



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:48 PM UTC

PDB ID : 4PJC / pdb_00004pjc
Title : Structure of human MR1-5-OP-RU in complex with human MAIT C-A11 TCR
Authors : Birkinshaw, R.W.; Rossjohn, J.
Deposited on : 2014-05-12
Resolution : 2.50 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

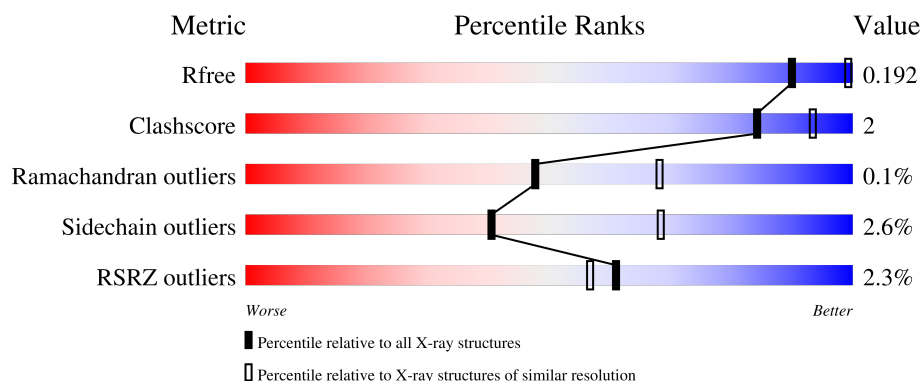
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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% 86% 11% ..
1	C	271	2% 83% 11% 6%
2	B	100	90% 6% .
2	D	100	% 84% 10% ..
3	E	205	8% 83% 8% 8%

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Mol	Chain	Length	Quality of chain
3	G	205	% 87% 9%
4	F	246	2% 89% 7%
4	H	246	92% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13281 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	264	Total	C	N	O	S	0	0	0
			2144	1376	370	387	11			
1	C	256	Total	C	N	O	S	0	0	0
			2085	1333	364	377	11			

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	96	Total	C	N	O	S	0	0	0
			765	492	131	140	2			
2	D	96	Total	C	N	O	S	0	0	0
			750	484	126	138	2			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called TCR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	188	Total	C	N	O	S	0	0	0
			1415	905	228	274	8			

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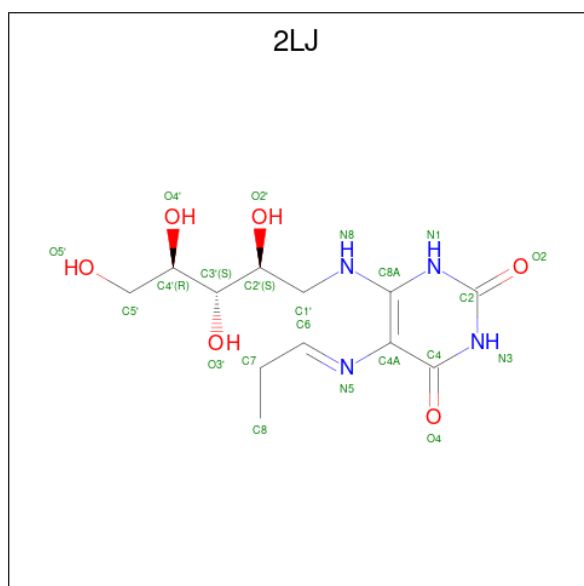
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	197	Total	C	N	O	S	0	0	0
			1532	968	249	306	9			

- Molecule 4 is a protein called TCR-beta.

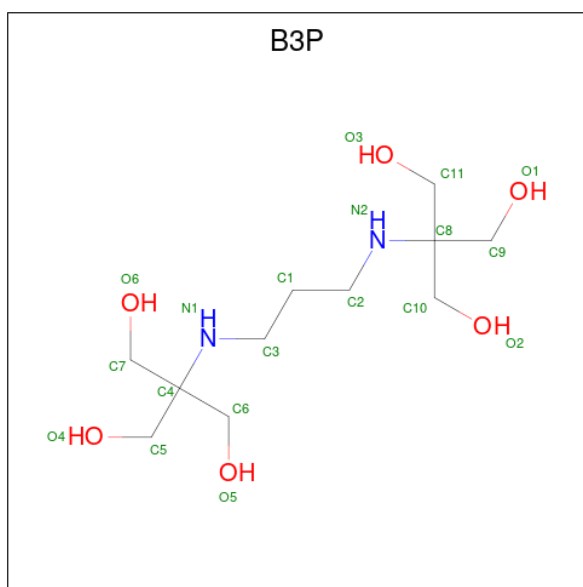
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	239	Total	C	N	O	S	0	0	0
			1812	1145	313	345	9			
4	H	240	Total	C	N	O	S	0	0	0
			1846	1163	319	355	9			

- Molecule 5 is 1-deoxy-1-({2,6-dioxo-5-[(E)-propylideneamino]-1,2,3,6-tetrahydropyrimidin-4-yl}amino)-D-ribose (CCD ID: 2LJ) (formula: C₁₂H₂₀N₄O₆).



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

- Molecule 6 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: C₁₁H₂₆N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			19	11	2	6		
6	C	1	Total	C	N	O	0	0
			19	11	2	6		

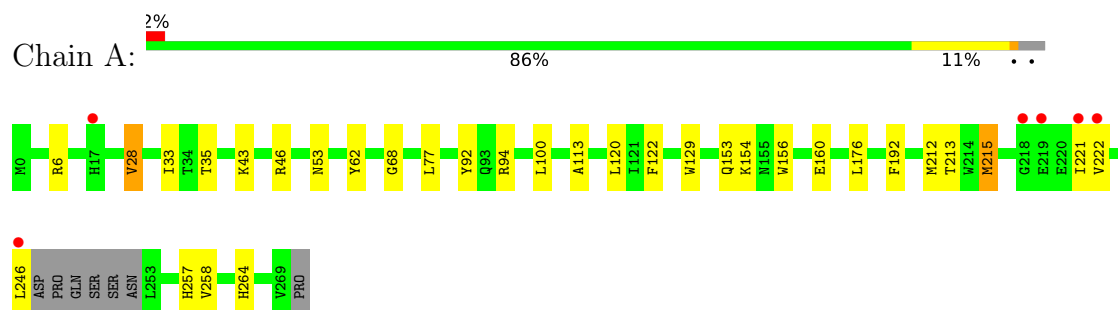
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	171	Total	O	0	0
			171	171		
7	B	75	Total	O	0	0
			75	75		
7	C	159	Total	O	0	0
			159	159		
7	D	34	Total	O	0	0
			34	34		
7	E	74	Total	O	0	0
			74	74		
7	F	79	Total	O	0	0
			79	79		
7	G	115	Total	O	0	0
			115	115		
7	H	143	Total	O	0	0
			143	143		

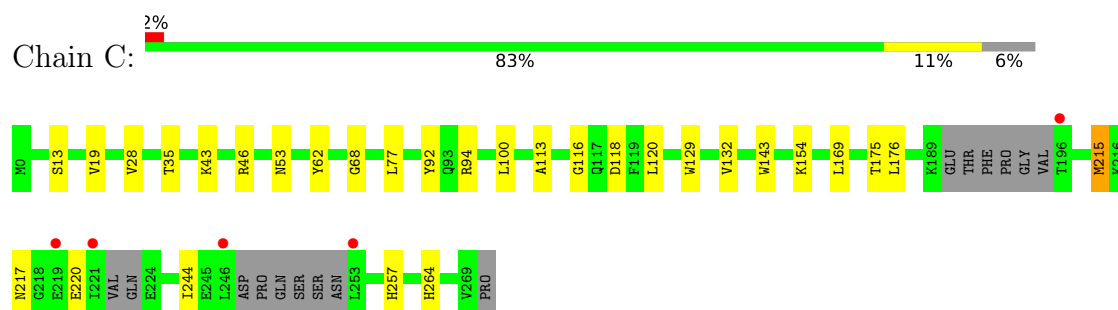
3 Residue-property plots [i](#)

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.

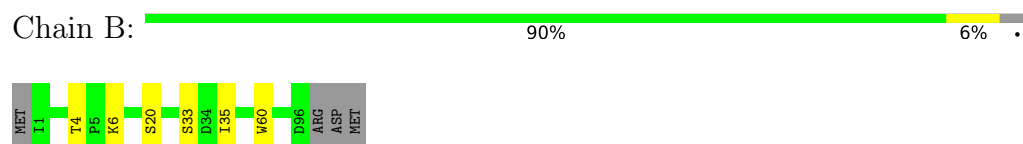
- Molecule 1: Major histocompatibility complex class I-related gene protein



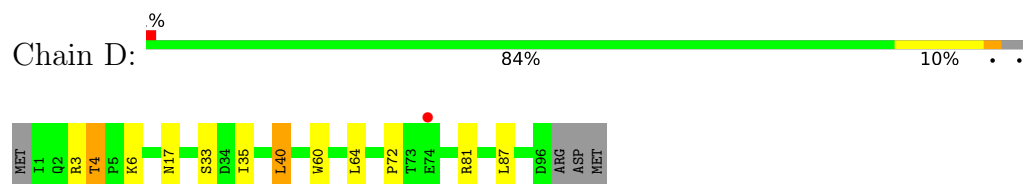
- Molecule 1: Major histocompatibility complex class I-related gene protein



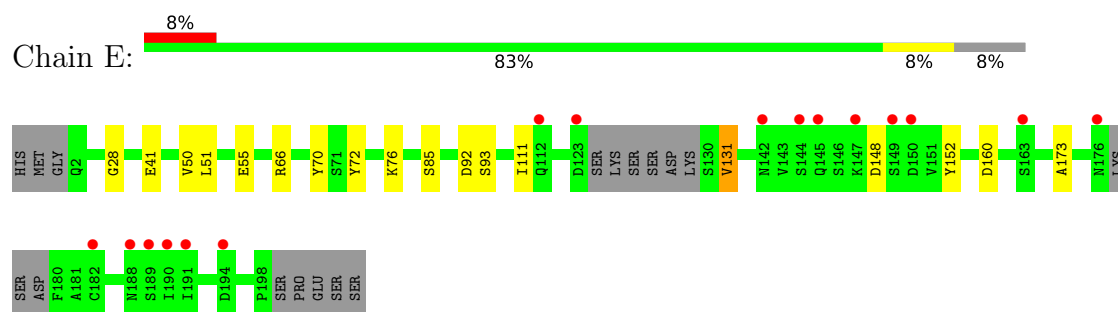
- Molecule 2: Beta-2-microglobulin



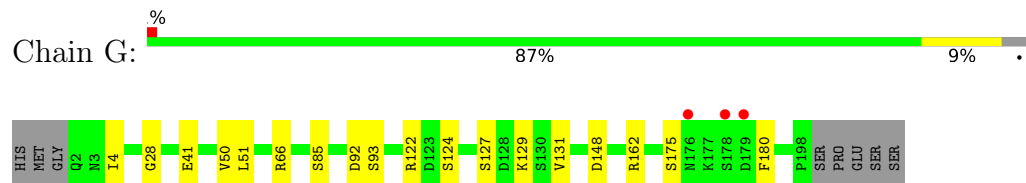
- Molecule 2: Beta-2-microglobulin



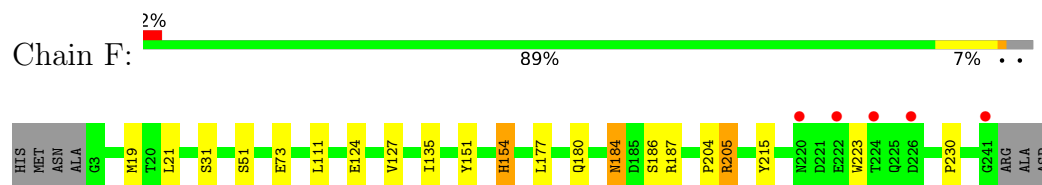
- Molecule 3: TCR-alpha



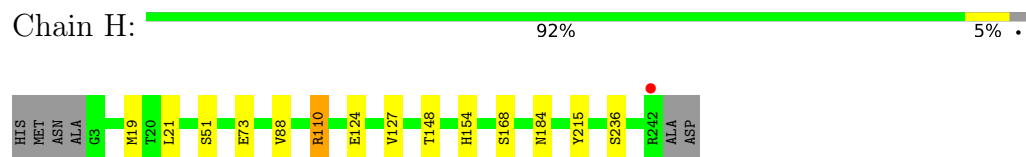
- Molecule 3: TCR-alpha



- 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	213.95Å 70.19Å 143.89Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	39.60 – 2.50 39.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.60-2.50) 100.0 (39.60-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.167 , 0.213 (Not available) , 0.192	Depositor DCC
R_{free} test set	3727 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13281	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: B3P, 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	0.85	0/2209	1.25	5/3005 (0.2%)
1	C	0.81	0/2147	1.31	8/2917 (0.3%)
2	B	0.77	0/788	1.21	2/1075 (0.2%)
2	D	0.77	0/773	1.25	5/1058 (0.5%)
3	E	0.84	0/1447	1.17	5/1970 (0.3%)
3	G	0.86	0/1566	1.22	2/2125 (0.1%)
4	F	0.82	0/1861	1.19	5/2546 (0.2%)
4	H	0.85	0/1895	1.20	3/2587 (0.1%)
All	All	0.83	0/12686	1.23	35/17283 (0.2%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	SER	N-CA-C	11.72	123.80	111.14
2	D	33	SER	N-CA-C	6.96	119.89	111.82
3	E	131	VAL	N-CA-C	6.80	118.27	108.48
4	F	154	HIS	CA-CB-CG	6.71	120.51	113.80
2	D	87	LEU	CA-C-N	6.42	129.40	120.29
2	D	87	LEU	C-N-CA	6.42	129.40	120.29
2	B	33	SER	N-CA-C	6.41	119.25	111.82
1	A	192	PHE	N-CA-C	-6.28	101.85	109.83
1	C	53	ASN	N-CA-C	6.23	120.95	113.23
1	C	19	VAL	CB-CA-C	6.07	116.87	110.37
1	A	28	VAL	N-CA-CB	6.05	119.30	111.67
1	C	28	VAL	N-CA-CB	5.86	119.05	111.67
3	E	92	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	176	LEU	N-CA-C	5.62	117.48	111.36
4	F	177	LEU	N-CA-CB	-5.61	101.76	110.57
1	C	176	LEU	N-CA-C	5.54	117.40	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	73	GLU	N-CA-C	5.53	118.48	109.59
4	H	73	GLU	N-CA-C	5.48	118.41	109.59
4	H	124	GLU	N-CA-C	-5.44	99.87	108.73
3	G	92	ASP	CA-CB-CG	5.43	118.03	112.60
3	E	148	ASP	CA-CB-CG	5.38	117.98	112.60
4	F	124	GLU	N-CA-C	-5.33	100.05	108.73
2	B	6	LYS	N-CA-C	-5.32	101.03	109.96
3	G	148	ASP	CA-CB-CG	5.31	117.91	112.60
2	D	4	THR	CB-CA-C	5.30	117.75	109.42
4	H	236	SER	N-CA-C	5.26	117.19	109.24
1	A	222	VAL	N-CA-C	-5.18	107.79	113.43
3	E	160	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	53	ASN	N-CA-C	5.06	120.44	113.97
1	C	220	GLU	N-CA-C	5.05	116.99	108.96
4	F	184	ASN	CA-CB-CG	5.03	117.63	112.60
1	C	175	THR	CA-C-N	5.01	127.41	120.29
1	C	175	THR	C-N-CA	5.01	127.41	120.29
3	E	111	ILE	CB-CA-C	5.01	117.11	111.80
2	D	6	LYS	N-CA-C	-5.01	101.55	109.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2144	0	2019	17	0
1	C	2085	0	1945	13	0
2	B	765	0	711	1	0
2	D	750	0	680	4	0
3	E	1415	0	1281	6	0
3	G	1532	0	1435	7	0
4	F	1812	0	1663	8	0
4	H	1846	0	1713	7	0
5	A	22	0	18	2	0
5	C	22	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	19	0	26	0	0
6	C	19	0	26	1	0
7	A	171	0	0	4	0
7	B	75	0	0	0	0
7	C	159	0	0	2	0
7	D	34	0	0	0	0
7	E	74	0	0	1	0
7	F	79	0	0	0	0
7	G	115	0	0	0	0
7	H	143	0	0	0	0
All	All	13281	0	11535	55	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 2.

All (55) 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:6:ARG:HD3	7:A:524:HOH:O	1.87	0.73
4:H:19:MET:HE3	4:H:21:LEU:HD23	1.74	0.68
3:G:28:GLY:HA3	3:G:93:SER:HB3	1.77	0.65
3:E:28:GLY:HA3	3:E:93:SER:HB3	1.78	0.65
1:A:94:ARG:HD3	7:A:440:HOH:O	1.97	0.64
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.85	0.58
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.87	0.56
4:H:19:MET:HE3	4:H:21:LEU:CD2	2.36	0.56
1:C:68:GLY:HA2	4:H:51:SER:HB3	1.87	0.55
5:A:301:2LJ:O4	5:A:301:2LJ:H1	2.07	0.55
1:C:264:HIS:HB2	7:C:408:HOH:O	2.06	0.55
1:A:264:HIS:HB2	7:A:424:HOH:O	2.07	0.54
1:A:68:GLY:HA2	4:F:51:SER:HB3	1.92	0.51
4:F:180:GLN:O	4:F:186:SER:HB2	2.12	0.50
2:D:40:LEU:HD11	2:D:81:ARG:HB2	1.94	0.50
4:H:154:HIS:HB3	4:H:215:TYR:HB2	1.93	0.49
3:G:124:SER:HB3	3:G:127:SER:HB3	1.95	0.49
1:A:212:MET:HG2	1:A:258:VAL:HG22	1.96	0.48
4:H:88:VAL:HG22	4:H:110:ARG:HG3	1.96	0.48
4:F:154:HIS:HB3	4:F:215:TYR:HB2	1.96	0.47
4:F:151:TYR:HB2	4:F:187:ARG:HG2	1.95	0.47
3:E:76:LYS:HG3	7:E:753:HOH:O	2.14	0.47
4:F:204:PRO:O	4:F:205:ARG:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LYS:HD3	3:G:51:LEU:HD11	1.97	0.47
4:F:21:LEU:HD21	4:F:111:LEU:HD11	1.98	0.46
1:C:94:ARG:HD3	7:C:419:HOH:O	2.16	0.45
1:C:116:GLY:O	2:D:3:ARG:NH2	2.49	0.45
1:A:43:LYS:HD2	1:A:62:TYR:HB3	1.99	0.44
1:C:113:ALA:HB2	2:D:60:TRP:CE2	2.53	0.44
1:C:43:LYS:HD2	1:C:62:TYR:HB3	1.99	0.44
1:A:122:PHE:HB2	1:A:129:TRP:CZ3	2.53	0.44
3:G:129:LYS:HE2	4:H:148:THR:HG21	2.00	0.43
1:C:35:THR:HG21	1:C:46:ARG:CZ	2.49	0.43
3:E:50:VAL:O	3:E:66:ARG:HD3	2.19	0.43
1:C:118:ASP:O	1:C:132:VAL:HG21	2.19	0.42
1:A:215:MET:HG3	1:A:257:HIS:CD2	2.54	0.42
2:D:17:ASN:HA	2:D:72:PRO:O	2.19	0.42
1:A:120:LEU:HD22	1:A:129:TRP:HB3	2.01	0.42
1:A:153:GLN:NE2	7:A:570:HOH:O	2.52	0.42
1:A:154:LYS:HD3	3:E:51:LEU:HD11	2.02	0.42
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.55	0.42
3:G:50:VAL:O	3:G:66:ARG:HD3	2.20	0.41
3:G:175:SER:HB3	3:G:180:PHE:CG	2.56	0.41
3:E:70:TYR:OH	3:E:72:TYR:HD2	2.04	0.41
1:C:143:TRP:CD1	6:C:302:B3P:H52	2.56	0.41
4:F:19:MET:HE3	4:F:21:LEU:HD23	2.01	0.41
1:C:120:LEU:HD22	1:C:129:TRP:HB3	2.02	0.41
3:E:152:TYR:O	3:E:173:ALA:HA	2.20	0.41
4:F:223:TRP:CZ2	4:F:230:PRO:HD3	2.56	0.41
1:A:43:LYS:HE3	5:A:301:2LJ:H1	1.87	0.41
1:A:28:VAL:HG23	1:A:33:ILE:HD13	2.03	0.41
1:A:35:THR:HG21	1:A:46:ARG:CZ	2.51	0.41
1:C:215:MET:HG3	1:C:257:HIS:CD2	2.55	0.41
3:G:162:ARG:HH11	4:H:168:SER:HA	1.86	0.41
1:A:156:TRP:HA	1:A:160:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/271 (96%)	253 (97%)	7 (3%)	0	100	100
1	C	248/271 (92%)	241 (97%)	7 (3%)	0	100	100
2	B	94/100 (94%)	93 (99%)	1 (1%)	0	100	100
2	D	94/100 (94%)	93 (99%)	1 (1%)	0	100	100
3	E	182/205 (89%)	179 (98%)	3 (2%)	0	100	100
3	G	195/205 (95%)	193 (99%)	2 (1%)	0	100	100
4	F	237/246 (96%)	232 (98%)	4 (2%)	1 (0%)	30	49
4	H	238/246 (97%)	235 (99%)	3 (1%)	0	100	100
All	All	1548/1644 (94%)	1519 (98%)	28 (2%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	205	ARG

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	223/241 (92%)	218 (98%)	5 (2%)	45	73
1	C	216/241 (90%)	211 (98%)	5 (2%)	44	72
2	B	82/95 (86%)	79 (96%)	3 (4%)	30	57
2	D	78/95 (82%)	74 (95%)	4 (5%)	21	43
3	E	143/182 (79%)	139 (97%)	4 (3%)	38	66
3	G	168/182 (92%)	163 (97%)	5 (3%)	36	64
4	F	186/211 (88%)	182 (98%)	4 (2%)	45	73
4	H	194/211 (92%)	191 (98%)	3 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1290/1458 (88%)	1257 (97%)	33 (3%)	40 68

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	213	THR
1	A	215	MET
1	A	221	ILE
1	A	246	LEU
2	B	4	THR
2	B	20	SER
2	B	35	ILE
1	C	100	LEU
1	C	169	LEU
1	C	215	MET
1	C	217	ASN
1	C	244	ILE
2	D	4	THR
2	D	35	ILE
2	D	40	LEU
2	D	64	LEU
3	E	41	GLU
3	E	55	GLU
3	E	85	SER
3	E	131	VAL
4	F	31	SER
4	F	127	VAL
4	F	135	ILE
4	F	184	ASN
3	G	4	ILE
3	G	41	GLU
3	G	85	SER
3	G	122	ARG
3	G	131	VAL
4	H	110	ARG
4	H	127	VAL
4	H	184	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	111	GLN
1	A	137	HIS
1	A	153	GLN
1	A	203	HIS
1	A	268	GLN
2	B	13	HIS
2	B	17	ASN
2	B	31	HIS
1	C	71	GLN
1	C	85	ASN
1	C	93	GLN
1	C	134	ASN
1	C	137	HIS
1	C	147	GLN
1	C	153	GLN
2	D	13	HIS
2	D	17	ASN
3	E	19	GLN
3	E	21	ASN
3	E	79	GLN
4	F	17	GLN
4	F	203	ASN
3	G	19	GLN
3	G	21	ASN
3	G	79	GLN
3	G	112	GLN
3	G	120	GLN
3	G	176	ASN
3	G	188	ASN
4	H	17	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	2LJ	C	301	1	22,22,22	1.59	3 (13%)	24,29,29	1.18	1 (4%)
6	B3P	A	302	-	18,18,18	0.44	0	23,23,23	1.44	3 (13%)
5	2LJ	A	301	1	22,22,22	1.49	2 (9%)	24,29,29	1.31	3 (12%)
6	B3P	C	302	-	18,18,18	0.61	0	23,23,23	1.10	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	2LJ	C	301	1	-	1/18/19/19	0/1/1/1
6	B3P	A	302	-	-	0/28/28/28	-
5	2LJ	A	301	1	-	1/18/19/19	0/1/1/1
6	B3P	C	302	-	-	4/28/28/28	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	2LJ	C8A-N8	5.61	1.41	1.32
5	C	301	2LJ	C8A-N8	5.58	1.41	1.32
5	C	301	2LJ	C7-C6	4.05	1.53	1.49
5	A	301	2LJ	C1'-C2'	3.49	1.57	1.52
5	C	301	2LJ	C1'-C2'	2.23	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	302	B3P	C2-N2-C8	5.06	123.57	116.17
6	C	302	B3P	C3-N1-C4	3.87	121.83	116.17
5	C	301	2LJ	C6-N5-C4A	3.77	126.53	121.17
5	A	301	2LJ	C6-N5-C4A	3.39	125.98	121.17
6	A	302	B3P	C3-N1-C4	2.72	120.15	116.17
5	A	301	2LJ	C2'-C1'-N8	2.42	118.25	111.53
5	A	301	2LJ	C1'-N8-C8A	-2.20	122.04	126.69
6	A	302	B3P	C5-C4-N1	-2.01	103.03	109.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	302	B3P	O3-C11-C8-C9
6	C	302	B3P	O3-C11-C8-C10
6	C	302	B3P	O3-C11-C8-N2
6	C	302	B3P	C1-C2-N2-C8
5	A	301	2LJ	N8-C1'-C2'-C3'
5	C	301	2LJ	N8-C1'-C2'-C3'

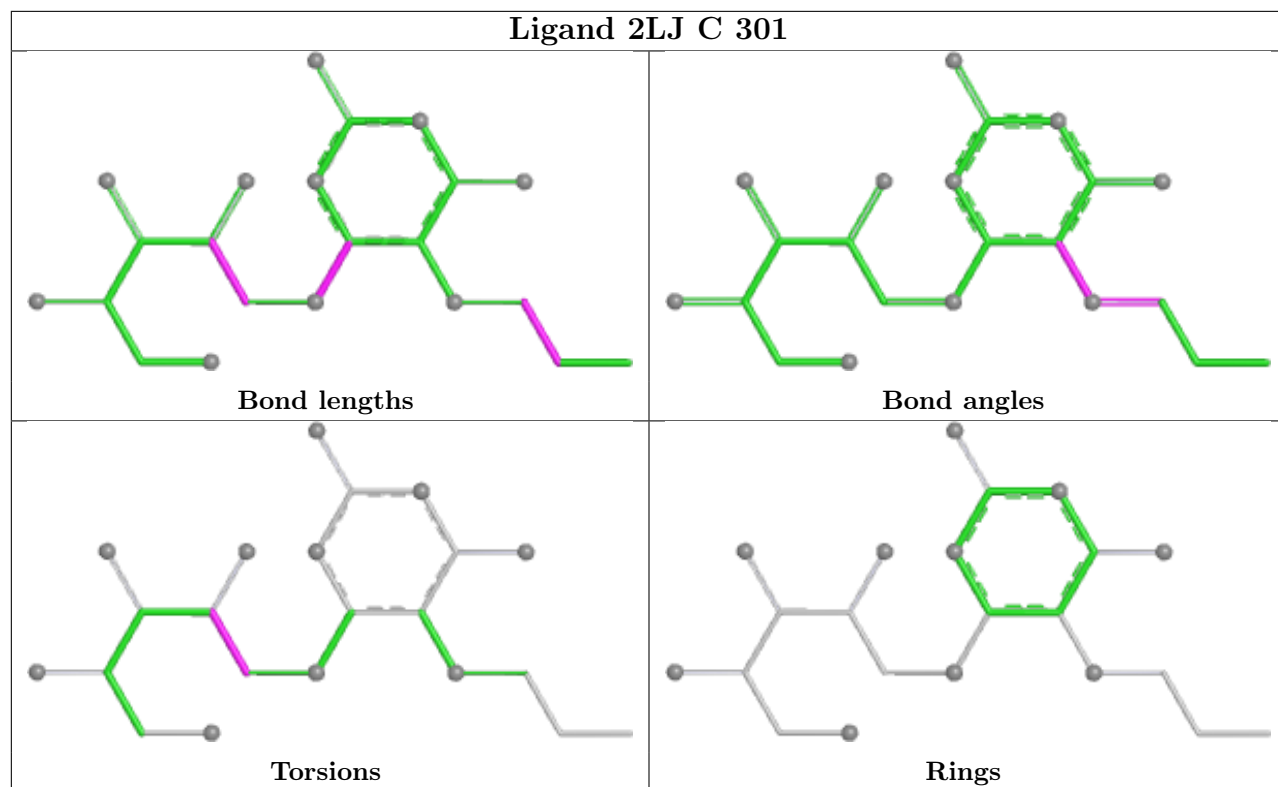
There are no ring outliers.

2 monomers are involved in 3 short contacts:

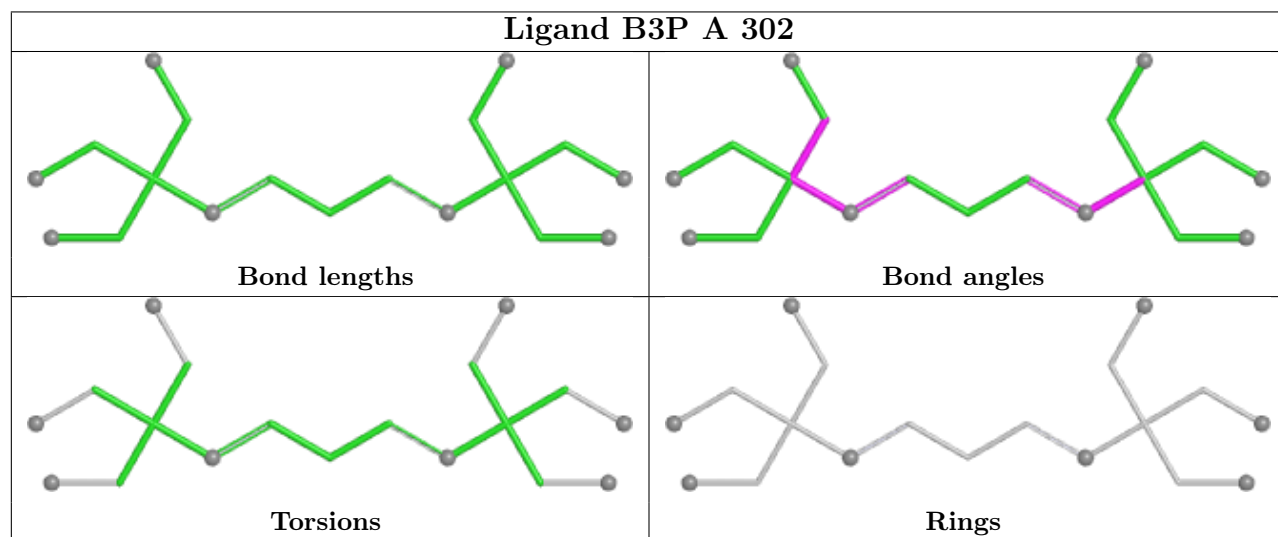
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	2LJ	2	0
6	C	302	B3P	1	0

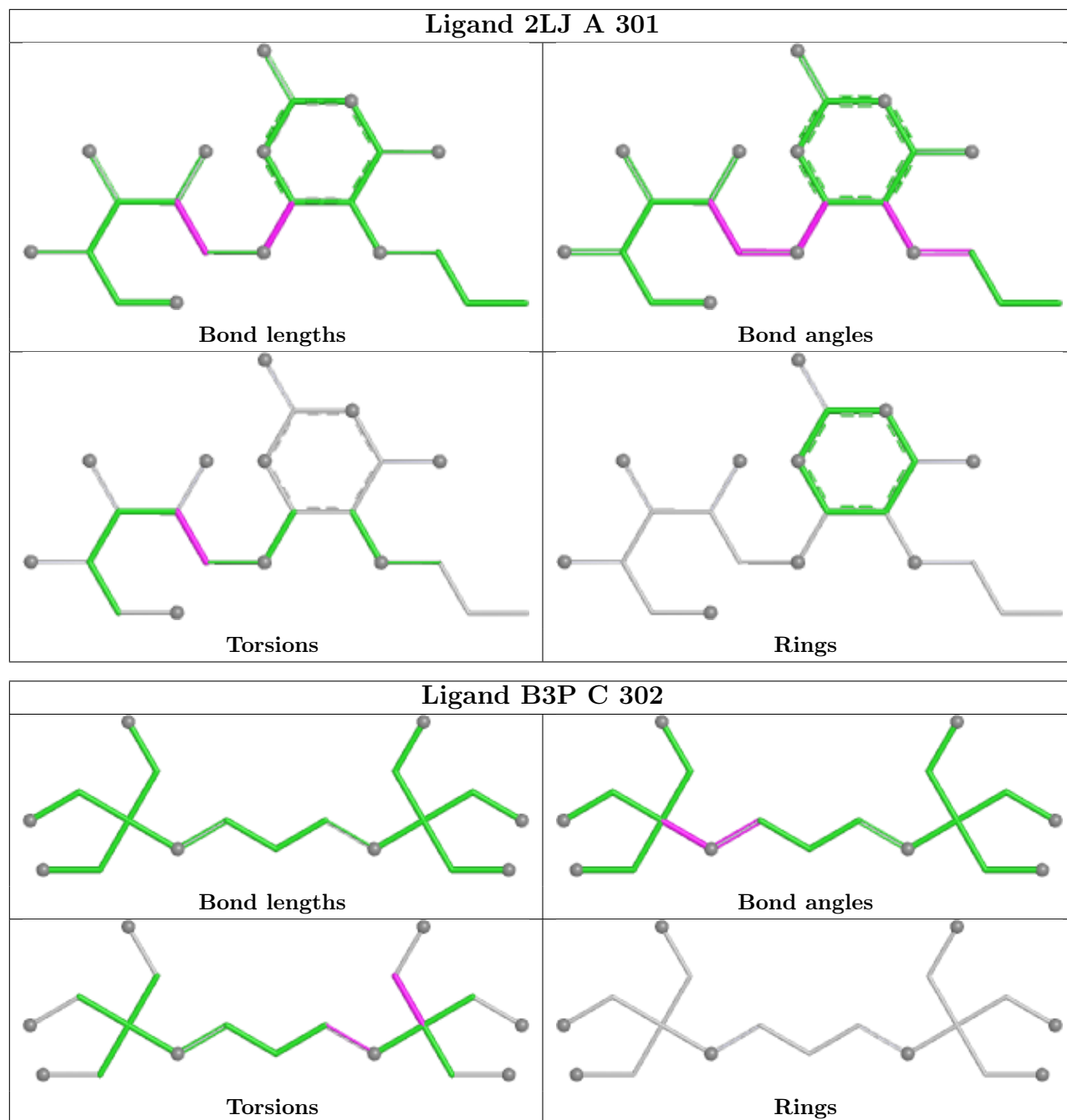
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 2LJ C 301



Ligand B3P A 302





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	264/271 (97%)	-0.48	6 (2%) 61 57	15, 27, 51, 71	0
1	C	256/271 (94%)	-0.37	5 (1%) 65 61	17, 30, 60, 79	0
2	B	96/100 (96%)	-0.42	0 100 100	18, 33, 54, 65	0
2	D	96/100 (96%)	0.12	1 (1%) 79 76	24, 49, 77, 91	0
3	E	188/205 (91%)	0.14	16 (8%) 16 14	17, 40, 77, 97	0
3	G	197/205 (96%)	-0.35	3 (1%) 72 68	18, 31, 59, 72	0
4	F	239/246 (97%)	-0.06	5 (2%) 63 59	20, 39, 69, 98	0
4	H	240/246 (97%)	-0.42	1 (0%) 88 86	18, 31, 49, 82	0
All	All	1576/1644 (95%)	-0.26	37 (2%) 61 57	15, 32, 68, 98	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	221	ILE	5.0
3	E	123	ASP	4.7
3	E	149	SER	3.5
3	E	188	ASN	3.5
1	A	222	VAL	3.3
4	F	241	GLY	3.2
4	F	222	GLU	3.1
3	E	163	SER	3.0
4	F	220	ASN	2.8
4	F	224	THR	2.7
3	E	176	ASN	2.7
3	E	182	CYS	2.7
1	C	246	LEU	2.7
3	E	191	ILE	2.6
3	G	176	ASN	2.5
3	E	112	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	142	ASN	2.4
1	A	221	ILE	2.4
4	F	226	ASP	2.4
3	E	190	ILE	2.3
3	E	150	ASP	2.3
3	E	194	ASP	2.3
4	H	242	ARG	2.3
1	C	219	GLU	2.3
3	E	147	LYS	2.3
1	C	196	THR	2.3
3	G	179	ASP	2.2
1	A	218	GLY	2.2
3	E	189	SER	2.2
3	E	145	GLN	2.1
1	A	219	GLU	2.1
2	D	74	GLU	2.1
1	A	246	LEU	2.1
3	G	178	SER	2.1
1	A	17	HIS	2.1
3	E	144	SER	2.0
1	C	253	LEU	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($\text{\AA}^2$)	Q<0.9
6	B3P	A	302	19/19	0.90	0.10	25,37,46,47	0
6	B3P	C	302	19/19	0.93	0.09	22,30,34,41	0

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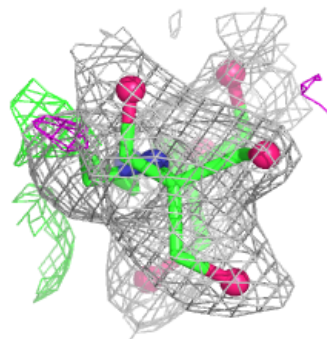
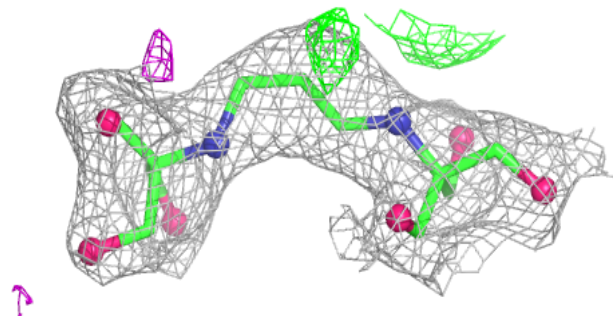
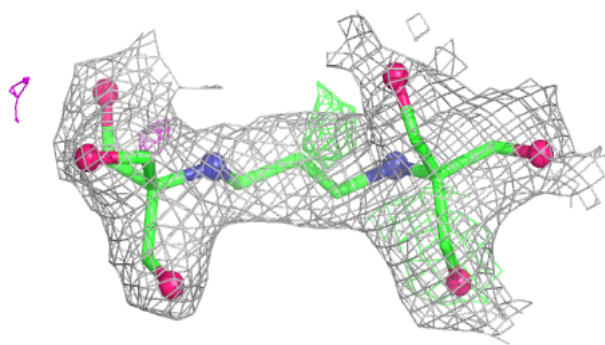
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	2LJ	A	301	22/22	0.97	0.06	14,18,21,23	0
5	2LJ	C	301	22/22	0.98	0.05	16,19,25,31	0

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.

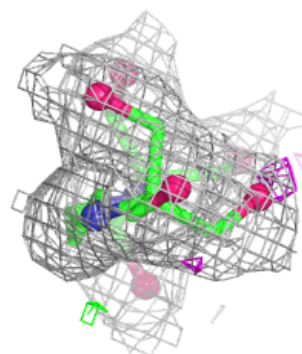
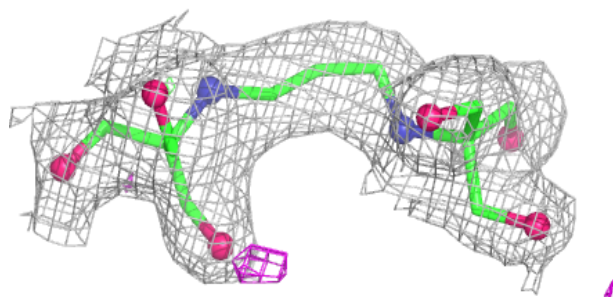
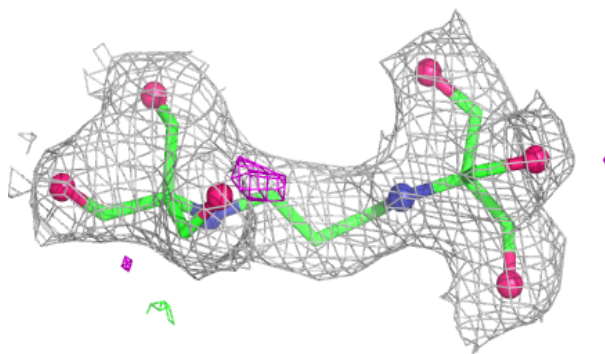
Electron density around B3P A 302:

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

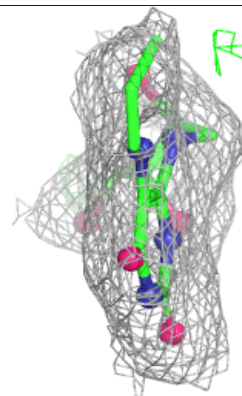
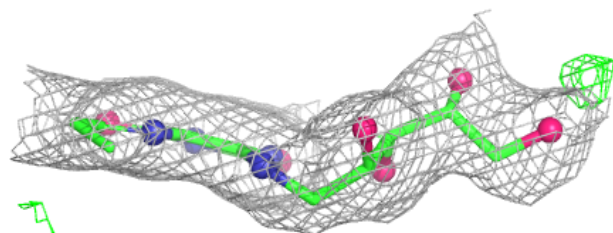
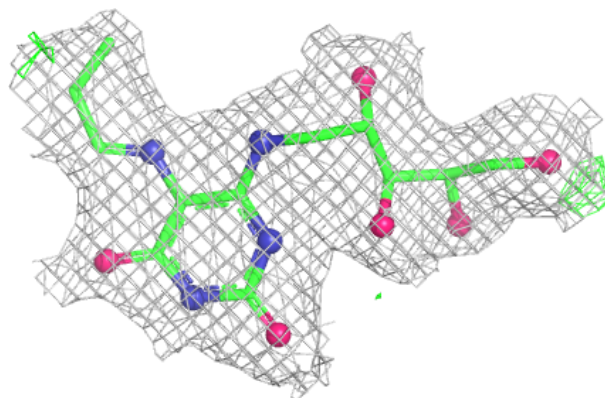


Electron density around B3P C 302:

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

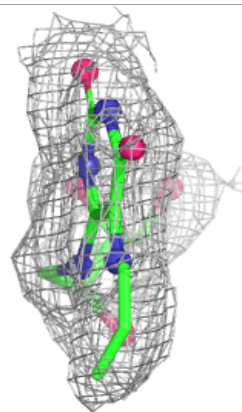
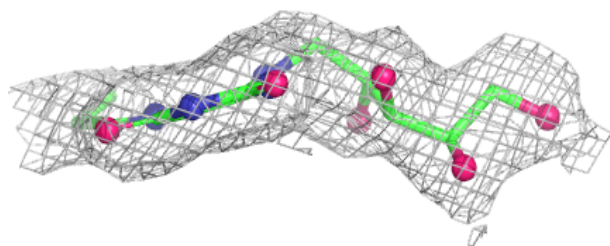
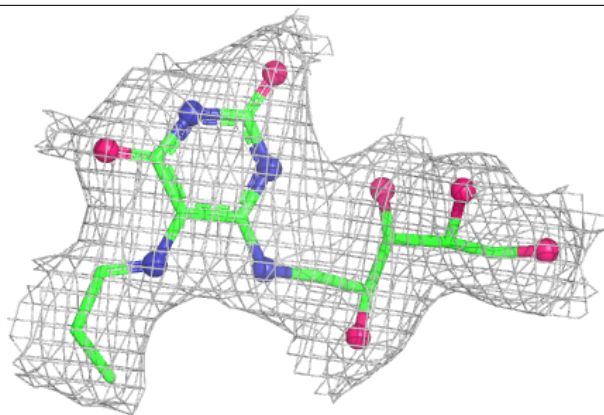
**Electron density around 2LJ A 301:**

$2mF_o-DF_c$ (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:

$2mF_o-DF_c$ (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.