

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	9F9M
Title	:	Crystal structure of MUS81-EME1 bound by compound 21.
Authors	:	Collie, G.W.
Deposited on	:	2024-05-08
Resolution	:	2.47 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	:	2.36.2
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)	:	2.36.2

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 2.47 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	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						
1	А	308	8%	9%	8% •	42%			
1	С	308	5%	%	12% •	41%			
2	В	326	² % 36%	6%		57%			
2	D	326	5%	6% •		58%			



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4941 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 Crossover junction endonuclease MUS81.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	170	Total	С	Ν	0	S	0	0	0
1	Л	179	1407	892	251	260	4	0	0	0
1	С	192	Total	С	Ν	0	S	0	0	
		100	1428	906	256	262	4			U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	244	GLY	-	expression tag	UNP Q96NY9
А	245	SER	-	expression tag	UNP Q96NY9
С	244	GLY	-	expression tag	UNP Q96NY9
С	245	SER	-	expression tag	UNP Q96NY9

• Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	В	120	Total	С	Ν	0	S	0	0	0
	D	159	1034	658	169	199	8	0	0	0
0	Л	197	Total	С	Ν	0	S	0	0	0
		137	1022	650	168	197	7	0		U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	245	GLY	-	expression tag	UNP Q96AY2
D	245	GLY	-	expression tag	UNP Q96AY2

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Mg 2 2	0	0





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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	2	Total Mg 2 2	0	0

• Molecule 4 is 5-oxidanyl-4-oxidanylidene-1-(4-piperazin-1-ylphenyl)pyridine-3-carboxylic acid (three-letter code: A1IA4) (formula: $C_{16}H_{17}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	Δ	1	Total	С	Ν	0	0	0	
4	A	L	23	16	3	4	0	0	
4	C	1	Total	С	Ν	0	0	0	
4	U			16	3	4	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: Crossover junction endonuclease MUS81







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	62.90Å 83.56 Å 91.53 Å	Deperitor
a, b, c, α , β , γ	90.00° 92.18° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	50.23 - 2.47	Depositor
Resolution (A)	50.23 - 2.47	EDS
% Data completeness	99.8 (50.23-2.47)	Depositor
(in resolution range)	99.9(50.23-2.47)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.71 (at 2.48 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
D D.	0.306 , 0.326	Depositor
Π, Π_{free}	0.298 , 0.324	DCC
R_{free} test set	1685 reflections (4.94%)	wwPDB-VP
Wilson B-factor $(Å^2)$	61.7	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32, 51.2	EDS
L-test for twinning ²	$< L >=0.54, < L^2>=0.38$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4941	wwPDB-VP
Average B, all atoms $(Å^2)$	75.0	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 53.29 % 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 4.3079e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: MG, $\rm A1IA4$

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		
	Cham RMSZ # Z		# Z > 5	RMSZ	# Z > 5	
1	А	0.36	0/1432	0.62	0/1941	
1	С	0.38	0/1454	0.60	0/1971	
2	В	0.34	0/1045	0.51	0/1423	
2	D	0.37	0/1032	0.55	0/1404	
All	All	0.37	0/4963	0.58	0/6739	

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	1407	0	1386	14	0
1	С	1428	0	1407	15	0
2	В	1034	0	1029	10	0
2	D	1022	0	1021	9	0
3	А	2	0	0	0	0
3	С	2	0	0	0	0
4	А	23	0	0	0	0
4	С	23	0	0	1	0
All	All	4941	0	4843	44	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 4.

All (44) 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:417:ARG:NH1	1:A:421:ARG:HH12	1.76	0.84	
2:B:291:VAL:HG13	2:B:313:LEU:HB3	1.67	0.76	
1:A:402:THR:HG21	1:A:408:SER:OG	1.87	0.73	
1:A:421:ARG:O	1:A:424:GLN:HG2	1.92	0.70	
2:D:310:PRO:HA	2:D:357:LYS:HG2	1.75	0.69	
2:D:291:VAL:HG13	2:D:313:LEU:HB3	1.76	0.66	
2:B:347:VAL:HG21	2:B:415:LEU:HD11	1.81	0.63	
2:B:360:SER:HA	2:B:422:GLN:HB3	1.82	0.62	
1:A:317:PRO:HG2	1:A:320:PRO:HA	1.84	0.59	
2:D:360:SER:HA	2:D:422:GLN:HB3	1.83	0.59	
2:D:260:LEU:HB2	2:D:289:CYS:HA	1.84	0.59	
1:C:264:PRO:HB3	1:C:425:GLY:HA2	1.85	0.57	
1:C:271:LEU:HD11	1:C:308:PHE:HB3	1.87	0.57	
1:A:417:ARG:NH1	1:A:421:ARG:NH1	2.50	0.56	
1:C:304:HIS:HD2	1:C:460:ASN:HA	1.71	0.56	
1:C:317:PRO:HG3	1:C:323:PRO:HB3	1.89	0.55	
1:A:348:ARG:O	1:A:352:GLN:HG3	2.09	0.53	
1:A:369:GLU:HG3	1:A:402:THR:HG22	1.91	0.53	
1:A:304:HIS:HD2	1:A:460:ASN:HA	1.75	0.51	
2:B:260:LEU:HB2	2:B:289:CYS:HA	1.91	0.51	
2:B:263:MET:SD	2:B:315:LEU:HD23	2.50	0.50	
1:A:432:PRO:O	1:A:458:ASP:OD2	2.30	0.50	
2:D:258:PRO:O	2:D:262:GLN:HG3	2.11	0.50	
2:B:252:ILE:HD11	2:B:443:VAL:HG12	1.94	0.49	
1:A:448:ASN:OD1	2:B:417:LEU:O	2.29	0.49	
1:C:385:LEU:O	1:C:389:THR:HG23	2.11	0.49	
1:C:304:HIS:CD2	1:C:460:ASN:HA	2.46	0.49	
1:C:348:ARG:NH2	4:C:603:A1IA4:C8	2.78	0.47	
1:A:392:GLN:NE2	2:B:422:GLN:HG2	2.30	0.46	
1:C:308:PHE:HB2	1:C:332:VAL:HB	1.98	0.46	
1:A:431:ARG:HD3	1:A:435:THR:C	2.37	0.45	
1:C:392:GLN:NE2	2:D:422:GLN:HG2	2.32	0.44	
1:C:353:LYS:O	1:C:357:LYS:HD3	2.17	0.44	
2:D:351:THR:HA	2:D:354:THR:HG22	1.98	0.44	
2:D:264:GLU:HG2	2:D:429:TRP:CZ2	2.52	0.44	
1:C:269:VAL:HA	1:C:311:VAL:O	2.18	0.43	
2:D:315:LEU:HD11	2:D:364:VAL:HG23	2.00	0.43	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:TRP:HB3	1:C:328:LEU:HD22	2.01	0.43
1:C:361:LEU:HD22	1:C:459:PHE:CE1	2.55	0.42
1:C:357:LYS:HD2	1:C:397:PHE:HE1	1.85	0.41
2:B:315:LEU:HD11	2:B:364:VAL:HG23	2.03	0.40
1:A:369:GLU:HG3	1:A:402:THR:CG2	2.51	0.40
1:C:400:LYS:HG3	1:C:411:TYR:CZ	2.57	0.40
1:A:398:PHE:HA	2:B:422:GLN:OE1	2.21	0.40

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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	171/308~(56%)	168~(98%)	1 (1%)	2(1%)	13	12
1	С	175/308~(57%)	166~(95%)	7 (4%)	2(1%)	14	14
2	В	131/326~(40%)	127~(97%)	3 (2%)	1 (1%)	19	22
2	D	129/326~(40%)	126~(98%)	3~(2%)	0	100	100
All	All	606/1268~(48%)	587 (97%)	14 (2%)	5 (1%)	19	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	432	PRO
1	С	432	PRO
1	А	433	TRP
2	В	355	ALA
1	С	433	TRP



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	151/260~(58%)	140~(93%)	11 (7%)		14	16
1	С	152/260~(58%)	134~(88%)	18 (12%)		5	4
2	В	110/275~(40%)	103~(94%)	7~(6%)		17	21
2	D	108/275~(39%)	99~(92%)	9 (8%)		11	12
All	All	521/1070~(49%)	476 (91%)	45 (9%)		10	11

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	268	ARG
1	А	354	PHE
1	А	355	ARG
1	А	358	ARG
1	А	364	ARG
1	А	400	LYS
1	А	402	THR
1	А	414	LEU
1	А	420	GLN
1	А	428	LEU
1	А	458	ASP
2	В	249	LEU
2	В	269	LEU
2	В	285	GLN
2	В	291	VAL
2	В	344	GLN
2	В	354	THR
2	В	414	ASP
1	С	260	LEU
1	С	269	VAL
1	С	270	LEU
1	С	288	LEU
1	С	296	VAL
1	C	334	ARG



Mol	Chain	Res	Type
1	С	351	GLU
1	С	384	LEU
1	С	400	LYS
1	С	402	THR
1	С	414	LEU
1	С	415	LEU
1	С	421	ARG
1	С	422	LEU
1	С	433	TRP
1	С	452	SER
1	С	455	THR
1	С	459	PHE
2	D	285	GLN
2	D	287	VAL
2	D	291	VAL
2	D	313	LEU
2	D	344	GLN
2	D	354	THR
2	D	366	GLN
2	D	414	ASP
2	D	439	PHE

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	304	HIS
1	А	352	GLN
1	А	420	GLN
1	С	304	HIS
1	С	352	GLN
1	С	420	GLN
2	D	366	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are 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 Trme Chain I		Dec	Tinle	Bo	ond leng	\mathbf{ths}	В	ond ang	les	
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	A1IA4	A	603	3	24,25,25	0.29	0	$32,\!35,\!35$	0.68	0
4	A1IA4	С	603	3	24,25,25	0.27	0	32,35,35	0.77	1 (3%)

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
4	A1IA4	А	603	3	-	4/12/20/20	0/3/3/3
4	A1IA4	С	603	3	-	0/12/20/20	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	С	603	A1IA4	C1-C5-C4	-2.00	116.23	118.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	603	A1IA4	C7-C6-N-C2
4	А	603	A1IA4	C11-C6-N-C2
4	А	603	A1IA4	C7-C6-N-C3



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Mol	Chain	Res	Type	Atoms
4	А	603	A1IA4	C11-C6-N-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	603	A1IA4	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	179/308~(58%)	0.98	25 (13%) 2 1	47, 79, 102, 124	0
1	С	183/308~(59%)	0.73	16 (8%) 10 7	46, 78, 100, 120	0
2	В	139/326~(42%)	0.67	8 (5%) 23 20	59, 74, 95, 101	0
2	D	137/326~(42%)	0.75	16 (11%) 4 3	54, 71, 92, 101	0
All	All	638/1268~(50%)	0.79	65 (10%) 6 4	46, 75, 98, 124	0

All (65) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	285	PRO	8.1
1	А	287	LEU	7.4
1	С	287	LEU	6.1
2	В	249	LEU	5.6
1	А	345	ILE	5.6
1	А	462	GLY	4.8
1	А	269	VAL	4.4
2	D	364	VAL	4.4
2	В	253	ILE	4.1
1	А	262	LEU	4.0
1	А	291	LEU	3.8
2	D	263	MET	3.6
1	С	300	VAL	3.4
1	С	260	LEU	3.3
1	А	384	LEU	3.2
2	В	280	CYS	3.2
1	С	435	THR	3.1
2	D	404	SER	3.1
1	А	295	HIS	3.0
2	В	252	ILE	2.9
1	А	342	SER	2.9



Mol	Chain	Res	Type	RSRZ
1	А	270	LEU	2.9
2	D	315	LEU	2.9
1	А	430	SER	2.8
1	А	296	VAL	2.8
1	С	259	PRO	2.8
1	С	279	ARG	2.8
1	А	337	LEU	2.8
1	А	324	GLY	2.7
1	С	271	LEU	2.7
2	D	321	PHE	2.7
2	D	425	ILE	2.7
1	С	290	GLU	2.7
1	А	294	LEU	2.6
2	В	278	CYS	2.6
2	В	279	ARG	2.6
1	А	343	SER	2.6
1	С	262	LEU	2.5
2	D	435	PHE	2.5
2	D	322	VAL	2.5
2	В	254	VAL	2.4
1	А	459	PHE	2.4
2	D	317	ARG	2.4
1	С	296	VAL	2.4
1	А	311	VAL	2.3
1	С	299	THR	2.3
1	С	350	ARG	2.3
1	А	341	CYS	2.3
1	А	447	PRO	2.2
1	С	295	HIS	2.2
2	D	252	ILE	2.2
2	D	429	TRP	2.2
1	А	260	LEU	2.1
2	В	316	LEU	2.1
1	А	259	PRO	2.1
1	A	412	LEU	2.1
2	D	295	ARG	2.1
2	D	362	VAL	2.1
2	D	361	LEU	2.1
1	А	428	LEU	2.1
2	D	365	ASP	2.0
1	А	448	ASN	2.0
1	С	294	LEU	2.0

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Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	288	LEU	2.0
2	D	346	PHE	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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	MG	А	602	1/1	0.72	0.21	97,97,97,97	0
4	A1IA4	С	603	23/23	0.82	0.24	97,99,102,102	0
4	A1IA4	А	603	23/23	0.84	0.21	89,91,95,95	0
3	MG	С	602	1/1	0.86	0.29	76,76,76,76	0
3	MG	С	601	1/1	0.93	0.30	69,69,69,69	0
3	MG	А	601	1/1	0.97	0.32	72,72,72,72	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.

