



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:57 pm BST

PDB ID : 6PUE
Title : Structure of human MAIT A-F7 TCR in complex with human MR1-4'D-5-OP-RU
Authors : Awad, W.; Rossjohn, J.
Deposited on : 2019-07-18
Resolution : 1.90 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 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

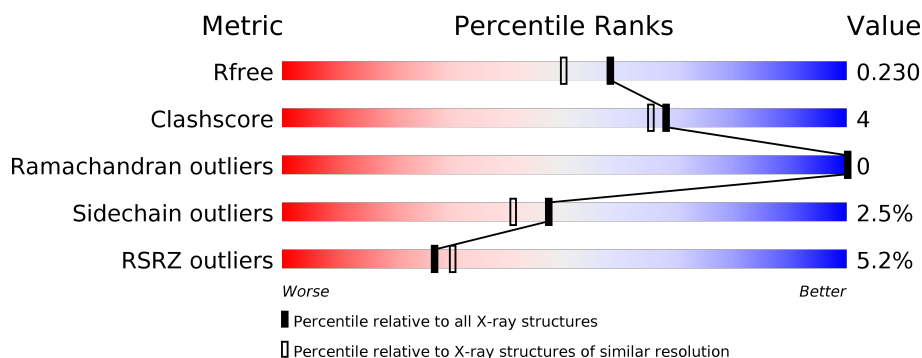
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>7%</div> <div>88%</div> <div>8%</div> <div>••</div> </div>
1	C	271	<div> <div>%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>
2	B	100	<div> <div>19%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>
2	F	100	<div> <div>2%</div> <div>91%</div> <div>9%</div> <div></div> </div>
3	D	204	<div> <div>14%</div> <div>81%</div> <div>10%</div> <div>• 7%</div> </div>
3	G	204	<div> <div></div> <div>92%</div> <div></div> <div>•••</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	246	<div><div></div><div>4%</div><div>89%</div><div>8%</div><div>..</div></div>
4	H	246	<div><div></div><div>%</div><div>87%</div><div>11%</div><div>..</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14767 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	6	0
			2189	1402	379	396	12			
1	C	265	Total	C	N	O	S	0	10	0
			2221	1426	382	401	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	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	96	Total	C	N	O	S	0	0	0
			770	495	129	144	2			
2	F	100	Total	C	N	O	S	0	2	0
			819	526	139	150	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 Human TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	190	Total	C	N	O	S	0	3	0
			1461	932	229	290	10			

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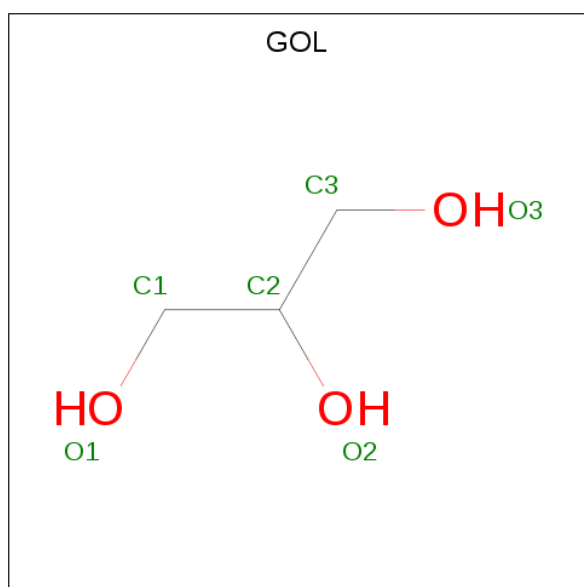
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	199	Total	C	N	O	S	0	13	0
			1610	1023	252	324	11			

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

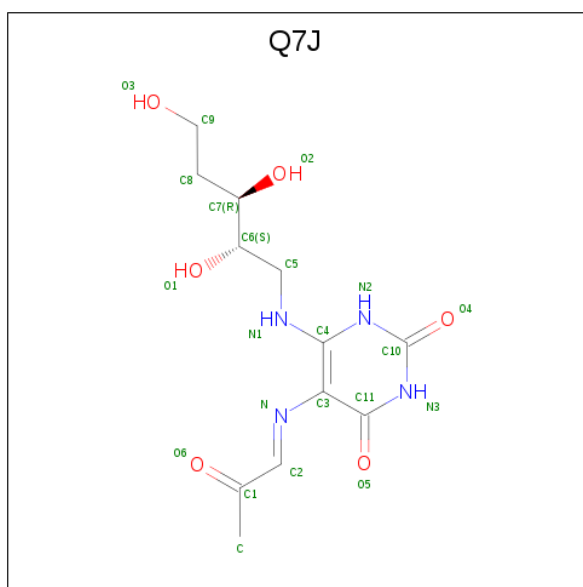
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	242	Total	C	N	O	S	0	12	0
			1934	1229	329	362	14			
4	H	243	Total	C	N	O	S	0	11	0
			1956	1236	336	371	13			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is 1,4-dideoxy-1-({2,6-dioxo-5-[(E)-(2-oxopropylidene)amino]-1,2,3,6-tetrahydropyrimidin-4-yl}amino)-D-erythro-pentitol (three-letter code: Q7J) (formula: $C_{12}H_{18}N_4O_6$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	1
			42	24	8	10		
6	C	1	Total	C	N	O	0	1
			42	24	8	10		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	258	Total	O	0	0
			258	258		
8	B	70	Total	O	0	0
			70	70		
8	C	336	Total	O	0	0
			336	336		
8	D	137	Total	O	0	0
			137	137		
8	E	193	Total	O	0	0
			193	193		
8	F	117	Total	O	0	0
			117	117		

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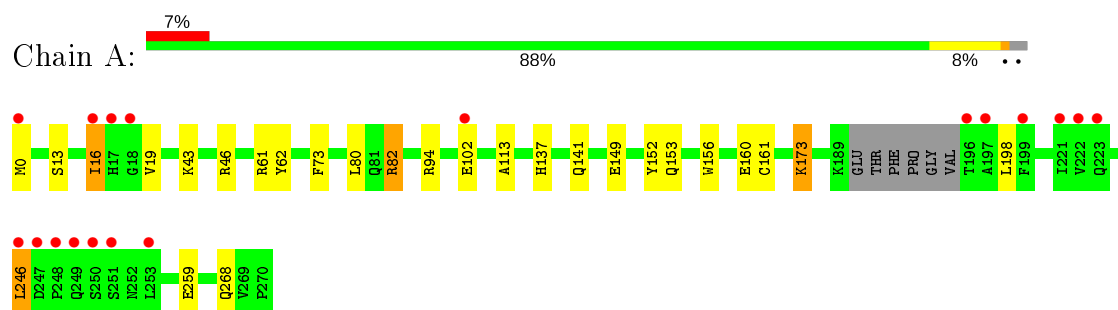
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	277	Total 277	O 277	0	0
8	H	328	Total 328	O 328	0	0

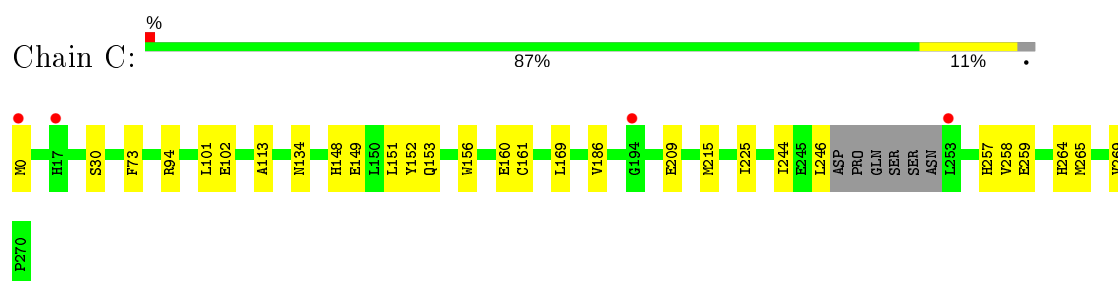
3 Residue-property plots [i](#)

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.

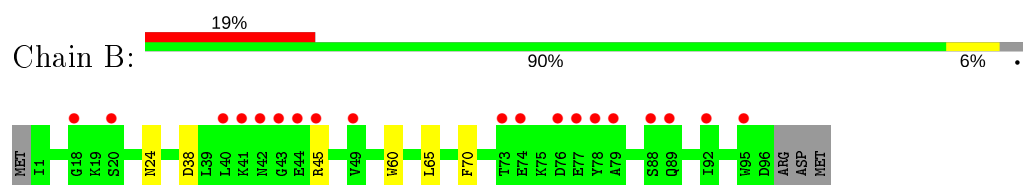
- Molecule 1: Major histocompatibility complex class I-related gene protein



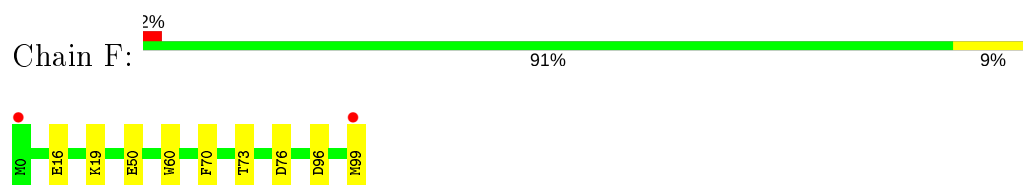
- Molecule 1: Major histocompatibility complex class I-related gene protein



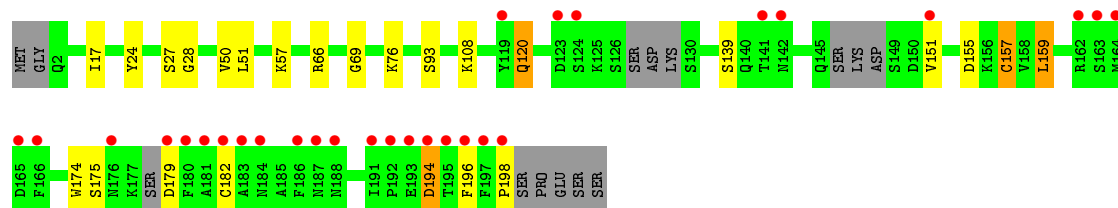
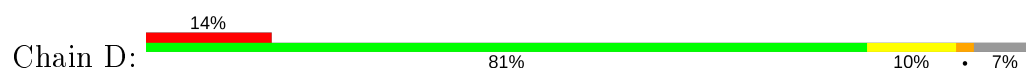
- Molecule 2: Beta-2-microglobulin



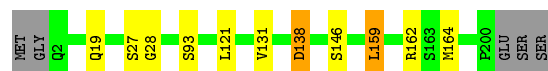
- Molecule 2: Beta-2-microglobulin



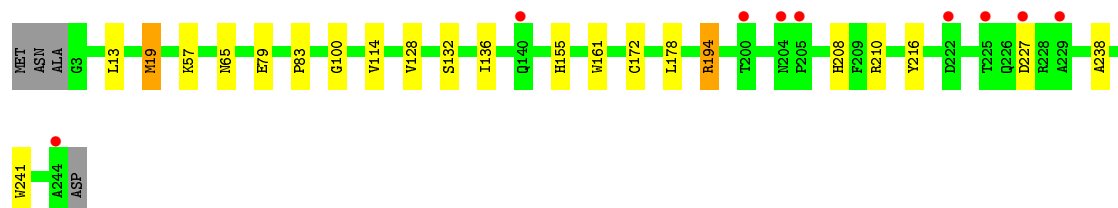
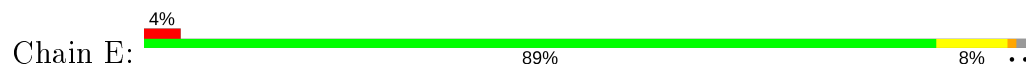
- Molecule 3: Human TCR alpha chain



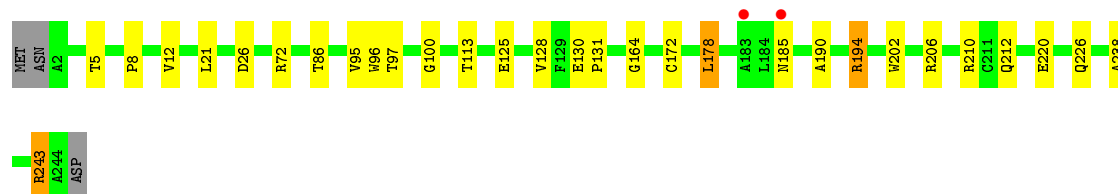
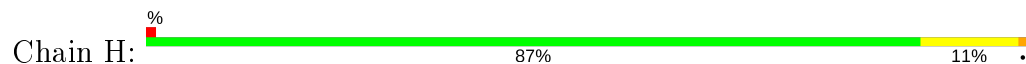
- Molecule 3: Human TCR alpha chain



- 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, α , β , γ	218.22Å 71.07Å 144.29Å 90.00° 104.77° 90.00°	Depositor
Resolution (Å)	45.64 – 1.90 46.51 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.64-1.90) 96.8 (46.51-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.199 , 0.232 0.198 , 0.230	Depositor DCC
R_{free} test set	8129 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.3	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	0.95	EDS
Total number of atoms	14767	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, Q7J, 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	0.38	0/2273	0.54	0/3090
1	C	0.41	0/2317	0.59	0/3150
2	B	0.32	0/793	0.52	0/1082
2	F	0.38	0/848	0.56	0/1151
3	D	0.37	0/1498	0.59	1/2032 (0.0%)
3	G	0.43	0/1684	0.62	1/2282 (0.0%)
4	E	0.38	0/2021	0.55	0/2750
4	H	0.44	0/2040	0.58	0/2773
All	All	0.40	0/13474	0.57	2/18310 (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	D	159	LEU	CA-CB-CG	7.38	132.27	115.30
3	G	159	LEU	CA-CB-CG	5.40	127.72	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	2189	0	2071	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2221	0	2128	19	0
2	B	770	0	707	3	0
2	F	819	0	775	4	0
3	D	1461	0	1341	15	0
3	G	1610	0	1547	6	0
4	E	1934	0	1846	15	0
4	H	1956	0	1870	27	0
5	A	6	0	8	0	0
6	A	42	0	0	1	0
6	C	42	0	0	1	0
7	H	1	0	0	0	0
8	A	258	0	0	6	1
8	B	70	0	0	0	0
8	C	336	0	0	8	1
8	D	137	0	0	1	0
8	E	193	0	0	0	0
8	F	117	0	0	1	0
8	G	277	0	0	3	0
8	H	328	0	0	15	0
All	All	14767	0	12293	97	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 (97) 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)
4:H:206[B]:ARG:NH1	8:H:402:HOH:O	2.05	0.89
4:H:72:ARG:NH1	8:H:403:HOH:O	2.13	0.81
4:H:212:GLN:OE1	8:H:401:HOH:O	1.99	0.80
1:C:30[B]:SER:OG	8:C:901:HOH:O	1.99	0.78
4:H:212:GLN:NE2	8:H:408:HOH:O	2.21	0.72
1:C:149:GLU:OE1	8:C:902:HOH:O	2.07	0.71
6:C:801[B]:Q7J:O3	8:C:903:HOH:O	2.08	0.70
3:G:138:ASP:OD1	8:G:301:HOH:O	2.10	0.70
1:C:134[A]:ASN:ND2	8:C:906:HOH:O	2.24	0.69
1:C:0:MET:HE1	1:C:169:LEU:HD13	1.75	0.69
3:G:19:GLN:NE2	8:G:303:HOH:O	2.25	0.69
1:C:148:HIS:ND1	8:C:909:HOH:O	2.28	0.67
6:A:302[B]:Q7J:O3	8:A:402:HOH:O	2.13	0.66
1:A:259:GLU:OE1	8:A:401:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:65[B]:ASN:ND2	4:E:79:GLU:OE2	2.28	0.66
4:H:97:THR:O	8:H:405:HOH:O	2.15	0.64
3:D:151:VAL:HG12	3:D:175:SER:HB2	1.81	0.61
3:D:174:TRP:HH2	4:E:178[B]:LEU:HD11	1.68	0.58
4:H:178:LEU:HD22	4:H:190:ALA:HB3	1.85	0.57
3:D:108:LYS:HG2	3:D:139:SER:HB3	1.89	0.55
1:A:82:ARG:NH1	8:A:410:HOH:O	2.40	0.55
1:C:151:LEU:HD22	3:D:51:LEU:HD12	1.88	0.54
1:A:13:SER:O	8:A:403:HOH:O	2.18	0.54
1:A:152:TYR:CD1	4:H:100:GLY:HA3	2.42	0.54
4:H:8:PRO:HD2	4:H:21:LEU:HD22	1.88	0.54
1:A:160:GLU:OE2	8:A:404:HOH:O	2.19	0.53
3:D:194:ASP:N	3:D:194:ASP:OD2	2.36	0.53
1:C:186:VAL:HG11	1:C:269:VAL:HG22	1.91	0.53
1:A:149:GLU:O	1:A:153[B]:GLN:HG2	2.09	0.52
1:A:198:LEU:HG	1:A:246:LEU:HD11	1.91	0.52
2:B:38:ASP:OD2	2:B:45:ARG:NH1	2.42	0.52
1:A:94:ARG:NH2	8:A:402:HOH:O	2.43	0.52
2:F:96[B]:ASP:OD2	8:F:101:HOH:O	2.19	0.51
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.45	0.51
4:E:128:VAL:HG23	4:E:238:ALA:HB3	1.91	0.51
1:C:94:ARG:NH2	8:C:903:HOH:O	2.43	0.51
4:H:72:ARG:NH2	8:H:414:HOH:O	2.36	0.51
3:G:28:GLY:HA3	3:G:93[A]:SER:OG	2.09	0.51
3:D:157:CYS:SG	4:E:172[B]:CYS:HB2	2.51	0.50
4:H:206[A]:ARG:HG3	8:H:402:HOH:O	2.11	0.49
4:E:172[B]:CYS:SG	4:E:194:ARG:HD3	2.53	0.49
4:H:130:GLU:OE1	4:H:243:ARG:NH2	2.45	0.49
1:A:137:HIS:O	1:A:141[A]:GLN:HG2	2.12	0.49
1:C:0:MET:O	1:C:102:GLU:HG3	2.13	0.49
3:D:28:GLY:HA3	3:D:93[B]:SER:OG	2.13	0.48
2:F:16:GLU:HB3	2:F:19:LYS:HG3	1.96	0.48
4:H:12:VAL:HG23	8:H:425:HOH:O	2.12	0.48
1:A:16:ILE:O	1:A:19:VAL:HG13	2.14	0.48
4:E:155:HIS:HB3	4:E:216:TYR:HB2	1.95	0.48
3:G:159:LEU:HB3	4:H:172[B]:CYS:SG	2.54	0.48
4:E:57[B]:LYS:HE2	4:E:57[B]:LYS:HB3	1.73	0.47
4:E:13:LEU:HD21	4:E:19[B]:MET:HG3	1.95	0.47
3:G:121[B]:LEU:HD12	3:G:131:VAL:HG12	1.97	0.46
1:C:113:ALA:HB2	2:F:60:TRP:CE2	2.51	0.46
3:D:196:PHE:CE2	3:D:198:PRO:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:185[A]:ASN:ND2	8:H:426:HOH:O	2.49	0.46
1:A:43:LYS:HD2	1:A:62:TYR:HB3	1.97	0.46
1:A:0:MET:O	1:A:102:GLU:HG3	2.16	0.45
3:G:164[A]:MET:HE3	8:G:521:HOH:O	2.17	0.45
3:D:151:VAL:HG12	3:D:175:SER:CB	2.47	0.45
3:D:120:GLN:HG2	3:D:182:CYS:SG	2.57	0.44
1:C:101:LEU:HD23	4:H:210:ARG:CZ	2.48	0.44
4:H:128:VAL:HG23	4:H:238:ALA:HB3	1.99	0.44
4:H:125:GLU:OE1	8:H:407:HOH:O	2.21	0.44
4:H:210:ARG:NE	8:H:401:HOH:O	2.25	0.43
4:H:95:VAL:HG12	4:H:96:TRP:CD1	2.53	0.43
1:C:258:VAL:HB	1:C:265[B]:MET:HG3	2.00	0.43
4:H:5[B]:THR:HG23	8:H:541:HOH:O	2.18	0.43
4:H:164:GLY:HA2	8:H:404:HOH:O	2.18	0.43
3:D:24:TYR:CZ	3:D:69:GLY:HA2	2.53	0.43
1:A:173:LYS:NZ	1:A:173:LYS:HB2	2.33	0.42
3:D:50:VAL:O	3:D:66:ARG:HD3	2.18	0.42
1:C:149:GLU:O	1:C:153[B]:GLN:HG2	2.19	0.42
4:H:210:ARG:NH1	8:H:404:HOH:O	2.14	0.42
1:C:215:MET:HG3	1:C:257:HIS:CD2	2.54	0.42
4:E:83:PRO:HA	4:E:114:VAL:HB	2.02	0.42
1:C:152:TYR:CD1	4:E:100:GLY:HA3	2.54	0.42
3:D:174:TRP:CH2	4:E:178[B]:LEU:HD11	2.51	0.42
4:H:26:ASP:HB3	4:H:72:ARG:HH21	1.85	0.42
4:E:208:HIS:HB2	4:E:241:TRP:CZ3	2.54	0.42
1:A:46:ARG:HD3	1:A:46:ARG:HA	1.74	0.41
4:H:226:GLN:NE2	8:H:406:HOH:O	2.21	0.41
1:A:156:TRP:CZ3	1:A:161:CYS:HB2	2.55	0.41
1:C:160:GLU:OE2	8:C:904:HOH:O	2.22	0.41
3:D:57:LYS:NZ	8:D:306:HOH:O	2.52	0.41
4:H:86:THR:HG23	4:H:113:THR:HA	2.02	0.41
1:C:225:ILE:HG12	1:C:244:ILE:HG22	2.03	0.41
4:E:132:SER:O	4:E:136:ILE:HG13	2.21	0.41
4:H:172[B]:CYS:SG	4:H:194:ARG:HD3	2.60	0.41
2:F:73:THR:OG1	2:F:76:ASP:OD1	2.32	0.41
4:H:131:PRO:HD2	4:H:202:TRP:CZ2	2.56	0.41
1:C:264:HIS:HB2	8:C:940:HOH:O	2.21	0.41
4:E:19[A]:MET:HE3	4:E:19[A]:MET:HB2	1.95	0.41
1:C:156:TRP:CZ3	1:C:161:CYS:HB2	2.56	0.40
4:E:161:TRP:HB2	4:E:210:ARG:CG	2.51	0.40
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:17:ILE:HG22	3:D:76:LYS:HA	2.04	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)
8:A:583:HOH:O	8:C:907:HOH:O[4_558]	2.17	0.03

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	267/271 (98%)	263 (98%)	4 (2%)	0	100	100
1	C	271/271 (100%)	268 (99%)	3 (1%)	0	100	100
2	B	94/100 (94%)	92 (98%)	2 (2%)	0	100	100
2	F	100/100 (100%)	100 (100%)	0	0	100	100
3	D	185/204 (91%)	180 (97%)	5 (3%)	0	100	100
3	G	210/204 (103%)	206 (98%)	4 (2%)	0	100	100
4	E	252/246 (102%)	247 (98%)	5 (2%)	0	100	100
4	H	252/246 (102%)	246 (98%)	6 (2%)	0	100	100
All	All	1631/1642 (99%)	1602 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	231/241 (96%)	223 (96%)	8 (4%)	36	27
1	C	238/241 (99%)	234 (98%)	4 (2%)	60	57
2	B	82/95 (86%)	81 (99%)	1 (1%)	71	70
2	F	89/95 (94%)	86 (97%)	3 (3%)	37	28
3	D	155/181 (86%)	148 (96%)	7 (4%)	27	18
3	G	184/181 (102%)	180 (98%)	4 (2%)	52	47
4	E	209/212 (99%)	205 (98%)	4 (2%)	57	53
4	H	214/212 (101%)	210 (98%)	4 (2%)	57	53
All	All	1402/1458 (96%)	1367 (98%)	35 (2%)	47	41

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	61	ARG
1	A	73	PHE
1	A	80	LEU
1	A	82	ARG
1	A	173	LYS
1	A	246	LEU
1	A	268	GLN
2	B	70	PHE
1	C	73	PHE
1	C	209	GLU
1	C	246	LEU
1	C	259	GLU
3	D	27	SER
3	D	120	GLN
3	D	155	ASP
3	D	157	CYS
3	D	159	LEU
3	D	179	ASP
3	D	194	ASP
4	E	19[A]	MET
4	E	19[B]	MET
4	E	194	ARG
4	E	227	ASP

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Mol	Chain	Res	Type
2	F	50	GLU
2	F	70	PHE
2	F	99	MET
3	G	27	SER
3	G	138	ASP
3	G	146	SER
3	G	162	ARG
4	H	178	LEU
4	H	194	ARG
4	H	220	GLU
4	H	243	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	C	177	GLN
3	D	120	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is 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
6	Q7J	C	801[B]	1	19,21,22	1.30	3 (15%)	20,27,29	4.40	6 (30%)
6	Q7J	A	302[A]	1	19,21,22	1.11	2 (10%)	20,27,29	4.31	5 (25%)
6	Q7J	A	302[B]	1	19,21,22	1.16	2 (10%)	20,27,29	4.34	5 (25%)
6	Q7J	C	801[A]	1	19,21,22	1.21	3 (15%)	20,27,29	4.49	8 (40%)
5	GOL	A	301	-	5,5,5	1.09	0	5,5,5	0.94	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
6	Q7J	C	801[B]	1	-	7/15/16/17	0/1/1/1
6	Q7J	A	302[A]	1	-	6/15/16/17	0/1/1/1
6	Q7J	A	302[B]	1	-	7/15/16/17	0/1/1/1
6	Q7J	C	801[A]	1	-	6/15/16/17	0/1/1/1
5	GOL	A	301	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	801[B]	Q7J	C11-N3	3.32	1.38	1.33
6	C	801[A]	Q7J	C11-N3	3.31	1.38	1.33
6	A	302[B]	Q7J	C11-N3	3.28	1.38	1.33
6	A	302[A]	Q7J	C11-N3	3.26	1.38	1.33
6	C	801[B]	Q7J	C1-C2	-3.14	1.46	1.49
6	A	302[B]	Q7J	C1-C2	-2.53	1.46	1.49
6	C	801[A]	Q7J	C1-C2	-2.48	1.46	1.49
6	C	801[B]	Q7J	C4-N1	2.33	1.38	1.34
6	A	302[A]	Q7J	C1-C2	-2.28	1.46	1.49
6	C	801[A]	Q7J	C4-N1	2.07	1.37	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	302[A]	Q7J	C11-N3-C10	13.96	126.92	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	801[A]	Q7J	C11-N3-C10	13.96	126.92	115.14
6	A	302[B]	Q7J	C11-N3-C10	13.94	126.91	115.14
6	C	801[B]	Q7J	C11-N3-C10	13.91	126.89	115.14
6	C	801[A]	Q7J	C11-C3-C4	10.28	121.25	114.53
6	C	801[B]	Q7J	C11-C3-C4	10.03	121.09	114.53
6	A	302[B]	Q7J	C11-C3-C4	9.92	121.02	114.53
6	A	302[A]	Q7J	C11-C3-C4	9.73	120.90	114.53
6	C	801[B]	Q7J	C3-C11-N3	-7.29	113.46	123.43
6	A	302[B]	Q7J	C3-C11-N3	-7.22	113.55	123.43
6	C	801[A]	Q7J	C3-C11-N3	-7.22	113.56	123.43
6	A	302[A]	Q7J	C3-C11-N3	-7.14	113.67	123.43
6	C	801[B]	Q7J	C10-N2-C4	4.60	124.33	113.80
6	A	302[B]	Q7J	C10-N2-C4	4.32	123.69	113.80
6	C	801[A]	Q7J	C10-N2-C4	4.26	123.56	113.80
6	A	302[A]	Q7J	C10-N2-C4	4.24	123.50	113.80
6	C	801[A]	Q7J	C5-N1-C4	-3.13	117.68	123.25
6	C	801[B]	Q7J	C-C1-C2	2.47	118.11	113.75
6	C	801[B]	Q7J	C4-C3-N	-2.39	112.23	125.02
6	A	302[B]	Q7J	C4-C3-N	-2.39	112.24	125.02
6	A	302[A]	Q7J	C4-C3-N	-2.27	112.89	125.02
6	C	801[A]	Q7J	C4-C3-N	-2.24	113.05	125.02
6	C	801[A]	Q7J	C-C1-C2	2.17	117.58	113.75
6	C	801[A]	Q7J	N1-C4-N2	2.06	121.13	118.50

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	801[B]	Q7J	C4-C3-N-C2
6	A	302[B]	Q7J	C4-C3-N-C2
6	C	801[A]	Q7J	C4-C3-N-C2
6	A	302[A]	Q7J	C4-C3-N-C2
6	A	302[A]	Q7J	N1-C5-C6-C7
5	A	301	GOL	O1-C1-C2-C3
6	C	801[B]	Q7J	C3-C4-N1-C5
6	C	801[B]	Q7J	N1-C5-C6-C7
6	A	302[B]	Q7J	N1-C5-C6-C7
6	C	801[A]	Q7J	N1-C5-C6-C7
6	A	302[B]	Q7J	C3-C4-N1-C5
6	C	801[A]	Q7J	C3-C4-N1-C5
6	A	302[A]	Q7J	C3-C4-N1-C5
6	C	801[B]	Q7J	N2-C4-N1-C5

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Mol	Chain	Res	Type	Atoms
6	A	302[B]	Q7J	N2-C4-N1-C5
6	A	302[A]	Q7J	N2-C4-N1-C5
6	C	801[B]	Q7J	C7-C8-C9-O3
5	A	301	GOL	O1-C1-C2-O2
6	C	801[A]	Q7J	N2-C4-N1-C5
6	C	801[B]	Q7J	C6-C7-C8-C9
6	A	302[B]	Q7J	O1-C6-C7-O2
6	C	801[A]	Q7J	O1-C6-C7-O2
6	A	302[A]	Q7J	O1-C6-C7-O2
6	C	801[B]	Q7J	C11-C3-N-C2
6	A	302[B]	Q7J	C11-C3-N-C2
6	C	801[A]	Q7J	C11-C3-N-C2
6	A	302[A]	Q7J	C11-C3-N-C2
6	A	302[B]	Q7J	C6-C7-C8-C9

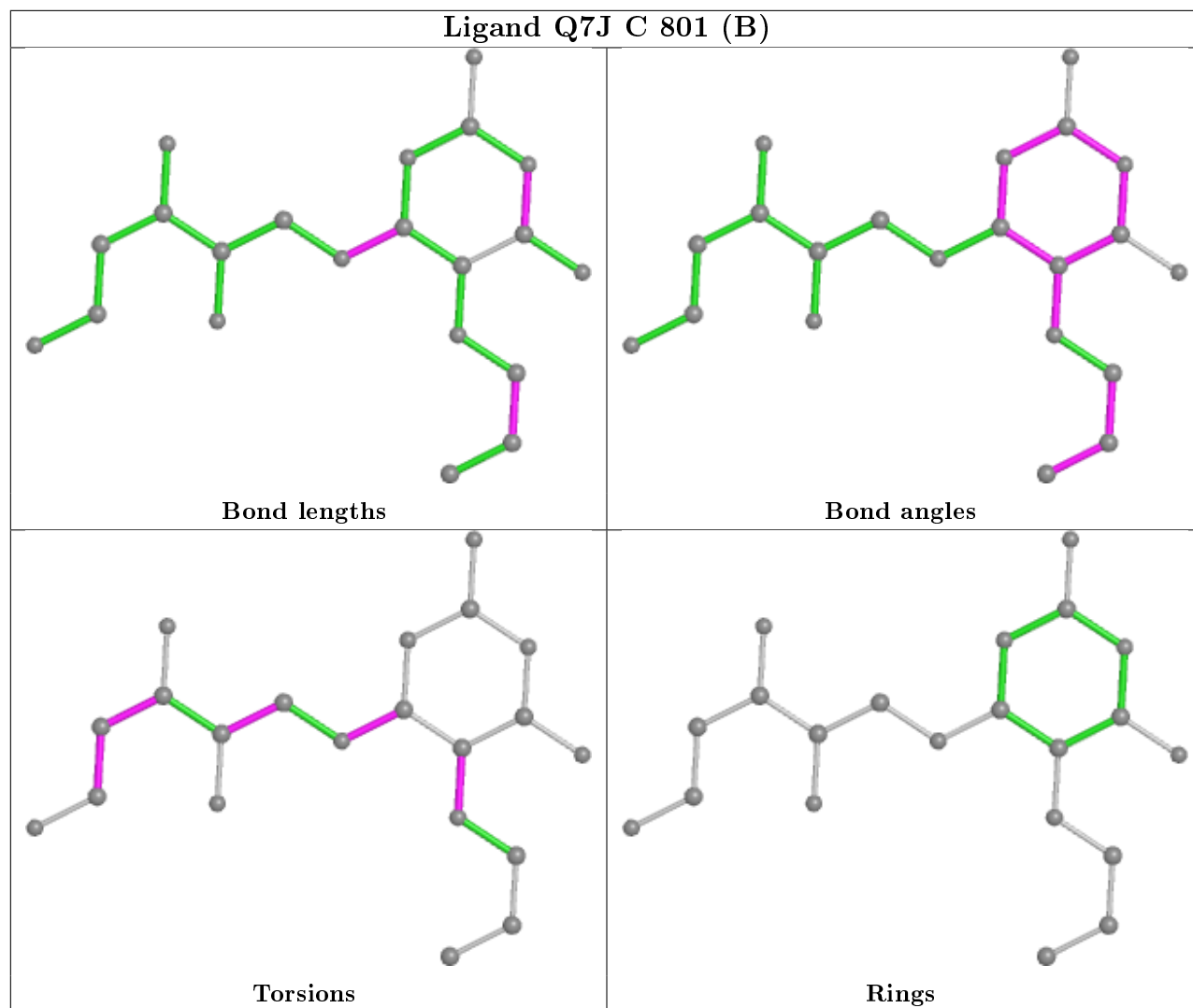
There are no ring outliers.

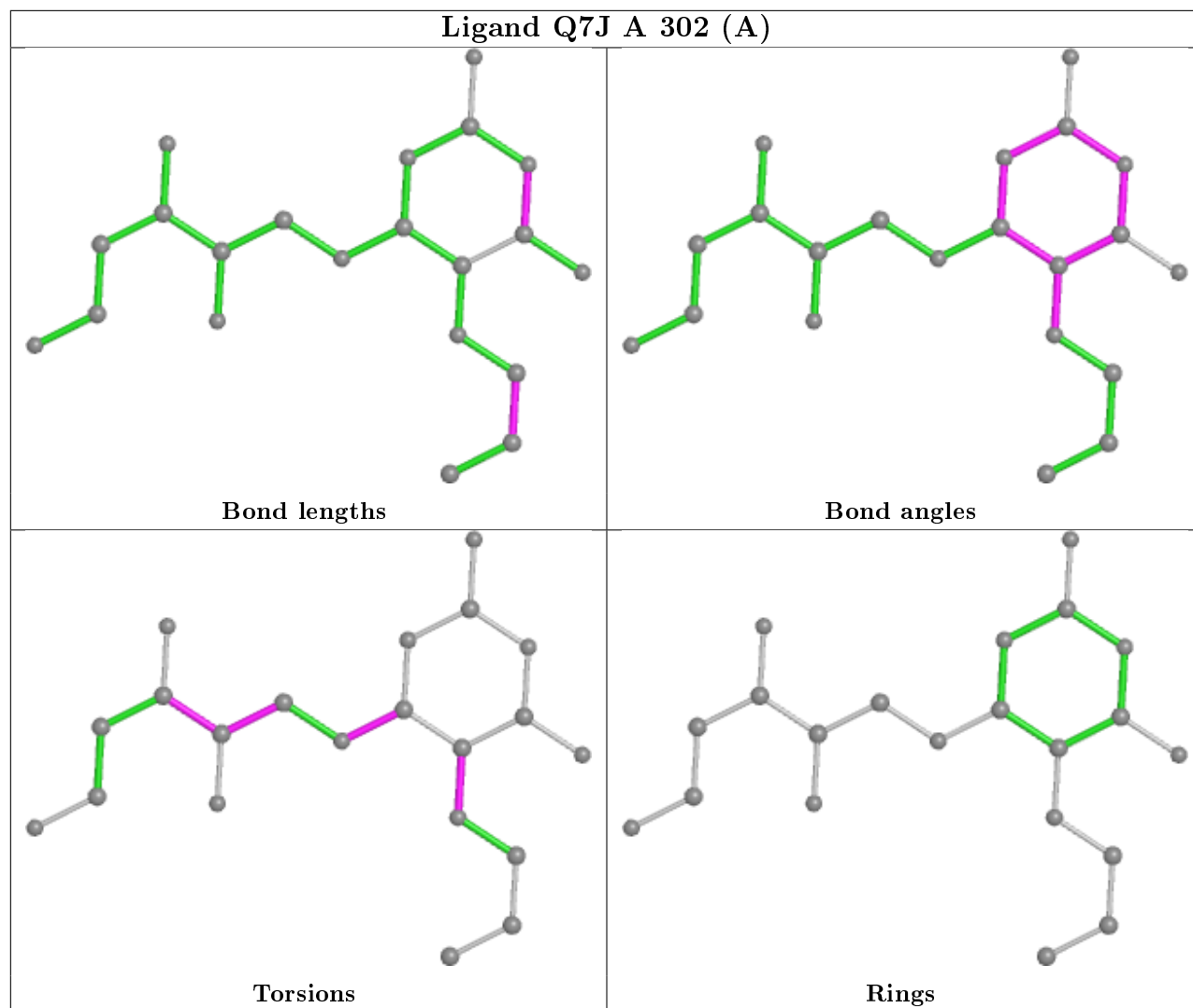
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	801[B]	Q7J	1	0
6	A	302[B]	Q7J	1	0

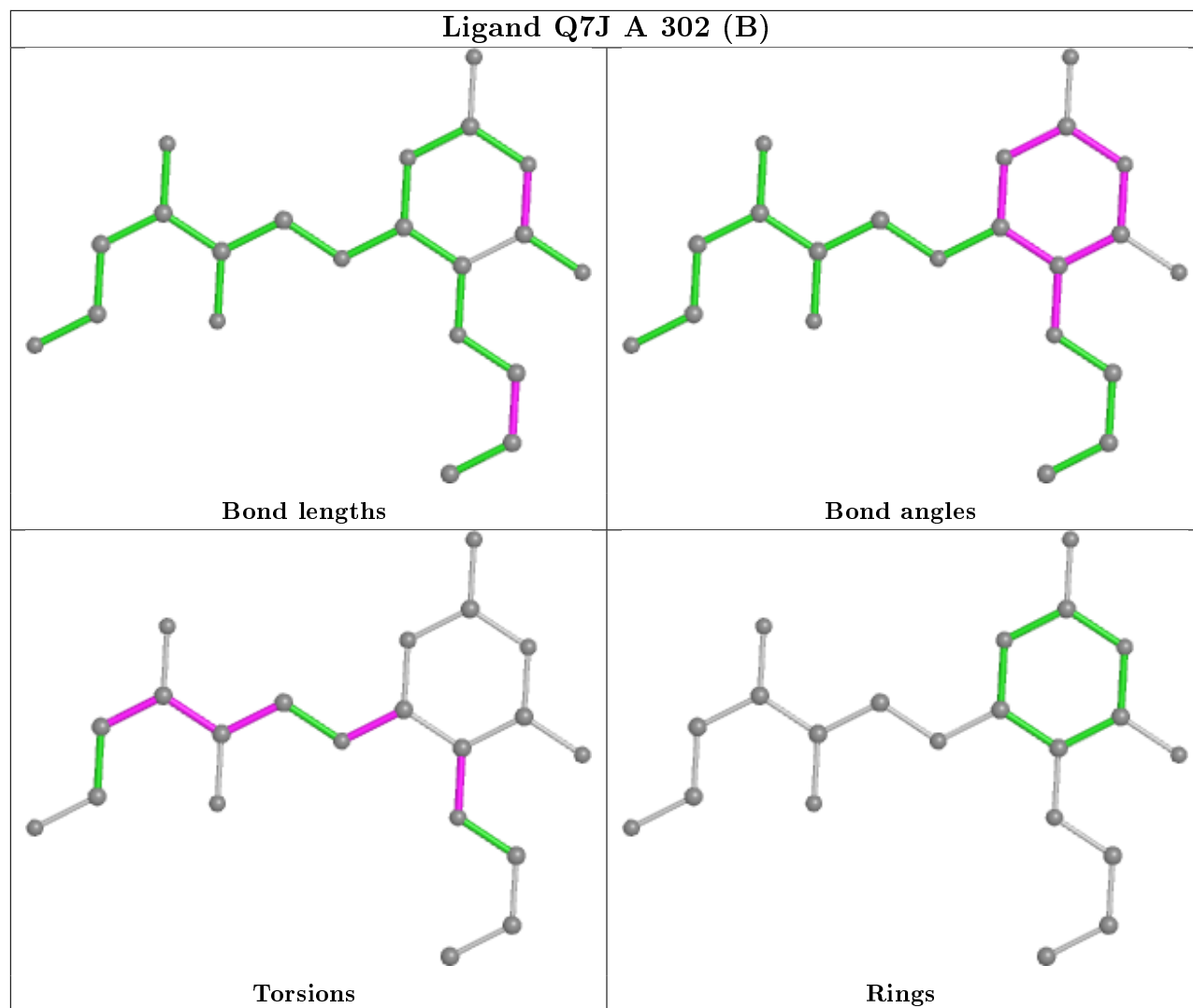
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

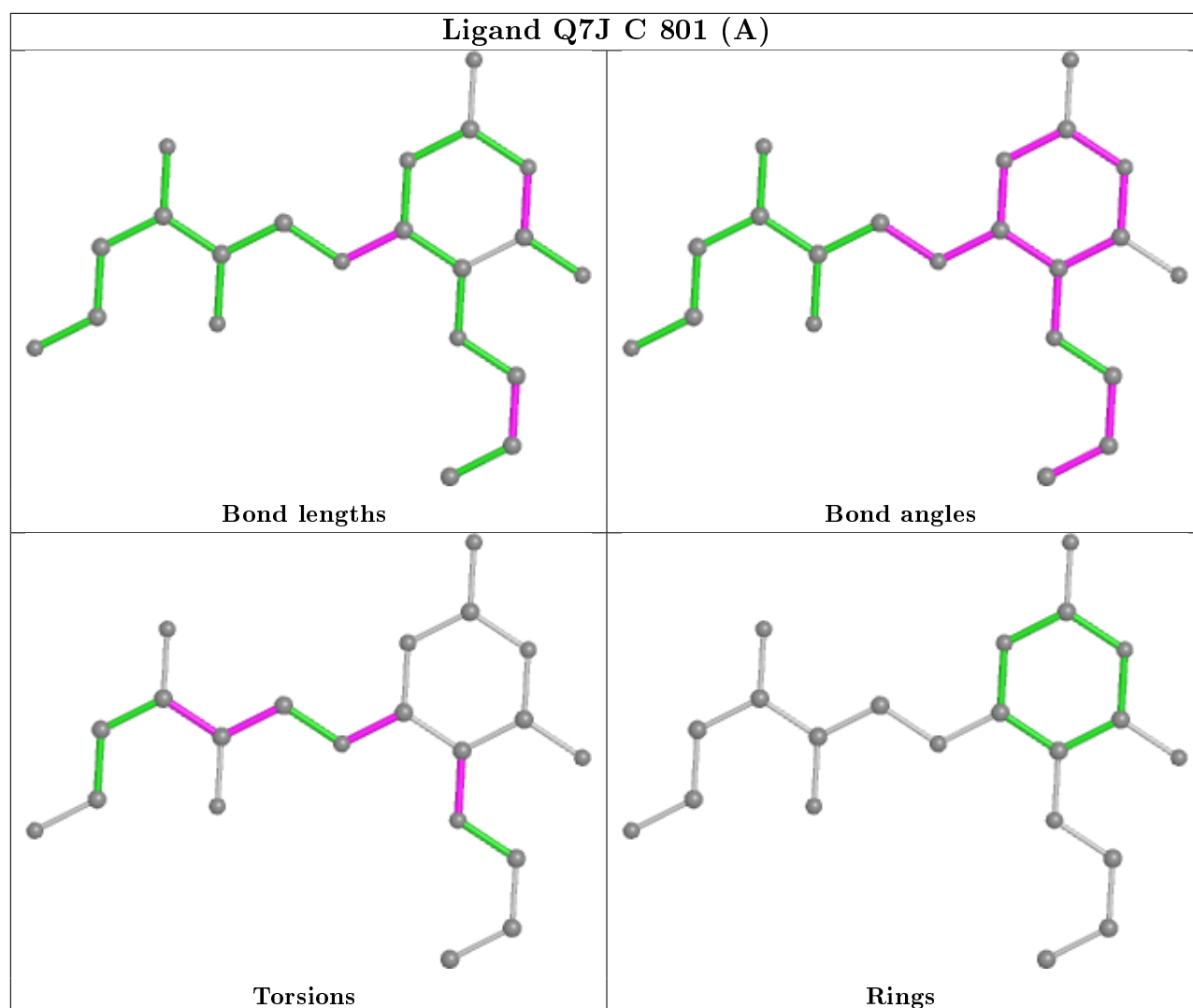
Ligand Q7J C 801 (B)





Ligand Q7J A 302 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/271 (97%)	0.03	18 (6%) 17 19	22, 33, 64, 79	5 (1%)
1	C	265/271 (97%)	-0.08	4 (1%) 73 76	20, 29, 51, 70	3 (1%)
2	B	96/100 (96%)	0.82	19 (19%) 1 1	27, 51, 76, 80	0
2	F	100/100 (100%)	0.01	2 (2%) 65 68	22, 36, 58, 66	4 (4%)
3	D	190/204 (93%)	0.61	29 (15%) 2 2	21, 42, 82, 96	2 (1%)
3	G	199/204 (97%)	-0.14	0 100 100	19, 28, 53, 62	4 (2%)
4	E	242/246 (98%)	0.02	9 (3%) 41 44	23, 37, 70, 95	3 (1%)
4	H	243/246 (98%)	-0.37	2 (0%) 86 87	20, 28, 44, 64	7 (2%)
All	All	1600/1642 (97%)	0.05	83 (5%) 27 30	19, 33, 67, 96	28 (1%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	180	PHE	5.7
1	A	221	ILE	5.2
3	D	183	ALA	5.2
3	D	196	PHE	5.1
1	A	247	ASP	4.6
4	H	183	ALA	4.4
3	D	197	PHE	4.4
4	E	244	ALA	4.4
3	D	187	ASN	4.3
3	D	164	MET	4.1
3	D	124	SER	4.0
3	D	192	PRO	3.8
4	E	205	PRO	3.8
3	D	163	SER	3.8
2	B	89	GLN	3.8
1	A	222	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	246	LEU	3.7
3	D	182	CYS	3.7
1	A	18	GLY	3.6
2	F	0	MET	3.6
2	B	43	GLY	3.6
1	A	250	SER	3.5
2	B	92	ILE	3.4
3	D	194	ASP	3.4
4	E	200	THR	3.4
2	B	78	TYR	3.4
3	D	195	THR	3.4
1	A	249	GLN	3.3
3	D	179	ASP	3.3
1	A	248	PRO	3.3
2	B	40	LEU	3.3
2	B	73	THR	3.3
2	B	77	GLU	3.2
4	E	227	ASP	3.2
3	D	188	ASN	3.1
1	A	253	LEU	3.1
1	A	17	HIS	3.1
3	D	165	ASP	3.0
3	D	193	GLU	3.0
4	E	225	THR	3.0
1	A	0	MET	3.0
2	B	76	ASP	3.0
1	A	223	GLN	2.9
4	H	185[A]	ASN	2.9
2	B	45	ARG	2.9
3	D	162	ARG	2.8
2	B	88	SER	2.8
2	B	79	ALA	2.8
1	A	16	ILE	2.8
1	A	196	THR	2.8
3	D	186	PHE	2.7
2	B	44	GLU	2.7
3	D	191	ILE	2.7
3	D	176	ASN	2.6
3	D	181	ALA	2.6
1	C	0	MET	2.6
2	B	74	GLU	2.6
4	E	222	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	151	VAL	2.5
1	A	197	ALA	2.5
3	D	184	ASN	2.4
1	A	251	SER	2.4
2	B	41	LYS	2.4
1	A	102	GLU	2.4
3	D	142	ASN	2.4
3	D	123	ASP	2.4
2	B	95	TRP	2.4
4	E	229	ALA	2.3
4	E	140[A]	GLN	2.3
2	B	42	ASN	2.3
1	C	194	GLY	2.2
1	A	199	PHE	2.2
3	D	166	PHE	2.2
3	D	119	TYR	2.2
3	D	198	PRO	2.2
2	B	20	SER	2.2
2	F	99	MET	2.1
2	B	49	VAL	2.1
3	D	141	THR	2.1
1	C	253	LEU	2.1
2	B	18	GLY	2.0
4	E	204	ASN	2.0
1	C	17	HIS	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

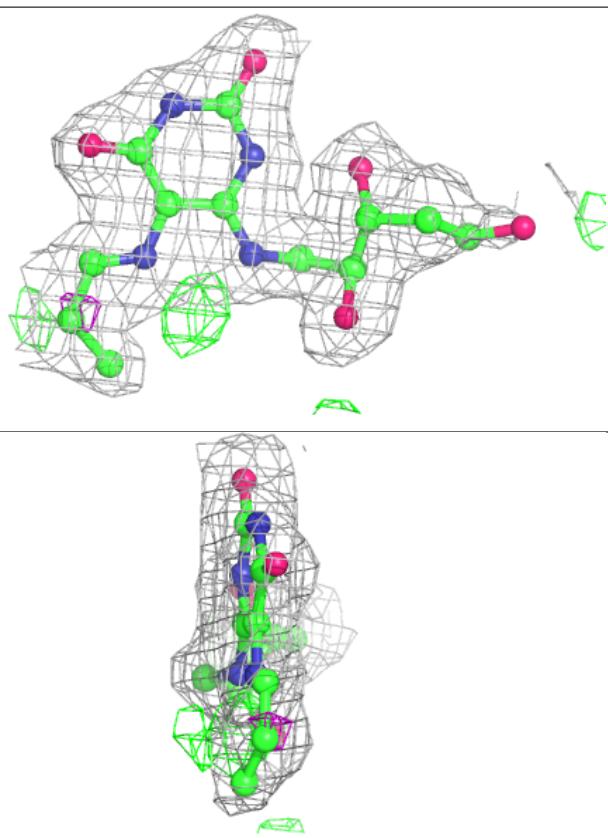
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	301	6/6	0.88	0.15	39,45,50,53	0
6	Q7J	A	302[B]	21/22	0.95	0.12	22,26,33,41	21
6	Q7J	A	302[A]	21/22	0.95	0.12	22,26,33,36	21
7	NA	H	301	1/1	0.98	0.05	30,30,30,30	0
6	Q7J	C	801[B]	21/22	0.98	0.18	21,24,27,30	21
6	Q7J	C	801[A]	21/22	0.98	0.18	20,24,27,28	21

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.

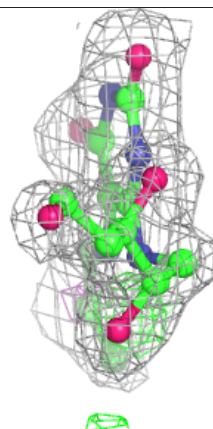
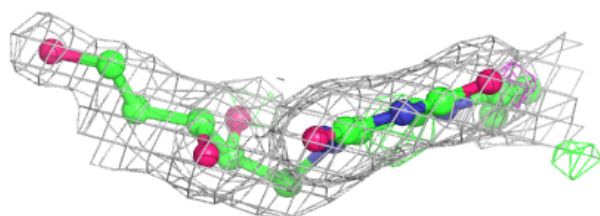
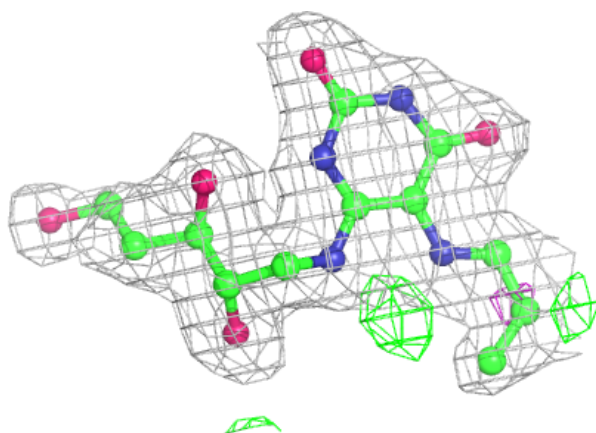
Electron density around Q7J A 302 (B):

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

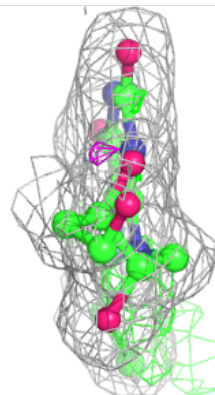
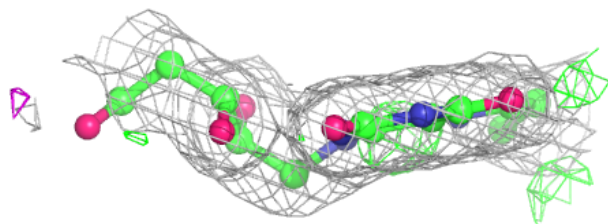
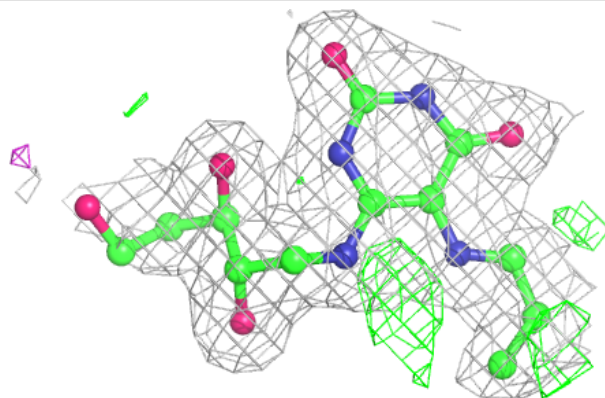


Electron density around Q7J A 302 (A):

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

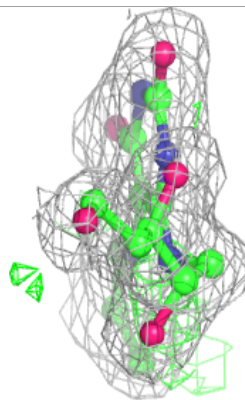
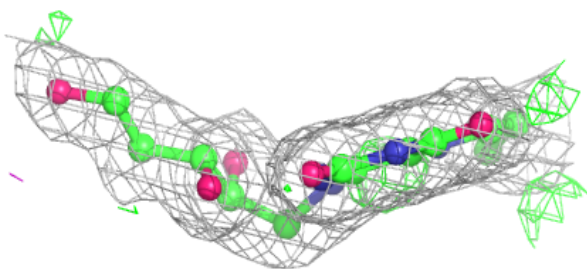
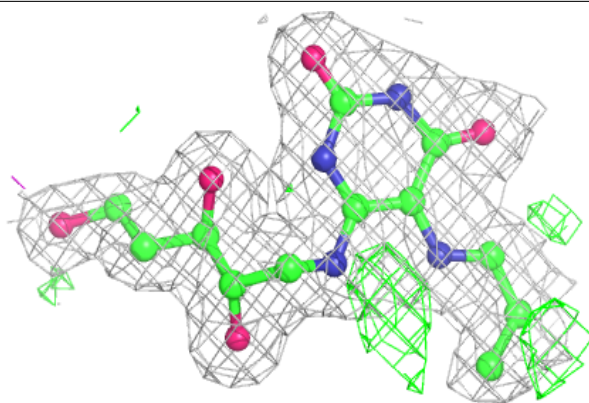
**Electron density around Q7J C 801 (B):**

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



Electron density around Q7J C 801 (A):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.