



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:41 AM UTC

PDB ID : 4NQE / pdb_00004nqe
Title : Crystal structure of TCR-MR1 ternary complex bound to 5-(2-oxoethylidene amino)-6-D-ribitylaminouracil
Authors : Birkinshaw, R.W.; Rossjohn, J.
Deposited on : 2013-11-25
Resolution : 2.10 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

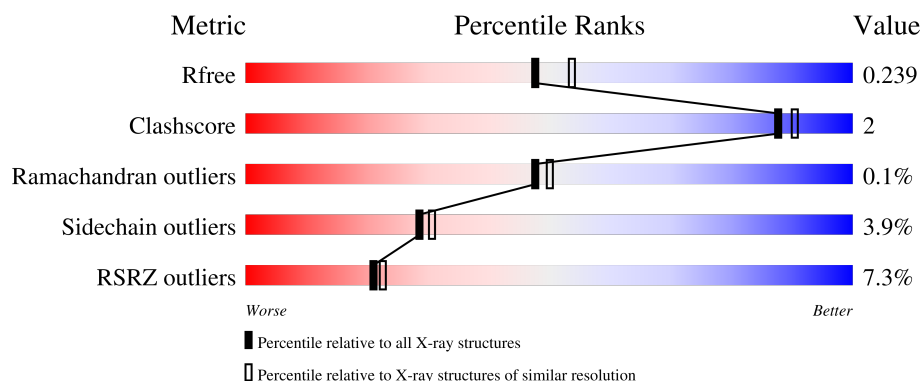
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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% 89% 8%
1	C	271	3% 83% 8% 8%
2	B	99	0% 94%
2	F	99	16% 91% 7%
3	D	203	3% 91% 7%

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Mol	Chain	Length	Quality of chain
3	G	203	23% 82% 10% 7%
4	E	245	2% 93% 6%
4	H	245	11% 84% 10% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13326 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
			2152	1380	373	388	11			
1	C	249	Total	C	N	O	S	0	1	0
			2044	1307	358	368	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q95460
A	261	SER	CYS	engineered mutation	UNP Q95460
C	0	MET	-	expression tag	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
			769	494	131	142	2			
2	F	97	Total	C	N	O	S	0	0	0
			766	492	130	142	2			

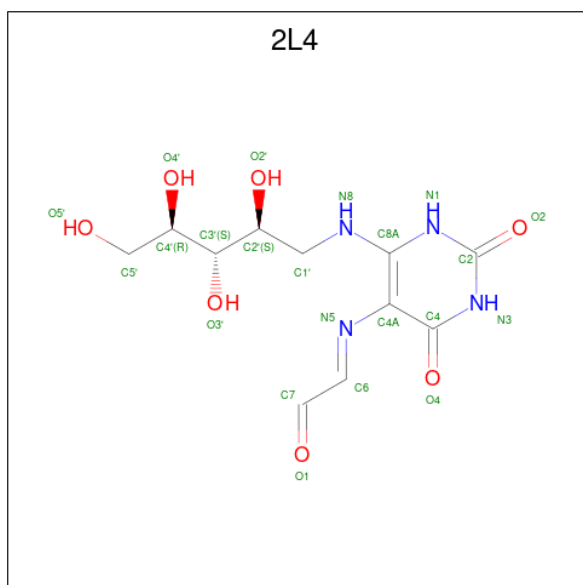
- Molecule 3 is a protein called TCR alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	200	Total	C	N	O	S	0	0	0
			1546	978	248	311	9			
3	G	189	Total	C	N	O	S	0	1	0
			1452	927	231	285	9			

- Molecule 4 is a protein called TCR beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	243	Total	C	N	O	S	0	2	0
			1913	1204	333	367	9			
4	H	231	Total	C	N	O	S	0	0	0
			1754	1109	298	338	9			

- Molecule 5 is 1-deoxy-1-({2,6-dioxo-5-[(E)-(2-oxoethylidene)amino]-1,2,3,6-tetrahydropyrimidin-4-yl}amino)-D-ribose (CCD ID: 2L4) (formula: C₁₁H₁₆N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	11	4	6		
5	C	1	Total	C	N	O	0	0
			21	11	4	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	159	Total	O	0	0
			159	159		
6	B	68	Total	O	0	0
			68	68		
6	C	162	Total	O	0	0
			162	162		
6	D	133	Total	O	0	0
			133	133		
6	E	197	Total	O	0	0
			197	197		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	40	Total	O	0	0
			40	40		
6	G	69	Total	O	0	0
			69	69		
6	H	60	Total	O	0	0
			60	60		

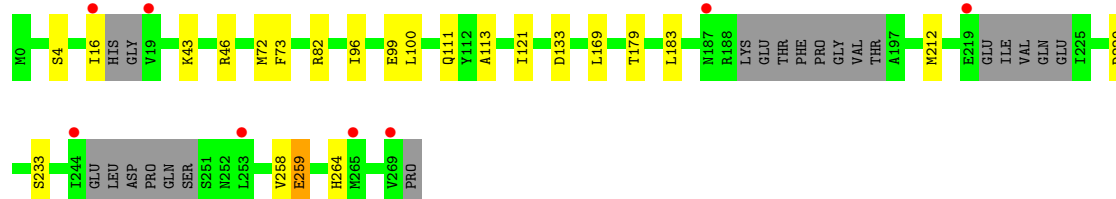
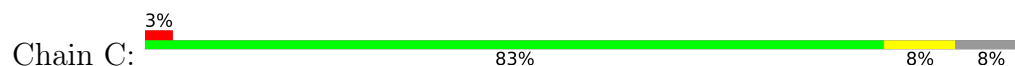
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

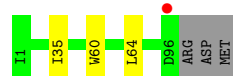
- Molecule 1: Major histocompatibility complex class I-related gene protein



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



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

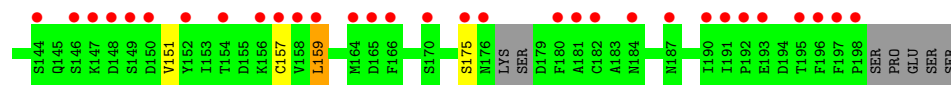
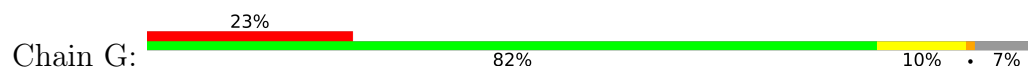


- Molecule 3: TCR alpha

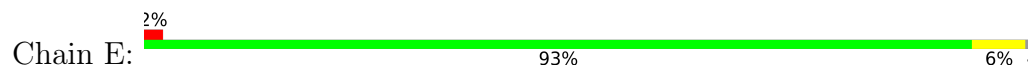




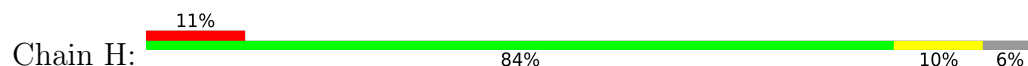
• Molecule 3: TCR alpha



• Molecule 4: TCR beta



• Molecule 4: TCR beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.11Å 70.60Å 143.86Å 90.00° 104.63° 90.00°	Depositor
Resolution (Å)	42.00 – 2.10 42.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (42.00-2.10) 98.4 (42.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.182 , 0.222 0.196 , 0.239	Depositor DCC
R_{free} test set	6147 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13326	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2L4

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	0.86	1/2218 (0.0%)	1.12	3/3017 (0.1%)
1	C	0.88	1/2106 (0.0%)	1.12	2/2859 (0.1%)
2	B	0.75	0/792	1.08	0/1080
2	F	0.84	0/789	1.11	1/1078 (0.1%)
3	D	0.86	0/1581	1.08	0/2145
3	G	0.87	0/1487	1.14	1/2018 (0.0%)
4	E	0.85	0/1971	1.09	2/2684 (0.1%)
4	H	0.79	0/1799	1.12	3/2456 (0.1%)
All	All	0.85	2/12743 (0.0%)	1.11	12/17337 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	ASP	CA-C	6.31	1.57	1.53
1	C	72	MET	SD-CE	5.80	1.94	1.79

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	92	ASP	CA-CB-CG	6.94	119.54	112.60
4	H	100	GLY	N-CA-C	6.34	120.34	112.73
1	C	133	ASP	CA-CB-CG	5.55	118.15	112.60
2	F	59	ASP	CA-CB-CG	5.40	118.00	112.60
4	H	98	GLY	CA-C-N	5.35	130.31	122.39
4	H	98	GLY	C-N-CA	5.35	130.31	122.39
1	A	14	ASP	CA-CB-CG	5.33	117.93	112.60
4	E	12	VAL	N-CA-CB	5.30	117.35	110.99
1	A	146	ASN	CA-CB-CG	5.30	117.90	112.60
1	A	229	ASP	CA-CB-CG	5.25	117.85	112.60
4	E	74	PHE	CA-CB-CG	5.09	118.89	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ASP	CA-CB-CG	5.01	117.61	112.60

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	2152	0	2028	10	0
1	C	2044	0	1926	10	0
2	B	769	0	715	1	0
2	F	766	0	700	3	0
3	D	1546	0	1456	3	0
3	G	1452	0	1360	12	0
4	E	1913	0	1799	8	0
4	H	1754	0	1621	8	0
5	A	21	0	15	1	0
5	C	21	0	15	2	0
6	A	159	0	0	2	0
6	B	68	0	0	0	0
6	C	162	0	0	1	0
6	D	133	0	0	0	0
6	E	197	0	0	1	0
6	F	40	0	0	0	0
6	G	69	0	0	0	0
6	H	60	0	0	0	0
All	All	13326	0	11635	49	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 (49) 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)
3:D:1:GLY:HA2	3:D:27:SER:H	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:GLY:N	3:G:27:SER:H	1.89	0.70
4:E:210:ARG:HH21	4:E:212:GLN:HE22	1.42	0.68
3:G:1:GLY:H2	3:G:27:SER:H	1.42	0.68
1:C:111:GLN:HG2	1:C:121:ILE:HG12	1.77	0.67
3:D:78:LEU:HG	3:D:107:ILE:HD12	1.79	0.64
1:C:259:GLU:HG3	1:C:264:HIS:CE1	2.34	0.62
6:C:441:HOH:O	4:E:97:THR:HG21	1.98	0.62
1:A:61:ARG:HG2	3:G:94:ASN:HB3	1.84	0.60
5:A:301:2L4:O4	5:A:301:2L4:H1	2.03	0.58
1:A:175:THR:HG23	6:A:491:HOH:O	2.04	0.57
4:E:210:ARG:HH21	4:E:212:GLN:NE2	2.02	0.56
4:H:155:HIS:HB3	4:H:216:TYR:HB2	1.89	0.54
4:E:128:VAL:HG23	4:E:238:ALA:HB3	1.90	0.53
1:C:113:ALA:HB2	2:F:60:TRP:CE2	2.43	0.53
1:A:151:LEU:HD22	3:G:51:LEU:HD12	1.89	0.53
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.89	0.53
1:C:96:ILE:HD13	5:C:301:2L4:H16	1.91	0.53
1:C:4:SER:HB3	1:C:99:GLU:HG2	1.92	0.51
4:E:200:THR:HG23	6:E:335:HOH:O	2.11	0.50
4:H:30:ASN:O	4:H:51:SER:HA	2.11	0.49
3:G:159:LEU:HB3	4:H:172:CYS:HB2	1.94	0.49
3:G:121:LEU:HB3	4:H:129:PHE:HB3	1.96	0.48
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.49	0.48
1:C:212:MET:HG2	1:C:258:VAL:HG22	1.95	0.48
4:E:210:ARG:HE	4:E:212:GLN:HE21	1.62	0.48
1:A:186:VAL:HG11	1:A:269:VAL:HG22	1.95	0.47
3:D:4:ILE:HD12	3:D:98:ILE:O	2.14	0.47
3:G:28:GLY:HA3	3:G:93[A]:SER:HB3	1.97	0.46
1:A:215:MET:HG3	1:A:257:HIS:CD2	2.51	0.46
1:C:43:LYS:HE3	5:C:301:2L4:H1	1.78	0.45
1:C:46:ARG:HA	1:C:46:ARG:HD3	1.68	0.45
1:C:259:GLU:HG3	1:C:264:HIS:ND1	2.33	0.44
2:F:24:ASN:HB3	2:F:65:LEU:HD11	2.00	0.44
1:C:233:SER:HB3	2:F:12:ARG:HG3	1.99	0.44
1:A:46:ARG:HD2	6:A:473:HOH:O	2.17	0.43
3:G:151:VAL:HA	3:G:175:SER:HB2	2.01	0.43
1:A:28:VAL:HG23	1:A:33:ILE:HD13	2.00	0.43
4:E:8:PRO:HD2	4:E:21:LEU:HD22	2.01	0.42
4:H:46:ILE:HG22	4:H:47:TYR:HD2	1.84	0.42
4:H:181:GLN:O	4:H:187:SER:HB2	2.20	0.42
3:G:89:ALA:HB1	3:G:97:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:78:LEU:HG	3:G:107:ILE:HD12	2.01	0.41
1:A:0:MET:HE3	1:A:177:GLN:CD	2.45	0.41
3:G:13:THR:O	3:G:16:ALA:HB3	2.20	0.41
4:H:70:ASN:HD22	4:H:72:ARG:H	1.69	0.41
4:H:148:ALA:HB2	4:H:213:VAL:HG21	2.03	0.41
3:G:18:VAL:HG12	3:G:78:LEU:HD11	2.03	0.40
4:E:2:ALA:HB3	4:E:26:ASP:OD2	2.20	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	260/271 (96%)	252 (97%)	8 (3%)	0	100	100
1	C	240/271 (89%)	237 (99%)	3 (1%)	0	100	100
2	B	94/99 (95%)	94 (100%)	0	0	100	100
2	F	95/99 (96%)	93 (98%)	2 (2%)	0	100	100
3	D	198/203 (98%)	195 (98%)	3 (2%)	0	100	100
3	G	184/203 (91%)	176 (96%)	7 (4%)	1 (0%)	24	22
4	E	243/245 (99%)	238 (98%)	5 (2%)	0	100	100
4	H	227/245 (93%)	224 (99%)	3 (1%)	0	100	100
All	All	1541/1636 (94%)	1509 (98%)	31 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	2	GLN

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	225/241 (93%)	218 (97%)	7 (3%)	35	39
1	C	215/241 (89%)	207 (96%)	8 (4%)	30	33
2	B	83/94 (88%)	81 (98%)	2 (2%)	43	49
2	F	81/94 (86%)	79 (98%)	2 (2%)	42	48
3	D	171/180 (95%)	161 (94%)	10 (6%)	18	16
3	G	156/180 (87%)	149 (96%)	7 (4%)	24	25
4	E	206/211 (98%)	202 (98%)	4 (2%)	50	58
4	H	184/211 (87%)	173 (94%)	11 (6%)	17	15
All	All	1321/1452 (91%)	1270 (96%)	51 (4%)	28	31

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	PHE
1	A	100	LEU
1	A	179	THR
1	A	215	MET
1	A	221	ILE
1	A	222	VAL
1	A	259	GLU
2	B	35	ILE
2	B	64	LEU
1	C	16	ILE
1	C	73	PHE
1	C	82	ARG
1	C	100	LEU
1	C	169	LEU
1	C	179	THR
1	C	183	LEU
1	C	259	GLU
3	D	41	GLU
3	D	55	GLU

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Mol	Chain	Res	Type
3	D	75	LEU
3	D	78	LEU
3	D	81	LYS
3	D	93	SER
3	D	121	LEU
3	D	122	ARG
3	D	125	LYS
3	D	179	ASP
4	E	9	LYS
4	E	79	GLU
4	E	97	THR
4	E	185	ASN
2	F	35	ILE
2	F	88	SER
3	G	27	SER
3	G	75	LEU
3	G	78	LEU
3	G	85	SER
3	G	131	VAL
3	G	157	CYS
3	G	159	LEU
4	H	18	SER
4	H	19	MET
4	H	21	LEU
4	H	70	ASN
4	H	78	LEU
4	H	97	THR
4	H	111	ARG
4	H	112	LEU
4	H	128	VAL
4	H	184	LEU
4	H	226	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	83	HIS
1	A	148	HIS
1	A	153	GLN
1	A	177	GLN
1	A	187	ASN

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Mol	Chain	Res	Type
1	A	239	GLN
1	A	268	GLN
2	B	17	ASN
2	B	31	HIS
2	B	51	HIS
1	C	64	GLN
1	C	93	GLN
3	D	19	GLN
3	D	21	ASN
3	D	37	GLN
3	D	140	GLN
4	E	22	GLN
4	E	37	GLN
4	E	212	GLN
4	E	214	GLN
2	F	8	GLN
3	G	19	GLN
3	G	21	ASN
3	G	37	GLN
3	G	145	GLN
4	H	37	GLN
4	H	65	ASN
4	H	70	ASN
4	H	120	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	2L4	C	301	1	20,21,22	1.38	3 (15%)	23,28,29	1.61	6 (26%)
5	2L4	A	301	1	20,21,22	1.09	1 (5%)	23,28,29	1.78	6 (26%)

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	2L4	C	301	1	-	2/17/18/19	0/1/1/1
5	2L4	A	301	1	-	2/17/18/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	301	2L4	C4A-C8A	3.34	1.48	1.43
5	A	301	2L4	C4A-C8A	2.21	1.46	1.43
5	C	301	2L4	C2-N1	-2.18	1.33	1.37
5	C	301	2L4	C4A-N5	2.15	1.41	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301	2L4	N3-C2-N1	4.21	122.36	115.74
5	A	301	2L4	C4-N3-C2	-3.66	121.33	126.37
5	C	301	2L4	N3-C2-N1	3.45	121.16	115.74
5	A	301	2L4	N1-C8A-N8	2.95	122.96	118.66
5	C	301	2L4	C6-N5-C4A	2.77	125.11	121.17
5	C	301	2L4	C1'-N8-C8A	-2.54	121.32	126.69
5	A	301	2L4	C4A-C4-N3	2.35	119.23	113.25
5	A	301	2L4	O4-C4-C4A	-2.34	120.35	126.53
5	C	301	2L4	C4-N3-C2	-2.31	123.18	126.37
5	C	301	2L4	C4A-C4-N3	2.16	118.76	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301	2L4	O2-C2-N1	-2.13	118.08	121.86
5	C	301	2L4	O2-C2-N1	-2.00	118.30	121.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	2L4	N1-C8A-N8-C1'
5	C	301	2L4	N1-C8A-N8-C1'
5	C	301	2L4	N8-C1'-C2'-C3'
5	A	301	2L4	N8-C1'-C2'-C3'

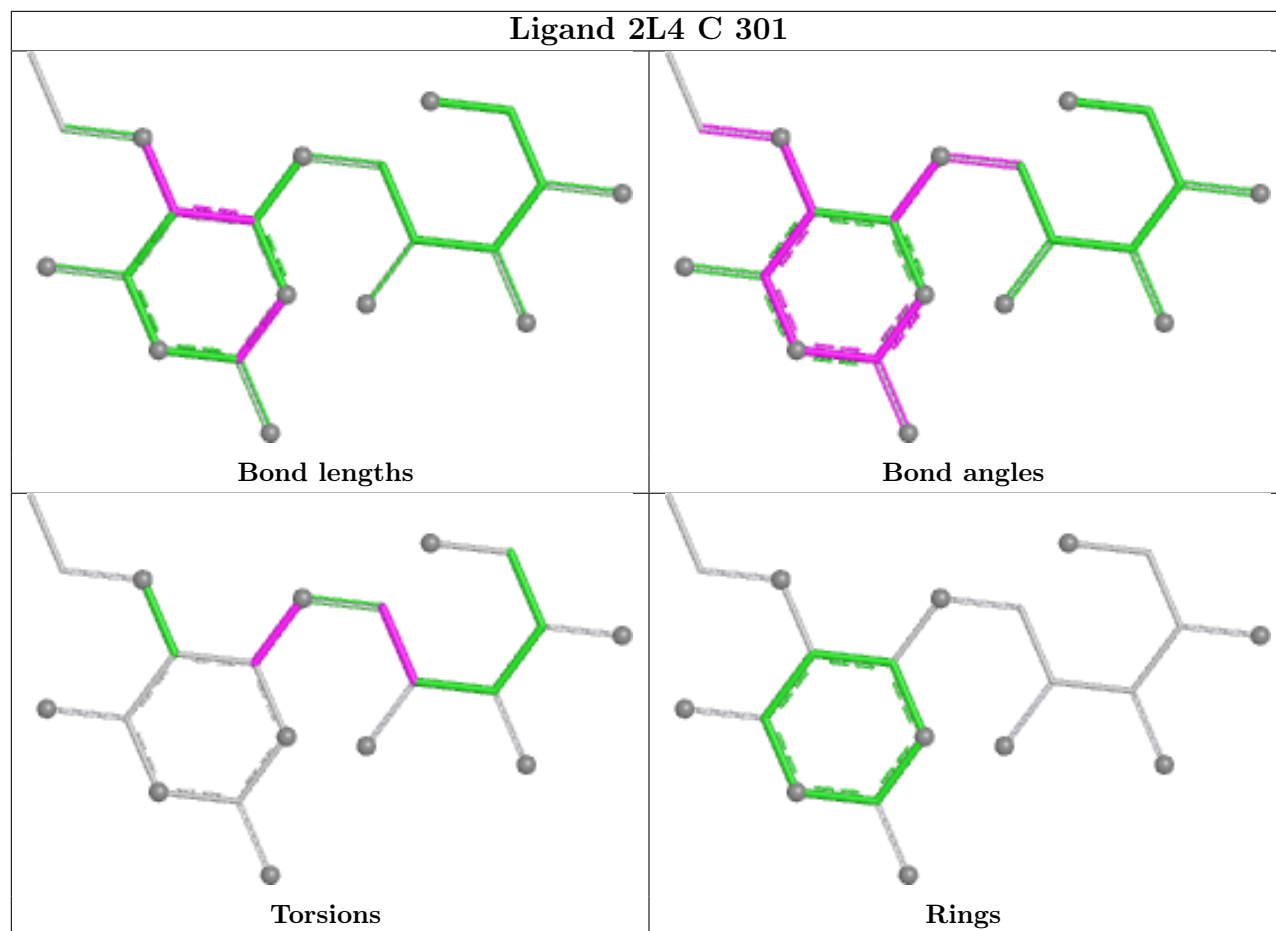
There are no ring outliers.

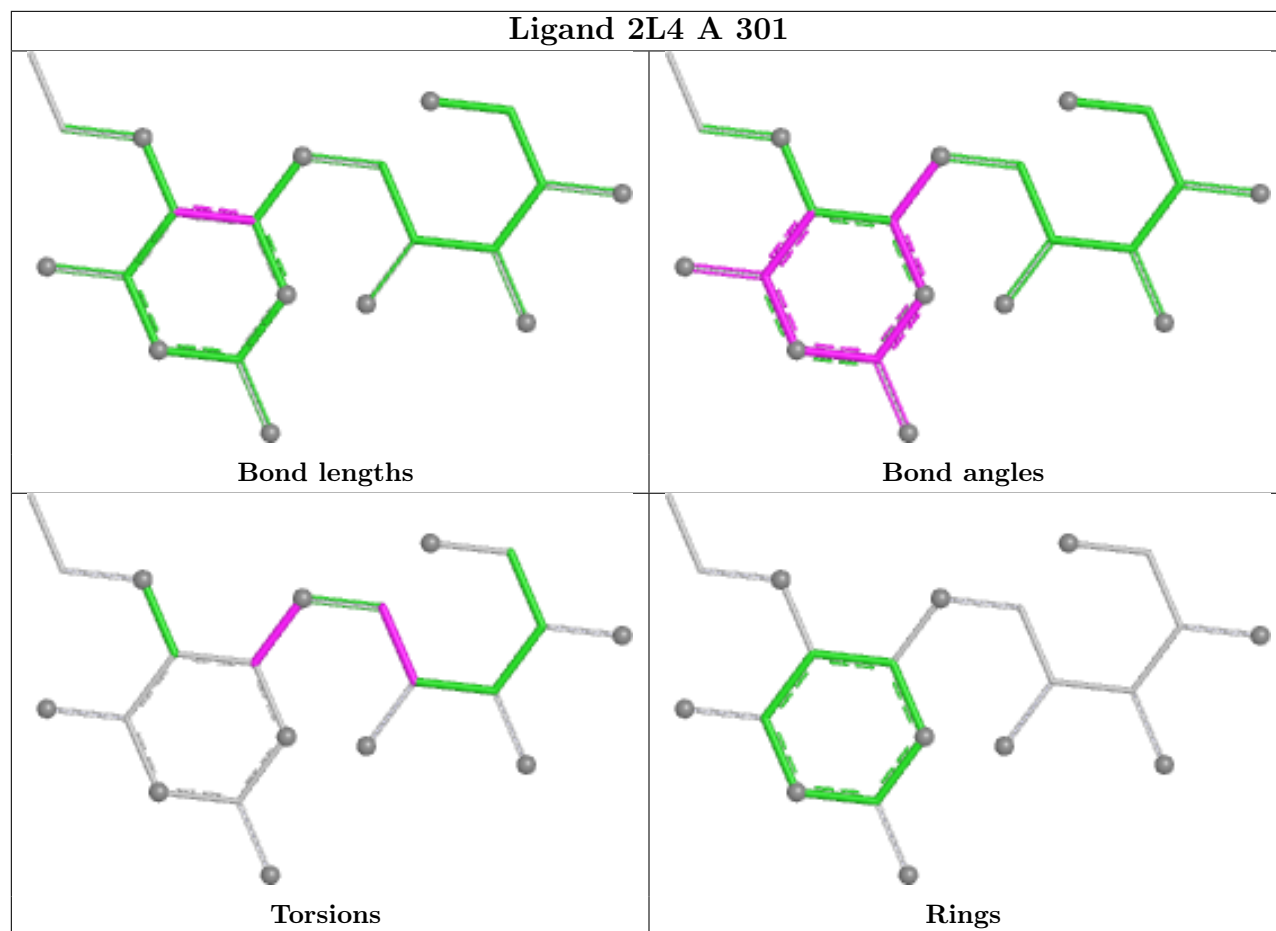
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	2L4	2	0
5	A	301	2L4	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 2L4 C 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/271 (97%)	0.00	6 (2%) 61 64	20, 31, 55, 75	0
1	C	249/271 (91%)	0.11	8 (3%) 50 53	16, 32, 58, 73	1 (0%)
2	B	96/99 (96%)	0.14	1 (1%) 79 81	19, 37, 60, 64	0
2	F	97/99 (97%)	1.00	16 (16%) 4 4	25, 51, 68, 76	0
3	D	200/203 (98%)	-0.14	7 (3%) 47 49	16, 27, 52, 67	0
3	G	189/203 (93%)	0.97	46 (24%) 2 2	21, 47, 88, 96	1 (0%)
4	E	243/245 (99%)	-0.26	5 (2%) 63 66	16, 26, 47, 80	3 (1%)
4	H	231/245 (94%)	0.84	26 (11%) 10 10	26, 47, 78, 89	0
All	All	1569/1636 (95%)	0.27	115 (7%) 21 22	16, 34, 71, 96	5 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	150	ASP	5.0
3	G	176	ASN	5.0
1	A	16	ILE	4.8
3	D	1	GLY	4.8
1	C	16	ILE	4.7
1	A	221	ILE	4.4
3	G	190	ILE	4.1
4	E	244	ALA	4.1
4	E	184	LEU	4.1
3	G	1	GLY	4.0
3	G	148	ASP	3.9
1	C	253	LEU	3.9
3	G	182	CYS	3.8
4	E	2	ALA	3.7
4	H	172	CYS	3.7
1	A	246	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
3	G	184	ASN	3.7
3	G	119	TYR	3.7
3	G	117	ALA	3.6
2	F	77	GLU	3.5
2	B	96	ASP	3.5
2	F	97	ARG	3.5
3	G	122	ARG	3.5
3	G	132	CYS	3.3
3	G	196	PHE	3.3
4	H	203	GLN	3.3
3	D	200	PRO	3.3
3	G	159	LEU	3.3
2	F	90	PRO	3.2
3	G	187	ASN	3.2
2	F	79	ALA	3.1
3	G	180	PHE	3.0
3	G	197	PHE	3.0
3	G	192	PRO	3.0
4	H	201	PHE	3.0
4	H	202	TRP	2.8
2	F	49	VAL	2.8
3	G	112	GLN	2.8
3	G	198	PRO	2.7
3	G	193	GLU	2.7
1	A	269	VAL	2.7
4	H	161	TRP	2.7
3	G	147	LYS	2.6
3	G	111	ILE	2.6
3	G	166	PHE	2.6
2	F	48	LYS	2.6
3	G	138	ASP	2.6
2	F	46	ILE	2.6
3	D	112	GLN	2.6
2	F	95	TRP	2.6
4	H	200	THR	2.6
2	F	72	PRO	2.6
4	E	243	ARG	2.5
3	D	163	SER	2.5
3	G	149	SER	2.5
3	G	195	THR	2.5
4	H	167	VAL	2.5
3	D	2	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	G	175	SER	2.5
3	G	114	PRO	2.5
4	H	144	LEU	2.5
3	G	118	VAL	2.4
4	H	227	ASP	2.4
4	H	221	ASN	2.4
4	H	162	VAL	2.4
1	A	17	HIS	2.4
2	F	1	ILE	2.4
3	G	191	ILE	2.4
3	G	157	CYS	2.4
2	F	78	TYR	2.3
2	F	74	GLU	2.3
4	H	226	GLN	2.3
3	G	152	TYR	2.3
1	C	219	GLU	2.3
4	H	116	GLU	2.3
4	H	171	VAL	2.3
4	H	220	GLU	2.3
4	H	134	ALA	2.3
3	G	165	ASP	2.3
2	F	39	LEU	2.3
4	H	224	TRP	2.3
1	C	269	VAL	2.2
4	H	229	ALA	2.2
3	D	179	ASP	2.2
2	F	40	LEU	2.2
3	G	170	SER	2.2
3	G	137	PHE	2.2
3	G	130	SER	2.2
4	H	169	SER	2.2
3	G	156	LYS	2.2
1	A	0	MET	2.2
4	H	225	THR	2.2
3	G	158	VAL	2.1
4	H	133	GLU	2.1
4	H	83	PRO	2.1
3	G	181	ALA	2.1
3	G	144	SER	2.1
1	C	265	MET	2.1
3	G	141	THR	2.1
3	G	4	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	E	183	ALA	2.1
1	C	244	ILE	2.1
4	H	199	ALA	2.1
3	G	164	MET	2.0
4	H	211	CYS	2.0
3	G	154	THR	2.0
4	H	139	THR	2.0
1	C	19	VAL	2.0
3	D	146	SER	2.0
3	G	146	SER	2.0
1	C	187	ASN	2.0
3	G	25	GLN	2.0
4	H	168	HIS	2.0
2	F	73	THR	2.0
2	F	18	GLY	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](#)

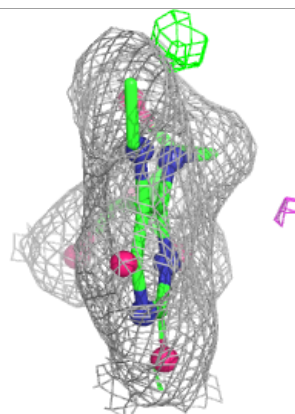
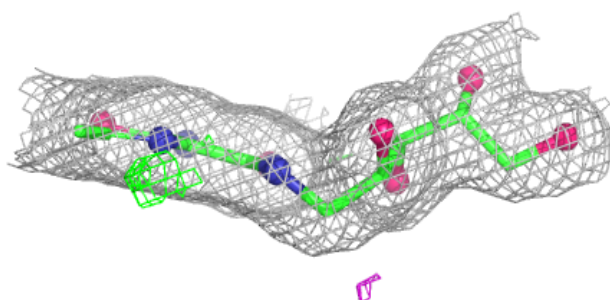
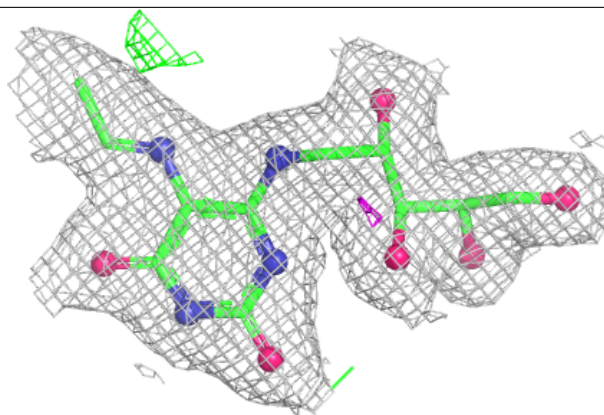
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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
5	2L4	A	301	21/22	0.97	0.05	19,23,29,30	0
5	2L4	C	301	21/22	0.97	0.05	17,22,28,30	0

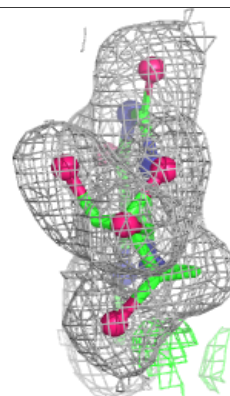
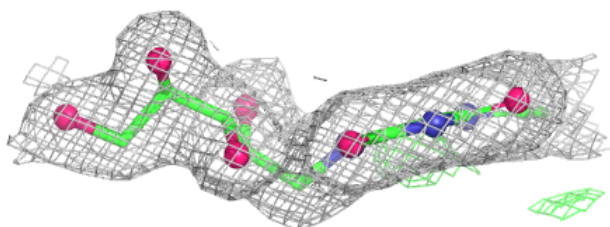
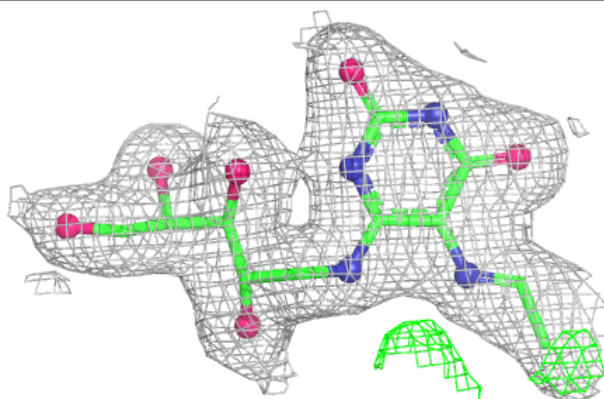
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2L4 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 2L4 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.