



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:58 PM UTC

PDB ID : 9Q75 / pdb_00009q75
Title : Crystal structure of T. cruzi EIF4E5 in complex with EIF4G1 peptide and cap-4.
Authors : Penteado, R.F.; Guimaraes, B.G.
Deposited on : 2025-08-22
Resolution : 1.77 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

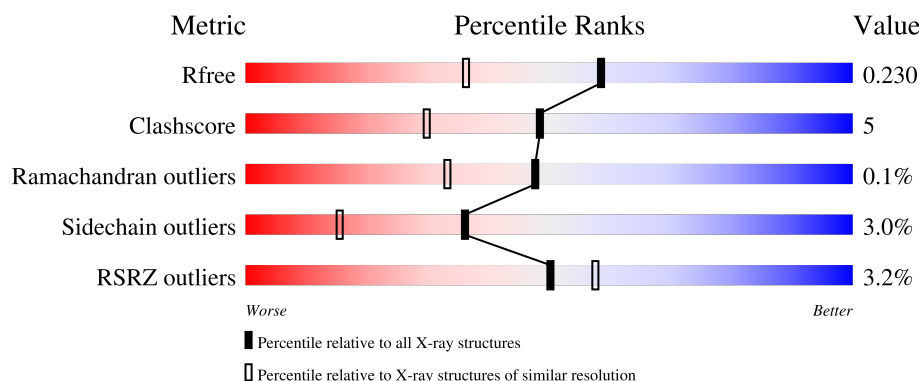
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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 $\leq 5\%$. 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	A	200	4% 81% 10% • 8%
1	C	200	2% 82% 9% • 8%
1	E	200	• 84% 8% • 8%
2	B	48	2% 79% 8% 12%
2	D	48	4% 75% 10% • 12%

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Mol	Chain	Length	Quality of chain
2	F	48	8% 77% 6% • 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6748 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 Putative Eukaryotic translation initiation factor 4E type 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	42	7	0
			1528	987	253	285	3			
1	C	185	Total	C	N	O	S	22	7	0
			1529	988	247	290	4			
1	E	185	Total	C	N	O	S	12	10	0
			1528	987	249	288	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	LYS	THR	conflict	UNP A0A2V2XI07
C	127	LYS	THR	conflict	UNP A0A2V2XI07
E	127	LYS	THR	conflict	UNP A0A2V2XI07

- Molecule 2 is a protein called Eukaryotic translation initiation factor 4 gamma 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	42	Total	C	N	O	S	3	3	0
			375	240	75	58	2			
2	D	42	Total	C	N	O	S	3	1	0
			361	232	69	58	2			
2	F	42	Total	C	N	O	S	13	0	0
			350	226	65	57	2			

There are 24 discrepancies between the modelled and reference sequences:

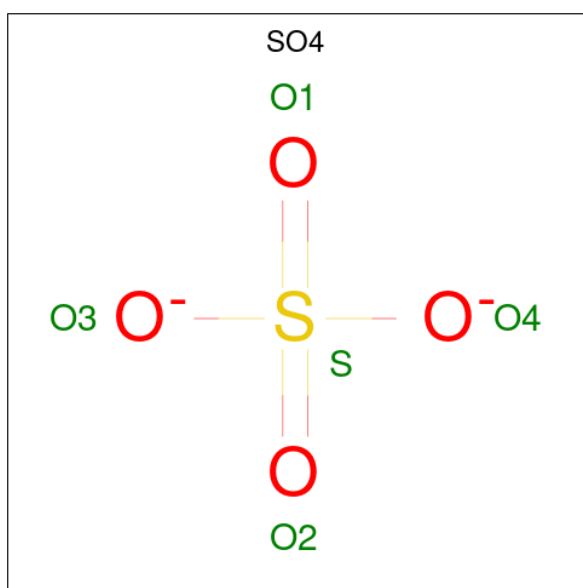
Chain	Residue	Modelled	Actual	Comment	Reference
B	106	MET	-	initiating methionine	UNP A0A2V2UXK5
B	107	GLY	-	expression tag	UNP A0A2V2UXK5
B	148	HIS	-	expression tag	UNP A0A2V2UXK5
B	149	HIS	-	expression tag	UNP A0A2V2UXK5
B	150	HIS	-	expression tag	UNP A0A2V2UXK5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	151	HIS	-	expression tag	UNP A0A2V2UXK5
B	152	HIS	-	expression tag	UNP A0A2V2UXK5
B	153	HIS	-	expression tag	UNP A0A2V2UXK5
D	106	MET	-	initiating methionine	UNP A0A2V2UXK5
D	107	GLY	-	expression tag	UNP A0A2V2UXK5
D	148	HIS	-	expression tag	UNP A0A2V2UXK5
D	149	HIS	-	expression tag	UNP A0A2V2UXK5
D	150	HIS	-	expression tag	UNP A0A2V2UXK5
D	151	HIS	-	expression tag	UNP A0A2V2UXK5
D	152	HIS	-	expression tag	UNP A0A2V2UXK5
D	153	HIS	-	expression tag	UNP A0A2V2UXK5
F	106	MET	-	initiating methionine	UNP A0A2V2UXK5
F	107	GLY	-	expression tag	UNP A0A2V2UXK5
F	148	HIS	-	expression tag	UNP A0A2V2UXK5
F	149	HIS	-	expression tag	UNP A0A2V2UXK5
F	150	HIS	-	expression tag	UNP A0A2V2UXK5
F	151	HIS	-	expression tag	UNP A0A2V2UXK5
F	152	HIS	-	expression tag	UNP A0A2V2UXK5
F	153	HIS	-	expression tag	UNP A0A2V2UXK5

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



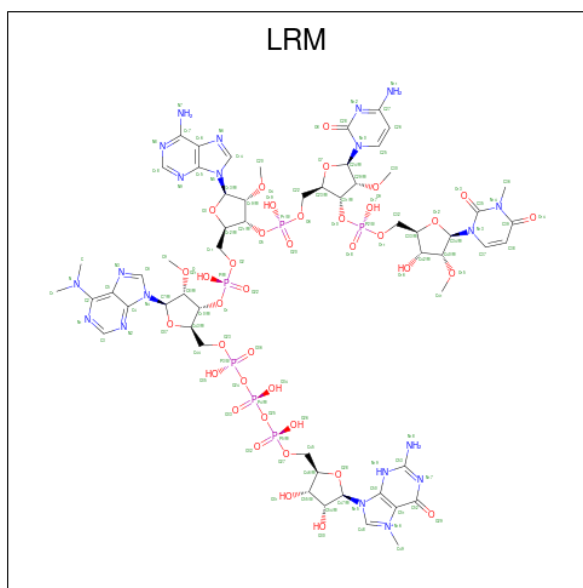
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-amino-9-[(2R,3R,4S,5R)-5-({[(R)-{[(R)-{(S)-{(2R,3R,4R,5R)-3-{[(R)-{[(2R,3R,4R,5R)-3-{[(S)-{[(2R,3R,4R,5R)-5-(4-amino-2-oxypyrimidin-1(2H)-yl)-3-{[(S)-hydroxy{[(2R,3R,4R,5R)-3-hydroxy-4-methoxy-5-(3-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-2-yl]methoxy}phosphoryl]oxy}-4-methoxytetrahydrofuran-2-yl]methoxy} (hydroxy)phosphoryl]oxy}-5-(6-amino-9H-purin-9-yl)-4-methoxytetrahydrofuran-2-yl]methoxy} (hydroxy)phosphoryl]oxy}-5-[6-(dimethylamino)-9H-purin-9-yl]-4-methoxytetrahydrofuran-2-yl}methoxy} (hydroxy)phosphoryl]oxy} (hydroxy)phosphoryl]oxy} (hydroxy)phosphoryl]oxy}methyl)-3,4-dihydroxytetrahydrofuran-2-yl]-7-methyl-6-oxo-6,9-dihydro-3H-purin-7-ium (CCD ID: LRM) (formula: C₅₆H₇₉N₂₀O₃₈P₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	1
			240	112	40	76	12		
4	E	1	Total	C	N	O	P	0	1
			240	112	40	76	12		

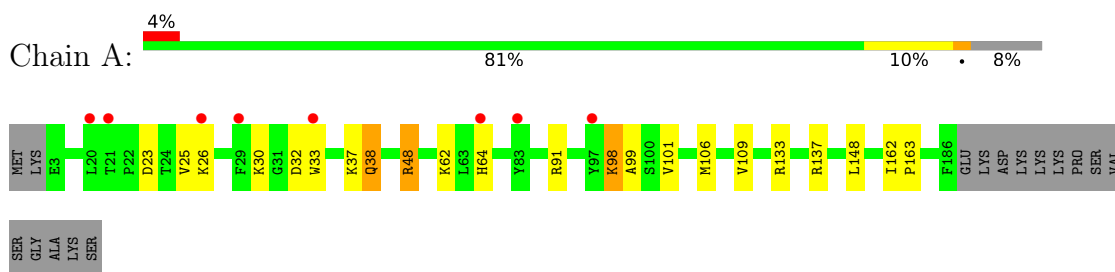
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total 143	O 143	0	0
5	C	168	Total 168	O 168	0	0
5	E	160	Total 160	O 160	0	0
5	B	30	Total 30	O 30	0	0
5	D	36	Total 36	O 36	0	0
5	F	35	Total 35	O 35	0	0

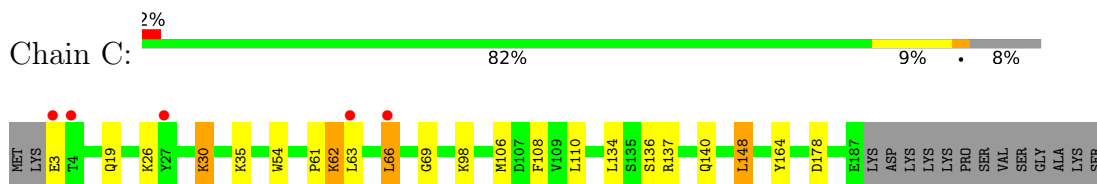
3 Residue-property plots

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.

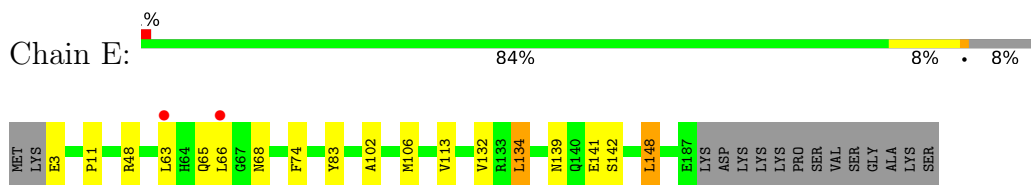
- Molecule 1: Putative Eukaryotic translation initiation factor 4E type 5



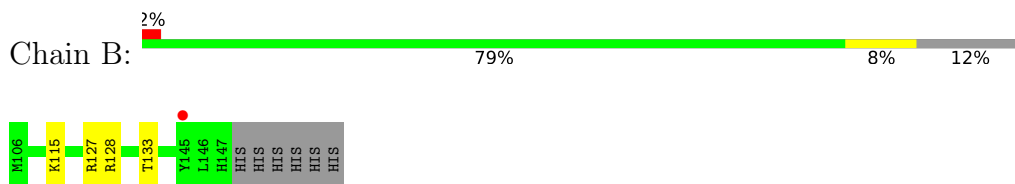
- Molecule 1: Putative Eukaryotic translation initiation factor 4E type 5



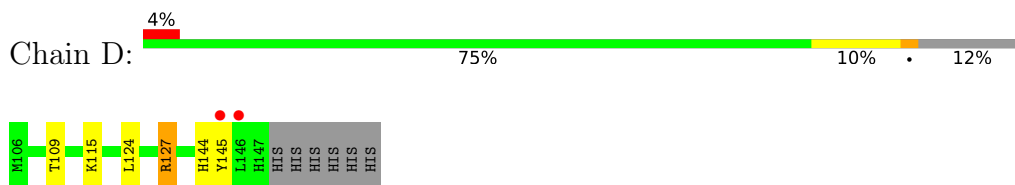
- Molecule 1: Putative Eukaryotic translation initiation factor 4E type 5



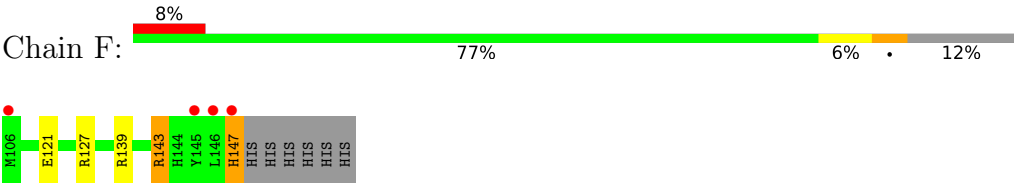
- Molecule 2: Eukaryotic translation initiation factor 4 gamma 1



- Molecule 2: Eukaryotic translation initiation factor 4 gamma 1



● Molecule 2: Eukaryotic translation initiation factor 4 gamma 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.38Å 88.89Å 110.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.21 – 1.77 25.21 – 1.77	Depositor EDS
% Data completeness (in resolution range)	79.0 (25.21-1.77) 79.4 (25.21-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.158 , 0.215 0.180 , 0.230	Depositor DCC
R_{free} test set	3398 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6748	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LRM

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	2/1579 (0.1%)	1.02	4/2142 (0.2%)
1	C	0.67	3/1575 (0.2%)	1.04	3/2138 (0.1%)
1	E	0.59	0/1599	1.03	3/2170 (0.1%)
2	B	0.74	1/395 (0.3%)	1.06	1/533 (0.2%)
2	D	0.74	1/373 (0.3%)	1.09	2/505 (0.4%)
2	F	0.77	1/362 (0.3%)	0.98	1/491 (0.2%)
All	All	0.68	8/5883 (0.1%)	1.04	14/7979 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	1
2	B	0	2
2	D	0	1
2	F	0	1
All	All	0	8

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	LYS	CG-CD	-12.32	1.15	1.52
2	B	115	LYS	CG-CD	-9.76	1.23	1.52
1	A	98	LYS	CG-CD	-8.82	1.25	1.52
2	F	147	HIS	CB-CG	8.44	1.61	1.50
1	C	140	GLN	CB-CG	-5.71	1.35	1.52
2	D	115	LYS	CG-CD	-5.45	1.36	1.52
1	C	35	LYS	CG-CD	-5.21	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	30	LYS	CG-CD	-5.19	1.36	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	GLN	CA-CB-CG	8.26	130.63	114.10
1	A	23	ASP	CA-CB-CG	7.71	120.31	112.60
1	A	38	GLN	CA-CB-CG	-6.24	101.62	114.10
2	D	115	LYS	CB-CG-CD	5.82	124.69	111.30
1	A	23	ASP	CB-CG-OD2	5.58	131.23	118.40
1	C	108	PHE	CA-CB-CG	-5.54	108.27	113.80
1	E	68	ASN	CB-CA-C	5.41	118.68	109.80
2	B	133	THR	CA-CB-OG1	-5.37	101.55	109.60
1	E	134	LEU	N-CA-CB	-5.33	101.58	110.80
1	C	35	LYS	CB-CG-CD	5.26	123.39	111.30
2	D	109	THR	CA-CB-OG1	-5.18	101.83	109.60
1	A	98	LYS	CB-CG-CD	5.07	122.95	111.30
1	E	65	GLN	CA-CB-CG	-5.05	104.00	114.10
2	F	139	ARG	CD-NE-CZ	5.03	131.44	124.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ARG	Sidechain
1	A	48[A]	ARG	Sidechain
1	A	91	ARG	Sidechain
2	B	127[A]	ARG	Sidechain
2	B	127[B]	ARG	Sidechain
1	C	137	ARG	Sidechain
2	D	127[A]	ARG	Sidechain
2	F	143	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	A	1528	0	1512	11	0
1	C	1529	0	1509	18	0
1	E	1528	0	1512	30	0
2	B	375	0	374	0	0
2	D	361	0	352	7	0
2	F	350	0	340	2	0
3	A	15	0	0	1	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
4	C	240	0	0	0	0
4	E	240	0	0	2	0
5	A	143	0	0	2	0
5	B	30	0	0	0	0
5	C	168	0	0	2	0
5	D	36	0	0	0	0
5	E	160	0	0	0	0
5	F	35	0	0	1	0
All	All	6748	0	5599	63	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 5.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106[B]:MET:HE2	1:E:148[B]:LEU:HD21	1.22	1.16
1:E:106[B]:MET:CE	1:E:148[B]:LEU:HD21	1.76	1.16
1:E:106[B]:MET:CE	1:E:148[B]:LEU:CD2	2.36	1.04
1:E:106[B]:MET:CE	1:E:148[B]:LEU:CG	2.37	1.02
1:E:106[B]:MET:HE1	1:E:148[B]:LEU:HG	1.45	0.98
1:E:106[B]:MET:HE1	1:E:148[B]:LEU:CD2	1.95	0.96
1:E:106[B]:MET:HE1	1:E:148[B]:LEU:CG	1.97	0.93
1:E:106[B]:MET:CE	1:E:148[B]:LEU:HG	2.00	0.91
1:A:48[B]:ARG:NH2	5:A:401:HOH:O	2.02	0.90
1:E:106[B]:MET:HE2	1:E:148[B]:LEU:CD2	2.00	0.85
1:E:106[B]:MET:CE	1:E:148[B]:LEU:HD11	2.14	0.77
1:C:61:PRO:HG3	2:D:145:TYR:CZ	2.22	0.75
1:E:106[B]:MET:CE	1:E:148[B]:LEU:CD1	2.65	0.73
1:C:63:LEU:HD13	1:C:106[B]:MET:CE	2.20	0.72
2:D:124:LEU:O	2:D:127[B]:ARG:HG3	1.92	0.69
2:F:143:ARG:HH12	2:F:147:HIS:HB3	1.57	0.69
1:C:106[B]:MET:CG	1:C:148:LEU:HD11	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:PRO:HG3	2:D:145:TYR:OH	1.96	0.65
1:E:106[B]:MET:HE2	1:E:148[B]:LEU:HD11	1.79	0.64
1:E:106[B]:MET:HE3	1:E:148[B]:LEU:HD11	1.79	0.64
1:E:139[A]:ASN:OD1	1:E:142:SER:N	2.30	0.63
1:C:106[B]:MET:HG2	1:C:148:LEU:HD11	1.80	0.63
1:A:106:MET:HG2	1:A:148[A]:LEU:HD11	1.80	0.63
1:C:164:TYR:OH	5:C:401:HOH:O	2.16	0.61
1:E:63:LEU:HD22	1:E:106[B]:MET:HG3	1.85	0.59
1:C:19:GLN:HG3	1:C:69:GLY:HA3	1.84	0.58
1:E:106[B]:MET:HE3	1:E:148[B]:LEU:CD1	2.32	0.58
1:C:54:TRP:CE3	2:D:127[A]:ARG:HD2	2.40	0.57
1:E:11:PRO:HB3	1:E:48[B]:ARG:HG2	1.86	0.57
1:C:63:LEU:HD13	1:C:106[B]:MET:HE3	1.87	0.57
1:C:66:LEU:CD1	1:C:136:SER:HB2	2.34	0.57
1:C:98[A]:LYS:NZ	5:C:408:HOH:O	2.37	0.56
1:A:109:VAL:HG11	1:A:148[B]:LEU:HD21	1.89	0.54
1:A:106:MET:CG	1:A:148[A]:LEU:HD11	2.38	0.53
1:E:83:TYR:OH	4:E:301[B]:LRM:O33	2.24	0.51
1:C:106[A]:MET:HA	1:C:148:LEU:HD21	1.94	0.50
1:E:106[B]:MET:HA	1:E:148[B]:LEU:HD11	1.93	0.50
2:F:127:ARG:NH1	5:F:201:HOH:O	2.40	0.50
1:A:162:ILE:HB	1:A:163[A]:PRO:HD3	1.94	0.50
2:D:144:HIS:HD2	2:D:145:TYR:CE1	2.30	0.50
1:E:83:TYR:OH	4:E:301[A]:LRM:O33	2.26	0.49
1:C:106[B]:MET:HA	1:C:148:LEU:HD21	1.95	0.49
1:E:106[B]:MET:HE2	1:E:148[B]:LEU:CD1	2.40	0.49
1:A:137:ARG:NH2	5:A:410:HOH:O	2.45	0.49
1:E:63:LEU:HD11	1:E:106[B]:MET:SD	2.53	0.48
1:E:113:VAL:HG21	1:E:132[B]:VAL:HG11	1.95	0.48
1:E:63:LEU:O	1:E:66:LEU:HG	2.14	0.48
1:E:113:VAL:HG11	1:E:132[A]:VAL:CG2	2.44	0.48
1:C:54:TRP:CZ3	2:D:127[A]:ARG:HD2	2.49	0.48
1:A:64[B]:HIS:CD2	1:A:99:ALA:HB1	2.50	0.47
1:A:106:MET:HE1	3:A:302:SO4:O3	2.15	0.47
1:A:109:VAL:HG11	1:A:148[B]:LEU:CD2	2.45	0.47
1:C:110:LEU:HD11	1:C:134[B]:LEU:HD11	1.97	0.47
1:E:102:ALA:O	1:E:106[B]:MET:HG2	2.15	0.46
1:C:63:LEU:HD13	1:C:106[B]:MET:SD	2.55	0.46
1:C:54:TRP:CZ3	2:D:127[A]:ARG:CD	2.99	0.45
1:E:63:LEU:HD13	1:E:106[A]:MET:SD	2.56	0.45
1:A:64[B]:HIS:NE2	1:A:99:ALA:HB1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG11	1:A:33:TRP:CD1	2.52	0.44
1:C:98[B]:LYS:HD2	1:C:178:ASP:OD1	2.19	0.43
1:E:74:PHE:HB2	1:E:132[B]:VAL:HG23	2.00	0.41
1:E:106[B]:MET:SD	1:E:134:LEU:CD1	3.09	0.41
1:E:113:VAL:HG11	1:E:132[A]:VAL:HG23	2.02	0.41

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	A	189/200 (94%)	184 (97%)	5 (3%)	0	100	100
1	C	190/200 (95%)	185 (97%)	4 (2%)	1 (0%)	24	11
1	E	193/200 (96%)	188 (97%)	5 (3%)	0	100	100
2	B	43/48 (90%)	43 (100%)	0	0	100	100
2	D	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
2	F	40/48 (83%)	40 (100%)	0	0	100	100
All	All	696/744 (94%)	680 (98%)	15 (2%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	62	LYS

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 analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/176 (96%)	162 (96%)	7 (4%)	27	8
1	C	170/176 (97%)	164 (96%)	6 (4%)	32	11
1	E	173/176 (98%)	169 (98%)	4 (2%)	44	25
2	B	38/41 (93%)	36 (95%)	2 (5%)	20	4
2	D	36/41 (88%)	36 (100%)	0	100	100
2	F	35/41 (85%)	34 (97%)	1 (3%)	37	16
All	All	621/651 (95%)	601 (97%)	20 (3%)	36	13

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	30	LYS
1	A	32	ASP
1	A	37	LYS
1	A	38	GLN
1	A	98	LYS
1	A	101	VAL
1	C	3	GLU
1	C	26	LYS
1	C	30	LYS
1	C	62	LYS
1	C	66	LEU
1	C	148	LEU
1	E	3	GLU
1	E	141	GLU
1	E	148[A]	LEU
1	E	148[B]	LEU
2	B	128[A]	ARG
2	B	128[B]	ARG
2	F	121	GLU

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

Mol	Chain	Res	Type
1	A	19	GLN
1	A	41	GLN

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Mol	Chain	Res	Type
1	A	65	GLN
1	E	170	ASN
2	B	144	HIS
2	D	144	HIS
2	F	144	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	LRM	C	301[B]	-	131,132,132	0.53	1 (0%)	180,204,204	0.69	3 (1%)
3	SO4	C	302	-	4,4,4	0.27	0	6,6,6	0.11	0
3	SO4	A	301	-	4,4,4	0.35	0	6,6,6	0.18	0
4	LRM	E	301[A]	-	131,132,132	0.57	1 (0%)	180,204,204	0.77	6 (3%)
3	SO4	A	303	-	4,4,4	0.31	0	6,6,6	0.09	0
3	SO4	E	302	-	4,4,4	0.23	0	6,6,6	0.18	0
4	LRM	E	301[B]	-	131,132,132	0.57	1 (0%)	180,204,204	0.73	6 (3%)
3	SO4	A	302	-	4,4,4	0.26	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LRM	C	301[A]	-	131,132,132	0.52	1 (0%)	180,204,204	0.82	7 (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	LRM	E	301[B]	-	-	12/89/169/169	0/13/13/13
4	LRM	C	301[B]	-	-	8/89/169/169	0/13/13/13
4	LRM	E	301[A]	-	-	8/89/169/169	0/13/13/13
4	LRM	C	301[A]	-	-	8/89/169/169	0/13/13/13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	301[A]	LRM	C48-N16	3.87	1.39	1.33
4	E	301[B]	LRM	C48-N16	3.79	1.39	1.33
4	C	301[B]	LRM	C48-N16	3.44	1.38	1.33
4	C	301[A]	LRM	C48-N16	3.40	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301[A]	LRM	O37-C7-N4	3.92	115.63	108.09
4	E	301[A]	LRM	C3-N1-C2	2.99	119.14	111.83
4	C	301[A]	LRM	C3-N1-C2	2.91	118.95	111.83
4	C	301[B]	LRM	C3-N1-C2	2.87	118.85	111.83
4	C	301[A]	LRM	C52-C51-N16	2.74	135.94	131.46
4	C	301[B]	LRM	C52-C51-N16	2.69	135.88	131.46
4	E	301[B]	LRM	N1-C2-N	2.68	120.12	116.86
4	E	301[B]	LRM	C3-N1-C2	2.64	118.27	111.83
4	E	301[A]	LRM	O37-C7-C8	-2.59	102.13	106.59
4	C	301[A]	LRM	O37-C7-C8	-2.50	102.28	106.59
4	E	301[B]	LRM	C52-C51-N16	2.48	135.52	131.46
4	C	301[A]	LRM	C10-C8-C7	-2.44	97.71	103.57
4	E	301[A]	LRM	C52-C51-N16	2.37	135.34	131.46
4	C	301[A]	LRM	O29-C52-N17	-2.27	116.45	120.27
4	E	301[A]	LRM	O37-C7-N4	2.26	112.43	108.09
4	C	301[B]	LRM	O29-C52-N17	-2.26	116.47	120.27
4	E	301[B]	LRM	C5-C2-N	-2.24	121.78	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	301[A]	LRM	C10-C8-C7	-2.23	98.23	103.57
4	C	301[A]	LRM	C43-O37-C7	-2.19	104.62	109.47
4	E	301[B]	LRM	O29-C52-N17	-2.06	116.80	120.27
4	E	301[B]	LRM	C37-N13-C35	-2.02	120.15	121.80
4	E	301[A]	LRM	C37-N13-C35	-2.02	120.15	121.80

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301[A]	LRM	C8-C7-N4-C6
4	C	301[A]	LRM	C10-O1-P-O2
4	C	301[B]	LRM	C5-C2-N-C
4	C	301[B]	LRM	C10-O1-P-O2
4	E	301[A]	LRM	C8-C7-N4-C6
4	E	301[A]	LRM	C44-O23-P3-O24
4	E	301[A]	LRM	C44-O23-P3-O36
4	E	301[B]	LRM	C5-C2-N-C
4	E	301[B]	LRM	N1-C2-N-C
4	E	301[B]	LRM	C10-O1-P-O22
4	E	301[B]	LRM	C10-O1-P-O2
4	E	301[B]	LRM	O37-C43-C44-O23
4	E	301[B]	LRM	C10-C43-C44-O23
4	C	301[A]	LRM	C8-C7-N4-C4
4	C	301[B]	LRM	N1-C2-N-C
4	E	301[A]	LRM	P3-O24-P4-O33
4	E	301[B]	LRM	C5-C2-N-C1
4	C	301[A]	LRM	P4-O25-P5-O32
4	C	301[A]	LRM	C10-O1-P-O21
4	E	301[B]	LRM	N1-C2-N-C1
4	E	301[A]	LRM	C44-O23-P3-O35
4	E	301[A]	LRM	C8-C7-N4-C4
4	E	301[A]	LRM	O2-C11-C12-C21
4	C	301[B]	LRM	C5-C2-N-C1
4	E	301[B]	LRM	C8-C10-O1-P
4	C	301[A]	LRM	P4-O25-P5-O26
4	C	301[B]	LRM	P4-O24-P3-O35
4	C	301[B]	LRM	C10-O1-P-O22
4	E	301[B]	LRM	P4-O24-P3-O35
4	E	301[B]	LRM	C43-C10-O1-P
4	C	301[A]	LRM	P4-O24-P3-O36
4	C	301[A]	LRM	P4-O24-P3-O35

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Mol	Chain	Res	Type	Atoms
4	C	301[B]	LRM	P4-O25-P5-O32
4	C	301[B]	LRM	P4-O25-P5-O26
4	E	301[A]	LRM	P4-O24-P3-O35
4	E	301[B]	LRM	P4-O24-P3-O36

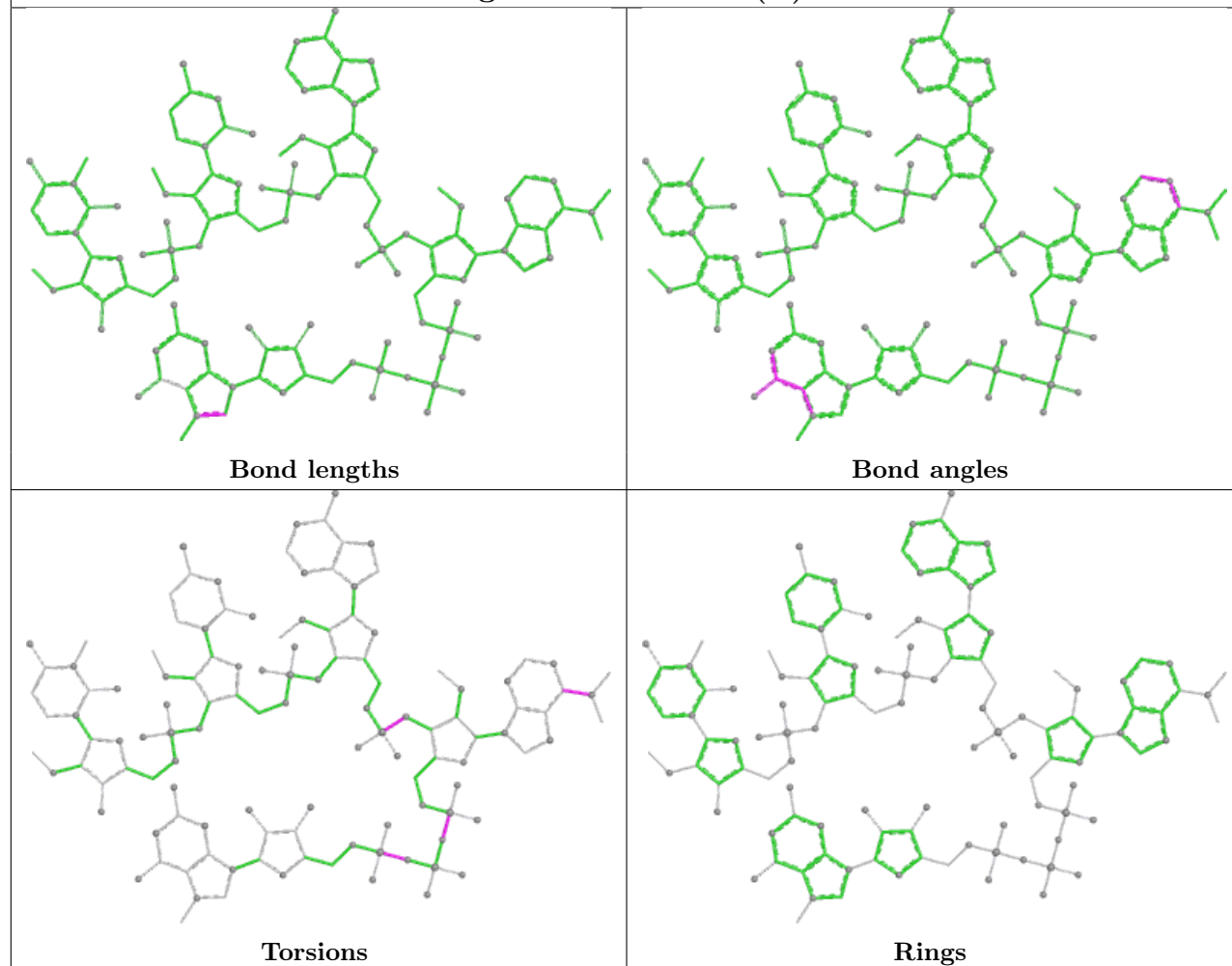
There are no ring outliers.

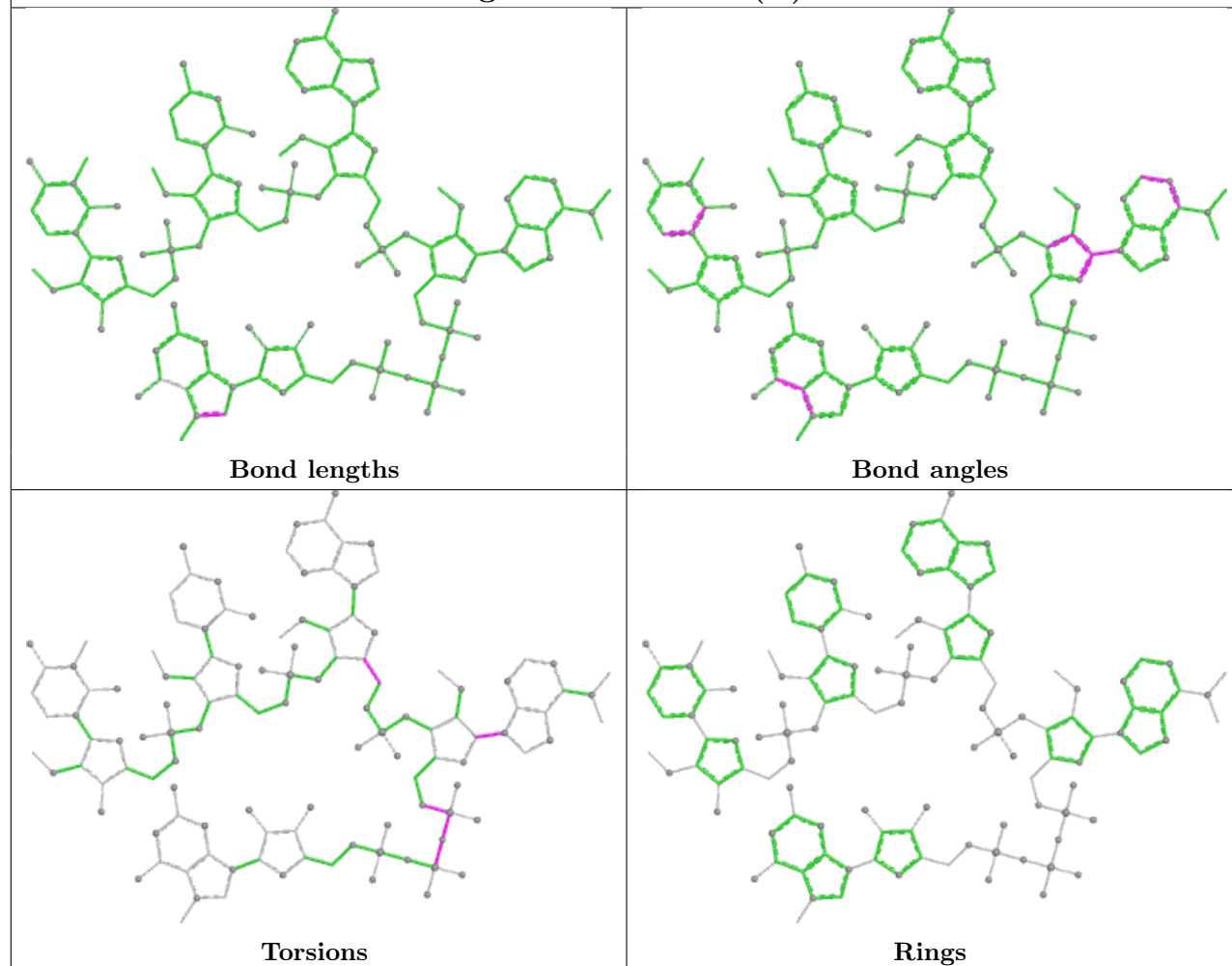
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	301[A]	LRM	1	0
4	E	301[B]	LRM	1	0
3	A	302	SO4	1	0

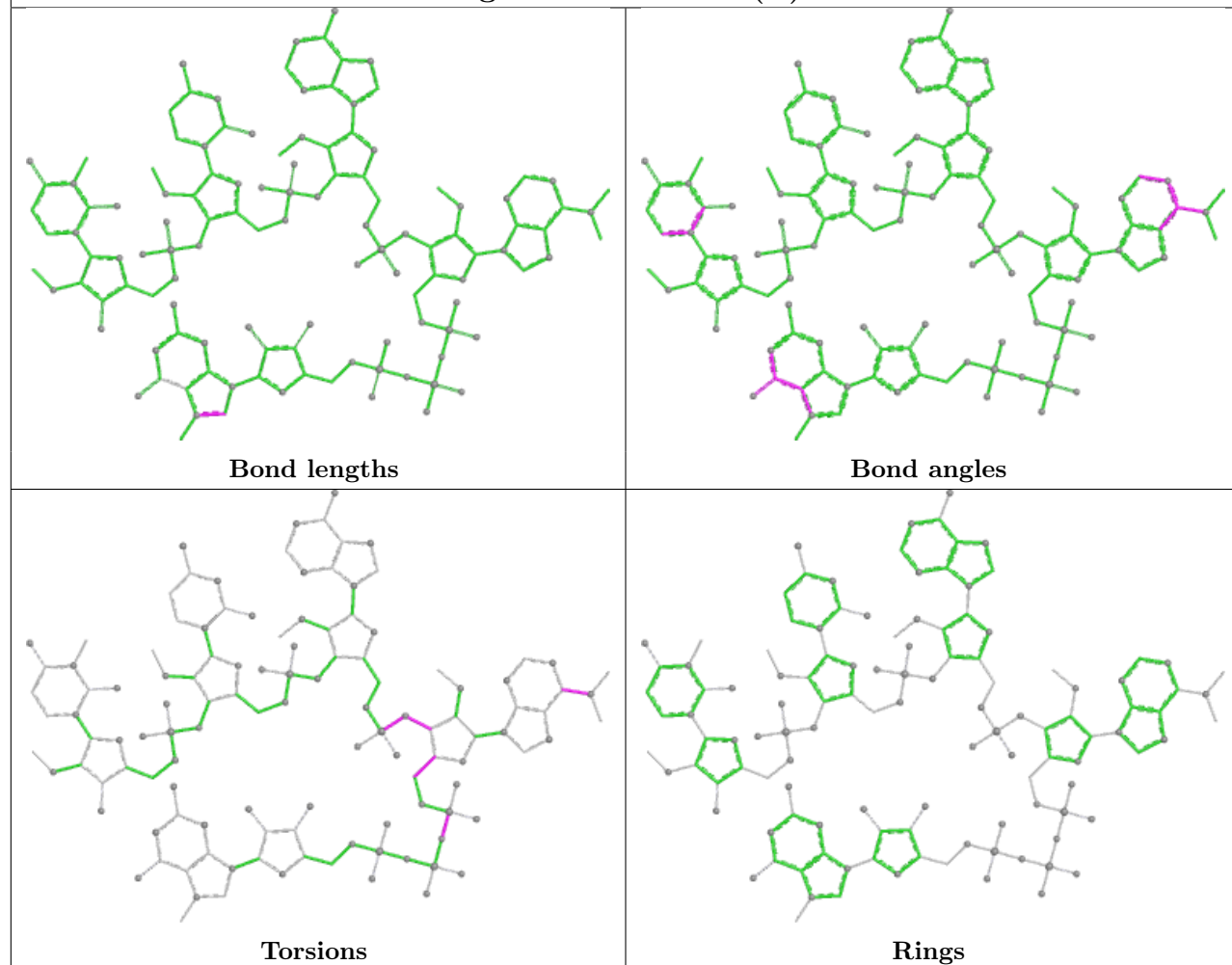
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

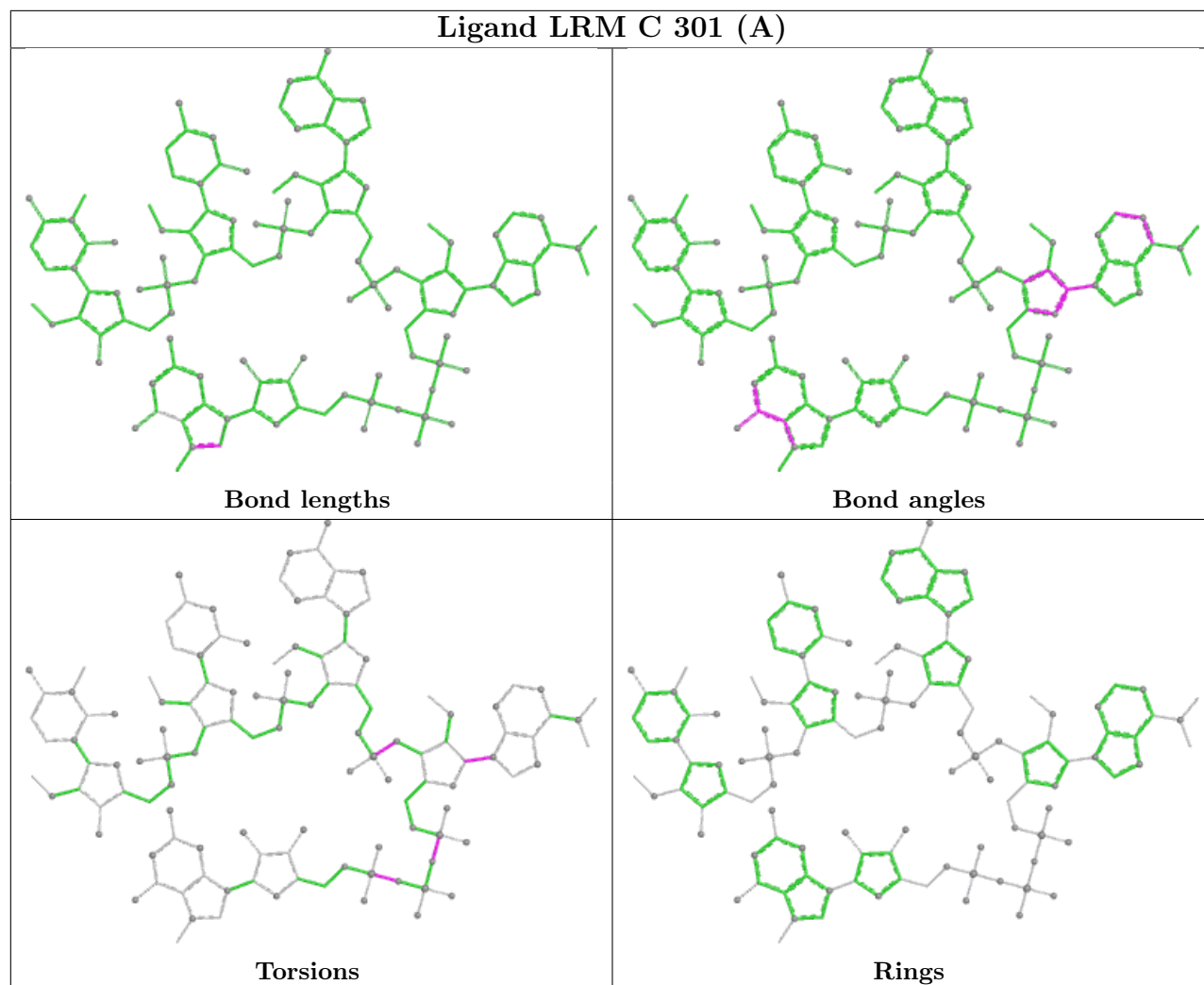
Ligand LRM C 301 (B)



Ligand LRM E 301 (A)

Ligand LRM E 301 (B)





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	A	184/200 (92%)	0.06	8 (4%)	40	45	10, 23, 56, 83	23 (12%)
1	C	185/200 (92%)	-0.11	5 (2%)	56	63	10, 22, 48, 93	14 (7%)
1	E	185/200 (92%)	-0.14	2 (1%)	78	84	12, 24, 48, 112	14 (7%)
2	B	42/48 (87%)	-0.00	1 (2%)	59	68	14, 21, 40, 72	5 (11%)
2	D	42/48 (87%)	-0.07	2 (4%)	35	41	11, 20, 33, 70	5 (11%)
2	F	42/48 (87%)	0.05	4 (9%)	14	15	15, 24, 42, 55	5 (11%)
All	All	680/744 (91%)	-0.06	22 (3%)	50	57	10, 23, 52, 112	66 (9%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	TRP	6.1
1	C	63	LEU	5.7
1	E	63	LEU	3.9
1	C	66	LEU	3.8
1	A	83	TYR	3.6
2	F	145	TYR	3.2
1	A	64[A]	HIS	3.2
1	E	66	LEU	3.1
1	C	3	GLU	3.1
2	D	145	TYR	2.9
1	A	29	PHE	2.8
1	C	4	THR	2.8
2	F	146	LEU	2.8
1	A	21	THR	2.5
1	A	97	TYR	2.3
2	F	147	HIS	2.3
1	A	20	LEU	2.3
2	D	146	LEU	2.3
1	C	27	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	26	LYS	2.2
2	B	145	TYR	2.1
2	F	106	MET	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

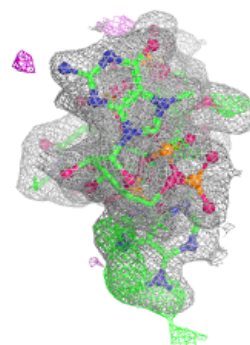
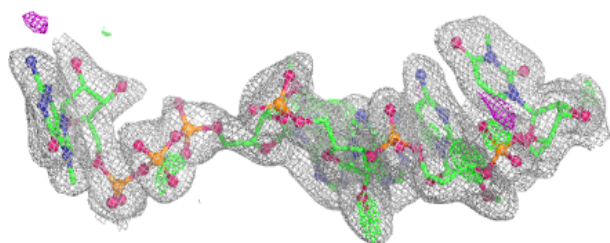
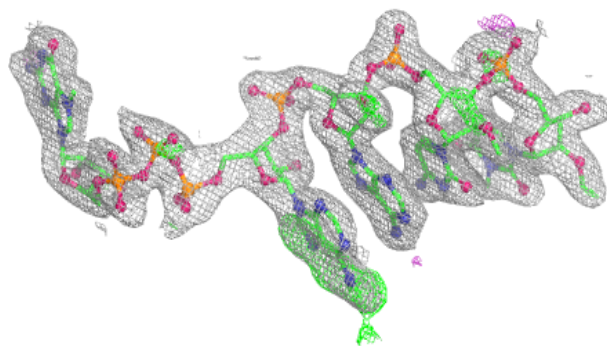
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	303	5/5	0.76	0.10	91,97,106,110	0
3	SO4	C	302	5/5	0.86	0.12	61,72,75,78	0
4	LRM	E	301[A]	120/120	0.92	0.09	24,30,46,58	120
4	LRM	E	301[B]	120/120	0.92	0.09	28,37,66,86	120
3	SO4	A	302	5/5	0.93	0.08	59,60,67,71	5
3	SO4	A	301	5/5	0.94	0.08	49,63,66,71	0
4	LRM	C	301[B]	120/120	0.95	0.08	24,35,66,72	120
3	SO4	E	302	5/5	0.95	0.07	44,56,62,65	0
4	LRM	C	301[A]	120/120	0.95	0.08	29,35,50,57	120

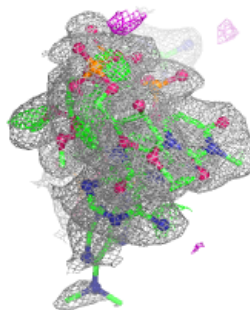
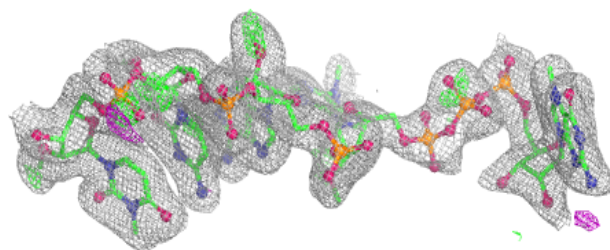
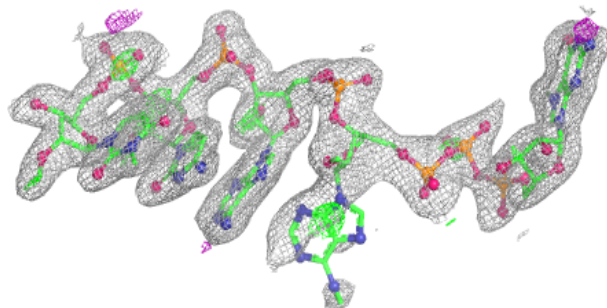
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LRM E 301 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

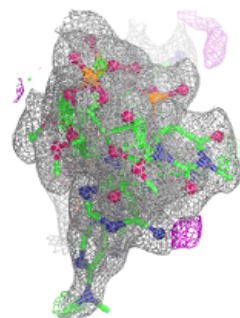
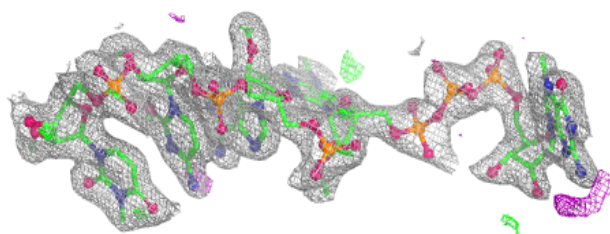
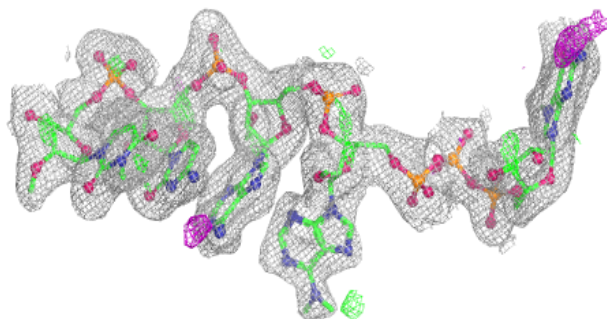
**Electron density around LRM E 301 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

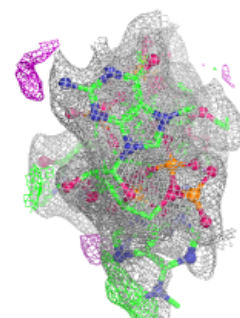
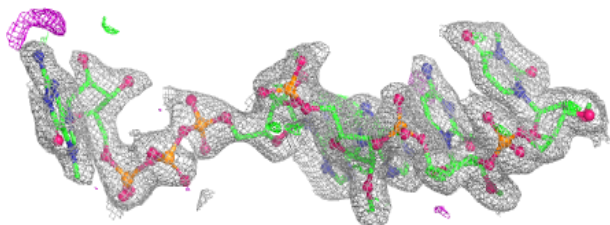
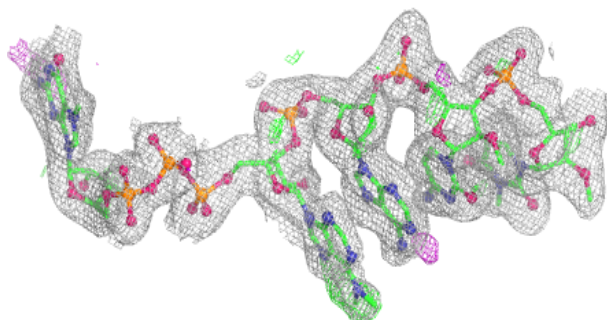


Electron density around LRM C 301 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LRM C 301 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.