



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:48 am GMT

PDB ID : 3UPN
Title : Structure of penicillin-binding protein A from *M. tuberculosis*: imipenem acyl-enzyme complex
Authors : Davies, C.; Fedorovich, A.
Deposited on : 2011-11-18
Resolution : 2.20 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

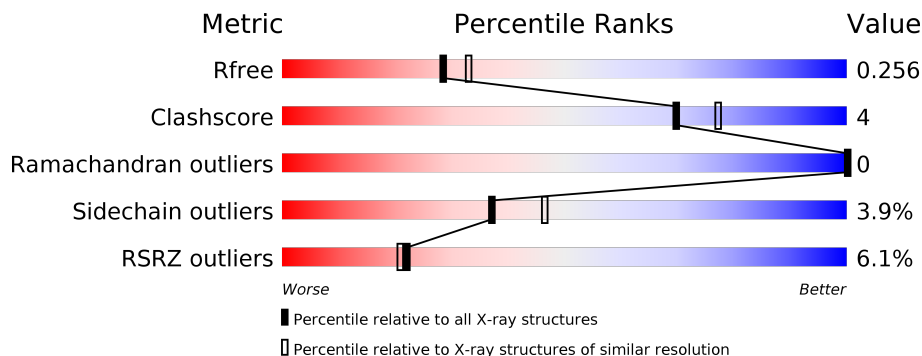
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	462	<div> <div>9%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	462	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</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
2	IM2	B	800	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6525 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.

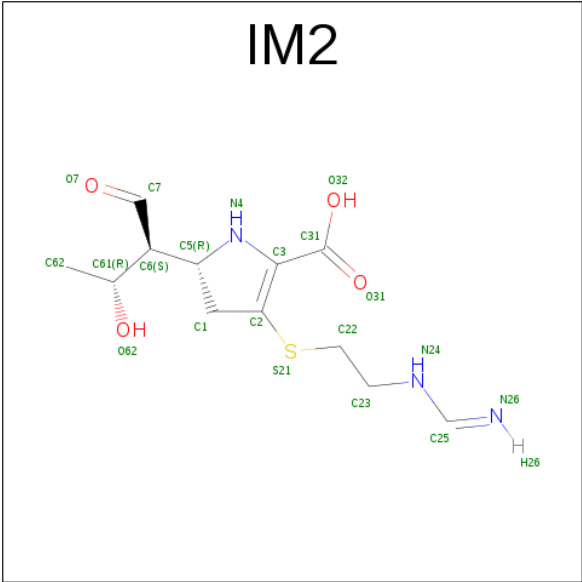
- Molecule 1 is a protein called Penicillin-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3214	2015	573	617	9			
1	B	436	Total	C	N	O	S	0	0	0
			3214	2013	574	618	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	EXPRESSION TAG	UNP P71586
A	31	ALA	-	EXPRESSION TAG	UNP P71586
A	32	MET	-	EXPRESSION TAG	UNP P71586
A	33	GLY	-	EXPRESSION TAG	UNP P71586
A	34	SER	-	EXPRESSION TAG	UNP P71586
A	384	ARG	GLY	SEE REMARK 999	UNP P71586
B	30	GLY	-	EXPRESSION TAG	UNP P71586
B	31	ALA	-	EXPRESSION TAG	UNP P71586
B	32	MET	-	EXPRESSION TAG	UNP P71586
B	33	GLY	-	EXPRESSION TAG	UNP P71586
B	34	SER	-	EXPRESSION TAG	UNP P71586
B	384	ARG	GLY	SEE REMARK 999	UNP P71586

- 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		

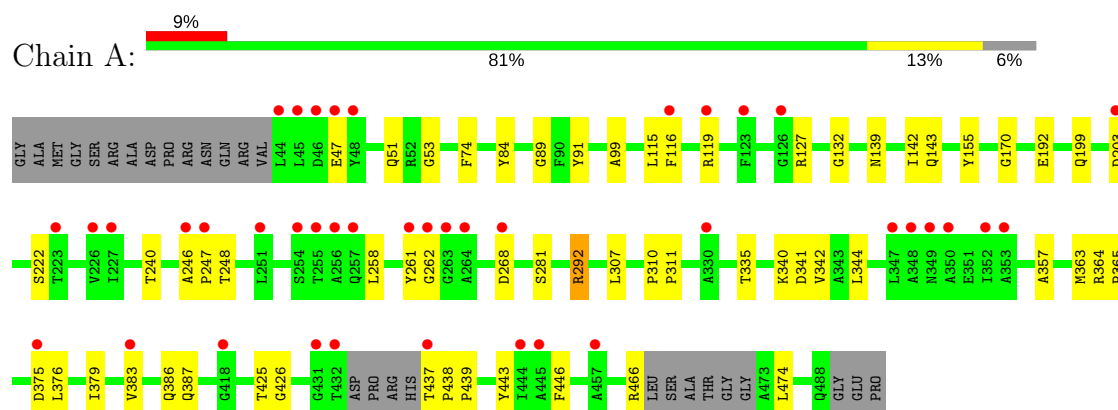
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	26	Total	O	0	0
			26	26		

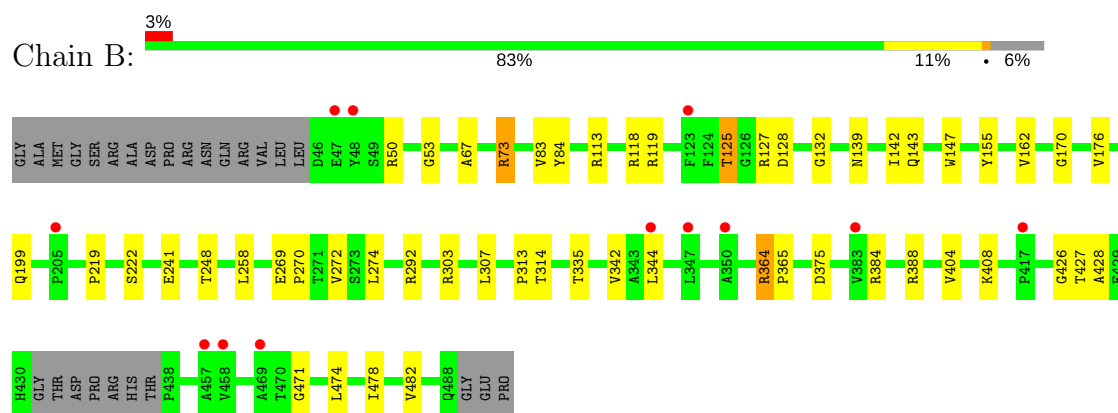
3 Residue-property plots [i](#)

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-binding protein A



• Molecule 1: Penicillin-binding protein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	122.80Å 122.80Å 101.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.35 – 2.20 37.35 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.35-2.20) 99.1 (37.35-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.258 0.209 , 0.256	Depositor DCC
R_{free} test set	2149 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6525	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.51	0/3280	0.60	0/4478
1	B	0.51	0/3281	0.61	0/4479
All	All	0.51	0/6561	0.60	0/8957

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 [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	3214	0	3209	30	0
1	B	3214	0	3206	25	1
2	A	20	0	14	0	0
2	B	20	0	14	3	0
3	A	31	0	0	0	0
3	B	26	0	0	0	0
All	All	6525	0	6443	54	1

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 4.

All (54) 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:292:ARG:HG3	1:A:292:ARG:HH11	1.46	0.79
1:B:427:THR:HG23	2:B:800:IM2:H222	1.68	0.74
1:B:427:THR:CG2	2:B:800:IM2:H222	2.23	0.69
1:A:292:ARG:CG	1:A:292:ARG:HH11	2.09	0.65
1:B:50:ARG:HH22	1:B:119:ARG:HD2	1.63	0.64
1:B:314:THR:HA	1:B:364:ARG:NH2	2.13	0.63
1:B:125:THR:HG23	1:B:127:ARG:HG3	1.85	0.58
1:A:199:GLN:NE2	1:A:203:ASP:OD2	2.39	0.55
1:B:170:GLY:O	1:B:365:PRO:HA	2.08	0.53
1:B:269:GLU:HB3	1:B:270:PRO:HD2	1.90	0.53
1:A:307:LEU:HD21	1:A:344:LEU:HD11	1.91	0.53
1:B:73:ARG:HH21	1:B:73:ARG:HG2	1.74	0.52
1:A:364:ARG:HB2	1:A:387:GLN:HG3	1.90	0.52
1:A:261:TYR:OH	1:A:466:ARG:HA	2.11	0.51
1:A:222:SER:HB2	1:A:426:GLY:HA3	1.94	0.49
1:A:292:ARG:NH1	1:A:292:ARG:HG3	2.19	0.49
1:A:335:THR:HG23	1:A:342:VAL:CG2	2.42	0.49
1:A:425:THR:HG22	1:A:443:TYR:HD1	1.78	0.48
1:B:139:ASN:HB3	1:B:142:ILE:HD12	1.93	0.48
1:A:155:TYR:HH	1:B:155:TYR:HH	1.62	0.47
1:A:340:LYS:HE3	1:A:341:ASP:OD2	2.13	0.47
1:B:67:ALA:HB1	1:B:73:ARG:NH1	2.30	0.47
1:A:261:TYR:HA	1:A:262:GLY:HA2	1.71	0.46
1:A:53:GLY:HA3	1:A:132:GLY:O	2.16	0.46
1:B:313:PRO:O	1:B:364:ARG:NH2	2.49	0.45
1:B:307:LEU:HD21	1:B:344:LEU:HD11	1.99	0.45
1:B:303:ARG:HA	1:B:307:LEU:O	2.17	0.44
1:B:335:THR:HG23	1:B:342:VAL:CG2	2.47	0.44
1:A:116:PHE:HD2	1:A:119:ARG:NH1	2.14	0.44
1:B:219:PRO:HB2	1:B:428:ALA:HB1	2.00	0.44
1:A:363:MET:SD	1:A:386:GLN:HG2	2.58	0.44
1:A:115:LEU:HD21	1:A:379:ILE:HD11	1.99	0.44
1:B:162:VAL:HB	1:B:176:VAL:HB	2.00	0.43
1:A:84:TYR:CE2	1:A:143:GLN:HG2	2.53	0.43
1:A:357:ALA:HB2	1:A:446:PHE:CG	2.53	0.43
1:A:170:GLY:O	1:A:365:PRO:HA	2.18	0.43
1:B:53:GLY:HA3	1:B:132:GLY:O	2.18	0.43
1:A:116:PHE:HD2	1:A:119:ARG:HH12	1.66	0.42
1:A:222:SER:HB2	1:A:426:GLY:CA	2.49	0.42
1:A:47:GLU:OE2	1:A:91:TYR:OH	2.35	0.42
1:B:471:GLY:HA2	2:B:800:IM2:H232	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:PRO:HA	1:A:439:PRO:HD3	1.97	0.42
1:A:246:ALA:HA	1:A:247:PRO:HD3	1.94	0.42
1:A:89:GLY:HA3	1:A:99:ALA:HB3	2.00	0.42
1:A:375:ASP:O	1:A:376:LEU:HB2	2.19	0.42
1:B:314:THR:HA	1:B:364:ARG:HH22	1.84	0.42
1:A:310:PRO:HA	1:A:311:PRO:HD3	1.97	0.42
1:B:478:ILE:O	1:B:482:VAL:HG23	2.19	0.42
1:A:51:GLN:HB2	1:A:74:PHE:CZ	2.55	0.42
1:B:83:VAL:HG22	1:B:147:TRP:CD1	2.54	0.41
1:B:222:SER:HB2	1:B:426:GLY:HA2	2.02	0.41
1:B:84:TYR:CE2	1:B:143:GLN:HG2	2.56	0.41
1:B:404:VAL:HG12	1:B:408:LYS:HE2	2.01	0.41
1:A:139:ASN:HB3	1:A:142:ILE:HD12	2.02	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ARG:NH1	1:B:375:ASP:OD1[6_445]	2.14	0.06

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	429/462 (93%)	418 (97%)	11 (3%)	0	100	100
1	B	432/462 (94%)	421 (98%)	11 (2%)	0	100	100
All	All	861/924 (93%)	839 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	331/350 (95%)	320 (97%)	11 (3%)	43	54
1	B	330/350 (94%)	315 (96%)	15 (4%)	32	39
All	All	661/700 (94%)	635 (96%)	26 (4%)	37	46

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ARG
1	A	192	GLU
1	A	240	THR
1	A	248	THR
1	A	258	LEU
1	A	268	ASP
1	A	281	SER
1	A	292	ARG
1	A	383	VAL
1	A	437	THR
1	A	474	LEU
1	B	73	ARG
1	B	118	ARG
1	B	125	THR
1	B	128	ASP
1	B	199	GLN
1	B	241	GLU
1	B	248	THR
1	B	258	LEU
1	B	272	VAL
1	B	274	LEU
1	B	292	ARG
1	B	364	ARG
1	B	384	ARG
1	B	388	ARG
1	B	474	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	189	HIS
1	B	242	GLN
1	B	488	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	800	1	14,20,20	2.04	4 (28%)	9,26,26	1.61	2 (22%)
2	IM2	B	800	1	14,20,20	1.89	4 (28%)	9,26,26	1.33	1 (11%)

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	800	1	-	0/13/32/32	0/1/1/1
2	IM2	B	800	1	-	0/13/32/32	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	IM2	C25-N24	-4.56	1.22	1.34
2	B	800	IM2	C25-N24	-4.07	1.24	1.34
2	B	800	IM2	C31-C3	-3.66	1.46	1.52
2	A	800	IM2	C31-C3	-3.55	1.46	1.52
2	B	800	IM2	C2-S21	-3.33	1.68	1.74
2	A	800	IM2	C2-S21	-3.09	1.68	1.74
2	B	800	IM2	C6-C7	2.10	1.53	1.49
2	A	800	IM2	C6-C7	2.56	1.54	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	IM2	C22-C23-N24	-3.00	105.92	112.45
2	A	800	IM2	C22-C23-N24	-2.88	106.19	112.45
2	A	800	IM2	O7-C7-C6	-2.77	117.77	125.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	IM2	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	435/462 (94%)	0.26	41 (9%) 9 8	28, 44, 70, 84	0
1	B	436/462 (94%)	0.01	12 (2%) 53 51	31, 44, 63, 78	0
All	All	871/924 (94%)	0.14	53 (6%) 22 21	28, 44, 66, 84	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	ALA	5.7
1	B	47	GLU	4.5
1	A	255	THR	4.4
1	A	432	THR	4.0
1	B	48	TYR	4.0
1	A	268	ASP	3.9
1	A	251	LEU	3.5
1	A	437	THR	3.4
1	A	352	ILE	3.3
1	A	383	VAL	3.2
1	B	469	ALA	3.2
1	A	261	TYR	3.1
1	A	350	ALA	3.1
1	A	347	LEU	3.1
1	A	349	ASN	3.1
1	A	119	ARG	3.1
1	A	44	LEU	2.9
1	B	123	PHE	2.9
1	B	417	PRO	2.9
1	A	375	ASP	2.9
1	A	444	ILE	2.8
1	B	350	ALA	2.8
1	A	116	PHE	2.8
1	A	247	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	264	ALA	2.7
1	A	45	LEU	2.7
1	A	418	GLY	2.7
1	B	457	ALA	2.6
1	A	348	ALA	2.6
1	A	263	GLY	2.6
1	A	431	GLY	2.5
1	A	457	ALA	2.5
1	A	46	ASP	2.3
1	A	330	ALA	2.3
1	A	123	PHE	2.3
1	A	353	ALA	2.3
1	A	47	GLU	2.3
1	A	262	GLY	2.2
1	A	203	ASP	2.2
1	A	257	GLN	2.2
1	B	458	VAL	2.2
1	A	445	ALA	2.2
1	A	226	VAL	2.1
1	B	205	PRO	2.1
1	A	126	GLY	2.1
1	A	223	THR	2.1
1	A	246	ALA	2.1
1	B	383	VAL	2.1
1	A	48	TYR	2.1
1	A	227	ILE	2.0
1	B	344	LEU	2.0
1	B	347	LEU	2.0
1	A	254	SER	2.0

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 [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	B	800	20/20	0.78	0.23	2.32	53,64,69,70	0
2	IM2	A	800	20/20	0.75	0.17	-0.03	56,66,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.