

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

Nov 15, 2022 – 12:57 pm GMT

PDB ID	:	7QA0
Title	:	Crystal structure of PqsR (MvfR) ligand-binding domain in complex with
		compound 1456
Authors	:	Schmelz, S.; Blankenfeldt, W.
Deposited on	:	2021-11-15
Resolution	:	2.67  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
NIGH TODATY	•	
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

# 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 2.67 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 <sub>free</sub>	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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				
			21%				
1	А	332	38%	23%	•	38%	
			19%				
1	В	332	36%	21%	•	40%	



#### 7QA0

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6159 atoms, of which 3014 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 Multiple virulence factor regulator MvfR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	Δ	206	Total	С	Н	Ν	0	$\mathbf{S}$	13	1	Ο
	11	200	3112	1003	1533	268	302	6	10	I	U
1	Р	100	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	0
	D	199	2948	962	1445	243	292	6	0	0	0

• Molecule 2 is {N}-[[2-(3-chloranyl-4-propan-2-yloxy-phenyl)-1,3-thiazol-5-yl]methyl]-2-(trifl uoromethyl)pyridin-4-amine (three-letter code: 9ZL) (formula:  $C_{19}H_{17}ClF_3N_3OS$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf				
0	Λ	1	Total	С	Cl	F	Η	Ν	Ο	S	0	0
	A		46	19	1	3	18	3	1	1	0	0
0	В	1	Total	С	Cl	F	Η	Ν	Ο	S	0	0
	D	1	46	19	1	3	18	3	1	1		0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	5	Total O 5 5	0	0
3	В	2	Total O 2 2	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: Multiple virulence factor regulator MvfR



#### 



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	109.13Å 119.82Å 114.03Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution(A)	54.57 - 2.67	Depositor
Resolution (A)	80.68 - 2.67	EDS
% Data completeness	50.8 (54.57-2.67)	Depositor
(in resolution range)	47.8 (80.68-2.67)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.07 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
P. P.	0.236 , $0.281$	Depositor
$\mathbf{n},  \mathbf{n}_{free}$	0.237 , $0.280$	DCC
$R_{free}$ test set	497 reflections $(4.54\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	62.6	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$   <  L  > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	6159	wwPDB-VP
Average B, all atoms $(Å^2)$	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.44% 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:  $9\mathrm{ZL}$ 

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.36	0/1612	0.64	0/2196	
1	В	0.43	0/1531	0.63	1/2090~(0.0%)	
All	All	0.40	0/3143	0.63	1/4286~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	285	LEU	CB-CG-CD2	-5.99	100.82	111.00

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	А	1579	1533	1533	60	0
1	В	1503	1445	1445	80	0
2	А	28	18	0	1	0
2	В	28	18	0	0	0
3	А	5	0	0	1	0
3	В	2	0	0	1	0
All	All	3145	3014	2978	135	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 22.

All (135) 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:159:ASN:OD1	1:B:185:SER:OG	1.77	1.02
1:B:178:LEU:HD13	1:B:189:LEU:HD23	1.50	0.91
1:A:108:CYS:SG	1:A:126:ARG:NH1	2.46	0.88
1:B:111:VAL:O	1:B:115:LEU:HD12	1.80	0.81
1:A:288:ALA:O	1:A:292:LEU:HD12	1.80	0.80
1:B:107:PHE:CE1	1:B:292:LEU:HD11	2.22	0.74
1:B:107:PHE:HE1	1:B:292:LEU:HD11	1.53	0.74
1:A:288:ALA:C	1:A:292:LEU:HD12	2.13	0.69
1:B:124:LEU:C	1:B:125:ILE:HD13	2.14	0.68
1:B:176:HIS:NE2	1:B:178:LEU:HD12	2.08	0.68
1:A:155:ILE:CG2	1:A:158:PHE:HB2	2.24	0.67
1:A:266:LYS:NZ	1:B:259:GLU:OE2	2.24	0.67
1:A:246:LEU:HD23	1:A:251:LEU:C	2.15	0.67
1:B:137:LYS:HE3	1:B:155:ILE:HD12	1.77	0.66
1:A:100:ASP:HA	1:A:127:THR:O	1.96	0.66
1:A:278:GLU:O	1:A:282:LEU:HD12	1.99	0.62
1:B:224:MET:O	1:B:228:VAL:HG23	2.00	0.62
1:A:155:ILE:HG22	1:A:158:PHE:HB2	1.81	0.61
1:B:105:PRO:O	1:B:109:ASP:OD2	2.18	0.61
1:A:224:MET:O	1:A:228:VAL:HG23	1.99	0.61
1:B:107:PHE:CE2	1:B:111:VAL:HG11	2.35	0.61
1:B:228:VAL:HG13	1:B:233:GLY:O	2.01	0.61
1:A:128:SER:HB2	1:A:197:LEU:HD21	1.83	0.60
1:B:227:LEU:O	1:B:232:VAL:HG23	2.00	0.60
1:A:98:LEU:HD11	1:A:127:THR:HG23	1.82	0.60
1:B:167:LYS:NZ	3:B:501:HOH:O	2.31	0.59
1:B:94:ASN:HB3	1:B:121:MET:HB3	1.83	0.59
1:B:167:LYS:HE2	1:B:261:GLY:O	2.02	0.59
1:A:178:LEU:HD11	1:A:192:TYR:CG	2.38	0.58
1:A:221:PHE:O	1:A:225:LEU:HD23	2.03	0.58
1:B:167:LYS:HE2	1:B:261:GLY:C	2.24	0.58
1:B:106:SER:HA	1:B:109:ASP:OD2	2.04	0.58
1:B:281:PHE:CE1	1:B:285:LEU:HD21	2.39	0.57
1:B:98:LEU:C	1:B:99:LEU:HD12	2.24	0.57
1:B:111:VAL:C	1:B:115:LEU:HD12	2.24	0.57
1:B:112:SER:HA	1:B:115:LEU:HD13	1.88	0.55
1:B:288:ALA:O	1:B:292:LEU:HD12	2.07	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:115:LEU:O	1:B:119:PHE:CD2	2.60	0.55
1:B:152:GLU:HB3	1:B:155:ILE:HD11	1.89	0.55
1:A:207:LEU:HB3	1:A:208:LEU:HD12	1.88	0.55
1:A:225:LEU:HD11	1:A:242[B]:VAL:HG12	1.89	0.55
1:B:241:PHE:O	1:B:245:ARG:NH2	2.40	0.54
1:A:259:GLU:OE1	1:B:266:LYS:HE2	2.07	0.54
1:A:133:LEU:HD21	1:A:270:TYR:CE1	2.42	0.54
1:A:246:LEU:HD13	1:A:253:VAL:HG13	1.89	0.53
1:A:129:PRO:HB2	1:A:208:LEU:HD21	1.90	0.53
1:B:184:HIS:CD2	1:B:254:LEU:O	2.62	0.53
1:B:281:PHE:HE1	1:B:285:LEU:HD21	1.73	0.53
1:B:103:ILE:CD1	1:B:147:ILE:HG22	2.38	0.53
1:A:151:GLU:HB3	1:A:268:TYR:CE2	2.44	0.52
1:B:148:THR:OG1	1:B:149:ILE:N	2.43	0.52
1:A:263:ILE:HG21	2:A:401:9ZL:S16	2.50	0.52
1:B:284:PHE:C	1:B:284:PHE:CD1	2.83	0.51
1:A:176:HIS:CD2	1:A:178:LEU:HD12	2.44	0.51
1:B:100:ASP:OD1	1:B:102:ALA:N	2.41	0.51
1:B:111:VAL:O	1:B:114:VAL:CG2	2.59	0.51
1:A:271:TYR:HB3	1:A:281:PHE:CZ	2.46	0.50
1:A:178:LEU:HD11	1:A:192:TYR:CD2	2.46	0.50
1:A:215:VAL:HG12	1:A:216:LEU:N	2.26	0.50
1:B:162:VAL:HG11	1:B:266:LYS:HD3	1.92	0.50
1:A:209:ARG:HG3	1:A:209:ARG:HH11	1.76	0.50
1:A:176:HIS:CD2	1:A:177:PRO:HD2	2.47	0.49
1:A:169:PHE:HE2	1:A:239:HIS:ND1	2.11	0.49
1:B:111:VAL:O	1:B:114:VAL:HG22	2.13	0.49
1:A:148:THR:OG1	1:A:149:ILE:N	2.45	0.49
1:B:271:TYR:CG	1:B:281:PHE:HE2	2.31	0.48
1:B:124:LEU:O	1:B:125:ILE:HD13	2.12	0.48
1:B:197:LEU:HD11	1:B:221:PHE:CE2	2.48	0.48
1:A:105:PRO:HD3	1:A:240:TYR:CD2	2.48	0.48
1:B:208:LEU:HD22	1:B:208:LEU:N	2.27	0.48
1:A:159:ASN:HD22	1:A:273:THR:HG22	1.77	0.48
1:B:103:ILE:HD12	1:B:147:ILE:HG22	1.94	0.48
1:B:271:TYR:CB	1:B:281:PHE:CE2	2.97	0.48
1:B:115:LEU:O	1:B:119:PHE:HD2	1.97	0.48
1:A:133:LEU:O	1:A:137:LYS:HG3	2.14	0.48
1:B:159:ASN:HB2	1:B:271:TYR:CE1	2.49	0.47
1:B:238:PRO:O	1:B:242:VAL:HG22	2.14	0.47
1:A:160:GLN:OE1	1:A:270:TYR:HE2	1.98	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:163:LEU:CD1	1:B:269:CYS:HB3	2.44	0.47
1:B:163:LEU:CD1	1:B:269:CYS:CB	2.93	0.47
1:B:271:TYR:CB	1:B:281:PHE:HE2	2.27	0.47
1:B:291:ARG:O	1:B:295:LEU:HD13	2.15	0.47
1:A:178:LEU:HD12	1:A:178:LEU:H	1.80	0.46
1:B:245:ARG:HG3	1:B:245:ARG:NH1	2.29	0.46
1:A:100:ASP:OD1	1:A:102:ALA:N	2.48	0.46
1:A:97:VAL:HG21	1:A:115:LEU:HD13	1.97	0.46
1:A:95:LEU:HD21	1:A:145:ILE:HD12	1.98	0.46
1:A:243:GLU:HG3	1:A:244:GLU:N	2.31	0.46
1:B:99:LEU:HD12	1:B:99:LEU:N	2.31	0.46
1:A:178:LEU:HD22	1:A:189:LEU:HD23	1.98	0.45
1:B:167:LYS:HE3	1:B:262:GLY:C	2.37	0.45
1:A:107:PHE:CZ	1:A:292:LEU:CD2	3.00	0.45
1:B:163:LEU:HD11	1:B:269:CYS:CB	2.46	0.45
1:A:215:VAL:CG1	1:A:216:LEU:N	2.79	0.45
1:B:115:LEU:HD12	1:B:115:LEU:H	1.81	0.45
1:A:100:ASP:OD1	1:A:100:ASP:C	2.55	0.45
1:B:100:ASP:OD1	1:B:100:ASP:C	2.55	0.44
1:B:111:VAL:HG23	1:B:112:SER:N	2.33	0.44
1:A:107:PHE:CZ	1:A:267:VAL:HG11	2.53	0.44
1:A:190:ALA:HA	1:A:212:SER:HB2	2.00	0.44
1:A:195:ILE:HD12	1:A:227:LEU:HD23	2.00	0.44
1:B:107:PHE:CZ	1:B:111:VAL:HG11	2.51	0.44
1:A:101:THR:O	1:A:240:TYR:OH	2.17	0.44
1:B:111:VAL:O	1:B:112:SER:C	2.56	0.44
1:B:107:PHE:C	1:B:107:PHE:CD2	2.91	0.44
1:B:163:LEU:HD11	1:B:269:CYS:HB3	1.99	0.44
1:B:176:HIS:ND1	1:B:177:PRO:HD2	2.33	0.43
1:B:111:VAL:C	1:B:115:LEU:CD1	2.85	0.43
1:B:133:LEU:HD13	1:B:152:GLU:HB2	2.00	0.43
1:A:98:LEU:HD11	1:A:127:THR:CG2	2.48	0.43
1:B:195:ILE:N	1:B:195:ILE:HD13	2.32	0.43
1:B:195:ILE:HD12	1:B:216:LEU:HD23	1.99	0.43
1:B:218:VAL:HG21	1:B:224:MET:HB2	2.01	0.43
1:A:256:GLU:O	1:A:260:PRO:HG3	2.19	0.43
1:A:97:VAL:HA	1:A:145:ILE:O	2.18	0.43
1:A:162:VAL:HB	1:B:259:GLU:HG2	2.01	0.43
1:A:101:THR:HG21	3:A:503:HOH:O	2.19	0.42
1:A:155:ILE:HG21	1:A:158:PHE:HB2	1.99	0.42
1:A:200:ARG:N	1:A:217:PHE:CE2	2.88	0.42



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:225:LEU:HD11	1:A:242[B]:VAL:CG1	2.49	0.42
1:B:178:LEU:HD11	1:B:192:TYR:CG	2.55	0.42
1:B:271:TYR:CG	1:B:281:PHE:CE2	3.08	0.42
1:A:243:GLU:CG	1:A:244:GLU:N	2.82	0.42
1:A:132:SER:OG	1:A:133:LEU:N	2.53	0.41
1:B:111:VAL:HA	1:B:114:VAL:CG2	2.50	0.41
1:B:220:ASN:ND2	1:B:223:ASP:OD2	2.53	0.41
1:B:132:SER:OG	1:B:133:LEU:N	2.54	0.41
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.84	0.41
1:B:193:ARG:HA	1:B:214:LYS:O	2.20	0.41
1:A:165:TYR:OH	1:B:264:ASP:HB2	2.21	0.41
1:A:289:ARG:O	1:A:293:ARG:HG3	2.21	0.41
1:B:111:VAL:CG2	1:B:112:SER:N	2.84	0.41
1:B:221:PHE:CE2	1:B:238:PRO:HD3	2.57	0.40
1:B:111:VAL:HA	1:B:114:VAL:HG22	2.03	0.40
1:B:122:VAL:HG12	1:B:124:LEU:CD1	2.52	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	Perce	ntiles
1	А	205/332~(62%)	200~(98%)	5(2%)	0	100	100
1	В	195/332~(59%)	191 (98%)	4 (2%)	0	100	100
All	All	400/664~(60%)	391 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.



#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	170/288~(59%)	160 (94%)	10 (6%)	19 40		
1	В	161/288~(56%)	146 (91%)	15 (9%)	9 19		
All	All	331/576~(58%)	306~(92%)	25~(8%)	13 28		

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	112	SER
1	А	139	ASP
1	А	140	ASN
1	А	179	CYS
1	А	182	SER
1	А	189	LEU
1	А	207	LEU
1	А	241	PHE
1	А	244	GLU
1	А	273	THR
1	В	106	SER
1	В	109	ASP
1	В	144	ASP
1	В	160	GLN
1	В	161	CYS
1	В	184	HIS
1	В	197	LEU
1	В	209	ARG
1	В	212	SER
1	В	222	ASP
1	В	241	PHE
1	В	264	ASP
1	В	280	SER
1	В	281	PHE
1	В	284	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such



sidechains are listed below:

Mol	Chain	Res	Type
1	А	176	HIS

#### 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)

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	Chain	ain Res	Dec	Timle	Bo	ond leng	$_{\rm ths}$	E	Bond ang	gles
	Chain		LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
2	9ZL	А	401	-	29,30,30	1.34	4 (13%)	32,43,43	2.16	11 (34%)
2	9ZL	В	401	-	29,30,30	1.40	6 (20%)	32,43,43	1.97	7 (21%)

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	9ZL	А	401	-	-	8/17/19/19	0/3/3/3
2	9ZL	В	401	-	-	12/17/19/19	0/3/3/3



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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	В	401	9ZL	C15-S16	-3.28	1.69	1.73
2	А	401	9ZL	C15-S16	-3.22	1.69	1.73
2	А	401	9ZL	C04-N11	2.99	1.47	1.38
2	В	401	9ZL	C04-N11	2.64	1.46	1.38
2	В	401	9ZL	C15-N14	2.50	1.35	1.31
2	А	401	9ZL	C22-CL1	2.20	1.78	1.73
2	А	401	9ZL	O25-C21	2.15	1.41	1.37
2	В	401	9ZL	C22-CL1	2.15	1.78	1.73
2	В	401	9ZL	O25-C21	2.10	1.41	1.37
2	В	401	9ZL	C12-S16	-2.05	1.69	1.73

All (10) bond length outliers are listed below:

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	401	9ZL	C13-C12-S16	-6.89	105.15	112.00
2	В	401	9ZL	C13-C12-S16	-6.26	105.78	112.00
2	В	401	9ZL	O25-C21-C22	4.36	119.97	116.13
2	А	401	9ZL	O25-C21-C22	3.99	119.64	116.13
2	В	401	9ZL	C07-C06-N01	3.92	119.32	114.61
2	В	401	9ZL	C02-N01-C06	3.51	122.30	117.49
2	А	401	9ZL	C21-C22-CL1	3.19	123.17	119.43
2	А	401	9ZL	C02-N01-C06	3.05	121.67	117.49
2	А	401	9ZL	C07-C06-N01	3.03	118.25	114.61
2	А	401	9ZL	F08-C07-C06	-2.88	107.55	112.47
2	А	401	9ZL	C03-C04-C05	-2.66	116.50	119.65
2	А	401	9ZL	C03-C02-N01	-2.46	120.90	123.96
2	В	401	9ZL	C03-C02-N01	-2.40	120.97	123.96
2	А	401	9ZL	C21-O25-C26	-2.39	114.93	119.53
2	В	401	9ZL	C05-C06-N01	-2.26	119.64	123.31
2	А	401	9ZL	F10-C07-C06	-2.15	108.79	112.47
2	A	401	9ZL	C19-C18-C23	2.07	121.09	118.16
2	В	401	9ZL	F09-C07-C06	-2.04	108.98	112.47

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	401	9ZL	N14-C15-C18-C19
2	В	401	9ZL	N14-C15-C18-C23
2	В	401	9ZL	C03-C04-N11-C17
2	В	401	9ZL	C05-C04-N11-C17



Mol	Chain	Res	Type	Atoms
2	А	401	9ZL	N01-C06-C07-F10
2	А	401	9ZL	C22-C21-O25-C26
2	А	401	9ZL	C05-C06-C07-F10
2	А	401	9ZL	N01-C06-C07-F09
2	В	401	9ZL	S16-C15-C18-C19
2	В	401	9ZL	S16-C15-C18-C23
2	В	401	9ZL	N01-C06-C07-F08
2	А	401	9ZL	N01-C06-C07-F08
2	В	401	9ZL	N01-C06-C07-F10
2	А	401	9ZL	C05-C06-C07-F09
2	В	401	9ZL	N01-C06-C07-F09
2	А	401	9ZL	C05-C06-C07-F08
2	В	401	9ZL	C05-C06-C07-F08
2	В	401	9ZL	C05-C06-C07-F10
2	В	401	9ZL	C05-C06-C07-F09
2	А	401	9ZL	C20-C21-O25-C26

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There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	401	9ZL	1	0

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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. 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		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	206/332~(62%)	1.61	70 (33%) 0	0	22, 55, 88, 109	0
1	В	199/332~(59%)	1.79	63 (31%) 0	0	24, 66, 109, 134	0
All	All	405/664~(60%)	1.70	133 (32%) 0	0	22, 60, 103, 134	0

All (133) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	В	183	LEU	12.8
1	В	178	LEU	11.7
1	В	184	HIS	10.0
1	В	188	SER	7.9
1	В	251	LEU	7.5
1	В	189	LEU	7.0
1	А	216	LEU	6.7
1	В	122	VAL	6.1
1	А	207	LEU	5.9
1	В	192	TYR	5.9
1	А	211	VAL	5.9
1	А	184	HIS	5.8
1	А	182	SER	5.6
1	В	136	ILE	5.5
1	А	251	LEU	5.4
1	А	183	LEU	5.4
1	В	116	LEU	5.4
1	А	270	TYR	5.1
1	В	186	ILE	5.1
1	В	182	SER	5.0
1	В	120	ASN	5.0
1	А	199	SER	4.9
1	A	171	VAL	4.8
1	В	124	LEU	4.6



Mol	Chain	Res	Type	RSRZ
1	А	93	ARG	4.5
1	В	252	ALA	4.4
1	В	295	LEU	4.4
1	А	186	ILE	4.4
1	В	107	PHE	4.3
1	В	216	LEU	4.2
1	А	282	LEU	4.2
1	В	153	LEU	4.0
1	В	241	PHE	4.0
1	В	155	ILE	4.0
1	А	208	LEU	4.0
1	А	236	ILE	3.9
1	А	254	LEU	3.9
1	A	145	ILE	3.9
1	А	201	SER	3.8
1	А	95	LEU	3.8
1	А	275	LEU	3.7
1	В	95	LEU	3.7
1	А	163	LEU	3.7
1	А	226	ARG	3.7
1	В	292	LEU	3.6
1	A	215	VAL	3.6
1	В	211	VAL	3.5
1	В	239	HIS	3.4
1	A	189	LEU	3.4
1	A	267	VAL	3.4
1	В	254	LEU	3.4
1	A	228	VAL	3.4
1	A	195	ILE	3.4
1	A	281	PHE	3.4
1	A	218	VAL	3.3
1	B	281	PHE	3.2
1	B	296	GLY	3.2
1	B	225	LEU	3.2
1	B	284	PHE	3.2
1	A	146	ALA	3.2
1	A	124	LEU	3.2
1	B	207	LEU	3.1
1	A	166	THR	3.1
1	B	99	LEU	3.1
1	A	225	LEU	3.0
1	B	270	TYR	3.0



Mol	Chain	Res	Type	RSRZ
1	В	240	TYR	3.0
1	А	257	LEU	3.0
1	В	265	THR	3.0
1	А	111	VAL	3.0
1	А	135	THR	2.9
1	А	227	LEU	2.9
1	В	250	THR	2.9
1	В	181	ALA	2.9
1	В	245	ARG	2.9
1	В	158	PHE	2.9
1	А	246	LEU	2.9
1	В	217	PHE	2.8
1	А	119	PHE	2.8
1	А	284	PHE	2.8
1	В	246	LEU	2.8
1	В	185	SER	2.7
1	А	295	LEU	2.7
1	А	271	TYR	2.7
1	А	204	HIS	2.7
1	В	257	LEU	2.7
1	А	122	VAL	2.7
1	А	285	LEU	2.7
1	В	119	PHE	2.7
1	В	149	ILE	2.6
1	В	133	LEU	2.6
1	В	137	LYS	2.6
1	В	103	ILE	2.6
1	В	145	ILE	2.5
1	А	169	PHE	2.5
1	А	292	LEU	2.5
1	В	193	ARG	2.5
1	В	208	LEU	2.5
1	A	241	PHE	2.5
1	А	147	ILE	2.4
1	В	176	HIS	2.4
1	A	99	LEU	2.4
1	A	136	ILE	2.4
1	A	165	TYR	2.4
1	A	153	LEU	2.3
1	В	159	ASN	2.3
1	A	107	PHE	2.3
1	А	221	PHE	2.3



Mol	Chain	Res	Type	RSRZ
1	В	195	ILE	2.3
1	А	98	LEU	2.3
1	А	112	SER	2.3
1	А	232	VAL	2.3
1	А	239	HIS	2.3
1	А	137	LYS	2.3
1	А	158	PHE	2.3
1	А	115	LEU	2.2
1	А	185	SER	2.2
1	В	93	ARG	2.2
1	В	232	VAL	2.2
1	В	143	ILE	2.2
1	А	197	LEU	2.2
1	А	242[A]	VAL	2.2
1	В	271	TYR	2.1
1	В	275	LEU	2.1
1	В	243	GLU	2.1
1	А	252	ALA	2.1
1	А	155	ILE	2.1
1	В	234	TRP	2.1
1	В	163	LEU	2.1
1	А	253	VAL	2.0
1	А	268	TYR	2.0
1	А	131	ASP	2.0
1	В	253	VAL	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	9ZL	А	401	28/28	0.90	0.54	$26,\!69,\!97,\!107$	0
2	9ZL	В	401	28/28	0.92	0.46	35,62,96,120	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.

