

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 7, 2024 - 12:30 am GMT

PDB ID	:	6F2W
Title	:	Bacterial asc transporter crystal structure in open to in conformation
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Deposited on	:	2017-11-27
Resolution	:	3.40  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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
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)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.40 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 of 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	А	444	<sup>2%</sup> 64%	30%		
2	В	134	% 63%	29%	•••	



#### 6F2W

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4259 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 Putative amino acid/polyamine transport protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	433	Total 3286	C 2218	N 504	O 552	S 12	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP A8UCQ5
А	436	GLY	-	expression tag	UNP A8UCQ5
А	437	GLY	-	expression tag	UNP A8UCQ5
А	438	GLY	-	expression tag	UNP A8UCQ5
А	439	LEU	-	expression tag	UNP A8UCQ5
А	440	GLU	-	expression tag	UNP A8UCQ5
А	441	VAL	-	expression tag	UNP A8UCQ5
А	442	LEU	-	expression tag	UNP A8UCQ5
А	443	PHE	-	expression tag	UNP A8UCQ5
А	444	GLN	-	expression tag	UNP A8UCQ5

• Molecule 2 is a protein called Nanobody 74.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	128	Total 965	C 595	N 179	0 187	${f S}$ $4$	0	0	0

• Molecule 3 is ALPHA-AMINOISOBUTYRIC ACID (three-letter code: AIB) (formula:  $C_4H_9NO_2$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total 7	C 4	N 1	O 2	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total Zn 1 1	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	85.64Å $85.64$ Å $321.63$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Perclution(Å)	24.96 - 3.40	Depositor
Resolution (A)	24.96 - 3.40	EDS
% Data completeness	83.0 (24.96-3.40)	Depositor
(in resolution range)	83.3 (24.96-3.40)	EDS
$R_{merge}$	0.10	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.22 (at 3.38 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0158, BUSTER 2.10.3, PHENIX dev-2880	Depositor
D D.	0.230 , $0.268$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.233 , $0.270$	DCC
$R_{free}$ test set	708 reflections $(4.90%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	110.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.23, 85.7	EDS
L-test for twinning <sup>2</sup>	$< L >=0.40, < L^2>=0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4259	wwPDB-VP
Average B, all atoms $(Å^2)$	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: ZN, AIB

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).

Mal	Chain	Bond	lengths	Bond angles		
10101	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.78	0/3369	0.94	1/4605~(0.0%)	
2	В	0.87	0/988	1.00	3/1339~(0.2%)	
All	All	0.80	0/4357	0.95	4/5944~(0.1%)	

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	А	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	34	MET	CG-SD-CE	-8.10	87.24	100.20
2	В	27	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	А	356	PHE	CB-CG-CD1	5.26	124.48	120.80
2	В	107	TYR	CB-CG-CD1	5.10	124.06	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	383	PHE	Peptide



### 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	А	3286	0	3495	72	0
2	В	965	0	910	21	0
3	А	7	0	6	0	0
4	В	1	0	0	0	0
All	All	4259	0	4411	88	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 10.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:77:VAL:HG21	1:A:364:ALA:HB1	1.67	0.77
2:B:22:CYS:HG	2:B:96:CYS:HG	1.26	0.72
1:A:165:GLY:HA2	1:A:266:LEU:HD21	1.76	0.67
1:A:362:PHE:HB2	1:A:392:ILE:HD13	1.78	0.64
1:A:104:ILE:HD11	1:A:338:ILE:HA	1.78	0.64
1:A:181:VAL:CG1	1:A:183:THR:HG22	2.28	0.63
1:A:27:THR:HG21	1:A:256:ASP:HA	1.81	0.62
2:B:29:PHE:HB3	2:B:77:ASN:HD22	1.63	0.62
1:A:316:ILE:HD13	1:A:321:ASN:HA	1.82	0.61
1:A:363:ILE:HG13	1:A:392:ILE:HD11	1.83	0.60
2:B:29:PHE:HB3	2:B:77:ASN:ND2	2.17	0.60
1:A:17:VAL:HG11	1:A:232:VAL:HG11	1.84	0.60
1:A:49:ILE:HD11	1:A:394:GLY:HA3	1.85	0.59
1:A:126:ILE:HG12	1:A:338:ILE:HD11	1.86	0.58
2:B:9:GLY:HA2	2:B:18:LEU:HD21	1.86	0.58
1:A:213:GLU:HG3	2:B:101:GLY:HA3	1.84	0.58
1:A:360:LEU:HA	1:A:363:ILE:HD12	1.85	0.58
1:A:230:SER:HA	1:A:233:MET:HB2	1.86	0.58
2:B:28:THR:HB	2:B:32:ARG:HE	1.70	0.57
2:B:91:THR:HG23	2:B:121:THR:HA	1.87	0.56
1:A:109:GLN:HE22	1:A:260:ALA:HB2	1.69	0.56
1:A:162:ILE:HG12	1:A:239:THR:HG22	1.87	0.56
2:B:30:SER:O	2:B:53:TRP:HE3	1.88	0.56



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:366:ILE:HG23	1·A·384·TYR·OH	2.05	0.55
1:A:355:TRP:HA	1:A:358:ILE:HB	1.87	0.54
2:B:53:TRP:CG	2:B:54:SEB:N	2.75	0.54
1:A:24:PHE:HE1	1:A:257:THR:HG22	1.71	0.54
1:A:364:ALA:HA	1:A:367:ILE:HD12	1.89	0.53
1:A:276:THR:HA	1:A:279:ILE:HD12	1.90	0.52
1:A:213:GLU:OE2	2:B:103:ALA:HB3	2.09	0.52
2:B:98:ALA:HB3	2:B:113:TYR:HB2	1.91	0.51
1:A:89:ALA:HB2	1:A:417:THR:HG22	1.94	0.50
1:A:284:PHE:HA	1:A:287:ILE:HD12	1.94	0.49
1:A:183:THR:HG23	1:A:184:HIS:CD2	2.48	0.48
1:A:165:GLY:HA3	1:A:242:ALA:HB1	1.95	0.48
1:A:357:PHE:HA	1:A:360:LEU:HD12	1.96	0.48
1:A:62:THR:HB	1:A:378:PRO:HD2	1.96	0.48
1:A:162:ILE:CG1	1:A:239:THR:HG22	2.44	0.47
2:B:12:VAL:HG23	2:B:122:VAL:HG22	1.95	0.47
2:B:95:HIS:ND1	2:B:117:GLY:HA3	2.29	0.47
1:A:22:ILE:HD13	1:A:158:LEU:HD21	1.95	0.47
1:A:385:PRO:O	1:A:389:LEU:HD13	2.15	0.47
1:A:181:VAL:HG11	1:A:183:THR:HG22	1.95	0.46
1:A:56:THR:HA	1:A:381:VAL:CG2	2.45	0.46
1:A:143:SER:HB3	1:A:292:ILE:HD11	1.97	0.45
1:A:195:ILE:HG13	1:A:351:VAL:HB	1.98	0.45
2:B:47:PHE:CD1	2:B:106:ASN:HA	2.51	0.45
1:A:84:PHE:CD1	1:A:306:MET:HB3	2.52	0.45
1:A:174:ILE:HA	1:A:177:VAL:HG13	1.99	0.45
1:A:297:VAL:HB	1:A:298:PRO:CD	2.46	0.45
2:B:112:VAL:HG23	2:B:113:TYR:CD2	2.52	0.45
1:A:48:ILE:HD13	1:A:48:ILE:HA	1.80	0.45
1:A:181:VAL:HG12	1:A:183:THR:HG22	1.98	0.45
1:A:84:PHE:CE2	1:A:424:TYR:HB2	2.51	0.45
1:A:363:ILE:HA	1:A:366:ILE:HD12	1.98	0.44
2:B:60:TYR:CE1	2:B:70:ILE:HG22	2.53	0.44
1:A:235:VAL:O	1:A:239:THR:HG23	2.18	0.44
1:A:90:GLN:HE21	1:A:95:TYR:HE2	1.65	0.44
1:A:155:LEU:O	1:A:159:VAL:HG23	2.17	0.44
1:A:84:PHE:CD2	1:A:424:TYR:HB2	2.53	0.44
1:A:136:ASN:HD21	1:A:292:ILE:HG13	1.83	0.44
1:A:361:THR:O	1:A:364:ALA:HB3	2.18	0.44
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.85	0.44
1:A:357:PHE:HD1	1:A:360:LEU:HD12	1.84	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:24:PHE:HZ	1:A:109:GLN:HB2	1.84	0.43
1:A:85:LEU:HD11	1:A:421:ILE:HD11	2.00	0.43
1:A:406:GLN:HB3	1:A:409:ASN:HB2	2.01	0.43
1:A:98:ASN:O	1:A:102:LEU:HD12	2.19	0.43
1:A:206:ASN:HD22	1:A:206:ASN:N	2.16	0.43
2:B:68:VAL:CG2	2:B:81:LEU:HG	2.50	0.42
1:A:102:LEU:O	1:A:105:ILE:HG22	2.20	0.42
1:A:108:THR:HA	1:A:121:ILE:HD12	2.00	0.42
1:A:24:PHE:CZ	1:A:109:GLN:HB2	2.55	0.42
1:A:213:GLU:CD	2:B:103:ALA:HB3	2.40	0.42
1:A:106:PHE:CD1	1:A:128:THR:HG21	2.55	0.41
1:A:34:GLY:HA3	1:A:184:HIS:CD2	2.55	0.41
1:A:66:GLN:HA	2:B:103:ALA:HB1	2.02	0.41
1:A:168:TYR:CD1	1:A:246:VAL:HG22	2.55	0.41
1:A:97:ALA:HA	1:A:100:ALA:HB3	2.03	0.41
1:A:105:ILE:HD13	1:A:343:PHE:CG	2.55	0.41
1:A:35:ALA:HB2	1:A:181:VAL:HG23	2.02	0.41
1:A:195:ILE:O	1:A:351:VAL:HG21	2.21	0.41
1:A:204:TRP:HH2	1:A:362:PHE:HZ	1.68	0.41
1:A:321:ASN:ND2	2:B:45:ARG:HH11	2.18	0.41
2:B:68:VAL:HG21	2:B:81:LEU:HG	2.03	0.41
1:A:409:ASN:HA	1:A:412:ILE:HD12	2.02	0.40
1:A:86:VAL:O	1:A:90:GLN:HG3	2.20	0.40
1:A:304:GLN:HB3	1:A:305:LYS:HE3	2.04	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	А	431/444~(97%)	380 (88%)	41 (10%)	10 (2%)	6 28



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	В	126/134~(94%)	116 (92%)	7~(6%)	3(2%)	6 28
All	All	557/578~(96%)	496 (89%)	48 (9%)	13 (2%)	6 28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	69	GLY
1	А	306	MET
1	А	206	ASN
2	В	91	THR
1	А	217	PRO
1	А	219	LYS
2	В	27	ARG
2	В	77	ASN
1	А	292	ILE
1	А	4	VAL
1	А	65	PRO
1	А	258	PRO
1	А	386	VAL

#### 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	А	348/356~(98%)	291~(84%)	57 (16%)	2 9
2	В	99/104~(95%)	84 (85%)	15~(15%)	3 11
All	All	447/460~(97%)	375~(84%)	72~(16%)	2 10

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	18	ILE
1	А	38	LEU
1	А	40	LEU



Mol	Chain	Res	Type
1	А	48	ILE
1	А	49	ILE
1	А	56	THR
1	А	57	VAL
1	А	66	GLN
1	А	70	MET
1	А	74	LEU
1	А	77	VAL
1	А	91	MET
1	А	127	LEU
1	А	135	VAL
1	А	145	TRP
1	А	160	VAL
1	А	176	LEU
1	А	205	ILE
1	А	206	ASN
1	А	210	LEU
1	А	213	GLU
1	А	220	MET
1	А	224	VAL
1	А	225	ILE
1	А	233	MET
1	А	248	ASP
1	А	250	SER
1	А	270	ILE
1	А	273	LYS
1	А	274	LEU
1	А	282	SER
1	А	292	ILE
1	А	297	VAL
1	А	305	LYS
1	A	306	MET
1	А	308	PRO
1	А	315	ARG
1	А	316	ILE
1	А	319	LYS
1	А	330	MET
1	А	338	ILE
1	А	345	GLN
1	А	348	ASP
1	A	368	LEU
1	А	374	ASP



Mol	Chain	Res	Type
1	А	375	ILE
1	А	380	ARG
1	А	387	ILE
1	А	392	ILE
1	А	398	ILE
1	А	401	ASN
1	А	403	LEU
1	А	408	LYS
1	А	409	ASN
1	А	426	TYR
1	А	428	LYS
1	А	429	LYS
2	В	1	GLN
2	В	12	VAL
2	В	27	ARG
2	В	31	SER
2	В	58	THR
2	В	71	SER
2	В	82	GLN
2	В	85	SER
2	В	87	LYS
2	В	93	VAL
2	В	100	ASN
2	В	121	THR
2	В	124	SER
2	В	126	HIS
2	В	128	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	90	GLN
1	А	109	GLN
1	А	136	ASN
1	А	147	GLN
1	А	184	HIS
1	А	206	ASN
1	А	240	ASN
1	А	288	ASN
1	А	345	GLN
1	А	406	GLN
1	А	409	ASN



Continued from previous page...

Mol	Chain	Res	Type
2	В	39	GLN
2	В	77	ASN

#### 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 monosaccharides 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	Tuno	Chain	Res	s Link	Bond lengths			Bond angles		
	туре				Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	AIB	А	501	-	2,6,6	1.15	0	$5,\!9,\!9$	4.46	2 (40%)

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	AIB	А	501	-	-	0/5/6/6	-

There are no bond length outliers.



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	501	AIB	CB2-CA-C	-8.34	88.45	108.84
3	А	501	AIB	CB1-CA-C	4.90	120.84	108.84

All (2) bond angle outliers are listed below:

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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,  $95^{th}$  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	А	433/444~(97%)	-0.26	11 (2%) 57 55	94, 142, 197, 246	1 (0%)
2	В	128/134~(95%)	-0.27	2 (1%) 72 70	84, 120, 183, 213	0
All	All	561/578~(97%)	-0.26	13 (2%) 60 59	84, 138, 196, 246	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	376	GLU	4.1
1	А	268	GLU	3.7
1	А	269	GLY	3.7
1	А	431	TYR	3.6
1	А	375	ILE	3.2
2	В	75	ALA	2.8
1	А	270	ILE	2.7
1	А	383	PHE	2.6
1	А	188	THR	2.3
2	В	41	PRO	2.3
1	А	80	ARG	2.2
1	А	374	ASP	2.2
1	А	189	SER	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 monosaccharides 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,  $95^{th}$  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	$B-factors(A^2)$	Q<0.9
3	AIB	А	501	7/7	0.95	0.28	132,149,154,160	0
4	ZN	В	201	1/1	0.98	0.04	$151,\!151,\!151,\!151,\!151$	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers (i)

There are no such residues in this entry.

