Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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:

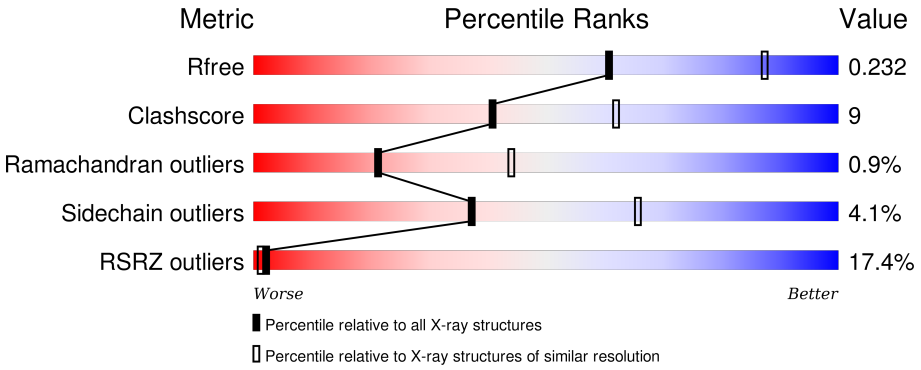
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

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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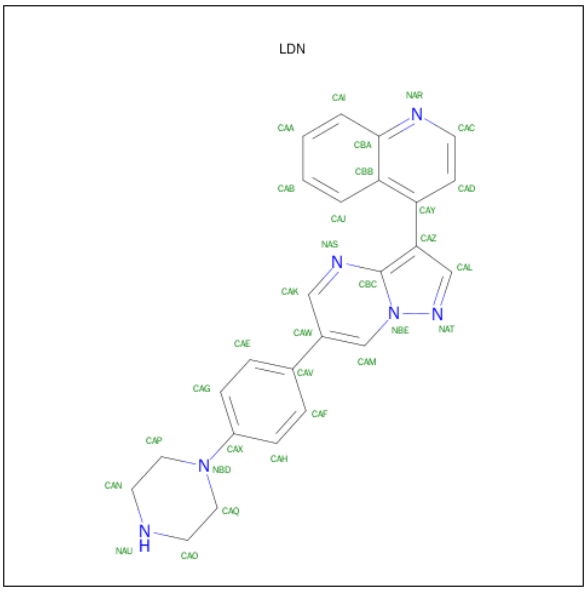
Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	EXPRESSION TAG	UNP P37023
M	-1	SER	-	EXPRESSION TAG	UNP P37023
M	0	MET	-	EXPRESSION TAG	UNP P37023
N	-1	SER	-	EXPRESSION TAG	UNP P37023
N	0	MET	-	EXPRESSION TAG	UNP P37023
O	-1	SER	-	EXPRESSION TAG	UNP P37023
O	0	MET	-	EXPRESSION TAG	UNP P37023
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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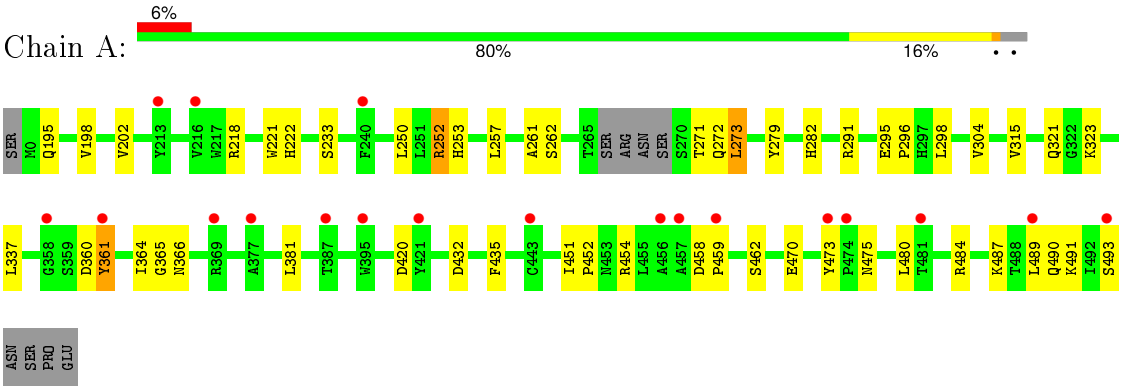
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	2	Total O 2 2	0	0
3	L	6	Total O 6 6	0	0
3	M	1	Total O 1 1	0	0
3	N	6	Total O 6 6	0	0
3	O	2	Total O 2 2	0	0
3	P	4	Total O 4 4	0	0
3	Q	8	Total O 8 8	0	0
3	R	5	Total O 5 5	0	0
3	S	6	Total O 6 6	0	0
3	T	5	Total O 5 5	0	0
3	U	9	Total O 9 9	0	0
3	V	2	Total O 2 2	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.

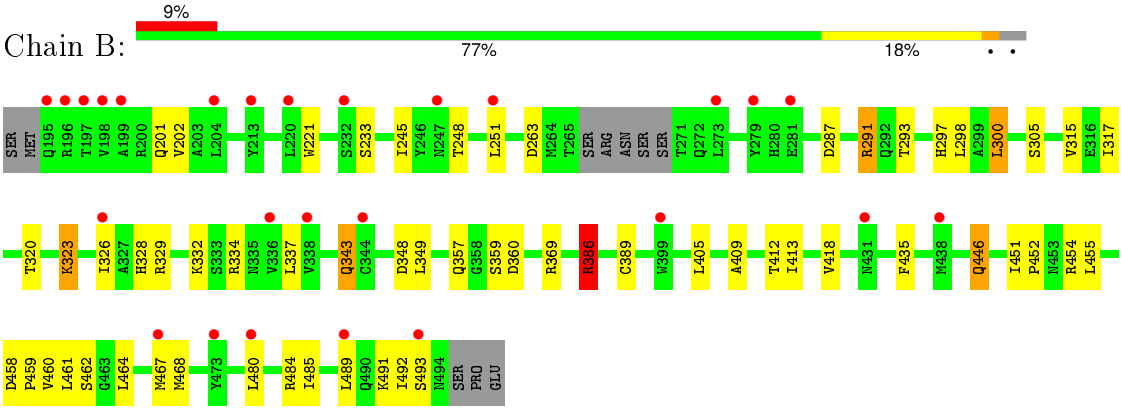
- Molecule 1: Serine/threonine-protein kinase receptor R3

Chain A:



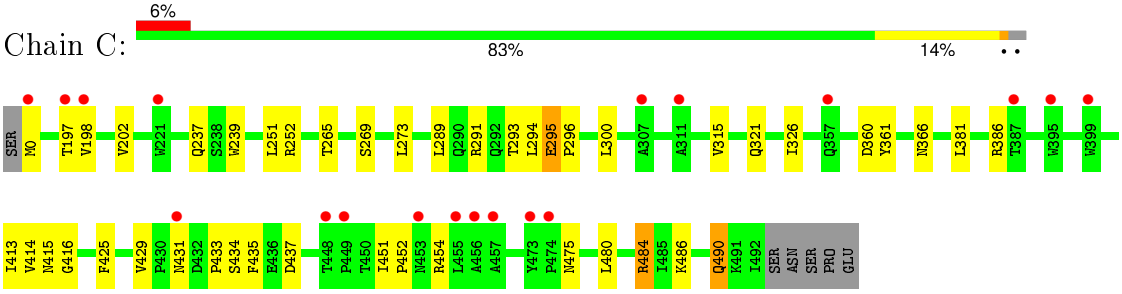
- Molecule 1: Serine/threonine-protein kinase receptor R3

Chain B:



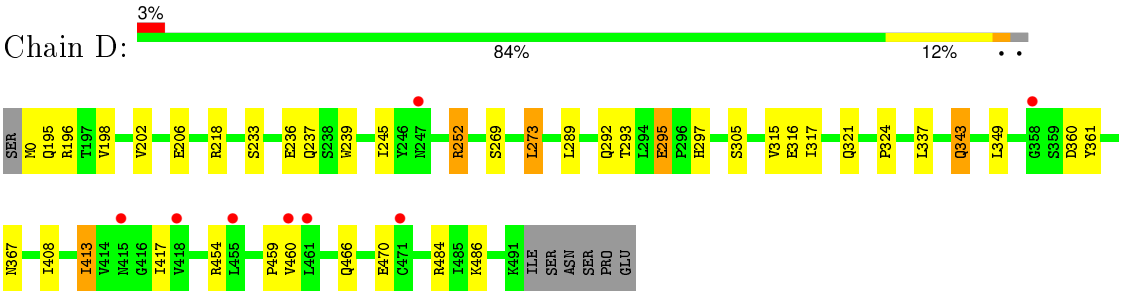
- Molecule 1: Serine/threonine-protein kinase receptor R3

Chain C:



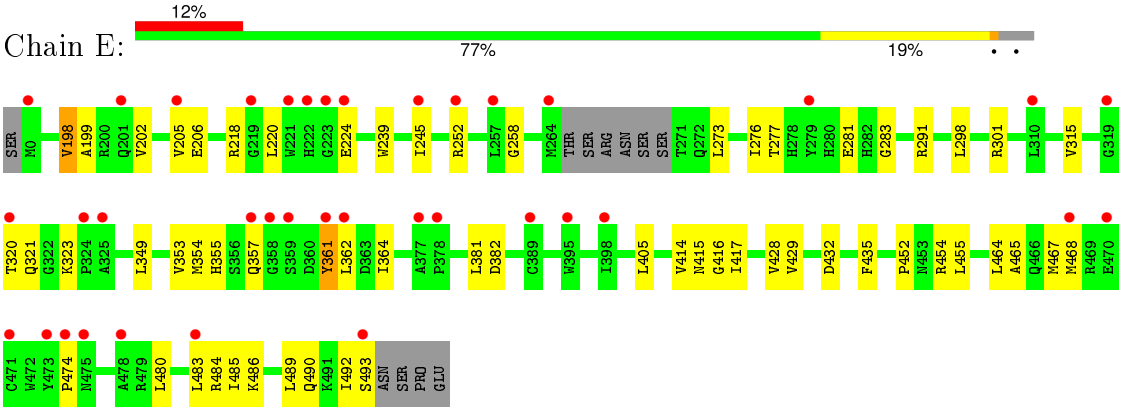
- Molecule 1: Serine/threonine-protein kinase receptor R3

Chain D:



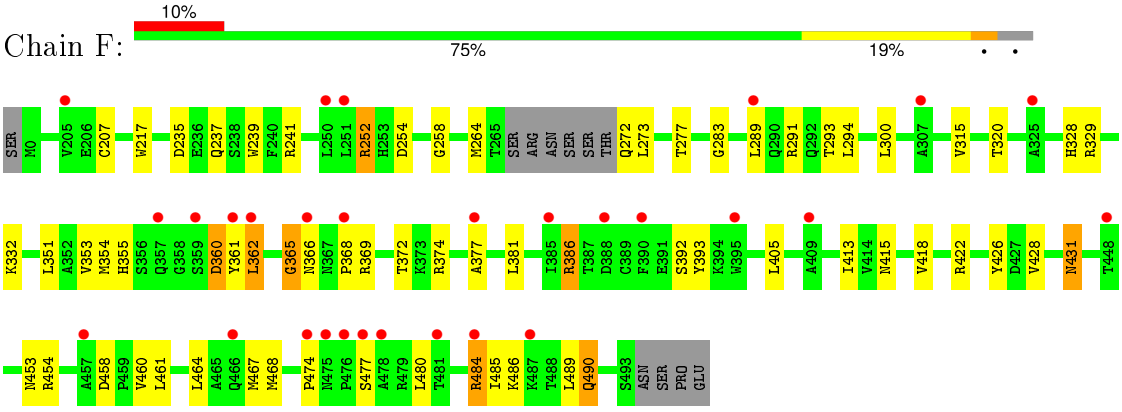
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain E:



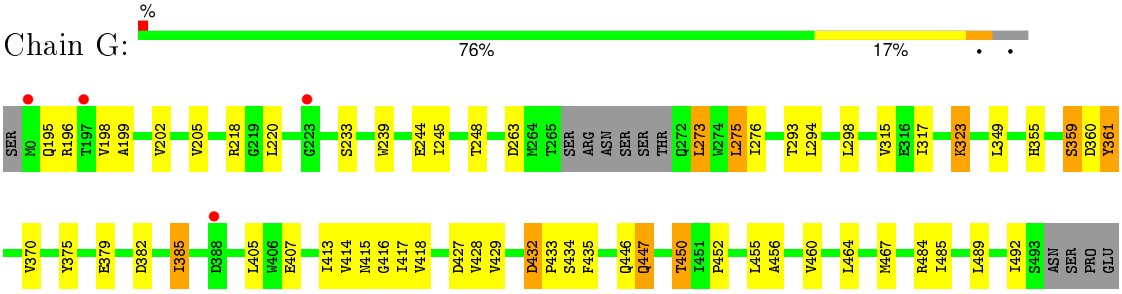
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain F:



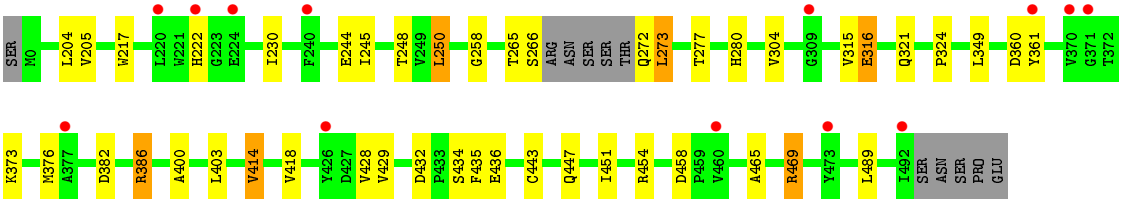
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain G:



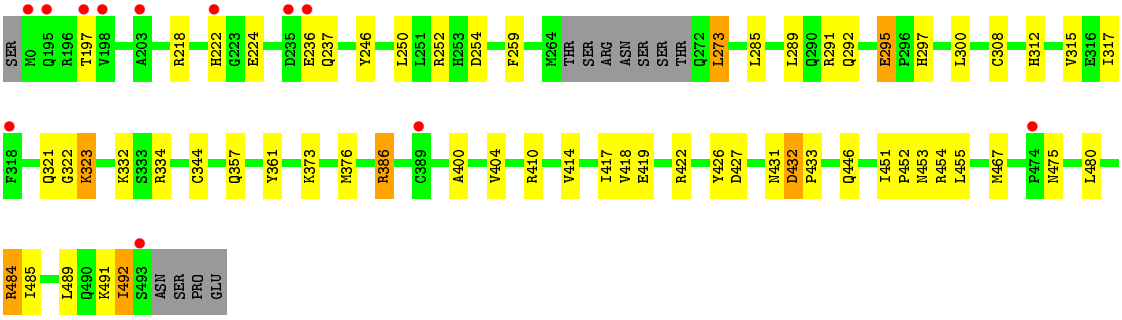
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain H:



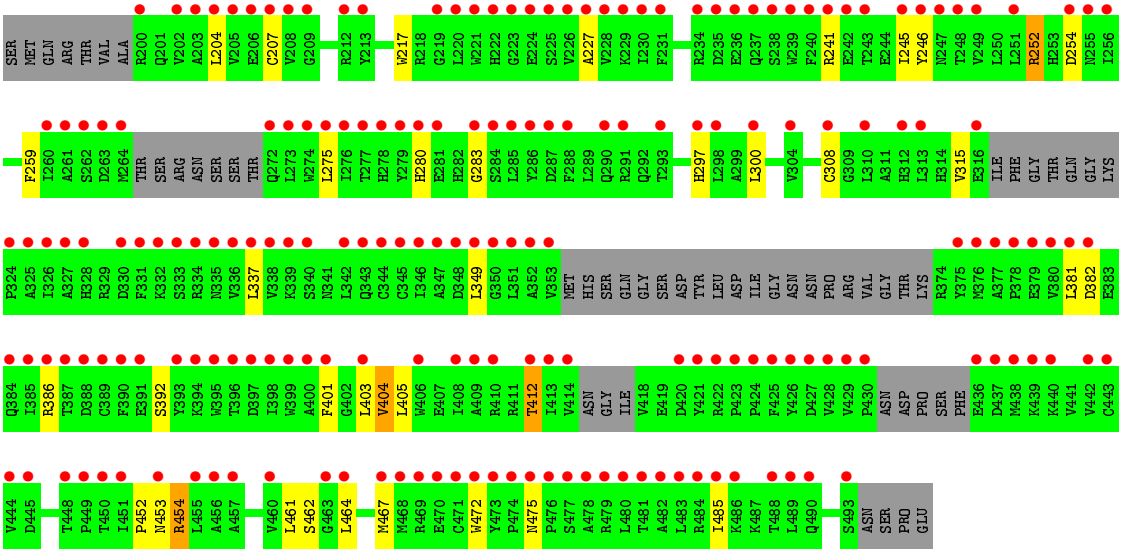
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain I:



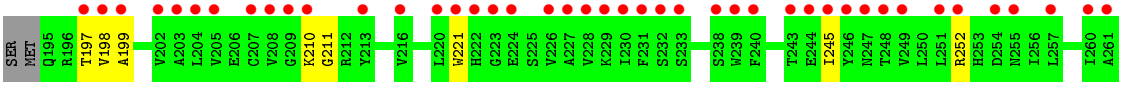
• Molecule 1: Serine/threonine-protein kinase receptor R3

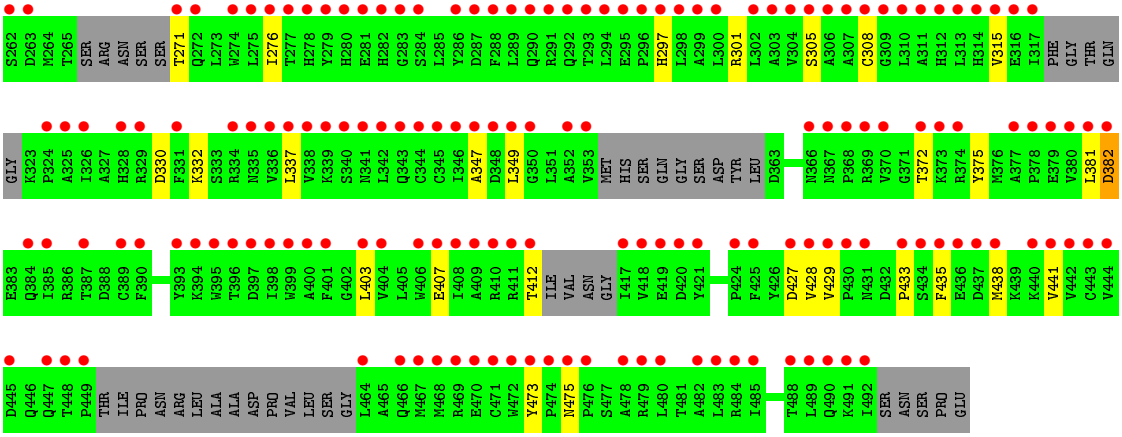
Chain J:



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

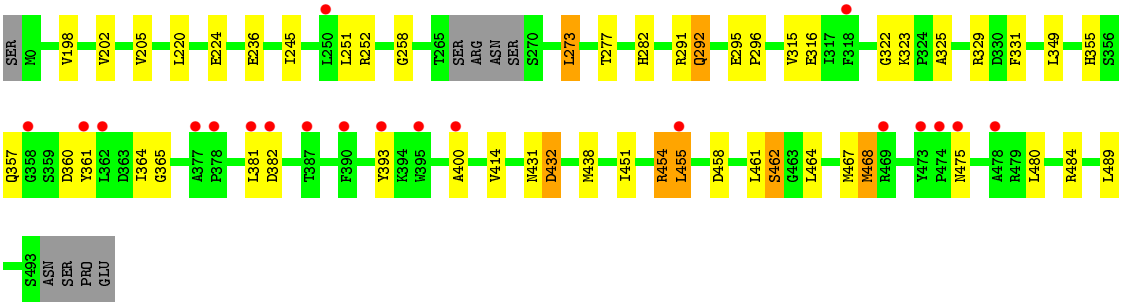
Chain K:





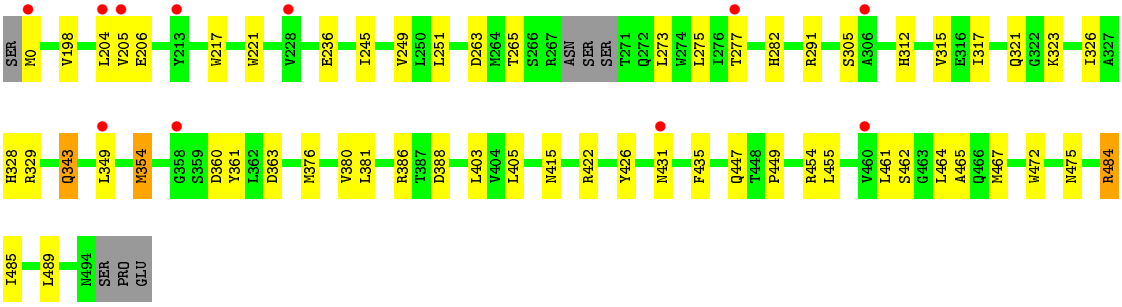
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain L:



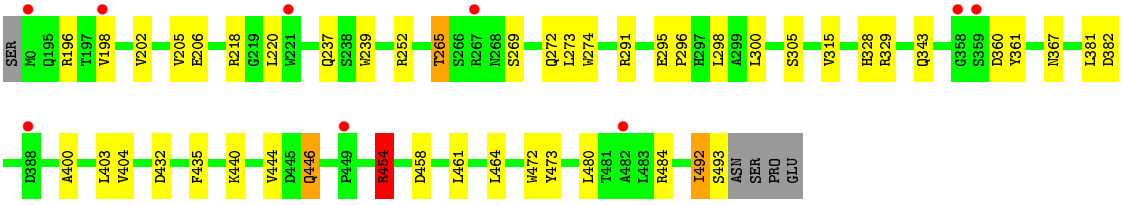
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain M:



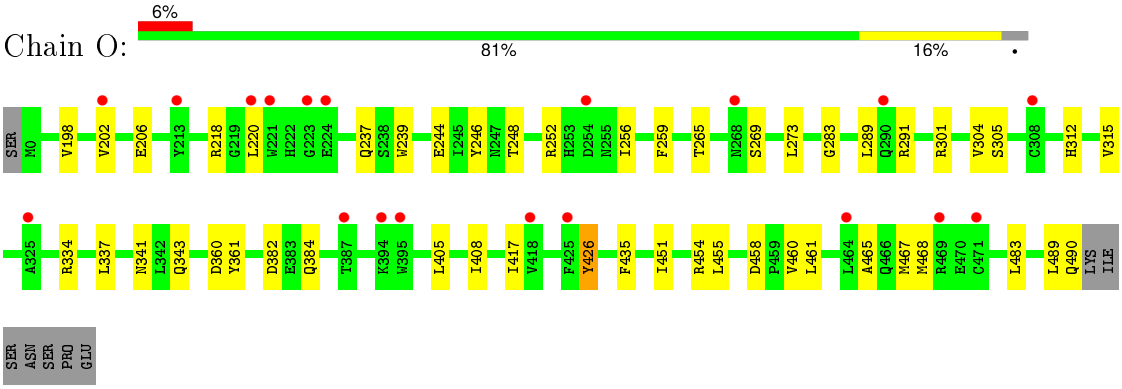
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain N:



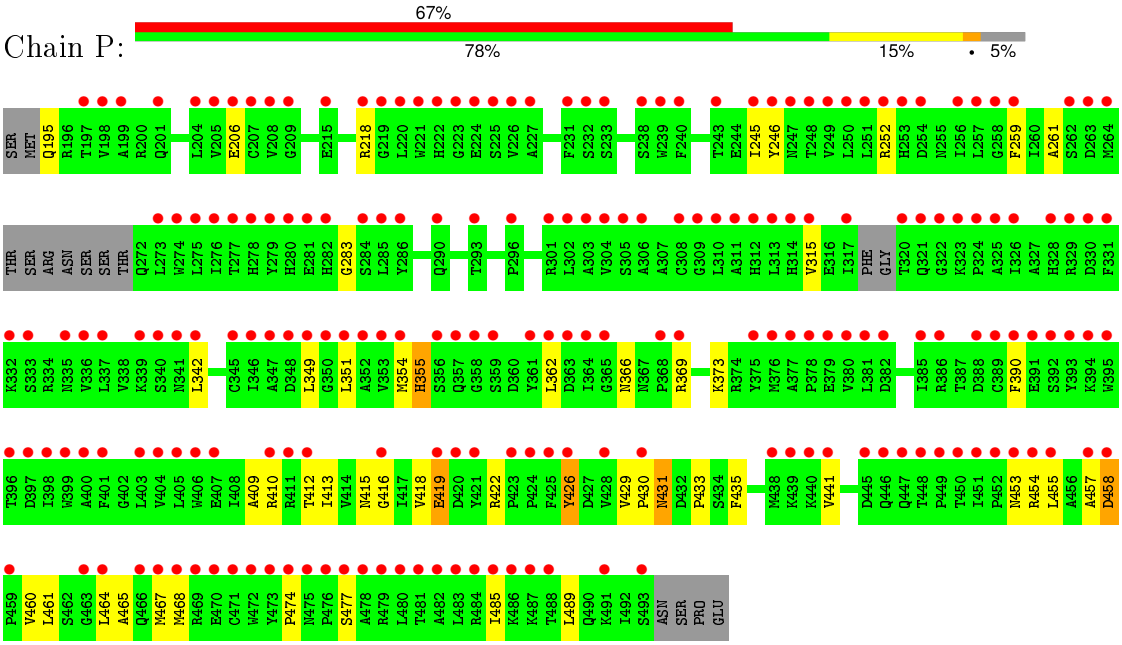
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain O:



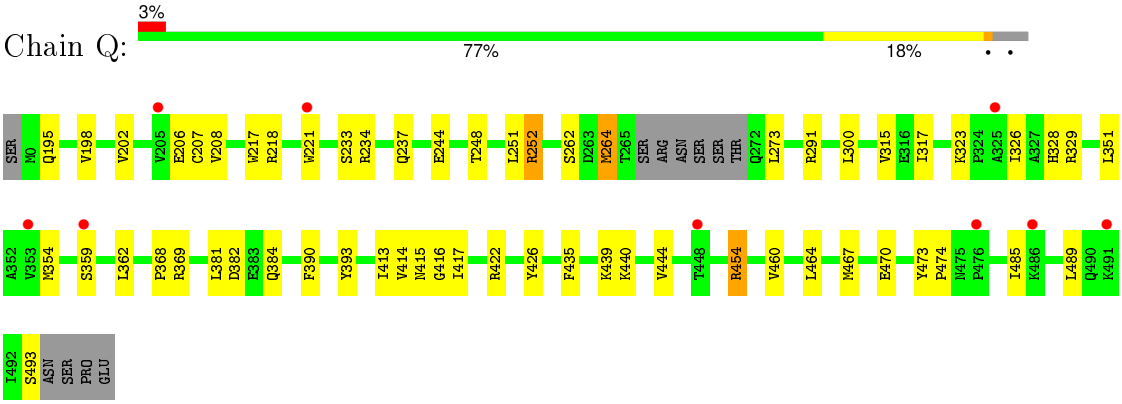
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain P:



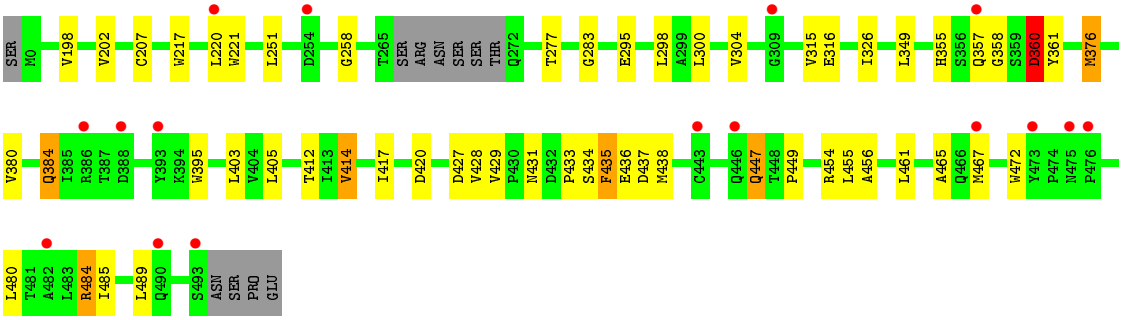
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain Q:



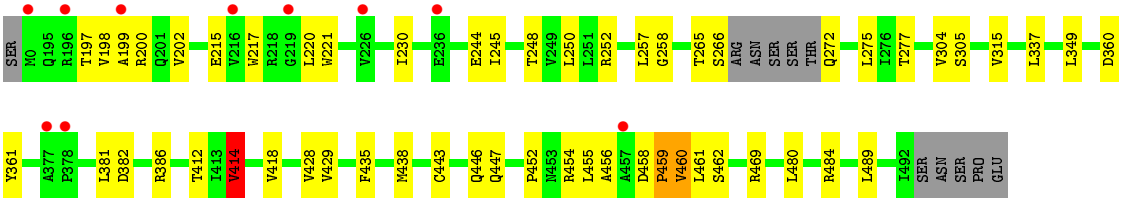
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain R:



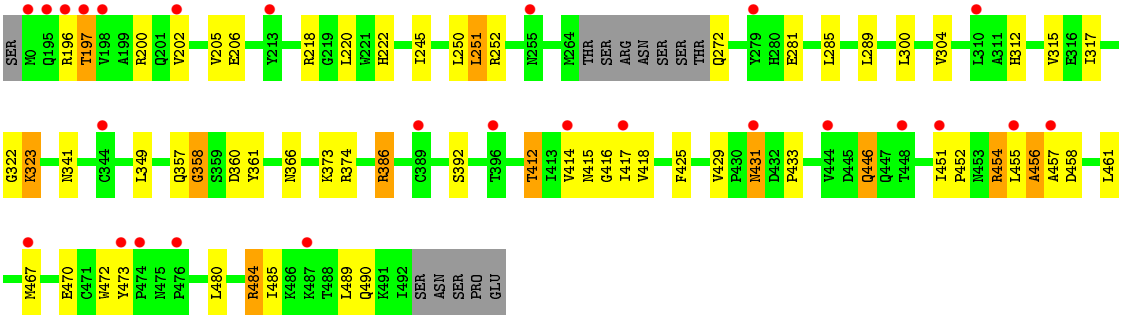
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain S:



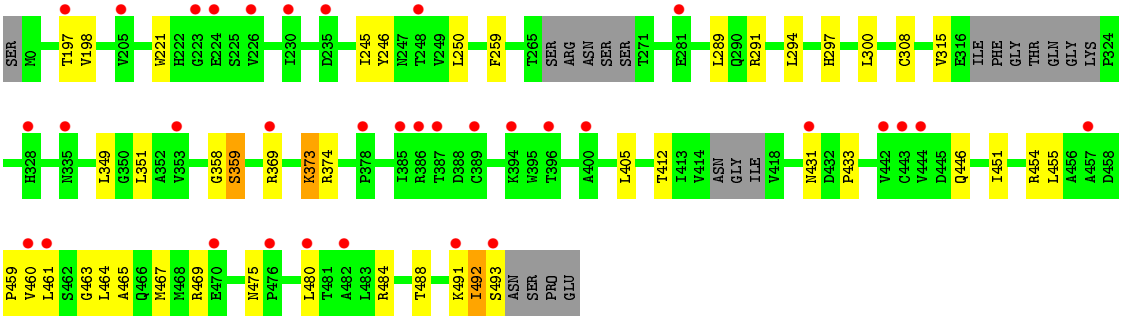
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain T:



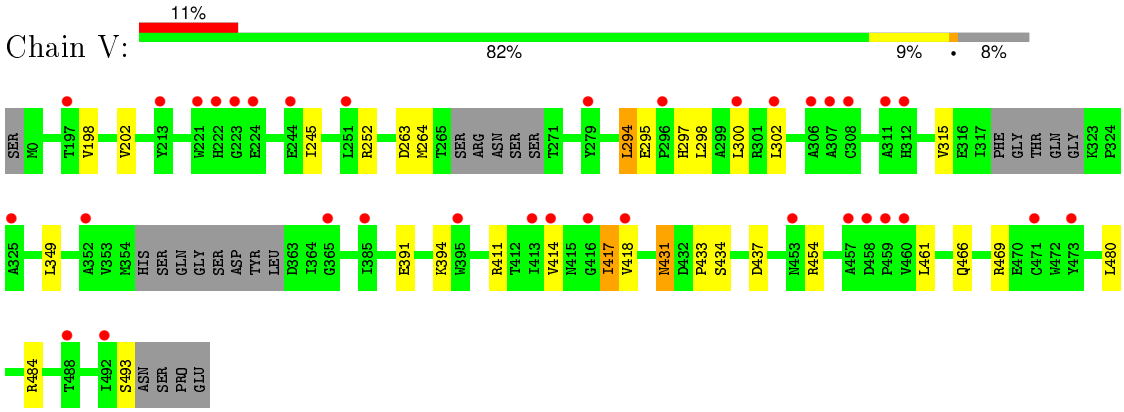
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain U:



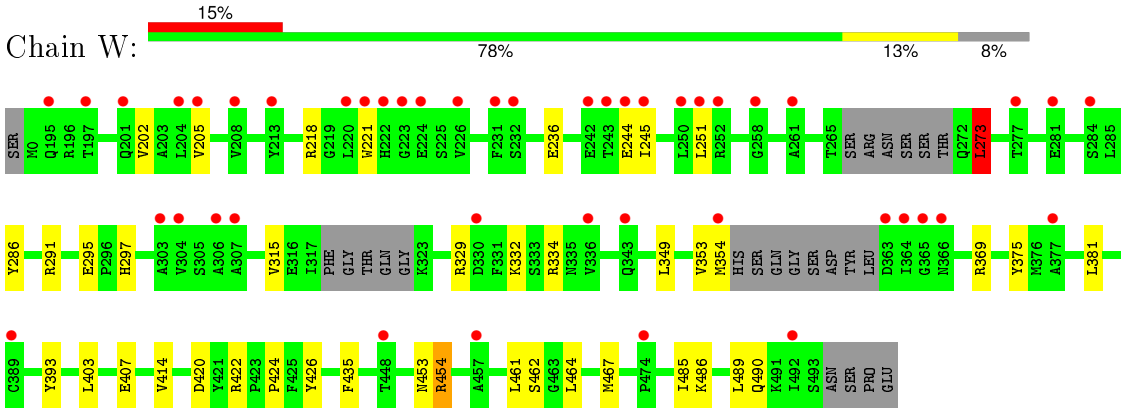
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain V:



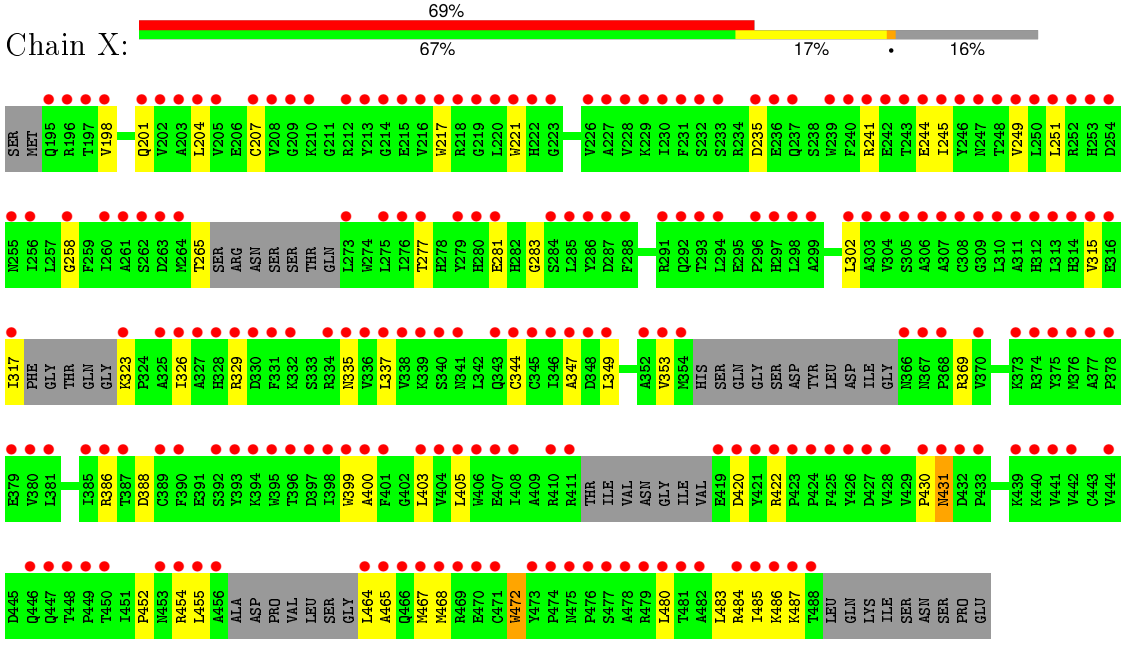
- Molecule 1: Serine/threonine-protein kinase receptor R3

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

All (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
1	W	273	LEU	CA-CB-CG	5.60	128.19	115.30
1	F	254	ASP	CB-CG-OD1	5.35	123.11	118.30
1	G	275	LEU	CA-CB-CG	5.28	127.44	115.30
1	F	254	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	T	251	LEU	CA-CB-CG	5.07	126.96	115.30

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.

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.

All (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
1:D:198:VAL:O	1:D:202:VAL:CG2	2.10	0.99
1:G:467:MET:CE	1:G:489:LEU:HD11	1.92	0.99
1:B:467:MET:HE1	1:B:489:LEU:HD11	1.44	0.98
1:T:480:LEU:HD22	1:T:484:ARG:HG2	1.49	0.95
1:P:412:THR:HG21	1:P:461:LEU:HD11	1.47	0.94
1:N:239:TRP:CD2	1:N:273:LEU:HD23	2.04	0.93
1:O:198:VAL:O	1:O:202:VAL:HG23	1.70	0.92
1:N:480:LEU:HD22	1:N:484:ARG:HG2	1.52	0.90
1:P:461:LEU:HD23	1:P:464:LEU:HD12	1.51	0.89
1:J:405:LEU:HD22	1:J:464:LEU:HD11	1.51	0.89
1:X:455:LEU:CD2	1:X:465:ALA:HB2	2.02	0.88
1:X:455:LEU:HD22	1:X:465:ALA:HB2	1.55	0.88
1:V:198:VAL:O	1:V:202:VAL:HG23	1.73	0.88
1:D:295:GLU:OE2	1:D:297:HIS:HB3	1.71	0.88
1:B:386:ARG:HB3	1:B:386:ARG:HH11	1.37	0.87
1:O:382:ASP:OD2	1:O:384:GLN:NE2	2.08	0.87
1:N:239:TRP:CE3	1:N:273:LEU:CD2	2.57	0.86
1:D:417:ILE:O	1:D:454:ARG:NH1	2.09	0.86
1:E:467:MET:HE1	1:E:489:LEU:HD11	1.58	0.84
1:N:239:TRP:CE3	1:N:273:LEU:HD23	2.12	0.84
1:T:470:GLU:HG2	1:T:473:TYR:OH	1.76	0.84
1:V:466:GLN:OE1	1:V:469:ARG:NH1	2.09	0.83
1:X:283:GLY:HA2	2:X:600:LDN:CAV	2.08	0.83
1:X:249:VAL:CG1	1:X:251:LEU:HD13	2.09	0.83
1:X:249:VAL:HG12	1:X:251:LEU:HD13	1.59	0.83
1:U:358:GLY:O	1:U:359:SER:O	1.97	0.83
1:E:464:LEU:HD23	1:E:489:LEU:HD21	1.61	0.82
1:S:480:LEU:HD22	1:S:484:ARG:HG2	1.60	0.82
1:G:464:LEU:HD23	1:G:489:LEU:HD21	1.62	0.82
1:C:486:LYS:HG2	1:C:490:GLN:OE1	1.79	0.81
1:B:455:LEU:HD12	1:B:461:LEU:HB3	1.62	0.81
1:F:477:SER:OG	1:J:382:ASP:HB3	1.80	0.80
1:X:480:LEU:HD22	1:X:484:ARG:HG2	1.63	0.80
1:G:467:MET:HE1	1:G:489:LEU:CD1	2.00	0.80
1:U:461:LEU:HD23	1:U:464:LEU:HD22	1.63	0.80
1:F:480:LEU:HD22	1:F:484:ARG:HG2	1.63	0.80
1:B:291:ARG:HH11	2:B:600:LDN:HANA	1.45	0.79
1:I:467:MET:HE1	1:I:489:LEU:HD11	1.62	0.79
1:G:464:LEU:CD2	1:G:489:LEU:HD21	2.12	0.78
1:R:412:THR:HG21	1:R:461:LEU:HD21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:464:LEU:HD23	1:Q:489:LEU:HD21	1.66	0.78
1:G:464:LEU:CD2	1:G:489:LEU:CD2	2.62	0.78
1:G:464:LEU:HD23	1:G:489:LEU:CD2	2.14	0.77
1:Q:198:VAL:HG13	1:Q:221:TRP:CE2	2.19	0.77
1:F:467:MET:HE1	1:F:489:LEU:HD11	1.66	0.77
1:U:300:LEU:HD13	1:U:460:VAL:HG13	1.65	0.77
1:W:236:GLU:HG2	1:W:273:LEU:HD21	1.67	0.76
1:X:467:MET:CE	1:X:485:ILE:HG23	2.16	0.76
1:T:412:THR:HG21	1:T:461:LEU:HD21	1.68	0.76
1:O:458:ASP:CB	1:O:461:LEU:HD12	2.17	0.75
1:O:252:ARG:NH1	1:T:317:ILE:HD13	2.01	0.75
1:P:195:GLN:HG2	1:P:261:ALA:CB	2.16	0.75
1:E:199:ALA:HB2	1:E:276:ILE:HD11	1.68	0.74
1:R:480:LEU:HD22	1:R:484:ARG:HG2	1.69	0.74
1:G:467:MET:CE	1:G:485:ILE:HG23	2.18	0.74
1:A:381:LEU:HA	1:A:435:PHE:CZ	2.23	0.74
1:A:291:ARG:HD2	1:F:291:ARG:CB	2.18	0.73
1:W:295:GLU:OE1	1:W:297:HIS:HB3	1.87	0.73
1:B:291:ARG:NH1	2:B:600:LDN:HANA	2.03	0.72
1:P:413:ILE:HG23	1:P:416:GLY:HA2	1.72	0.72
1:P:412:THR:HG21	1:P:461:LEU:CD1	2.18	0.72
1:D:293:THR:HB	1:D:413:ILE:HD11	1.70	0.72
1:O:460:VAL:O	1:O:461:LEU:HD23	1.90	0.71
1:N:239:TRP:CD2	1:N:273:LEU:CD2	2.73	0.71
1:X:483:LEU:HD11	1:X:487:LYS:HE3	1.70	0.71
1:P:461:LEU:CD2	1:P:464:LEU:HD12	2.20	0.71
1:E:467:MET:CE	1:E:485:ILE:HG23	2.20	0.71
1:X:480:LEU:HD22	1:X:484:ARG:CG	2.20	0.71
1:M:467:MET:HE1	1:M:489:LEU:HD11	1.72	0.71
1:P:195:GLN:HG2	1:P:261:ALA:HB1	1.73	0.71
1:L:198:VAL:O	1:L:202:VAL:HG23	1.90	0.71
1:X:337:LEU:HD11	2:X:600:LDN:HAJ	1.73	0.71
1:A:480:LEU:HD22	1:A:484:ARG:HG2	1.73	0.70
1:I:414:VAL:HG13	1:I:454:ARG:HD2	1.73	0.70
1:Q:198:VAL:HG13	1:Q:221:TRP:CZ2	2.26	0.70
1:Q:351:LEU:HD21	1:Q:369:ARG:O	1.92	0.70
1:I:295:GLU:CD	1:I:297:HIS:HB3	2.12	0.70
1:P:467:MET:CE	1:P:485:ILE:HG23	2.22	0.70
1:W:454:ARG:HG2	1:W:454:ARG:O	1.90	0.70
1:E:353:VAL:HB	1:E:362:LEU:HD11	1.73	0.69
1:I:222:HIS:O	1:I:224:GLU:OE2	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ILE:N	1:D:317:ILE:HD12	2.07	0.69
1:N:239:TRP:CE2	1:N:273:LEU:HD23	2.27	0.69
1:T:281:GLU:O	2:T:600:LDN:HAQA	1.91	0.69
1:N:206:GLU:OE1	1:N:218:ARG:NH1	2.26	0.69
1:Q:467:MET:CE	1:Q:485:ILE:HG23	2.22	0.69
1:T:374:ARG:NH1	1:T:431:ASN:O	2.26	0.69
1:N:446:GLN:HB2	1:R:395:TRP:HH2	1.58	0.68
1:M:317:ILE:HG21	1:N:252:ARG:HD2	1.75	0.68
1:K:330:ASP:OD1	1:K:372:THR:OG1	2.09	0.68
1:F:300:LEU:HD12	1:F:460:VAL:HG13	1.75	0.68
1:M:236:GLU:HG2	1:M:273:LEU:HD11	1.74	0.68
1:Q:207:CYS:HB2	1:Q:217:TRP:CZ2	2.28	0.68
1:S:460:VAL:HG12	1:S:461:LEU:HD23	1.75	0.68
1:J:386:ARG:NH1	1:J:392:SER:OG	2.27	0.68
1:Q:206:GLU:OE2	1:Q:218:ARG:NH1	2.27	0.67
1:D:239:TRP:CE3	1:D:273:LEU:CD2	2.78	0.67
1:S:217:TRP:CZ2	1:X:430:PRO:CB	2.72	0.67
1:X:405:LEU:HD22	1:X:464:LEU:HD22	1.76	0.67
1:K:332:LYS:HB2	1:K:375:TYR:CE2	2.29	0.67
1:M:321:GLN:O	1:N:252:ARG:NE	2.28	0.67
1:Q:326:ILE:HG12	1:Q:354:MET:HG2	1.77	0.67
1:K:199:ALA:HB2	1:K:276:ILE:HD11	1.77	0.67
1:F:353:VAL:HB	1:F:362:LEU:HD11	1.77	0.67
1:F:293:THR:OG1	1:F:413:ILE:HD11	1.95	0.66
1:W:329:ARG:HE	1:W:353:VAL:HG13	1.60	0.66
1:C:239:TRP:CE3	1:C:273:LEU:HD23	2.30	0.66
1:J:254:ASP:OD1	1:W:490:GLN:HB3	1.94	0.66
1:X:467:MET:SD	1:X:485:ILE:HG23	2.35	0.66
1:B:293:THR:OG1	1:B:413:ILE:HD11	1.95	0.66
1:C:239:TRP:CE3	1:C:273:LEU:CD2	2.79	0.66
1:L:236:GLU:HG2	1:L:273:LEU:HD21	1.76	0.66
1:N:305:SER:HB3	1:N:343:GLN:HG2	1.78	0.66
1:X:337:LEU:HD11	2:X:600:LDN:CAJ	2.25	0.66
1:O:283:GLY:HA2	2:O:600:LDN:CAV	2.26	0.65
1:D:486:LYS:NZ	1:I:254:ASP:OD1	2.28	0.65
1:T:304:VAL:HA	1:T:489:LEU:HD12	1.77	0.65
1:G:427:ASP:OD1	1:G:428:VAL:HG13	1.96	0.65
1:I:236:GLU:HG2	1:I:273:LEU:HD21	1.79	0.65
1:F:422:ARG:HD2	1:F:426:TYR:CD1	2.31	0.65
1:R:434:SER:O	1:R:437:ASP:N	2.29	0.65
1:F:351:LEU:HD21	1:F:369:ARG:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:251:LEU:HD11	1:X:326:ILE:CD1	2.27	0.65
1:C:480:LEU:HD22	1:C:484:ARG:HG2	1.79	0.65
1:G:233:SER:HB2	1:K:210:LYS:C	2.16	0.65
1:L:382:ASP:OD2	1:P:477:SER:OG	2.15	0.65
1:F:467:MET:CE	1:F:485:ILE:HG23	2.26	0.65
1:B:287:ASP:O	1:B:291:ARG:HD3	1.97	0.65
1:H:382:ASP:OD1	1:H:443:CYS:SG	2.54	0.65
1:R:428:VAL:HG23	1:R:429:VAL:HG13	1.78	0.64
1:L:295:GLU:HG2	1:L:296:PRO:HD2	1.80	0.64
1:A:218:ARG:HD2	1:A:279:TYR:CE2	2.33	0.64
1:Q:264:MET:HG3	1:Q:273:LEU:CD2	2.28	0.64
1:U:463:GLY:HA3	1:U:492:ILE:HD11	1.80	0.64
1:K:428:VAL:HG21	1:K:441:VAL:HG11	1.80	0.63
1:E:489:LEU:HA	1:E:492:ILE:HD12	1.79	0.63
1:N:461:LEU:HD23	1:N:464:LEU:HD12	1.79	0.63
1:L:205:VAL:O	1:Q:416:GLY:HA2	1.99	0.63
1:E:464:LEU:CD2	1:E:489:LEU:HD21	2.28	0.63
1:X:315:VAL:O	1:X:323:LYS:NZ	2.31	0.63
1:S:275:LEU:HD13	1:S:277:THR:HG23	1.80	0.62
1:U:455:LEU:HD13	1:U:465:ALA:HB2	1.81	0.62
1:K:347:ALA:HB1	2:K:600:LDN:CAI	2.30	0.62
1:H:428:VAL:HG11	1:H:447:GLN:NE2	2.15	0.62
1:P:355:HIS:HB3	1:P:390:PHE:HB2	1.81	0.62
1:R:251:LEU:HD21	1:R:349:LEU:HD21	1.81	0.62
1:M:464:LEU:HD23	1:M:489:LEU:HD21	1.81	0.62
1:J:412:THR:HG21	1:J:461:LEU:HD11	1.81	0.61
1:J:204:LEU:HD22	1:J:217:TRP:CB	2.30	0.61
1:I:480:LEU:HD22	1:I:484:ARG:HG2	1.81	0.61
1:U:300:LEU:CD2	1:U:493:SER:HA	2.31	0.61
1:M:467:MET:CE	1:M:485:ILE:HG23	2.30	0.61
1:B:405:LEU:HD11	1:B:467:MET:HE3	1.82	0.61
1:D:198:VAL:C	1:D:202:VAL:HG23	2.14	0.61
1:D:239:TRP:CE3	1:D:273:LEU:HD22	2.35	0.61
1:A:458:ASP:O	1:A:462:SER:HB3	2.01	0.61
1:U:198:VAL:HG22	1:U:221:TRP:HZ2	1.66	0.61
1:H:428:VAL:HG11	1:H:447:GLN:HE22	1.64	0.60
1:L:414:VAL:HG12	1:L:454:ARG:HH11	1.65	0.60
1:H:273:LEU:H	1:H:273:LEU:HD22	1.65	0.60
1:P:283:GLY:HA2	2:P:600:LDN:CAF	2.31	0.60
1:T:467:MET:CE	1:T:485:ILE:HG23	2.31	0.60
1:B:386:ARG:HB3	1:B:386:ARG:NH1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:ALA:HB2	1:K:276:ILE:CD1	2.32	0.59
1:T:315:VAL:HG13	1:T:315:VAL:O	2.02	0.59
1:F:374:ARG:NH1	1:F:431:ASN:O	2.35	0.59
1:P:464:LEU:HD21	1:P:489:LEU:HD11	1.82	0.59
1:W:461:LEU:HD23	1:W:464:LEU:HB2	1.84	0.59
1:H:273:LEU:HD22	1:H:273:LEU:N	2.18	0.59
1:J:467:MET:CE	1:J:485:ILE:HG23	2.32	0.59
1:P:355:HIS:HB2	1:P:362:LEU:HD12	1.84	0.59
1:S:460:VAL:HG12	1:S:461:LEU:N	2.17	0.59
1:H:250:LEU:HD21	1:H:321:GLN:OE1	2.03	0.59
1:P:206:GLU:CB	1:P:218:ARG:HH12	2.15	0.59
1:K:381:LEU:HD11	1:K:438:MET:HB3	1.84	0.58
1:U:374:ARG:NH1	1:U:431:ASN:O	2.36	0.58
1:G:450:THR:CG2	1:I:453:ASN:H	2.16	0.58
1:F:474:PRO:HB3	1:J:475:ASN:HB2	1.86	0.58
1:G:467:MET:SD	1:G:485:ILE:HG23	2.42	0.58
1:D:252:ARG:HD3	1:I:321:GLN:O	2.03	0.58
1:F:235:ASP:OD2	1:F:369:ARG:NH2	2.37	0.58
1:W:464:LEU:HD13	1:W:489:LEU:HD21	1.84	0.58
1:B:386:ARG:CB	1:B:386:ARG:HH11	2.14	0.58
1:B:405:LEU:HD11	1:B:467:MET:CE	2.33	0.58
1:R:428:VAL:HG11	1:R:447:GLN:OE1	2.04	0.58
1:I:417:ILE:HG22	1:I:418:VAL:N	2.19	0.58
1:P:465:ALA:HA	1:P:468:MET:HE3	1.86	0.58
1:Q:381:LEU:HA	1:Q:435:PHE:CZ	2.38	0.58
1:C:239:TRP:CD2	1:C:273:LEU:HD23	2.38	0.57
1:S:386:ARG:NH1	1:T:446:GLN:HB2	2.20	0.57
1:O:301:ARG:NH2	1:O:341:ASN:O	2.37	0.57
1:J:227:ALA:HB1	2:J:600:LDN:HAD	1.86	0.57
1:Q:207:CYS:HB2	1:Q:217:TRP:CE2	2.39	0.57
1:B:409:ALA:HB2	1:B:468:MET:HE2	1.86	0.57
1:A:195:GLN:HB3	1:A:261:ALA:HB1	1.87	0.57
1:I:250:LEU:HD11	1:I:252:ARG:NH1	2.20	0.57
1:Q:440:LYS:HA	1:Q:444:VAL:HG23	1.86	0.57
1:S:428:VAL:HG23	1:S:429:VAL:HG13	1.87	0.57
1:B:412:THR:HG21	1:B:461:LEU:HD21	1.85	0.57
1:X:420:ASP:CB	1:X:422:ARG:HH21	2.17	0.57
1:W:251:LEU:HD21	1:W:349:LEU:HD21	1.85	0.57
1:W:369:ARG:NH2	3:W:142:HOH:O	2.25	0.57
1:D:206:GLU:OE1	1:D:218:ARG:NH1	2.38	0.56
1:S:265:THR:O	1:S:266:SER:OG	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:379:GLU:CG	1:G:385:ILE:HG23	2.35	0.56
1:I:317:ILE:HG22	1:I:322:GLY:HA2	1.87	0.56
1:U:373:LYS:HG3	1:U:433:PRO:O	2.04	0.56
1:X:452:PRO:HD2	1:X:455:LEU:HD13	1.86	0.56
1:U:358:GLY:O	1:U:359:SER:C	2.44	0.56
1:N:300:LEU:HD21	1:N:493:SER:HB3	1.87	0.56
1:R:455:LEU:CD2	1:R:465:ALA:HB2	2.35	0.56
1:M:405:LEU:HD11	1:M:467:MET:CE	2.35	0.56
1:G:450:THR:HG22	1:I:453:ASN:HB2	1.87	0.56
1:E:405:LEU:HD22	1:E:464:LEU:HD22	1.86	0.56
1:X:405:LEU:HD11	1:X:467:MET:CE	2.36	0.56
1:L:236:GLU:HG2	1:L:273:LEU:CD2	2.36	0.56
1:G:450:THR:HG21	1:I:452:PRO:HA	1.85	0.56
1:A:198:VAL:O	1:A:202:VAL:HG23	2.05	0.56
1:N:239:TRP:CZ3	1:N:273:LEU:HD23	2.40	0.56
1:G:428:VAL:HG23	1:G:429:VAL:HG13	1.87	0.56
1:T:414:VAL:HG11	1:T:454:ARG:HG3	1.86	0.56
1:U:480:LEU:HD22	1:U:484:ARG:HG2	1.87	0.56
1:F:474:PRO:CB	1:J:475:ASN:HB2	2.36	0.56
1:S:265:THR:O	1:S:272:GLN:N	2.39	0.55
1:C:237:GLN:HG2	1:C:366:ASN:O	2.05	0.55
1:R:414:VAL:HG11	1:R:454:ARG:HG2	1.87	0.55
1:F:477:SER:OG	1:J:382:ASP:CB	2.54	0.55
1:C:293:THR:OG1	1:C:413:ILE:HD11	2.07	0.55
1:X:400:ALA:HA	1:X:403:LEU:HD12	1.87	0.55
1:V:263:ASP:OD2	1:V:264:MET:N	2.39	0.55
1:E:452:PRO:HD2	1:E:455:LEU:HD13	1.89	0.55
1:W:375:TYR:OH	1:W:407:GLU:OE2	2.17	0.55
1:N:454:ARG:O	1:N:454:ARG:CG	2.54	0.55
1:U:412:THR:HG21	1:U:461:LEU:HD21	1.89	0.55
1:C:239:TRP:CZ3	1:C:273:LEU:HD23	2.41	0.55
1:R:414:VAL:HG13	1:R:454:ARG:NH1	2.22	0.55
1:M:305:SER:HB3	1:M:343:GLN:HG3	1.88	0.55
1:X:347:ALA:HB3	2:X:600:LDN:CAB	2.37	0.55
1:P:410:ARG:NH1	1:P:419:GLU:OE2	2.39	0.55
1:F:464:LEU:HD23	1:F:489:LEU:HD21	1.88	0.55
1:X:483:LEU:HD12	1:X:486:LYS:HE2	1.89	0.55
1:M:467:MET:SD	1:M:485:ILE:HG23	2.47	0.55
2:F:600:LDN:HAJ	2:F:600:LDN:CBC	2.36	0.55
1:T:452:PRO:HD2	1:T:455:LEU:HD13	1.89	0.55
1:C:315:VAL:HG13	1:C:315:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:285:LEU:O	1:T:289:LEU:HG	2.06	0.55
1:M:251:LEU:HD11	1:M:326:ILE:CD1	2.36	0.55
1:H:434:SER:OG	1:H:436:GLU:HG2	2.07	0.55
1:H:414:VAL:HG13	1:H:454:ARG:CG	2.37	0.55
1:E:298:LEU:HD12	1:E:298:LEU:O	2.07	0.55
1:Q:329:ARG:HD3	1:Q:393:TYR:CD1	2.41	0.55
1:L:431:ASN:OD1	1:L:432:ASP:N	2.40	0.55
1:F:239:TRP:CE3	1:F:273:LEU:HD13	2.41	0.54
1:G:199:ALA:HB2	1:G:276:ILE:HD11	1.88	0.54
1:S:414:VAL:HG21	1:S:454:ARG:HG3	1.89	0.54
1:R:283:GLY:HA2	2:R:600:LDN:CAV	2.37	0.54
1:J:452:PRO:O	1:J:454:ARG:N	2.41	0.54
1:N:295:GLU:HG2	1:N:296:PRO:HD2	1.89	0.54
1:O:315:VAL:HG13	1:O:315:VAL:O	2.06	0.54
1:O:426:TYR:H	1:O:426:TYR:HD2	1.52	0.54
1:E:354:MET:O	1:E:362:LEU:HD12	2.07	0.54
1:Q:467:MET:SD	1:Q:485:ILE:HG23	2.48	0.54
1:N:305:SER:CB	1:N:343:GLN:HG2	2.37	0.54
1:G:199:ALA:HB2	1:G:276:ILE:CD1	2.37	0.54
1:R:198:VAL:O	1:R:202:VAL:HG23	2.07	0.54
1:P:413:ILE:HG23	1:P:416:GLY:CA	2.37	0.54
1:A:291:ARG:NH2	3:A:105:HOH:O	2.41	0.54
1:R:298:LEU:HD12	1:R:298:LEU:O	2.07	0.54
1:Q:195:GLN:OE1	1:Q:262:SER:N	2.39	0.54
1:M:403:LEU:HD23	1:M:472:TRP:CZ2	2.43	0.53
1:P:429:VAL:HG13	1:P:441:VAL:HG21	1.91	0.53
1:A:470:GLU:HA	1:A:473:TYR:CE2	2.43	0.53
1:U:300:LEU:HD22	1:U:493:SER:HA	1.89	0.53
1:N:315:VAL:O	1:N:315:VAL:HG13	2.07	0.53
2:V:600:LDN:CBC	2:V:600:LDN:HAJ	2.38	0.53
1:L:455:LEU:O	1:L:461:LEU:CB	2.56	0.53
1:X:283:GLY:CA	2:X:600:LDN:CAV	2.86	0.53
1:K:347:ALA:HB3	2:K:600:LDN:CAA	2.38	0.53
1:G:418:VAL:HG13	1:G:418:VAL:O	2.08	0.53
1:Q:473:TYR:CZ	1:U:446:GLN:OE1	2.62	0.53
1:D:237:GLN:HG2	1:D:367:ASN:HA	1.89	0.53
1:B:386:ARG:HD2	1:B:389:CYS:HB2	1.90	0.53
1:T:470:GLU:HG2	1:T:473:TYR:CZ	2.44	0.53
1:E:199:ALA:HB2	1:E:276:ILE:CD1	2.38	0.53
1:K:428:VAL:HG23	1:K:429:VAL:HG13	1.91	0.53
1:Q:474:PRO:HB2	1:U:475:ASN:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:464:LEU:CD2	1:P:489:LEU:HD11	2.39	0.53
1:N:239:TRP:CE3	1:N:273:LEU:HD22	2.41	0.53
1:O:455:LEU:HD13	1:O:465:ALA:HB2	1.89	0.53
1:P:467:MET:HE3	1:P:485:ILE:HG23	1.90	0.53
1:W:381:LEU:HA	1:W:435:PHE:CZ	2.44	0.53
1:G:434:SER:O	1:G:435:PHE:C	2.47	0.52
1:G:417:ILE:HG21	1:I:427:ASP:O	2.09	0.52
1:S:197:THR:O	1:S:199:ALA:N	2.42	0.52
1:X:337:LEU:HD21	2:X:600:LDN:CBC	2.38	0.52
1:O:426:TYR:CD2	1:O:426:TYR:N	2.77	0.52
1:L:329:ARG:HD3	1:L:393:TYR:CD1	2.45	0.52
1:V:315:VAL:O	1:V:315:VAL:HG13	2.08	0.52
1:D:239:TRP:CD2	1:D:273:LEU:CD2	2.92	0.52
1:N:300:LEU:CD2	1:N:492:ILE:O	2.57	0.52
1:K:473:TYR:CE1	1:K:475:ASN:HB3	2.44	0.52
1:X:468:MET:O	1:X:472:TRP:CD1	2.62	0.52
1:I:410:ARG:NH1	1:I:419:GLU:OE2	2.42	0.52
1:B:446:GLN:HA	1:B:446:GLN:OE1	2.08	0.52
1:J:412:THR:CG2	1:J:461:LEU:HD11	2.39	0.52
1:R:202:VAL:HG22	1:R:221:TRP:HB2	1.91	0.52
1:G:294:LEU:HD22	1:G:298:LEU:HG	1.92	0.52
1:Q:422:ARG:HD2	1:Q:426:TYR:CD1	2.45	0.52
1:R:315:VAL:O	1:R:315:VAL:HG13	2.08	0.52
1:X:249:VAL:HG11	1:X:251:LEU:HD13	1.90	0.52
1:K:428:VAL:HG23	1:K:441:VAL:HG21	1.91	0.52
1:M:422:ARG:HD2	1:M:426:TYR:CD1	2.45	0.52
1:T:251:LEU:HD21	1:T:349:LEU:HD21	1.91	0.52
1:D:337:LEU:HD21	2:D:600:LDN:HAJ	1.90	0.52
1:O:417:ILE:HG22	1:O:454:ARG:HH11	1.75	0.52
1:G:375:TYR:OH	1:G:407:GLU:OE2	2.22	0.52
1:U:300:LEU:HD13	1:U:460:VAL:CG1	2.36	0.52
1:O:206:GLU:OE1	1:O:218:ARG:NH1	2.42	0.52
1:C:434:SER:OG	1:C:437:ASP:CG	2.47	0.52
1:C:360:ASP:HA	1:C:361:TYR:C	2.30	0.52
1:N:446:GLN:HB2	1:R:395:TRP:CH2	2.42	0.52
1:B:458:ASP:O	1:B:462:SER:HB2	2.09	0.52
1:X:347:ALA:HB3	2:X:600:LDN:CAA	2.39	0.52
1:O:305:SER:HB3	1:O:343:GLN:HG2	1.91	0.52
1:C:386:ARG:HB2	1:C:386:ARG:CZ	2.40	0.52
1:F:464:LEU:O	1:F:468:MET:HG3	2.10	0.52
1:K:375:TYR:OH	1:K:407:GLU:OE2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HD13	1:A:321:GLN:OE1	2.10	0.52
1:R:376:MET:HG2	1:R:380:VAL:CG1	2.39	0.52
1:L:381:LEU:HD11	1:L:438:MET:HB3	1.92	0.52
1:X:455:LEU:HD23	1:X:465:ALA:HB2	1.91	0.51
1:I:236:GLU:HG2	1:I:273:LEU:CD2	2.40	0.51
1:X:241:ARG:NH1	1:X:244:GLU:OE1	2.43	0.51
1:I:373:LYS:HA	1:I:376:MET:HG3	1.92	0.51
1:N:440:LYS:HA	1:N:444:VAL:HG23	1.92	0.51
1:B:460:VAL:HG12	1:B:492:ILE:HG22	1.93	0.51
1:M:328:HIS:O	1:M:329:ARG:HB2	2.10	0.51
1:D:239:TRP:CD2	1:D:273:LEU:HD23	2.45	0.51
1:M:305:SER:HB3	1:M:343:GLN:CG	2.41	0.51
1:M:275:LEU:HD13	1:M:277:THR:HG23	1.92	0.51
1:D:360:ASP:HA	1:D:361:TYR:C	2.30	0.51
1:S:215:GLU:OE2	1:X:431:ASN:HB3	2.10	0.51
1:A:298:LEU:HD12	1:A:298:LEU:O	2.10	0.51
1:U:198:VAL:HG22	1:U:221:TRP:CZ2	2.46	0.51
1:X:399:TRP:NE1	1:X:403:LEU:HD11	2.26	0.51
1:K:473:TYR:HE1	1:K:475:ASN:HB3	1.76	0.51
1:B:251:LEU:HD21	1:B:326:ILE:CD1	2.41	0.51
1:N:198:VAL:O	1:N:202:VAL:HG23	2.11	0.51
1:Q:315:VAL:HG13	1:Q:315:VAL:O	2.10	0.51
1:F:477:SER:CB	1:J:382:ASP:HB3	2.41	0.51
1:M:455:LEU:HD22	1:M:461:LEU:HB3	1.93	0.51
1:B:467:MET:HE1	1:B:489:LEU:CD1	2.28	0.51
1:N:239:TRP:CZ3	1:N:273:LEU:CD2	2.93	0.51
1:T:315:VAL:CG1	1:T:315:VAL:O	2.59	0.51
1:O:304:VAL:HA	1:O:489:LEU:HD13	1.93	0.51
1:E:480:LEU:HD22	1:E:484:ARG:HG2	1.92	0.51
1:V:295:GLU:OE2	1:V:297:HIS:HB3	2.10	0.51
1:E:414:VAL:HG11	1:E:454:ARG:HG2	1.93	0.51
1:B:467:MET:SD	1:B:485:ILE:HG23	2.51	0.51
1:S:459:PRO:O	1:S:460:VAL:C	2.49	0.51
1:W:329:ARG:HD3	1:W:393:TYR:CD1	2.45	0.51
1:R:455:LEU:HD23	1:R:465:ALA:HB2	1.92	0.51
1:A:202:VAL:HG22	1:A:221:TRP:HB2	1.93	0.51
1:C:289:LEU:CD2	1:C:294:LEU:HD11	2.40	0.51
1:U:351:LEU:HD21	1:U:369:ARG:O	2.10	0.51
1:R:467:MET:HE1	1:R:489:LEU:HD21	1.92	0.51
1:O:360:ASP:HA	1:O:361:TYR:C	2.31	0.51
1:X:283:GLY:HA3	2:X:600:LDN:CAG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:360:ASP:HA	1:N:361:TYR:C	2.31	0.50
1:P:430:PRO:O	1:P:431:ASN:O	2.29	0.50
1:T:206:GLU:OE2	1:T:218:ARG:NH1	2.44	0.50
1:E:415:ASN:O	1:E:417:ILE:HD12	2.11	0.50
1:U:451:ILE:HD12	1:U:469:ARG:HE	1.76	0.50
1:B:412:THR:HG21	1:B:461:LEU:HD11	1.94	0.50
1:S:197:THR:O	1:S:200:ARG:N	2.45	0.50
1:B:317:ILE:HG21	1:C:252:ARG:HD2	1.93	0.50
1:S:460:VAL:HG12	1:S:461:LEU:CD2	2.41	0.50
1:C:295:GLU:HG2	1:C:296:PRO:HD2	1.92	0.50
1:H:250:LEU:HD23	1:H:321:GLN:HA	1.92	0.50
1:G:417:ILE:CG2	1:I:427:ASP:O	2.59	0.50
1:V:417:ILE:HG22	1:V:454:ARG:HH11	1.77	0.50
1:P:252:ARG:HB3	1:P:252:ARG:CZ	2.42	0.50
1:F:315:VAL:O	1:F:315:VAL:HG13	2.11	0.50
2:T:600:LDN:HAJ	2:T:600:LDN:CBC	2.41	0.50
1:H:428:VAL:HG23	1:H:429:VAL:HG13	1.94	0.50
1:I:417:ILE:CG2	1:I:418:VAL:N	2.75	0.50
1:B:317:ILE:HG21	1:C:252:ARG:CD	2.42	0.50
1:L:322:GLY:O	1:L:323:LYS:HB3	2.12	0.50
1:R:434:SER:O	1:R:436:GLU:N	2.45	0.50
1:F:289:LEU:HD21	1:F:294:LEU:HD11	1.94	0.50
1:T:451:ILE:HD11	1:T:472:TRP:HZ3	1.77	0.50
1:X:235:ASP:OD1	1:X:369:ARG:HD3	2.11	0.49
1:I:446:GLN:O	1:I:446:GLN:HG3	2.12	0.49
1:B:386:ARG:CB	1:B:386:ARG:NH1	2.75	0.49
1:K:337:LEU:HD11	2:K:600:LDN:CAJ	2.42	0.49
1:L:451:ILE:HG23	1:L:455:LEU:HD13	1.94	0.49
1:H:400:ALA:HA	1:H:403:LEU:HD12	1.94	0.49
1:S:360:ASP:HA	1:S:361:TYR:C	2.32	0.49
1:C:197:THR:O	1:C:197:THR:HG22	2.11	0.49
1:V:434:SER:OG	1:V:437:ASP:OD2	2.30	0.49
1:C:434:SER:HG	1:C:437:ASP:CG	2.15	0.49
1:M:275:LEU:HD13	1:M:277:THR:CG2	2.43	0.49
1:X:467:MET:HE3	1:X:485:ILE:HG23	1.94	0.49
1:J:252:ARG:HD3	1:W:486:LYS:NZ	2.26	0.49
1:U:315:VAL:HG13	1:U:315:VAL:O	2.11	0.49
1:S:217:TRP:CH2	1:X:430:PRO:CB	2.84	0.49
1:E:428:VAL:HG23	1:E:429:VAL:HG13	1.94	0.49
1:L:315:VAL:HG13	1:L:315:VAL:O	2.11	0.49
1:S:315:VAL:HG13	1:S:315:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:LEU:HD11	1:C:326:ILE:CD1	2.42	0.49
1:A:490:GLN:O	1:A:493:SER:N	2.38	0.49
1:X:455:LEU:HB3	1:X:465:ALA:HB2	1.94	0.49
1:T:417:ILE:O	1:T:454:ARG:NH1	2.46	0.49
1:G:359:SER:O	1:G:361:TYR:N	2.46	0.49
1:W:315:VAL:O	1:W:315:VAL:HG13	2.12	0.49
2:D:600:LDN:HAJ	2:D:600:LDN:CBC	2.43	0.49
1:W:205:VAL:HG11	1:W:218:ARG:HH22	1.78	0.49
1:P:412:THR:O	1:P:418:VAL:HG23	2.13	0.49
1:H:386:ARG:NH1	1:I:446:GLN:HB2	2.28	0.49
1:S:452:PRO:HB2	1:S:455:LEU:HD13	1.95	0.49
1:C:425:PHE:O	1:C:429:VAL:HG22	2.13	0.49
1:X:283:GLY:HA2	2:X:600:LDN:CAF	2.43	0.48
1:M:447:GLN:OE1	1:Q:454:ARG:HA	2.13	0.48
1:E:205:VAL:HG21	1:E:220:LEU:HG	1.93	0.48
1:B:452:PRO:HB2	1:B:454:ARG:HB3	1.95	0.48
1:W:467:MET:CE	1:W:485:ILE:HG23	2.44	0.48
1:P:206:GLU:CB	1:P:218:ARG:NH1	2.76	0.48
1:T:197:THR:CG2	1:T:200:ARG:CB	2.92	0.48
1:A:361:TYR:CZ	1:M:0:MET:HA	2.48	0.48
1:R:207:CYS:HB2	1:R:217:TRP:CZ2	2.49	0.48
1:B:332:LYS:HE3	1:B:334:ARG:HB2	1.94	0.48
1:L:291:ARG:NH2	2:L:600:LDN:HNAU	2.10	0.48
1:P:315:VAL:HG13	1:P:315:VAL:O	2.13	0.48
1:O:490:GLN:OE1	1:T:341:ASN:ND2	2.47	0.48
1:H:434:SER:O	1:H:435:PHE:C	2.51	0.48
1:G:452:PRO:HB2	1:G:455:LEU:HD13	1.95	0.48
1:H:265:THR:HG23	1:H:266:SER:N	2.28	0.48
1:K:198:VAL:HG13	1:K:221:TRP:CZ2	2.48	0.48
1:G:317:ILE:HB	1:G:323:LYS:HG3	1.94	0.48
1:K:428:VAL:HG21	1:K:441:VAL:CG1	2.44	0.48
1:P:354:MET:HA	1:P:390:PHE:CE1	2.48	0.48
1:T:250:LEU:HD11	1:T:252:ARG:NH1	2.29	0.48
1:S:456:ALA:HA	1:S:462:SER:OG	2.13	0.48
1:R:403:LEU:HD22	1:R:449:PRO:HG2	1.94	0.48
1:M:198:VAL:HG13	1:M:221:TRP:NE1	2.28	0.48
1:A:315:VAL:O	1:A:315:VAL:HG13	2.12	0.48
1:T:418:VAL:O	1:T:418:VAL:HG13	2.14	0.48
1:M:236:GLU:HG2	1:M:273:LEU:CD1	2.41	0.48
1:D:198:VAL:O	1:D:202:VAL:N	2.44	0.48
1:C:486:LYS:HE2	1:C:490:GLN:HE22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:362:LEU:HD13	1:Q:390:PHE:HB2	1.96	0.48
1:T:414:VAL:O	1:T:416:GLY:N	2.47	0.48
1:B:460:VAL:HG12	1:B:492:ILE:CG2	2.44	0.48
1:V:391:GLU:OE2	1:V:394:LYS:NZ	2.43	0.48
1:G:245:ILE:HG21	1:G:349:LEU:HD23	1.95	0.48
1:D:316:GLU:HG3	1:D:324:PRO:HA	1.95	0.48
2:C:600:LDN:CBC	2:C:600:LDN:HAJ	2.43	0.48
1:E:315:VAL:HG13	1:E:315:VAL:O	2.13	0.48
1:N:446:GLN:CD	1:R:395:TRP:HZ3	2.17	0.48
1:Q:264:MET:HG3	1:Q:273:LEU:HD22	1.95	0.48
1:T:245:ILE:HG21	1:T:349:LEU:HD23	1.96	0.48
1:L:325:ALA:N	1:L:355:HIS:O	2.40	0.48
1:D:305:SER:HB3	1:D:343:GLN:HG2	1.96	0.48
1:N:446:GLN:CB	1:R:395:TRP:CH2	2.97	0.48
1:F:329:ARG:HD3	1:F:393:TYR:CD1	2.49	0.48
1:H:258:GLY:O	1:H:277:THR:HB	2.14	0.48
1:F:207:CYS:HB2	1:F:217:TRP:CZ2	2.48	0.48
1:Q:237:GLN:CD	1:Q:368:PRO:HD3	2.34	0.48
1:I:432:ASP:O	1:I:433:PRO:C	2.52	0.47
1:I:315:VAL:O	1:I:315:VAL:HG13	2.14	0.47
1:M:403:LEU:HD22	1:M:449:PRO:HG2	1.95	0.47
1:H:316:GLU:HG2	1:H:324:PRO:HA	1.96	0.47
1:F:237:GLN:CD	1:F:368:PRO:HD3	2.34	0.47
1:I:400:ALA:O	1:I:404:VAL:HG23	2.14	0.47
1:V:298:LEU:HD12	1:V:302:LEU:HD13	1.96	0.47
1:L:467:MET:HE1	1:L:489:LEU:HD21	1.95	0.47
1:H:360:ASP:HA	1:H:361:TYR:C	2.35	0.47
1:T:386:ARG:H	1:T:386:ARG:HE	1.62	0.47
1:U:488:THR:O	1:U:491:LYS:HB2	2.14	0.47
1:N:400:ALA:O	1:N:404:VAL:HG23	2.14	0.47
1:Q:198:VAL:HG22	1:Q:221:TRP:CZ2	2.49	0.47
1:F:467:MET:SD	1:F:485:ILE:HG23	2.54	0.47
1:S:230:ILE:CG2	1:S:272:GLN:OE1	2.62	0.47
1:B:315:VAL:HG13	1:B:315:VAL:O	2.14	0.47
1:A:304:VAL:HA	1:A:489:LEU:HD13	1.97	0.47
1:E:467:MET:SD	1:E:485:ILE:HG23	2.55	0.47
1:I:467:MET:CE	1:I:485:ILE:HG23	2.44	0.47
1:O:465:ALA:HA	1:O:468:MET:HE3	1.96	0.47
1:E:455:LEU:HD23	1:E:465:ALA:HB2	1.97	0.47
1:F:458:ASP:CB	1:F:461:LEU:HD12	2.44	0.47
2:U:600:LDN:HAJ	2:U:600:LDN:CBC	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:312:HIS:O	1:T:323:LYS:HE3	2.15	0.47
1:I:446:GLN:NE2	1:I:446:GLN:HA	2.29	0.47
1:I:491:LYS:O	1:I:492:ILE:C	2.52	0.47
1:S:381:LEU:HD11	1:S:438:MET:HB3	1.96	0.47
1:B:248:THR:C	1:C:321:GLN:NE2	2.68	0.47
1:N:298:LEU:HD12	1:N:298:LEU:O	2.14	0.47
1:O:256:ILE:CD1	1:O:312:HIS:HD1	2.28	0.47
1:K:347:ALA:CB	2:K:600:LDN:CAA	2.93	0.47
1:J:283:GLY:HA2	2:J:600:LDN:CAM	2.45	0.47
1:A:195:GLN:OE1	1:A:262:SER:N	2.46	0.47
1:Q:440:LYS:HA	1:Q:444:VAL:CG2	2.45	0.47
1:B:328:HIS:O	1:B:329:ARG:HB2	2.15	0.47
1:F:332:LYS:HD3	1:F:372:THR:OG1	2.15	0.47
1:R:304:VAL:HA	1:R:489:LEU:HD13	1.97	0.47
1:X:198:VAL:HA	1:X:221:TRP:NE1	2.30	0.47
1:X:317:ILE:HD12	1:X:323:LYS:HG2	1.95	0.47
1:R:403:LEU:HD23	1:R:472:TRP:NE1	2.30	0.47
1:L:467:MET:CE	1:L:489:LEU:HD21	2.45	0.47
1:S:202:VAL:HG22	1:S:221:TRP:HB2	1.97	0.47
1:E:283:GLY:HA2	2:E:600:LDN:CAV	2.45	0.47
1:T:386:ARG:NE	1:T:386:ARG:H	2.13	0.46
1:X:302:LEU:HD22	1:X:344:CYS:SG	2.55	0.46
1:B:202:VAL:HG22	1:B:221:TRP:HB2	1.97	0.46
1:G:447:GLN:OE1	1:I:454:ARG:HA	2.14	0.46
1:K:305:SER:HA	1:K:308:CYS:SG	2.55	0.46
1:F:241:ARG:HD3	1:F:365:GLY:HA3	1.96	0.46
1:I:467:MET:SD	1:I:485:ILE:HG23	2.55	0.46
1:P:195:GLN:CG	1:P:261:ALA:CB	2.92	0.46
1:N:446:GLN:CB	1:R:395:TRP:HH2	2.26	0.46
1:K:332:LYS:HD3	1:K:372:THR:OG1	2.15	0.46
1:J:227:ALA:CB	2:J:600:LDN:HAD	2.44	0.46
1:I:446:GLN:HE21	1:I:446:GLN:HA	1.79	0.46
1:T:197:THR:HG23	1:T:200:ARG:CB	2.45	0.46
1:C:381:LEU:HD23	1:C:435:PHE:CE1	2.50	0.46
1:G:293:THR:OG1	1:G:413:ILE:HD11	2.15	0.46
1:W:464:LEU:CD1	1:W:489:LEU:HD21	2.45	0.46
1:I:332:LYS:HE3	1:I:334:ARG:HB2	1.98	0.46
1:S:428:VAL:HG11	1:S:447:GLN:OE1	2.15	0.46
1:V:418:VAL:HA	1:V:454:ARG:HH12	1.81	0.46
1:M:354:MET:HB2	1:M:363:ASP:HB3	1.97	0.46
1:L:464:LEU:O	1:L:468:MET:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ILE:HG22	1:A:365:GLY:O	2.15	0.46
1:Q:317:ILE:HD12	1:Q:323:LYS:HD3	1.97	0.46
1:O:455:LEU:HD22	1:O:461:LEU:HB3	1.97	0.46
1:G:379:GLU:HG3	1:G:385:ILE:HG23	1.97	0.46
1:R:315:VAL:CG1	1:R:315:VAL:O	2.64	0.46
1:R:207:CYS:HB2	1:R:217:TRP:CE2	2.51	0.46
1:W:403:LEU:HD22	1:W:424:PRO:HB3	1.97	0.46
2:W:600:LDN:CBC	2:W:600:LDN:HAJ	2.46	0.46
1:O:256:ILE:HD12	1:O:312:HIS:HD1	1.80	0.46
1:M:245:ILE:HG21	1:M:349:LEU:HD23	1.98	0.46
1:E:198:VAL:O	1:E:202:VAL:HG23	2.16	0.46
1:E:206:GLU:CB	3:E:113:HOH:O	2.63	0.46
1:M:204:LEU:HB3	1:M:217:TRP:CE3	2.50	0.46
1:H:204:LEU:HD13	1:H:217:TRP:CG	2.51	0.46
1:B:464:LEU:HD23	1:B:489:LEU:HD21	1.98	0.46
1:R:251:LEU:HD21	1:R:349:LEU:CD2	2.45	0.46
1:B:409:ALA:HB2	1:B:468:MET:CE	2.45	0.46
1:N:300:LEU:HD22	1:N:492:ILE:O	2.15	0.46
1:R:414:VAL:HG21	1:R:454:ARG:CG	2.46	0.46
1:C:315:VAL:CG1	1:C:315:VAL:O	2.63	0.46
1:B:315:VAL:O	1:B:323:LYS:NZ	2.49	0.46
1:H:245:ILE:HG21	1:H:349:LEU:HD23	1.97	0.46
1:K:315:VAL:O	1:K:315:VAL:HG13	2.15	0.46
1:N:403:LEU:HD23	1:N:472:TRP:NE1	2.30	0.46
1:X:283:GLY:CA	2:X:600:LDN:CAE	2.93	0.46
1:X:281:GLU:O	2:X:600:LDN:HAH	2.16	0.46
1:X:483:LEU:CD1	1:X:487:LYS:HE3	2.43	0.46
1:M:405:LEU:HD11	1:M:467:MET:HE3	1.97	0.46
1:B:293:THR:CB	1:B:413:ILE:HD11	2.46	0.46
1:T:315:VAL:O	1:T:323:LYS:NZ	2.48	0.46
1:W:245:ILE:HG21	1:W:349:LEU:HD23	1.98	0.46
1:D:315:VAL:HG13	1:D:315:VAL:O	2.15	0.46
1:H:414:VAL:CG1	1:H:454:ARG:HG2	2.46	0.46
1:W:420:ASP:OD2	1:W:422:ARG:CZ	2.64	0.46
1:G:460:VAL:HA	1:G:492:ILE:HG21	1.98	0.46
1:X:283:GLY:HA3	2:X:600:LDN:CAE	2.46	0.45
1:X:337:LEU:CD1	2:X:600:LDN:HAJ	2.45	0.45
1:D:317:ILE:N	1:D:317:ILE:CD1	2.75	0.45
1:L:382:ASP:CG	1:P:477:SER:HG	2.17	0.45
1:R:427:ASP:C	1:T:417:ILE:HD12	2.37	0.45
1:X:335:ASN:HA	2:X:600:LDN:HAA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:LEU:HG	1:F:369:ARG:HG2	1.97	0.45
1:F:272:GLN:O	1:F:273:LEU:HD23	2.16	0.45
1:P:409:ALA:HB1	1:P:455:LEU:HD22	1.97	0.45
1:B:305:SER:CB	1:B:343:GLN:HG2	2.46	0.45
1:H:414:VAL:HG13	1:H:454:ARG:HG2	1.98	0.45
1:O:315:VAL:CG1	1:O:315:VAL:O	2.64	0.45
2:E:600:LDN:CBC	2:E:600:LDN:HAJ	2.46	0.45
1:T:317:ILE:HG22	1:T:322:GLY:HA2	1.98	0.45
1:M:305:SER:CB	1:M:343:GLN:CG	2.95	0.45
1:F:289:LEU:CD2	1:F:294:LEU:HD11	2.46	0.45
1:F:328:HIS:O	1:F:329:ARG:HB2	2.15	0.45
1:B:467:MET:SD	1:B:489:LEU:HG	2.56	0.45
1:D:239:TRP:CE2	1:D:273:LEU:HD23	2.50	0.45
1:C:293:THR:CB	1:C:413:ILE:HD11	2.47	0.45
1:H:315:VAL:O	1:H:315:VAL:HG13	2.15	0.45
1:X:405:LEU:HD11	1:X:467:MET:HE2	1.99	0.45
1:O:451:ILE:HG23	1:O:455:LEU:HD12	1.98	0.45
1:K:199:ALA:CB	1:K:276:ILE:HD11	2.44	0.45
1:F:355:HIS:NE2	1:F:360:ASP:OD2	2.47	0.45
1:J:403:LEU:HD23	1:J:472:TRP:CZ2	2.52	0.45
1:M:484:ARG:HA	1:M:484:ARG:HD2	1.77	0.45
1:X:455:LEU:HD22	1:X:465:ALA:CB	2.39	0.45
1:P:195:GLN:HG2	1:P:261:ALA:CA	2.46	0.45
1:N:315:VAL:CG1	1:N:315:VAL:O	2.64	0.45
1:R:467:MET:CE	1:R:489:LEU:HD21	2.47	0.45
1:E:320:THR:HG22	1:E:321:GLN:N	2.30	0.45
1:R:357:GLN:O	1:R:358:GLY:C	2.55	0.45
1:C:451:ILE:O	1:C:452:PRO:C	2.53	0.45
1:B:435:PHE:CD2	1:B:435:PHE:O	2.70	0.45
1:O:337:LEU:HD21	2:O:600:LDN:CBC	2.47	0.45
1:T:489:LEU:O	1:T:490:GLN:C	2.55	0.45
1:G:485:ILE:O	1:G:489:LEU:HD12	2.17	0.45
1:B:480:LEU:HD22	1:B:484:ARG:HG2	1.99	0.45
1:D:239:TRP:CD2	1:D:273:LEU:HD22	2.52	0.45
1:K:427:ASP:OD1	1:K:428:VAL:HG13	2.16	0.45
1:A:257:LEU:HD13	1:A:337:LEU:HD13	1.99	0.45
1:N:265:THR:HG21	1:N:274:TRP:CE2	2.52	0.45
1:P:351:LEU:HD21	1:P:369:ARG:O	2.17	0.45
1:K:375:TYR:HD1	1:K:403:LEU:HD12	1.82	0.44
2:O:600:LDN:CBC	2:O:600:LDN:HAJ	2.47	0.44
2:P:600:LDN:HAM	2:P:600:LDN:HAF	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:414:VAL:HG21	1:R:454:ARG:HG3	1.98	0.44
1:E:281:GLU:O	2:E:600:LDN:HAH	2.18	0.44
1:I:467:MET:HE1	1:I:489:LEU:CD1	2.41	0.44
1:Q:251:LEU:HD11	1:Q:326:ILE:CD1	2.48	0.44
1:M:381:LEU:HA	1:M:435:PHE:CZ	2.52	0.44
1:F:252:ARG:O	1:F:252:ARG:HG2	2.16	0.44
1:U:455:LEU:HD22	1:U:461:LEU:HB3	1.99	0.44
1:N:458:ASP:CB	1:N:461:LEU:HD12	2.47	0.44
1:A:273:LEU:HD22	1:A:273:LEU:N	2.32	0.44
1:O:283:GLY:CA	2:O:600:LDN:CAV	2.94	0.44
1:S:258:GLY:O	1:S:277:THR:HB	2.17	0.44
1:C:386:ARG:NH1	1:C:386:ARG:HB2	2.33	0.44
1:R:405:LEU:HD11	1:R:467:MET:CE	2.47	0.44
1:E:381:LEU:HD23	1:E:435:PHE:CE1	2.52	0.44
1:E:357:GLN:HG2	1:E:357:GLN:O	2.17	0.44
1:E:467:MET:HE1	1:E:489:LEU:CD1	2.39	0.44
1:U:461:LEU:HA	1:U:464:LEU:HD13	1.99	0.44
1:S:414:VAL:CG1	1:S:461:LEU:HD12	2.47	0.44
1:D:239:TRP:CE3	1:D:273:LEU:HD23	2.52	0.44
1:X:315:VAL:HG13	1:X:315:VAL:O	2.17	0.44
1:B:251:LEU:HA	1:B:251:LEU:HD23	1.84	0.44
1:K:198:VAL:HG13	1:K:221:TRP:CH2	2.52	0.44
1:H:304:VAL:HA	1:H:489:LEU:HD13	1.99	0.44
1:B:245:ILE:HG21	1:B:349:LEU:HD23	2.00	0.44
1:X:386:ARG:HG2	1:X:388:ASP:OD1	2.17	0.44
1:X:245:ILE:HG21	1:X:349:LEU:HD23	2.00	0.44
1:P:245:ILE:HG21	1:P:349:LEU:HD23	1.99	0.44
1:O:198:VAL:O	1:O:202:VAL:CG2	2.55	0.44
1:N:205:VAL:HG11	1:N:218:ARG:NH2	2.33	0.44
1:G:432:ASP:O	1:G:433:PRO:C	2.55	0.44
1:C:414:VAL:O	1:C:416:GLY:N	2.51	0.44
1:C:431:ASN:OD1	1:C:431:ASN:N	2.51	0.44
1:D:245:ILE:HG21	1:D:349:LEU:HD23	1.99	0.44
1:Q:264:MET:HG3	1:Q:273:LEU:HD21	1.99	0.44
1:R:251:LEU:HD11	1:R:326:ILE:CD1	2.48	0.44
1:P:410:ARG:NH2	1:P:426:TYR:OH	2.50	0.44
1:V:417:ILE:HA	1:V:417:ILE:HD12	1.82	0.44
1:B:337:LEU:HD21	2:B:600:LDN:CBC	2.48	0.44
1:I:312:HIS:O	1:I:323:LYS:NZ	2.44	0.44
1:H:414:VAL:HG13	1:H:454:ARG:HD2	2.00	0.44
1:R:467:MET:CE	1:R:485:ILE:HG23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:206:GLU:HG2	1:Q:208:VAL:HG13	2.00	0.44
1:L:295:GLU:HG2	1:L:296:PRO:CD	2.47	0.44
2:P:600:LDN:HAQA	2:P:600:LDN:HAH	1.82	0.44
1:L:480:LEU:HD22	1:L:484:ARG:HG2	2.00	0.44
1:I:422:ARG:HD2	1:I:426:TYR:CD1	2.53	0.43
1:M:315:VAL:O	1:M:315:VAL:HG13	2.17	0.43
1:X:455:LEU:HB3	1:X:465:ALA:CB	2.48	0.43
1:V:315:VAL:O	1:V:315:VAL:CG1	2.65	0.43
1:L:292:GLN:NE2	2:Q:600:LDN:HAOA	2.33	0.43
1:M:386:ARG:HG2	1:M:388:ASP:OD1	2.19	0.43
1:A:475:ASN:HB2	1:E:474:PRO:HB2	1.99	0.43
1:J:315:VAL:HG13	1:J:315:VAL:O	2.18	0.43
1:C:454:ARG:CG	1:C:454:ARG:O	2.66	0.43
1:I:285:LEU:O	1:I:289:LEU:HG	2.18	0.43
1:Q:202:VAL:HG22	1:Q:221:TRP:HB2	2.00	0.43
1:R:403:LEU:HD23	1:R:472:TRP:CE2	2.53	0.43
1:O:289:LEU:HD11	1:O:408:ILE:HA	1.98	0.43
1:J:401:PHE:O	1:J:404:VAL:HG12	2.18	0.43
1:M:462:SER:O	1:M:465:ALA:HB3	2.18	0.43
1:G:414:VAL:O	1:G:416:GLY:N	2.51	0.43
1:W:414:VAL:CG2	1:W:454:ARG:CZ	2.96	0.43
1:S:275:LEU:HD13	1:S:277:THR:CG2	2.46	0.43
1:X:235:ASP:OD1	1:X:369:ARG:CD	2.67	0.43
1:W:420:ASP:OD2	1:W:422:ARG:NH2	2.51	0.43
1:G:239:TRP:CE3	1:G:273:LEU:HD12	2.53	0.43
2:A:600:LDN:HAJ	2:A:600:LDN:CBC	2.49	0.43
1:F:486:LYS:HG2	1:F:490:GLN:HE22	1.83	0.43
1:E:405:LEU:HD11	1:E:467:MET:CE	2.48	0.43
1:G:233:SER:OG	1:K:211:GLY:HA2	2.19	0.43
1:N:461:LEU:HD23	1:N:464:LEU:CD1	2.46	0.43
1:U:198:VAL:HG13	1:U:221:TRP:CE2	2.53	0.43
1:E:218:ARG:NH1	3:E:113:HOH:O	2.52	0.43
1:S:443:CYS:O	1:S:446:GLN:OE1	2.36	0.43
1:Q:244:GLU:O	1:Q:248:THR:HB	2.19	0.43
2:G:600:LDN:HAQA	2:G:600:LDN:HAH	1.77	0.43
1:F:454:ARG:CG	1:F:454:ARG:O	2.66	0.43
1:L:245:ILE:HG21	1:L:349:LEU:HD23	2.01	0.43
1:B:300:LEU:HD23	1:B:489:LEU:HD22	2.00	0.43
1:G:273:LEU:N	1:G:273:LEU:HD22	2.33	0.43
1:A:366:ASN:ND2	1:M:263:ASP:OD2	2.52	0.43
1:K:381:LEU:HD23	1:K:435:PHE:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:315:VAL:O	1:Q:315:VAL:CG1	2.67	0.43
1:R:316:GLU:CD	1:R:357:GLN:H	2.22	0.43
1:W:332:LYS:HE3	1:W:334:ARG:HB2	2.01	0.43
1:G:198:VAL:O	1:G:202:VAL:N	2.51	0.43
1:E:239:TRP:CE3	1:E:273:LEU:HD13	2.53	0.43
1:C:239:TRP:CE3	1:C:273:LEU:HD22	2.53	0.43
1:I:451:ILE:HA	1:I:452:PRO:HD2	1.83	0.43
1:F:283:GLY:HA2	2:F:600:LDN:CAV	2.49	0.43
1:N:381:LEU:HA	1:N:435:PHE:CZ	2.53	0.43
1:M:305:SER:CB	1:M:343:GLN:HG3	2.48	0.43
1:H:418:VAL:HA	1:H:454:ARG:NH1	2.34	0.43
1:F:237:GLN:OE1	1:F:366:ASN:O	2.36	0.43
1:E:258:GLY:O	1:E:277:THR:HB	2.19	0.43
1:U:405:LEU:HD11	1:U:467:MET:CE	2.48	0.43
1:U:405:LEU:HD11	1:U:467:MET:HE3	2.01	0.43
1:T:205:VAL:HG21	1:T:220:LEU:HD23	1.99	0.43
1:G:315:VAL:O	1:G:315:VAL:HG13	2.19	0.43
1:P:283:GLY:CA	2:P:600:LDN:CAF	2.96	0.42
2:F:600:LDN:HAH	2:F:600:LDN:HAQA	1.82	0.42
1:W:422:ARG:HD2	1:W:426:TYR:CD1	2.52	0.42
1:L:364:ILE:HG22	1:L:365:GLY:O	2.18	0.42
1:T:373:LYS:HD3	1:T:433:PRO:O	2.19	0.42
1:E:252:ARG:HB3	1:E:252:ARG:NH1	2.33	0.42
1:D:459:PRO:CD	1:D:460:VAL:H	2.32	0.42
1:R:431:ASN:O	1:R:433:PRO:HD3	2.18	0.42
1:N:205:VAL:HG21	1:N:220:LEU:HG	2.00	0.42
1:K:245:ILE:HG21	1:K:349:LEU:HD23	2.01	0.42
1:H:465:ALA:O	1:H:469:ARG:HG2	2.19	0.42
1:E:465:ALA:HA	1:E:468:MET:HE3	2.01	0.42
2:L:600:LDN:HAJ	2:L:600:LDN:CBC	2.48	0.42
1:R:316:GLU:OE1	1:R:357:GLN:HB2	2.20	0.42
1:D:0:MET:O	1:D:196:ARG:N	2.52	0.42
1:P:457:ALA:O	1:P:458:ASP:CB	2.67	0.42
1:A:451:ILE:O	1:A:452:PRO:C	2.56	0.42
1:M:282:HIS:HA	1:M:291:ARG:NH2	2.34	0.42
1:V:431:ASN:O	1:V:433:PRO:HD3	2.19	0.42
2:N:600:LDN:HAQA	2:N:600:LDN:HAH	1.75	0.42
2:X:600:LDN:HAQA	2:X:600:LDN:HAH	1.91	0.42
1:O:283:GLY:HA3	2:O:600:LDN:CAE	2.50	0.42
1:A:221:TRP:NE1	1:A:222:HIS:CE1	2.87	0.42
1:Q:382:ASP:HB3	1:Q:384:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:205:VAL:HG12	1:M:206:GLU:HG3	2.02	0.42
1:U:289:LEU:CD2	1:U:294:LEU:HD11	2.50	0.42
1:G:355:HIS:C	1:G:355:HIS:ND1	2.72	0.42
1:J:412:THR:HG21	1:J:461:LEU:HD21	2.00	0.42
1:N:300:LEU:HD21	1:N:492:ILE:O	2.19	0.42
2:W:600:LDN:NAS	2:W:600:LDN:HAJ	2.34	0.42
1:J:403:LEU:HD23	1:J:472:TRP:CE2	2.54	0.42
1:L:316:GLU:CD	1:L:357:GLN:H	2.23	0.42
1:R:258:GLY:O	1:R:277:THR:HB	2.20	0.42
1:F:377:ALA:O	1:F:381:LEU:HD12	2.20	0.42
1:O:405:LEU:HD11	1:O:467:MET:CE	2.50	0.42
1:N:237:GLN:HG2	1:N:367:ASN:HA	2.01	0.42
1:H:244:GLU:O	1:H:248:THR:HB	2.18	0.42
1:U:245:ILE:HG21	1:U:349:LEU:HD23	2.00	0.42
1:D:466:GLN:O	1:D:470:GLU:HG3	2.20	0.42
1:I:467:MET:CE	1:I:489:LEU:HD21	2.49	0.42
1:A:315:VAL:O	1:A:315:VAL:CG1	2.68	0.42
1:N:473:TYR:CE1	1:R:384:GLN:NE2	2.88	0.42
1:R:360:ASP:N	1:R:360:ASP:OD1	2.48	0.42
1:M:312:HIS:O	1:M:323:LYS:CE	2.67	0.42
1:L:475:ASN:HB2	1:P:474:PRO:HB3	2.01	0.42
1:Q:328:HIS:O	1:Q:329:ARG:HB2	2.20	0.42
2:D:600:LDN:HAF	2:D:600:LDN:HAM	1.80	0.42
1:S:315:VAL:CG1	1:S:315:VAL:O	2.68	0.42
1:T:386:ARG:NE	1:T:392:SER:OG	2.52	0.42
1:T:425:PHE:O	1:T:429:VAL:HG22	2.19	0.42
1:H:373:LYS:HA	1:H:376:MET:HG3	2.01	0.42
1:W:467:MET:SD	1:W:489:LEU:HG	2.60	0.42
1:D:252:ARG:NH1	1:I:317:ILE:HD13	2.35	0.42
1:J:337:LEU:HD22	2:J:600:LDN:NAT	2.34	0.42
1:A:452:PRO:C	1:A:454:ARG:H	2.23	0.42
1:G:244:GLU:O	1:G:248:THR:HB	2.19	0.42
1:U:246:TYR:CD1	1:U:259:PHE:HB2	2.55	0.42
1:A:295:GLU:HG2	1:A:296:PRO:HD2	2.02	0.42
1:G:484:ARG:NH1	3:G:10:HOH:O	2.51	0.42
1:B:300:LEU:HD11	1:B:493:SER:HA	2.02	0.42
2:P:600:LDN:HAJ	2:P:600:LDN:CBC	2.49	0.42
1:S:257:LEU:HD13	1:S:337:LEU:HD13	2.01	0.42
1:W:202:VAL:HG22	1:W:221:TRP:HB2	2.02	0.42
1:R:434:SER:O	1:R:435:PHE:C	2.58	0.41
1:P:422:ARG:CB	1:P:426:TYR:CD1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:376:MET:HG2	1:R:380:VAL:HG11	2.01	0.41
1:J:252:ARG:HD3	1:W:486:LYS:CE	2.50	0.41
1:U:315:VAL:CG1	1:U:315:VAL:O	2.68	0.41
1:L:282:HIS:O	1:L:291:ARG:NH2	2.53	0.41
1:P:409:ALA:HB1	1:P:455:LEU:CD2	2.50	0.41
1:L:475:ASN:HB2	1:P:474:PRO:CB	2.49	0.41
1:R:427:ASP:OD1	1:R:428:VAL:HG13	2.21	0.41
1:S:275:LEU:CD1	1:S:277:THR:CG2	2.98	0.41
1:J:280:HIS:O	2:J:600:LDN:HAM	2.20	0.41
1:W:315:VAL:CG1	1:W:315:VAL:O	2.68	0.41
1:L:251:LEU:HD21	1:L:349:LEU:HD21	2.02	0.41
1:E:252:ARG:CZ	1:E:252:ARG:HB3	2.50	0.41
1:S:245:ILE:HG21	1:S:349:LEU:HD23	2.00	0.41
1:V:245:ILE:HG21	1:V:349:LEU:HD23	2.03	0.41
1:E:245:ILE:HG21	1:E:349:LEU:HD23	2.02	0.41
1:D:236:GLU:HG2	1:D:273:LEU:HD13	2.01	0.41
1:C:239:TRP:CD2	1:C:273:LEU:CD2	3.02	0.41
1:R:434:SER:C	1:R:436:GLU:N	2.73	0.41
1:K:381:LEU:HD11	1:K:438:MET:CB	2.50	0.41
1:Q:467:MET:HE3	1:Q:485:ILE:HG23	2.02	0.41
2:V:600:LDN:NAS	2:V:600:LDN:HAJ	2.35	0.41
1:L:315:VAL:CG1	1:L:315:VAL:O	2.69	0.41
1:X:204:LEU:HD22	1:X:217:TRP:CB	2.49	0.41
1:Q:415:ASN:O	1:Q:417:ILE:HD12	2.20	0.41
1:B:300:LEU:HD11	1:B:493:SER:CA	2.50	0.41
1:B:455:LEU:HD12	1:B:461:LEU:CB	2.43	0.41
1:P:195:GLN:CG	1:P:261:ALA:HB1	2.45	0.41
1:F:315:VAL:CG1	1:F:315:VAL:O	2.68	0.41
1:Q:362:LEU:HA	1:Q:362:LEU:HD12	1.90	0.41
1:F:258:GLY:O	1:F:277:THR:HB	2.21	0.41
1:E:486:LYS:O	1:E:490:GLN:HG3	2.20	0.41
1:I:246:TYR:CD1	1:I:259:PHE:HB2	2.55	0.41
1:L:331:PHE:O	1:L:400:ALA:HB1	2.21	0.41
1:E:464:LEU:CD2	1:E:489:LEU:CD2	2.98	0.41
1:B:348:ASP:HB2	2:B:600:LDN:HAI	2.03	0.41
1:I:414:VAL:CG1	1:I:454:ARG:HD2	2.48	0.41
1:S:460:VAL:CG1	1:S:461:LEU:HD23	2.45	0.41
1:T:414:VAL:C	1:T:416:GLY:N	2.74	0.41
1:H:414:VAL:HG13	1:H:454:ARG:CD	2.50	0.41
1:C:0:MET:CB	1:C:197:THR:HB	2.50	0.41
1:B:315:VAL:CG1	1:B:315:VAL:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:VAL:O	1:C:202:VAL:HG23	2.20	0.41
1:J:245:ILE:HG21	1:J:349:LEU:HD23	2.02	0.41
1:F:405:LEU:HD11	1:F:467:MET:CE	2.50	0.41
1:Q:206:GLU:HG2	1:Q:208:VAL:CG1	2.51	0.41
1:M:251:LEU:HD11	1:M:326:ILE:HD12	2.02	0.41
2:W:600:LDN:HAH	2:W:600:LDN:HAQA	1.81	0.41
1:U:289:LEU:HD21	1:U:294:LEU:HD11	2.02	0.41
1:T:357:GLN:O	1:T:358:GLY:C	2.59	0.41
1:G:405:LEU:HD11	1:G:467:MET:CE	2.50	0.41
1:H:386:ARG:NH2	1:I:446:GLN:OE1	2.54	0.41
1:E:315:VAL:O	1:E:315:VAL:CG1	2.69	0.41
1:W:286:TYR:HB2	1:W:334:ARG:HG2	2.02	0.41
1:E:490:GLN:O	1:E:493:SER:N	2.52	0.41
1:O:244:GLU:O	1:O:248:THR:HB	2.20	0.41
1:S:304:VAL:HA	1:S:489:LEU:HD13	2.02	0.41
1:X:329:ARG:HH11	1:X:353:VAL:CG1	2.34	0.41
1:V:252:ARG:HG2	1:V:252:ARG:HH11	1.86	0.41
1:D:289:LEU:HD11	1:D:408:ILE:HA	2.03	0.41
1:X:480:LEU:HD22	1:X:484:ARG:HG3	1.99	0.41
1:J:467:MET:HE1	1:J:485:ILE:HG23	2.03	0.41
1:S:386:ARG:NH1	1:T:446:GLN:CB	2.84	0.41
1:S:230:ILE:HG21	1:S:272:GLN:OE1	2.21	0.41
1:Q:470:GLU:HG2	1:Q:473:TYR:OH	2.21	0.41
1:L:467:MET:HE1	1:L:489:LEU:HD11	2.03	0.41
1:T:456:ALA:O	1:T:458:ASP:N	2.54	0.41
1:P:246:TYR:CD1	1:P:259:PHE:HB2	2.55	0.41
1:O:239:TRP:CE3	1:O:273:LEU:HD23	2.56	0.41
1:L:220:LEU:HD12	1:L:224:GLU:O	2.21	0.41
1:S:244:GLU:O	1:S:248:THR:HB	2.20	0.41
1:X:258:GLY:O	1:X:277:THR:HB	2.21	0.41
1:L:458:ASP:O	1:L:462:SER:HB2	2.21	0.41
1:X:454:ARG:O	1:X:454:ARG:HG3	2.21	0.41
1:I:317:ILE:HD12	1:I:323:LYS:HD3	2.03	0.41
1:B:460:VAL:HA	1:B:492:ILE:HG21	2.03	0.41
1:D:315:VAL:CG1	1:D:315:VAL:O	2.69	0.41
1:F:355:HIS:NE2	1:F:360:ASP:HA	2.36	0.41
1:F:386:ARG:HG2	1:F:392:SER:OG	2.21	0.41
1:J:246:TYR:CD1	1:J:259:PHE:HB2	2.56	0.41
1:S:418:VAL:HG13	1:S:418:VAL:O	2.21	0.41
2:I:600:LDN:CBC	2:I:600:LDN:HAJ	2.50	0.41
1:B:451:ILE:O	1:B:452:PRO:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:403:LEU:HD23	1:R:472:TRP:CZ2	2.56	0.40
1:V:294:LEU:CD1	1:V:411:ARG:HB3	2.51	0.40
1:I:295:GLU:HG2	1:I:297:HIS:H	1.86	0.40
1:C:431:ASN:O	1:C:433:PRO:CD	2.69	0.40
2:G:600:LDN:HAF	2:G:600:LDN:HAM	1.84	0.40
1:D:459:PRO:HD2	1:D:460:VAL:HG23	2.02	0.40
1:S:304:VAL:HG13	1:S:305:SER:N	2.36	0.40
1:N:328:HIS:O	1:N:329:ARG:HB2	2.21	0.40
1:H:230:ILE:CG2	1:H:272:GLN:OE1	2.70	0.40
1:M:376:MET:HG2	1:M:380:VAL:HG11	2.04	0.40
1:G:195:GLN:O	1:G:196:ARG:C	2.59	0.40
1:O:246:TYR:CD1	1:O:259:PHE:HB2	2.56	0.40
1:A:487:LYS:O	1:A:491:LYS:HG3	2.21	0.40
1:B:298:LEU:HD12	1:B:298:LEU:O	2.20	0.40
1:I:295:GLU:HG2	1:I:297:HIS:N	2.36	0.40
1:N:464:LEU:HD23	1:N:464:LEU:N	2.34	0.40
2:V:600:LDN:HAP	2:V:600:LDN:HAG	1.84	0.40
1:X:468:MET:O	1:X:472:TRP:NE1	2.54	0.40
1:E:414:VAL:HG11	1:E:454:ARG:CG	2.51	0.40
1:X:207:CYS:HB2	1:X:217:TRP:CE2	2.56	0.40
1:G:464:LEU:HD21	1:G:489:LEU:CD2	2.45	0.40
1:U:412:THR:HG21	1:U:461:LEU:CD2	2.50	0.40
1:M:305:SER:CB	1:M:343:GLN:HG2	2.51	0.40
1:N:440:LYS:HA	1:N:444:VAL:CG2	2.51	0.40
2:W:600:LDN:HAF	2:W:600:LDN:HAM	1.80	0.40
1:B:305:SER:HB3	1:B:343:GLN:CG	2.52	0.40
1:R:433:PRO:HB2	1:R:438:MET:HG2	2.03	0.40
1:J:241:ARG:HE	1:J:245:ILE:HD11	1.86	0.40
1:O:239:TRP:CE3	1:O:273:LEU:CD2	3.04	0.40
1:R:355:HIS:C	1:R:355:HIS:ND1	2.74	0.40
1:B:464:LEU:HD23	1:B:464:LEU:HA	1.94	0.40
1:M:249:VAL:HG12	1:M:251:LEU:HD13	2.02	0.40
1:C:434:SER:OG	1:C:437:ASP:OD2	2.39	0.40
2:L:600:LDN:HAH	2:L:600:LDN:HAQA	1.87	0.40
1:F:490:GLN:HE21	1:F:490:GLN:HB2	1.57	0.40
1:G:205:VAL:HG11	1:G:218:ARG:NH2	2.37	0.40
1:L:258:GLY:O	1:L:277:THR:HB	2.21	0.40
1:A:252:ARG:HE	1:A:253:HIS:N	2.19	0.40

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	P	433	PRO
1	U	359	SER
1	D	195	GLN
1	F	320	THR
1	F	453	ASN
1	L	462	SER
1	N	492	ILE
1	P	454	ARG
1	S	198	VAL
1	S	459	PRO
1	S	460	VAL
1	T	358	GLY
1	T	415	ASN
1	T	457	ALA
1	A	459	PRO
1	B	357	GLN
1	B	360	ASP
1	C	269	SER
1	D	269	SER
1	E	198	VAL
1	E	361	TYR
1	G	456	ALA
1	J	454	ARG
1	N	269	SER

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Mol	Chain	Res	Type
1	O	269	SER
1	P	355	HIS
1	R	435	PHE
1	T	196	ARG
1	F	365	GLY
1	I	357	GLN
1	M	415	ASN
1	M	454	ARG
1	P	453	ASN
1	P	460	VAL
1	R	456	ALA
1	S	435	PHE
1	T	456	ALA
1	V	431	ASN
1	W	453	ASN
1	B	459	PRO
1	C	415	ASN
1	F	431	ASN
1	N	196	ARG
1	N	454	ARG
1	P	435	PHE
1	U	459	PRO
1	K	433	PRO
1	Q	460	VAL
1	P	458	ASP
1	S	414	VAL
1	V	414	VAL
1	E	364	ILE
1	G	432	ASP

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	231/267 (86%)	225 (97%)	6 (3%)	54 81
1	D	232/267 (87%)	223 (96%)	9 (4%)	39 67
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

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	SER
1	A	252	ARG
1	A	271	THR
1	A	272	GLN
1	A	273	LEU
1	A	323	LYS
1	A	360	ASP

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Mol	Chain	Res	Type
1	A	361	TYR
1	A	420	ASP
1	A	432	ASP
1	B	201	GLN
1	B	233	SER
1	B	263	ASP
1	B	291	ARG
1	B	297	HIS
1	B	300	LEU
1	B	323	LYS
1	B	343	GLN
1	B	359	SER
1	B	369	ARG
1	B	386	ARG
1	B	418	VAL
1	B	446	GLN
1	B	491	LYS
1	C	265	THR
1	C	291	ARG
1	C	295	GLU
1	C	300	LEU
1	C	475	ASN
1	C	484	ARG
1	D	233	SER
1	D	252	ARG
1	D	273	LEU
1	D	292	GLN
1	D	295	GLU
1	D	321	GLN
1	D	343	GLN
1	D	413	ILE
1	D	484	ARG
1	E	224	GLU
1	E	291	ARG
1	E	323	LYS
1	E	355	HIS
1	E	361	TYR
1	E	382	ASP
1	E	432	ASP
1	E	483	LEU
1	F	252	ARG
1	F	264	MET

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Mol	Chain	Res	Type
1	F	354	MET
1	F	360	ASP
1	F	361	TYR
1	F	362	LEU
1	F	386	ARG
1	F	415	ASN
1	F	418	VAL
1	F	428	VAL
1	F	484	ARG
1	F	490	GLN
1	G	220	LEU
1	G	263	ASP
1	G	273	LEU
1	G	275	LEU
1	G	323	LYS
1	G	360	ASP
1	G	361	TYR
1	G	370	VAL
1	G	382	ASP
1	G	385	ILE
1	G	446	GLN
1	G	447	GLN
1	G	450	THR
1	H	222	HIS
1	H	250	LEU
1	H	273	LEU
1	H	316	GLU
1	H	386	ARG
1	H	414	VAL
1	H	432	ASP
1	H	451	ILE
1	H	458	ASP
1	H	469	ARG
1	I	197	THR
1	I	218	ARG
1	I	237	GLN
1	I	273	LEU
1	I	291	ARG
1	I	292	GLN
1	I	295	GLU
1	I	300	LEU
1	I	323	LYS

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Mol	Chain	Res	Type
1	I	361	TYR
1	I	386	ARG
1	I	431	ASN
1	I	432	ASP
1	I	455	LEU
1	I	475	ASN
1	I	484	ARG
1	I	492	ILE
1	J	252	ARG
1	J	275	LEU
1	J	297	HIS
1	J	300	LEU
1	J	308	CYS
1	J	381	LEU
1	J	404	VAL
1	J	412	THR
1	J	462	SER
1	K	197	THR
1	K	252	ARG
1	K	271	THR
1	K	297	HIS
1	K	301	ARG
1	K	382	ASP
1	K	412	THR
1	L	252	ARG
1	L	273	LEU
1	L	292	GLN
1	L	360	ASP
1	L	361	TYR
1	L	432	ASP
1	L	454	ARG
1	L	455	LEU
1	L	468	MET
1	M	265	THR
1	M	343	GLN
1	M	354	MET
1	M	360	ASP
1	M	361	TYR
1	M	431	ASN
1	M	475	ASN
1	M	484	ARG
1	N	265	THR

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Mol	Chain	Res	Type
1	N	272	GLN
1	N	291	ARG
1	N	382	ASP
1	N	432	ASP
1	N	446	GLN
1	N	454	ARG
1	O	220	LEU
1	O	237	GLN
1	O	265	THR
1	O	291	ARG
1	O	334	ARG
1	O	426	TYR
1	O	435	PHE
1	O	483	LEU
1	P	342	LEU
1	P	366	ASN
1	P	415	ASN
1	P	419	GLU
1	P	426	TYR
1	Q	233	SER
1	Q	234	ARG
1	Q	252	ARG
1	Q	264	MET
1	Q	291	ARG
1	Q	300	LEU
1	Q	359	SER
1	Q	413	ILE
1	Q	414	VAL
1	Q	439	LYS
1	Q	454	ARG
1	Q	493	SER
1	R	295	GLU
1	R	300	LEU
1	R	360	ASP
1	R	361	TYR
1	R	376	MET
1	R	384	GLN
1	R	414	VAL
1	R	417	ILE
1	R	420	ASP
1	R	447	GLN
1	R	484	ARG

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Mol	Chain	Res	Type
1	S	250	LEU
1	S	382	ASP
1	S	412	THR
1	S	414	VAL
1	S	458	ASP
1	S	469	ARG
1	T	197	THR
1	T	202	VAL
1	T	222	HIS
1	T	272	GLN
1	T	300	LEU
1	T	323	LYS
1	T	360	ASP
1	T	361	TYR
1	T	366	ASN
1	T	386	ARG
1	T	412	THR
1	T	431	ASN
1	T	446	GLN
1	T	454	ARG
1	T	484	ARG
1	U	197	THR
1	U	250	LEU
1	U	297	HIS
1	U	373	LYS
1	U	454	ARG
1	U	492	ILE
1	V	294	LEU
1	V	300	LEU
1	V	417	ILE
1	V	461	LEU
1	V	493	SER
1	W	244	GLU
1	W	273	LEU
1	W	291	ARG
1	W	354	MET
1	W	454	ARG
1	W	462	SER
1	X	201	GLN
1	X	265	THR
1	X	431	ASN
1	X	472	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	282	HIS
1	B	282	HIS
1	C	282	HIS
1	C	321	GLN
1	D	282	HIS
1	F	490	GLN
1	H	247	ASN
1	L	292	GLN
1	O	384	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
2	M	600	LDN	CAZ-CAY	-3.95	1.39	1.49
2	P	600	LDN	CAZ-CAY	-3.88	1.40	1.49
2	D	600	LDN	CAV-CAW	-3.81	1.39	1.49
2	F	600	LDN	CAZ-CAY	-3.80	1.40	1.49
2	U	600	LDN	CAZ-CAY	-3.73	1.40	1.49
2	K	600	LDN	CAZ-CAY	-3.72	1.40	1.49
2	A	600	LDN	CAZ-CAY	-3.72	1.40	1.49
2	R	600	LDN	CAZ-CAY	-3.63	1.40	1.49
2	F	600	LDN	CAV-CAW	-3.63	1.39	1.49
2	V	600	LDN	CAZ-CAY	-3.61	1.40	1.49
2	D	600	LDN	CAZ-CAY	-3.56	1.40	1.49
2	G	600	LDN	CAZ-CAY	-3.54	1.40	1.49
2	T	600	LDN	CAZ-CAY	-3.53	1.40	1.49
2	H	600	LDN	CAV-CAW	-3.51	1.39	1.49
2	W	600	LDN	CAV-CAW	-3.51	1.39	1.49
2	Q	600	LDN	CAZ-CAY	-3.48	1.41	1.49
2	N	600	LDN	CAZ-CAY	-3.47	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	600	LDN	CAV-CAW	-3.47	1.40	1.49
2	E	600	LDN	CAZ-CAY	-3.45	1.41	1.49
2	L	600	LDN	CAZ-CAY	-3.42	1.41	1.49
2	H	600	LDN	CAZ-CAY	-3.40	1.41	1.49
2	O	600	LDN	CAZ-CAY	-3.39	1.41	1.49
2	S	600	LDN	CAZ-CAY	-3.38	1.41	1.49
2	N	600	LDN	CAV-CAW	-3.36	1.40	1.49
2	L	600	LDN	CAV-CAW	-3.31	1.40	1.49
2	A	600	LDN	CAV-CAW	-3.28	1.40	1.49
2	U	600	LDN	CAV-CAW	-3.27	1.40	1.49
2	J	600	LDN	CAV-CAW	-3.25	1.40	1.49
2	I	600	LDN	CAV-CAW	-3.24	1.40	1.49
2	S	600	LDN	CAV-CAW	-3.23	1.40	1.49
2	T	600	LDN	CAV-CAW	-3.21	1.40	1.49
2	Q	600	LDN	CAV-CAW	-3.21	1.40	1.49
2	C	600	LDN	CAV-CAW	-3.17	1.40	1.49
2	B	600	LDN	CAV-CAW	-3.17	1.40	1.49
2	G	600	LDN	CAV-CAW	-3.12	1.40	1.49
2	M	600	LDN	CAV-CAW	-3.10	1.41	1.49
2	B	600	LDN	CAZ-CAY	-3.07	1.42	1.49
2	P	600	LDN	CAV-CAW	-3.00	1.41	1.49
2	O	600	LDN	CAV-CAW	-2.95	1.41	1.49
2	I	600	LDN	CBA-NAR	-2.77	1.32	1.37
2	V	600	LDN	CAV-CAW	-2.77	1.41	1.49
2	L	600	LDN	CBB-CBA	-2.75	1.38	1.42
2	E	600	LDN	CAV-CAW	-2.66	1.42	1.49
2	H	600	LDN	CBA-NAR	-2.63	1.32	1.37
2	R	600	LDN	CAV-CAW	-2.58	1.42	1.49
2	J	600	LDN	CBB-CBA	-2.41	1.38	1.42
2	W	600	LDN	CBB-CBA	-2.37	1.39	1.42
2	A	600	LDN	CBB-CBA	-2.33	1.39	1.42
2	T	600	LDN	CAI-CBA	-2.09	1.38	1.41
2	U	600	LDN	CBB-CBA	-2.06	1.39	1.42
2	K	600	LDN	CAV-CAW	-2.06	1.43	1.49
2	W	600	LDN	CAQ-NBD	2.01	1.49	1.46
2	P	600	LDN	CAA-CAI	2.02	1.41	1.36
2	T	600	LDN	CAQ-NBD	2.04	1.49	1.46
2	D	600	LDN	CAD-CAY	2.09	1.42	1.38
2	L	600	LDN	CAQ-NBD	2.11	1.49	1.46
2	X	600	LDN	CAQ-NBD	2.11	1.49	1.46
2	S	600	LDN	CAP-NBD	2.17	1.50	1.46
2	R	600	LDN	CAQ-NBD	2.18	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	600	LDN	CAQ-NBD	2.19	1.50	1.46
2	C	600	LDN	CAQ-NBD	2.23	1.50	1.46
2	K	600	LDN	CAK-NAS	2.27	1.35	1.31
2	K	600	LDN	CAP-NBD	2.27	1.50	1.46
2	R	600	LDN	CAP-NBD	2.28	1.50	1.46
2	I	600	LDN	CAX-NBD	2.32	1.45	1.38
2	O	600	LDN	CAP-NBD	2.38	1.50	1.46
2	M	600	LDN	CAQ-NBD	2.42	1.50	1.46
2	P	600	LDN	CAQ-NBD	2.45	1.50	1.46
2	A	600	LDN	CAP-NBD	2.45	1.50	1.46
2	F	600	LDN	CAP-NBD	2.53	1.50	1.46
2	E	600	LDN	CAP-NBD	2.57	1.50	1.46
2	K	600	LDN	CAX-NBD	2.64	1.46	1.38
2	K	600	LDN	CAQ-NBD	2.67	1.50	1.46
2	O	600	LDN	CAQ-NBD	2.74	1.50	1.46
2	M	600	LDN	CAP-NBD	3.22	1.51	1.46

All (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
2	F	600	LDN	CAW-CAK-NAS	-4.11	120.26	125.46
2	L	600	LDN	CAW-CAK-NAS	-4.09	120.28	125.46
2	B	600	LDN	CAW-CAK-NAS	-4.04	120.36	125.46
2	P	600	LDN	CAW-CAK-NAS	-3.98	120.43	125.46
2	T	600	LDN	CAW-CAK-NAS	-3.87	120.56	125.46
2	W	600	LDN	CAW-CAK-NAS	-3.87	120.57	125.46
2	Q	600	LDN	CAW-CAK-NAS	-3.74	120.73	125.46
2	J	600	LDN	CAD-CAC-NAR	-3.74	118.66	124.56
2	X	600	LDN	CAW-CAK-NAS	-3.71	120.77	125.46
2	D	600	LDN	CAW-CAK-NAS	-3.70	120.79	125.46
2	G	600	LDN	CAW-CAK-NAS	-3.67	120.82	125.46
2	T	600	LDN	CAH-CAX-NBD	-3.61	116.53	121.38
2	N	600	LDN	CAW-CAK-NAS	-3.51	121.02	125.46
2	M	600	LDN	CAD-CAC-NAR	-3.37	119.24	124.56
2	U	600	LDN	CAW-CAK-NAS	-3.27	121.33	125.46
2	H	600	LDN	CAW-CAK-NAS	-3.22	121.39	125.46
2	S	600	LDN	CAW-CAK-NAS	-3.22	121.39	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	600	LDN	CAH-CAX-NBD	-3.17	117.13	121.38
2	C	600	LDN	CAH-CAX-NBD	-3.13	117.18	121.38
2	K	600	LDN	CAW-CAK-NAS	-3.06	121.59	125.46
2	W	600	LDN	CAN-CAP-NBD	-2.99	103.34	110.70
2	W	600	LDN	CAD-CAC-NAR	-2.99	119.84	124.56
2	R	600	LDN	CAW-CAK-NAS	-2.97	121.71	125.46
2	X	600	LDN	CAD-CAC-NAR	-2.94	119.92	124.56
2	D	600	LDN	CAD-CAC-NAR	-2.93	119.94	124.56
2	J	600	LDN	CAO-CAQ-NBD	-2.90	103.56	110.70
2	A	600	LDN	CAO-CAQ-NBD	-2.89	103.59	110.70
2	M	600	LDN	CAW-CAK-NAS	-2.87	121.83	125.46
2	T	600	LDN	CAD-CAC-NAR	-2.85	120.07	124.56
2	G	600	LDN	CBB-CBA-NAR	-2.83	119.87	122.88
2	I	600	LDN	CBB-CBA-NAR	-2.76	119.95	122.88
2	E	600	LDN	CAW-CAK-NAS	-2.72	122.02	125.46
2	I	600	LDN	CAC-CAD-CAY	-2.68	117.87	119.98
2	B	600	LDN	CAD-CAC-NAR	-2.68	120.34	124.56
2	C	600	LDN	CAD-CAC-NAR	-2.68	120.34	124.56
2	L	600	LDN	CAD-CAC-NAR	-2.66	120.36	124.56
2	P	600	LDN	CAD-CAC-NAR	-2.64	120.40	124.56
2	U	600	LDN	CBB-CBA-NAR	-2.60	120.11	122.88
2	T	600	LDN	CAF-CAV-CAW	-2.54	116.83	121.39
2	Q	600	LDN	CAD-CAC-NAR	-2.51	120.61	124.56
2	U	600	LDN	CAD-CAC-NAR	-2.50	120.62	124.56
2	A	600	LDN	CAD-CAC-NAR	-2.50	120.62	124.56
2	V	600	LDN	CAW-CAK-NAS	-2.45	122.36	125.46
2	H	600	LDN	CAD-CAC-NAR	-2.45	120.70	124.56
2	X	600	LDN	CAN-CAP-NBD	-2.43	104.72	110.70
2	M	600	LDN	CBB-CBA-NAR	-2.43	120.29	122.88
2	O	600	LDN	CAW-CAK-NAS	-2.43	122.39	125.46
2	W	600	LDN	CAH-CAX-NBD	-2.37	118.20	121.38
2	C	600	LDN	CBB-CBA-NAR	-2.33	120.40	122.88
2	P	600	LDN	CAH-CAX-NBD	-2.32	118.26	121.38
2	R	600	LDN	CBB-CBA-NAR	-2.27	120.47	122.88
2	E	600	LDN	CAD-CAC-NAR	-2.25	121.02	124.56
2	K	600	LDN	CAD-CAC-NAR	-2.25	121.02	124.56
2	J	600	LDN	CBB-CBA-NAR	-2.23	120.51	122.88
2	R	600	LDN	CAC-CAD-CAY	-2.20	118.25	119.98
2	N	600	LDN	CAD-CAC-NAR	-2.18	121.12	124.56
2	S	600	LDN	CAD-CAC-NAR	-2.18	121.13	124.56
2	W	600	LDN	CBB-CBA-NAR	-2.16	120.58	122.88
2	G	600	LDN	CAB-CAA-CAI	-2.15	117.33	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	600	LDN	CAD-CAC-NAR	-2.11	121.23	124.56
2	H	600	LDN	CBB-CBA-NAR	-2.10	120.64	122.88
2	R	600	LDN	CAP-CAN-NAU	-2.10	105.64	111.55
2	T	600	LDN	CAM-CAW-CAV	-2.10	115.48	120.56
2	O	600	LDN	CAG-CAX-NBD	-2.08	118.58	121.38
2	C	600	LDN	CAE-CAG-CAX	-2.06	117.70	120.36
2	N	600	LDN	CAF-CAV-CAW	-2.05	117.71	121.39
2	J	600	LDN	CAG-CAX-NBD	-2.05	118.63	121.38
2	F	600	LDN	CBB-CBA-NAR	-2.04	120.71	122.88
2	W	600	LDN	CAM-CAW-CAV	-2.02	115.66	120.56
2	U	600	LDN	CAZ-CAY-CBB	-2.01	118.58	121.44
2	F	600	LDN	CAD-CAC-NAR	-2.01	121.39	124.56
2	P	600	LDN	CAY-CBB-CBA	2.01	118.51	117.46
2	V	600	LDN	CAQ-NBD-CAP	2.01	115.81	111.59
2	V	600	LDN	CAC-NAR-CBA	2.01	120.28	116.87
2	J	600	LDN	CAY-CBB-CBA	2.06	118.53	117.46
2	G	600	LDN	CAI-CBA-CBB	2.07	121.40	119.07
2	O	600	LDN	CAZ-CAY-CBB	2.09	124.43	121.44
2	M	600	LDN	CAQ-NBD-CAX	2.11	123.58	117.92
2	E	600	LDN	CAM-CAW-CAK	2.13	117.85	115.45
2	T	600	LDN	CAC-NAR-CBA	2.14	120.50	116.87
2	Q	600	LDN	CAC-NAR-CBA	2.17	120.55	116.87
2	K	600	LDN	CAC-NAR-CBA	2.19	120.58	116.87
2	N	600	LDN	CAZ-CAY-CBB	2.23	124.62	121.44
2	K	600	LDN	CAE-CAV-CAW	2.24	125.42	121.39
2	Q	600	LDN	CAM-CAW-CAK	2.27	118.00	115.45
2	S	600	LDN	CAM-CAW-CAK	2.28	118.01	115.45
2	H	600	LDN	CAI-CBA-CBB	2.29	121.65	119.07
2	M	600	LDN	CAY-CBB-CBA	2.32	118.67	117.46
2	P	600	LDN	CAC-NAR-CBA	2.32	120.80	116.87
2	C	600	LDN	CAY-CBB-CBA	2.37	118.70	117.46
2	N	600	LDN	CAC-NAR-CBA	2.38	120.91	116.87
2	T	600	LDN	CAJ-CBB-CBA	2.40	120.77	118.33
2	R	600	LDN	CAC-NAR-CBA	2.41	120.96	116.87
2	F	600	LDN	CAC-NAR-CBA	2.42	120.97	116.87
2	B	600	LDN	CAM-CAW-CAK	2.43	118.17	115.45
2	H	600	LDN	CAK-NAS-CBC	2.43	120.08	116.86
2	L	600	LDN	CAC-NAR-CBA	2.43	121.00	116.87
2	B	600	LDN	CAC-NAR-CBA	2.43	121.00	116.87
2	N	600	LDN	CAG-CAX-NBD	2.44	124.66	121.38
2	D	600	LDN	CAQ-NBD-CAX	2.45	124.48	117.92
2	R	600	LDN	CAZ-CAY-CBB	2.45	124.93	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	600	LDN	CAM-CAW-CAK	2.47	118.23	115.45
2	H	600	LDN	CAY-CBB-CBA	2.55	118.79	117.46
2	M	600	LDN	CAM-CAW-CAK	2.55	118.31	115.45
2	K	600	LDN	CAY-CBB-CBA	2.56	118.80	117.46
2	D	600	LDN	CAY-CBB-CBA	2.57	118.80	117.46
2	M	600	LDN	CAH-CAX-NBD	2.59	124.86	121.38
2	G	600	LDN	CAM-CAW-CAK	2.62	118.39	115.45
2	T	600	LDN	CAK-CAW-CAV	2.63	126.73	121.90
2	W	600	LDN	CAK-NAS-CBC	2.65	120.37	116.86
2	I	600	LDN	CAY-CBB-CBA	2.77	118.91	117.46
2	A	600	LDN	CAC-NAR-CBA	2.77	121.56	116.87
2	I	600	LDN	CAM-CAW-CAK	2.77	118.56	115.45
2	V	600	LDN	CAY-CBB-CBA	2.77	118.91	117.46
2	B	600	LDN	CAZ-CAY-CBB	2.80	125.43	121.44
2	V	600	LDN	CAK-NAS-CBC	2.81	120.58	116.86
2	D	600	LDN	CAM-CAW-CAK	2.84	118.64	115.45
2	A	600	LDN	CAY-CBB-CBA	2.84	118.94	117.46
2	O	600	LDN	CAM-CAW-CAK	2.85	118.65	115.45
2	T	600	LDN	CAY-CBB-CBA	2.88	118.97	117.46
2	D	600	LDN	CAC-NAR-CBA	2.90	121.79	116.87
2	G	600	LDN	CAC-NAR-CBA	2.91	121.81	116.87
2	Q	600	LDN	CAY-CBB-CBA	2.96	119.00	117.46
2	O	600	LDN	CAK-NAS-CBC	2.99	120.81	116.86
2	I	600	LDN	CAC-NAR-CBA	3.04	122.03	116.87
2	X	600	LDN	CAC-NAR-CBA	3.04	122.03	116.87
2	C	600	LDN	CAC-NAR-CBA	3.07	122.07	116.87
2	E	600	LDN	CAK-NAS-CBC	3.07	120.92	116.86
2	H	600	LDN	CAC-NAR-CBA	3.08	122.09	116.87
2	S	600	LDN	CAY-CBB-CBA	3.13	119.09	117.46
2	U	600	LDN	CAC-NAR-CBA	3.14	122.19	116.87
2	P	600	LDN	CAQ-NBD-CAP	3.14	118.19	111.59
2	X	600	LDN	CAQ-NBD-CAP	3.17	118.24	111.59
2	F	600	LDN	CAQ-NBD-CAP	3.17	118.25	111.59
2	U	600	LDN	CAK-NAS-CBC	3.19	121.08	116.86
2	U	600	LDN	CAM-CAW-CAK	3.22	119.06	115.45
2	U	600	LDN	CAY-CBB-CBA	3.23	119.15	117.46
2	T	600	LDN	CAQ-NBD-CAP	3.25	118.41	111.59
2	H	600	LDN	CAM-CAW-CAK	3.25	119.10	115.45
2	J	600	LDN	CAQ-NBD-CAP	3.30	118.53	111.59
2	U	600	LDN	CAQ-NBD-CAP	3.31	118.54	111.59
2	N	600	LDN	CAQ-NBD-CAP	3.32	118.57	111.59
2	W	600	LDN	CAC-NAR-CBA	3.35	122.55	116.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	600	LDN	CAM-CAW-CAK	3.37	119.23	115.45
2	N	600	LDN	CAM-CAW-CAK	3.39	119.25	115.45
2	M	600	LDN	CAQ-NBD-CAP	3.42	118.77	111.59
2	X	600	LDN	CAM-CAW-CAK	3.45	119.32	115.45
2	M	600	LDN	CAK-NAS-CBC	3.45	121.43	116.86
2	K	600	LDN	CAK-CAW-CAV	3.45	128.24	121.90
2	M	600	LDN	CAC-NAR-CBA	3.45	122.72	116.87
2	X	600	LDN	CAK-NAS-CBC	3.47	121.45	116.86
2	A	600	LDN	CAQ-NBD-CAP	3.48	118.90	111.59
2	F	600	LDN	CAM-CAW-CAK	3.51	119.39	115.45
2	S	600	LDN	CAK-NAS-CBC	3.51	121.51	116.86
2	W	600	LDN	CAQ-NBD-CAP	3.54	119.02	111.59
2	G	600	LDN	CAQ-NBD-CAP	3.56	119.06	111.59
2	J	600	LDN	CAC-NAR-CBA	3.58	122.94	116.87
2	N	600	LDN	CAY-CBB-CBA	3.58	119.33	117.46
2	D	600	LDN	CAQ-NBD-CAP	3.61	119.18	111.59
2	H	600	LDN	CAZ-CAY-CBB	3.63	126.61	121.44
2	E	600	LDN	CAY-CBB-CBA	3.65	119.37	117.46
2	A	600	LDN	CAM-CAW-CAK	3.67	119.57	115.45
2	W	600	LDN	CAM-CAW-CAK	3.70	119.61	115.45
2	E	600	LDN	CAQ-NBD-CAP	3.71	119.38	111.59
2	Q	600	LDN	CAQ-NBD-CAP	3.72	119.41	111.59
2	C	600	LDN	CAK-NAS-CBC	3.81	121.90	116.86
2	I	600	LDN	CAK-NAS-CBC	3.81	121.91	116.86
2	A	600	LDN	CAK-NAS-CBC	3.82	121.91	116.86
2	F	600	LDN	CAY-CBB-CBA	3.82	119.45	117.46
2	Q	600	LDN	CAZ-CAY-CBB	3.82	126.88	121.44
2	N	600	LDN	CAK-NAS-CBC	3.87	121.99	116.86
2	F	600	LDN	CAK-NAS-CBC	3.88	121.99	116.86
2	R	600	LDN	CAY-CBB-CBA	3.88	119.49	117.46
2	J	600	LDN	CAK-NAS-CBC	3.90	122.02	116.86
2	K	600	LDN	CAK-NAS-CBC	3.94	122.08	116.86
2	R	600	LDN	CAK-NAS-CBC	3.98	122.12	116.86
2	B	600	LDN	CAY-CBB-CBA	4.01	119.56	117.46
2	J	600	LDN	CAM-CAW-CAK	4.09	120.04	115.45
2	X	600	LDN	CAZ-CAY-CBB	4.12	127.31	121.44
2	B	600	LDN	CAK-NAS-CBC	4.14	122.34	116.86
2	D	600	LDN	CAK-NAS-CBC	4.28	122.52	116.86
2	K	600	LDN	CAZ-CAY-CBB	4.31	127.59	121.44
2	H	600	LDN	CAQ-NBD-CAP	4.36	120.75	111.59
2	G	600	LDN	CAK-NAS-CBC	4.37	122.64	116.86
2	G	600	LDN	CAZ-CAY-CBB	4.37	127.67	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	600	LDN	CAK-NAS-CBC	4.38	122.65	116.86
2	L	600	LDN	CAK-NAS-CBC	4.49	122.81	116.86
2	L	600	LDN	CAY-CBB-CBA	4.52	119.82	117.46
2	T	600	LDN	CAK-NAS-CBC	4.56	122.89	116.86
2	G	600	LDN	CAY-CBB-CBA	4.61	119.87	117.46
2	P	600	LDN	CAK-NAS-CBC	4.62	122.97	116.86
2	O	600	LDN	CAY-CBB-CBA	4.79	119.96	117.46
2	O	600	LDN	CAQ-NBD-CAP	4.88	121.84	111.59
2	C	600	LDN	CAQ-NBD-CAP	4.95	121.99	111.59
2	I	600	LDN	CAQ-NBD-CAP	5.06	122.21	111.59
2	S	600	LDN	CAQ-NBD-CAP	5.08	122.25	111.59
2	B	600	LDN	CAQ-NBD-CAP	5.13	122.37	111.59
2	L	600	LDN	CAQ-NBD-CAP	5.20	122.50	111.59
2	R	600	LDN	CAQ-NBD-CAP	5.45	123.03	111.59
2	G	600	LDN	CAL-NAT-NBE	7.01	108.97	103.70
2	U	600	LDN	CAL-NAT-NBE	7.43	109.29	103.70
2	H	600	LDN	CAL-NAT-NBE	7.75	109.53	103.70
2	D	600	LDN	CAL-NAT-NBE	8.17	109.84	103.70
2	B	600	LDN	CAL-NAT-NBE	8.34	109.97	103.70
2	M	600	LDN	CAL-NAT-NBE	8.38	110.00	103.70
2	T	600	LDN	CAL-NAT-NBE	8.39	110.01	103.70
2	S	600	LDN	CAL-NAT-NBE	8.40	110.02	103.70
2	F	600	LDN	CAL-NAT-NBE	8.42	110.03	103.70
2	K	600	LDN	CAL-NAT-NBE	8.75	110.29	103.70
2	A	600	LDN	CAL-NAT-NBE	8.78	110.31	103.70
2	N	600	LDN	CAL-NAT-NBE	8.83	110.35	103.70
2	W	600	LDN	CAL-NAT-NBE	8.89	110.39	103.70
2	X	600	LDN	CAL-NAT-NBE	8.90	110.39	103.70
2	O	600	LDN	CAL-NAT-NBE	9.17	110.60	103.70
2	R	600	LDN	CAL-NAT-NBE	9.23	110.64	103.70
2	E	600	LDN	CAL-NAT-NBE	9.34	110.73	103.70
2	L	600	LDN	CAL-NAT-NBE	9.38	110.76	103.70
2	J	600	LDN	CAL-NAT-NBE	9.64	110.95	103.70
2	C	600	LDN	CAL-NAT-NBE	9.70	111.00	103.70
2	V	600	LDN	CAL-NAT-NBE	9.76	111.04	103.70
2	Q	600	LDN	CAL-NAT-NBE	9.82	111.09	103.70
2	P	600	LDN	CAL-NAT-NBE	9.87	111.13	103.70
2	I	600	LDN	CAL-NAT-NBE	9.99	111.22	103.70

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
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

All (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
1	X	242	GLU	13.6
1	P	309	GLY	13.3
1	X	405	LEU	12.7
1	J	387	THR	12.5
1	K	296	PRO	12.1
1	P	472	TRP	12.0
1	B	195	GLN	11.5
1	X	220	LEU	11.4
1	P	473	TYR	10.8
1	J	445	ASP	10.7
1	P	401	PHE	10.4
1	X	331	PHE	10.4
1	J	424	PRO	10.3
1	X	203	ALA	10.3
1	K	337	LEU	10.1
1	P	221	TRP	10.1
1	J	438	MET	10.0
1	P	325	ALA	9.9
1	P	320	THR	9.7
1	P	476	PRO	9.6
1	J	478	ALA	9.5
1	J	351	LEU	9.4
1	P	308	CYS	9.4
1	P	483	LEU	9.4
1	X	375	TYR	9.3
1	K	239	TRP	9.3
1	X	251	LEU	9.2
1	X	396	THR	9.2
1	K	306	ALA	9.1
1	P	352	ALA	9.1
1	K	385	ILE	9.1
1	J	353	VAL	9.1

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Mol	Chain	Res	Type	RSRZ
1	J	444	VAL	9.1
1	K	309	GLY	9.1
1	X	205	VAL	9.1
1	K	368	PRO	9.0
1	X	228	VAL	9.0
1	X	304	VAL	9.0
1	P	400	ALA	8.9
1	X	407	GLU	8.8
1	K	251	LEU	8.8
1	X	480	LEU	8.8
1	P	396	THR	8.7
1	J	328	HIS	8.7
1	P	377	ALA	8.6
1	P	245	ILE	8.6
1	K	279	TYR	8.6
1	X	213	TYR	8.5
1	X	250	LEU	8.5
1	K	312	HIS	8.4
1	X	474	PRO	8.4
1	P	378	PRO	8.4
1	J	449	PRO	8.3
1	J	248	THR	8.3
1	J	335	ASN	8.2
1	P	381	LEU	8.2
1	X	421	TYR	8.2
1	J	421	TYR	8.2
1	K	488	THR	8.1
1	J	325	ALA	8.1
1	X	471	CYS	8.1
1	P	223	GLY	8.1
1	X	261	ALA	8.0
1	J	285	LEU	8.0
1	X	367	ASN	7.9
1	K	492	ILE	7.9
1	P	395	TRP	7.9
1	J	460	VAL	7.9
1	K	243	THR	7.8
1	X	330	ASP	7.7
1	P	205	VAL	7.7
1	J	331	PHE	7.7
1	J	393	TYR	7.7
1	J	482	ALA	7.7

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Mol	Chain	Res	Type	RSRZ
1	X	279	TYR	7.6
1	J	414	VAL	7.6
1	X	404	VAL	7.6
1	J	477	SER	7.6
1	K	408	ILE	7.6
1	X	230	ILE	7.6
1	X	285	LEU	7.6
1	X	239	TRP	7.6
1	K	381	LEU	7.5
1	P	376	MET	7.5
1	X	406	TRP	7.5
1	K	399	TRP	7.5
1	X	399	TRP	7.5
1	X	376	MET	7.4
1	X	426	TYR	7.4
1	X	337	LEU	7.4
1	K	299	ALA	7.4
1	P	257	LEU	7.3
1	K	304	VAL	7.3
1	X	280	HIS	7.3
1	J	205	VAL	7.3
1	J	425	PHE	7.3
1	M	0	MET	7.2
1	X	428	VAL	7.2
1	X	243	THR	7.2
1	P	279	TYR	7.2
1	W	220	LEU	7.2
1	J	474	PRO	7.2
1	P	321	GLN	7.1
1	P	249	VAL	7.1
1	K	373	LYS	7.1
1	X	476	PRO	7.0
1	K	472	TRP	7.0
1	K	471	CYS	7.0
1	P	335	ASN	6.9
1	K	396	THR	6.9
1	W	195	GLN	6.9
1	K	398	ILE	6.9
1	X	229	LYS	6.8
1	X	281	GLU	6.8
1	P	393	TYR	6.8
1	P	222	HIS	6.8

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Mol	Chain	Res	Type	RSRZ
1	J	245	ILE	6.8
1	P	310	LEU	6.8
1	P	359	SER	6.8
1	P	478	ALA	6.8
1	D	460	VAL	6.8
1	P	224	GLU	6.7
1	P	470	GLU	6.7
1	X	408	ILE	6.7
1	P	346	ILE	6.7
1	X	419	GLU	6.7
1	X	442	VAL	6.7
1	P	225	SER	6.7
1	J	400	ALA	6.7
1	P	480	LEU	6.7
1	K	305	SER	6.6
1	X	334	ARG	6.6
1	X	377	ALA	6.6
1	X	482	ALA	6.6
1	P	447	GLN	6.6
1	K	303	ALA	6.6
1	S	219	GLY	6.5
1	J	471	CYS	6.5
1	J	220	LEU	6.5
1	K	425	PHE	6.5
1	X	201	GLN	6.5
1	K	222	HIS	6.5
1	P	246	TYR	6.5
1	X	468	MET	6.5
1	W	457	ALA	6.5
1	X	486	LYS	6.4
1	X	215	GLU	6.4
1	J	428	VAL	6.4
1	P	207	CYS	6.4
1	X	449	PRO	6.4
1	X	262	SER	6.4
1	K	297	HIS	6.4
1	K	271	THR	6.4
1	K	338	VAL	6.4
1	K	393	TYR	6.4
1	X	310	LEU	6.4
1	J	401	PHE	6.3
1	P	219	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
1	P	302	LEU	6.3
1	K	421	TYR	6.2
1	P	326	ILE	6.2
1	J	261	ALA	6.2
1	X	354	MET	6.2
1	P	403	LEU	6.2
1	P	348	ASP	6.2
1	X	298	LEU	6.2
1	P	364	ILE	6.2
1	K	311	ALA	6.2
1	J	448	THR	6.1
1	P	252	ARG	6.1
1	X	390	PHE	6.1
1	K	328	HIS	6.1
1	K	281	GLU	6.1
1	P	204	LEU	6.1
1	K	378	PRO	6.1
1	P	347	ALA	6.1
1	J	287	ASP	6.1
1	J	337	LEU	6.1
1	X	394	LYS	6.1
1	K	209	GLY	6.1
1	P	306	ALA	6.1
1	K	307	ALA	6.0
1	P	281	GLU	6.0
1	K	403	LEU	6.0
1	K	485	ILE	6.0
1	I	0	MET	6.0
1	X	197	THR	6.0
1	X	314	HIS	6.0
1	X	221	TRP	6.0
1	J	423	PRO	6.0
1	K	300	LEU	6.0
1	J	442	VAL	6.0
1	J	313	LEU	6.0
1	P	276	ILE	5.9
1	K	310	LEU	5.9
1	X	464	LEU	5.9
1	P	375	TYR	5.9
1	J	326	ILE	5.9
1	X	284	SER	5.9
1	K	229	LYS	5.9

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Mol	Chain	Res	Type	RSRZ
1	V	223	GLY	5.9
1	J	231	PHE	5.8
1	P	423	PRO	5.8
1	J	489	LEU	5.8
1	X	395	TRP	5.8
1	J	345	CYS	5.8
1	X	389	CYS	5.8
1	X	401	PHE	5.8
1	X	393	TYR	5.8
1	J	246	TYR	5.7
1	J	310	LEU	5.7
1	J	470	GLU	5.7
1	K	352	ALA	5.7
1	E	358	GLY	5.7
1	P	441	VAL	5.7
1	A	456	ALA	5.7
1	J	241	ARG	5.7
1	K	395	TRP	5.7
1	X	223	GLY	5.6
1	P	303	ALA	5.6
1	J	349	LEU	5.6
1	E	325	ALA	5.6
1	X	329	ARG	5.6
1	P	206	GLU	5.6
1	J	426	TYR	5.6
1	K	224	GLU	5.6
1	J	472	TRP	5.5
1	X	453	ASN	5.5
1	P	351	LEU	5.5
1	X	425	PHE	5.5
1	J	202	VAL	5.5
1	K	246	TYR	5.5
1	K	474	PRO	5.5
1	K	445	ASP	5.5
1	P	239	TRP	5.5
1	K	410	ARG	5.5
1	C	221	TRP	5.5
1	P	398	ILE	5.5
1	K	295	GLU	5.4
1	X	293	THR	5.4
1	J	385	ILE	5.4
1	P	448	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	J	389	CYS	5.4
1	P	340	SER	5.4
1	P	468	MET	5.3
1	J	334	ARG	5.3
1	K	470	GLU	5.3
1	K	449	PRO	5.3
1	K	325	ALA	5.3
1	P	254	ASP	5.3
1	X	231	PHE	5.3
1	P	198	VAL	5.3
1	X	308	CYS	5.3
1	X	467	MET	5.3
1	K	480	LEU	5.3
1	P	337	LEU	5.2
1	K	377	ALA	5.2
1	E	474	PRO	5.2
1	V	492	ILE	5.2
1	K	288	PHE	5.2
1	J	255	ASN	5.2
1	J	223	GLY	5.2
1	X	400	ALA	5.2
1	X	432	ASP	5.2
1	P	368	PRO	5.2
1	J	437	ASP	5.2
1	X	202	VAL	5.2
1	X	374	ARG	5.2
1	K	226	VAL	5.1
1	J	243	THR	5.1
1	K	448	THR	5.1
1	J	235	ASP	5.1
1	B	220	LEU	5.1
1	X	387	THR	5.1
1	P	311	ALA	5.1
1	J	480	LEU	5.1
1	K	308	CYS	5.1
1	L	387	THR	5.1
1	P	446	GLN	5.0
1	P	481	THR	5.0
1	X	448	THR	5.0
1	K	366	ASN	5.0
1	K	438	MET	5.0
1	K	419	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	P	392	SER	5.0
1	K	198	VAL	5.0
1	J	390	PHE	5.0
1	K	275	LEU	5.0
1	J	484	ARG	5.0
1	X	327	ALA	5.0
1	X	313	LEU	5.0
1	J	226	VAL	5.0
1	X	287	ASP	4.9
1	P	238	SER	4.9
1	P	394	LYS	4.9
1	X	286	TYR	4.9
1	P	475	ASN	4.9
1	X	439	LYS	4.9
1	K	199	ALA	4.9
1	J	375	TYR	4.9
1	P	380	VAL	4.9
1	X	381	LEU	4.9
1	X	303	ALA	4.9
1	B	493	SER	4.9
1	J	300	LEU	4.9
1	J	352	ALA	4.9
1	P	449	PRO	4.9
1	W	201	GLN	4.9
1	K	412	THR	4.9
1	X	368	PRO	4.9
1	J	350	GLY	4.8
1	X	398	ILE	4.8
1	X	226	VAL	4.8
1	K	491	LYS	4.8
1	X	222	HIS	4.8
1	J	476	PRO	4.8
1	P	324	PRO	4.8
1	P	248	THR	4.8
1	P	263	ASP	4.8
1	X	246	TYR	4.8
1	W	366	ASN	4.8
1	X	245	ILE	4.8
1	K	220	LEU	4.7
1	X	380	VAL	4.7
1	X	456	ALA	4.7
1	P	220	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	X	336	VAL	4.7
1	P	438	MET	4.7
1	K	244	GLU	4.7
1	K	400	ALA	4.7
1	X	455	LEU	4.7
1	J	475	ASN	4.7
1	K	336	VAL	4.7
1	E	0	MET	4.6
1	P	440	LYS	4.6
1	K	483	LEU	4.6
1	U	400	ALA	4.6
1	P	313	LEU	4.6
1	P	314	HIS	4.6
1	J	473	TYR	4.6
1	P	390	PHE	4.6
1	J	247	ASN	4.6
1	K	428	VAL	4.6
1	J	324	PRO	4.5
1	J	376	MET	4.5
1	X	340	SER	4.5
1	K	342	LEU	4.5
1	P	304	VAL	4.5
1	J	276	ILE	4.5
1	J	281	GLU	4.5
1	P	349	LEU	4.5
1	J	396	THR	4.5
1	W	213	TYR	4.5
1	F	388	ASP	4.5
1	X	385	ILE	4.5
1	B	199	ALA	4.5
1	K	231	PHE	4.5
1	U	460	VAL	4.5
1	J	420	ASP	4.5
1	P	466	GLN	4.5
1	X	204	LEU	4.5
1	C	453	ASN	4.4
1	X	277	THR	4.4
1	X	338	VAL	4.4
1	J	346	ILE	4.4
1	X	309	GLY	4.4
1	X	339	LYS	4.4
1	P	404	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	J	348	ASP	4.4
1	K	468	MET	4.4
1	O	224	GLU	4.4
1	X	276	ILE	4.4
1	K	475	ASN	4.4
1	P	280	HIS	4.3
1	P	209	GLY	4.3
1	X	392	SER	4.3
1	K	343	GLN	4.3
1	V	473	TYR	4.3
1	X	219	GLY	4.3
1	P	479	ARG	4.3
1	K	221	TRP	4.3
1	K	290	GLN	4.3
1	F	385	ILE	4.3
1	J	450	THR	4.3
1	X	332	LYS	4.3
1	U	224	GLU	4.3
1	K	420	ASP	4.3
1	K	205	VAL	4.3
1	P	199	ALA	4.3
1	J	464	LEU	4.3
1	K	443	CYS	4.3
1	X	288	PHE	4.2
1	K	429	VAL	4.2
1	L	377	ALA	4.2
1	J	213	TYR	4.2
1	X	258	GLY	4.2
1	X	441	VAL	4.2
1	P	457	ALA	4.2
1	X	479	ARG	4.2
1	P	386	ARG	4.2
1	J	486	LYS	4.2
1	J	280	HIS	4.2
1	X	207	CYS	4.2
1	P	358	GLY	4.2
1	X	240	PHE	4.2
1	X	470	GLU	4.2
1	R	388	ASP	4.2
1	X	254	ASP	4.2
1	P	332	LYS	4.1
1	J	262	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	P	469	ARG	4.1
1	J	456	ALA	4.1
1	P	290	GLN	4.1
1	X	348	ASP	4.1
1	X	216	VAL	4.1
1	J	312	HIS	4.1
1	X	410	ARG	4.1
1	J	397	ASP	4.1
1	X	345	CYS	4.1
1	X	292	GLN	4.1
1	E	493	SER	4.1
1	K	418	VAL	4.1
1	X	218	ARG	4.1
1	X	249	VAL	4.1
1	P	218	ARG	4.1
1	P	391	GLU	4.1
1	K	407	GLU	4.1
1	P	322	GLY	4.1
1	X	260	ILE	4.0
1	X	297	HIS	4.0
1	J	224	GLU	4.0
1	J	490	GLN	4.0
1	X	328	HIS	4.0
1	J	457	ALA	4.0
1	X	307	ALA	4.0
1	N	267	ARG	4.0
1	K	406	TRP	4.0
1	K	282	HIS	4.0
1	T	198	VAL	4.0
1	X	315	VAL	4.0
1	U	223	GLY	4.0
1	P	357	GLN	4.0
1	J	204	LEU	4.0
1	K	228	VAL	4.0
1	J	378	PRO	4.0
1	P	285	LEU	4.0
1	K	324	PRO	4.0
1	P	331	PHE	4.0
1	K	387	THR	3.9
1	P	250	LEU	3.9
1	U	387	THR	3.9
1	K	478	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	K	467	MET	3.9
1	X	353	VAL	3.9
1	P	463	GLY	3.9
1	X	466	GLN	3.9
1	J	279	TYR	3.9
1	K	331	PHE	3.9
1	K	341	ASN	3.9
1	K	230	ILE	3.9
1	J	222	HIS	3.9
1	X	275	LEU	3.9
1	K	347	ALA	3.9
1	P	482	ALA	3.9
1	J	406	TRP	3.9
1	N	388	ASP	3.8
1	K	466	GLN	3.8
1	X	256	ILE	3.8
1	J	483	LEU	3.8
1	E	361	TYR	3.8
1	X	475	ASN	3.8
1	W	204	LEU	3.8
1	X	341	ASN	3.8
1	J	379	GLU	3.8
1	W	281	GLU	3.8
1	F	361	TYR	3.8
1	J	398	ILE	3.8
1	L	455	LEU	3.8
1	X	253	HIS	3.8
1	X	241	ARG	3.8
1	J	254	ASP	3.8
1	X	294	LEU	3.8
1	U	493	SER	3.8
1	X	217	TRP	3.8
1	J	277	THR	3.8
1	P	488	THR	3.8
1	T	474	PRO	3.8
1	J	200	ARG	3.8
1	X	422	ARG	3.8
1	K	245	ILE	3.7
1	K	284	SER	3.7
1	F	475	ASN	3.7
1	K	249	VAL	3.7
1	S	226	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	V	251	LEU	3.7
1	B	196	ARG	3.7
1	C	307	ALA	3.7
1	W	205	VAL	3.7
1	K	427	ASP	3.7
1	E	223	GLY	3.7
1	K	257	LEU	3.7
1	X	481	THR	3.7
1	V	459	PRO	3.7
1	K	315	VAL	3.7
1	P	330	ASP	3.7
1	P	243	THR	3.7
1	K	484	ARG	3.7
1	X	252	ARG	3.7
1	J	493	SER	3.7
1	K	490	GLN	3.7
1	J	274	TRP	3.7
1	K	367	ASN	3.7
1	V	453	ASN	3.7
1	K	389	CYS	3.7
1	J	347	ALA	3.7
1	X	478	ALA	3.7
1	K	444	VAL	3.7
1	K	476	PRO	3.7
1	J	394	LYS	3.6
1	V	325	ALA	3.6
1	X	233	SER	3.6
1	T	197	THR	3.6
1	K	394	LYS	3.6
1	F	395	TRP	3.6
1	J	230	ILE	3.6
1	K	283	GLY	3.6
1	P	452	PRO	3.6
1	T	487	LYS	3.6
1	X	431	ASN	3.6
1	X	427	ASP	3.6
1	W	474	PRO	3.6
1	E	205	VAL	3.6
1	K	287	ASP	3.6
1	J	256	ILE	3.6
1	J	225	SER	3.6
1	W	258	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	W	222	HIS	3.6
1	V	308	CYS	3.6
1	I	203	ALA	3.5
1	K	340	SER	3.5
1	C	455	LEU	3.5
1	X	444	VAL	3.5
1	P	233	SER	3.5
1	J	336	VAL	3.5
1	L	358	GLY	3.5
1	M	358	GLY	3.5
1	J	488	THR	3.5
1	K	294	LEU	3.5
1	S	377	ALA	3.5
1	X	311	ALA	3.5
1	L	473	TYR	3.5
1	K	345	CYS	3.5
1	K	441	VAL	3.5
1	P	424	PRO	3.5
1	X	214	GLY	3.5
1	X	306	ALA	3.5
1	K	247	ASN	3.5
1	X	296	PRO	3.5
1	E	471	CYS	3.5
1	K	479	ARG	3.5
1	K	437	ASP	3.5
1	W	303	ALA	3.5
1	K	208	VAL	3.5
1	P	253	HIS	3.5
1	P	312	HIS	3.5
1	E	475	ASN	3.4
1	K	424	PRO	3.4
1	P	363	ASP	3.4
1	K	272	GLN	3.4
1	P	293	THR	3.4
1	U	385	ILE	3.4
1	P	264	MET	3.4
1	T	195	GLN	3.4
1	X	423	PRO	3.4
1	J	399	TRP	3.4
1	P	353	VAL	3.4
1	P	258	GLY	3.4
1	X	397	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	P	467	MET	3.4
1	P	484	ARG	3.4
1	K	213	TYR	3.4
1	K	293	THR	3.4
1	X	440	LYS	3.4
1	J	290	GLN	3.4
1	V	224	GLU	3.4
1	J	219	GLY	3.4
1	X	232	SER	3.4
1	E	245	ILE	3.4
1	K	326	ILE	3.4
1	W	364	ILE	3.4
1	K	233	SER	3.4
1	X	208	VAL	3.4
1	J	410	ARG	3.4
1	F	362	LEU	3.4
1	F	359	SER	3.4
1	T	202	VAL	3.4
1	U	205	VAL	3.4
1	I	389	CYS	3.3
1	J	469	ARG	3.3
1	K	204	LEU	3.3
1	J	395	TRP	3.3
1	J	228	VAL	3.3
1	P	419	GLU	3.3
1	K	382	ASP	3.3
1	P	428	VAL	3.3
1	B	204	LEU	3.3
1	J	273	LEU	3.3
1	P	382	ASP	3.3
1	H	220	LEU	3.3
1	J	275	LEU	3.3
1	P	412	THR	3.3
1	W	389	CYS	3.3
1	V	418	VAL	3.3
1	K	302	LEU	3.3
1	J	242	GLU	3.3
1	J	436	GLU	3.3
1	R	475	ASN	3.3
1	P	305	SER	3.3
1	J	479	ARG	3.3
1	P	365	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	U	378	PRO	3.3
1	J	286	TYR	3.3
1	W	197	THR	3.3
1	J	203	ALA	3.3
1	J	340	SER	3.3
1	J	429	VAL	3.2
1	K	298	LEU	3.2
1	K	263	ASP	3.2
1	L	393	TYR	3.2
1	U	248	THR	3.2
1	K	379	GLU	3.2
1	X	326	ILE	3.2
1	K	210	LYS	3.2
1	H	460	VAL	3.2
1	K	202	VAL	3.2
1	N	358	GLY	3.2
1	T	467	MET	3.2
1	U	476	PRO	3.2
1	J	240	PHE	3.2
1	P	342	LEU	3.2
1	P	389	CYS	3.2
1	J	221	TRP	3.2
1	L	395	TRP	3.2
1	P	425	PHE	3.2
1	X	430	PRO	3.2
1	J	284	SER	3.2
1	K	409	ALA	3.2
1	O	213	TYR	3.2
1	X	346	ILE	3.2
1	C	449	PRO	3.2
1	K	353	VAL	3.2
1	P	406	TRP	3.2
1	X	198	VAL	3.2
1	P	385	ILE	3.2
1	J	283	GLY	3.2
1	K	482	ALA	3.2
1	M	213	TYR	3.2
1	K	203	ALA	3.2
1	F	250	LEU	3.1
1	X	487	LYS	3.1
1	J	443	CYS	3.1
1	V	414	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	434	SER	3.1
1	W	232	SER	3.1
1	L	478	ALA	3.1
1	N	482	ALA	3.1
1	P	278	HIS	3.1
1	X	347	ALA	3.1
1	J	391	GLU	3.1
1	X	195	GLN	3.1
1	K	350	GLY	3.1
1	K	227	ALA	3.1
1	M	277	THR	3.1
1	P	450	THR	3.1
1	C	431	ASN	3.1
1	K	262	SER	3.1
1	P	493	SER	3.1
1	K	348	ASP	3.1
1	P	397	ASP	3.1
1	K	464	LEU	3.1
1	X	378	PRO	3.1
1	P	336	VAL	3.1
1	K	255	ASN	3.1
1	X	403	LEU	3.1
1	I	493	SER	3.1
1	K	374	ARG	3.1
1	P	341	ASN	3.1
1	K	346	ILE	3.1
1	P	356	SER	3.1
1	X	305	SER	3.1
1	X	473	TYR	3.1
1	J	236	GLU	3.1
1	O	290	GLN	3.1
1	J	234	ARG	3.0
1	P	454	ARG	3.0
1	K	207	CYS	3.0
1	B	198	VAL	3.0
1	J	249	VAL	3.0
1	P	282	HIS	3.0
1	J	293	THR	3.0
1	K	313	LEU	3.0
1	E	201	GLN	3.0
1	X	237	GLN	3.0
1	J	338	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	427	ASP	3.0
1	L	382	ASP	3.0
1	P	247	ASN	3.0
1	J	467	MET	3.0
1	I	195	GLN	3.0
1	K	280	HIS	3.0
1	J	412	THR	3.0
1	X	477	SER	3.0
1	X	485	ILE	3.0
1	K	278	HIS	3.0
1	A	457	ALA	3.0
1	K	489	LEU	3.0
1	J	333	SER	3.0
1	A	474	PRO	3.0
1	V	296	PRO	3.0
1	P	486	LYS	3.0
1	P	277	THR	3.0
1	P	477	SER	3.0
1	K	291	ARG	3.0
1	K	417	ILE	3.0
1	J	239	TRP	3.0
1	P	421	TYR	3.0
1	C	457	ALA	3.0
1	F	477	SER	3.0
1	K	277	THR	3.0
1	C	0	MET	3.0
1	J	468	MET	3.0
1	K	254	ASP	3.0
1	U	444	VAL	3.0
1	P	453	ASN	3.0
1	X	343	GLN	3.0
1	U	369	ARG	2.9
1	G	388	ASP	2.9
1	K	276	ILE	2.9
1	P	315	VAL	2.9
1	X	379	GLU	2.9
1	I	198	VAL	2.9
1	K	370	VAL	2.9
1	P	329	ARG	2.9
1	F	448	THR	2.9
1	O	387	THR	2.9
1	W	330	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	219	GLY	2.9
1	E	468	MET	2.9
1	C	197	THR	2.9
1	U	491	LYS	2.9
1	B	247	ASN	2.9
1	F	478	ALA	2.9
1	U	197	THR	2.9
1	X	411	ARG	2.9
1	J	332	LYS	2.9
1	K	232	SER	2.9
1	M	204	LEU	2.9
1	P	273	LEU	2.9
1	J	308	CYS	2.9
1	P	388	ASP	2.9
1	X	235	ASP	2.9
1	W	252	ARG	2.9
1	E	279	TYR	2.9
1	P	455	LEU	2.8
1	K	238	SER	2.8
1	K	252	ARG	2.8
1	W	224	GLU	2.8
1	W	245	ILE	2.8
1	J	208	VAL	2.8
1	P	251	LEU	2.8
1	P	262	SER	2.8
1	X	227	ALA	2.8
1	P	286	TYR	2.8
1	V	279	TYR	2.8
1	J	316	GLU	2.8
1	X	291	ARG	2.8
1	O	254	ASP	2.8
1	U	442	VAL	2.8
1	T	396	THR	2.8
1	K	390	PHE	2.8
1	P	275	LEU	2.8
1	P	350	GLY	2.8
1	W	304	VAL	2.8
1	K	401	PHE	2.8
1	T	448	THR	2.8
1	X	236	GLU	2.8
1	H	361	TYR	2.8
1	O	220	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	339	LYS	2.8
1	X	248	THR	2.8
1	J	403	LEU	2.8
1	Q	205	VAL	2.8
1	X	210	LYS	2.8
1	X	447	GLN	2.8
1	J	388	ASP	2.8
1	R	473	TYR	2.8
1	J	304	VAL	2.8
1	K	369	ARG	2.8
1	O	308	CYS	2.8
1	W	208	VAL	2.8
1	H	377	ALA	2.8
1	D	455	LEU	2.7
1	L	362	LEU	2.7
1	F	205	VAL	2.7
1	P	208	VAL	2.7
1	E	257	LEU	2.7
1	J	260	ILE	2.7
1	C	456	ALA	2.7
1	F	476	PRO	2.7
1	J	229	LYS	2.7
1	X	424	PRO	2.7
1	H	473	TYR	2.7
1	K	274	TRP	2.7
1	V	300	LEU	2.7
1	J	440	LYS	2.7
1	B	281	GLU	2.7
1	J	453	ASN	2.7
1	K	404	VAL	2.7
1	X	264	MET	2.7
1	X	263	ASP	2.7
1	J	422	ARG	2.7
1	K	430	PRO	2.7
1	P	301	ARG	2.7
1	P	274	TRP	2.7
1	T	389	CYS	2.7
1	V	302	LEU	2.7
1	K	473	TYR	2.7
1	P	426	TYR	2.7
1	F	466	GLN	2.7
1	U	226	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	W	244	GLU	2.7
1	B	431	ASN	2.7
1	K	286	TYR	2.7
1	W	242	GLU	2.7
1	X	302	LEU	2.7
1	C	473	TYR	2.7
1	C	474	PRO	2.7
1	P	227	ALA	2.7
1	U	457	ALA	2.7
1	F	487	LYS	2.6
1	P	416	GLY	2.6
1	C	198	VAL	2.6
1	D	418	VAL	2.6
1	K	260	ILE	2.6
1	X	299	ALA	2.6
1	X	247	ASN	2.6
1	X	312	HIS	2.6
1	E	319	GLY	2.6
1	K	380	VAL	2.6
1	S	199	ALA	2.6
1	C	399	TRP	2.6
1	K	397	ASP	2.6
1	P	317	ILE	2.6
1	B	473	TYR	2.6
1	L	361	TYR	2.6
1	P	201	GLN	2.6
1	V	471	CYS	2.6
1	J	381	LEU	2.6
1	X	273	LEU	2.6
1	X	420	ASP	2.6
1	P	439	LYS	2.6
1	L	474	PRO	2.6
1	P	411	ARG	2.6
1	X	325	ALA	2.6
1	I	236	GLU	2.6
1	P	379	GLU	2.6
1	E	362	LEU	2.6
1	J	463	GLY	2.6
1	B	344	CYS	2.6
1	K	329	ARG	2.6
1	J	384	GLN	2.6
1	E	359	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	W	448	THR	2.6
1	K	314	HIS	2.6
1	P	328	HIS	2.6
1	K	334	ARG	2.6
1	M	228	VAL	2.6
1	P	296	PRO	2.6
1	X	255	ASN	2.5
1	T	344	CYS	2.5
1	A	387	THR	2.5
1	R	254	ASP	2.5
1	A	473	TYR	2.5
1	T	473	TYR	2.5
1	P	491	LYS	2.5
1	J	485	ILE	2.5
1	P	256	ILE	2.5
1	L	475	ASN	2.5
1	O	325	ALA	2.5
1	W	250	LEU	2.5
1	X	335	ASN	2.5
1	S	236	GLU	2.5
1	X	316	GLU	2.5
1	R	493	SER	2.5
1	R	309	GLY	2.5
1	R	386	ARG	2.5
1	K	289	LEU	2.5
1	J	380	VAL	2.5
1	O	418	VAL	2.5
1	E	320	THR	2.5
1	U	431	ASN	2.5
1	A	216	VAL	2.5
1	C	311	ALA	2.5
1	F	377	ALA	2.5
1	S	216	VAL	2.5
1	R	467	MET	2.5
1	H	309	GLY	2.5
1	E	324	PRO	2.5
1	B	338	VAL	2.5
1	O	464	LEU	2.5
1	P	405	LEU	2.5
1	F	325	ALA	2.5
1	J	207	CYS	2.5
1	K	436	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	U	443	CYS	2.5
1	A	361	TYR	2.5
1	J	330	ASP	2.5
1	K	339	LYS	2.4
1	J	377	ALA	2.4
1	K	261	ALA	2.4
1	K	248	THR	2.4
1	K	411	ARG	2.4
1	V	488	THR	2.4
1	P	284	SER	2.4
1	G	0	MET	2.4
1	K	335	ASN	2.4
1	H	240	PHE	2.4
1	L	250	LEU	2.4
1	K	442	VAL	2.4
1	M	205	VAL	2.4
1	V	385	ILE	2.4
1	W	377	ALA	2.4
1	K	372	THR	2.4
1	E	395	TRP	2.4
1	X	386	ARG	2.4
1	V	352	ALA	2.4
1	I	197	THR	2.4
1	K	431	ASN	2.4
1	O	268	ASN	2.4
1	E	378	PRO	2.4
1	N	449	PRO	2.4
1	X	196	ARG	2.4
1	J	413	ILE	2.4
1	Q	491	LYS	2.4
1	A	481	THR	2.4
1	W	365	GLY	2.4
1	J	382	ASP	2.4
1	B	489	LEU	2.4
1	J	237	GLN	2.4
1	P	430	PRO	2.4
1	V	395	TRP	2.4
1	X	344	CYS	2.4
1	W	243	THR	2.4
1	T	255	ASN	2.4
1	R	490	GLN	2.4
1	A	421	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	464	LEU	2.4
1	J	297	HIS	2.4
1	W	284	SER	2.4
1	J	291	ARG	2.4
1	O	469	ARG	2.4
1	U	235	ASP	2.4
1	E	357	GLN	2.4
1	S	378	PRO	2.4
1	T	0	MET	2.4
1	W	354	MET	2.4
1	V	458	ASP	2.4
1	W	363	ASP	2.4
1	R	446	GLN	2.4
1	T	431	ASN	2.4
1	E	483	LEU	2.3
1	P	240	PHE	2.3
1	B	336	VAL	2.3
1	L	400	ALA	2.3
1	P	369	ARG	2.3
1	P	485	ILE	2.3
1	U	328	HIS	2.3
1	F	474	PRO	2.3
1	J	238	SER	2.3
1	V	221	TRP	2.3
1	E	398	ILE	2.3
1	G	197	THR	2.3
1	A	240	PHE	2.3
1	X	212	ARG	2.3
1	P	399	TRP	2.3
1	P	420	ASP	2.3
1	W	221	TRP	2.3
1	J	408	ILE	2.3
1	J	439	LYS	2.3
1	A	369	ARG	2.3
1	F	484	ARG	2.3
1	J	212	ARG	2.3
1	X	454	ARG	2.3
1	J	288	PHE	2.3
1	A	395	TRP	2.3
1	R	482	ALA	2.3
1	O	202	VAL	2.3
1	T	417	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	298	LEU	2.3
1	E	389	CYS	2.3
1	V	244	GLU	2.3
1	V	306	ALA	2.3
1	B	279	TYR	2.3
1	M	460	VAL	2.3
1	D	461	LEU	2.3
1	U	461	LEU	2.3
1	L	390	PHE	2.3
1	K	316	GLU	2.3
1	N	0	MET	2.3
1	U	335	ASN	2.3
1	U	482	ALA	2.3
1	N	198	VAL	2.3
1	C	448	THR	2.3
1	P	197	THR	2.3
1	V	213	TYR	2.3
1	K	447	GLN	2.3
1	P	362	LEU	2.3
1	W	251	LEU	2.3
1	A	459	PRO	2.3
1	L	378	PRO	2.3
1	P	459	PRO	2.3
1	J	327	ALA	2.3
1	X	352	ALA	2.3
1	X	484	ARG	2.3
1	K	344	CYS	2.3
1	V	413	ILE	2.3
1	X	488	THR	2.3
1	K	384	GLN	2.3
1	X	349	LEU	2.2
1	B	232	SER	2.2
1	D	415	ASN	2.2
1	J	409	ALA	2.2
1	B	399	TRP	2.2
1	C	357	GLN	2.2
1	U	396	THR	2.2
1	X	244	GLU	2.2
1	P	445	ASP	2.2
1	O	223	GLY	2.2
1	V	416	GLY	2.2
1	E	473	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	251	LEU	2.2
1	J	344	CYS	2.2
1	T	455	LEU	2.2
1	W	231	PHE	2.2
1	O	394	LYS	2.2
1	D	247	ASN	2.2
1	A	358	GLY	2.2
1	A	377	ALA	2.2
1	Q	325	ALA	2.2
1	V	312	HIS	2.2
1	B	467	MET	2.2
1	B	197	THR	2.2
1	N	221	TRP	2.2
1	V	197	THR	2.2
1	F	251	LEU	2.2
1	U	480	LEU	2.2
1	O	471	CYS	2.2
1	P	232	SER	2.2
1	T	476	PRO	2.2
1	G	223	GLY	2.2
1	J	227	ALA	2.2
1	V	311	ALA	2.2
1	B	438	MET	2.2
1	E	264	MET	2.2
1	B	326	ILE	2.2
1	E	221	TRP	2.2
1	F	481	THR	2.2
1	P	410	ARG	2.2
1	Q	448	THR	2.2
1	A	213	TYR	2.2
1	P	259	PHE	2.2
1	R	476	PRO	2.2
1	E	470	GLU	2.2
1	U	281	GLU	2.2
1	F	409	ALA	2.2
1	T	457	ALA	2.2
1	V	457	ALA	2.2
1	U	353	VAL	2.2
1	U	386	ARG	2.2
1	V	460	VAL	2.2
1	J	455	LEU	2.2
1	E	224	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	357	GLN	2.2
1	F	368	PRO	2.2
1	I	318	PHE	2.2
1	K	433	PRO	2.2
1	P	361	TYR	2.2
1	P	407	GLU	2.2
1	X	446	GLN	2.2
1	V	222	HIS	2.2
1	P	226	VAL	2.2
1	S	0	MET	2.2
1	T	451	ILE	2.2
1	N	359	SER	2.2
1	J	430	PRO	2.2
1	L	318	PHE	2.2
1	Q	476	PRO	2.2
1	K	440	LYS	2.2
1	L	469	ARG	2.2
1	D	471	CYS	2.2
1	P	354	MET	2.2
1	O	395	TRP	2.1
1	W	343	GLN	2.1
1	A	493	SER	2.1
1	X	317	ILE	2.1
1	M	431	ASN	2.1
1	E	252	ARG	2.1
1	J	278	HIS	2.1
1	J	263	ASP	2.1
1	C	387	THR	2.1
1	P	345	CYS	2.1
1	U	389	CYS	2.1
1	W	336	VAL	2.1
1	O	221	TRP	2.1
1	F	390	PHE	2.1
1	X	433	PRO	2.1
1	J	386	ARG	2.1
1	J	272	GLN	2.1
1	S	457	ALA	2.1
1	U	394	LYS	2.1
1	Q	353	VAL	2.1
1	X	370	VAL	2.1
1	D	358	GLY	2.1
1	P	451	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	366	ASN	2.1
1	P	231	PHE	2.1
1	P	215	GLU	2.1
1	J	343	GLN	2.1
1	E	377	ALA	2.1
1	I	235	ASP	2.1
1	W	307	ALA	2.1
1	B	251	LEU	2.1
1	E	310	LEU	2.1
1	W	226	VAL	2.1
1	J	451	ILE	2.1
1	P	339	LYS	2.1
1	H	222	HIS	2.1
1	I	222	HIS	2.1
1	R	357	GLN	2.1
1	T	213	TYR	2.1
1	T	279	TYR	2.1
1	F	457	ALA	2.1
1	W	306	ALA	2.1
1	B	480	LEU	2.1
1	K	349	LEU	2.1
1	X	209	GLY	2.1
1	J	264	MET	2.1
1	I	474	PRO	2.1
1	X	469	ARG	2.1
1	J	209	GLY	2.1
1	H	224	GLU	2.1
1	R	220	LEU	2.1
1	J	481	THR	2.1
1	K	197	THR	2.1
1	O	425	PHE	2.1
1	W	492	ILE	2.1
1	H	426	TYR	2.1
1	H	370	VAL	2.1
1	T	444	VAL	2.1
1	H	492	ILE	2.1
1	U	230	ILE	2.1
1	P	458	ASP	2.1
1	Q	486	LYS	2.1
1	S	196	ARG	2.1
1	J	206	GLU	2.1
1	M	306	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	310	LEU	2.0
1	X	450	THR	2.0
1	C	395	TRP	2.0
1	X	323	LYS	2.0
1	F	307	ALA	2.0
1	Q	359	SER	2.0
1	V	307	ALA	2.0
1	B	273	LEU	2.0
1	J	342	LEU	2.0
1	R	443	CYS	2.0
1	K	216	VAL	2.0
1	P	487	LYS	2.0
1	K	317	ILE	2.0
1	K	435	PHE	2.0
1	U	470	GLU	2.0
1	E	222	HIS	2.0
1	V	365	GLY	2.0
1	W	223	GLY	2.0
1	A	489	LEU	2.0
1	B	213	TYR	2.0
1	F	289	LEU	2.0
1	L	381	LEU	2.0
1	R	393	TYR	2.0
1	K	469	ARG	2.0
1	T	196	ARG	2.0
1	T	414	VAL	2.0
1	Q	221	TRP	2.0
1	H	371	GLY	2.0
1	K	292	GLN	2.0
1	P	323	LYS	2.0
1	P	333	SER	2.0
1	X	373	LYS	2.0
1	E	478	ALA	2.0
1	M	349	LEU	2.0
1	W	261	ALA	2.0
1	W	277	THR	2.0
1	A	443	CYS	2.0
1	K	240	PHE	2.0

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
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 (i)

There are no such residues in this entry.