



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:19 AM GMT

PDB ID : 3OGK  
Title : Structure of COI1-ASK1 in complex with coronatine and an incomplete 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 : 2010-08-16  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

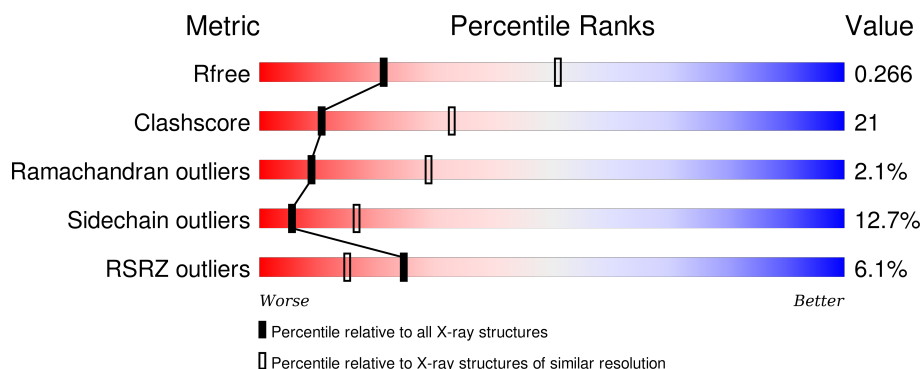
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.



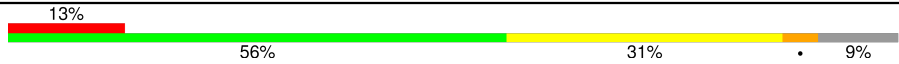

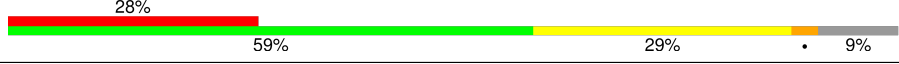
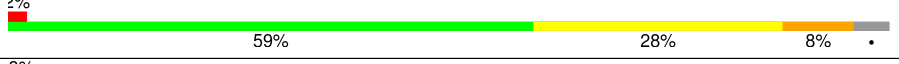

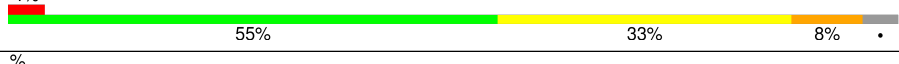
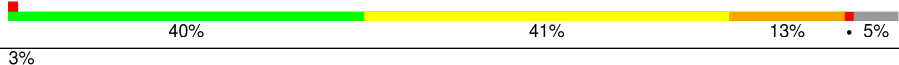

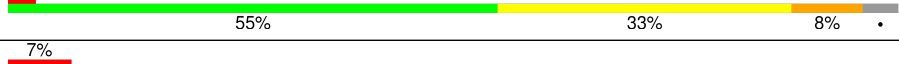



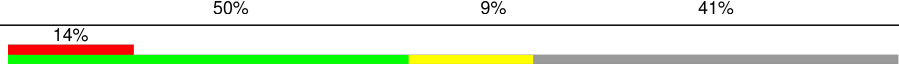
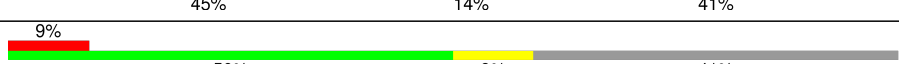
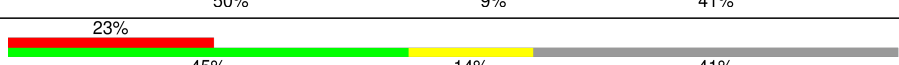

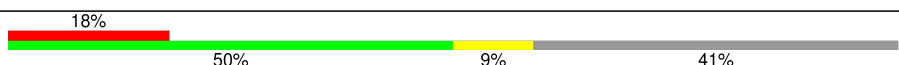

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	<div> <div>6%</div> <div>56%</div> <div>31%</div> <div>•</div> <div>9%</div> </div>
1	C	160	<div> <div>18%</div> <div>54%</div> <div>30%</div> <div>6%</div> <div>9%</div> </div>
1	E	160	<div> <div>3%</div> <div>58%</div> <div>29%</div> <div>•</div> <div>9%</div> </div>
1	G	160	<div> <div>4%</div> <div>58%</div> <div>28%</div> <div>5%</div> <div>9%</div> </div>
1	I	160	<div> <div>12%</div> <div>49%</div> <div>36%</div> <div>5%</div> <div>9%</div> </div>

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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	22	
3	R	22	
3	S	22	
3	U	22	
3	V	22	
3	W	22	
3	X	22	

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	B	1100	X	-	-	-
4	OGK	D	1100	X	-	-	-
4	OGK	H	1100	X	-	-	-
4	OGK	L	1100	X	-	X	-
5	PO4	B	1102	-	X	-	-
5	PO4	B	1103	-	-	X	-
5	PO4	D	1103	-	-	X	-

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

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46526 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	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	C	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	E	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	G	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	I	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	K	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	M	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	O	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	D	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	F	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	H	562	Total	C	N	O	S	0	0	0
			4486	2840	779	831	36			
2	J	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	L	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			

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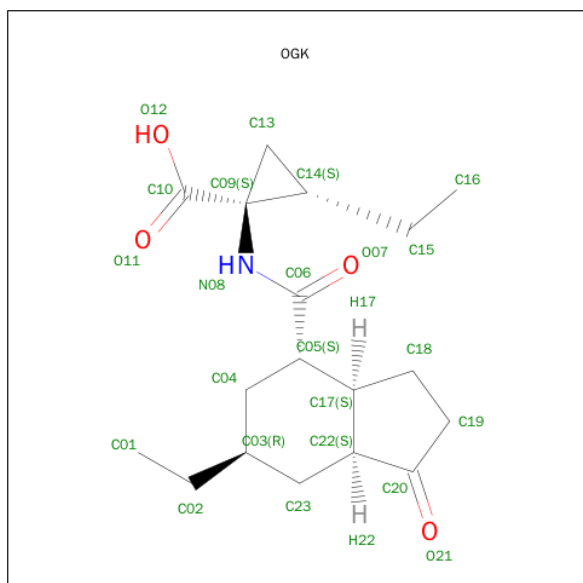
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	P	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			

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

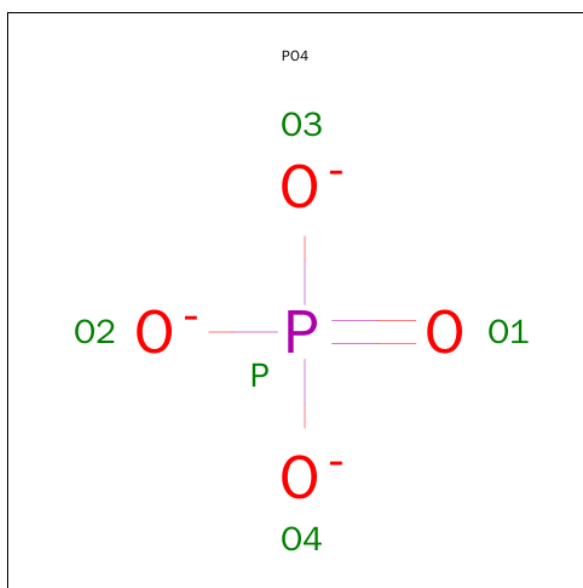
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	R	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	S	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	U	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	V	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	W	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	X	13	Total	C	N	O	0	0	0
			119	74	29	16			

- Molecule 4 is (1S,2S)-2-ETHYL-1-([[(3AS,4S,6R,7AS)-6-ETHYL-1-OXOOCTAHYDR O-1H-INDEN-4-YL]CARBONYL}AMINO)CYCLOPROPANECARBOXYLIC ACID (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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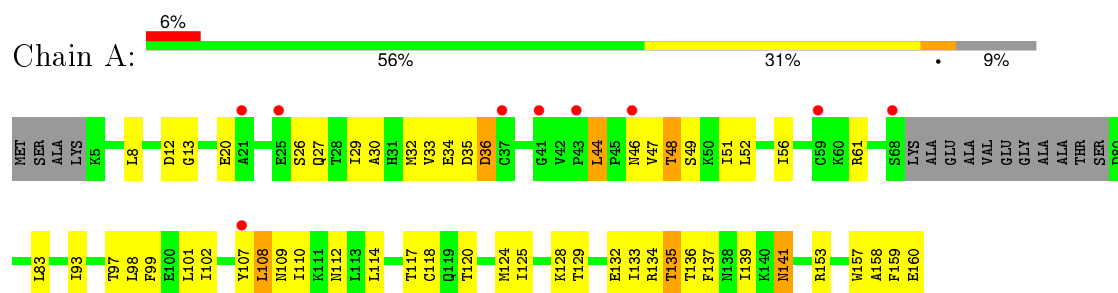
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		

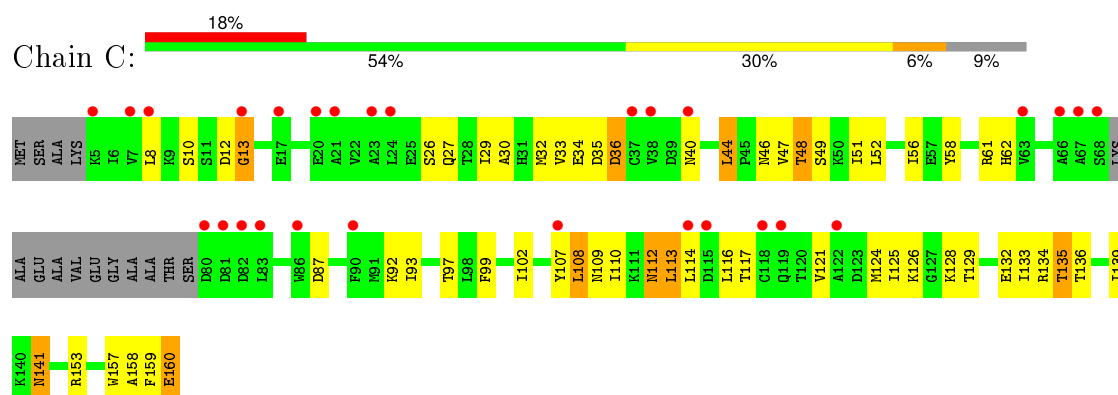
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

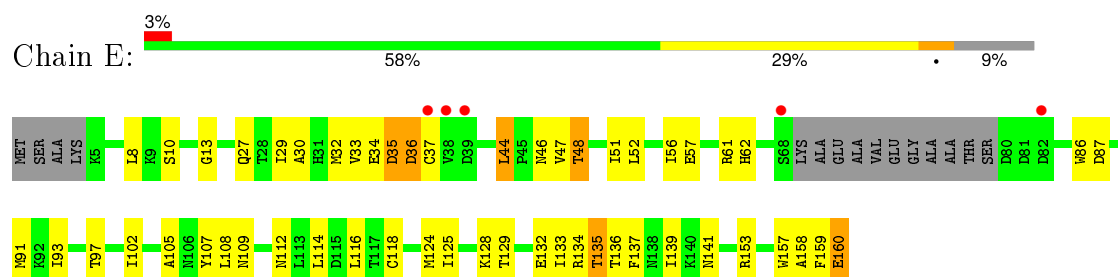
- Molecule 1: SKP1-like protein 1A



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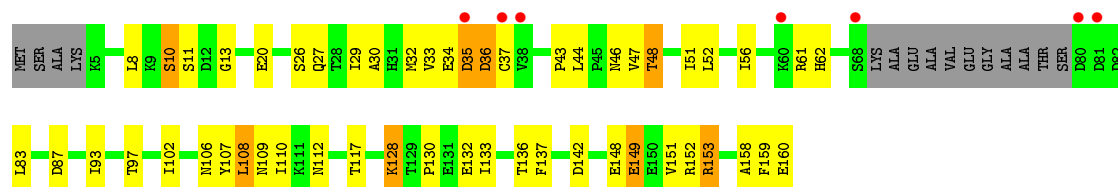


- Molecule 1: SKP1-like protein 1A

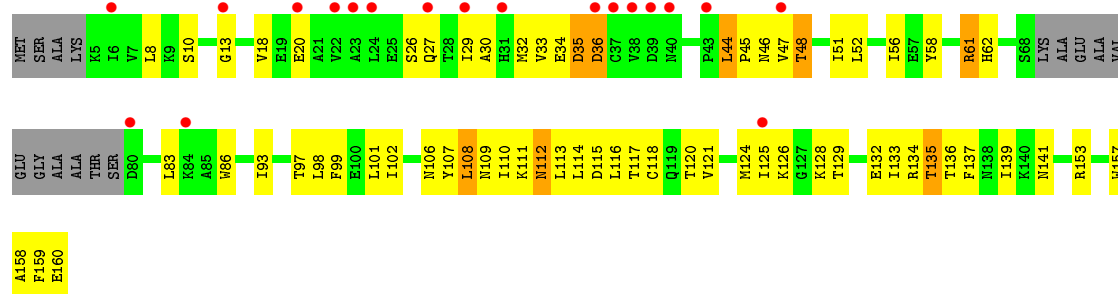


- Molecule 1: SKP1-like protein 1A

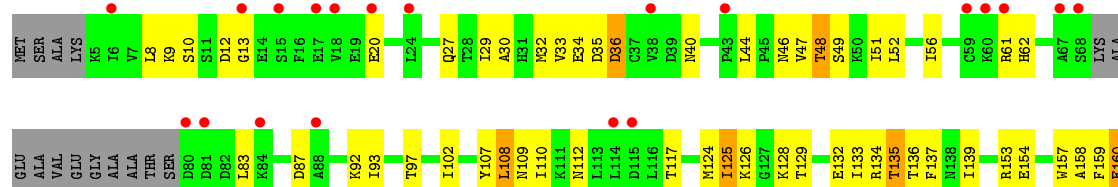




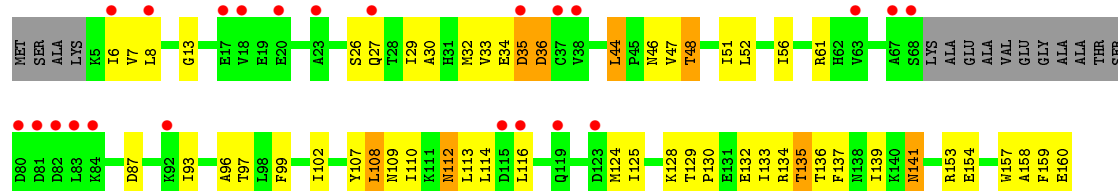
• Molecule 1: SKP1-like protein 1A



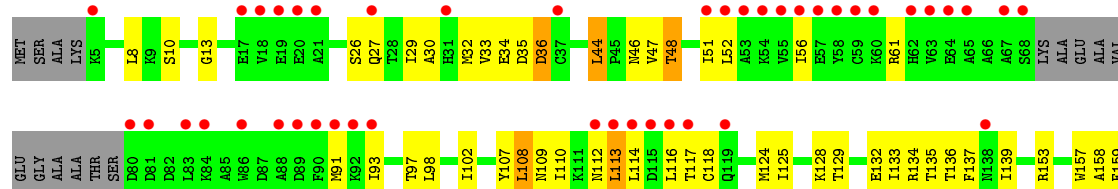
• Molecule 1: SKP1-like protein 1A



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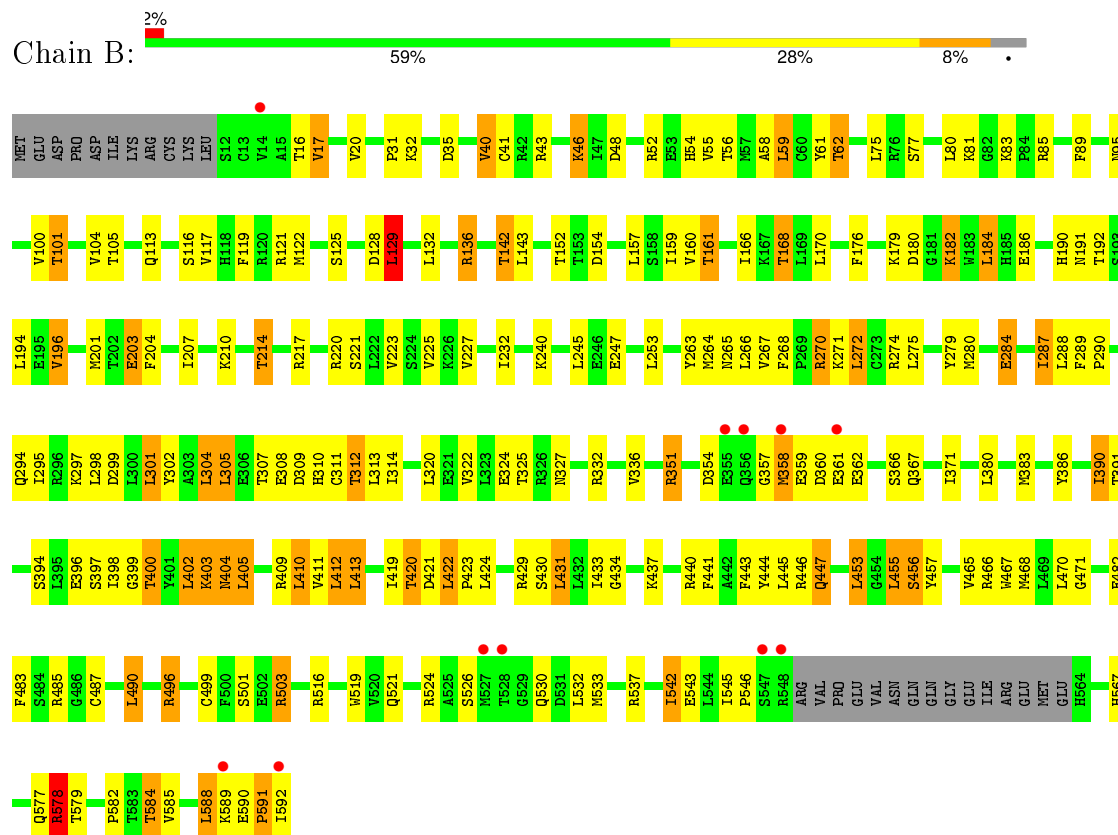


• Molecule 1: SKP1-like protein 1A

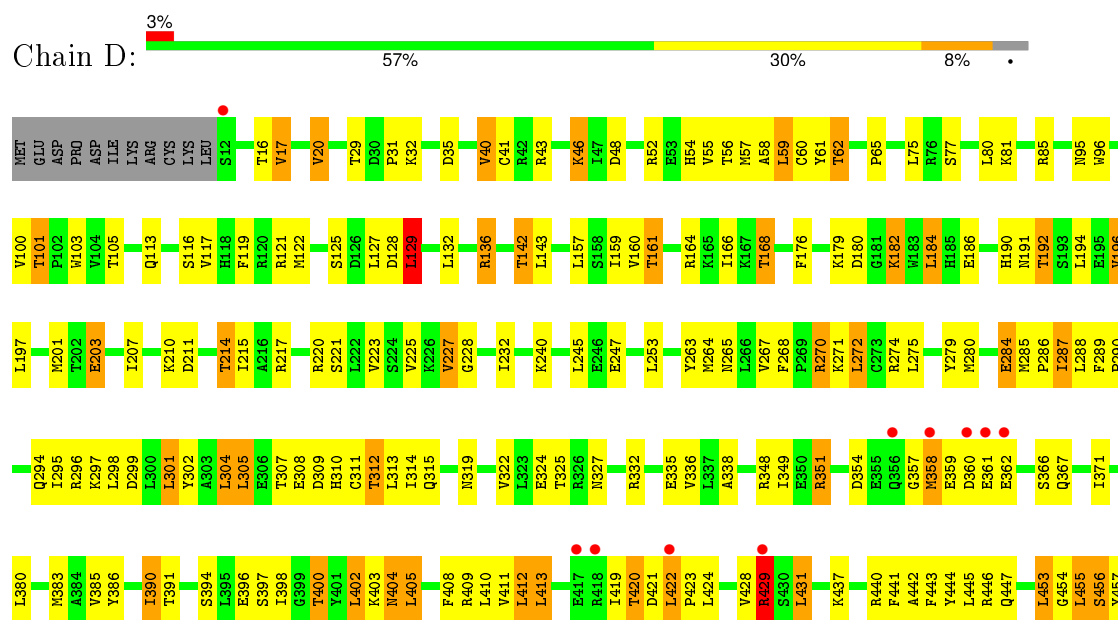


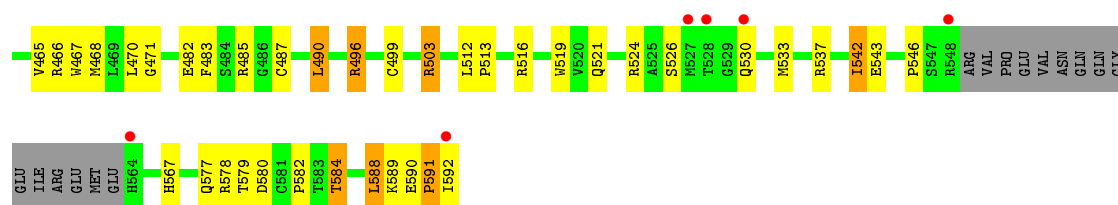
E160

- Molecule 2: Coronatine-insensitive protein 1

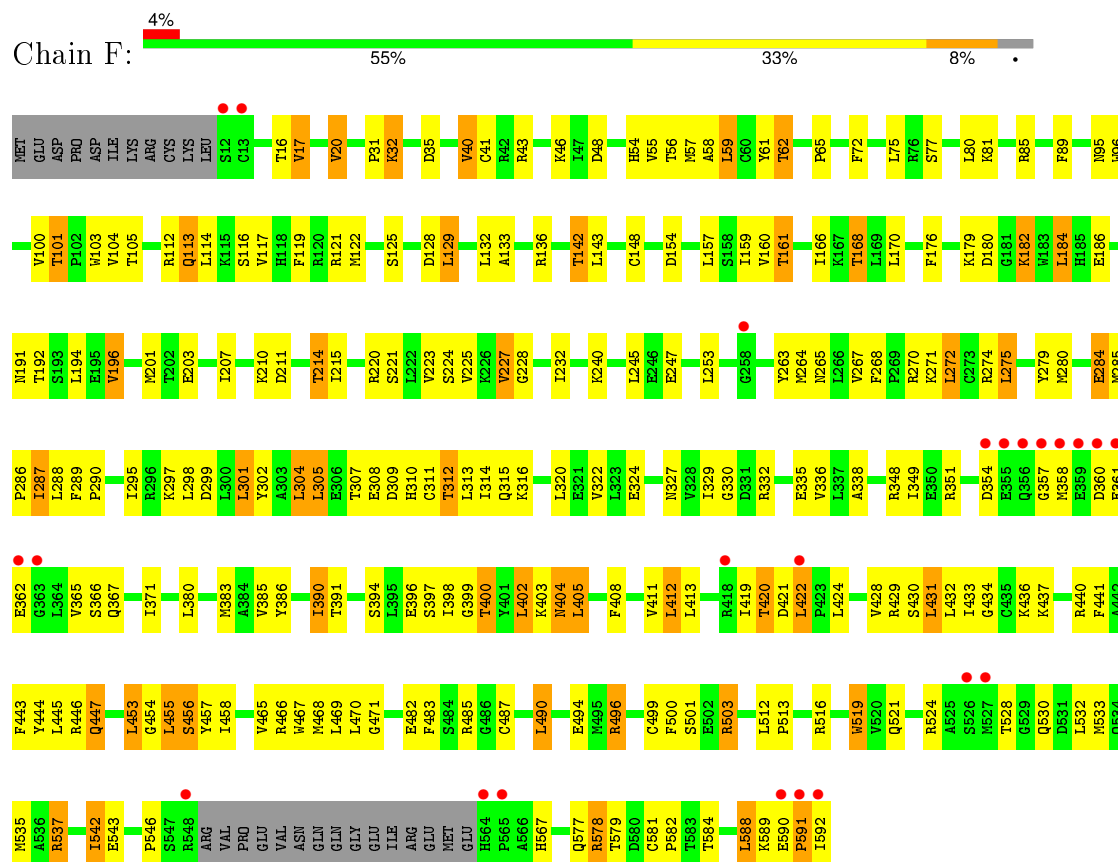


- Molecule 2: Coronatine-insensitive protein 1



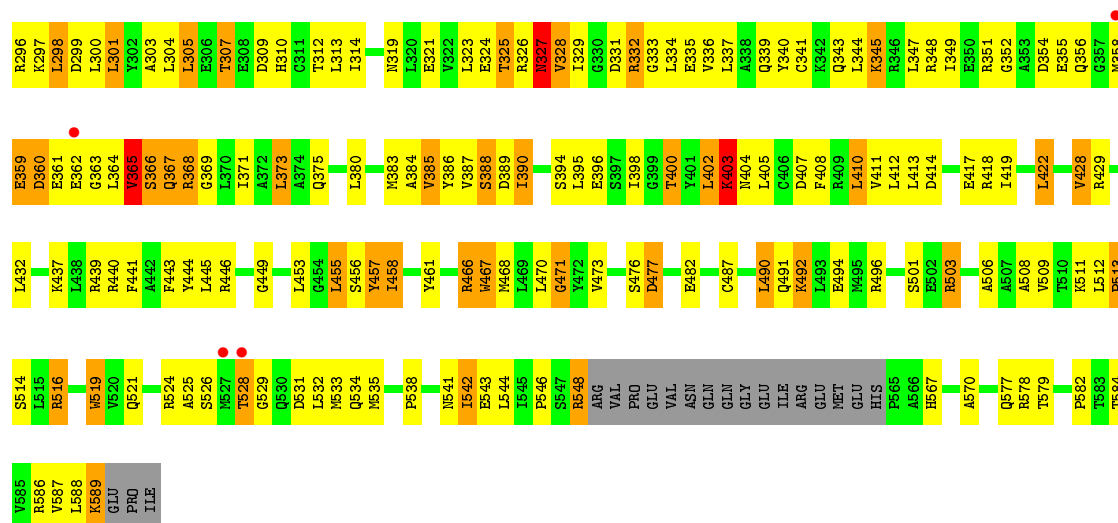


• Molecule 2: Coronatine-insensitive protein 1

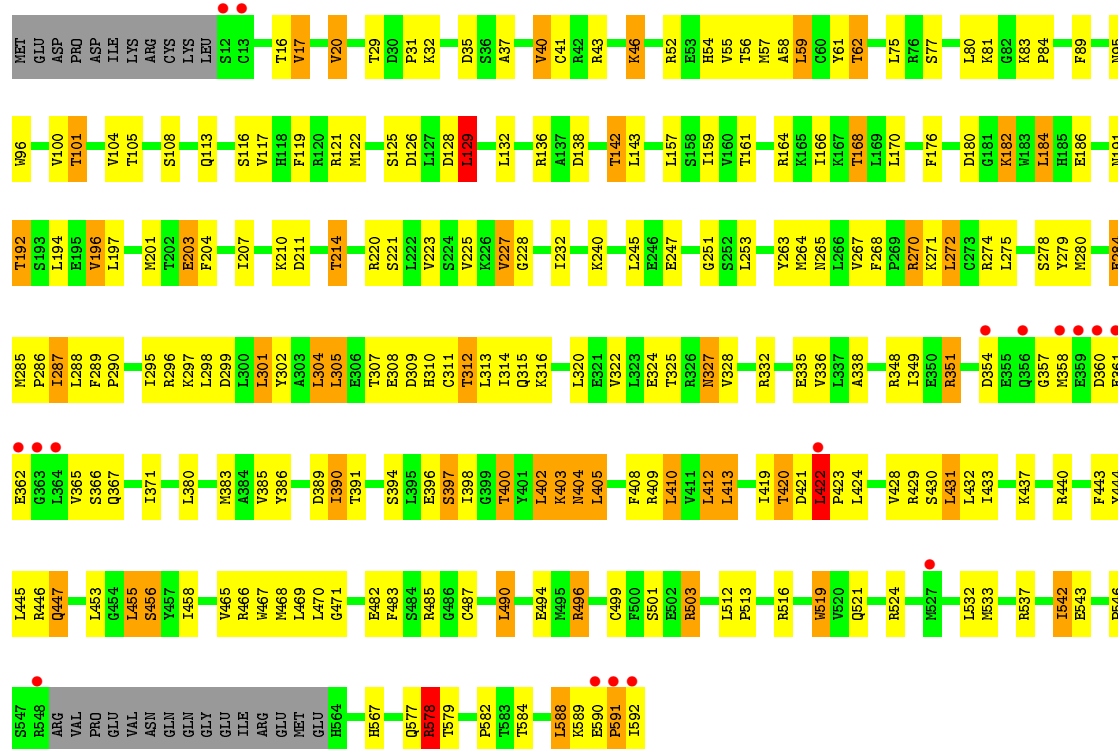


• Molecule 2: Coronatine-insensitive protein 1



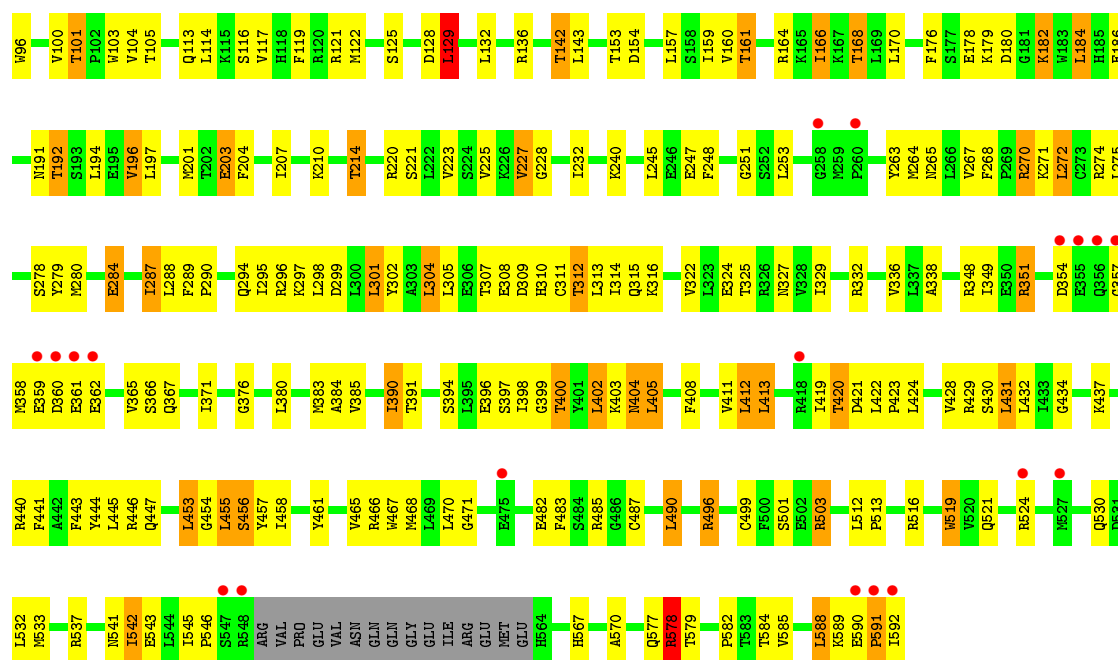


• Molecule 2: Coronatine-insensitive protein 1

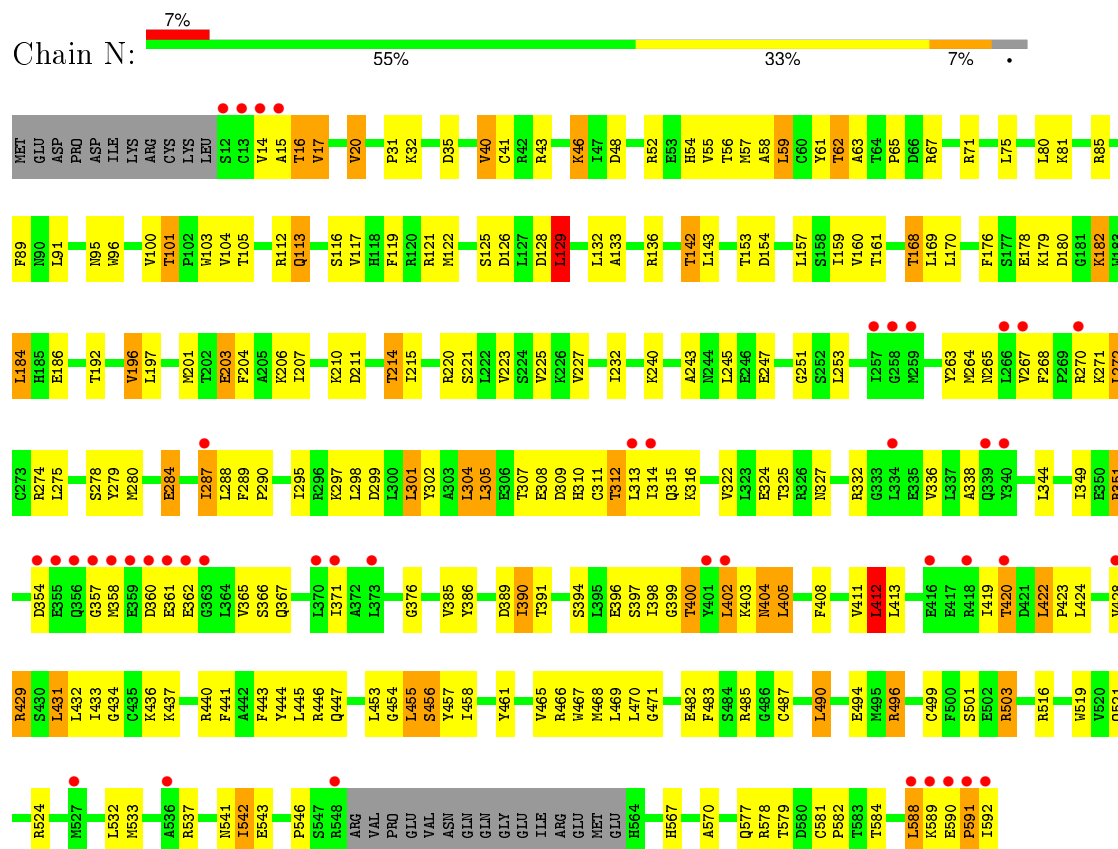


• Molecule 2: Coronatine-insensitive protein 1





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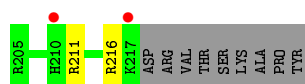


• Molecule 2: Coronatine-insensitive protein 1

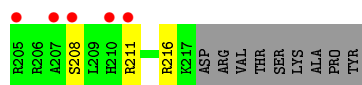




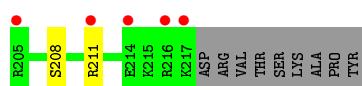




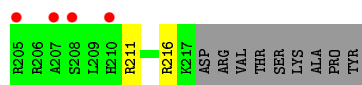
- Molecule 3: JAZ1 incomplete degron peptide



- Molecule 3: JAZ1 incomplete degron peptide



- Molecule 3: JAZ1 incomplete degron peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.85Å 221.46Å 148.47Å 90.00° 104.49° 90.00°	Depositor
Resolution (Å)	49.63 – 2.80 49.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.7 (49.63-2.80) 93.7 (49.63-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.225 , 0.268 0.224 , 0.266	Depositor DCC
$R_{free}$ test set	9332 reflections (5.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 186238 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	46526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.53	0/1168	0.61	0/1579
1	C	0.59	2/1168 (0.2%)	0.65	0/1579
1	E	0.62	0/1168	0.66	0/1579
1	G	0.64	0/1168	0.69	0/1579
1	I	0.54	1/1168 (0.1%)	0.61	0/1579
1	K	0.50	0/1168	0.62	0/1579
1	M	0.55	0/1168	0.63	0/1579
1	O	0.60	0/1168	0.63	0/1579
2	B	0.70	0/4603	0.79	4/6212 (0.1%)
2	D	0.67	1/4603 (0.0%)	0.79	2/6212 (0.0%)
2	F	0.63	1/4603 (0.0%)	0.78	1/6212 (0.0%)
2	H	0.77	0/4566	0.99	11/6161 (0.2%)
2	J	0.62	0/4603	0.78	4/6212 (0.1%)
2	L	0.59	0/4603	0.77	3/6212 (0.0%)
2	N	0.68	0/4603	0.79	3/6212 (0.0%)
2	P	0.64	0/4603	0.77	1/6212 (0.0%)
3	Q	0.36	0/120	0.62	0/155
3	R	0.42	0/120	0.64	0/155
3	S	0.40	0/120	0.58	0/155
3	U	0.41	0/120	0.61	0/155
3	V	0.46	0/120	0.57	0/155
3	W	0.44	0/120	0.60	0/155
3	X	0.43	0/120	0.59	0/155
All	All	0.64	5/46971 (0.0%)	0.78	29/63362 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	60	CYS	CB-SG	-6.18	1.71	1.82
2	F	148	CYS	CB-SG	-5.77	1.72	1.81
1	C	114	LEU	N-CA	5.58	1.57	1.46
1	I	118	CYS	CB-SG	-5.14	1.73	1.81
1	C	113	LEU	C-N	5.06	1.45	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	129	LEU	CA-CB-CG	10.65	139.79	115.30
2	B	129	LEU	CA-CB-CG	10.24	138.86	115.30
2	D	129	LEU	CA-CB-CG	9.72	137.66	115.30
2	N	129	LEU	CA-CB-CG	9.63	137.46	115.30
2	P	129	LEU	CA-CB-CG	9.35	136.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	365	VAL	Peptide

## 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	1152	0	1122	42	0
1	C	1152	0	1122	58	0
1	E	1152	0	1122	46	0
1	G	1152	0	1122	51	0
1	I	1152	0	1122	55	2
1	K	1152	0	1122	49	0
1	M	1152	0	1122	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1152	0	1122	44	0
2	B	4521	0	4564	169	0
2	D	4521	0	4564	197	2
2	F	4521	0	4564	194	0
2	H	4486	0	4534	354	0
2	J	4521	0	4564	190	0
2	L	4521	0	4564	195	0
2	N	4521	0	4564	219	0
2	P	4521	0	4564	190	0
3	Q	119	0	131	2	0
3	R	119	0	131	2	0
3	S	119	0	131	3	0
3	U	119	0	131	2	0
3	V	119	0	131	4	0
3	W	119	0	131	2	0
3	X	119	0	131	2	0
4	B	23	0	26	6	0
4	D	23	0	26	2	0
4	F	23	0	27	8	0
4	H	23	0	26	8	0
4	J	23	0	27	7	0
4	L	23	0	27	11	0
4	N	23	0	27	7	0
4	P	23	0	27	7	0
5	B	20	0	0	3	0
5	D	20	0	0	3	0
5	F	20	0	0	2	0
5	H	20	0	0	6	0
5	J	20	0	0	2	0
5	L	20	0	0	1	0
5	N	20	0	0	3	0
5	P	20	0	0	3	0
All	All	46526	0	46588	1980	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 21.

The worst 5 of 1980 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:168:THR:HB	2:H:196:VAL:HG13	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:305:LEU:HD23	2:H:305:LEU:H	1.24	1.01
1:M:102:ILE:HG21	2:N:20:VAL:HG22	1.43	1.00
2:H:364:LEU:HB3	2:H:365:VAL:HG22	1.41	1.00
2:B:444:TYR:HA	2:B:471:GLY:HA3	1.47	0.97

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]	2.03	0.17
2:D:429:ARG:NH1	1:I:86:TRP:CE3[2_555]	2.06	0.14

## 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	141/160 (88%)	115 (82%)	21 (15%)	5 (4%)	4	15
1	C	141/160 (88%)	115 (82%)	21 (15%)	5 (4%)	4	15
1	E	141/160 (88%)	117 (83%)	21 (15%)	3 (2%)	9	29
1	G	141/160 (88%)	119 (84%)	18 (13%)	4 (3%)	6	21
1	I	141/160 (88%)	116 (82%)	21 (15%)	4 (3%)	6	21
1	K	141/160 (88%)	118 (84%)	19 (14%)	4 (3%)	6	21
1	M	141/160 (88%)	114 (81%)	22 (16%)	5 (4%)	4	15
1	O	141/160 (88%)	114 (81%)	23 (16%)	4 (3%)	6	21
2	B	562/592 (95%)	509 (91%)	44 (8%)	9 (2%)	12	38
2	D	562/592 (95%)	508 (90%)	44 (8%)	10 (2%)	11	34
2	F	562/592 (95%)	509 (91%)	44 (8%)	9 (2%)	12	38
2	H	558/592 (94%)	475 (85%)	63 (11%)	20 (4%)	4	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	562/592 (95%)	508 (90%)	44 (8%)	10 (2%)	11	34
2	L	562/592 (95%)	508 (90%)	46 (8%)	8 (1%)	14	42
2	N	562/592 (95%)	505 (90%)	49 (9%)	8 (1%)	14	42
2	P	562/592 (95%)	503 (90%)	49 (9%)	10 (2%)	11	34
3	Q	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	R	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	S	11/22 (50%)	9 (82%)	2 (18%)	0	100	100
3	U	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	V	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	W	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	X	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
All	All	5697/6170 (92%)	5022 (88%)	557 (10%)	118 (2%)	9	29

5 of 118 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	271	LYS
2	B	404	ASN
2	B	420	THR
2	D	271	LYS
2	D	420	THR

### 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	128/137 (93%)	121 (94%)	7 (6%)	27	59
1	C	128/137 (93%)	119 (93%)	9 (7%)	19	47
1	E	128/137 (93%)	119 (93%)	9 (7%)	19	47
1	G	128/137 (93%)	118 (92%)	10 (8%)	16	41
1	I	128/137 (93%)	120 (94%)	8 (6%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	128/137 (93%)	118 (92%)	10 (8%)	16	41
1	M	128/137 (93%)	121 (94%)	7 (6%)	27	59
1	O	128/137 (93%)	120 (94%)	8 (6%)	22	53
2	B	498/523 (95%)	424 (85%)	74 (15%)	4	11
2	D	498/523 (95%)	428 (86%)	70 (14%)	4	12
2	F	498/523 (95%)	427 (86%)	71 (14%)	4	12
2	H	494/523 (94%)	402 (81%)	92 (19%)	2	6
2	J	498/523 (95%)	426 (86%)	72 (14%)	4	11
2	L	498/523 (95%)	428 (86%)	70 (14%)	4	12
2	N	498/523 (95%)	432 (87%)	66 (13%)	5	14
2	P	498/523 (95%)	433 (87%)	65 (13%)	5	15
3	Q	12/20 (60%)	12 (100%)	0	100	100
3	R	12/20 (60%)	12 (100%)	0	100	100
3	S	12/20 (60%)	12 (100%)	0	100	100
3	U	12/20 (60%)	12 (100%)	0	100	100
3	V	12/20 (60%)	12 (100%)	0	100	100
3	W	12/20 (60%)	12 (100%)	0	100	100
3	X	12/20 (60%)	12 (100%)	0	100	100
All	All	5088/5420 (94%)	4440 (87%)	648 (13%)	5	16

5 of 648 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	272	LEU
2	J	104	VAL
2	P	136	ARG
2	H	307	THR
2	H	467	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	319	ASN
2	J	294	GLN
2	P	109	ASN

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Mol	Chain	Res	Type
2	H	343	GLN
1	I	31	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no 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	-	22,25,25	6.37	9 (40%)	25,38,38	2.72	10 (40%)
5	PO4	B	1101	-	4,4,4	2.95	3 (75%)	6,6,6	0.30	0
5	PO4	B	1102	-	4,4,4	3.05	4 (100%)	6,6,6	0.26	0
5	PO4	B	1103	-	4,4,4	2.74	3 (75%)	6,6,6	0.32	0
5	PO4	B	1104	-	4,4,4	2.87	3 (75%)	6,6,6	0.32	0
4	OGK	D	1100	-	22,25,25	6.33	8 (36%)	25,38,38	3.06	12 (48%)
5	PO4	D	1101	-	4,4,4	3.00	3 (75%)	6,6,6	0.33	0
5	PO4	D	1102	-	4,4,4	3.12	3 (75%)	6,6,6	0.28	0
5	PO4	D	1103	-	4,4,4	2.62	3 (75%)	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PO4	D	1104	-	4,4,4	2.93	3 (75%)	6,6,6	0.33	0
4	OGK	F	1100	-	22,25,25	6.41	8 (36%)	25,38,38	2.58	13 (52%)
5	PO4	F	1101	-	4,4,4	3.04	4 (100%)	6,6,6	0.35	0
5	PO4	F	1102	-	4,4,4	3.11	3 (75%)	6,6,6	0.27	0
5	PO4	F	1103	-	4,4,4	2.74	3 (75%)	6,6,6	0.28	0
5	PO4	F	1104	-	4,4,4	3.07	3 (75%)	6,6,6	0.31	0
4	OGK	H	1100	-	22,25,25	6.28	8 (36%)	25,38,38	2.69	13 (52%)
5	PO4	H	1101	-	4,4,4	3.10	4 (100%)	6,6,6	0.32	0
5	PO4	H	1102	-	4,4,4	3.25	3 (75%)	6,6,6	0.29	0
5	PO4	H	1103	-	4,4,4	3.01	4 (100%)	6,6,6	0.27	0
5	PO4	H	1104	-	4,4,4	2.96	3 (75%)	6,6,6	0.39	0
4	OGK	J	1100	-	22,25,25	6.17	8 (36%)	25,38,38	2.64	12 (48%)
5	PO4	J	1101	-	4,4,4	3.09	3 (75%)	6,6,6	0.29	0
5	PO4	J	1102	-	4,4,4	3.12	3 (75%)	6,6,6	0.28	0
5	PO4	J	1103	-	4,4,4	2.75	3 (75%)	6,6,6	0.29	0
5	PO4	J	1104	-	4,4,4	2.82	3 (75%)	6,6,6	0.27	0
4	OGK	L	1100	-	22,25,25	6.40	9 (40%)	25,38,38	3.23	15 (60%)
5	PO4	L	1101	-	4,4,4	2.89	3 (75%)	6,6,6	0.34	0
5	PO4	L	1102	-	4,4,4	3.02	3 (75%)	6,6,6	0.27	0
5	PO4	L	1103	-	4,4,4	2.99	3 (75%)	6,6,6	0.27	0
5	PO4	L	1104	-	4,4,4	2.89	3 (75%)	6,6,6	0.27	0
4	OGK	N	1100	-	22,25,25	6.34	8 (36%)	25,38,38	2.51	7 (28%)
5	PO4	N	1101	-	4,4,4	3.06	3 (75%)	6,6,6	0.32	0
5	PO4	N	1102	-	4,4,4	2.98	3 (75%)	6,6,6	0.27	0
5	PO4	N	1103	-	4,4,4	2.89	3 (75%)	6,6,6	0.30	0
5	PO4	N	1104	-	4,4,4	3.05	3 (75%)	6,6,6	0.29	0
4	OGK	P	1100	-	22,25,25	6.52	9 (40%)	25,38,38	3.09	11 (44%)
5	PO4	P	1101	-	4,4,4	2.97	3 (75%)	6,6,6	0.30	0
5	PO4	P	1102	-	4,4,4	3.09	3 (75%)	6,6,6	0.28	0
5	PO4	P	1103	-	4,4,4	2.93	3 (75%)	6,6,6	0.29	0
5	PO4	P	1104	-	4,4,4	3.09	3 (75%)	6,6,6	0.30	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	B	1100	-	1/1/9/10	0/13/52/52	0/2/3/3
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
4	OGK	D	1100	-	1/1/9/10	0/13/52/52	0/2/3/3
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	F	1100	-	-	0/13/52/52	0/2/3/3
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	H	1100	-	1/1/9/10	0/13/52/52	0/2/3/3
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	J	1100	-	-	0/13/52/52	0/2/3/3
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	L	1100	-	1/1/9/10	0/13/52/52	0/2/3/3
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
4	OGK	N	1100	-	-	0/13/52/52	0/2/3/3
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	P	1100	-	-	0/13/52/52	0/2/3/3
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

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1100	OGK	C13-C09	-22.54	1.27	1.51
4	P	1100	OGK	C13-C09	-22.22	1.27	1.51
4	L	1100	OGK	C13-C09	-21.98	1.28	1.51
4	F	1100	OGK	C13-C09	-21.73	1.28	1.51
4	H	1100	OGK	C13-C09	-21.66	1.28	1.51

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1100	OGK	C13-C14-C09	-7.72	56.76	60.38
4	L	1100	OGK	C13-C14-C09	-6.77	57.21	60.38
4	P	1100	OGK	C13-C14-C09	-6.74	57.22	60.38
4	H	1100	OGK	C13-C14-C09	-6.61	57.28	60.38
4	P	1100	OGK	C13-C09-N08	-6.49	108.01	117.71

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1100	OGK	C05
4	L	1100	OGK	C05
4	D	1100	OGK	C05
4	H	1100	OGK	C03

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1100	OGK	6	0
5	B	1101	PO4	1	0
5	B	1103	PO4	2	0
4	D	1100	OGK	2	0
5	D	1101	PO4	1	0
5	D	1103	PO4	2	0
4	F	1100	OGK	8	0
5	F	1101	PO4	1	0
5	F	1103	PO4	1	0
4	H	1100	OGK	8	0
5	H	1101	PO4	2	0
5	H	1103	PO4	4	0
5	H	1104	PO4	1	0
4	J	1100	OGK	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1103	PO4	2	0
4	L	1100	OGK	11	0
5	L	1103	PO4	1	0
4	N	1100	OGK	7	0
5	N	1101	PO4	1	0
5	N	1103	PO4	2	0
4	P	1100	OGK	7	0
5	P	1101	PO4	1	0
5	P	1103	PO4	2	0

## 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, 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	145/160 (90%)	0.51	9 (6%) 24 15	27, 72, 133, 163	0
1	C	145/160 (90%)	0.93	28 (19%) 2 1	26, 75, 134, 163	0
1	E	145/160 (90%)	0.28	5 (3%) 49 36	28, 70, 133, 161	0
1	G	145/160 (90%)	0.09	7 (4%) 34 23	27, 66, 134, 161	0
1	I	145/160 (90%)	0.57	19 (13%) 5 2	29, 73, 134, 163	0
1	K	145/160 (90%)	0.65	20 (13%) 4 2	28, 75, 134, 165	0
1	M	145/160 (90%)	0.87	23 (15%) 3 1	32, 75, 133, 162	0
1	O	145/160 (90%)	1.28	44 (30%) 1 0	32, 76, 134, 164	0
2	B	566/592 (95%)	-0.08	11 (1%) 70 59	21, 45, 107, 175	0
2	D	566/592 (95%)	-0.07	16 (2%) 56 44	21, 46, 110, 176	0
2	F	566/592 (95%)	-0.15	23 (4%) 41 29	20, 49, 111, 177	0
2	H	562/592 (94%)	-0.54	5 (0%) 85 79	19, 38, 91, 171	0
2	J	566/592 (95%)	-0.23	17 (3%) 54 41	22, 49, 110, 177	0
2	L	566/592 (95%)	-0.26	20 (3%) 48 35	21, 50, 111, 176	0
2	N	566/592 (95%)	0.26	43 (7%) 17 9	24, 53, 112, 178	0
2	P	566/592 (95%)	0.09	37 (6%) 22 13	23, 54, 114, 176	0
3	Q	13/22 (59%)	0.71	0 100 100	79, 102, 125, 126	0
3	R	13/22 (59%)	2.22	7 (53%) 0 0	86, 109, 128, 129	0
3	S	13/22 (59%)	1.29	3 (23%) 1 1	89, 108, 129, 131	0
3	U	13/22 (59%)	1.19	2 (15%) 3 1	87, 111, 128, 130	0
3	V	13/22 (59%)	1.45	5 (38%) 0 0	88, 111, 128, 128	0
3	W	13/22 (59%)	1.47	5 (38%) 0 0	88, 111, 128, 129	0
3	X	13/22 (59%)	1.42	4 (30%) 1 0	89, 110, 128, 129	0
All	All	5775/6170 (93%)	0.06	353 (6%) 25 15	19, 53, 119, 178	0

The worst 5 of 353 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	592	ILE	17.2
2	F	592	ILE	13.3
2	D	12	SER	13.1
2	N	591	PRO	11.1
2	P	12	SER	10.4

## 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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	PO4	P	1104	5/5	0.83	0.22	6.12	30,51,77,101	0
5	PO4	N	1104	5/5	0.94	0.24	5.39	32,59,102,105	0
5	PO4	H	1102	5/5	0.79	0.24	4.40	58,70,91,138	0
5	PO4	H	1104	5/5	0.92	0.19	2.60	23,27,62,87	0
5	PO4	J	1103	5/5	0.99	0.18	2.42	34,39,48,64	0
5	PO4	N	1103	5/5	0.97	0.22	1.96	40,60,78,102	0
5	PO4	L	1104	5/5	0.96	0.17	1.68	54,54,85,104	0
5	PO4	N	1102	5/5	0.91	0.23	1.26	78,89,102,114	0
5	PO4	L	1103	5/5	0.97	0.21	1.15	31,41,62,72	0
5	PO4	N	1101	5/5	0.95	0.20	0.83	47,54,57,87	0
4	OGK	H	1100	23/23	0.97	0.17	0.81	23,41,56,62	0
5	PO4	L	1101	5/5	0.97	0.18	0.30	34,39,58,68	0
5	PO4	P	1102	5/5	0.93	0.19	0.08	70,91,121,132	0
4	OGK	J	1100	23/23	0.96	0.18	0.02	24,36,51,65	0
5	PO4	P	1101	5/5	0.98	0.18	-0.10	47,50,65,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PO4	D	1103	5/5	0.98	0.19	-0.17	28,30,38,79	0
4	OGK	L	1100	23/23	0.97	0.17	-0.21	31,43,62,67	0
4	OGK	P	1100	23/23	0.97	0.16	-0.22	40,52,64,68	0
4	OGK	F	1100	23/23	0.96	0.18	-0.24	23,41,50,70	0
5	PO4	F	1103	5/5	0.97	0.18	-0.26	32,36,48,80	0
4	OGK	N	1100	23/23	0.93	0.17	-0.36	33,54,73,77	0
5	PO4	D	1102	5/5	0.94	0.15	-0.70	48,60,103,128	0
5	PO4	F	1101	5/5	0.98	0.15	-0.77	25,37,47,70	0
5	PO4	B	1103	5/5	0.98	0.16	-0.79	23,25,30,45	0
5	PO4	J	1101	5/5	0.98	0.14	-0.81	42,53,62,65	0
5	PO4	D	1101	5/5	0.98	0.16	-0.90	29,32,43,57	0
4	OGK	D	1100	23/23	0.97	0.14	-0.91	24,32,41,45	0
5	PO4	F	1104	5/5	0.95	0.16	-1.05	28,33,60,69	0
5	PO4	P	1103	5/5	0.96	0.15	-1.06	55,56,64,76	0
5	PO4	J	1102	5/5	0.96	0.12	-1.30	54,71,85,106	0
5	PO4	B	1101	5/5	0.98	0.13	-1.84	31,37,44,44	0
4	OGK	B	1100	23/23	0.98	0.14	-1.88	14,26,38,48	0
5	PO4	D	1104	5/5	0.93	0.15	-	32,38,82,83	0
5	PO4	J	1104	5/5	0.97	0.14	-	44,46,72,76	0
5	PO4	H	1101	5/5	0.94	0.15	-	65,65,83,99	0
5	PO4	H	1103	5/5	0.95	0.19	-	45,60,71,83	0
5	PO4	B	1102	5/5	0.98	0.14	-	51,71,81,85	0
5	PO4	B	1104	5/5	0.96	0.13	-	23,44,66,67	0
5	PO4	L	1102	5/5	0.93	0.18	-	56,67,112,139	0
5	PO4	F	1102	5/5	0.83	0.24	-	67,80,101,127	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.