



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:21 AM GMT

PDB ID : 3OEE
Title : Structure of four mutant forms of yeast F1 ATPase: alpha-F405S
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.
Deposited on : 2010-08-12
Resolution : 2.74 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 ⓘ symbol.

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

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

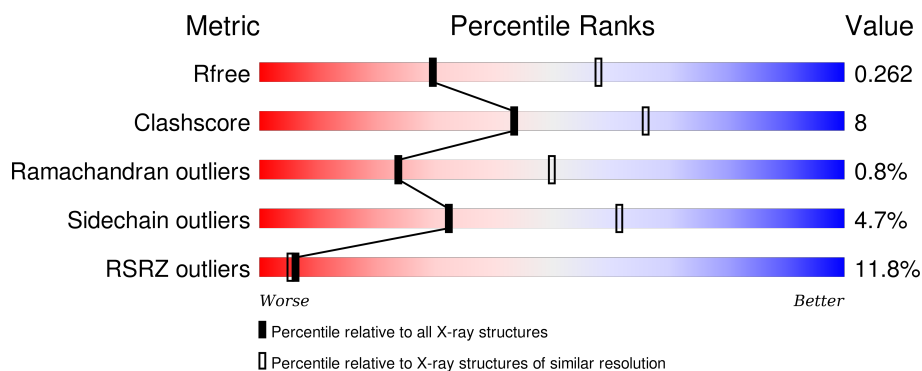
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
1	J	510	
1	K	510	

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Mol	Chain	Length	Quality of chain
1	L	510	
1	S	510	
1	T	510	
1	U	510	
2	D	484	
2	E	484	
2	F	484	
2	M	484	
2	N	484	
2	O	484	
2	V	484	
2	W	484	
2	X	484	
3	G	278	
3	P	278	
3	Y	278	
4	H	138	
4	Q	138	
4	Z	138	
5	I	61	
5	I	61	
5	R	61	

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
7	MG	D	700	-	-	-	X
7	MG	F	700	-	-	-	X
7	MG	O	700	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 72675 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3659	2308	648	700	3			
1	B	483	Total	C	N	O	S	0	0	0
			3664	2311	649	701	3			
1	C	484	Total	C	N	O	S	0	0	0
			3675	2319	650	703	3			
1	J	481	Total	C	N	O	S	0	0	0
			3650	2303	646	698	3			
1	K	486	Total	C	N	O	S	0	0	0
			3679	2320	652	704	3			
1	L	482	Total	C	N	O	S	0	0	0
			3659	2308	648	700	3			
1	S	477	Total	C	N	O	S	0	0	0
			3622	2287	642	690	3			
1	T	478	Total	C	N	O	S	0	0	0
			3632	2293	643	693	3			
1	U	481	Total	C	N	O	S	0	0	0
			3650	2302	646	699	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
B	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
C	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
J	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
K	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
L	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
S	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
T	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
U	405	SER	PHE	ENGINEERED MUTATION	UNP P07251

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3545	2248	603	688	6			
2	E	468	Total	C	N	O	S	0	0	0
			3504	2223	598	677	6			
2	F	469	Total	C	N	O	S	0	0	0
			3527	2238	602	681	6			
2	M	470	Total	C	N	O	S	0	0	0
			3535	2243	600	686	6			
2	N	470	Total	C	N	O	S	0	0	0
			3541	2245	602	688	6			
2	O	468	Total	C	N	O	S	0	0	0
			3534	2242	602	684	6			
2	V	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	W	467	Total	C	N	O	S	0	0	0
			3531	2240	601	684	6			
2	X	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	ALA	-	EXPRESSION TAG	UNP P00830
D	-4	SER	-	EXPRESSION TAG	UNP P00830
D	-3	HIS	-	EXPRESSION TAG	UNP P00830
D	-2	HIS	-	EXPRESSION TAG	UNP P00830
D	-1	HIS	-	EXPRESSION TAG	UNP P00830
D	0	HIS	-	EXPRESSION TAG	UNP P00830
D	1	HIS	-	EXPRESSION TAG	UNP P00830
D	2	HIS	-	EXPRESSION TAG	UNP P00830
E	-5	ALA	-	EXPRESSION TAG	UNP P00830
E	-4	SER	-	EXPRESSION TAG	UNP P00830
E	-3	HIS	-	EXPRESSION TAG	UNP P00830
E	-2	HIS	-	EXPRESSION TAG	UNP P00830
E	-1	HIS	-	EXPRESSION TAG	UNP P00830
E	0	HIS	-	EXPRESSION TAG	UNP P00830
E	1	HIS	-	EXPRESSION TAG	UNP P00830
E	2	HIS	-	EXPRESSION TAG	UNP P00830
F	-5	ALA	-	EXPRESSION TAG	UNP P00830
F	-4	SER	-	EXPRESSION TAG	UNP P00830
F	-3	HIS	-	EXPRESSION TAG	UNP P00830
F	-2	HIS	-	EXPRESSION TAG	UNP P00830
F	-1	HIS	-	EXPRESSION TAG	UNP P00830
F	0	HIS	-	EXPRESSION TAG	UNP P00830

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	HIS	-	EXPRESSION TAG	UNP P00830
F	2	HIS	-	EXPRESSION TAG	UNP P00830
M	-5	ALA	-	EXPRESSION TAG	UNP P00830
M	-4	SER	-	EXPRESSION TAG	UNP P00830
M	-3	HIS	-	EXPRESSION TAG	UNP P00830
M	-2	HIS	-	EXPRESSION TAG	UNP P00830
M	-1	HIS	-	EXPRESSION TAG	UNP P00830
M	0	HIS	-	EXPRESSION TAG	UNP P00830
M	1	HIS	-	EXPRESSION TAG	UNP P00830
M	2	HIS	-	EXPRESSION TAG	UNP P00830
N	-5	ALA	-	EXPRESSION TAG	UNP P00830
N	-4	SER	-	EXPRESSION TAG	UNP P00830
N	-3	HIS	-	EXPRESSION TAG	UNP P00830
N	-2	HIS	-	EXPRESSION TAG	UNP P00830
N	-1	HIS	-	EXPRESSION TAG	UNP P00830
N	0	HIS	-	EXPRESSION TAG	UNP P00830
N	1	HIS	-	EXPRESSION TAG	UNP P00830
N	2	HIS	-	EXPRESSION TAG	UNP P00830
O	-5	ALA	-	EXPRESSION TAG	UNP P00830
O	-4	SER	-	EXPRESSION TAG	UNP P00830
O	-3	HIS	-	EXPRESSION TAG	UNP P00830
O	-2	HIS	-	EXPRESSION TAG	UNP P00830
O	-1	HIS	-	EXPRESSION TAG	UNP P00830
O	0	HIS	-	EXPRESSION TAG	UNP P00830
O	1	HIS	-	EXPRESSION TAG	UNP P00830
O	2	HIS	-	EXPRESSION TAG	UNP P00830
V	-5	ALA	-	EXPRESSION TAG	UNP P00830
V	-4	SER	-	EXPRESSION TAG	UNP P00830
V	-3	HIS	-	EXPRESSION TAG	UNP P00830
V	-2	HIS	-	EXPRESSION TAG	UNP P00830
V	-1	HIS	-	EXPRESSION TAG	UNP P00830
V	0	HIS	-	EXPRESSION TAG	UNP P00830
V	1	HIS	-	EXPRESSION TAG	UNP P00830
V	2	HIS	-	EXPRESSION TAG	UNP P00830
W	-5	ALA	-	EXPRESSION TAG	UNP P00830
W	-4	SER	-	EXPRESSION TAG	UNP P00830
W	-3	HIS	-	EXPRESSION TAG	UNP P00830
W	-2	HIS	-	EXPRESSION TAG	UNP P00830
W	-1	HIS	-	EXPRESSION TAG	UNP P00830
W	0	HIS	-	EXPRESSION TAG	UNP P00830
W	1	HIS	-	EXPRESSION TAG	UNP P00830
W	2	HIS	-	EXPRESSION TAG	UNP P00830

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-5	ALA	-	EXPRESSION TAG	UNP P00830
X	-4	SER	-	EXPRESSION TAG	UNP P00830
X	-3	HIS	-	EXPRESSION TAG	UNP P00830
X	-2	HIS	-	EXPRESSION TAG	UNP P00830
X	-1	HIS	-	EXPRESSION TAG	UNP P00830
X	0	HIS	-	EXPRESSION TAG	UNP P00830
X	1	HIS	-	EXPRESSION TAG	UNP P00830
X	2	HIS	-	EXPRESSION TAG	UNP P00830

- Molecule 3 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	266	Total	C	N	O	S	0	0	0
			2055	1291	359	395	10			
3	P	244	Total	C	N	O	S	0	0	0
			1850	1162	323	356	9			
3	Y	200	Total	C	N	O	S	0	0	0
			1517	944	273	291	9			

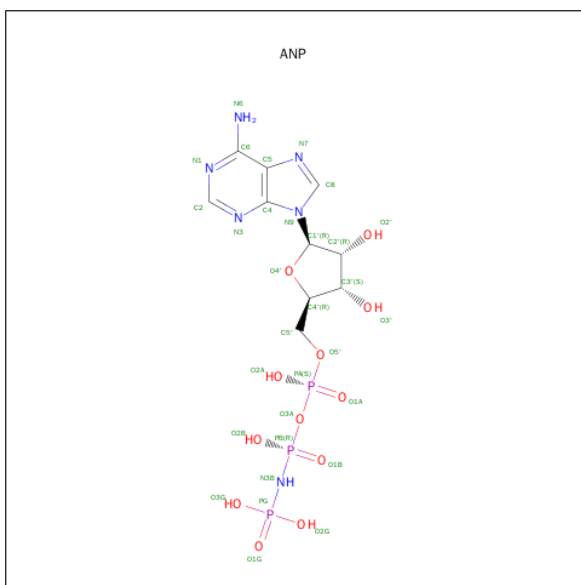
- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	122	Total	C	N	O	S	0	0	0
			795	497	138	158	2			
4	Q	83	Total	C	N	O		0	0	0
			441	267	88	86				
4	Z	17	Total	C	N	O		0	0	0
			85	51	17	17				

- Molecule 5 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	49	Total	C	N	O	0	0	0
			339	212	57	70			
5	R	34	Total	C	N	O	0	0	0
			175	104	34	37			
5	1	27	Total	C	N	O	0	0	0
			145	86	31	28			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	D	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	F	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	J	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	K	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	L	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	M	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	O	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	S	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	T	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	U	1	Total 31	C 10	N 6	O 12	P 3	0	0
6	V	1	Total 31	C 10	N 6	O 12	P 3	0	0

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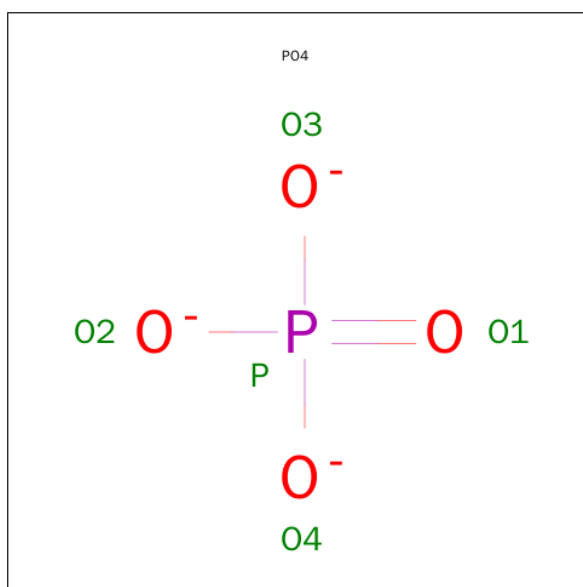
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	X	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	K	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	V	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		
7	T	1	Total	Mg	0	0
			1	1		
7	U	1	Total	Mg	0	0
			1	1		
7	X	1	Total	Mg	0	0
			1	1		
7	O	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		
7	S	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		
7	M	1	Total	Mg	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	O	P	0	0
			5	4	1		
8	N	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	10	Total	O	0	0
			10	10		
9	B	9	Total	O	0	0
			9	9		
9	C	3	Total	O	0	0
			3	3		
9	D	11	Total	O	0	0
			11	11		
9	E	10	Total	O	0	0
			10	10		
9	F	8	Total	O	0	0
			8	8		
9	G	2	Total	O	0	0
			2	2		
9	J	3	Total	O	0	0
			3	3		
9	K	5	Total	O	0	0
			5	5		
9	L	8	Total	O	0	0
			8	8		

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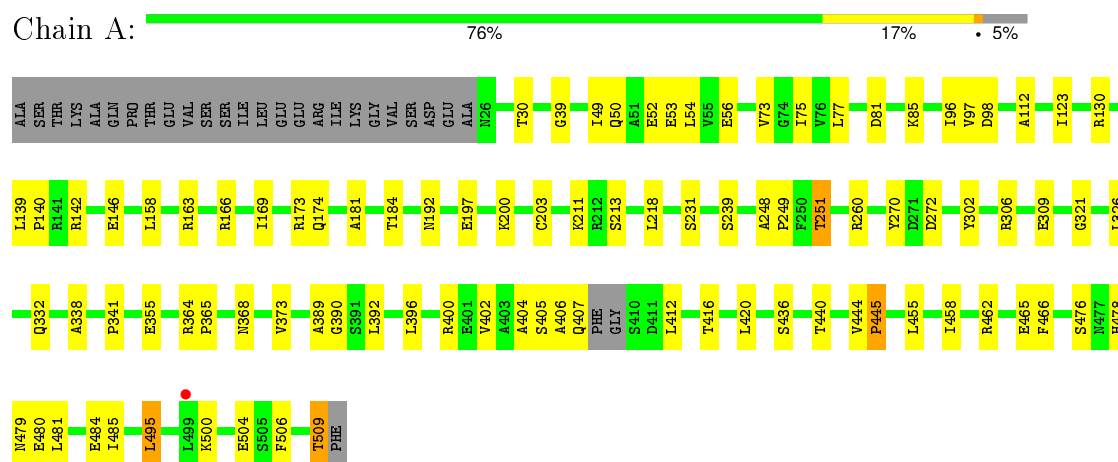
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	4	Total 4	O 4	0	0
9	N	3	Total 3	O 3	0	0
9	O	5	Total 5	O 5	0	0
9	P	2	Total 2	O 2	0	0
9	X	1	Total 1	O 1	0	0

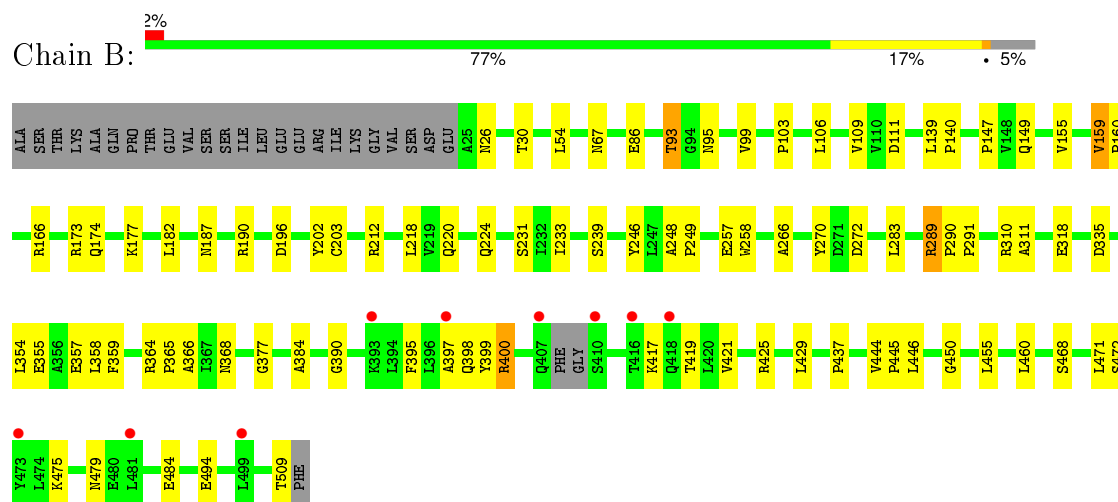
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

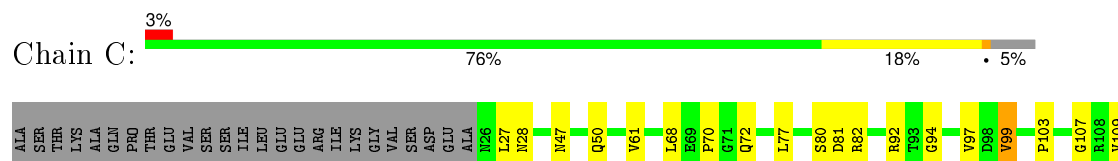
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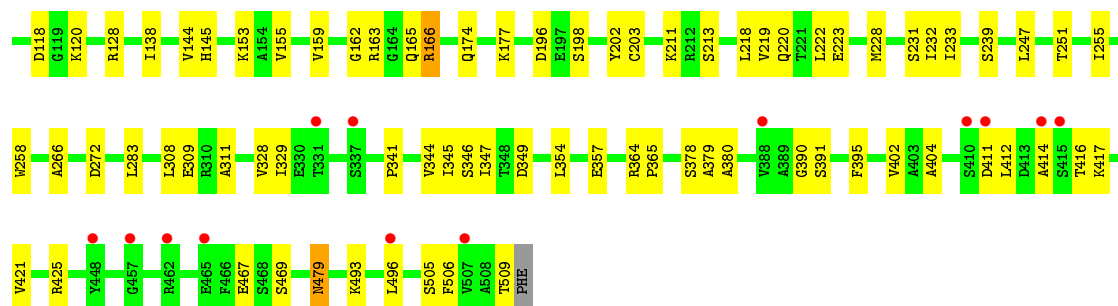


• Molecule 1: ATP synthase subunit alpha

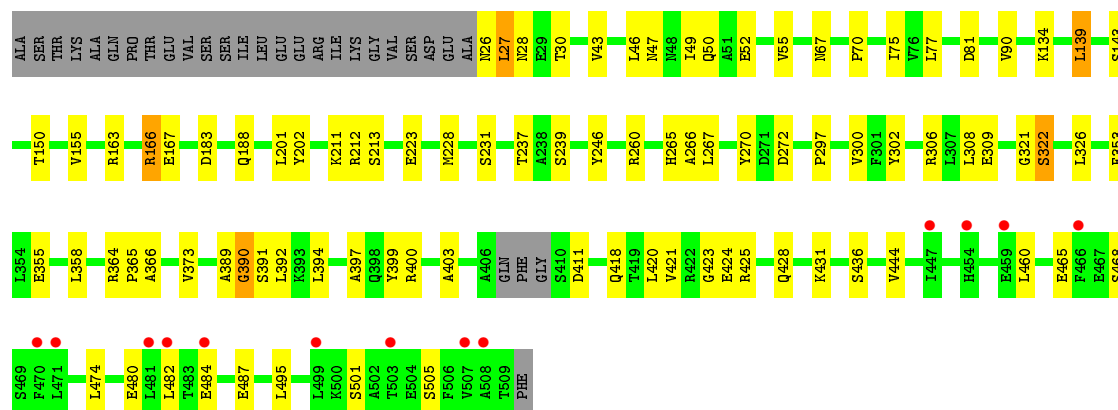
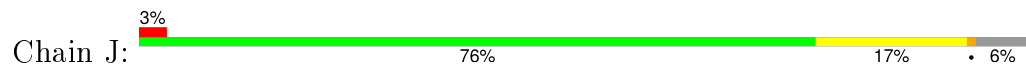


• Molecule 1: ATP synthase subunit alpha

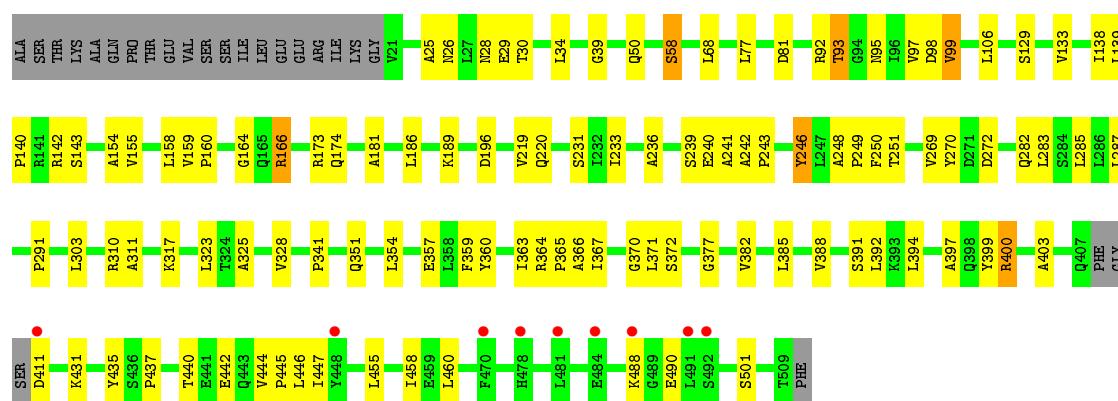




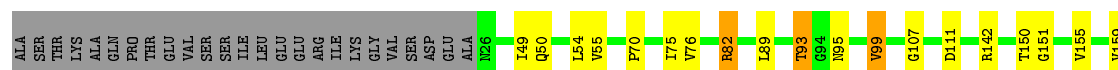
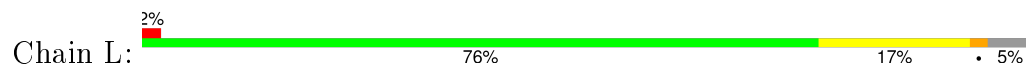
• Molecule 1: ATP synthase subunit alpha

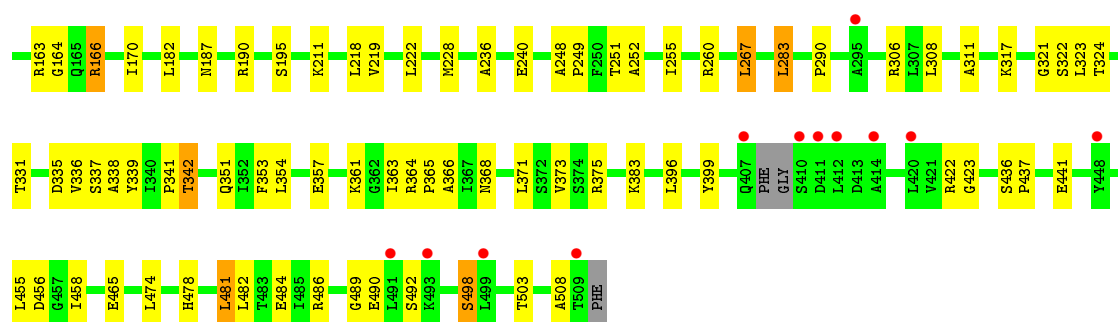


• Molecule 1: ATP synthase subunit alpha

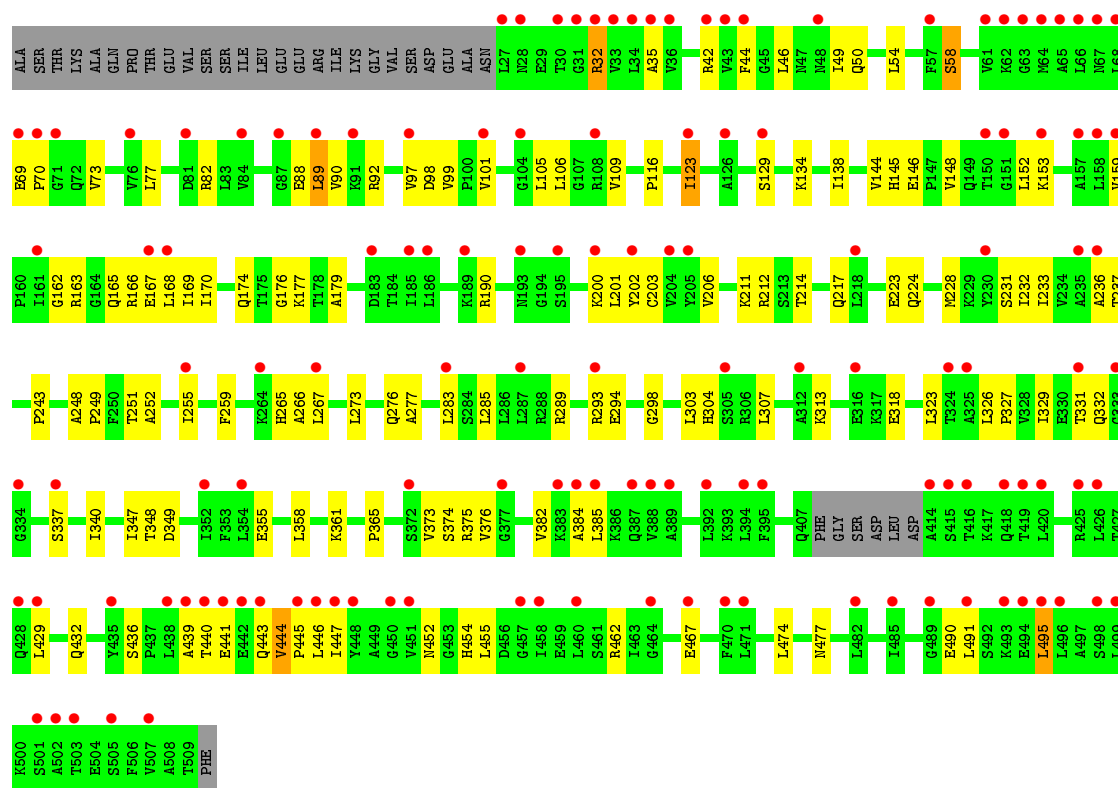


• Molecule 1: ATP synthase subunit alpha

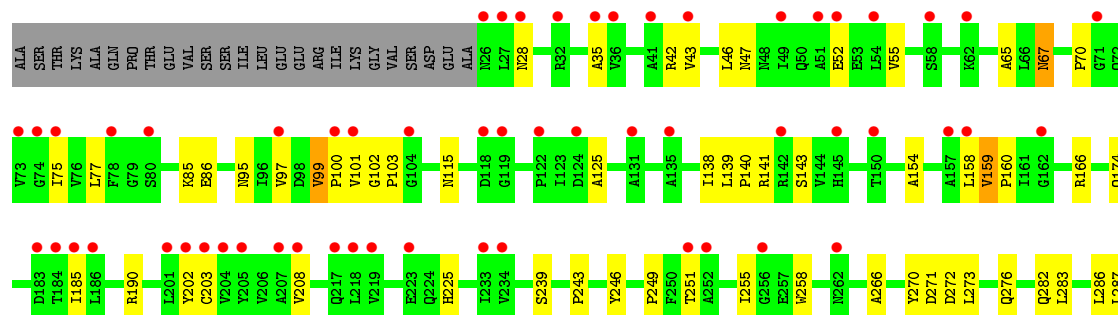
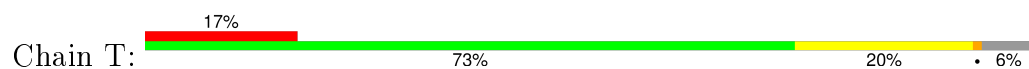


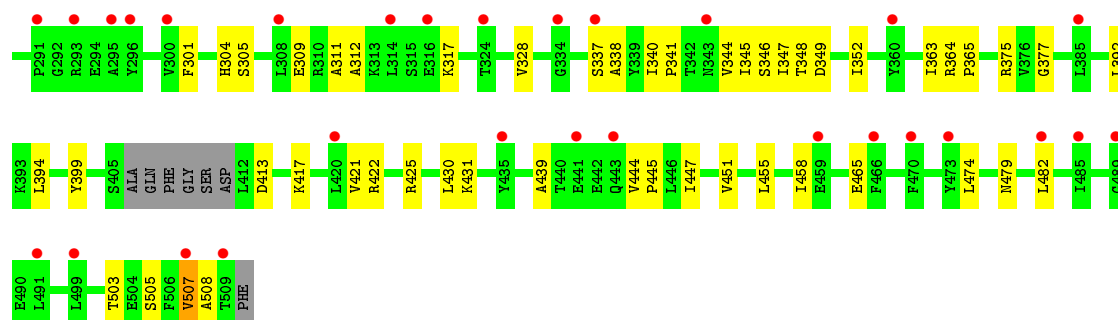


• Molecule 1: ATP synthase subunit alpha

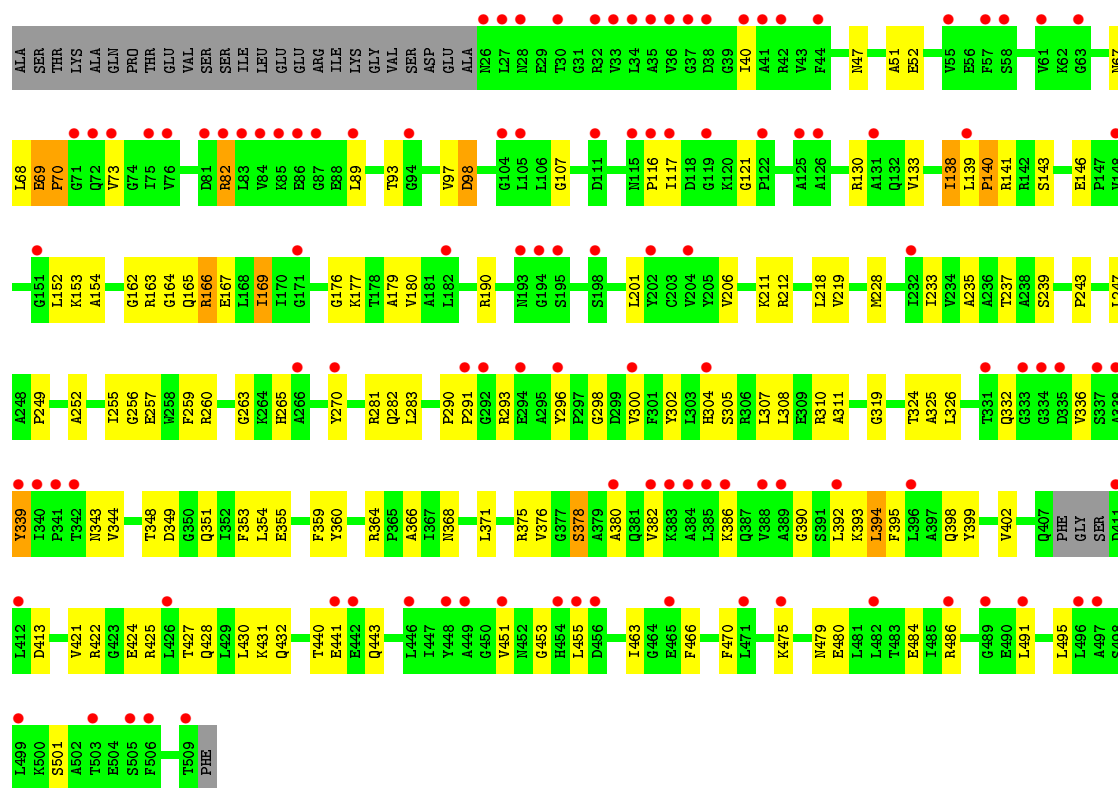


• Molecule 1: ATP synthase subunit alpha

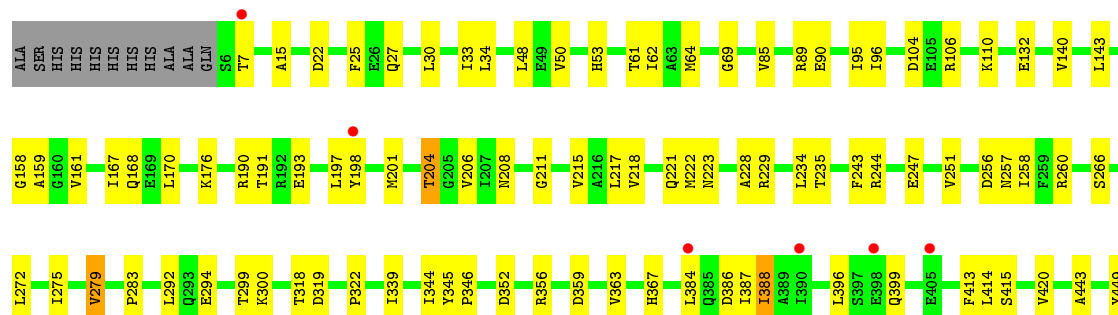
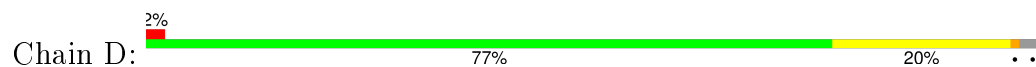


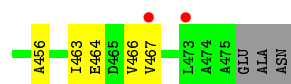


• Molecule 1: ATP synthase subunit alpha

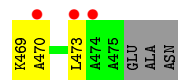
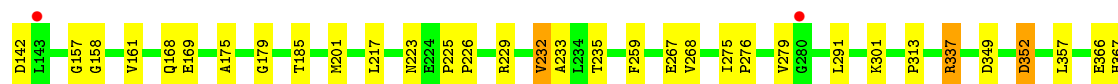
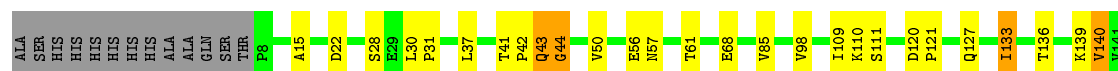
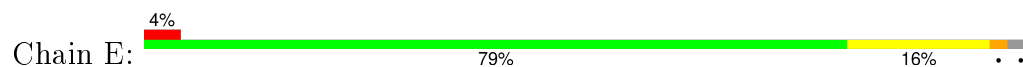


• Molecule 2: ATP synthase subunit beta

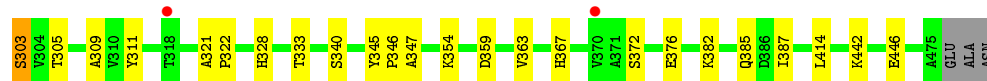
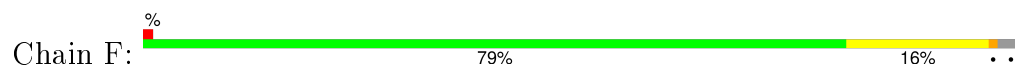




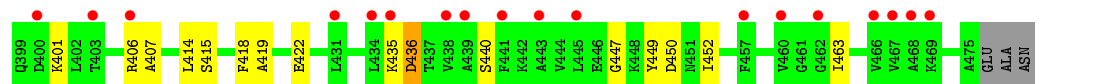
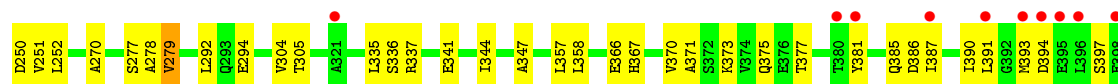
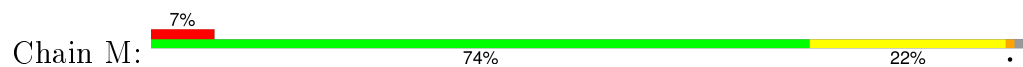
- Molecule 2: ATP synthase subunit beta



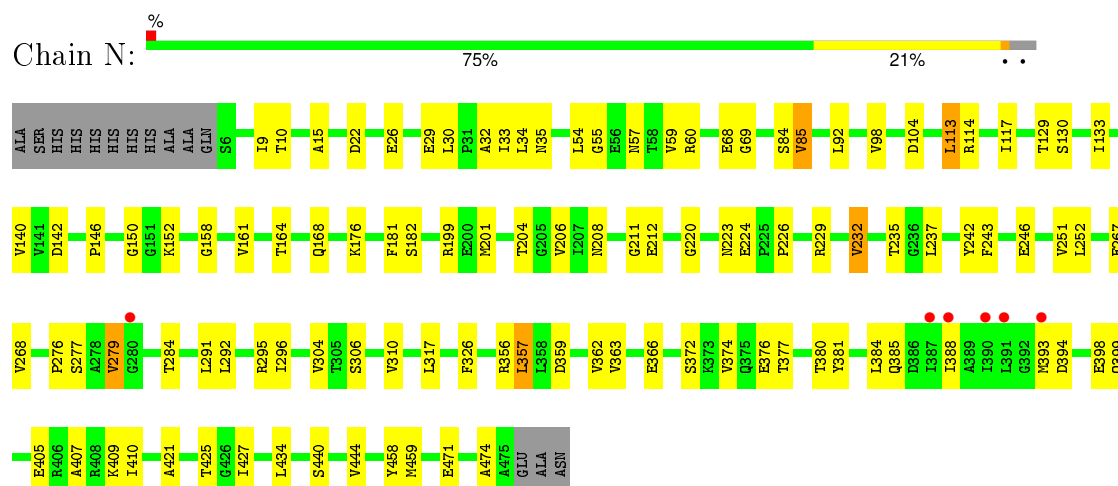
- Molecule 2: ATP synthase subunit beta



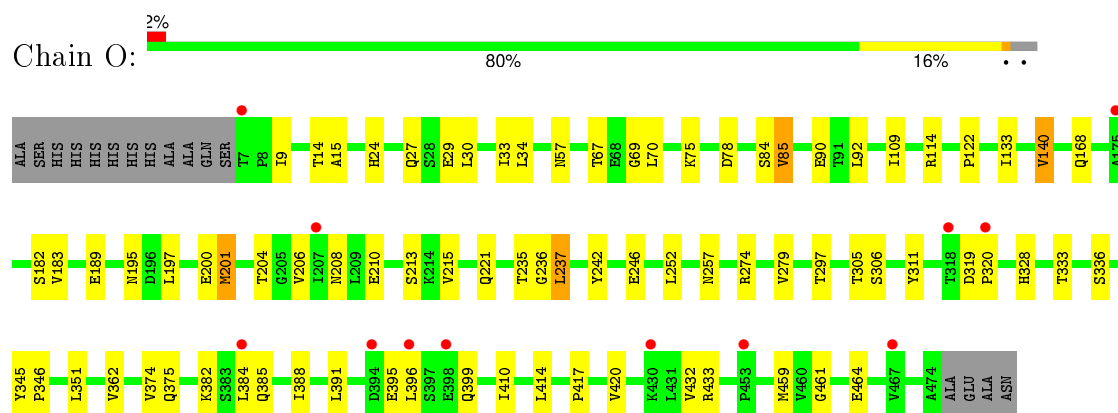
- Molecule 2: ATP synthase subunit beta



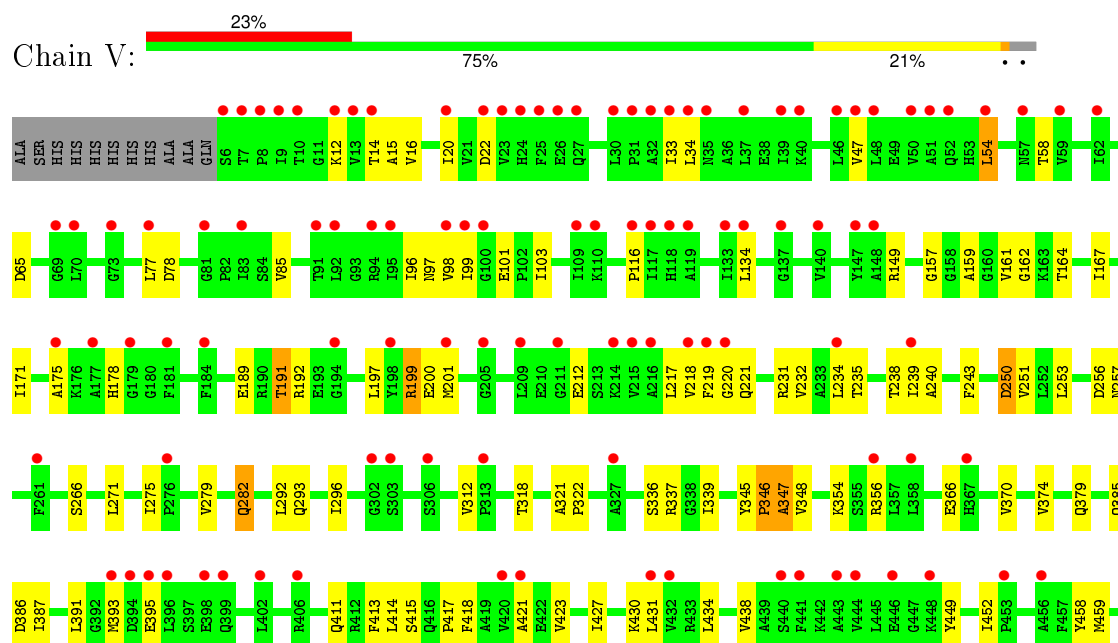
- Molecule 2: ATP synthase subunit beta

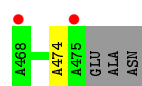


- Molecule 2: ATP synthase subunit beta

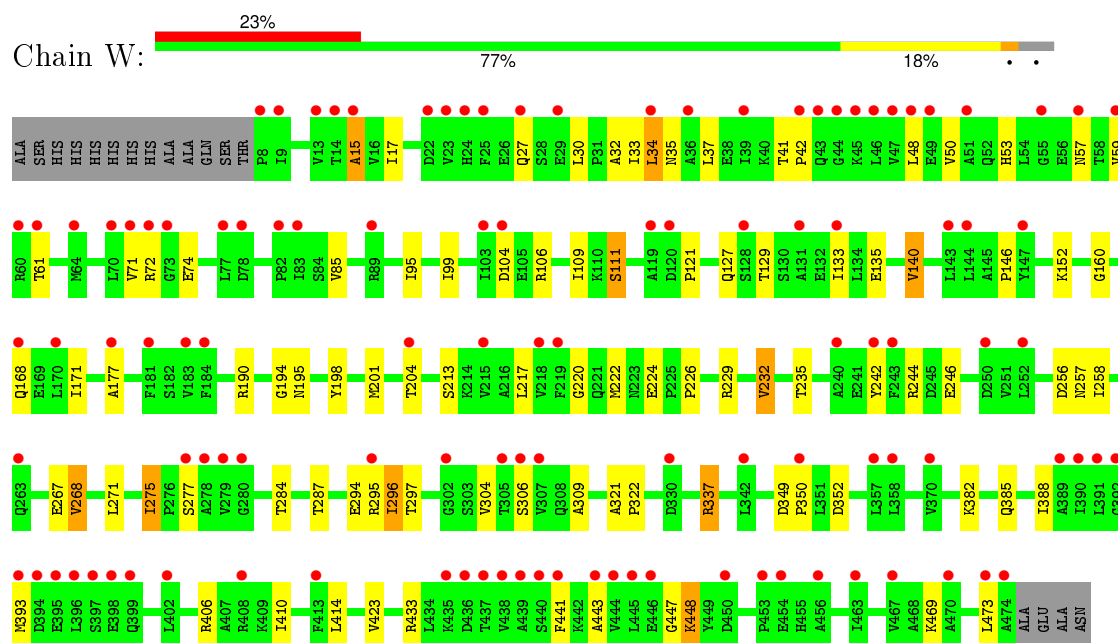


- Molecule 2: ATP synthase subunit beta

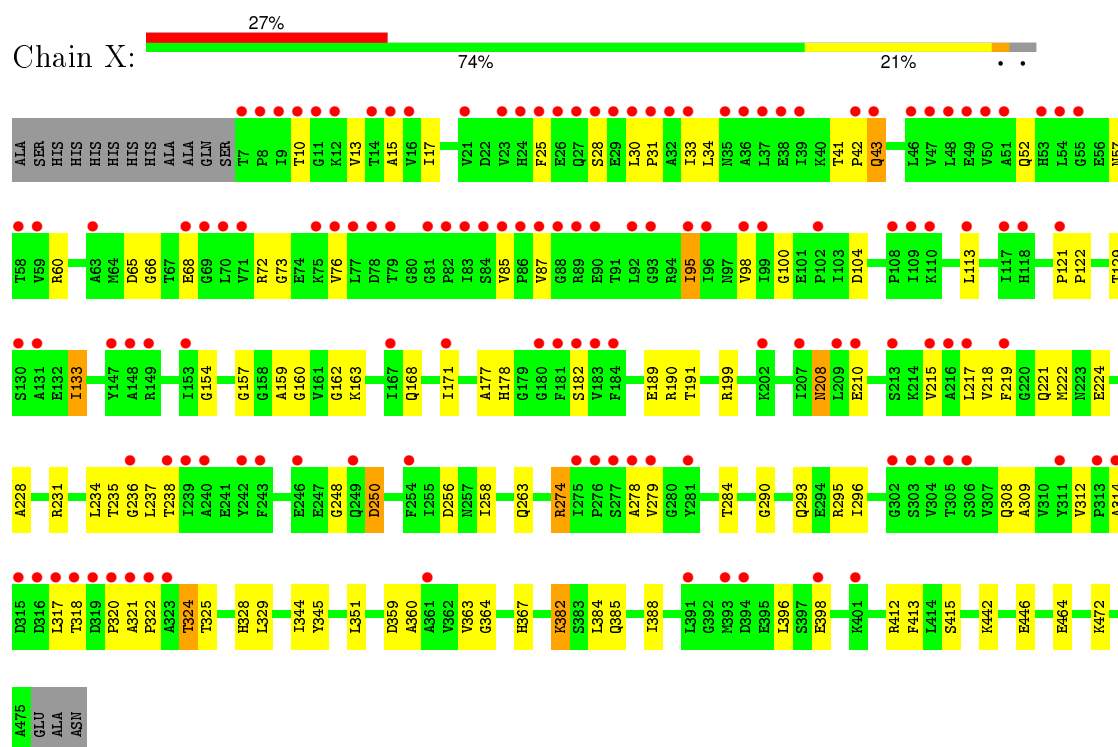




• Molecule 2: ATP synthase subunit beta

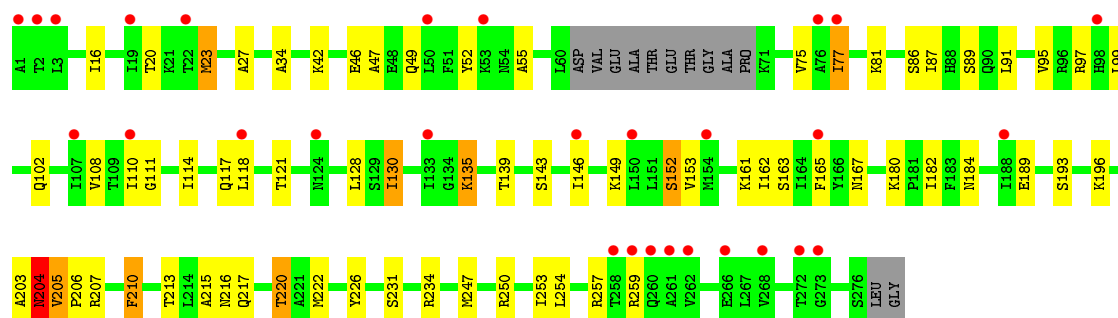


• Molecule 2: ATP synthase subunit beta

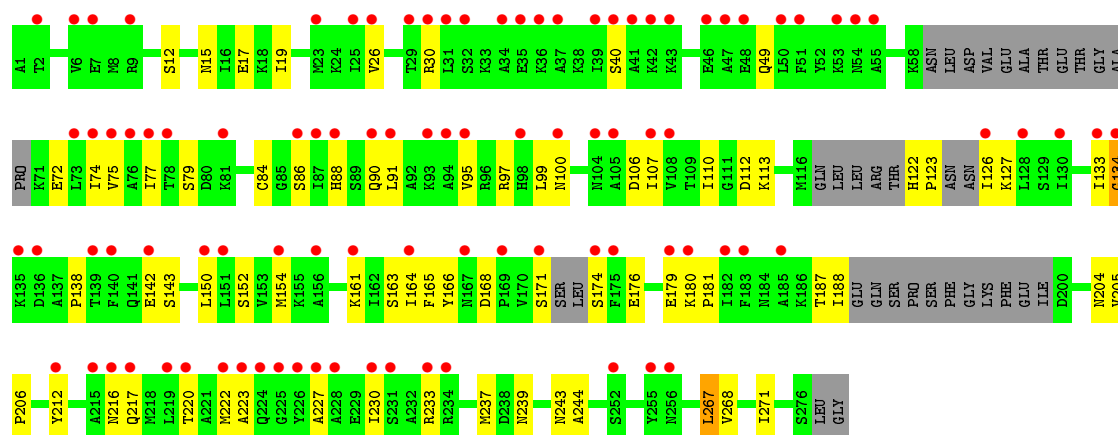


• Molecule 3: ATP synthase subunit gamma

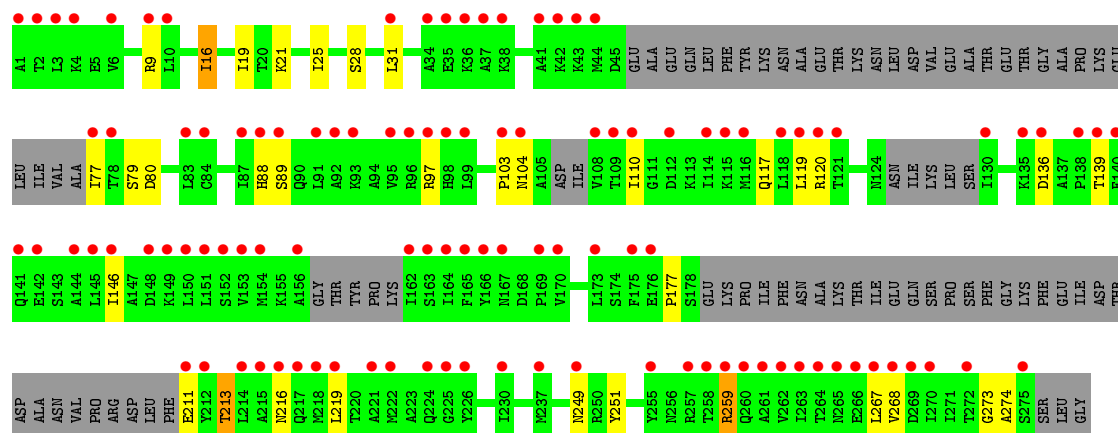
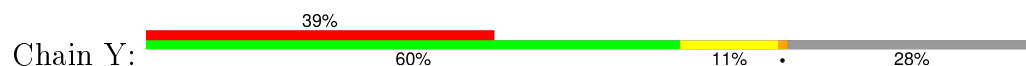




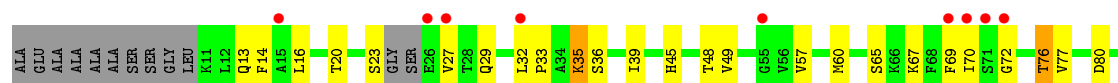
• Molecule 3: ATP synthase subunit gamma

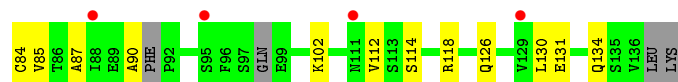


• Molecule 3: ATP synthase subunit gamma

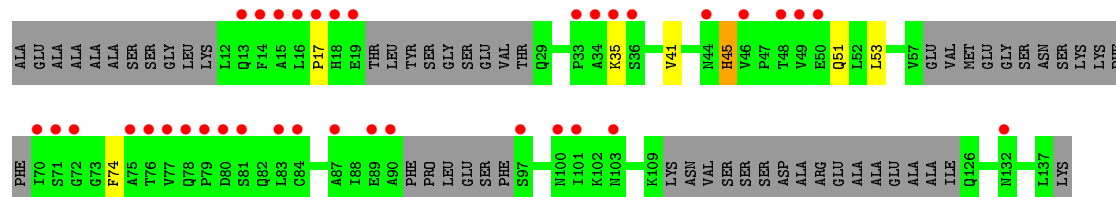


• Molecule 4: ATP synthase subunit delta

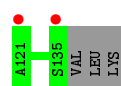
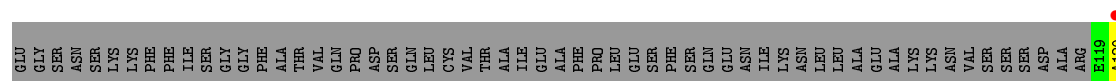




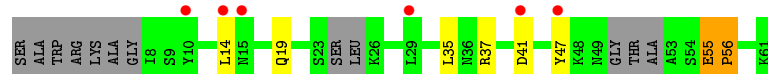
• Molecule 4: ATP synthase subunit delta



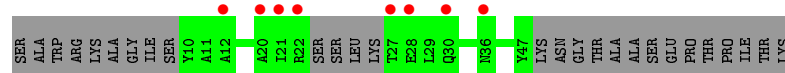
• Molecule 4: ATP synthase subunit delta



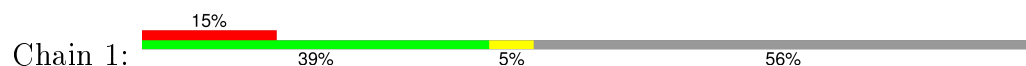
• Molecule 5: ATP synthase subunit epsilon



• Molecule 5: ATP synthase subunit epsilon



• Molecule 5: ATP synthase subunit epsilon



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.43Å 288.58Å 187.17Å 90.00° 101.37° 90.00°	Depositor
Resolution (Å)	20.00 – 2.74 67.14 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.74) 98.6 (67.14-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.212 , 0.259 0.213 , 0.262	Depositor DCC
R_{free} test set	5965 reflections (2.06%)	DCC
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 295714 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	72675	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ANP, MG

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	0.52	0/3712	0.67	0/5024
1	B	0.51	0/3717	0.66	1/5031 (0.0%)
1	C	0.43	0/3730	0.61	0/5049
1	J	0.43	0/3703	0.61	0/5012
1	K	0.46	0/3732	0.63	0/5052
1	L	0.45	0/3712	0.62	1/5024 (0.0%)
1	S	0.40	0/3675	0.57	0/4973
1	T	0.40	0/3685	0.55	0/4987
1	U	0.41	0/3703	0.58	0/5013
2	D	0.48	0/3601	0.65	0/4884
2	E	0.51	0/3560	0.65	0/4834
2	F	0.44	0/3583	0.63	0/4862
2	M	0.42	0/3591	0.61	0/4872
2	N	0.50	0/3597	0.64	0/4880
2	O	0.47	0/3590	0.65	0/4869
2	V	0.40	0/3605	0.57	0/4889
2	W	0.43	0/3587	0.56	0/4863
2	X	0.40	0/3599	0.56	0/4881
3	G	0.39	0/2080	0.55	0/2798
3	P	0.40	0/1867	0.54	0/2509
3	Y	0.38	0/1527	0.53	0/2048
4	H	0.40	0/804	0.58	0/1101
4	Q	0.39	0/440	0.50	0/603
4	Z	0.43	0/84	0.59	0/116
5	1	0.36	0/143	0.53	0/195
5	I	0.46	0/343	0.58	0/470
5	R	0.41	0/173	0.52	0/239
All	All	0.45	0/73143	0.61	2/99078 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	283	LEU	CA-CB-CG	6.71	130.74	115.30
1	B	111	ASP	CB-CG-OD1	5.54	123.28	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	3659	0	3743	54	0
1	B	3664	0	3748	50	0
1	C	3675	0	3759	53	0
1	J	3650	0	3735	41	0
1	K	3679	0	3754	71	0
1	L	3659	0	3743	52	0
1	S	3622	0	3716	90	0
1	T	3632	0	3724	72	0
1	U	3650	0	3730	99	0
2	D	3545	0	3614	64	0
2	E	3504	0	3550	53	0
2	F	3527	0	3592	49	0
2	M	3535	0	3599	66	0
2	N	3541	0	3604	63	0
2	O	3534	0	3606	52	0
2	V	3549	0	3620	75	0
2	W	3531	0	3605	59	0
2	X	3543	0	3615	92	0
3	G	2055	0	2123	44	0
3	P	1850	0	1892	49	0
3	Y	1517	0	1561	20	0
4	H	795	0	670	19	0
4	Q	441	0	234	3	0
4	Z	85	0	45	0	0
5	1	145	0	87	2	0
5	I	339	0	280	4	0
5	R	175	0	100	0	0
6	A	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	31	0	13	2	0
6	C	31	0	13	0	0
6	D	31	0	13	1	0
6	F	31	0	13	2	0
6	J	31	0	13	0	0
6	K	31	0	13	1	0
6	L	31	0	13	0	0
6	M	31	0	13	5	0
6	O	31	0	13	0	0
6	S	31	0	13	4	0
6	T	31	0	13	1	0
6	U	31	0	13	4	0
6	V	31	0	13	4	0
6	X	31	0	13	6	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	O	1	0	0	0	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
7	U	1	0	0	0	0
7	V	1	0	0	0	0
7	X	1	0	0	0	0
8	E	5	0	0	0	0
8	N	5	0	0	0	0
9	A	10	0	0	0	0
9	B	9	0	0	0	0
9	C	3	0	0	0	0
9	D	11	0	0	0	0
9	E	10	0	0	0	0
9	F	8	0	0	0	0
9	G	2	0	0	1	0
9	J	3	0	0	0	0
9	K	5	0	0	0	0
9	L	8	0	0	0	0
9	M	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	3	0	0	0	0
9	O	5	0	0	0	0
9	P	2	0	0	0	0
9	X	1	0	0	0	0
All	All	72675	0	73244	1182	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.24	1.08
2:O:84:SER:HB3	2:O:114:ARG:HH11	1.18	1.07
1:L:336:VAL:HG11	1:L:353:PHE:HE2	1.23	1.03
2:X:95:ILE:HD12	2:X:104:ASP:HB3	1.43	1.01
1:A:112:ALA:O	1:A:251:THR:HG21	1.61	1.01
3:P:88:HIS:CD2	3:P:113:LYS:HB2	1.97	0.98
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.46	0.97
5:I:55:GLU:CB	5:I:56:PRO:HD3	1.95	0.96
2:O:84:SER:CB	2:O:114:ARG:HH11	1.79	0.95
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.52	0.92
2:M:160:GLY:H	6:M:600:ANP:HNB1	1.15	0.90
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.54	0.90
2:V:449:TYR:HD1	2:V:452:ILE:HD11	1.39	0.88
1:K:186:LEU:O	1:K:189:LYS:HE3	1.73	0.88
2:V:47:VAL:HG21	2:V:99:ILE:HG21	1.55	0.87
1:C:97:VAL:HG11	1:C:247:LEU:HD21	1.56	0.87
1:U:69:GLU:HB3	1:U:70:PRO:HD2	1.55	0.86
2:M:25:PHE:HB2	2:M:30:LEU:HD23	1.56	0.84
1:L:336:VAL:HG11	1:L:353:PHE:CE2	2.12	0.83
2:W:27:GLN:HG3	2:W:57:ASN:HD21	1.42	0.83
2:F:41:THR:HB	2:F:42:PRO:HD2	1.60	0.83
1:B:26:ASN:O	1:B:30:THR:HB	1.78	0.83
1:A:444:VAL:HG22	1:A:445:PRO:HD3	1.62	0.82
2:X:258:ILE:HD13	2:X:308:GLN:OE1	1.80	0.81
1:B:93:THR:HG22	1:B:95:ASN:H	1.45	0.81
3:P:88:HIS:HD2	3:P:113:LYS:HB2	1.40	0.81
3:G:110:ILE:HG12	3:G:130:ILE:HG13	1.62	0.81
2:X:160:GLY:H	6:X:600:ANP:HNB1	1.29	0.81
1:U:212:ARG:HG2	1:U:237:THR:HG21	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:246:TYR:CE2	1:K:283:LEU:CD1	2.64	0.80
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.63	0.80
1:U:354:LEU:HA	1:U:366:ALA:O	1.80	0.80
1:S:98:ASP:HB2	1:S:129:SER:O	1.82	0.79
2:F:363:VAL:HB	2:F:367:HIS:CD2	2.16	0.79
2:D:176:LYS:HD3	2:D:204:THR:HG22	1.64	0.79
2:O:84:SER:CB	2:O:114:ARG:NH1	2.45	0.79
1:S:212:ARG:HG3	1:S:237:THR:HG21	1.63	0.79
1:S:444:VAL:HG23	1:S:445:PRO:HD3	1.65	0.78
3:G:89:SER:HA	3:G:117:GLN:HE21	1.48	0.78
1:T:143:SER:H	2:X:199:ARG:HH22	1.33	0.77
1:C:138:ILE:HD12	2:D:191:THR:HG23	1.65	0.77
3:P:95:VAL:O	3:P:99:LEU:HB2	1.84	0.77
1:T:239:SER:HB3	2:W:294:GLU:HG3	1.66	0.76
1:L:93:THR:HG22	1:L:95:ASN:H	1.50	0.76
1:J:211:LYS:HE3	1:J:213:SER:OG	1.86	0.76
3:G:108:VAL:HG22	3:G:128:LEU:HB3	1.67	0.76
2:N:384:LEU:O	2:N:388:ILE:HG12	1.86	0.75
2:F:363:VAL:HB	2:F:367:HIS:HD2	1.51	0.75
1:B:147:PRO:HB2	1:B:149:GLN:HE21	1.49	0.75
1:U:441:GLU:HG2	1:U:486:ARG:HB2	1.70	0.74
2:N:85:VAL:CG1	2:N:235:THR:HG23	2.18	0.74
1:L:290:PRO:HB2	2:M:270:ALA:HB1	1.71	0.73
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.70	0.73
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.70	0.73
3:Y:16:ILE:HA	3:Y:19:ILE:HG22	1.69	0.72
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.71	0.72
2:E:136:THR:HG22	2:E:142:ASP:OD1	1.89	0.72
2:D:234:LEU:HD23	2:D:292:LEU:HD13	1.70	0.72
1:C:341:PRO:O	1:C:345:ILE:HG13	1.89	0.72
3:Y:79:SER:HB3	3:Y:88:HIS:HE1	1.53	0.72
4:H:126:GLN:O	4:H:130:LEU:HG	1.90	0.71
2:E:133:ILE:HD13	2:E:357:LEU:HD12	1.72	0.71
1:A:302:TYR:O	1:A:306:ARG:HB2	1.90	0.71
1:S:166:ARG:HH22	2:W:190:ARG:HD3	1.55	0.71
1:C:239:SER:HB3	2:F:294:GLU:HG3	1.73	0.71
3:P:180:LYS:NZ	3:P:220:THR:HB	2.06	0.71
3:P:88:HIS:CD2	3:P:113:LYS:CB	2.74	0.70
2:O:9:ILE:HG23	2:O:27:GLN:HE21	1.56	0.70
1:L:481:LEU:HD21	1:L:498:SER:HB3	1.73	0.70
1:C:92:ARG:HH21	1:C:94:GLY:HA2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:97:ASN:HD21	2:V:101:GLU:HB2	1.57	0.70
2:M:371:ALA:O	2:M:375:GLN:HG3	1.92	0.70
1:L:54:LEU:O	1:L:93:THR:HB	1.92	0.69
2:V:77:LEU:HG	2:V:78:ASP:H	1.58	0.69
2:M:50:VAL:HA	2:M:61:THR:HG22	1.74	0.69
2:W:226:PRO:HB2	2:W:268:VAL:HG23	1.75	0.69
1:C:107:GLY:HA2	1:C:228:MET:O	1.92	0.69
2:N:229:ARG:NH2	2:N:267:GLU:OE1	2.26	0.69
1:J:309:GLU:HG3	2:N:223:ASN:HB3	1.75	0.69
1:L:383:LYS:HG2	1:L:490:GLU:HG3	1.73	0.69
2:D:244:ARG:HD2	2:D:299:THR:HG22	1.75	0.69
2:V:178:HIS:CE1	2:V:250:ASP:HB3	2.28	0.68
2:O:84:SER:HB2	2:O:114:ARG:NH1	2.07	0.68
1:S:148:VAL:HG23	1:S:163:ARG:HG2	1.76	0.68
2:O:9:ILE:HD12	2:O:9:ILE:H	1.58	0.68
1:T:35:ALA:HB3	1:T:42:ARG:NH1	2.09	0.68
1:T:77:LEU:O	1:T:243:PRO:HG2	1.94	0.68
5:I:55:GLU:CB	5:I:56:PRO:CD	2.70	0.67
1:A:481:LEU:O	1:A:485:ILE:HG13	1.94	0.67
2:V:85:VAL:HG11	2:V:235:THR:HG23	1.75	0.67
2:F:250:ASP:OD1	2:F:303:SER:HB3	1.94	0.67
2:X:321:ALA:HB3	2:X:322:PRO:HD2	1.77	0.67
3:P:187:THR:O	3:P:188:ILE:HG13	1.94	0.67
1:J:260:ARG:O	1:J:321:GLY:HA3	1.94	0.67
2:M:160:GLY:N	6:M:600:ANP:HNB1	1.92	0.67
2:N:142:ASP:HB3	2:N:434:LEU:HD12	1.77	0.66
1:T:138:ILE:HD13	2:X:95:ILE:HG21	1.75	0.66
1:K:138:ILE:HD12	1:K:138:ILE:N	2.11	0.66
1:C:412:LEU:HB3	1:C:416:THR:OG1	1.96	0.66
2:X:208:ASN:HD22	2:X:210:GLU:H	1.44	0.66
1:U:378:SER:HB3	1:U:386:LYS:HG3	1.78	0.66
2:D:456:ALA:O	2:D:466:VAL:HG13	1.96	0.66
1:K:388:VAL:HG12	1:K:447:ILE:HG22	1.78	0.65
2:D:197:LEU:O	2:D:201:MET:HG2	1.96	0.65
2:X:160:GLY:N	6:X:600:ANP:HNB1	1.95	0.65
1:A:174:GLN:HA	6:A:600:ANP:HNB1	1.60	0.65
2:E:168:GLN:HE21	2:E:201:MET:HG2	1.61	0.65
2:V:47:VAL:HG21	2:V:99:ILE:HD13	1.77	0.65
2:O:9:ILE:HG23	2:O:27:GLN:NE2	2.11	0.65
2:F:140:VAL:HG13	2:F:414:LEU:HD22	1.79	0.65
3:G:77:ILE:HG21	3:G:222:MET:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:465:ASP:O	2:E:469:LYS:HB2	1.97	0.65
2:V:15:ALA:HB3	2:V:22:ASP:HB2	1.79	0.65
2:V:162:GLY:HA2	6:V:600:ANP:O1A	1.97	0.65
1:U:349:ASP:O	1:U:375:ARG:HB2	1.97	0.64
2:V:275:ILE:HG23	3:Y:274:ALA:HB2	1.79	0.64
1:K:98:ASP:HB2	1:K:129:SER:O	1.97	0.64
4:H:35:LYS:HG2	4:H:36:SER:H	1.62	0.64
1:L:187:ASN:OD1	1:L:190:ARG:NH1	2.30	0.64
2:X:321:ALA:HB3	2:X:322:PRO:CD	2.27	0.64
4:H:48:THR:H	4:H:77:VAL:HB	1.62	0.64
2:D:319:ASP:O	2:D:322:PRO:HD2	1.97	0.64
2:X:384:LEU:O	2:X:388:ILE:HG12	1.97	0.64
1:K:93:THR:HG22	1:K:95:ASN:H	1.63	0.64
1:B:140:PRO:HB3	1:B:318:GLU:HG3	1.79	0.63
1:L:422:ARG:HG3	1:L:456:ASP:OD1	1.98	0.63
2:V:449:TYR:HD1	2:V:452:ILE:CD1	2.10	0.63
1:U:263:GLY:HA2	1:U:319:GLY:O	1.98	0.63
2:O:140:VAL:HG13	2:O:414:LEU:HD22	1.80	0.63
3:P:138:PRO:HG3	3:P:223:ALA:HA	1.80	0.63
2:M:90:GLU:HG3	2:M:111:SER:CB	2.28	0.63
1:J:26:ASN:O	1:J:27:LEU:HB2	1.99	0.63
1:S:69:GLU:HG2	1:S:70:PRO:HD2	1.79	0.63
1:B:54:LEU:O	1:B:93:THR:HB	1.99	0.63
2:N:30:LEU:HD11	2:N:57:ASN:HA	1.80	0.63
1:S:177:LYS:HB2	6:S:600:ANP:O1B	1.99	0.63
1:U:153:LYS:HE2	1:U:432:GLN:HB2	1.81	0.63
3:G:118:LEU:HA	3:G:121:THR:HG22	1.81	0.62
1:T:479:ASN:HA	1:T:482:LEU:HD12	1.81	0.62
2:E:168:GLN:HE21	2:E:201:MET:CG	2.12	0.62
2:M:234:LEU:CD2	2:M:292:LEU:HD13	2.29	0.62
1:T:85:LYS:HE2	2:W:32:ALA:HB2	1.80	0.62
1:T:455:LEU:HA	1:T:458:ILE:HD13	1.80	0.62
1:U:166:ARG:HD3	1:U:308:LEU:O	1.99	0.62
2:N:425:THR:O	2:N:427:ILE:HD12	1.99	0.62
3:P:26:VAL:O	3:P:30:ARG:HD2	1.99	0.62
2:N:33:ILE:O	2:N:34:LEU:HB2	1.99	0.62
1:L:338:ALA:O	1:L:342:THR:OG1	2.18	0.62
1:U:281:ARG:HH12	2:X:278:ALA:HB2	1.65	0.62
3:G:189:GLU:OE2	3:G:206:PRO:HG2	2.00	0.62
1:C:166:ARG:HD2	1:C:308:LEU:O	2.00	0.62
1:U:212:ARG:CG	1:U:237:THR:HG21	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:55:VAL:HG21	1:J:75:ILE:HD13	1.82	0.61
1:S:355:GLU:HB2	1:S:358:LEU:HD12	1.82	0.61
1:B:355:GLU:HG3	1:B:368:ASN:HD22	1.63	0.61
1:K:246:TYR:CE2	1:K:283:LEU:HD12	2.35	0.61
2:D:258:ILE:HD11	2:D:292:LEU:HD21	1.81	0.61
1:K:246:TYR:HE2	1:K:283:LEU:CD1	2.11	0.61
2:D:221:GLN:HA	2:D:221:GLN:OE1	2.01	0.61
3:G:193:SER:HB3	3:G:196:LYS:HG3	1.81	0.61
2:V:47:VAL:CG2	2:V:99:ILE:HD13	2.29	0.61
2:N:296:ILE:HD13	2:N:306:SER:HB2	1.82	0.61
3:G:180:LYS:NZ	3:G:220:THR:HG22	2.15	0.61
3:P:239:ASN:O	3:P:243:ASN:ND2	2.32	0.61
1:B:109:VAL:HG13	1:B:233:ILE:HB	1.83	0.61
1:S:349:ASP:O	1:S:375:ARG:HB2	2.01	0.61
2:D:25:PHE:HB2	2:D:30:LEU:HD23	1.82	0.61
3:Y:213:THR:HA	3:Y:216:ASN:HB3	1.82	0.61
1:S:266:ALA:O	1:S:323:LEU:HA	2.00	0.61
2:V:189:GLU:HG3	2:V:221:GLN:OE1	2.00	0.61
2:O:85:VAL:CG1	2:O:235:THR:HG23	2.30	0.61
1:S:243:PRO:HG3	1:S:283:LEU:HD21	1.81	0.61
1:U:466:PHE:O	1:U:470:PHE:HB2	2.01	0.61
3:P:150:LEU:O	3:P:154:MET:HB2	2.01	0.61
1:U:176:GLY:HA2	6:U:600:ANP:O5'	2.00	0.61
1:L:375:ARG:HH12	2:M:160:GLY:HA2	1.65	0.60
2:W:160:GLY:HA3	2:W:337:ARG:NH2	2.16	0.60
2:F:33:ILE:O	2:F:34:LEU:HB2	2.01	0.60
1:J:358:LEU:HB2	1:J:366:ALA:HB1	1.83	0.60
1:U:69:GLU:HB3	1:U:70:PRO:CD	2.28	0.60
1:T:101:VAL:HG12	1:T:255:ILE:HA	1.83	0.60
2:O:168:GLN:HB3	2:O:420:VAL:HG11	1.84	0.60
1:B:290:PRO:HB3	2:F:276:PRO:HG3	1.83	0.60
2:N:310:VAL:HG11	2:N:326:PHE:HE1	1.67	0.60
2:M:144:LEU:O	2:M:358:LEU:HD22	2.01	0.60
2:O:84:SER:HB3	2:O:114:ARG:NH1	2.00	0.60
2:E:226:PRO:HB2	2:E:268:VAL:HG23	1.83	0.60
1:J:265:HIS:ND1	1:J:322:SER:HB3	2.17	0.60
1:L:368:ASN:ND2	1:L:371:LEU:HD12	2.17	0.60
2:V:220:GLY:HA3	2:V:232:VAL:HG11	1.84	0.59
1:K:382:VAL:HG11	1:K:440:THR:HG21	1.84	0.59
2:F:165:VAL:HG23	6:F:600:ANP:O1A	2.01	0.59
1:L:441:GLU:OE2	1:L:486:ARG:HD3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:243:PRO:HA	1:K:246:TYR:CD2	2.37	0.59
3:G:213:THR:HG23	3:G:217:GLN:HE21	1.68	0.59
1:S:249:PRO:HB2	1:S:307:LEU:HD21	1.84	0.59
1:U:304:HIS:CE1	1:U:343:ASN:HB3	2.37	0.59
2:W:48:LEU:HB3	2:W:61:THR:HB	1.85	0.59
2:X:87:VAL:HG22	2:X:113:LEU:O	2.02	0.59
2:N:98:VAL:HB	2:N:232:VAL:HG13	1.83	0.59
3:P:122:HIS:N	3:P:123:PRO:HD3	2.17	0.59
1:L:76:VAL:HG11	1:L:283:LEU:HG	1.84	0.59
2:M:33:ILE:O	2:M:34:LEU:HB2	2.03	0.59
1:J:143:SER:OG	2:N:199:ARG:NH1	2.36	0.59
1:T:458:ILE:H	1:T:458:ILE:HD12	1.68	0.59
2:N:220:GLY:HA3	2:N:232:VAL:HG11	1.84	0.59
2:O:242:TYR:CE1	2:O:246:GLU:HG3	2.36	0.59
2:W:388:ILE:HD12	2:W:393:MET:HG2	1.85	0.58
2:O:417:PRO:HG3	2:O:459:MET:HG3	1.84	0.58
2:M:344:ILE:HG23	2:M:415:SER:HB3	1.84	0.58
1:S:46:LEU:HG	1:S:49:ILE:HB	1.85	0.58
1:U:359:PHE:CE1	1:U:364:ARG:HD3	2.39	0.58
2:M:197:LEU:O	2:M:201:MET:HG2	2.02	0.58
3:G:91:LEU:HD23	3:G:114:ILE:HD13	1.86	0.58
1:T:346:SER:HA	6:X:600:ANP:O1G	2.04	0.58
2:N:220:GLY:CA	2:N:232:VAL:HG11	2.33	0.58
2:O:391:LEU:HB3	2:O:395:GLU:HG3	1.86	0.58
2:O:122:PRO:HG2	2:O:297:THR:HG21	1.84	0.58
2:D:204:THR:HB	2:D:206:VAL:HG23	1.85	0.58
3:Y:9:ARG:HD3	3:Y:251:TYR:HE1	1.69	0.58
1:C:144:VAL:CG1	1:C:162:GLY:HA3	2.32	0.58
1:K:138:ILE:H	1:K:138:ILE:HD12	1.67	0.58
2:M:148:ALA:HB2	2:M:357:LEU:HD11	1.84	0.58
1:U:302:TYR:HA	1:U:305:SER:OG	2.03	0.58
2:F:293:GLN:HA	2:F:293:GLN:OE1	2.04	0.58
1:B:358:LEU:HB2	1:B:366:ALA:HB1	1.86	0.58
2:D:143:LEU:O	2:D:367:HIS:HE1	1.87	0.58
2:N:15:ALA:HB3	2:N:22:ASP:HB2	1.86	0.58
1:U:360:TYR:CZ	2:X:351:LEU:O	2.57	0.57
2:X:325:THR:O	2:X:328:HIS:HB2	2.03	0.57
2:D:234:LEU:CD2	2:D:292:LEU:HD13	2.34	0.57
1:L:364:ARG:HA	1:L:365:PRO:C	2.24	0.57
2:W:168:GLN:HE21	2:W:201:MET:HG2	1.69	0.57
2:F:140:VAL:CG1	2:F:414:LEU:HD22	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:208:VAL:HG11	1:T:276:GLN:HB2	1.86	0.57
1:A:478:HIS:HB3	1:A:481:LEU:HG	1.86	0.57
2:N:359:ASP:O	2:N:363:VAL:HG22	2.03	0.57
1:C:144:VAL:HG11	1:C:162:GLY:HA3	1.86	0.57
2:W:177:ALA:HB1	2:W:433:ARG:HH22	1.68	0.57
1:U:375:ARG:NH1	6:V:600:ANP:HNB1	2.02	0.57
2:F:293:GLN:HG3	2:F:328:HIS:CG	2.39	0.57
1:K:154:ALA:HB1	1:K:367:ILE:HD12	1.86	0.57
2:E:406:ARG:HD3	2:E:450:ASP:OD1	2.05	0.57
1:L:187:ASN:O	1:L:190:ARG:HG3	2.05	0.57
1:U:51:ALA:O	1:U:52:GLU:HB2	2.05	0.57
3:G:95:VAL:O	3:G:99:LEU:HB3	2.05	0.56
2:W:95:ILE:HB	2:W:104:ASP:HB3	1.86	0.56
4:H:29:GLN:O	4:H:60:MET:HB2	2.05	0.56
2:N:405:GLU:HG2	2:N:409:LYS:HE2	1.87	0.56
1:T:305:SER:HB2	2:X:222:MET:HB2	1.87	0.56
1:K:236:ALA:HA	1:K:240:GLU:OE1	2.05	0.56
2:N:85:VAL:HG11	2:N:235:THR:CG2	2.35	0.56
1:S:249:PRO:HG2	1:S:276:GLN:NE2	2.21	0.56
2:F:345:TYR:HA	2:F:346:PRO:C	2.25	0.56
2:N:381:TYR:O	2:N:385:GLN:HG2	2.04	0.56
1:K:364:ARG:HA	1:K:365:PRO:C	2.25	0.56
4:H:16:LEU:HD11	4:H:90:ALA:HB3	1.87	0.56
2:V:346:PRO:O	2:V:347:ALA:HB3	2.04	0.56
3:Y:79:SER:HB3	3:Y:88:HIS:CE1	2.39	0.56
1:A:270:TYR:O	1:A:272:ASP:HA	2.05	0.56
2:D:33:ILE:O	2:D:34:LEU:HB2	2.05	0.56
1:B:147:PRO:HB2	1:B:149:GLN:NE2	2.19	0.56
2:O:206:VAL:HG12	2:O:215:VAL:HG12	1.88	0.56
1:K:99:VAL:HG11	1:K:251:THR:HB	1.87	0.56
3:P:40:SER:HB3	4:Q:17:PRO:O	2.06	0.56
2:N:84:SER:O	2:N:114:ARG:NH1	2.39	0.56
2:O:30:LEU:HD21	2:O:57:ASN:HA	1.88	0.56
1:B:395:PHE:HE1	1:B:419:THR:HG22	1.71	0.56
2:E:425:THR:HB	2:E:427:ILE:HD12	1.86	0.56
2:V:266:SER:N	2:V:282:GLN:HE21	2.02	0.56
1:B:139:LEU:HD22	2:F:104:ASP:HA	1.88	0.56
1:S:289:ARG:HE	2:W:17:ILE:HG22	1.70	0.56
1:S:217:GLN:OE1	2:V:356:ARG:NH2	2.39	0.56
2:E:157:GLY:HA2	2:E:337:ARG:HH22	1.71	0.56
3:P:168:ASP:N	3:P:176:GLU:O	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:197:LEU:O	2:O:201:MET:HG2	2.06	0.56
1:K:68:LEU:O	2:O:15:ALA:HA	2.06	0.56
1:K:138:ILE:H	1:K:138:ILE:CD1	2.20	0.55
1:U:166:ARG:CD	1:U:308:LEU:O	2.54	0.55
3:Y:9:ARG:HD3	3:Y:251:TYR:CE1	2.41	0.55
1:B:166:ARG:HD3	1:B:311:ALA:HB3	1.87	0.55
2:D:50:VAL:HA	2:D:61:THR:HG22	1.86	0.55
2:M:170:LEU:O	2:M:174:ILE:HG12	2.07	0.55
2:D:222:MET:HA	2:D:229:ARG:HD2	1.88	0.55
1:B:212:ARG:HG2	2:E:127:GLN:HG3	1.88	0.55
2:X:162:GLY:HA2	6:X:600:ANP:O1A	2.06	0.55
3:P:180:LYS:HZ3	3:P:220:THR:HB	1.72	0.55
4:H:69:PHE:O	4:H:90:ALA:HA	2.06	0.55
2:N:32:ALA:O	2:N:35:ASN:HB2	2.07	0.55
1:U:336:VAL:HG11	1:U:353:PHE:HE1	1.71	0.55
2:W:41:THR:HB	2:W:42:PRO:CD	2.37	0.55
2:M:64:MET:CE	2:M:228:ALA:HA	2.37	0.55
2:O:75:LYS:NZ	2:X:177:ALA:HB1	2.21	0.55
2:X:33:ILE:HG22	2:X:34:LEU:HG	1.87	0.55
1:U:441:GLU:CG	1:U:486:ARG:HB2	2.36	0.55
2:O:204:THR:OG1	2:O:206:VAL:HG23	2.06	0.55
1:S:236:ALA:HB2	1:S:248:ALA:HB2	1.89	0.55
1:A:309:GLU:HG3	2:E:223:ASN:HB3	1.88	0.55
1:U:68:LEU:HD13	1:U:73:VAL:HG13	1.88	0.55
3:G:162:ILE:HB	3:G:182:ILE:HB	1.88	0.55
1:A:462:ARG:HD2	1:A:465:GLU:OE2	2.06	0.55
3:G:49:GLN:HA	3:G:52:TYR:HD1	1.72	0.55
2:D:339:ILE:HG22	2:D:344:ILE:HB	1.86	0.55
2:D:7:THR:HG23	2:D:7:THR:O	2.06	0.55
2:E:175:ALA:O	2:E:179:GLY:HA2	2.07	0.55
1:C:309:GLU:HG3	2:D:223:ASN:HB3	1.87	0.55
1:K:220:GLN:HB2	2:N:129:THR:HB	1.87	0.55
1:T:70:PRO:HD3	2:X:15:ALA:HB2	1.87	0.55
1:J:212:ARG:HG3	1:J:237:THR:HG21	1.89	0.55
1:S:70:PRO:HD3	2:W:15:ALA:HB2	1.88	0.55
3:G:180:LYS:HE3	3:G:217:GLN:HB3	1.89	0.54
1:U:378:SER:HB2	1:U:386:LYS:HE2	1.90	0.54
2:O:75:LYS:HZ1	2:X:177:ALA:HB1	1.73	0.54
2:V:345:TYR:HA	2:V:347:ALA:N	2.22	0.54
2:M:134:LEU:HD13	2:M:149:ARG:HH12	1.73	0.54
1:T:447:ILE:O	1:T:451:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:253:LEU:HD23	2:V:296:ILE:HG23	1.89	0.54
2:X:191:THR:HA	2:X:221:GLN:HG3	1.90	0.54
1:U:475:LYS:HA	1:U:479:ASN:HD22	1.72	0.54
2:X:168:GLN:HA	2:X:171:ILE:HD12	1.89	0.54
2:X:442:LYS:HG2	2:X:446:GLU:OE2	2.07	0.54
2:N:226:PRO:HB2	2:N:268:VAL:HG23	1.89	0.54
2:D:388:ILE:HG22	2:D:388:ILE:O	2.08	0.54
1:S:101:VAL:HG12	1:S:255:ILE:HG12	1.89	0.54
3:P:97:ARG:HA	3:P:100:ASN:HD22	1.72	0.54
3:P:233:ARG:O	3:P:237:MET:HG2	2.08	0.54
1:B:357:GLU:HA	1:B:357:GLU:OE1	2.08	0.54
1:T:166:ARG:HH22	2:X:190:ARG:HD3	1.73	0.54
1:T:138:ILE:CD1	2:X:95:ILE:HG21	2.38	0.54
1:S:159:VAL:HG12	1:S:374:SER:HB2	1.90	0.54
1:K:173:ARG:HG3	1:K:173:ARG:HH11	1.72	0.54
2:X:367:HIS:HD2	2:X:367:HIS:O	1.91	0.54
1:K:154:ALA:CB	1:K:367:ILE:HD12	2.38	0.54
1:J:77:LEU:CD1	1:J:81:ASP:HB3	2.37	0.54
2:O:382:LYS:HA	2:O:385:GLN:HG2	1.88	0.54
2:X:133:ILE:HD12	2:X:133:ILE:H	1.73	0.54
2:F:30:LEU:HD11	2:F:57:ASN:OD1	2.08	0.53
1:B:203:CYS:HB2	1:B:231:SER:HB3	1.89	0.53
1:S:361:LYS:HE3	2:V:379:GLN:HG3	1.90	0.53
1:A:389:ALA:O	1:A:390:GLY:C	2.47	0.53
2:V:434:LEU:O	2:V:438:VAL:HG23	2.09	0.53
2:X:237:LEU:HD21	2:X:295:ARG:HB2	1.89	0.53
1:C:346:SER:HB3	2:D:260:ARG:HH22	1.74	0.53
1:T:344:VAL:HA	1:T:347:ILE:HD12	1.90	0.53
1:S:332:GLN:HB3	2:V:318:THR:HB	1.90	0.53
2:W:133:ILE:HD12	2:W:146:PRO:HB2	1.89	0.53
1:B:450:GLY:HA2	1:B:455:LEU:HD12	1.89	0.53
1:A:484:GLU:HG2	1:A:495:LEU:HD11	1.91	0.53
1:S:89:LEU:HG	1:S:90:VAL:N	2.23	0.53
1:L:99:VAL:HG11	1:L:251:THR:HB	1.90	0.53
1:L:222:LEU:CB	1:L:228:MET:HE2	2.38	0.53
1:T:301:PHE:HB3	2:X:263:GLN:HE22	1.73	0.53
3:G:184:ASN:HA	3:G:210:PHE:CD1	2.44	0.53
1:U:117:ILE:HD11	1:U:235:ALA:HB3	1.91	0.53
2:W:109:ILE:HG22	2:W:111:SER:HB2	1.90	0.53
4:H:13:GLN:HG2	4:H:23:SER:HA	1.89	0.53
1:T:103:PRO:HD3	1:T:258:TRP:CH2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:90:GLU:HG3	2:M:111:SER:HB3	1.89	0.53
2:M:436:ASP:O	2:M:440:SER:N	2.38	0.53
2:W:35:ASN:O	2:W:50:VAL:HG23	2.09	0.53
1:S:200:LYS:HD2	1:S:202:TYR:OH	2.08	0.53
1:T:100:PRO:HB3	1:T:125:ALA:HB2	1.90	0.53
1:T:337:SER:O	2:X:314:ALA:HA	2.09	0.53
2:D:89:ARG:NH1	2:D:247:GLU:OE2	2.41	0.53
1:S:50:GLN:HG2	2:W:71:VAL:HG22	1.91	0.53
2:M:406:ARG:HH21	2:M:447:GLY:HA3	1.74	0.53
3:G:87:ILE:HG23	3:G:167:ASN:HD22	1.73	0.53
2:V:266:SER:HA	2:V:282:GLN:HG3	1.90	0.53
2:W:127:GLN:HE22	2:W:297:THR:HG21	1.74	0.53
1:T:35:ALA:HB1	2:W:53:HIS:O	2.09	0.53
1:S:169:ILE:HD11	1:S:326:LEU:HB3	1.90	0.52
2:N:237:LEU:HD22	2:N:292:LEU:HD12	1.91	0.52
4:H:57:VAL:O	4:H:67:LYS:HA	2.08	0.52
2:M:136:THR:HB	2:M:138:ILE:HD12	1.91	0.52
1:A:54:LEU:HD13	1:A:97:VAL:HG22	1.91	0.52
1:K:250:PHE:HZ	1:K:303:LEU:HD12	1.75	0.52
2:W:406:ARG:NH1	2:W:447:GLY:HA2	2.25	0.52
1:S:249:PRO:HG2	1:S:276:GLN:HE21	1.75	0.52
2:E:158:GLY:H	2:E:337:ARG:HH12	1.56	0.52
2:N:243:PHE:HB2	2:N:251:VAL:HG21	1.92	0.52
1:K:29:GLU:OE2	1:K:92:ARG:NH1	2.42	0.52
1:A:444:VAL:HG22	1:A:445:PRO:CD	2.37	0.52
1:T:102:GLY:HA2	1:T:258:TRP:CE2	2.44	0.52
1:A:500:LYS:O	1:A:504:GLU:HG3	2.09	0.52
2:M:15:ALA:HB3	2:M:22:ASP:HB2	1.90	0.52
2:M:25:PHE:HB2	2:M:30:LEU:CD2	2.34	0.52
1:S:298:GLY:HA3	2:W:271:LEU:HG	1.92	0.52
3:G:259:ARG:HD2	9:G:279:HOH:O	2.10	0.52
1:T:340:ILE:HB	1:T:341:PRO:HD3	1.92	0.52
3:P:72:GLU:HG3	3:P:161:LYS:HB3	1.91	0.52
2:D:206:VAL:HG12	2:D:215:VAL:HG12	1.90	0.52
1:L:236:ALA:HA	1:L:240:GLU:OE2	2.10	0.52
1:S:174:GLN:HB3	2:V:354:LYS:HD3	1.92	0.52
3:G:89:SER:HA	3:G:117:GLN:NE2	2.22	0.52
1:T:166:ARG:O	1:T:348:THR:HB	2.10	0.52
1:S:293:ARG:O	1:S:294:GLU:HB2	2.09	0.52
2:V:164:THR:O	2:V:167:ILE:HG22	2.10	0.52
3:G:139:THR:HG21	5:I:37:ARG:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:VAL:HA	1:B:159:VAL:HG23	1.92	0.51
1:L:50:GLN:HB3	2:M:69:GLY:HA2	1.92	0.51
1:T:138:ILE:CD1	2:X:95:ILE:HD13	2.39	0.51
1:C:28:ASN:HA	1:C:47:ASN:HB2	1.92	0.51
1:A:85:LYS:HG2	2:D:53:HIS:HE1	1.75	0.51
1:J:302:TYR:O	1:J:306:ARG:HB2	2.10	0.51
1:K:166:ARG:HG3	1:K:325:ALA:HB3	1.92	0.51
1:K:370:GLY:H	1:K:400:ARG:NH1	2.09	0.51
2:E:403:THR:O	2:E:407:ALA:N	2.43	0.51
2:F:189:GLU:O	2:F:221:GLN:HB3	2.09	0.51
2:E:169:GLU:OE1	2:E:420:VAL:HG22	2.09	0.51
1:L:151:GLY:HA3	1:L:437:PRO:HB2	1.93	0.51
1:T:349:ASP:HA	1:T:375:ARG:HD2	1.91	0.51
1:C:166:ARG:HD3	1:C:311:ALA:HB3	1.91	0.51
1:U:336:VAL:HG11	1:U:353:PHE:CE1	2.46	0.51
1:T:507:VAL:HG12	1:T:508:ALA:N	2.26	0.51
1:C:174:GLN:HB3	2:F:354:LYS:HD3	1.92	0.51
1:S:152:LEU:HA	1:S:432:GLN:OE1	2.09	0.51
1:B:202:TYR:O	1:B:266:ALA:HA	2.10	0.51
2:E:349:ASP:HB3	2:E:352:ASP:HB2	1.92	0.51
1:A:39:GLY:HA2	1:A:77:LEU:HD12	1.90	0.51
2:O:345:TYR:HA	2:O:346:PRO:C	2.31	0.51
2:W:410:ILE:HG23	2:W:441:PHE:HE2	1.75	0.51
1:B:160:PRO:O	1:B:377:GLY:HA3	2.09	0.51
1:A:173:ARG:NH2	2:D:352:ASP:OD1	2.44	0.51
1:U:399:TYR:OH	1:U:424:GLU:HG3	2.10	0.51
2:W:469:LYS:O	2:W:473:LEU:HG	2.10	0.51
2:E:37:LEU:HD12	2:E:61:THR:HG21	1.93	0.51
1:J:223:GLU:HG3	1:J:228:MET:HG3	1.93	0.51
2:W:321:ALA:HB3	2:W:322:PRO:CD	2.40	0.51
2:V:20:ILE:HG13	2:V:271:LEU:HB2	1.93	0.51
2:D:363:VAL:HB	2:D:367:HIS:CD2	2.45	0.51
1:S:159:VAL:CG1	1:S:374:SER:HB2	2.41	0.51
1:J:77:LEU:HD12	1:J:81:ASP:HB3	1.92	0.51
1:K:435:TYR:C	1:K:437:PRO:HD3	2.30	0.51
1:U:152:LEU:HA	1:U:432:GLN:OE1	2.11	0.51
1:S:144:VAL:HG11	1:S:162:GLY:HA3	1.91	0.51
2:E:470:ALA:HA	2:E:473:LEU:HD12	1.93	0.51
1:U:139:LEU:C	1:U:141:ARG:H	2.14	0.51
1:C:344:VAL:HA	1:C:347:ILE:HD12	1.93	0.51
3:G:204:ASN:N	3:G:204:ASN:OD1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:157:GLY:O	2:X:163:LYS:HD3	2.11	0.51
1:U:375:ARG:CZ	6:V:600:ANP:HNB1	2.24	0.51
1:S:384:ALA:O	1:S:491:LEU:HD12	2.11	0.51
1:B:475:LYS:O	1:B:479:ASN:HB2	2.12	0.51
2:V:98:VAL:HG13	2:V:99:ILE:HG23	1.91	0.50
2:D:104:ASP:O	2:D:106:ARG:HG3	2.12	0.50
1:S:82:ARG:HB2	2:V:34:LEU:HD12	1.93	0.50
2:N:201:MET:HG2	2:N:206:VAL:CG2	2.41	0.50
2:F:298:THR:HG23	2:F:303:SER:HA	1.92	0.50
1:A:402:VAL:O	1:A:405:SER:HB2	2.11	0.50
1:T:99:VAL:HG11	1:T:251:THR:HB	1.93	0.50
3:G:253:ILE:HG22	3:G:257:ARG:NH1	2.26	0.50
1:U:164:GLY:N	1:U:324:THR:OG1	2.43	0.50
1:T:444:VAL:HG22	1:T:445:PRO:HD3	1.93	0.50
1:K:219:VAL:HG22	1:K:233:ILE:HG13	1.93	0.50
1:L:150:THR:HG21	1:L:155:VAL:HG11	1.92	0.50
2:O:140:VAL:HG13	2:O:414:LEU:HB3	1.94	0.50
2:E:30:LEU:HD21	2:E:57:ASN:HA	1.93	0.50
3:G:161:LYS:HE2	3:G:163:SER:OG	2.11	0.50
1:U:97:VAL:HG11	1:U:247:LEU:HD21	1.93	0.50
1:K:158:LEU:HD21	1:K:392:LEU:HG	1.93	0.50
2:D:279:VAL:HG12	2:D:279:VAL:O	2.11	0.50
1:K:138:ILE:CD1	1:K:138:ILE:N	2.75	0.50
2:X:256:ASP:HA	2:X:309:ALA:HB3	1.93	0.50
3:G:247:MET:HG2	3:G:250:ARG:NH2	2.26	0.50
2:O:14:THR:HG21	2:O:24:HIS:HB2	1.92	0.50
1:S:385:LEU:HD11	1:S:447:ILE:HD12	1.92	0.50
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.93	0.50
2:D:90:GLU:HG3	2:D:110:LYS:O	2.11	0.50
1:S:446:LEU:HD21	1:S:467:GLU:HA	1.94	0.50
1:S:277:ALA:HB2	1:S:304:HIS:HE1	1.77	0.50
1:S:211:LYS:HE3	1:S:214:THR:OG1	2.11	0.50
2:N:85:VAL:HG13	2:N:235:THR:HG23	1.92	0.50
2:F:442:LYS:HG2	2:F:446:GLU:OE2	2.11	0.50
1:C:109:VAL:HG13	1:C:233:ILE:HB	1.94	0.50
2:M:381:TYR:O	2:M:385:GLN:HG3	2.12	0.50
1:L:375:ARG:HH11	6:M:600:ANP:C5'	2.24	0.50
1:S:101:VAL:HA	1:S:105:LEU:HD11	1.93	0.50
2:E:109:ILE:C	2:E:111:SER:H	2.14	0.50
3:Y:28:SER:O	3:Y:31:LEU:HB3	2.12	0.50
2:D:208:ASN:ND2	2:D:211:GLY:HA3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:384:LEU:O	2:O:388:ILE:HG12	2.12	0.50
1:A:239:SER:HB3	2:D:294:GLU:HG3	1.94	0.50
1:J:399:TYR:CD1	1:J:423:GLY:HA3	2.46	0.50
3:Y:89:SER:HA	3:Y:117:GLN:HE21	1.77	0.50
2:M:377:THR:HG22	2:M:407:ALA:HB2	1.94	0.50
1:T:166:ARG:NH2	2:X:190:ARG:HD3	2.27	0.49
1:S:165:GLN:NE2	1:S:374:SER:OG	2.44	0.49
1:K:30:THR:HG23	2:X:464:GLU:OE2	2.12	0.49
2:M:143:LEU:O	2:M:367:HIS:HE1	1.95	0.49
1:C:203:CYS:O	1:C:231:SER:HA	2.12	0.49
1:T:283:LEU:O	1:T:287:LEU:HD12	2.12	0.49
2:N:224:GLU:O	2:N:229:ARG:NH1	2.41	0.49
1:K:166:ARG:CD	1:K:311:ALA:HB3	2.42	0.49
1:A:405:SER:C	1:A:407:GLN:H	2.16	0.49
1:B:429:LEU:HD21	1:B:446:LEU:O	2.12	0.49
2:E:425:THR:HB	2:E:427:ILE:CD1	2.42	0.49
2:M:97:ASN:C	2:M:97:ASN:OD1	2.51	0.49
2:F:96:ILE:HG22	2:F:97:ASN:N	2.27	0.49
1:B:248:ALA:HB3	1:B:249:PRO:HD3	1.94	0.49
2:O:140:VAL:CG1	2:O:414:LEU:HD22	2.42	0.49
1:T:208:VAL:HG21	1:T:249:PRO:HD3	1.94	0.49
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.94	0.49
2:M:335:LEU:HA	2:M:347:ALA:O	2.12	0.49
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.94	0.49
1:L:331:THR:HG21	1:L:336:VAL:HG12	1.95	0.49
3:P:107:ILE:HG13	3:P:126:ILE:HA	1.94	0.49
2:W:53:HIS:CD2	2:W:59:VAL:HG12	2.47	0.49
3:G:77:ILE:HG12	3:G:165:PHE:O	2.12	0.49
4:H:131:GLU:HA	4:H:134:GLN:HE21	1.77	0.49
3:G:149:LYS:HA	3:G:152:SER:HB2	1.94	0.49
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.95	0.49
1:T:421:VAL:O	1:T:425:ARG:HG2	2.13	0.49
1:U:68:LEU:HB2	2:V:16:VAL:HG23	1.95	0.49
1:S:99:VAL:HG21	1:S:251:THR:HG23	1.95	0.49
1:C:77:LEU:HD12	1:C:81:ASP:HB3	1.95	0.49
2:E:98:VAL:HG23	2:E:232:VAL:HA	1.93	0.49
2:W:242:TYR:CE1	2:W:246:GLU:HG3	2.47	0.49
1:K:138:ILE:O	2:O:195:ASN:ND2	2.45	0.49
4:H:35:LYS:HD3	4:H:35:LYS:H	1.77	0.49
3:P:212:TYR:O	3:P:216:ASN:HB2	2.13	0.49
1:U:332:GLN:HB3	2:X:318:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:HA	1:A:365:PRO:C	2.33	0.49
2:M:387:ILE:HG23	2:M:391:LEU:HD12	1.94	0.49
1:A:197:GLU:HA	1:A:200:LYS:HD2	1.95	0.49
2:X:344:ILE:HG23	2:X:415:SER:HB3	1.94	0.49
3:P:74:ILE:HG23	3:P:165:PHE:CD2	2.47	0.49
3:P:267:LEU:O	3:P:271:ILE:HD12	2.13	0.49
2:X:52:GLN:HE22	2:X:60:ARG:HH11	1.61	0.49
3:G:42:LYS:O	3:G:46:GLU:HG2	2.13	0.49
1:S:347:ILE:HA	2:W:222:MET:SD	2.53	0.49
2:M:138:ILE:HG12	2:M:418:PHE:CE1	2.47	0.48
1:T:444:VAL:CG2	1:T:445:PRO:HD3	2.41	0.48
2:D:176:LYS:HD3	2:D:204:THR:CG2	2.40	0.48
1:K:455:LEU:HA	1:K:458:ILE:HD12	1.94	0.48
1:C:232:ILE:HD13	1:C:255:ILE:CG2	2.42	0.48
1:K:155:VAL:HA	1:K:159:VAL:HG23	1.95	0.48
1:A:158:LEU:HD21	1:A:392:LEU:HG	1.94	0.48
1:S:166:ARG:NH2	2:W:190:ARG:HD3	2.27	0.48
1:C:222:LEU:HB2	1:C:228:MET:HE2	1.94	0.48
1:S:429:LEU:HD11	1:S:455:LEU:HD12	1.95	0.48
1:S:145:HIS:H	1:S:313:LYS:HZ3	1.62	0.48
2:E:396:LEU:HB3	2:E:401:LYS:HB3	1.95	0.48
2:D:190:ARG:O	2:D:193:GLU:HB2	2.13	0.48
1:B:220:GLN:HG3	1:B:224:GLN:NE2	2.29	0.48
3:P:86:SER:HB2	3:P:90:GLN:HG3	1.96	0.48
2:X:218:VAL:HG21	2:X:236:GLY:CA	2.43	0.48
2:E:185:THR:HG21	2:E:233:ALA:HA	1.96	0.48
2:D:345:TYR:HA	2:D:346:PRO:C	2.33	0.48
1:U:455:LEU:HD22	1:U:463:ILE:HD12	1.96	0.48
3:G:34:ALA:HB2	3:G:226:TYR:HE2	1.79	0.48
2:X:52:GLN:HE22	2:X:60:ARG:NH1	2.11	0.48
1:C:145:HIS:HA	1:C:379:ALA:O	2.13	0.48
2:D:64:MET:CE	2:D:228:ALA:HA	2.43	0.48
1:A:455:LEU:HD21	1:A:466:PHE:CE1	2.48	0.48
1:B:384:ALA:HB1	1:B:444:VAL:HG11	1.96	0.48
1:S:106:LEU:HD21	1:S:259:PHE:CZ	2.49	0.48
1:T:43:VAL:HG21	1:T:75:ILE:HD12	1.95	0.48
2:V:293:GLN:HA	2:V:296:ILE:HD12	1.96	0.48
1:B:335:ASP:HB2	3:G:257:ARG:NH1	2.29	0.48
1:U:392:LEU:HD13	1:U:451:VAL:HG22	1.96	0.48
1:K:50:GLN:HB3	2:O:69:GLY:HA2	1.95	0.48
1:S:153:LYS:HG2	1:S:443:GLN:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:432:VAL:HG12	2:O:433:ARG:H	1.79	0.48
1:K:285:LEU:CD1	2:N:277:SER:HB3	2.44	0.48
2:O:237:LEU:O	2:O:237:LEU:HD12	2.14	0.48
1:U:332:GLN:HB3	2:X:318:THR:CG2	2.44	0.48
1:C:99:VAL:HG11	1:C:251:THR:HB	1.96	0.48
2:V:157:GLY:HA3	2:V:161:VAL:HG21	1.94	0.48
2:V:279:VAL:HG12	2:V:279:VAL:O	2.14	0.48
2:V:391:LEU:HG	3:Y:19:ILE:HD11	1.96	0.47
1:A:484:GLU:HB3	1:A:495:LEU:HD21	1.95	0.47
1:L:211:LYS:HD3	2:O:328:HIS:HA	1.95	0.47
1:U:282:GLN:CD	2:X:284:THR:HA	2.34	0.47
1:T:86:GLU:HB3	2:W:30:LEU:HD13	1.95	0.47
1:J:202:TYR:O	1:J:266:ALA:HA	2.14	0.47
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.96	0.47
6:S:600:ANP:O2A	6:S:600:ANP:N3B	2.46	0.47
3:G:213:THR:CG2	3:G:217:GLN:HE21	2.26	0.47
1:K:291:PRO:HG2	3:P:268:VAL:HG22	1.97	0.47
1:U:428:GLN:HA	1:U:431:LYS:HE3	1.96	0.47
1:B:187:ASN:OD1	1:B:437:PRO:HB2	2.14	0.47
2:X:224:GLU:HB3	2:X:228:ALA:HB3	1.96	0.47
2:N:279:VAL:HG12	2:N:279:VAL:O	2.14	0.47
3:G:110:ILE:HD11	3:G:146:ILE:HG21	1.96	0.47
1:U:293:ARG:HB3	1:U:339:TYR:CE2	2.48	0.47
1:A:260:ARG:O	1:A:321:GLY:HA3	2.14	0.47
1:J:139:LEU:HD13	2:N:104:ASP:HA	1.97	0.47
1:L:375:ARG:NH1	6:M:600:ANP:H5'1	2.30	0.47
2:X:163:LYS:H	6:X:600:ANP:PB	2.38	0.47
2:D:258:ILE:HD11	2:D:292:LEU:CD2	2.44	0.47
3:P:166:TYR:HE1	3:P:180:LYS:HG2	1.80	0.47
2:O:9:ILE:HB	2:O:78:ASP:HB3	1.95	0.47
2:V:346:PRO:O	2:V:347:ALA:CB	2.62	0.47
2:V:240:ALA:HB2	2:V:253:LEU:HD13	1.96	0.47
1:S:146:GLU:H	1:S:313:LYS:HZ3	1.62	0.47
2:D:190:ARG:HB2	2:D:193:GLU:HG3	1.96	0.47
1:B:444:VAL:N	1:B:445:PRO:CD	2.77	0.47
1:U:296:TYR:CD2	1:U:300:VAL:HG21	2.50	0.47
2:N:68:GLU:CD	2:N:68:GLU:H	2.17	0.47
1:U:290:PRO:HA	1:U:291:PRO:HD3	1.80	0.47
1:T:270:TYR:O	1:T:272:ASP:HA	2.15	0.47
1:J:424:GLU:HB3	1:J:460:LEU:CD1	2.45	0.47
2:W:140:VAL:HG22	2:W:414:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:474:LEU:HD13	1:T:482:LEU:HD21	1.97	0.47
3:G:55:ALA:HA	3:G:193:SER:HB2	1.96	0.47
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.97	0.47
1:T:338:ALA:HB3	1:T:341:PRO:HG2	1.96	0.47
1:S:174:GLN:HB3	2:V:354:LYS:CD	2.44	0.47
2:O:67:THR:HB	2:O:70:LEU:HD12	1.96	0.47
2:X:217:LEU:HB3	2:X:219:PHE:HE2	1.79	0.47
2:V:97:ASN:ND2	2:V:101:GLU:HB2	2.27	0.47
2:X:321:ALA:CB	2:X:322:PRO:CD	2.92	0.47
1:J:43:VAL:HG21	1:J:75:ILE:HD12	1.97	0.47
2:N:152:LYS:HE3	2:N:296:ILE:HB	1.97	0.47
2:V:346:PRO:HG3	2:V:418:PHE:CZ	2.50	0.47
2:M:64:MET:HE1	2:M:228:ALA:HA	1.97	0.47
1:S:32:ARG:HD2	1:S:89:LEU:HD12	1.96	0.47
2:M:96:ILE:HG22	2:M:97:ASN:O	2.15	0.47
1:K:174:GLN:HA	6:K:600:ANP:HNB1	1.80	0.47
2:X:65:ASP:CG	2:X:66:GLY:H	2.18	0.47
3:P:227:ALA:HA	3:P:230:ILE:HG22	1.96	0.47
1:T:52:GLU:HA	1:T:65:ALA:O	2.14	0.47
2:N:30:LEU:HD22	2:N:59:VAL:HG13	1.97	0.47
2:V:191:THR:HA	2:V:221:GLN:HG3	1.96	0.47
1:S:232:ILE:HG21	1:S:255:ILE:HG21	1.96	0.47
1:S:382:VAL:HG11	1:S:440:THR:HG21	1.97	0.47
1:A:396:LEU:O	1:A:400:ARG:HG3	2.15	0.47
1:T:474:LEU:HB3	1:T:482:LEU:HD11	1.96	0.47
2:V:189:GLU:HG2	2:V:256:ASP:O	2.15	0.47
1:U:394:LEU:HD11	2:V:458:TYR:OH	2.15	0.47
1:T:174:GLN:HA	6:T:600:ANP:HNB1	1.80	0.47
1:J:397:ALA:HA	1:J:400:ARG:NH2	2.30	0.47
2:W:220:GLY:HA3	2:W:232:VAL:HG21	1.97	0.47
2:M:198:TYR:CZ	2:M:202:LYS:HE2	2.50	0.47
2:M:132:GLU:HG2	2:M:149:ARG:HG3	1.97	0.47
1:A:77:LEU:CD1	1:A:81:ASP:HB3	2.44	0.47
2:E:30:LEU:HA	2:E:31:PRO:HD2	1.72	0.47
2:D:62:ILE:HD11	2:D:272:LEU:HD11	1.96	0.47
1:S:452:ASN:HB3	1:S:454:HIS:HE1	1.80	0.47
3:P:17:GLU:HB2	3:P:244:ALA:HB1	1.97	0.47
2:N:471:GLU:HA	2:N:474:ALA:HB2	1.97	0.47
1:U:166:ARG:HD3	1:U:311:ALA:HB3	1.96	0.46
1:S:32:ARG:HH11	1:S:89:LEU:HB2	1.79	0.46
1:U:260:ARG:NH1	1:U:310:ARG:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:179:ALA:CB	6:S:600:ANP:H8	2.45	0.46
1:S:491:LEU:HD23	1:S:495:LEU:HB3	1.96	0.46
1:A:455:LEU:HD23	1:A:458:ILE:HD12	1.98	0.46
2:N:133:ILE:HD12	2:N:146:PRO:HB2	1.97	0.46
1:A:96:ILE:CG2	2:E:68:GLU:OE2	2.63	0.46
2:F:182:SER:O	2:F:215:VAL:HA	2.15	0.46
2:W:95:ILE:HD11	2:W:198:TYR:CD1	2.50	0.46
1:T:166:ARG:HG2	1:T:311:ALA:HB3	1.96	0.46
2:V:346:PRO:HB2	2:V:348:VAL:HG23	1.97	0.46
2:X:217:LEU:HB3	2:X:219:PHE:CE2	2.50	0.46
2:X:178:HIS:NE2	2:X:250:ASP:O	2.48	0.46
2:X:360:ALA:O	2:X:364:GLY:N	2.46	0.46
2:N:150:GLY:HA2	2:N:304:VAL:O	2.15	0.46
2:W:135:GLU:OE2	2:W:433:ARG:HD3	2.16	0.46
1:A:169:ILE:HD11	1:A:326:LEU:HD13	1.97	0.46
2:F:171:ILE:O	2:F:175:ALA:HB3	2.16	0.46
1:A:338:ALA:HB3	1:A:341:PRO:HD2	1.98	0.46
1:T:160:PRO:O	1:T:377:GLY:HA3	2.16	0.46
1:U:252:ALA:HA	1:U:255:ILE:HD12	1.98	0.46
1:J:428:GLN:HA	1:J:431:LYS:HG3	1.97	0.46
2:X:279:VAL:O	2:X:279:VAL:HG12	2.15	0.46
2:M:30:LEU:HD22	2:M:59:VAL:HG13	1.97	0.46
1:U:291:PRO:HD2	3:Y:273:GLY:HA2	1.98	0.46
1:S:54:LEU:HD13	1:S:97:VAL:HG22	1.98	0.46
1:K:160:PRO:O	1:K:377:GLY:HA3	2.15	0.46
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.46	0.46
2:M:449:TYR:HD1	2:M:452:ILE:CD1	2.28	0.46
1:K:142:ARG:HG2	1:K:143:SER:N	2.30	0.46
1:U:153:LYS:HA	1:U:443:GLN:OE1	2.15	0.46
2:W:296:ILE:HG21	2:W:306:SER:HB2	1.98	0.46
2:D:167:ILE:HA	2:D:170:LEU:HD12	1.98	0.46
4:H:112:VAL:C	4:H:114:SER:HB3	2.36	0.46
3:P:180:LYS:HZ1	3:P:220:THR:HB	1.78	0.46
1:A:405:SER:O	1:A:407:GLN:N	2.49	0.46
1:T:185:ILE:HG12	1:T:203:CYS:SG	2.56	0.46
1:B:364:ARG:HA	1:B:365:PRO:C	2.35	0.46
1:S:138:ILE:HD12	2:W:194:GLY:HA3	1.96	0.46
2:M:30:LEU:HD11	2:M:57:ASN:HA	1.98	0.46
1:T:35:ALA:HB3	1:T:42:ARG:HH12	1.80	0.46
1:U:166:ARG:HD2	1:U:308:LEU:HB3	1.97	0.46
1:B:187:ASN:OD1	1:B:190:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HG21	2:E:68:GLU:CD	2.36	0.46
1:A:96:ILE:HG21	2:E:68:GLU:OE2	2.16	0.46
1:A:52:GLU:HB2	2:E:68:GLU:HG3	1.98	0.46
2:M:337:ARG:HG2	2:M:341:GLU:OE2	2.16	0.46
1:A:211:LYS:HE3	1:A:213:SER:OG	2.16	0.46
1:B:270:TYR:O	1:B:272:ASP:HA	2.15	0.46
1:J:270:TYR:O	1:J:272:ASP:HA	2.16	0.46
1:U:368:ASN:ND2	1:U:371:LEU:HD12	2.31	0.46
1:K:242:ALA:N	1:K:243:PRO:CD	2.79	0.46
1:U:349:ASP:HB3	2:V:192:ARG:HH21	1.80	0.46
2:W:321:ALA:HB3	2:W:322:PRO:HD3	1.97	0.46
1:A:407:GLN:HE21	2:D:384:LEU:HD21	1.81	0.46
1:A:192:ASN:HA	1:A:200:LYS:HG2	1.97	0.46
3:P:17:GLU:HB2	3:P:244:ALA:CB	2.46	0.46
2:X:13:VAL:O	2:X:73:GLY:N	2.47	0.46
1:T:139:LEU:HB3	1:T:140:PRO:HD3	1.97	0.46
1:B:421:VAL:HG13	1:B:425:ARG:HH12	1.81	0.46
1:L:455:LEU:HA	1:L:458:ILE:HD12	1.98	0.46
1:T:345:ILE:HG22	2:X:159:ALA:HB1	1.97	0.46
3:P:171:SER:HG	3:P:174:SER:N	2.13	0.46
1:T:138:ILE:HD12	2:X:95:ILE:HD13	1.97	0.46
2:D:299:THR:OG1	2:D:300:LYS:N	2.49	0.46
3:P:77:ILE:HD13	3:P:222:MET:HG3	1.97	0.46
2:M:90:GLU:CG	2:M:111:SER:HB3	2.45	0.46
1:S:77:LEU:O	1:S:243:PRO:HG2	2.16	0.46
1:U:177:LYS:NZ	6:U:600:ANP:O1B	2.43	0.46
1:J:46:LEU:O	1:J:49:ILE:HG22	2.16	0.46
1:K:363:ILE:HA	1:K:431:LYS:HE2	1.98	0.46
2:E:41:THR:HB	2:E:42:PRO:HD2	1.98	0.46
1:J:166:ARG:HD2	1:J:308:LEU:O	2.16	0.46
2:V:134:LEU:HB2	2:V:149:ARG:HG3	1.98	0.46
1:S:223:GLU:HG3	1:S:228:MET:HG3	1.98	0.46
2:X:312:VAL:HG11	2:X:317:LEU:HD23	1.98	0.46
2:F:257:ASN:HD21	2:F:311:TYR:N	2.14	0.46
1:K:243:PRO:HA	1:K:246:TYR:HD2	1.81	0.45
3:P:77:ILE:HG21	3:P:222:MET:HG2	1.98	0.45
1:U:344:VAL:O	1:U:348:THR:HG23	2.16	0.45
2:X:43:GLN:HA	2:X:43:GLN:HE21	1.82	0.45
2:N:310:VAL:HG11	2:N:326:PHE:CE1	2.49	0.45
1:B:86:GLU:HB3	2:E:30:LEU:HD13	1.98	0.45
1:L:363:ILE:O	1:L:366:ALA:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:133:ILE:HD11	2:O:362:VAL:HG12	1.98	0.45
1:T:273:LEU:HD22	1:T:304:HIS:CD2	2.51	0.45
2:O:33:ILE:O	2:O:34:LEU:HB2	2.16	0.45
2:O:182:SER:O	2:O:215:VAL:HA	2.16	0.45
1:S:82:ARG:HH11	2:V:34:LEU:HB2	1.81	0.45
2:E:396:LEU:HD13	2:E:401:LYS:HA	1.98	0.45
2:D:140:VAL:HG23	2:D:414:LEU:HD22	1.97	0.45
1:T:309:GLU:CG	2:X:222:MET:HG3	2.47	0.45
1:C:211:LYS:HE3	1:C:213:SER:OG	2.16	0.45
1:U:107:GLY:HA2	1:U:228:MET:HG3	1.99	0.45
1:C:165:GLN:HG3	1:C:349:ASP:HB2	1.98	0.45
2:E:140:VAL:HG13	2:E:414:LEU:HB3	1.98	0.45
1:L:375:ARG:HH11	6:M:600:ANP:H5'2	1.81	0.45
1:K:283:LEU:CD2	1:K:287:LEU:HD12	2.46	0.45
2:W:34:LEU:H	2:W:50:VAL:HB	1.80	0.45
1:U:282:GLN:OE1	2:X:284:THR:HA	2.16	0.45
1:U:201:LEU:HA	1:U:265:HIS:O	2.16	0.45
1:S:168:LEU:HB2	1:S:348:THR:HG21	1.98	0.45
1:U:239:SER:HB3	2:X:290:GLY:O	2.16	0.45
1:B:103:PRO:HD3	1:B:258:TRP:CH2	2.51	0.45
1:K:283:LEU:CD2	1:K:287:LEU:CD1	2.95	0.45
2:M:90:GLU:CG	2:M:111:SER:CB	2.93	0.45
2:F:159:ALA:HA	6:F:600:ANP:O1G	2.16	0.45
3:G:23:MET:O	3:G:27:ALA:HB2	2.17	0.45
2:D:168:GLN:HB3	2:D:420:VAL:HG11	1.98	0.45
1:S:201:LEU:HA	1:S:265:HIS:O	2.17	0.45
1:J:353:PHE:CE2	1:J:355:GLU:HG3	2.51	0.45
1:C:329:ILE:HA	1:C:329:ILE:HD13	1.88	0.45
2:N:317:LEU:HD22	2:N:326:PHE:HE2	1.81	0.45
2:W:33:ILE:O	2:W:34:LEU:HB2	2.16	0.45
1:L:357:GLU:OE2	1:L:361:LYS:NZ	2.47	0.45
1:J:421:VAL:O	1:J:425:ARG:HD2	2.17	0.45
1:C:92:ARG:NH2	1:C:94:GLY:HA2	2.26	0.45
1:U:375:ARG:NH1	6:V:600:ANP:N3B	2.65	0.45
1:U:176:GLY:HA2	6:U:600:ANP:PA	2.57	0.45
1:U:339:TYR:HE1	1:U:343:ASN:HD21	1.65	0.45
2:N:242:TYR:CE1	2:N:246:GLU:HG3	2.51	0.45
2:D:96:ILE:O	2:D:218:VAL:HA	2.16	0.45
1:U:206:VAL:HG11	1:U:249:PRO:HA	1.98	0.45
1:J:167:GLU:O	1:J:326:LEU:HA	2.16	0.45
1:C:364:ARG:HA	1:C:365:PRO:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:74:ILE:HG21	3:P:95:VAL:HG13	1.99	0.45
1:L:478:HIS:HB3	1:L:481:LEU:HB2	1.99	0.45
3:G:87:ILE:HG23	3:G:167:ASN:ND2	2.31	0.45
1:T:503:THR:O	1:T:507:VAL:HG23	2.16	0.45
1:B:471:LEU:O	1:B:475:LYS:HG3	2.17	0.45
2:V:33:ILE:O	2:V:34:LEU:HB2	2.17	0.45
1:S:109:VAL:HG22	1:S:233:ILE:HB	1.99	0.45
1:A:506:PHE:O	1:A:509:THR:HG22	2.17	0.45
1:T:375:ARG:NH2	2:X:160:GLY:HA2	2.32	0.45
1:S:165:GLN:NE2	1:S:167:GLU:OE1	2.50	0.45
1:U:139:LEU:O	1:U:141:ARG:N	2.47	0.45
2:X:359:ASP:O	2:X:363:VAL:HG22	2.17	0.45
1:A:203:CYS:O	1:A:231:SER:HA	2.17	0.45
1:L:248:ALA:HB3	1:L:249:PRO:HD3	1.99	0.45
1:L:252:ALA:HA	1:L:255:ILE:HD12	1.99	0.44
2:V:197:LEU:HA	2:V:200:GLU:HG2	2.00	0.44
1:U:69:GLU:CB	1:U:70:PRO:HD2	2.36	0.44
1:K:400:ARG:HA	1:K:403:ALA:HB3	1.99	0.44
1:C:174:GLN:CB	2:F:354:LYS:HD3	2.48	0.44
2:M:93:GLY:HA2	2:M:207:ILE:HG12	1.99	0.44
3:P:204:ASN:C	3:P:206:PRO:HD2	2.38	0.44
2:F:41:THR:HB	2:F:42:PRO:CD	2.39	0.44
2:F:359:ASP:O	2:F:363:VAL:HG22	2.18	0.44
1:L:383:LYS:HB3	1:L:489:GLY:O	2.17	0.44
2:D:201:MET:CE	2:D:217:LEU:HD21	2.48	0.44
2:X:388:ILE:HD11	2:X:396:LEU:HD11	1.99	0.44
1:K:155:VAL:HA	1:K:159:VAL:CG2	2.48	0.44
1:A:98:ASP:HA	1:A:130:ARG:HA	2.00	0.44
2:W:382:LYS:HA	2:W:385:GLN:HG3	1.99	0.44
1:U:382:VAL:HG21	1:U:440:THR:HG21	1.99	0.44
2:X:163:LYS:HE2	2:X:163:LYS:HB2	1.82	0.44
2:X:274:ARG:NH2	2:X:284:THR:OG1	2.50	0.44
1:K:181:ALA:HB1	1:K:269:VAL:HG21	1.99	0.44
4:Q:51:GLN:HG3	4:Q:74:PHE:CE2	2.52	0.44
1:U:98:ASP:HB3	1:U:130:ARG:HA	1.99	0.44
1:J:201:LEU:HD11	1:J:267:LEU:HB2	1.98	0.44
1:C:395:PHE:CD1	1:C:395:PHE:C	2.90	0.44
1:S:162:GLY:N	1:S:165:GLN:OE1	2.50	0.44
1:S:152:LEU:HD22	1:S:365:PRO:HG3	2.00	0.44
4:Q:41:VAL:HG23	4:Q:45:HIS:HB2	2.00	0.44
2:O:257:ASN:HD21	2:O:311:TYR:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:133:ILE:HD12	3:P:134:GLY:N	2.32	0.44
2:N:33:ILE:O	2:N:34:LEU:CB	2.65	0.44
1:B:290:PRO:HA	1:B:291:PRO:HD2	1.90	0.44
2:N:237:LEU:HD21	2:N:295:ARG:HB2	1.99	0.44
1:B:220:GLN:HE21	1:B:224:GLN:HE21	1.66	0.44
1:A:455:LEU:HA	1:A:458:ILE:HD12	1.99	0.44
1:K:442:GLU:C	1:K:445:PRO:HD2	2.38	0.44
2:M:140:VAL:HA	2:M:414:LEU:HD22	1.99	0.44
1:J:484:GLU:HB3	1:J:495:LEU:HD21	1.99	0.44
2:M:54:LEU:HD11	2:M:60:ARG:HB2	1.98	0.44
2:E:225:PRO:O	2:E:226:PRO:C	2.56	0.44
2:W:242:TYR:CD1	2:W:246:GLU:HG3	2.53	0.44
1:S:203:CYS:O	1:S:231:SER:HA	2.17	0.44
1:U:270:TYR:CE1	1:U:307:LEU:HD11	2.53	0.44
1:K:488:LYS:HB3	1:K:490:GLU:H	1.81	0.44
2:M:89:ARG:HH11	2:M:181:PHE:HZ	1.64	0.44
1:C:155:VAL:HG13	1:C:159:VAL:HG23	1.99	0.44
4:H:45:HIS:HD2	4:H:77:VAL:HG21	1.82	0.44
2:N:296:ILE:HD13	2:N:306:SER:CB	2.45	0.44
2:W:37:LEU:HD12	2:W:61:THR:HG21	1.99	0.44
2:X:367:HIS:CD2	2:X:367:HIS:O	2.71	0.44
1:S:452:ASN:HB3	1:S:454:HIS:CE1	2.53	0.44
2:F:182:SER:HA	2:F:252:LEU:O	2.17	0.44
1:U:395:PHE:O	1:U:398:GLN:HB2	2.18	0.44
2:W:121:PRO:HG3	2:W:295:ARG:HG3	2.00	0.44
2:E:139:LYS:NZ	2:E:413:PHE:O	2.49	0.44
1:K:77:LEU:O	1:K:243:PRO:HG2	2.18	0.44
3:G:213:THR:CG2	3:G:217:GLN:NE2	2.81	0.44
1:B:166:ARG:CD	1:B:311:ALA:HB3	2.47	0.44
2:D:48:LEU:HD13	2:D:61:THR:OG1	2.17	0.44
4:H:57:VAL:HG21	4:H:70:ILE:HD12	2.00	0.44
3:G:204:ASN:HB2	3:G:207:ARG:HB3	1.98	0.44
2:N:168:GLN:HE21	2:N:201:MET:HG3	1.82	0.44
3:G:143:SER:OG	3:G:215:ALA:O	2.34	0.44
2:N:92:LEU:HD11	2:N:181:PHE:CE2	2.53	0.44
1:S:337:SER:HB3	3:Y:259:ARG:HH11	1.83	0.44
3:P:75:VAL:HB	3:P:164:ILE:HD13	2.00	0.44
2:V:231:ARG:HD2	2:V:234:LEU:HD12	1.99	0.44
2:N:26:GLU:O	2:N:29:GLU:HB2	2.18	0.44
1:K:34:LEU:O	2:N:55:GLY:HA2	2.17	0.44
2:F:190:ARG:HH11	2:F:190:ARG:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:279:VAL:HG12	2:M:279:VAL:O	2.18	0.44
3:G:95:VAL:O	3:G:99:LEU:CB	2.64	0.43
1:U:139:LEU:N	1:U:140:PRO:CD	2.80	0.43
1:C:68:LEU:O	2:D:15:ALA:HA	2.17	0.43
2:F:247:GLU:CB	2:F:249:GLN:HG2	2.48	0.43
1:T:202:TYR:O	1:T:266:ALA:HA	2.18	0.43
1:T:190:ARG:HE	1:T:439:ALA:HB2	1.83	0.43
3:Y:77:ILE:HA	3:Y:110:ILE:HB	2.00	0.43
1:K:164:GLY:HA2	1:K:323:LEU:O	2.18	0.43
3:Y:211:GLU:O	5:1:11:ALA:HB2	2.18	0.43
2:D:191:THR:HA	2:D:221:GLN:HG3	1.99	0.43
1:S:148:VAL:HG12	1:S:148:VAL:O	2.18	0.43
4:H:35:LYS:HG2	4:H:36:SER:N	2.31	0.43
1:K:397:ALA:HA	1:K:400:ARG:HD2	1.99	0.43
1:B:421:VAL:O	1:B:425:ARG:HG2	2.18	0.43
2:F:258:ILE:HD11	2:F:292:LEU:HD21	2.00	0.43
2:E:43:GLN:HG2	2:E:44:GLY:N	2.33	0.43
2:X:293:GLN:HA	2:X:296:ILE:HD12	2.00	0.43
1:C:414:ALA:HA	1:C:417:LYS:HE2	1.99	0.43
4:H:32:LEU:HD21	4:H:85:VAL:HG22	2.00	0.43
1:S:385:LEU:HD12	1:S:444:VAL:HG13	1.99	0.43
2:D:64:MET:HE1	2:D:228:ALA:HA	2.00	0.43
1:S:138:ILE:O	2:W:195:ASN:ND2	2.44	0.43
1:C:493:LYS:H	1:C:493:LYS:HD2	1.83	0.43
1:S:58:SER:HB2	1:S:88:GLU:HG3	2.00	0.43
2:M:252:LEU:HD23	2:M:305:THR:HB	1.99	0.43
2:V:96:ILE:HB	2:V:218:VAL:HG22	1.99	0.43
1:U:154:ALA:HA	1:U:430:LEU:HD22	2.01	0.43
1:U:165:GLN:NE2	1:U:167:GLU:OE1	2.50	0.43
2:V:159:ALA:O	2:V:337:ARG:NH2	2.45	0.43
2:E:419:ALA:HA	2:E:429:GLY:HA3	2.00	0.43
1:C:202:TYR:O	1:C:266:ALA:HA	2.18	0.43
2:X:182:SER:HB2	2:X:215:VAL:HB	1.99	0.43
2:M:277:SER:OG	2:M:278:ALA:N	2.50	0.43
1:K:139:LEU:HB3	1:K:140:PRO:HD3	2.01	0.43
1:C:219:VAL:HB	1:C:228:MET:CE	2.48	0.43
1:L:107:GLY:HA2	1:L:228:MET:O	2.19	0.43
2:W:71:VAL:O	2:W:74:GLU:HB2	2.18	0.43
2:E:31:PRO:HB2	2:E:50:VAL:HG21	2.00	0.43
1:L:166:ARG:HD2	1:L:308:LEU:O	2.17	0.43
1:C:80:SER:OG	1:C:82:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:367:HIS:CD2	2:E:434:LEU:HD11	2.53	0.43
2:V:417:PRO:HD2	2:V:430:LYS:HB2	2.00	0.43
1:C:177:LYS:HG2	1:C:354:LEU:HD12	2.00	0.43
1:L:311:ALA:HA	1:L:323:LEU:HB3	1.99	0.43
1:C:421:VAL:HG13	1:C:425:ARG:NH1	2.33	0.43
1:U:146:GLU:O	1:U:162:GLY:HA2	2.19	0.43
2:M:64:MET:HE3	2:M:228:ALA:HA	2.00	0.43
2:O:388:ILE:CD1	2:O:396:LEU:HD11	2.49	0.43
1:U:116:PRO:HG3	1:U:121:GLY:O	2.19	0.43
2:X:41:THR:HB	2:X:42:PRO:HD2	2.00	0.43
2:V:201:MET:SD	2:V:217:LEU:HD21	2.59	0.43
1:B:174:GLN:HA	6:B:600:ANP:HNB1	1.82	0.43
2:X:121:PRO:HA	2:X:122:PRO:HD2	1.84	0.43
1:K:249:PRO:HB3	1:K:270:TYR:CD1	2.54	0.43
2:V:199:ARG:CZ	2:V:199:ARG:HB3	2.48	0.43
2:X:382:LYS:HA	2:X:385:GLN:HG2	1.99	0.43
1:U:211:LYS:HD3	2:X:328:HIS:O	2.18	0.43
1:L:219:VAL:HG22	1:L:228:MET:HE1	2.00	0.43
3:Y:139:THR:HG21	5:1:37:ARG:HA	2.00	0.43
1:L:182:LEU:HD13	1:L:218:LEU:HD11	2.00	0.43
3:G:135:LYS:HB2	3:G:135:LYS:HE2	1.74	0.43
2:E:275:ILE:HA	2:E:276:PRO:HD3	1.86	0.43
1:J:188:GLN:CD	1:J:201:LEU:HD23	2.39	0.43
1:K:272:ASP:HB2	1:K:328:VAL:O	2.19	0.43
3:P:106:ASP:HB3	3:P:127:LYS:HG3	2.01	0.43
1:T:159:VAL:HG21	1:T:352:ILE:HG12	2.01	0.43
2:M:366:GLU:O	2:M:370:VAL:HG23	2.19	0.43
2:M:24:HIS:CE1	2:M:25:PHE:O	2.72	0.42
1:K:93:THR:HG22	1:K:95:ASN:N	2.31	0.42
2:O:206:VAL:HG12	2:O:215:VAL:CG1	2.48	0.42
1:S:105:LEU:HD23	1:S:123:ILE:HG21	2.00	0.42
1:U:133:VAL:HB	1:U:310:ARG:NH2	2.34	0.42
2:N:440:SER:O	2:N:444:VAL:HG23	2.19	0.42
2:N:357:LEU:HD13	2:N:362:VAL:HG11	2.01	0.42
3:G:203:ALA:O	3:G:205:VAL:N	2.52	0.42
2:O:374:VAL:HG13	2:O:410:ILE:HG21	2.01	0.42
1:C:479:ASN:O	1:C:479:ASN:ND2	2.49	0.42
1:U:441:GLU:CD	1:U:486:ARG:HD3	2.40	0.42
1:K:442:GLU:O	1:K:446:LEU:HG	2.19	0.42
1:J:239:SER:HB3	2:M:294:GLU:HG3	2.00	0.42
2:W:244:ARG:HD3	2:W:304:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:N	1:A:140:PRO:HD2	2.34	0.42
1:J:389:ALA:O	1:J:390:GLY:C	2.58	0.42
1:C:272:ASP:HB2	1:C:328:VAL:O	2.20	0.42
1:U:422:ARG:NH1	1:U:453:GLY:HA3	2.33	0.42
2:V:321:ALA:HB3	2:V:322:PRO:CD	2.49	0.42
2:W:256:ASP:HA	2:W:257:ASN:HA	1.85	0.42
2:E:120:ASP:HA	2:E:121:PRO:HD3	1.92	0.42
2:V:387:ILE:HG23	2:V:391:LEU:HD12	2.00	0.42
3:Y:79:SER:OG	3:Y:80:ASP:N	2.53	0.42
1:C:239:SER:HB2	2:F:291:LEU:HD23	2.02	0.42
1:U:360:TYR:OH	2:X:351:LEU:O	2.31	0.42
1:K:139:LEU:HD12	1:K:139:LEU:HA	1.86	0.42
2:M:172:ASN:ND2	2:M:419:ALA:HB3	2.34	0.42
2:F:49:GLU:CD	2:F:231:ARG:HE	2.22	0.42
2:F:372:SER:O	2:F:376:GLU:HG3	2.19	0.42
2:O:351:LEU:HD23	2:O:375:GLN:HG2	2.01	0.42
2:X:472:LYS:HD2	2:X:472:LYS:HA	1.81	0.42
2:X:351:LEU:HD12	2:X:382:LYS:HE3	2.01	0.42
1:J:52:GLU:CD	2:N:68:GLU:HG3	2.40	0.42
1:J:424:GLU:HB3	1:J:460:LEU:HD11	2.01	0.42
1:A:248:ALA:HB3	1:A:249:PRO:HD3	2.00	0.42
3:P:49:GLN:HG3	3:P:217:GLN:NE2	2.34	0.42
2:M:209:LEU:O	2:M:210:GLU:HG3	2.20	0.42
1:B:67:ASN:O	1:B:67:ASN:OD1	2.37	0.42
3:P:180:LYS:HA	3:P:181:PRO:HD3	1.77	0.42
1:S:176:GLY:HA2	6:S:600:ANP:O5'	2.18	0.42
2:X:189:GLU:O	2:X:221:GLN:HB3	2.19	0.42
2:M:373:LYS:O	2:M:377:THR:OG1	2.38	0.42
4:H:72:GLY:HA3	5:I:14:LEU:HD21	1.99	0.42
2:D:275:ILE:O	2:D:283:PRO:HG3	2.20	0.42
1:J:474:LEU:HD13	1:J:482:LEU:HD21	2.01	0.42
2:X:25:PHE:CZ	2:X:31:PRO:HG3	2.55	0.42
2:V:239:ILE:O	2:V:243:PHE:HD2	2.01	0.42
2:F:256:ASP:HA	2:F:309:ALA:HB3	2.02	0.42
2:M:221:GLN:OE1	2:M:221:GLN:HA	2.19	0.42
3:G:75:VAL:HA	3:G:108:VAL:O	2.19	0.42
3:P:166:TYR:CE1	3:P:180:LYS:HG2	2.54	0.42
2:V:77:LEU:CG	2:V:78:ASP:H	2.23	0.42
1:S:144:VAL:HB	1:S:376:VAL:HG11	2.01	0.42
2:X:218:VAL:HG21	2:X:236:GLY:HA2	2.02	0.42
1:U:257:GLU:HG2	1:U:260:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:206:VAL:HG22	1:S:252:ALA:CB	2.49	0.42
1:J:50:GLN:HB3	2:N:69:GLY:HA2	2.02	0.42
1:J:297:PRO:HD2	1:J:300:VAL:HB	2.02	0.42
1:T:363:ILE:HA	1:T:431:LYS:HE2	2.00	0.42
1:U:428:GLN:O	1:U:431:LYS:HB2	2.20	0.42
2:O:252:LEU:HD23	2:O:305:THR:HB	2.02	0.42
1:C:118:ASP:CG	1:C:120:LYS:HG3	2.40	0.42
1:A:355:GLU:OE2	1:A:368:ASN:ND2	2.44	0.42
2:N:458:TYR:CE2	2:N:459:MET:HG2	2.55	0.42
2:D:158:GLY:O	2:D:161:VAL:HG22	2.18	0.42
2:F:88:GLY:O	2:F:91:THR:OG1	2.34	0.42
2:V:171:ILE:O	2:V:175:ALA:HB3	2.19	0.42
2:X:320:PRO:O	2:X:324:THR:OG1	2.34	0.42
1:A:440:THR:O	1:A:444:VAL:HG13	2.20	0.42
3:P:74:ILE:HB	3:P:107:ILE:HG22	2.02	0.42
2:W:160:GLY:HA3	2:W:337:ARG:HH22	1.82	0.42
2:D:243:PHE:O	2:D:247:GLU:HB3	2.20	0.42
2:O:189:GLU:O	2:O:221:GLN:HB3	2.19	0.42
2:M:84:SER:HB2	2:M:114:ARG:NH2	2.35	0.42
2:W:258:ILE:HG22	2:W:309:ALA:O	2.20	0.42
1:U:293:ARG:HB3	1:U:339:TYR:HE2	1.85	0.42
1:L:222:LEU:HB3	1:L:228:MET:HE2	2.01	0.42
2:E:50:VAL:HA	2:E:61:THR:HG22	2.01	0.42
2:V:415:SER:HB2	2:V:459:MET:H	1.85	0.42
1:U:491:LEU:HA	1:U:495:LEU:HD12	2.01	0.42
2:F:9:ILE:HG23	2:F:27:GLN:NE2	2.34	0.42
1:J:391:SER:O	1:J:394:LEU:N	2.51	0.42
1:J:501:SER:O	1:J:505:SER:HB2	2.20	0.42
3:P:12:SER:O	3:P:15:ASN:HB2	2.20	0.42
1:L:399:TYR:CD1	1:L:423:GLY:HA3	2.55	0.42
1:K:241:ALA:HB1	1:K:243:PRO:HD2	2.02	0.41
1:S:285:LEU:HD22	2:V:275:ILE:HG22	2.02	0.41
2:V:345:TYR:HA	2:V:346:PRO:C	2.41	0.41
2:O:432:VAL:HG12	2:O:433:ARG:N	2.34	0.41
1:L:49:ILE:HD11	1:L:55:VAL:CG1	2.49	0.41
1:T:271:ASP:HA	1:T:272:ASP:HA	1.66	0.41
2:O:33:ILE:HG22	2:O:34:LEU:HG	2.02	0.41
1:S:168:LEU:HD12	1:S:327:PRO:O	2.20	0.41
1:K:354:LEU:HA	1:K:366:ALA:O	2.20	0.41
2:D:463:ILE:O	2:D:467:VAL:HG23	2.19	0.41
1:B:182:LEU:HD13	1:B:218:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:138:ILE:HD13	2:V:103:ILE:HD12	2.02	0.41
1:K:39:GLY:HA2	1:K:81:ASP:OD1	2.19	0.41
2:F:84:SER:HB3	2:F:114:ARG:HH11	1.85	0.41
1:T:143:SER:N	2:X:199:ARG:HH22	2.09	0.41
3:P:91:LEU:HD11	3:P:165:PHE:HB3	2.02	0.41
1:U:153:LYS:HB2	1:U:153:LYS:HE3	1.88	0.41
1:S:106:LEU:HD21	1:S:259:PHE:HZ	1.84	0.41
1:U:480:GLU:O	1:U:484:GLU:HB2	2.20	0.41
1:K:282:GLN:NE2	2:N:284:THR:HG22	2.34	0.41
3:Y:21:LYS:O	3:Y:25:ILE:HG12	2.20	0.41
1:L:474:LEU:HB3	1:L:482:LEU:HD21	2.02	0.41
1:K:246:TYR:CE2	1:K:283:LEU:HD13	2.53	0.41
1:U:179:ALA:N	6:U:600:ANP:O1A	2.52	0.41
3:G:111:GLY:O	3:G:114:ILE:HG22	2.21	0.41
2:V:418:PHE:HB2	2:V:421:ALA:CB	2.50	0.41
1:B:239:SER:HB2	2:E:291:LEU:HD23	2.01	0.41
1:U:169:ILE:HD11	1:U:326:LEU:HB3	2.02	0.41
2:F:382:LYS:HA	2:F:385:GLN:HG2	2.02	0.41
2:X:231:ARG:HA	2:X:234:LEU:HD12	2.02	0.41
2:N:85:VAL:HG22	2:N:117:ILE:HG22	2.03	0.41
2:M:84:SER:HB2	2:M:114:ARG:HH21	1.85	0.41
3:G:47:ALA:HB1	4:H:84:CYS:HB3	2.03	0.41
1:A:146:GLU:O	1:A:163:ARG:HG3	2.20	0.41
1:B:257:GLU:OE2	1:B:310:ARG:NE	2.34	0.41
2:V:411:GLN:HA	2:V:414:LEU:HD12	2.02	0.41
1:B:398:GLN:C	1:B:400:ARG:N	2.72	0.41
1:A:49:ILE:HG13	1:A:53:GLU:CD	2.41	0.41
2:D:256:ASP:HA	2:D:257:ASN:HA	1.81	0.41
3:P:77:ILE:HG12	3:P:110:ILE:HB	2.01	0.41
1:U:166:ARG:HG2	1:U:325:ALA:HB3	2.01	0.41
2:W:267:GLU:O	2:W:271:LEU:N	2.52	0.41
1:A:455:LEU:HD21	1:A:466:PHE:CZ	2.55	0.41
1:L:267:LEU:HB2	1:L:324:THR:HB	2.01	0.41
2:M:158:GLY:O	2:M:163:LYS:NZ	2.54	0.41
1:S:35:ALA:HB3	1:S:42:ARG:HH11	1.86	0.41
1:A:181:ALA:O	1:A:184:THR:HB	2.20	0.41
1:A:332:GLN:HB3	2:D:318:THR:HB	2.02	0.41
1:T:46:LEU:O	2:X:72:ARG:NH2	2.53	0.41
1:J:150:THR:HG21	1:J:155:VAL:HG11	2.02	0.41
1:C:378:SER:C	1:C:380:ALA:H	2.24	0.41
2:W:201:MET:SD	2:W:217:LEU:HD21	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:354:LEU:HA	1:L:366:ALA:O	2.21	0.41
1:L:164:GLY:HA2	1:L:323:LEU:O	2.21	0.41
4:H:72:GLY:O	4:H:87:ALA:HA	2.20	0.41
1:L:396:LEU:HA	1:L:399:TYR:HB3	2.02	0.41
1:K:25:ALA:O	1:K:28:ASN:ND2	2.54	0.41
1:L:170:ILE:HD11	1:L:341:PRO:HB3	2.03	0.41
3:G:16:ILE:O	3:G:20:THR:HG23	2.19	0.41
2:D:159:ALA:HA	6:D:600:ANP:O1G	2.20	0.41
2:D:443:ALA:HB1	2:D:449:TYR:HE2	1.86	0.41
1:T:28:ASN:HA	1:T:47:ASN:H	1.86	0.41
2:N:54:LEU:HD21	2:N:60:ARG:HB2	2.02	0.41
1:T:158:LEU:HD21	1:T:392:LEU:HG	2.02	0.41
1:T:67:ASN:HB2	2:X:17:ILE:HG12	2.02	0.41
1:U:176:GLY:O	1:U:180:VAL:HG23	2.19	0.41
2:E:399:GLN:O	2:E:403:THR:HG23	2.20	0.41
2:W:220:GLY:N	2:W:232:VAL:HG11	2.35	0.41
1:U:398:GLN:O	1:U:402:VAL:HG23	2.21	0.41
2:F:27:GLN:HG2	2:F:27:GLN:H	1.67	0.41
2:F:340:SER:HB3	2:F:347:ALA:CB	2.51	0.41
2:O:90:GLU:O	2:O:109:ILE:HG23	2.21	0.41
1:T:364:ARG:HA	1:T:365:PRO:C	2.41	0.41
2:N:208:ASN:ND2	2:N:211:GLY:HA3	2.36	0.41
2:X:154:GLY:HA3	2:X:329:LEU:HD13	2.01	0.41
1:J:364:ARG:HA	1:J:365:PRO:C	2.40	0.41
1:U:82:ARG:HG3	1:U:82:ARG:H	1.49	0.41
2:E:201:MET:SD	2:E:217:LEU:HD21	2.61	0.41
2:E:398:GLU:HA	2:E:401:LYS:HE2	2.02	0.41
3:P:205:VAL:N	3:P:206:PRO:CD	2.84	0.41
1:T:141:ARG:NH1	1:T:312:ALA:HB2	2.36	0.41
2:F:168:GLN:O	2:F:172:ASN:HB2	2.20	0.41
2:V:116:PRO:O	2:V:238:THR:HG21	2.21	0.41
2:E:381:TYR:O	2:E:385:GLN:HG2	2.21	0.41
2:F:207:ILE:HA	2:F:213:SER:HB3	2.01	0.41
1:S:73:VAL:HG23	2:W:72:ARG:HH22	1.86	0.41
2:X:345:TYR:HB3	6:X:600:ANP:C6	2.50	0.41
2:V:385:GLN:C	2:V:387:ILE:H	2.24	0.41
3:P:187:THR:C	3:P:188:ILE:HG13	2.41	0.41
3:G:95:VAL:HG11	3:G:118:LEU:HD21	2.03	0.41
2:V:256:ASP:HA	2:V:257:ASN:HA	1.73	0.41
1:C:144:VAL:HG22	1:C:163:ARG:O	2.21	0.41
2:V:418:PHE:HB2	2:V:421:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:219:VAL:HG13	1:L:228:MET:HE3	2.03	0.41
1:K:250:PHE:CZ	1:K:303:LEU:HD12	2.55	0.41
1:K:26:ASN:O	2:X:464:GLU:OE1	2.39	0.41
2:N:276:PRO:HD2	3:P:271:ILE:HD11	2.02	0.41
1:T:272:ASP:HB3	1:T:328:VAL:HB	2.02	0.41
1:B:417:LYS:O	1:B:421:VAL:HG23	2.21	0.41
1:B:359:PHE:HZ	6:B:600:ANP:O4'	2.04	0.41
2:N:377:THR:HG22	2:N:407:ALA:HB2	2.01	0.41
2:W:443:ALA:O	2:W:448:LYS:HB2	2.21	0.41
2:W:275:ILE:HG12	2:W:275:ILE:H	1.55	0.41
1:S:329:ILE:HD12	1:S:340:ILE:HG22	2.03	0.41
1:T:154:ALA:HB2	1:T:430:LEU:HB3	2.03	0.41
2:X:30:LEU:HD21	2:X:57:ASN:HA	2.03	0.41
1:U:256:GLY:HA2	1:U:259:PHE:HD2	1.85	0.41
2:D:359:ASP:OD1	2:D:359:ASP:C	2.59	0.41
2:N:113:LEU:HD22	2:N:113:LEU:HA	1.78	0.41
1:C:219:VAL:HB	1:C:228:MET:HE1	2.03	0.41
3:P:138:PRO:HG3	3:P:222:MET:O	2.21	0.41
1:B:289:ARG:HA	1:B:290:PRO:HD3	1.92	0.41
2:X:190:ARG:O	2:X:221:GLN:NE2	2.51	0.41
1:S:293:ARG:HA	3:Y:267:LEU:HD12	2.03	0.41
1:A:50:GLN:HB2	1:A:53:GLU:HB2	2.02	0.41
1:L:260:ARG:O	1:L:321:GLY:HA3	2.21	0.41
1:C:50:GLN:HB3	2:D:69:GLY:HA2	2.03	0.41
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.48	0.41
2:N:374:VAL:HG13	2:N:410:ILE:HG21	2.02	0.41
2:M:164:THR:O	2:M:167:ILE:HG22	2.21	0.41
1:C:402:VAL:C	1:C:404:ALA:H	2.25	0.41
2:O:319:ASP:O	2:O:320:PRO:C	2.59	0.41
2:M:393:MET:O	2:M:401:LYS:HE2	2.21	0.41
1:K:239:SER:HB2	2:N:291:LEU:HD23	2.03	0.41
2:W:349:ASP:HA	2:W:350:PRO:HD2	1.92	0.41
2:X:398:GLU:HG3	3:Y:120:ARG:HE	1.85	0.41
2:M:90:GLU:HG3	2:M:111:SER:CA	2.50	0.40
2:W:48:LEU:HB3	2:W:61:THR:CB	2.50	0.40
2:X:33:ILE:O	2:X:34:LEU:HB2	2.21	0.40
2:V:157:GLY:H	2:V:312:VAL:HG23	1.86	0.40
1:C:493:LYS:HA	1:C:496:LEU:HD12	2.03	0.40
1:K:248:ALA:HB3	1:K:249:PRO:HD3	2.02	0.40
2:V:54:LEU:HD13	2:V:58:THR:HG22	2.04	0.40
1:T:413:ASP:O	1:T:417:LYS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:421:VAL:O	1:U:425:ARG:HD2	2.20	0.40
2:M:184:PHE:HB3	2:M:217:LEU:HD23	2.02	0.40
1:B:177:LYS:HG2	1:B:354:LEU:HD12	2.03	0.40
2:V:336:SER:HB3	2:V:339:ILE:HG13	2.02	0.40
2:F:121:PRO:HA	2:F:122:PRO:HD3	1.86	0.40
2:D:201:MET:HE2	2:D:217:LEU:HD21	2.03	0.40
1:S:273:LEU:HD13	1:S:304:HIS:CD2	2.55	0.40
1:U:219:VAL:HB	1:U:228:MET:CE	2.51	0.40
2:V:197:LEU:HD23	2:V:219:PHE:HZ	1.86	0.40
2:X:10:THR:HA	2:X:76:VAL:O	2.20	0.40
1:C:103:PRO:HD3	1:C:258:TRP:CZ2	2.56	0.40
1:C:153:LYS:NZ	1:C:467:GLU:OE1	2.51	0.40
2:O:92:LEU:HB3	2:O:213:SER:O	2.22	0.40
2:M:26:GLU:O	2:M:27:GLN:C	2.59	0.40
1:U:376:VAL:HG11	1:U:380:ALA:HB2	2.02	0.40
2:V:395:GLU:HG3	2:V:395:GLU:O	2.21	0.40
1:L:111:ASP:C	1:L:111:ASP:OD1	2.60	0.40
2:W:168:GLN:HA	2:W:171:ILE:HD12	2.03	0.40
2:X:189:GLU:O	2:X:222:MET:HG2	2.21	0.40
1:U:68:LEU:HB2	2:V:16:VAL:CG2	2.51	0.40
1:T:55:VAL:HG21	1:T:75:ILE:HD13	2.03	0.40
1:C:99:VAL:O	1:C:128:ARG:HA	2.22	0.40
1:K:444:VAL:N	1:K:445:PRO:CD	2.84	0.40
3:Y:110:ILE:HD11	3:Y:146:ILE:HG21	2.02	0.40
1:A:73:VAL:HG12	1:A:75:ILE:HG13	2.04	0.40
1:S:170:ILE:HG12	1:S:331:THR:HG23	2.02	0.40
1:C:469:SER:HB3	1:C:506:PHE:HZ	1.86	0.40
2:D:95:ILE:HD11	2:D:198:TYR:CE1	2.56	0.40
2:N:182:SER:HA	2:N:252:LEU:O	2.20	0.40
1:K:133:VAL:H	1:K:310:ARG:NH1	2.20	0.40
1:T:282:GLN:O	1:T:286:LEU:HG	2.21	0.40
2:O:183:VAL:HG11	2:O:236:GLY:O	2.21	0.40
1:J:28:ASN:HA	1:J:47:ASN:HB2	2.04	0.40
1:U:243:PRO:HA	1:U:283:LEU:HD11	2.03	0.40
1:S:116:PRO:HB3	1:S:123:ILE:HD11	2.04	0.40
2:E:109:ILE:O	2:E:111:SER:N	2.47	0.40
1:U:355:GLU:OE2	1:U:368:ASN:ND2	2.54	0.40
2:M:244:ARG:HD3	2:M:304:VAL:HG23	2.03	0.40
1:S:190:ARG:CZ	1:S:439:ALA:HB2	2.51	0.40
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.56	0.40
4:H:49:VAL:HG22	4:H:76:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:370:VAL:O	2:V:374:VAL:HG23	2.21	0.40
1:B:139:LEU:HD23	2:F:105:GLU:OE2	2.22	0.40
2:F:252:LEU:HD23	2:F:305:THR:HB	2.04	0.40
3:P:79:SER:HB2	3:P:134:GLY:HA3	2.04	0.40
3:P:163:SER:HB3	3:P:179:GLU:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/510 (94%)	456 (95%)	19 (4%)	3 (1%)	30	57
1	B	479/510 (94%)	455 (95%)	21 (4%)	3 (1%)	30	57
1	C	482/510 (94%)	448 (93%)	31 (6%)	3 (1%)	30	57
1	J	477/510 (94%)	449 (94%)	23 (5%)	5 (1%)	19	43
1	K	482/510 (94%)	446 (92%)	32 (7%)	4 (1%)	24	50
1	L	478/510 (94%)	451 (94%)	23 (5%)	4 (1%)	24	50
1	S	473/510 (93%)	434 (92%)	39 (8%)	0	100	100
1	T	474/510 (93%)	430 (91%)	42 (9%)	2 (0%)	39	68
1	U	477/510 (94%)	423 (89%)	48 (10%)	6 (1%)	15	35
2	D	468/484 (97%)	435 (93%)	30 (6%)	3 (1%)	30	57
2	E	466/484 (96%)	429 (92%)	30 (6%)	7 (2%)	13	30
2	F	467/484 (96%)	432 (92%)	34 (7%)	1 (0%)	52	80
2	M	468/484 (97%)	431 (92%)	32 (7%)	5 (1%)	17	40
2	N	468/484 (97%)	438 (94%)	27 (6%)	3 (1%)	30	57
2	O	466/484 (96%)	430 (92%)	34 (7%)	2 (0%)	39	68
2	V	468/484 (97%)	433 (92%)	31 (7%)	4 (1%)	21	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	465/484 (96%)	425 (91%)	36 (8%)	4 (1%)	21	47
2	X	467/484 (96%)	419 (90%)	45 (10%)	3 (1%)	30	57
3	G	262/278 (94%)	240 (92%)	19 (7%)	3 (1%)	17	40
3	P	232/278 (84%)	210 (90%)	20 (9%)	2 (1%)	21	47
3	Y	188/278 (68%)	173 (92%)	13 (7%)	2 (1%)	17	40
4	H	114/138 (83%)	91 (80%)	20 (18%)	3 (3%)	7	15
4	Q	73/138 (53%)	61 (84%)	9 (12%)	3 (4%)	3	7
4	Z	15/138 (11%)	10 (67%)	4 (27%)	1 (7%)	1	2
5	1	23/61 (38%)	18 (78%)	4 (17%)	1 (4%)	3	6
5	I	43/61 (70%)	39 (91%)	2 (5%)	2 (5%)	3	5
5	R	30/61 (49%)	21 (70%)	9 (30%)	0	100	100
All	All	9483/10377 (91%)	8727 (92%)	677 (7%)	79 (1%)	24	50

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	152	SER
3	G	204	ASN
4	H	118	ARG
5	I	55	GLU
5	I	56	PRO
1	J	392	LEU
1	T	507	VAL
1	U	298	GLY
1	A	406	ALA
1	B	196	ASP
1	C	390	GLY
2	E	279	VAL
2	E	366	GLU
4	H	102	LYS
1	J	27	LEU
1	J	390	GLY
1	J	403	ALA
1	K	196	ASP
1	L	82	ARG
2	M	250	ASP
3	P	134	GLY
1	T	97	VAL

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Mol	Chain	Res	Type
1	U	390	GLY
2	V	347	ALA
2	X	28	SER
3	Y	103	PRO
1	A	479	ASN
3	G	135	LYS
1	L	335	ASP
1	L	508	ALA
2	M	27	GLN
2	M	279	VAL
3	P	152	SER
4	Q	35	LYS
1	U	70	PRO
2	V	474	ALA
1	B	397	ALA
2	D	388	ILE
2	E	110	LYS
1	K	58	SER
2	M	463	ILE
2	N	421	ALA
1	U	140	PRO
2	W	277	SER
2	W	284	THR
4	Z	120	ALA
1	A	404	ALA
2	D	27	GLN
2	E	28	SER
4	H	33	PRO
1	K	359	PHE
1	L	339	TYR
2	M	175	ALA
2	N	279	VAL
4	Q	45	HIS
2	V	212	GLU
2	W	15	ALA
2	W	34	LEU
1	C	196	ASP
2	N	158	GLY
2	E	461	GLY
2	E	463	ILE
1	U	69	GLU
2	X	248	GLY

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Mol	Chain	Res	Type
2	F	279	VAL
2	O	279	VAL
2	O	461	GLY
4	Q	53	LEU
2	X	100	GLY
3	Y	177	PRO
1	B	390	GLY
1	K	97	VAL
1	C	70	PRO
2	D	279	VAL
1	U	138	ILE
5	1	34	VAL
2	E	44	GLY
1	J	70	PRO
2	V	346	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/412 (94%)	371 (96%)	17 (4%)	35	64
1	B	388/412 (94%)	372 (96%)	16 (4%)	37	67
1	C	390/412 (95%)	374 (96%)	16 (4%)	37	67
1	J	387/412 (94%)	366 (95%)	21 (5%)	27	54
1	K	388/412 (94%)	366 (94%)	22 (6%)	25	51
1	L	388/412 (94%)	363 (94%)	25 (6%)	22	45
1	S	384/412 (93%)	364 (95%)	20 (5%)	29	56
1	T	386/412 (94%)	373 (97%)	13 (3%)	44	74
1	U	387/412 (94%)	365 (94%)	22 (6%)	25	51
2	D	379/390 (97%)	368 (97%)	11 (3%)	50	79
2	E	370/390 (95%)	359 (97%)	11 (3%)	48	78
2	F	375/390 (96%)	357 (95%)	18 (5%)	31	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	377/390 (97%)	362 (96%)	15 (4%)	38	68
2	N	378/390 (97%)	356 (94%)	22 (6%)	25	50
2	O	378/390 (97%)	364 (96%)	14 (4%)	41	71
2	V	380/390 (97%)	363 (96%)	17 (4%)	34	63
2	W	378/390 (97%)	359 (95%)	19 (5%)	30	58
2	X	379/390 (97%)	365 (96%)	14 (4%)	41	71
3	G	225/236 (95%)	209 (93%)	16 (7%)	18	39
3	P	197/236 (84%)	191 (97%)	6 (3%)	48	78
3	Y	163/236 (69%)	153 (94%)	10 (6%)	23	47
4	H	65/112 (58%)	57 (88%)	8 (12%)	6	13
4	Q	8/112 (7%)	8 (100%)	0	100	100
5	1	2/48 (4%)	2 (100%)	0	100	100
5	I	28/48 (58%)	24 (86%)	4 (14%)	4	9
5	R	3/48 (6%)	3 (100%)	0	100	100
All	All	7571/8294 (91%)	7214 (95%)	357 (5%)	32	61

All (357) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	56	GLU
1	A	123	ILE
1	A	142	ARG
1	A	166	ARG
1	A	218	LEU
1	A	251	THR
1	A	373	VAL
1	A	412	LEU
1	A	416	THR
1	A	420	LEU
1	A	436	SER
1	A	445	PRO
1	A	476	SER
1	A	480	GLU
1	A	495	LEU
1	A	509	THR
1	B	93	THR

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Mol	Chain	Res	Type
1	B	99	VAL
1	B	106	LEU
1	B	159	VAL
1	B	173	ARG
1	B	246	TYR
1	B	283	LEU
1	B	289	ARG
1	B	399	TYR
1	B	400	ARG
1	B	460	LEU
1	B	468	SER
1	B	472	SER
1	B	484	GLU
1	B	494	GLU
1	B	509	THR
1	C	27	LEU
1	C	61	VAL
1	C	72	GLN
1	C	99	VAL
1	C	166	ARG
1	C	198	SER
1	C	218	LEU
1	C	220	GLN
1	C	223	GLU
1	C	283	LEU
1	C	357	GLU
1	C	391	SER
1	C	411	ASP
1	C	479	ASN
1	C	505	SER
1	C	509	THR
2	D	132	GLU
2	D	204	THR
2	D	251	VAL
2	D	266	SER
2	D	356	ARG
2	D	386	ASP
2	D	387	ILE
2	D	396	LEU
2	D	399	GLN
2	D	413	PHE
2	D	464	GLU

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Mol	Chain	Res	Type
2	E	43	GLN
2	E	56	GLU
2	E	133	ILE
2	E	140	VAL
2	E	161	VAL
2	E	232	VAL
2	E	301	LYS
2	E	337	ARG
2	E	352	ASP
2	E	386	ASP
2	E	399	GLN
2	F	28	SER
2	F	68	GLU
2	F	84	SER
2	F	85	VAL
2	F	133	ILE
2	F	140	VAL
2	F	149	ARG
2	F	201	MET
2	F	208	ASN
2	F	210	GLU
2	F	237	LEU
2	F	246	GLU
2	F	250	ASP
2	F	279	VAL
2	F	292	LEU
2	F	303	SER
2	F	333	THR
2	F	387	ILE
3	G	23	MET
3	G	77	ILE
3	G	81	LYS
3	G	86	SER
3	G	97	ARG
3	G	102	GLN
3	G	130	ILE
3	G	153	VAL
3	G	204	ASN
3	G	205	VAL
3	G	210	PHE
3	G	216	ASN
3	G	220	THR

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Mol	Chain	Res	Type
3	G	231	SER
3	G	234	ARG
3	G	254	LEU
4	H	14	PHE
4	H	20	THR
4	H	27	VAL
4	H	35	LYS
4	H	39	ILE
4	H	65	SER
4	H	76	THR
4	H	80	ASP
5	I	19	GLN
5	I	35	LEU
5	I	41	ASP
5	I	47	TYR
1	J	30	THR
1	J	67	ASN
1	J	90	VAL
1	J	134	LYS
1	J	139	LEU
1	J	163	ARG
1	J	166	ARG
1	J	183	ASP
1	J	231	SER
1	J	246	TYR
1	J	322	SER
1	J	373	VAL
1	J	411	ASP
1	J	418	GLN
1	J	420	LEU
1	J	436	SER
1	J	444	VAL
1	J	465	GLU
1	J	468	SER
1	J	480	GLU
1	J	487	GLU
1	K	58	SER
1	K	93	THR
1	K	99	VAL
1	K	106	LEU
1	K	166	ARG
1	K	231	SER

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Mol	Chain	Res	Type
1	K	246	TYR
1	K	317	LYS
1	K	341	PRO
1	K	351	GLN
1	K	357	GLU
1	K	360	TYR
1	K	371	LEU
1	K	372	SER
1	K	385	LEU
1	K	391	SER
1	K	394	LEU
1	K	399	TYR
1	K	400	ARG
1	K	411	ASP
1	K	460	LEU
1	K	501	SER
1	L	70	PRO
1	L	82	ARG
1	L	89	LEU
1	L	93	THR
1	L	99	VAL
1	L	142	ARG
1	L	159	VAL
1	L	163	ARG
1	L	166	ARG
1	L	195	SER
1	L	267	LEU
1	L	306	ARG
1	L	317	LYS
1	L	322	SER
1	L	337	SER
1	L	342	THR
1	L	351	GLN
1	L	373	VAL
1	L	436	SER
1	L	465	GLU
1	L	481	LEU
1	L	484	GLU
1	L	492	SER
1	L	498	SER
1	L	503	THR
2	M	10	THR

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Mol	Chain	Res	Type
2	M	113	LEU
2	M	134	LEU
2	M	149	ARG
2	M	206	VAL
2	M	251	VAL
2	M	336	SER
2	M	386	ASP
2	M	390	ILE
2	M	394	ASP
2	M	397	SER
2	M	422	GLU
2	M	435	LYS
2	M	436	ASP
2	M	450	ASP
2	N	9	ILE
2	N	10	THR
2	N	85	VAL
2	N	113	LEU
2	N	130	SER
2	N	140	VAL
2	N	161	VAL
2	N	164	THR
2	N	176	LYS
2	N	204	THR
2	N	212	GLU
2	N	232	VAL
2	N	356	ARG
2	N	357	LEU
2	N	366	GLU
2	N	372	SER
2	N	376	GLU
2	N	380	THR
2	N	393	MET
2	N	394	ASP
2	N	398	GLU
2	N	399	GLN
2	O	29	GLU
2	O	85	VAL
2	O	140	VAL
2	O	200	GLU
2	O	201	MET
2	O	208	ASN

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Mol	Chain	Res	Type
2	O	210	GLU
2	O	237	LEU
2	O	274	ARG
2	O	306	SER
2	O	333	THR
2	O	336	SER
2	O	399	GLN
2	O	464	GLU
3	P	19	ILE
3	P	84	CYS
3	P	112	ASP
3	P	142	GLU
3	P	143	SER
3	P	267	LEU
1	S	32	ARG
1	S	44	PHE
1	S	58	SER
1	S	89	LEU
1	S	92	ARG
1	S	123	ILE
1	S	134	LYS
1	S	224	GLN
1	S	267	LEU
1	S	303	LEU
1	S	318	GLU
1	S	373	VAL
1	S	436	SER
1	S	441	GLU
1	S	444	VAL
1	S	462	ARG
1	S	474	LEU
1	S	477	ASN
1	S	490	GLU
1	S	495	LEU
1	T	67	ASN
1	T	95	ASN
1	T	99	VAL
1	T	115	ASN
1	T	159	VAL
1	T	225	HIS
1	T	246	TYR
1	T	317	LYS

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Mol	Chain	Res	Type
1	T	394	LEU
1	T	399	TYR
1	T	422	ARG
1	T	465	GLU
1	T	505	SER
1	U	40	ILE
1	U	47	ASN
1	U	67	ASN
1	U	82	ARG
1	U	89	LEU
1	U	93	THR
1	U	98	ASP
1	U	143	SER
1	U	163	ARG
1	U	166	ARG
1	U	169	ILE
1	U	190	ARG
1	U	218	LEU
1	U	233	ILE
1	U	339	TYR
1	U	351	GLN
1	U	378	SER
1	U	393	LYS
1	U	394	LEU
1	U	413	ASP
1	U	427	THR
1	U	501	SER
2	V	12	LYS
2	V	14	THR
2	V	54	LEU
2	V	65	ASP
2	V	191	THR
2	V	199	ARG
2	V	250	ASP
2	V	251	VAL
2	V	282	GLN
2	V	292	LEU
2	V	366	GLU
2	V	386	ASP
2	V	393	MET
2	V	413	PHE
2	V	423	VAL

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Mol	Chain	Res	Type
2	V	427	ILE
2	V	431	LEU
2	W	99	ILE
2	W	106	ARG
2	W	111	SER
2	W	129	THR
2	W	140	VAL
2	W	152	LYS
2	W	204	THR
2	W	213	SER
2	W	224	GLU
2	W	229	ARG
2	W	232	VAL
2	W	268	VAL
2	W	275	ILE
2	W	287	THR
2	W	296	ILE
2	W	337	ARG
2	W	352	ASP
2	W	423	VAL
2	W	448	LYS
2	X	43	GLN
2	X	68	GLU
2	X	95	ILE
2	X	98	VAL
2	X	129	THR
2	X	133	ILE
2	X	208	ASN
2	X	238	THR
2	X	250	ASP
2	X	274	ARG
2	X	324	THR
2	X	382	LYS
2	X	412	ARG
2	X	413	PHE
3	Y	16	ILE
3	Y	97	ARG
3	Y	104	ASN
3	Y	119	LEU
3	Y	136	ASP
3	Y	213	THR
3	Y	219	LEU

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Mol	Chain	Res	Type
3	Y	249	ASN
3	Y	259	ARG
3	Y	268	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	452	ASN
1	B	149	GLN
1	B	224	GLN
1	B	368	ASN
1	B	454	HIS
1	C	145	HIS
1	C	174	GLN
2	D	52	GLN
2	D	178	HIS
2	D	195	ASN
2	D	208	ASN
2	D	367	HIS
2	E	168	GLN
2	E	399	GLN
2	F	43	GLN
2	F	208	ASN
2	F	367	HIS
3	G	54	ASN
3	G	59	ASN
3	G	117	GLN
3	G	217	GLN
4	H	45	HIS
4	H	134	GLN
5	I	19	GLN
1	J	145	HIS
1	K	28	ASN
1	K	149	GLN
1	K	428	GLN
1	L	132	GLN
1	L	145	HIS
1	L	225	HIS
2	M	195	ASN
2	M	328	HIS
2	M	367	HIS

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Mol	Chain	Res	Type
2	M	379	GLN
2	M	385	GLN
2	N	168	GLN
2	O	27	GLN
2	O	52	GLN
2	O	328	HIS
3	P	88	HIS
3	P	100	ASN
3	P	216	ASN
3	P	239	ASN
3	P	243	ASN
1	S	387	GLN
1	S	443	GLN
1	S	454	HIS
1	T	28	ASN
1	T	47	ASN
1	T	48	ASN
1	T	67	ASN
1	T	428	GLN
1	U	220	GLN
1	U	265	HIS
1	U	407	GLN
1	U	479	ASN
2	V	282	GLN
2	W	57	ASN
2	W	127	GLN
2	W	168	GLN
2	W	221	GLN
2	X	43	GLN
2	X	52	GLN
2	X	208	ASN
2	X	263	GLN
3	Y	102	GLN
3	Y	117	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 ⓘ

Of 32 ligands modelled in this entry, 15 are monoatomic - leaving 17 for Mogul analysis.

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	$\# Z > 2$
6	ANP	A	600	7	27,33,33	1.82	8 (29%)	30,52,52	2.55	8 (26%)
6	ANP	B	600	7	27,33,33	2.00	9 (33%)	30,52,52	2.09	5 (16%)
6	ANP	C	600	7	27,33,33	2.06	7 (25%)	30,52,52	2.33	7 (23%)
6	ANP	D	600	7	27,33,33	1.93	7 (25%)	30,52,52	2.33	7 (23%)
8	PO4	E	800	-	4,4,4	0.15	0	6,6,6	0.29	0
6	ANP	F	600	7	27,33,33	1.93	7 (25%)	30,52,52	2.56	9 (30%)
6	ANP	J	600	7	27,33,33	1.94	8 (29%)	30,52,52	2.22	4 (13%)
6	ANP	K	600	7	27,33,33	1.86	7 (25%)	30,52,52	2.01	5 (16%)
6	ANP	L	600	7	27,33,33	1.90	8 (29%)	30,52,52	2.32	5 (16%)
6	ANP	M	600	7	27,33,33	2.02	8 (29%)	30,52,52	2.12	7 (23%)
8	PO4	N	800	-	4,4,4	0.31	0	6,6,6	0.28	0
6	ANP	O	600	7	27,33,33	1.90	8 (29%)	30,52,52	2.23	8 (26%)
6	ANP	S	600	7	27,33,33	2.31	8 (29%)	30,52,52	3.28	9 (30%)
6	ANP	T	600	7	27,33,33	2.29	8 (29%)	30,52,52	2.26	9 (30%)
6	ANP	U	600	7	27,33,33	1.92	6 (22%)	30,52,52	2.34	8 (26%)
6	ANP	V	600	7	27,33,33	2.10	8 (29%)	30,52,52	2.29	9 (30%)
6	ANP	X	600	7	27,33,33	2.13	6 (22%)	30,52,52	1.97	6 (20%)

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
6	ANP	A	600	7	-	2/12/38/38	0/3/3/3
6	ANP	B	600	7	-	1/12/38/38	0/3/3/3
6	ANP	C	600	7	-	1/12/38/38	0/3/3/3
6	ANP	D	600	7	-	1/12/38/38	0/3/3/3
8	PO4	E	800	-	-	0/0/0/0	0/0/0/0
6	ANP	F	600	7	-	1/12/38/38	0/3/3/3
6	ANP	J	600	7	-	1/12/38/38	0/3/3/3
6	ANP	K	600	7	-	2/12/38/38	0/3/3/3
6	ANP	L	600	7	-	2/12/38/38	0/3/3/3
6	ANP	M	600	7	-	0/12/38/38	0/3/3/3
8	PO4	N	800	-	-	0/0/0/0	0/0/0/0
6	ANP	O	600	7	-	2/12/38/38	0/3/3/3
6	ANP	S	600	7	-	0/12/38/38	0/3/3/3
6	ANP	T	600	7	-	0/12/38/38	0/3/3/3
6	ANP	U	600	7	-	0/12/38/38	0/3/3/3
6	ANP	V	600	7	-	0/12/38/38	0/3/3/3
6	ANP	X	600	7	-	0/12/38/38	0/3/3/3

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	600	ANP	PG-O2G	-2.98	1.48	1.56
6	A	600	ANP	PG-O2G	-2.82	1.48	1.56
6	F	600	ANP	PG-O2G	-2.73	1.49	1.56
6	B	600	ANP	PG-O3G	-2.65	1.49	1.56
6	K	600	ANP	PG-O3G	-2.61	1.49	1.56
6	L	600	ANP	PG-O2G	-2.49	1.49	1.56
6	O	600	ANP	PG-O2G	-2.43	1.49	1.56
6	B	600	ANP	PG-O2G	-2.42	1.50	1.56
6	L	600	ANP	PG-O3G	-2.36	1.50	1.56
6	A	600	ANP	PG-O3G	-2.34	1.50	1.56
6	D	600	ANP	PG-O3G	-2.28	1.50	1.56
6	J	600	ANP	PG-O2G	-2.24	1.50	1.56
6	J	600	ANP	PB-O2B	-2.20	1.50	1.56
6	F	600	ANP	PG-O3G	-2.19	1.50	1.56
6	D	600	ANP	PG-O2G	-2.19	1.50	1.56
6	B	600	ANP	PB-O2B	-2.15	1.50	1.56
6	C	600	ANP	PG-O2G	-2.05	1.51	1.56
6	M	600	ANP	PG-O2G	-2.04	1.51	1.56
6	B	600	ANP	O4'-C1'	2.01	1.43	1.41
6	L	600	ANP	PB-O3A	2.01	1.61	1.59
6	X	600	ANP	PB-O3A	2.04	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	600	ANP	C2-N3	2.07	1.35	1.32
6	A	600	ANP	PB-O3A	2.07	1.61	1.59
6	O	600	ANP	O4'-C1'	2.08	1.43	1.41
6	T	600	ANP	C2-N3	2.12	1.35	1.32
6	M	600	ANP	C2-N3	2.13	1.36	1.32
6	M	600	ANP	PB-O3A	2.25	1.61	1.59
6	O	600	ANP	PB-O3A	2.26	1.61	1.59
6	S	600	ANP	PB-O3A	2.29	1.61	1.59
6	J	600	ANP	O4'-C1'	2.36	1.44	1.41
6	S	600	ANP	C2-N3	2.36	1.36	1.32
6	C	600	ANP	PB-O3A	2.43	1.62	1.59
6	T	600	ANP	O4'-C1'	2.43	1.44	1.41
6	V	600	ANP	O4'-C1'	2.45	1.44	1.41
6	V	600	ANP	PB-O3A	2.45	1.62	1.59
6	S	600	ANP	O4'-C1'	2.48	1.44	1.41
6	T	600	ANP	PB-O3A	2.61	1.62	1.59
6	L	600	ANP	C5-C4	2.69	1.46	1.40
6	U	600	ANP	PB-O3A	2.73	1.62	1.59
6	C	600	ANP	C5-C4	2.90	1.47	1.40
6	A	600	ANP	PG-O1G	3.09	1.49	1.46
6	K	600	ANP	C5-C4	3.12	1.47	1.40
6	J	600	ANP	C5-C4	3.13	1.47	1.40
6	K	600	ANP	PG-O1G	3.14	1.49	1.46
6	B	600	ANP	C5-C4	3.20	1.47	1.40
6	V	600	ANP	C5-C4	3.24	1.47	1.40
6	F	600	ANP	C5-C4	3.26	1.47	1.40
6	A	600	ANP	PB-O1B	3.29	1.49	1.46
6	A	600	ANP	C5-C4	3.30	1.47	1.40
6	D	600	ANP	C5-C4	3.34	1.48	1.40
6	S	600	ANP	C5-C4	3.34	1.48	1.40
6	T	600	ANP	C5-C4	3.35	1.48	1.40
6	O	600	ANP	PB-O1B	3.37	1.50	1.46
6	U	600	ANP	C5-C4	3.44	1.48	1.40
6	M	600	ANP	C5-C4	3.44	1.48	1.40
6	B	600	ANP	PG-O1G	3.45	1.50	1.46
6	A	600	ANP	PG-N3B	3.51	1.72	1.63
6	K	600	ANP	PB-O1B	3.52	1.50	1.46
6	O	600	ANP	C5-C4	3.54	1.48	1.40
6	L	600	ANP	PB-O1B	3.56	1.50	1.46
6	U	600	ANP	PB-O1B	3.56	1.50	1.46
6	U	600	ANP	PB-N3B	3.64	1.73	1.63
6	X	600	ANP	C5-C4	3.64	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	ANP	PB-N3B	3.64	1.73	1.63
6	M	600	ANP	PG-N3B	3.67	1.73	1.63
6	O	600	ANP	PB-N3B	3.71	1.73	1.63
6	F	600	ANP	PB-N3B	3.73	1.73	1.63
6	F	600	ANP	PG-N3B	3.75	1.73	1.63
6	O	600	ANP	PG-O1G	3.75	1.50	1.46
6	J	600	ANP	PG-N3B	3.76	1.73	1.63
6	O	600	ANP	PG-N3B	3.77	1.73	1.63
6	B	600	ANP	PB-O1B	3.79	1.50	1.46
6	J	600	ANP	PB-N3B	3.79	1.73	1.63
6	D	600	ANP	PB-O1B	3.79	1.50	1.46
6	J	600	ANP	PB-O1B	3.81	1.50	1.46
6	C	600	ANP	PB-N3B	3.86	1.73	1.63
6	K	600	ANP	PB-N3B	3.88	1.73	1.63
6	D	600	ANP	PG-N3B	3.91	1.73	1.63
6	L	600	ANP	PG-N3B	3.93	1.73	1.63
6	U	600	ANP	PG-O1G	3.93	1.50	1.46
6	L	600	ANP	PB-N3B	3.97	1.73	1.63
6	D	600	ANP	PB-N3B	4.00	1.73	1.63
6	F	600	ANP	PG-O1G	4.01	1.50	1.46
6	K	600	ANP	PG-N3B	4.03	1.74	1.63
6	L	600	ANP	PG-O1G	4.04	1.50	1.46
6	U	600	ANP	PG-N3B	4.04	1.74	1.63
6	C	600	ANP	PG-N3B	4.09	1.74	1.63
6	M	600	ANP	PB-N3B	4.10	1.74	1.63
6	D	600	ANP	PG-O1G	4.17	1.50	1.46
6	B	600	ANP	PG-N3B	4.19	1.74	1.63
6	V	600	ANP	PB-N3B	4.22	1.74	1.63
6	V	600	ANP	PG-N3B	4.23	1.74	1.63
6	F	600	ANP	PB-O1B	4.25	1.51	1.46
6	M	600	ANP	PB-O1B	4.28	1.51	1.46
6	X	600	ANP	PG-N3B	4.31	1.74	1.63
6	B	600	ANP	PB-N3B	4.36	1.74	1.63
6	V	600	ANP	PB-O1B	4.38	1.51	1.46
6	X	600	ANP	PB-N3B	4.39	1.75	1.63
6	C	600	ANP	PB-O1B	4.40	1.51	1.46
6	M	600	ANP	PG-O1G	4.46	1.51	1.46
6	T	600	ANP	PB-O1B	4.47	1.51	1.46
6	S	600	ANP	PG-N3B	4.52	1.75	1.63
6	J	600	ANP	PG-O1G	4.55	1.51	1.46
6	X	600	ANP	PB-O1B	4.56	1.51	1.46
6	S	600	ANP	PB-N3B	4.57	1.75	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	600	ANP	PG-O1G	4.71	1.51	1.46
6	T	600	ANP	PB-N3B	4.90	1.76	1.63
6	T	600	ANP	PG-N3B	4.92	1.76	1.63
6	S	600	ANP	PB-O1B	5.02	1.51	1.46
6	C	600	ANP	PG-O1G	5.17	1.52	1.46
6	X	600	ANP	PG-O1G	5.29	1.52	1.46
6	T	600	ANP	PG-O1G	5.72	1.52	1.46
6	S	600	ANP	PG-O1G	5.94	1.52	1.46

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	600	ANP	C4'-O4'-C1'	-11.78	96.78	109.72
6	L	600	ANP	N3-C2-N1	-7.88	122.86	128.89
6	D	600	ANP	N3-C2-N1	-7.83	122.90	128.89
6	C	600	ANP	N3-C2-N1	-7.60	123.07	128.89
6	A	600	ANP	O1G-PG-N3B	-7.31	100.69	111.90
6	K	600	ANP	N3-C2-N1	-7.26	123.33	128.89
6	T	600	ANP	N3-C2-N1	-7.03	123.51	128.89
6	J	600	ANP	N3-C2-N1	-6.96	123.56	128.89
6	S	600	ANP	PA-O3A-PB	-6.93	109.44	132.67
6	B	600	ANP	N3-C2-N1	-6.79	123.70	128.89
6	V	600	ANP	N3-C2-N1	-6.78	123.70	128.89
6	A	600	ANP	N3-C2-N1	-6.71	123.75	128.89
6	S	600	ANP	N3-C2-N1	-6.59	123.85	128.89
6	F	600	ANP	N3-C2-N1	-6.55	123.88	128.89
6	M	600	ANP	N3-C2-N1	-6.54	123.89	128.89
6	O	600	ANP	N3-C2-N1	-6.53	123.89	128.89
6	V	600	ANP	O1G-PG-N3B	-6.52	101.90	111.90
6	L	600	ANP	O1G-PG-N3B	-6.39	102.11	111.90
6	F	600	ANP	O1G-PG-N3B	-6.13	102.50	111.90
6	F	600	ANP	C2'-C1'-N9	-6.08	105.01	114.29
6	J	600	ANP	O1G-PG-N3B	-6.00	102.70	111.90
6	U	600	ANP	N3-C2-N1	-5.76	124.48	128.89
6	X	600	ANP	N3-C2-N1	-5.64	124.58	128.89
6	U	600	ANP	O1G-PG-N3B	-5.60	103.31	111.90
6	U	600	ANP	O1B-PB-N3B	-5.10	104.08	111.90
6	C	600	ANP	O1G-PG-N3B	-5.02	104.19	111.90
6	B	600	ANP	O1G-PG-N3B	-5.00	104.23	111.90
6	S	600	ANP	O1G-PG-N3B	-4.86	104.44	111.90
6	D	600	ANP	C2'-C1'-N9	-4.78	106.99	114.29
6	T	600	ANP	O1G-PG-N3B	-4.65	104.77	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	600	ANP	O1G-PG-N3B	-4.61	104.83	111.90
6	X	600	ANP	O1G-PG-N3B	-4.39	105.17	111.90
6	T	600	ANP	PA-O3A-PB	-4.34	118.11	132.67
6	O	600	ANP	O1G-PG-N3B	-4.13	105.57	111.90
6	M	600	ANP	O1G-PG-N3B	-4.03	105.72	111.90
6	A	600	ANP	C2'-C1'-N9	-4.01	108.17	114.29
6	A	600	ANP	O1B-PB-N3B	-3.93	105.87	111.90
6	K	600	ANP	O1G-PG-N3B	-3.62	106.34	111.90
6	U	600	ANP	PA-O3A-PB	-3.60	120.59	132.67
6	O	600	ANP	C4-C5-N7	-3.49	106.27	109.48
6	A	600	ANP	C4-C5-N7	-3.49	106.27	109.48
6	T	600	ANP	O1B-PB-N3B	-3.48	106.56	111.90
6	C	600	ANP	C2'-C1'-N9	-3.38	109.13	114.29
6	J	600	ANP	C4-C5-N7	-3.37	106.38	109.48
6	X	600	ANP	C4-C5-N7	-3.28	106.46	109.48
6	B	600	ANP	C2'-C1'-N9	-3.28	109.29	114.29
6	C	600	ANP	C4-C5-N7	-3.25	106.49	109.48
6	V	600	ANP	C4-C5-N7	-3.24	106.50	109.48
6	X	600	ANP	PA-O3A-PB	-3.15	122.12	132.67
6	M	600	ANP	C2'-C1'-N9	-3.05	109.63	114.29
6	V	600	ANP	C2'-C1'-N9	-3.04	109.65	114.29
6	O	600	ANP	C2'-C1'-N9	-2.97	109.75	114.29
6	V	600	ANP	PA-O3A-PB	-2.96	122.73	132.67
6	U	600	ANP	C4-C5-N7	-2.91	106.80	109.48
6	L	600	ANP	C2'-C1'-N9	-2.90	109.86	114.29
6	O	600	ANP	O1B-PB-N3B	-2.84	107.54	111.90
6	K	600	ANP	C4-C5-N7	-2.75	106.95	109.48
6	F	600	ANP	PA-O3A-PB	-2.73	123.52	132.67
6	D	600	ANP	PA-O3A-PB	-2.72	123.55	132.67
6	T	600	ANP	C2'-C1'-N9	-2.60	110.32	114.29
6	X	600	ANP	O1B-PB-N3B	-2.51	108.05	111.90
6	B	600	ANP	C4-C5-N7	-2.49	107.19	109.48
6	F	600	ANP	C4-C5-N7	-2.40	107.27	109.48
6	T	600	ANP	C4-C5-N7	-2.33	107.34	109.48
6	S	600	ANP	C4-C5-N7	-2.26	107.40	109.48
6	M	600	ANP	C4-C5-N7	-2.21	107.45	109.48
6	M	600	ANP	O1B-PB-N3B	-2.17	108.57	111.90
6	L	600	ANP	O1B-PB-N3B	-2.09	108.70	111.90
6	V	600	ANP	O1B-PB-N3B	-2.07	108.72	111.90
6	A	600	ANP	O2B-PB-O3A	2.10	114.60	105.09
6	T	600	ANP	O4'-C1'-N9	2.11	112.51	108.10
6	F	600	ANP	O4'-C1'-N9	2.12	112.53	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	600	ANP	O3G-PG-O2G	2.13	113.89	107.58
6	A	600	ANP	C2-N1-C6	2.13	122.58	118.77
6	T	600	ANP	O3G-PG-O2G	2.15	113.95	107.58
6	C	600	ANP	O4'-C1'-N9	2.23	112.77	108.10
6	D	600	ANP	O3G-PG-O2G	2.27	114.30	107.58
6	U	600	ANP	O3G-PG-O2G	2.27	114.31	107.58
6	C	600	ANP	O3G-PG-O2G	2.32	114.45	107.58
6	S	600	ANP	O3G-PG-O2G	2.35	114.55	107.58
6	V	600	ANP	O3G-PG-O2G	2.46	114.86	107.58
6	V	600	ANP	O4'-C1'-N9	2.47	113.26	108.10
6	F	600	ANP	O2B-PB-O3A	2.52	116.53	105.09
6	D	600	ANP	C2-N1-C6	2.57	123.36	118.77
6	O	600	ANP	O2B-PB-O3A	2.58	116.82	105.09
6	F	600	ANP	O3G-PG-O2G	2.59	115.25	107.58
6	U	600	ANP	O3A-PB-N3B	2.62	113.66	106.44
6	S	600	ANP	O4'-C1'-N9	2.66	113.68	108.10
6	V	600	ANP	O2B-PB-O1B	2.71	115.65	110.00
6	M	600	ANP	O3G-PG-O2G	2.98	116.41	107.58
6	O	600	ANP	O3G-PG-O2G	3.32	117.41	107.58
6	B	600	ANP	O2B-PB-O1B	3.46	117.22	110.00
6	T	600	ANP	O2B-PB-O1B	3.68	117.69	110.00
6	K	600	ANP	O2B-PB-O1B	3.71	117.75	110.00
6	X	600	ANP	O2B-PB-O1B	3.84	118.02	110.00
6	D	600	ANP	O2B-PB-O1B	3.94	118.23	110.00
6	U	600	ANP	O2B-PB-O1B	4.00	118.35	110.00
6	S	600	ANP	O2B-PB-O1B	4.01	118.38	110.00
6	S	600	ANP	C2'-C1'-N9	4.03	120.46	114.29
6	L	600	ANP	O2B-PB-O1B	4.16	118.69	110.00
6	O	600	ANP	O2B-PB-O1B	4.52	119.43	110.00
6	C	600	ANP	O2B-PB-O1B	4.62	119.64	110.00
6	J	600	ANP	O2B-PB-O1B	4.74	119.89	110.00
6	M	600	ANP	O2B-PB-O1B	4.93	120.28	110.00
6	A	600	ANP	O2B-PB-O1B	5.02	120.47	110.00
6	F	600	ANP	O2B-PB-O1B	5.02	120.48	110.00

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	600	ANP	O1B-PB-N3B-PG
6	O	600	ANP	O1B-PB-N3B-PG
6	L	600	ANP	O1B-PB-N3B-PG

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Mol	Chain	Res	Type	Atoms
6	F	600	ANP	O1G-PG-N3B-PB
6	C	600	ANP	O1B-PB-N3B-PG
6	J	600	ANP	O1G-PG-N3B-PB
6	A	600	ANP	O1G-PG-N3B-PB
6	D	600	ANP	O1G-PG-N3B-PB
6	K	600	ANP	O1B-PB-N3B-PG
6	L	600	ANP	O1G-PG-N3B-PB
6	O	600	ANP	O1G-PG-N3B-PB
6	K	600	ANP	O1G-PG-N3B-PB
6	B	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	600	ANP	1	0
6	B	600	ANP	2	0
6	D	600	ANP	1	0
6	F	600	ANP	2	0
6	K	600	ANP	1	0
6	M	600	ANP	5	0
6	S	600	ANP	4	0
6	T	600	ANP	1	0
6	U	600	ANP	4	0
6	V	600	ANP	4	0
6	X	600	ANP	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	482/510 (94%)	0.03	1 (0%) 95 96	37, 55, 89, 139	0
1	B	483/510 (94%)	0.15	9 (1%) 70 72	35, 58, 109, 138	0
1	C	484/510 (94%)	0.20	13 (2%) 58 60	47, 74, 127, 169	0
1	J	481/510 (94%)	0.18	13 (2%) 58 60	45, 72, 114, 155	0
1	K	486/510 (95%)	0.17	9 (1%) 70 72	41, 64, 116, 150	0
1	L	482/510 (94%)	0.17	12 (2%) 61 63	46, 62, 113, 162	0
1	S	477/510 (93%)	1.35	134 (28%) 1 0	95, 123, 165, 179	0
1	T	478/510 (93%)	0.92	86 (17%) 2 1	93, 120, 148, 167	0
1	U	481/510 (94%)	1.32	111 (23%) 1 1	85, 120, 151, 163	0
2	D	470/484 (97%)	0.18	8 (1%) 73 75	43, 66, 102, 136	0
2	E	468/484 (96%)	0.22	19 (4%) 41 42	36, 61, 129, 168	0
2	F	469/484 (96%)	0.04	5 (1%) 82 84	42, 75, 98, 120	0
2	M	470/484 (97%)	0.45	32 (6%) 20 20	51, 81, 139, 168	0
2	N	470/484 (97%)	0.08	6 (1%) 79 81	42, 62, 117, 157	0
2	O	468/484 (96%)	0.20	12 (2%) 59 62	44, 70, 103, 129	0
2	V	470/484 (97%)	1.24	110 (23%) 1 1	85, 123, 151, 172	0
2	W	467/484 (96%)	1.20	113 (24%) 1 1	92, 107, 138, 156	0
2	X	469/484 (96%)	1.45	133 (28%) 1 0	66, 125, 158, 176	0
3	G	266/278 (95%)	0.74	29 (10%) 7 6	49, 102, 128, 137	0
3	P	244/278 (87%)	1.80	95 (38%) 0 0	50, 117, 137, 152	0
3	Y	200/278 (71%)	2.36	108 (54%) 0 0	89, 116, 141, 152	0
4	H	122/138 (88%)	0.68	13 (10%) 8 6	96, 126, 153, 160	0
4	Q	83/138 (60%)	1.95	36 (43%) 0 0	113, 135, 153, 156	0
4	Z	17/138 (12%)	0.59	3 (17%) 2 1	134, 138, 144, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	1	27/61 (44%)	1.40	9 (33%) 0 0	119, 126, 131, 136	0
5	I	49/61 (80%)	0.46	6 (12%) 5 5	98, 111, 131, 143	0
5	R	34/61 (55%)	1.04	8 (23%) 1 1	107, 118, 147, 152	0
All	All	9597/10377 (92%)	0.62	1133 (11%) 6 5	35, 90, 146, 179	0

All (1133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	37	LEU	11.8
1	S	43	VAL	10.8
2	X	83	ILE	10.4
2	X	217	LEU	9.9
1	T	203	CYS	9.5
1	T	36	VAL	9.2
1	U	36	VAL	8.9
2	X	209	LEU	8.9
4	Q	15	ALA	8.6
1	U	388	VAL	8.5
1	U	37	GLY	8.5
3	P	53	LYS	8.4
2	X	30	LEU	8.4
2	X	32	ALA	8.3
4	Q	49	VAL	8.3
2	X	77	LEU	8.2
2	E	457	PHE	8.2
2	X	39	ILE	8.1
1	U	392	LEU	7.8
3	Y	108	VAL	7.8
1	U	499	LEU	7.7
2	X	46	LEU	7.7
3	P	47	ALA	7.7
2	V	432	VAL	7.7
1	S	44	PHE	7.7
1	S	385	LEU	7.6
2	X	7	THR	7.6
2	X	31	PRO	7.6
3	Y	95	VAL	7.5
2	V	46	LEU	7.4
2	M	467	VAL	7.4
4	Q	83	LEU	7.3
4	Q	84	CYS	7.3

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Mol	Chain	Res	Type	RSRZ
3	Y	164	ILE	7.2
2	X	63	ALA	7.2
1	T	207	ALA	7.1
1	T	202	TYR	6.9
2	X	210	GLU	6.9
3	P	126	ILE	6.9
2	X	54	LEU	6.9
1	U	27	LEU	6.9
3	Y	212	TYR	6.8
3	P	95	VAL	6.8
2	W	59	VAL	6.8
1	U	35	ALA	6.7
4	Q	90	ALA	6.7
4	Q	77	VAL	6.6
3	Y	146	ILE	6.6
1	T	124	ASP	6.6
1	U	125	ALA	6.6
3	Y	145	LEU	6.6
3	P	36	LYS	6.5
2	V	33	ILE	6.5
1	U	34	LEU	6.5
1	S	388	VAL	6.5
2	M	457	PHE	6.5
3	P	93	LYS	6.4
1	U	266	ALA	6.4
1	U	85	LYS	6.3
2	V	198	TYR	6.3
1	S	447	ILE	6.2
1	U	384	ALA	6.2
3	P	164	ILE	6.2
2	W	444	VAL	6.2
1	U	30	THR	6.2
1	U	32	ARG	6.2
2	X	28	SER	6.2
3	P	25	ILE	6.1
3	P	29	THR	6.1
1	S	81	ASP	6.1
3	Y	36	LYS	6.1
2	X	23	VAL	6.1
2	W	305	THR	6.1
2	X	53	HIS	6.0
2	X	43	GLN	6.0

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Mol	Chain	Res	Type	RSRZ
3	Y	110	ILE	6.0
2	V	52	GLN	6.0
1	U	84	VAL	5.9
1	J	499	LEU	5.9
1	S	414	ALA	5.9
3	P	39	ILE	5.9
2	W	389	ALA	5.8
2	X	87	VAL	5.8
4	Q	72	GLY	5.8
3	Y	165	PHE	5.8
2	X	8	PRO	5.8
2	W	391	LEU	5.8
2	V	22	ASP	5.7
2	W	23	VAL	5.7
1	S	446	LEU	5.7
1	T	491	LEU	5.7
2	X	246	GLU	5.7
1	S	61	VAL	5.6
1	S	457	GLY	5.6
1	S	448	TYR	5.6
1	T	205	TYR	5.6
2	W	143	LEU	5.6
3	P	34	ALA	5.5
4	Q	48	THR	5.5
2	W	9	ILE	5.5
1	U	131	ALA	5.5
3	Y	78	THR	5.5
3	P	100	ASN	5.5
5	R	21	ILE	5.4
2	W	82	PRO	5.4
2	V	6	SER	5.4
2	V	9	ILE	5.4
1	U	89	LEU	5.4
1	U	26	ASN	5.4
2	X	238	THR	5.4
2	W	83	ILE	5.4
2	V	116	PRO	5.3
3	Y	91	LEU	5.3
1	S	68	LEU	5.3
1	S	460	LEU	5.3
2	W	47	VAL	5.3
3	Y	261	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
2	X	24	HIS	5.3
2	M	466	VAL	5.3
4	H	72	GLY	5.3
2	X	29	GLU	5.3
1	U	75	ILE	5.3
2	X	304	VAL	5.3
1	U	194	GLY	5.3
1	S	438	LEU	5.3
2	V	175	ALA	5.2
5	R	30	GLN	5.2
3	Y	120	ARG	5.2
3	P	182	ILE	5.2
3	Y	211	GLU	5.2
1	T	26	ASN	5.2
2	W	395	GLU	5.2
3	Y	99	LEU	5.2
2	V	7	THR	5.2
1	S	389	ALA	5.1
2	W	119	ALA	5.1
2	W	394	ASP	5.1
1	S	352	ILE	5.1
2	W	103	ILE	5.1
2	W	133	ILE	5.1
2	X	207	ILE	5.1
2	V	39	ILE	5.1
2	W	219	PHE	5.1
4	H	129	VAL	5.1
1	S	493	LYS	5.1
2	V	34	LEU	5.1
1	S	503	THR	5.1
1	U	454	HIS	5.1
3	Y	83	LEU	5.0
1	S	33	VAL	5.0
2	X	239	ILE	5.0
2	V	179	GLY	5.0
3	Y	140	PHE	5.0
2	X	76	VAL	5.0
2	W	342	LEU	5.0
2	V	30	LEU	5.0
2	X	70	LEU	5.0
1	U	482	LEU	5.0
2	V	134	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
2	V	62	ILE	5.0
1	T	150	THR	4.9
1	S	491	LEU	4.9
1	U	61	VAL	4.9
2	W	473	LEU	4.9
2	W	390	ILE	4.9
1	U	509	THR	4.9
1	S	418	GLN	4.9
3	Y	266	GLU	4.9
2	V	393	MET	4.9
2	W	77	LEU	4.9
3	Y	150	LEU	4.9
2	V	94	ARG	4.9
2	X	181	PHE	4.9
2	W	437	THR	4.8
2	X	184	PHE	4.8
2	W	8	PRO	4.8
2	N	387	ILE	4.8
2	W	440	SER	4.8
3	Y	230	ILE	4.8
2	X	48	LEU	4.8
2	X	79	THR	4.8
1	U	41	ALA	4.7
2	V	32	ALA	4.7
2	X	36	ALA	4.7
2	X	38	GLU	4.7
3	Y	130	ILE	4.7
1	T	234	VAL	4.7
1	S	202	TYR	4.7
2	V	25	PHE	4.7
2	W	306	SER	4.7
3	G	165	PHE	4.7
3	P	46	GLU	4.7
1	U	83	LEU	4.7
2	D	467	VAL	4.7
2	V	91	THR	4.7
1	U	44	PHE	4.7
2	V	81	GLY	4.7
2	X	180	GLY	4.6
3	P	91	LEU	4.6
1	U	71	GLY	4.6
1	S	70	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	S	499	LEU	4.6
3	Y	153	VAL	4.6
2	W	57	ASN	4.6
3	Y	148	ASP	4.6
1	S	34	LEU	4.6
2	X	27	GLN	4.6
4	Q	79	PRO	4.6
2	V	99	ILE	4.5
4	Z	135	SER	4.5
2	V	10	THR	4.5
3	Y	265	ASN	4.5
4	Q	50	GLU	4.5
2	V	50	VAL	4.5
3	Y	264	THR	4.5
2	W	474	ALA	4.5
5	1	9	SER	4.5
3	Y	166	TYR	4.5
1	S	167	GLU	4.5
2	W	55	GLY	4.5
1	S	387	GLN	4.5
1	U	122	PRO	4.5
1	S	392	LEU	4.5
2	X	50	VAL	4.5
3	Y	2	THR	4.5
4	Q	70	ILE	4.5
1	B	410	SER	4.5
1	U	119	GLY	4.5
2	V	83	ILE	4.4
2	V	118	HIS	4.4
1	U	232	ILE	4.4
2	X	254	PHE	4.4
2	V	100	GLY	4.4
2	W	46	LEU	4.4
3	P	171	SER	4.4
2	X	391	LEU	4.4
2	M	387	ILE	4.4
2	X	75	LYS	4.3
1	T	35	ALA	4.3
3	Y	103	PRO	4.3
2	O	7	THR	4.3
1	K	411	ASP	4.3
3	Y	156	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	S	57	PHE	4.3
2	V	218	VAL	4.3
2	W	413	PHE	4.3
1	S	324	THR	4.3
2	E	466	VAL	4.3
1	U	126	ALA	4.3
2	W	34	LEU	4.2
4	H	95	SER	4.2
1	S	204	VAL	4.2
2	W	22	ASP	4.2
1	S	157	ALA	4.2
1	U	380	ALA	4.2
2	V	117	ILE	4.2
4	H	70	ILE	4.2
4	H	88	ILE	4.2
3	Y	269	ASP	4.2
3	P	37	ALA	4.2
1	U	72	GLN	4.2
2	X	183	VAL	4.2
1	S	502	ALA	4.2
3	P	133	ILE	4.2
1	C	457	GLY	4.2
1	S	27	LEU	4.2
1	U	385	LEU	4.2
3	Y	225	GLY	4.2
1	T	54	LEU	4.2
3	Y	151	LEU	4.2
2	X	78	ASP	4.2
2	V	13	VAL	4.2
1	K	488	LYS	4.1
3	Y	37	ALA	4.1
2	V	440	SER	4.1
2	V	443	ALA	4.1
1	S	420	LEU	4.1
1	S	485	ILE	4.1
2	X	35	ASN	4.1
1	T	204	VAL	4.1
3	Y	175	PHE	4.1
2	W	71	VAL	4.1
3	Y	96	ARG	4.1
1	S	419	THR	4.1
2	X	14	THR	4.1

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Mol	Chain	Res	Type	RSRZ
4	Q	89	GLU	4.1
1	U	87	GLY	4.1
3	Y	104	ASN	4.0
2	W	144	LEU	4.0
1	U	195	SER	4.0
1	S	63	GLY	4.0
4	Q	71	SER	4.0
2	W	307	VAL	4.0
2	W	131	ALA	4.0
2	V	98	VAL	4.0
3	Y	170	VAL	4.0
3	Y	92	ALA	4.0
2	X	88	GLY	4.0
4	Q	17	PRO	4.0
2	W	398	GLU	4.0
1	T	51	ALA	4.0
2	M	445	LEU	4.0
4	H	15	ALA	4.0
4	Q	34	ALA	4.0
2	W	45	LYS	4.0
4	H	26	GLU	4.0
3	Y	87	ILE	4.0
1	T	218	LEU	4.0
2	E	473	LEU	4.0
2	V	303	SER	4.0
2	X	147	TYR	3.9
3	P	76	ALA	3.9
1	U	57	PHE	3.9
1	S	205	TYR	3.9
3	P	31	LEU	3.9
1	U	63	GLY	3.9
3	Y	141	GLN	3.9
2	X	113	LEU	3.9
3	G	76	ALA	3.9
2	D	390	ILE	3.9
3	P	234	ARG	3.9
2	X	71	VAL	3.9
4	Q	103	ASN	3.9
3	Y	42	LYS	3.8
3	Y	114	ILE	3.8
1	U	441	GLU	3.8
1	S	429	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	U	338	ALA	3.8
2	X	9	ILE	3.8
2	M	391	LEU	3.8
2	V	394	ASP	3.8
2	V	8	PRO	3.8
2	X	16	VAL	3.8
1	T	49	ILE	3.8
1	U	496	LEU	3.8
2	W	358	LEU	3.8
2	W	15	ALA	3.8
2	X	314	ALA	3.8
1	U	76	VAL	3.8
2	X	92	LEU	3.8
4	H	32	LEU	3.8
2	W	397	SER	3.8
1	U	270	TYR	3.8
2	M	441	PHE	3.8
2	V	421	ALA	3.8
2	W	51	ALA	3.8
3	P	48	GLU	3.8
3	G	258	THR	3.8
3	Y	1	ALA	3.8
3	Y	263	ILE	3.8
1	S	32	ARG	3.8
3	P	35	GLU	3.7
1	U	40	ILE	3.7
2	M	462	GLY	3.7
2	V	14	THR	3.7
1	U	42	ARG	3.7
2	X	279	VAL	3.7
1	T	186	LEU	3.7
3	P	128	LEU	3.7
2	W	128	SER	3.7
1	T	142	ARG	3.7
1	S	195	SER	3.7
1	T	27	LEU	3.7
3	Y	222	MET	3.7
3	P	220	THR	3.7
2	V	453	PRO	3.7
2	X	68	GLU	3.7
1	U	148	VAL	3.7
2	V	140	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	S	482	LEU	3.7
2	V	70	LEU	3.7
2	X	51	ALA	3.6
1	U	503	THR	3.6
2	V	31	PRO	3.6
1	U	33	VAL	3.6
1	U	55	VAL	3.6
3	Y	262	VAL	3.6
3	Y	77	ILE	3.6
3	P	108	VAL	3.6
3	Y	218	MET	3.6
1	L	509	THR	3.6
1	S	62	LYS	3.6
1	T	183	ASP	3.6
2	X	42	PRO	3.6
3	P	185	ALA	3.6
2	X	219	PHE	3.6
2	W	445	LEU	3.6
3	P	174	SER	3.6
3	Y	173	LEU	3.6
2	X	302	GLY	3.6
2	W	64	MET	3.6
1	T	184	THR	3.6
2	M	439	ALA	3.6
1	S	443	GLN	3.6
2	V	69	GLY	3.6
2	V	367	HIS	3.6
2	W	240	ALA	3.5
2	D	473	LEU	3.5
1	U	82	ARG	3.5
2	X	249	GLN	3.5
3	Y	116	MET	3.5
3	Y	275	SER	3.5
5	1	12	ALA	3.5
1	S	151	GLY	3.5
4	H	27	VAL	3.5
1	S	415	SER	3.5
2	X	69	GLY	3.5
4	Q	35	LYS	3.5
2	W	43	GLN	3.5
1	U	455	LEU	3.5
5	1	11	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	N	388	ILE	3.5
2	E	474	ALA	3.5
2	V	57	ASN	3.5
2	X	82	PRO	3.5
2	V	27	GLN	3.5
1	S	64	MET	3.5
3	Y	260	GLN	3.5
4	Q	75	ALA	3.5
1	S	435	TYR	3.5
2	M	438	VAL	3.5
3	P	30	ARG	3.4
3	P	32	SER	3.4
1	U	139	LEU	3.4
2	W	39	ILE	3.4
2	X	171	ILE	3.4
1	U	86	GLU	3.4
3	P	228	ALA	3.4
1	U	296	TYR	3.4
2	X	215	VAL	3.4
4	Q	46	VAL	3.4
1	U	117	ILE	3.4
3	P	87	ILE	3.4
3	Y	118	LEU	3.4
2	V	475	ALA	3.4
2	W	120	ASP	3.4
3	P	23	MET	3.4
2	V	181	PHE	3.4
2	V	219	PHE	3.4
2	W	396	LEU	3.4
2	V	148	ALA	3.4
3	P	227	ALA	3.4
3	Y	268	VAL	3.4
1	T	473	TYR	3.4
2	X	26	GLU	3.4
2	X	117	ILE	3.4
3	P	151	LEU	3.4
3	P	77	ILE	3.4
3	P	223	ALA	3.4
3	Y	217	GLN	3.4
2	V	12	LYS	3.4
2	X	21	VAL	3.4
5	R	22	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	U	291	PRO	3.3
2	X	81	GLY	3.3
2	X	109	ILE	3.3
3	Y	215	ALA	3.3
1	U	335	ASP	3.3
3	Y	93	LYS	3.3
3	G	262	VAL	3.3
2	V	395	GLU	3.3
2	W	25	PHE	3.3
4	H	55	GLY	3.3
2	W	370	VAL	3.3
1	S	66	LEU	3.3
1	T	489	GLY	3.3
1	S	150	THR	3.3
2	V	446	GLU	3.3
3	Y	35	GLU	3.3
1	T	135	ALA	3.3
1	S	495	LEU	3.3
1	T	420	LEU	3.3
2	X	243	PHE	3.3
2	X	317	LEU	3.3
1	U	505	SER	3.3
1	K	484	GLU	3.3
3	P	175	PHE	3.3
3	Y	119	LEU	3.3
3	Y	214	LEU	3.3
5	1	13	TYR	3.3
5	1	15	ASN	3.3
1	S	89	LEU	3.2
1	T	78	PHE	3.2
2	V	396	LEU	3.2
2	W	42	PRO	3.2
3	Y	109	THR	3.2
2	W	29	GLU	3.2
2	E	467	VAL	3.2
1	S	498	SER	3.2
3	Y	149	LYS	3.2
3	Y	88	HIS	3.2
5	1	44	TYR	3.2
1	T	75	ILE	3.2
3	Y	3	LEU	3.2
2	W	250	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	X	108	PRO	3.2
3	Y	6	VAL	3.2
2	V	398	GLU	3.2
3	P	54	ASN	3.2
3	P	81	LYS	3.2
3	Y	97	ARG	3.2
2	D	7	THR	3.2
2	V	119	ALA	3.2
1	T	158	LEU	3.2
1	U	341	PRO	3.2
3	Y	154	MET	3.2
2	E	453	PRO	3.2
2	W	450	ASP	3.2
1	U	337	SER	3.2
2	W	168	GLN	3.2
2	V	23	VAL	3.2
3	P	180	LYS	3.2
1	S	65	ALA	3.2
4	Q	76	THR	3.2
1	U	446	LEU	3.1
2	M	394	ASP	3.1
2	W	89	ARG	3.1
1	T	122	PRO	3.1
1	T	119	GLY	3.1
2	X	148	ALA	3.1
2	W	436	ASP	3.1
2	V	444	VAL	3.1
3	P	225	GLY	3.1
3	Y	142	GLU	3.1
3	Y	144	ALA	3.1
1	S	496	LEU	3.1
1	U	396	LEU	3.1
2	X	99	ILE	3.1
3	Y	138	PRO	3.1
1	S	71	GLY	3.1
2	V	220	GLY	3.1
2	X	130	SER	3.1
2	M	403	THR	3.1
2	V	214	LYS	3.1
3	G	146	ILE	3.1
1	S	183	ASP	3.1
1	T	131	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	V	216	ALA	3.1
2	W	14	THR	3.1
1	J	471	LEU	3.1
3	P	73	LEU	3.1
2	X	33	ILE	3.1
1	S	489	GLY	3.1
2	E	458	TYR	3.1
2	V	73	GLY	3.1
2	O	398	GLU	3.1
1	T	314	LEU	3.1
2	V	261	PHE	3.1
2	V	356	ARG	3.1
3	Y	38	LYS	3.1
1	S	235	ALA	3.1
1	S	236	ALA	3.1
3	P	105	ALA	3.1
2	W	277	SER	3.1
2	X	276	PRO	3.1
1	S	153	LYS	3.0
3	G	2	THR	3.0
3	G	50	LEU	3.0
2	E	390	ILE	3.0
3	P	231	SER	3.0
1	S	69	GLU	3.0
2	W	27	GLN	3.0
2	X	47	VAL	3.0
4	Q	78	GLN	3.0
2	W	104	ASP	3.0
2	V	327	ALA	3.0
2	X	323	ALA	3.0
2	X	213	SER	3.0
1	J	447	ILE	3.0
1	T	118	ASP	3.0
1	U	411	ASP	3.0
3	P	86	SER	3.0
1	T	208	VAL	3.0
3	P	136	ASP	3.0
1	U	442	GLU	3.0
2	V	51	ALA	3.0
1	S	255	ILE	3.0
2	X	242	TYR	3.0
1	T	509	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	456	ALA	3.0
2	V	194	GLY	3.0
2	W	24	HIS	3.0
1	U	105	LEU	3.0
2	V	54	LEU	3.0
2	X	361	ALA	3.0
3	P	50	LEU	3.0
1	S	470	PHE	3.0
1	S	383	LYS	3.0
5	I	16	VAL	3.0
2	W	147	TYR	3.0
2	W	357	LEU	3.0
3	P	219	LEU	3.0
2	X	10	THR	3.0
2	V	110	LYS	3.0
1	L	412	LEU	2.9
2	V	441	PHE	2.9
2	W	302	GLY	2.9
2	W	70	LEU	2.9
1	S	30	THR	2.9
2	X	305	THR	2.9
2	W	78	ASP	2.9
1	U	304	HIS	2.9
2	V	215	VAL	2.9
2	X	85	VAL	2.9
2	V	26	GLU	2.9
2	V	48	LEU	2.9
3	Y	226	TYR	2.9
4	Q	36	SER	2.9
4	Q	87	ALA	2.9
5	I	10	TYR	2.9
2	X	313	PRO	2.9
1	U	383	LYS	2.9
2	X	12	LYS	2.9
2	W	60	ARG	2.9
3	P	230	ILE	2.9
5	I	15	ASN	2.9
1	S	337	SER	2.9
1	S	384	ALA	2.9
1	S	104	GLY	2.9
2	O	320	PRO	2.9
3	P	216	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	98	HIS	2.9
1	B	499	LEU	2.9
2	V	177	ALA	2.9
2	X	318	THR	2.9
2	X	275	ILE	2.9
1	S	36	VAL	2.9
3	P	150	LEU	2.9
2	V	399	GLN	2.9
1	S	42	ARG	2.9
2	M	468	ALA	2.9
1	U	465	GLU	2.9
1	U	489	GLY	2.9
2	W	242	TYR	2.9
5	R	28	GLU	2.9
1	U	115	ASN	2.9
3	Y	163	SER	2.9
1	U	151	GLY	2.9
2	M	443	ALA	2.9
2	W	184	PHE	2.9
3	P	51	PHE	2.9
4	Q	14	PHE	2.9
1	S	67	ASN	2.9
3	P	42	LYS	2.9
1	S	186	LEU	2.8
1	S	287	LEU	2.8
2	M	143	LEU	2.8
1	S	87	GLY	2.8
2	W	36	ALA	2.8
1	S	445	PRO	2.8
2	W	441	PHE	2.8
5	I	47	TYR	2.8
5	1	10	TYR	2.8
2	X	316	ASP	2.8
4	H	111	ASN	2.8
1	S	129	SER	2.8
2	W	48	LEU	2.8
2	W	435	LYS	2.8
3	Y	219	LEU	2.8
2	X	102	PRO	2.8
1	S	316	GLU	2.8
1	B	473	TYR	2.8
1	T	360	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	410	SER	2.8
2	V	201	MET	2.8
2	W	463	ILE	2.8
3	Y	162	ILE	2.8
3	G	1	ALA	2.8
3	Y	224	GLN	2.8
3	P	43	LYS	2.8
1	U	412	LEU	2.8
2	X	55	GLY	2.8
2	X	96	ILE	2.8
2	W	467	VAL	2.8
2	X	59	VAL	2.8
2	X	98	VAL	2.8
2	V	35	ASN	2.8
3	P	233	ARG	2.8
2	V	37	LEU	2.8
2	X	95	ILE	2.8
1	J	507	VAL	2.8
1	C	462	ARG	2.8
1	B	397	ALA	2.8
1	K	481	LEU	2.8
2	V	209	LEU	2.8
2	W	446	GLU	2.8
1	S	293	ARG	2.8
1	T	41	ALA	2.8
2	W	456	ALA	2.8
3	G	261	ALA	2.8
2	W	204	THR	2.8
3	P	169	PRO	2.8
1	U	182	LEU	2.7
2	V	302	GLY	2.7
1	S	168	LEU	2.7
3	Y	259	ARG	2.7
3	G	133	ILE	2.7
1	T	101	VAL	2.7
2	M	393	MET	2.7
1	J	470	PHE	2.7
1	S	189	LYS	2.7
2	X	121	PRO	2.7
1	T	256	GLY	2.7
1	A	499	LEU	2.7
3	Y	31	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	V	147	TYR	2.7
3	Y	270	ILE	2.7
1	S	193	ASN	2.7
2	W	439	ALA	2.7
3	P	156	ALA	2.7
3	P	183	PHE	2.7
3	P	252	SER	2.7
1	S	442	GLU	2.7
3	P	7	GLU	2.7
3	P	212	TYR	2.7
3	P	255	TYR	2.7
1	L	407	GLN	2.7
1	S	312	ALA	2.7
1	T	71	GLY	2.7
1	T	295	ALA	2.7
2	X	240	ALA	2.7
2	X	321	ALA	2.7
3	P	217	GLN	2.7
3	Y	139	THR	2.7
3	Y	258	THR	2.7
3	Y	89	SER	2.7
2	X	118	HIS	2.7
3	G	77	ILE	2.7
3	P	74	ILE	2.7
2	O	467	VAL	2.7
2	W	72	ARG	2.7
1	T	157	ALA	2.7
1	S	200	LYS	2.7
2	O	430	LYS	2.7
2	N	391	LEU	2.7
2	V	234	LEU	2.7
2	X	153	ILE	2.7
1	S	76	VAL	2.7
1	U	204	VAL	2.7
1	U	491	LEU	2.7
2	W	392	GLY	2.7
2	X	11	GLY	2.7
2	X	236	GLY	2.7
2	X	319	ASP	2.7
1	U	448	TYR	2.7
1	U	389	ALA	2.7
1	S	48	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	U	193	ASN	2.6
2	W	295	ARG	2.6
2	V	211	GLY	2.6
1	S	185	ILE	2.6
2	V	95	ILE	2.6
3	G	268	VAL	2.6
2	N	393	MET	2.6
2	X	86	PRO	2.6
1	S	218	LEU	2.6
1	C	411	ASP	2.6
1	S	123	ILE	2.6
1	T	185	ILE	2.6
2	X	49	GLU	2.6
4	Z	121	ALA	2.6
1	S	91	LYS	2.6
2	F	318	THR	2.6
2	O	396	LEU	2.6
3	P	90	GLN	2.6
2	V	24	HIS	2.6
1	S	494	GLU	2.6
3	P	179	GLU	2.6
4	Q	80	ASP	2.6
1	T	233	ILE	2.6
1	U	300	VAL	2.6
2	V	47	VAL	2.6
3	P	75	VAL	2.6
1	L	448	TYR	2.6
3	P	256	ASN	2.6
1	B	393	LYS	2.6
1	T	62	LYS	2.6
1	S	505	SER	2.6
1	B	407	GLN	2.6
1	S	507	VAL	2.6
1	T	32	ARG	2.6
1	T	100	PRO	2.6
1	S	158	LEU	2.6
2	O	207	ILE	2.6
2	X	131	ALA	2.6
3	P	215	ALA	2.6
1	T	262	ASN	2.6
2	N	280	GLY	2.6
2	X	89	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	S	467	GLU	2.6
3	Y	4	LYS	2.6
1	J	481	LEU	2.6
2	W	44	GLY	2.6
2	W	73	GLY	2.6
5	R	27	THR	2.6
2	F	214	LYS	2.6
3	P	135	LYS	2.6
3	Y	135	LYS	2.6
4	H	69	PHE	2.6
4	Q	101	ILE	2.6
2	X	278	ALA	2.5
1	U	471	LEU	2.5
4	Q	44	ASN	2.5
1	S	264	LYS	2.5
2	M	6	SER	2.5
1	J	508	ALA	2.5
1	U	449	ALA	2.5
3	P	41	ALA	2.5
3	Y	237	MET	2.5
4	Q	18	HIS	2.5
3	Y	152	SER	2.5
1	U	334	GLY	2.5
1	S	267	LEU	2.5
2	X	277	SER	2.5
1	S	333	GLY	2.5
1	T	162	GLY	2.5
1	U	506	PHE	2.5
1	C	414	ALA	2.5
1	S	471	LEU	2.5
1	T	219	VAL	2.5
2	X	149	ARG	2.5
1	L	410	SER	2.5
3	Y	9	ARG	2.5
2	V	276	PRO	2.5
1	U	28	ASN	2.5
2	V	92	LEU	2.5
3	Y	267	LEU	2.5
2	X	202	LYS	2.5
4	H	71	SER	2.5
2	X	394	ASP	2.5
2	V	77	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	W	443	ALA	2.5
2	X	167	ILE	2.5
3	G	188	ILE	2.5
1	U	198	SER	2.5
4	Q	13	GLN	2.5
1	J	482	LEU	2.5
1	L	491	LEU	2.5
4	Q	16	LEU	2.5
3	Y	84	CYS	2.5
1	S	395	PHE	2.5
2	W	453	PRO	2.5
3	Y	167	ASN	2.5
1	S	354	LEU	2.4
2	M	396	LEU	2.4
2	V	306	SER	2.4
3	Y	43	LYS	2.4
1	T	43	VAL	2.4
1	T	485	ILE	2.4
2	M	398	GLU	2.4
2	M	406	ARG	2.4
1	S	428	GLN	2.4
2	W	61	THR	2.4
3	Y	255	TYR	2.4
2	W	183	VAL	2.4
3	P	224	GLN	2.4
1	S	334	GLY	2.4
1	S	440	THR	2.4
1	L	411	ASP	2.4
1	U	81	ASP	2.4
1	T	316	GLU	2.4
1	U	294	GLU	2.4
1	S	394	LEU	2.4
2	M	431	LEU	2.4
2	W	402	LEU	2.4
1	S	97	VAL	2.4
1	U	382	VAL	2.4
2	V	109	ILE	2.4
3	Y	34	ALA	2.4
1	T	251	THR	2.4
3	Y	121	THR	2.4
3	Y	257	ARG	2.4
1	T	482	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	140	PHE	2.4
4	Q	33	PRO	2.4
3	G	107	ILE	2.4
1	K	492	SER	2.4
2	X	182	SER	2.4
3	G	272	THR	2.4
5	1	33	SER	2.4
2	M	400	ASP	2.4
2	X	110	LYS	2.4
3	P	154	MET	2.4
1	S	325	ALA	2.4
2	V	420	VAL	2.4
3	Y	41	ALA	2.4
5	R	12	ALA	2.4
5	R	20	ALA	2.4
1	U	58	SER	2.4
1	J	484	GLU	2.4
2	E	403	THR	2.4
2	W	454	GLU	2.4
3	P	78	THR	2.4
2	O	394	ASP	2.4
2	W	399	GLN	2.4
1	K	491	LEU	2.4
1	T	291	PRO	2.4
2	M	8	PRO	2.4
3	P	222	MET	2.4
1	S	230	TYR	2.4
2	V	468	ALA	2.4
1	C	415	SER	2.4
2	W	49	GLU	2.4
2	O	318	THR	2.4
2	V	313	PRO	2.3
3	G	150	LEU	2.3
5	I	29	LEU	2.3
1	U	292	GLY	2.3
2	V	205	GLY	2.3
2	M	435	LYS	2.3
2	W	215	VAL	2.3
3	P	40	SER	2.3
4	Q	97	SER	2.3
4	Z	120	ALA	2.3
2	V	184	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	V	431	LEU	2.3
3	G	118	LEU	2.3
1	U	386	LYS	2.3
2	X	401	LYS	2.3
1	T	443	GLN	2.3
2	V	20	ILE	2.3
2	X	315	ASP	2.3
2	X	90	GLU	2.3
2	E	143	LEU	2.3
2	X	322	PRO	2.3
2	X	393	MET	2.3
1	T	58	SER	2.3
2	X	15	ALA	2.3
1	T	52	GLU	2.3
1	T	104	GLY	2.3
3	P	9	ARG	2.3
1	U	497	ALA	2.3
1	T	324	THR	2.3
1	U	475	LYS	2.3
2	D	398	GLU	2.3
2	M	469	LYS	2.3
2	W	13	VAL	2.3
3	P	161	LYS	2.3
1	S	377	GLY	2.3
2	E	391	LEU	2.3
1	K	470	PHE	2.3
1	T	466	PHE	2.3
1	T	252	ALA	2.3
3	P	167	ASN	2.3
3	P	2	THR	2.3
1	S	464	GLY	2.3
2	V	137	GLY	2.3
1	U	456	ASP	2.3
2	X	303	SER	2.3
1	C	448	TYR	2.3
2	E	452	ILE	2.3
2	M	381	TYR	2.3
3	P	226	TYR	2.3
1	U	104	GLY	2.3
1	L	493	LYS	2.3
1	T	499	LEU	2.3
1	U	426	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	X	25	PHE	2.3
3	Y	112	ASP	2.3
1	S	28	ASN	2.3
1	S	108	ARG	2.3
1	S	331	THR	2.3
1	S	458	ILE	2.3
1	T	293	ARG	2.2
3	Y	44	MET	2.2
2	V	59	VAL	2.2
2	M	9	ILE	2.2
2	V	133	ILE	2.2
2	W	330	ASP	2.2
3	Y	115	LYS	2.2
1	L	295	ALA	2.2
1	L	414	ALA	2.2
1	S	126	ALA	2.2
1	T	459	GLU	2.2
1	U	202	TYR	2.2
5	I	14	LEU	2.2
2	O	453	PRO	2.2
2	W	408	ARG	2.2
3	Y	169	PRO	2.2
2	M	395	GLU	2.2
3	P	55	ALA	2.2
1	T	73	VAL	2.2
2	E	410	ILE	2.2
1	T	308	LEU	2.2
2	W	252	LEU	2.2
1	S	372	SER	2.2
1	S	501	SER	2.2
3	Y	216	ASN	2.2
2	W	218	VAL	2.2
1	C	331	THR	2.2
2	F	176	LYS	2.2
2	V	406	ARG	2.2
1	U	111	ASP	2.2
1	K	448	TYR	2.2
2	D	198	TYR	2.2
2	V	358	LEU	2.2
1	T	337	SER	2.2
1	T	441	GLU	2.2
2	E	470	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	M	380	THR	2.2
2	V	239	ILE	2.2
2	X	58	THR	2.2
3	G	22	THR	2.2
2	E	424	PHE	2.2
2	E	449	TYR	2.2
2	X	281	TYR	2.2
1	J	454	HIS	2.2
2	O	175	ALA	2.2
1	U	73	VAL	2.2
3	Y	272	THR	2.2
1	S	283	LEU	2.2
2	N	390	ILE	2.2
3	G	19	ILE	2.2
1	J	466	PHE	2.2
3	P	104	ASN	2.2
2	W	470	ALA	2.2
3	P	94	ALA	2.2
1	S	101	VAL	2.2
2	W	438	VAL	2.2
3	G	260	GLN	2.1
2	F	28	SER	2.1
1	S	31	GLY	2.1
3	P	98	HIS	2.1
4	Q	19	GLU	2.1
5	I	41	ASP	2.1
1	C	388	VAL	2.1
1	S	416	THR	2.1
1	S	451	VAL	2.1
1	T	507	VAL	2.1
1	S	161	ILE	2.1
1	S	305	SER	2.1
3	G	273	GLY	2.1
1	T	28	ASN	2.1
3	G	259	ARG	2.1
3	P	88	HIS	2.1
1	C	496	LEU	2.1
2	M	434	LEU	2.1
2	E	280	GLY	2.1
3	Y	98	HIS	2.1
1	S	35	ALA	2.1
2	M	321	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	V	456	ALA	2.1
2	X	216	ALA	2.1
3	Y	136	ASP	2.1
3	Y	221	ALA	2.1
1	B	481	LEU	2.1
1	J	503	THR	2.1
3	P	6	VAL	2.1
2	W	393	MET	2.1
3	G	154	MET	2.1
1	T	470	PHE	2.1
2	W	350	PRO	2.1
2	W	177	ALA	2.1
1	C	507	VAL	2.1
1	T	97	VAL	2.1
1	T	201	LEU	2.1
1	T	334	GLY	2.1
1	U	331	THR	2.1
2	F	370	VAL	2.1
1	T	223	GLU	2.1
1	U	340	ILE	2.1
3	G	124	ASN	2.1
4	Q	100	ASN	2.1
1	T	145	HIS	2.1
1	U	339	TYR	2.1
2	W	278	ALA	2.1
2	O	384	LEU	2.1
2	V	40	LYS	2.1
2	V	402	LEU	2.1
3	G	3	LEU	2.1
3	G	266	GLU	2.1
3	Y	10	LEU	2.1
1	U	451	VAL	2.1
1	B	418	GLN	2.1
1	K	478	HIS	2.1
1	U	38	ASP	2.1
2	V	448	LYS	2.1
1	S	441	GLU	2.1
1	U	171	GLY	2.1
1	U	333	GLY	2.1
2	X	93	GLY	2.1
3	P	134	GLY	2.1
1	L	420	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	80	SER	2.1
2	E	444	VAL	2.1
5	R	36	ASN	2.1
2	D	405	GLU	2.1
1	T	74	GLY	2.1
1	S	426	LEU	2.0
2	W	170	LEU	2.0
1	T	217	GLN	2.0
1	T	343	ASN	2.0
3	Y	249	ASN	2.0
2	M	460	VAL	2.0
1	U	116	PRO	2.0
3	P	107	ILE	2.0
3	P	130	ILE	2.0
1	U	94	GLY	2.0
2	W	280	GLY	2.0
1	C	337	SER	2.0
2	X	84	SER	2.0
4	Q	81	SER	2.0
1	C	465	GLU	2.0
1	U	486	ARG	2.0
1	S	450	GLY	2.0
1	T	385	LEU	2.0
1	T	435	TYR	2.0
2	D	384	LEU	2.0
3	G	53	LYS	2.0
4	Q	132	ASN	2.0
1	J	459	GLU	2.0
1	S	84	VAL	2.0
1	S	159	VAL	2.0
2	X	398	GLU	2.0
3	P	26	VAL	2.0
3	P	139	THR	2.0
2	X	320	PRO	2.0
3	G	110	ILE	2.0
2	W	263	GLN	2.0
2	X	306	SER	2.0
1	L	499	LEU	2.0
1	S	439	ALA	2.0
1	T	296	TYR	2.0
2	X	311	TYR	2.0
1	S	425	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
3	P	142	GLU	2.0
3	Y	176	GLU	2.0
1	B	416	THR	2.0
1	T	300	VAL	2.0
1	U	342	THR	2.0
2	W	279	VAL	2.0
2	W	181	PHE	2.0
2	W	243	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	MG	D	700	1/1	0.95	0.32	13.06	57,57,57,57	0
7	MG	O	700	1/1	0.93	0.25	3.22	55,55,55,55	0
7	MG	F	700	1/1	0.91	0.27	3.21	56,56,56,56	0
6	ANP	B	600	31/31	0.96	0.23	1.72	53,63,65,65	0
6	ANP	K	600	31/31	0.97	0.22	1.08	51,60,62,63	0
6	ANP	A	600	31/31	0.96	0.22	0.97	50,60,62,62	0
6	ANP	L	600	31/31	0.97	0.23	0.72	57,61,63,64	0
6	ANP	J	600	31/31	0.95	0.20	0.60	58,73,81,82	0
6	ANP	O	600	31/31	0.96	0.21	0.54	58,62,72,72	0
6	ANP	C	600	31/31	0.95	0.21	0.39	60,70,72,73	0
6	ANP	D	600	31/31	0.97	0.19	0.09	62,66,69,71	0
8	PO4	E	800	5/5	0.83	0.15	0.09	101,101,102,103	0
6	ANP	F	600	31/31	0.97	0.19	-0.01	58,65,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	ANP	M	600	31/31	0.95	0.20	-0.05	64,77,78,78	0
8	PO4	N	800	5/5	0.94	0.14	-0.29	96,97,97,97	0
6	ANP	U	600	31/31	0.93	0.21	-0.42	71,74,77,79	0
7	MG	X	700	1/1	0.92	0.20	-0.73	65,65,65,65	0
6	ANP	V	600	31/31	0.93	0.16	-0.75	77,85,87,88	0
6	ANP	S	600	31/31	0.88	0.16	-0.81	74,79,82,83	0
6	ANP	T	600	31/31	0.94	0.12	-1.62	75,82,84,85	0
6	ANP	X	600	31/31	0.96	0.15	-1.92	75,79,83,85	0
7	MG	L	700	1/1	0.98	0.44	-	52,52,52,52	0
7	MG	U	700	1/1	0.93	0.23	-	75,75,75,75	0
7	MG	C	700	1/1	0.94	0.33	-	56,56,56,56	0
7	MG	S	700	1/1	0.90	0.08	-	64,64,64,64	0
7	MG	T	700	1/1	0.87	0.07	-	65,65,65,65	0
7	MG	V	700	1/1	0.97	0.10	-	67,67,67,67	0
7	MG	M	700	1/1	0.97	0.28	-	57,57,57,57	0
7	MG	B	700	1/1	0.91	0.35	-	50,50,50,50	0
7	MG	J	700	1/1	0.97	0.37	-	52,52,52,52	0
7	MG	K	700	1/1	0.96	0.36	-	47,47,47,47	0
7	MG	A	700	1/1	0.98	0.40	-	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.