



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:23 PM BST

PDB ID : 6XQP
Title : Structure of human D462-E4 TCR in complex with human MR1-5-OP-RU
Authors : Awad, W.; Rossjohn, J.
Deposited on : 2020-07-10
Resolution : 2.90 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 : 2.13
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) : 2.13

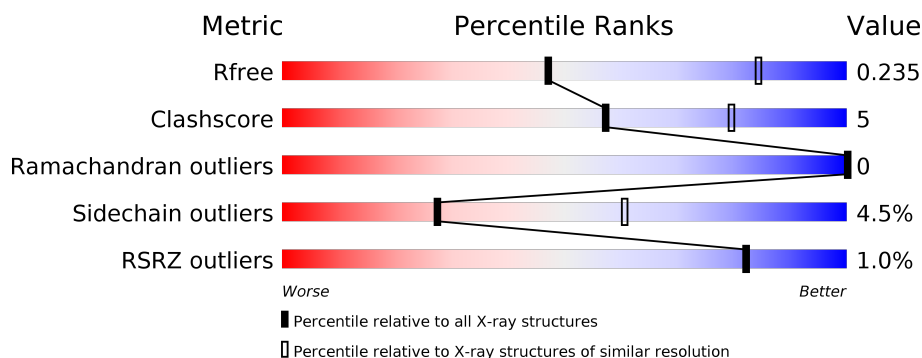
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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>0%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	271	<div> <div></div> <div> <div>77%</div> <div>15%</div> <div>•</div> <div>6%</div> </div> </div>
2	B	100	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>•</div> </div> </div>
2	D	100	<div> <div></div> <div> <div>90%</div> <div>10%</div> </div> </div>
3	E	205	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>•</div> <div>6%</div> </div> </div>
3	G	205	<div> <div></div> <div> <div>83%</div> <div>11%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	248	
4	H	248	

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
5	2LJ	A	301[B]	X	-	-	-
5	2LJ	C	301[A]	X	-	-	-
7	BR	G	301	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12963 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	243	Total	C	N	O	S	0	0	0
			1978	1268	343	358	9			
1	C	254	Total	C	N	O	S	0	1	0
			2099	1343	366	380	10			

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	100	Total	C	N	O	S	0	1	0
			812	517	138	153	4			
2	D	100	Total	C	N	O	S	0	0	0
			809	515	137	154	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769
D	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called TRAV12-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	193	Total	C	N	O	S	0	0	0
			1452	911	238	293	10			

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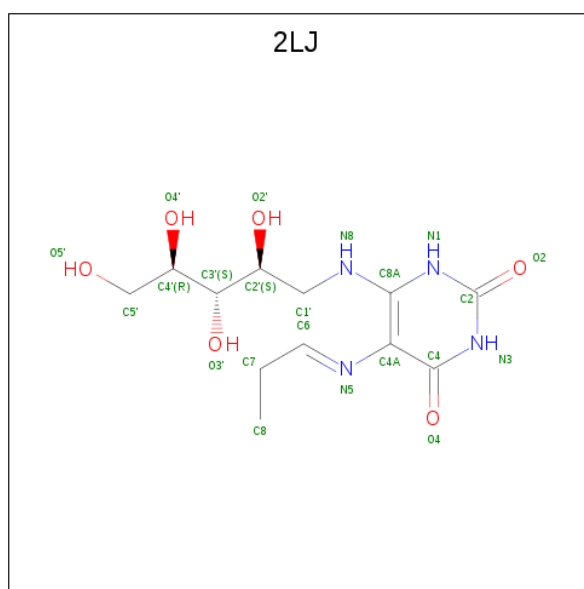
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	194	Total	C	N	O	S	0	0	0
			1483	926	245	302	10			

- Molecule 4 is a protein called TRBV29-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	246	Total	C	N	O	S	0	1	0
			1930	1211	336	374	9			
4	H	246	Total	C	N	O	S	0	1	0
			1932	1212	334	377	9			

- Molecule 5 is 1-deoxy-1-({2,6-dioxo-5-[(E)-propylideneamino]-1,2,3,6-tetrahydropyrimidin-4-yl}amino)-D-ribose (three-letter code: 2LJ) (formula: $C_{12}H_{20}N_4O_6$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			44	24	8	12		
5	C	1	Total	C	N	O	0	1
			44	24	8	12		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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	C	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		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Br	0	0
			1	1		
7	E	1	Total	Br	0	0
			1	1		

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

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	2	Total Cl 2 2	0	0
9	F	2	Total Cl 2 2	0	0

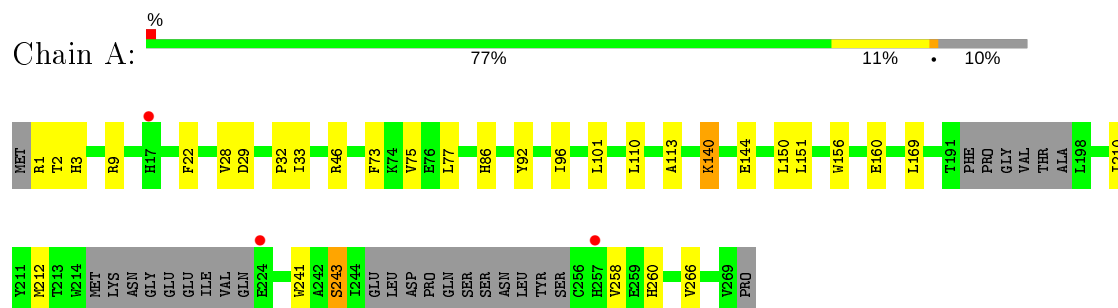
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	54	Total O 54 54	0	0
10	B	11	Total O 11 11	0	0
10	C	63	Total O 63 63	0	0
10	D	20	Total O 20 20	0	0
10	E	29	Total O 29 29	0	0
10	F	60	Total O 60 60	0	0
10	G	36	Total O 36 36	0	0
10	H	58	Total O 58 58	0	0

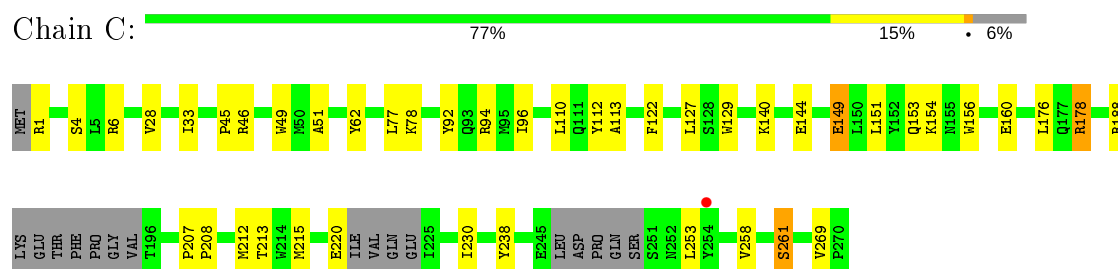
3 Residue-property plots [i](#)

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.

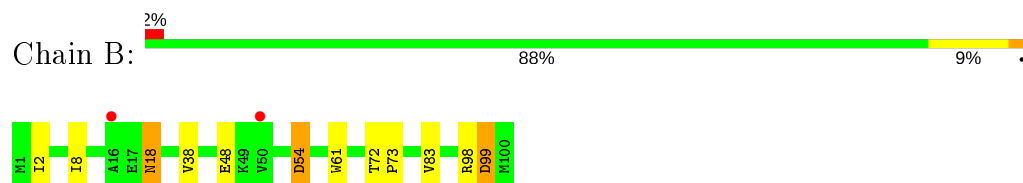
- Molecule 1: Major histocompatibility complex class I-related gene protein



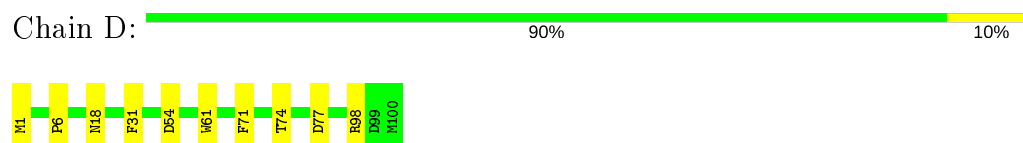
- Molecule 1: Major histocompatibility complex class I-related gene protein



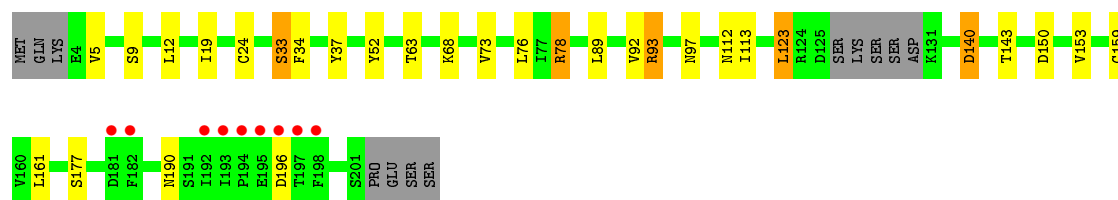
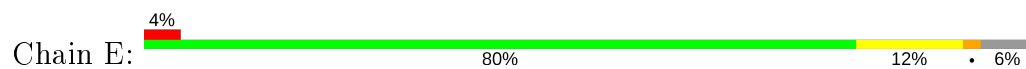
- Molecule 2: Beta-2-microglobulin



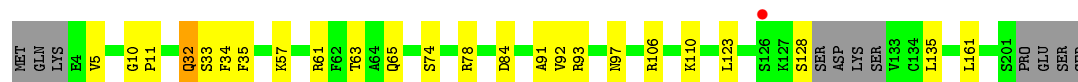
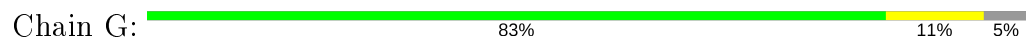
- Molecule 2: Beta-2-microglobulin



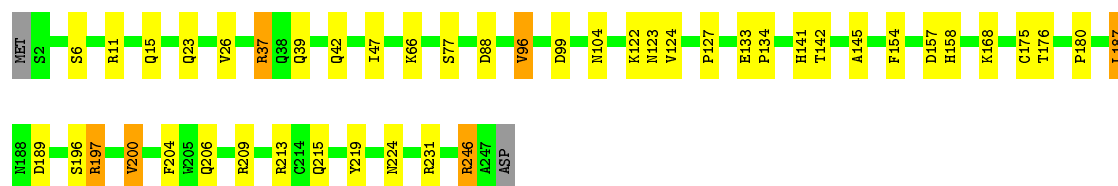
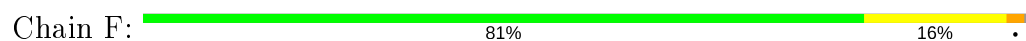
- Molecule 3: TRAV12-2 alpha chain



- Molecule 3: TRAV12-2 alpha chain



- Molecule 4: TRBV29-1



- Molecule 4: TRBV29-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.88Å 113.43Å 209.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.81 – 2.90 48.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.81-2.90) 100.0 (48.23-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.190 , 0.235 0.191 , 0.235	Depositor DCC
R_{free} test set	2819 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12963	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 2.59% 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, CL, NA, BR, 2LJ

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	0/2038	0.45	0/2773
1	C	0.27	0/2165	0.45	0/2941
2	B	0.28	0/835	0.45	0/1137
2	D	0.28	0/832	0.46	0/1133
3	E	0.25	0/1483	0.43	0/2015
3	G	0.25	0/1514	0.44	0/2054
4	F	0.27	0/1981	0.45	0/2699
4	H	0.27	0/1983	0.46	0/2702
All	All	0.27	0/12831	0.45	0/17454

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	1978	0	1842	22	0
1	C	2099	0	1981	29	0
2	B	812	0	746	6	0
2	D	809	0	744	6	0
3	E	1452	0	1331	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1483	0	1371	13	0
4	F	1930	0	1850	23	0
4	H	1932	0	1849	14	0
5	A	44	0	35	6	0
5	C	44	0	36	6	0
6	A	6	0	8	1	0
6	C	18	0	24	1	0
6	F	6	0	8	1	0
6	H	12	0	16	1	0
7	E	1	0	0	0	0
7	G	1	0	0	2	0
8	F	1	0	0	0	0
9	F	2	0	0	0	0
9	H	2	0	0	1	0
10	A	54	0	0	0	0
10	B	11	0	0	0	0
10	C	63	0	0	1	0
10	D	20	0	0	0	0
10	E	29	0	0	1	0
10	F	60	0	0	2	0
10	G	36	0	0	1	0
10	H	58	0	0	0	0
All	All	12963	0	11841	121	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (121) 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:32:PRO:HB2	1:A:46:ARG:HG2	1.70	0.73
3:G:33:SER:HB3	3:G:93:ARG:HG2	1.70	0.72
1:C:78:LYS:HE3	6:C:304:GOL:H2	1.73	0.70
3:G:93:ARG:HD3	3:G:97:ASN:HA	1.75	0.67
3:E:93:ARG:HD3	3:E:97:ASN:HA	1.77	0.66
3:G:61:ARG:NH2	3:G:84:ASP:OD2	2.29	0.65
3:G:63:THR:OG1	3:G:78:ARG:NH2	2.30	0.65
1:A:2:THR:HG23	1:A:101:LEU:HA	1.78	0.64
1:A:96:ILE:HG13	1:A:110:LEU:HB2	1.79	0.64
3:G:123:LEU:HD11	3:G:135:LEU:HD12	1.79	0.63
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:68:LYS:NZ	10:E:401:HOH:O	2.32	0.63
1:C:208:PRO:HG3	1:C:238:TYR:CE1	2.34	0.63
4:H:16:ARG:NH1	4:H:119:GLU:OE2	2.31	0.62
1:C:261:SER:OG	1:C:261:SER:O	2.17	0.61
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.82	0.61
1:C:212:MET:HG2	1:C:258:VAL:HG22	1.82	0.61
2:D:18:ASN:OD1	2:D:98:ARG:NH1	2.35	0.60
3:E:63:THR:HB	3:E:76:LEU:HB2	1.83	0.59
1:C:160:GLU:OE2	3:G:32:GLN:NE2	2.30	0.59
4:F:124:VAL:O	4:F:231:ARG:NH2	2.36	0.58
4:F:209:ARG:NH1	10:F:402:HOH:O	2.36	0.58
4:F:200:VAL:HG22	6:F:301:GOL:H12	1.86	0.57
3:E:161:LEU:HB3	4:F:175:CYS:HB2	1.88	0.56
4:H:15:GLN:HG2	4:H:121:LEU:HG	1.88	0.56
1:A:156:TRP:CZ2	5:A:301[B]:2LJ:H9	2.40	0.56
3:G:65:GLN:HB2	3:G:74:SER:HB2	1.88	0.56
3:E:159:CYS:HB2	4:F:197:ARG:HH11	1.71	0.55
1:C:96:ILE:HG13	1:C:110:LEU:HB2	1.88	0.55
1:C:178:ARG:NH2	10:C:402:HOH:O	2.31	0.55
1:A:28:VAL:HG23	1:A:33:ILE:HD13	1.88	0.55
4:F:200:VAL:HG13	4:F:204:PHE:HB3	1.89	0.55
1:C:1:ARG:NH1	1:C:207:PRO:HG3	2.22	0.54
1:C:153:GLN:NE2	5:C:301[B]:2LJ:O5'	2.41	0.54
2:B:99:ASP:OD1	2:B:99:ASP:N	2.39	0.54
4:H:39:GLN:HB3	4:H:42:GLN:HG3	1.90	0.54
1:A:210:ILE:HG21	1:A:212:MET:HE3	1.90	0.53
1:C:208:PRO:HG3	1:C:238:TYR:CZ	2.44	0.53
4:F:134:PRO:HG2	4:F:145:ALA:HB1	1.90	0.53
2:B:18:ASN:OD1	2:B:18:ASN:N	2.30	0.53
4:F:213:ARG:NH2	10:F:401:HOH:O	2.35	0.53
4:F:39:GLN:HB3	4:F:42:GLN:HG3	1.91	0.53
3:E:113:ILE:HG13	3:E:140:ASP:HA	1.92	0.52
4:F:99:ASP:OD1	4:F:104:ASN:ND2	2.36	0.52
4:F:176:THR:HG23	4:F:196:SER:HB2	1.92	0.52
1:C:113:ALA:HB2	2:D:61:TRP:CE2	2.45	0.52
3:E:150:ASP:HB3	3:E:153:VAL:HG12	1.93	0.51
4:F:37:ARG:HB3	4:F:47:ILE:HD11	1.92	0.51
3:E:24:CYS:HB3	3:E:73:VAL:HG23	1.92	0.51
3:E:33:SER:HB3	3:E:52:TYR:CE1	2.47	0.50
3:E:196:ASP:OD1	3:E:196:ASP:N	2.40	0.50
1:A:46:ARG:NH2	2:B:54:ASP:HB2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ALA:HB2	2:B:61:TRP:CE2	2.47	0.50
1:A:9:ARG:HD3	1:A:22:PHE:HZ	1.77	0.49
4:F:66:LYS:NZ	4:F:88:ASP:OD2	2.44	0.49
1:C:49:TRP:CH2	1:C:176:LEU:HD11	2.47	0.49
4:H:127:PRO:HB3	4:H:154:PHE:CD1	2.47	0.49
1:C:94:ARG:HG3	1:C:112:TYR:CE2	2.47	0.48
5:A:301[B]:2LJ:H1	5:A:301[B]:2LJ:O4	2.12	0.48
4:F:187:LEU:HD12	4:F:189:ASP:OD1	2.13	0.48
1:C:215:MET:HG2	1:C:220:GLU:HG2	1.94	0.48
4:H:133:GLU:OE2	4:H:246:ARG:NH2	2.46	0.48
2:D:74:THR:OG1	2:D:77:ASP:OD2	2.28	0.48
4:F:127:PRO:HB3	4:F:154:PHE:CD1	2.48	0.48
3:G:34:PHE:HD2	3:G:92:VAL:HG22	1.79	0.47
4:F:11[B]:ARG:HD2	4:F:219:TYR:CG	2.50	0.47
4:F:213:ARG:NH1	4:F:215:GLN:OE1	2.47	0.47
5:A:301[A]:2LJ:O4	5:A:301[A]:2LJ:H1	2.13	0.47
5:A:301[A]:2LJ:H19	5:A:301[A]:2LJ:H8	1.38	0.47
3:G:35:PHE:HB2	3:G:91:ALA:HB3	1.97	0.47
3:E:34:PHE:HD1	3:E:92:VAL:HG22	1.81	0.46
10:G:403:HOH:O	9:H:304:CL:CL	2.58	0.46
4:F:157:ASP:HB2	4:F:180:PRO:HG2	1.97	0.46
1:A:156:TRP:CZ2	5:A:301[A]:2LJ:H9	2.51	0.46
4:H:26:VAL:HG21	4:H:96:VAL:HG21	1.97	0.46
1:C:156:TRP:CZ2	5:C:301[B]:2LJ:H9	2.51	0.46
4:H:39:GLN:HG3	4:H:40:PRO:HD2	1.98	0.45
1:C:28:VAL:HG23	1:C:33:ILE:HD13	1.98	0.45
1:A:212:MET:HG2	1:A:258:VAL:HG22	1.98	0.45
1:C:149:GLU:HG2	4:H:103:GLY:HA3	1.98	0.45
1:C:62:TYR:CE1	5:C:301[B]:2LJ:H3	2.52	0.45
1:C:149:GLU:HG2	4:H:104:ASN:H	1.80	0.45
3:G:161:LEU:HB3	4:H:175:CYS:HB2	1.99	0.45
1:C:122:PHE:HB2	1:C:129:TRP:CH2	2.53	0.44
5:A:301[B]:2LJ:H19	5:A:301[B]:2LJ:H8	1.46	0.44
1:C:4:SER:OG	1:C:6[B]:ARG:NH2	2.50	0.44
4:F:158:HIS:HB3	4:F:219:TYR:HB2	1.99	0.44
2:D:1:MET:H1	4:F:168:LYS:HE3	1.82	0.44
1:C:62:TYR:CE1	5:C:301[A]:2LJ:H3	2.53	0.44
4:H:151:ALA:HB2	4:H:216:VAL:HG21	2.00	0.44
3:E:19:ILE:HG12	3:E:78:ARG:HA	2.00	0.44
1:A:156:TRP:CD1	1:A:160:GLU:HB3	2.53	0.43
3:G:57:LYS:CE	7:G:301:BR:BR	3.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:HG13	1:A:260:HIS:HB2	1.99	0.43
2:B:73:PRO:HB2	2:B:98:ARG:HH21	1.82	0.43
4:H:11:ARG:HD2	4:H:219:TYR:CG	2.53	0.43
2:B:38:VAL:HG22	2:B:83:VAL:HG22	2.01	0.43
1:C:45:PRO:HG3	1:C:51:ALA:HB2	2.01	0.43
1:A:241:TRP:HZ3	1:A:243:SER:HB3	1.84	0.43
1:A:75:VAL:HG22	6:A:302:GOL:H31	2.00	0.43
1:A:210:ILE:HD13	1:A:212:MET:HE2	2.01	0.42
1:C:140:LYS:NZ	1:C:144:GLU:OE2	2.48	0.42
3:G:57:LYS:HE3	7:G:301:BR:BR	2.74	0.42
4:H:204:PHE:HA	6:H:302:GOL:H2	2.01	0.42
1:C:208:PRO:O	1:C:230:ILE:HD13	2.18	0.42
5:C:301[A]:2LJ:O4	5:C:301[A]:2LJ:H1	2.17	0.42
4:F:206:GLN:HA	4:F:246:ARG:O	2.19	0.42
3:E:123:LEU:HB3	4:F:133:GLU:O	2.20	0.42
1:C:156:TRP:CZ2	5:C:301[A]:2LJ:H9	2.55	0.42
3:G:10:GLY:HA3	3:G:11:PRO:HD3	1.85	0.42
1:C:127:LEU:HD21	1:C:154:LYS:HD2	2.02	0.42
1:A:140:LYS:NZ	1:A:144:GLU:OE1	2.51	0.41
1:A:3:HIS:ND1	1:A:29:ASP:OD2	2.53	0.41
3:E:37:TYR:HB2	3:E:89:LEU:HB2	2.01	0.41
2:D:6:PRO:HB3	2:D:31:PHE:HB3	2.03	0.41
4:F:26:VAL:HG21	4:F:96:VAL:HG21	2.03	0.41
1:A:86:HIS:HE1	4:H:168:LYS:HE3	1.85	0.41
1:A:144:GLU:HA	1:A:150:LEU:HD11	2.02	0.41
3:E:153:VAL:HA	3:E:177:SER:HB2	2.02	0.40
1:A:169:LEU:HA	1:A:169:LEU:HD23	1.87	0.40
1:C:46:ARG:NH1	2:D:54:ASP:HB2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/271 (87%)	231 (98%)	4 (2%)	0	100	100
1	C	247/271 (91%)	239 (97%)	8 (3%)	0	100	100
2	B	99/100 (99%)	98 (99%)	1 (1%)	0	100	100
2	D	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	E	189/205 (92%)	185 (98%)	4 (2%)	0	100	100
3	G	190/205 (93%)	185 (97%)	5 (3%)	0	100	100
4	F	245/248 (99%)	240 (98%)	5 (2%)	0	100	100
4	H	245/248 (99%)	241 (98%)	4 (2%)	0	100	100
All	All	1548/1648 (94%)	1515 (98%)	33 (2%)	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	206/241 (86%)	200 (97%)	6 (3%)	42	76
1	C	222/241 (92%)	214 (96%)	8 (4%)	35	69
2	B	88/95 (93%)	81 (92%)	7 (8%)	12	33
2	D	88/95 (93%)	87 (99%)	1 (1%)	73	92
3	E	157/182 (86%)	146 (93%)	11 (7%)	15	41
3	G	164/182 (90%)	159 (97%)	5 (3%)	41	75
4	F	216/219 (99%)	201 (93%)	15 (7%)	15	41
4	H	217/219 (99%)	209 (96%)	8 (4%)	34	68
All	All	1358/1474 (92%)	1297 (96%)	61 (4%)	27	61

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	73	PHE

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Mol	Chain	Res	Type
1	A	140	LYS
1	A	151	LEU
1	A	243	SER
1	A	266	VAL
2	B	2	ILE
2	B	8	ILE
2	B	18	ASN
2	B	48	GLU
2	B	54	ASP
2	B	72	THR
2	B	99	ASP
1	C	149	GLU
1	C	151	LEU
1	C	178	ARG
1	C	188	ARG
1	C	213	THR
1	C	253	LEU
1	C	261	SER
1	C	269	VAL
2	D	71	PHE
3	E	5	VAL
3	E	9	SER
3	E	12	LEU
3	E	33	SER
3	E	78	ARG
3	E	93	ARG
3	E	112	ASN
3	E	123	LEU
3	E	140	ASP
3	E	143	THR
3	E	190	ASN
4	F	6	SER
4	F	15	GLN
4	F	23	GLN
4	F	37	ARG
4	F	77	SER
4	F	96	VAL
4	F	122	LYS
4	F	123	ASN
4	F	141	HIS
4	F	142	THR
4	F	187	LEU

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Mol	Chain	Res	Type
4	F	197	ARG
4	F	200	VAL
4	F	224	ASN
4	F	246	ARG
3	G	5	VAL
3	G	32	GLN
3	G	106	ARG
3	G	110	LYS
3	G	128	SER
4	H	96	VAL
4	H	118	LEU
4	H	187	LEU
4	H	188	ASN
4	H	189	ASP
4	H	191	ARG
4	H	203	THR
4	H	246	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	C	153	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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	GOL	C	304	-	5,5,5	0.90	0	5,5,5	0.98	0
5	2LJ	C	301[B]	1	20,22,22	1.25	3 (15%)	22,29,29	4.16	6 (27%)
6	GOL	H	301	-	5,5,5	0.92	0	5,5,5	0.98	0
5	2LJ	C	301[A]	1	20,22,22	1.31	3 (15%)	22,29,29	4.17	6 (27%)
6	GOL	F	301	-	5,5,5	0.91	0	5,5,5	0.98	0
6	GOL	C	302	-	5,5,5	0.89	0	5,5,5	1.00	0
5	2LJ	A	301[A]	1	20,22,22	1.55	2 (10%)	22,29,29	4.31	8 (36%)
6	GOL	A	302	-	5,5,5	0.92	0	5,5,5	0.99	0
5	2LJ	A	301[B]	1	20,22,22	1.36	2 (10%)	22,29,29	4.22	7 (31%)
6	GOL	C	303	-	5,5,5	0.91	0	5,5,5	1.00	0
6	GOL	H	302	-	5,5,5	0.91	0	5,5,5	1.00	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	GOL	C	304	-	-	2/4/4/4	-
5	2LJ	C	301[B]	1	-	10/18/19/19	0/1/1/1
6	GOL	H	301	-	-	0/4/4/4	-
5	2LJ	C	301[A]	1	1/1/3/5	10/18/19/19	0/1/1/1
6	GOL	F	301	-	-	2/4/4/4	-
6	GOL	C	302	-	-	3/4/4/4	-
5	2LJ	A	301[A]	1	-	8/18/19/19	0/1/1/1
6	GOL	A	302	-	-	0/4/4/4	-
5	2LJ	A	301[B]	1	1/1/3/5	9/18/19/19	0/1/1/1
6	GOL	C	303	-	-	0/4/4/4	-
6	GOL	H	302	-	-	0/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301[A]	2LJ	C8A-N8	5.12	1.42	1.34
5	A	301[B]	2LJ	C8A-N8	4.14	1.41	1.34
5	A	301[A]	2LJ	C4-N3	3.33	1.38	1.33
5	A	301[B]	2LJ	C4-N3	3.32	1.38	1.33
5	C	301[B]	2LJ	C4-N3	3.30	1.38	1.33
5	C	301[A]	2LJ	C4-N3	3.28	1.38	1.33
5	C	301[B]	2LJ	C7-C6	-3.17	1.45	1.49
5	C	301[A]	2LJ	C7-C6	-3.15	1.46	1.49
5	C	301[A]	2LJ	C8A-N8	2.77	1.38	1.34
5	C	301[B]	2LJ	C8A-N8	2.00	1.37	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301[A]	2LJ	C4-N3-C2	13.97	126.93	115.14
5	A	301[B]	2LJ	C4-N3-C2	13.96	126.93	115.14
5	C	301[B]	2LJ	C4-N3-C2	13.86	126.84	115.14
5	C	301[A]	2LJ	C4-N3-C2	13.85	126.84	115.14
5	C	301[A]	2LJ	C4-C4A-C8A	9.19	120.54	114.53
5	C	301[B]	2LJ	C4-C4A-C8A	9.19	120.54	114.53
5	A	301[B]	2LJ	C4-C4A-C8A	8.81	120.29	114.53
5	A	301[A]	2LJ	C4-C4A-C8A	8.76	120.26	114.53
5	C	301[B]	2LJ	C4A-C4-N3	-7.09	113.73	123.43
5	C	301[A]	2LJ	C4A-C4-N3	-7.09	113.73	123.43
5	A	301[B]	2LJ	C4A-C4-N3	-7.00	113.86	123.43
5	A	301[A]	2LJ	C4A-C4-N3	-6.96	113.91	123.43
5	A	301[A]	2LJ	C1'-N8-C8A	-5.46	113.53	123.25
5	A	301[A]	2LJ	C2-N1-C8A	5.01	125.27	113.80
5	A	301[B]	2LJ	C2-N1-C8A	4.93	125.08	113.80
5	A	301[B]	2LJ	C1'-N8-C8A	-4.89	114.54	123.25
5	C	301[A]	2LJ	C2-N1-C8A	4.86	124.91	113.80
5	C	301[B]	2LJ	C2-N1-C8A	4.66	124.47	113.80
5	C	301[B]	2LJ	C1'-N8-C8A	-4.30	115.59	123.25
5	C	301[A]	2LJ	C1'-N8-C8A	-4.29	115.63	123.25
5	A	301[A]	2LJ	C4A-C8A-N8	2.89	126.64	121.76
5	C	301[B]	2LJ	C8A-C4A-N5	-2.51	111.62	125.02
5	C	301[A]	2LJ	C8A-C4A-N5	-2.38	112.32	125.02
5	A	301[B]	2LJ	C4A-C8A-N8	2.36	125.74	121.76
5	A	301[A]	2LJ	N8-C8A-N1	-2.29	115.57	118.50
5	A	301[A]	2LJ	C8A-C4A-N5	-2.16	113.48	125.02
5	A	301[B]	2LJ	C8A-C4A-N5	-2.14	113.58	125.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	301[A]	2LJ	C4'
5	A	301[B]	2LJ	C4'

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	304	GOL	O1-C1-C2-C3
5	C	301[B]	2LJ	N8-C1'-C2'-O2'
5	C	301[B]	2LJ	C1'-C2'-C3'-O3'
5	C	301[B]	2LJ	C1'-C2'-C3'-C4'
5	C	301[A]	2LJ	N8-C1'-C2'-O2'
5	C	301[A]	2LJ	C1'-C2'-C3'-O3'
5	C	301[A]	2LJ	C1'-C2'-C3'-C4'
6	F	301	GOL	C1-C2-C3-O3
6	C	302	GOL	O1-C1-C2-O2
6	C	302	GOL	O1-C1-C2-C3
5	A	301[A]	2LJ	N8-C1'-C2'-O2'
5	A	301[A]	2LJ	N8-C1'-C2'-C3'
5	A	301[A]	2LJ	C1'-C2'-C3'-O3'
5	A	301[A]	2LJ	C1'-C2'-C3'-C4'
5	A	301[B]	2LJ	N8-C1'-C2'-O2'
5	A	301[B]	2LJ	N8-C1'-C2'-C3'
5	A	301[B]	2LJ	O4'-C4'-C5'-O5'
5	C	301[B]	2LJ	C8A-C4A-N5-C6
5	C	301[A]	2LJ	C8A-C4A-N5-C6
5	A	301[A]	2LJ	C8A-C4A-N5-C6
5	A	301[B]	2LJ	C8A-C4A-N5-C6
5	C	301[A]	2LJ	C3'-C4'-C5'-O5'
5	A	301[B]	2LJ	C3'-C4'-C5'-O5'
5	A	301[A]	2LJ	O2'-C2'-C3'-O3'
5	A	301[A]	2LJ	O2'-C2'-C3'-C4'
5	C	301[A]	2LJ	O4'-C4'-C5'-O5'
5	C	301[B]	2LJ	N8-C1'-C2'-C3'
5	C	301[A]	2LJ	N8-C1'-C2'-C3'
6	C	302	GOL	C1-C2-C3-O3
6	C	304	GOL	O1-C1-C2-O2
6	F	301	GOL	O2-C2-C3-O3
5	C	301[B]	2LJ	O2'-C2'-C3'-C4'
5	C	301[A]	2LJ	O2'-C2'-C3'-O3'
5	C	301[B]	2LJ	O2'-C2'-C3'-O3'
5	C	301[A]	2LJ	O2'-C2'-C3'-C4'
5	C	301[B]	2LJ	O4'-C4'-C5'-O5'
5	C	301[B]	2LJ	C3'-C4'-C5'-O5'

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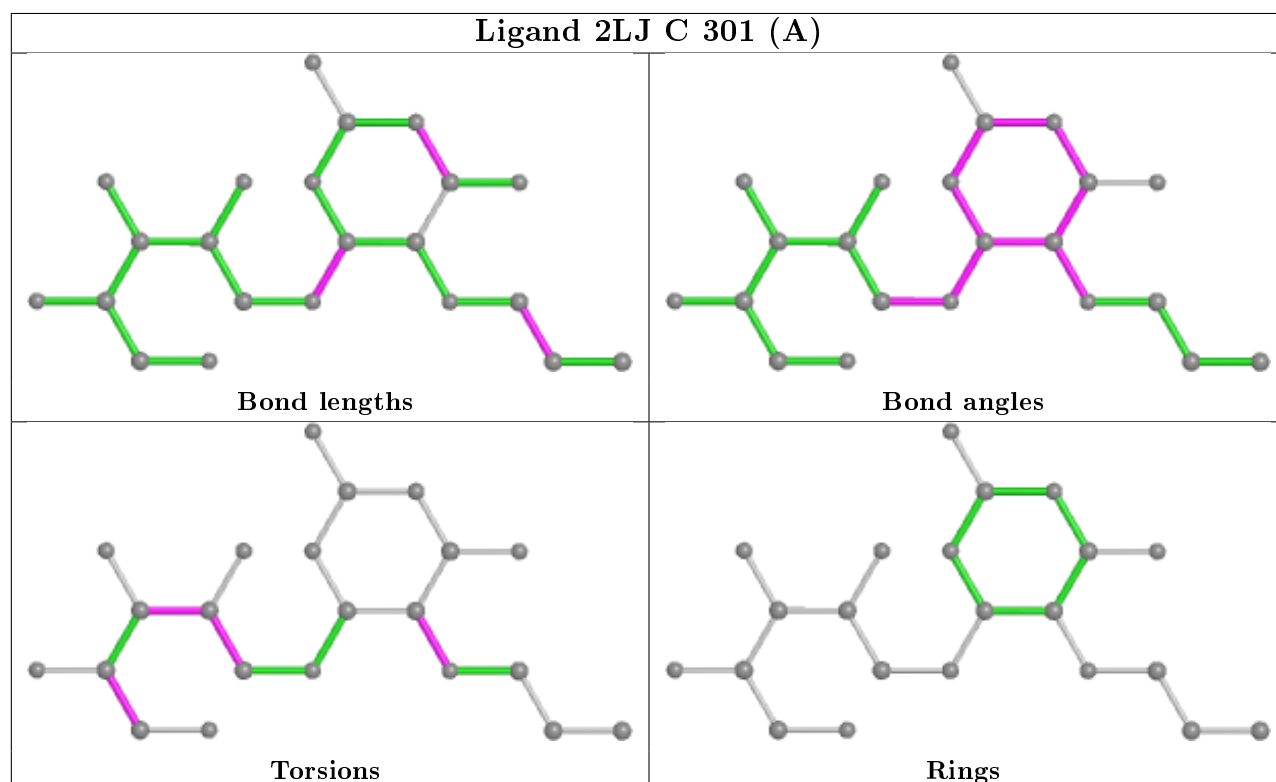
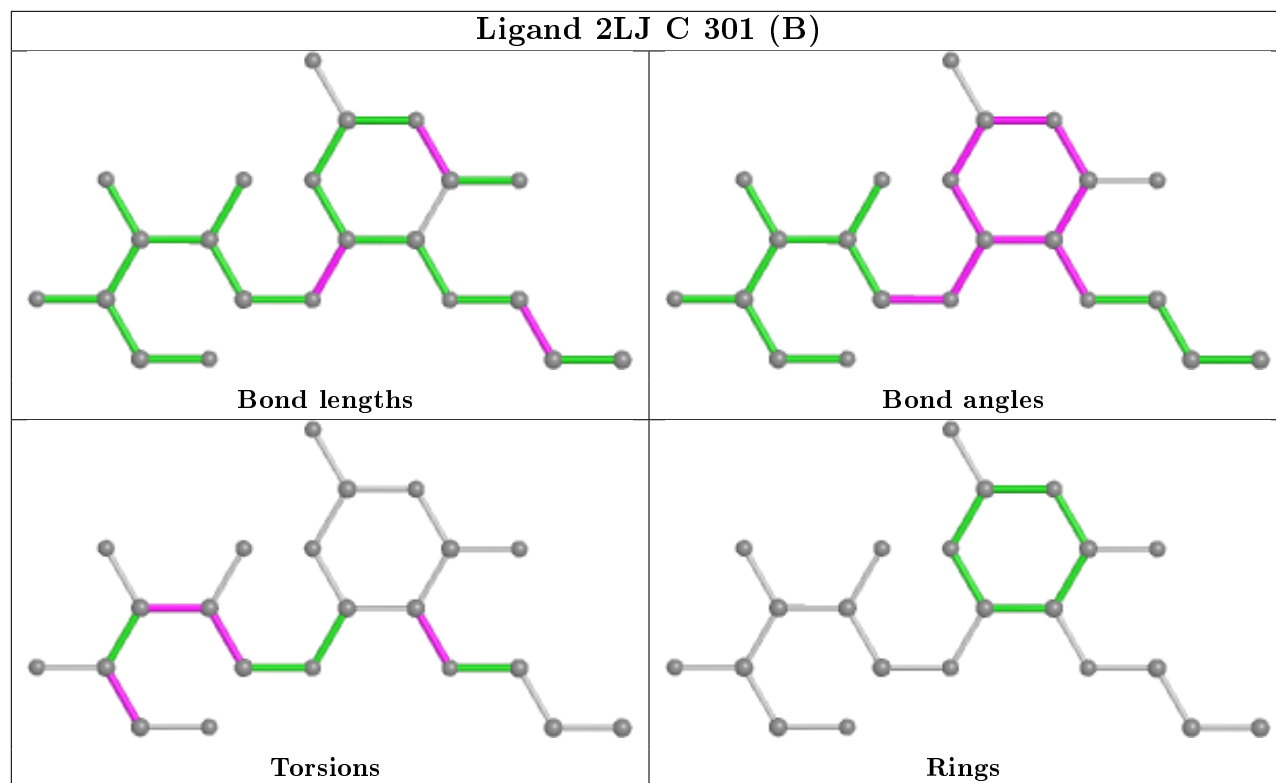
Mol	Chain	Res	Type	Atoms
5	A	301[B]	2LJ	O2'-C2'-C3'-O3'
5	C	301[B]	2LJ	C4-C4A-N5-C6
5	C	301[A]	2LJ	C4-C4A-N5-C6
5	A	301[A]	2LJ	C4-C4A-N5-C6
5	A	301[B]	2LJ	C4-C4A-N5-C6
5	A	301[B]	2LJ	O2'-C2'-C3'-C4'
5	A	301[B]	2LJ	C1'-C2'-C3'-O3'

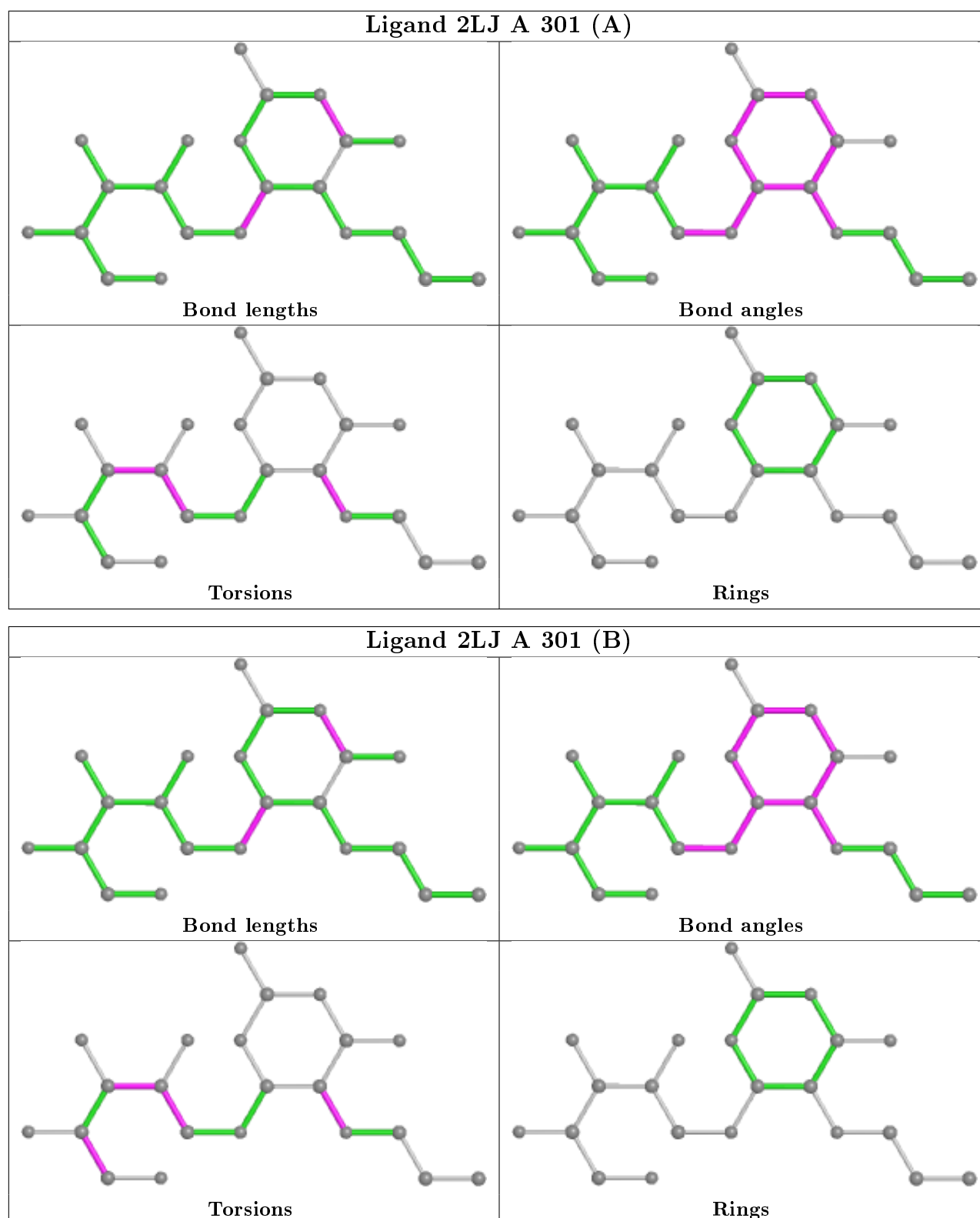
There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	304	GOL	1	0
5	C	301[B]	2LJ	3	0
5	C	301[A]	2LJ	3	0
6	F	301	GOL	1	0
5	A	301[A]	2LJ	3	0
6	A	302	GOL	1	0
5	A	301[B]	2LJ	3	0
6	H	302	GOL	1	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	243/271 (89%)	-0.17	3 (1%) 79 79	22, 40, 81, 101	0
1	C	254/271 (93%)	-0.27	1 (0%) 92 93	20, 35, 71, 92	1 (0%)
2	B	100/100 (100%)	0.25	2 (2%) 65 63	32, 60, 85, 102	0
2	D	100/100 (100%)	-0.16	0 100 100	27, 47, 80, 100	0
3	E	193/205 (94%)	0.18	9 (4%) 31 28	24, 53, 83, 109	0
3	G	194/205 (94%)	-0.16	1 (0%) 91 91	22, 42, 68, 84	0
4	F	246/248 (99%)	-0.39	0 100 100	18, 33, 57, 86	0
4	H	246/248 (99%)	-0.42	0 100 100	18, 29, 53, 92	0
All	All	1576/1648 (95%)	-0.19	16 (1%) 82 82	18, 39, 77, 109	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	192	ILE	3.2
3	E	195	GLU	3.1
1	A	224	GLU	3.0
3	E	182	PHE	2.7
2	B	16	ALA	2.6
3	E	197	THR	2.5
3	E	196	ASP	2.5
3	E	193	ILE	2.3
3	E	181	ASP	2.2
3	G	126	SER	2.2
2	B	50	VAL	2.2
1	A	257	HIS	2.1
3	E	198	PHE	2.1
1	A	17	HIS	2.1
1	C	254	TYR	2.1
3	E	194	PRO	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 monosaccharides in this entry.

6.4 Ligands ⓘ

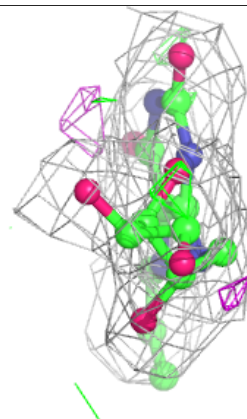
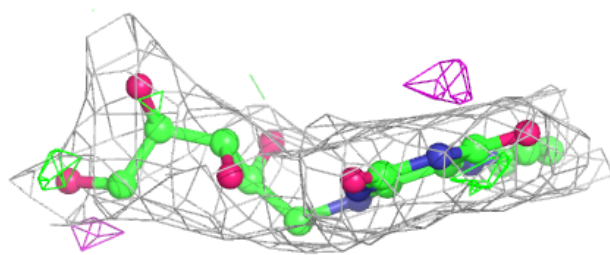
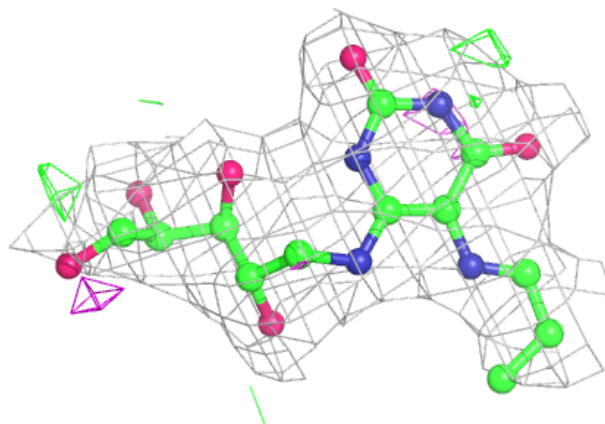
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	H	301	6/6	0.86	0.22	46,58,68,77	0
6	GOL	A	302	6/6	0.89	0.21	32,44,47,55	0
6	GOL	C	303	6/6	0.89	0.28	40,48,53,55	0
6	GOL	C	304	6/6	0.91	0.23	28,55,64,71	0
6	GOL	F	301	6/6	0.91	0.18	41,44,50,51	0
6	GOL	C	302	6/6	0.92	0.21	53,54,59,62	0
6	GOL	H	302	6/6	0.93	0.21	26,44,49,58	0
5	2LJ	C	301[B]	22/22	0.96	0.20	20,26,31,34	22
5	2LJ	A	301[B]	22/22	0.96	0.18	26,31,35,37	22
5	2LJ	C	301[A]	22/22	0.96	0.20	21,26,32,35	22
5	2LJ	A	301[A]	22/22	0.96	0.18	26,31,36,36	22
8	NA	F	302	1/1	0.98	0.28	19,19,19,19	0
9	CL	F	304	1/1	0.98	0.15	32,32,32,32	0
9	CL	F	303	1/1	0.99	0.19	16,16,16,16	0
7	BR	G	301	1/1	0.99	0.08	58,58,58,58	0
9	CL	H	303	1/1	0.99	0.17	19,19,19,19	0
9	CL	H	304	1/1	0.99	0.13	19,19,19,19	0
7	BR	E	301	1/1	1.00	0.05	61,61,61,61	0

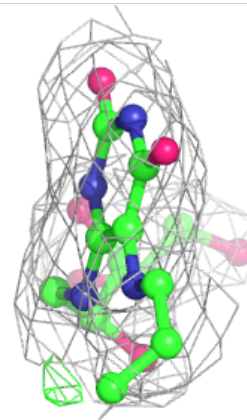
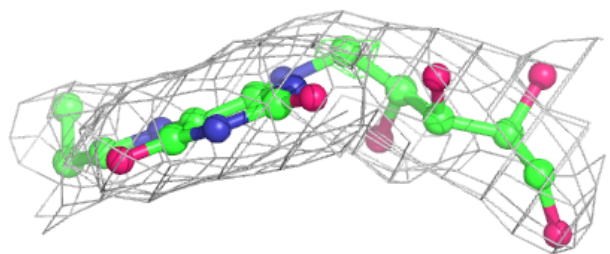
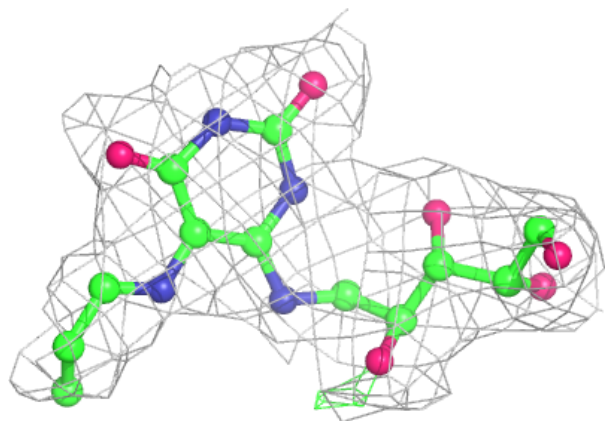
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2LJ C 301 (B):

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

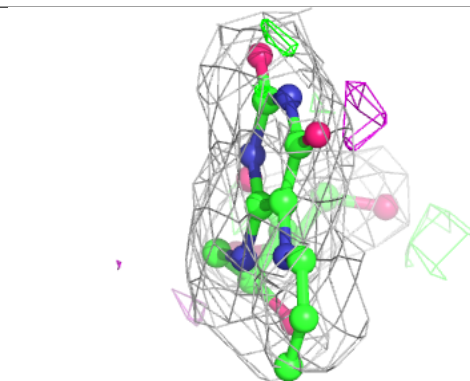
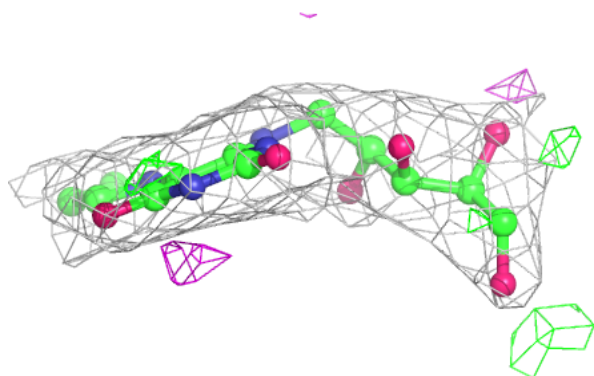
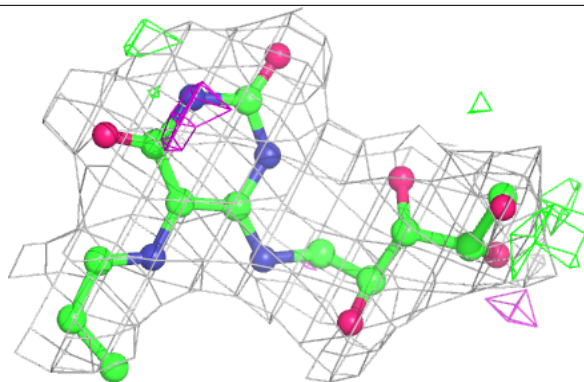
**Electron density around 2LJ A 301 (B):**

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

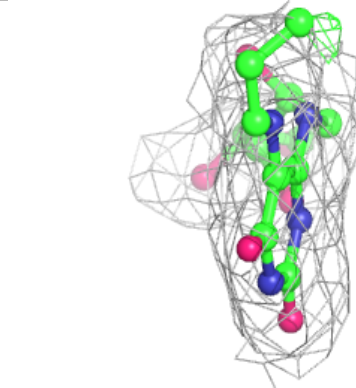
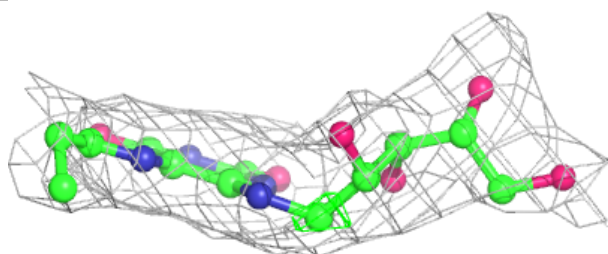
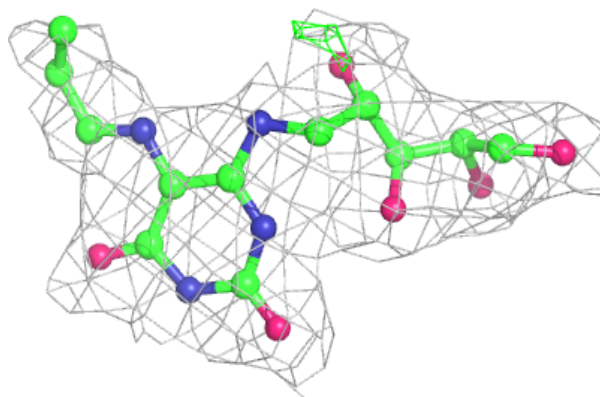


Electron density around 2LJ C 301 (A):

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

**Electron density around 2LJ A 301 (A):**

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



6.5 Other polymers

There are no such residues in this entry.