



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 11:21 AM UTC

PDB ID : 3OGL / pdb_00003ogl
Title : Structure of COI1-ASK1 in complex with JA-isoleucine and the JAZ1 degron
Authors : Sheard, L.B.; Tan, X.; Mao, H.; Withers, J.; Ben-Nissan, G.; Hinds, T.R.;
Hsu, F.; Sharon, M.; Browse, J.; He, S.Y.; Rizo, J.; Howe, G.A.; Zheng, N.
Deposited on : 2010-08-17
Resolution : 3.18 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

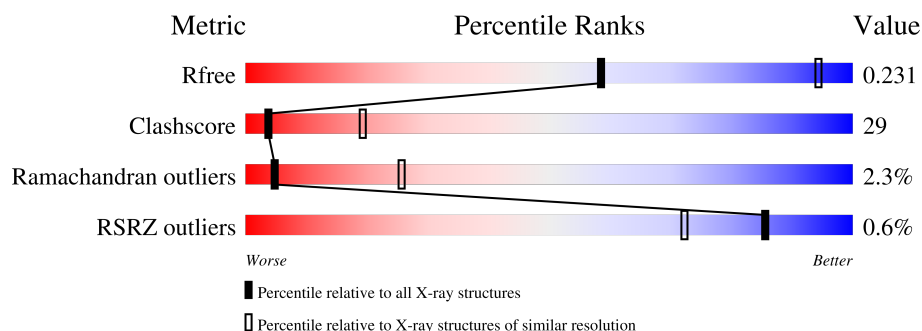
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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.



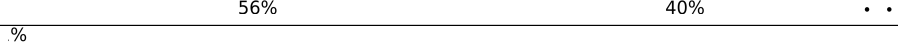
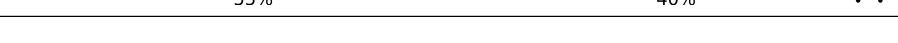
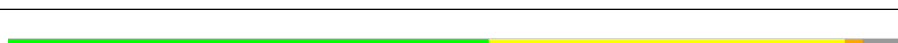
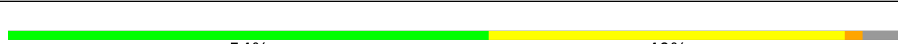
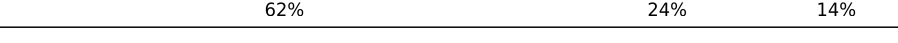
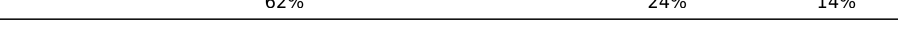
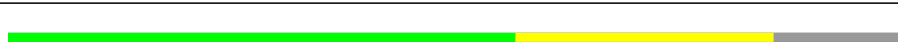
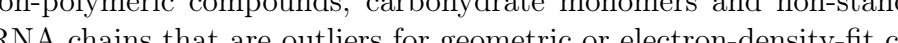
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	160	49% 40% 10%
1	C	160	51% 38% 10%
1	E	160	52% 36% 10%
1	G	160	48% 39% 10%
1	I	160	46% 40% 10%
1	K	160	50% 38% 10%

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Mol	Chain	Length	Quality of chain
1	M	160	
1	O	160	
2	B	592	
2	D	592	
2	F	592	
2	H	592	
2	J	592	
2	L	592	
2	N	592	
2	P	592	
3	Q	21	
3	R	21	
3	S	21	
3	U	21	
3	V	21	
3	W	21	
3	X	21	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	7JA	B	1100	-	-	X	-
4	7JA	D	1100	-	-	X	-
4	7JA	F	1100	-	-	X	-
4	7JA	H	1100	-	-	X	-
4	7JA	J	1100	-	-	X	-
4	7JA	L	1100	-	-	X	-
4	7JA	N	1100	-	-	X	-
4	7JA	P	1100	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	B	1101	-	X	-	-
5	PO4	B	1102	-	X	-	-
5	PO4	B	1103	-	X	X	-
5	PO4	B	1104	-	X	-	-
5	PO4	D	1101	-	X	-	-
5	PO4	D	1102	-	X	-	-
5	PO4	D	1103	-	X	X	-
5	PO4	F	1101	-	X	-	-
5	PO4	F	1102	-	X	-	-
5	PO4	F	1103	-	X	X	-
5	PO4	F	1104	-	X	-	-
5	PO4	H	1101	-	X	-	-
5	PO4	H	1102	-	X	-	-
5	PO4	H	1103	-	X	X	-
5	PO4	H	1104	-	X	-	-
5	PO4	J	1101	-	X	-	-
5	PO4	J	1102	-	X	-	-
5	PO4	J	1103	-	X	X	-
5	PO4	J	1104	-	X	-	-
5	PO4	L	1101	-	X	-	-
5	PO4	L	1102	-	X	-	-
5	PO4	L	1103	-	X	X	-
5	PO4	L	1104	-	X	-	-
5	PO4	N	1101	-	X	-	-
5	PO4	N	1102	-	X	-	-
5	PO4	N	1103	-	X	X	-
5	PO4	N	1104	-	X	-	-
5	PO4	P	1101	-	X	-	-
5	PO4	P	1102	-	X	-	-
5	PO4	P	1103	-	X	X	-
5	PO4	P	1104	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 46877 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 SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	C	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	E	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	G	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	I	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	K	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	M	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	O	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			

- Molecule 2 is a protein called Coronatine-insensitive protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	D	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	F	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	H	562	Total	C	N	O	S	0	0	0
			4486	2840	779	831	36			
2	J	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	L	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			

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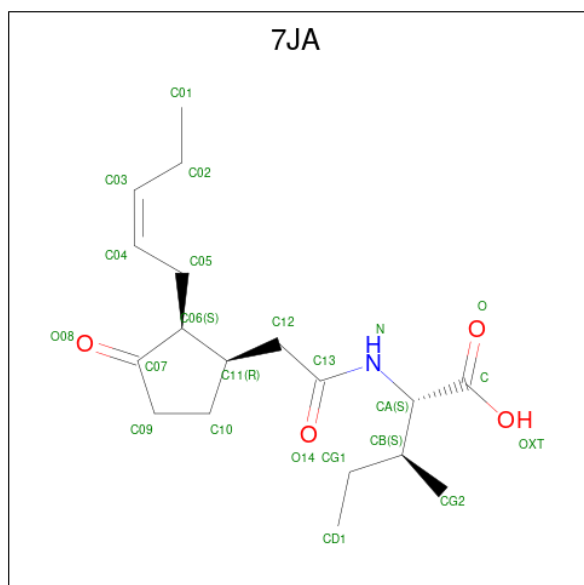
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	P	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			

- Molecule 3 is a protein called JAZ1 incomplete degron peptide.

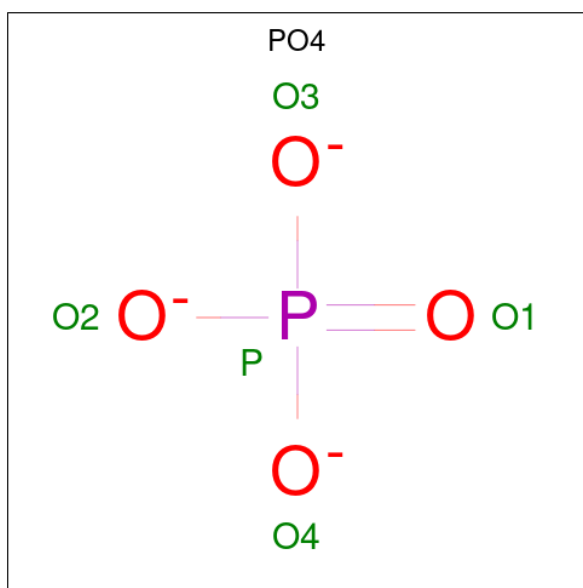
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	R	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	S	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	U	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	V	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	W	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	X	18	Total	C	N	O	0	0	0
			156	99	34	23			

- Molecule 4 is N-((1R,2S)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetyl)-L-isoleucine (CCD ID: 7JA) (formula: C₁₈H₂₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			23	18	1	4		
4	D	1	Total	C	N	O	0	0
			23	18	1	4		
4	F	1	Total	C	N	O	0	0
			23	18	1	4		
4	H	1	Total	C	N	O	0	0
			23	18	1	4		
4	J	1	Total	C	N	O	0	0
			23	18	1	4		
4	L	1	Total	C	N	O	0	0
			23	18	1	4		
4	N	1	Total	C	N	O	0	0
			23	18	1	4		
4	P	1	Total	C	N	O	0	0
			23	18	1	4		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		

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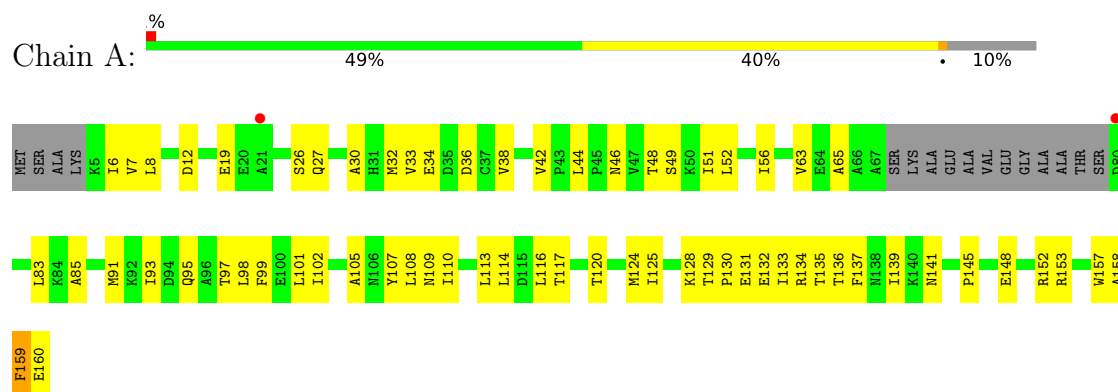
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		

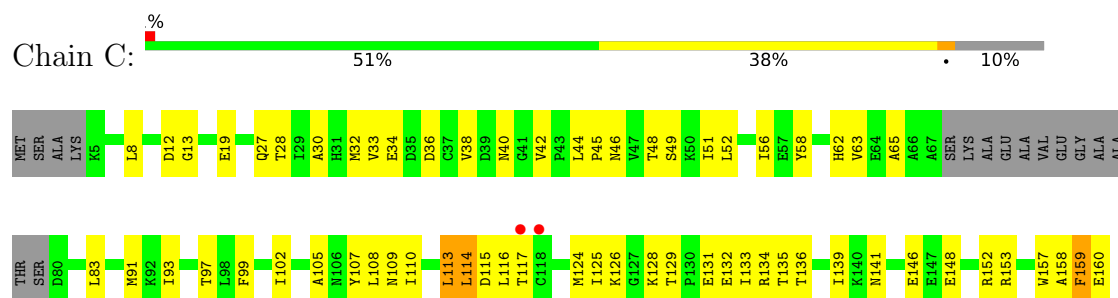
3 Residue-property plots [i](#)

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.

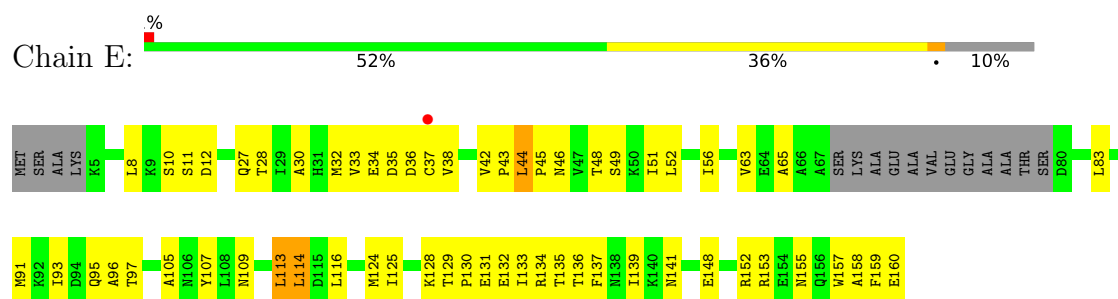
- Molecule 1: SKP1-like protein 1A



- Molecule 1: SKP1-like protein 1A

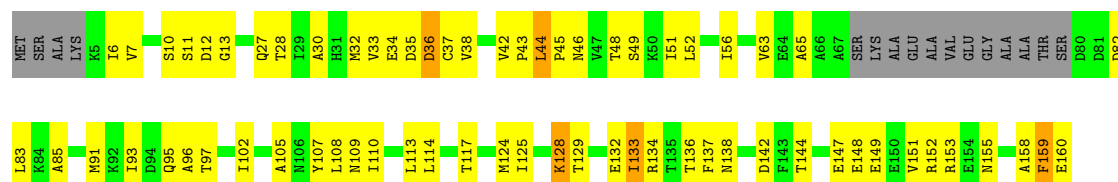


- Molecule 1: SKP1-like protein 1A

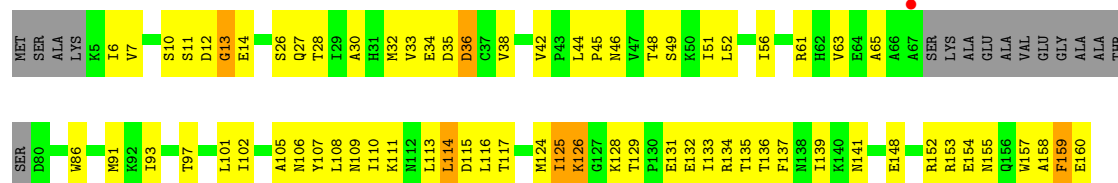


- Molecule 1: SKP1-like protein 1A

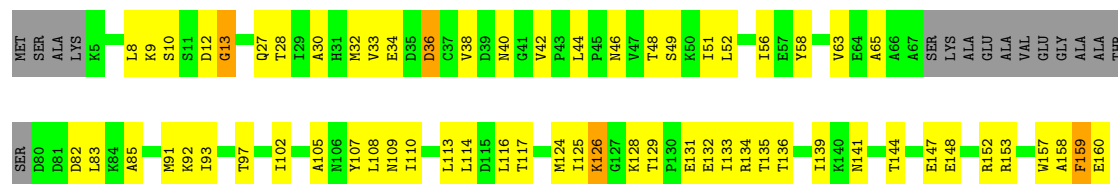




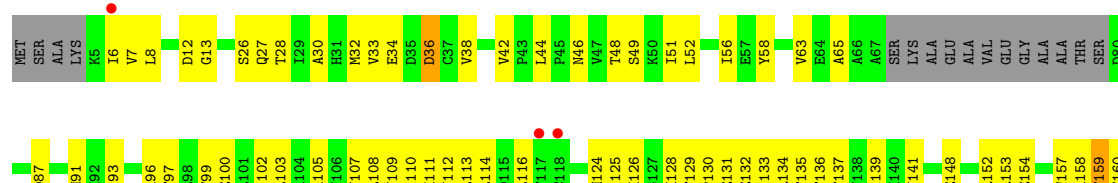
- Molecule 1: SKP1-like protein 1A



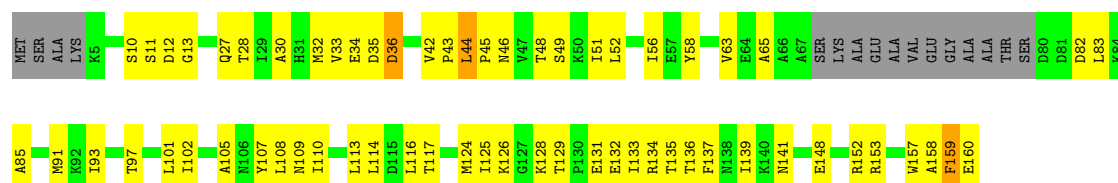
- Molecule 1: SKP1-like protein 1A



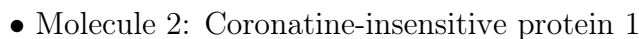
- Molecule 1: SKP1-like protein 1A



- Molecule 1: SKP1-like protein 1A



- Molecule 2: Coronatine-insensitive protein 1



VAL	ASN	GLN	GLN	GLY	GLY	ILE	ARG	GLU	GLU	MET	E563	H564	P565	A566	H567	R578	T579	D580	G581	P582	T583	T584	L588	K589	E590	P591	I592
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

• Molecule 2: Coronatine-insensitive protein 1

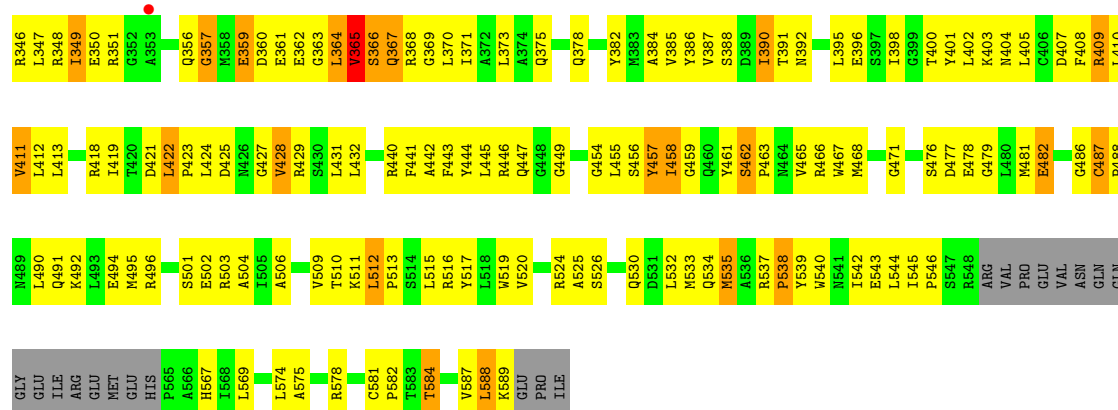


MET	GLU	ASP	PRO	ASP	ILE	LYS	ARG	CYS	LYS	LEU	S12	C13	V14	V17	V20	T21	E22	Q23	V24	P31	K32	V40	C41	K46	I47	E50	H54	V55	T56	M57	A58	L59	C60	V61	T62	F72	L75	R76	S77	L80	K83	P84	B85	L91	I92	P93	E94																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										

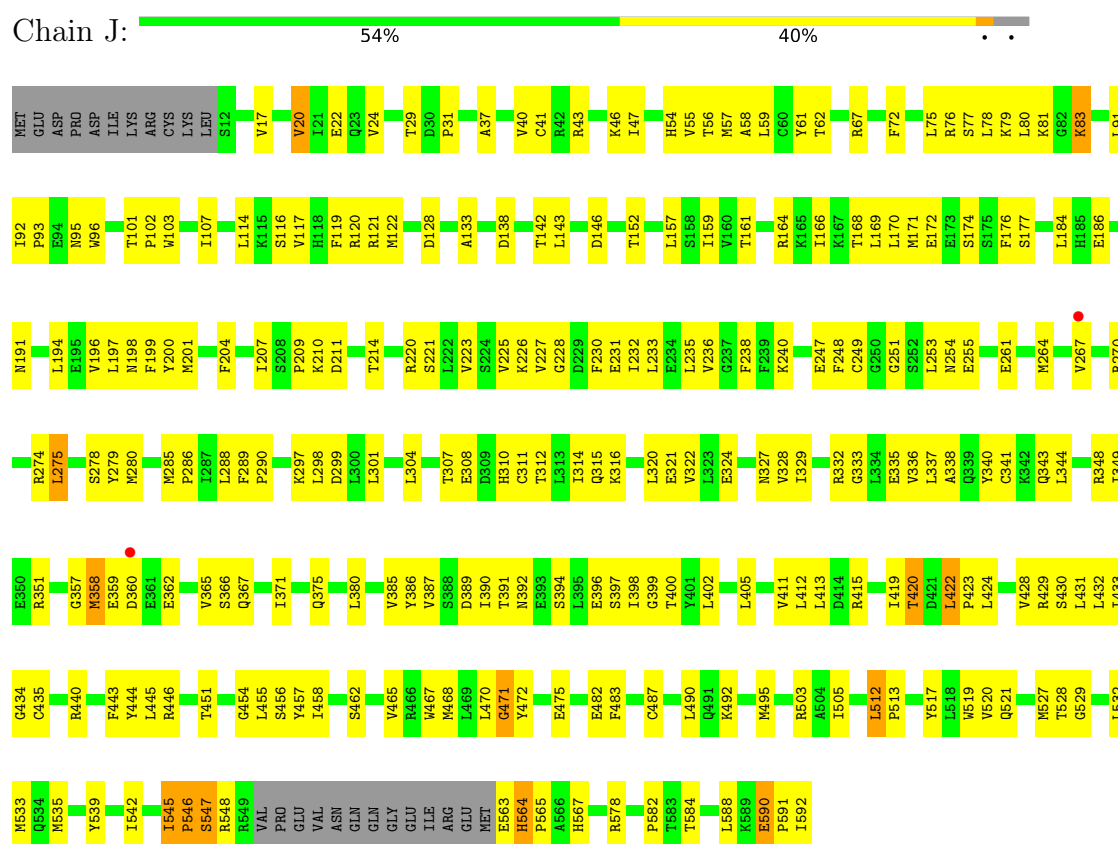
• Molecule 2: Coronatine-insensitive protein 1



M280	M283	M285	P286	L288	F289	P290	F291	A292				T295	K297	L298	D299	L300	L301	A302	A303	L304	L305	E306	T307	E308	D309	H310	C311	T312	L313	I314	K316	C317	L320	E321	L322	L323	E324	R326	N327	V328	C329	G330	D331	G332	G333	V336	L337	C341	K342	Q343	L344	K345								
F204	A205	K206	I207	D211	L212	E213	T214	L215	A216			R220	S224	V225	K226	V227	G228	D229	E231	L232	L233	E234	L235	V236	G237	F238	E247	F248	C249	G250		L253	N254	E255	D256	T257	G258	M259	P260	E261	K262	Y263		L266	V267	F268	P269	R270	K271	L272	C273	R274	L277	S278	Y279					
R136	A137	D138	D139	L140	E141	L142	L143	K144	L145	D146	K147		F151	T152	T153		L156		I159	V160	Q161	H162	C163	R164		T168	L169	G170	Y171	V172	P173	T174	E175	F176	E177	I178	K179	D180	G181	L182	L183	H184	E185	L186	L187	A188	Q189	H190	F191	V192	S193		V196	L197	N198	F199	Y200	M201	T202	E203
R67		R71	F72	P73	N74	L75	R76	S77	L78	K79		K83	P84	R85	A86	M87	M88	F89	N90	L91	I92	P93	E94	N95	G96	G97	L98	H99	V100	T101	S102	W103		E106	I107	S108	N109	N110	L111	R112	Q113	L114	K115	L116	V117	H118	F119	R120	M121	M122	I123	V124	S125	D126	L127	A128	L129		A135	
MET	GLU	ASP	PRO	ASP	ILE	LYS	ARG	CYS	LYS	LEU	S12		T16	V17	D18	D19	V20	I21	E22	Q23	V24	M25		I28		P31	K32	D33	R34	D35	S36	A37	S38	L39	V40			R43	W44		L47	D48	S49	T51	R52	E53	H54	V55	R56	M57	A58	L59	C60	Y61	T62	G63	T64	P65	D66	

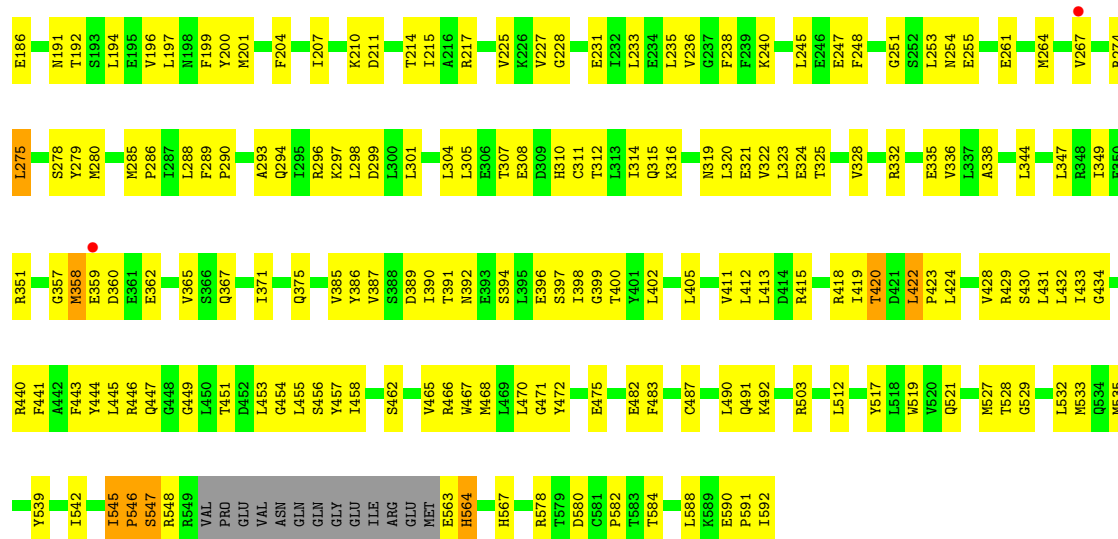


• Molecule 2: Coronatine-insensitive protein 1



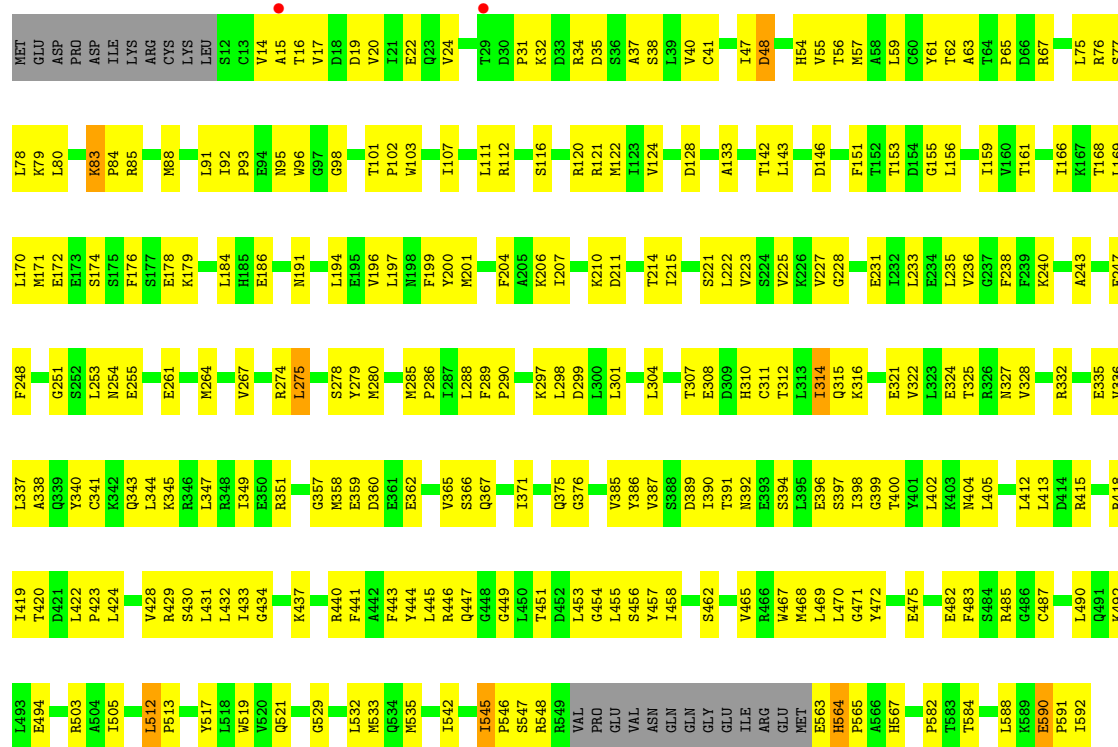
• Molecule 2: Coronatine-insensitive protein 1





• Molecule 2: Coronatine-insensitive protein 1

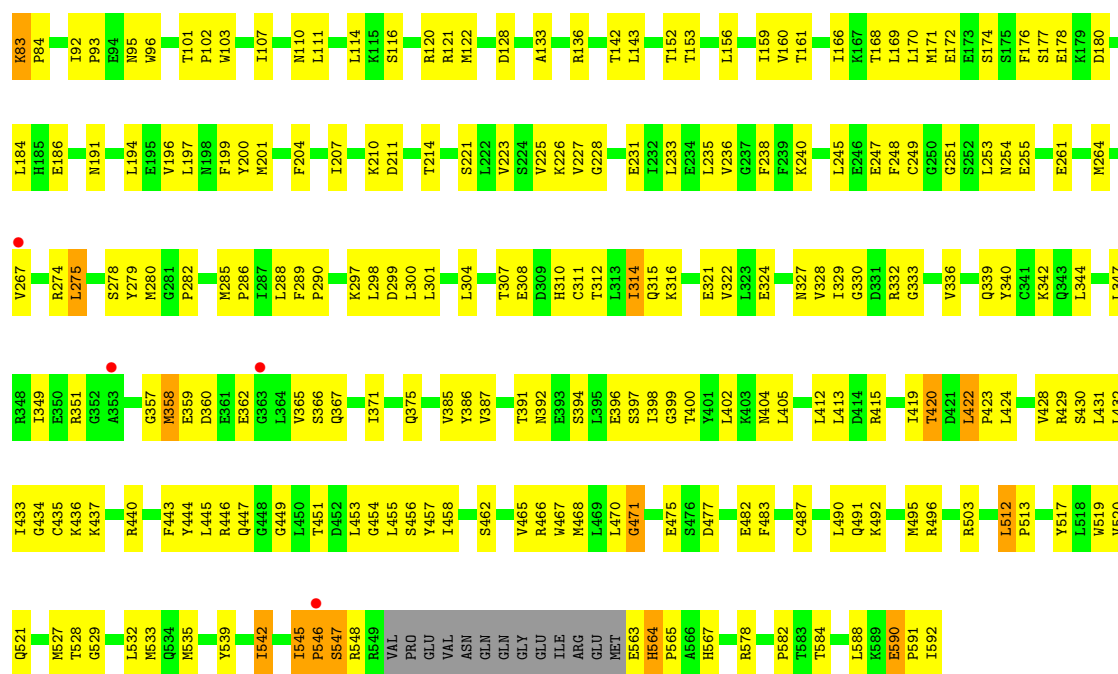
Chain N: 53% 42%



• Molecule 2: Coronatine-insensitive protein 1

Chain P: 53% 40%





- Molecule 3: JAZ1 incomplete degnon peptide

Chain Q: 62% 24% 14%



- Molecule 3: JAZ1 incomplete degnon peptide

Chain R: 62% 24% 14%



- Molecule 3: JAZ1 incomplete degnon peptide

Chain S: 62% 24% 14%



- Molecule 3: JAZ1 incomplete degnon peptide

Chain U: 62% 24% 14%



- Molecule 3: JAZ1 incomplete degnon peptide

Chain V:  62% 24% 14%



- Molecule 3: JAZ1 incomplete degron peptide

Chain W:  67% 19% 14%



- Molecule 3: JAZ1 incomplete degron peptide

Chain X:  57% 29% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.35Å 220.82Å 148.67Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	49.68 – 3.18 49.68 – 3.18	Depositor EDS
% Data completeness (in resolution range)	91.1 (49.68-3.18) 91.1 (49.68-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.215 , 0.263 (Not available) , 0.231	Depositor DCC
R_{free} test set	2000 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.8	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	0.92	EDS
Total number of atoms	46877	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: 7JA, PO4

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	0.63	0/1162	0.88	1/1571 (0.1%)
1	C	0.71	2/1162 (0.2%)	0.91	4/1571 (0.3%)
1	E	0.73	2/1162 (0.2%)	0.98	5/1571 (0.3%)
1	G	0.71	0/1162	1.01	6/1571 (0.4%)
1	I	0.61	0/1162	0.92	4/1571 (0.3%)
1	K	0.62	0/1162	0.90	1/1571 (0.1%)
1	M	0.62	0/1162	0.89	1/1571 (0.1%)
1	O	0.62	0/1162	0.91	3/1571 (0.2%)
2	B	0.78	1/4623 (0.0%)	1.07	25/6238 (0.4%)
2	D	0.75	0/4623	1.07	15/6238 (0.2%)
2	F	0.68	0/4623	1.05	19/6238 (0.3%)
2	H	0.78	1/4566 (0.0%)	1.23	38/6161 (0.6%)
2	J	0.69	0/4623	1.06	19/6238 (0.3%)
2	L	0.67	0/4623	1.06	19/6238 (0.3%)
2	N	0.71	0/4623	1.08	20/6238 (0.3%)
2	P	0.65	1/4623 (0.0%)	1.07	20/6238 (0.3%)
3	Q	0.66	0/158	0.83	0/208
3	R	0.60	0/158	0.85	0/208
3	S	0.53	0/158	0.79	0/208
3	U	0.58	0/158	0.80	0/208
3	V	0.49	0/158	0.83	0/208
3	W	0.56	0/158	0.80	0/208
3	X	0.57	0/158	0.77	0/208
All	All	0.70	7/47329 (0.0%)	1.05	200/63851 (0.3%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	114	LEU	N-CA	7.21	1.56	1.47
1	C	113	LEU	C-N	6.70	1.44	1.33
1	E	113	LEU	C-N	-6.18	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	542	ILE	CA-CB	5.45	1.61	1.54
2	B	59	LEU	CA-C	-5.22	1.47	1.52

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	114	LEU	N-CA-C	-9.90	101.08	113.55
2	F	545	ILE	CA-C-N	9.84	132.14	119.84
2	F	545	ILE	C-N-CA	9.84	132.14	119.84
2	P	545	ILE	CA-C-N	9.67	131.92	119.84
2	P	545	ILE	C-N-CA	9.67	131.92	119.84

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	1146	0	1117	64	0
1	C	1146	0	1117	69	0
1	E	1146	0	1117	66	0
1	G	1146	0	1117	64	0
1	I	1146	0	1117	66	2
1	K	1146	0	1117	62	0
1	M	1146	0	1117	99	0
1	O	1146	0	1117	60	0
2	B	4541	0	4583	239	0
2	D	4541	0	4583	250	2
2	F	4541	0	4583	243	0
2	H	4486	0	4534	456	0
2	J	4541	0	4583	250	0
2	L	4541	0	4583	256	0
2	N	4541	0	4583	285	0
2	P	4541	0	4583	244	0
3	Q	156	0	171	5	0
3	R	156	0	171	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	156	0	171	5	0
3	U	156	0	171	5	0
3	V	156	0	171	5	0
3	W	156	0	171	4	0
3	X	156	0	171	5	0
4	B	23	0	29	16	0
4	D	23	0	28	15	0
4	F	23	0	28	19	0
4	H	23	0	29	21	0
4	J	23	0	28	17	0
4	L	23	0	28	16	0
4	N	23	0	28	17	0
4	P	23	0	28	15	0
5	B	20	0	0	2	0
5	D	20	0	0	3	0
5	F	20	0	0	4	0
5	H	20	0	0	3	0
5	J	20	0	0	2	0
5	L	20	0	0	3	0
5	N	20	0	0	2	0
5	P	20	0	0	3	0
All	All	46877	0	46974	2702	2

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 29.

The worst 5 of 2702 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)
2:B:168:THR:HB	2:B:196:VAL:HG13	1.28	1.14
2:L:168:THR:HB	2:L:196:VAL:HG13	1.22	1.14
2:F:168:THR:HB	2:F:196:VAL:HG13	1.27	1.13
4:J:1100:7JA:H12	4:J:1100:7JA:H04	1.29	1.13
1:G:151:VAL:HG11	2:H:39:LEU:HD21	1.28	1.13

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:429:ARG:NH2	1:I:61:ARG:NH1[2_555]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:429:ARG:NH1	1:I:86:TRP:CE3[2_555]	2.14	0.06

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	G	140/160 (88%)	114 (81%)	22 (16%)	4 (3%)	3	21
1	I	140/160 (88%)	117 (84%)	20 (14%)	3 (2%)	5	27
1	K	140/160 (88%)	117 (84%)	19 (14%)	4 (3%)	3	21
1	M	109/160 (68%)	88 (81%)	18 (16%)	3 (3%)	4	22
1	O	140/160 (88%)	112 (80%)	25 (18%)	3 (2%)	5	27
2	B	36/592 (6%)	30 (83%)	6 (17%)	0	100	100
2	D	24/592 (4%)	21 (88%)	3 (12%)	0	100	100
2	H	558/592 (94%)	430 (77%)	98 (18%)	30 (5%)	1	10
2	J	564/592 (95%)	504 (89%)	52 (9%)	8 (1%)	9	36
2	L	536/592 (90%)	480 (90%)	50 (9%)	6 (1%)	11	41
2	N	65/592 (11%)	57 (88%)	7 (11%)	1 (2%)	8	35
2	P	564/592 (95%)	500 (89%)	56 (10%)	8 (1%)	9	36
3	S	4/21 (19%)	4 (100%)	0	0	100	100
3	U	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	V	14/21 (67%)	13 (93%)	1 (7%)	0	100	100
3	W	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	X	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
All	All	3082/5049 (61%)	2632 (85%)	380 (12%)	70 (2%)	5	26

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	36	ASP
2	H	97	GLY
2	H	200	TYR
2	H	269	PRO
2	H	270	ARG

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

40 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	PO4	F	1101	-	4,4,4	4.38	4 (100%)	6,6,6	1.69	2 (33%)
5	PO4	B	1104	-	4,4,4	4.43	4 (100%)	6,6,6	1.03	0
4	7JA	L	1100	-	23,23,23	2.04	5 (21%)	25,30,30	1.88	5 (20%)
5	PO4	J	1104	-	4,4,4	4.34	4 (100%)	6,6,6	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	7JA	P	1100	-	23,23,23	2.03	5 (21%)	25,30,30	2.06	6 (24%)
4	7JA	N	1100	-	23,23,23	2.18	6 (26%)	25,30,30	2.04	6 (24%)
5	PO4	J	1101	-	4,4,4	4.27	4 (100%)	6,6,6	0.95	0
5	PO4	L	1104	-	4,4,4	4.33	4 (100%)	6,6,6	0.81	0
4	7JA	H	1100	-	23,23,23	1.62	5 (21%)	25,30,30	2.02	8 (32%)
5	PO4	P	1102	-	4,4,4	4.47	4 (100%)	6,6,6	0.49	0
5	PO4	B	1101	-	4,4,4	4.42	4 (100%)	6,6,6	0.70	0
5	PO4	D	1104	-	4,4,4	4.33	3 (75%)	6,6,6	1.13	0
5	PO4	B	1102	-	4,4,4	4.33	4 (100%)	6,6,6	0.69	0
4	7JA	F	1100	-	23,23,23	2.10	5 (21%)	25,30,30	2.12	5 (20%)
5	PO4	P	1104	-	4,4,4	4.40	4 (100%)	6,6,6	1.05	0
5	PO4	N	1102	-	4,4,4	4.55	4 (100%)	6,6,6	0.75	0
5	PO4	H	1101	-	4,4,4	4.54	4 (100%)	6,6,6	1.05	1 (16%)
5	PO4	F	1102	-	4,4,4	4.58	4 (100%)	6,6,6	0.38	0
5	PO4	N	1103	-	4,4,4	4.31	4 (100%)	6,6,6	1.16	0
5	PO4	F	1103	-	4,4,4	4.20	4 (100%)	6,6,6	0.73	0
5	PO4	H	1104	-	4,4,4	4.41	4 (100%)	6,6,6	1.91	1 (16%)
4	7JA	B	1100	-	23,23,23	1.66	4 (17%)	25,30,30	2.11	6 (24%)
5	PO4	F	1104	-	4,4,4	4.31	4 (100%)	6,6,6	1.32	0
5	PO4	P	1103	-	4,4,4	4.44	4 (100%)	6,6,6	0.96	0
5	PO4	B	1103	-	4,4,4	4.12	4 (100%)	6,6,6	0.74	0
4	7JA	D	1100	-	23,23,23	2.11	5 (21%)	25,30,30	2.02	5 (20%)
5	PO4	D	1102	-	4,4,4	4.32	4 (100%)	6,6,6	0.28	0
5	PO4	D	1103	-	4,4,4	4.23	4 (100%)	6,6,6	0.91	0
5	PO4	J	1103	-	4,4,4	4.37	4 (100%)	6,6,6	0.78	0
5	PO4	L	1101	-	4,4,4	4.18	4 (100%)	6,6,6	0.81	0
5	PO4	L	1103	-	4,4,4	4.44	4 (100%)	6,6,6	0.64	0
5	PO4	L	1102	-	4,4,4	4.45	4 (100%)	6,6,6	0.32	0
5	PO4	D	1101	-	4,4,4	4.22	4 (100%)	6,6,6	0.89	0
5	PO4	H	1103	-	4,4,4	4.37	4 (100%)	6,6,6	0.68	0
5	PO4	J	1102	-	4,4,4	4.55	4 (100%)	6,6,6	0.43	0
5	PO4	H	1102	-	4,4,4	4.55	4 (100%)	6,6,6	0.65	0
5	PO4	P	1101	-	4,4,4	4.44	4 (100%)	6,6,6	0.72	0
5	PO4	N	1104	-	4,4,4	4.53	4 (100%)	6,6,6	1.00	0
5	PO4	N	1101	-	4,4,4	4.27	4 (100%)	6,6,6	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	7JA	J	1100	-	23,23,23	2.11	6 (26%)	25,30,30	2.08	6 (24%)

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
4	7JA	B	1100	-	-	6/23/36/36	0/1/1/1
4	7JA	F	1100	-	-	7/23/36/36	0/1/1/1
4	7JA	L	1100	-	-	7/23/36/36	0/1/1/1
4	7JA	D	1100	-	-	8/23/36/36	0/1/1/1
4	7JA	P	1100	-	-	7/23/36/36	0/1/1/1
4	7JA	J	1100	-	-	5/23/36/36	0/1/1/1
4	7JA	N	1100	-	-	7/23/36/36	0/1/1/1
4	7JA	H	1100	-	-	12/23/36/36	0/1/1/1

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1102	PO4	P-O1	7.07	1.67	1.50
5	P	1103	PO4	P-O1	7.00	1.66	1.50
5	J	1104	PO4	P-O1	6.97	1.66	1.50
4	N	1100	7JA	O-C	6.96	1.42	1.22
5	P	1104	PO4	P-O1	6.92	1.66	1.50

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	1100	7JA	CB-CA-N	-6.37	98.25	111.35
4	J	1100	7JA	CB-CA-N	-5.79	99.44	111.35
4	D	1100	7JA	CB-CA-N	-5.78	99.46	111.35
4	B	1100	7JA	CB-CA-N	-5.76	99.51	111.35
4	F	1100	7JA	CB-CA-N	-5.59	99.86	111.35

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

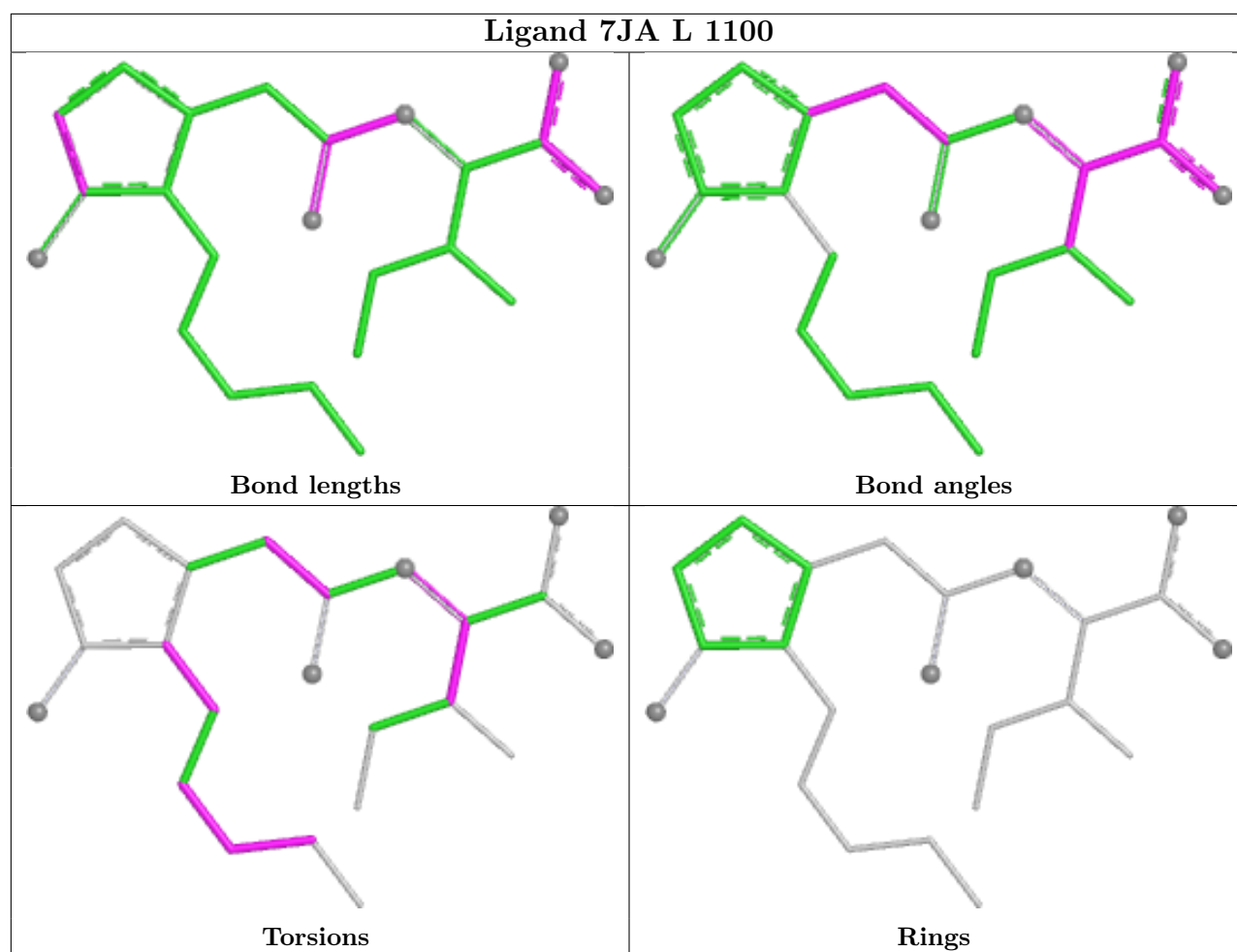
Mol	Chain	Res	Type	Atoms
4	B	1100	7JA	C11-C12-C13-N
4	B	1100	7JA	C11-C12-C13-O14
4	D	1100	7JA	C11-C12-C13-N
4	D	1100	7JA	C11-C12-C13-O14
4	F	1100	7JA	C11-C12-C13-N

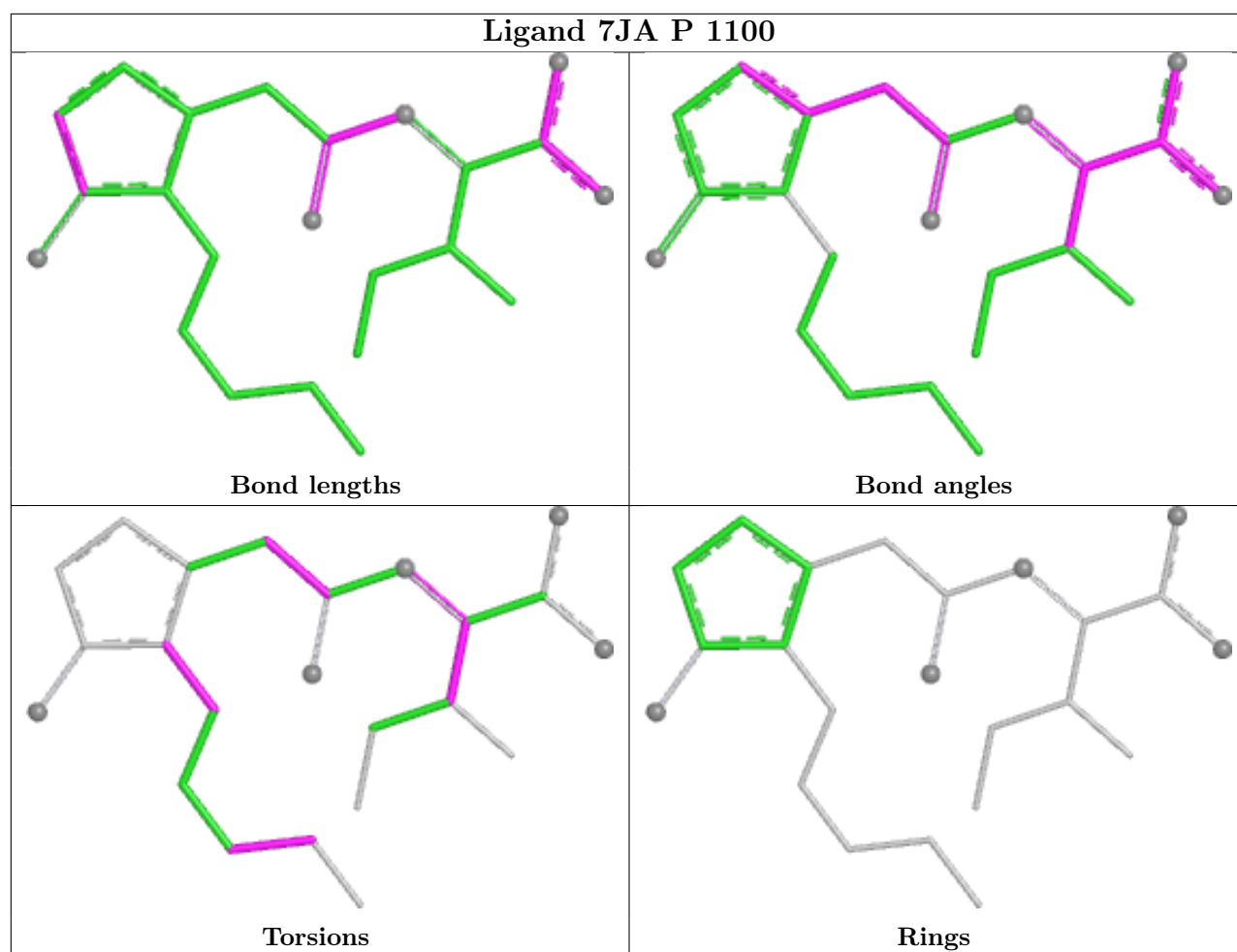
There are no ring outliers.

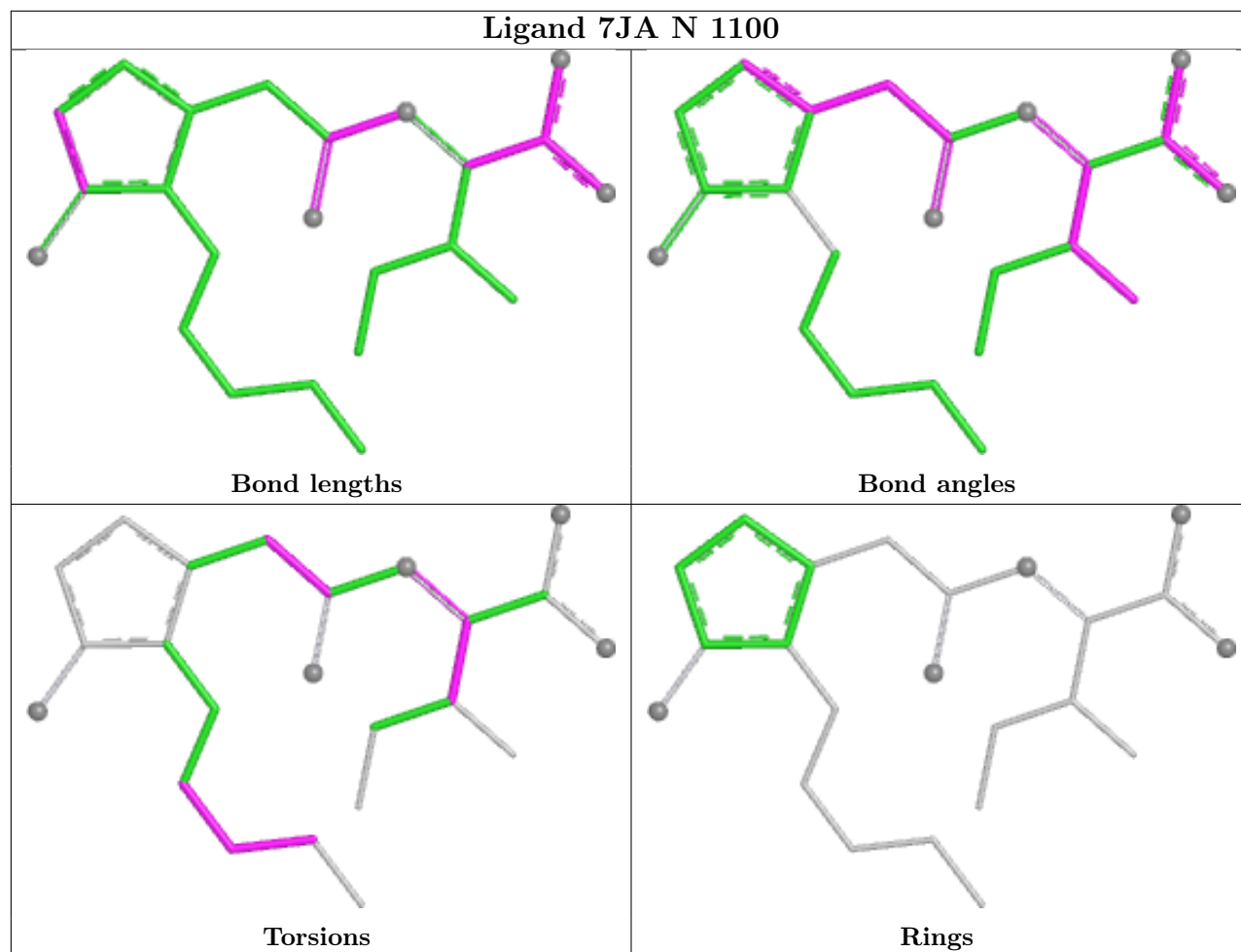
18 monomers are involved in 158 short contacts:

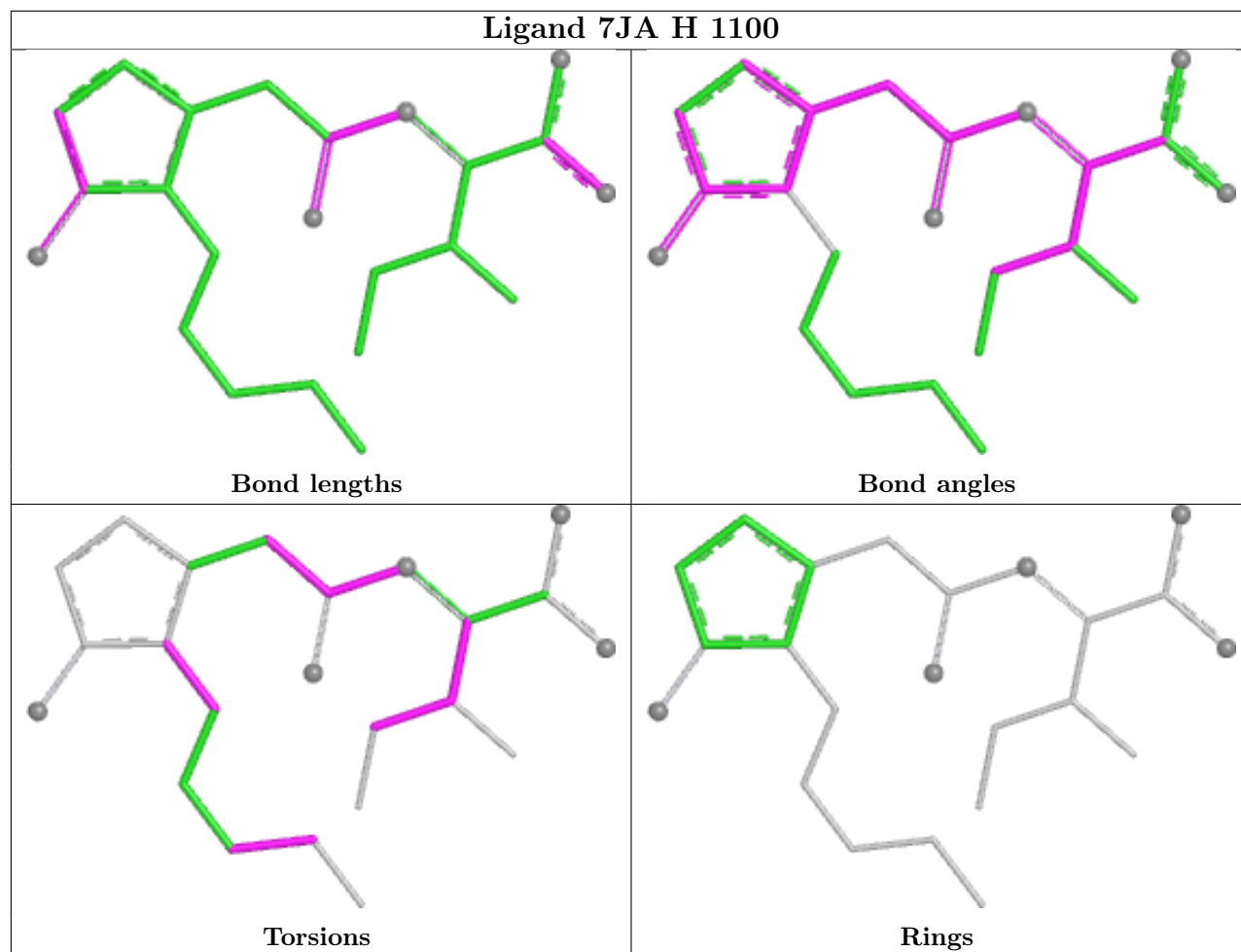
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1101	PO4	1	0
4	L	1100	7JA	16	0
4	P	1100	7JA	15	0
4	N	1100	7JA	17	0
4	H	1100	7JA	21	0
4	F	1100	7JA	19	0
5	N	1103	PO4	2	0
5	F	1103	PO4	3	0
4	B	1100	7JA	16	0
5	P	1103	PO4	3	0
5	B	1103	PO4	2	0
4	D	1100	7JA	15	0
5	D	1103	PO4	3	0
5	J	1103	PO4	2	0
5	L	1101	PO4	1	0
5	L	1103	PO4	2	0
5	H	1103	PO4	3	0
4	J	1100	7JA	17	0

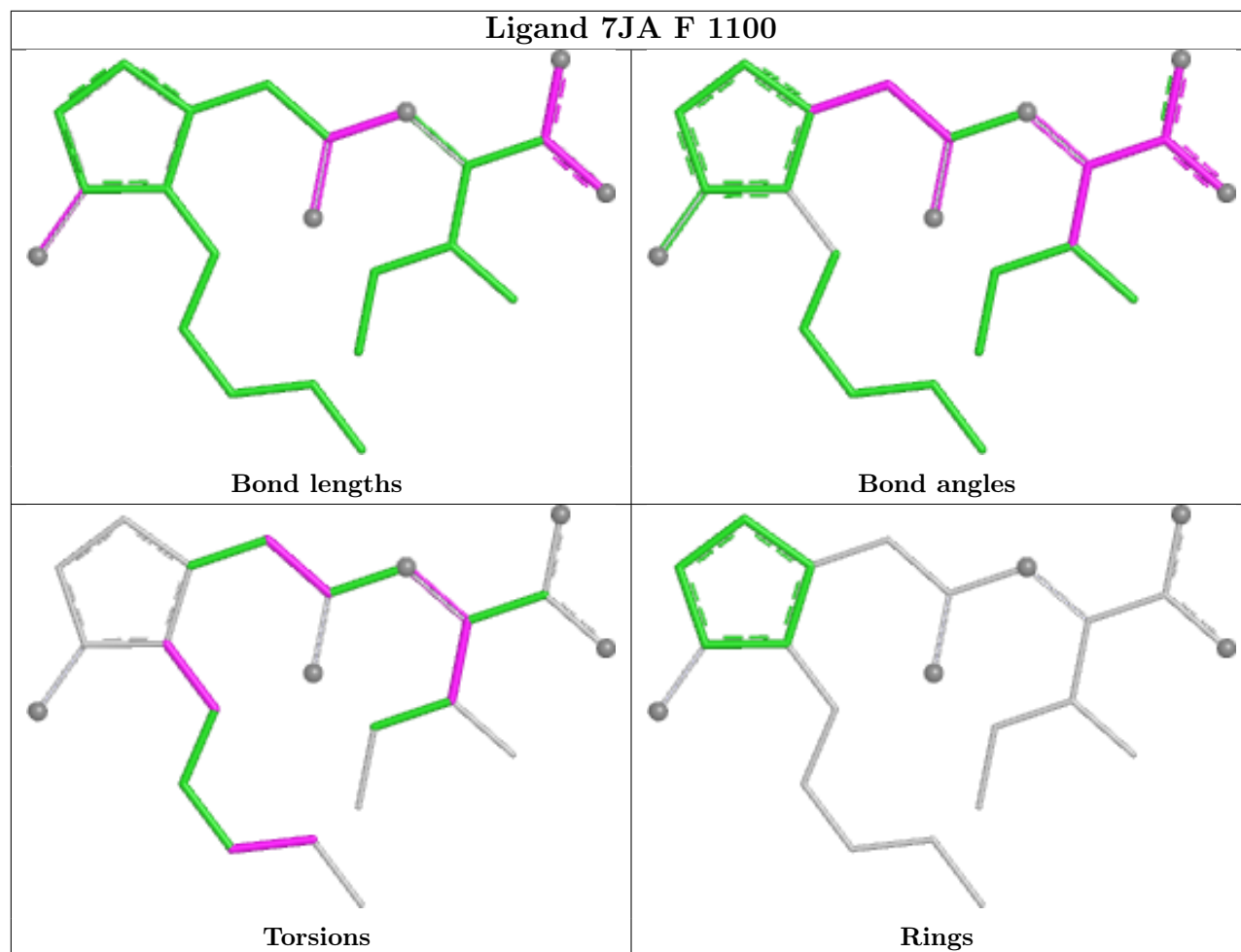
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

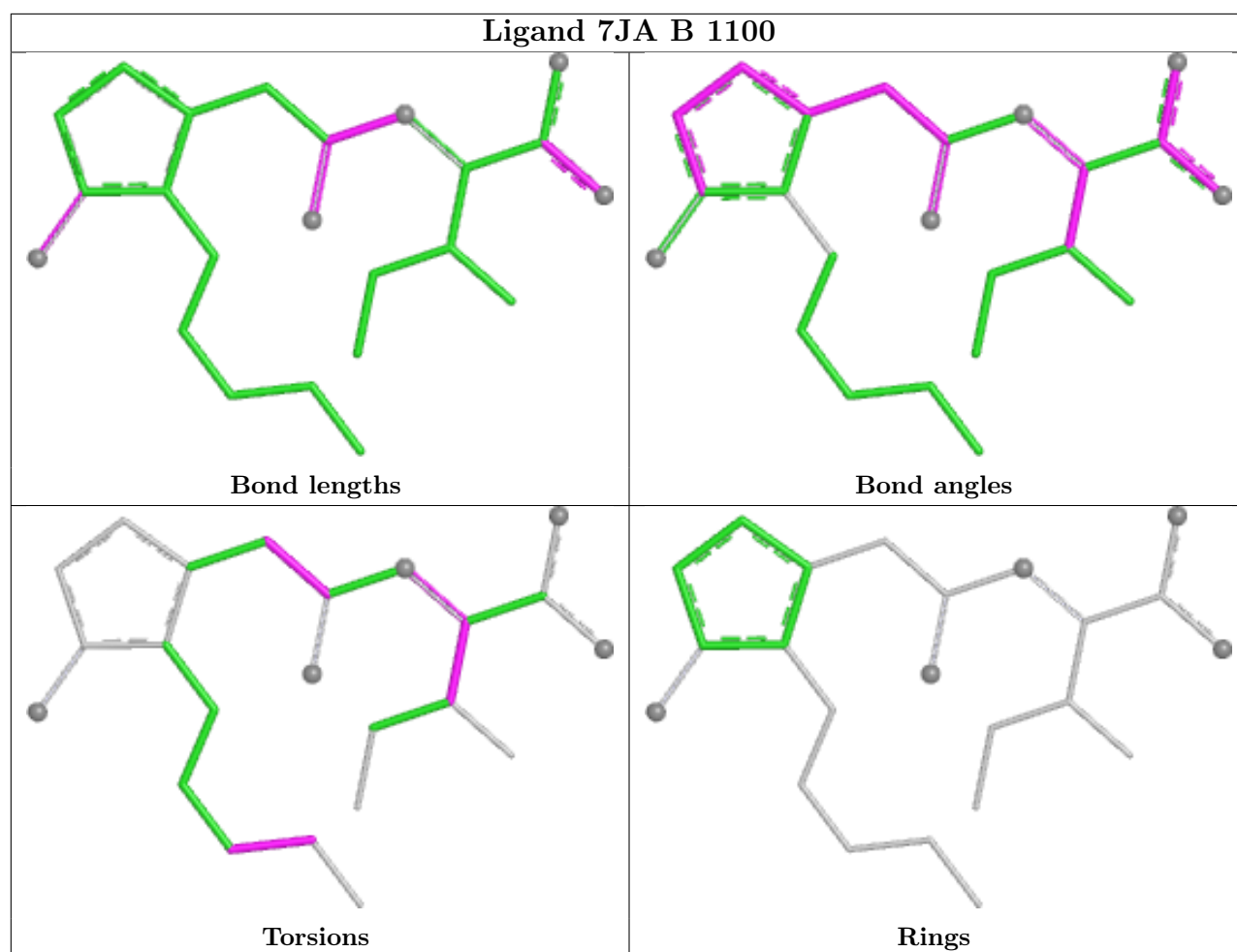


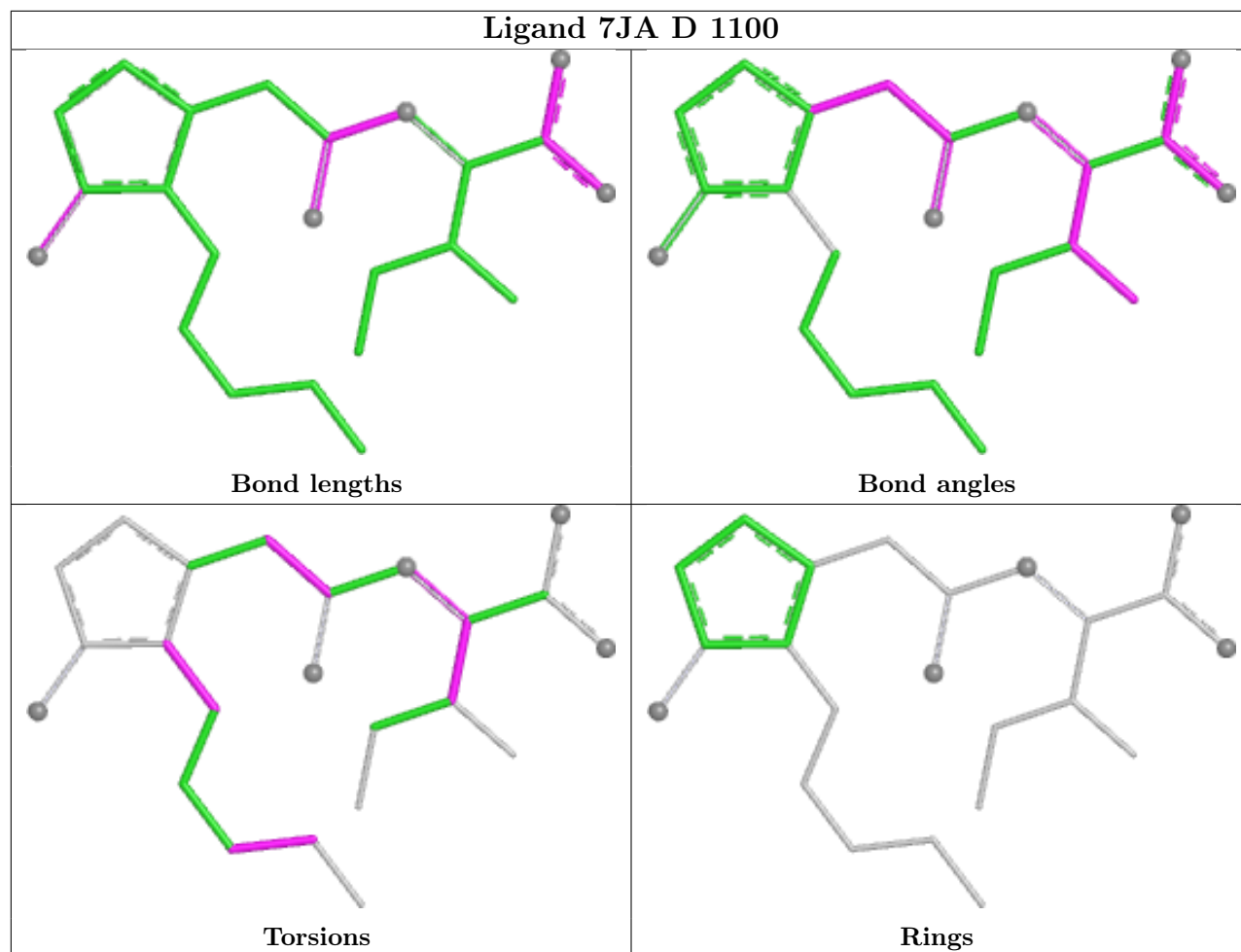


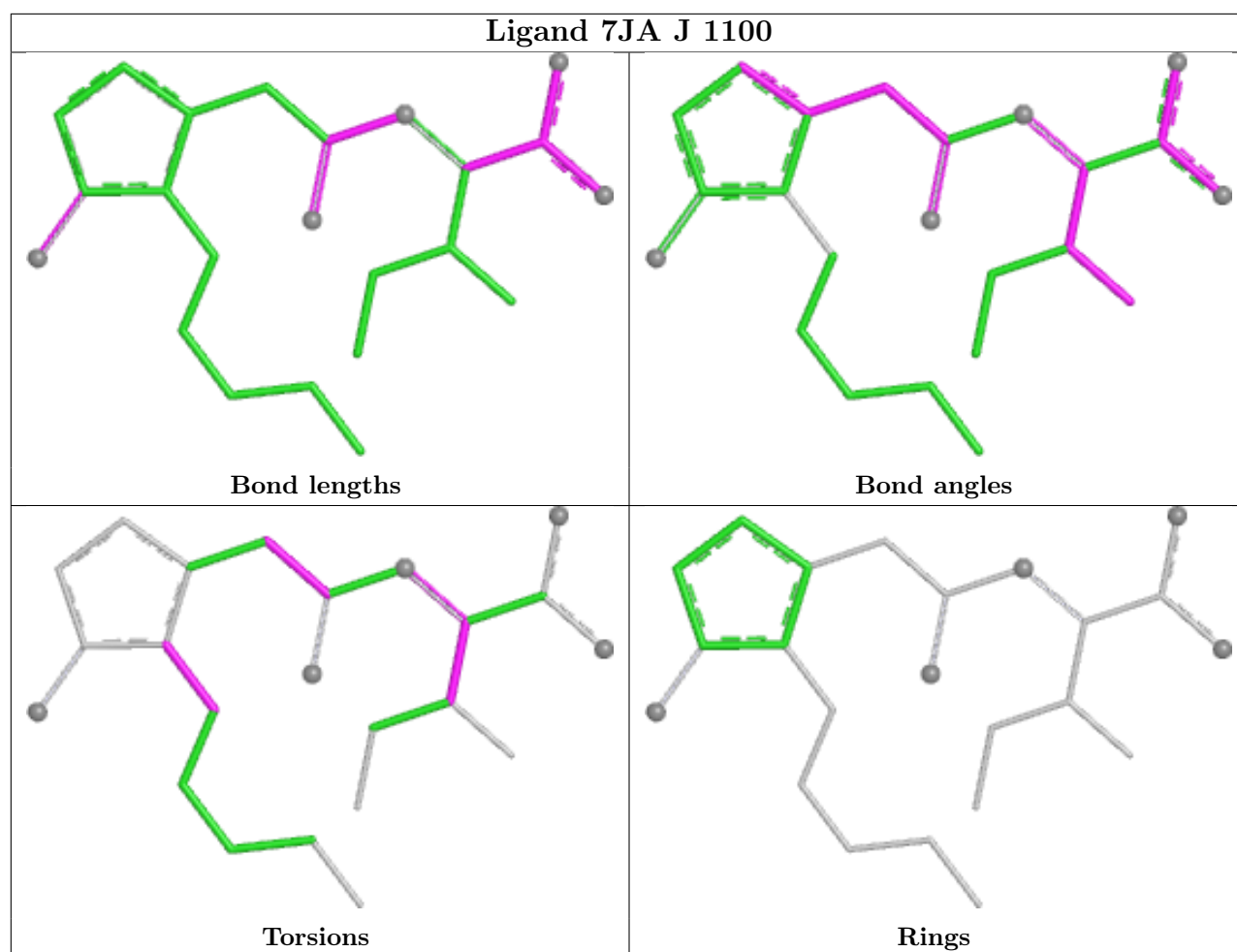












5.7 Other polymers [i](#)

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	144/160 (90%)	0.10	2 (1%) 73 53	38, 87, 141, 157	0
1	C	144/160 (90%)	0.12	2 (1%) 73 53	40, 90, 140, 159	0
1	E	144/160 (90%)	0.16	1 (0%) 84 69	41, 85, 136, 157	0
1	G	144/160 (90%)	-0.20	0 100 100	37, 81, 136, 156	0
1	I	144/160 (90%)	0.12	1 (0%) 84 69	43, 88, 138, 160	0
1	K	144/160 (90%)	-0.05	0 100 100	43, 89, 140, 158	0
1	M	144/160 (90%)	0.22	3 (2%) 63 42	45, 89, 139, 163	0
1	O	144/160 (90%)	0.01	0 100 100	43, 88, 138, 159	0
2	B	568/592 (95%)	-0.17	5 (0%) 81 64	31, 60, 122, 191	0
2	D	568/592 (95%)	-0.19	3 (0%) 87 75	33, 61, 124, 190	0
2	F	568/592 (95%)	-0.25	7 (1%) 76 57	32, 63, 125, 191	0
2	H	562/592 (94%)	-0.66	1 (0%) 91 85	29, 57, 106, 169	0
2	J	568/592 (95%)	-0.30	2 (0%) 88 78	33, 64, 124, 194	0
2	L	568/592 (95%)	-0.32	2 (0%) 88 78	33, 64, 125, 192	0
2	N	568/592 (95%)	0.10	2 (0%) 88 78	33, 69, 126, 194	0
2	P	568/592 (95%)	-0.13	4 (0%) 84 69	34, 68, 126, 192	0
3	Q	18/21 (85%)	-0.05	0 100 100	61, 77, 108, 128	0
3	R	18/21 (85%)	-0.02	0 100 100	63, 78, 108, 131	0
3	S	18/21 (85%)	-0.35	0 100 100	64, 78, 109, 129	0
3	U	18/21 (85%)	0.15	0 100 100	60, 80, 109, 130	0
3	V	18/21 (85%)	-0.21	0 100 100	61, 81, 108, 132	0
3	W	18/21 (85%)	0.13	0 100 100	66, 83, 110, 132	0
3	X	18/21 (85%)	-0.18	0 100 100	65, 81, 109, 131	0
All	All	5816/6163 (94%)	-0.18	35 (0%) 85 72	29, 68, 128, 194	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	360	ASP	3.3
1	C	118	CYS	3.2
1	C	117	THR	3.1
2	N	15	ALA	2.9
2	D	429	ARG	2.7

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	PO4	H	1102	5/5	0.78	0.13	72,73,108,121	0
5	PO4	N	1102	5/5	0.80	0.12	64,78,83,116	0
5	PO4	P	1102	5/5	0.85	0.14	63,72,83,106	0
5	PO4	N	1104	5/5	0.86	0.10	56,57,89,100	0
5	PO4	F	1102	5/5	0.86	0.11	56,74,78,96	0
5	PO4	B	1102	5/5	0.87	0.09	49,75,81,91	0
5	PO4	D	1102	5/5	0.88	0.10	55,73,86,95	0
5	PO4	H	1101	5/5	0.89	0.07	65,80,94,96	0
5	PO4	H	1104	5/5	0.90	0.09	57,64,69,95	0
5	PO4	D	1104	5/5	0.91	0.11	49,60,85,91	0
5	PO4	P	1104	5/5	0.91	0.08	50,58,89,93	0
5	PO4	J	1102	5/5	0.92	0.08	53,74,83,101	0
5	PO4	L	1104	5/5	0.92	0.08	52,60,91,94	0
4	7JA	N	1100	23/23	0.92	0.13	49,61,73,86	0
4	7JA	B	1100	23/23	0.93	0.16	34,55,70,87	0
5	PO4	J	1104	5/5	0.93	0.11	57,60,82,86	0
5	PO4	L	1102	5/5	0.93	0.05	64,67,83,96	0

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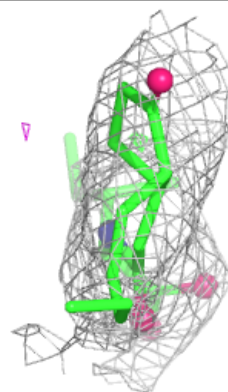
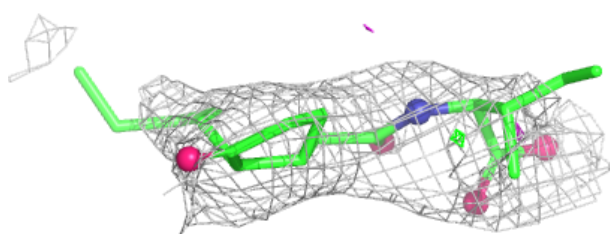
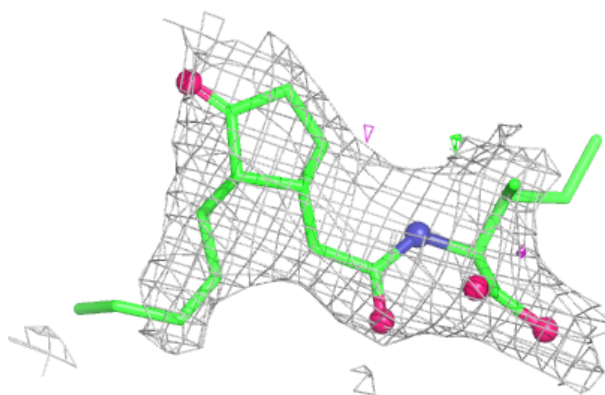
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	P	1103	5/5	0.93	0.08	47,55,70,76	0
4	7JA	H	1100	23/23	0.93	0.12	38,62,77,81	0
5	PO4	N	1103	5/5	0.94	0.07	48,51,62,80	0
5	PO4	F	1104	5/5	0.94	0.08	48,54,80,83	0
4	7JA	J	1100	23/23	0.94	0.13	39,55,72,83	0
5	PO4	N	1101	5/5	0.94	0.08	42,48,74,75	0
4	7JA	P	1100	23/23	0.94	0.12	47,59,73,85	0
4	7JA	L	1100	23/23	0.95	0.10	42,58,72,86	0
4	7JA	F	1100	23/23	0.95	0.12	42,56,70,88	0
5	PO4	B	1104	5/5	0.95	0.07	47,63,91,96	0
5	PO4	P	1101	5/5	0.96	0.05	40,51,70,73	0
5	PO4	B	1101	5/5	0.96	0.06	35,48,61,72	0
5	PO4	F	1101	5/5	0.96	0.07	40,41,55,77	0
4	7JA	D	1100	23/23	0.96	0.10	37,55,68,85	0
5	PO4	L	1103	5/5	0.97	0.06	45,48,58,71	0
5	PO4	D	1101	5/5	0.97	0.05	42,45,58,71	0
5	PO4	F	1103	5/5	0.97	0.05	44,47,48,69	0
5	PO4	L	1101	5/5	0.97	0.05	36,48,65,73	0
5	PO4	D	1103	5/5	0.97	0.07	38,46,52,75	0
5	PO4	H	1103	5/5	0.98	0.04	35,56,67,68	0
5	PO4	J	1103	5/5	0.98	0.04	42,45,52,68	0
5	PO4	J	1101	5/5	0.98	0.06	37,45,66,73	0
5	PO4	B	1103	5/5	0.99	0.06	41,45,51,66	0

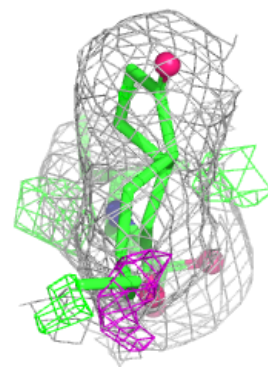
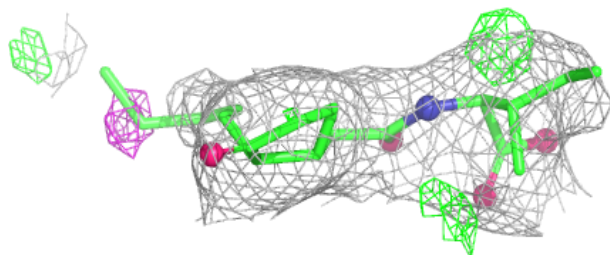
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7JA N 1100:

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

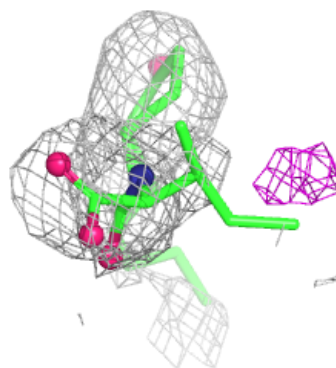
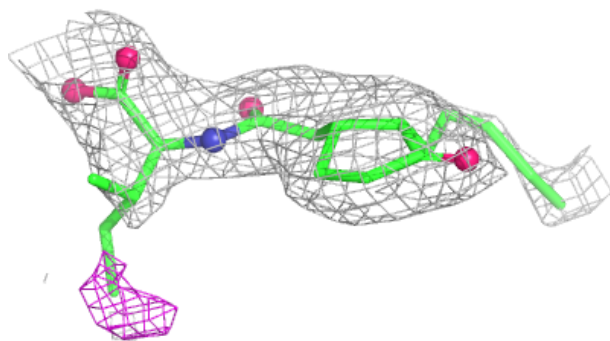
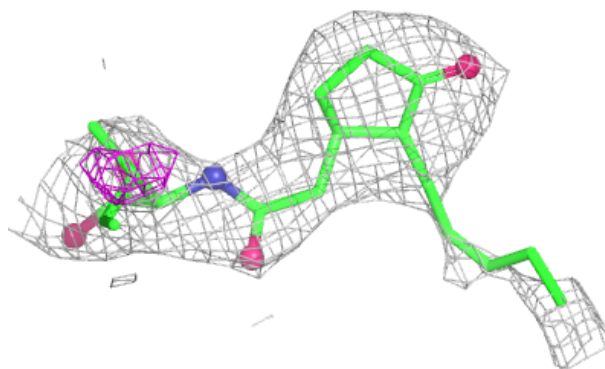
**Electron density around 7JA B 1100:**

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

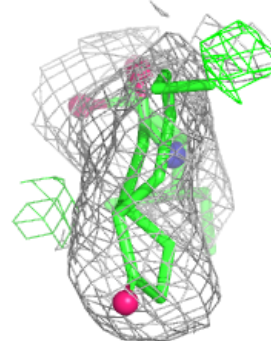
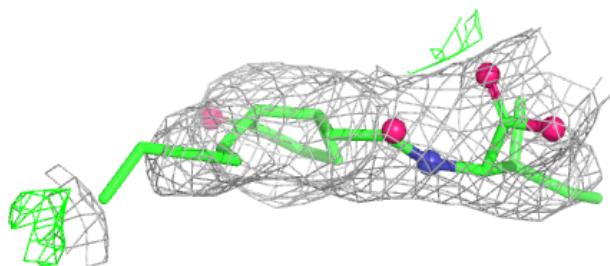
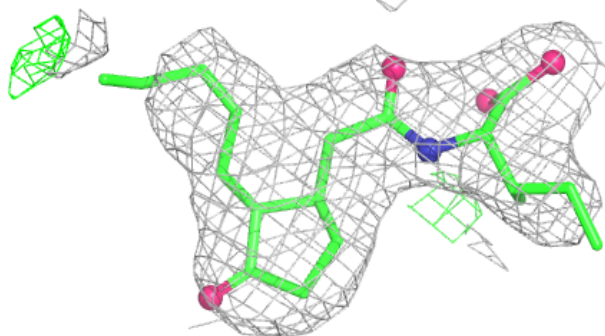


Electron density around 7JA H 1100:

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

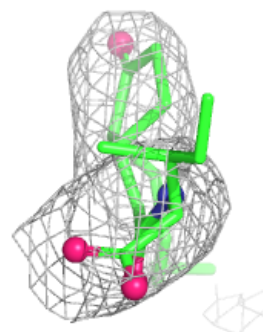
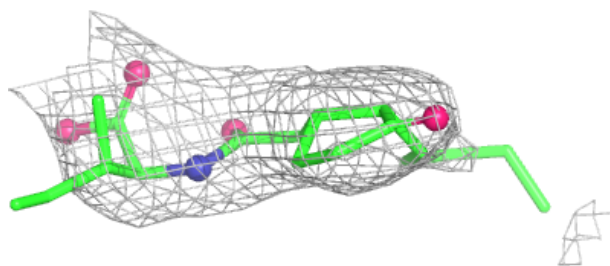
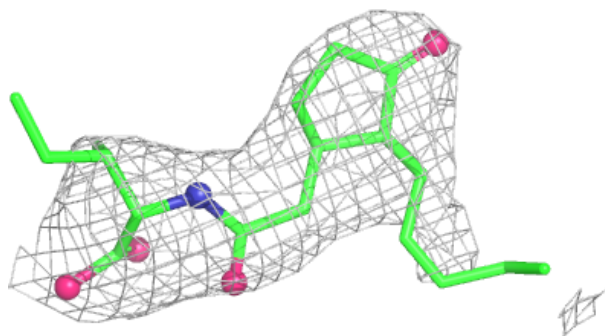
**Electron density around 7JA J 1100:**

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

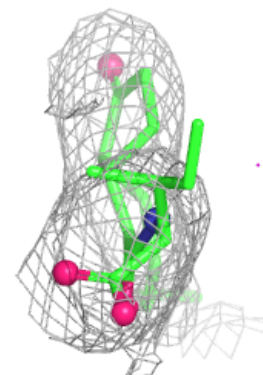
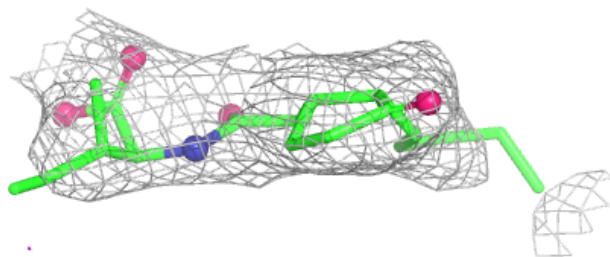


Electron density around 7JA P 1100:

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

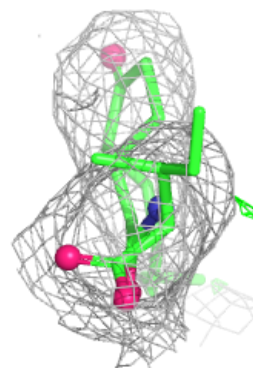
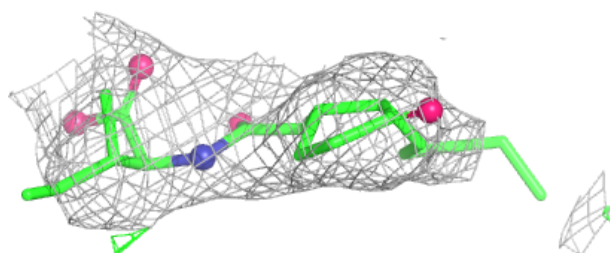
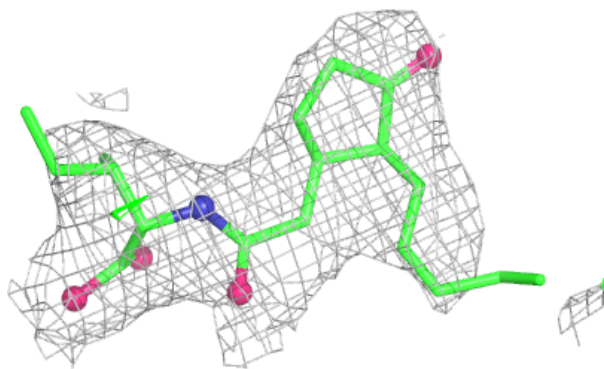
**Electron density around 7JA L 1100:**

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

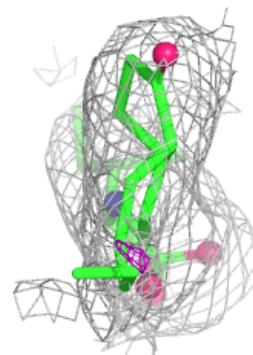
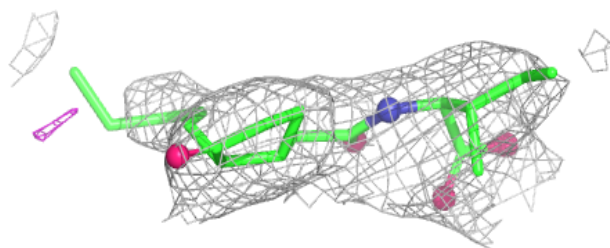


Electron density around 7JA F 1100:

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

**Electron density around 7JA D 1100:**

$2mF_o-DF_c$ (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.