



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:53 PM UTC

PDB ID : 3OGM / pdb_00003ogm
Title : Structure of COI1-ASK1 in complex with coronatine and the JAZ1 degra
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 : 3.34 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

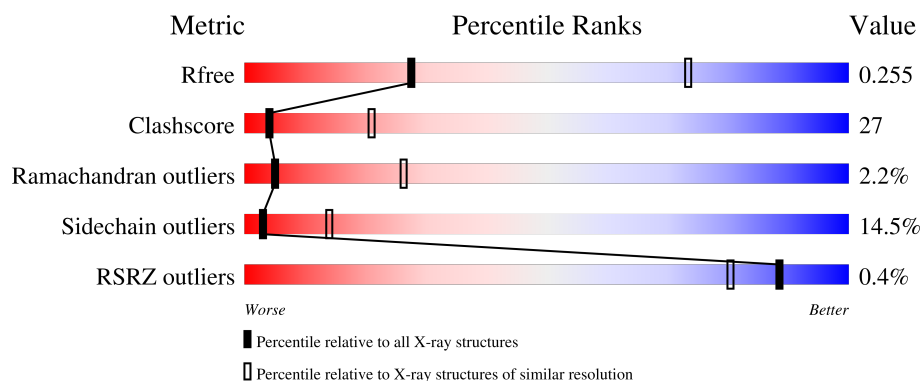
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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	% 48% 36% 6% 10%
1	C	160	50% 32% 8% 10%
1	E	160	% 49% 34% 7% 10%
1	G	160	48% 36% 6% 10%
1	I	160	% 45% 37% 8% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	160	
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	OGK	H	4100	X	-	X	-
5	PO4	B	1101	-	X	-	-
5	PO4	B	1102	-	X	-	-
5	PO4	B	1103	-	X	-	-
5	PO4	B	1104	-	X	-	-
5	PO4	D	1101	-	X	-	-
5	PO4	D	1102	-	X	-	-

Continued on next page...

Continued from previous page...

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

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			

Continued on next page...

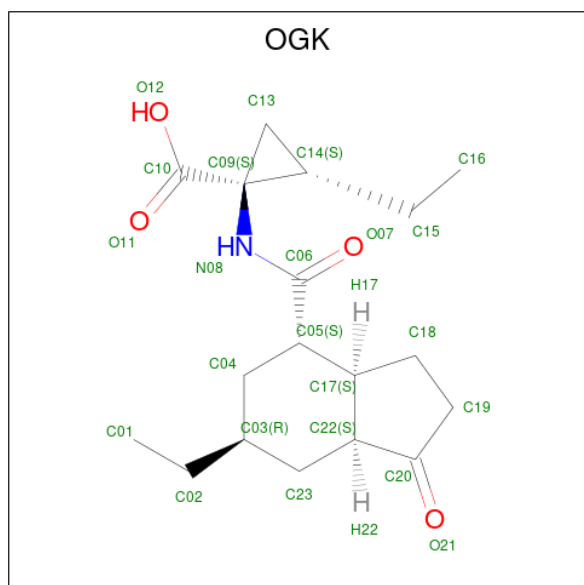
Continued from previous page...

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 degran peptide.

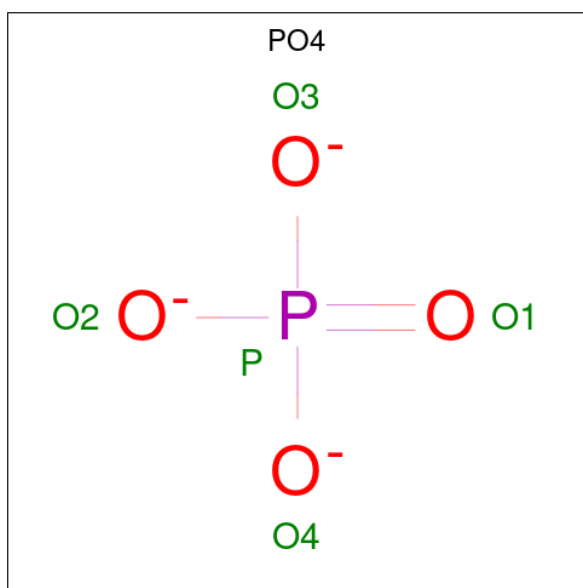
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	R	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	S	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	U	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	V	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	W	18	Total	C	N	O	0	0	0
			156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

- Molecule 4 is (1S,2S)-2-ethyl-1-([(3aS,4S,6R,7aS)-6-ethyl-1-oxooctahydro-1H-inden-4-yl]carbonyl)amino)cyclopropanecarboxylic acid (CCD ID: OGK) (formula: C₁₈H₂₇NO₄).



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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

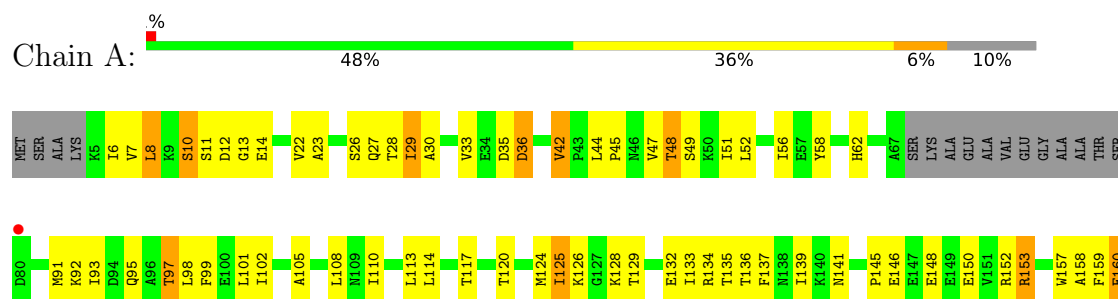
Continued from previous page...

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		

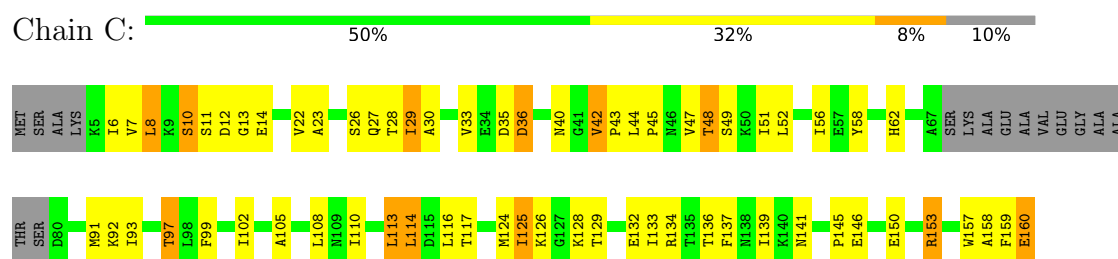
3 Residue-property plots

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.

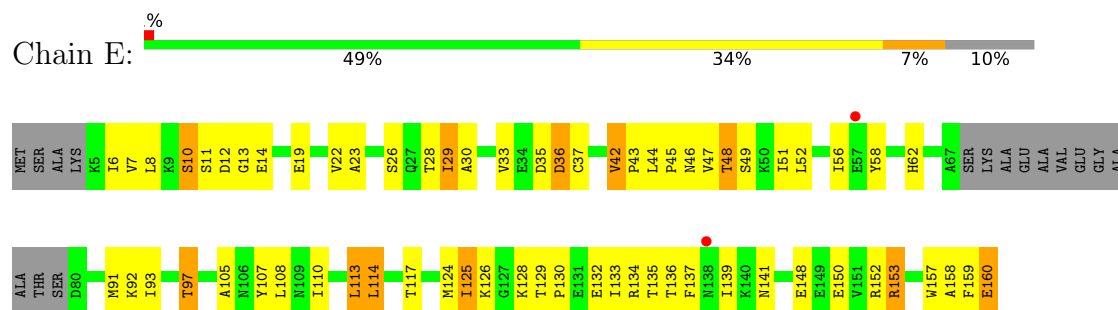
• Molecule 1: SKP1-like protein 1A



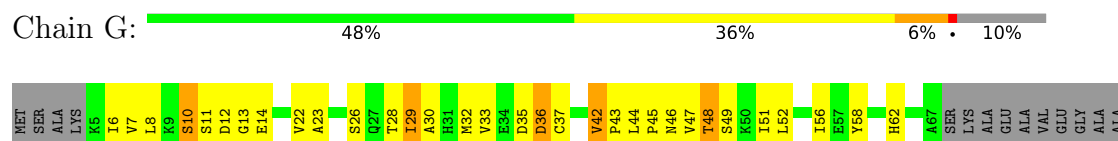
• Molecule 1: SKP1-like protein 1A



• Molecule 1: SKP1-like protein 1A

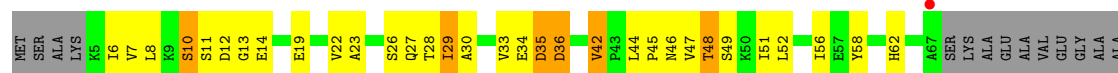
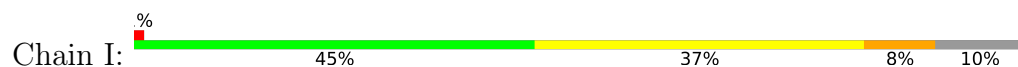


• Molecule 1: SKP1-like protein 1A





- Molecule 1: SKP1-like protein 1A



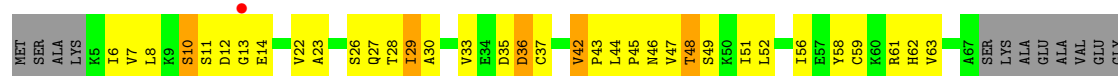
- Molecule 1: SKP1-like protein 1A



- Molecule 1: SKP1-like protein 1A

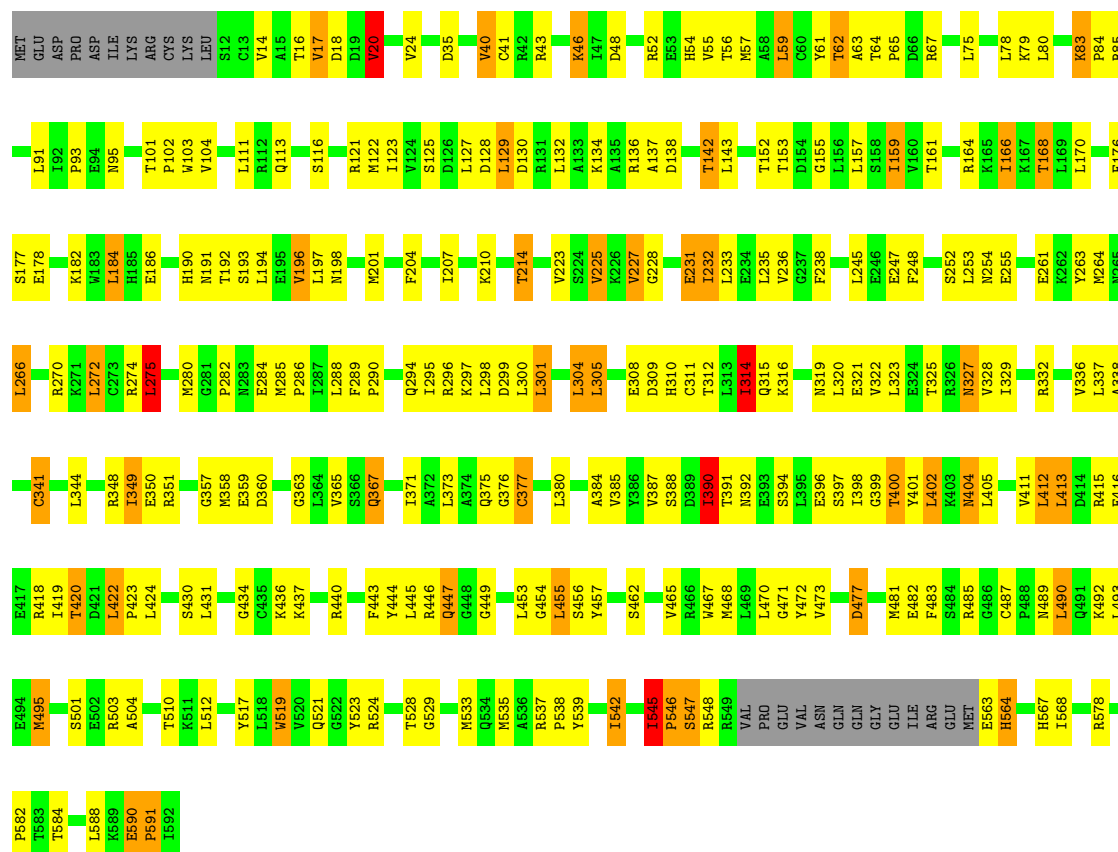


- Molecule 1: SKP1-like protein 1A



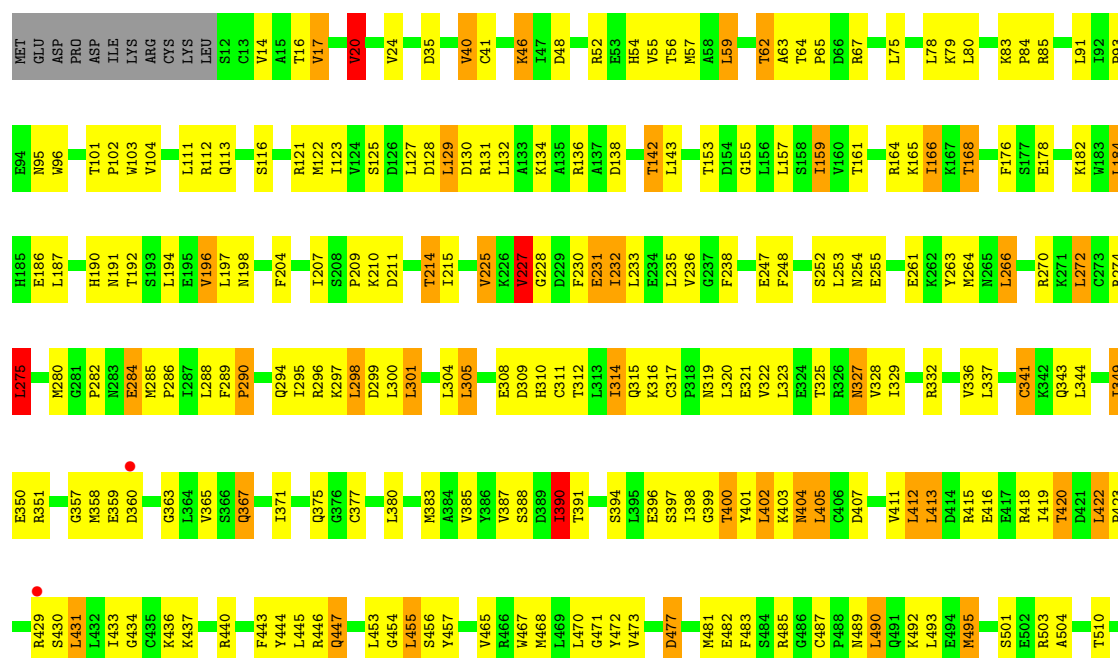
- Molecule 2: Coronatine-insensitive protein 1

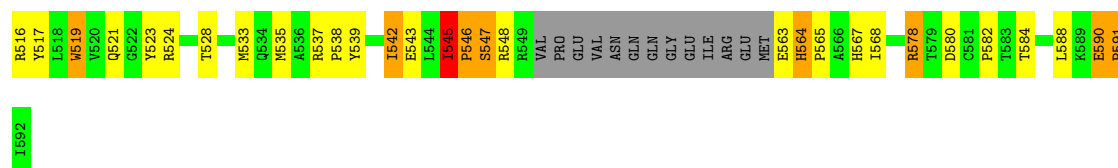




• Molecule 2: Coronatine-insensitive protein 1

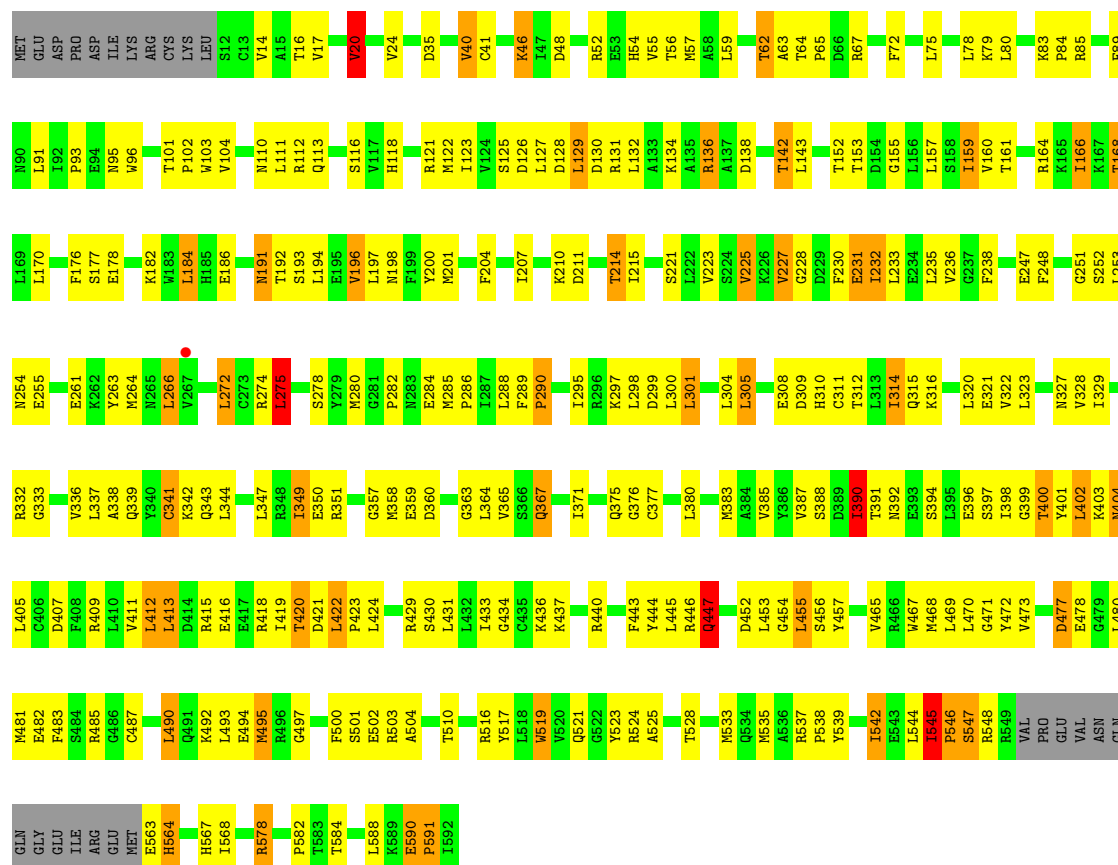
Chain D: 52% 35% 8%





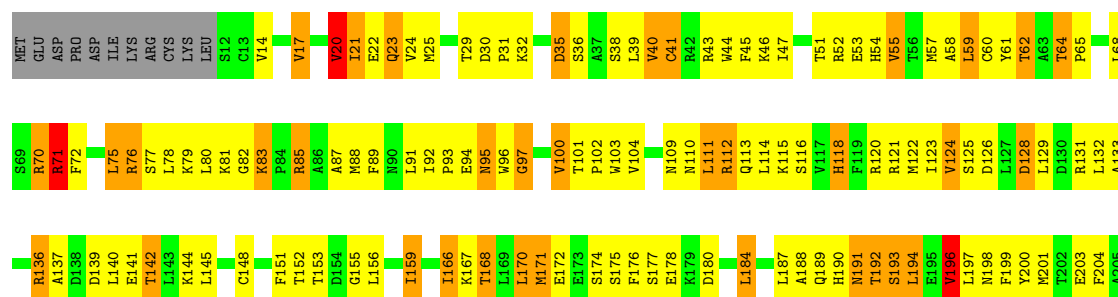
• Molecule 2: Coronatine-insensitive protein 1

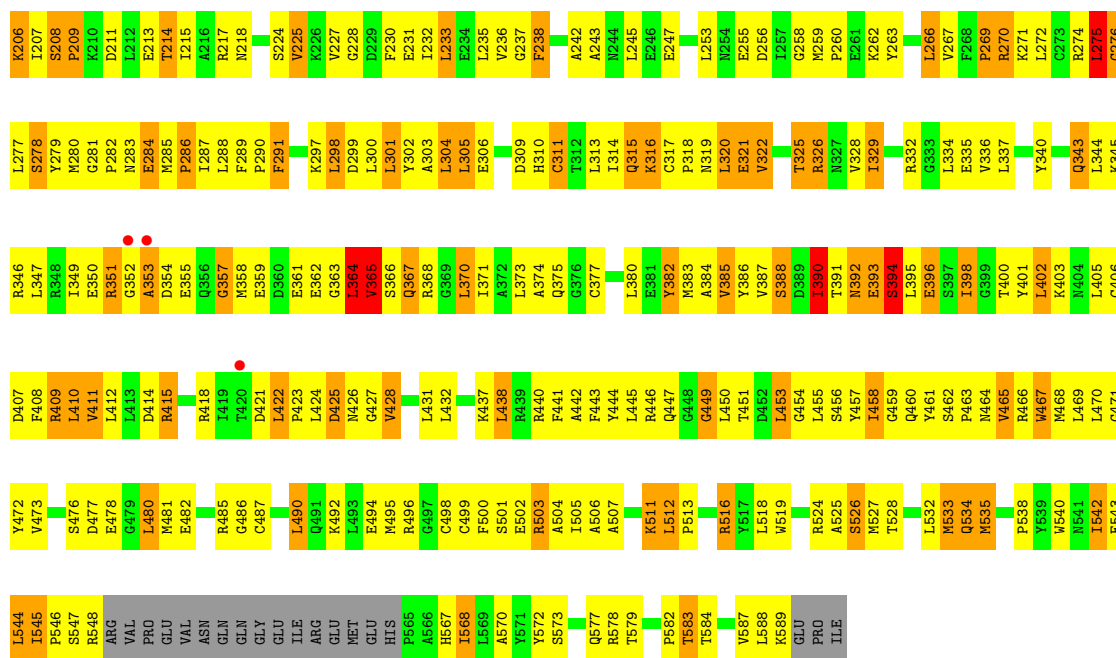
Chain F: 48% 40% 8% • •



• Molecule 2: Coronatine-insensitive protein 1

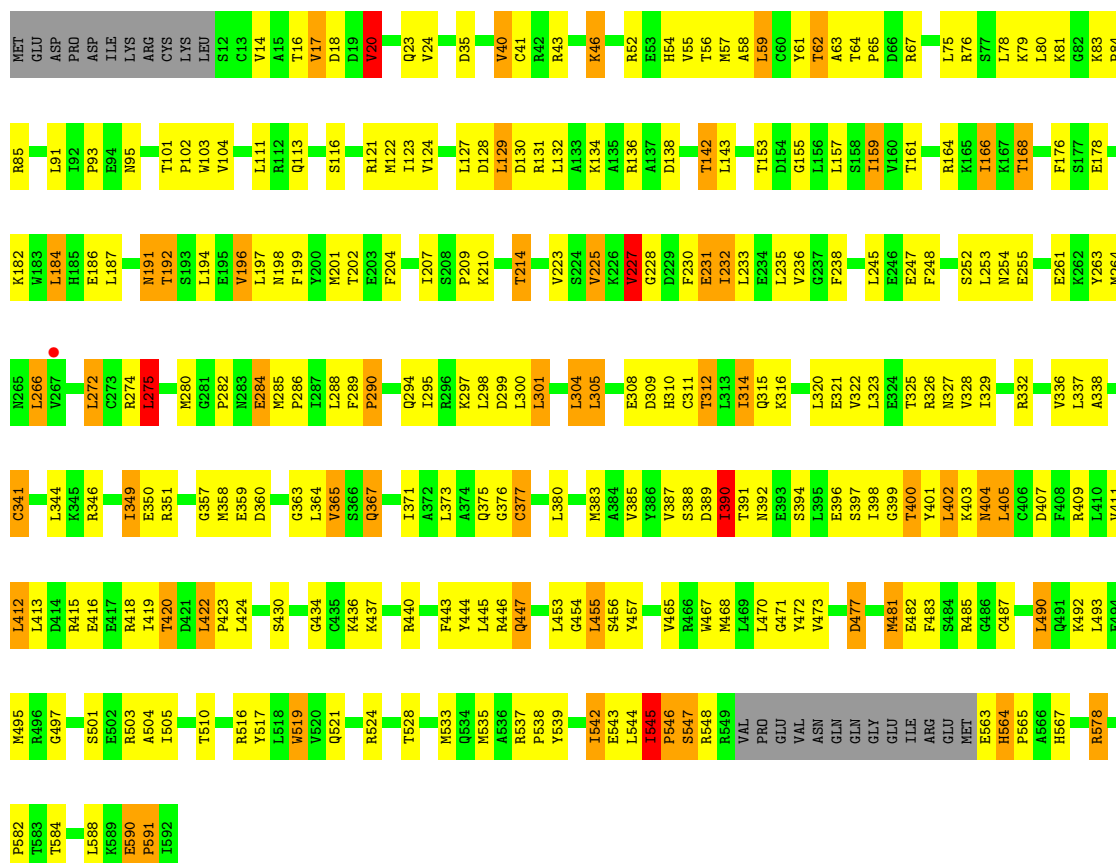
Chain H: 30% 46% 18% 5%





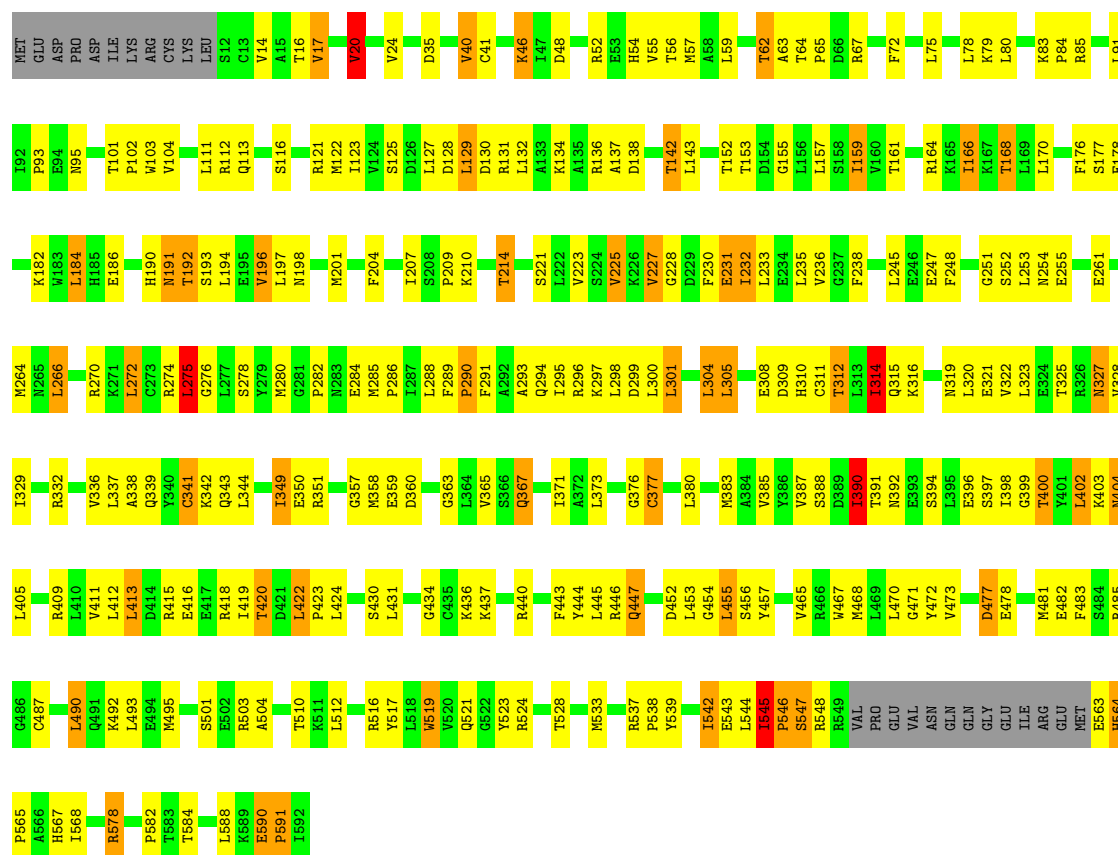
• Molecule 2: Coronatine-insensitive protein 1

Chain J: 51% 36% 9% . .



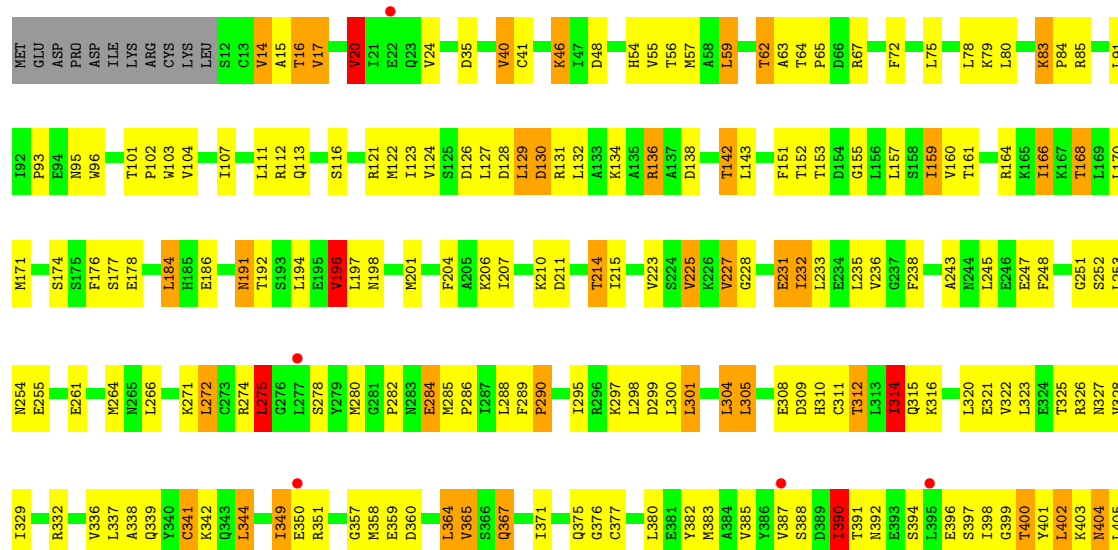
• Molecule 2: Coronatine-insensitive protein 1

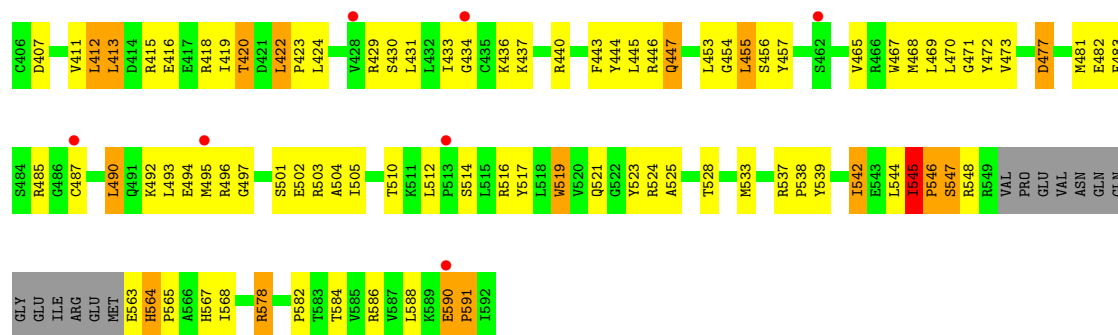
Chain L: 



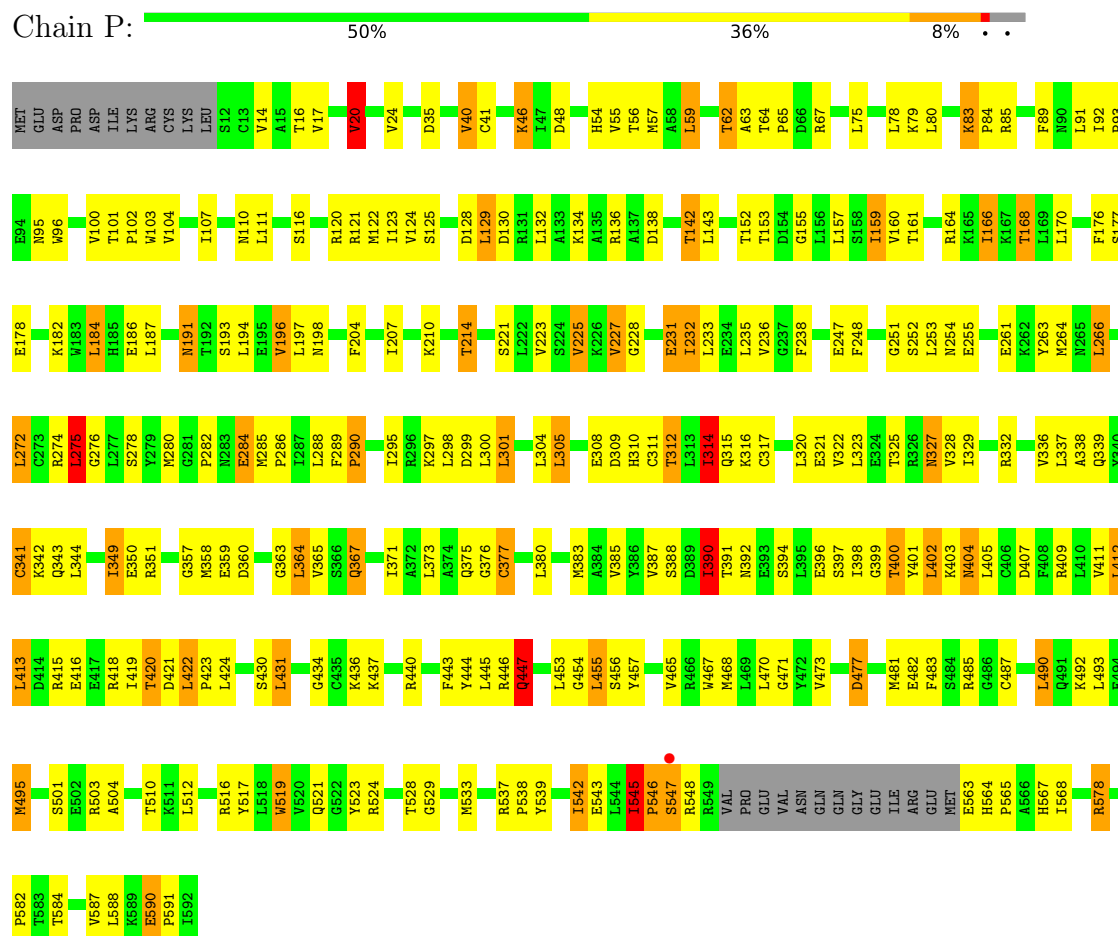
• Molecule 2: Coronatine-insensitive protein 1

Chain N: 

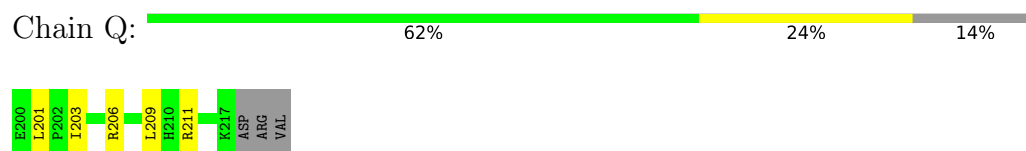




• Molecule 2: Coronatine-insensitive protein 1



• Molecule 3: JAZ1 degron peptide



• Molecule 3: JAZ1 degron peptide





- Molecule 3: JAZ1 degron peptide



- Molecule 3: JAZ1 degron peptide



- Molecule 3: JAZ1 degron peptide



- Molecule 3: JAZ1 degron peptide



- Molecule 3: JAZ1 degron peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.17Å 220.76Å 149.54Å 90.00° 104.45° 90.00°	Depositor
Resolution (Å)	49.94 – 3.34 49.94 – 3.34	Depositor EDS
% Data completeness (in resolution range)	85.8 (49.94-3.34) 85.8 (49.94-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.226 , 0.270 0.214 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.2	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	0.91	EDS
Total number of atoms	46877	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: PO4, OGK

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	0.55	0/1162	0.86	0/1571
1	C	0.62	2/1162 (0.2%)	0.86	0/1571
1	E	0.57	1/1162 (0.1%)	0.93	2/1571 (0.1%)
1	G	0.64	0/1162	0.94	2/1571 (0.1%)
1	I	0.58	0/1162	0.88	2/1571 (0.1%)
1	K	0.58	0/1162	0.89	0/1571
1	M	0.60	0/1162	0.90	1/1571 (0.1%)
1	O	0.55	0/1162	0.88	2/1571 (0.1%)
2	B	0.63	0/4623	0.98	15/6238 (0.2%)
2	D	0.66	0/4623	0.96	11/6238 (0.2%)
2	F	0.59	0/4623	0.96	10/6238 (0.2%)
2	H	0.74	0/4566	1.19	29/6161 (0.5%)
2	J	0.63	0/4623	0.96	11/6238 (0.2%)
2	L	0.58	0/4623	0.96	14/6238 (0.2%)
2	N	0.69	0/4623	1.00	13/6238 (0.2%)
2	P	0.58	0/4623	0.96	15/6238 (0.2%)
3	Q	0.50	0/158	0.84	0/208
3	R	0.54	0/158	0.82	0/208
3	S	0.48	0/158	0.84	0/208
3	U	0.64	0/158	0.81	0/208
3	V	0.48	0/158	0.85	0/208
3	W	0.53	0/158	0.85	0/208
3	X	0.53	0/158	0.79	0/208
All	All	0.63	3/47329 (0.0%)	0.98	127/63851 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	LEU	C-N	6.15	1.41	1.33
1	C	114	LEU	N-CA	5.67	1.53	1.46
1	E	113	LEU	C-N	-5.60	1.26	1.33

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	83	LYS	CA-C-N	11.19	131.16	119.85
2	H	83	LYS	C-N-CA	11.19	131.16	119.85
1	G	159	PHE	N-CA-C	8.97	123.53	108.90
2	H	583	THR	N-CA-C	-8.45	103.16	113.97
1	E	114	LEU	N-CA-C	-8.37	103.20	113.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1146	0	1117	63	0
1	C	1146	0	1117	60	0
1	E	1146	0	1117	73	0
1	G	1146	0	1117	67	0
1	I	1146	0	1117	71	0
1	K	1146	0	1117	58	0
1	M	1146	0	1117	91	0
1	O	1146	0	1117	72	0
2	B	4541	0	4583	230	0
2	D	4541	0	4583	234	0
2	F	4541	0	4583	229	0
2	H	4486	0	4534	459	0
2	J	4541	0	4583	237	0
2	L	4541	0	4583	237	0
2	N	4541	0	4583	281	0
2	P	4541	0	4583	234	0
3	Q	156	0	171	7	0
3	R	156	0	171	5	0
3	S	156	0	171	5	0
3	U	156	0	171	7	0
3	V	156	0	171	5	0
3	W	156	0	171	7	0
3	X	156	0	171	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	23	0	27	7	0
4	D	23	0	27	7	0
4	F	23	0	27	7	0
4	H	23	0	27	16	0
4	J	23	0	27	7	0
4	L	23	0	27	7	0
4	N	23	0	27	6	0
4	P	23	0	27	8	0
5	B	20	0	0	3	0
5	D	20	0	0	2	0
5	F	20	0	0	2	0
5	H	20	0	0	3	0
5	J	20	0	0	2	0
5	L	20	0	0	2	0
5	N	20	0	0	3	0
5	P	20	0	0	3	0
All	All	46877	0	46964	2577	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 27.

The worst 5 of 2577 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:H:116:SER:HB2	2:H:142:THR:HG23	1.35	1.09
2:P:168:THR:HB	2:P:196:VAL:HG13	1.35	1.08
2:D:168:THR:HB	2:D:196:VAL:HG13	1.35	1.08
2:J:168:THR:HB	2:J:196:VAL:HG13	1.35	1.06
2:L:168:THR:HB	2:L:196:VAL:HG13	1.35	1.06

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	140/160 (88%)	115 (82%)	20 (14%)	5 (4%)	2	18
1	C	140/160 (88%)	116 (83%)	19 (14%)	5 (4%)	2	18
1	E	140/160 (88%)	118 (84%)	17 (12%)	5 (4%)	2	18
1	G	140/160 (88%)	113 (81%)	21 (15%)	6 (4%)	2	14
1	I	140/160 (88%)	117 (84%)	17 (12%)	6 (4%)	2	14
1	K	140/160 (88%)	116 (83%)	19 (14%)	5 (4%)	2	18
1	M	140/160 (88%)	115 (82%)	20 (14%)	5 (4%)	2	18
1	O	140/160 (88%)	115 (82%)	19 (14%)	6 (4%)	2	14
2	B	564/592 (95%)	501 (89%)	57 (10%)	6 (1%)	11	40
2	D	564/592 (95%)	503 (89%)	53 (9%)	8 (1%)	9	34
2	F	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	10	37
2	H	558/592 (94%)	426 (76%)	95 (17%)	37 (7%)	1	7
2	J	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	10	37
2	L	564/592 (95%)	501 (89%)	55 (10%)	8 (1%)	9	34
2	N	564/592 (95%)	502 (89%)	55 (10%)	7 (1%)	10	37
2	P	564/592 (95%)	500 (89%)	58 (10%)	6 (1%)	11	40
3	Q	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	R	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	S	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	U	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	V	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	W	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	X	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
All	All	5738/6163 (93%)	4968 (87%)	641 (11%)	129 (2%)	5	26

5 of 129 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
2	B	420	THR
2	B	546	PRO
2	D	420	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	546	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	127/137 (93%)	111 (87%)	16 (13%)	4	19
1	C	127/137 (93%)	112 (88%)	15 (12%)	5	21
1	E	127/137 (93%)	111 (87%)	16 (13%)	4	19
1	G	127/137 (93%)	109 (86%)	18 (14%)	3	14
1	I	127/137 (93%)	111 (87%)	16 (13%)	4	19
1	K	127/137 (93%)	112 (88%)	15 (12%)	5	21
1	M	127/137 (93%)	110 (87%)	17 (13%)	4	16
1	O	127/137 (93%)	112 (88%)	15 (12%)	5	21
2	B	500/523 (96%)	428 (86%)	72 (14%)	3	14
2	D	500/523 (96%)	427 (85%)	73 (15%)	3	14
2	F	500/523 (96%)	426 (85%)	74 (15%)	3	13
2	H	494/523 (94%)	393 (80%)	101 (20%)	1	5
2	J	500/523 (96%)	427 (85%)	73 (15%)	3	14
2	L	500/523 (96%)	427 (85%)	73 (15%)	3	14
2	N	500/523 (96%)	426 (85%)	74 (15%)	3	13
2	P	500/523 (96%)	427 (85%)	73 (15%)	3	14
3	Q	16/19 (84%)	16 (100%)	0	100	100
3	R	16/19 (84%)	15 (94%)	1 (6%)	16	45
3	S	16/19 (84%)	15 (94%)	1 (6%)	16	45
3	U	16/19 (84%)	15 (94%)	1 (6%)	16	45
3	V	16/19 (84%)	15 (94%)	1 (6%)	16	45
3	W	16/19 (84%)	16 (100%)	0	100	100
3	X	16/19 (84%)	16 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5122/5413 (95%)	4377 (86%)	745 (14%)	3 14

5 of 745 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	477	ASP
1	M	44	LEU
3	U	217	LYS
2	J	473	VAL
2	L	214	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 151 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	491	GLN
2	P	254	ASN
1	M	141	ASN
2	N	564	HIS
2	P	567	HIS

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	H	1101	-	4,4,4	4.52	4 (100%)	6,6,6	0.66	0
5	PO4	F	1101	-	4,4,4	4.30	4 (100%)	6,6,6	1.28	0
5	PO4	L	1103	-	4,4,4	4.32	4 (100%)	6,6,6	0.79	0
4	OGK	B	1100	-	25,25,25	6.97	11 (44%)	31,38,38	2.47	14 (45%)
5	PO4	N	1101	-	4,4,4	4.59	3 (75%)	6,6,6	1.52	1 (16%)
4	OGK	F	3100	-	25,25,25	6.97	11 (44%)	31,38,38	2.45	12 (38%)
5	PO4	P	1104	-	4,4,4	4.34	4 (100%)	6,6,6	0.76	0
5	PO4	B	1104	-	4,4,4	4.29	4 (100%)	6,6,6	0.71	0
5	PO4	J	1101	-	4,4,4	4.21	4 (100%)	6,6,6	1.02	0
5	PO4	J	1102	-	4,4,4	4.38	4 (100%)	6,6,6	0.61	0
5	PO4	P	1101	-	4,4,4	4.26	4 (100%)	6,6,6	0.86	0
4	OGK	D	2100	-	25,25,25	7.09	11 (44%)	31,38,38	2.55	14 (45%)
4	OGK	J	5100	-	25,25,25	7.09	12 (48%)	31,38,38	2.50	14 (45%)
5	PO4	D	1103	-	4,4,4	4.42	4 (100%)	6,6,6	0.75	0
4	OGK	H	4100	-	25,25,25	6.90	11 (44%)	31,38,38	2.59	15 (48%)
5	PO4	L	1101	-	4,4,4	4.33	4 (100%)	6,6,6	0.90	0
5	PO4	D	1102	-	4,4,4	4.30	4 (100%)	6,6,6	0.34	0
5	PO4	N	1102	-	4,4,4	4.42	4 (100%)	6,6,6	0.55	0
5	PO4	N	1104	-	4,4,4	4.41	4 (100%)	6,6,6	0.72	0
5	PO4	N	1103	-	4,4,4	4.28	3 (75%)	6,6,6	1.40	1 (16%)
5	PO4	H	1104	-	4,4,4	4.46	4 (100%)	6,6,6	1.15	1 (16%)
5	PO4	F	1102	-	4,4,4	4.67	4 (100%)	6,6,6	0.58	0
5	PO4	F	1104	-	4,4,4	4.58	4 (100%)	6,6,6	0.71	0
5	PO4	H	1102	-	4,4,4	4.41	4 (100%)	6,6,6	0.83	0
5	PO4	B	1101	-	4,4,4	4.21	4 (100%)	6,6,6	0.85	0
5	PO4	F	1103	-	4,4,4	4.32	4 (100%)	6,6,6	0.79	0
5	PO4	J	1103	-	4,4,4	4.26	4 (100%)	6,6,6	0.67	0
5	PO4	P	1103	-	4,4,4	4.25	4 (100%)	6,6,6	0.76	0
5	PO4	J	1104	-	4,4,4	4.35	4 (100%)	6,6,6	0.69	0
5	PO4	L	1102	-	4,4,4	4.36	4 (100%)	6,6,6	0.36	0
5	PO4	L	1104	-	4,4,4	4.50	4 (100%)	6,6,6	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	P	1102	-	4,4,4	4.32	4 (100%)	6,6,6	0.60	0
4	OGK	P	8100	-	25,25,25	7.06	11 (44%)	31,38,38	2.47	12 (38%)
4	OGK	L	6100	-	25,25,25	6.92	11 (44%)	31,38,38	2.44	13 (41%)
5	PO4	B	1102	-	4,4,4	4.35	4 (100%)	6,6,6	0.60	0
5	PO4	B	1103	-	4,4,4	4.31	4 (100%)	6,6,6	0.49	0
4	OGK	N	7100	-	25,25,25	6.69	11 (44%)	31,38,38	2.50	10 (32%)
5	PO4	D	1101	-	4,4,4	4.07	4 (100%)	6,6,6	1.09	0
5	PO4	H	1103	-	4,4,4	4.59	4 (100%)	6,6,6	0.64	0
5	PO4	D	1104	-	4,4,4	4.33	4 (100%)	6,6,6	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OGK	D	2100	-	-	9/19/52/52	0/3/3/3
4	OGK	J	5100	-	-	9/19/52/52	0/3/3/3
4	OGK	B	1100	-	-	10/19/52/52	0/3/3/3
4	OGK	P	8100	-	-	9/19/52/52	0/3/3/3
4	OGK	L	6100	-	-	9/19/52/52	0/3/3/3
4	OGK	H	4100	-	1/1/9/10	10/19/52/52	0/3/3/3
4	OGK	F	3100	-	-	10/19/52/52	0/3/3/3
4	OGK	N	7100	-	-	10/19/52/52	0/3/3/3

The worst 5 of 215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	5100	OGK	C13-C09	-22.76	1.27	1.51
4	D	2100	OGK	C13-C09	-22.66	1.27	1.51
4	P	8100	OGK	C13-C09	-22.40	1.28	1.51
4	F	3100	OGK	C13-C09	-22.34	1.28	1.51
4	B	1100	OGK	C13-C09	-22.09	1.28	1.51

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	7100	OGK	C04-C05-C17	6.09	121.81	110.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	5100	OGK	C13-C14-C09	-5.99	57.22	60.30
4	F	3100	OGK	C13-C14-C09	-5.78	57.33	60.30
4	P	8100	OGK	C13-C14-C09	-5.70	57.37	60.30
4	B	1100	OGK	C04-C05-C17	5.68	121.01	110.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	4100	OGK	C03

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1100	OGK	C17-C05-C06-O07
4	B	1100	OGK	C17-C05-C06-N08
4	B	1100	OGK	N08-C09-C10-O11
4	B	1100	OGK	N08-C09-C10-O12
4	B	1100	OGK	C14-C09-C10-O11

There are no ring outliers.

27 monomers are involved in 85 short contacts:

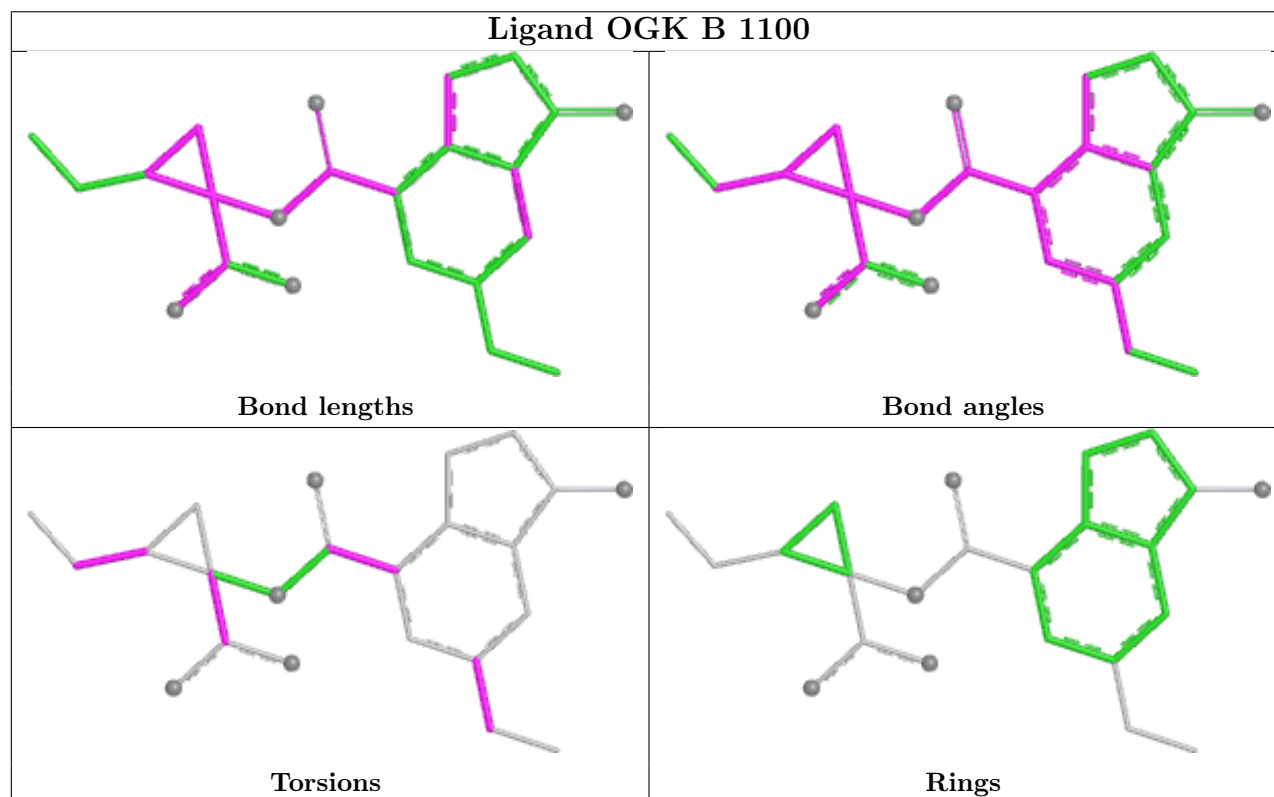
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1101	PO4	1	0
5	F	1101	PO4	1	0
5	L	1103	PO4	1	0
4	B	1100	OGK	7	0
5	N	1101	PO4	1	0
4	F	3100	OGK	7	0
5	J	1101	PO4	1	0
5	P	1101	PO4	1	0
4	D	2100	OGK	7	0
4	J	5100	OGK	7	0
5	D	1103	PO4	1	0
4	H	4100	OGK	16	0
5	L	1101	PO4	1	0
5	N	1102	PO4	1	0
5	N	1103	PO4	1	0
5	H	1102	PO4	1	0
5	B	1101	PO4	1	0
5	F	1103	PO4	1	0
5	J	1103	PO4	1	0

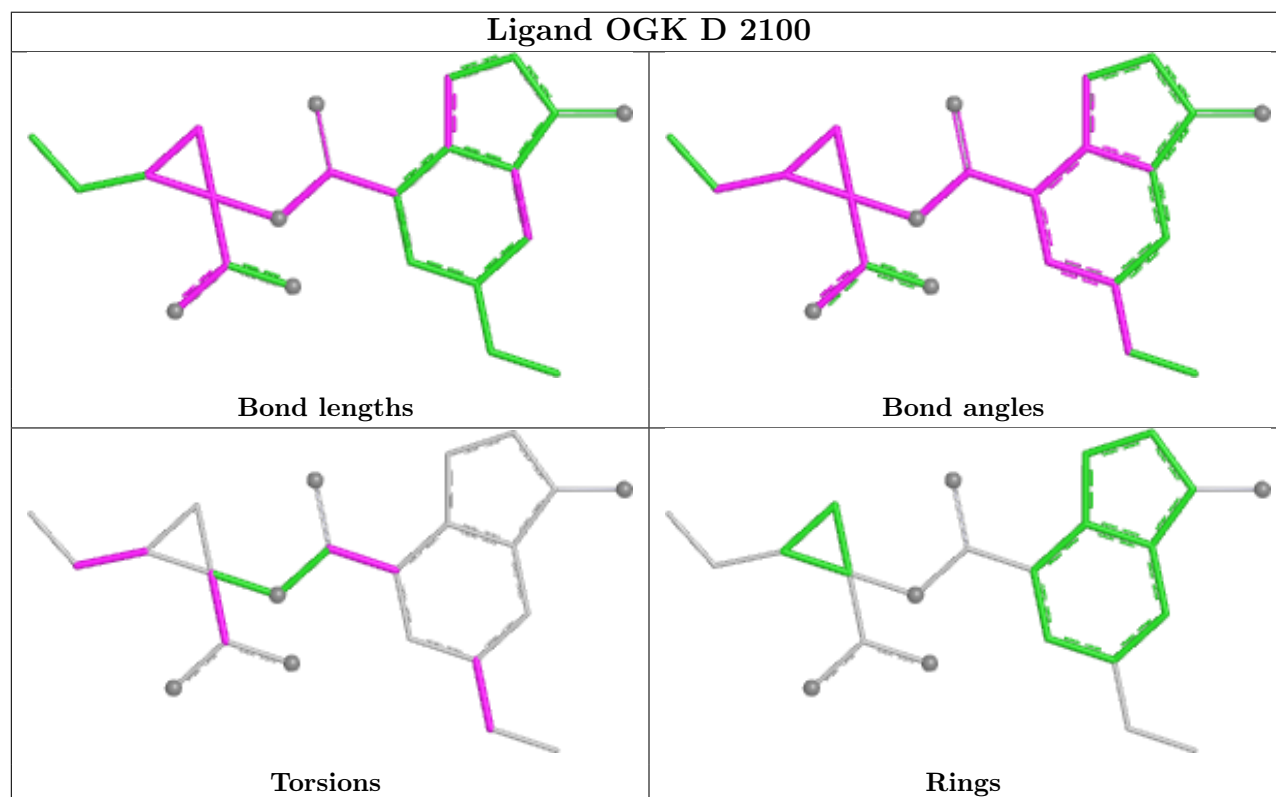
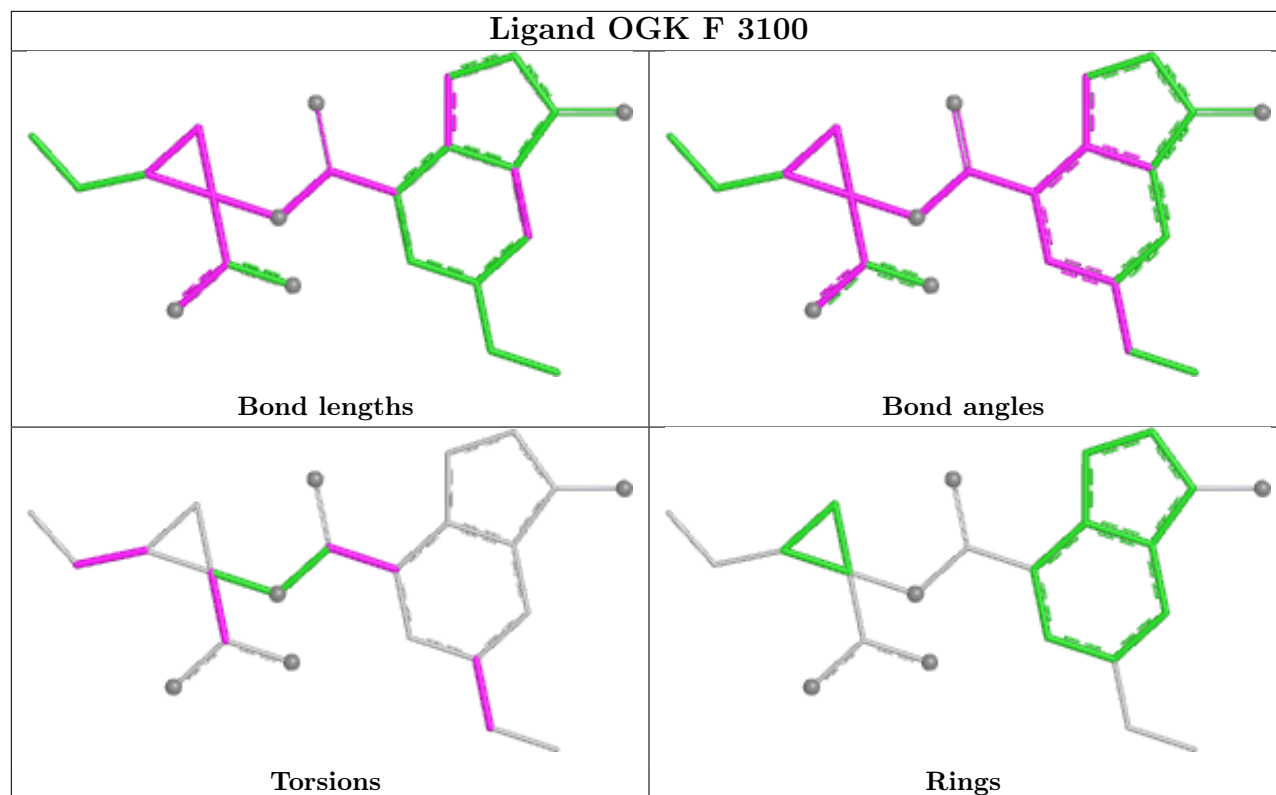
Continued on next page...

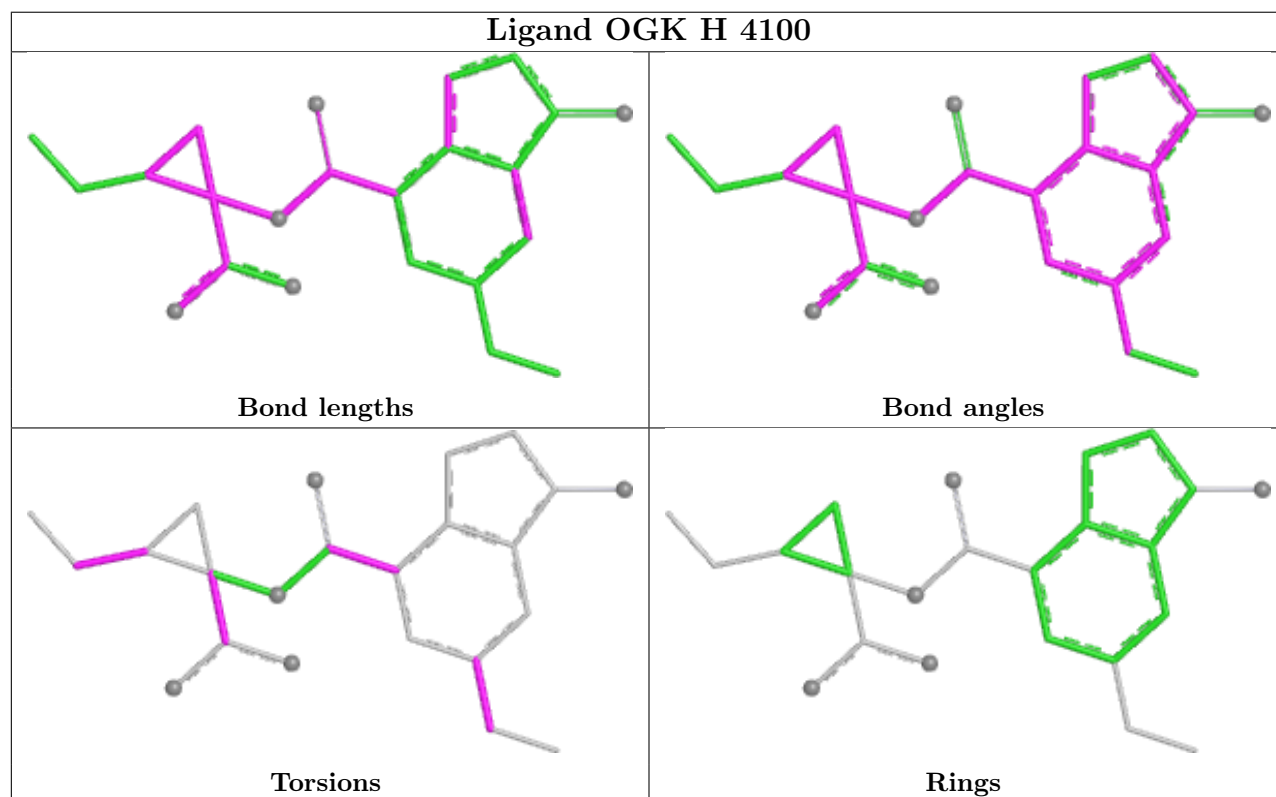
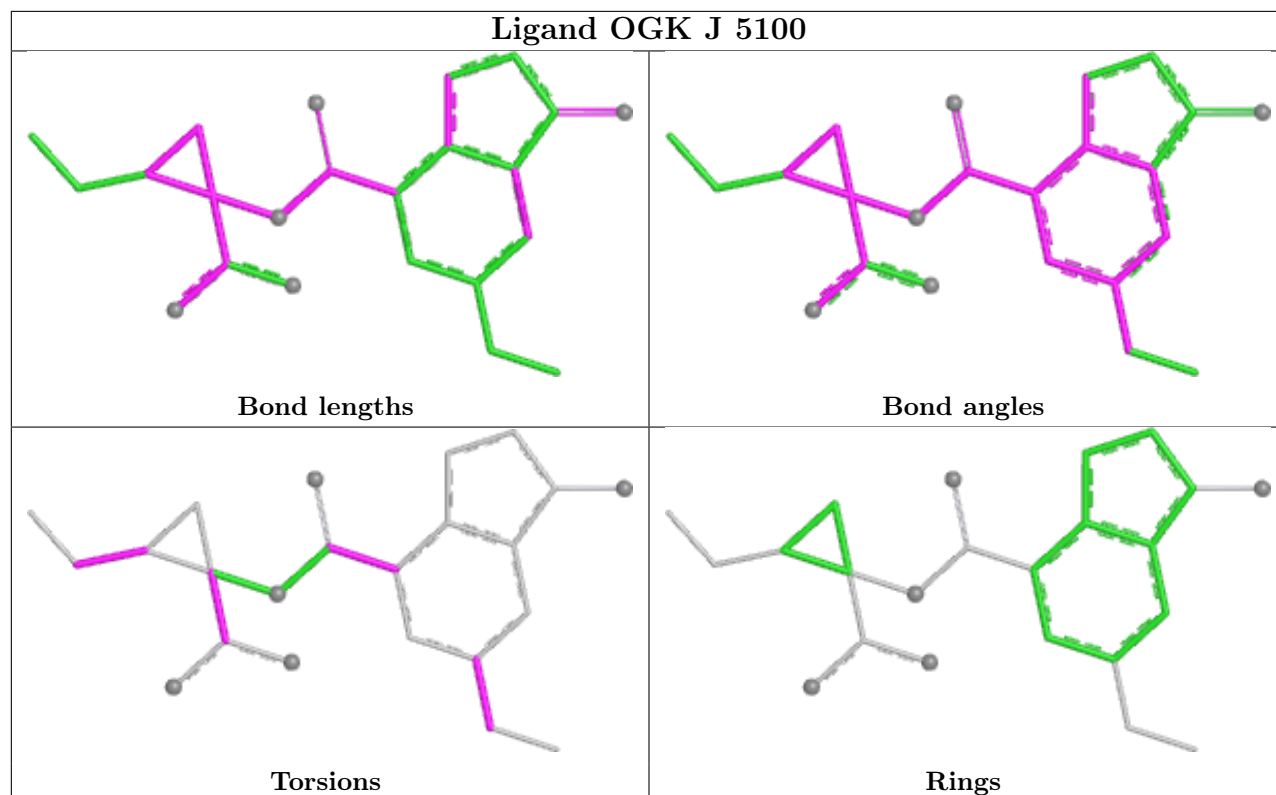
Continued from previous page...

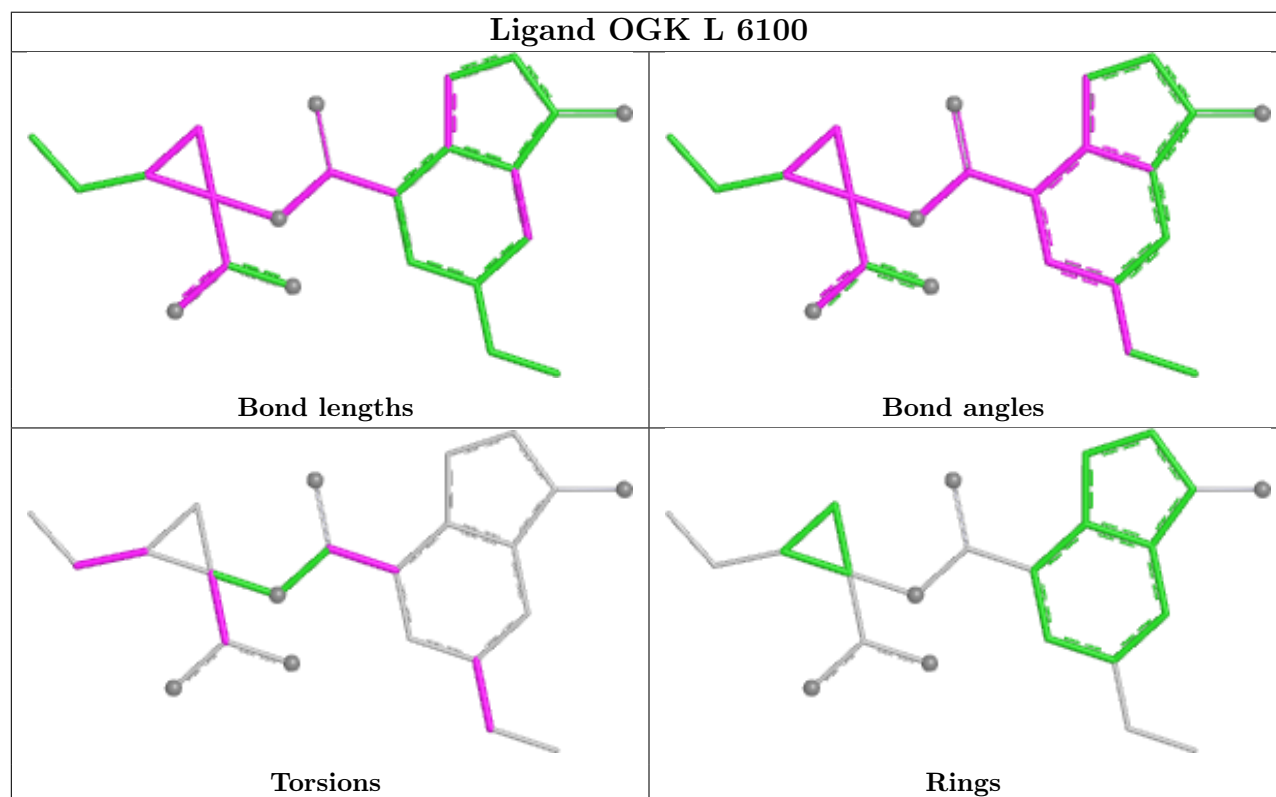
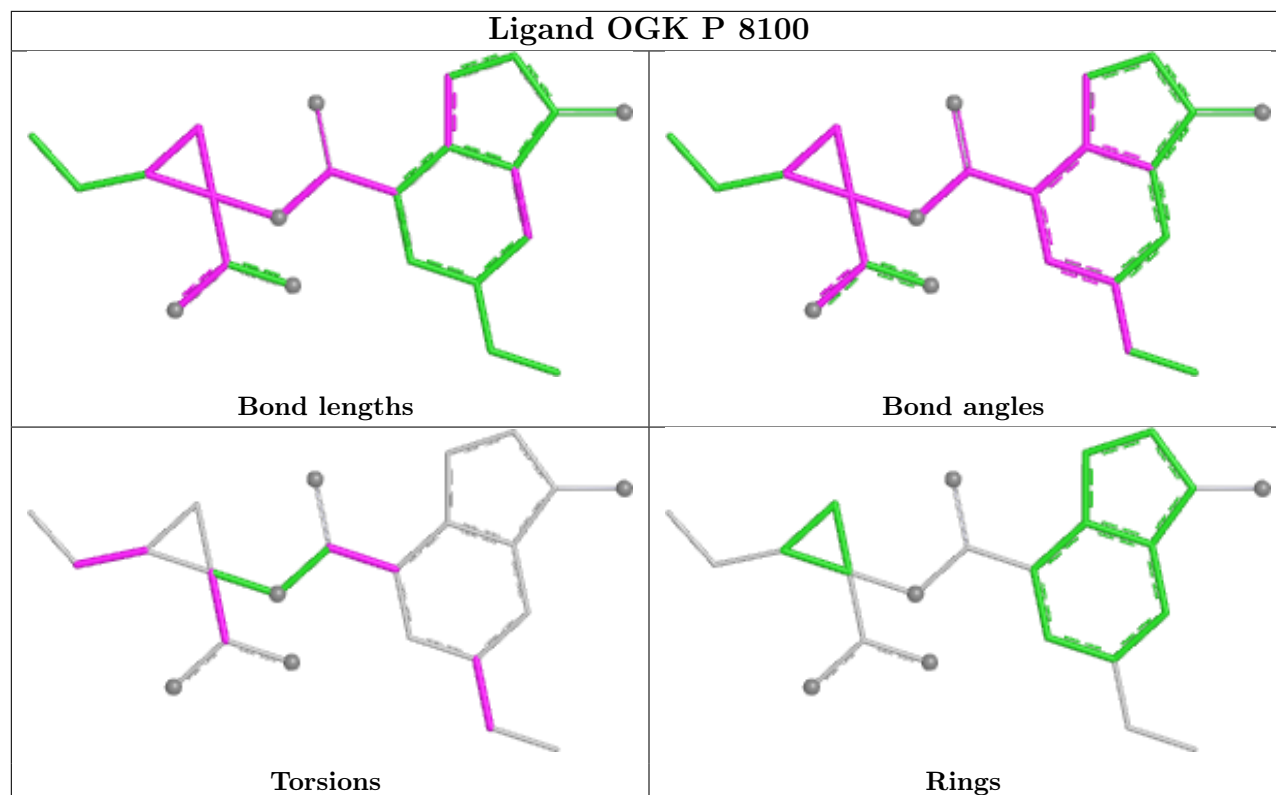
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	1103	PO4	2	0
4	P	8100	OGK	8	0
4	L	6100	OGK	7	0
5	B	1102	PO4	1	0
5	B	1103	PO4	1	0
4	N	7100	OGK	6	0
5	D	1101	PO4	1	0
5	H	1103	PO4	1	0

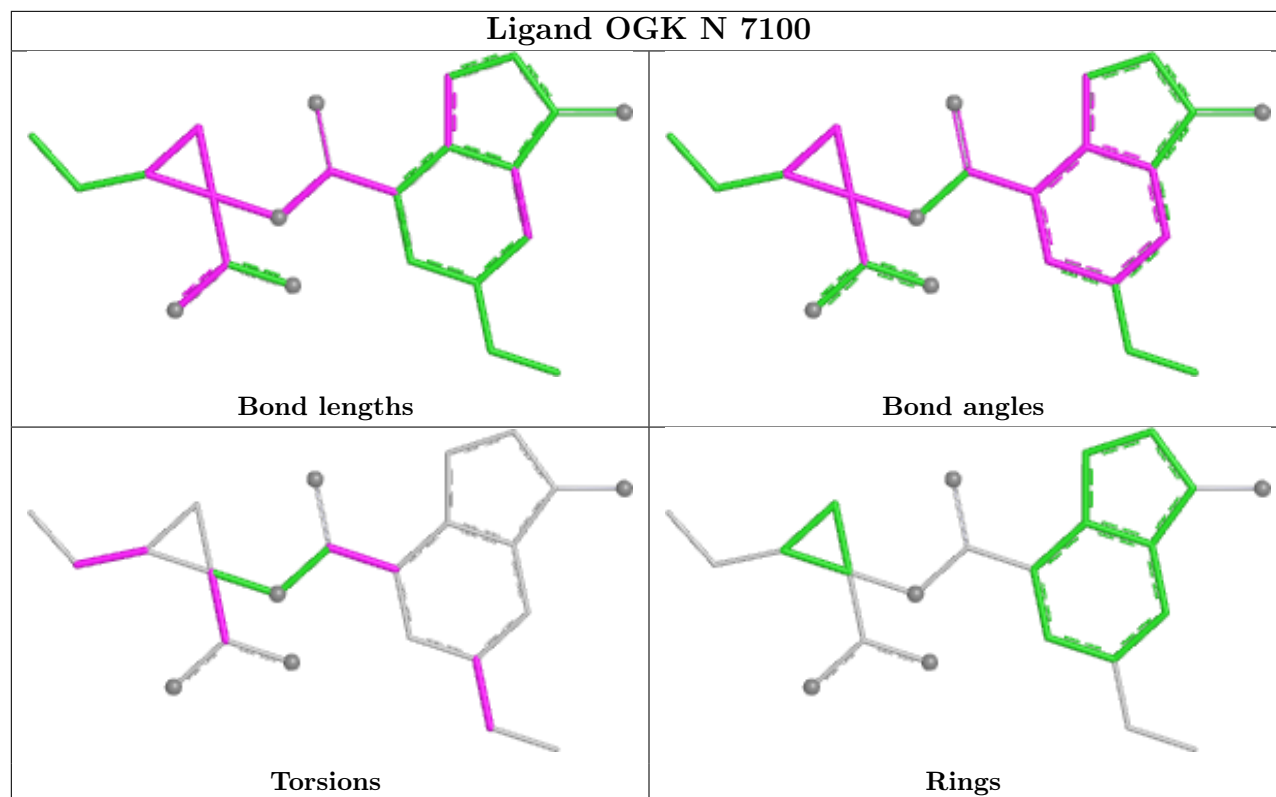
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [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%)	-0.02	1 (0%) 84 71	50, 100, 151, 168	0
1	C	144/160 (90%)	-0.08	0 100 100	50, 102, 153, 170	0
1	E	144/160 (90%)	0.11	2 (1%) 73 56	54, 101, 151, 171	0
1	G	144/160 (90%)	-0.13	0 100 100	49, 96, 149, 170	0
1	I	144/160 (90%)	0.10	1 (0%) 84 71	50, 100, 150, 170	0
1	K	144/160 (90%)	-0.12	0 100 100	53, 102, 152, 170	0
1	M	144/160 (90%)	0.24	0 100 100	55, 102, 152, 175	0
1	O	144/160 (90%)	-0.10	1 (0%) 84 71	51, 101, 151, 173	0
2	B	568/592 (95%)	-0.22	0 100 100	38, 76, 136, 201	0
2	D	568/592 (95%)	-0.10	2 (0%) 88 80	38, 75, 135, 200	0
2	F	568/592 (95%)	-0.19	1 (0%) 91 87	40, 79, 136, 202	0
2	H	562/592 (94%)	-0.53	3 (0%) 87 77	34, 73, 127, 191	0
2	J	568/592 (95%)	-0.20	1 (0%) 91 87	39, 77, 136, 204	0
2	L	568/592 (95%)	-0.30	0 100 100	41, 79, 135, 202	0
2	N	568/592 (95%)	0.39	12 (2%) 63 45	41, 82, 137, 206	0
2	P	568/592 (95%)	-0.24	1 (0%) 91 87	40, 80, 138, 204	0
3	Q	18/21 (85%)	-0.09	0 100 100	72, 93, 116, 143	0
3	R	18/21 (85%)	0.15	0 100 100	71, 88, 115, 145	0
3	S	18/21 (85%)	-0.22	0 100 100	73, 93, 117, 143	0
3	U	18/21 (85%)	0.06	0 100 100	71, 88, 112, 143	0
3	V	18/21 (85%)	-0.16	0 100 100	75, 93, 115, 143	0
3	W	18/21 (85%)	0.42	0 100 100	80, 96, 119, 143	0
3	X	18/21 (85%)	-0.27	0 100 100	76, 91, 119, 143	0
All	All	5816/6163 (94%)	-0.13	25 (0%) 88 80	34, 82, 141, 206	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	462	SER	3.9
2	H	353	ALA	3.6
2	H	352	GLY	3.4
2	N	428	VAL	3.2
1	E	138	ASN	3.1

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	N	1104	5/5	0.81	0.12	82,83,118,122	0
5	PO4	N	1103	5/5	0.82	0.12	56,56,74,85	0
5	PO4	P	1102	5/5	0.85	0.17	72,87,98,108	0
5	PO4	N	1102	5/5	0.86	0.09	78,90,92,113	0
4	OGK	N	7100	23/23	0.86	0.18	65,79,100,104	0
5	PO4	F	1104	5/5	0.87	0.11	72,81,117,120	0
5	PO4	H	1104	5/5	0.87	0.09	54,57,114,134	0
5	PO4	F	1102	5/5	0.88	0.12	64,90,96,109	0
5	PO4	N	1101	5/5	0.88	0.09	51,59,80,82	0
5	PO4	B	1102	5/5	0.89	0.10	70,84,93,100	0
5	PO4	D	1102	5/5	0.91	0.11	66,79,93,93	0
5	PO4	D	1104	5/5	0.91	0.10	72,73,107,122	0
5	PO4	L	1104	5/5	0.91	0.09	76,78,119,123	0
5	PO4	B	1104	5/5	0.91	0.09	68,79,102,119	0
5	PO4	P	1103	5/5	0.91	0.07	50,58,73,85	0
5	PO4	J	1102	5/5	0.92	0.06	67,86,95,104	0
5	PO4	P	1104	5/5	0.92	0.08	73,75,110,121	0

Continued on next page...

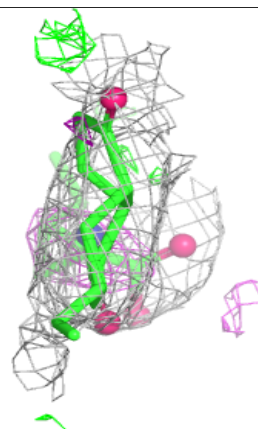
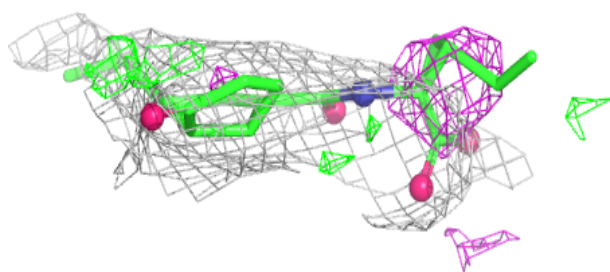
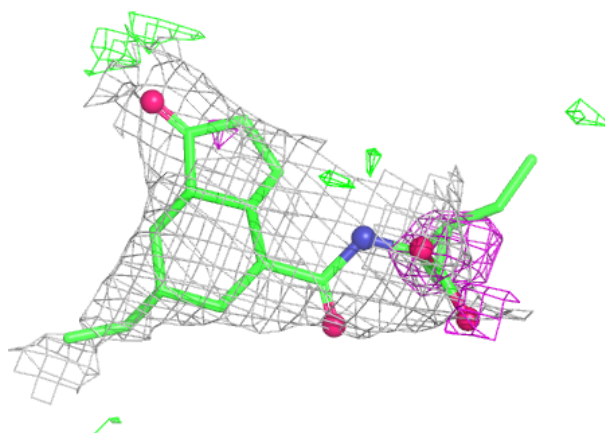
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OGK	H	4100	23/23	0.93	0.10	44,71,85,98	0
5	PO4	F	1101	5/5	0.93	0.10	52,58,68,88	0
4	OGK	B	1100	23/23	0.94	0.11	62,73,87,93	0
5	PO4	J	1101	5/5	0.94	0.07	50,55,74,79	0
4	OGK	J	5100	23/23	0.94	0.11	59,67,88,93	0
5	PO4	L	1102	5/5	0.94	0.07	73,82,96,100	0
4	OGK	P	8100	23/23	0.95	0.12	64,75,88,90	0
4	OGK	F	3100	23/23	0.95	0.11	64,72,91,94	0
5	PO4	B	1103	5/5	0.96	0.08	54,54,61,76	0
5	PO4	B	1101	5/5	0.96	0.06	58,59,65,75	0
5	PO4	D	1101	5/5	0.96	0.07	51,55,63,80	0
5	PO4	J	1104	5/5	0.96	0.08	76,81,112,117	0
5	PO4	P	1101	5/5	0.96	0.07	57,62,74,75	0
4	OGK	D	2100	23/23	0.96	0.12	60,72,81,86	0
5	PO4	L	1103	5/5	0.96	0.06	52,56,69,89	0
5	PO4	H	1102	5/5	0.96	0.05	58,59,72,88	0
5	PO4	J	1103	5/5	0.97	0.05	53,53,64,77	0
4	OGK	L	6100	23/23	0.97	0.09	62,71,90,92	0
5	PO4	L	1101	5/5	0.97	0.04	48,58,74,76	0
5	PO4	H	1103	5/5	0.97	0.05	38,47,52,77	0
5	PO4	F	1103	5/5	0.97	0.06	53,57,73,86	0
5	PO4	D	1103	5/5	0.97	0.06	48,52,55,81	0
5	PO4	H	1101	5/5	0.97	0.05	36,45,63,88	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.

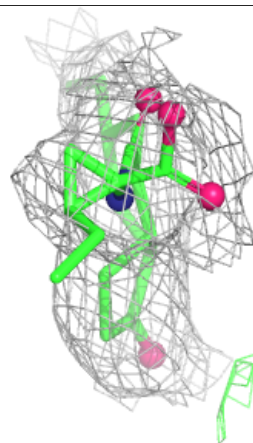
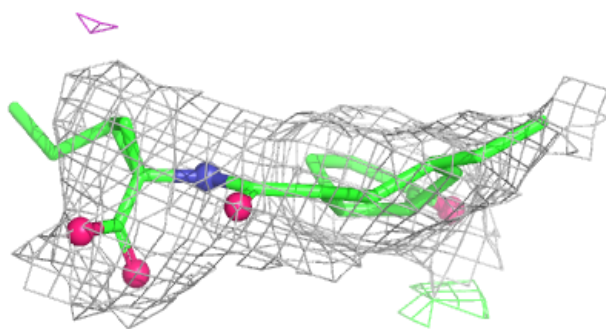
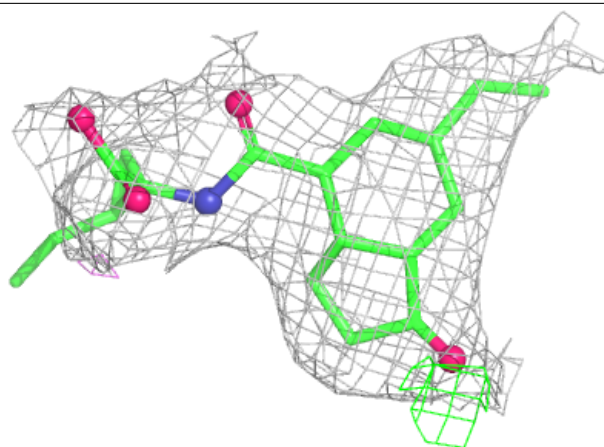
Electron density around OGK N 7100:

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

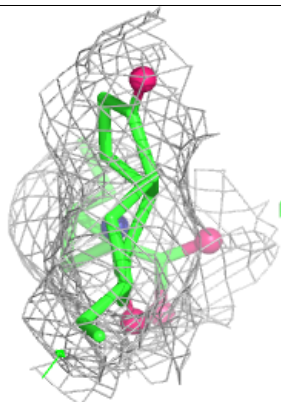
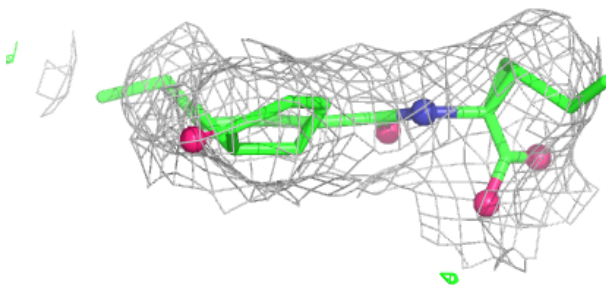
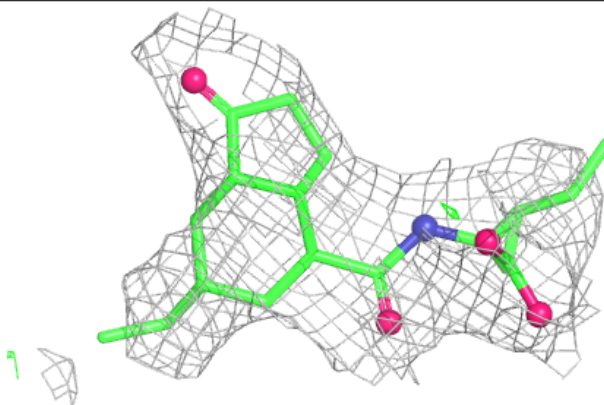


Electron density around OGK H 4100:

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

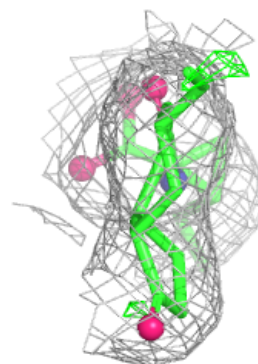
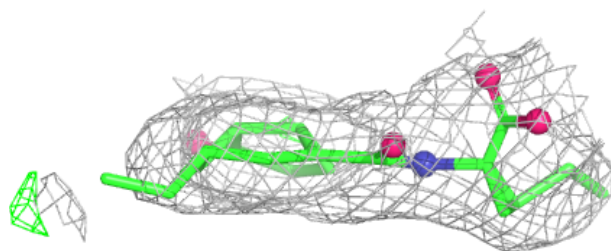
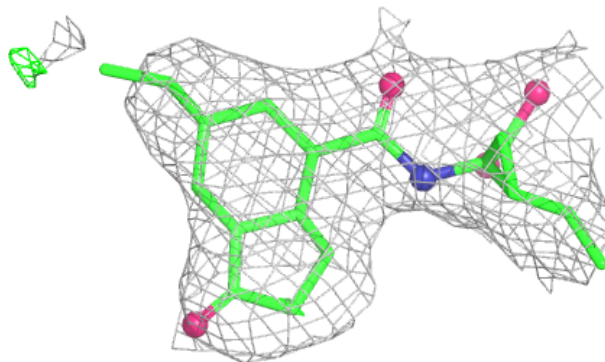
**Electron density around OGK B 1100:**

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

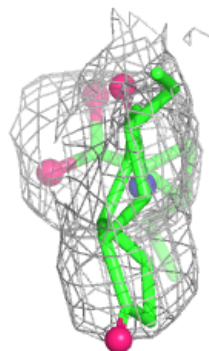
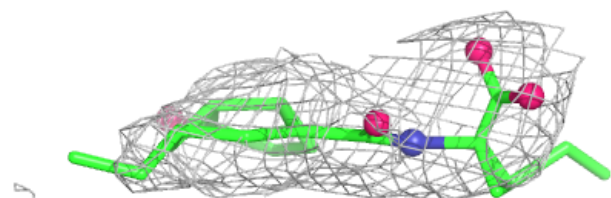
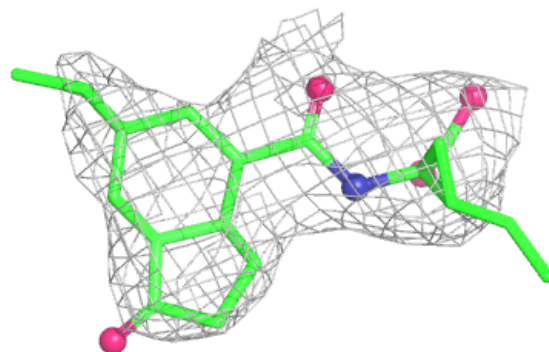


Electron density around OGK J 5100:

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

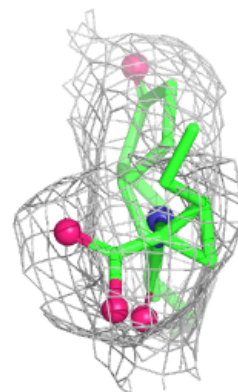
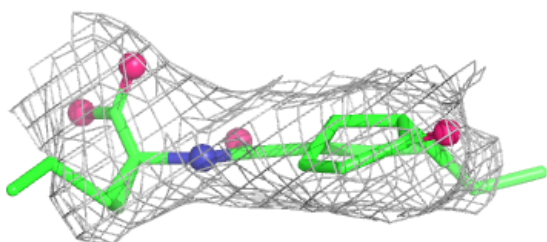
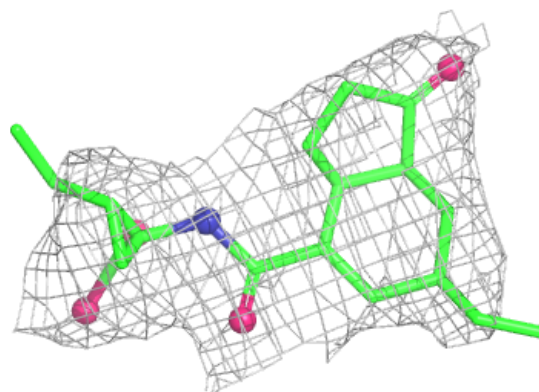
**Electron density around OGK P 8100:**

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

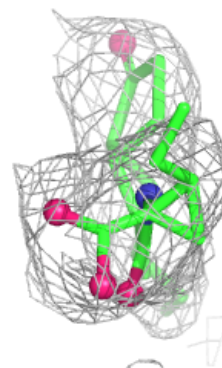
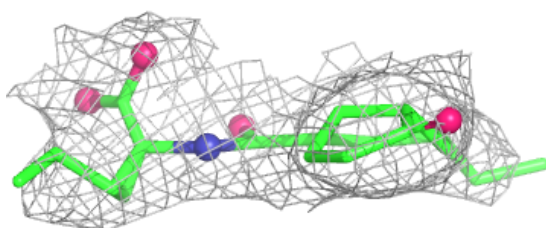
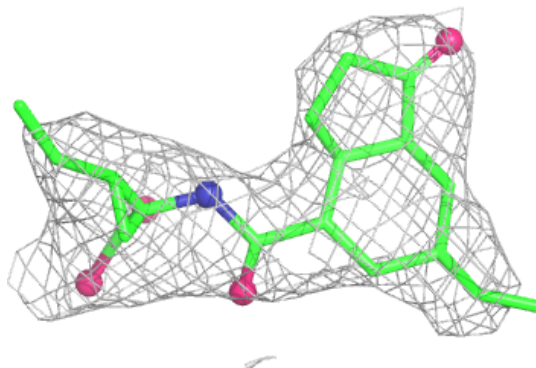


Electron density around OGK F 3100:

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

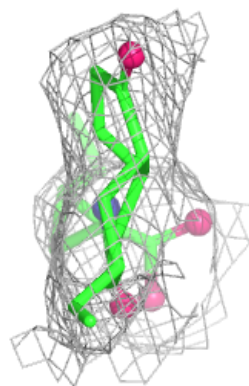
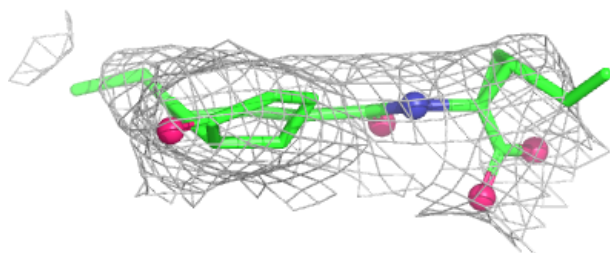
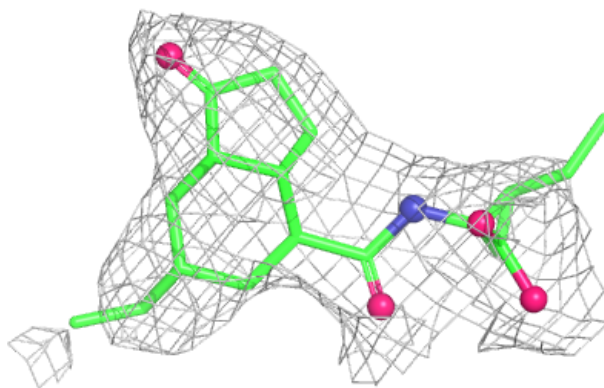
**Electron density around OGK D 2100:**

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



Electron density around OGK L 6100:

$2mF_o-DF_c$ (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.