

Full wwPDB X-ray Structure Validation Report (i)

Dec 20, 2021 – 03:17 pm GMT

PDB ID	:	70UM
Title	:	BDM88855 inhibitor bound to the transmembrane domain of AcrB-R971A
Authors	:	Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on	:	2021-06-12
Resolution	:	2.45 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 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 as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
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)	:	2.24

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 2.45 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.



Motric	Whole archive	Similar resolution
IVIEUTIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	
			9%	
1	А	1057	94%	
			5%	
1	В	1057	94%	• •
			3%	
1	С	1057	93%	• •
			9%	
2	D	169	92%	8%
			24%	
2	Ε	169	91%	9%



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
3	LMT	В	1107	-	-	-	Х
9	EDO	С	1114	-	-	-	Х



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2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 27129 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1 A	1024	Total	С	Ν	Ο	\mathbf{S}	0	2	0
	A	1054	7881	5071	1302	1464	44	0		U
1	1 B	1034	Total	С	Ν	Ο	S	0	2	0
			7866	5061	1298	1463	44			
1	1 0	1099	Total	С	Ν	Ο	S	0	1	0
	1099	7852	5054	1294	1460	44	0	L	0	

• Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Chain	Residue	Modelled	Actual Comment		Reference
A	971	ALA	ARG	engineered mutation	UNP P31224
А	1050	LEU	-	expression tag	UNP P31224
А	1051	GLU	-	expression tag	UNP P31224
А	1052	HIS	-	expression tag	UNP P31224
А	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
А	1056	HIS	-	expression tag	UNP P31224
А	1057	HIS	-	expression tag	UNP P31224
В	971	ALA	ARG	engineered mutation	UNP P31224
В	1050	LEU	-	expression tag	UNP P31224
В	1051	GLU	-	expression tag	UNP P31224
В	1052	HIS	-	expression tag	UNP P31224
В	1053	HIS	-	expression tag	UNP P31224
В	1054	HIS	-	expression tag	UNP P31224
В	1055	HIS	-	expression tag	UNP P31224
В	1056	HIS	-	expression tag	UNP P31224
В	1057	HIS	-	expression tag	UNP P31224
С	971	ALA	ARG	engineered mutation	UNP P31224
С	1050	LEU	-	expression tag	UNP P31224
С	1051	GLU	-	expression tag	UNP P31224
С	1052	HIS	-	expression tag	UNP P31224
С	1053	HIS	_	expression tag	UNP P31224

There are 27 discrepancies between the modelled and reference sequences:



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Chain	Residue	Modelled	Actual	Comment	Reference					
С	1054	HIS	-	expression tag	UNP P31224					
С	1055	HIS	-	expression tag	UNP P31224					
С	1056	HIS	-	expression tag	UNP P31224					
С	1057	HIS	-	expression tag	UNP P31224					

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• Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	D 155	155	Total	С	N	0	S	0	0	0
			1173	739	205	228	1	_	Ŭ	_
9	F	154	Total	С	Ν	Ο	\mathbf{S}	0	0	0
		104	1167	736	204	226	1	0	0	0

• Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $\rm C_{24}H_{46}O_{11}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C O 35 24 11	0	0
3	А	1	Total C O 35 24 11	0	0
3	А	1	Total C O 35 24 11	0	0
3	В	1	Total C O 35 24 11	0	0
3	В	1	Total C O 35 24 11	0	0



α \cdot \cdot \cdot	C		
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		1	1 0

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total C O 35 24 11	0	0
3	С	1	Total C O 35 24 11	0	0

• Molecule 4 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C 14 14	0	0

• Molecule 5 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total C N O 14 12 1 1	0	0
5	С	1	Total C N O 14 12 1 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 7 is 3-chloranyl-2-piperazin-1-yl-quinoline (three-letter code: 1K8) (formula: $C_{13}H_{14}ClN_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
7	А	1	Total	С	Cl	Ν	0	0
	1	17	13	1	3	0		
7	Р	1	Total	С	Cl	Ν	0	0
	D	L	17	13	1	3	0	0

• Molecule 8 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	Total C 10 10	0	0
8	А	1	Total C 10 10	0	0
8	В	1	Total C 10 10	0	0
8	С	1	Total C 10 10	0	0

• Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	А	1	TotalCO422	0	0
9	В	1	TotalCO422	0	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	D	1	$\begin{array}{c cc} Total & C & O \\ 4 & 2 & 2 \end{array}$	0	0
9	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
10	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	С	1	Total C 8 8	0	0
11	С	1	Total C 8 8	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	С	1	Total C 8 8	0	0
11	С	1	Total C 8 8	0	0

• Molecule 12 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: $C_{21}H_{44}NO_7P$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
19	С	1	Total	С	Ν	0	Р	0	0
12	U	T	30	21	1	7	1	0	0

• Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	А	220	Total O 220 220	0	0
13	В	180	Total O 180 180	0	0
13	С	239	Total O 239 239	0	0
13	D	24	$\begin{array}{cc} \text{Total} & \text{O} \\ 24 & 24 \end{array}$	0	0
13	Ε	8	Total O 8 8	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: Multidrug efflux pump subunit AcrB











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	146.21Å 161.63Å 244.44Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	49.51 - 2.45	Depositor
Itesolution (A)	49.51 - 2.45	EDS
% Data completeness	$100.0 \ (49.51-2.45)$	Depositor
(in resolution range)	$100.0 \ (49.51-2.45)$	EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.68 (at 2.45 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
P. P.	0.228 , 0.256	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.230 , 0.255	DCC
R_{free} test set	10468 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	43.5	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$ < L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27129	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities 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: C14, GOL, LMT, SO4, DDQ, EDO, LPX, 1K8, D10, OCT

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
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.67	0/8032	0.70	0/10905
1	В	0.67	0/8016	0.70	0/10886
1	С	0.67	0/8002	0.70	0/10868
2	D	0.68	0/1192	0.70	0/1621
2	Е	0.68	0/1186	0.71	0/1613
All	All	0.67	0/26428	0.70	0/35893

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	А	7881	0	8040	15	0
1	В	7866	0	8014	19	0
1	С	7852	0	8000	23	0
2	D	1173	0	1156	0	0
2	Е	1167	0	1151	0	0
3	А	105	0	138	0	0
3	В	105	0	138	0	0
3	С	35	0	46	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	А	14	0	30	0	0
5	А	14	0	27	0	0
5	С	14	0	27	0	0
6	А	6	0	8	0	0
6	В	6	0	8	0	0
6	С	6	0	8	0	0
7	А	17	0	0	0	0
7	В	17	0	0	0	0
8	А	20	0	44	0	0
8	В	10	0	22	0	0
8	С	10	0	22	0	0
9	А	12	0	18	0	0
9	В	28	0	42	0	0
9	С	20	0	30	0	0
9	D	4	0	6	0	0
9	Е	4	0	6	0	0
10	В	5	0	0	0	0
10	С	5	0	0	0	0
11	С	32	0	72	1	0
12	С	30	0	43	0	0
13	А	220	0	0	0	0
13	В	180	0	0	0	0
13	С	239	0	0	0	0
13	D	24	0	0	0	0
13	Е	8	0	0	0	0
All	All	27129	0	27096	51	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 1.

All (51) 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 (\AA)	overlap (Å)
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.83	0.61
1:C:901:VAL:O	1:C:904:VAL:HG12	2.01	0.61
1:A:356:TYR:HA	1:A:365:THR:HG21	1.83	0.61
1:C:151:GLN:NE2	1:C:279:ALA:O	2.35	0.59
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.84	0.59
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.88	0.54
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.89	0.54
1:C:935:ILE:HD11	11:C:1108:OCT:H81	1.91	0.52



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.94	0.49	
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.28	0.48	
1:B:173:GLY:O	1:C:71:GLY:HA3	2.13	0.48	
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.96	0.47	
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.96	0.47	
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.95	0.47	
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.95	0.47	
1:A:108:GLN:NE2	1:B:109:ASN:O	2.48	0.46	
1:B:897:ILE:N	1:B:898:PRO:CD	2.78	0.46	
1:C:330:THR:N	1:C:331:PRO:CD	2.79	0.46	
1:C:115:MET:HB2	1:C:116:PRO:HD3	1.98	0.46	
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.98	0.46	
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.98	0.45	
1:C:336:SER:O	1:C:340:VAL:HG23	2.16	0.45	
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.98	0.45	
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.98	0.45	
1:C:987:MET:HA	1:C:1008:MET:CE	2.47	0.44	
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.52	0.44	
1:C:453:PHE:CE1	1:C:474:ILE:HG21	2.53	0.44	
1:B:330:THR:N	1:B:331:PRO:CD	2.81	0.44	
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.99	0.44	
1:A:330:THR:N	1:A:331:PRO:CD	2.81	0.43	
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.53	0.43	
1:B:314:GLU:HB2	1:B:315:PRO:HD3	2.01	0.43	
1:B:489:THR:N	1:B:490:PRO:CD	2.82	0.43	
1:B:126:GLY:HA3	1:C:116:PRO:HB3	2.01	0.43	
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.19	0.43	
1:A:115:MET:HB2	1:A:116:PRO:HD3	2.01	0.43	
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.48	0.43	
1:A:987:MET:N	1:A:988:PRO:CD	2.82	0.43	
1:A:777:ALA:O	1:A:781:MET:HG2	2.20	0.42	
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.82	0.42	
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.83	0.42	
1:A:897:ILE:N	1:A:898:PRO:CD	2.83	0.41	
1:B:115:MET:N	1:B:116:PRO:CD	2.83	0.41	
1:B:873:ALA:HB3	1:B:874:PRO:HD3	2.02	0.41	
1:B:973:ARG:N	1:B:974:PRO:HD2	2.35	0.41	
1:C:407:ASP:HA	1:C:978:THR:HG22	2.02	0.41	
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.56	0.41	
1:A:110:LYS:NZ	1:C:130:GLU:OE1	2.53	0.40	
1:B:303:ALA:CB	1:B:330:THR:HG21	2.52	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:VAL:HG23	1:C:453:PHE:CD1	2.56	0.40
1:A:684:LEU:O	1:A:824:SER:HA	2.22	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	entiles
1	А	1032/1057~(98%)	997~(97%)	31 (3%)	4 (0%)	34	41
1	В	1034/1057~(98%)	1013 (98%)	21 (2%)	0	100	100
1	С	1032/1057~(98%)	1008 (98%)	24 (2%)	0	100	100
2	D	153/169~(90%)	150 (98%)	3 (2%)	0	100	100
2	Ε	152/169~(90%)	147 (97%)	5(3%)	0	100	100
All	All	3403/3509~(97%)	3315 (97%)	84 (2%)	4 (0%)	51	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	1038	GLU
1	А	1037	ASN
1	А	867	ARG
1	А	538	THR

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



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	844/862~(98%)	837~(99%)	7 (1%)	81	88
1	В	841/862~(98%)	833 (99%)	8 (1%)	76	84
1	С	839/862~(97%)	830 (99%)	9 (1%)	73	82
2	D	120/132~(91%)	120 (100%)	0	100	100
2	Ε	119/132~(90%)	119 (100%)	0	100	100
All	All	2763/2850 (97%)	2739~(99%)	24 (1%)	78	86

analysed, and the total number of residues.

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	11	PHE
1	А	49	TYR
1	А	130	GLU
1	А	407	ASP
1	А	575	MET
1	А	674	LEU
1	А	835	LYS
1	В	11	PHE
1	В	49	TYR
1	В	330	THR
1	В	544	LEU
1	В	610	PHE
1	В	801	PHE
1	В	881	LEU
1	В	1030	ARG
1	С	11	PHE
1	С	49	TYR
1	С	239	ARG
1	С	252	LYS
1	С	546	LEU
1	С	778	LYS
1	С	850	LYS
1	С	919	ARG
1	С	1032	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



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)

43 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).

Mal	Type	Chain	Dog	Link	Bo	ond leng	ths	Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	1K8	А	1106	-	19,19,19	2.66	4 (21%)	24,26,26	1.29	2 (8%)
9	EDO	С	1105	-	3,3,3	0.05	0	2,2,2	0.17	0
9	EDO	В	1104	-	3,3,3	0.06	0	2,2,2	0.16	0
9	EDO	С	1107	-	3,3,3	0.06	0	2,2,2	0.18	0
11	OCT	С	1104	-	7,7,7	0.12	0	6,6,6	0.09	0
9	EDO	С	1114	-	3,3,3	0.06	0	2,2,2	0.16	0
9	EDO	В	1108	-	3,3,3	0.05	0	2,2,2	0.17	0
9	EDO	В	1103	-	3,3,3	0.06	0	2,2,2	0.18	0
11	OCT	C	1109	-	7,7,7	0.12	0	6,6,6	0.05	0
3	LMT	А	1107	-	36,36,36	0.49	1 (2%)	47,47,47	0.67	1 (2%)
3	LMT	С	1101	-	36,36,36	0.42	0	47,47,47	0.47	0
10	SO4	В	1114	-	4,4,4	0.39	0	6,6,6	0.05	0
3	LMT	В	1101	-	36,36,36	0.45	0	47,47,47	0.56	0
8	D10	С	1103	-	9,9,9	0.10	0	8,8,8	0.05	0
6	GOL	С	1111	-	$5,\!5,\!5$	0.10	0	$5,\!5,\!5$	0.30	0
9	EDO	С	1110	-	3,3,3	0.06	0	2,2,2	0.19	0
12	LPX	С	1106	-	29,29,29	0.29	0	31,33,33	0.36	0



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	Bond angles		
	Type	Ullaili	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	D	201	-	3,3,3	0.07	0	2,2,2	0.18	0
5	DDQ	А	1104	-	10,13,13	0.13	0	12,15,15	0.21	0
9	EDO	В	1110	-	3,3,3	0.07	0	2,2,2	0.17	0
9	EDO	А	1109	-	3,3,3	0.07	0	2,2,2	0.17	0
6	GOL	А	1105	-	$5,\!5,\!5$	0.09	0	$5,\!5,\!5$	0.29	0
7	1K8	В	1113	-	19,19,19	2.71	4 (21%)	24,26,26	1.30	3 (12%)
3	LMT	В	1102	-	36,36,36	0.46	0	47,47,47	0.72	0
4	C14	А	1103	-	13,13,13	0.09	0	12,12,12	0.07	0
9	EDO	А	1110	-	3,3,3	0.07	0	2,2,2	0.21	0
3	LMT	А	1101	-	36,36,36	0.47	0	47,47,47	0.62	0
8	D10	А	1108	-	9,9,9	0.10	0	8,8,8	0.07	0
8	D10	А	1111	-	9,9,9	0.10	0	8,8,8	0.06	0
9	EDO	В	1112	-	3,3,3	0.06	0	2,2,2	0.19	0
8	D10	В	1111	-	9,9,9	0.11	0	8,8,8	0.08	0
11	OCT	С	1108	-	7,7,7	0.11	0	$6,\!6,\!6$	0.06	0
11	OCT	С	1112	-	7,7,7	0.11	0	$6,\!6,\!6$	0.07	0
9	EDO	В	1109	-	3, 3, 3	0.07	0	$2,\!2,\!2$	0.16	0
3	LMT	В	1107	-	36,36,36	0.51	1 (2%)	47,47,47	0.78	1 (2%)
9	EDO	В	1106	-	3,3,3	0.06	0	2,2,2	0.24	0
10	SO4	С	1115	-	4,4,4	0.39	0	$6,\!6,\!6$	0.05	0
3	LMT	А	1102	-	36,36,36	0.45	0	47,47,47	0.58	0
9	EDO	Е	201	-	3,3,3	0.06	0	2,2,2	0.18	0
9	EDO	А	1112	-	3,3,3	0.07	0	2,2,2	0.20	0
9	EDO	С	1113	-	3,3,3	0.07	0	2,2,2	0.21	0
5	DDQ	С	1102	-	10,13,13	0.12	0	$12,\!15,\!15$	0.27	0
6	GOL	В	1105	-	$5,\!5,\!5$	0.09	0	$5,\!5,\!5$	0.25	0

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
7	1K8	А	1106	-	-	2/4/12/12	0/3/3/3
9	EDO	С	1105	-	-	0/1/1/1	-
9	EDO	В	1104	-	-	1/1/1/1	-
9	EDO	С	1107	-	-	1/1/1/1	-
11	OCT	С	1104	-	-	2/5/5/5	-
9	EDO	С	1114	-	-	1/1/1/1	-
9	EDO	В	1108	-	-	0/1/1/1	-
9	EDO	B	1103	-	-	1/1/1/1	-
11	OCT	С	1109	-	-	2/5/5/5	-



7	O	U	Μ	I

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	А	1107	-	-	15/21/61/61	0/2/2/2
3	LMT	С	1101	-	-	8/21/61/61	0/2/2/2
3	LMT	В	1101	-	-	6/21/61/61	0/2/2/2
8	D10	С	1103	-	-	1/7/7/7	-
6	GOL	С	1111	-	-	1/4/4/4	-
9	EDO	С	1110	-	-	1/1/1/1	-
12	LPX	С	1106	-	-	16/31/31/31	-
9	EDO	D	201	-	-	0/1/1/1	-
5	DDQ	А	1104	-	-	3/11/11/11	-
9	EDO	В	1110	-	-	1/1/1/1	-
9	EDO	А	1109	-	-	0/1/1/1	-
6	GOL	А	1105	-	-	0/4/4/4	-
7	1K8	В	1113	-	-	2/4/12/12	0/3/3/3
3	LMT	В	1102	-	-	7/21/61/61	0/2/2/2
4	C14	А	1103	-	-	4/11/11/11	-
9	EDO	А	1110	-	-	1/1/1/1	-
3	LMT	А	1101	-	-	8/21/61/61	0/2/2/2
8	D10	А	1108	-	-	1/7/7/7	-
8	D10	А	1111	-	-	5/7/7/7	-
9	EDO	В	1112	-	-	0/1/1/1	-
8	D10	В	1111	-	-	4/7/7/7	-
11	OCT	С	1108	-	-	1/5/5/5	-
11	OCT	С	1112	-	-	4/5/5/5	-
9	EDO	В	1109	-	-	1/1/1/1	-
3	LMT	В	1107	-	-	10/21/61/61	0/2/2/2
9	EDO	В	1106	-	-	1/1/1/1	-
3	LMT	А	1102	-	-	12/21/61/61	0/2/2/2
9	EDO	Е	201	-	-	1/1/1/1	-
9	EDO	А	1112	-	-	1/1/1/1	-
9	EDO	С	1113	-	-	0/1/1/1	-
5	DDQ	С	1102	-	-	5/11/11/11	-
6	GOL	В	1105	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
7	В	1113	1K8	C9-C8	8.73	1.50	1.39
7	А	1106	1K8	C9-C8	8.62	1.50	1.39
7	В	1113	1K8	C11-C12	4.59	1.49	1.42



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
7	А	1106	1K8	C11-C12	4.51	1.49	1.42
7	В	1113	1K8	C8-N13	4.16	1.36	1.31
7	А	1106	1K8	C8-N13	3.93	1.35	1.31
7	А	1106	1K8	C9-CL1	2.71	1.80	1.73
7	В	1113	1K8	C9-CL1	2.63	1.79	1.73
3	А	1107	LMT	O1'-C1'	2.06	1.43	1.40
3	В	1107	LMT	O1'-C1'	2.03	1.43	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
7	А	1106	1K8	C4-N3-C2	3.99	120.31	111.52
7	В	1113	1K8	C4-N3-C2	3.32	118.86	111.52
7	А	1106	1K8	C8-N13-C12	2.71	121.84	116.11
7	В	1113	1K8	C8-N13-C12	2.69	121.80	116.11
3	В	1107	LMT	C1B-O5B-C5B	2.09	117.79	113.69
7	В	1113	1K8	C9-C8-N13	-2.08	119.16	122.70
3	А	1107	LMT	C1'-O5'-C5'	2.07	117.75	113.69

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
3	А	1101	LMT	C2'-C1'-O1'-C1
3	А	1101	LMT	O5'-C1'-O1'-C1
3	А	1102	LMT	C2'-C1'-O1'-C1
3	А	1102	LMT	O5'-C1'-O1'-C1
3	А	1107	LMT	C2'-C1'-O1'-C1
3	А	1107	LMT	O5'-C1'-O1'-C1
3	В	1101	LMT	C2'-C1'-O1'-C1
3	В	1101	LMT	O5'-C1'-O1'-C1
3	В	1101	LMT	C2-C1-O1'-C1'
3	В	1102	LMT	O5B-C1B-O1B-C4'
5	А	1104	DDQ	N1-C1-C2-C3
7	А	1106	1K8	C9-C8-N3-C2
7	А	1106	1K8	N13-C8-N3-C2
7	В	1113	1K8	C9-C8-N3-C2
12	С	1106	LPX	O7-C6-O6-C5
12	С	1106	LPX	C7-C6-O6-C5
3	A	1101	LMT	C5'-C4'-O1B-C1B
3	С	1101	LMT	O5'-C5'-C6'-O6'
3	В	1107	LMT	C2B-C1B-O1B-C4'

All (132) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	В	1107	LMT	O5B-C1B-O1B-C4'
12	С	1106	LPX	O1-C3-C4-O5
3	А	1102	LMT	O5'-C5'-C6'-O6'
3	А	1107	LMT	O5'-C5'-C6'-O6'
3	С	1101	LMT	C4'-C5'-C6'-O6'
7	В	1113	1K8	N13-C8-N3-C2
3	А	1107	LMT	O5B-C5B-C6B-O6B
3	А	1102	LMT	C4'-C5'-C6'-O6'
3	А	1107	LMT	C4B-C5B-C6B-O6B
12	С	1106	LPX	C6-C7-C8-C9
12	С	1106	LPX	C4-C5-O6-C6
3	С	1101	LMT	O1'-C1-C2-C3
12	С	1106	LPX	O5-C4-C5-O6
12	С	1106	LPX	C3-O1-P1-O2
3	В	1107	LMT	O5B-C5B-C6B-O6B
12	С	1106	LPX	C10-C11-C12-C13
12	С	1106	LPX	C3-C4-C5-O6
3	В	1107	LMT	C4-C5-C6-C7
5	А	1104	DDQ	C6-C7-C8-C9
5	С	1102	DDQ	C2-C3-C4-C5
3	А	1107	LMT	C7-C8-C9-C10
6	В	1105	GOL	O1-C1-C2-C3
6	С	1111	GOL	O1-C1-C2-C3
3	В	1102	LMT	C6-C7-C8-C9
3	В	1107	LMT	C5-C6-C7-C8
3	С	1101	LMT	C5-C6-C7-C8
8	В	1111	D10	C6-C7-C8-C9
3	В	1102	LMT	C11-C10-C9-C8
8	В	1111	D10	C2-C3-C4-C5
3	В	1107	LMT	C2-C1-O1'-C1'
3	С	1101	LMT	C2-C1-O1'-C1'
8	А	1111	D10	C2-C3-C4-C5
11	С	1109	OCT	C2-C3-C4-C5
12	С	1106	LPX	C11-C12-C13-C14
3	В	1102	LMT	C3-C4-C5-C6
6	В	1105	GOL	01-C1-C2-O2
8	А	1111	D10	C3-C4-C5-C6
5	A	1104	DDQ	C3-C4-C5-C6
3	А	1107	LMT	C4'-C5'-C6'-O6'
3	A	1101	LMT	C3-C4-C5-C6
5	С	1102	DDQ	C3-C4-C5-C6
9	А	1110	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	В	1109	EDO	O1-C1-C2-O2
9	Е	201	EDO	O1-C1-C2-O2
3	С	1101	LMT	C1-C2-C3-C4
3	А	1107	LMT	C3-C4-C5-C6
3	А	1102	LMT	C11-C10-C9-C8
3	А	1102	LMT	C4-C5-C6-C7
4	А	1103	C14	C09-C10-C11-C12
3	В	1102	LMT	C5'-C4'-O1B-C1B
3	В	1101	LMT	O5'-C5'-C6'-O6'
12	С	1106	LPX	O1-C3-C4-C5
3	В	1102	LMT	O5B-C5B-C6B-O6B
3	В	1107	LMT	O1'-C1-C2-C3
4	А	1103	C14	C06-C07-C08-C09
3	А	1102	LMT	C9-C10-C11-C12
3	В	1102	LMT	C3'-C4'-O1B-C1B
9	В	1104	EDO	O1-C1-C2-O2
3	А	1101	LMT	C9-C10-C11-C12
3	А	1102	LMT	O1'-C1-C2-C3
11	С	1104	OCT	C5-C6-C7-C8
5	С	1102	DDQ	N1-C1-C2-C3
8	А	1111	D10	C5-C6-C7-C8
11	С	1112	OCT	C2-C3-C4-C5
3	А	1102	LMT	C2-C1-O1'-C1'
3	А	1107	LMT	C2-C1-O1'-C1'
8	В	1111	D10	C7-C8-C9-C10
11	С	1112	OCT	C1-C2-C3-C4
3	А	1102	LMT	C3-C4-C5-C6
3	В	1107	LMT	C11-C10-C9-C8
11	С	1109	OCT	C4-C5-C6-C7
3	С	1101	LMT	C9-C10-C11-C12
3	А	1102	LMT	C4B-C5B-C6B-O6B
3	А	1107	LMT	C2-C3-C4-C5
11	C	1112	OCT	C4-C5-C6-C7
12	С	1106	LPX	C16-C17-C18-C19
3	A	1107	LMT	C5-C6-C7-C8
8	С	1103	D10	C6-C7-C8-C9
11	С	1104	OCT	C2-C3-C4-C5
3	A	1107	LMT	O1'-C1-C2-C3
12	С	1106	LPX	C1-O2-P1-O1
12	С	1106	LPX	C4-C3-O1-P1
12	С	1106	LPX	C3-O1-P1-O3
9	С	1107	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	А	1107	LMT	C6-C7-C8-C9
8	А	1111	D10	C1-C2-C3-C4
3	В	1107	LMT	C3-C4-C5-C6
4	А	1103	C14	C10-C11-C12-C13
8	В	1111	D10	C3-C4-C5-C6
3	В	1107	LMT	C1-C2-C3-C4
3	В	1101	LMT	O1'-C1-C2-C3
11	С	1108	OCT	C4-C5-C6-C7
9	С	1110	EDO	O1-C1-C2-O2
9	С	1114	EDO	O1-C1-C2-O2
12	С	1106	LPX	C14-C15-C16-C17
4	А	1103	C14	C01-C02-C03-C04
8	А	1111	D10	C6-C7-C8-C9
3	А	1101	LMT	C2-C3-C4-C5
3	А	1102	LMT	C2-C3-C4-C5
3	В	1101	LMT	C7-C8-C9-C10
11	С	1112	OCT	C3-C4-C5-C6
8	А	1108	D10	C7-C8-C9-C10
5	С	1102	DDQ	C7-C8-C9-C10
3	А	1107	LMT	C9-C10-C11-C12
3	А	1101	LMT	O1'-C1-C2-C3
3	А	1101	LMT	C3'-C4'-O1B-C1B
5	С	1102	DDQ	C5-C6-C7-C8
9	А	1112	EDO	O1-C1-C2-O2
9	В	1103	EDO	O1-C1-C2-O2
9	В	1106	EDO	01-C1-C2-O2
9	В	1110	EDO	O1-C1-C2-O2
3	A	1107	LMT	C1-C2-C3-C4
3	С	1101	LMT	C11-C10-C9-C8

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There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	С	1108	OCT	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	$OWAB(Å^2)$	Q<0.9
1	А	1034/1057~(97%)	0.56	94 (9%) 9 6	34, 53, 98, 114	0
1	В	1034/1057~(97%)	0.37	57 (5%) 25 22	35, 54, 68, 78	0
1	С	1033/1057~(97%)	0.19	32 (3%) 49 45	34, 43, 61, 69	0
2	D	155/169~(91%)	0.47	16 (10%) 6 4	41, 52, 67, 77	0
2	Ε	154/169~(91%)	1.38	41 (26%) 0 0	50, 64, 84, 93	0
All	All	3410/3509~(97%)	0.42	240 (7%) 16 13	34, 50, 79, 114	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Е	34	MET	6.7
2	Е	66	LEU	6.5
1	А	868	LEU	6.2
2	Е	35	ALA	6.2
1	В	600	THR	6.0
2	Е	68	LYS	5.9
1	А	515	TRP	5.6
2	Е	27	ASP	5.6
1	В	606	VAL	5.4
1	В	635	ALA	5.4
2	Ε	31	ARG	5.4
1	А	1040	ILE	5.3
1	А	833	PRO	5.3
2	D	165	LEU	5.3
1	В	597	TYR	5.2
1	А	511	GLY	5.1
1	В	641	GLU	5.1
1	В	657	GLN	5.1
1	В	603	LYS	5.0
1	С	497	LEU	5.0



IOUM

Mol	Chain	Res	Type	RSRZ
1	В	655	PHE	5.0
1	А	678	THR	5.0
1	А	500	ILE	4.9
1	А	510	LYS	4.9
1	А	513	PHE	4.8
2	Е	33	LEU	4.8
1	А	712	MET	4.8
2	Е	69	ASN	4.8
1	А	869	SER	4.7
1	В	653	ARG	4.7
1	А	834	GLY	4.7
2	D	161	LEU	4.7
1	В	993	THR	4.6
2	Е	67	LEU	4.6
1	А	421	ALA	4.6
1	А	713	LEU	4.6
2	Е	32	ILE	4.5
1	В	558	ARG	4.5
1	В	599	LEU	4.5
2	Е	64	GLU	4.5
2	Е	36	ASN	4.4
1	А	424	GLY	4.4
2	Е	30	VAL	4.4
1	А	255	GLN	4.3
1	В	596	HIS	4.3
1	В	1033	PHE	4.3
1	С	510	LYS	4.3
1	А	556	PHE	4.3
1	А	514	GLY	4.2
2	Е	62	ILE	4.2
2	D	150	PHE	4.2
1	А	512	PHE	4.2
2	D	164	ILE	4.2
1	С	811	TYR	4.2
1	А	525	HIS	4.1
1	А	657	GLN	4.1
1	А	432	ARG	4.1
1	С	362	PHE	4.0
1	В	554	TYR	4.0
1	А	535	LEU	4.0
1	А	557	VAL	4.0
1	А	711	ASP	3.9



IOUM

Mol	Chain	Res	Type	RSRZ
1	С	500	ILE	3.9
1	А	707	ALA	3.9
1	А	430	ALA	3.8
2	D	162	ALA	3.8
2	D	163	GLU	3.8
1	В	656	SER	3.8
1	В	593	GLU	3.8
1	А	509	LYS	3.8
2	Е	102	ASN	3.7
2	Е	73	VAL	3.7
2	Е	101	LYS	3.7
2	D	159	GLU	3.7
2	Е	60	LEU	3.7
1	А	431	THR	3.7
2	Ε	63	VAL	3.6
1	А	558	ARG	3.6
2	Е	70	GLY	3.6
2	Е	29	GLU	3.6
1	А	993	THR	3.6
2	Е	61	GLU	3.6
1	В	636	ASP	3.6
1	А	836	SER	3.5
1	В	561	SER	3.5
2	D	154	ILE	3.5
1	С	739	LEU	3.5
2	Е	99	LEU	3.5
1	В	637	ARG	3.5
1	А	425	LEU	3.4
1	А	516	PHE	3.4
1	В	633	ASP	3.4
1	А	554	TYR	3.4
1	А	533	GLY	3.4
1	A	521	GLU	3.4
1	А	835	LYS	3.4
1	A	965	LEU	3.3
1	С	511	GLY	3.3
2	Е	28	ASP	3.3
1	А	420	MET	3.3
1	А	422	GLU	3.3
2	Е	13	ASP	3.3
1	А	526	HIS	3.2
1	В	659	LYS	3.2



IOUM

Mol	Chain	Res	Type	RSRZ
1	А	867	ARG	3.2
2	Е	106	VAL	3.2
1	В	642	ASN	3.2
1	А	831	ALA	3.2
1	А	918	PHE	3.2
1	В	638	PRO	3.2
1	А	423	GLU	3.2
1	А	508	GLY	3.2
1	А	497	LEU	3.2
2	Е	65	VAL	3.2
1	В	508	GLY	3.1
1	А	704	ALA	3.1
1	A	716	VAL	3.1
1	А	709	HIS	3.1
1	A	520	PHE	3.1
1	А	1037	ASN	3.0
2	D	166	GLN	3.0
2	Ε	97	GLU	3.0
2	Ε	40	VAL	3.0
1	С	498	LYS	3.0
1	А	536	ARG	2.9
1	А	942	ALA	2.9
2	D	117	LEU	2.9
1	В	575	MET	2.9
1	С	558	ARG	2.9
2	D	129	VAL	2.9
1	В	513	PHE	2.9
2	D	28	ASP	2.9
2	E	22	ALA	2.9
2	Е	38	ALA	2.9
1	А	429	GLU	2.9
1	А	677	ALA	2.8
1	А	839	GLU	2.8
2	Е	37	GLY	2.8
1	В	598	TYR	2.8
1	А	842	GLU	2.8
1	А	499	PRO	2.8
2	D	160	ASP	2.8
1	А	1035	ARG	2.8
1	С	804	PHE	2.8
1	А	838	GLY	2.8
1	В	640	GLU	2.8



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Mol	Chain	Res	Type	RSRZ
1	В	563	PHE	2.8
1	А	710	PRO	2.8
1	В	660	ASP	2.8
1	А	498	LYS	2.7
1	А	541	TYR	2.7
1	А	495	THR	2.7
1	А	517	ASN	2.7
1	С	425	LEU	2.7
1	А	832	ALA	2.7
1	В	255	GLN	2.7
1	В	658	ILE	2.7
1	А	518	ARG	2.7
1	В	834	GLY	2.7
1	В	618	ALA	2.6
1	А	427	PRO	2.6
1	С	737	GLN	2.6
1	А	496	MET	2.6
2	Е	165	LEU	2.6
1	В	634	TRP	2.6
1	С	918	PHE	2.6
1	В	602	GLU	2.6
1	С	363	ARG	2.5
1	С	733	GLN	2.5
1	В	832	ALA	2.5
2	Е	115	THR	2.5
1	В	601	LYS	2.5
1	В	836	SER	2.5
1	С	707	ALA	2.5
1	А	846	GLN	2.4
1	В	1034	SER	2.4
1	С	361	ASN	2.4
1	С	255	GLN	2.4
1	С	499	PRO	2.4
1	А	446	ALA	2.4
1	В	501	ALA	2.4
1	В	651	ALA	2.4
1	В	654	ALA	2.4
1	A	426	PRO	2.4
1	С	736	ALA	2.4
1	А	866	GLU	2.4
1	С	513	PHE	2.4
2	Е	59	HIS	2.4



Mol	Chain	Res	Type	RSRZ
1	А	963	ALA	2.4
1	В	711	ASP	2.4
1	С	253	VAL	2.4
2	Е	95	ILE	2.3
1	А	494	ALA	2.3
1	А	11	PHE	2.3
1	С	803	ALA	2.3
1	В	604	ASN	2.3
2	Е	74	ASN	2.3
1	В	712	MET	2.3
1	С	515	TRP	2.3
1	А	618	ALA	2.3
2	Е	98	VAL	2.3
2	D	139	VAL	2.3
1	А	872	GLN	2.3
2	D	158	ASN	2.2
1	В	196	PHE	2.2
1	А	417	GLU	2.2
1	А	538	THR	2.2
1	А	529	ASP	2.2
1	А	871	ASN	2.2
1	С	508	GLY	2.2
1	А	118	LEU	2.2
1	А	542	LEU	2.2
1	А	575	MET	2.1
1	В	639	GLY	2.1
1	В	512	PHE	2.1
2	D	126	LEU	2.1
1	А	519	MET	2.1
1	С	501	ALA	2.1
1	С	65	ILE	2.1
1	С	1033	PHE	2.1
1	В	649	MET	2.1
1	С	496	MET	2.1
2	Е	71	ALA	2.1
2	Е	159	GLU	2.1
1	А	122	VAL	2.1
1	А	527	TYR	2.1
1	С	730	ASP	2.0
1	В	595	THR	2.0
1	А	360	GLN	2.0
2	Е	100	LEU	2.0



Mol	Chain	Res	Type	RSRZ
1	В	607	GLU	2.0
1	В	629	VAL	2.0
1	А	617	PHE	2.0
1	В	352	PHE	2.0
1	В	615	PHE	2.0
1	С	512	PHE	2.0
1	А	540	ARG	2.0
1	В	867	ARG	2.0
1	С	801	PHE	2.0
1	А	1039	ASP	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(Å ²)	Q<0.9
12	LPX	С	1106	30/30	0.67	0.35	$57,\!68,\!75,\!75$	0
5	DDQ	С	1102	14/14	0.69	0.25	58,64,66,67	0
3	LMT	А	1101	35/35	0.71	0.23	65,78,83,85	0
9	EDO	С	1114	4/4	0.72	0.43	$57,\!57,\!57,\!57$	0
7	1K8	В	1113	17/17	0.72	0.30	45,47,48,49	17
3	LMT	В	1102	35/35	0.73	0.36	64,66,71,72	0
5	DDQ	А	1104	14/14	0.73	0.33	66,73,80,80	0
4	C14	А	1103	14/14	0.74	0.22	55,57,60,60	0
3	LMT	В	1107	35/35	0.74	0.41	$59,\!64,\!68,\!68$	0
8	D10	А	1108	10/10	0.76	0.23	59,60,61,62	0
8	D10	В	1111	10/10	0.77	0.30	66,68,70,71	0
11	OCT	С	1109	8/8	0.79	0.27	55, 56, 58, 58	0
6	GOL	В	1105	6/6	0.79	0.22	58, 59, 59, 59	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LMT	А	1102	35/35	0.80	0.28	$56,\!59,\!62,\!63$	0
11	OCT	С	1108	8/8	0.81	0.28	48,49,50,50	0
9	EDO	В	1109	4/4	0.81	0.26	$57,\!57,\!58,\!58$	0
3	LMT	А	1107	35/35	0.81	0.39	64,67,71,73	0
9	EDO	А	1112	4/4	0.83	0.17	42,42,42,42	0
9	EDO	В	1106	4/4	0.85	0.21	53,54,54,54	0
8	D10	А	1111	10/10	0.85	0.23	69,74,80,81	0
9	EDO	В	1104	4/4	0.85	0.31	$55,\!55,\!56,\!56$	0
9	EDO	Е	201	4/4	0.87	0.27	61,62,62,64	0
9	EDO	С	1113	4/4	0.87	0.34	56, 56, 56, 56	0
6	GOL	А	1105	6/6	0.87	0.23	48,48,48,49	0
9	EDO	D	201	4/4	0.87	0.26	$55,\!56,\!56,\!56$	0
9	EDO	А	1109	4/4	0.88	0.15	$59,\!60,\!60,\!61$	0
9	EDO	С	1110	4/4	0.88	0.19	52,52,52,53	0
3	LMT	В	1101	35/35	0.88	0.32	70,72,75,75	0
9	EDO	А	1110	4/4	0.89	0.34	60,60,61,61	0
11	OCT	С	1104	8/8	0.90	0.25	$49,\!50,\!51,\!51$	0
9	EDO	В	1112	4/4	0.90	0.21	$59,\!59,\!59,\!60$	0
8	D10	С	1103	10/10	0.91	0.18	$49,\!49,\!50,\!51$	0
9	EDO	В	1110	4/4	0.91	0.14	75,76,76,76	0
3	LMT	С	1101	35/35	0.91	0.22	$57,\!61,\!63,\!64$	0
9	EDO	В	1108	4/4	0.91	0.25	$53,\!53,\!53,\!54$	0
9	EDO	С	1105	4/4	0.92	0.40	$57,\!57,\!57,\!57$	0
6	GOL	С	1111	6/6	0.92	0.18	43,44,44,44	0
7	1K8	А	1106	17/17	0.93	0.24	$67,\!72,\!77,\!77$	0
9	EDO	В	1103	4/4	0.93	0.21	$4\overline{9,49,49,50}$	0
9	EDO	С	1107	4/4	0.94	0.26	47,47,47,47	0
10	SO4	В	1114	5/5	0.94	0.24	85,85,85,85	0
10	SO4	С	1115	5/5	0.95	0.16	75,75,75,76	0
11	OCT	C	1112	8/8	0.96	0.12	51,52,53,54	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.

