

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

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PDB ID	:	8JX6
Title	:	Deep-Sea Helicase 9 (DSH9)
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Deposited on	:	2023-06-30
Resolution	:	2.10  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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.34
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)	:	2.34

# 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 2.10 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	5197(2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	457	8%	13%	••
1	В	457	7%84%	14%	••

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	TLA	В	501	-	Х	-	-



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7918 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 Deep-Sea Helicase 9.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	447	Total 3616	C 2329	N 577	O 695	$\begin{array}{c} \mathrm{S} \\ 15 \end{array}$	0	2	0
1	В	451	Total 3626	C 2327	N 583	O 702	S 14	0	1	0

• Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula:  $C_4H_6O_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total         C         O           10         4         6	0	0
2	В	1	Total         C         O           10         4         6	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Mg 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	332	Total O 332 332	0	0
4	В	323	Total         O           323         323	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.



• Molecule 1: Deep-Sea Helicase 9



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	56.81Å 126.84Å 150.72Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	19.99 - 2.10	Depositor
	19.99 - 2.10	EDS
% Data completeness	94.2 (19.99-2.10)	Depositor
(in resolution range)	94.2 (19.99-2.10)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.50 (at 2.09 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R R.	0.201 , 0.241	Depositor
II, II, <i>free</i>	0.200 , $0.241$	DCC
$R_{free}$ test set	2987 reflections $(4.93%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	37.9	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32 , $41.9$	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	0.96	EDS
Total number of atoms	7918	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 28.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8246e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: TLA, MG

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		Bo	nd lengths	Bond angles		
	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
1	А	0.27	0/3686	0.49	3/4978~(0.1%)	
1	В	0.32	2/3695~(0.1%)	0.52	2/4995~(0.0%)	
All	All	0.30	2/7381~(0.0%)	0.51	5/9973~(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	В	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
1	В	10	GLU	CG-CD	-7.09	1.41	1.51
1	В	10	GLU	CD-OE1	-5.22	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	В	176	LEU	CA-CB-CG	8.03	133.77	115.30
1	А	223	LYS	CD-CE-NZ	6.47	126.58	111.70
1	А	241	GLU	CA-CB-CG	5.58	125.67	113.40
1	В	10	GLU	CA-CB-CG	5.44	125.38	113.40
1	А	241	GLU	N-CA-CB	5.30	120.14	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	В	176	LEU	Peptide
1	В	9	THR	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	3616	0	3557	32	1
1	В	3626	0	3554	45	1
2	А	10	0	4	3	0
2	В	10	0	4	0	0
3	В	1	0	0	0	0
4	А	332	0	0	3	0
4	В	323	0	0	4	0
All	All	7918	0	7119	77	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 5.

All (77) 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:139:VAL:HG22	1:A:166:ILE:HD11	1.68	0.73
1:B:11:GLU:O	1:B:15:ILE:N	2.17	0.67
1:B:10:GLU:HG3	1:B:11:GLU:HG3	1.77	0.65
1:B:10:GLU:CG	1:B:11:GLU:H	1.97	0.64
1:A:108:HIS:NE2	1:A:392:GLU:OE2	2.30	0.64
1:A:428:ARG:NH2	4:A:606:HOH:O	2.30	0.64
1:B:8:ALA:O	1:B:13:ARG:NH2	2.33	0.62
1:B:373:LYS:NZ	4:B:604:HOH:O	2.32	0.61
1:B:10:GLU:OE1	1:B:199:LYS:HG3	2.01	0.59
1:B:10:GLU:HG2	1:B:11:GLU:OE1	2.03	0.59
1:B:10:GLU:OE1	1:B:199:LYS:CG	2.50	0.59
1:A:222:GLN:HG3	1:A:224:THR:HG23	1.86	0.58
1:B:105:LYS:NZ	4:B:610:HOH:O	2.37	0.56
1:A:208:ILE:HG22	1:A:243:ILE:HG13	1.89	0.54
1:B:81:LEU:HD22	1:B:86:ILE:HD12	1.91	0.53



			Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:212:LYS:HG3	1:A:243:ILE:HD12	1.90	0.52
1:B:182:GLU:N	1:B:182:GLU:OE1	2.39	0.52
1:B:331:LYS:HE3	1:B:331:LYS:HA	1.91	0.52
1:A:42:ALA:HA	2:A:501:TLA:H2	1.92	0.51
1:B:428:ARG:HA	1:B:431:ARG:HE	1.75	0.51
1:B:11:GLU:OE2	1:B:196:LYS:O	2.29	0.50
1:B:11:GLU:OE1	1:B:197:LEU:HA	2.12	0.49
1:B:396:LYS:NZ	4:B:603:HOH:O	2.30	0.49
1:A:69:PRO:HG3	1:A:147:MET:HG2	1.94	0.49
1:A:328:ASP:O	1:A:330:ASP:N	2.46	0.49
1:B:432:ASP:OD2	1:B:436:ARG:NH2	2.46	0.49
1:B:128:ASN:C	1:B:128:ASN:HD22	2.17	0.48
1:A:265:THR:HG22	1:A:417:TYR:HB2	1.95	0.48
1:B:191:ASP:OD2	1:B:191:ASP:N	2.44	0.48
1:A:186:ILE:HA	1:A:189:LYS:HG3	1.96	0.47
1:A:227:PRO:HD2	1:A:231:ASP:OD2	2.14	0.47
1:B:51:ALA:O	1:B:86:ILE:HD11	2.14	0.47
1:A:39:GLN:HG3	4:A:667:HOH:O	2.13	0.47
1:B:388:PHE:O	1:B:392:GLU:HG2	2.14	0.47
1:A:291:ILE:HG21	1:A:337:ILE:HD12	1.97	0.47
1:B:376:LYS:HA	1:B:380:ARG:HG3	1.98	0.46
1:A:128:ASN:HD22	1:A:131:ASN:HB2	1.81	0.46
1:B:332:PHE:CE1	1:B:360:GLU:HB3	2.51	0.45
1:A:34:GLU:HA	1:A:166:ILE:HG22	1.98	0.45
1:A:293[B]:ASP:N	1:A:293[B]:ASP:OD1	2.49	0.45
1:B:246:LEU:HD11	1:B:450:PHE:HB3	1.98	0.45
1:B:209:ILE:HA	1:B:243:ILE:HD11	1.99	0.45
1:A:259:ASP:O	1:A:263:LYS:HE2	2.18	0.44
1:B:11:GLU:CD	1:B:196:LYS:O	2.56	0.44
1:A:228:SER:HB2	1:A:424:ASP:OD2	2.17	0.44
1:B:292:CYS:SG	1:B:294:LYS:HG2	2.57	0.44
1:B:420:MET:HG3	1:B:451:ILE:HG23	1.99	0.44
1:A:81:LEU:HD22	1:A:86:ILE:HD12	2.00	0.44
1:A:177:LEU:HD11	1:A:185:SER:HB2	2.00	0.44
1:B:111:ALA:HB3	1:B:115:THR:HG22	2.00	0.44
1:A:454:ASP:OXT	4:A:601:HOH:O	2.21	0.43
1:B:186:ILE:HA	1:B:189:LYS:HG3	2.00	0.43
1:A:67:THR:HA	1:A:96:GLY:O	2.19	0.43
1:A:176:LEU:HD11	1:A:437:LEU:HA	2.00	0.43
1:A:134:LEU:HD23	1:A:163:ARG:HD3	1.99	0.43
1:A:46:LYS:NZ	2:A:501:TLA:O11	2.52	0.42

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A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:268:TYR:CE1	1:A:437:LEU:HD11	2.54	0.42
1:B:245:LEU:HD13	1:B:245:LEU:HA	1.85	0.42
1:B:46:LYS:HB3	1:B:46:LYS:HE2	1.74	0.42
1:B:241:GLU:HG3	1:B:242:GLY:N	2.34	0.42
1:A:4:ASP:OD2	1:A:7:SER:HB2	2.19	0.42
1:B:10:GLU:HG3	1:B:11:GLU:H	1.78	0.42
1:B:128:ASN:ND2	1:B:129:LYS:O	2.52	0.42
1:B:4:ASP:N	1:B:4:ASP:OD1	2.52	0.42
1:A:365:LEU:HD21	1:A:391:LYS:HG3	2.01	0.42
1:B:341:LYS:HD3	1:B:341:LYS:H	1.85	0.41
1:B:175:GLN:O	1:B:436:ARG:HD3	2.21	0.41
1:B:321:ALA:HB2	1:B:340:LYS:HG3	2.02	0.41
1:B:67:THR:HA	1:B:96:GLY:O	2.20	0.41
1:A:420:MET:HE3	1:A:423:LEU:HD12	2.02	0.41
1:B:75:ARG:HH21	1:B:343[B]:GLU:HG3	1.86	0.41
1:B:341:LYS:H	1:B:341:LYS:CD	2.34	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.83	0.40
1:B:435:LEU:HD23	1:B:435:LEU:HA	1.79	0.40
1:A:43:GLY:H	2:A:501:TLA:H2	1.85	0.40
1:B:82:LYS:NZ	4:B:637:HOH:O	2.54	0.40
1:B:271:LYS:O	1:B:275:GLN:HG3	2.21	0.40

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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:A:162:ASP:OD2	1:B:336:LYS:NZ[3_454]	2.15	0.05

### 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	Percer	ntiles
1	А	445/457 (97%)	435~(98%)	9(2%)	1 (0%)	47	49
1	В	450/457~(98%)	441 (98%)	8 (2%)	1 (0%)	47	49
All	All	895/914~(98%)	876 (98%)	17 (2%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	329	ILE
1	В	237	THR

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	alysed Rotameric Outliers		Percentiles	
1	А	396/411~(96%)	385~(97%)	11 (3%)	43 47	
1	В	396/411~(96%)	384 (97%)	12 (3%)	41 44	
All	All	792/822~(96%)	769~(97%)	23~(3%)	42 46	

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	7	SER
1	А	107	ASP
1	А	181	ASP
1	А	223	LYS
1	А	239	ASP
1	А	298	VAL
1	А	320	VAL
1	А	341	LYS
1	А	373	LYS
1	А	381	SER
1	А	424	ASP
1	В	21	LYS
1	В	47	THR
1	В	105	LYS



Mol	Chain	Res	
1	D	110	
1	В	112	ASP
1	В	128	ASN
1	В	176	LEU
1	В	177	LEU
1	В	179	VAL
1	В	221	ASP
1	В	237	THR
1	В	239	ASP
1	В	435	LEU

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

Mol	Chain	Res	Type
1	В	100	HIS
1	В	128	ASN
1	В	230	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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 Turo	Chain Boy	Dog	Bos	Dog	Dec	Dec	Dec	Dec	Dec	Bos	Bos	Dog	Dec	Dec	Dec	Deg Link	Bond lengths			Bond angles		
INIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2												
2	TLA	А	501	-	9,9,9	1.33	0	12,12,12	1.43	2 (16%)												
2	TLA	В	501	-	9,9,9	1.30	0	12,12,12	1.45	2 (16%)												

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	TLA	А	501	-	-	4/12/12/12	-
2	TLA	В	501	-	-	12/12/12/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$\mathbf{Ideal}(^{o})$
2	А	501	TLA	O4-C4-C3	-2.66	114.65	121.63
2	В	501	TLA	O1-C1-C2	-2.57	114.87	121.63
2	А	501	TLA	O1-C1-C2	-2.52	115.02	121.63
2	В	501	TLA	O4-C4-C3	-2.44	115.22	121.63

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	501	TLA	C1-C2-C3-C4
2	А	501	TLA	O2-C2-C3-O3
2	В	501	TLA	C1-C2-C3-O3
2	В	501	TLA	C1-C2-C3-C4
2	В	501	TLA	O2-C2-C3-O3
2	В	501	TLA	O2-C2-C3-C4
2	А	501	TLA	C1-C2-C3-O3
2	А	501	TLA	O2-C2-C3-C4
2	В	501	TLA	O1-C1-C2-O2
2	В	501	TLA	O11-C1-C2-O2
2	В	501	TLA	O3-C3-C4-O4
2	В	501	TLA	O3-C3-C4-O41
2	В	501	TLA	C2-C3-C4-O4
2	В	501	TLA	C2-C3-C4-O41
2	В	501	TLA	O1-C1-C2-C3



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Mol	Chain	Res	Type	Atoms
2	В	501	TLA	O11-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	501	TLA	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 (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	447/457~(97%)	0.36	36 (8%) 12 15	25, 44, 87, 142	0
1	В	451/457~(98%)	0.33	30 (6%) 17 22	27, 45, 81, 123	0
All	All	898/914 (98%)	0.34	66 (7%) 15 19	25, 45, 83, 142	0

All (66) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	В	179	VAL	8.6
1	А	120	THR	7.8
1	В	237	THR	7.5
1	В	180	ASP	7.5
1	А	130	PHE	7.4
1	А	111	ALA	7.1
1	А	110	PHE	6.2
1	В	130	PHE	6.2
1	А	239	ASP	6.2
1	А	237	THR	5.6
1	А	240	THR	5.6
1	А	179	VAL	5.5
1	В	177	LEU	5.5
1	А	133	CYS	5.4
1	В	236	ILE	5.3
1	А	345	GLY	5.3
1	А	119	VAL	5.2
1	А	236	ILE	4.9
1	В	240	THR	4.6
1	А	180	ASP	4.6
1	A	109	GLY	4.2
1	A	132	GLU	4.1
1	В	10	GLU	4.1
1	A	241	GLU	4.0



Mol	Chain	Res	Type	RSRZ
1	В	11	GLU	4.0
1	А	183	ASP	3.8
1	В	260	PHE	3.8
1	А	206	ASP	3.8
1	А	260	PHE	3.8
1	В	250	VAL	3.8
1	А	205	GLU	3.7
1	В	133	CYS	3.7
1	А	330	ASP	3.4
1	В	118	ASN	3.3
1	В	132	GLU	3.3
1	В	346	GLU	3.2
1	А	121	THR	3.1
1	A	346	GLU	2.9
1	В	417	TYR	2.8
1	А	247	LYS	2.8
1	В	345	GLY	2.8
1	В	112	ASP	2.8
1	А	4	ASP	2.8
1	А	122	LYS	2.8
1	А	178	PRO	2.7
1	В	183	ASP	2.7
1	В	4	ASP	2.7
1	В	343[A]	GLU	2.6
1	А	190	ASP	2.6
1	В	238	GLU	2.6
1	А	177	LEU	2.6
1	В	117	ASP	2.6
1	В	376	LYS	2.5
1	В	139	VAL	2.4
1	B	113	ASP	2.4
1	A	6	SER	2.4
1	В	181	ASP	2.3
1	В	206	ASP	2.3
1	В	241	GLU	2.3
1	A	222	GLN	2.3
1	А	390	LEU	2.2
1	А	238	GLU	2.2
1	A	297	LEU	2.1
1	В	239	ASP	2.1
1	A	139	VAL	2.1
1	А	221	ASP	2.0

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### 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	$B-factors(Å^2)$	Q < 0.9
2	TLA	В	501	10/10	0.84	0.22	$65,\!75,\!83,\!101$	0
2	TLA	А	501	10/10	0.89	0.23	58,73,82,89	0
3	MG	В	502	1/1	0.99	0.13	25,25,25,25	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.

