wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:49 AM GMT

PDB ID	:	3MY0
Title	:	Crystal structure of the ACVRL1 (ALK1) kinase domain bound to LDN-193189
Authors	:	Chaikuad, A.; Alfano, I.; Cooper, C.; Mahajan, P.; Daga, N.; Sanvitale, C.; Fedorov, O.; Petrie, K.; Savitsky, P.; Gileadi, O.; Sethi, R.; Krojer, T.; Muniz, J.R.C.; Pike, A.C.W.; Vollmar, M.; Carpenter, C.P.; Ugochukwu, E.; Knapp, S.; von Delft, F.; Weigelt, J.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Bullock, A.; Structural Genomics Consortium (SGC)
Deposited on	:	2010-05-08
Resolution	:	2.65 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

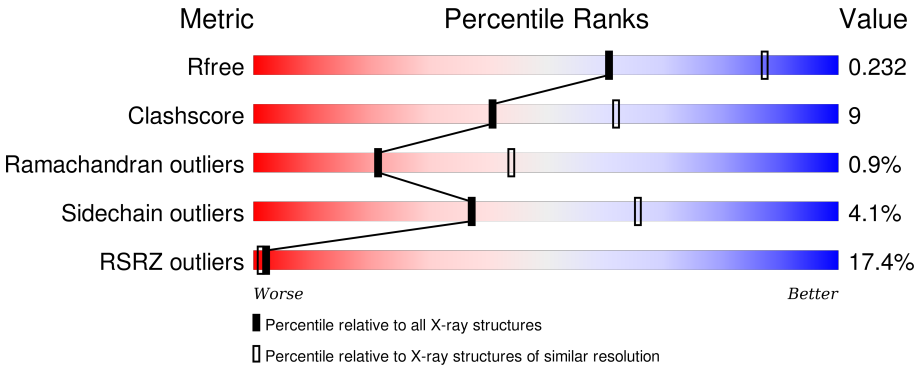
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 >=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 <=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	305	6% 80% 16%
1	B	305	9% 77% 18%
1	C	305	6% 83% 14%
1	D	305	3% 84% 12%
1	E	305	12% 77% 19%

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Mol	Chain	Length	Quality of chain
1	F	305	10% 75% 19%
1	G	305	% 76% 17%
1	H	305	4% 81% 13%
1	I	305	4% 76% 18%
1	J	305	63% 70% 11% 17%
1	K	305	66% 74% 11% 14%
1	L	305	7% 80% 15%
1	M	305	4% 78% 18%
1	N	305	3% 83% 14%
1	O	305	6% 81% 16%
1	P	305	67% 78% 15% 5%
1	Q	305	3% 77% 18%
1	R	305	5% 78% 16%
1	S	305	3% 78% 17%
1	T	305	9% 75% 17%
1	U	305	11% 79% 13% 7%
1	V	305	11% 82% 9% 8%
1	W	305	15% 78% 13% 8%
1	X	305	69% 67% 17% 16%

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
2	LDN	X	600	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 53931 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 Serine/threonine-protein kinase receptor R3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2295	1461	403	418	13			
1	B	295	Total	C	N	O	S	0	0	0
			2303	1470	402	418	13			
1	C	299	Total	C	N	O	S	0	0	0
			2285	1457	401	414	13			
1	D	298	Total	C	N	O	S	0	0	0
			2284	1454	396	421	13			
1	E	294	Total	C	N	O	S	0	0	0
			2251	1446	390	403	12			
1	F	294	Total	C	N	O	S	0	0	0
			2239	1430	396	401	12			
1	G	294	Total	C	N	O	S	0	0	0
			2269	1455	388	413	13			
1	H	294	Total	C	N	O	S	0	0	0
			2233	1428	390	402	13			
1	I	293	Total	C	N	O	S	0	0	0
			2286	1463	399	411	13			
1	J	252	Total	C	N	O	S	0	0	0
			1898	1215	329	342	12			
1	K	261	Total	C	N	O	S	0	0	0
			1937	1241	336	348	12			
1	L	296	Total	C	N	O	S	0	0	0
			2312	1474	406	419	13			
1	M	298	Total	C	N	O	S	0	0	0
			2325	1485	405	422	13			
1	N	300	Total	C	N	O	S	0	0	0
			2295	1464	402	416	13			
1	O	297	Total	C	N	O	S	0	0	0
			2279	1451	398	417	13			
1	P	290	Total	C	N	O	S	0	0	0
			2103	1337	370	385	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	294	Total	C	N	O	S	0	0	0
			2262	1447	399	404	12			
1	R	294	Total	C	N	O	S	0	0	0
			2258	1449	387	409	13			
1	S	294	Total	C	N	O	S	0	0	0
			2236	1430	391	402	13			
1	T	292	Total	C	N	O	S	0	0	0
			2256	1443	391	409	13			
1	U	285	Total	C	N	O	S	0	0	0
			2154	1378	377	386	13			
1	V	282	Total	C	N	O	S	0	0	0
			2122	1358	370	381	13			
1	W	281	Total	C	N	O	S	0	0	0
			2211	1414	386	398	13			
1	X	257	Total	C	N	O	S	0	0	0
			1968	1266	337	354	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P37023
A	0	MET	-	EXPRESSION TAG	UNP P37023
B	-1	SER	-	EXPRESSION TAG	UNP P37023
B	0	MET	-	EXPRESSION TAG	UNP P37023
C	-1	SER	-	EXPRESSION TAG	UNP P37023
C	0	MET	-	EXPRESSION TAG	UNP P37023
D	-1	SER	-	EXPRESSION TAG	UNP P37023
D	0	MET	-	EXPRESSION TAG	UNP P37023
E	-1	SER	-	EXPRESSION TAG	UNP P37023
E	0	MET	-	EXPRESSION TAG	UNP P37023
F	-1	SER	-	EXPRESSION TAG	UNP P37023
F	0	MET	-	EXPRESSION TAG	UNP P37023
G	-1	SER	-	EXPRESSION TAG	UNP P37023
G	0	MET	-	EXPRESSION TAG	UNP P37023
H	-1	SER	-	EXPRESSION TAG	UNP P37023
H	0	MET	-	EXPRESSION TAG	UNP P37023
I	-1	SER	-	EXPRESSION TAG	UNP P37023
I	0	MET	-	EXPRESSION TAG	UNP P37023
J	-1	SER	-	EXPRESSION TAG	UNP P37023
J	0	MET	-	EXPRESSION TAG	UNP P37023
K	-1	SER	-	EXPRESSION TAG	UNP P37023
K	0	MET	-	EXPRESSION TAG	UNP P37023
L	-1	SER	-	EXPRESSION TAG	UNP P37023

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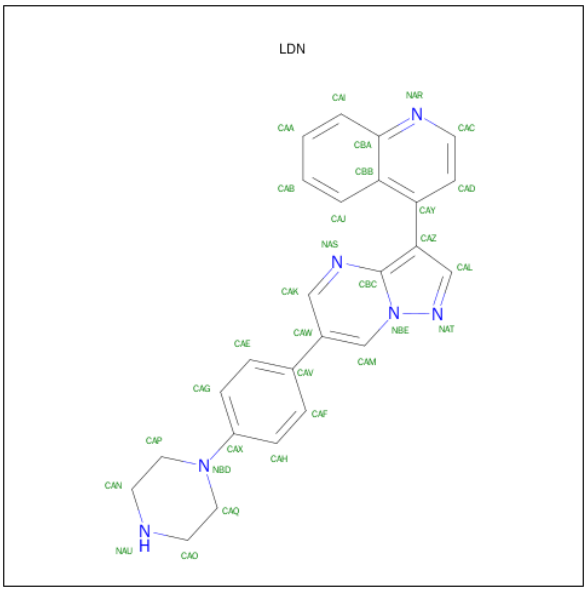
Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	EXPRESSION TAG	UNP P37023
M	-1	SER	-	EXPRESSION TAG	UNP P37023
M	0	MET	-	EXPRESSION TAG	UNP P37023
N	-1	SER	-	EXPRESSION TAG	UNP P37023
N	0	MET	-	EXPRESSION TAG	UNP P37023
O	-1	SER	-	EXPRESSION TAG	UNP P37023
O	0	MET	-	EXPRESSION TAG	UNP P37023
P	-1	SER	-	EXPRESSION TAG	UNP P37023
P	0	MET	-	EXPRESSION TAG	UNP P37023
Q	-1	SER	-	EXPRESSION TAG	UNP P37023
Q	0	MET	-	EXPRESSION TAG	UNP P37023
R	-1	SER	-	EXPRESSION TAG	UNP P37023
R	0	MET	-	EXPRESSION TAG	UNP P37023
S	-1	SER	-	EXPRESSION TAG	UNP P37023
S	0	MET	-	EXPRESSION TAG	UNP P37023
T	-1	SER	-	EXPRESSION TAG	UNP P37023
T	0	MET	-	EXPRESSION TAG	UNP P37023
U	-1	SER	-	EXPRESSION TAG	UNP P37023
U	0	MET	-	EXPRESSION TAG	UNP P37023
V	-1	SER	-	EXPRESSION TAG	UNP P37023
V	0	MET	-	EXPRESSION TAG	UNP P37023
W	-1	SER	-	EXPRESSION TAG	UNP P37023
W	0	MET	-	EXPRESSION TAG	UNP P37023
X	-1	SER	-	EXPRESSION TAG	UNP P37023
X	0	MET	-	EXPRESSION TAG	UNP P37023

- Molecule 2 is 4-[6-(4-PIPERAZIN-1-YLPHENYL)PYRAZOLO[1,5-A]PYRIMIDIN-3-YL]QUINOLINE (three-letter code: LDN) (formula: $C_{25}H_{22}N_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 31 25 6	0	0
2	B	1	Total C N 31 25 6	0	0
2	C	1	Total C N 31 25 6	0	0
2	D	1	Total C N 31 25 6	0	0
2	E	1	Total C N 31 25 6	0	0
2	F	1	Total C N 31 25 6	0	0
2	G	1	Total C N 31 25 6	0	0
2	H	1	Total C N 31 25 6	0	0
2	I	1	Total C N 31 25 6	0	0
2	J	1	Total C N 31 25 6	0	0
2	K	1	Total C N 31 25 6	0	0
2	L	1	Total C N 31 25 6	0	0
2	M	1	Total C N 31 25 6	0	0
2	N	1	Total C N 31 25 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	O	1	Total C N 31 25 6	0	0
2	P	1	Total C N 31 25 6	0	0
2	Q	1	Total C N 31 25 6	0	0
2	R	1	Total C N 31 25 6	0	0
2	S	1	Total C N 31 25 6	0	0
2	T	1	Total C N 31 25 6	0	0
2	U	1	Total C N 31 25 6	0	0
2	V	1	Total C N 31 25 6	0	0
2	W	1	Total C N 31 25 6	0	0
2	X	1	Total C N 31 25 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	12	Total O 12 12	0	0
3	C	11	Total O 11 11	0	0
3	D	7	Total O 7 7	0	0
3	E	4	Total O 4 4	0	0
3	F	8	Total O 8 8	0	0
3	G	6	Total O 6 6	0	0
3	H	6	Total O 6 6	0	0
3	I	3	Total O 3 3	0	0

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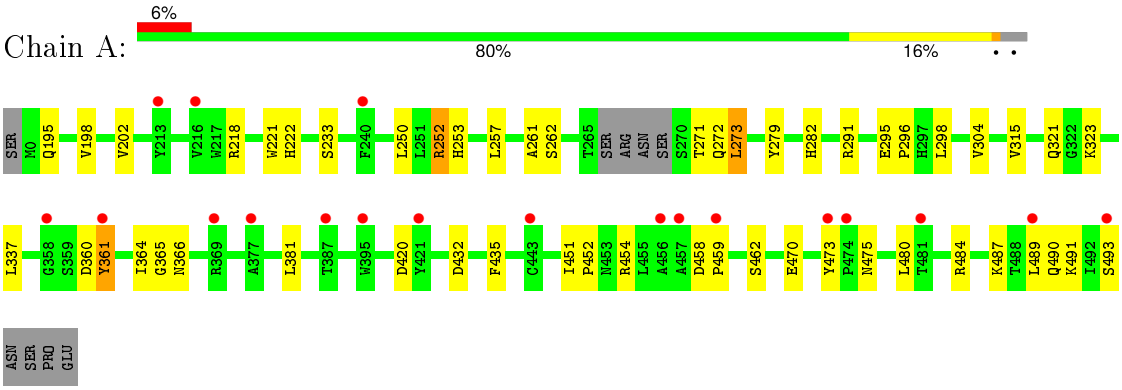
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	2	Total O 2 2	0	0
3	L	6	Total O 6 6	0	0
3	M	1	Total O 1 1	0	0
3	N	6	Total O 6 6	0	0
3	O	2	Total O 2 2	0	0
3	P	4	Total O 4 4	0	0
3	Q	8	Total O 8 8	0	0
3	R	5	Total O 5 5	0	0
3	S	6	Total O 6 6	0	0
3	T	5	Total O 5 5	0	0
3	U	9	Total O 9 9	0	0
3	V	2	Total O 2 2	0	0
3	W	9	Total O 9 9	0	0

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.

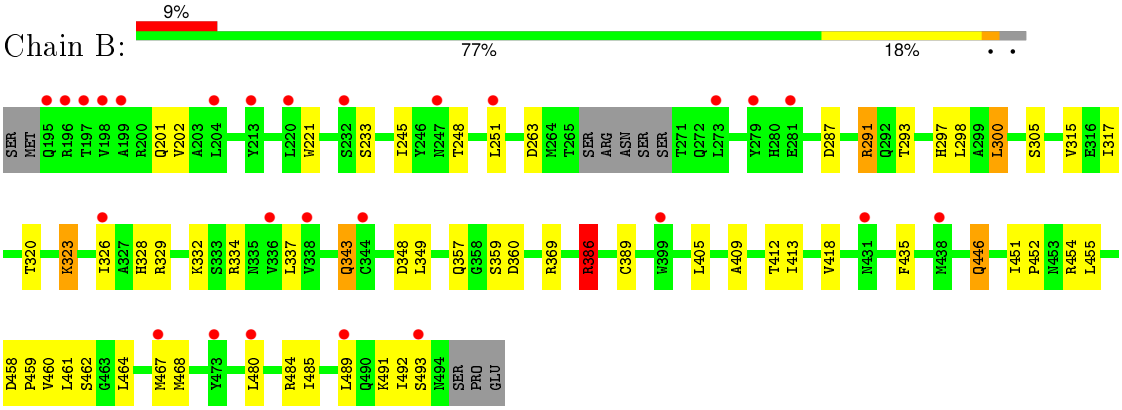
- Molecule 1: Serine/threonine-protein kinase receptor R3

Chain A:



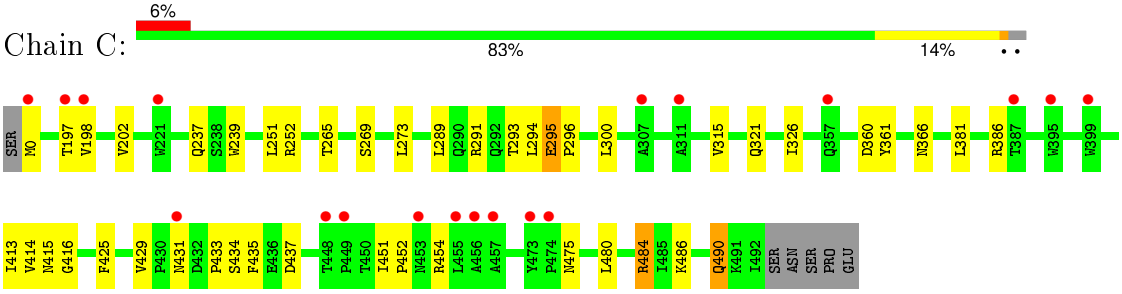
- Molecule 1: Serine/threonine-protein kinase receptor R3

Chain B:



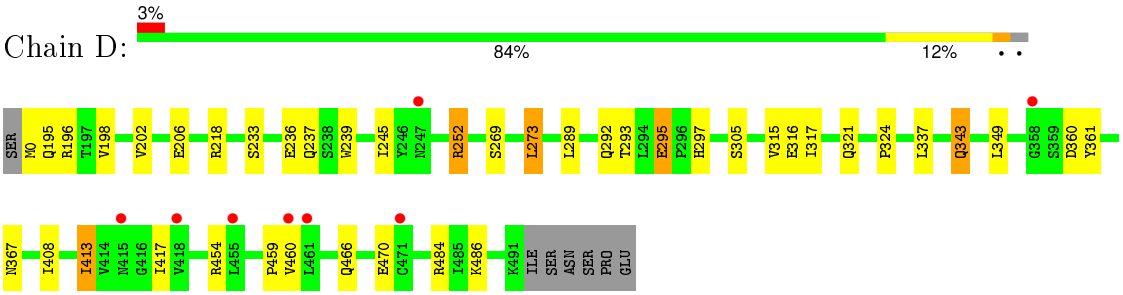
- Molecule 1: Serine/threonine-protein kinase receptor R3

Chain C:



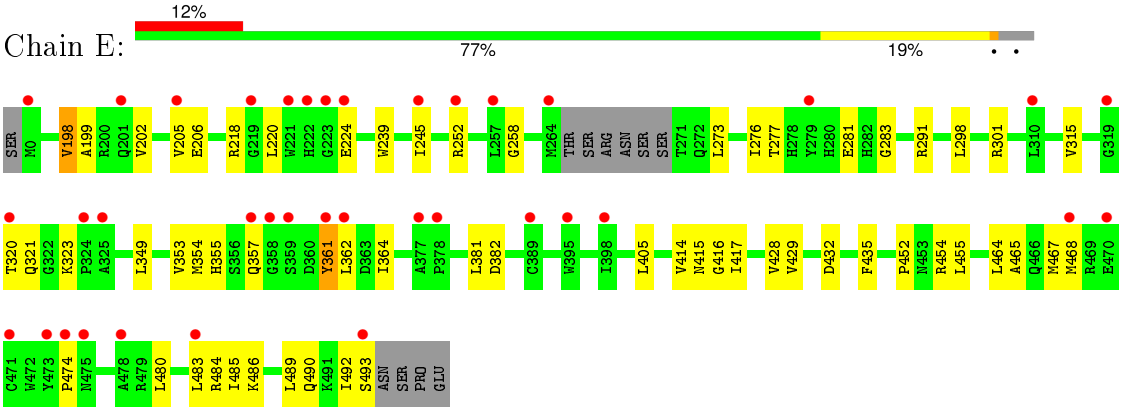
- Molecule 1: Serine/threonine-protein kinase receptor R3

Chain D:



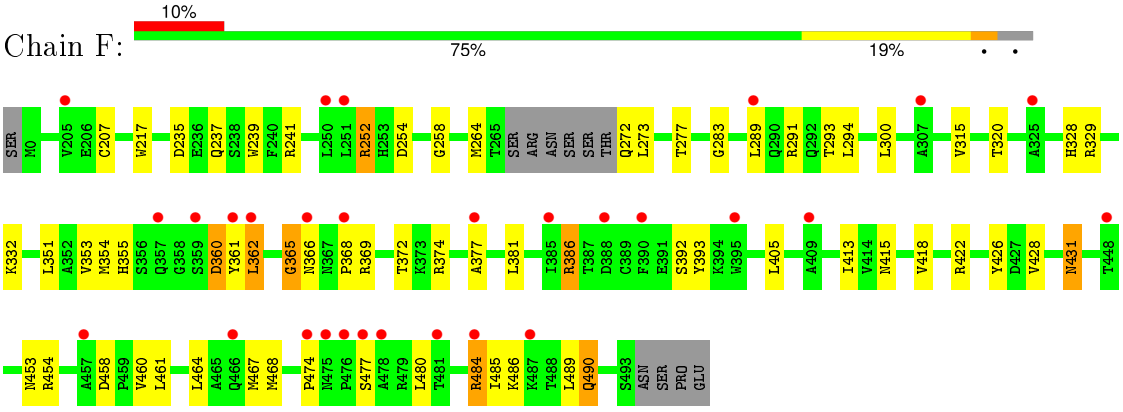
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain E:



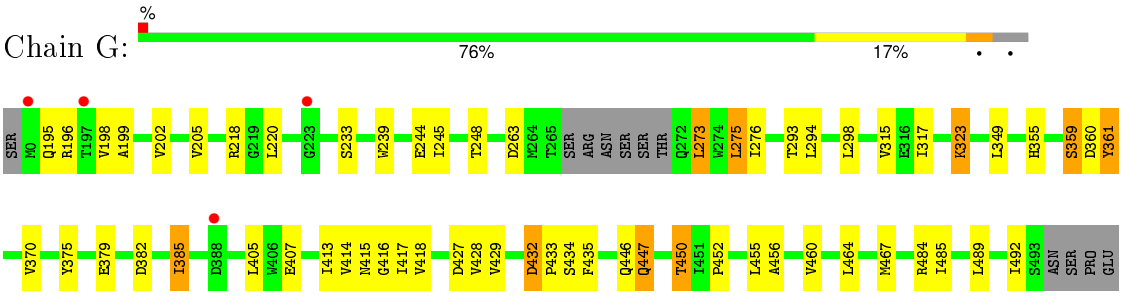
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain F:



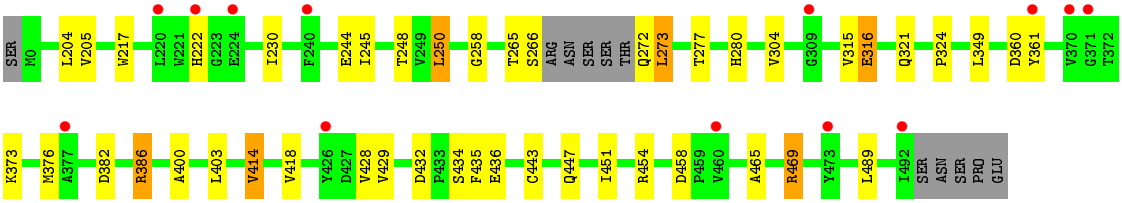
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain G:

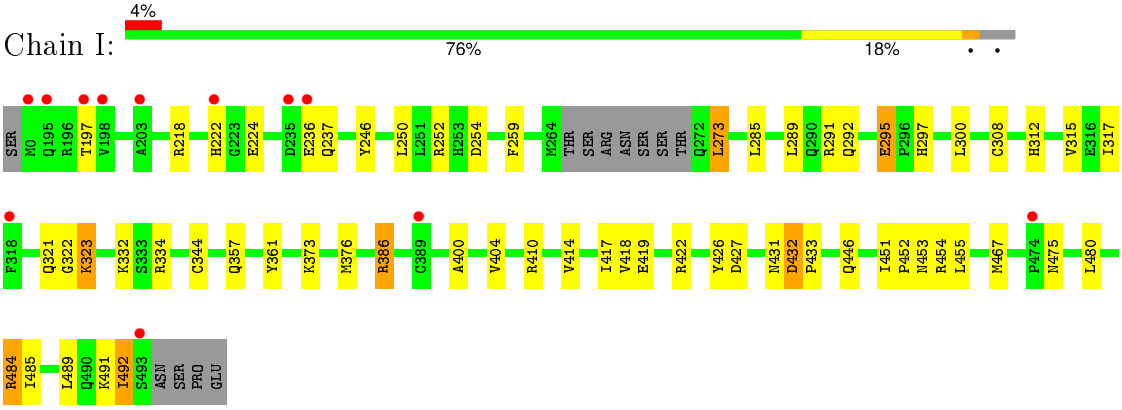


• Molecule 1: Serine/threonine-protein kinase receptor R3

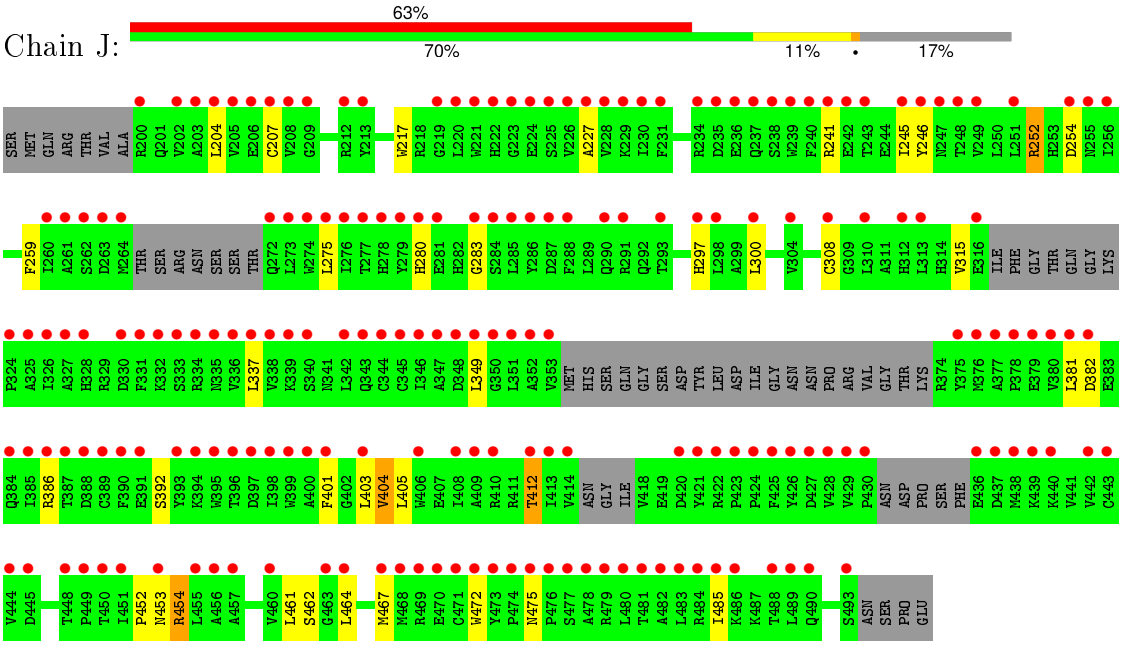
Chain H:



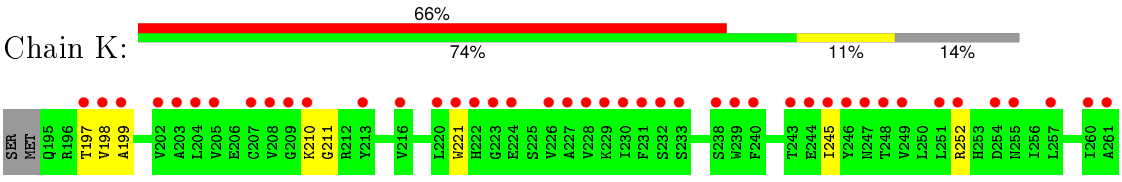
• Molecule 1: Serine/threonine-protein kinase receptor R3

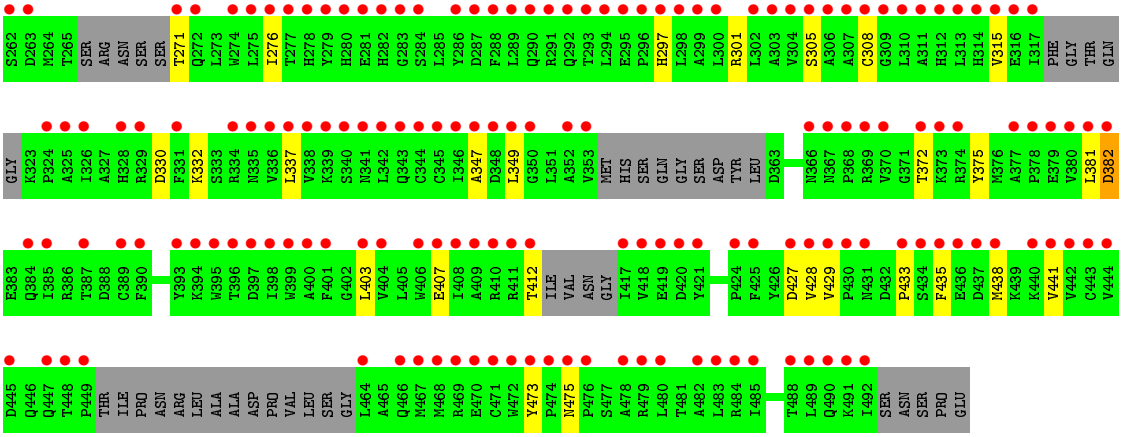


• Molecule 1: Serine/threonine-protein kinase receptor R3



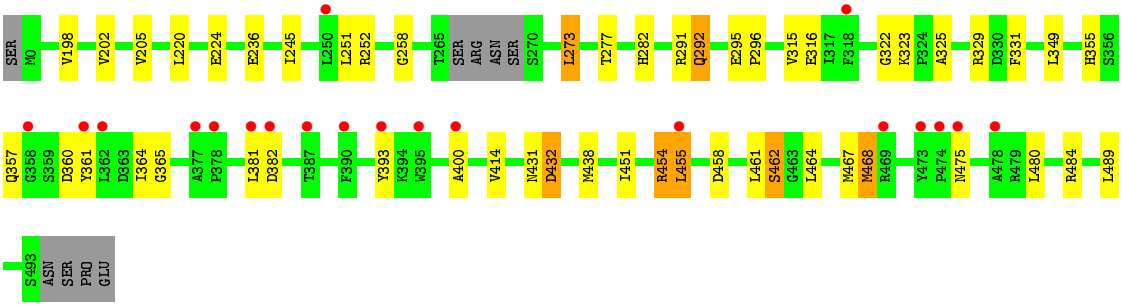
• Molecule 1: Serine/threonine-protein kinase receptor R3





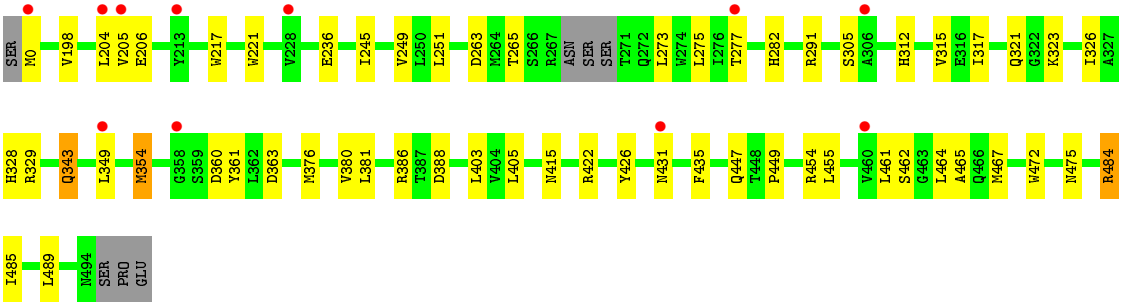
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain L:



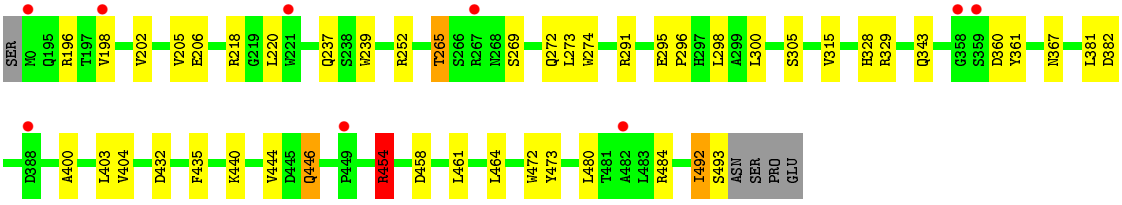
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain M:



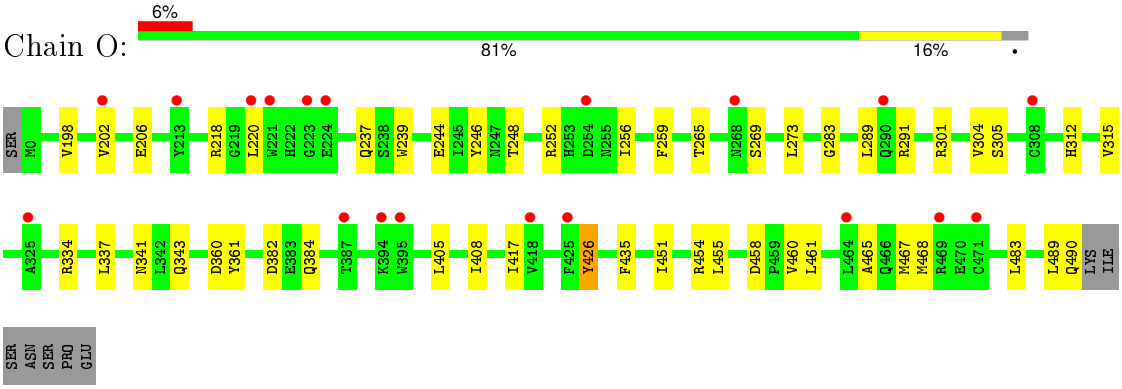
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain N:



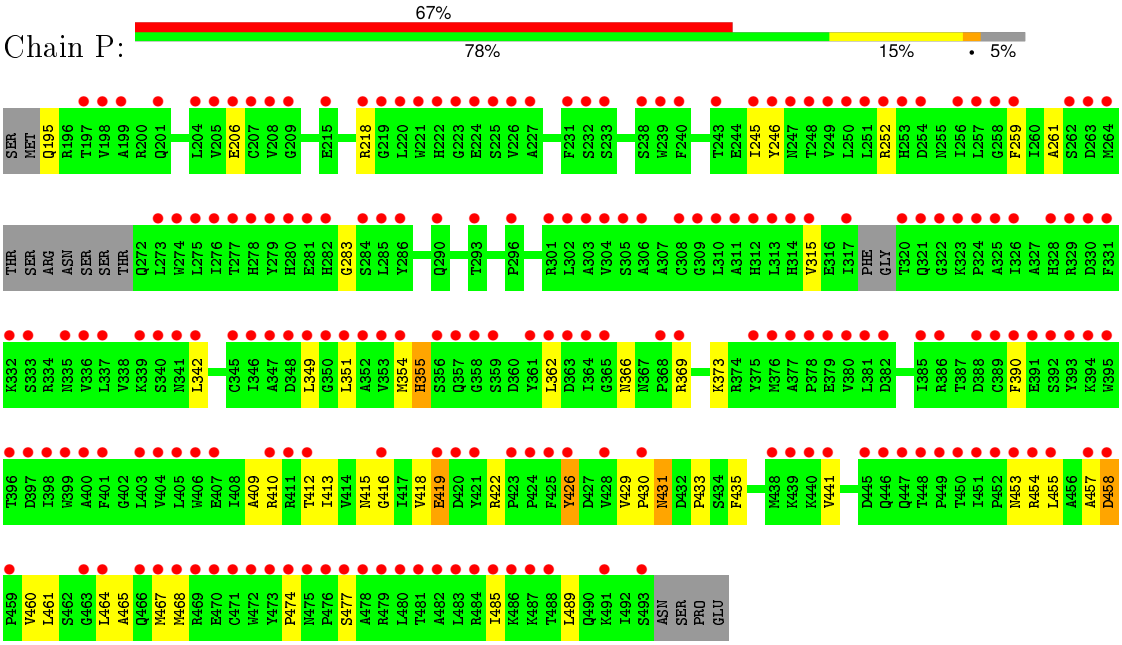
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain O:



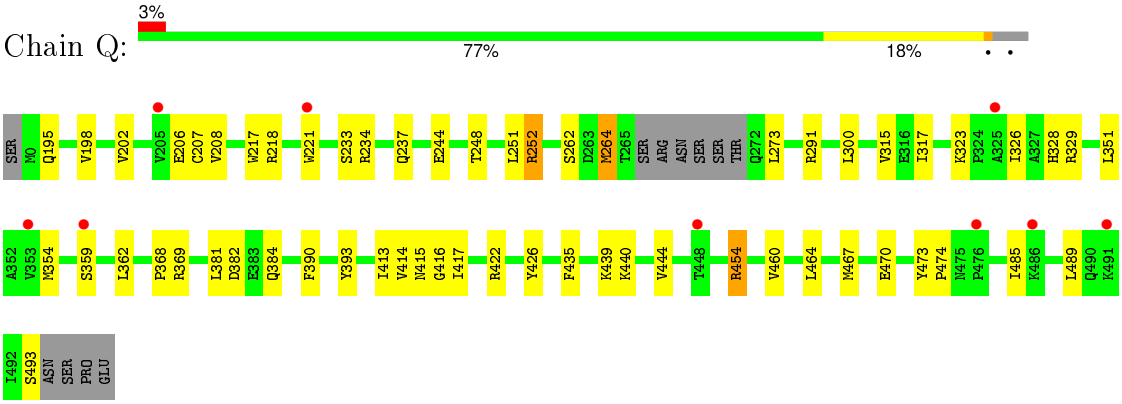
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain P:



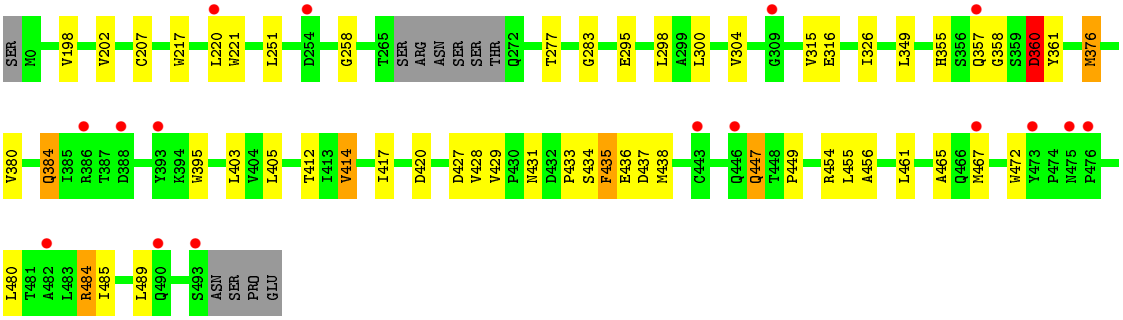
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain Q:



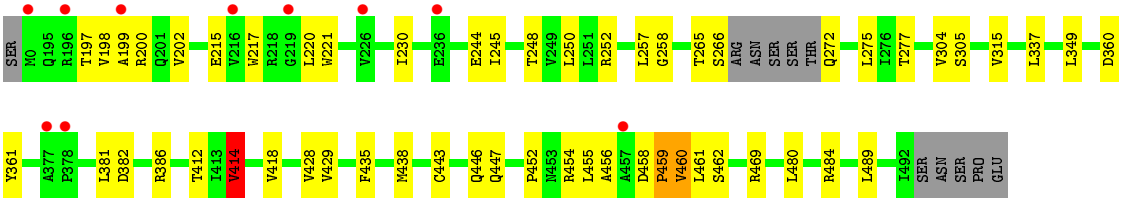
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain R:



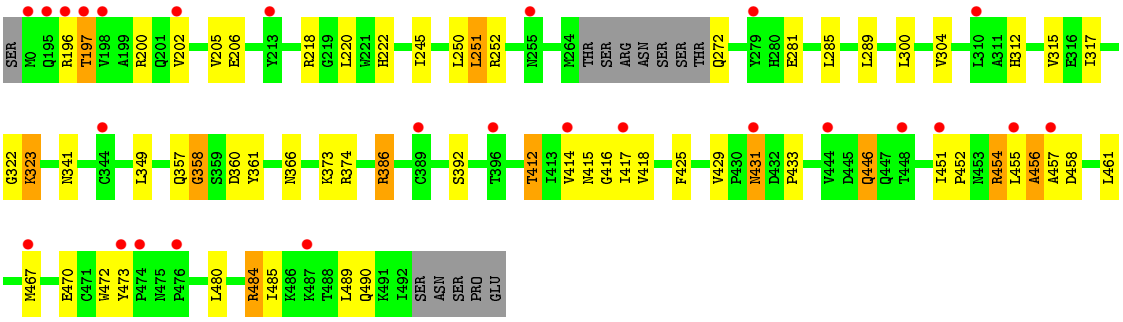
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain S:



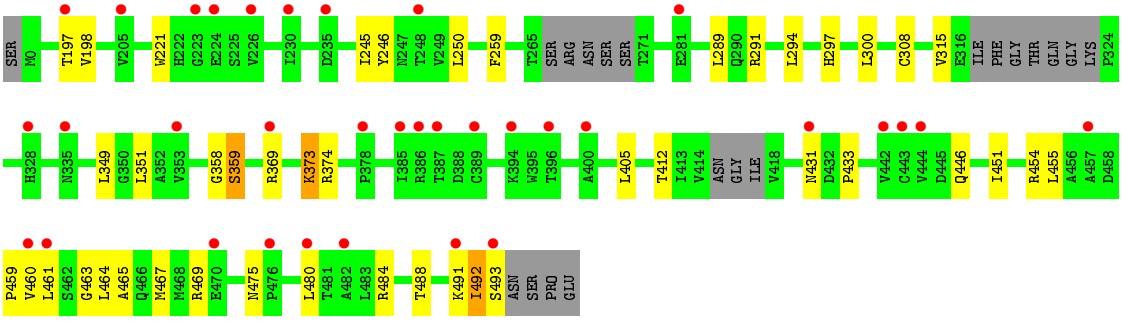
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain T:



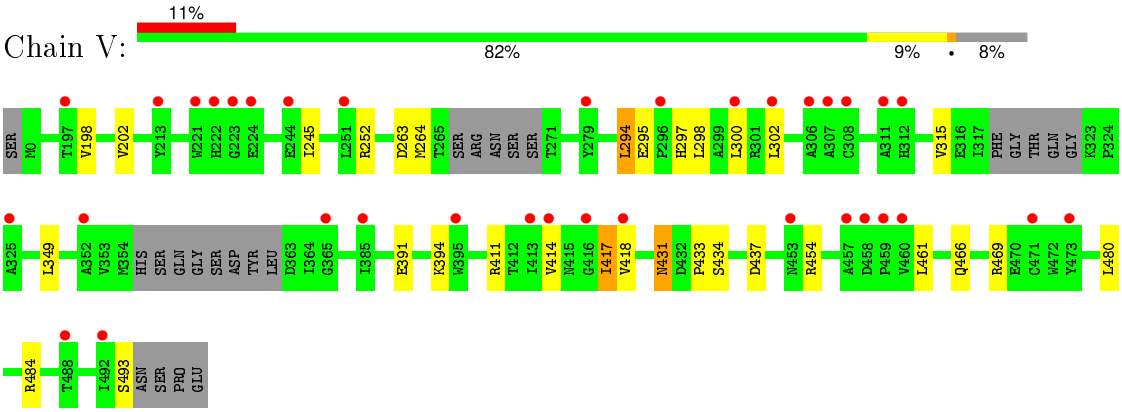
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain U:



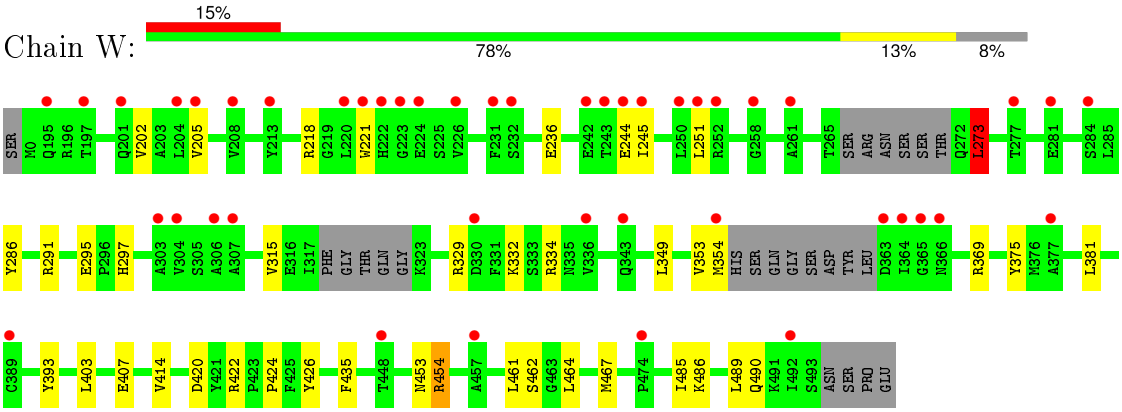
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain V:



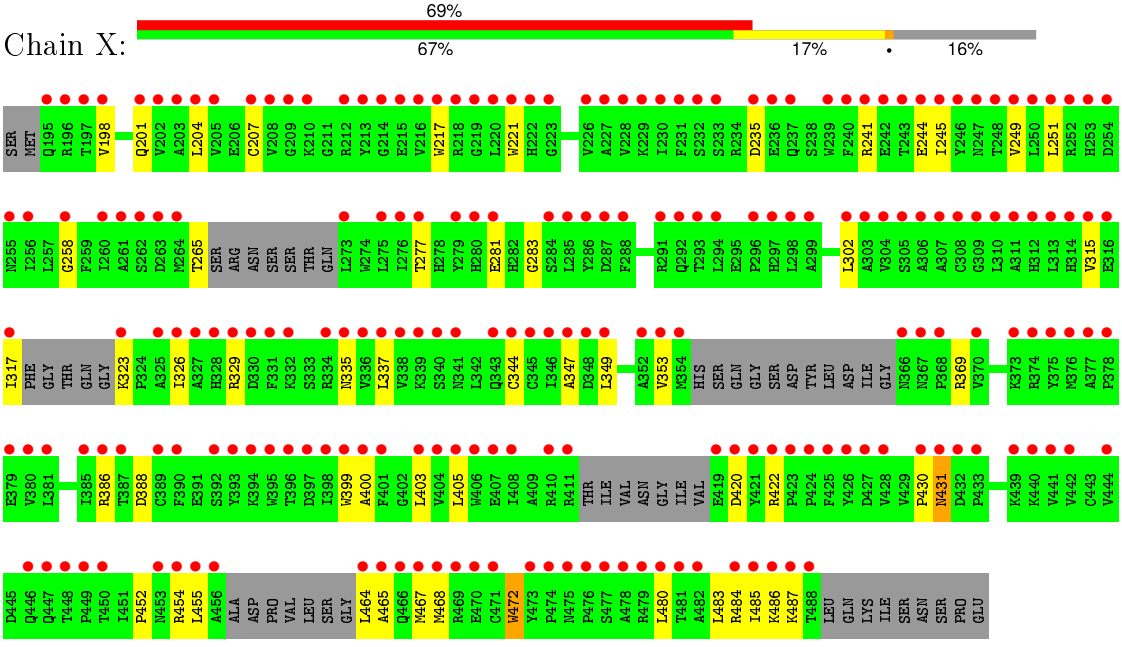
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain W:



• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	118.77Å 118.77Å 510.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.99 – 2.65 58.99 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (58.99-2.65) 99.8 (58.99-2.65)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.6.0066	Depositor
R, R_{free}	0.207 , 0.247 0.208 , 0.232	Depositor DCC
R_{free} test set	11716 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.2	EDS
Estimated twinning fraction	0.357 for H, K, L 0.147 for H+K, -K, -L 0.352 for -H, -K, L 0.145 for H, -H-K, -L 0.457 for -h,-k,l 0.316 for h,-h-k,-l 0.315 for -k,-h,-l	Xtriage
Reported twinning fraction	0.357 for H, K, L 0.147 for H+K, -K, -L 0.352 for -H, -K, L 0.145 for H, -H-K, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 233740 reflections	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	53931	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.52 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.7713e-03.The detected translational NCS is most likely*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

also responsible for the elevated intensity ratio.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDN

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	0.57	2/2352 (0.1%)	0.66	0/3204
1	B	0.57	0/2359	0.70	1/3212 (0.0%)
1	C	0.55	0/2342	0.67	0/3195
1	D	0.58	0/2340	0.67	0/3192
1	E	0.59	0/2308	0.70	1/3150 (0.0%)
1	F	0.52	0/2296	0.64	2/3133 (0.1%)
1	G	0.67	0/2326	0.72	1/3173 (0.0%)
1	H	0.57	0/2289	0.68	0/3124
1	I	0.69	2/2343 (0.1%)	0.73	1/3191 (0.0%)
1	J	0.39	0/1942	0.54	0/2645
1	K	0.39	0/1984	0.55	0/2709
1	L	0.57	0/2369	0.66	0/3226
1	M	0.61	0/2381	0.70	0/3243
1	N	0.63	0/2352	0.69	0/3209
1	O	0.55	0/2335	0.65	0/3185
1	P	0.43	0/2150	0.56	0/2942
1	Q	0.57	0/2319	0.69	0/3160
1	R	0.55	0/2315	0.67	1/3160 (0.0%)
1	S	0.60	0/2292	0.68	1/3128 (0.0%)
1	T	0.53	0/2311	0.64	1/3149 (0.0%)
1	U	0.57	1/2206 (0.0%)	0.62	0/3009
1	V	0.56	0/2174	0.62	0/2969
1	W	0.59	0/2263	0.67	1/3079 (0.0%)
1	X	0.39	0/2014	0.53	0/2743
All	All	0.56	5/54362 (0.0%)	0.66	10/74130 (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
1	B	0	1
1	C	0	1
1	H	0	1
1	R	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	HIS	CG-CD2	6.62	1.47	1.35
1	U	308	CYS	CB-SG	6.13	1.92	1.82
1	I	308	CYS	CB-SG	-6.00	1.72	1.81
1	I	344	CYS	CB-SG	-5.45	1.73	1.81
1	A	282	HIS	CE1-NE2	5.33	1.45	1.32

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	386	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	S	220	LEU	CA-CB-CG	6.52	130.30	115.30
1	E	301	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	R	220	LEU	CA-CB-CG	6.07	129.26	115.30
1	I	386	ARG	NE-CZ-NH1	5.78	123.19	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	320	THR	Peptide
1	C	490	GLN	Peptide
1	H	280	HIS	Sidechain
1	R	360	ASP	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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2295	0	2191	29	0
1	B	2303	0	2224	53	1
1	C	2285	0	2171	36	0
1	D	2284	0	2161	34	0
1	E	2251	0	2153	42	1
1	F	2239	0	2112	45	0
1	G	2269	0	2174	47	1
1	H	2233	0	2106	31	1
1	I	2286	0	2215	45	0
1	J	1898	0	1760	29	1
1	K	1937	0	1740	29	1
1	L	2312	0	2228	36	0
1	M	2325	0	2254	41	0
1	N	2295	0	2190	45	0
1	O	2279	0	2161	33	0
1	P	2103	0	1917	41	0
1	Q	2262	0	2164	40	1
1	R	2258	0	2157	52	0
1	S	2236	0	2118	41	1
1	T	2256	0	2171	41	0
1	U	2154	0	2023	32	1
1	V	2122	0	1976	17	0
1	W	2211	0	2148	29	0
1	X	1968	0	1848	62	0
2	A	31	0	22	1	0
2	B	31	0	22	4	0
2	C	31	0	22	1	0
2	D	31	0	22	3	0
2	E	31	0	22	3	0
2	F	31	0	22	3	0
2	G	31	0	22	2	0
2	H	31	0	22	0	0
2	I	31	0	22	1	0
2	J	31	0	22	5	0
2	K	31	0	22	4	0
2	L	31	0	22	3	0
2	M	31	0	22	0	0
2	N	31	0	22	1	0
2	O	31	0	22	5	0
2	P	31	0	22	5	0
2	Q	31	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	31	0	22	1	1
2	S	31	0	22	0	0
2	T	31	0	22	2	0
2	U	31	0	22	1	0
2	V	31	0	22	3	0
2	W	31	0	22	4	0
2	X	31	0	22	15	0
3	A	4	0	0	1	0
3	B	12	0	0	0	0
3	C	11	0	0	0	0
3	D	7	0	0	0	0
3	E	4	0	0	2	0
3	F	8	0	0	0	0
3	G	6	0	0	1	0
3	H	6	0	0	0	0
3	I	3	0	0	0	0
3	J	2	0	0	0	0
3	L	6	0	0	0	0
3	M	1	0	0	0	0
3	N	6	0	0	0	0
3	O	2	0	0	0	0
3	P	4	0	0	0	0
3	Q	8	0	0	0	0
3	R	5	0	0	0	0
3	S	6	0	0	0	0
3	T	5	0	0	0	0
3	U	9	0	0	0	0
3	V	2	0	0	0	0
3	W	9	0	0	1	0
All	All	53931	0	50890	903	5

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 9.

The worst 5 of 903 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)
1:D:198:VAL:O	1:D:202:VAL:HG23	1.17	1.27
1:S:217:TRP:CZ2	1:X:430:PRO:HB3	1.88	1.09
1:S:217:TRP:CH2	1:X:430:PRO:HB3	1.94	1.01
1:V:480:LEU:HD22	1:V:484:ARG:HG2	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:467:MET:HE1	1:G:489:LEU:HD11	1.04	1.00

All (5) 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)
1:E:416:GLY:CA	1:H:205:VAL:O[1_445]	2.08	0.12
1:Q:252:ARG:NH2	1:S:252:ARG:O[1_665]	2.08	0.12
1:B:386:ARG:NH2	1:K:382:ASP:O[1_655]	2.10	0.10
1:G:416:GLY:O	1:J:207:CYS:N[1_455]	2.12	0.08
1:U:291:ARG:O	2:R:600:LDN:NAU[1_655]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/305 (96%)	279 (96%)	12 (4%)	1 (0%)	46	72
1	B	291/305 (95%)	277 (95%)	11 (4%)	3 (1%)	19	41
1	C	297/305 (97%)	277 (93%)	18 (6%)	2 (1%)	26	51
1	D	296/305 (97%)	277 (94%)	17 (6%)	2 (1%)	26	51
1	E	290/305 (95%)	272 (94%)	15 (5%)	3 (1%)	19	41
1	F	290/305 (95%)	276 (95%)	10 (3%)	4 (1%)	14	31
1	G	290/305 (95%)	272 (94%)	14 (5%)	4 (1%)	14	31
1	H	290/305 (95%)	270 (93%)	20 (7%)	0	100	100
1	I	289/305 (95%)	271 (94%)	17 (6%)	1 (0%)	46	72
1	J	240/305 (79%)	231 (96%)	7 (3%)	2 (1%)	24	47
1	K	249/305 (82%)	242 (97%)	6 (2%)	1 (0%)	39	65
1	L	292/305 (96%)	279 (96%)	12 (4%)	1 (0%)	46	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	294/305 (96%)	280 (95%)	12 (4%)	2 (1%)	26 51
1	N	298/305 (98%)	277 (93%)	17 (6%)	4 (1%)	15 33
1	O	295/305 (97%)	278 (94%)	16 (5%)	1 (0%)	46 72
1	P	284/305 (93%)	260 (92%)	15 (5%)	9 (3%)	5 10
1	Q	290/305 (95%)	279 (96%)	10 (3%)	1 (0%)	46 72
1	R	290/305 (95%)	275 (95%)	13 (4%)	2 (1%)	26 51
1	S	290/305 (95%)	270 (93%)	15 (5%)	5 (2%)	11 25
1	T	288/305 (94%)	274 (95%)	9 (3%)	5 (2%)	11 25
1	U	277/305 (91%)	267 (96%)	8 (3%)	2 (1%)	26 51
1	V	274/305 (90%)	258 (94%)	14 (5%)	2 (1%)	26 51
1	W	273/305 (90%)	261 (96%)	11 (4%)	1 (0%)	39 65
1	X	245/305 (80%)	239 (98%)	6 (2%)	0	100 100
All	All	6804/7320 (93%)	6441 (95%)	305 (4%)	58 (1%)	21 44

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	359	SER
1	G	415	ASN
1	J	453	ASN
1	P	373	LYS
1	P	431	ASN

5.3.2 Protein sidechains (i)

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	236/267 (88%)	226 (96%)	10 (4%)	36 64
1	B	240/267 (90%)	226 (94%)	14 (6%)	25 48
1	C	231/267 (86%)	225 (97%)	6 (3%)	54 81
1	D	232/267 (87%)	223 (96%)	9 (4%)	39 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	228/267 (85%)	220 (96%)	8 (4%)	43	71
1	F	222/267 (83%)	210 (95%)	12 (5%)	27	52
1	G	234/267 (88%)	221 (94%)	13 (6%)	26	50
1	H	222/267 (83%)	212 (96%)	10 (4%)	34	61
1	I	238/267 (89%)	221 (93%)	17 (7%)	18	38
1	J	185/267 (69%)	176 (95%)	9 (5%)	31	58
1	K	180/267 (67%)	173 (96%)	7 (4%)	39	67
1	L	240/267 (90%)	231 (96%)	9 (4%)	40	68
1	M	243/267 (91%)	235 (97%)	8 (3%)	45	73
1	N	234/267 (88%)	227 (97%)	7 (3%)	48	77
1	O	231/267 (86%)	223 (96%)	8 (4%)	43	71
1	P	198/267 (74%)	193 (98%)	5 (2%)	55	82
1	Q	228/267 (85%)	216 (95%)	12 (5%)	28	54
1	R	231/267 (86%)	220 (95%)	11 (5%)	31	59
1	S	224/267 (84%)	218 (97%)	6 (3%)	52	80
1	T	233/267 (87%)	218 (94%)	15 (6%)	22	43
1	U	212/267 (79%)	206 (97%)	6 (3%)	51	79
1	V	207/267 (78%)	202 (98%)	5 (2%)	57	82
1	W	231/267 (86%)	225 (97%)	6 (3%)	54	81
1	X	194/267 (73%)	190 (98%)	4 (2%)	61	85
All	All	5354/6408 (84%)	5137 (96%)	217 (4%)	37	66

5 of 217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	492	ILE
1	L	454	ARG
1	U	454	ARG
1	J	297	HIS
1	K	271	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	321	GLN
1	D	282	HIS
1	H	247	ASN
1	C	282	HIS
1	F	490	GLN

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

24 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	$\#\|Z\| > 2$
2	LDN	A	600	-	31,36,36	1.36	4 (12%)	40,51,51	2.17	9 (22%)
2	LDN	B	600	-	31,36,36	1.16	2 (6%)	40,51,51	2.18	9 (22%)
2	LDN	C	600	-	31,36,36	1.39	3 (9%)	40,51,51	2.36	11 (27%)
2	LDN	D	600	-	31,36,36	1.37	3 (9%)	40,51,51	2.05	9 (22%)
2	LDN	E	600	-	31,36,36	1.25	3 (9%)	40,51,51	2.03	7 (17%)
2	LDN	F	600	-	31,36,36	1.41	3 (9%)	40,51,51	2.09	9 (22%)
2	LDN	G	600	-	31,36,36	1.17	2 (6%)	40,51,51	2.14	11 (27%)
2	LDN	H	600	-	31,36,36	1.26	3 (9%)	40,51,51	2.05	11 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LDN	I	600	-	31,36,36	1.48	5 (16%)	40,51,51	2.35	9 (22%)
2	LDN	J	600	-	31,36,36	1.27	3 (9%)	40,51,51	2.42	11 (27%)
2	LDN	K	600	-	31,36,36	1.46	6 (19%)	40,51,51	2.18	9 (22%)
2	LDN	L	600	-	31,36,36	1.39	4 (12%)	40,51,51	2.32	8 (20%)
2	LDN	M	600	-	31,36,36	1.44	4 (12%)	40,51,51	2.18	12 (30%)
2	LDN	N	600	-	31,36,36	1.33	2 (6%)	40,51,51	2.19	12 (30%)
2	LDN	O	600	-	31,36,36	1.40	4 (12%)	40,51,51	2.19	8 (20%)
2	LDN	P	600	-	31,36,36	1.37	4 (12%)	40,51,51	2.21	8 (20%)
2	LDN	Q	600	-	31,36,36	1.26	2 (6%)	40,51,51	2.24	9 (22%)
2	LDN	R	600	-	31,36,36	1.29	4 (12%)	40,51,51	2.24	10 (25%)
2	LDN	S	600	-	31,36,36	1.22	3 (9%)	40,51,51	2.04	7 (17%)
2	LDN	T	600	-	31,36,36	1.33	4 (12%)	40,51,51	2.25	12 (30%)
2	LDN	U	600	-	31,36,36	1.37	3 (9%)	40,51,51	1.95	10 (25%)
2	LDN	V	600	-	31,36,36	1.13	2 (6%)	40,51,51	1.95	7 (17%)
2	LDN	W	600	-	31,36,36	1.36	4 (12%)	40,51,51	2.22	11 (27%)
2	LDN	X	600	-	31,36,36	1.31	3 (9%)	40,51,51	2.21	9 (22%)

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
2	LDN	A	600	-	-	0/11/20/20	0/6/6/6
2	LDN	B	600	-	-	0/11/20/20	0/6/6/6
2	LDN	C	600	-	-	0/11/20/20	0/6/6/6
2	LDN	D	600	-	-	0/11/20/20	0/6/6/6
2	LDN	E	600	-	-	0/11/20/20	0/6/6/6
2	LDN	F	600	-	-	0/11/20/20	0/6/6/6
2	LDN	G	600	-	-	0/11/20/20	0/6/6/6
2	LDN	H	600	-	-	0/11/20/20	0/6/6/6
2	LDN	I	600	-	-	0/11/20/20	0/6/6/6
2	LDN	J	600	-	-	0/11/20/20	0/6/6/6
2	LDN	K	600	-	-	0/11/20/20	0/6/6/6
2	LDN	L	600	-	-	0/11/20/20	0/6/6/6
2	LDN	M	600	-	-	0/11/20/20	0/6/6/6
2	LDN	N	600	-	-	0/11/20/20	0/6/6/6
2	LDN	O	600	-	-	0/11/20/20	0/6/6/6
2	LDN	P	600	-	-	0/11/20/20	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDN	Q	600	-	-	0/11/20/20	0/6/6/6
2	LDN	R	600	-	-	0/11/20/20	0/6/6/6
2	LDN	S	600	-	-	0/11/20/20	0/6/6/6
2	LDN	T	600	-	-	0/11/20/20	0/6/6/6
2	LDN	U	600	-	-	0/11/20/20	0/6/6/6
2	LDN	V	600	-	-	0/11/20/20	0/6/6/6
2	LDN	W	600	-	-	0/11/20/20	0/6/6/6
2	LDN	X	600	-	-	0/11/20/20	0/6/6/6

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	600	LDN	CAZ-CAY	-4.48	1.38	1.49
2	W	600	LDN	CAZ-CAY	-4.23	1.39	1.49
2	X	600	LDN	CAZ-CAY	-4.17	1.39	1.49
2	C	600	LDN	CAZ-CAY	-4.16	1.39	1.49
2	J	600	LDN	CAZ-CAY	-3.95	1.39	1.49

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	600	LDN	CAW-CAK-NAS	-4.88	119.29	125.46
2	M	600	LDN	CAG-CAX-NBD	-4.42	115.44	121.38
2	A	600	LDN	CAW-CAK-NAS	-4.35	119.95	125.46
2	C	600	LDN	CAW-CAK-NAS	-4.26	120.07	125.46
2	I	600	LDN	CAW-CAK-NAS	-4.21	120.14	125.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	LDN	1	0
2	B	600	LDN	4	0
2	C	600	LDN	1	0
2	D	600	LDN	3	0
2	E	600	LDN	3	0
2	F	600	LDN	3	0
2	G	600	LDN	2	0
2	I	600	LDN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	600	LDN	5	0
2	K	600	LDN	4	0
2	L	600	LDN	3	0
2	N	600	LDN	1	0
2	O	600	LDN	5	0
2	P	600	LDN	5	0
2	Q	600	LDN	1	0
2	R	600	LDN	1	1
2	T	600	LDN	2	0
2	U	600	LDN	1	0
2	V	600	LDN	3	0
2	W	600	LDN	4	0
2	X	600	LDN	15	0

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^{th} 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	296/305 (97%)	0.72	19 (6%) 23 20	24, 39, 54, 64	0
1	B	295/305 (96%)	0.84	26 (8%) 12 9	31, 43, 58, 70	0
1	C	299/305 (98%)	0.68	19 (6%) 23 20	24, 40, 58, 70	0
1	D	298/305 (97%)	0.55	8 (2%) 58 56	25, 37, 51, 64	0
1	E	294/305 (96%)	0.84	37 (12%) 5 3	26, 36, 51, 69	0
1	F	294/305 (96%)	0.85	29 (9%) 9 7	28, 44, 68, 87	0
1	G	294/305 (96%)	0.27	4 (1%) 78 76	15, 27, 43, 58	0
1	H	294/305 (96%)	0.65	13 (4%) 38 36	27, 40, 57, 63	0
1	I	293/305 (96%)	0.40	12 (4%) 41 39	16, 27, 45, 55	0
1	J	252/305 (82%)	3.62	192 (76%) 0 0	62, 82, 101, 113	0
1	K	261/305 (85%)	3.71	202 (77%) 0 0	29, 88, 105, 112	0
1	L	296/305 (97%)	0.76	20 (6%) 20 18	26, 40, 53, 70	0
1	M	298/305 (97%)	0.55	11 (3%) 45 44	25, 35, 58, 65	0
1	N	300/305 (98%)	0.39	9 (3%) 54 52	17, 30, 50, 68	0
1	O	297/305 (97%)	0.80	19 (6%) 23 20	29, 44, 59, 79	0
1	P	290/305 (95%)	3.65	204 (70%) 0 0	35, 79, 99, 110	0
1	Q	294/305 (96%)	0.74	9 (3%) 52 51	27, 39, 55, 68	0
1	R	294/305 (96%)	0.70	16 (5%) 29 27	26, 41, 56, 71	0
1	S	294/305 (96%)	0.40	10 (3%) 49 47	15, 33, 53, 71	0
1	T	292/305 (95%)	0.73	26 (8%) 12 9	32, 44, 57, 67	0
1	U	285/305 (93%)	0.84	34 (11%) 6 4	28, 39, 53, 66	0
1	V	282/305 (92%)	0.89	35 (12%) 5 4	26, 39, 55, 69	0
1	W	281/305 (92%)	1.10	45 (16%) 3 1	28, 39, 54, 68	0
1	X	257/305 (84%)	4.27	210 (81%) 0 0	44, 90, 111, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	6930/7320 (94%)	1.16	1209 (17%)	2	1	15, 40, 90, 129	0

The worst 5 of 1209 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	223	GLY	17.6
1	P	471	CYS	16.3
1	X	366	ASN	15.6
1	P	474	PRO	14.7
1	X	465	ALA	14.6

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^{th} 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^2)	Q<0.9
2	LDN	D	600	31/31	0.86	0.24	0.77	27,34,40,43	0
2	LDN	I	600	31/31	0.88	0.23	0.75	24,27,39,40	0
2	LDN	V	600	31/31	0.86	0.28	0.72	26,31,44,46	0
2	LDN	M	600	31/31	0.88	0.25	0.64	30,35,40,48	0
2	LDN	B	600	31/31	0.91	0.28	0.47	27,34,41,41	0
2	LDN	W	600	31/31	0.84	0.30	0.37	33,38,42,44	0
2	LDN	Q	600	31/31	0.88	0.24	0.35	25,31,39,45	0
2	LDN	G	600	31/31	0.89	0.23	0.27	21,26,36,36	0
2	LDN	E	600	31/31	0.89	0.23	0.23	29,33,37,38	0
2	LDN	U	600	31/31	0.87	0.24	0.20	26,31,44,45	0
2	LDN	N	600	31/31	0.92	0.20	0.11	21,26,34,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	LDN	L	600	31/31	0.92	0.23	0.03	27,32,36,37	0
2	LDN	F	600	31/31	0.92	0.21	-0.12	23,29,32,34	0
2	LDN	S	600	31/31	0.91	0.21	-0.12	20,27,45,50	0
2	LDN	A	600	31/31	0.92	0.21	-0.30	24,36,47,50	0
2	LDN	O	600	31/31	0.88	0.22	-0.41	26,33,40,46	0
2	LDN	C	600	31/31	0.93	0.20	-0.47	27,33,42,45	0
2	LDN	P	600	31/31	0.71	0.35	-0.48	41,50,55,55	0
2	LDN	J	600	31/31	0.73	0.34	-0.49	35,46,52,56	0
2	LDN	R	600	31/31	0.92	0.19	-0.68	25,31,36,38	0
2	LDN	X	600	31/31	0.64	0.38	-0.70	34,52,63,64	0
2	LDN	K	600	31/31	0.69	0.36	-0.76	36,48,53,59	0
2	LDN	H	600	31/31	0.94	0.18	-0.83	24,27,39,42	0
2	LDN	T	600	31/31	0.91	0.17	-1.26	30,39,45,45	0

6.5 Other polymers

There are no such residues in this entry.