



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:33 PM UTC

PDB ID : 6K2M / pdb_00006k2m
Title : Crystal structure of the complex of Proliferating Cell Nuclear Antigen from *Leishmania donovani* with arginine at 3.19 Å resolution.
Authors : Viswanathan, V.; Iqbal, N.; Sharma, S.; Singh, T.P.
Deposited on : 2019-05-15
Resolution : 3.19 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:

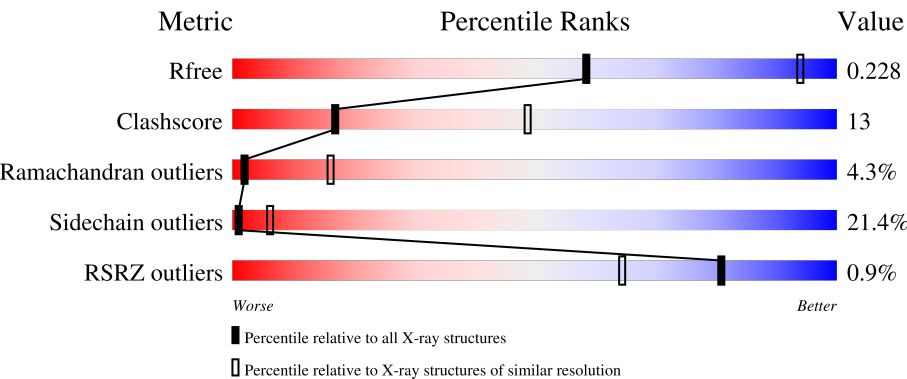
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	302	% 55%21%6%18%
1	B	302	% 52%24%6%18%
1	C	302	% 45%30%6%18%
1	D	302	49%27%6%17%
1	E	302	% 54%22%9%15%

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Mol	Chain	Length	Quality of chain
1	F	302	% 46% 27% 8% • 18%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11702 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	D	251	Total	C	N	O	S	0	0	0
			1941	1222	320	384	15			
1	E	258	Total	C	N	O	S	0	0	0
			1988	1251	332	390	15			
1	B	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	C	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	F	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP B5TV91
A	-8	SER	-	expression tag	UNP B5TV91
A	-7	GLY	-	expression tag	UNP B5TV91
A	-6	ARG	-	expression tag	UNP B5TV91
A	-5	PRO	-	expression tag	UNP B5TV91
A	-4	VAL	-	expression tag	UNP B5TV91
A	-3	LEU	-	expression tag	UNP B5TV91
A	-2	GLY	-	expression tag	UNP B5TV91
A	-1	SER	-	expression tag	UNP B5TV91
A	0	SER	-	expression tag	UNP B5TV91
D	-9	HIS	-	expression tag	UNP B5TV91
D	-8	SER	-	expression tag	UNP B5TV91
D	-7	GLY	-	expression tag	UNP B5TV91
D	-6	ARG	-	expression tag	UNP B5TV91
D	-5	PRO	-	expression tag	UNP B5TV91
D	-4	VAL	-	expression tag	UNP B5TV91
D	-3	LEU	-	expression tag	UNP B5TV91

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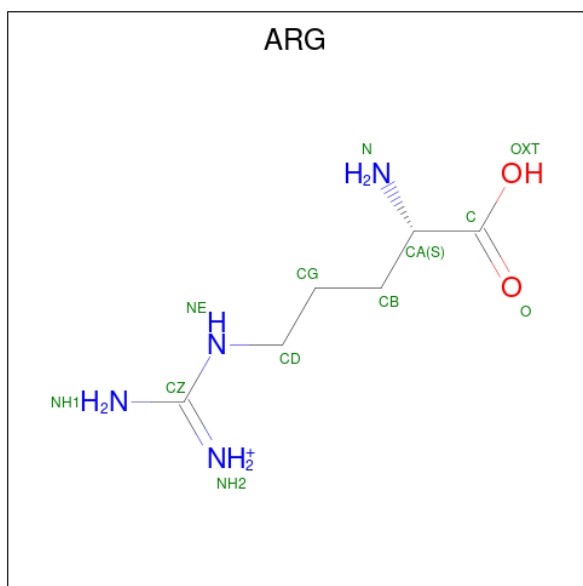
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP B5TV91
D	-1	SER	-	expression tag	UNP B5TV91
D	0	SER	-	expression tag	UNP B5TV91
E	-9	HIS	-	expression tag	UNP B5TV91
E	-8	SER	-	expression tag	UNP B5TV91
E	-7	GLY	-	expression tag	UNP B5TV91
E	-6	ARG	-	expression tag	UNP B5TV91
E	-5	PRO	-	expression tag	UNP B5TV91
E	-4	VAL	-	expression tag	UNP B5TV91
E	-3	LEU	-	expression tag	UNP B5TV91
E	-2	GLY	-	expression tag	UNP B5TV91
E	-1	SER	-	expression tag	UNP B5TV91
E	0	SER	-	expression tag	UNP B5TV91
B	-9	HIS	-	expression tag	UNP B5TV91
B	-8	SER	-	expression tag	UNP B5TV91
B	-7	GLY	-	expression tag	UNP B5TV91
B	-6	ARG	-	expression tag	UNP B5TV91
B	-5	PRO	-	expression tag	UNP B5TV91
B	-4	VAL	-	expression tag	UNP B5TV91
B	-3	LEU	-	expression tag	UNP B5TV91
B	-2	GLY	-	expression tag	UNP B5TV91
B	-1	SER	-	expression tag	UNP B5TV91
B	0	SER	-	expression tag	UNP B5TV91
C	-9	HIS	-	expression tag	UNP B5TV91
C	-8	SER	-	expression tag	UNP B5TV91
C	-7	GLY	-	expression tag	UNP B5TV91
C	-6	ARG	-	expression tag	UNP B5TV91
C	-5	PRO	-	expression tag	UNP B5TV91
C	-4	VAL	-	expression tag	UNP B5TV91
C	-3	LEU	-	expression tag	UNP B5TV91
C	-2	GLY	-	expression tag	UNP B5TV91
C	-1	SER	-	expression tag	UNP B5TV91
C	0	SER	-	expression tag	UNP B5TV91
F	-9	HIS	-	expression tag	UNP B5TV91
F	-8	SER	-	expression tag	UNP B5TV91
F	-7	GLY	-	expression tag	UNP B5TV91
F	-6	ARG	-	expression tag	UNP B5TV91
F	-5	PRO	-	expression tag	UNP B5TV91
F	-4	VAL	-	expression tag	UNP B5TV91
F	-3	LEU	-	expression tag	UNP B5TV91
F	-2	GLY	-	expression tag	UNP B5TV91
F	-1	SER	-	expression tag	UNP B5TV91

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP B5TV91

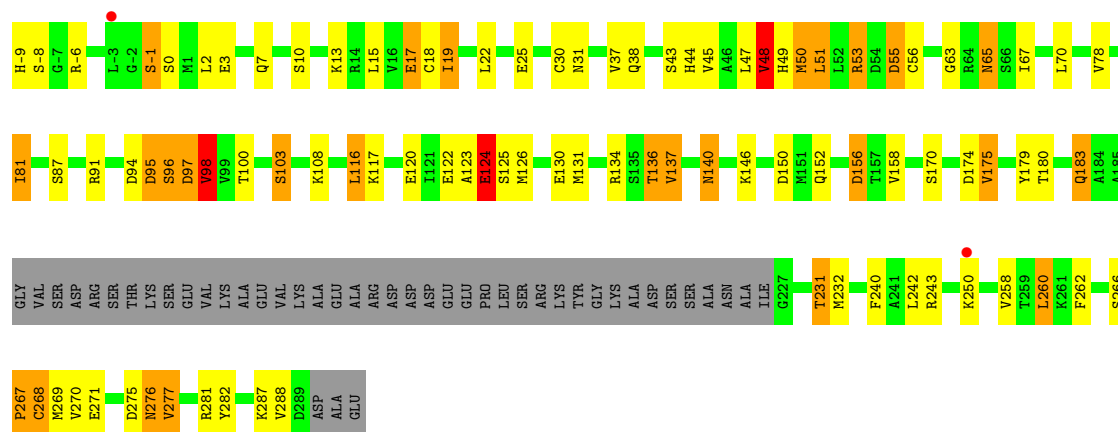
- Molecule 2 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



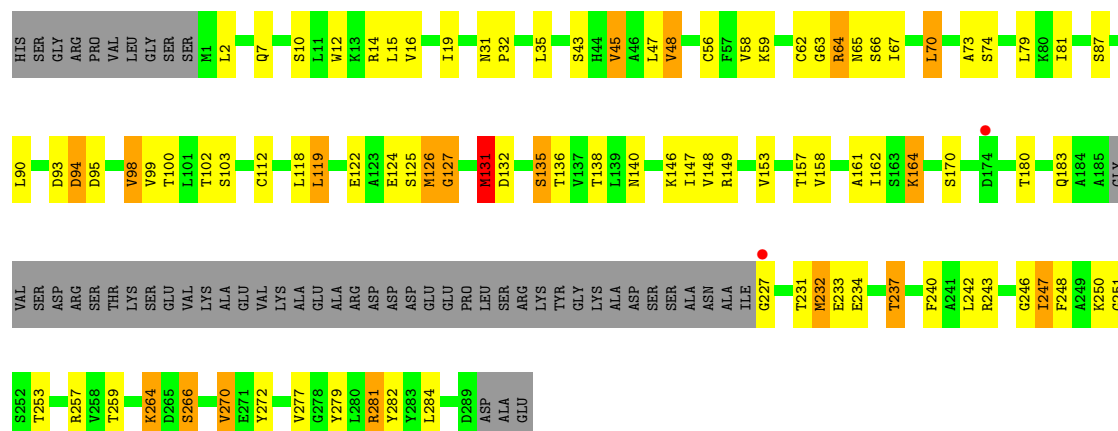
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		
2	E	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 3 is water.

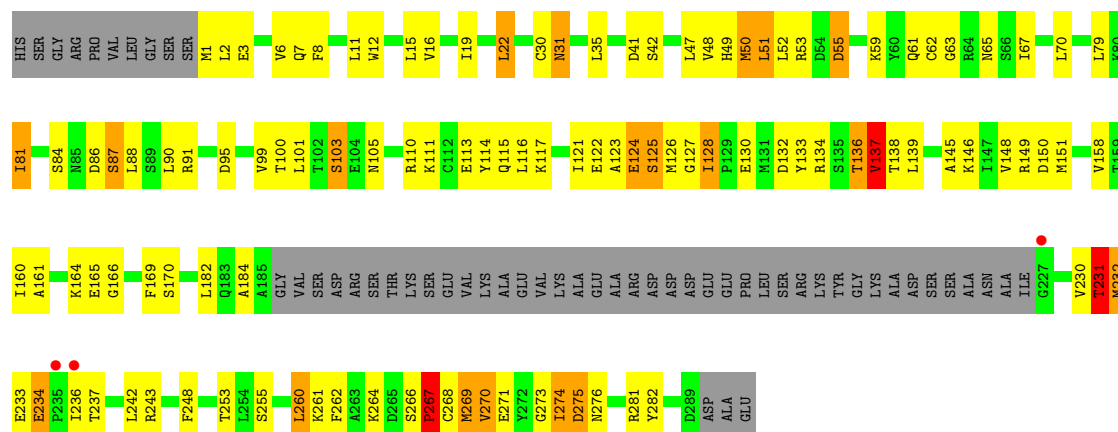
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	D	22	Total	O	0	0
			22	22		
3	E	8	Total	O	0	0
			8	8		
3	B	8	Total	O	0	0
			8	8		
3	C	10	Total	O	0	0
			10	10		
3	F	9	Total	O	0	0
			9	9		



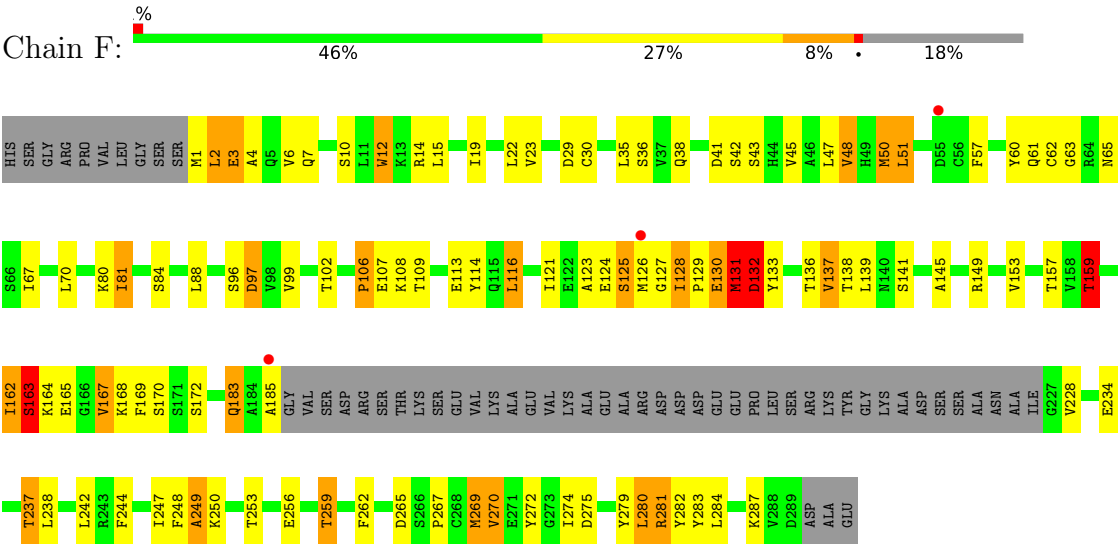
● Molecule 1: Proliferating cell nuclear antigen



● Molecule 1: Proliferating cell nuclear antigen



● Molecule 1: Proliferating cell nuclear antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.93Å 150.59Å 171.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.63 – 3.19 106.63 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (106.63-3.19) 99.4 (106.63-3.19)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.167 , 0.227 (Not available) , 0.228	Depositor DCC
R_{free} test set	3020 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	111.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 93.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11702	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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

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	1.03	0/1947	1.52	8/2627 (0.3%)
1	B	1.08	0/1947	1.49	6/2627 (0.2%)
1	C	1.06	0/1947	1.52	5/2627 (0.2%)
1	D	1.11	0/1969	1.50	4/2657 (0.2%)
1	E	1.08	0/2018	1.52	9/2723 (0.3%)
1	F	1.11	1/1947 (0.1%)	1.49	7/2627 (0.3%)
All	All	1.08	1/11775 (0.0%)	1.51	39/15888 (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	1
1	B	0	2
1	C	0	2
1	D	0	3
1	E	0	1
1	F	0	3
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	270	VAL	C-O	5.36	1.29	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ASN	CA-C-N	7.02	130.68	120.71
1	B	65	ASN	C-N-CA	7.02	130.68	120.71
1	F	159	THR	CA-CB-OG1	-6.59	99.72	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	55	ASP	CA-CB-CG	6.41	119.01	112.60
1	E	49	HIS	CB-CA-C	6.28	119.78	110.62
1	A	136	THR	CA-CB-OG1	-6.22	100.28	109.60
1	E	231	THR	CB-CA-C	6.20	119.82	111.70
1	D	159	THR	CA-CB-OG1	-6.07	100.49	109.60
1	A	124	GLU	CA-C-N	6.04	128.29	120.44
1	A	124	GLU	C-N-CA	6.04	128.29	120.44
1	E	140	ASN	CB-CA-C	6.04	119.74	109.72
1	E	275	ASP	CB-CA-C	-5.84	108.83	115.79
1	F	133	TYR	CA-C-N	5.80	128.53	120.63
1	F	133	TYR	C-N-CA	5.80	128.53	120.63
1	A	95	ASP	CB-CA-C	-5.76	98.96	110.42
1	F	141	SER	CA-C-N	5.64	128.30	120.63
1	F	141	SER	C-N-CA	5.64	128.30	120.63
1	C	55	ASP	CA-C-N	5.60	128.82	120.31
1	C	55	ASP	C-N-CA	5.60	128.82	120.31
1	F	132	ASP	CA-CB-CG	5.54	118.14	112.60
1	E	97	ASP	CA-CB-CG	5.45	118.05	112.60
1	E	17	GLU	N-CA-C	-5.42	104.77	111.33
1	D	145	ALA	O-C-N	5.38	127.82	122.12
1	A	179	TYR	CB-CA-C	5.29	118.84	109.89
1	C	267	PRO	N-CA-CB	-5.29	97.69	103.25
1	C	55	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	245	MET	CA-C-N	5.21	125.72	119.94
1	A	245	MET	C-N-CA	5.21	125.72	119.94
1	E	180	THR	CB-CA-C	5.17	118.17	110.62
1	A	152	GLN	CA-C-O	-5.14	115.10	120.55
1	F	272	TYR	CB-CA-C	5.12	119.14	110.79
1	E	183	GLN	CA-C-O	-5.12	115.98	121.56
1	C	138	THR	CB-CA-C	5.09	118.20	109.80
1	D	252	SER	N-CA-C	-5.05	106.37	112.54
1	B	98	VAL	CA-C-N	5.05	128.13	120.75
1	B	98	VAL	C-N-CA	5.05	128.13	120.75
1	E	48	VAL	N-CA-CB	5.05	117.52	110.56
1	B	164	LYS	CA-C-N	5.03	127.02	120.28
1	B	164	LYS	C-N-CA	5.03	127.02	120.28

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	131	MET	Peptide
1	B	232	MET	Peptide
1	C	266	SER	Peptide
1	C	95	ASP	Peptide
1	D	1	MET	Peptide
1	D	119	LEU	Peptide
1	D	48	VAL	Peptide
1	E	38	GLN	Peptide
1	F	125	SER	Peptide
1	F	132	ASP	Peptide
1	F	62	CYS	Peptide

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	1919	0	1914	40	0
1	B	1919	0	1914	45	0
1	C	1919	0	1914	63	0
1	D	1941	0	1929	51	0
1	E	1988	0	1982	41	0
1	F	1919	0	1914	57	0
2	A	12	0	12	0	0
2	E	12	0	12	1	0
3	A	16	0	0	1	0
3	B	8	0	0	1	0
3	C	10	0	0	1	0
3	D	22	0	0	1	0
3	E	8	0	0	0	0
3	F	9	0	0	2	0
All	All	11702	0	11591	295	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 13.

All (295) 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:B:124:GLU:HB2	1:B:126:MET:SD	1.95	1.06
1:A:1:MET:N	1:A:94:ASP:OD2	2.00	0.93
1:A:22:LEU:HD12	1:A:48:VAL:HG22	1.61	0.82
1:C:2:LEU:HD23	1:C:3:GLU:N	1.94	0.81
1:A:126:MET:HE3	1:A:126:MET:HA	1.63	0.81
1:A:1:MET:CA	1:A:94:ASP:OD2	2.30	0.79
1:D:56:CYS:HB2	1:D:277:VAL:HG13	1.64	0.79
1:F:130:GLU:O	1:F:131:MET:O	2.01	0.78
1:D:125:SER:O	1:D:127:GLY:N	2.20	0.74
1:A:15:LEU:HD22	1:A:50:MET:HE3	1.67	0.74
1:A:95:ASP:OD1	1:A:96:SER:N	2.21	0.73
1:D:48:VAL:HG13	1:D:282:TYR:CE1	2.25	0.72
1:A:1:MET:HA	1:A:94:ASP:OD2	1.90	0.71
1:E:276:ASN:N	1:E:276:ASN:HD22	1.86	0.71
1:C:31:ASN:ND2	1:C:65:ASN:OD1	2.23	0.70
1:F:70:LEU:HD21	1:F:99:VAL:HG11	1.74	0.70
1:C:70:LEU:HD21	1:C:99:VAL:HG11	1.77	0.67
1:F:183:GLN:HG2	1:F:185:ALA:HB2	1.77	0.67
1:E:276:ASN:HD22	1:E:276:ASN:H	1.42	0.65
1:B:118:LEU:C	1:B:119:LEU:HD23	2.22	0.64
1:A:130:GLU:OE2	1:A:130:GLU:HA	1.97	0.64
1:D:49:HIS:ND1	1:D:128:ILE:HD11	2.13	0.63
1:C:22:LEU:HD12	1:C:48:VAL:CG2	2.28	0.63
1:F:116:LEU:N	1:F:116:LEU:HD23	2.13	0.63
1:A:105:ASN:HD22	1:A:106:PRO:HD2	1.64	0.63
1:D:56:CYS:HA	1:D:277:VAL:HG22	1.81	0.62
1:D:7:GLN:NE2	1:D:8:PHE:CE1	2.68	0.61
1:E:242:LEU:O	1:E:243:ARG:C	2.43	0.61
1:D:118:LEU:N	1:D:118:LEU:HD23	2.16	0.61
1:B:48:VAL:HG13	1:B:282:TYR:CE1	2.36	0.61
1:D:20:ASN:HB3	3:D:307:HOH:O	2.01	0.60
1:C:274:ILE:O	1:C:274:ILE:HG22	2.00	0.60
1:C:248:PHE:CD1	1:C:282:TYR:CG	2.89	0.60
1:A:18:CYS:HB3	1:A:282:TYR:OH	2.01	0.60
1:E:126:MET:SD	2:E:301:ARG:HD2	2.41	0.60
1:C:87:SER:O	1:C:103:SER:HA	2.00	0.60
1:D:125:SER:O	1:D:126:MET:C	2.44	0.60
1:C:81:ILE:HD11	1:C:114:TYR:CZ	2.38	0.59
1:C:116:LEU:N	1:C:116:LEU:HD12	2.17	0.59
1:F:38:GLN:CD	1:F:128:ILE:HD11	2.28	0.59
1:F:96:SER:O	1:F:97:ASP:OD1	2.21	0.59
1:A:10:SER:HB3	1:A:14:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:ASN:H	1:E:276:ASN:ND2	2.00	0.58
1:F:248:PHE:CD1	1:F:282:TYR:CG	2.91	0.58
1:C:49:HIS:ND1	1:C:128:ILE:HD11	2.19	0.57
1:B:103:SER:HB3	1:B:112:CYS:HB2	1.85	0.57
1:F:269:MET:HB2	1:F:283:TYR:CD1	2.39	0.57
1:E:51:LEU:C	1:E:51:LEU:HD12	2.29	0.57
1:B:149:ARG:HD2	3:B:308:HOH:O	2.04	0.57
1:F:2:LEU:HD23	1:F:3:GLU:N	2.19	0.57
1:D:48:VAL:HG13	1:D:282:TYR:CD1	2.40	0.56
1:F:244:PHE:HA	1:F:247:ILE:HD12	1.87	0.56
1:D:249:ALA:HA	1:D:272:TYR:OH	2.05	0.56
1:D:266:SER:O	1:D:267:PRO:O	2.23	0.56
1:F:38:GLN:HA	1:F:48:VAL:O	2.06	0.56
1:A:48:VAL:HG13	1:A:282:TYR:CE1	2.41	0.56
1:A:158:VAL:H	1:A:242:LEU:HG	1.72	0.55
1:E:276:ASN:N	1:E:276:ASN:ND2	2.55	0.55
1:B:58:VAL:HG23	1:B:59:LYS:H	1.72	0.55
1:D:27:ASN:HD21	1:D:121:ILE:HG22	1.71	0.55
1:C:90:LEU:HD11	1:C:99:VAL:CG2	2.37	0.55
1:A:160:ILE:HG12	1:A:169:PHE:CD1	2.41	0.54
1:C:50:MET:HE2	1:C:52:LEU:HG	1.89	0.54
1:F:162:ILE:HD11	1:F:262:PHE:CE2	2.42	0.54
1:B:270:VAL:HG22	1:B:282:TYR:HB2	1.89	0.54
1:C:30:CYS:SG	1:C:35:LEU:CD2	2.96	0.54
1:A:50:MET:HE2	1:A:52:LEU:HG	1.89	0.54
1:E:2:LEU:HD12	1:E:3:GLU:N	2.23	0.53
1:F:81:ILE:HD11	1:F:114:TYR:CE1	2.44	0.53
1:D:53:ARG:O	1:D:56:CYS:HB3	2.08	0.52
1:B:227:GLY:O	1:B:257:ARG:NH2	2.42	0.52
1:C:243:ARG:HB2	3:C:302:HOH:O	2.09	0.52
1:F:51:LEU:HB2	1:F:279:TYR:CZ	2.44	0.52
1:D:118:LEU:N	1:D:118:LEU:CD2	2.73	0.52
1:E:269:MET:HE3	1:E:271:GLU:HB2	1.92	0.52
1:A:98:VAL:CG1	1:A:99:VAL:N	2.73	0.52
1:D:25:GLU:HB2	1:D:121:ILE:HD11	1.92	0.52
1:D:31:ASN:ND2	1:D:65:ASN:OD1	2.40	0.52
1:F:2:LEU:HD23	1:F:3:GLU:H	1.74	0.52
1:A:264:LYS:HG3	3:A:407:HOH:O	2.11	0.51
1:B:131:MET:SD	1:B:266:SER:HB3	2.51	0.51
1:D:119:LEU:HA	1:D:120:GLU:HG3	1.91	0.51
1:E:95:ASP:O	1:E:97:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLN:C	1:C:116:LEU:HD12	2.35	0.51
1:B:48:VAL:HG13	1:B:282:TYR:CD1	2.46	0.51
1:C:166:GLY:HA3	1:C:182:LEU:O	2.11	0.51
1:F:248:PHE:O	1:F:250:LYS:N	2.44	0.51
1:C:30:CYS:SG	1:C:35:LEU:HD23	2.51	0.51
1:F:81:ILE:HD11	1:F:114:TYR:CZ	2.46	0.51
1:E:179:TYR:CE2	1:F:113:GLU:HB3	2.45	0.51
1:D:158:VAL:HB	1:D:242:LEU:HD21	1.93	0.51
1:C:132:ASP:CG	1:C:133:TYR:H	2.19	0.51
1:F:124:GLU:HG3	3:F:301:HOH:O	2.11	0.51
1:C:90:LEU:HD11	1:C:99:VAL:HG21	1.92	0.50
1:D:269:MET:HE3	1:D:271:GLU:HB2	1.94	0.50
1:C:30:CYS:O	1:C:62:CYS:SG	2.70	0.50
1:D:144:PHE:O	1:D:148:VAL:HG13	2.12	0.50
1:E:13:LYS:O	1:E:17:GLU:HG2	2.12	0.50
1:F:70:LEU:HD21	1:F:99:VAL:CG1	2.40	0.50
1:B:147:ILE:HG12	1:B:180:THR:HG21	1.93	0.50
1:E:97:ASP:O	1:E:98:VAL:HG23	2.12	0.50
1:B:279:TYR:CZ	1:B:281:ARG:NH2	2.80	0.50
1:C:233:GLU:O	1:C:234:GLU:CB	2.59	0.50
1:C:269:MET:HE3	1:C:271:GLU:HB2	1.94	0.50
1:E:78:VAL:O	1:E:81:ILE:HG12	2.11	0.49
1:C:248:PHE:CE1	1:C:282:TYR:HB3	2.47	0.49
1:D:22:LEU:HD23	1:D:48:VAL:HG22	1.94	0.49
1:B:126:MET:CG	1:B:127:GLY:H	2.25	0.49
1:F:88:LEU:HD12	1:F:102:THR:O	2.12	0.49
1:D:99:VAL:HG12	1:D:118:LEU:HD21	1.94	0.49
1:E:78:VAL:HG21	1:E:116:LEU:HD11	1.93	0.49
1:C:116:LEU:N	1:C:116:LEU:CD1	2.74	0.49
1:F:237:THR:O	1:F:238:LEU:HG	2.13	0.49
1:B:119:LEU:HD23	1:B:119:LEU:N	2.26	0.49
1:C:133:TYR:HB3	1:C:261:LYS:HB3	1.93	0.49
1:E:123:ALA:O	1:E:124:GLU:C	2.55	0.49
1:E:156:ASP:OD1	1:E:156:ASP:N	2.45	0.49
1:E:174:ASP:O	1:E:175:VAL:C	2.56	0.49
1:D:135:SER:HA	1:D:232:MET:HA	1.95	0.49
1:B:16:VAL:HG21	1:B:79:LEU:CD1	2.43	0.49
1:F:30:CYS:SG	1:F:35:LEU:CD2	3.01	0.48
1:D:78:VAL:O	1:D:81:ILE:HG12	2.14	0.48
1:F:23:VAL:HG12	1:F:41:ASP:HA	1.94	0.48
1:D:37:VAL:HG23	1:D:50:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ASN:ND2	1:D:74:SER:OG	2.46	0.48
1:C:22:LEU:HD12	1:C:48:VAL:HG22	1.94	0.48
1:C:158:VAL:HB	1:C:242:LEU:HD21	1.94	0.48
1:C:275:ASP:OD1	1:C:276:ASN:OD1	2.31	0.48
1:D:48:VAL:CG1	1:D:282:TYR:CE1	2.95	0.48
1:F:128:ILE:HG22	1:F:128:ILE:O	2.13	0.48
1:E:56:CYS:O	1:E:56:CYS:SG	2.72	0.48
1:A:2:LEU:HD12	1:A:3:GLU:N	2.28	0.48
1:F:159:THR:O	1:F:159:THR:HG22	2.12	0.48
1:A:51:LEU:HD23	1:A:279:TYR:CE2	2.49	0.47
1:C:51:LEU:HD12	1:C:52:LEU:N	2.29	0.47
1:C:230:VAL:HG12	1:C:231:THR:N	2.30	0.47
1:A:129:PRO:O	1:A:130:GLU:C	2.56	0.47
1:D:49:HIS:HB2	1:D:128:ILE:HD11	1.96	0.47
1:F:12:TRP:HA	1:F:12:TRP:CE3	2.49	0.47
1:B:43:SER:OG	1:B:45:VAL:CG2	2.62	0.47
1:E:260:LEU:HB2	1:E:262:PHE:HE1	1.79	0.47
1:B:31:ASN:HB3	1:B:32:PRO:HD2	1.97	0.47
1:B:248:PHE:CD1	1:B:282:TYR:CG	3.02	0.47
1:C:6:VAL:HG12	1:C:7:GLN:N	2.30	0.47
1:F:138:THR:OG1	1:F:259:THR:HG23	2.14	0.47
1:D:129:PRO:HB2	1:D:131:MET:HE2	1.97	0.47
1:C:86:ASP:OD2	1:C:110:ARG:NH2	2.48	0.47
1:B:161:ALA:HA	1:B:237:THR:HB	1.98	0.46
1:E:15:LEU:HD13	1:E:50:MET:HE2	1.97	0.46
1:C:165:GLU:OE1	1:C:165:GLU:N	2.45	0.46
1:B:242:LEU:O	1:B:243:ARG:C	2.58	0.46
1:C:160:ILE:HG12	1:C:169:PHE:CD1	2.51	0.46
1:C:260:LEU:HD22	1:C:270:VAL:HB	1.96	0.46
1:A:19:ILE:HG13	1:A:72:LEU:HD13	1.97	0.46
1:A:38:GLN:O	1:A:38:GLN:CG	2.64	0.46
1:A:71:ASN:OD1	1:A:73:ALA:HB3	2.16	0.46
1:A:126:MET:HA	1:A:126:MET:CE	2.33	0.46
1:E:53:ARG:HB3	1:E:55:ASP:OD1	2.16	0.46
1:B:233:GLU:C	1:B:234:GLU:HG2	2.39	0.46
1:C:132:ASP:CG	1:C:133:TYR:N	2.74	0.46
1:A:126:MET:N	1:A:126:MET:SD	2.89	0.46
1:B:232:MET:HG2	1:B:233:GLU:N	2.31	0.46
1:E:19:ILE:HD12	1:E:37:VAL:HG11	1.98	0.46
1:F:2:LEU:CD2	1:F:3:GLU:N	2.79	0.46
1:F:280:LEU:HD21	1:F:282:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:HA	1:A:232:MET:HA	1.98	0.46
1:E:65:ASN:OD1	1:E:65:ASN:N	2.49	0.46
1:F:269:MET:SD	1:F:281:ARG:HG2	2.56	0.46
1:A:10:SER:HB3	1:A:14:ARG:HH12	1.80	0.45
1:B:125:SER:O	1:B:127:GLY:N	2.50	0.45
1:C:16:VAL:HG21	1:C:79:LEU:CD1	2.46	0.45
1:F:163:SER:O	1:F:164:LYS:C	2.59	0.45
1:B:14:ARG:HD2	1:B:253:THR:O	2.16	0.45
1:C:124:GLU:OE1	1:C:126:MET:O	2.34	0.45
1:D:274:ILE:HG22	1:D:274:ILE:O	2.16	0.45
1:F:14:ARG:HD2	1:F:253:THR:O	2.16	0.45
1:E:136:THR:CG2	1:E:137:VAL:N	2.79	0.45
1:C:233:GLU:O	1:C:234:GLU:HB2	2.16	0.45
1:C:65:ASN:ND2	1:C:65:ASN:O	2.49	0.45
1:B:251:GLY:HA3	1:B:272:TYR:CE2	2.52	0.45
1:C:125:SER:OG	1:C:126:MET:N	2.49	0.45
1:F:125:SER:O	1:F:127:GLY:N	2.49	0.45
1:F:248:PHE:HA	1:F:282:TYR:CE2	2.52	0.45
1:A:134:ARG:H	1:A:134:ARG:HG2	1.64	0.44
1:C:145:ALA:O	1:C:148:VAL:HG22	2.18	0.44
1:C:255:SER:HB2	1:C:273:GLY:O	2.17	0.44
1:E:150:ASP:HB3	1:F:81:ILE:HD12	1.98	0.44
1:D:101:LEU:O	1:D:113:GLU:HA	2.16	0.44
1:D:147:ILE:O	1:D:151:MET:HG2	2.17	0.44
1:E:19:ILE:CD1	1:E:37:VAL:HG11	2.48	0.44
1:C:7:GLN:NE2	1:C:8:PHE:CE1	2.86	0.44
1:B:10:SER:CB	1:B:14:ARG:HH21	2.31	0.44
1:C:81:ILE:O	1:C:81:ILE:HG13	2.17	0.44
1:A:9:ALA:O	1:A:10:SER:C	2.61	0.44
1:A:269:MET:HE3	1:A:271:GLU:HB2	2.00	0.44
1:E:158:VAL:HB	1:E:242:LEU:HD21	2.00	0.44
1:F:60:TYR:CD2	1:F:61:GLN:N	2.85	0.44
1:D:46:ALA:HA	1:D:283:TYR:O	2.18	0.44
1:D:50:MET:HE2	1:D:50:MET:HB3	1.92	0.43
1:D:145:ALA:HA	1:D:249:ALA:HB1	2.00	0.43
1:A:154:PHE:O	1:A:173:GLY:HA3	2.18	0.43
1:C:15:LEU:HD13	1:C:50:MET:HE3	2.00	0.43
1:A:38:GLN:HG3	1:A:126:MET:HE2	2.01	0.43
1:B:248:PHE:CD1	1:B:282:TYR:CD1	3.06	0.43
1:A:48:VAL:HG13	1:A:282:TYR:CD1	2.54	0.43
1:D:127:GLY:O	1:D:128:ILE:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:GLU:O	1:E:122:GLU:HG2	2.18	0.43
1:B:12:TRP:HA	1:B:12:TRP:CE3	2.52	0.43
1:F:36:SER:HA	1:F:50:MET:O	2.18	0.43
1:F:45:VAL:O	1:F:45:VAL:CG1	2.66	0.43
1:D:279:TYR:CD1	1:D:279:TYR:C	2.97	0.43
1:F:265:ASP:N	1:F:265:ASP:OD1	2.51	0.43
1:D:38:GLN:HA	1:D:48:VAL:O	2.19	0.43
1:B:248:PHE:CE1	1:B:282:TYR:HB3	2.53	0.43
1:D:276:ASN:N	1:D:276:ASN:OD1	2.51	0.43
1:A:105:ASN:ND2	1:A:106:PRO:HD2	2.31	0.43
1:D:7:GLN:NE2	1:D:8:PHE:CZ	2.87	0.43
1:D:56:CYS:HB2	1:D:277:VAL:CG1	2.43	0.43
1:F:4:ALA:HB1	1:F:57:PHE:CE2	2.53	0.43
1:C:2:LEU:HD23	1:C:2:LEU:C	2.44	0.42
1:F:123:ALA:HB1	3:F:301:HOH:O	2.19	0.42
1:F:183:GLN:HG2	1:F:185:ALA:CB	2.48	0.42
1:C:70:LEU:CD2	1:C:99:VAL:HG11	2.48	0.42
1:D:90:LEU:HD11	1:D:99:VAL:HG21	2.00	0.42
1:D:150:ASP:O	1:D:153:VAL:HG13	2.19	0.42
1:E:0:SER:HB2	1:E:91:ARG:NH1	2.34	0.42
1:F:128:ILE:O	1:F:129:PRO:C	2.61	0.42
1:A:23:VAL:HG23	1:A:72:LEU:HD12	2.01	0.42
1:B:70:LEU:HD12	1:B:70:LEU:HA	1.82	0.42
1:C:232:MET:HG2	1:C:233:GLU:N	2.35	0.42
1:F:2:LEU:CD1	1:F:30:CYS:SG	3.08	0.42
1:A:5:GLN:HA	1:A:89:SER:HA	2.01	0.42
1:E:240:PHE:CE1	1:E:268:CYS:HB3	2.54	0.42
1:C:230:VAL:CG1	1:C:231:THR:N	2.82	0.42
1:D:9:ALA:O	1:D:10:SER:C	2.63	0.42
1:F:51:LEU:CB	1:F:279:TYR:CE2	3.03	0.42
1:F:242:LEU:HD23	1:F:242:LEU:HA	1.93	0.42
1:D:125:SER:C	1:D:127:GLY:N	2.77	0.42
1:E:136:THR:CG2	1:E:231:THR:HG22	2.50	0.42
1:B:90:LEU:CD1	1:B:99:VAL:HG13	2.49	0.42
1:A:136:THR:CG2	1:A:137:VAL:N	2.83	0.42
1:C:81:ILE:HD11	1:C:114:TYR:CE1	2.54	0.42
1:E:48:VAL:HG13	1:E:282:TYR:CE1	2.55	0.42
1:C:51:LEU:HD12	1:C:51:LEU:C	2.45	0.42
1:C:88:LEU:HD11	1:C:101:LEU:HB3	2.02	0.42
1:C:127:GLY:O	1:C:128:ILE:HB	2.20	0.42
1:F:137:VAL:HG21	1:F:167:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ASP:O	1:B:94:ASP:C	2.62	0.42
1:B:48:VAL:CG1	1:B:282:TYR:CE1	3.03	0.41
1:B:232:MET:HE2	1:B:232:MET:HB3	1.97	0.41
1:F:14:ARG:HD2	1:F:253:THR:HB	2.01	0.41
1:C:12:TRP:HA	1:C:12:TRP:CE3	2.54	0.41
1:A:87:SER:O	1:A:103:SER:HA	2.20	0.41
1:D:264:LYS:O	1:D:266:SER:N	2.53	0.41
1:B:43:SER:OG	1:B:45:VAL:HG22	2.20	0.41
1:F:45:VAL:O	1:F:45:VAL:HG12	2.19	0.41
1:E:43:SER:O	1:E:44:HIS:C	2.62	0.41
1:B:90:LEU:HD12	1:B:90:LEU:C	2.45	0.41
1:D:266:SER:O	1:D:267:PRO:C	2.61	0.41
1:E:45:VAL:HG22	1:E:45:VAL:O	2.20	0.41
1:E:70:LEU:HD23	1:E:70:LEU:HA	1.91	0.41
1:E:266:SER:O	1:E:267:PRO:C	2.63	0.41
1:C:22:LEU:HD22	1:C:41:ASP:HB3	2.02	0.41
1:D:71:ASN:HD21	1:D:73:ALA:HB3	1.85	0.41
1:E:123:ALA:O	1:E:124:GLU:O	2.38	0.41
1:B:131:MET:SD	1:B:266:SER:CB	3.09	0.41
1:C:262:PHE:CD1	1:C:262:PHE:N	2.89	0.41
1:A:266:SER:O	1:A:267:PRO:C	2.64	0.41
1:D:279:TYR:CE2	1:D:281:ARG:NH2	2.89	0.41
1:E:258:VAL:HG13	1:E:258:VAL:O	2.20	0.41
1:B:232:MET:HG2	1:B:234:GLU:H	1.86	0.41
1:B:246:GLY:O	1:B:247:ILE:C	2.63	0.41
1:C:161:ALA:HA	1:C:237:THR:HG22	2.02	0.41
1:C:232:MET:CG	1:C:233:GLU:N	2.82	0.41
1:F:57:PHE:CD1	1:F:57:PHE:N	2.89	0.41
1:F:70:LEU:HD23	1:F:70:LEU:HA	1.92	0.41
1:F:145:ALA:HA	1:F:249:ALA:HB1	2.02	0.41
1:D:49:HIS:HB2	1:D:128:ILE:CD1	2.51	0.41
1:C:79:LEU:HD21	1:C:88:LEU:HD21	2.03	0.41
1:F:15:LEU:HD22	1:F:50:MET:HE3	2.03	0.41
1:E:87:SER:O	1:E:103:SER:HA	2.21	0.40
1:B:58:VAL:HG23	1:B:59:LYS:N	2.36	0.40
1:B:158:VAL:O	1:B:158:VAL:HG13	2.21	0.40
1:C:136:THR:CG2	1:C:137:VAL:N	2.84	0.40
1:A:164:LYS:H	1:A:164:LYS:HE2	1.85	0.40
1:B:164:LYS:HE3	1:B:164:LYS:HB2	1.87	0.40
1:C:151:MET:HA	1:C:151:MET:HE2	2.03	0.40
1:B:56:CYS:HB2	1:B:277:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LEU:HD12	1:C:52:LEU:C	2.45	0.40
1:F:60:TYR:O	1:F:61:GLN:HG3	2.21	0.40
1:F:248:PHE:CD1	1:F:282:TYR:CD2	3.09	0.40
1:E:277:VAL:O	1:E:277:VAL:HG13	2.21	0.40
1:B:87:SER:O	1:B:103:SER:HA	2.21	0.40
1:B:240:PHE:HD2	1:B:284:LEU:HD23	1.87	0.40
1:F:139:LEU:H	1:F:139:LEU:HD23	1.87	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	A	244/302 (81%)	209 (86%)	28 (12%)	7 (3%)	3	24
1	B	244/302 (81%)	214 (88%)	21 (9%)	9 (4%)	2	18
1	C	244/302 (81%)	195 (80%)	35 (14%)	14 (6%)	1	11
1	D	247/302 (82%)	215 (87%)	24 (10%)	8 (3%)	3	21
1	E	254/302 (84%)	210 (83%)	32 (13%)	12 (5%)	2	14
1	F	244/302 (81%)	203 (83%)	27 (11%)	14 (6%)	1	11
All	All	1477/1812 (82%)	1246 (84%)	167 (11%)	64 (4%)	2	16

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	95	ASP
1	D	95	ASP
1	D	126	MET
1	D	231	THR

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Mol	Chain	Res	Type
1	D	265	ASP
1	D	267	PRO
1	E	96	SER
1	E	98	VAL
1	E	124	GLU
1	E	125	SER
1	E	131	MET
1	B	94	ASP
1	B	126	MET
1	B	135	SER
1	C	84	SER
1	C	234	GLU
1	C	267	PRO
1	F	126	MET
1	F	130	GLU
1	F	131	MET
1	F	132	ASP
1	A	105	ASN
1	A	122	GLU
1	A	130	GLU
1	D	64	ARG
1	E	63	GLY
1	E	95	ASP
1	E	267	PRO
1	B	62	CYS
1	B	63	GLY
1	C	275	ASP
1	F	84	SER
1	F	165	GLU
1	F	249	ALA
1	F	275	ASP
1	E	-1	SER
1	E	10	SER
1	B	64	ARG
1	C	59	LYS
1	C	91	ARG
1	C	231	THR
1	F	63	GLY
1	D	10	SER
1	E	-6	ARG
1	B	264	LYS
1	C	61	GLN

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Mol	Chain	Res	Type
1	C	123	ALA
1	C	128	ILE
1	F	10	SER
1	A	164	LYS
1	D	132	ASP
1	B	127	GLY
1	C	137	VAL
1	C	184	ALA
1	F	163	SER
1	A	228	VAL
1	B	73	ALA
1	C	63	GLY
1	F	267	PRO
1	C	274	ILE
1	F	274	ILE
1	E	175	VAL
1	F	106	PRO

5.3.2 Protein sidechains ⓘ

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	216/259 (83%)	175 (81%)	41 (19%)	1	9
1	B	216/259 (83%)	174 (81%)	42 (19%)	1	8
1	C	216/259 (83%)	171 (79%)	45 (21%)	1	7
1	D	218/259 (84%)	170 (78%)	48 (22%)	1	6
1	E	224/259 (86%)	175 (78%)	49 (22%)	1	5
1	F	216/259 (83%)	163 (76%)	53 (24%)	1	3
All	All	1306/1554 (84%)	1028 (79%)	278 (21%)	1	6

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU

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Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	GLN
1	A	15	LEU
1	A	19	ILE
1	A	22	LEU
1	A	30	CYS
1	A	38	GLN
1	A	41	ASP
1	A	48	VAL
1	A	50	MET
1	A	53	ARG
1	A	80	LYS
1	A	81	ILE
1	A	90	LEU
1	A	99	VAL
1	A	102	THR
1	A	103	SER
1	A	104	GLU
1	A	105	ASN
1	A	116	LEU
1	A	120	GLU
1	A	126	MET
1	A	132	ASP
1	A	134	ARG
1	A	137	VAL
1	A	140	ASN
1	A	153	VAL
1	A	162	ILE
1	A	163	SER
1	A	164	LYS
1	A	167	VAL
1	A	170	SER
1	A	171	SER
1	A	179	TYR
1	A	229	GLU
1	A	231	THR
1	A	232	MET
1	A	234	GLU
1	A	260	LEU
1	A	270	VAL
1	D	1	MET
1	D	6	VAL

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Mol	Chain	Res	Type
1	D	19	ILE
1	D	25	GLU
1	D	30	CYS
1	D	35	LEU
1	D	45	VAL
1	D	47	LEU
1	D	48	VAL
1	D	53	ARG
1	D	56	CYS
1	D	59	LYS
1	D	66	SER
1	D	78	VAL
1	D	80	LYS
1	D	84	SER
1	D	88	LEU
1	D	97	ASP
1	D	98	VAL
1	D	111	LYS
1	D	116	LEU
1	D	118	LEU
1	D	125	SER
1	D	128	ILE
1	D	130	GLU
1	D	134	ARG
1	D	136	THR
1	D	137	VAL
1	D	140	ASN
1	D	148	VAL
1	D	152	GLN
1	D	153	VAL
1	D	159	THR
1	D	164	LYS
1	D	231	THR
1	D	234	GLU
1	D	237	THR
1	D	250	LYS
1	D	253	THR
1	D	256	GLU
1	D	260	LEU
1	D	267	PRO
1	D	270	VAL
1	D	276	ASN

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Mol	Chain	Res	Type
1	D	277	VAL
1	D	287	LYS
1	D	288	VAL
1	D	290	ASP
1	E	-9	HIS
1	E	-8	SER
1	E	-1	SER
1	E	7	GLN
1	E	18	CYS
1	E	19	ILE
1	E	22	LEU
1	E	25	GLU
1	E	30	CYS
1	E	31	ASN
1	E	47	LEU
1	E	48	VAL
1	E	50	MET
1	E	51	LEU
1	E	53	ARG
1	E	55	ASP
1	E	65	ASN
1	E	67	ILE
1	E	81	ILE
1	E	94	ASP
1	E	96	SER
1	E	98	VAL
1	E	100	THR
1	E	103	SER
1	E	108	LYS
1	E	116	LEU
1	E	117	LYS
1	E	120	GLU
1	E	124	GLU
1	E	130	GLU
1	E	134	ARG
1	E	136	THR
1	E	137	VAL
1	E	140	ASN
1	E	146	LYS
1	E	152	GLN
1	E	156	ASP
1	E	170	SER

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Mol	Chain	Res	Type
1	E	183	GLN
1	E	232	MET
1	E	250	LYS
1	E	260	LEU
1	E	268	CYS
1	E	270	VAL
1	E	276	ASN
1	E	277	VAL
1	E	281	ARG
1	E	287	LYS
1	E	288	VAL
1	B	2	LEU
1	B	7	GLN
1	B	15	LEU
1	B	19	ILE
1	B	35	LEU
1	B	45	VAL
1	B	47	LEU
1	B	48	VAL
1	B	64	ARG
1	B	66	SER
1	B	67	ILE
1	B	70	LEU
1	B	74	SER
1	B	81	ILE
1	B	95	ASP
1	B	98	VAL
1	B	100	THR
1	B	102	THR
1	B	119	LEU
1	B	122	GLU
1	B	131	MET
1	B	132	ASP
1	B	135	SER
1	B	136	THR
1	B	138	THR
1	B	140	ASN
1	B	146	LYS
1	B	148	VAL
1	B	153	VAL
1	B	157	THR
1	B	162	ILE

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Mol	Chain	Res	Type
1	B	170	SER
1	B	183	GLN
1	B	231	THR
1	B	237	THR
1	B	247	ILE
1	B	250	LYS
1	B	259	THR
1	B	264	LYS
1	B	266	SER
1	B	270	VAL
1	B	281	ARG
1	C	1	MET
1	C	11	LEU
1	C	19	ILE
1	C	22	LEU
1	C	31	ASN
1	C	42	SER
1	C	47	LEU
1	C	50	MET
1	C	51	LEU
1	C	53	ARG
1	C	55	ASP
1	C	67	ILE
1	C	81	ILE
1	C	87	SER
1	C	100	THR
1	C	103	SER
1	C	105	ASN
1	C	111	LYS
1	C	113	GLU
1	C	117	LYS
1	C	121	ILE
1	C	122	GLU
1	C	124	GLU
1	C	125	SER
1	C	130	GLU
1	C	134	ARG
1	C	136	THR
1	C	137	VAL
1	C	139	LEU
1	C	146	LYS
1	C	149	ARG

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Mol	Chain	Res	Type
1	C	150	ASP
1	C	164	LYS
1	C	170	SER
1	C	231	THR
1	C	232	MET
1	C	236	ILE
1	C	253	THR
1	C	260	LEU
1	C	264	LYS
1	C	267	PRO
1	C	268	CYS
1	C	269	MET
1	C	270	VAL
1	C	281	ARG
1	F	1	MET
1	F	2	LEU
1	F	3	GLU
1	F	6	VAL
1	F	7	GLN
1	F	12	TRP
1	F	19	ILE
1	F	22	LEU
1	F	29	ASP
1	F	42	SER
1	F	43	SER
1	F	47	LEU
1	F	48	VAL
1	F	50	MET
1	F	51	LEU
1	F	65	ASN
1	F	67	ILE
1	F	80	LYS
1	F	81	ILE
1	F	97	ASP
1	F	106	PRO
1	F	107	GLU
1	F	108	LYS
1	F	109	THR
1	F	116	LEU
1	F	121	ILE
1	F	128	ILE
1	F	131	MET

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Mol	Chain	Res	Type
1	F	136	THR
1	F	137	VAL
1	F	149	ARG
1	F	153	VAL
1	F	157	THR
1	F	159	THR
1	F	162	ILE
1	F	163	SER
1	F	167	VAL
1	F	168	LYS
1	F	169	PHE
1	F	170	SER
1	F	172	SER
1	F	183	GLN
1	F	228	VAL
1	F	234	GLU
1	F	237	THR
1	F	256	GLU
1	F	259	THR
1	F	269	MET
1	F	270	VAL
1	F	280	LEU
1	F	281	ARG
1	F	284	LEU
1	F	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	152	GLN
1	D	7	GLN
1	D	27	ASN
1	D	71	ASN
1	D	115	GLN
1	D	183	GLN
1	E	5	GLN
1	E	7	GLN
1	E	27	ASN
1	E	276	ASN
1	B	38	GLN
1	B	85	ASN

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Mol	Chain	Res	Type
1	B	115	GLN
1	F	20	ASN
1	F	38	GLN
1	F	61	GLN
1	F	85	ASN
1	F	276	ASN

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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ARG	A	301	-	10,11,11	0.87	1 (10%)	9,13,13	1.69	2 (22%)
2	ARG	E	301	-	10,11,11	0.94	0	9,13,13	1.98	3 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARG	A	301	-	-	5/11/11/11	-
2	ARG	E	301	-	-	1/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ARG	OXT-C	-2.22	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	ARG	OXT-C-O	-4.46	113.97	124.08
2	A	301	ARG	OXT-C-O	-3.13	116.99	124.08
2	A	301	ARG	CB-CG-CD	2.30	118.70	112.07
2	E	301	ARG	CB-CA-C	2.21	116.30	110.45
2	E	301	ARG	CG-CD-NE	2.07	118.01	112.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ARG	O-C-CA-N
2	A	301	ARG	OXT-C-CA-N
2	E	301	ARG	CA-CB-CG-CD
2	A	301	ARG	O-C-CA-CB
2	A	301	ARG	OXT-C-CA-CB
2	A	301	ARG	NE-CD-CG-CB

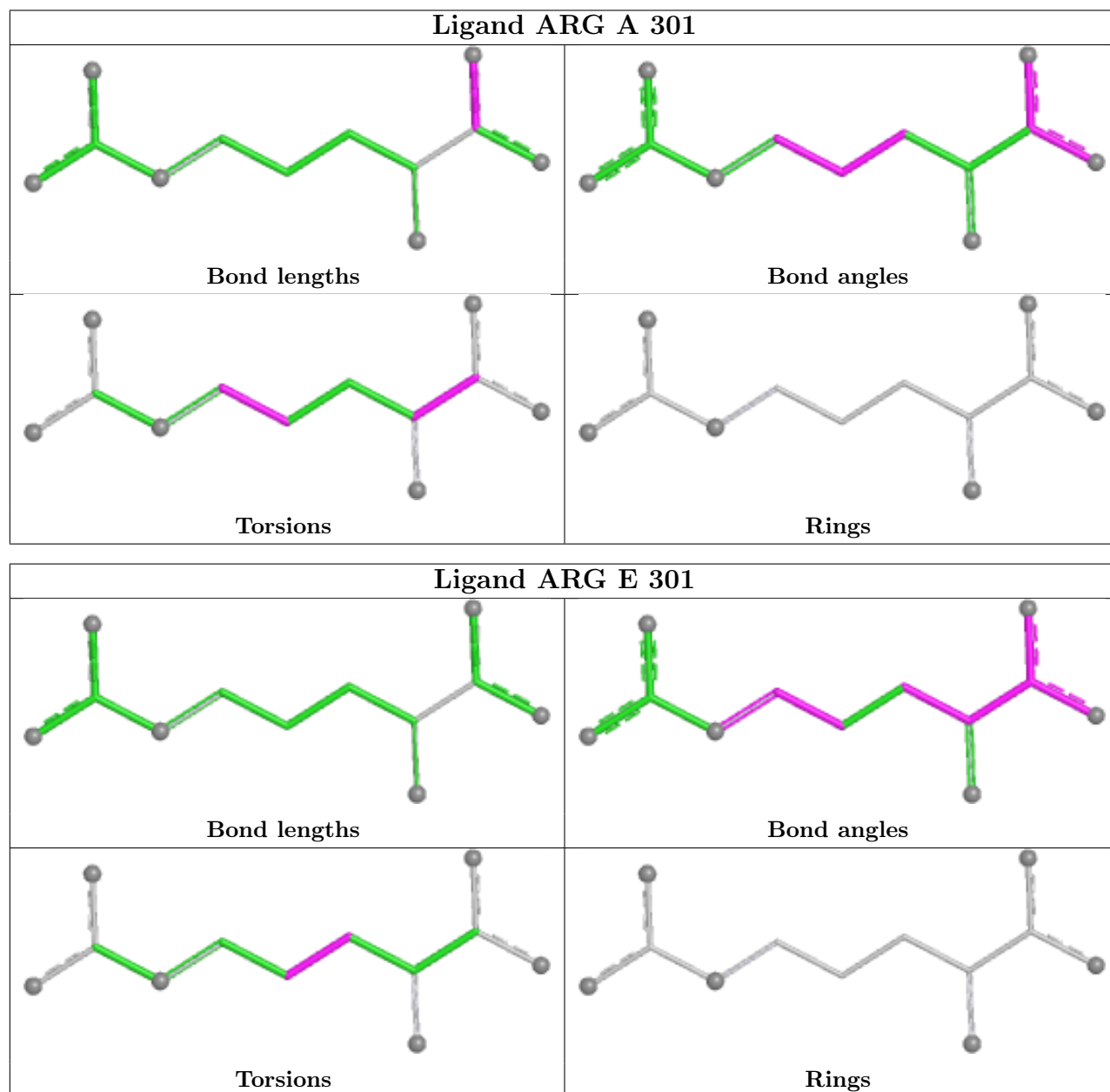
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	ARG	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.



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	248/302 (82%)	-0.56	2 (0%)	82 67	69, 103, 155, 205	0
1	B	248/302 (82%)	-0.45	2 (0%)	82 67	82, 118, 168, 200	0
1	C	248/302 (82%)	-0.38	3 (1%)	76 58	86, 118, 174, 201	0
1	D	251/302 (83%)	-0.48	1 (0%)	88 79	75, 112, 163, 208	0
1	E	258/302 (85%)	-0.50	2 (0%)	82 67	77, 108, 171, 203	0
1	F	248/302 (82%)	-0.26	3 (1%)	76 58	91, 126, 181, 214	0
All	All	1501/1812 (82%)	-0.44	13 (0%)	81 64	69, 115, 171, 214	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	126	MET	3.5
1	D	126	MET	3.0
1	C	227	GLY	2.9
1	A	227	GLY	2.8
1	B	227	GLY	2.7
1	F	185	ALA	2.6
1	A	185	ALA	2.6
1	C	236	ILE	2.5
1	C	235	PRO	2.5
1	F	55	ASP	2.4
1	E	250	LYS	2.3
1	E	-3	LEU	2.2
1	B	174	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

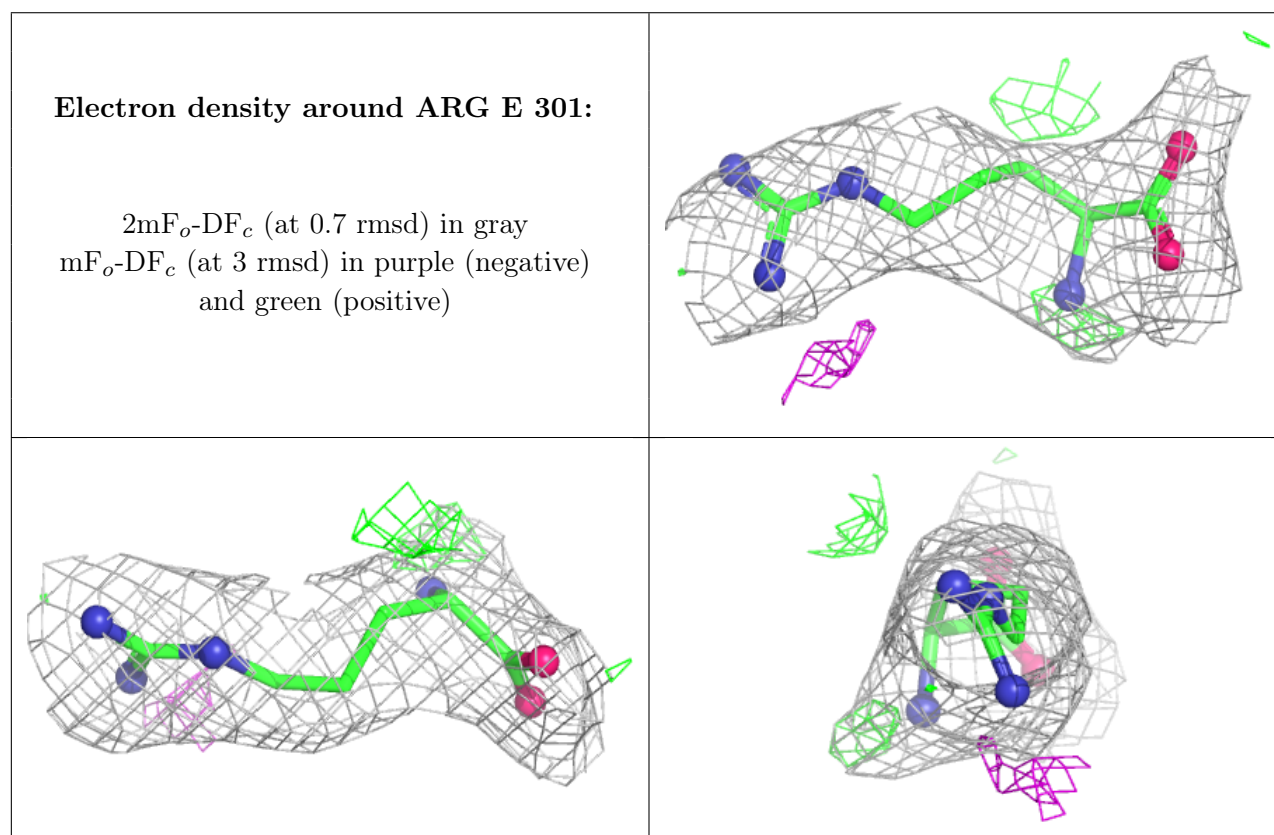
There are no oligosaccharides in this entry.

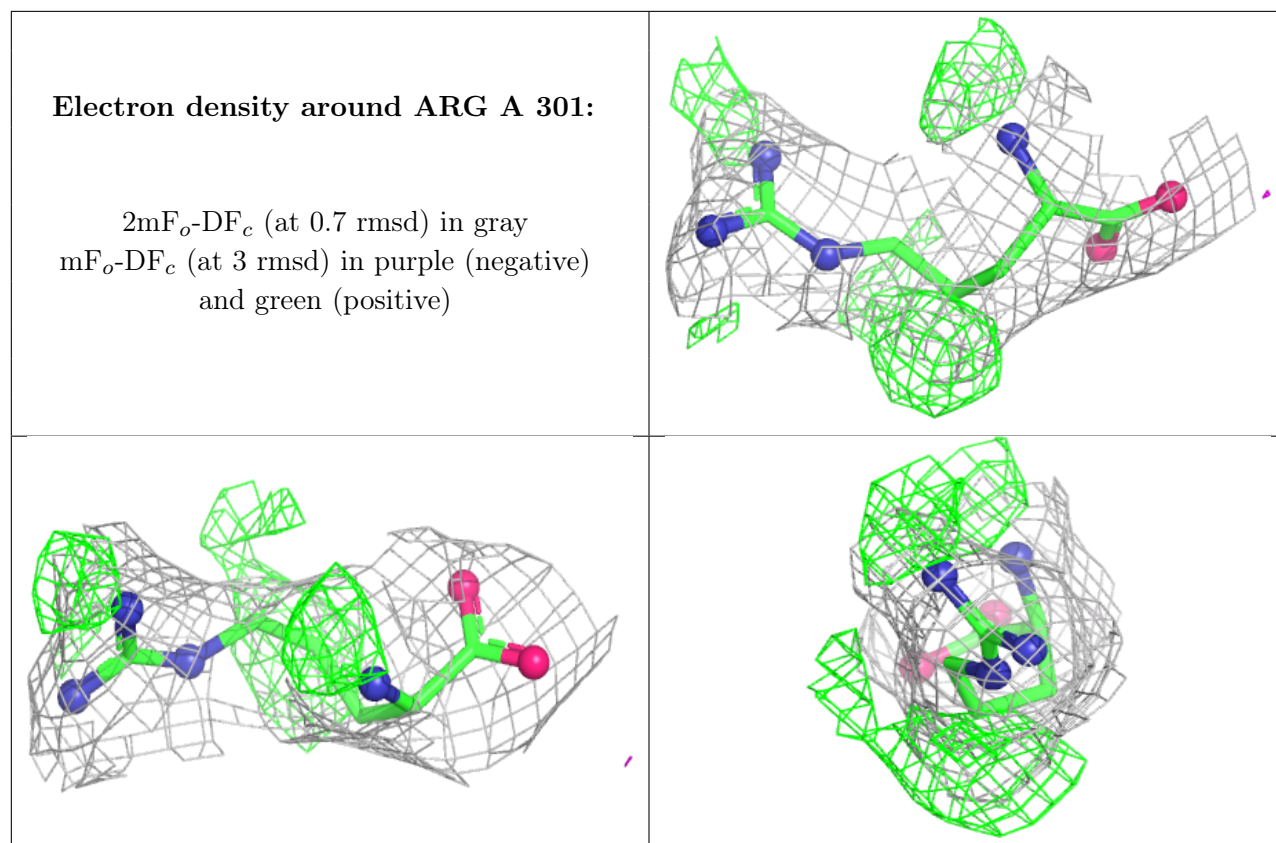
6.4 Ligands [i](#)

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
2	ARG	E	301	12/12	0.77	0.15	113,136,147,152	0
2	ARG	A	301	12/12	0.80	0.16	112,145,153,162	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.