



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 05:28 PM GMT

PDB ID : 3OGM  
Title : Structure of COI1-ASK1 in complex with coronatine 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 : 3.34 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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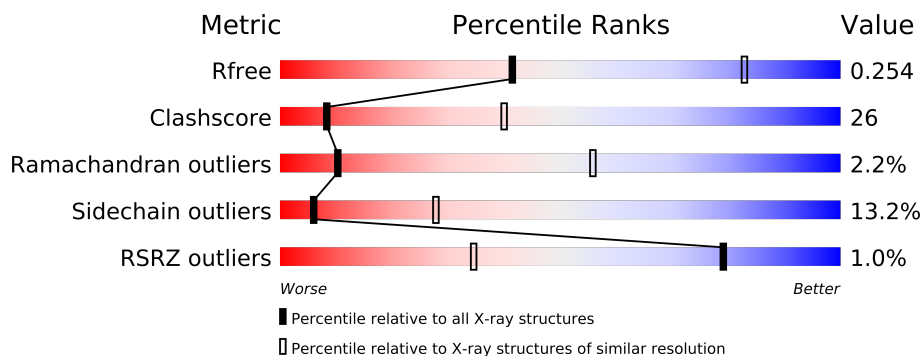
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1421 (3.48-3.20)
Clashscore	79885	1077 (3.46-3.22)
Ramachandran outliers	78287	1053 (3.46-3.22)
Sidechain outliers	78261	1052 (3.46-3.22)
RSRZ outliers	66119	1422 (3.48-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	160	
1	C	160	
1	E	160	
1	G	160	
1	I	160	
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	

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Mol	Chain	Length	Quality of chain
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 that are outliers for geometric or electron-density-fit criteria:

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

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46877 atoms, of which 0 are hydrogen and 0 are deuterium.

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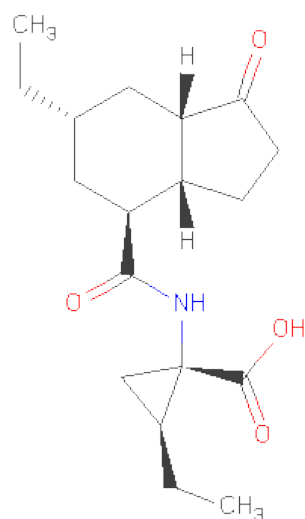
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	P	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			

- Molecule 3 is a protein called JAZ1 degron peptide.

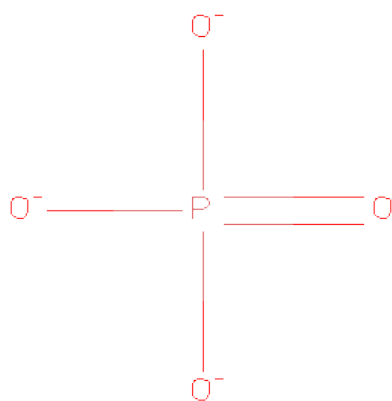
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	R	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	S	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	U	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	V	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	W	18	Total	C	N	O	0	0	0
			156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

- Molecule 4 is (1S,2S)-2-ETHYL-1-({[(3AS,4S,6R,7AS)-6-ETHYL-1-OXOOCTAHYDRO-1H-INDEN-4-YL]CARBONYL}AMINO)CYCLOPROPANECARBOXYLICACID (three-letter code: OGK) (formula: C<sub>18</sub>H<sub>27</sub>NO<sub>4</sub>).



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 (three-letter code: PO4) (formula: O<sub>4</sub>P).



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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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		

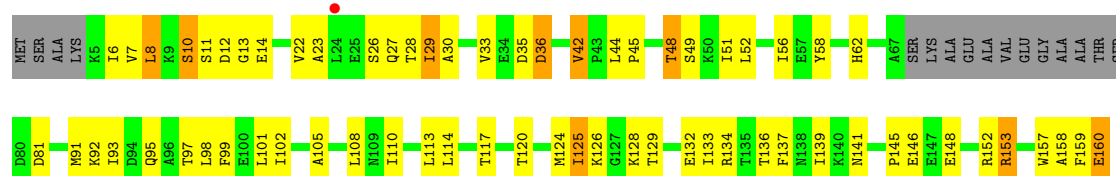


### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

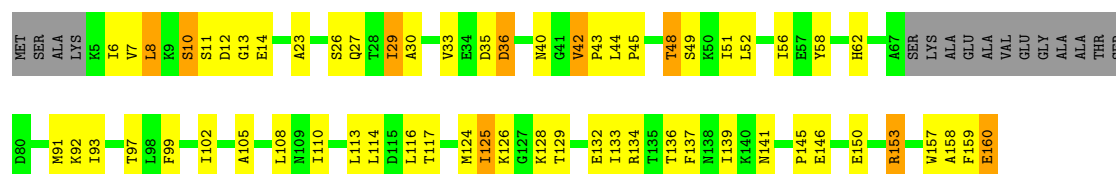
- Molecule 1: SKP1-like protein 1A

Chain A: 



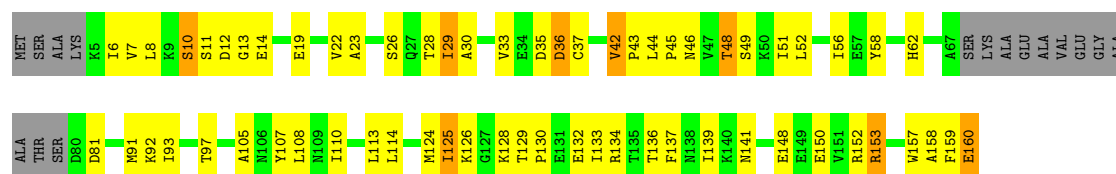
- Molecule 1: SKP1-like protein 1A

Chain C: 



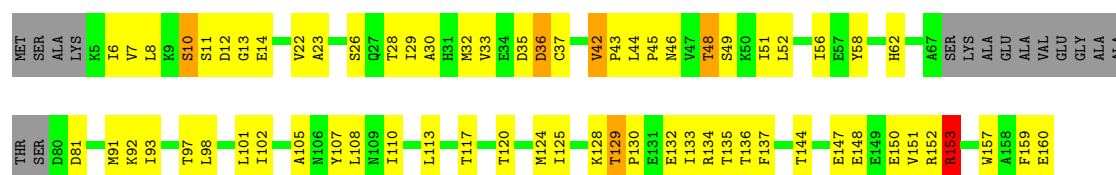
- Molecule 1: SKP1-like protein 1A

Chain E: 



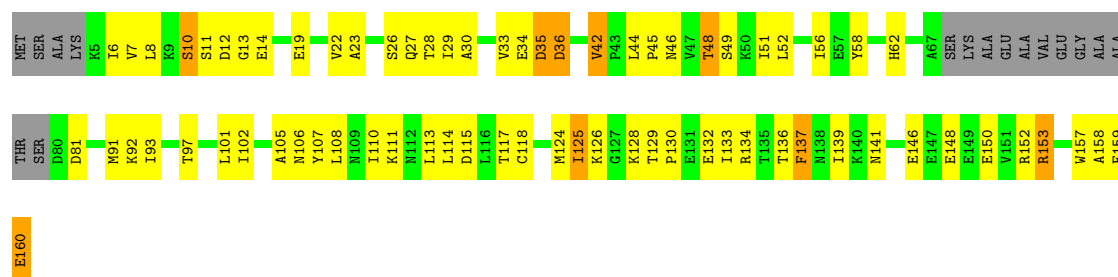
- Molecule 1: SKP1-like protein 1A

Chain G: 



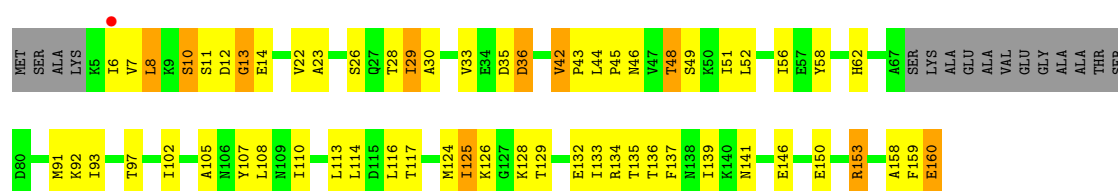
- Molecule 1: SKP1-like protein 1A

Chain I:



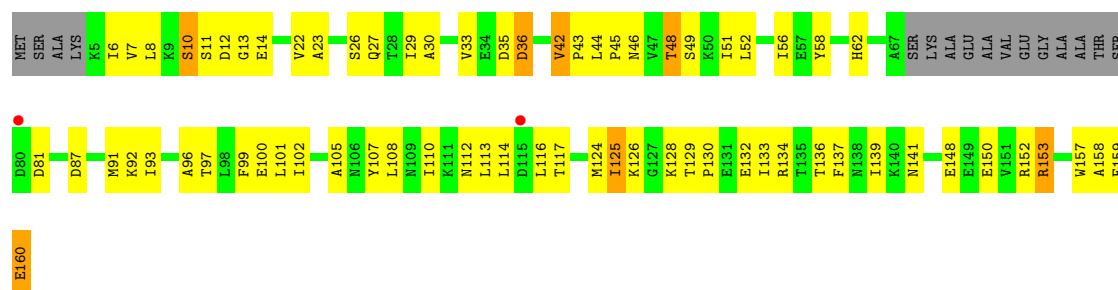
- Molecule 1: SKP1-like protein 1A

Chain K:



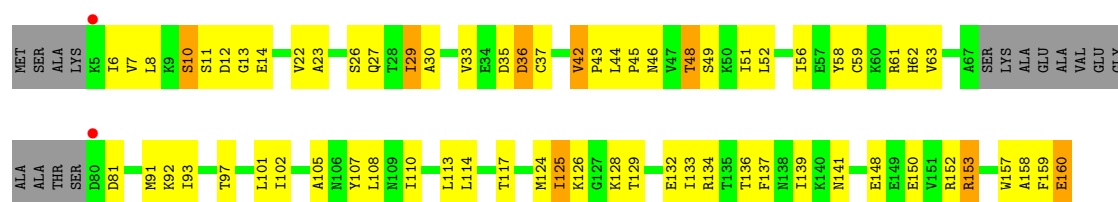
- Molecule 1: SKP1-like protein 1A

Chain M:



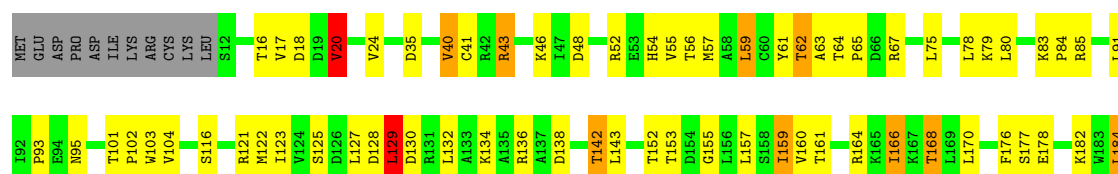
- Molecule 1: SKP1-like protein 1A

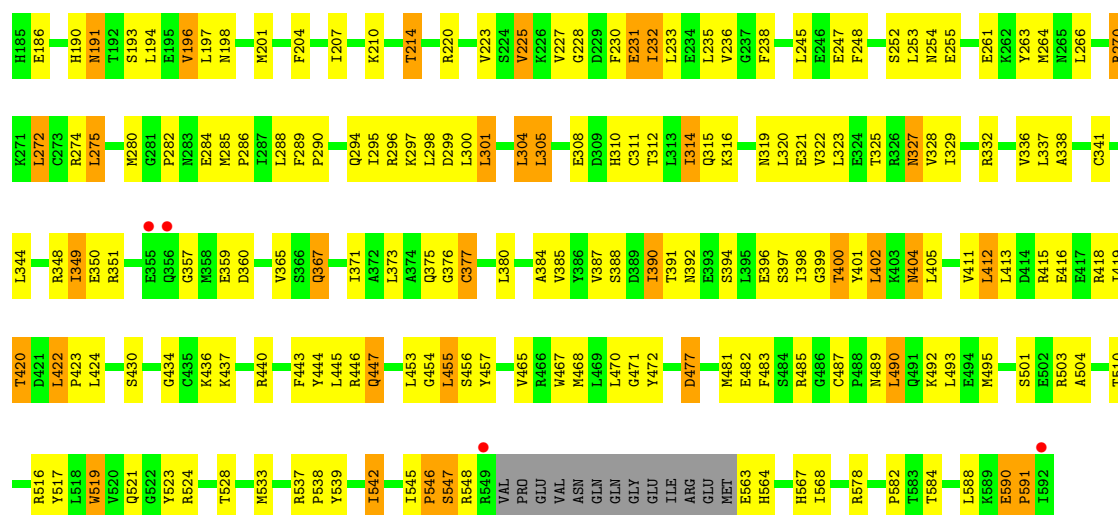
Chain O:



- Molecule 2: Coronatine-insensitive protein 1

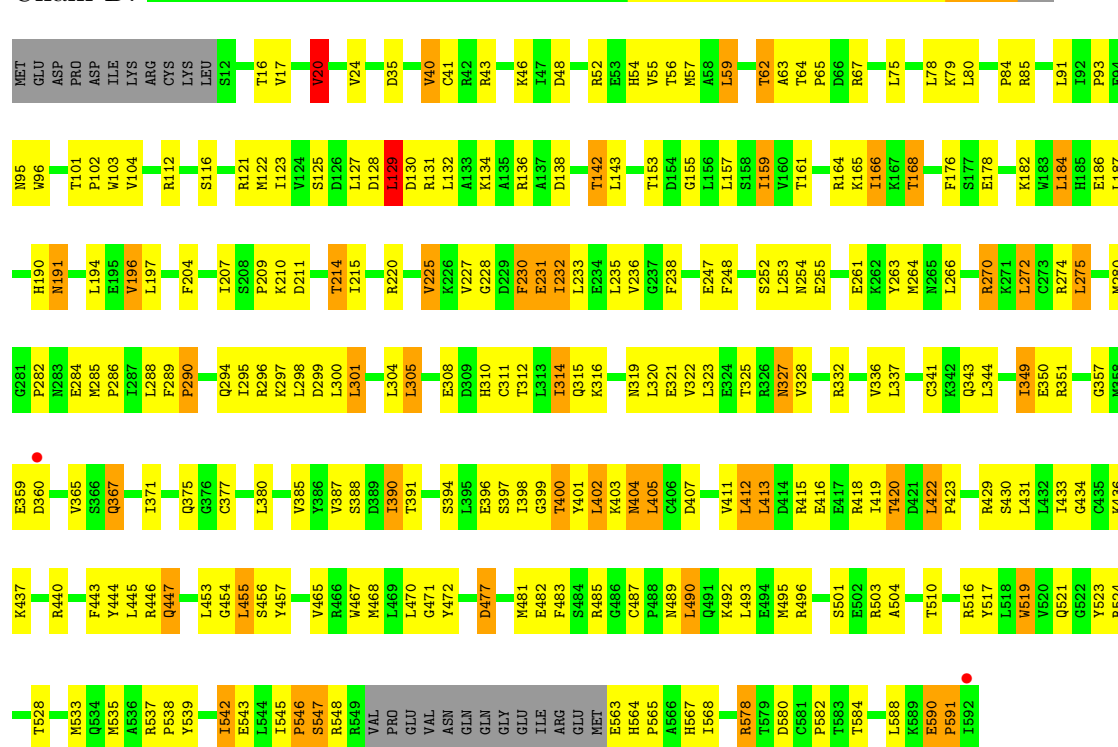
Chain B:





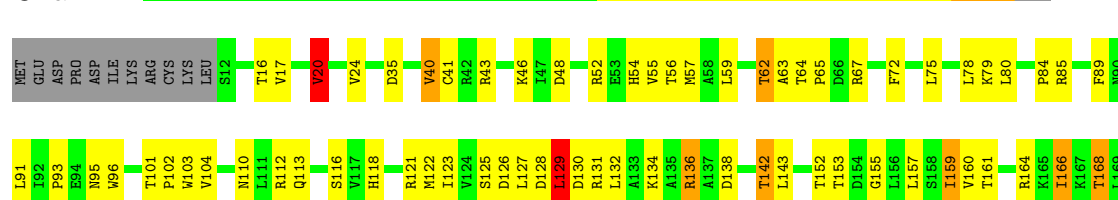
• Molecule 2: Coronatine-insensitive protein 1

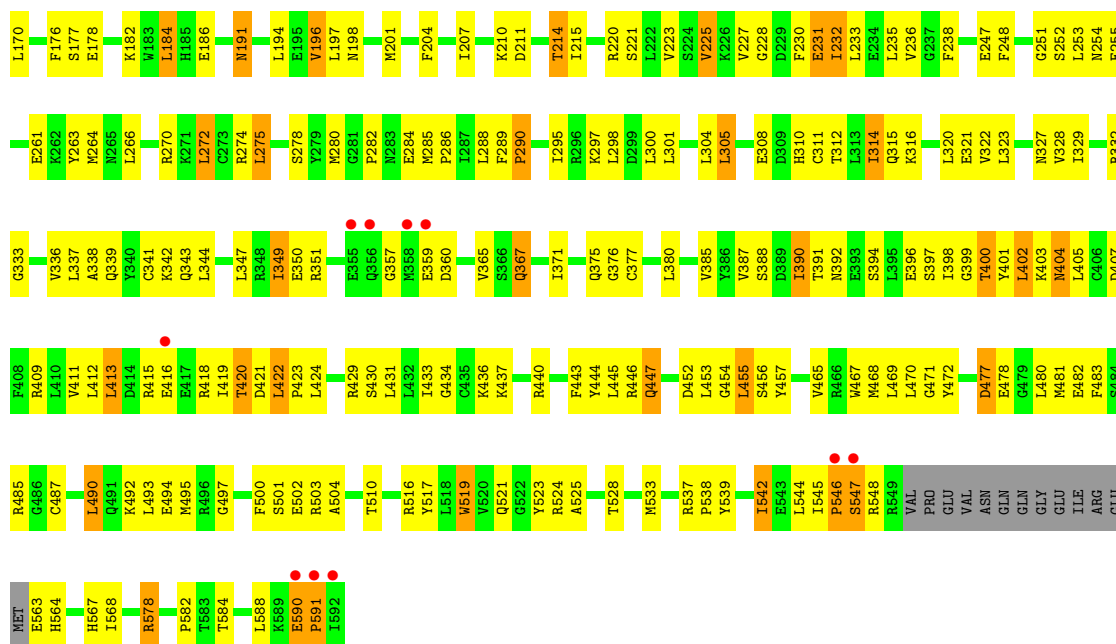
Chain D:



• Molecule 2: Coronatine-insensitive protein 1

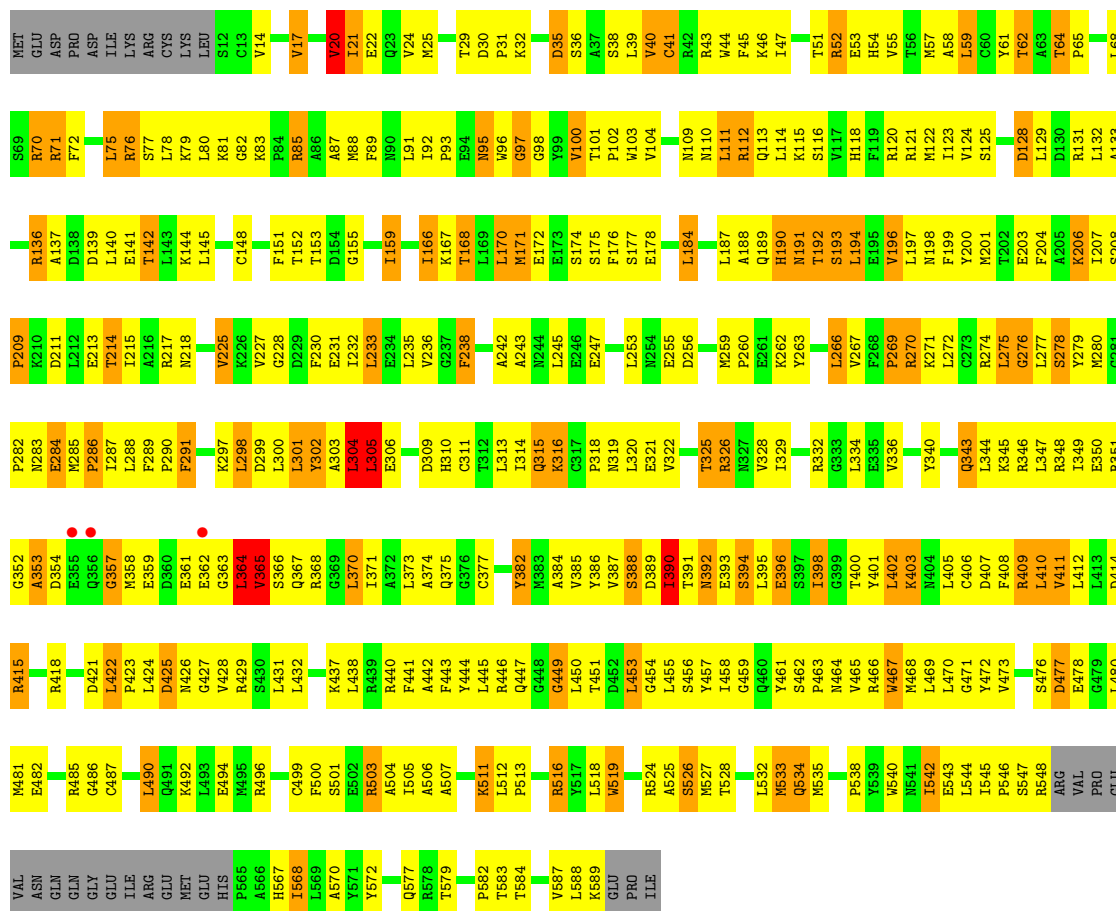
Chain F:





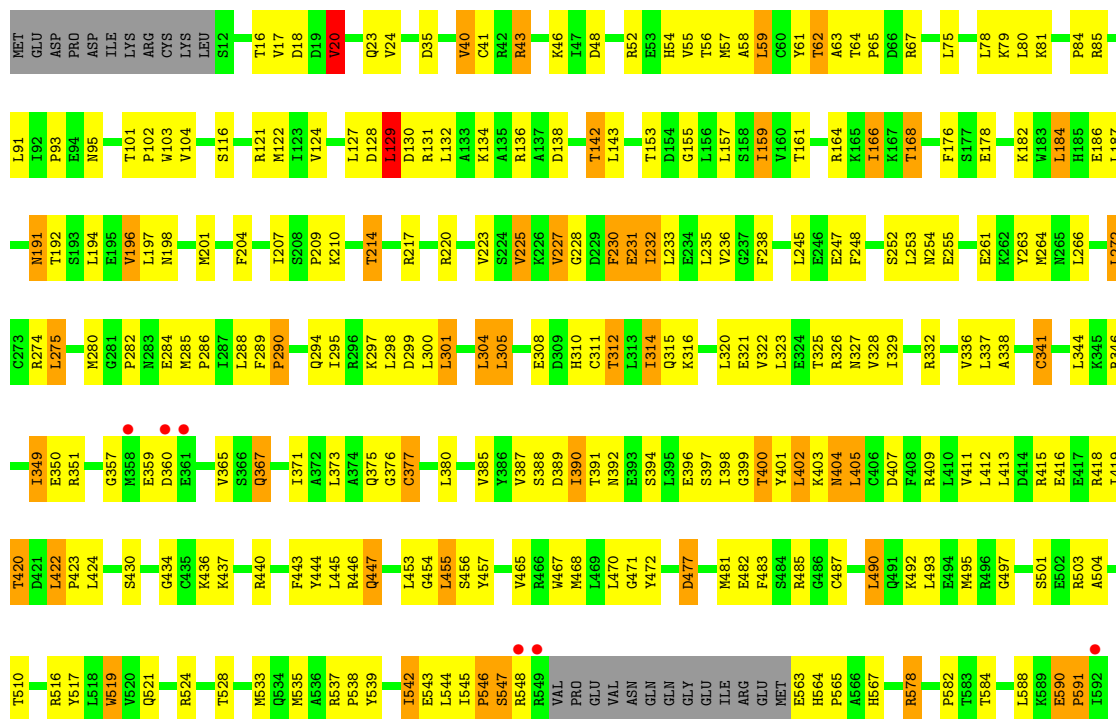
• Molecule 2: Coronatine-insensitive protein 1

Chain H:



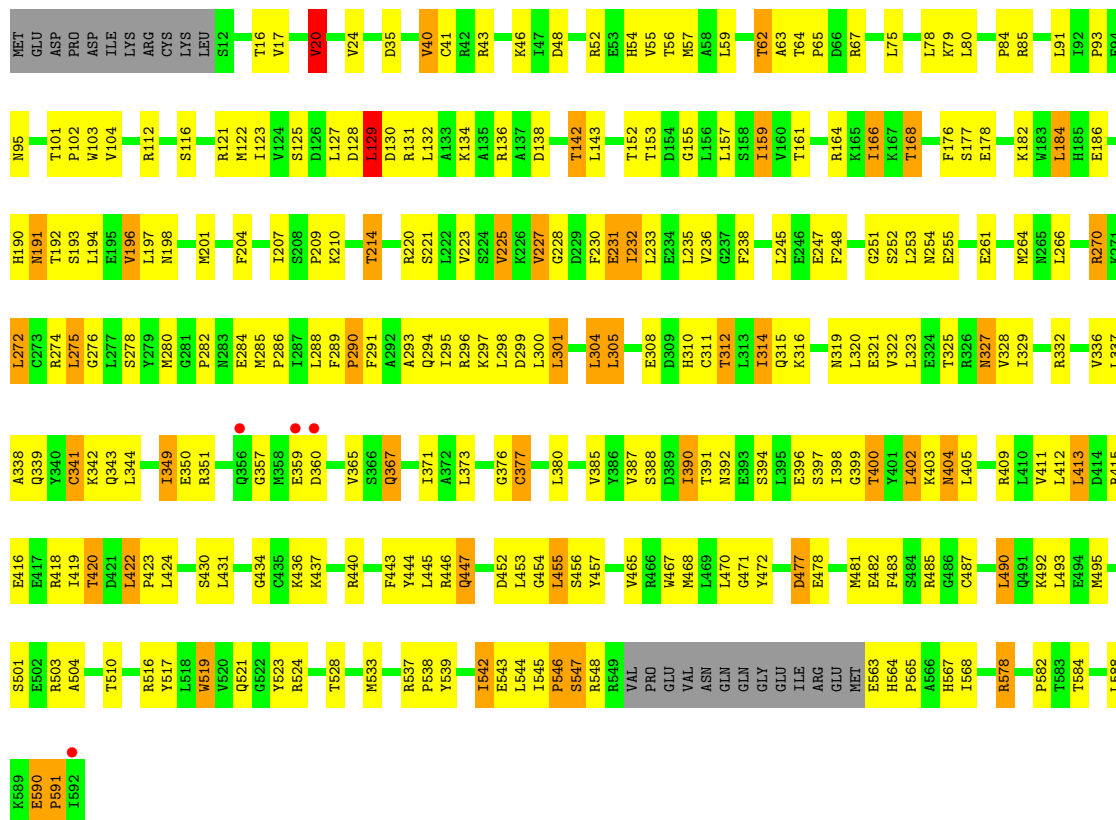
• Molecule 2: Coronatine-insensitive protein 1

## Chain J:



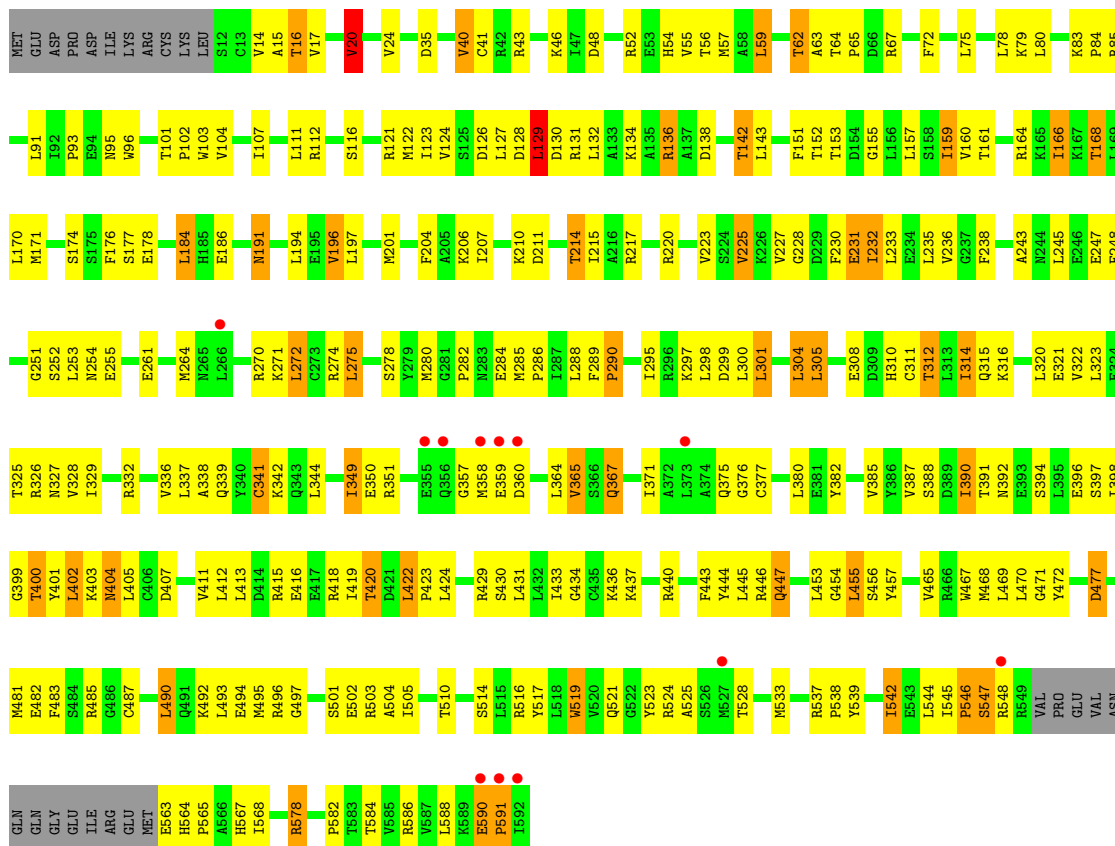
## • Molecule 2: Coronatine-insensitive protein 1

## Chain L:



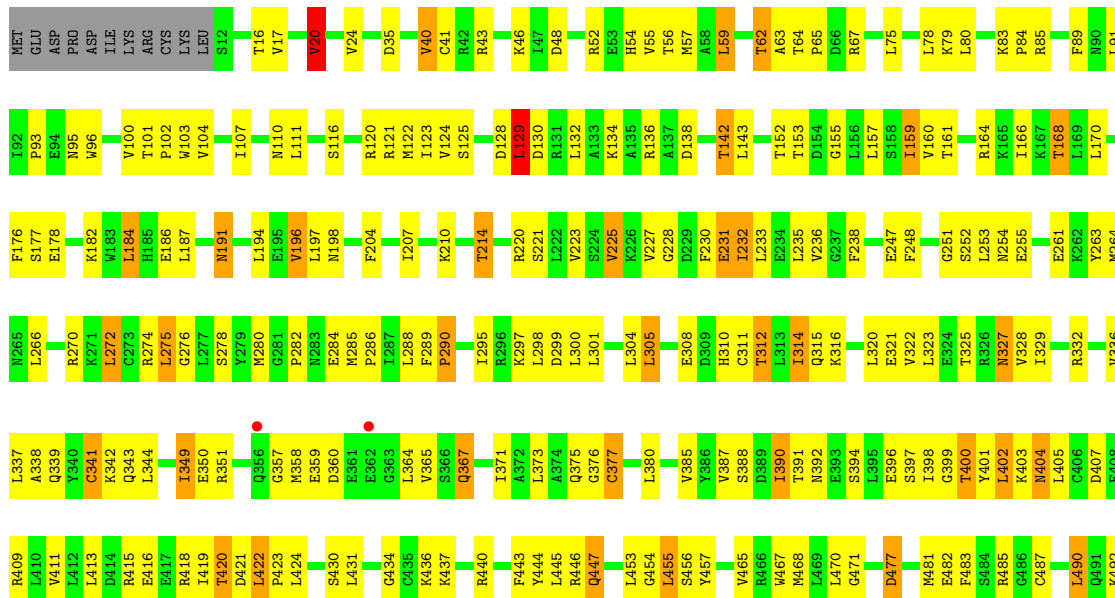
• Molecule 2: Coronatine-insensitive protein 1

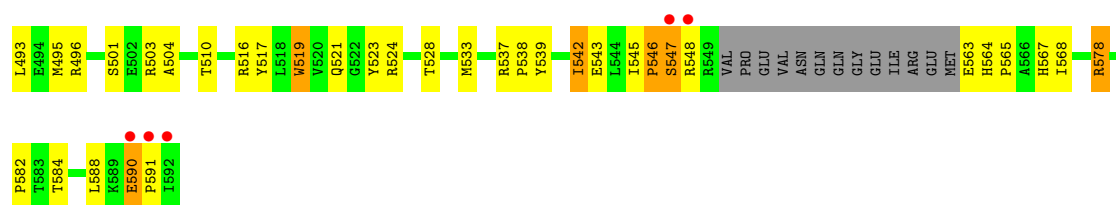
Chain N: 



• Molecule 2: Coronatine-insensitive protein 1

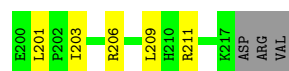
Chain P: 





- Molecule 3: JAZ1 degron peptide

Chain Q:



- Molecule 3: JAZ1 degron peptide

Chain R:



- Molecule 3: JAZ1 degron peptide

Chain S:



- Molecule 3: JAZ1 degron peptide

Chain U:



- Molecule 3: JAZ1 degron peptide

Chain V:



- Molecule 3: JAZ1 degron peptide

Chain W:



- Molecule 3: JAZ1 degron peptide

Chain X:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 85.9 (49.94-3.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.226 , 0.270 0.213 , 0.254	Depositor DCC
$R_{free}$ test set	1871 reflections (1.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 23.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 103078 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	46877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.



## 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	0.44	0/1162	0.56	0/1571
1	C	0.45	0/1162	0.58	0/1571
1	E	0.45	0/1162	0.59	0/1571
1	G	0.52	0/1162	0.63	0/1571
1	I	0.44	0/1162	0.57	0/1571
1	K	0.43	0/1162	0.57	0/1571
1	M	0.50	0/1162	0.59	0/1571
1	O	0.45	0/1162	0.56	0/1571
2	B	0.49	0/4623	0.63	1/6238 (0.0%)
2	D	0.50	0/4623	0.64	1/6238 (0.0%)
2	F	0.46	0/4623	0.64	1/6238 (0.0%)
2	H	0.58	0/4566	0.83	2/6161 (0.0%)
2	J	0.49	0/4623	0.64	1/6238 (0.0%)
2	L	0.45	0/4623	0.63	1/6238 (0.0%)
2	N	0.58	0/4623	0.67	1/6238 (0.0%)
2	P	0.47	0/4623	0.63	1/6238 (0.0%)
3	Q	0.42	0/158	0.53	0/208
3	R	0.39	0/158	0.52	0/208
3	S	0.38	0/158	0.55	0/208
3	U	0.46	0/158	0.55	0/208
3	V	0.41	0/158	0.54	0/208
3	W	0.43	0/158	0.57	0/208
3	X	0.40	0/158	0.53	0/208
All	All	0.50	0/47329	0.65	9/63851 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	129	LEU	CA-CB-CG	7.63	132.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	129	LEU	CA-CB-CG	7.51	132.58	115.30
2	L	129	LEU	CA-CB-CG	7.50	132.54	115.30
2	B	129	LEU	CA-CB-CG	7.40	132.32	115.30
2	N	129	LEU	CA-CB-CG	7.21	131.87	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1146	0	1117	63	0
1	C	1146	0	1117	57	0
1	E	1146	0	1117	69	0
1	G	1146	0	1117	65	0
1	I	1146	0	1117	69	0
1	K	1146	0	1117	55	0
1	M	1146	0	1117	86	0
1	O	1146	0	1117	69	0
2	B	4541	0	4583	222	0
2	D	4541	0	4583	225	0
2	F	4541	0	4583	219	0
2	H	4486	0	4534	431	0
2	J	4541	0	4583	226	0
2	L	4541	0	4583	233	0
2	N	4541	0	4583	271	0
2	P	4541	0	4583	224	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	6	0
3	V	156	0	171	5	0
3	W	156	0	171	7	0
3	X	156	0	171	5	0

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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	2465	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

The worst 5 of 2465 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:L:168:THR:HB	2:L:196:VAL:HG13	1.35	1.06
2:J:168:THR:HB	2:J:196:VAL:HG13	1.35	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/160 (88%)	115 (82%)	20 (14%)	5 (4%)	5	42
1	C	140/160 (88%)	116 (83%)	19 (14%)	5 (4%)	5	42
1	E	140/160 (88%)	118 (84%)	17 (12%)	5 (4%)	5	42
1	G	140/160 (88%)	113 (81%)	21 (15%)	6 (4%)	4	35
1	I	140/160 (88%)	117 (84%)	17 (12%)	6 (4%)	4	35
1	K	140/160 (88%)	116 (83%)	19 (14%)	5 (4%)	5	42
1	M	140/160 (88%)	115 (82%)	20 (14%)	5 (4%)	5	42
1	O	140/160 (88%)	115 (82%)	19 (14%)	6 (4%)	4	35
2	B	564/592 (95%)	501 (89%)	57 (10%)	6 (1%)	21	72
2	D	564/592 (95%)	503 (89%)	53 (9%)	8 (1%)	16	66
2	F	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	19	70
2	H	558/592 (94%)	426 (76%)	95 (17%)	37 (7%)	2	21
2	J	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	19	70
2	L	564/592 (95%)	501 (89%)	55 (10%)	8 (1%)	16	66
2	N	564/592 (95%)	502 (89%)	55 (10%)	7 (1%)	19	70
2	P	564/592 (95%)	500 (89%)	58 (10%)	6 (1%)	21	72
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%)	10	56

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
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%)	114 (90%)	13 (10%)	11	42
1	C	127/137 (93%)	115 (91%)	12 (9%)	13	47
1	E	127/137 (93%)	113 (89%)	14 (11%)	9	38
1	G	127/137 (93%)	113 (89%)	14 (11%)	9	38
1	I	127/137 (93%)	114 (90%)	13 (10%)	11	42
1	K	127/137 (93%)	114 (90%)	13 (10%)	11	42
1	M	127/137 (93%)	114 (90%)	13 (10%)	11	42
1	O	127/137 (93%)	113 (89%)	14 (11%)	9	38
2	B	500/523 (96%)	433 (87%)	67 (13%)	6	27
2	D	500/523 (96%)	432 (86%)	68 (14%)	5	26
2	F	500/523 (96%)	433 (87%)	67 (13%)	6	27
2	H	494/523 (94%)	397 (80%)	97 (20%)	2	9
2	J	500/523 (96%)	433 (87%)	67 (13%)	6	27
2	L	500/523 (96%)	431 (86%)	69 (14%)	5	25
2	N	500/523 (96%)	432 (86%)	68 (14%)	5	26
2	P	500/523 (96%)	434 (87%)	66 (13%)	6	28
3	Q	16/19 (84%)	16 (100%)	0	100	100
3	R	16/19 (84%)	16 (100%)	0	100	100
3	S	16/19 (84%)	16 (100%)	0	100	100
3	U	16/19 (84%)	16 (100%)	0	100	100
3	V	16/19 (84%)	16 (100%)	0	100	100
3	W	16/19 (84%)	16 (100%)	0	100	100
3	X	16/19 (84%)	16 (100%)	0	100	100
All	All	5122/5413 (95%)	4447 (87%)	675 (13%)	6	28

5 of 675 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	301	LEU

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Mol	Chain	Res	Type
2	J	132	LEU
2	P	136	ARG
2	H	343	GLN
2	H	516	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	110	ASN
2	J	23	GLN
2	P	109	ASN
2	H	310	HIS
2	H	489	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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
4	OGK	B	1100	-	25,25,25	7.08	10 (40%)	38,38,38	3.83	19 (50%)
5	PO4	B	1101	-	4,4,4	2.54	3 (75%)	6,6,6	0.32	0
5	PO4	B	1102	-	4,4,4	2.59	3 (75%)	6,6,6	0.31	0
5	PO4	B	1103	-	4,4,4	2.60	3 (75%)	6,6,6	0.31	0
5	PO4	B	1104	-	4,4,4	2.57	3 (75%)	6,6,6	0.31	0
5	PO4	D	1101	-	4,4,4	2.49	3 (75%)	6,6,6	0.35	0
5	PO4	D	1102	-	4,4,4	2.55	3 (75%)	6,6,6	0.30	0
5	PO4	D	1103	-	4,4,4	2.64	3 (75%)	6,6,6	0.32	0
5	PO4	D	1104	-	4,4,4	2.63	3 (75%)	6,6,6	0.32	0
4	OGK	D	2100	-	25,25,25	7.22	10 (40%)	38,38,38	3.80	18 (47%)
5	PO4	F	1101	-	4,4,4	2.56	3 (75%)	6,6,6	0.36	0
5	PO4	F	1102	-	4,4,4	2.76	3 (75%)	6,6,6	0.31	0
5	PO4	F	1103	-	4,4,4	2.63	3 (75%)	6,6,6	0.32	0
5	PO4	F	1104	-	4,4,4	2.74	3 (75%)	6,6,6	0.31	0
4	OGK	F	3100	-	25,25,25	7.09	11 (44%)	38,38,38	3.83	16 (42%)
5	PO4	H	1101	-	4,4,4	2.79	3 (75%)	6,6,6	0.31	0
5	PO4	H	1102	-	4,4,4	2.68	3 (75%)	6,6,6	0.32	0
5	PO4	H	1103	-	4,4,4	2.79	3 (75%)	6,6,6	0.31	0
5	PO4	H	1104	-	4,4,4	2.77	3 (75%)	6,6,6	0.35	0
4	OGK	H	4100	-	25,25,25	7.01	11 (44%)	38,38,38	3.64	19 (50%)
5	PO4	J	1101	-	4,4,4	2.60	3 (75%)	6,6,6	0.34	0
5	PO4	J	1102	-	4,4,4	2.66	3 (75%)	6,6,6	0.31	0
5	PO4	J	1103	-	4,4,4	2.50	3 (75%)	6,6,6	0.31	0
5	PO4	J	1104	-	4,4,4	2.52	3 (75%)	6,6,6	0.31	0
4	OGK	J	5100	-	25,25,25	7.22	11 (44%)	38,38,38	3.71	18 (47%)
5	PO4	L	1101	-	4,4,4	2.69	3 (75%)	6,6,6	0.33	0
5	PO4	L	1102	-	4,4,4	2.65	3 (75%)	6,6,6	0.30	0
5	PO4	L	1103	-	4,4,4	2.56	3 (75%)	6,6,6	0.32	0
5	PO4	L	1104	-	4,4,4	2.71	3 (75%)	6,6,6	0.31	0
4	OGK	L	6100	-	25,25,25	7.04	11 (44%)	38,38,38	3.68	17 (44%)
5	PO4	N	1101	-	4,4,4	2.90	3 (75%)	6,6,6	0.37	0
5	PO4	N	1102	-	4,4,4	2.68	3 (75%)	6,6,6	0.31	0
5	PO4	N	1103	-	4,4,4	2.57	3 (75%)	6,6,6	0.35	0
5	PO4	N	1104	-	4,4,4	2.71	3 (75%)	6,6,6	0.32	0
4	OGK	N	7100	-	25,25,25	6.81	10 (40%)	38,38,38	3.67	16 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PO4	P	1101	-	4,4,4	2.56	3 (75%)	6,6,6	0.33	0
5	PO4	P	1102	-	4,4,4	2.62	3 (75%)	6,6,6	0.31	0
5	PO4	P	1103	-	4,4,4	2.55	3 (75%)	6,6,6	0.32	0
5	PO4	P	1104	-	4,4,4	2.61	3 (75%)	6,6,6	0.32	0
4	OGK	P	8100	-	25,25,25	7.20	10 (40%)	38,38,38	3.72	18 (47%)

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	B	1100	-	-	0/19/52/52	0/0/3/3
5	PO4	B	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1104	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	D	2100	-	-	0/19/52/52	0/0/3/3
5	PO4	F	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	F	3100	-	-	0/19/52/52	0/0/3/3
5	PO4	H	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	H	4100	-	1/1/9/10	0/19/52/52	0/0/3/3
5	PO4	J	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	J	5100	-	-	0/19/52/52	0/0/3/3
5	PO4	L	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1104	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OGK	L	6100	-	-	0/19/52/52	0/0/3/3
5	PO4	N	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	N	7100	-	-	0/19/52/52	0/0/3/3
5	PO4	P	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	P	8100	-	-	0/19/52/52	0/0/3/3

The worst 5 of 180 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	5100	OGK	C13-C09	-23.21	1.27	1.51
4	D	2100	OGK	C13-C09	-23.11	1.27	1.51
4	P	8100	OGK	C13-C09	-22.84	1.28	1.51
4	F	3100	OGK	C13-C09	-22.78	1.28	1.51
4	B	1100	OGK	C13-C09	-22.53	1.28	1.51

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1100	OGK	C15-C14-C09	-16.31	99.15	122.07
4	F	3100	OGK	C15-C14-C09	-16.25	99.23	122.07
4	D	2100	OGK	C15-C14-C09	-15.66	100.06	122.07
4	J	5100	OGK	C15-C14-C09	-15.40	100.43	122.07
4	L	6100	OGK	C15-C14-C09	-15.27	100.61	122.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	4100	OGK	C03

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	144/160 (90%)	0.26	1 (0%) 84 43	50, 100, 151, 168	0
1	C	144/160 (90%)	0.22	0 100 100	50, 102, 153, 170	0
1	E	144/160 (90%)	0.15	0 100 100	54, 101, 151, 171	0
1	G	144/160 (90%)	0.02	0 100 100	49, 96, 149, 170	0
1	I	144/160 (90%)	0.12	0 100 100	50, 100, 150, 170	0
1	K	144/160 (90%)	0.23	1 (0%) 84 43	53, 102, 152, 170	0
1	M	144/160 (90%)	0.34	2 (1%) 72 26	55, 102, 152, 175	0
1	O	144/160 (90%)	0.28	2 (1%) 72 26	51, 101, 151, 173	0
2	B	568/592 (95%)	-0.13	4 (0%) 84 43	38, 76, 136, 201	0
2	D	568/592 (95%)	-0.08	2 (0%) 90 58	38, 75, 135, 200	0
2	F	568/592 (95%)	-0.09	10 (1%) 65 22	40, 79, 136, 202	0
2	H	562/592 (94%)	-0.18	3 (0%) 88 52	34, 73, 127, 191	0
2	J	568/592 (95%)	-0.12	6 (1%) 77 32	39, 77, 136, 204	0
2	L	568/592 (95%)	-0.13	4 (0%) 84 43	41, 79, 135, 202	0
2	N	568/592 (95%)	0.18	12 (2%) 60 19	41, 82, 137, 206	0
2	P	568/592 (95%)	-0.09	7 (1%) 75 30	40, 80, 138, 204	0
3	Q	18/21 (85%)	-0.10	0 100 100	72, 93, 116, 143	0
3	R	18/21 (85%)	-0.08	0 100 100	71, 88, 115, 145	0
3	S	18/21 (85%)	-0.24	0 100 100	73, 93, 117, 143	0
3	U	18/21 (85%)	-0.17	0 100 100	71, 88, 112, 143	0
3	V	18/21 (85%)	-0.03	1 (5%) 24 6	75, 93, 115, 143	0
3	W	18/21 (85%)	0.17	1 (5%) 24 6	80, 96, 119, 143	0
3	X	18/21 (85%)	-0.11	1 (5%) 24 6	76, 91, 119, 143	0
All	All	5816/6163 (94%)	-0.02	57 (0%) 79 34	34, 82, 141, 206	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	591	PRO	6.0
2	N	590	GLU	5.9
2	N	592	ILE	4.6
2	B	549	ARG	4.4
2	P	362	GLU	4.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	PO4	J	1102	5/5	0.39	17.65	67,86,95,104	0
5	PO4	F	1102	5/5	0.33	7.86	64,90,96,109	0
5	PO4	L	1102	5/5	0.38	5.81	73,82,96,100	0
5	PO4	H	1104	5/5	0.29	5.41	54,57,114,134	0
5	PO4	H	1103	5/5	0.18	5.20	38,47,52,77	0
5	PO4	N	1102	5/5	0.34	4.56	78,90,92,113	0
5	PO4	L	1103	5/5	0.32	3.99	52,56,69,89	0
5	PO4	L	1101	5/5	0.32	3.48	48,58,74,76	0
5	PO4	H	1101	5/5	0.20	3.17	36,45,63,88	0
5	PO4	B	1101	5/5	0.24	3.16	58,59,65,75	0
5	PO4	H	1102	5/5	0.29	3.08	58,59,72,88	0
5	PO4	J	1101	5/5	0.25	3.00	50,55,74,79	0
5	PO4	B	1102	5/5	0.26	2.71	70,84,93,100	0
5	PO4	F	1103	5/5	0.30	2.48	53,57,73,86	0
5	PO4	P	1101	5/5	0.24	2.40	57,62,74,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PO4	B	1104	5/5	0.25	2.28	68,79,102,119	0
5	PO4	N	1103	5/5	0.33	2.21	56,56,74,85	0
5	PO4	F	1101	5/5	0.23	2.17	52,58,68,88	0
5	PO4	B	1103	5/5	0.28	2.15	54,54,61,76	0
5	PO4	D	1101	5/5	0.28	1.76	51,55,63,80	0
5	PO4	J	1104	5/5	0.26	1.69	76,81,112,117	0
5	PO4	L	1104	5/5	0.24	1.64	76,78,119,123	0
5	PO4	D	1103	5/5	0.30	1.63	48,52,55,81	0
5	PO4	D	1102	5/5	0.23	1.61	66,79,93,93	0
4	OGK	H	4100	23/23	0.26	1.38	44,71,85,98	0
5	PO4	J	1103	5/5	0.24	1.15	53,53,64,77	0
4	OGK	P	8100	23/23	0.26	0.95	64,75,88,90	0
5	PO4	P	1104	5/5	0.21	0.90	73,75,110,121	0
5	PO4	D	1104	5/5	0.23	0.81	72,73,107,122	0
4	OGK	J	5100	23/23	0.25	0.65	59,67,88,93	0
5	PO4	N	1104	5/5	0.24	0.63	82,83,118,122	0
5	PO4	P	1103	5/5	0.22	0.58	50,58,73,85	0
4	OGK	D	2100	23/23	0.26	0.54	60,72,81,86	0
4	OGK	B	1100	23/23	0.23	0.46	62,73,87,93	0
4	OGK	F	3100	23/23	0.23	0.46	64,72,91,94	0
5	PO4	N	1101	5/5	0.29	0.39	51,59,80,82	0
4	OGK	L	6100	23/23	0.22	0.29	62,71,90,92	0
4	OGK	N	7100	23/23	0.29	0.23	65,79,100,104	0
5	PO4	F	1104	5/5	0.21	0.14	72,81,117,120	0
5	PO4	P	1102	5/5	0.16	-2.18	72,87,98,108	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.