



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:10 am BST

PDB ID : 6PUC  
Title : Structure of human MAIT A-F7 TCR in complex with human MR1-5-OP-RU  
Authors : Awad, W.; Rossjohn, J.  
Deposited on : 2019-07-18  
Resolution : 1.85 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

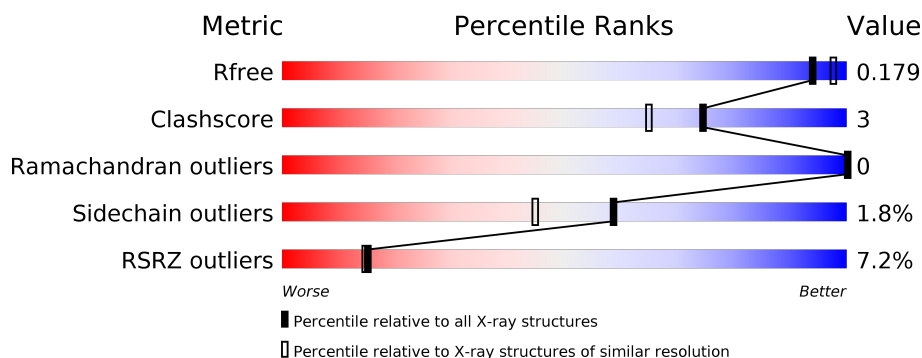
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	271	<div> <div>3%</div> <div>89%</div> <div>9%</div> <div>•</div> </div>
1	C	271	<div> <div>2%</div> <div>91%</div> <div>6%</div> <div>••</div> </div>
2	B	100	<div> <div>27%</div> <div>94%</div> <div>••</div> </div>
2	F	100	<div> <div>95%</div> <div>••</div> </div>
3	D	204	<div> <div>21%</div> <div>80%</div> <div>10%</div> <div>•</div> <div>8%</div> </div>
3	G	204	<div> <div>%</div> <div>93%</div> <div>5%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	246	<div><div></div><div>11%</div><div>90%</div><div>7% ..</div></div>
4	H	246	<div><div></div><div>%</div><div>91%</div><div>8% .</div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14696 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	14	0
			2231	1435	385	397	14			
1	C	267	Total	C	N	O	S	0	14	0
			2257	1455	382	406	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	conflict	UNP Q95460

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	1	0
			774	498	131	142	3			
2	F	99	Total	C	N	O	S	0	3	0
			814	524	138	149	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Human TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	188	Total	C	N	O	S	0	4	0
			1439	927	228	274	10			

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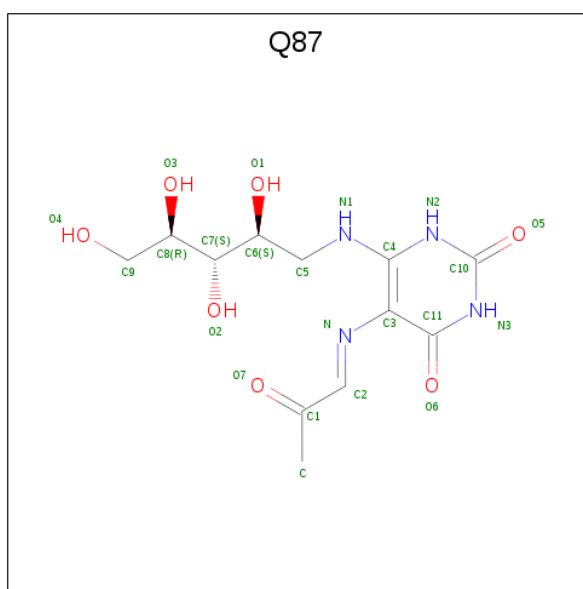
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	199	Total	C	N	O	S	0	18	0
			1613	1030	249	322	12			

- Molecule 4 is a protein called Human TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	241	Total	C	N	O	S	0	9	0
			1867	1181	312	362	12			
4	H	244	Total	C	N	O	S	0	13	0
			1953	1240	332	367	14			

- Molecule 5 is 1-deoxy-1-({2,6-dioxo-5-[(E)-(2-oxopropylidene)amino]-1,2,3,6-tetrahydropyrimidin-4-yl}amino)-D-ribose (three-letter code: Q87) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			22	12	4	6		
5	C	1	Total	C	N	O	0	0
			22	12	4	6		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	F	1	Total	Cl	0	0
			1	1		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	Na	0	0
			1	1		
8	F	1	Total	Na	0	0
			1	1		

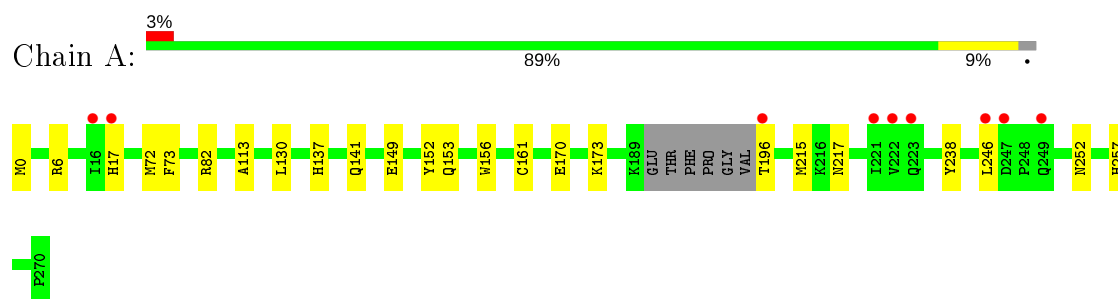
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	299	Total 299	O 299	0	0
9	B	80	Total 80	O 80	0	0
9	C	309	Total 309	O 309	0	0
9	D	135	Total 135	O 135	0	0
9	E	132	Total 132	O 132	0	0
9	F	116	Total 116	O 116	0	0
9	G	264	Total 264	O 264	0	0
9	H	347	Total 347	O 347	0	0

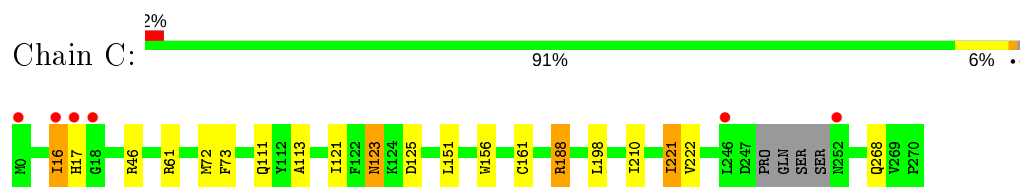
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

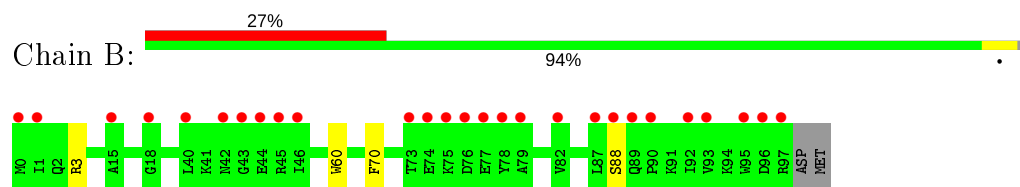
- Molecule 1: Major histocompatibility complex class I-related gene protein



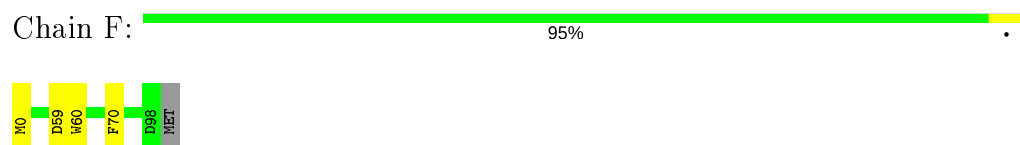
- Molecule 1: Major histocompatibility complex class I-related gene protein



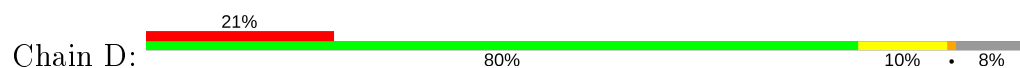
- Molecule 2: Beta-2-microglobulin



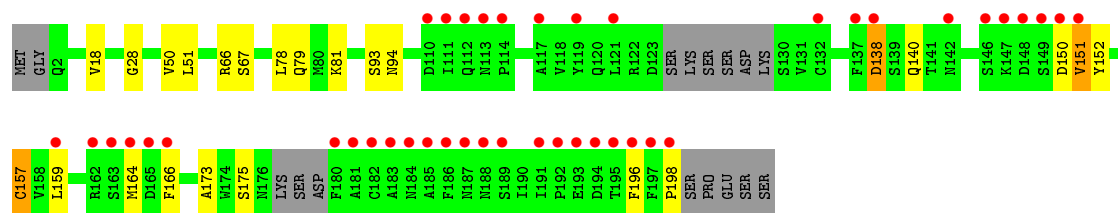
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Human TCR alpha chain



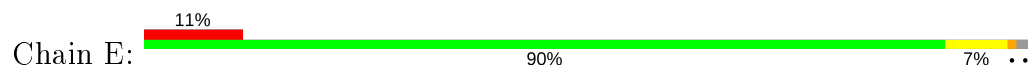




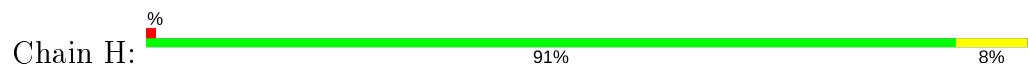
• Molecule 3: Human TCR alpha chain



• Molecule 4: Human TCR beta chain



• Molecule 4: Human TCR beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.97Å 70.25Å 143.63Å 90.00° 104.81° 90.00°	Depositor
Resolution (Å)	48.34 – 1.85 48.34 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.34-1.85) 99.9 (48.34-1.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.159 , 0.178 0.161 , 0.179	Depositor DCC
$R_{free}$ test set	9025 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, Q87, NA

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	0.41	0/2340	0.57	0/3179
1	C	0.40	0/2367	0.58	0/3216
2	B	0.33	0/800	0.51	0/1092
2	F	0.35	0/846	0.56	0/1151
3	D	0.37	0/1483	0.57	0/2016
3	G	0.45	0/1702	0.61	2/2309 (0.1%)
4	E	0.35	0/1939	0.55	0/2647
4	H	0.46	0/2047	0.59	0/2787
All	All	0.40	0/13524	0.57	2/18397 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	159[A]	LEU	CA-CB-CG	5.32	127.54	115.30
3	G	159[B]	LEU	CA-CB-CG	5.32	127.54	115.30

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	A	2231	0	2139	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2257	0	2168	17	0
2	B	774	0	703	2	0
2	F	814	0	773	2	0
3	D	1439	0	1336	16	0
3	G	1613	0	1568	9	0
4	E	1867	0	1723	18	0
4	H	1953	0	1862	18	0
5	A	22	0	0	0	0
5	C	22	0	0	0	0
6	A	6	0	8	0	0
6	C	6	0	8	0	0
6	F	6	0	8	0	0
7	A	1	0	0	0	0
7	F	1	0	0	0	0
8	F	1	0	0	0	0
8	H	1	0	0	0	0
9	A	299	0	0	5	0
9	B	80	0	0	1	0
9	C	309	0	0	3	0
9	D	135	0	0	0	0
9	E	132	0	0	3	0
9	F	116	0	0	1	0
9	G	264	0	0	3	1
9	H	347	0	0	5	0
All	All	14696	0	12296	81	1

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 3.

All (81) 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:A:153[B]:GLN:NE2	9:A:401:HOH:O	2.04	0.89
3:G:96[B]:GLN:NE2	9:G:301:HOH:O	2.08	0.86
1:A:6[A]:ARG:NH1	9:A:402:HOH:O	2.13	0.81
1:A:217:ASN:HD21	1:A:252:ASN:HD22	1.36	0.73
4:H:99:GLU:OE1	9:H:401:HOH:O	2.06	0.73
1:C:268[B]:GLN:NE2	9:C:402:HOH:O	2.17	0.73
4:H:65[B]:ASN:OD1	9:H:402:HOH:O	2.10	0.68
4:E:13:LEU:HD21	4:E:19[B]:MET:HG3	1.76	0.68
4:E:73:GLU:OE2	9:E:301:HOH:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268[B]:GLN:OE1	9:C:401:HOH:O	2.15	0.65
2:B:3:ARG:HD2	9:B:148:HOH:O	1.99	0.62
4:H:65[B]:ASN:ND2	9:H:404:HOH:O	2.31	0.62
2:F:59:ASP:OD2	9:F:201:HOH:O	2.16	0.61
1:A:153[B]:GLN:HG3	9:A:632:HOH:O	2.00	0.59
1:C:222:VAL:HA	4:H:200[B]:THR:HG21	1.86	0.58
1:C:61[A]:ARG:HG2	3:D:94:ASN:HB3	1.85	0.58
4:E:28:ASN:ND2	9:E:303:HOH:O	2.36	0.58
1:A:149[B]:GLU:OE1	4:H:99:GLU:HB2	2.03	0.57
1:C:123:ASN:HD22	1:C:125:ASP:H	1.52	0.57
1:A:215:MET:HG3	1:A:257:HIS:CD2	2.42	0.54
4:E:131:PRO:HD3	4:E:144:LEU:HD23	1.89	0.54
4:E:13:LEU:HD11	4:E:19[B]:MET:HE2	1.90	0.53
1:C:123:ASN:C	1:C:123:ASN:HD22	2.12	0.53
4:E:99[A]:GLU:OE2	9:E:302:HOH:O	2.19	0.53
4:E:172[B]:CYS:SG	4:E:194:ARG:HD3	2.49	0.52
3:G:28:GLY:HA3	3:G:93[B]:SER:OG	2.09	0.52
3:D:157:CYS:SG	4:E:172[B]:CYS:HB2	2.50	0.52
3:D:28:GLY:HA3	3:D:93[B]:SER:OG	2.10	0.52
4:H:8:PRO:HD2	4:H:21:LEU:HD22	1.91	0.51
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.45	0.51
1:A:215:MET:HG3	1:A:257:HIS:NE2	2.26	0.51
1:C:72[B]:MET:HG3	4:E:96:TRP:CZ2	2.46	0.51
3:G:140:GLN:NE2	9:G:308:HOH:O	2.43	0.51
3:D:166:PHE:CZ	4:E:141:LYS:HE3	2.47	0.50
1:A:137:HIS:O	1:A:141[B]:GLN:HG2	2.11	0.50
4:E:154:ASP:OD1	4:E:177:PRO:HG2	2.11	0.49
4:E:174:ASP:HB2	4:E:191:LEU:HD12	1.94	0.49
1:C:210:ILE:O	4:H:206[A]:ARG:HD2	2.13	0.48
4:H:12[B]:VAL:HG23	9:H:405:HOH:O	2.12	0.48
1:A:238:TYR:OH	9:A:403:HOH:O	2.20	0.48
3:D:151:VAL:HA	3:D:175:SER:HB2	1.96	0.47
1:C:113:ALA:HB2	2:F:60:TRP:CE2	2.50	0.46
3:G:17[B]:ILE:HD12	9:G:497:HOH:O	2.16	0.46
1:A:196:THR:HG22	1:A:246:LEU:HD12	1.98	0.45
4:H:19[B]:MET:SD	4:H:112:LEU:HD21	2.56	0.44
3:D:18:VAL:HG12	3:D:78:LEU:HD21	1.99	0.44
1:C:151:LEU:HD22	3:D:51:LEU:HD12	1.99	0.44
4:E:136:ILE:HG23	4:E:199:ALA:HB1	1.99	0.44
1:A:170:GLU:OE1	1:A:173:LYS:HE3	2.18	0.43
3:D:138:ASP:OD1	3:D:140:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:HG12	1:C:17:HIS:N	2.33	0.43
4:E:128:VAL:HG23	4:E:238:ALA:HB3	2.00	0.43
1:A:152:TYR:CD1	4:H:100:GLY:HA3	2.53	0.43
1:C:156:TRP:CZ3	1:C:161:CYS:HB2	2.54	0.43
4:E:131:PRO:HG2	4:E:142:ALA:HB1	2.01	0.43
3:D:150:ASP:O	3:D:175:SER:OG	2.22	0.43
1:A:217:ASN:HD21	1:A:252:ASN:ND2	2.10	0.43
3:D:166:PHE:CE2	4:E:141:LYS:HE3	2.54	0.42
1:C:111:GLN:HG2	1:C:121:ILE:HG23	2.00	0.42
3:G:166:PHE:CE1	4:H:141:LYS:HE2	2.55	0.42
4:H:208:HIS:NE2	4:H:239:GLU:OE1	2.34	0.42
1:C:221:ILE:HG22	4:H:200[A]:THR:HG21	2.02	0.42
3:D:152:TYR:O	3:D:173:ALA:HA	2.19	0.42
3:D:159:LEU:HB3	4:E:172[B]:CYS:SG	2.60	0.42
4:H:1:ASN:HA	9:H:617:HOH:O	2.19	0.42
1:C:188:ARG:HB2	1:C:198:LEU:HD23	2.02	0.41
1:A:72[B]:MET:HE1	9:A:649:HOH:O	2.20	0.41
3:G:166:PHE:CD1	4:H:141:LYS:HE2	2.55	0.41
3:D:50:VAL:O	3:D:66:ARG:HD3	2.21	0.41
4:H:186:ASP:N	4:H:186:ASP:OD1	2.54	0.41
3:D:79:GLN:OE1	3:D:81:LYS:HE2	2.21	0.41
4:H:128[A]:VAL:HG23	4:H:238:ALA:HB3	2.02	0.41
1:C:46:ARG:HD2	9:C:653:HOH:O	2.20	0.40
3:D:196:PHE:CE2	3:D:198:PRO:HG3	2.56	0.40
3:D:28:GLY:HA3	3:D:93[A]:SER:HB3	2.03	0.40
3:G:5:ASP:HB2	3:G:23[A]:THR:HG23	2.03	0.40
3:G:157:CYS:SG	4:H:172[B]:CYS:HB2	2.61	0.40
1:A:156:TRP:CZ3	1:A:161:CYS:HB2	2.56	0.40
1:C:123:ASN:ND2	1:C:125:ASP:H	2.16	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:468:HOH:O	9:G:552:HOH:O[4_548]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	275/271 (102%)	271 (98%)	4 (2%)	0	100	100
1	C	277/271 (102%)	274 (99%)	3 (1%)	0	100	100
2	B	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
2	F	100/100 (100%)	99 (99%)	1 (1%)	0	100	100
3	D	186/204 (91%)	182 (98%)	4 (2%)	0	100	100
3	G	215/204 (105%)	211 (98%)	4 (2%)	0	100	100
4	E	248/246 (101%)	246 (99%)	2 (1%)	0	100	100
4	H	256/246 (104%)	253 (99%)	3 (1%)	0	100	100
All	All	1654/1642 (101%)	1632 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	238/241 (99%)	232 (98%)	6 (2%)	47	31
1	C	243/241 (101%)	237 (98%)	6 (2%)	47	31
2	B	80/95 (84%)	78 (98%)	2 (2%)	47	31
2	F	89/95 (94%)	87 (98%)	2 (2%)	52	36
3	D	149/181 (82%)	144 (97%)	5 (3%)	37	19
3	G	189/181 (104%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	196/212 (92%)	193 (98%)	3 (2%)	65	53
4	H	212/212 (100%)	208 (98%)	4 (2%)	57	43
All	All	1396/1458 (96%)	1368 (98%)	28 (2%)	59	40

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	17	HIS
1	A	73	PHE
1	A	82	ARG
1	A	130[A]	LEU
1	A	130[B]	LEU
2	B	70	PHE
2	B	88	SER
1	C	16	ILE
1	C	73[A]	PHE
1	C	73[B]	PHE
1	C	123	ASN
1	C	188	ARG
1	C	221	ILE
3	D	67	SER
3	D	138	ASP
3	D	151	VAL
3	D	157	CYS
3	D	164	MET
4	E	19[A]	MET
4	E	19[B]	MET
4	E	194	ARG
2	F	0	MET
2	F	70	PHE
4	H	132	SER
4	H	194	ARG
4	H	206[A]	ARG
4	H	206[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS

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Mol	Chain	Res	Type
1	A	252	ASN
1	C	123	ASN
4	E	163	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	Q87	A	301	1	20,22,23	1.21	3 (15%)	22,29,31	4.24	6 (27%)
6	GOL	F	101	-	5,5,5	1.05	0	5,5,5	0.99	0
6	GOL	A	302	-	5,5,5	0.76	0	5,5,5	1.05	0
5	Q87	C	301	1	20,22,23	1.42	4 (20%)	22,29,31	4.15	7 (31%)
6	GOL	C	302	-	5,5,5	0.82	0	5,5,5	0.91	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
5	Q87	A	301	1	-	3/18/19/20	0/1/1/1
6	GOL	F	101	-	-	0/4/4/4	-
6	GOL	A	302	-	-	0/4/4/4	-
5	Q87	C	301	1	-	3/18/19/20	0/1/1/1
6	GOL	C	302	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	301	Q87	C1-C2	-3.37	1.45	1.49
5	C	301	Q87	C4-N1	3.24	1.39	1.34
5	A	301	Q87	C11-N3	3.21	1.38	1.33
5	C	301	Q87	C11-N3	3.01	1.38	1.33
5	A	301	Q87	C1-C2	-2.58	1.46	1.49
5	A	301	Q87	C4-N1	2.24	1.38	1.34
5	C	301	Q87	C3-N	-2.16	1.39	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	301	Q87	C11-N3-C10	14.05	127.00	115.14
5	A	301	Q87	C11-N3-C10	13.73	126.73	115.14
5	A	301	Q87	C11-C3-C4	10.72	121.54	114.53
5	C	301	Q87	C11-C3-C4	9.53	120.77	114.53
5	A	301	Q87	C3-C11-N3	-7.24	113.53	123.43
5	C	301	Q87	C3-C11-N3	-6.86	114.06	123.43
5	A	301	Q87	C10-N2-C4	4.34	123.74	113.80
5	C	301	Q87	C10-N2-C4	4.32	123.69	113.80
5	C	301	Q87	C6-C5-N1	2.61	119.01	111.52
5	A	301	Q87	C4-C3-N	-2.33	112.56	125.02
5	C	301	Q87	C4-C3-N	-2.32	112.63	125.02
5	A	301	Q87	C6-C5-N1	2.29	118.11	111.52
5	C	301	Q87	O1-C6-C7	2.10	114.21	109.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	Q87	C4-C3-N-C2
5	A	301	Q87	C4-C3-N-C2
5	C	301	Q87	N1-C5-C6-C7
5	A	301	Q87	N1-C5-C6-C7

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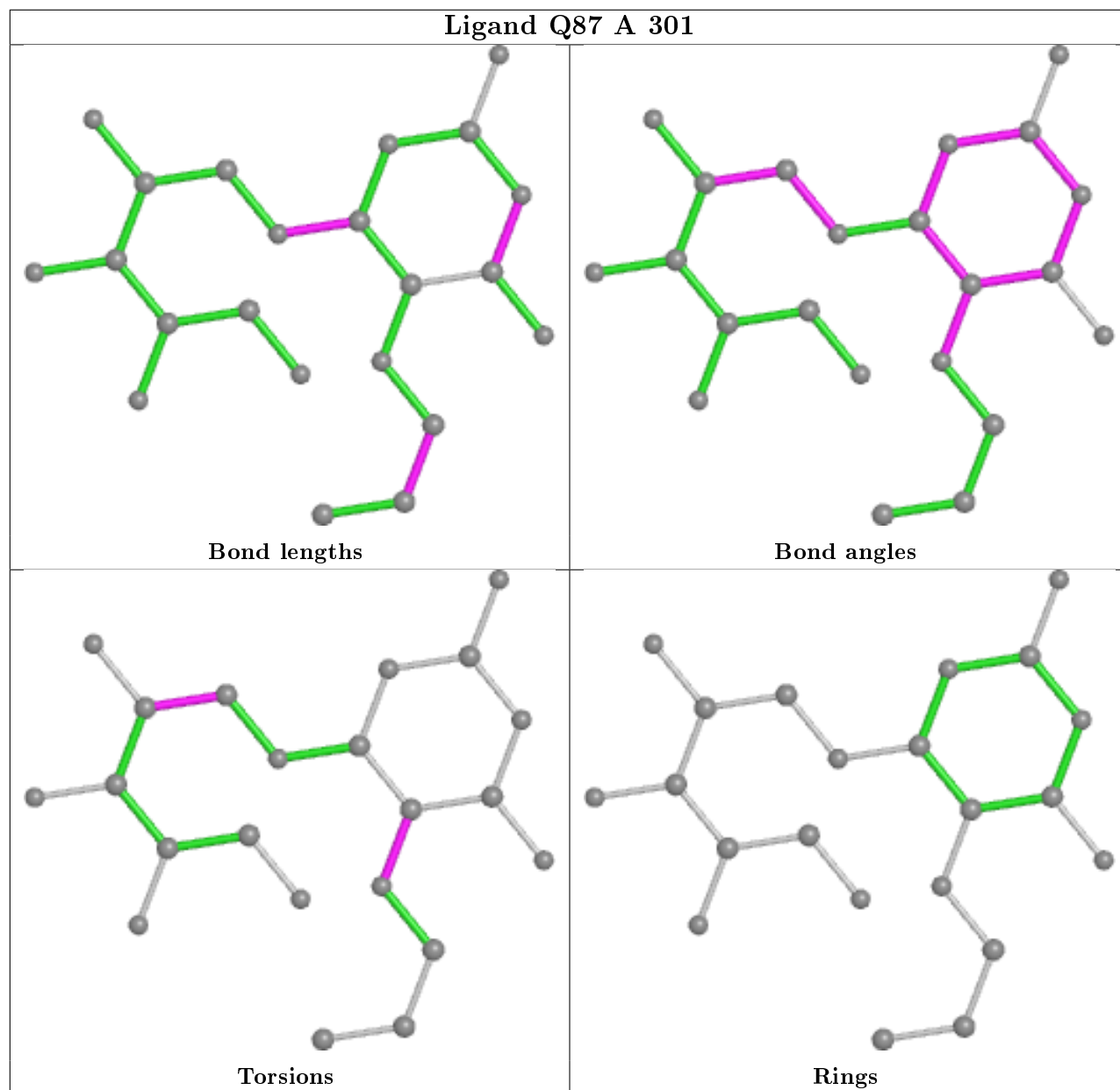
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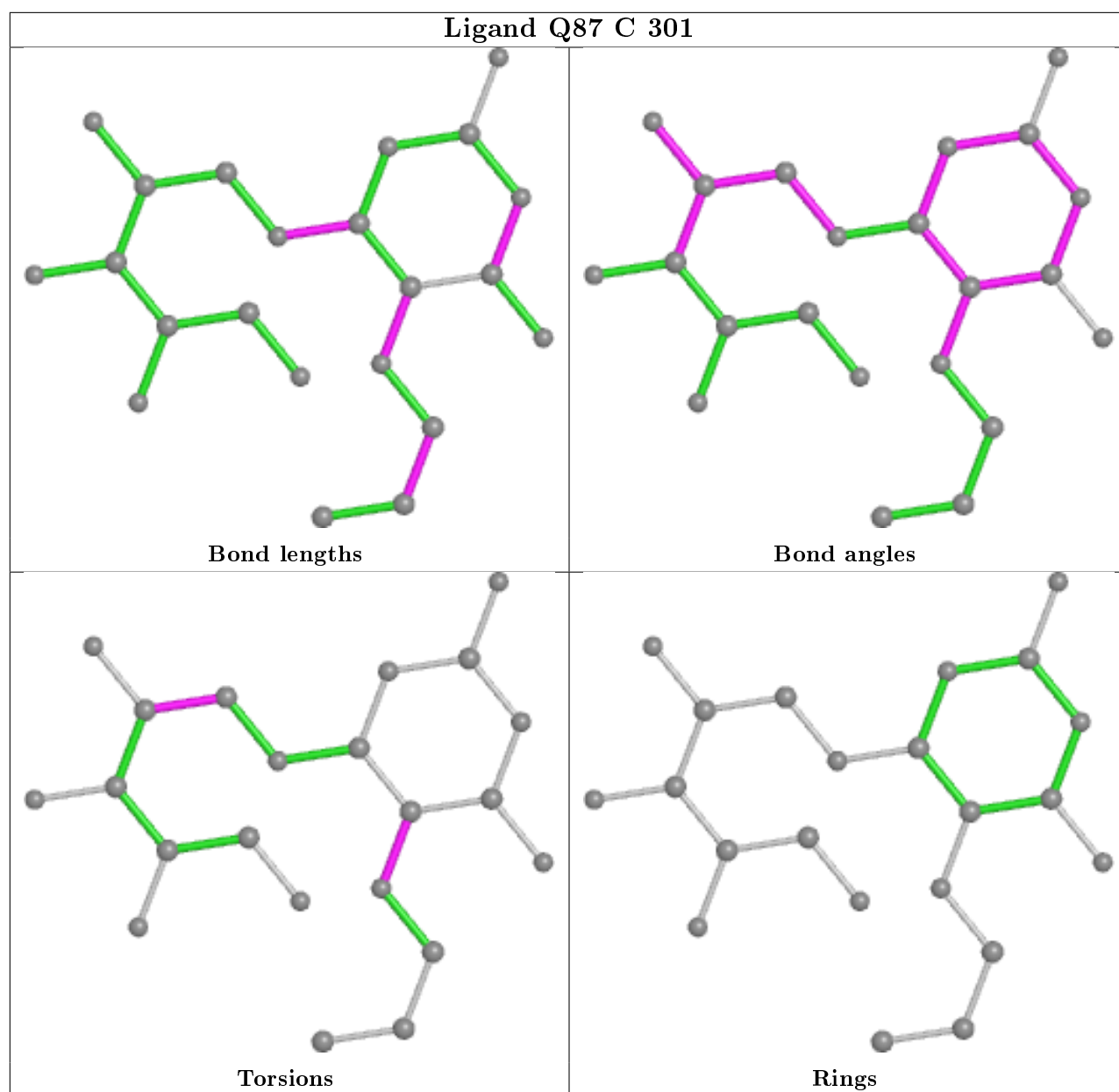
Mol	Chain	Res	Type	Atoms
5	C	301	Q87	C11-C3-N-C2
5	A	301	Q87	C11-C3-N-C2

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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	265/271 (97%)	-0.17	9 (3%) 45 42	21, 34, 69, 83	4 (1%)
1	C	267/271 (98%)	-0.20	6 (2%) 62 61	23, 32, 59, 83	7 (2%)
2	B	98/100 (98%)	1.03	27 (27%) 0 0	28, 55, 75, 83	1 (1%)
2	F	99/100 (99%)	-0.16	0 100 100	25, 38, 58, 63	4 (4%)
3	D	188/204 (92%)	0.80	42 (22%) 0 0	27, 47, 87, 107	5 (2%)
3	G	199/204 (97%)	-0.41	3 (1%) 73 74	19, 29, 49, 74	4 (2%)
4	E	241/246 (97%)	0.28	27 (11%) 5 5	30, 48, 84, 98	1 (0%)
4	H	244/246 (99%)	-0.18	2 (0%) 86 86	21, 29, 46, 64	2 (0%)
All	All	1601/1642 (97%)	0.05	116 (7%) 15 15	19, 35, 74, 107	28 (1%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	191	ILE	7.5
3	D	197	PHE	6.8
3	D	147	LYS	6.5
2	B	78	TYR	5.5
3	D	181	ALA	5.3
3	D	180	PHE	5.2
3	D	119	TYR	5.0
3	D	164	MET	4.9
1	A	222	VAL	4.8
4	E	224	TRP	4.7
2	B	43	GLY	4.6
3	D	183	ALA	4.5
3	D	196	PHE	4.4
3	D	148	ASP	4.4
4	E	200	THR	4.4
1	C	16	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
3	D	192	PRO	4.4
3	D	188	ASN	4.3
3	D	113	ASN	4.3
3	D	163	SER	4.3
3	D	198	PRO	4.2
3	D	185	ALA	4.1
3	D	166	PHE	4.1
3	D	112	GLN	4.0
2	B	76	ASP	4.0
1	A	221	ILE	3.9
4	E	204	ASN	3.9
1	A	196	THR	3.9
4	E	136	ILE	3.9
2	B	95	TRP	3.9
2	B	79	ALA	3.9
4	E	199	ALA	3.7
2	B	42	ASN	3.7
3	D	195	THR	3.7
3	D	187	ASN	3.7
4	E	167	VAL	3.6
4	E	225	THR	3.6
4	E	227	ASP	3.6
1	C	17	HIS	3.6
3	D	151	VAL	3.6
2	B	75	LYS	3.5
2	B	73	THR	3.5
3	D	146	SER	3.5
4	E	164	GLY	3.5
2	B	92	ILE	3.5
1	C	252	ASN	3.5
4	E	202	TRP	3.5
2	B	97	ARG	3.5
3	D	149	SER	3.5
3	G	179	ASP	3.4
4	E	198	SER	3.4
2	B	74	GLU	3.4
4	E	207	ASN	3.4
4	E	221	ASN	3.4
2	B	46	ILE	3.4
4	E	205	PRO	3.3
3	D	117	ALA	3.3
4	E	137	SER	3.3

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Mol	Chain	Res	Type	RSRZ
4	E	197	VAL	3.2
4	E	219	SER	3.2
4	E	140	GLN	3.2
3	D	193	GLU	3.1
4	E	203	GLN	3.1
3	D	121	LEU	3.1
4	E	142	ALA	3.1
3	D	138	ASP	3.0
1	C	246	LEU	3.0
3	D	184	ASN	3.0
3	D	189	SER	2.9
2	B	18	GLY	2.9
2	B	88	SER	2.9
4	H	2	ALA	2.9
2	B	45	ARG	2.8
2	B	77	GLU	2.8
2	B	96	ASP	2.8
4	E	209	PHE	2.7
4	E	223	GLU	2.7
3	D	132	CYS	2.7
3	D	182	CYS	2.7
4	E	228	ARG	2.7
2	B	1	ILE	2.7
4	E	222	ASP	2.6
1	A	223	GLN	2.6
3	D	110	ASP	2.6
2	B	87	LEU	2.6
2	B	89	GLN	2.5
3	D	194	ASP	2.5
3	D	165	ASP	2.5
1	A	17	HIS	2.4
3	D	142	ASN	2.4
2	B	0	MET	2.4
1	A	247	ASP	2.4
3	D	114	PRO	2.3
1	A	246	LEU	2.3
3	D	150	ASP	2.3
3	D	162	ARG	2.3
3	D	137	PHE	2.3
3	D	186	PHE	2.3
4	E	132	SER	2.3
3	D	159	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	249	GLN	2.3
2	B	90	PRO	2.2
3	G	146[A]	SER	2.2
4	E	232	VAL	2.2
2	B	44	GLU	2.2
1	C	18	GLY	2.1
2	B	40	LEU	2.1
4	H	206[A]	ARG	2.1
3	D	111	ILE	2.1
2	B	93	VAL	2.1
1	A	16	ILE	2.1
3	G	163	SER	2.1
2	B	82	VAL	2.1
1	C	0	MET	2.0
4	E	210	ARG	2.0
2	B	15	ALA	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 carbohydrates 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	CL	A	303	1/1	0.86	0.11	70,70,70,70	0
6	GOL	F	101	6/6	0.88	0.15	34,43,50,51	0
6	GOL	C	302	6/6	0.90	0.12	39,56,62,64	0
6	GOL	A	302	6/6	0.91	0.18	27,42,51,54	6
5	Q87	A	301	22/23	0.97	0.09	18,21,25,27	0
5	Q87	C	301	22/23	0.98	0.12	22,24,27,29	0
8	NA	F	102	1/1	0.98	0.20	39,39,39,39	1

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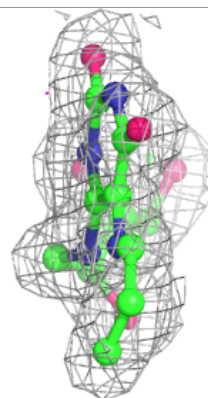
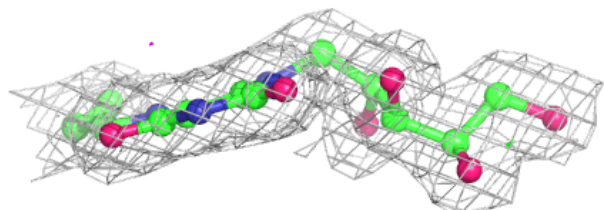
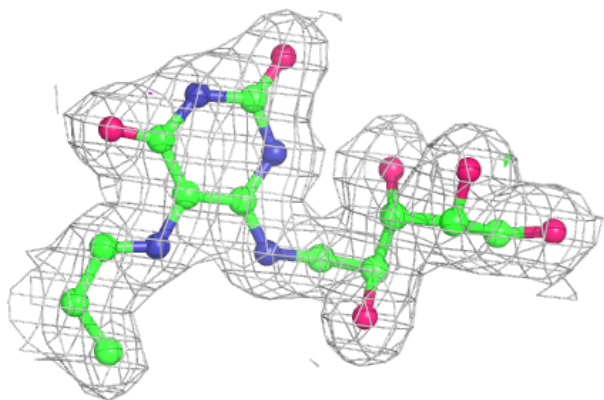
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CL	F	103	1/1	0.98	0.05	41,41,41,41	0
8	NA	H	301	1/1	1.00	0.08	33,33,33,33	0

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.

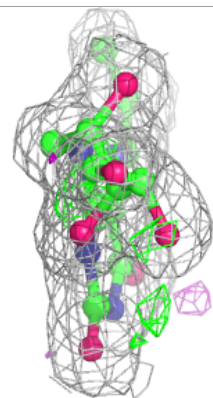
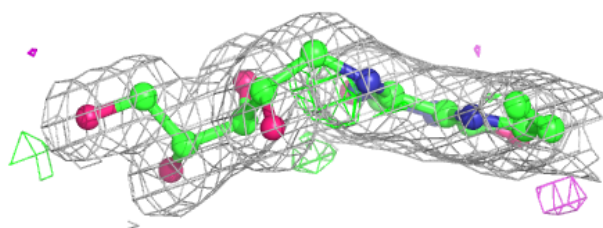
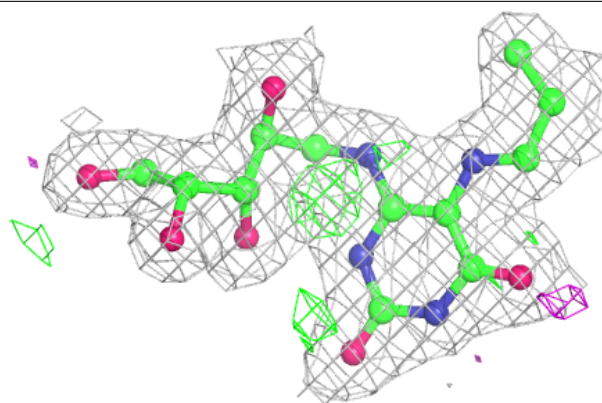
**Electron density around Q87 A 301:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Q87 C 301:**

$2mF_o-DF_c$  (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.