:THR:HG22	1:A:466:THR:OG1	2.12	0.49
1:A:313:TYR:CE1	1:A:419:GLN:HB2	2.48	0.49
1:B:510:ASP:O	1:B:549:ARG:HD3	2.13	0.48
1:B:473:ARG:O	1:B:488:ARG:NH2	2.46	0.48
1:A:148:ILE:HG21	1:A:184:PRO:HB3	1.94	0.47
1:A:514:GLN:HB2	1:A:517:GLN:HG2	1.96	0.47
1:B:298:ARG:H	1:B:390:GLN:NE2	1.99	0.46
1:B:72:PHE:HB3	1:B:140:ILE:HD12	1.96	0.46
1:A:640:TYR:HD1	1:A:732:VAL:HG23	1.81	0.46
1:A:298:ARG:H	1:A:390:GLN:NE2	2.03	0.46
1:A:137:LYS:NZ	1:B:256:HIS:HD2	2.14	0.46
1:A:558:ILE:HB	1:A:567:TYR:HB3	1.98	0.46
1:B:229:ILE:HD12	1:B:231:LEU:H	1.80	0.45
1:B:371:VAL:O	1:B:372:LYS:HB2	2.17	0.45
1:A:144:TYR:O	1:A:148:ILE:HG13	2.18	0.44
1:A:29:LEU:HD22	1:A:266:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLY:O	1:A:552:PRO:HA	2.18	0.44
1:B:528:THR:N	1:B:529:PRO:CD	2.81	0.43
1:B:310:PHE:O	1:B:334:GLN:NE2	2.52	0.42
1:A:303:HIS:HD2	1:A:373:ASP:OD1	2.02	0.42
1:B:483:ALA:HB1	1:B:491:VAL:HG11	2.01	0.42
1:B:191:ASN:HB3	1:B:194:VAL:HG12	2.02	0.42
1:B:145:VAL:HG22	1:B:157:ILE:HG12	2.01	0.42
1:B:356:ASN:HD21	1:B:704:ARG:N	2.12	0.42
1:B:704:ARG:O	1:B:705:ARG:CB	2.65	0.42
1:A:483:ALA:HA	1:A:488:ARG:HG2	2.01	0.42
1:B:323:LYS:HB3	1:B:330:GLU:HB2	2.02	0.41
1:A:72:PHE:HB3	1:A:140:ILE:HD12	2.02	0.41
1:A:484:LEU:HD23	1:A:645:ILE:HG21	2.01	0.41
1:A:316:THR:HG22	1:A:389:VAL:HG21	2.02	0.41
1:A:383:LYS:HB3	1:A:384:THR:H	1.66	0.41
1:B:496:LEU:HD23	1:B:522:TYR:HD1	1.86	0.41
1:A:356:ASN:OD1	1:A:704:ARG:HB2	2.21	0.40
1:A:380:ASN:HB2	1:A:383:LYS:O	2.21	0.40
1:B:210:MET:HB3	1:B:216:ILE:HG12	2.03	0.40
1:B:166:ASN:HB2	1:B:234:PRO:HD3	2.03	0.40
1:B:195:ASN:HB3	1:B:198:ARG:HB3	2.03	0.40
1:A:319:ALA:HB1	1:A:331:ALA:HB1	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	590/731 (81%)	564 (96%)	23 (4%)	3 (0%)	34	55
1	B	588/731 (80%)	562 (96%)	24 (4%)	2 (0%)	46	68
All	All	1178/1462 (81%)	1126 (96%)	47 (4%)	5 (0%)	39	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	ALA
1	A	383	LYS
1	B	349	ALA
1	B	705	ARG
1	A	379	PRO

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	490/608 (81%)	465 (95%)	25 (5%)	29	52
1	B	487/608 (80%)	467 (96%)	20 (4%)	37	63
All	All	977/1216 (80%)	932 (95%)	45 (5%)	33	57

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	PHE
1	A	133	GLN
1	A	139	ASP
1	A	195	ASN
1	A	198	ARG
1	A	240	ASN
1	A	263	ASP
1	A	275	LYS
1	A	311	ARG
1	A	352	TYR
1	A	394	VAL
1	A	401	ILE
1	A	421	LYS
1	A	447	ARG
1	A	470	SER
1	A	481	ARG
1	A	511	PHE
1	A	556	GLN

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Mol	Chain	Res	Type
1	A	568	GLU
1	A	579	ILE
1	A	635	LYS
1	A	650	ILE
1	A	675	ASP
1	A	685	ASN
1	A	732	VAL
1	B	27	LYS
1	B	35	ASP
1	B	53	LYS
1	B	59	PHE
1	B	68	ASP
1	B	135	LEU
1	B	142	SER
1	B	189	LYS
1	B	209	ARG
1	B	218	GLN
1	B	225	VAL
1	B	240	ASN
1	B	520	ARG
1	B	556	GLN
1	B	626	GLN
1	B	627	TYR
1	B	650	ILE
1	B	700	THR
1	B	710	ILE
1	B	733	ARG

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	235	ASN
1	A	295	HIS
1	A	303	HIS
1	A	325	ASN
1	A	390	GLN
1	A	551	GLN
1	A	556	GLN
1	A	629	GLN
1	A	652	HIS
1	B	212	GLN
1	B	256	HIS

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Mol	Chain	Res	Type
1	B	356	ASN
1	B	390	GLN
1	B	469	ASN
1	B	514	GLN
1	B	551	GLN
1	B	556	GLN
1	B	629	GLN
1	B	674	ASN
1	B	722	GLN

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](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	IM2	A	998	1	13,20,20	1.00	1 (7%)	10,26,26	1.26	1 (10%)
2	IM2	B	999	1	13,20,20	1.02	1 (7%)	10,26,26	0.97	1 (10%)

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
2	IM2	A	998	1	-	0/13/32/32	0/1/1/1
2	IM2	B	999	1	-	0/13/32/32	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	IM2	C31-C3	-2.53	1.47	1.52
2	B	999	IM2	C31-C3	-2.36	1.48	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	IM2	C62-C61-C6	2.26	115.49	112.19
2	A	998	IM2	C62-C61-C6	2.91	116.44	112.19

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

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, 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	598/731 (81%)	0.20	32 (5%) 29 33	31, 53, 88, 122	0
1	B	595/731 (81%)	0.11	19 (3%) 51 56	21, 46, 93, 120	0
All	All	1193/1462 (81%)	0.15	51 (4%) 39 44	21, 50, 93, 122	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	VAL	6.5
1	A	382	ALA	5.8
1	A	363	SER	4.8
1	B	225	VAL	4.8
1	B	226	ALA	4.7
1	B	465	TRP	4.5
1	A	327	SER	4.5
1	B	190	TYR	4.3
1	A	362	PRO	3.9
1	A	626	GLN	3.9
1	B	511	PHE	3.9
1	B	462	ILE	3.7
1	B	194	VAL	3.7
1	B	470	SER	3.7
1	A	329	PHE	3.7
1	B	460	ILE	3.6
1	A	381	GLU	3.5
1	A	345	GLY	3.5
1	A	190	TYR	3.4
1	B	707	TYR	3.3
1	A	565	VAL	3.2
1	B	464	LYS	3.2
1	A	360	ALA	3.1
1	A	735	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	463	GLY	3.0
1	A	465	TRP	3.0
1	A	343	TRP	2.9
1	A	328	SER	2.9
1	A	341	VAL	2.9
1	A	734	LEU	2.9
1	A	562	TYR	2.8
1	A	326	SER	2.8
1	B	198	ARG	2.6
1	A	369	VAL	2.5
1	A	348	TRP	2.5
1	B	53	LYS	2.3
1	B	219	ALA	2.3
1	A	347	SER	2.3
1	A	733	ARG	2.3
1	A	367	GLN	2.3
1	A	512	GLY	2.3
1	A	364	ARG	2.3
1	B	51	GLU	2.3
1	B	228	PRO	2.2
1	A	340	THR	2.2
1	A	361	ALA	2.2
1	A	654	THR	2.2
1	B	562	TYR	2.1
1	B	459	PRO	2.1
1	A	627	TYR	2.0
1	A	342	GLN	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(\AA^2)	Q<0.9
2	IM2	A	998	20/20	0.91	0.21	2.33	52,76,95,95	0
2	IM2	B	999	20/20	0.93	0.18	0.06	46,70,98,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.