



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:54 AM UTC

PDB ID : 9O05 / pdb_00009o05
Title : Structure of human MAIT A-F7 TCR in complex with human MR1-riboflavin
Authors : Abdelaal, M.; Rossjohn, J.; Awad, W.
Deposited on : 2025-04-02
Resolution : 1.95 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

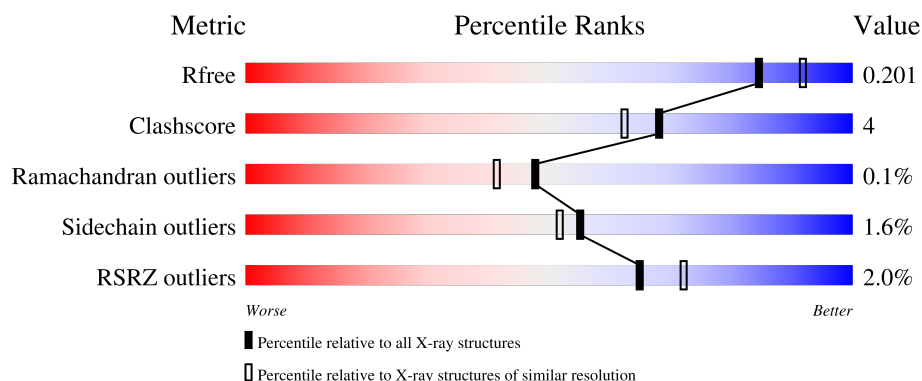
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



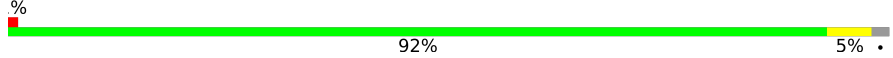
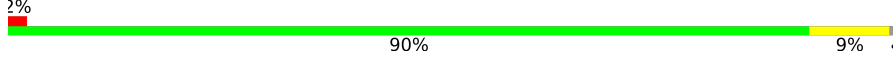
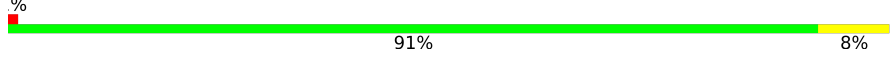
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	271	2% 88% 10% .
1	C	271	2% 86% 11% .
2	B	100	94% . .
2	F	100	% 92% 8%
3	D	204	5% 84% 8% 7%

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Mol	Chain	Length	Quality of chain
3	G	204	 92% 5%
4	E	246	 90% 9%
4	H	246	 91% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	A	302	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14760 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	9	0
			2211	1418	381	398	14			
1	C	266	Total	C	N	O	S	0	13	0
			2255	1449	383	411	12			

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	engineered mutation	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	engineered mutation	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
			791	508	133	147	3			
2	F	100	Total	C	N	O	S	0	2	0
			831	531	140	156	4			

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 TCR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	189	Total	C	N	O	S	0	5	0
			1455	934	230	281	10			

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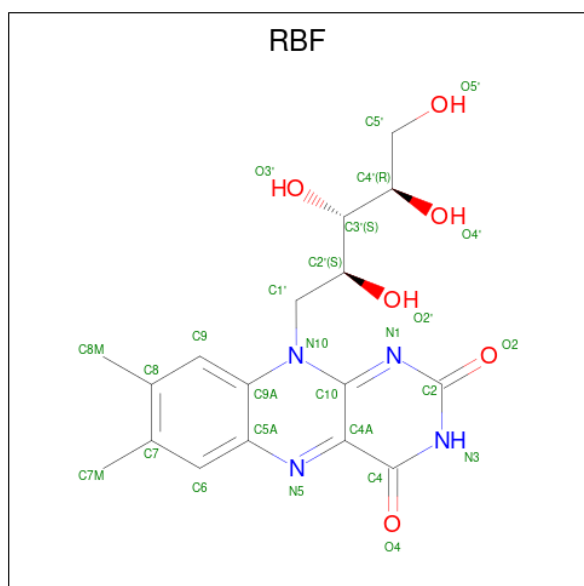
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	200	Total	C	N	O	S	0	13	0
			1624	1029	259	325	11			

- Molecule 4 is a protein called TCR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	243	Total	C	N	O	S	0	6	0
			1906	1204	323	369	10			
4	H	245	Total	C	N	O	S	0	12	0
			1970	1244	337	376	13			

- Molecule 5 is RIBOFLAVIN (CCD ID: RBF) (formula: $C_{17}H_{20}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			27	17	4	6		
5	C	1	Total	C	N	O	0	0
			27	17	4	6		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total	Na	0	0
			1	1		

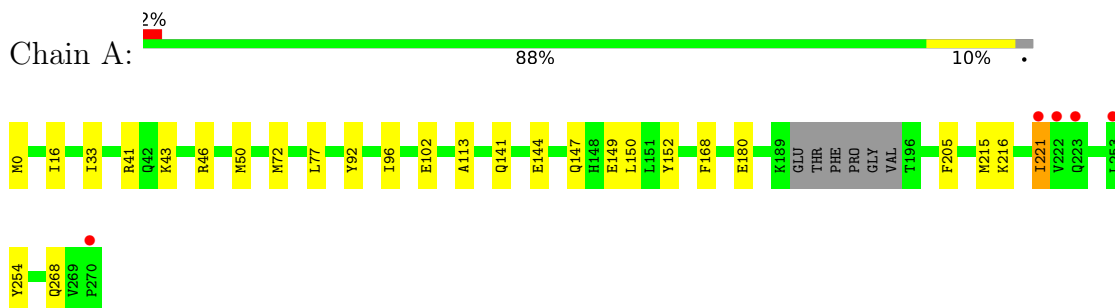
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	279	Total	O	0	0
			279	279		
10	B	75	Total	O	0	0
			75	75		
10	C	294	Total	O	0	0
			294	294		
10	D	145	Total	O	0	0
			145	145		
10	E	172	Total	O	0	0
			172	172		
10	F	125	Total	O	0	0
			125	125		
10	G	240	Total	O	0	0
			240	240		
10	H	287	Total	O	0	0
			287	287		

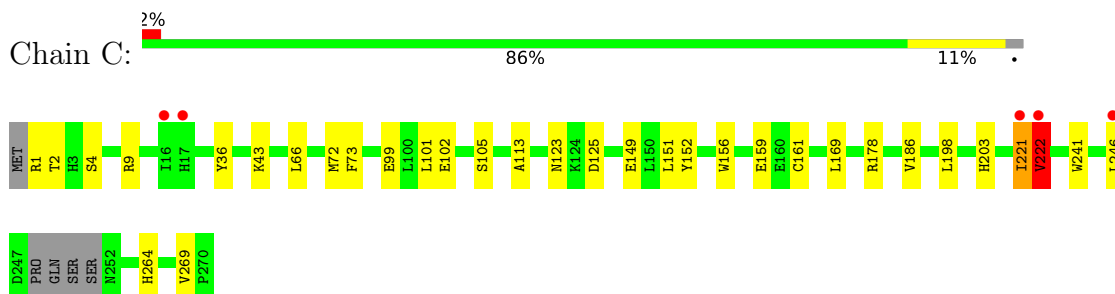
3 Residue-property plots

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.

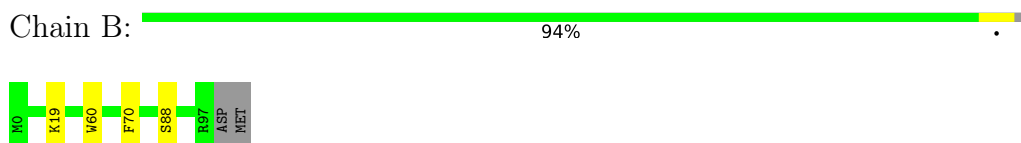
- Molecule 1: Major histocompatibility complex class I-related gene protein



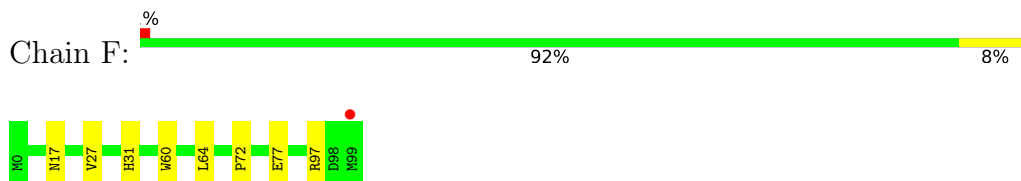
- Molecule 1: Major histocompatibility complex class I-related gene protein



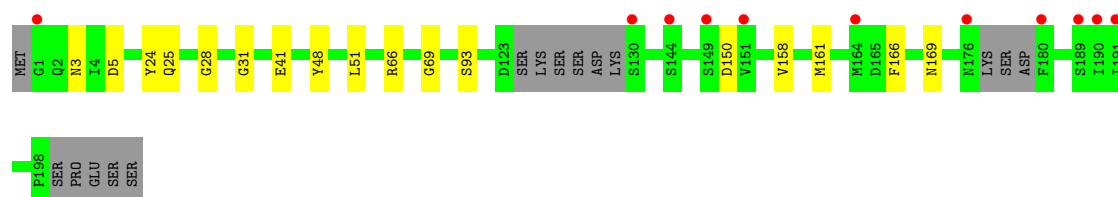
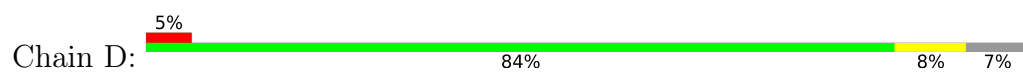
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



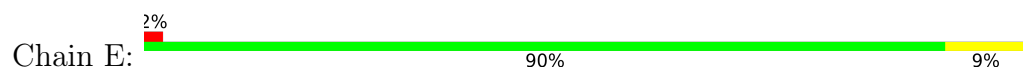
- Molecule 3: TCR-alpha



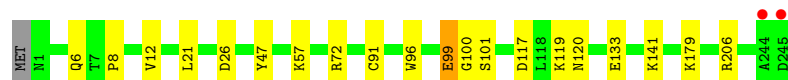
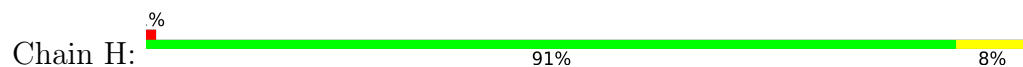
• Molecule 3: TCR-alpha



• Molecule 4: TCR-beta



• Molecule 4: TCR-beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	217.38Å 70.77Å 143.63Å 90.00° 104.70° 90.00°	Depositor
Resolution (Å)	47.01 – 1.95 47.01 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.01-1.95) 98.7 (47.01-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.164 , 0.201 0.165 , 0.201	Depositor DCC
R_{free} test set	7580 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14760	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/2304	0.46	0/3130
1	C	0.29	0/2359	0.48	0/3207
2	B	0.21	0/817	0.40	0/1113
2	F	0.23	0/857	0.43	0/1165
3	D	0.26	0/1502	0.45	0/2041
3	G	0.28	0/1695	0.50	0/2297
4	E	0.25	0/1975	0.46	0/2692
4	H	0.29	0/2054	0.51	0/2795
All	All	0.27	0/13563	0.47	0/18440

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2211	0	2121	21	0
1	C	2255	0	2158	26	0
2	B	791	0	729	2	0
2	F	831	0	782	5	0
3	D	1455	0	1351	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1624	0	1567	8	0
4	E	1906	0	1775	14	0
4	H	1970	0	1871	15	0
5	A	27	0	20	3	0
5	C	27	0	20	1	0
6	A	4	0	3	3	0
6	C	4	0	3	0	0
7	A	6	0	8	0	0
7	C	6	0	8	1	0
7	E	6	0	8	0	0
7	F	12	0	16	0	0
7	G	6	0	8	0	0
8	A	1	0	0	0	0
9	H	1	0	0	0	0
10	A	279	0	0	4	0
10	B	75	0	0	1	0
10	C	294	0	0	10	1
10	D	145	0	0	1	0
10	E	172	0	0	3	1
10	F	125	0	0	2	0
10	G	240	0	0	2	0
10	H	287	0	0	6	0
All	All	14760	0	12448	93	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 4.

All (93) 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:41[B]:ARG:NH1	10:A:401:HOH:O	2.09	0.84
1:C:125:ASP:OD1	10:C:402:HOH:O	2.07	0.73
1:C:125:ASP:O	10:C:401:HOH:O	2.05	0.73
4:H:133:GLU:OE2	10:H:401:HOH:O	2.07	0.72
4:H:206[B]:ARG:HG3	10:H:443:HOH:O	1.91	0.70
4:H:179:LYS:NZ	10:H:403:HOH:O	2.26	0.69
3:D:66[B]:ARG:NH1	10:D:301:HOH:O	2.19	0.66
1:A:43:LYS:HE2	6:A:302:ACT:OXT	1.97	0.65
3:G:184[A]:ASN:ND2	10:G:404:HOH:O	2.29	0.65
1:C:198:LEU:HD13	1:C:269:VAL:HG21	1.82	0.61
1:A:141:GLN:NE2	10:A:404:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LYS:NZ	5:C:301:RBF:N5	2.51	0.59
4:H:99:GLU:OE1	4:H:101:SER:N	2.37	0.58
3:D:28:GLY:HA3	3:D:93[A]:SER:OG	2.05	0.56
4:H:6:GLN:HB3	4:H:91[B]:CYS:SG	2.45	0.56
3:G:28:GLY:HA3	3:G:93[A]:SER:OG	2.05	0.56
1:A:221:ILE:H	1:A:221:ILE:HD13	1.70	0.56
4:H:12[A]:VAL:HG23	10:H:420:HOH:O	2.06	0.55
4:H:8:PRO:HD2	4:H:21:LEU:HD22	1.88	0.54
1:C:125:ASP:OD2	10:C:403:HOH:O	2.18	0.54
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.91	0.53
4:E:119:LYS:HG2	4:E:226:GLN:HE21	1.74	0.53
1:C:9:ARG:NH1	10:C:410:HOH:O	2.40	0.53
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.43	0.53
4:E:183:ALA:O	10:E:401:HOH:O	2.19	0.53
1:A:72[A]:MET:HE1	10:A:566:HOH:O	2.08	0.52
1:C:72[B]:MET:HE1	10:C:489:HOH:O	2.10	0.52
4:H:26:ASP:HB3	4:H:72:ARG:HH21	1.75	0.51
1:C:123:ASN:ND2	10:C:413:HOH:O	2.43	0.51
3:G:28:GLY:HA3	3:G:93[B]:SER:HB3	1.94	0.50
1:A:43:LYS:NZ	5:A:301:RBF:O4	2.45	0.50
10:C:543:HOH:O	4:E:97[B]:THR:HG21	2.12	0.49
3:D:161:MET:HE2	3:D:166:PHE:CD2	2.48	0.49
4:E:181:GLN:O	4:E:187:SER:HB2	2.11	0.49
1:A:152:TYR:CD1	4:H:100:GLY:HA3	2.47	0.49
4:H:141:LYS:NZ	10:H:414:HOH:O	2.46	0.49
1:A:168:PHE:CZ	6:A:302:ACT:H2	2.47	0.48
2:B:19:LYS:NZ	10:B:104:HOH:O	2.46	0.48
3:G:2:GLN:HG2	3:G:26:THR:HA	1.94	0.48
3:G:4[A]:ILE:HD11	3:G:90:VAL:HB	1.96	0.48
1:C:36:TYR:HB2	1:C:66:LEU:HD13	1.97	0.47
2:F:31:HIS:HD2	10:F:244:HOH:O	1.96	0.47
1:C:101:LEU:HD12	1:C:105[A]:SER:OG	2.14	0.46
1:A:96:ILE:HD13	5:A:301:RBF:HC51	1.98	0.46
1:A:50:MET:CE	6:A:302:ACT:H3	2.45	0.46
1:C:241:TRP:HE1	7:C:303:GOL:H31	1.81	0.46
4:E:174:ASP:HB2	4:E:191:LEU:HD12	1.97	0.46
1:C:4:SER:HB3	1:C:99:GLU:HG2	1.98	0.46
3:D:24:TYR:CZ	3:D:69:GLY:HA2	2.51	0.46
1:A:149:GLU:OE2	4:H:99:GLU:HB2	2.16	0.45
3:D:3:ASN:ND2	3:D:5:ASP:OD2	2.34	0.45
1:A:216:LYS:HE2	1:A:254:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72[A]:MET:HG3	4:H:96:TRP:CZ2	2.52	0.45
3:G:194:ASP:OD2	10:G:401:HOH:O	2.21	0.45
4:H:117[A]:ASP:OD1	4:H:119:LYS:HG3	2.18	0.44
1:C:152:TYR:CD1	4:E:100:GLY:HA3	2.53	0.44
1:C:1:ARG:NH2	1:C:178:ARG:O	2.36	0.44
1:C:36:TYR:CB	1:C:66:LEU:HD13	2.48	0.43
4:E:204:ASN:HB3	4:E:207:ASN:ND2	2.34	0.43
1:C:102:GLU:O	10:C:404:HOH:O	2.21	0.43
3:D:158:VAL:HG22	3:D:169:ASN:OD1	2.19	0.43
1:C:113:ALA:HB2	2:F:60:TRP:CE2	2.54	0.43
4:E:19[B]:MET:HE3	4:E:19[B]:MET:HB2	1.87	0.43
1:C:221:ILE:O	1:C:222:VAL:HG22	2.19	0.43
1:C:159:GLU:HB3	10:C:628:HOH:O	2.19	0.43
1:C:264[A]:HIS:CD2	10:C:627:HOH:O	2.71	0.43
4:H:47:TYR:CD1	4:H:57:LYS:HA	2.54	0.43
4:E:208:HIS:ND1	10:E:404:HOH:O	2.36	0.42
1:A:46:ARG:HD3	1:A:46:ARG:HA	1.73	0.42
1:C:151:LEU:HD22	3:D:51:LEU:HD12	2.01	0.42
4:H:12[B]:VAL:HG13	10:H:420:HOH:O	2.18	0.42
5:A:301:RBF:HC52	5:A:301:RBF:HC2'	1.73	0.42
1:C:123:ASN:HD21	1:C:125:ASP:HB2	1.85	0.42
4:E:140:GLN:HG3	10:E:531:HOH:O	2.19	0.42
1:A:0:MET:O	1:A:102:GLU:HG3	2.20	0.42
1:A:180:GLU:O	1:A:205:PHE:HA	2.19	0.42
1:A:144:GLU:HA	1:A:150:LEU:HD11	2.01	0.42
3:G:121:LEU:HD11	3:G:133:LEU:HB2	2.02	0.42
1:A:33:ILE:HB	1:A:50:MET:HG3	2.02	0.41
1:C:203:HIS:HD2	10:F:271:HOH:O	2.03	0.41
4:E:208:HIS:HB2	4:E:241:TRP:CH2	2.54	0.41
3:D:31:GLY:HA3	3:D:48:TYR:CE1	2.55	0.41
4:E:155:HIS:HB3	4:E:216:TYR:HB2	2.02	0.41
3:G:121:LEU:HD13	3:G:131:VAL:HG12	2.02	0.41
1:C:156:TRP:CZ3	1:C:161:CYS:HB2	2.55	0.41
1:C:186:VAL:HG11	1:C:269:VAL:HG22	2.02	0.41
2:F:27:VAL:HB	2:F:64[A]:LEU:HD12	2.02	0.41
2:F:77:GLU:CD	2:F:97:ARG:HH21	2.29	0.41
1:C:149:GLU:HG3	4:E:99:GLU:OE2	2.21	0.41
4:E:154:ASP:CG	4:E:177:PRO:HG3	2.46	0.41
3:D:28:GLY:HA3	3:D:93[B]:SER:HB3	2.03	0.40
1:A:147:GLN:OE1	10:A:402:HOH:O	2.22	0.40
2:F:17:ASN:HA	2:F:72:PRO:O	2.22	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)
10:C:608:HOH:O	10:E:529:HOH:O[4_547]	2.10	0.10

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	270/271 (100%)	267 (99%)	3 (1%)	0	100	100
1	C	275/271 (102%)	270 (98%)	4 (2%)	1 (0%)	30	21
2	B	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
2	F	100/100 (100%)	100 (100%)	0	0	100	100
3	D	188/204 (92%)	180 (96%)	8 (4%)	0	100	100
3	G	211/204 (103%)	208 (99%)	3 (1%)	0	100	100
4	E	247/246 (100%)	242 (98%)	5 (2%)	0	100	100
4	H	255/246 (104%)	252 (99%)	3 (1%)	0	100	100
All	All	1643/1642 (100%)	1615 (98%)	27 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	222	VAL

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	238/241 (99%)	234 (98%)	4 (2%)	53	49
1	C	244/241 (101%)	237 (97%)	7 (3%)	37	29
2	B	84/95 (88%)	82 (98%)	2 (2%)	43	36
2	F	92/95 (97%)	92 (100%)	0	100	100
3	D	152/181 (84%)	149 (98%)	3 (2%)	48	43
3	G	187/181 (103%)	183 (98%)	4 (2%)	47	41
4	E	203/212 (96%)	201 (99%)	2 (1%)	68	67
4	H	214/212 (101%)	211 (99%)	3 (1%)	59	56
All	All	1414/1458 (97%)	1389 (98%)	25 (2%)	55	47

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	215	MET
1	A	221	ILE
1	A	268	GLN
2	B	70	PHE
2	B	88	SER
1	C	2	THR
1	C	73	PHE
1	C	169[A]	LEU
1	C	169[B]	LEU
1	C	221	ILE
1	C	222	VAL
1	C	246	LEU
3	D	25	GLN
3	D	41	GLU
3	D	150	ASP
4	E	22	GLN
4	E	221	ASN
3	G	93[A]	SER
3	G	93[B]	SER
3	G	138[A]	ASP
3	G	138[B]	ASP
4	H	99	GLU
4	H	120[A]	ASN
4	H	120[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	177	GLN
1	C	93	GLN
1	C	203	HIS
3	D	19	GLN
3	D	21	ASN
3	D	37	GLN
4	E	37	GLN
2	F	17	ASN
2	F	31	HIS
3	G	94	ASN
3	G	120	GLN
4	H	168	HIS
4	H	181	GLN
4	H	226	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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
7	GOL	A	303	-	5,5,5	0.32	0	5,5,5	0.50	0
7	GOL	C	303	-	5,5,5	0.32	0	5,5,5	0.23	0
5	RBF	A	301	-	29,29,29	0.24	0	42,43,43	0.53	1 (2%)
7	GOL	E	301	-	5,5,5	0.23	0	5,5,5	0.49	0
6	ACT	C	302	-	3,3,3	0.99	0	3,3,3	1.42	0
7	GOL	F	102	-	5,5,5	0.17	0	5,5,5	0.52	0
5	RBF	C	301	-	29,29,29	0.19	0	42,43,43	0.47	1 (2%)
7	GOL	F	101	-	5,5,5	0.33	0	5,5,5	0.36	0
6	ACT	A	302	-	3,3,3	1.04	0	3,3,3	1.32	0
7	GOL	G	301	-	5,5,5	0.36	0	5,5,5	0.59	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
7	GOL	A	303	-	-	0/4/4/4	-
7	GOL	C	303	-	-	3/4/4/4	-
5	RBF	A	301	-	-	1/14/14/14	0/3/3/3
7	GOL	E	301	-	-	1/4/4/4	-
7	GOL	F	102	-	-	2/4/4/4	-
5	RBF	C	301	-	-	0/14/14/14	0/3/3/3
7	GOL	F	101	-	-	0/4/4/4	-
7	GOL	G	301	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	301	RBF	C2'-C1'-N10	2.27	120.92	110.20
5	A	301	RBF	C2'-C1'-N10	2.01	119.72	110.20

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	303	GOL	C1-C2-C3-O3
7	F	102	GOL	O1-C1-C2-O2
7	F	102	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	G	301	GOL	C1-C2-C3-O3
7	E	301	GOL	O1-C1-C2-C3
7	C	303	GOL	O2-C2-C3-O3
7	G	301	GOL	O2-C2-C3-O3
7	C	303	GOL	O1-C1-C2-O2
5	A	301	RBF	C2'-C3'-C4'-C5'

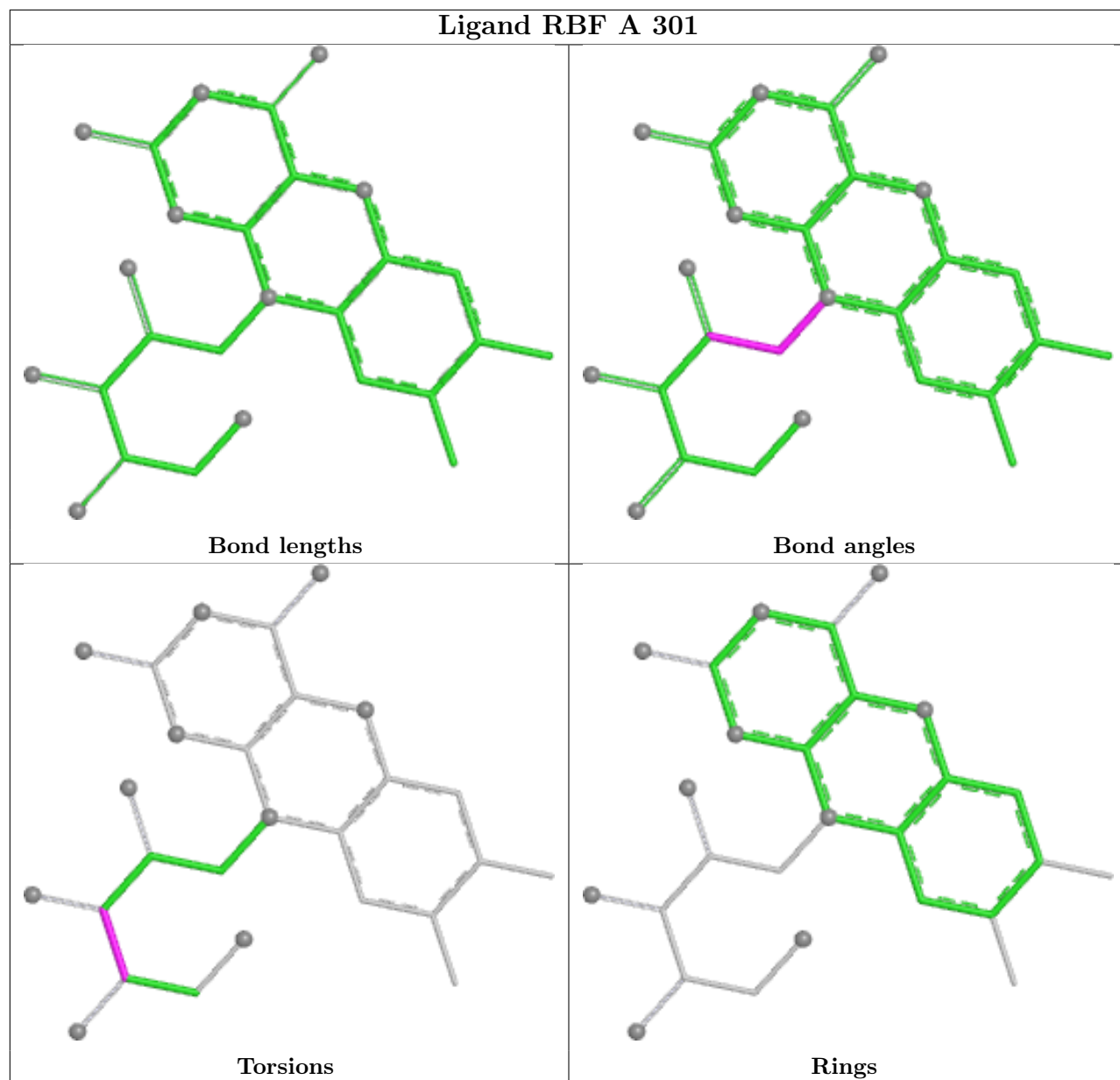
There are no ring outliers.

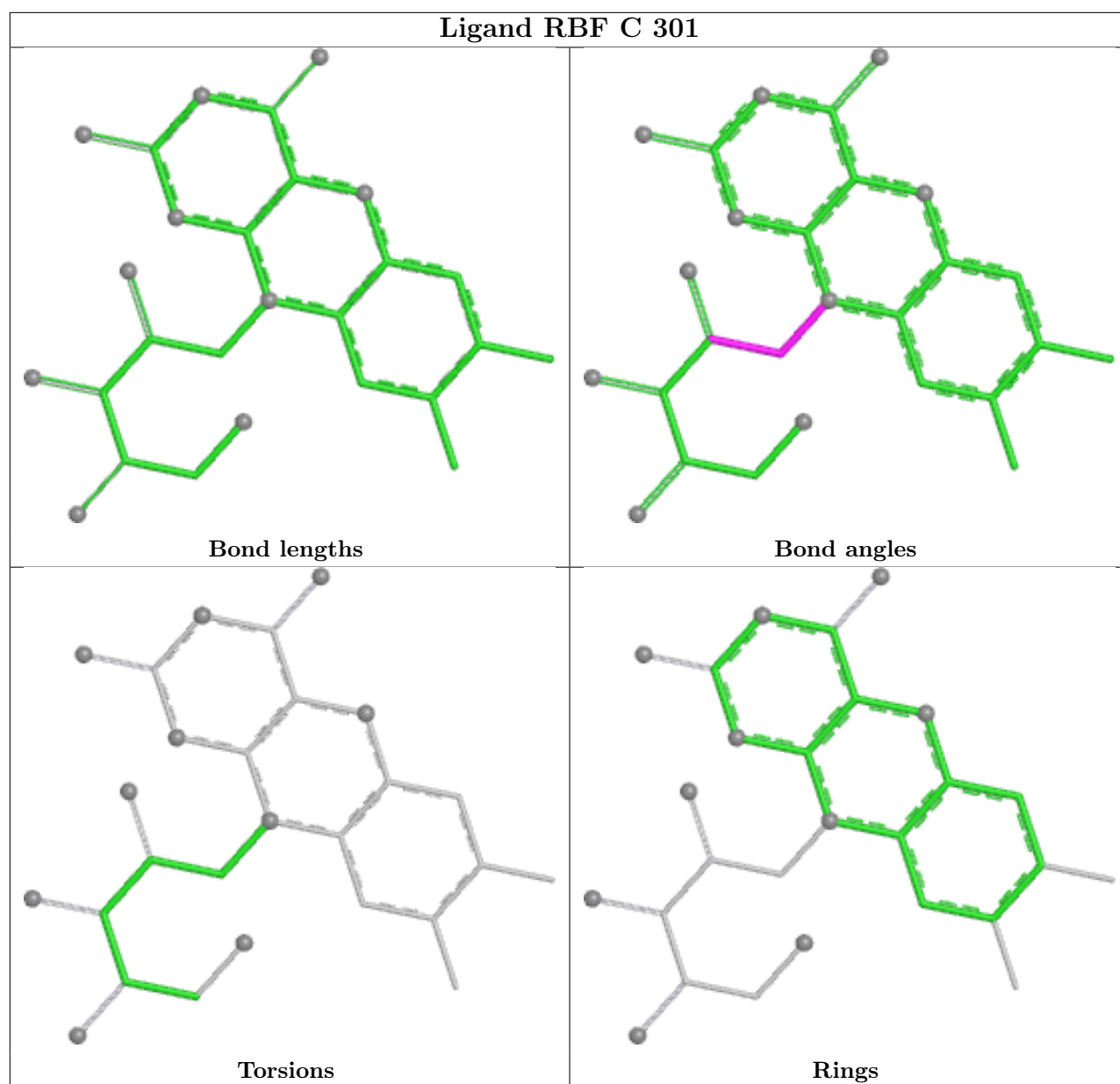
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	303	GOL	1	0
5	A	301	RBF	3	0
5	C	301	RBF	1	0
6	A	302	ACT	3	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 RBF A 301





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	265/271 (97%)	-0.11	5 (1%) 66 74	19, 37, 72, 84	12 (4%)
1	C	266/271 (98%)	-0.13	5 (1%) 66 74	19, 33, 58, 78	23 (8%)
2	B	98/100 (98%)	0.22	0 100 100	33, 56, 77, 81	1 (1%)
2	F	100/100 (100%)	-0.10	1 (1%) 79 84	16, 41, 63, 69	2 (2%)
3	D	189/204 (92%)	0.34	11 (5%) 29 33	20, 44, 81, 98	9 (4%)
3	G	200/204 (98%)	-0.21	2 (1%) 79 84	17, 33, 56, 68	19 (9%)
4	E	243/246 (98%)	0.16	6 (2%) 58 65	22, 43, 83, 110	14 (5%)
4	H	245/246 (99%)	-0.22	2 (0%) 82 86	21, 35, 52, 81	20 (8%)
All	All	1606/1642 (97%)	-0.03	32 (1%) 65 72	16, 37, 73, 110	100 (6%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	245	ASP	4.4
1	C	222	VAL	4.1
1	A	221	ILE	3.9
1	C	221	ILE	3.9
3	D	149	SER	3.6
3	D	191	ILE	3.5
3	G	200	PRO	3.4
1	A	222	VAL	3.4
4	E	245	ASP	3.3
1	C	246	LEU	3.1
1	A	253	LEU	2.9
3	G	27	SER	2.7
3	D	180	PHE	2.7
3	D	151	VAL	2.7
3	D	1	GLY	2.5
2	F	99	MET	2.3

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Mol	Chain	Res	Type	RSRZ
4	E	164	GLY	2.3
3	D	189	SER	2.3
4	E	162	VAL	2.3
1	C	16	ILE	2.3
3	D	190	ILE	2.2
1	A	270	PRO	2.2
4	H	244	ALA	2.2
4	E	244	ALA	2.2
4	E	161	TRP	2.1
4	E	241	TRP	2.1
3	D	130	SER	2.1
3	D	164	MET	2.1
1	A	223	GLN	2.1
3	D	176	ASN	2.1
1	C	17	HIS	2.0
3	D	144	SER	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.

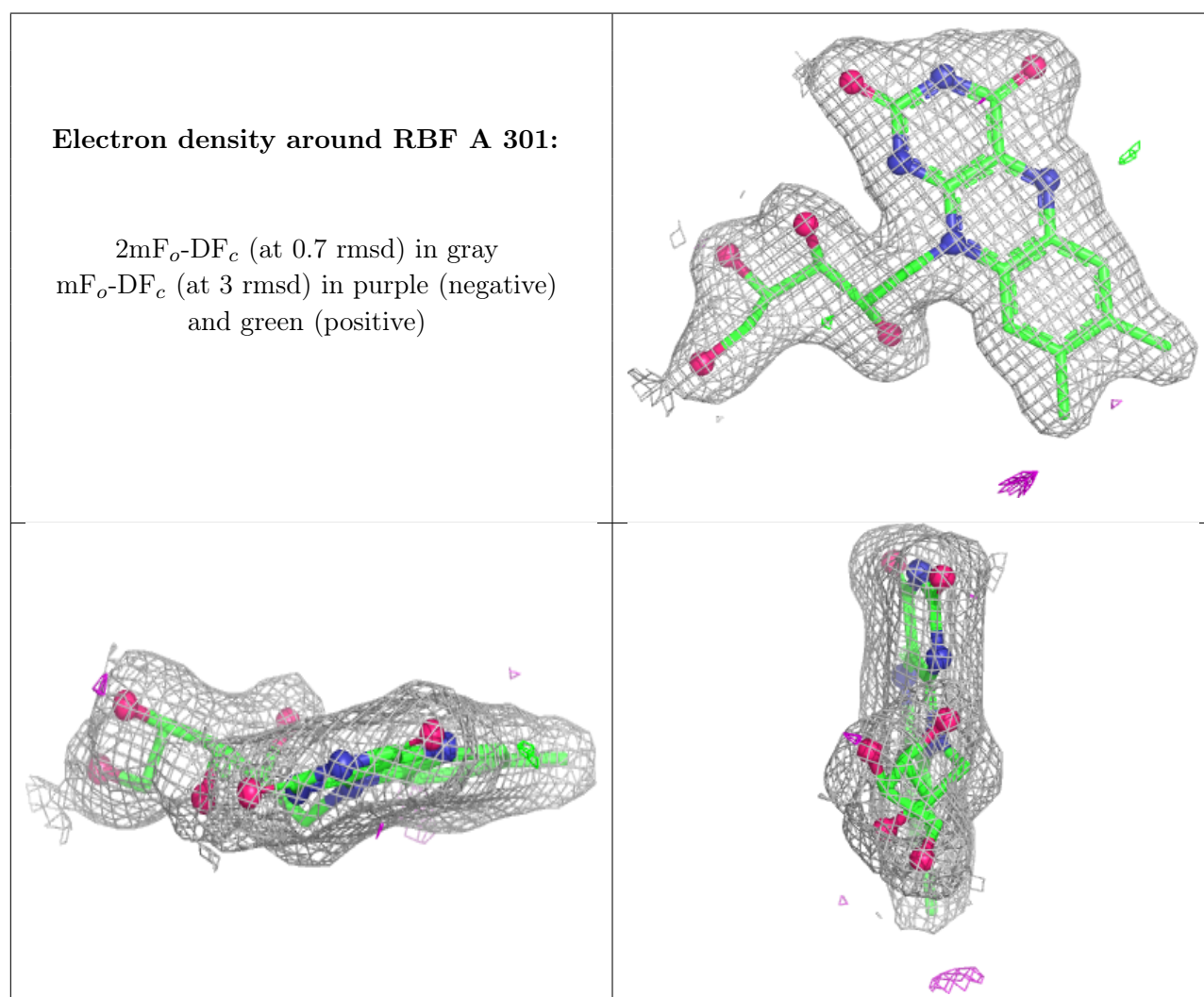
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	G	301	6/6	0.84	0.15	36,40,47,56	6
7	GOL	E	301	6/6	0.86	0.14	55,57,58,66	0
7	GOL	C	303	6/6	0.87	0.12	47,49,54,59	0
8	CL	A	304	1/1	0.90	0.17	67,67,67,67	0
6	ACT	A	302	4/4	0.92	0.12	32,37,39,44	0
7	GOL	A	303	6/6	0.93	0.10	37,46,48,48	0
7	GOL	F	102	6/6	0.94	0.10	33,40,46,48	0

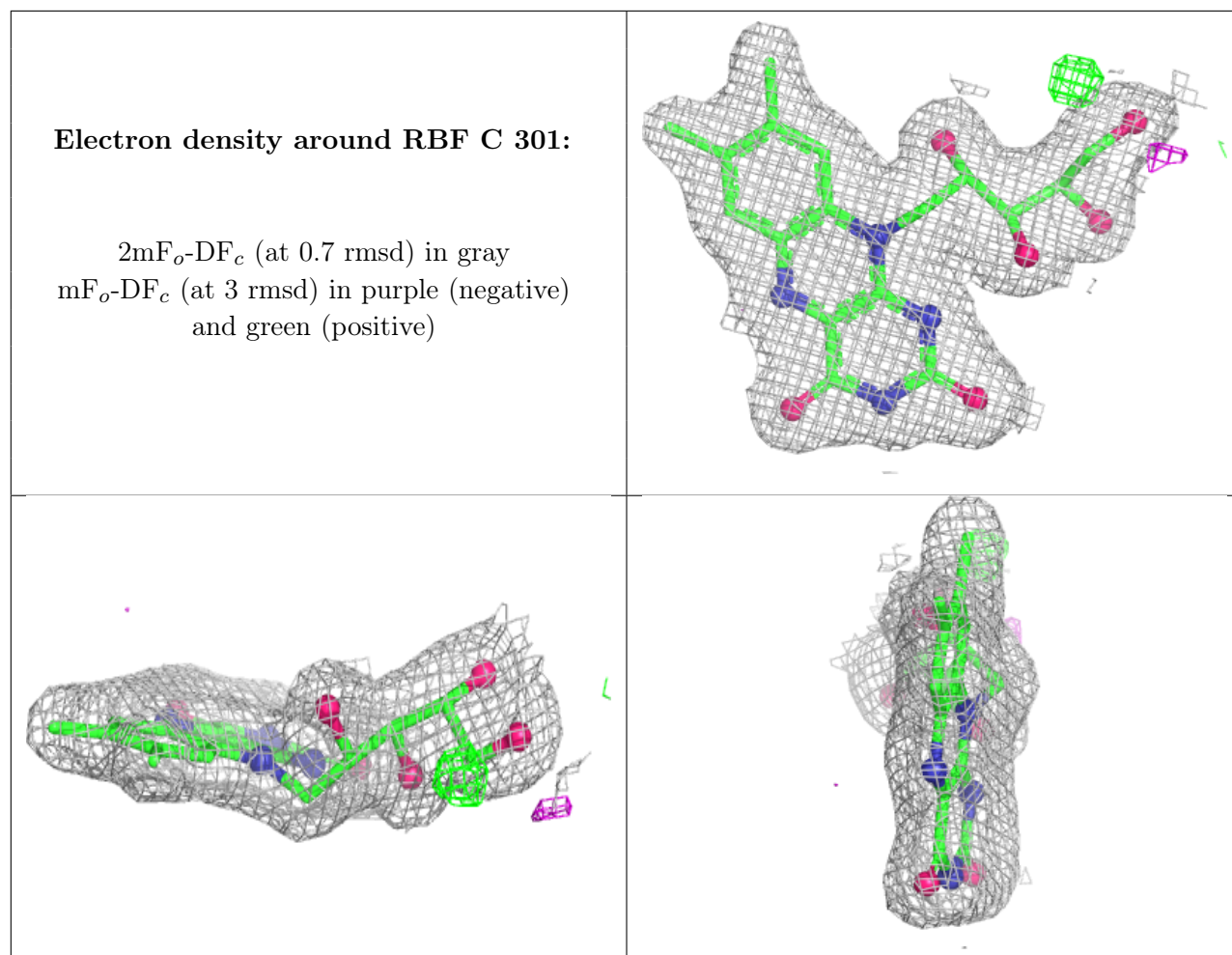
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	RBF	A	301	27/27	0.96	0.06	26,30,36,42	0
5	RBF	C	301	27/27	0.97	0.05	27,30,36,40	0
6	ACT	C	302	4/4	0.97	0.07	32,32,35,42	4
9	NA	H	301	1/1	0.97	0.04	39,39,39,39	0
7	GOL	F	101	6/6	0.98	0.07	33,34,42,43	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.