

Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 - 11:06 am BST

PDB ID	:	9F9A
Title	:	Crystal structure of MUS81-EME1 bound by compound 12.
Authors	:	Collie, G.W.
Deposited on	:	2024-05-07
Resolution	:	2.91 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 2.91 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.



Motria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462(2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	Qual	lity of chain	
1	А	308	49%	10% •	40%
1	С	308	48%	11% •	40%
1	Е	308	48%	12% ·	39%
1	G	308	42%	17% ·	40%
2	В	326	3% 39% · ·		58%



α \cdot 1	C		
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Mol	Chain	Length	Quality of chain				
2	D	326	32%	10% •	57%		
2	F	326	^{2%}	10% •	57%		
2	Н	326	.% -	10% •	58%		



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10093 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	195	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	165	1458	924	265	265	4	0	0	0
1	C	186	Total	С	Ν	0	S	0	0	0
	U	160	1468	929	267	268	4	0	0	0
1	F	197	Total	С	Ν	0	S	0	0	0
		107	1472	933	267	268	4	0	0	0
1	C	195	Total	С	Ν	0	S	0	0	0
	G	100	1458	924	265	265	4		0	U

• Molecule 1 is a protein called Crossover junction endonuclease MUS81.

There are 8 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
Е	244	GLY	-	expression tag	UNP Q96NY9
E	245	SER	-	expression tag	UNP Q96NY9
G	244	GLY	-	expression tag	UNP Q96NY9
G	245	SER	-	expression tag	UNP Q96NY9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	р	128	Total	С	Ν	0	S	0	0	0
	D	130	1031	653	170	200	8	0	0	0
9	л	120	Total	С	Ν	0	S	0	0	0
	D	159	1045	664	172	201	8	0	0	0
9	Б	120	Total	С	Ν	0	S	0	0	0
	Г	159	1045	664	172	201	8	0	0	0
9	ц	127	Total	С	Ν	0	S	0	0	0
	11	107	1024	648	169	199	8		0	U





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

There are 4 discrepancies between the modelled and reference sequences:

• Molecule 3 is 2-naphthalen-2-yl-5-oxidanyl-6-oxidanylidene-1H-pyrimidine-4-carboxylic acid (three-letter code: A1IA6) (formula: $C_{15}H_{10}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Δ	1	Total	С	Ν	Ο	0	0
0	Л	T	21	15	2	4	0	0
3	С	1	Total	С	Ν	Ο	0	0
0	U	T	21	15	2	4	0	0
3	F	1	Total	С	Ν	Ο	0	0
0	Ľ	1	21	15	2	4	0	0
3	С	1	Total	С	Ν	Ο	0	0
5	G	1	21	15	2	4	0	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Mg 2 2	0	0
4	С	2	Total Mg 2 2	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Е	2	Total Mg 2 2	0	0
4	G	2	Total Mg 2 2	0	0



GLY SER ALA ALA GLU LEU LEU LEU ALA GLU VAL CLV VAL CLN GLN

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





LEU SER ARG ARG CILEU CILEU CILEU CILEU PRO CILN LEU LEU LEU LEU LEU ASP SER ASP ASP





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	111.87Å 124.35Å 217.57Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	83.17 - 2.91	Depositor
Resolution (A)	83.17 - 2.91	EDS
% Data completeness	60.8 (83.17 - 2.91)	Depositor
(in resolution range)	$60.8 \ (83.17 - 2.91)$	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.76 (at 2.91 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
B B.	0.243 , 0.278	Depositor
II, II free	0.243 , 0.280	DCC
R_{free} test set	2051 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	72.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31 , 47.4	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10093	wwPDB-VP
Average B, all atoms $(Å^2)$	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.13% 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: MG, $\rm A1IA6$

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	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.38	0/1486	0.62	0/2014
1	С	0.38	0/1496	0.63	0/2028
1	Е	0.34	0/1501	0.59	0/2036
1	G	0.35	0/1486	0.57	0/2014
2	В	0.30	0/1040	0.51	0/1413
2	D	0.33	0/1056	0.54	0/1436
2	F	0.32	0/1056	0.50	0/1436
2	Н	0.31	0/1033	0.47	0/1403
All	All	0.34	0/10154	0.56	0/13780

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	1458	0	1446	16	0
1	С	1468	0	1457	17	0
1	Е	1472	0	1460	23	0
1	G	1458	0	1446	26	0
2	В	1031	0	1036	3	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1045	0	1046	19	0
2	F	1045	0	1046	15	0
2	Н	1024	0	1027	20	0
3	А	21	0	0	0	0
3	С	21	0	0	0	0
3	Ε	21	0	0	0	0
3	G	21	0	0	0	0
4	А	2	0	0	0	0
4	С	2	0	0	0	0
4	Ε	2	0	0	0	0
4	G	2	0	0	0	0
All	All	10093	0	9964	132	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 7.

All (132) 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:C:304:HIS:CD2	1:C:305:VAL:HG12	2.10	0.85
1:E:335:LYS:NZ	1:E:352:GLN:HE22	1.73	0.84
2:D:258:PRO:HD2	2:D:284:ALA:HA	1.61	0.82
2:D:310:PRO:HA	2:D:357:LYS:HG2	1.64	0.78
2:F:253:ILE:HD11	2:F:306:TRP:CE2	2.22	0.75
1:G:308:PHE:HB2	1:G:332:VAL:HB	1.69	0.74
1:G:341:CYS:O	1:G:345:ILE:HG12	1.87	0.74
2:D:258:PRO:CD	2:D:284:ALA:HA	2.16	0.74
1:E:335:LYS:HZ3	1:E:352:GLN:NE2	1.86	0.74
1:E:335:LYS:NZ	1:E:352:GLN:NE2	2.35	0.74
1:E:335:LYS:HZ3	1:E:352:GLN:HE22	1.32	0.73
2:H:254:VAL:HG22	2:H:293:TRP:CD1	2.27	0.70
2:D:252:ILE:HD11	2:D:293:TRP:CD1	2.27	0.70
2:B:291:VAL:HG13	2:B:313:LEU:HB3	1.74	0.68
2:H:254:VAL:HG22	2:H:293:TRP:NE1	2.08	0.68
2:F:291:VAL:HG13	2:F:313:LEU:HB3	1.76	0.66
1:E:304:HIS:CD2	1:E:305:VAL:HG12	2.31	0.66
1:E:341:CYS:O	1:E:345:ILE:HG12	1.96	0.65
2:H:258:PRO:HD2	2:H:284:ALA:HA	1.78	0.65
1:E:431:ARG:HD3	1:E:435:THR:HA	1.79	0.65
2:D:315:LEU:HD11	2:D:432:LEU:HD11	1.78	0.64
2:H:254:VAL:HG22	2:H:293:TRP:HE1	1.63	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:308:PHE:HB2	1:E:332:VAL:HB	1.81	0.62
1:E:348:ARG:O	1:E:352:GLN:HG3	2.00	0.60
1:E:414:LEU:HB3	2:F:413:VAL:HG21	1.83	0.60
1:A:364:ARG:NH2	1:A:395:ASP:O	2.35	0.60
2:D:354:THR:HG23	2:D:357:LYS:H	1.68	0.57
2:B:252:ILE:HG13	2:B:295:ARG:HG2	1.86	0.57
1:C:335:LYS:HG3	1:C:366:TYR:OH	2.04	0.57
2:H:315:LEU:HD21	2:H:432:LEU:HD21	1.85	0.57
2:F:363:ILE:HB	2:F:425:ILE:HG12	1.86	0.56
2:D:364:VAL:HG13	2:D:426:VAL:HG23	1.87	0.56
1:G:305:VAL:HG22	1:G:356:LEU:HD12	1.85	0.56
1:G:345:ILE:HD11	1:G:379:LEU:HD13	1.88	0.56
1:C:269:VAL:HG13	1:C:420:GLN:HG2	1.87	0.56
1:A:345:ILE:HD11	1:A:379:LEU:HD13	1.86	0.56
1:E:400:LYS:HG3	1:E:411:TYR:CE1	2.42	0.55
1:E:304:HIS:NE2	1:E:305:VAL:HG12	2.22	0.55
1:G:405:ILE:HD12	1:G:405:ILE:H	1.72	0.54
2:D:252:ILE:HD11	2:D:293:TRP:HD1	1.71	0.52
2:F:346:PHE:O	2:F:350:ILE:HG13	2.09	0.52
1:A:341:CYS:O	1:A:345:ILE:HG12	2.09	0.52
1:E:369:GLU:HA	1:E:402:THR:HG23	1.92	0.52
1:G:363:ARG:HH21	1:G:448:ASN:HD22	1.56	0.52
1:E:263:ARG:HA	1:E:427:THR:HG23	1.90	0.52
2:H:249:LEU:HD13	2:H:278:CYS:HB3	1.92	0.52
1:C:308:PHE:HB2	1:C:332:VAL:HB	1.91	0.51
2:H:291:VAL:HG13	2:H:313:LEU:HB3	1.92	0.51
1:C:332:VAL:HG22	1:C:365:VAL:HB	1.92	0.51
2:D:292:THR:HG22	2:D:293:TRP:H	1.75	0.51
1:E:363:ARG:NH1	1:E:448:ASN:ND2	2.59	0.51
1:C:287:LEU:HD12	1:C:409:ALA:HB2	1.92	0.50
1:E:333:GLU:HB2	1:E:356:LEU:HD11	1.94	0.50
1:A:297:THR:H	1:C:316:ASN:HD21	1.60	0.49
1:A:305:VAL:HG11	1:A:359:CYS:HB2	1.94	0.49
2:D:261:LEU:HD12	2:D:282:ILE:HG21	1.93	0.49
1:G:363:ARG:HH21	1:G:448:ASN:ND2	2.10	0.49
1:C:327:VAL:HG22	1:C:361:LEU:HD21	1.95	0.49
2:H:350:ILE:HG21	2:H:359:LEU:HD13	1.95	0.48
2:F:292:THR:HG21	2:F:357:LYS:HZ3	1.78	0.48
1:E:327:VAL:HG11	1:E:459:PHE:HB2	1.94	0.48
1:G:402:THR:HG21	1:G:408:SER:OG	2.14	0.48
2:D:291:VAL:HG13	2:D:313:LEU:HB3	1.96	0.48



Interatomic Clash						
Atom-1	Atom-2	distance (Å)	overlap (Å)			
2:H:260:LEU:HD11	2:H:315:LEU:HD13	1.96	0.48			
1:A:335:LYS:NZ	1:A:352:GLN:NE2	2.62	0.47			
1:G:263:ARG:HA	1:G:427:THR:HG23	1.97	0.47			
1:A:369:GLU:O	1:A:370:GLU:HB2	2.15	0.47			
2:H:260:LEU:HD13	2:H:289:CYS:HA	1.97	0.47			
1:A:340:LEU:HD23	1:A:384:LEU:HD12	1.97	0.46			
1:C:345:ILE:HD11	1:C:379:LEU:HD13	1.96	0.46			
2:D:347:VAL:HG21	2:D:415:LEU:HD11	1.98	0.46			
2:F:253:ILE:HB	2:F:294:ARG:HB2	1.98	0.46			
2:D:363:ILE:HB	2:D:425:ILE:HG12	1.97	0.46			
1:A:338:ASP:HA	1:A:377:LEU:HD21	1.98	0.46			
1:C:369:GLU:HA	1:C:402:THR:HG22	1.96	0.46			
2:D:315:LEU:HD21	2:D:432:LEU:HD21	1.97	0.46			
1:A:335:LYS:NZ	1:A:352:GLN:HE22	2.14	0.46			
1:G:269:VAL:HG13	1:G:420:GLN:HG2	1.98	0.46			
1:E:335:LYS:HZ1	1:E:352:GLN:NE2	2.11	0.45			
1:E:354:PHE:HE1	1:E:355:ARG:NH1	2.13	0.45			
1:G:428:LEU:HD12	1:G:451:CYS:HA	1.99	0.45			
1:C:333:GLU:HB2	1:C:356:LEU:HD21	1.98	0.45			
2:H:261:LEU:HD11	2:H:282:ILE:HD12	1.98	0.45			
1:G:331:ILE:HB	1:G:361:LEU:HD23	1.99	0.45			
1:G:369:GLU:O	1:G:370:GLU:HB2	2.17	0.45			
1:C:392:GLN:NE2	2:D:422:GLN:HG2	2.32	0.45			
2:F:253:ILE:HD11	2:F:306:TRP:CD2	2.51	0.45			
1:G:400:LYS:HG3	1:G:411:TYR:CE1	2.51	0.45			
1:G:337:LEU:HB3	1:G:377:LEU:HD11	1.98	0.44			
1:C:336:ARG:HG3	1:C:369:GLU:HB3	1.98	0.44			
1:C:304:HIS:HD2	1:C:305:VAL:HG12	1.76	0.44			
2:D:441:LYS:O	2:D:445:GLU:OE2	2.35	0.44			
1:E:335:LYS:HG3	1:E:366:TYR:OH	2.18	0.44			
2:F:321:PHE:HE2	2:F:408:ALA:HB1	1.82	0.44			
1:G:271:LEU:HD13	1:G:310:TRP:NE1	2.33	0.44			
1:C:329:ASP:HA	1:C:361:LEU:HG	2.00	0.44			
1:G:354:PHE:HA	1:G:357:LYS:HG2	2.00	0.43			
1:C:283:HIS:CD2	1:E:436:PRO:HD2	2.53	0.43			
1:C:335:LYS:NZ	1:C:352:GLN:HE22	2.17	0.43			
2:B:354:THR:OG1	2:B:357:LYS:HD2	2.17	0.43			
1:A:317:PRO:HG2	1:A:320:PRO:HA	2.01	0.43			
2:D:322:VAL:O	2:D:325:ILE:HG13	2.18	0.43			
1:E:327:VAL:HG11	1:E:459:PHE:CB	2.49	0.43			
1:G:400:LYS:HG3	1:G:411:TYR:CZ	2.55	0.42			



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:260:LEU:HD11	2:H:315:LEU:HD22	2.00	0.42
2:H:422:GLN:HE21	2:H:422:GLN:HB2	1.65	0.42
2:H:256:LEU:HD22	2:H:260:LEU:HD23	2.01	0.42
1:A:335:LYS:HZ3	1:A:352:GLN:NE2	2.17	0.42
2:F:354:THR:HG23	2:F:357:LYS:H	1.85	0.42
1:G:369:GLU:HA	1:G:402:THR:HG22	2.00	0.42
2:F:311:THR:HG23	2:F:358:ALA:HB3	2.01	0.42
1:A:287:LEU:HD12	1:A:409:ALA:HB2	2.02	0.42
1:E:400:LYS:HG3	1:E:411:TYR:CZ	2.55	0.42
2:F:310:PRO:HA	2:F:357:LYS:HG2	2.02	0.41
2:H:354:THR:HG23	2:H:357:LYS:H	1.85	0.41
1:A:423:TYR:CZ	1:A:449:PRO:HB2	2.56	0.41
2:D:310:PRO:CA	2:D:357:LYS:HG2	2.42	0.41
2:F:261:LEU:HA	2:F:266:GLY:HA3	2.03	0.41
2:H:265:GLY:HA3	2:H:429:TRP:CD2	2.55	0.41
2:H:311:THR:HG23	2:H:358:ALA:HB3	2.02	0.41
2:H:322:VAL:O	2:H:325:ILE:HG13	2.20	0.41
1:G:262:LEU:HD22	1:G:267:TYR:HB3	2.02	0.41
1:G:335:LYS:NZ	1:G:352:GLN:HE22	2.18	0.41
2:F:292:THR:HG22	2:F:293:TRP:H	1.86	0.41
1:G:326:LEU:HB3	1:G:453:LEU:HB2	2.01	0.41
1:A:283:HIS:CE1	1:G:329:ASP:OD1	2.74	0.41
1:G:414:LEU:HB3	2:H:413:VAL:HG21	2.02	0.41
1:A:400:LYS:HG3	1:A:411:TYR:CZ	2.55	0.41
2:D:260:LEU:HD11	2:D:315:LEU:HD22	2.03	0.41
1:G:401:ARG:HH22	2:H:435:PHE:HE1	1.68	0.41
1:G:267:TYR:HA	1:G:314:GLU:HA	2.02	0.40
2:F:422:GLN:HE21	2:F:422:GLN:HB2	1.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	179/308~(58%)	172 (96%)	5(3%)	2(1%)	14 41
1	С	180/308~(58%)	169 (94%)	10 (6%)	1 (1%)	25 57
1	E	181/308~(59%)	172 (95%)	7 (4%)	2(1%)	14 41
1	G	179/308~(58%)	164 (92%)	13 (7%)	2(1%)	14 41
2	В	130/326~(40%)	125~(96%)	4(3%)	1 (1%)	19 49
2	D	131/326~(40%)	121 (92%)	7 (5%)	3~(2%)	6 22
2	F	131/326~(40%)	118 (90%)	12 (9%)	1 (1%)	19 49
2	Н	129/326~(40%)	121 (94%)	8 (6%)	0	100 100
All	All	1240/2536~(49%)	1162 (94%)	66~(5%)	12 (1%)	15 43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	432	PRO
1	А	282	GLY
2	D	307	VAL
1	Е	282	GLY
1	Е	432	PRO
1	А	432	PRO
2	F	307	VAL
1	G	432	PRO
2	В	355	ALA
1	G	282	GLY
2	D	445	GLU
2	D	282	ILE

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	156/260~(60%)	147 (94%)	9~(6%)	20 48
1	С	158/260~(61%)	140 (89%)	18 (11%)	5 17
1	Е	158/260~(61%)	146 (92%)	12 (8%)	13 35



Mol	Chain	Analysed	Rotameric	Outliers	Pe	erce	entiles
1	G	156/260~(60%)	138 (88%)	18 (12%)		5	16
2	В	111/275~(40%)	104 (94%)	7~(6%)		18	44
2	D	112/275~(41%)	101 (90%)	11 (10%)		8	23
2	F	112/275~(41%)	99~(88%)	13 (12%)		5	16
2	Н	110/275~(40%)	101 (92%)	9~(8%)		11	31
All	All	1073/2140~(50%)	976 (91%)	97(9%)		9	27

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All (97) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	269	VAL
1	А	275	ILE
1	А	279	ARG
1	А	295	HIS
1	А	370	GLU
1	А	384	LEU
1	А	400	LYS
1	А	402	THR
1	А	422	LEU
2	В	249	LEU
2	В	285	GLN
2	В	287	VAL
2	В	291	VAL
2	В	344	GLN
2	В	354	THR
2	В	422	GLN
1	С	269	VAL
1	С	275	ILE
1	С	299	THR
1	С	304	HIS
1	С	315	THR
1	С	335	LYS
1	С	351	GLU
1	С	355	ARG
1	С	356	LEU
1	С	384	LEU
1	С	400	LYS
1	С	402	THR
1	С	405	ILE
1	С	408	SER



Mol	Chain	Res	Type
1	С	417	ARG
1	С	422	LEU
1	С	433	TRP
1	С	448	ASN
2	D	249	LEU
2	D	252	ILE
2	D	291	VAL
2	D	319	GLU
2	D	344	GLN
2	D	361	LEU
2	D	365	ASP
2	D	406	VAL
2	D	410	GLU
2	D	424	GLN
2	D	445	GLU
1	Е	269	VAL
1	Е	275	ILE
1	Е	288	LEU
1	Е	294	LEU
1	Е	304	HIS
1	Е	335	LYS
1	Е	337	LEU
1	Е	366	TYR
1	Е	379	LEU
1	Е	408	SER
1	Е	421	ARG
1	Е	422	LEU
2	F	249	LEU
2	F	251	HIS
2	F	252	ILE
2	F	268	GLN
2	F	279	ARG
2	F	291	VAL
2	F	344	GLN
2	F	360	SER
2	F	361	LEU
2	F	366	GLN
2	F	410	GLU
2	F	422	GLN
2	F	424	GLN
1	G	269	VAL
1	G	275	ILE

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Mol	Chain	Res	Type
1	G	288	LEU
1	G	290	GLU
1	G	300	VAL
1	G	301	ARG
1	G	335	LYS
1	G	338	ASP
1	G	364	ARG
1	G	378	SER
1	G	379	LEU
1	G	384	LEU
1	G	402	THR
1	G	421	ARG
1	G	422	LEU
1	G	433	TRP
1	G	455	THR
1	G	460	ASN
2	Н	263	MET
2	Н	276	MET
2	Н	279	ARG
2	Н	291	VAL
2	Н	309	GLU
2	Н	311	THR
2	Н	344	GLN
2	Н	422	GLN
2	Н	424	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	283	HIS
1	А	304	HIS
1	А	352	GLN
1	А	392	GLN
1	А	448	ASN
1	С	283	HIS
1	С	304	HIS
1	С	316	ASN
1	С	352	GLN
1	С	448	ASN
1	Е	352	GLN
1	Е	448	ASN
1	G	292	GLN



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Mol	Chain	Res	Type
1	G	352	GLN
1	G	448	ASN
2	Н	251	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)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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).

Mal Trupa		Chain	Dec	Tink	Bo	ond lengths		Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1IA6	Е	601	4	21,23,23	0.33	0	26,33,33	0.45	0
3	A1IA6	А	601	4	21,23,23	0.33	0	26,33,33	0.41	0
3	A1IA6	С	601	4	21,23,23	0.23	0	26,33,33	0.48	0
3	A1IA6	G	601	4	21,23,23	0.23	0	26,33,33	0.41	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
3	A1IA6	Е	601	4	-	3/8/8/8	0/3/3/3
3	A1IA6	А	601	4	-	0/8/8/8	0/3/3/3
3	A1IA6	С	601	4	-	4/8/8/8	0/3/3/3
3	A1IA6	G	601	4	-	6/8/8/8	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
3	G	601	A1IA6	O1-C-C1-C2
3	G	601	A1IA6	N-C4-C5-C14
3	G	601	A1IA6	N-C4-C5-C6
3	G	601	A1IA6	N1-C4-C5-C6
3	G	601	A1IA6	N1-C4-C5-C14
3	G	601	A1IA6	O1-C-C1-N1
3	С	601	A1IA6	N-C4-C5-C6
3	Е	601	A1IA6	N-C4-C5-C6
3	С	601	A1IA6	N-C4-C5-C14
3	Е	601	A1IA6	N-C4-C5-C14
3	С	601	A1IA6	N1-C4-C5-C14
3	C	601	A1IA6	N1-C4-C5-C6
3	Е	601	A1IA6	N1-C4-C5-C6

All (13) torsion outliers are listed below:

There are no ring outliers.

No monomer is involved in short contacts.

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









5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	185/308~(60%)	0.13	1 (0%) 91 91	35, 57, 80, 88	0
1	С	186/308~(60%)	0.03	0 100 100	39, 58, 76, 82	0
1	Ε	187/308~(60%)	0.06	1 (0%) 91 91	40, 67, 93, 101	0
1	G	185/308~(60%)	0.11	0 100 100	43, 70, 95, 101	0
2	В	138/326~(42%)	0.59	11 (7%) 12 10	66, 87, 111, 122	0
2	D	139/326~(42%)	0.32	6 (4%) 35 32	60, 85, 104, 108	0
2	F	139/326~(42%)	0.36	6 (4%) 35 32	62, 87, 104, 109	0
2	Н	137/326~(42%)	0.24	4 (2%) 51 48	64, 90, 106, 113	0
All	All	1296/2536~(51%)	0.21	29 (2%) 62 60	35, 76, 102, 122	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	261	LEU	3.9
2	В	260	LEU	3.8
2	В	344	GLN	3.0
1	А	448	ASN	3.0
2	F	279	ARG	2.9
2	В	343	LEU	2.8
2	F	253	ILE	2.7
2	В	254	VAL	2.6
2	D	260	LEU	2.6
2	F	282	ILE	2.5
2	Н	347	VAL	2.4
2	D	276	MET	2.4
2	Н	248	CYS	2.4
2	В	252	ILE	2.4
2	В	361	LEU	2.4
2	В	429	TRP	2.3



Mol	Chain	Res	Type	RSRZ
2	F	281	VAL	2.3
1	Е	435	THR	2.3
2	В	261	LEU	2.3
2	D	289	CYS	2.3
2	D	291	VAL	2.2
2	D	362	VAL	2.2
2	Н	315	LEU	2.1
2	Н	279	ARG	2.1
2	В	358	ALA	2.1
2	F	315	LEU	2.0
2	В	256	LEU	2.0
2	В	315	LEU	2.0
2	F	249	LEU	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
4	MG	С	602	1/1	0.93	0.24	$51,\!51,\!51,\!51$	0
3	A1IA6	С	601	21/21	0.94	0.23	66,67,67,67	0
3	A1IA6	А	601	21/21	0.95	0.23	53,54,54,54	0
4	MG	G	603	1/1	0.95	0.15	24,24,24,24	0
3	A1IA6	Е	601	21/21	0.96	0.21	60,61,63,63	0
4	MG	E	602	1/1	0.96	0.24	33,33,33,33	0
4	MG	А	602	1/1	0.96	0.25	37,37,37,37	0
3	A1IA6	G	601	21/21	0.97	0.21	61,62,64,64	0
4	MG	Е	603	1/1	0.98	0.18	29,29,29,29	0
4	MG	G	602	1/1	0.98	0.18	42,42,42,42	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
4	MG	С	603	1/1	0.98	0.17	$38,\!38,\!38,\!38$	0
4	MG	А	603	1/1	0.99	0.20	$27,\!27,\!27,\!27$	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.

