



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:15 AM UTC

PDB ID : 6EA8 / pdb_00006ea8
Title : Structure of VACV poxin in pre-reactive state with nonhydrolyzable 2'3' cGAMP
Authors : Eaglesham, J.B.; Kranzusch, P.J.
Deposited on : 2018-08-02
Resolution : 2.60 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

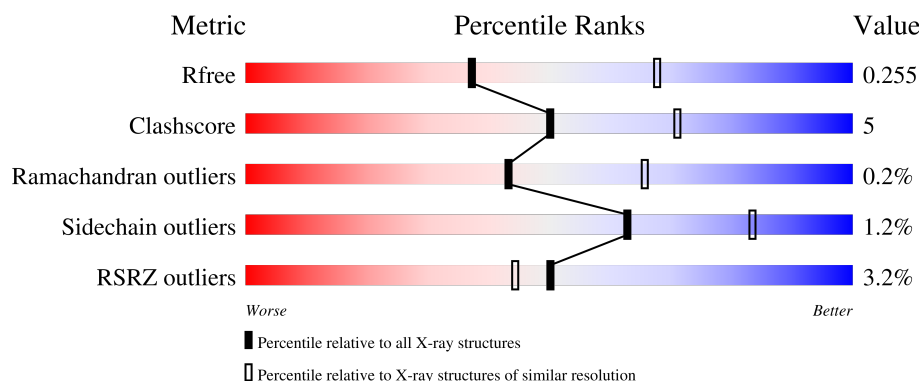
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	220	0.2% 77% 11% 11%
1	B	220	2% 80% 8% 11%
1	C	220	0.2% 80% 9% 11%
1	D	220	2% 79% 10% 11%
1	E	220	0.2% 77% 11% 11%

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Mol	Chain	Length	Quality of chain
1	F	220	2%74%14%12%
1	G	220	4%77%11%12%
1	H	220	4%74%14%11%
1	I	220	5%67%15%18%
1	J	220	6%70%12%18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15611 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 Protein B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1552	994	261	285	12			
1	B	195	Total	C	N	O	S	0	0	0
			1552	994	261	285	12			
1	C	195	Total	C	N	O	S	0	0	0
			1552	994	261	285	12			
1	D	195	Total	C	N	O	S	0	0	0
			1552	994	261	285	12			
1	E	195	Total	C	N	O	S	0	0	0
			1552	994	261	285	12			
1	F	194	Total	C	N	O	S	0	0	0
			1546	991	260	283	12			
1	G	194	Total	C	N	O	S	0	0	0
			1546	991	260	283	12			
1	H	195	Total	C	N	O	S	0	0	0
			1552	994	261	285	12			
1	I	181	Total	C	N	O	S	0	0	0
			1460	935	247	267	11			
1	J	180	Total	C	N	O	S	0	0	0
			1455	932	246	266	11			

There are 10 discrepancies between the modelled and reference sequences:

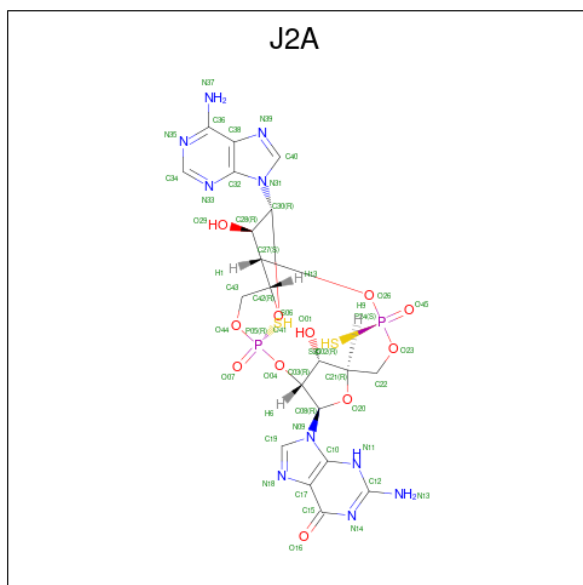
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q01225
B	0	SER	-	expression tag	UNP Q01225
D	0	SER	-	expression tag	UNP Q01225
E	0	SER	-	expression tag	UNP Q01225
F	0	SER	-	expression tag	UNP Q01225
G	0	SER	-	expression tag	UNP Q01225
H	0	SER	-	expression tag	UNP Q01225
J	0	SER	-	expression tag	UNP Q01225
C	0	SER	-	expression tag	UNP Q01225

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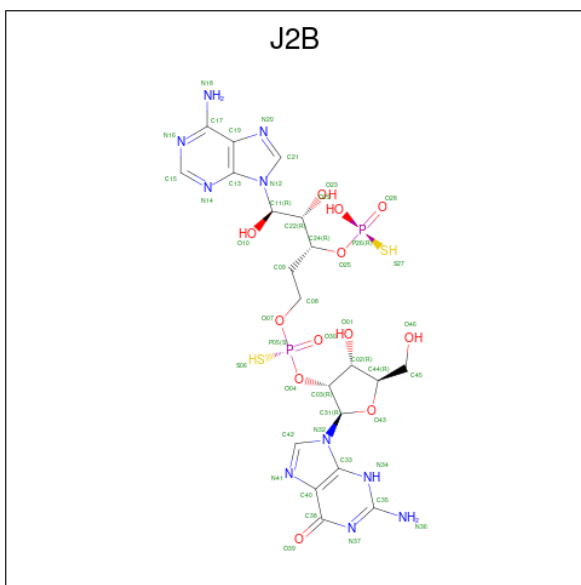
Chain	Residue	Modelled	Actual	Comment	Reference
I	0	SER	-	expression tag	UNP Q01225

- Molecule 2 is (2S,5R,7R,8R,10R,12aR,14R,15R,15aS,16R)-7-(2-amino-6-oxo-3,6-dihydro-9H-purin-9-yl)-14-(6-amino-9H-purin-9-yl)-15,16-dihydroxy-2,10-disulfanyloctahydro-2H,10H,12H-5,8-methano-2lambda 5 ,10lambda 5 -furo[3,2-l][1,3,6,9,11,2,10]pentaoadiphosphacyclotetradecine-2,10-dione (CCD ID: J2A) (formula: C₂₀H₂₄N₁₀O₁₁P₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			45	20	10	11	2	2		
2	F	1	Total	C	N	O	P	S	0	0
			45	20	10	11	2	2		

- Molecule 3 is O-[(1R,2R,3R)-5-{[(S)-{[(2R,3R,4R,5R)-2-(2-amino-6-oxo-3,6-dihydro-9H-purin-9-yl)-4-hydroxy-5-(hydroxymethyl)tetrahydro furan-3-yl]oxy}(sulfanyl)phosphoryl]oxy}-1-(6-amino-9H-purin-9-yl)-1,2-dihydroxypentan-3-yl] dihydrogen (R)-phosphorothioate (CCD ID: J2B) (formula: C₂₀H₂₈N₁₀O₁₂P₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	H	1	Total 46	C 20	N 10	O 12	P 2	S 2	0	0

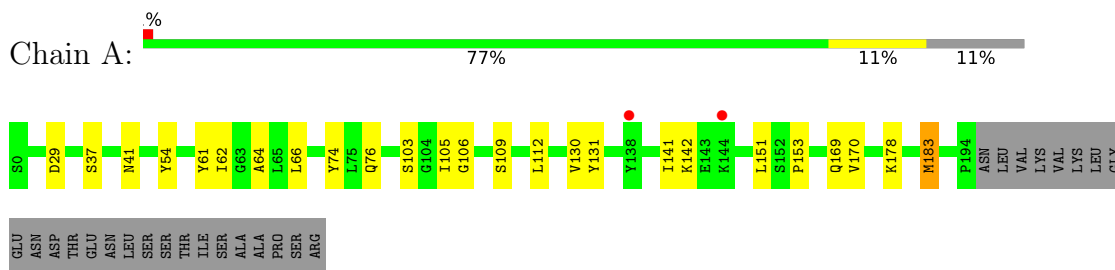
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	22	Total O 22 22	0	0
4	B	28	Total O 28 28	0	0
4	C	46	Total O 46 46	0	0
4	D	25	Total O 25 25	0	0
4	E	20	Total O 20 20	0	0
4	F	3	Total O 3 3	0	0
4	G	9	Total O 9 9	0	0
4	H	1	Total O 1 1	0	0
4	J	2	Total O 2 2	0	0

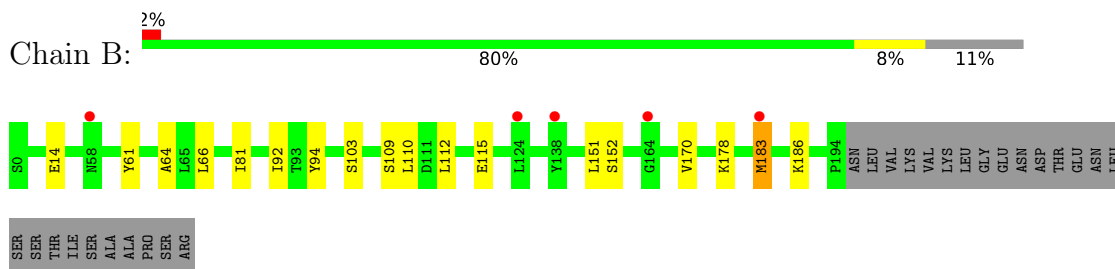
3 Residue-property plots [i](#)

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.

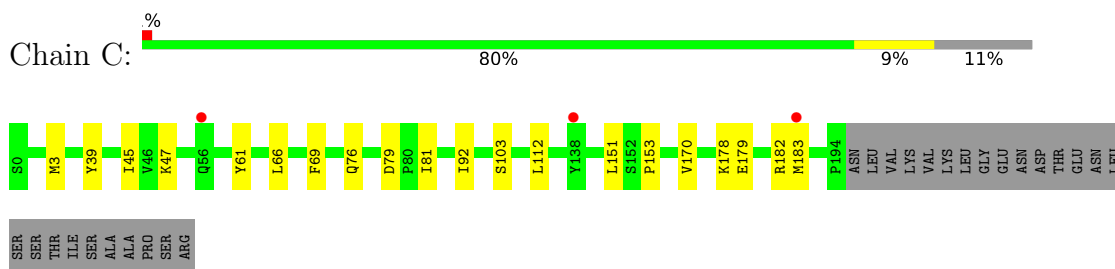
- Molecule 1: Protein B2



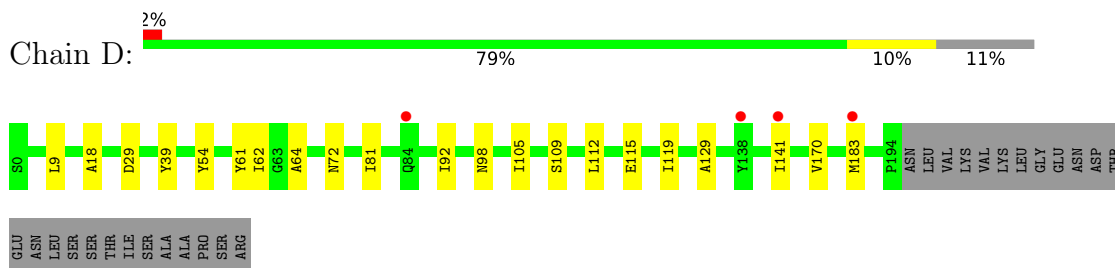
- Molecule 1: Protein B2



- Molecule 1: Protein B2

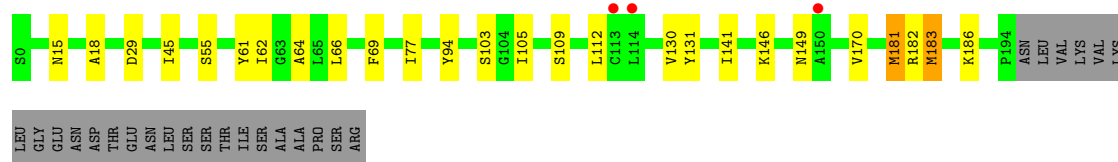


- Molecule 1: Protein B2



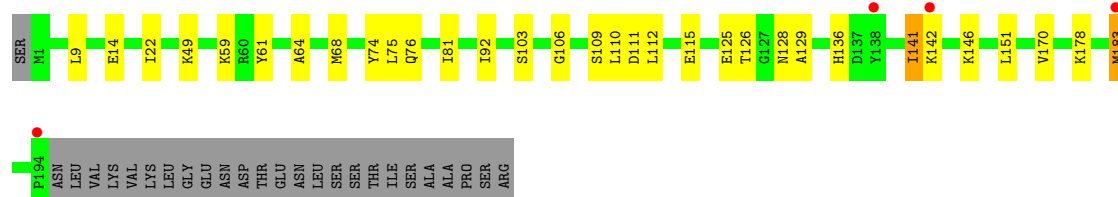
● Molecule 1: Protein B2

Chain E: 



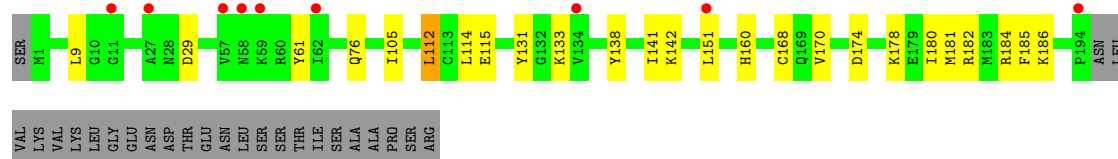
● Molecule 1: Protein B2

Chain F: 



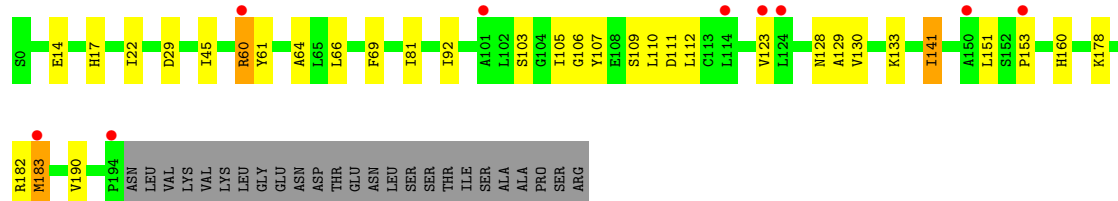
● Molecule 1: Protein B2

Chain G: 



● Molecule 1: Protein B2

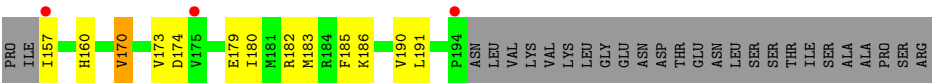
Chain H: 



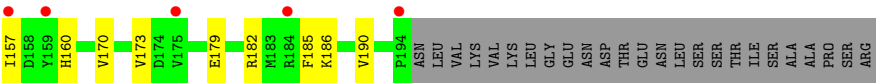
● Molecule 1: Protein B2

Chain I: 





● Molecule 1: Protein B2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.43Å 92.33Å 257.09Å 90.00° 93.66° 90.00°	Depositor
Resolution (Å)	49.48 – 2.60 49.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.48-2.60) 98.7 (49.48-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.218 , 0.252 0.222 , 0.255	Depositor DCC
R_{free} test set	1981 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15611	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5652e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: J2B, J2A

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	0.12	0/1592	0.33	0/2156
1	B	0.12	0/1592	0.33	0/2156
1	C	0.15	0/1592	0.35	0/2156
1	D	0.12	0/1592	0.31	0/2156
1	E	0.11	0/1592	0.31	0/2156
1	F	0.11	0/1586	0.31	0/2148
1	G	0.10	0/1586	0.30	0/2148
1	H	0.11	0/1592	0.28	0/2156
1	I	0.09	0/1496	0.28	0/2021
1	J	0.08	0/1491	0.27	0/2014
All	All	0.11	0/15711	0.31	0/21267

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

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	1552	0	1516	17	0
1	B	1552	0	1516	12	0
1	C	1552	0	1516	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1552	0	1516	14	0
1	E	1552	0	1516	18	0
1	F	1546	0	1511	21	0
1	G	1546	0	1511	19	0
1	H	1552	0	1516	26	0
1	I	1460	0	1417	22	0
1	J	1455	0	1412	21	0
2	A	45	0	0	2	0
2	F	45	0	0	2	0
3	H	46	0	0	9	0
4	A	22	0	0	2	0
4	B	28	0	0	2	0
4	C	46	0	0	2	0
4	D	25	0	0	1	0
4	E	20	0	0	1	0
4	F	3	0	0	0	0
4	G	9	0	0	1	0
4	H	1	0	0	0	0
4	J	2	0	0	2	0
All	All	15611	0	14947	161	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 (161) 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:H:301:J2B:O10	3:H:301:J2B:C09	1.66	1.20
1:B:94:TYR:OH	4:B:301:HOH:O	1.97	0.83
1:C:39:TYR:OH	1:C:79:ASP:OD2	1.99	0.80
1:B:152:SER:O	4:B:302:HOH:O	1.99	0.80
1:H:60:ARG:NH1	3:H:301:J2B:N20	2.32	0.77
1:H:60:ARG:NH1	3:H:301:J2B:C21	2.48	0.76
1:G:115:GLU:HB3	1:H:153:PRO:HG3	1.69	0.75
1:J:61:TYR:HB3	1:J:112:LEU:HB2	1.69	0.74
1:J:30:VAL:O	4:J:301:HOH:O	2.05	0.74
1:F:76:GLN:HE22	1:J:6:ALA:H	1.34	0.74
1:H:60:ARG:HH12	3:H:301:J2B:C21	2.02	0.73
1:H:130:VAL:O	1:H:182:ARG:NH1	2.21	0.69
1:E:77:ILE:O	4:E:302:HOH:O	2.08	0.69
1:C:76:GLN:HB3	1:C:79:ASP:OD2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:ASN:OD1	1:F:146:LYS:NZ	2.28	0.67
1:J:4:PHE:O	4:J:302:HOH:O	2.13	0.66
1:E:149:ASN:ND2	1:F:14:GLU:OE2	2.29	0.66
1:I:186:LYS:NZ	1:J:106:GLY:O	2.29	0.65
1:B:151:LEU:O	1:B:178:LYS:NZ	2.22	0.64
1:D:129:ALA:HB3	1:D:141:ILE:HG12	1.80	0.64
1:I:170:VAL:HB	1:I:183:MET:HE2	1.78	0.64
1:I:130:VAL:O	1:I:182:ARG:NH1	2.29	0.63
1:C:76:GLN:NE2	4:C:302:HOH:O	2.22	0.63
1:I:111:ASP:HB2	1:J:182:ARG:HB3	1.82	0.62
1:I:174:ASP:HB3	1:I:180:ILE:HD11	1.82	0.62
1:H:64:ALA:HA	1:H:109:SER:HA	1.82	0.61
1:A:151:LEU:O	1:A:178:LYS:NZ	2.30	0.61
1:I:106:GLY:O	1:J:186:LYS:NZ	2.34	0.60
1:F:76:GLN:HE21	1:J:9:LEU:HD12	1.66	0.60
1:G:174:ASP:HB3	1:G:180:ILE:HD11	1.82	0.60
1:F:61:TYR:HB3	1:F:112:LEU:HB3	1.84	0.59
1:A:169:GLN:NE2	2:A:301:J2A:S06	2.64	0.59
1:G:182:ARG:HB3	1:H:111:ASP:HB2	1.84	0.59
1:F:9:LEU:HD21	1:J:9:LEU:HD21	1.84	0.59
1:D:9:LEU:HD21	1:G:9:LEU:HD21	1.85	0.58
1:G:29:ASP:HA	1:G:105:ILE:HB	1.84	0.58
1:G:133:LYS:HG3	1:G:160:HIS:CE1	2.38	0.58
1:J:64:ALA:HA	1:J:109:SER:HA	1.86	0.58
1:B:61:TYR:HB3	1:B:112:LEU:HB2	1.86	0.58
1:E:130:VAL:O	1:E:182:ARG:NH2	2.37	0.57
1:I:22:ILE:HD12	1:I:103:SER:HB3	1.86	0.57
1:B:110:LEU:HD13	1:B:183:MET:HE1	1.85	0.57
1:J:130:VAL:O	1:J:182:ARG:NH1	2.35	0.57
1:C:61:TYR:HB3	1:C:112:LEU:HB2	1.86	0.57
1:F:74:TYR:HE2	1:F:76:GLN:HG3	1.70	0.57
2:F:301:J2A:S25	2:F:301:J2A:O29	2.63	0.57
1:I:61:TYR:HB3	1:I:112:LEU:HB2	1.87	0.57
1:H:133:LYS:HG3	1:H:160:HIS:CE1	2.39	0.56
1:I:170:VAL:HG12	1:I:183:MET:HG2	1.87	0.56
1:G:151:LEU:O	1:G:178:LYS:NZ	2.39	0.55
1:F:110:LEU:HD13	1:F:183:MET:HE1	1.89	0.55
1:I:64:ALA:HA	1:I:109:SER:HA	1.88	0.55
1:G:138:TYR:OH	3:H:301:J2B:S27	2.58	0.55
1:G:168:CYS:HB2	1:G:185:PHE:HB2	1.88	0.55
1:D:170:VAL:HB	1:D:183:MET:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LEU:HD13	1:C:103:SER:HA	1.90	0.54
1:F:59:LYS:HD3	1:F:115:GLU:HG2	1.89	0.54
1:A:153:PRO:HG3	1:B:115:GLU:HB3	1.90	0.54
1:G:76:GLN:OE1	4:G:301:HOH:O	2.18	0.54
1:H:151:LEU:HB2	1:H:178:LYS:HD2	1.89	0.53
1:E:130:VAL:N	2:F:301:J2A:S06	2.76	0.53
1:I:96:HIS:ND1	1:I:191:LEU:O	2.41	0.53
1:H:45:ILE:HD13	1:H:69:PHE:HB3	1.91	0.53
1:A:74:TYR:OH	4:A:401:HOH:O	2.17	0.53
1:I:186:LYS:HG3	1:J:107:TYR:HA	1.90	0.53
1:I:107:TYR:HA	1:J:186:LYS:HG3	1.91	0.52
1:G:186:LYS:NZ	1:H:106:GLY:O	2.43	0.52
1:A:106:GLY:O	1:B:186:LYS:NZ	2.42	0.51
1:B:64:ALA:HA	1:B:109:SER:HA	1.92	0.51
1:H:29:ASP:HA	1:H:105:ILE:HB	1.92	0.51
1:D:112:LEU:HD12	1:D:119:ILE:HD12	1.91	0.51
1:B:81:ILE:HD11	1:B:92:ILE:HD13	1.92	0.51
1:G:61:TYR:HB3	1:G:112:LEU:HB2	1.92	0.50
1:D:29:ASP:HA	1:D:105:ILE:HB	1.94	0.50
1:E:170:VAL:HB	1:E:183:MET:HG3	1.94	0.50
1:E:186:LYS:NZ	1:F:106:GLY:O	2.42	0.50
1:A:130:VAL:N	2:A:301:J2A:S06	2.84	0.50
1:G:142:LYS:NZ	1:H:14:GLU:O	2.41	0.50
1:H:22:ILE:HD12	1:H:103:SER:HB3	1.92	0.49
1:I:179:GLU:OE1	1:I:182:ARG:NH1	2.45	0.49
1:C:153:PRO:HG2	1:D:115:GLU:HB3	1.94	0.49
1:F:125:GLU:O	1:F:128:ASN:HB2	2.13	0.49
1:I:29:ASP:HA	1:I:105:ILE:HB	1.94	0.49
1:G:184:ARG:NE	3:H:301:J2B:S06	2.80	0.49
1:H:17:HIS:HA	3:H:301:J2B:O28	2.11	0.49
1:F:136:HIS:H	1:F:141:ILE:HD11	1.77	0.48
1:D:81:ILE:HD11	1:D:92:ILE:HD13	1.94	0.48
1:C:45:ILE:HD13	1:C:69:PHE:HB3	1.96	0.48
1:I:73:GLU:OE1	1:I:73:GLU:N	2.46	0.48
1:J:66:LEU:HD13	1:J:103:SER:HA	1.96	0.47
1:F:64:ALA:HA	1:F:109:SER:HA	1.96	0.47
1:E:61:TYR:HB3	1:E:112:LEU:HB2	1.95	0.47
1:E:146:LYS:HA	1:E:149:ASN:HD22	1.80	0.47
1:B:66:LEU:HD13	1:B:103:SER:HA	1.97	0.47
1:E:18:ALA:HB1	1:E:62:ILE:HD13	1.97	0.47
1:I:133:LYS:HG3	1:I:160:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:ARG:CZ	3:H:301:J2B:C19	2.93	0.47
1:E:66:LEU:HD13	1:E:103:SER:HA	1.97	0.47
1:A:131:TYR:HB2	1:A:141:ILE:HG23	1.98	0.46
1:H:129:ALA:HB3	1:H:141:ILE:HG21	1.96	0.46
1:B:170:VAL:HB	1:B:183:MET:HG2	1.97	0.46
1:A:29:ASP:HA	1:A:105:ILE:HB	1.98	0.46
1:H:128:ASN:OD1	1:H:129:ALA:N	2.49	0.46
1:A:170:VAL:HB	1:A:183:MET:HE2	1.98	0.46
1:H:151:LEU:HD22	1:H:178:LYS:HB2	1.98	0.46
1:J:179:GLU:OE1	1:J:182:ARG:NH1	2.49	0.46
1:D:72:ASN:OD1	1:D:98:ASN:ND2	2.50	0.45
1:E:45:ILE:HD13	1:E:69:PHE:HB3	1.98	0.45
1:E:64:ALA:HA	1:E:109:SER:HA	1.99	0.45
1:J:22:ILE:HD12	1:J:103:SER:HB3	1.99	0.45
1:J:157:ILE:N	1:J:173:VAL:O	2.49	0.45
1:H:61:TYR:HB3	1:H:112:LEU:HB2	1.99	0.45
1:D:18:ALA:HB1	1:D:62:ILE:HD13	1.98	0.45
1:F:81:ILE:HD11	1:F:92:ILE:HD13	1.99	0.45
1:G:186:LYS:HG3	1:H:107:TYR:HA	1.99	0.45
1:G:61:TYR:HB2	1:G:114:LEU:HD11	1.98	0.45
1:J:18:ALA:HB1	1:J:62:ILE:HD13	1.99	0.45
1:H:66:LEU:HD13	1:H:103:SER:HA	1.99	0.45
1:F:142:LYS:O	1:F:146:LYS:HG2	2.18	0.44
1:A:66:LEU:HD13	1:A:103:SER:HA	1.99	0.44
1:C:170:VAL:HB	1:C:183:MET:HG2	1.98	0.44
1:G:133:LYS:HG3	1:G:160:HIS:NE2	2.32	0.44
1:C:81:ILE:HD11	1:C:92:ILE:HD13	1.99	0.44
1:C:47:LYS:HA	4:C:310:HOH:O	2.18	0.44
1:I:133:LYS:HG3	1:I:160:HIS:NE2	2.32	0.44
1:H:81:ILE:HD11	1:H:92:ILE:HD13	1.99	0.43
1:F:129:ALA:HB3	1:F:141:ILE:HD13	2.00	0.43
1:E:131:TYR:HB2	1:E:141:ILE:HG23	2.00	0.43
1:A:76:GLN:NE2	4:A:401:HOH:O	2.25	0.43
1:H:60:ARG:NH1	3:H:301:J2B:C19	2.81	0.43
1:F:151:LEU:O	1:F:178:LYS:NZ	2.30	0.43
1:H:110:LEU:HD13	1:H:183:MET:HE1	2.00	0.43
1:J:133:LYS:HG3	1:J:160:HIS:NE2	2.34	0.42
1:D:64:ALA:HA	1:D:109:SER:HA	2.00	0.42
1:A:54:TYR:HA	1:A:62:ILE:O	2.20	0.42
1:A:183:MET:HB3	1:B:183:MET:HE3	2.01	0.42
1:C:179:GLU:OE2	1:C:182:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:HB	1:A:183:MET:HG3	2.00	0.42
1:E:29:ASP:HA	1:E:105:ILE:HB	2.02	0.42
1:F:49:LYS:HB3	1:F:68:MET:HE2	2.00	0.42
1:D:61:TYR:HB3	1:D:112:LEU:HB2	2.02	0.42
1:F:22:ILE:HD12	1:F:103:SER:HB3	2.01	0.42
1:I:18:ALA:HB1	1:I:62:ILE:HD13	2.01	0.42
1:I:81:ILE:HD11	1:I:92:ILE:HD13	2.01	0.42
1:A:37:SER:HA	1:A:41:ASN:O	2.19	0.42
1:H:60:ARG:HG3	1:H:61:TYR:N	2.31	0.42
1:A:61:TYR:HB3	1:A:112:LEU:HB2	2.01	0.41
1:E:181:MET:HG2	1:E:182:ARG:N	2.34	0.41
1:I:185:PHE:HE1	1:J:185:PHE:HE1	1.68	0.41
1:C:3:MET:HA	1:C:3:MET:HE2	2.02	0.41
1:E:55:SER:HB3	1:E:94:TYR:OH	2.21	0.41
1:C:151:LEU:O	1:C:178:LYS:NZ	2.32	0.41
1:E:182:ARG:HB3	1:F:111:ASP:HB2	2.01	0.41
1:I:157:ILE:N	1:I:173:VAL:O	2.54	0.41
1:D:54:TYR:HA	1:D:62:ILE:O	2.20	0.41
1:D:39:TYR:N	4:D:306:HOH:O	2.54	0.41
1:F:76:GLN:NE2	1:J:6:ALA:H	2.11	0.41
1:G:131:TYR:HB2	1:G:141:ILE:HG23	2.03	0.41
1:G:181:MET:HE3	1:G:181:MET:HB3	1.88	0.41
1:A:64:ALA:HA	1:A:109:SER:HA	2.03	0.41
1:D:129:ALA:CB	1:D:141:ILE:HG12	2.51	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	193/220 (88%)	186 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	193/220 (88%)	187 (97%)	6 (3%)	0	100	100
1	C	193/220 (88%)	187 (97%)	6 (3%)	0	100	100
1	D	193/220 (88%)	187 (97%)	6 (3%)	0	100	100
1	E	193/220 (88%)	185 (96%)	8 (4%)	0	100	100
1	F	192/220 (87%)	181 (94%)	9 (5%)	2 (1%)	12	28
1	G	192/220 (87%)	185 (96%)	7 (4%)	0	100	100
1	H	193/220 (88%)	184 (95%)	9 (5%)	0	100	100
1	I	175/220 (80%)	169 (97%)	5 (3%)	1 (1%)	21	42
1	J	174/220 (79%)	167 (96%)	7 (4%)	0	100	100
All	All	1891/2200 (86%)	1818 (96%)	70 (4%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	75	LEU
1	F	126	THR
1	I	20	PRO

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	167/189 (88%)	165 (99%)	2 (1%)	63	83
1	B	167/189 (88%)	165 (99%)	2 (1%)	63	83
1	C	167/189 (88%)	167 (100%)	0	100	100
1	D	167/189 (88%)	167 (100%)	0	100	100
1	E	167/189 (88%)	165 (99%)	2 (1%)	63	83
1	F	166/189 (88%)	163 (98%)	3 (2%)	51	76
1	G	166/189 (88%)	164 (99%)	2 (1%)	63	83
1	H	167/189 (88%)	162 (97%)	5 (3%)	36	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	156/189 (82%)	154 (99%)	2 (1%)	61	82
1	J	156/189 (82%)	154 (99%)	2 (1%)	61	82
All	All	1646/1890 (87%)	1626 (99%)	20 (1%)	63	83

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LYS
1	A	183	MET
1	B	14	GLU
1	B	183	MET
1	E	181	MET
1	E	183	MET
1	F	141	ILE
1	F	170	VAL
1	F	183	MET
1	G	112	LEU
1	G	170	VAL
1	H	60	ARG
1	H	123	VAL
1	H	141	ILE
1	H	183	MET
1	H	190	VAL
1	I	170	VAL
1	I	190	VAL
1	J	170	VAL
1	J	190	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	72	ASN
1	A	82	HIS
1	A	176	HIS
1	C	28	ASN
1	C	84	GLN
1	D	98	ASN
1	E	84	GLN
1	E	149	ASN

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Mol	Chain	Res	Type
1	F	76	GLN
1	F	82	HIS
1	G	15	ASN
1	G	28	ASN
1	G	72	ASN
1	H	82	HIS
1	I	72	ASN
1	I	82	HIS
1	J	28	ASN
1	J	82	HIS

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 ⓘ

3 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	$\# Z > 2$
3	J2B	H	301	-	44,50,50	3.73	23 (52%)	52,76,76	2.02	17 (32%)
2	J2A	A	301	-	45,51,51	2.17	11 (24%)	60,80,80	1.76	12 (20%)
2	J2A	F	301	-	45,51,51	2.18	13 (28%)	60,80,80	1.76	12 (20%)

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
3	J2B	H	301	-	-	9/29/51/51	0/5/5/5
2	J2A	A	301	-	-	2/26/62/62	0/6/7/7
2	J2A	F	301	-	-	5/26/62/62	0/6/7/7

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	J2B	C02-C03	-11.50	1.27	1.53
3	H	301	J2B	O10-C11	-8.05	1.30	1.40
3	H	301	J2B	C09-C24	-7.95	1.34	1.52
2	A	301	J2A	C10-N11	7.24	1.49	1.37
2	F	301	J2A	C10-N11	7.15	1.49	1.37
3	H	301	J2B	C33-N34	6.77	1.49	1.37
3	H	301	J2B	O43-C44	-6.64	1.30	1.45
3	H	301	J2B	C31-N32	-5.08	1.33	1.47
3	H	301	J2B	C02-C44	5.08	1.65	1.53
3	H	301	J2B	C35-N37	5.03	1.45	1.33
3	H	301	J2B	C35-N36	4.95	1.45	1.34
3	H	301	J2B	O43-C31	4.86	1.53	1.42
2	F	301	J2A	C12-N13	4.81	1.45	1.34
2	A	301	J2A	C12-N13	4.75	1.45	1.34
3	H	301	J2B	C17-N18	4.61	1.46	1.34
2	A	301	J2A	C12-N14	4.54	1.44	1.33
2	F	301	J2A	C12-N14	4.53	1.44	1.33
2	F	301	J2A	C36-N37	4.41	1.45	1.34
2	A	301	J2A	C36-N37	4.38	1.45	1.34
3	H	301	J2B	O23-C22	-4.22	1.32	1.43
3	H	301	J2B	C35-N34	3.93	1.47	1.37
2	A	301	J2A	C12-N11	3.64	1.46	1.37
2	F	301	J2A	C12-N11	3.62	1.46	1.37
3	H	301	J2B	C38-N37	3.39	1.43	1.38
2	A	301	J2A	C15-C17	3.10	1.54	1.45
2	F	301	J2A	C15-C17	3.05	1.53	1.45
2	F	301	J2A	C15-N14	2.96	1.43	1.38
2	A	301	J2A	C15-N14	2.88	1.42	1.38
2	F	301	J2A	C02-C03	-2.83	1.46	1.53
3	H	301	J2B	C38-C40	2.83	1.53	1.45
2	A	301	J2A	C02-C03	-2.71	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	J2A	O16-C15	-2.67	1.18	1.23
2	F	301	J2A	O16-C15	-2.65	1.18	1.23
3	H	301	J2B	C21-N12	-2.60	1.33	1.37
3	H	301	J2B	O39-C38	-2.57	1.19	1.23
3	H	301	J2B	C33-N32	-2.48	1.34	1.37
2	F	301	J2A	C28-C27	-2.45	1.47	1.53
2	A	301	J2A	C28-C27	-2.42	1.47	1.53
2	A	301	J2A	C17-N18	-2.41	1.34	1.39
3	H	301	J2B	C40-N41	-2.39	1.34	1.39
2	F	301	J2A	C17-N18	-2.34	1.34	1.39
3	H	301	J2B	P26-O28	2.23	1.51	1.46
3	H	301	J2B	C19-N20	-2.23	1.35	1.39
2	F	301	J2A	C10-N09	-2.09	1.35	1.37
3	H	301	J2B	P26-O29	-2.08	1.51	1.56
3	H	301	J2B	C42-N32	-2.07	1.32	1.37
2	F	301	J2A	C40-N31	-2.01	1.34	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	301	J2B	N16-C15-N14	-5.59	120.12	128.58
2	A	301	J2A	C38-C32-N33	-5.05	119.76	126.72
3	H	301	J2B	C19-C13-N14	-4.93	119.93	126.72
2	F	301	J2A	C38-C32-N33	-4.82	120.08	126.72
2	F	301	J2A	N35-C34-N33	-4.52	121.74	128.58
2	A	301	J2A	N35-C34-N33	-4.22	122.19	128.58
2	F	301	J2A	N31-C40-N39	-4.02	108.23	113.94
2	A	301	J2A	C17-C10-N09	4.00	108.10	106.25
2	A	301	J2A	N31-C40-N39	-3.86	108.45	113.94
2	F	301	J2A	C17-C10-N09	3.82	108.01	106.25
3	H	301	J2B	C15-N14-C13	3.79	121.08	111.83
3	H	301	J2B	C13-C19-N20	-3.74	106.31	110.58
3	H	301	J2B	C19-N20-C21	3.42	108.82	103.45
2	A	301	J2A	C34-N33-C32	3.38	120.07	111.83
2	F	301	J2A	C34-N33-C32	3.35	120.02	111.83
3	H	301	J2B	N12-C21-N20	-3.28	109.28	113.94
2	A	301	J2A	C38-N39-C40	3.25	108.56	103.45
2	F	301	J2A	N33-C32-N31	3.17	132.56	127.17
2	F	301	J2A	C38-N39-C40	3.16	108.42	103.45
2	A	301	J2A	N33-C32-N31	3.16	132.53	127.17
3	H	301	J2B	N14-C13-N12	3.14	132.50	127.17
2	A	301	J2A	C32-C38-N39	-2.99	107.17	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	J2A	C32-C38-N39	-2.83	107.35	110.58
3	H	301	J2B	C09-C24-C22	-2.79	102.73	114.72
3	H	301	J2B	C03-C02-C44	2.78	107.98	101.99
2	F	301	J2A	N09-C19-N18	-2.76	108.28	113.40
2	F	301	J2A	C32-N31-C40	2.76	108.64	105.74
2	A	301	J2A	N09-C19-N18	-2.66	108.47	113.40
3	H	301	J2B	C44-O43-C31	-2.60	103.72	109.47
3	H	301	J2B	C15-N16-C17	2.42	122.70	118.73
2	A	301	J2A	C32-N31-C40	2.26	108.12	105.74
3	H	301	J2B	C08-C09-C24	-2.20	109.82	113.22
2	A	301	J2A	C19-N18-C17	2.18	108.14	104.26
3	H	301	J2B	C13-N12-C21	2.16	108.01	105.74
2	A	301	J2A	C03-C08-N09	-2.16	110.14	114.24
2	F	301	J2A	C19-N18-C17	2.14	108.08	104.26
3	H	301	J2B	O10-C11-C22	-2.13	102.81	107.93
2	F	301	J2A	P05-O04-C03	-2.11	115.34	121.80
3	H	301	J2B	C42-N41-C40	2.10	107.99	104.26
3	H	301	J2B	C45-C44-C02	-2.02	110.33	115.10
3	H	301	J2B	C17-C19-N20	2.01	135.96	132.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

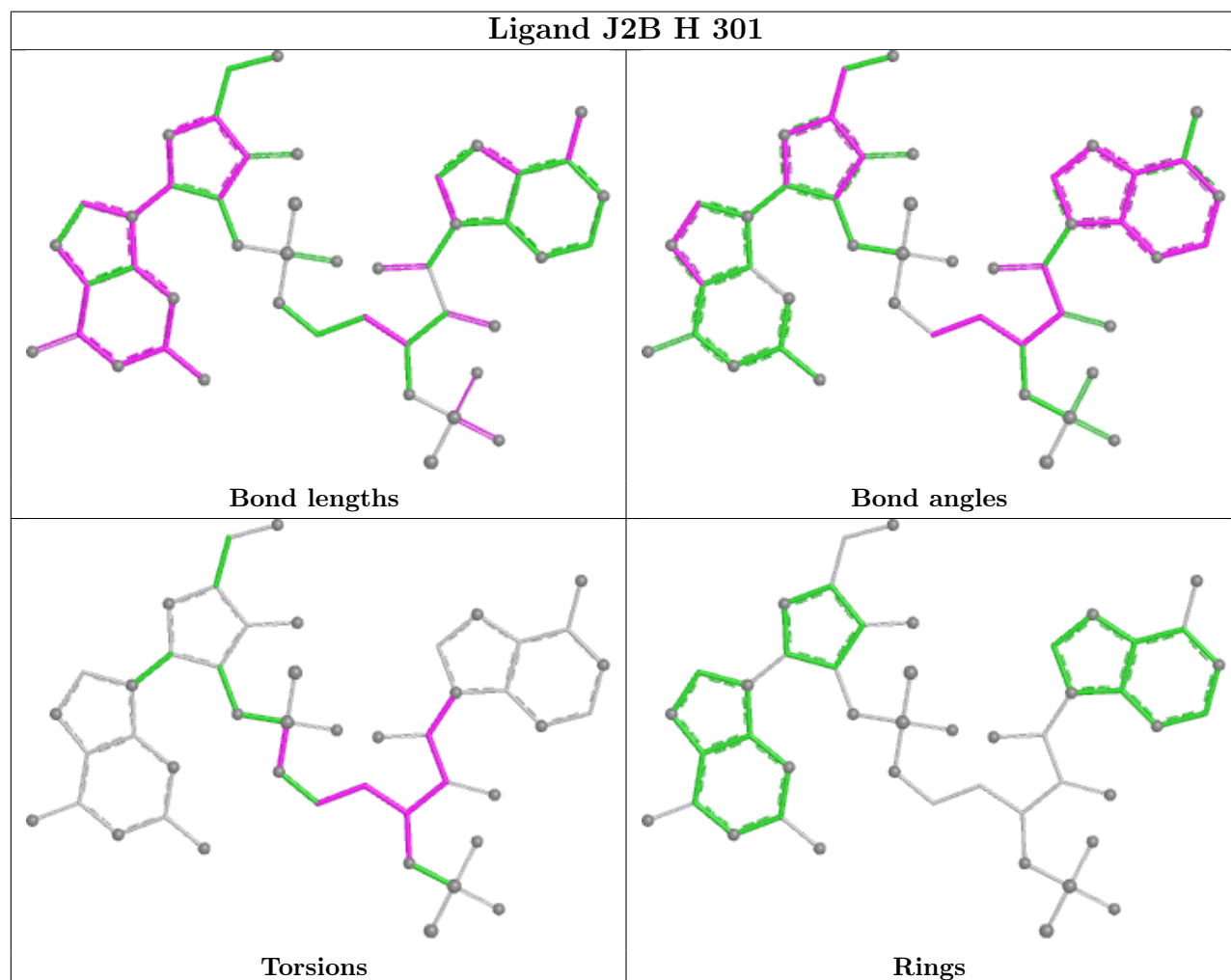
Mol	Chain	Res	Type	Atoms
3	H	301	J2B	C22-C11-N12-C21
3	H	301	J2B	O23-C22-C24-C09
3	H	301	J2B	C09-C24-O25-P26
3	H	301	J2B	C22-C24-O25-P26
2	F	301	J2A	C27-C42-C43-O44
2	F	301	J2A	O41-C42-C43-O44
3	H	301	J2B	O07-C08-C09-C24
3	H	301	J2B	C08-O07-P05-O30
2	A	301	J2A	C27-C42-C43-O44
2	A	301	J2A	O41-C42-C43-O44
2	F	301	J2A	C43-O44-P05-O07
3	H	301	J2B	O10-C11-C22-O23
2	F	301	J2A	C03-O04-P05-O44
2	F	301	J2A	C03-O04-P05-O07
3	H	301	J2B	C08-C09-C24-O25
3	H	301	J2B	C11-C22-C24-C09

There are no ring outliers.

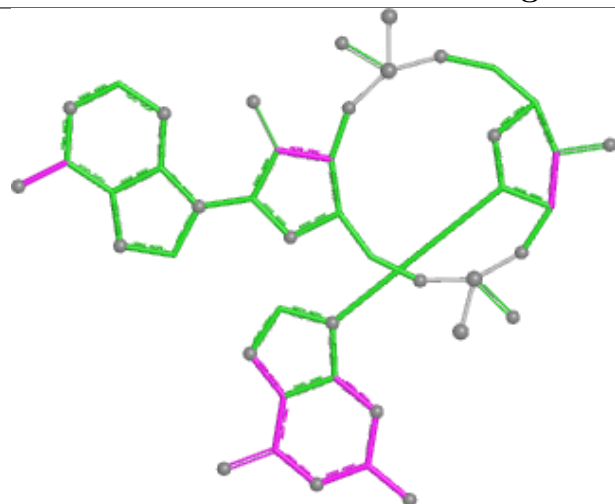
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	301	J2B	9	0
2	A	301	J2A	2	0
2	F	301	J2A	2	0

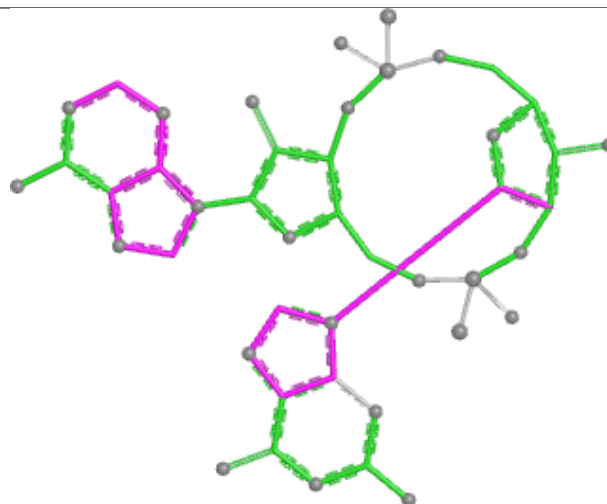
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



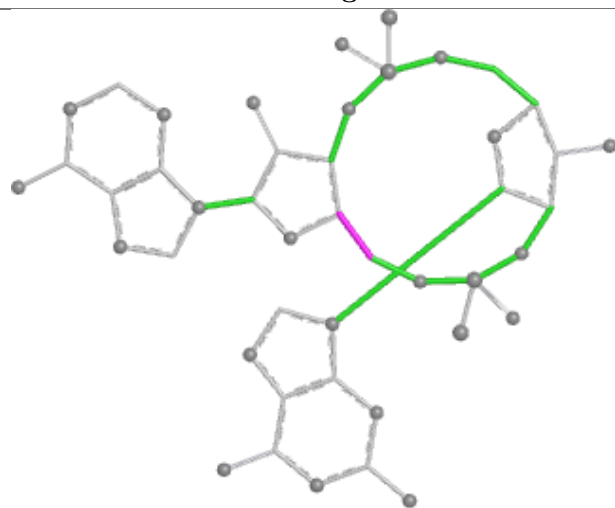
Ligand J2A A 301



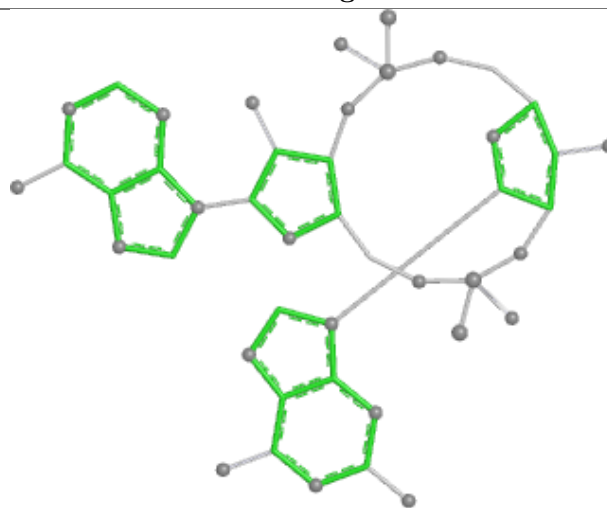
Bond lengths



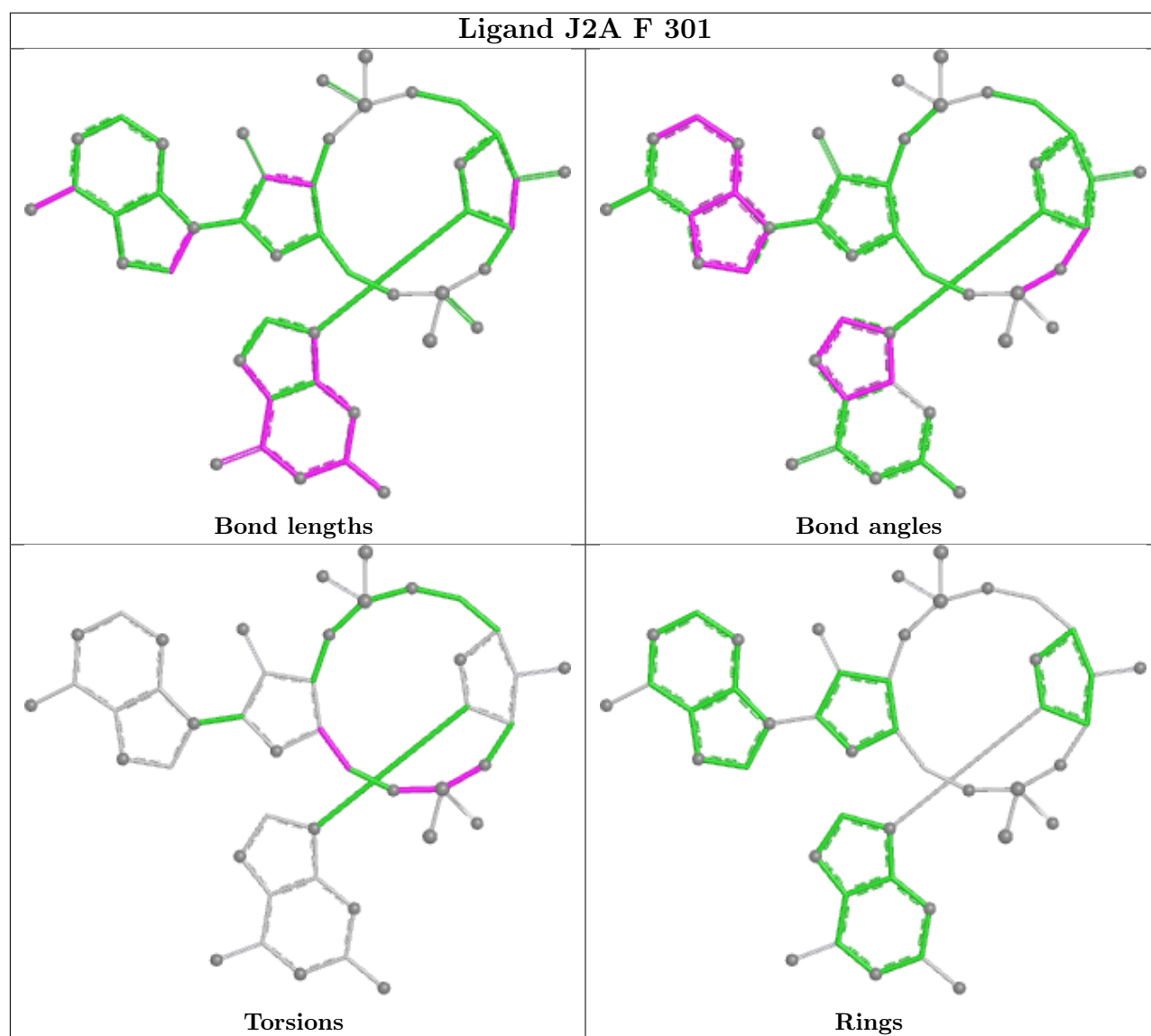
Bond angles



Torsions



Rings



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	195/220 (88%)	0.02	2 (1%) 79 76	39, 63, 101, 132	0
1	B	195/220 (88%)	0.03	5 (2%) 57 51	47, 63, 93, 109	0
1	C	195/220 (88%)	-0.10	3 (1%) 72 68	40, 55, 90, 116	0
1	D	195/220 (88%)	0.13	4 (2%) 63 58	47, 69, 112, 125	0
1	E	195/220 (88%)	0.24	3 (1%) 72 68	53, 83, 135, 153	0
1	F	194/220 (88%)	0.45	4 (2%) 63 58	81, 107, 130, 172	0
1	G	194/220 (88%)	0.53	9 (4%) 37 32	64, 100, 148, 156	0
1	H	195/220 (88%)	0.71	9 (4%) 37 32	90, 118, 171, 182	0
1	I	181/220 (82%)	0.74	10 (5%) 30 25	101, 126, 176, 192	0
1	J	180/220 (81%)	0.74	13 (7%) 21 17	113, 135, 176, 192	0
All	All	1919/2200 (87%)	0.34	62 (3%) 50 44	39, 94, 155, 192	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	194	PRO	4.5
1	H	194	PRO	4.4
1	I	194	PRO	4.0
1	F	194	PRO	3.7
1	D	141	ILE	3.6
1	B	138	TYR	3.6
1	D	138	TYR	3.4
1	E	150	ALA	3.3
1	J	130	VAL	3.3
1	I	112	LEU	3.2
1	J	112	LEU	3.1
1	H	150	ALA	3.0
1	G	62	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	120	HIS	2.9
1	C	138	TYR	2.9
1	J	159	TYR	2.9
1	C	183	MET	2.8
1	I	84	GLN	2.8
1	H	101	ALA	2.8
1	I	150	ALA	2.8
1	G	194	PRO	2.7
1	J	157	ILE	2.7
1	B	124	LEU	2.6
1	J	175	VAL	2.6
1	H	60	ARG	2.6
1	J	146	LYS	2.6
1	G	27	ALA	2.6
1	F	138	TYR	2.5
1	E	113	CYS	2.5
1	A	138	TYR	2.5
1	I	175	VAL	2.5
1	J	138	TYR	2.5
1	I	12	TYR	2.4
1	B	183	MET	2.4
1	D	183	MET	2.4
1	H	153	PRO	2.4
1	F	142	LYS	2.4
1	I	157	ILE	2.4
1	H	183	MET	2.4
1	J	184	ARG	2.4
1	D	84	GLN	2.4
1	H	123	VAL	2.3
1	I	39	TYR	2.3
1	I	138	TYR	2.3
1	J	33	TYR	2.3
1	B	58	ASN	2.3
1	H	124	LEU	2.3
1	B	164	GLY	2.3
1	E	114	LEU	2.3
1	F	183	MET	2.2
1	A	144	LYS	2.2
1	C	56	GLN	2.2
1	H	114	LEU	2.2
1	J	120	HIS	2.1
1	G	59	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	57	VAL	2.1
1	J	94	TYR	2.1
1	G	151	LEU	2.0
1	G	58	ASN	2.0
1	G	134	VAL	2.0
1	J	102	LEU	2.0
1	G	11	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](#)

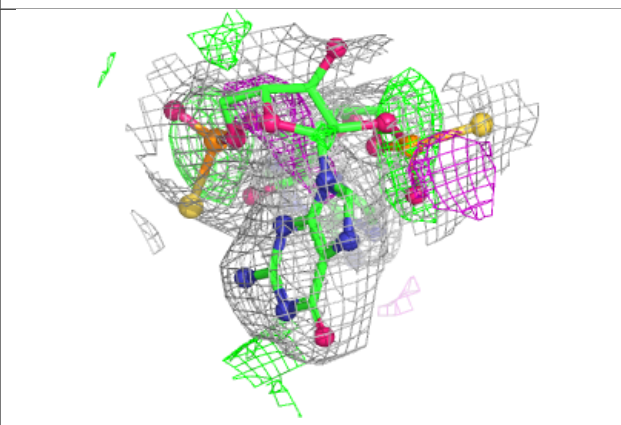
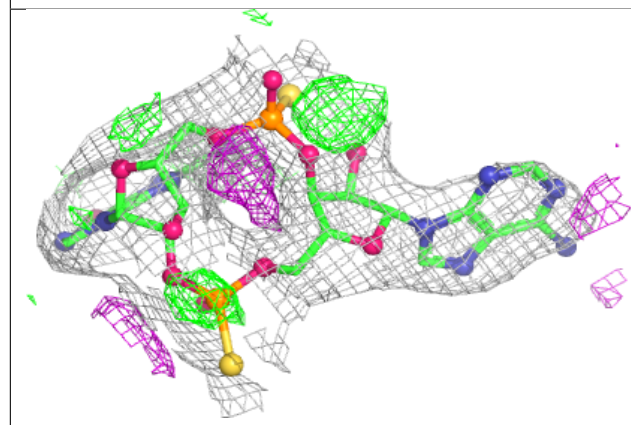
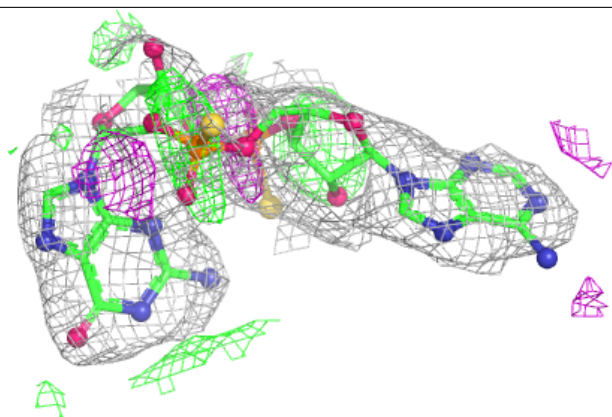
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	J2A	F	301	45/45	0.81	0.15	96,129,148,203	0
2	J2A	A	301	45/45	0.85	0.14	69,81,97,112	0
3	J2B	H	301	46/46	0.88	0.12	92,109,172,188	0

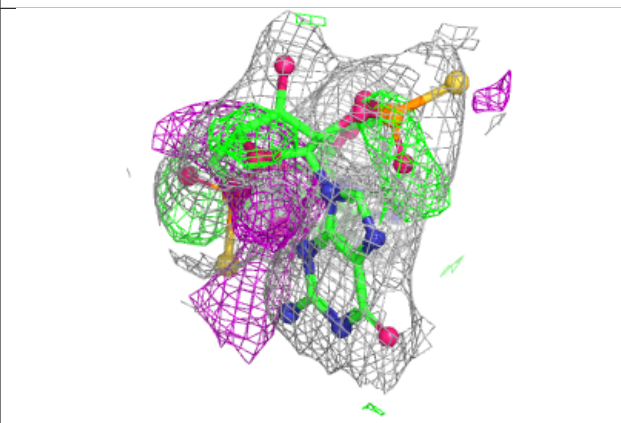
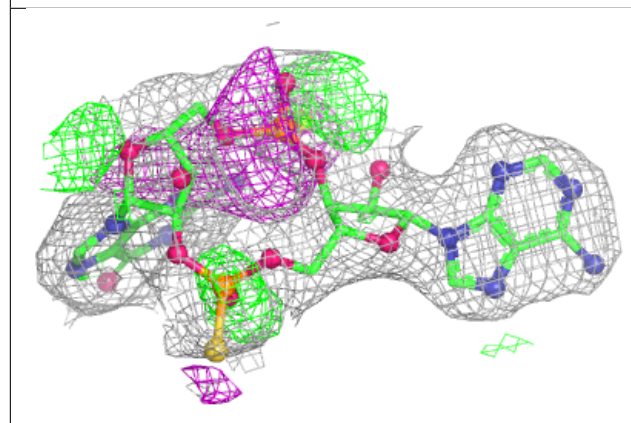
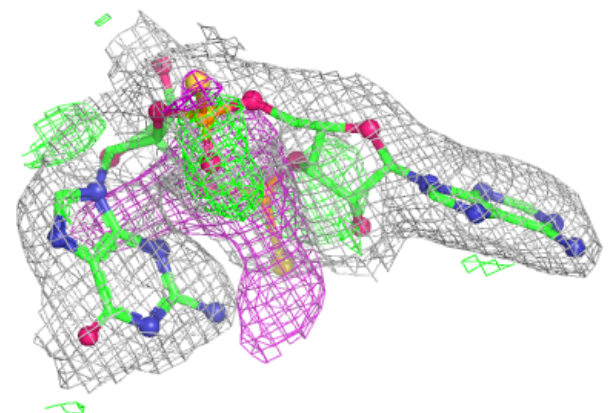
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around J2A F 301:

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

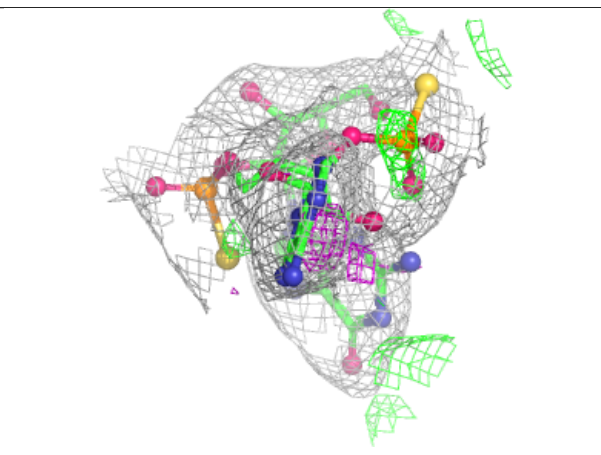
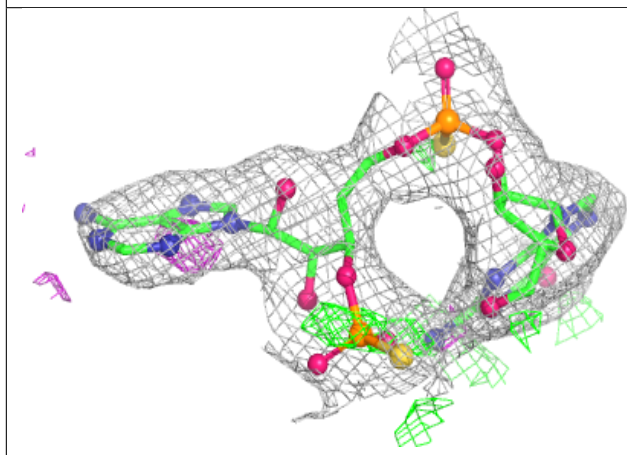
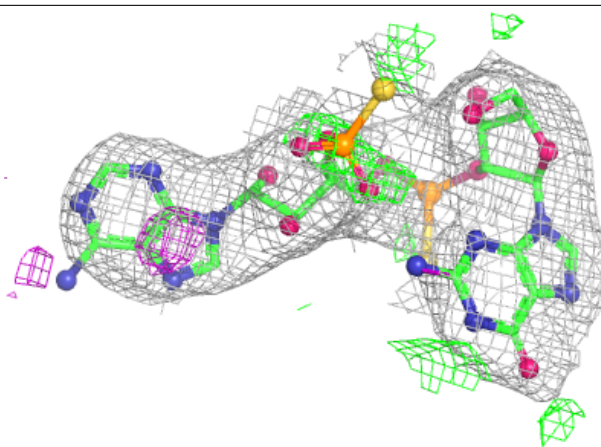
**Electron density around J2A A 301:**

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



Electron density around J2B H 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.