Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:25 AM GMT

PDB ID	:	3OFN
Title	:	Structure of four mutant forms of yeast F1 ATPase: alpha-N67I
Authors	:	Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.
Deposited on	:	2010-08-15
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

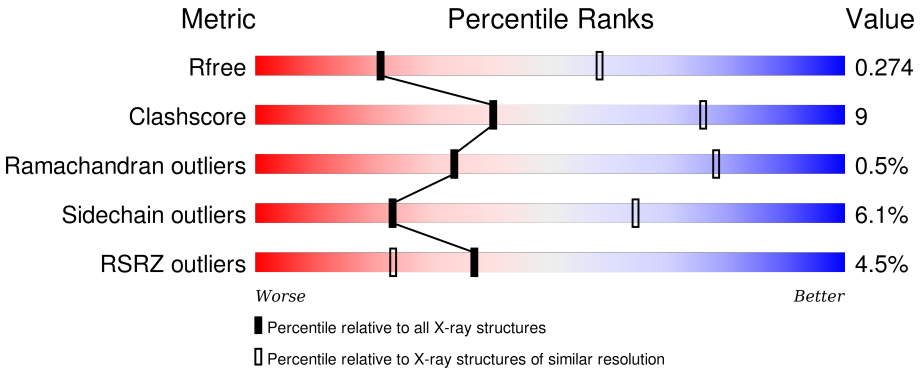
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	69% 24% • 5%
1	B	510	3% 72% 22% • 5%
1	C	510	2% 78% 15% • 5%
1	J	510	4% 74% 19% • 5%
1	K	510	7% 74% 21% 5%

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Mol	Chain	Length	Quality of chain
1	L	510	3% 71% 22% 6%
1	S	510	% 76% 17% 5%
1	T	510	% 75% 19% 5%
1	U	510	5% 76% 18% 5%
2	D	484	2% 74% 22%
2	E	484	3% 70% 24%
2	F	484	2% 73% 24%
2	M	484	5% 69% 24% 5%
2	N	484	10% 69% 25%
2	O	484	6% 78% 18%
2	V	484	6% 53% 20% 26%
2	W	484	% 77% 18%
2	X	484	% 76% 21%
3	G	278	67% 28%
3	P	278	15% 71% 24%
3	Y	278	11% 30% 11% 59%
4	H	138	64% 20% 12%
4	Q	138	27% 64% 9% 27%
5	I	61	2% 61% 21% 8% 10%
5	R	61	8% 70% 20% 10%

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	M	700	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MG	O	700	-	-	-	X
7	MG	X	700	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 70481 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	485	Total	C	N	O	S	0	0	0
			3691	2336	650	702	3			
1	B	486	Total	C	N	O	S	0	0	0
			3690	2336	648	703	3			
1	C	484	Total	C	N	O	S	0	0	0
			3680	2327	649	701	3			
1	J	482	Total	C	N	O	S	0	0	0
			3664	2316	647	698	3			
1	K	483	Total	C	N	O	S	0	0	0
			3578	2255	634	686	3			
1	L	479	Total	C	N	O	S	0	0	0
			3608	2282	637	686	3			
1	S	483	Total	C	N	O	S	0	0	0
			3642	2302	640	697	3			
1	T	484	Total	C	N	O	S	0	0	0
			3639	2296	642	698	3			
1	U	485	Total	C	N	O	S	0	0	0
			3511	2205	619	684	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
B	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
C	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
J	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
K	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
L	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
S	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
T	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
U	67	ILE	ASN	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	469	Total	C	N	O	S	0	0	0
			3511	2226	598	681	6			
2	F	469	Total	C	N	O	S	0	0	0
			3539	2245	603	685	6			
2	M	460	Total	C	N	O	S	0	0	0
			3436	2180	584	667	5			
2	N	463	Total	C	N	O	S	0	0	0
			3403	2160	573	665	5			
2	O	469	Total	C	N	O	S	0	0	0
			3449	2191	581	671	6			
2	V	360	Total	C	N	O	S	0	0	0
			2582	1625	439	515	3			
2	W	468	Total	C	N	O	S	0	0	0
			3468	2198	590	674	6			
2	X	469	Total	C	N	O	S	0	0	0
			3447	2181	588	673	5			

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	268	Total	C	N	O	S	0	0	0
			2064	1297	358	399	10			
3	P	268	Total	C	N	O	S	0	0	0
			1869	1163	320	380	6			
3	Y	115	Total	C	N	O	S	0	0	0
			790	482	141	163	4			

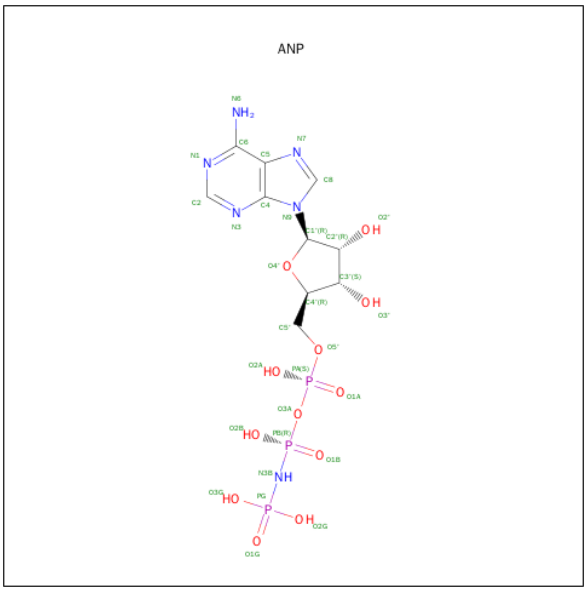
- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	122	Total	C	N	O	S	0	0	0
			815	513	139	161	2			
4	Q	101	Total	C	N	O	S	0	0	0
			625	389	110	125	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	55	Total	C	N	O	0	0	0
			388	242	68	78			
5	R	55	Total	C	N	O	0	0	0
			367	227	66	74			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

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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).

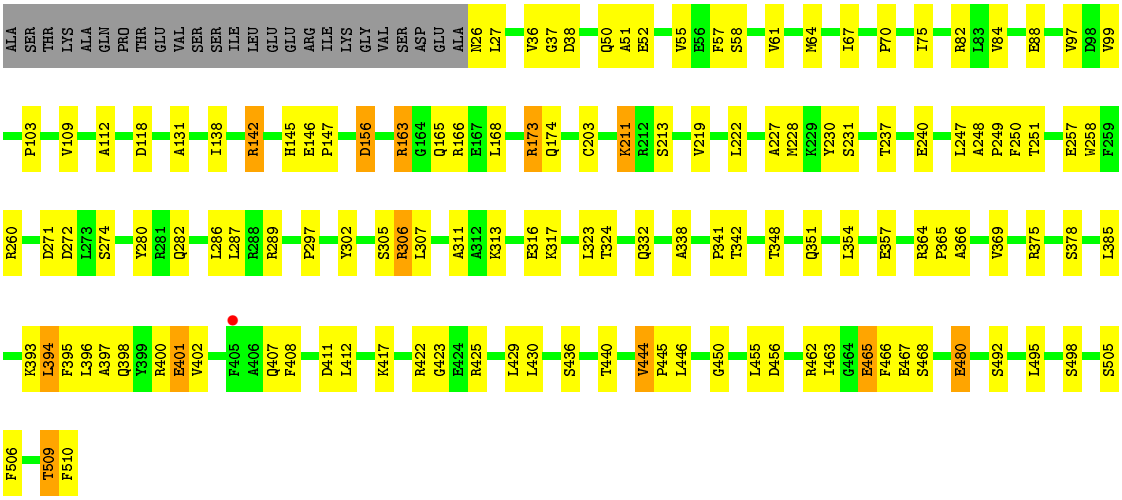
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	K	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	V	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		
7	T	1	Total	Mg	0	0
			1	1		
7	U	1	Total	Mg	0	0
			1	1		
7	X	1	Total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

3 Residue-property plots (i)

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

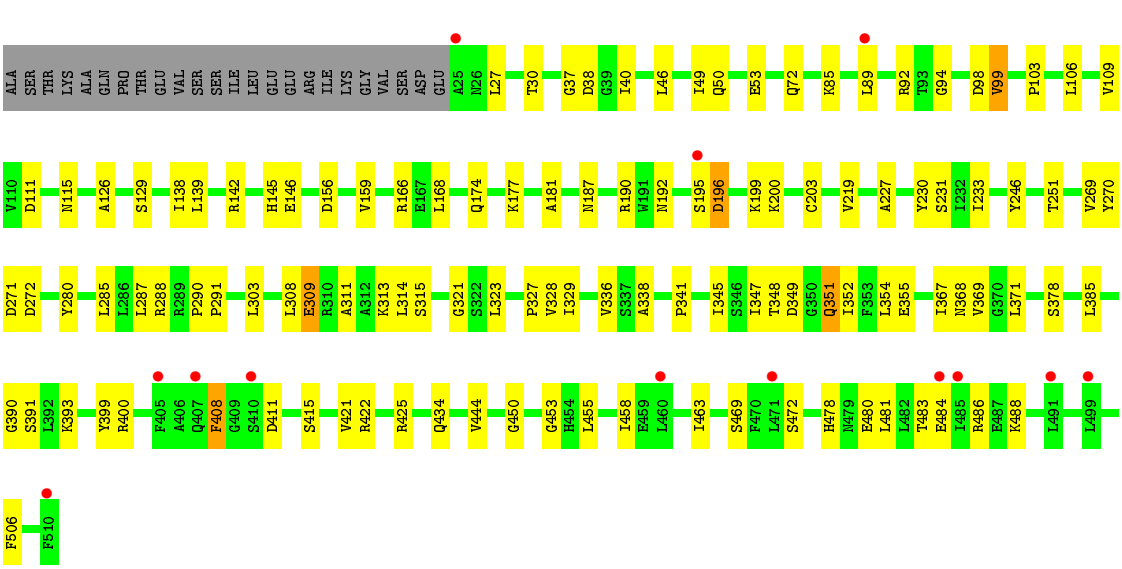
- Molecule 1: ATP synthase subunit alpha

Chain A:



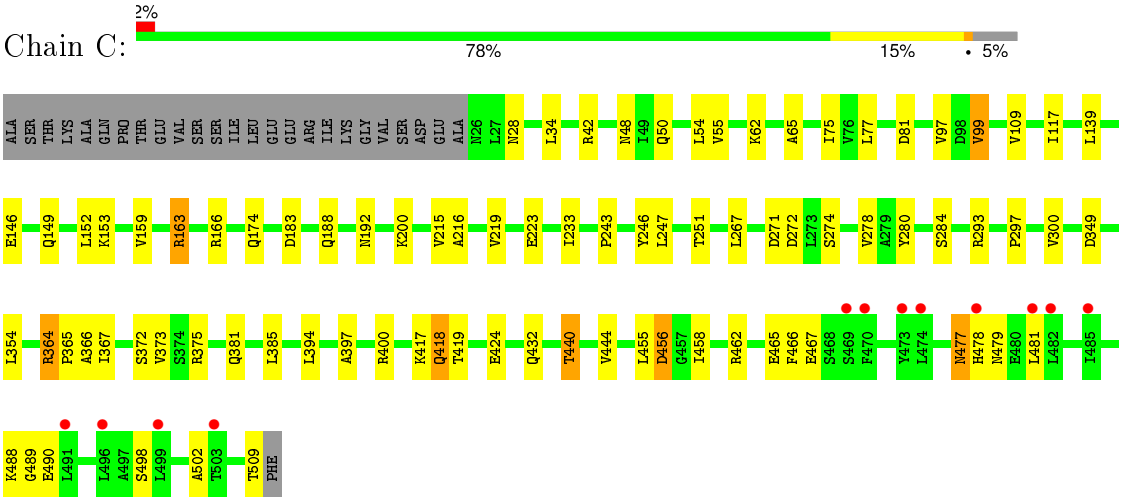
- Molecule 1: ATP synthase subunit alpha

Chain B:



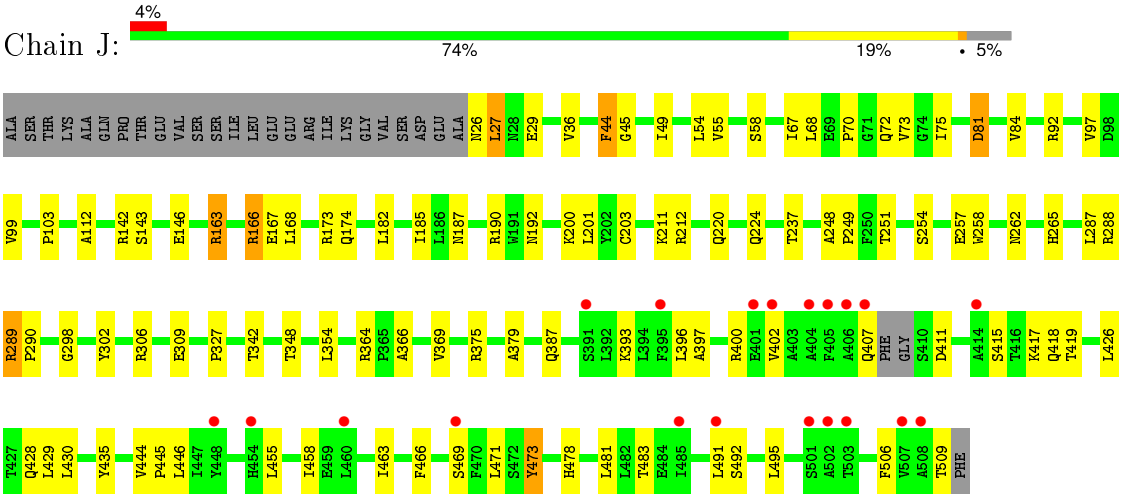
• Molecule 1: ATP synthase subunit alpha

Chain C:



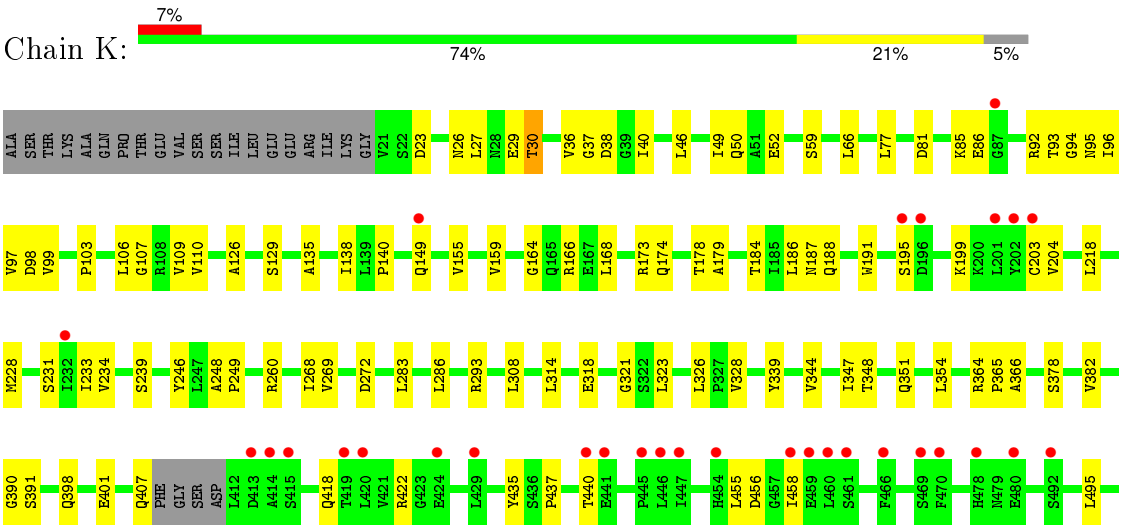
• Molecule 1: ATP synthase subunit alpha

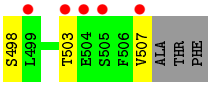
Chain J:



• Molecule 1: ATP synthase subunit alpha

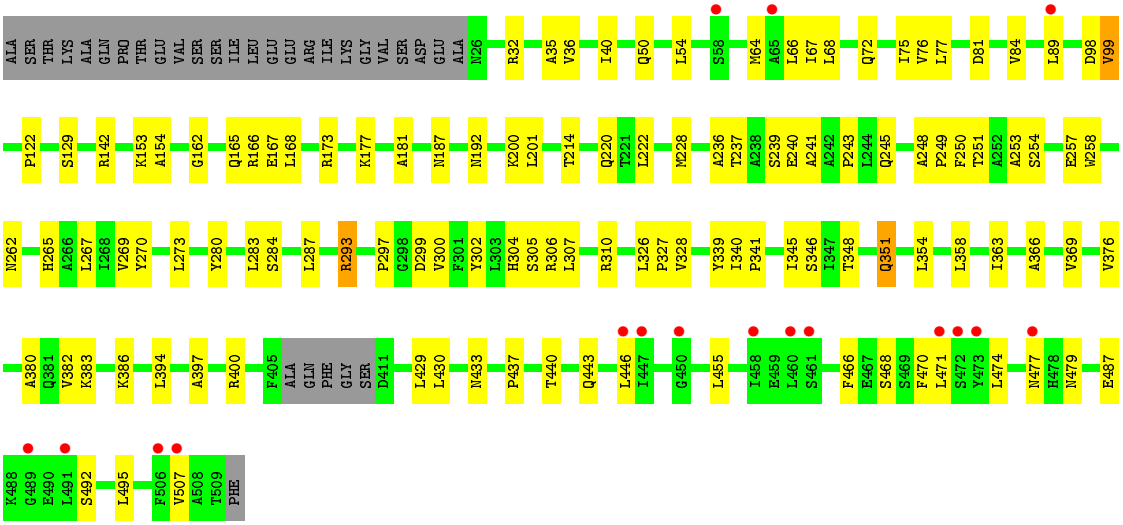
Chain K:





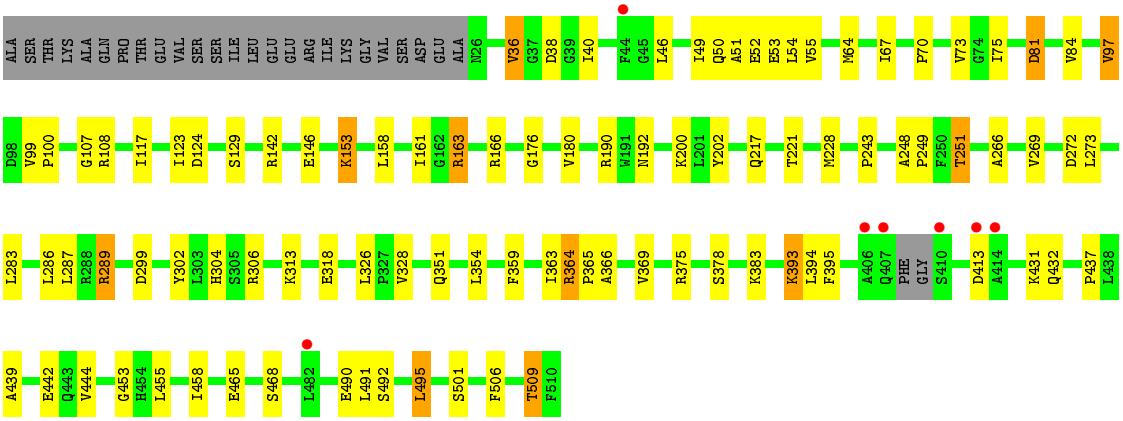
• Molecule 1: ATP synthase subunit alpha

Chain L:



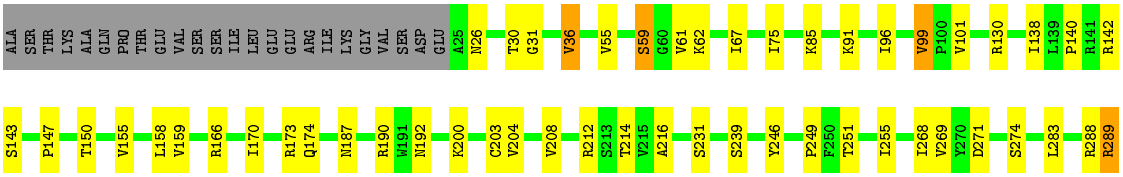
• Molecule 1: ATP synthase subunit alpha

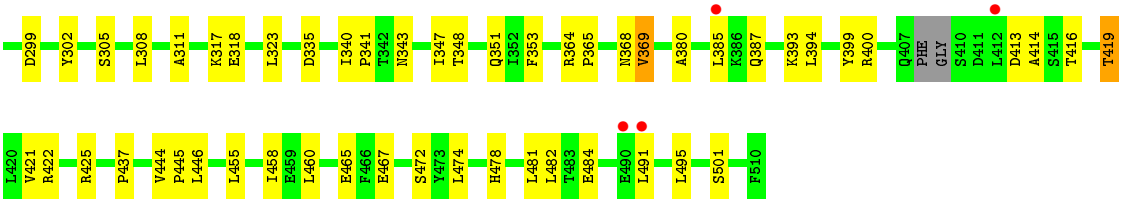
Chain S:

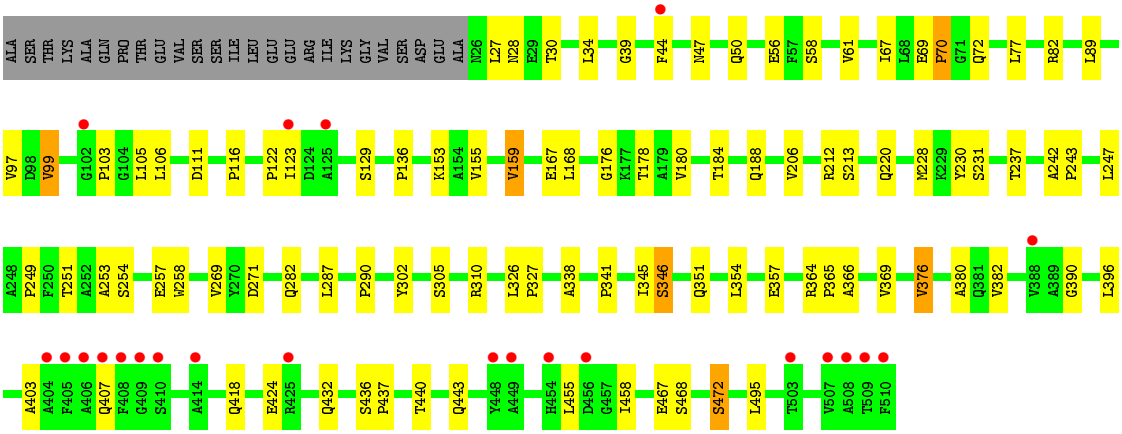


• Molecule 1: ATP synthase subunit alpha

Chain T:





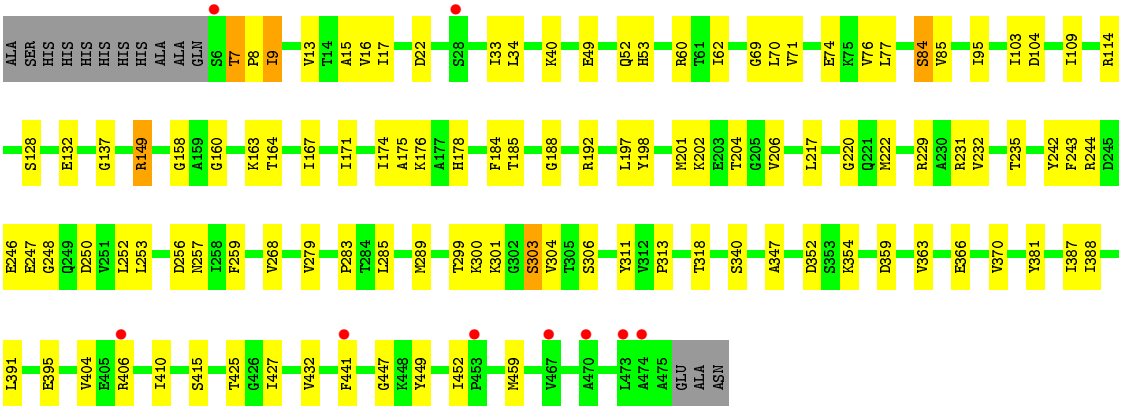


• Molecule 1: ATP synthase subunit alpha

Chain U:

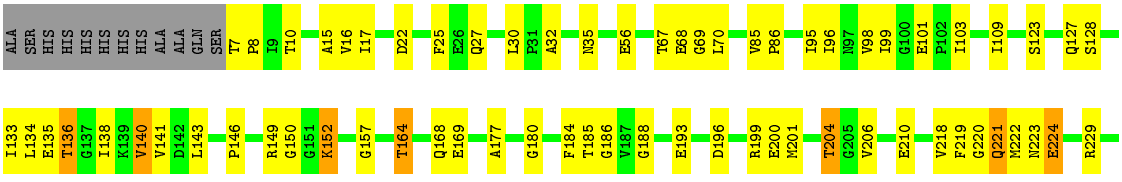
• Molecule 2: ATP synthase subunit beta

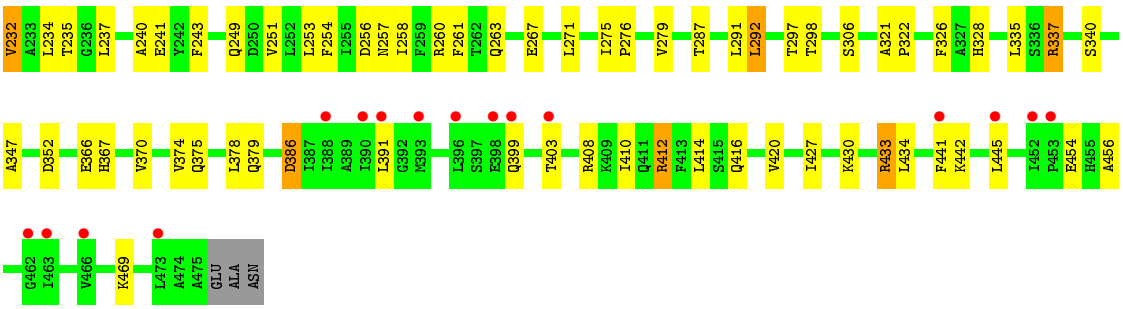
Chain D:



• Molecule 2: ATP synthase subunit beta

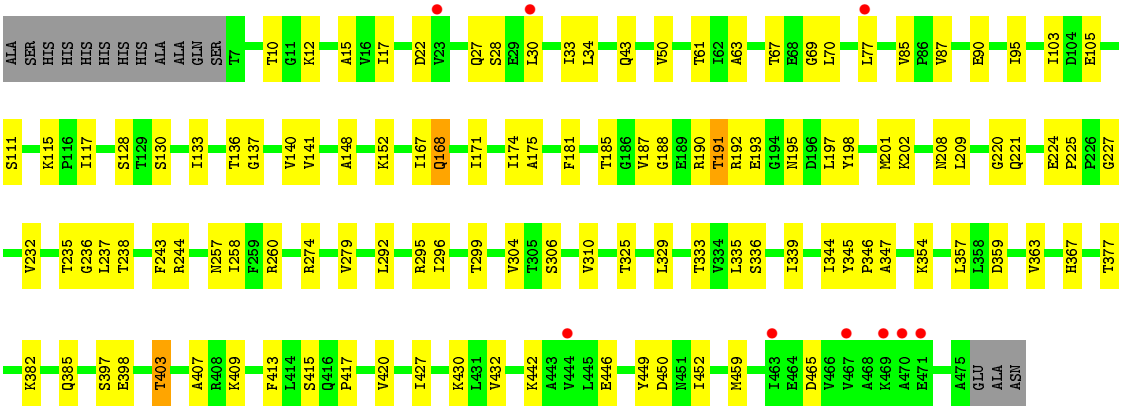
Chain E:





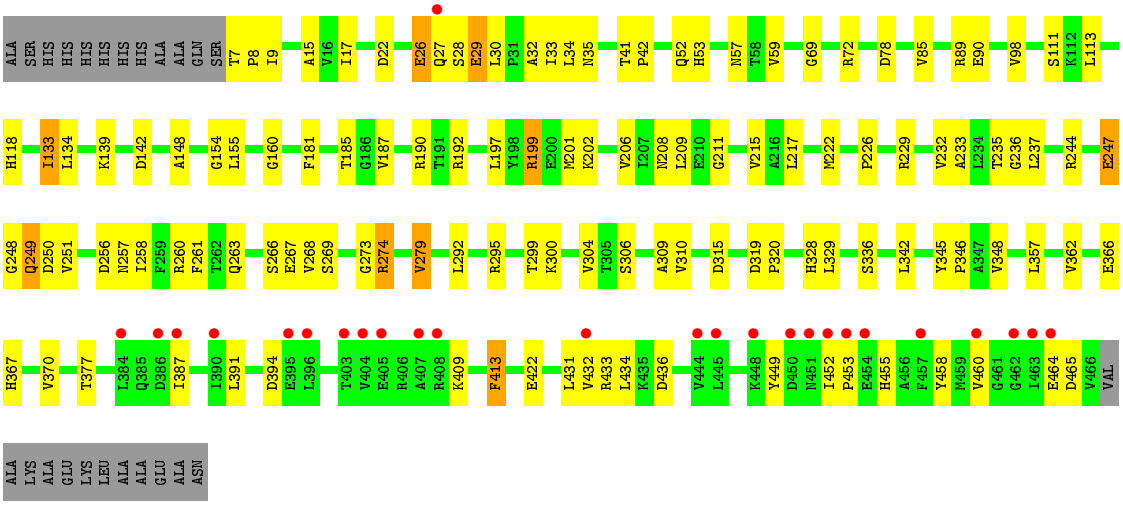
• Molecule 2: ATP synthase subunit beta

Chain F:



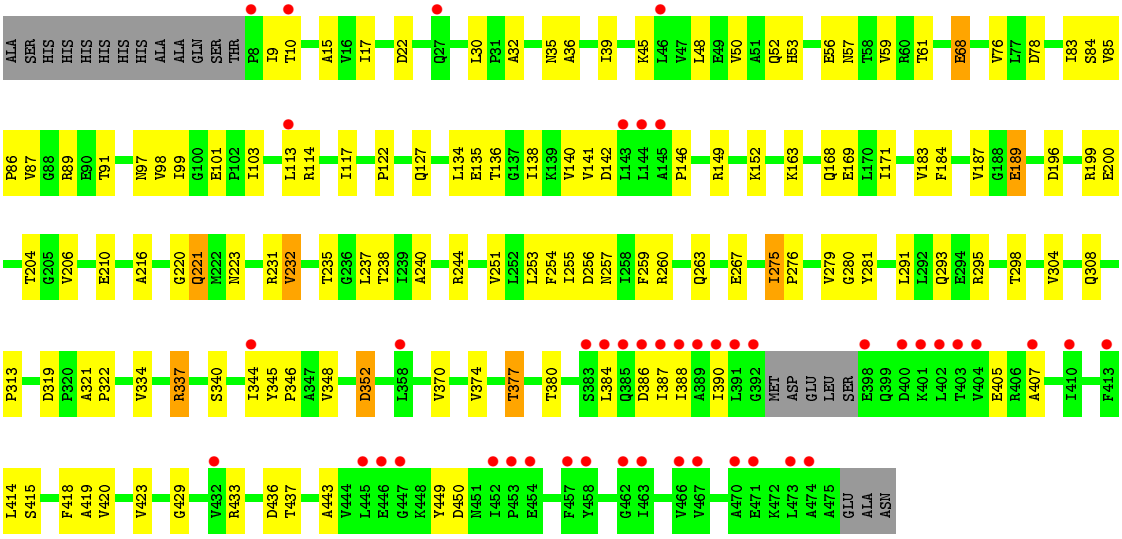
• Molecule 2: ATP synthase subunit beta

Chain M:



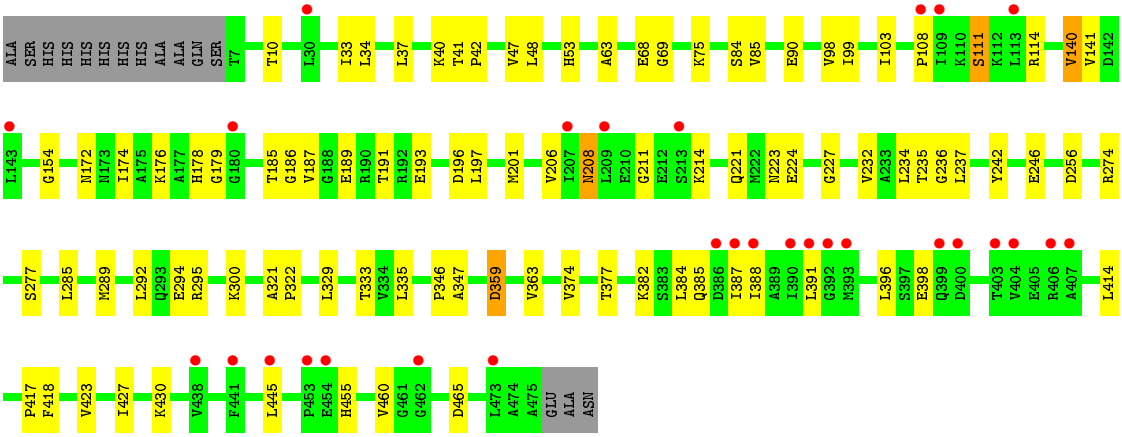
• Molecule 2: ATP synthase subunit beta

Chain N:



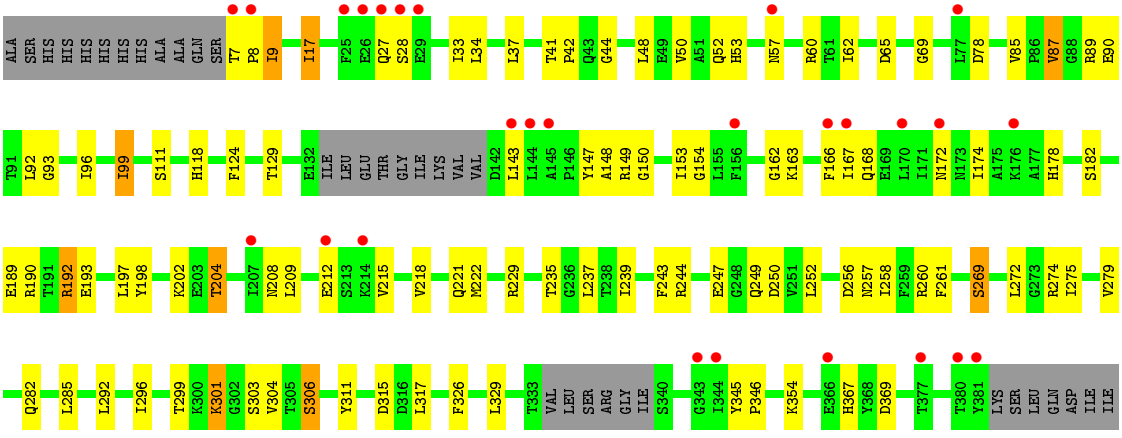
• Molecule 2: ATP synthase subunit beta

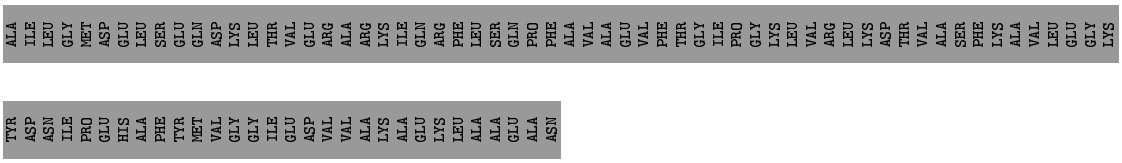
Chain O:



• Molecule 2: ATP synthase subunit beta

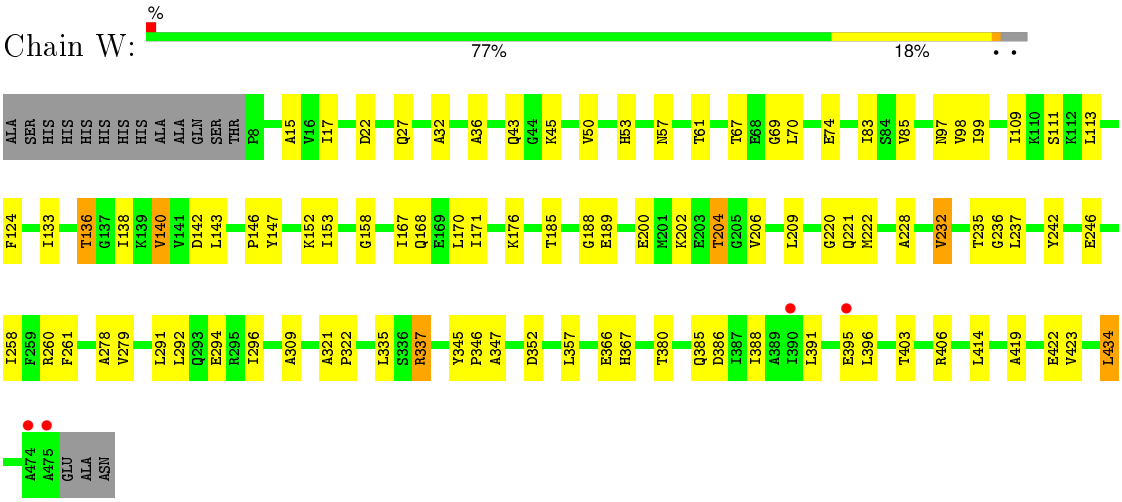
Chain V:





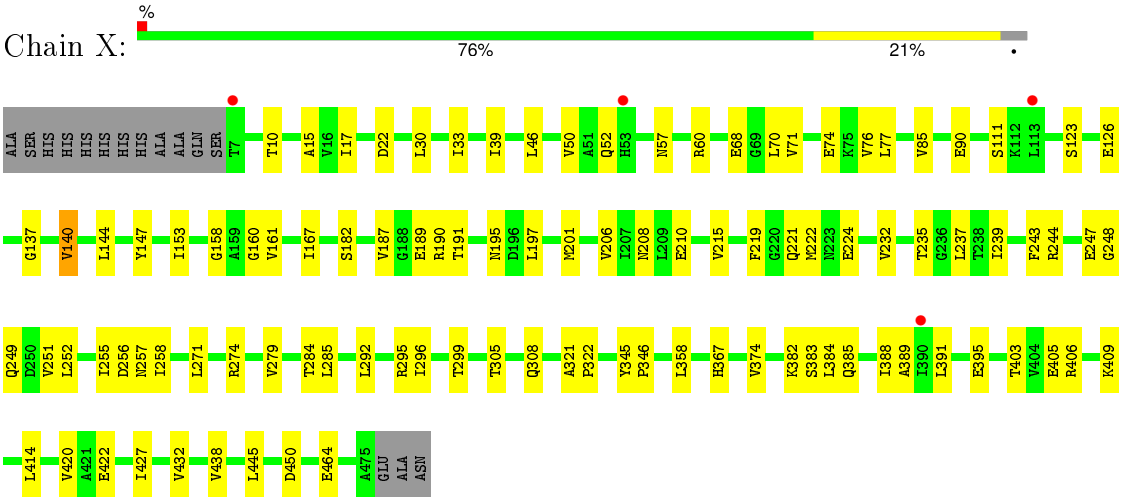
• Molecule 2: ATP synthase subunit beta

Chain W:



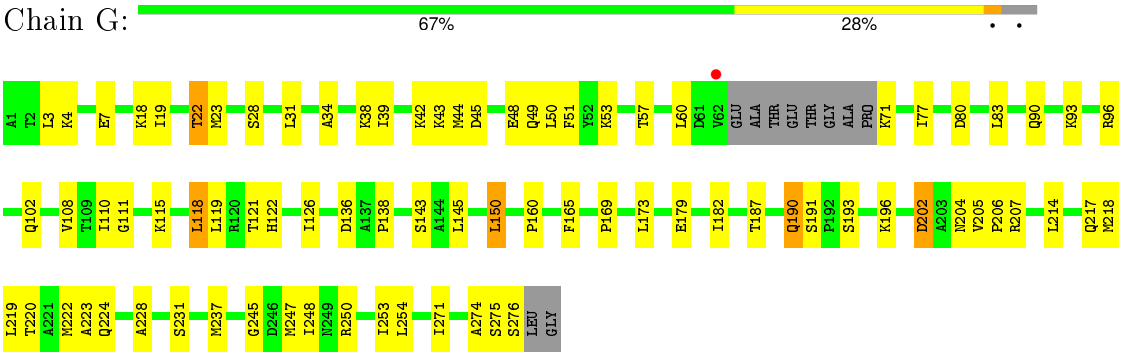
• Molecule 2: ATP synthase subunit beta

Chain X:



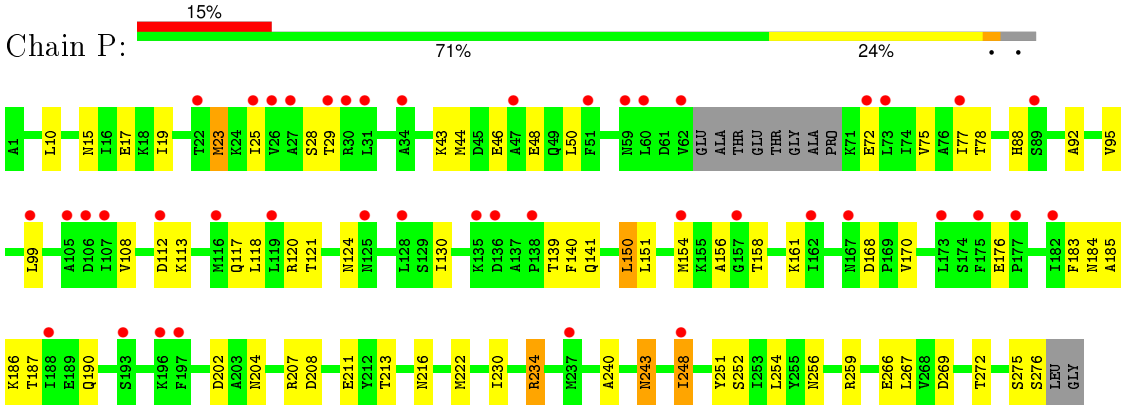
• Molecule 3: ATP synthase subunit gamma

Chain G:



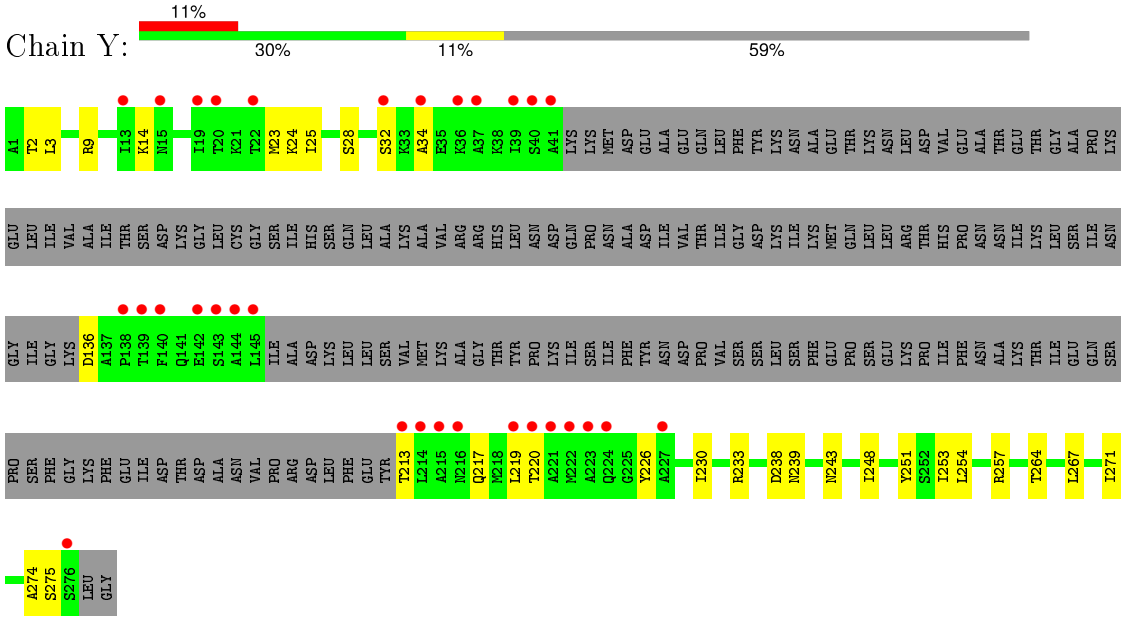
• Molecule 3: ATP synthase subunit gamma

Chain P:



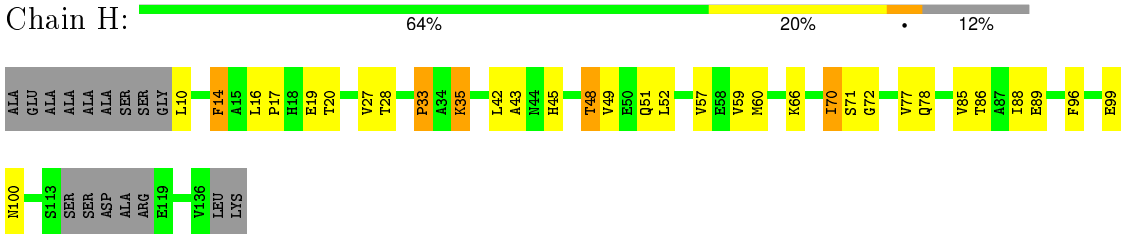
• Molecule 3: ATP synthase subunit gamma

Chain Y:



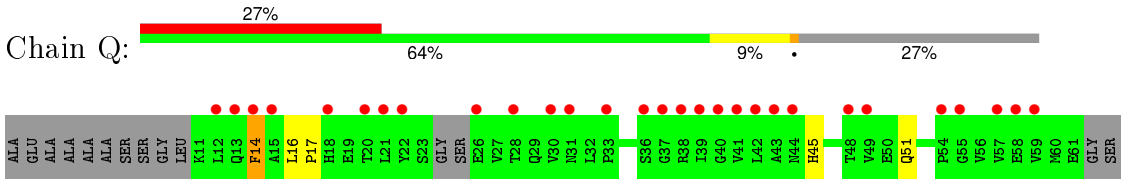
• Molecule 4: ATP synthase subunit delta

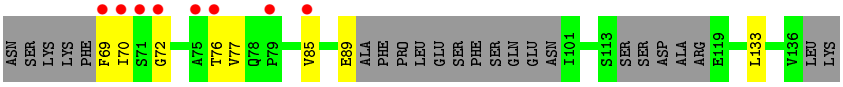
Chain H:



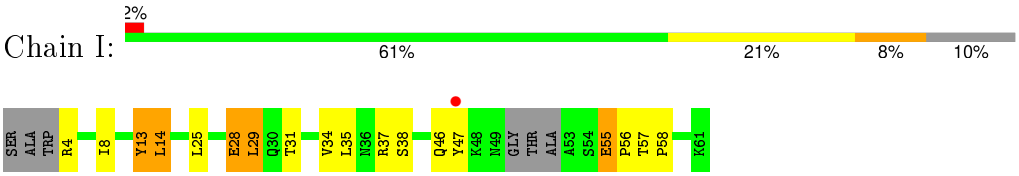
• Molecule 4: ATP synthase subunit delta

Chain Q:

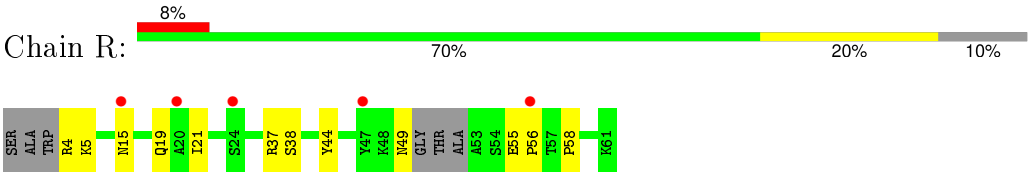




• Molecule 5: ATP synthase subunit epsilon



• Molecule 5: ATP synthase subunit epsilon



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	112.02Å 290.62Å 188.47Å 90.00° 102.34° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 49.63 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.00-3.20) 91.2 (49.63-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.210 , 0.276 0.211 , 0.274	Depositor DCC
R_{free} test set	3554 reflections (2.05%)	DCC
Wilson B-factor (Å^2)	90.9	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	2 of 176635 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	70481	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.43	0/3748	0.60	0/5073
1	B	0.40	0/3747	0.57	0/5073
1	C	0.41	0/3736	0.57	0/5057
1	J	0.39	0/3718	0.56	0/5032
1	K	0.37	0/3630	0.53	0/4926
1	L	0.40	0/3662	0.57	0/4963
1	S	0.41	0/3696	0.57	0/5008
1	T	0.39	0/3693	0.57	0/5006
1	U	0.37	0/3564	0.53	0/4850
2	D	0.41	0/3601	0.57	0/4884
2	E	0.43	0/3567	0.57	0/4846
2	F	0.40	0/3595	0.59	0/4876
2	M	0.42	0/3492	0.57	0/4747
2	N	0.38	0/3457	0.56	0/4708
2	O	0.38	0/3505	0.56	0/4774
2	V	0.42	0/2623	0.56	0/3585
2	W	0.43	0/3524	0.59	0/4796
2	X	0.39	0/3503	0.56	0/4774
3	G	0.39	0/2089	0.58	0/2812
3	P	0.36	0/1892	0.50	0/2586
3	Y	0.39	0/791	0.54	0/1077
4	H	0.45	0/827	0.63	0/1133
4	Q	0.40	0/629	0.50	0/866
5	I	0.48	0/393	0.69	0/537
5	R	0.45	0/372	0.51	0/510
All	All	0.40	0/71054	0.57	0/96499

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3691	0	3777	84	0
1	B	3690	0	3771	66	0
1	C	3680	0	3768	47	0
1	J	3664	0	3752	68	0
1	K	3578	0	3577	59	0
1	L	3608	0	3668	66	0
1	S	3642	0	3697	58	0
1	T	3639	0	3673	63	0
1	U	3511	0	3411	49	0
2	D	3545	0	3614	64	0
2	E	3511	0	3549	80	0
2	F	3539	0	3611	68	0
2	M	3436	0	3459	78	0
2	N	3403	0	3385	77	0
2	O	3449	0	3435	52	0
2	V	2582	0	2492	67	0
2	W	3468	0	3463	59	0
2	X	3447	0	3402	61	0
3	G	2064	0	2125	46	0
3	P	1869	0	1710	36	0
3	Y	790	0	735	17	0
4	H	815	0	712	26	0
4	Q	625	0	501	6	0
5	I	388	0	344	18	0
5	R	367	0	301	8	0
6	A	31	0	13	0	0
6	B	31	0	13	2	0
6	C	31	0	13	3	0
6	D	31	0	13	2	0
6	F	31	0	13	3	0
6	J	31	0	13	3	0
6	K	31	0	13	1	0
6	L	31	0	13	0	0
6	M	31	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	31	0	13	0	0
6	S	31	0	13	0	0
6	T	31	0	13	2	0
6	U	31	0	13	0	0
6	V	31	0	13	2	0
6	X	31	0	13	2	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
All	All	70481	0	70127	1222	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 9.

All (1222) 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)
6:F:600:ANP:H8	6:F:600:ANP:H5'1	1.26	1.16
3:G:96:ARG:HE	3:G:121:THR:HG21	1.25	1.01
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.42	1.00
5:I:31:THR:HG22	5:I:34:VAL:HG23	1.45	0.98
1:T:289:ARG:HH11	1:T:289:ARG:HG2	1.23	0.98
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.46	0.96
2:V:85:VAL:HG11	2:V:235:THR:HG23	1.47	0.95
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.48	0.95
4:H:72:GLY:HA3	5:I:14:LEU:HD21	1.47	0.95
1:A:397:ALA:HA	1:A:400:ARG:NE	1.81	0.94
2:F:192:ARG:HG2	2:F:192:ARG:HH11	1.31	0.92
2:M:160:GLY:H	6:M:600:ANP:HNB1	1.11	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:168:GLN:NE2	2:W:204:THR:HG21	1.84	0.92
2:W:168:GLN:HE21	2:W:204:THR:HG21	1.34	0.89
2:N:68:GLU:HG2	2:N:68:GLU:O	1.69	0.89
5:I:46:GLN:HB3	5:I:56:PRO:HG2	1.55	0.89
1:A:112:ALA:O	1:A:251:THR:HG21	1.71	0.88
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.56	0.88
1:A:397:ALA:HA	1:A:400:ARG:CZ	2.04	0.87
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.54	0.87
4:H:35:LYS:HD2	4:H:51:GLN:HG3	1.55	0.86
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.57	0.86
2:D:160:GLY:H	6:D:600:ANP:HNB1	1.22	0.86
1:A:142:ARG:HA	2:E:199:ARG:HH12	1.40	0.85
2:X:197:LEU:O	2:X:201:MET:HG2	1.77	0.85
4:H:14:PHE:HZ	4:H:70:ILE:HD11	1.41	0.84
1:S:369:VAL:HG13	1:S:393:LYS:HD3	1.60	0.84
1:J:289:ARG:HD3	1:J:290:PRO:HD2	1.59	0.83
2:F:50:VAL:HA	2:F:61:THR:HG22	1.62	0.82
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.60	0.82
2:D:244:ARG:HD3	2:D:304:VAL:HG23	1.60	0.81
1:A:146:GLU:HB2	1:A:163:ARG:HG3	1.63	0.81
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.62	0.80
2:D:149:ARG:NH2	2:D:178:HIS:NE2	2.30	0.80
1:A:142:ARG:HG2	2:E:199:ARG:HH22	1.47	0.79
3:G:219:LEU:HD21	4:H:17:PRO:HB3	1.64	0.79
2:M:249:GLN:HE21	2:M:249:GLN:HA	1.48	0.79
1:U:212:ARG:HG3	1:U:237:THR:HG21	1.62	0.79
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.66	0.78
1:J:174:GLN:HA	6:J:600:ANP:HNB1	1.46	0.78
1:T:369:VAL:HG12	1:T:393:LYS:HD2	1.64	0.77
1:S:190:ARG:NH1	1:S:439:ALA:HB2	1.99	0.77
1:T:289:ARG:HG2	1:T:289:ARG:NH1	1.97	0.77
1:T:174:GLN:HA	6:T:600:ANP:HNB1	1.49	0.77
2:M:160:GLY:N	6:M:600:ANP:HNB1	1.81	0.77
1:K:495:LEU:HA	1:K:498:SER:HB3	1.66	0.76
1:A:351:GLN:HE22	1:A:375:ARG:HH12	1.31	0.76
3:P:72:GLU:HG3	3:P:161:LYS:HB3	1.66	0.76
2:M:449:TYR:HD1	2:M:452:ILE:HD12	1.50	0.76
1:A:282:GLN:HG3	2:D:283:PRO:O	1.86	0.76
2:D:299:THR:HG23	2:D:301:LYS:H	1.51	0.76
2:O:174:ILE:HG22	2:O:178:HIS:HB2	1.69	0.75
1:S:289:ARG:HA	1:S:289:ARG:HH11	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:221:GLN:HB2	2:E:223:ASN:OD1	1.87	0.74
1:J:44:PHE:HD2	1:J:45:GLY:N	1.85	0.74
1:C:97:VAL:HG11	1:C:247:LEU:HD21	1.70	0.74
5:I:55:GLU:CB	5:I:56:PRO:HD3	2.17	0.74
2:N:39:ILE:HD11	2:N:48:LEU:HD11	1.68	0.74
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.69	0.74
5:I:4:ARG:HG3	5:I:13:TYR:CE2	2.23	0.73
2:F:190:ARG:HB2	2:F:193:GLU:HG3	1.69	0.73
2:V:190:ARG:HB2	2:V:193:GLU:HG3	1.71	0.73
2:X:391:LEU:HB3	2:X:395:GLU:HG3	1.70	0.73
2:W:189:GLU:HA	2:W:260:ARG:HH21	1.54	0.73
1:B:455:LEU:HD23	1:B:458:ILE:HD12	1.71	0.72
5:I:28:GLU:O	5:I:29:LEU:HD13	1.88	0.72
1:A:394:LEU:O	1:A:397:ALA:HB3	1.90	0.72
2:D:7:THR:HG23	2:D:8:PRO:HD3	1.70	0.72
1:T:187:ASN:OD1	1:T:190:ARG:NH1	2.22	0.72
2:N:337:ARG:HA	2:N:340:SER:HB3	1.71	0.72
2:F:382:LYS:HA	2:F:385:GLN:HG2	1.72	0.72
3:P:230:ILE:O	3:P:234:ARG:HG2	1.89	0.72
5:I:31:THR:HG22	5:I:34:VAL:CG2	2.19	0.71
2:D:222:MET:HA	2:D:229:ARG:HD2	1.72	0.71
2:O:189:GLU:O	2:O:221:GLN:HB3	1.91	0.71
2:F:202:LYS:HE3	2:F:209:LEU:HD11	1.72	0.71
3:Y:25:ILE:HA	3:Y:28:SER:HB2	1.71	0.71
2:O:237:LEU:HD21	2:O:295:ARG:HB2	1.73	0.71
1:B:287:LEU:O	1:B:288:ARG:HB2	1.91	0.71
2:F:192:ARG:NH1	2:F:192:ARG:HG2	2.02	0.71
1:U:99:VAL:HG11	1:U:251:THR:HB	1.72	0.71
1:S:36:VAL:HG12	2:V:53:HIS:HB2	1.72	0.71
2:F:148:ALA:HA	2:F:357:LEU:HD11	1.71	0.70
2:V:154:GLY:HA3	2:V:329:LEU:HD13	1.72	0.70
1:B:174:GLN:HA	6:B:600:ANP:HNB1	1.56	0.70
1:L:397:ALA:HA	1:L:400:ARG:CZ	2.20	0.70
2:E:140:VAL:HG13	2:E:414:LEU:HD22	1.74	0.70
2:M:197:LEU:O	2:M:201:MET:HG2	1.91	0.70
1:B:85:LYS:HE2	2:E:32:ALA:HB2	1.73	0.69
2:F:221:GLN:OE1	2:F:221:GLN:HA	1.92	0.69
3:G:57:THR:HA	3:G:191:SER:HB3	1.72	0.69
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.75	0.69
2:W:242:TYR:CZ	2:W:246:GLU:HG2	2.27	0.69
3:P:118:LEU:HA	3:P:121:THR:HG22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:158:GLY:O	2:X:161:VAL:HG22	1.91	0.69
2:N:419:ALA:HA	2:N:429:GLY:HA3	1.75	0.69
1:L:305:SER:HB2	2:M:222:MET:HB2	1.75	0.69
1:K:187:ASN:HB2	1:K:437:PRO:HB3	1.75	0.68
5:I:46:GLN:HB3	5:I:56:PRO:CG	2.22	0.68
1:A:369:VAL:HB	1:A:400:ARG:NH1	2.09	0.68
1:L:239:SER:HB3	2:O:294:GLU:HG3	1.76	0.68
2:N:220:GLY:HA3	2:N:232:VAL:HG21	1.74	0.68
2:N:384:LEU:HD22	2:N:387:ILE:HD11	1.74	0.68
1:S:383:LYS:HD3	1:S:490:GLU:OE2	1.94	0.67
1:L:187:ASN:OD1	1:L:437:PRO:HB2	1.94	0.67
3:G:51:PHE:CE1	4:H:49:VAL:HG21	2.29	0.67
2:F:398:GLU:HA	2:F:398:GLU:OE1	1.94	0.67
1:A:397:ALA:O	1:A:400:ARG:HG3	1.95	0.67
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.76	0.67
2:N:244:ARG:HD3	2:N:304:VAL:HG23	1.77	0.66
2:V:9:ILE:HB	2:V:78:ASP:HB3	1.77	0.66
2:E:169:GLU:OE1	2:E:420:VAL:HG22	1.95	0.66
1:L:98:ASP:HB2	1:L:129:SER:O	1.95	0.66
2:M:249:GLN:HG3	2:M:250:ASP:H	1.61	0.66
2:N:189:GLU:OE2	2:N:221:GLN:HA	1.96	0.66
2:W:202:LYS:HD3	2:W:209:LEU:HD11	1.78	0.66
1:K:92:ARG:HH21	1:K:94:GLY:HA2	1.60	0.66
2:W:50:VAL:HA	2:W:61:THR:HG22	1.77	0.66
1:J:168:LEU:HD12	1:J:327:PRO:O	1.96	0.66
2:D:250:ASP:OD2	2:D:303:SER:HB2	1.96	0.65
3:G:45:ASP:OD1	3:G:220:THR:HG21	1.96	0.65
1:B:422:ARG:HH21	1:B:453:GLY:HA3	1.61	0.65
2:V:244:ARG:HD3	2:V:304:VAL:HG23	1.77	0.65
1:J:44:PHE:CD2	1:J:45:GLY:N	2.65	0.65
2:M:133:ILE:HG12	2:M:134:LEU:N	2.10	0.65
2:M:15:ALA:HB3	2:M:22:ASP:HB2	1.78	0.65
2:X:237:LEU:HD13	2:X:296:ILE:HG12	1.77	0.65
1:B:203:CYS:HB2	1:B:231:SER:HB3	1.78	0.65
2:O:398:GLU:HB2	3:P:120:ARG:HD3	1.79	0.65
2:F:115:LYS:HE3	2:F:238:THR:HG22	1.78	0.64
2:D:160:GLY:N	6:D:600:ANP:HNB1	1.91	0.64
3:P:141:GLN:HG3	5:R:15:ASN:HD21	1.62	0.64
2:D:9:ILE:H	2:D:9:ILE:HD12	1.61	0.64
2:O:41:THR:HB	2:O:42:PRO:HD2	1.79	0.64
1:U:69:GLU:HB3	1:U:70:PRO:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:204:THR:OG1	2:N:420:VAL:HB	1.97	0.64
2:N:53:HIS:HD2	2:N:59:VAL:HG12	1.62	0.64
5:I:46:GLN:O	5:I:56:PRO:HD2	1.97	0.64
2:X:30:LEU:HD21	2:X:57:ASN:HA	1.78	0.64
2:V:174:ILE:O	2:V:178:HIS:HB2	1.98	0.63
1:T:416:THR:HA	1:T:419:THR:HG23	1.80	0.63
1:T:239:SER:HB2	2:W:291:LEU:HD23	1.80	0.63
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.78	0.63
1:L:369:VAL:HB	1:L:400:ARG:HH12	1.63	0.63
3:Y:9:ARG:HD3	3:Y:251:TYR:CE1	2.32	0.63
2:W:142:ASP:HB3	2:W:434:LEU:HD12	1.79	0.63
1:S:243:PRO:HG3	1:S:283:LEU:HD21	1.80	0.63
1:A:168:LEU:HB2	1:A:348:THR:HG21	1.79	0.63
1:B:142:ARG:HB2	1:B:315:SER:HA	1.80	0.63
1:K:166:ARG:HD3	1:K:308:LEU:O	1.99	0.63
1:K:248:ALA:HB3	1:K:249:PRO:HD3	1.81	0.63
2:E:221:GLN:H	2:E:221:GLN:HE21	1.47	0.63
1:T:174:GLN:HA	6:T:600:ANP:N3B	2.14	0.62
1:K:455:LEU:HA	1:K:458:ILE:HD12	1.79	0.62
1:B:369:VAL:H	1:B:400:ARG:HH12	1.47	0.62
1:B:338:ALA:HB3	1:B:341:PRO:HG2	1.81	0.62
2:M:237:LEU:HD21	2:M:295:ARG:HB2	1.81	0.62
1:A:109:VAL:HB	1:A:118:ASP:HB3	1.81	0.62
2:O:47:VAL:HG21	2:O:99:ILE:HG21	1.81	0.62
2:E:152:LYS:HD3	2:E:328:HIS:O	1.99	0.62
2:F:377:THR:HG23	2:F:403:THR:HG22	1.81	0.62
2:E:98:VAL:HG23	2:E:232:VAL:HA	1.80	0.62
2:W:258:ILE:HG22	2:W:309:ALA:O	2.00	0.62
1:J:393:LYS:O	1:J:397:ALA:HB2	1.99	0.62
1:J:248:ALA:HB3	1:J:249:PRO:HD3	1.80	0.62
2:V:243:PHE:HB3	2:V:249:GLN:HE21	1.64	0.62
2:W:158:GLY:H	2:W:337:ARG:HH12	1.47	0.62
4:H:16:LEU:HD12	4:H:19:GLU:HB3	1.82	0.62
2:M:201:MET:HE3	2:M:217:LEU:HD21	1.82	0.61
3:P:130:ILE:HD13	5:R:44:TYR:HB3	1.81	0.61
1:A:174:GLN:HB3	2:D:354:LYS:HD2	1.82	0.61
2:O:387:ILE:HG23	2:O:391:LEU:HD12	1.80	0.61
2:N:390:ILE:HG21	3:P:28:SER:HB3	1.82	0.61
6:F:600:ANP:C5'	6:F:600:ANP:H8	2.18	0.61
2:X:160:GLY:H	6:X:600:ANP:HNB1	1.47	0.61
2:M:7:THR:N	2:M:8:PRO:HD3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:367:HIS:CD2	2:M:434:LEU:HD21	2.35	0.61
1:U:153:LYS:HG2	1:U:432:GLN:OE1	2.00	0.61
1:U:67:ILE:HD12	1:U:287:LEU:HD22	1.81	0.61
2:N:344:ILE:HG23	2:N:415:SER:HB3	1.81	0.61
2:M:346:PRO:HB2	2:M:348:VAL:HG23	1.83	0.61
1:L:369:VAL:HB	1:L:400:ARG:NH1	2.15	0.61
2:X:382:LYS:HA	2:X:385:GLN:HG2	1.82	0.61
2:N:135:GLU:OE2	2:N:433:ARG:HD3	2.01	0.61
3:Y:136:ASP:HB3	3:Y:226:TYR:HE1	1.65	0.61
2:D:128:SER:HB2	2:D:300:LYS:HG2	1.83	0.61
2:N:255:ILE:HB	2:N:308:GLN:HG2	1.82	0.61
2:E:185:THR:HA	2:E:218:VAL:O	2.01	0.61
3:P:184:ASN:HD21	3:P:186:LYS:HD3	1.65	0.60
1:J:469:SER:O	1:J:473:TYR:HB3	2.02	0.60
2:F:141:VAL:HG22	2:F:333:THR:HG21	1.82	0.60
2:M:229:ARG:NH2	2:M:267:GLU:OE1	2.28	0.60
2:E:337:ARG:HA	2:E:340:SER:HB3	1.83	0.60
2:X:147:TYR:CE1	2:X:153:ILE:HG21	2.36	0.60
1:B:174:GLN:HA	6:B:600:ANP:N3B	2.16	0.60
1:T:364:ARG:HA	1:T:365:PRO:C	2.22	0.60
2:O:382:LYS:HA	2:O:385:GLN:HG2	1.82	0.60
2:E:168:GLN:NE2	2:E:201:MET:HA	2.16	0.60
4:H:52:LEU:HD11	4:H:85:VAL:HG13	1.82	0.60
2:V:243:PHE:HA	2:V:247:GLU:HG3	1.84	0.60
2:X:244:ARG:O	2:X:248:GLY:HA2	2.01	0.60
1:U:455:LEU:HA	1:U:458:ILE:HD12	1.82	0.60
1:U:345:ILE:HG12	1:U:351:GLN:HG2	1.83	0.60
1:A:145:HIS:CD2	1:A:146:GLU:HG3	2.37	0.59
2:W:136:THR:HG23	2:W:138:ILE:H	1.67	0.59
3:G:60:LEU:HD23	3:G:187:THR:HA	1.84	0.59
1:S:40:ILE:HD12	1:S:287:LEU:HG	1.83	0.59
2:V:143:LEU:HA	2:V:367:HIS:CE1	2.37	0.59
2:O:242:TYR:CE1	2:O:246:GLU:HG3	2.37	0.59
2:N:98:VAL:HG13	2:N:99:ILE:HG23	1.84	0.59
1:U:67:ILE:HG12	2:V:17:ILE:HG23	1.83	0.59
2:N:86:PRO:HD3	2:N:114:ARG:NH1	2.18	0.59
2:E:204:THR:CG2	2:E:206:VAL:HG22	2.32	0.59
1:B:483:THR:HG23	1:B:486:ARG:HH12	1.66	0.59
1:A:26:ASN:O	1:A:27:LEU:HB2	2.02	0.59
1:U:354:LEU:HA	1:U:366:ALA:O	2.02	0.59
1:J:44:PHE:HD2	1:J:45:GLY:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:26:ASN:O	1:J:27:LEU:HB2	2.02	0.59
1:U:376:VAL:HG11	1:U:380:ALA:HB3	1.84	0.59
6:F:600:ANP:C8	6:F:600:ANP:H5'1	2.17	0.59
2:N:334:VAL:HG21	2:N:352:ASP:HB3	1.85	0.59
5:I:55:GLU:CB	5:I:56:PRO:CD	2.80	0.59
1:S:54:LEU:HD12	1:S:64:MET:HB3	1.85	0.59
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.36	0.59
1:L:382:VAL:HG11	1:L:440:THR:HG21	1.85	0.58
2:X:384:LEU:O	2:X:388:ILE:HG12	2.02	0.58
1:A:425:ARG:HD3	1:A:456:ASP:HA	1.84	0.58
4:H:27:VAL:CG1	4:H:59:VAL:HG13	2.33	0.58
1:T:478:HIS:HB3	1:T:481:LEU:HG	1.84	0.58
2:F:336:SER:HB3	2:F:339:ILE:HD12	1.83	0.58
1:C:55:VAL:HG21	1:C:75:ILE:HD13	1.86	0.58
2:F:152:LYS:HD2	2:F:296:ILE:O	2.02	0.58
1:B:92:ARG:HH21	1:B:94:GLY:HA2	1.67	0.58
2:X:140:VAL:HG13	2:X:414:LEU:HD22	1.84	0.58
2:V:269:SER:OG	2:V:282:GLN:HB3	2.03	0.58
2:V:299:THR:HG23	2:V:301:LYS:H	1.67	0.58
1:C:50:GLN:HB3	2:D:69:GLY:HA2	1.86	0.58
1:T:455:LEU:HA	1:T:458:ILE:HD12	1.86	0.58
2:V:172:ASN:OD1	2:V:204:THR:HG21	2.03	0.58
1:C:354:LEU:HA	1:C:366:ALA:O	2.04	0.58
2:E:86:PRO:HG2	2:E:109:ILE:HD13	1.85	0.58
2:X:221:GLN:HA	2:X:221:GLN:OE1	2.04	0.58
1:B:159:VAL:HG21	1:B:352:ILE:HG12	1.86	0.58
1:C:146:GLU:HB2	1:C:163:ARG:HD2	1.86	0.58
2:F:171:ILE:O	2:F:175:ALA:HB3	2.02	0.58
1:U:382:VAL:HG11	1:U:440:THR:HG21	1.86	0.58
1:C:174:GLN:HA	6:C:600:ANP:HNB1	1.68	0.58
1:S:192:ASN:HA	1:S:200:LYS:HG2	1.86	0.58
1:T:96:ILE:HG13	1:T:130:ARG:NH2	2.18	0.58
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.85	0.58
2:N:50:VAL:HA	2:N:61:THR:HG22	1.85	0.58
2:M:201:MET:CE	2:M:217:LEU:HD21	2.34	0.58
1:B:46:LEU:O	1:B:49:ILE:HG22	2.03	0.58
2:V:202:LYS:NZ	2:V:209:LEU:HD21	2.19	0.58
1:C:99:VAL:HG11	1:C:251:THR:HB	1.85	0.58
2:W:98:VAL:HG13	2:W:99:ILE:HG23	1.86	0.58
1:K:85:LYS:HG2	2:N:53:HIS:HE1	1.68	0.57
1:L:429:LEU:HD21	1:L:446:LEU:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:ILE:HG22	2:D:103:ILE:HG13	1.86	0.57
1:A:396:LEU:O	1:A:400:ARG:HG3	2.04	0.57
2:N:39:ILE:HG12	2:N:76:VAL:HG22	1.86	0.57
2:E:168:GLN:HE21	2:E:201:MET:HA	1.68	0.57
1:L:284:SER:OG	1:L:297:PRO:HG3	2.04	0.57
1:B:272:ASP:HB2	1:B:328:VAL:O	2.04	0.57
2:W:419:ALA:O	2:W:422:GLU:HB2	2.04	0.57
2:W:188:GLY:C	2:W:260:ARG:HE	2.07	0.57
2:N:168:GLN:HA	2:N:171:ILE:HD12	1.86	0.57
1:L:345:ILE:HG23	1:L:351:GLN:HG2	1.85	0.57
2:O:208:ASN:ND2	2:O:211:GLY:H	2.03	0.57
1:A:222:LEU:HD12	1:A:228:MET:HE2	1.85	0.57
1:J:81:ASP:HB2	2:M:33:ILE:HD12	1.87	0.57
2:O:197:LEU:O	2:O:201:MET:HG2	2.04	0.57
1:L:358:LEU:HB2	1:L:366:ALA:HB1	1.85	0.57
1:J:492:SER:HB2	1:J:495:LEU:H	1.69	0.57
1:A:369:VAL:CG1	1:A:393:LYS:HG3	2.35	0.57
4:H:14:PHE:CZ	4:H:70:ILE:HD11	2.32	0.57
2:M:367:HIS:HD2	2:M:434:LEU:HD21	1.68	0.57
4:H:27:VAL:HG11	4:H:59:VAL:HG13	1.86	0.57
1:A:305:SER:HB2	2:E:222:MET:HG2	1.86	0.57
1:A:369:VAL:HG12	1:A:393:LYS:HG3	1.86	0.56
1:A:302:TYR:O	1:A:306:ARG:HB2	2.04	0.56
3:G:96:ARG:HG2	3:G:122:HIS:HE1	1.70	0.56
2:D:204:THR:HB	2:D:206:VAL:HG23	1.88	0.56
1:A:50:GLN:HB3	2:E:69:GLY:HA2	1.87	0.56
1:S:38:ASP:HB3	1:S:286:LEU:HD22	1.86	0.56
2:D:366:GLU:O	2:D:370:VAL:HG23	2.05	0.56
3:G:44:MET:CE	4:H:86:THR:HB	2.36	0.56
2:M:90:GLU:HG3	2:M:111:SER:HA	1.88	0.56
1:L:302:TYR:O	1:L:306:ARG:HG2	2.06	0.56
2:V:243:PHE:HA	2:V:247:GLU:CG	2.35	0.56
2:N:15:ALA:HB3	2:N:22:ASP:HB2	1.87	0.56
1:U:364:ARG:HA	1:U:365:PRO:C	2.25	0.56
2:D:201:MET:CE	2:D:217:LEU:HD21	2.34	0.56
3:G:50:LEU:HG	4:H:78:GLN:NE2	2.20	0.56
2:V:258:ILE:O	2:V:261:PHE:HB3	2.05	0.56
2:O:234:LEU:HD23	2:O:292:LEU:HD13	1.86	0.56
2:M:142:ASP:HB3	2:M:434:LEU:HD12	1.87	0.56
1:L:273:LEU:HB3	1:L:304:HIS:NE2	2.21	0.56
2:M:148:ALA:HA	2:M:357:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:34:ALA:O	3:G:38:LYS:HB2	2.06	0.56
1:S:51:ALA:HB3	2:W:69:GLY:H	1.70	0.56
1:K:138:ILE:HD13	2:O:103:ILE:HD12	1.88	0.56
2:V:154:GLY:HA3	2:V:329:LEU:CD1	2.36	0.56
1:T:99:VAL:HG11	1:T:251:THR:HB	1.87	0.56
2:M:258:ILE:HG22	2:M:310:VAL:HG22	1.88	0.55
1:L:192:ASN:HA	1:L:200:LYS:HG2	1.87	0.55
2:E:95:ILE:HG22	2:E:103:ILE:HG13	1.88	0.55
1:S:36:VAL:HG13	2:V:33:ILE:HD11	1.88	0.55
2:V:143:LEU:HA	2:V:367:HIS:HE1	1.70	0.55
1:L:297:PRO:HB2	1:L:299:ASP:OD1	2.07	0.55
1:U:105:LEU:HG	1:U:123:ILE:HG21	1.87	0.55
2:W:133:ILE:HD12	2:W:146:PRO:HB2	1.89	0.55
2:O:41:THR:HB	2:O:42:PRO:CD	2.37	0.55
1:T:85:LYS:HE2	2:W:32:ALA:HB2	1.88	0.55
3:P:272:THR:O	3:P:275:SER:HB2	2.06	0.55
1:J:302:TYR:O	1:J:306:ARG:HB2	2.06	0.55
1:K:85:LYS:HE2	2:N:32:ALA:HB2	1.89	0.55
2:D:415:SER:HB2	2:D:459:MET:H	1.71	0.55
2:E:164:THR:HB	2:E:200:GLU:OE1	2.06	0.55
2:N:337:ARG:HE	2:N:337:ARG:H	1.54	0.55
1:L:397:ALA:HA	1:L:400:ARG:NH2	2.21	0.55
1:U:69:GLU:HB3	1:U:70:PRO:CD	2.37	0.55
1:J:81:ASP:N	1:J:81:ASP:OD1	2.36	0.55
1:A:97:VAL:HG11	1:A:247:LEU:HD13	1.89	0.55
2:M:366:GLU:O	2:M:370:VAL:HG23	2.07	0.55
3:P:140:PHE:HE2	3:P:216:ASN:HD22	1.55	0.55
2:D:171:ILE:O	2:D:175:ALA:HB3	2.07	0.55
2:E:234:LEU:HD23	2:E:292:LEU:HD12	1.89	0.55
1:T:343:ASN:O	1:T:347:ILE:HG13	2.07	0.55
1:B:109:VAL:HG22	1:B:233:ILE:HB	1.88	0.55
3:G:138:PRO:HG3	3:G:223:ALA:HA	1.89	0.55
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.88	0.55
1:J:288:ARG:NH2	2:M:273:GLY:O	2.39	0.55
1:S:455:LEU:CD2	1:S:458:ILE:HD12	2.37	0.54
1:U:346:SER:HB3	2:V:260:ARG:HH12	1.72	0.54
2:E:243:PHE:HB2	2:E:251:VAL:HG21	1.88	0.54
1:A:401:GLU:HG3	1:A:402:VAL:N	2.22	0.54
2:E:188:GLY:HA3	2:E:260:ARG:HD2	1.88	0.54
2:M:433:ARG:O	2:M:436:ASP:HB2	2.07	0.54
1:L:142:ARG:HA	2:M:199:ARG:NH2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:192:ASN:HA	1:T:200:LYS:HG2	1.90	0.54
1:K:46:LEU:O	1:K:49:ILE:HG22	2.07	0.54
1:L:68:LEU:HB3	2:M:72:ARG:HD3	1.89	0.54
1:K:293:ARG:HD2	1:K:339:TYR:CD1	2.42	0.54
1:T:308:LEU:HD12	1:T:347:ILE:HG21	1.90	0.54
1:K:260:ARG:O	1:K:321:GLY:HA3	2.08	0.54
2:M:89:ARG:NH1	2:M:247:GLU:OE1	2.40	0.54
1:A:57:PHE:HB2	1:A:61:VAL:HG12	1.89	0.54
1:L:250:PHE:CD1	1:L:307:LEU:HD13	2.41	0.54
1:J:455:LEU:HD23	1:J:458:ILE:HD12	1.88	0.54
2:F:90:GLU:HG3	2:F:111:SER:HA	1.89	0.54
2:W:345:TYR:HA	2:W:346:PRO:C	2.28	0.54
1:S:52:GLU:O	1:S:97:VAL:HG23	2.08	0.54
1:C:174:GLN:HB2	2:F:354:LYS:HE2	1.90	0.54
1:T:348:THR:O	2:X:190:ARG:NH2	2.40	0.54
1:C:153:LYS:NZ	1:C:467:GLU:OE1	2.40	0.54
1:A:174:GLN:CB	2:D:354:LYS:HD2	2.38	0.54
2:N:321:ALA:HB3	2:N:322:PRO:CD	2.38	0.54
3:G:28:SER:HA	3:G:31:LEU:HB2	1.90	0.54
2:M:244:ARG:HD3	2:M:304:VAL:HG23	1.90	0.54
2:E:16:VAL:HG21	2:E:70:LEU:HB3	1.88	0.54
1:L:470:PHE:CE2	1:L:474:LEU:HD11	2.42	0.54
3:G:205:VAL:N	3:G:206:PRO:CD	2.71	0.54
1:A:369:VAL:HB	1:A:400:ARG:HH12	1.72	0.53
1:J:174:GLN:HA	6:J:600:ANP:N3B	2.20	0.53
1:B:166:ARG:NH2	1:B:349:ASP:OD1	2.41	0.53
1:J:387:GLN:NE2	1:J:491:LEU:HB2	2.23	0.53
2:D:95:ILE:HG22	2:D:103:ILE:CG1	2.39	0.53
2:V:33:ILE:O	2:V:34:LEU:HB2	2.08	0.53
1:K:50:GLN:HB3	2:O:69:GLY:HA2	1.89	0.53
2:V:89:ARG:HG2	2:V:92:LEU:HD12	1.91	0.53
2:V:198:TYR:O	2:V:202:LYS:HG2	2.08	0.53
1:J:29:GLU:O	1:J:92:ARG:HG3	2.09	0.53
2:V:87:VAL:HG12	2:V:239:ILE:HA	1.90	0.53
1:J:397:ALA:HA	1:J:400:ARG:NH2	2.24	0.53
2:M:89:ARG:HH11	2:M:181:PHE:HZ	1.54	0.53
1:K:38:ASP:HB3	1:K:286:LEU:HD22	1.89	0.53
1:L:293:ARG:HD2	1:L:339:TYR:CD2	2.43	0.53
1:T:142:ARG:NH1	1:T:143:SER:O	2.41	0.53
1:C:77:LEU:CD1	1:C:81:ASP:HB3	2.38	0.53
1:T:101:VAL:HG12	1:T:255:ILE:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:GLU:HG3	1:B:368:ASN:HB2	1.90	0.53
2:W:189:GLU:CA	2:W:260:ARG:HH21	2.20	0.53
2:F:87:VAL:HG11	2:F:115:LYS:HE2	1.89	0.53
1:C:481:LEU:HD21	1:C:498:SER:HB3	1.91	0.53
3:G:218:MET:O	3:G:222:MET:HG3	2.08	0.53
5:R:55:GLU:CB	5:R:56:PRO:CD	2.86	0.53
2:D:242:TYR:CE1	2:D:246:GLU:HG3	2.44	0.53
5:I:4:ARG:HG3	5:I:13:TYR:CD2	2.44	0.53
5:I:46:GLN:C	5:I:56:PRO:HD2	2.30	0.52
1:L:358:LEU:HB3	1:L:363:ILE:HD12	1.89	0.52
1:C:381:GLN:HE21	1:C:385:LEU:HG	1.74	0.52
3:P:88:HIS:CE1	3:P:113:LYS:HB2	2.43	0.52
2:X:52:GLN:HG2	2:X:60:ARG:HB3	1.90	0.52
2:X:126:GLU:O	2:X:299:THR:HA	2.08	0.52
2:N:84:SER:O	2:N:114:ARG:NH2	2.41	0.52
1:L:280:TYR:CE2	1:L:297:PRO:HG2	2.45	0.52
3:G:44:MET:HE2	4:H:86:THR:HB	1.91	0.52
2:V:41:THR:HB	2:V:42:PRO:CD	2.39	0.52
3:Y:14:LYS:HA	3:Y:248:ILE:HD11	1.91	0.52
2:M:9:ILE:HB	2:M:78:ASP:HB3	1.91	0.52
2:E:136:THR:HG21	2:E:141:VAL:HB	1.91	0.52
1:B:49:ILE:HG13	1:B:53:GLU:CD	2.30	0.52
1:K:203:CYS:HB2	1:K:231:SER:HA	1.91	0.52
1:L:201:LEU:HD21	1:L:267:LEU:HB2	1.90	0.52
2:D:33:ILE:O	2:D:34:LEU:HB2	2.09	0.52
1:J:298:GLY:O	2:N:267:GLU:HG2	2.09	0.52
1:L:40:ILE:CD1	1:L:76:VAL:HG12	2.40	0.52
2:X:206:VAL:HG12	2:X:215:VAL:HG12	1.92	0.52
2:E:123:SER:O	2:E:127:GLN:HG2	2.09	0.52
2:X:39:ILE:HG12	2:X:76:VAL:HG22	1.91	0.52
2:D:243:PHE:HD1	2:D:247:GLU:HG3	1.75	0.52
2:X:345:TYR:HA	2:X:346:PRO:C	2.30	0.52
1:L:341:PRO:O	1:L:345:ILE:HG13	2.09	0.52
1:C:109:VAL:HG13	1:C:233:ILE:HB	1.91	0.52
2:W:391:LEU:HD22	2:W:395:GLU:HG3	1.92	0.52
1:T:368:ASN:C	1:T:368:ASN:OD1	2.48	0.52
1:B:450:GLY:HA2	1:B:455:LEU:HD12	1.91	0.52
1:J:473:TYR:CE2	1:J:506:PHE:HB2	2.45	0.52
2:W:36:ALA:HB2	2:W:83:ILE:HG13	1.91	0.52
2:W:237:LEU:HD22	2:W:292:LEU:HD12	1.91	0.52
4:H:72:GLY:CA	5:I:14:LEU:HD21	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:NH2	2:D:352:ASP:OD1	2.43	0.52
2:O:417:PRO:HG2	2:O:430:LYS:HG2	1.91	0.52
2:V:174:ILE:HG22	2:V:252:LEU:HD11	1.92	0.52
3:G:49:GLN:HE21	3:G:217:GLN:HE22	1.56	0.52
2:M:28:SER:C	2:M:30:LEU:H	2.12	0.52
2:O:384:LEU:O	2:O:388:ILE:HG12	2.09	0.52
3:G:45:ASP:CG	3:G:220:THR:HG21	2.29	0.51
2:D:259:PHE:CE1	2:D:313:PRO:HG3	2.45	0.51
5:I:31:THR:CG2	5:I:34:VAL:HG23	2.30	0.51
1:J:289:ARG:HH11	1:J:289:ARG:HA	1.76	0.51
1:J:309:GLU:HG3	2:N:223:ASN:HB3	1.91	0.51
2:M:279:VAL:HG12	2:M:279:VAL:O	2.09	0.51
2:D:197:LEU:O	2:D:201:MET:HG2	2.10	0.51
1:L:250:PHE:CE1	1:L:307:LEU:HB2	2.45	0.51
1:B:227:ALA:HA	1:B:230:TYR:CE2	2.46	0.51
1:B:168:LEU:HB2	1:B:348:THR:HG21	1.92	0.51
2:V:192:ARG:HH11	2:V:193:GLU:HG2	1.75	0.51
2:V:189:GLU:O	2:V:221:GLN:HB3	2.10	0.51
1:L:50:GLN:HB3	2:M:69:GLY:HA2	1.93	0.51
2:X:367:HIS:CD2	2:X:438:VAL:HG21	2.45	0.51
2:V:96:ILE:O	2:V:218:VAL:HA	2.10	0.51
1:A:444:VAL:N	1:A:445:PRO:HD2	2.26	0.51
1:L:222:LEU:HB2	1:L:228:MET:HE2	1.93	0.51
3:Y:24:LYS:HG3	3:Y:238:ASP:HB2	1.93	0.51
1:K:390:GLY:O	1:K:391:SER:HB2	2.11	0.51
1:S:354:LEU:HA	1:S:366:ALA:O	2.11	0.51
1:J:166:ARG:O	1:J:348:THR:HB	2.11	0.51
1:B:166:ARG:CD	1:B:308:LEU:O	2.59	0.51
2:X:239:ILE:O	2:X:243:PHE:HD2	1.94	0.51
1:J:396:LEU:O	1:J:400:ARG:HG3	2.11	0.51
1:T:311:ALA:HA	1:T:323:LEU:HB3	1.92	0.51
1:C:397:ALA:HA	1:C:400:ARG:NH2	2.26	0.51
2:M:98:VAL:HG23	2:M:232:VAL:HA	1.93	0.51
3:P:240:ALA:HA	3:P:243:ASN:HB3	1.93	0.51
2:W:143:LEU:O	2:W:367:HIS:HE1	1.93	0.51
2:W:335:LEU:HA	2:W:347:ALA:O	2.11	0.51
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.93	0.51
2:D:137:GLY:HA2	2:D:432:VAL:O	2.11	0.51
2:W:200:GLU:O	2:W:204:THR:HB	2.11	0.51
2:E:456:ALA:HA	2:E:469:LYS:HD3	1.91	0.51
3:P:168:ASP:HB3	3:P:176:GLU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:248:ALA:HB3	1:L:249:PRO:HD3	1.93	0.50
2:F:133:ILE:HD11	2:F:363:VAL:HG12	1.92	0.50
2:V:182:SER:HB2	2:V:215:VAL:HG23	1.92	0.50
1:J:146:GLU:HB2	1:J:163:ARG:HG3	1.93	0.50
2:E:253:LEU:O	2:E:306:SER:HA	2.11	0.50
1:T:26:ASN:O	1:T:30:THR:HB	2.11	0.50
2:X:255:ILE:HD12	2:X:308:GLN:HG2	1.93	0.50
2:F:67:THR:HB	2:F:70:LEU:HD12	1.93	0.50
2:M:185:THR:OG1	2:M:236:GLY:HA3	2.12	0.50
3:P:48:GLU:OE1	3:P:213:THR:HA	2.11	0.50
1:S:70:PRO:HD3	2:W:15:ALA:HB2	1.93	0.50
1:J:201:LEU:HA	1:J:265:HIS:O	2.11	0.50
1:B:422:ARG:NH2	1:B:453:GLY:HA3	2.24	0.50
2:N:321:ALA:HB3	2:N:322:PRO:HD3	1.94	0.50
1:U:82:ARG:HA	2:X:33:ILE:HB	1.94	0.50
1:S:50:GLN:HB2	1:S:53:GLU:HB2	1.94	0.50
2:O:398:GLU:HB2	3:P:120:ARG:CD	2.40	0.50
2:D:201:MET:HE2	2:D:217:LEU:HD21	1.94	0.50
1:S:146:GLU:HB2	1:S:163:ARG:HG3	1.94	0.50
1:L:167:GLU:O	1:L:327:PRO:HD2	2.12	0.50
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.93	0.50
1:S:67:ILE:HG12	2:W:17:ILE:HG23	1.93	0.50
2:W:189:GLU:HA	2:W:260:ARG:NH2	2.25	0.50
2:F:237:LEU:HD21	2:F:295:ARG:HB2	1.93	0.50
2:M:357:LEU:HB3	2:M:362:VAL:HG11	1.94	0.50
2:N:9:ILE:HB	2:N:78:ASP:HB3	1.94	0.50
1:J:444:VAL:N	1:J:445:PRO:HD2	2.27	0.50
1:S:369:VAL:CG1	1:S:393:LYS:HD3	2.39	0.50
2:N:36:ALA:HB2	2:N:83:ILE:HG13	1.94	0.50
1:S:176:GLY:O	1:S:180:VAL:HG23	2.12	0.50
1:K:149:GLN:HG3	1:K:191:TRP:CH2	2.46	0.50
1:C:455:LEU:HA	1:C:458:ILE:HD12	1.94	0.50
1:J:167:GLU:O	1:J:327:PRO:HD2	2.11	0.50
2:M:155:LEU:HB2	2:M:309:ALA:HA	1.93	0.50
2:V:222:MET:HA	2:V:229:ARG:HD2	1.94	0.50
3:G:50:LEU:HG	4:H:78:GLN:HE21	1.77	0.50
1:U:242:ALA:HB3	1:U:243:PRO:HD3	1.94	0.50
4:H:78:GLN:HA	4:H:78:GLN:OE1	2.12	0.49
2:O:417:PRO:HG2	2:O:430:LYS:CG	2.42	0.49
1:S:302:TYR:O	1:S:306:ARG:HB2	2.12	0.49
3:G:108:VAL:HG11	3:G:150:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:136:THR:HG23	2:E:138:ILE:H	1.77	0.49
2:M:319:ASP:OD1	2:M:320:PRO:HD2	2.12	0.49
1:T:59:SER:HB2	1:T:61:VAL:HG12	1.93	0.49
1:B:181:ALA:HB1	1:B:269:VAL:HG11	1.94	0.49
2:W:188:GLY:O	2:W:222:MET:HG3	2.11	0.49
2:O:234:LEU:CD2	2:O:292:LEU:HD13	2.43	0.49
2:D:410:ILE:HG23	2:D:441:PHE:HE2	1.77	0.49
1:L:67:ILE:HG12	2:M:17:ILE:HG23	1.94	0.49
2:F:63:ALA:O	2:F:227:GLY:HA3	2.12	0.49
2:E:237:LEU:O	2:E:241:GLU:HG3	2.13	0.49
2:W:168:GLN:HA	2:W:171:ILE:HD12	1.94	0.49
1:J:289:ARG:HE	2:N:17:ILE:CG2	2.24	0.49
1:T:239:SER:HB3	2:W:294:GLU:HG3	1.93	0.49
2:V:37:LEU:HB2	2:V:48:LEU:HB2	1.95	0.49
1:L:253:ALA:O	1:L:257:GLU:HG3	2.11	0.49
1:U:282:GLN:NE2	2:X:284:THR:HA	2.28	0.49
1:J:212:ARG:HG3	1:J:237:THR:HG21	1.95	0.49
2:M:202:LYS:NZ	2:M:209:LEU:HD11	2.27	0.49
2:F:137:GLY:HA2	2:F:432:VAL:O	2.12	0.49
2:M:249:GLN:HG3	2:M:250:ASP:N	2.28	0.49
2:N:168:GLN:HG2	2:N:206:VAL:HG21	1.95	0.49
2:X:10:THR:HG22	2:X:77:LEU:HA	1.94	0.49
1:U:403:ALA:O	1:U:407:GLN:HG2	2.11	0.49
1:T:421:VAL:O	1:T:425:ARG:HG2	2.13	0.49
2:D:381:TYR:HD1	2:D:404:VAL:HG22	1.76	0.49
2:M:258:ILE:CG2	2:M:310:VAL:HG22	2.42	0.49
2:N:97:ASN:HD21	2:N:101:GLU:HB2	1.78	0.49
1:A:338:ALA:HB3	1:A:341:PRO:HG2	1.94	0.49
2:W:147:TYR:CE1	2:W:153:ILE:HG21	2.48	0.49
2:O:285:LEU:C	2:O:285:LEU:HD23	2.33	0.49
1:K:138:ILE:HD12	1:K:138:ILE:N	2.27	0.49
2:V:52:GLN:HE22	2:V:60:ARG:HD2	1.78	0.49
1:S:248:ALA:HB3	1:S:249:PRO:HD3	1.94	0.49
1:A:311:ALA:HA	1:A:323:LEU:HD23	1.94	0.49
1:S:99:VAL:HG21	1:S:251:THR:HG23	1.94	0.49
6:V:600:ANP:O5'	6:V:600:ANP:H8	2.12	0.49
1:K:239:SER:HB2	2:N:291:LEU:HD23	1.93	0.49
2:D:184:PHE:C	2:D:184:PHE:CD1	2.85	0.49
2:E:427:ILE:HD12	2:E:427:ILE:H	1.78	0.49
2:D:244:ARG:O	2:D:248:GLY:HA2	2.13	0.49
1:T:413:ASP:HB3	1:T:416:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:185:THR:OG1	2:O:236:GLY:HA3	2.13	0.49
2:D:406:ARG:HH21	2:D:447:GLY:HA3	1.77	0.49
1:A:38:ASP:O	1:A:286:LEU:HD13	2.13	0.49
3:Y:213:THR:HG22	3:Y:217:GLN:HG2	1.95	0.49
2:F:237:LEU:HD22	2:F:292:LEU:HD12	1.95	0.49
2:X:374:VAL:HG23	2:X:445:LEU:HD11	1.94	0.49
2:V:90:GLU:HB2	2:V:111:SER:HB3	1.94	0.49
3:P:183:PHE:HB3	3:P:187:THR:HB	1.95	0.49
1:J:182:LEU:HA	1:J:185:ILE:HD12	1.94	0.49
2:N:384:LEU:O	2:N:388:ILE:HG12	2.12	0.48
1:K:293:ARG:HD2	1:K:339:TYR:CG	2.48	0.48
1:L:99:VAL:CG1	1:L:251:THR:HB	2.43	0.48
1:S:491:LEU:HD23	1:S:495:LEU:HD13	1.94	0.48
2:W:27:GLN:HA	2:W:57:ASN:ND2	2.28	0.48
2:D:174:ILE:O	2:D:178:HIS:HB2	2.13	0.48
2:E:140:VAL:CG1	2:E:414:LEU:HD22	2.41	0.48
3:P:150:LEU:O	3:P:154:MET:HB2	2.13	0.48
1:K:164:GLY:HA2	1:K:323:LEU:O	2.13	0.48
2:M:391:LEU:HD21	3:P:23:MET:SD	2.52	0.48
1:L:201:LEU:HA	1:L:265:HIS:O	2.12	0.48
2:V:221:GLN:OE1	2:V:221:GLN:HA	2.12	0.48
1:L:177:LYS:HD2	1:L:328:VAL:HG13	1.94	0.48
4:Q:69:PHE:CZ	4:Q:133:LEU:HA	2.47	0.48
1:C:28:ASN:HB3	1:C:48:ASN:ND2	2.29	0.48
2:D:359:ASP:O	2:D:363:VAL:HG22	2.13	0.48
2:E:370:VAL:HG13	2:E:445:LEU:HD12	1.95	0.48
2:F:168:GLN:HB3	2:F:420:VAL:HG11	1.96	0.48
2:F:188:GLY:O	2:F:260:ARG:HG3	2.14	0.48
2:E:375:GLN:O	2:E:379:GLN:HB2	2.14	0.48
1:U:155:VAL:HG13	1:U:159:VAL:HG23	1.94	0.48
1:B:168:LEU:HD11	1:B:329:ILE:HB	1.94	0.48
2:F:191:THR:HA	2:F:221:GLN:HG3	1.94	0.48
3:G:245:GLY:HA2	3:G:248:ILE:HD12	1.96	0.48
1:S:364:ARG:HA	1:S:365:PRO:C	2.33	0.48
2:N:256:ASP:HA	2:N:257:ASN:HA	1.63	0.48
2:O:374:VAL:HG23	2:O:445:LEU:HD11	1.95	0.48
1:S:36:VAL:HG21	1:S:84:VAL:HB	1.94	0.48
2:M:90:GLU:HG3	2:M:111:SER:CA	2.44	0.48
2:X:187:VAL:HG22	2:X:232:VAL:HG13	1.95	0.48
1:B:99:VAL:HG11	1:B:251:THR:HB	1.95	0.48
1:B:345:ILE:HG12	1:B:351:GLN:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:15:ASN:O	3:P:19:ILE:HG12	2.13	0.48
3:G:42:LYS:HE3	3:G:224:GLN:OE1	2.14	0.48
1:J:55:VAL:HG21	1:J:75:ILE:HD13	1.95	0.48
2:E:143:LEU:HD21	2:E:374:VAL:HG21	1.94	0.48
2:W:388:ILE:HD11	2:W:396:LEU:HD11	1.96	0.48
1:A:332:GLN:HB3	2:D:318:THR:CG2	2.43	0.48
1:U:58:SER:HB3	1:U:89:LEU:HB3	1.94	0.48
1:J:258:TRP:O	1:J:262:ASN:ND2	2.47	0.48
1:T:173:ARG:HB3	1:T:173:ARG:HH11	1.78	0.48
1:K:186:LEU:HD11	1:K:435:TYR:HD1	1.79	0.48
1:B:166:ARG:HD3	1:B:308:LEU:O	2.13	0.48
2:F:359:ASP:O	2:F:363:VAL:HG22	2.14	0.48
2:M:185:THR:HG21	2:M:233:ALA:HA	1.96	0.48
1:A:37:GLY:O	1:A:38:ASP:HB2	2.13	0.48
1:J:103:PRO:HD3	1:J:258:TRP:CZ2	2.48	0.48
1:K:364:ARG:HA	1:K:365:PRO:C	2.34	0.48
2:N:136:THR:HG23	2:N:138:ILE:H	1.79	0.48
1:J:354:LEU:HA	1:J:366:ALA:O	2.13	0.48
2:M:208:ASN:ND2	2:M:211:GLY:HA3	2.28	0.48
4:H:16:LEU:HB2	4:H:19:GLU:O	2.13	0.48
1:L:236:ALA:CB	1:L:245:GLN:HA	2.44	0.48
1:B:192:ASN:HA	1:B:200:LYS:HG2	1.94	0.48
1:A:317:LYS:O	1:A:317:LYS:HG2	2.13	0.48
1:J:402:VAL:HG12	1:J:402:VAL:O	2.14	0.48
4:H:33:PRO:HD2	4:H:52:LEU:HD22	1.95	0.47
1:S:54:LEU:HD13	1:S:97:VAL:HG22	1.96	0.47
1:C:418:GLN:HG3	1:C:419:THR:N	2.29	0.47
1:U:436:SER:N	1:U:437:PRO:HD3	2.29	0.47
1:S:107:GLY:HA2	1:S:228:MET:O	2.14	0.47
2:O:98:VAL:HG23	2:O:232:VAL:HA	1.96	0.47
1:L:153:LYS:HG2	1:L:443:GLN:HG2	1.96	0.47
2:O:174:ILE:O	2:O:178:HIS:N	2.39	0.47
1:J:168:LEU:HB2	1:J:348:THR:HG21	1.96	0.47
1:S:299:ASP:HB2	1:S:302:TYR:HB3	1.95	0.47
2:E:150:GLY:HA3	2:E:298:THR:OG1	2.14	0.47
3:G:193:SER:HB3	3:G:196:LYS:CE	2.44	0.47
1:T:36:VAL:HG13	2:W:53:HIS:HB2	1.95	0.47
2:D:109:ILE:O	2:D:109:ILE:HG22	2.14	0.47
1:A:446:LEU:HD21	1:A:467:GLU:HA	1.96	0.47
1:L:77:LEU:HD12	1:L:81:ASP:HB3	1.95	0.47
1:C:477:ASN:N	1:C:477:ASN:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:136:THR:HG22	2:W:142:ASP:OD1	2.15	0.47
2:M:345:TYR:HA	2:M:346:PRO:C	2.34	0.47
2:V:275:ILE:HG23	3:Y:274:ALA:HB2	1.97	0.47
1:A:395:PHE:CZ	1:A:422:ARG:HB3	2.49	0.47
2:D:164:THR:HA	2:D:167:ILE:HG22	1.95	0.47
1:B:115:ASN:ND2	1:B:115:ASN:H	2.12	0.47
3:G:96:ARG:HG2	3:G:122:HIS:CE1	2.50	0.47
3:Y:25:ILE:HA	3:Y:28:SER:CB	2.40	0.47
1:U:376:VAL:CG1	1:U:380:ALA:HB3	2.45	0.47
1:A:64:MET:SD	1:A:97:VAL:HG21	2.54	0.47
2:V:41:THR:HB	2:V:42:PRO:HD2	1.96	0.47
1:S:351:GLN:HE22	1:S:375:ARG:HH12	1.63	0.47
2:D:40:LYS:HG3	2:D:40:LYS:O	2.13	0.47
1:L:167:GLU:O	1:L:326:LEU:HA	2.14	0.47
3:G:193:SER:HB3	3:G:196:LYS:HE2	1.97	0.47
2:W:167:ILE:O	2:W:170:LEU:HB2	2.14	0.47
1:L:154:ALA:HA	1:L:430:LEU:HD22	1.96	0.47
1:L:237:THR:HB	1:L:240:GLU:HG3	1.97	0.47
3:P:46:GLU:O	3:P:50:LEU:CB	2.62	0.47
2:O:335:LEU:HA	2:O:347:ALA:O	2.14	0.47
2:X:71:VAL:O	2:X:74:GLU:HB2	2.14	0.47
2:E:180:GLY:HA2	2:E:249:GLN:NE2	2.30	0.47
2:E:204:THR:HG22	2:E:206:VAL:HG22	1.96	0.47
2:X:160:GLY:N	6:X:600:ANP:HNB1	2.11	0.47
1:A:219:VAL:HG13	1:A:228:MET:HE3	1.97	0.47
1:T:166:ARG:HH22	2:X:190:ARG:HD3	1.80	0.47
1:A:412:LEU:HB3	1:A:417:LYS:HB2	1.97	0.47
1:T:67:ILE:HG12	2:X:17:ILE:HG23	1.97	0.47
1:B:177:LYS:HG2	1:B:354:LEU:HD12	1.95	0.47
2:F:10:THR:HG22	2:F:77:LEU:HA	1.97	0.47
2:F:10:THR:N	2:F:27:GLN:HE22	2.13	0.47
1:U:97:VAL:HG11	1:U:247:LEU:HD21	1.97	0.47
1:A:462:ARG:HD2	1:A:465:GLU:OE2	2.13	0.47
4:H:45:HIS:HD2	4:H:77:VAL:HG21	1.79	0.47
2:N:117:ILE:HA	2:N:238:THR:OG1	2.15	0.47
4:H:10:LEU:HB2	4:H:43:ALA:HA	1.96	0.47
1:T:491:LEU:HA	1:T:495:LEU:HD23	1.97	0.47
1:T:55:VAL:HG21	1:T:75:ILE:HD13	1.96	0.47
1:A:138:ILE:HD11	2:E:221:GLN:CG	2.45	0.47
1:C:243:PRO:O	1:C:247:LEU:HB2	2.14	0.47
2:E:157:GLY:HA2	2:E:337:ARG:HH22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASN:ND2	1:B:371:LEU:HD22	2.29	0.47
2:D:13:VAL:HG23	2:D:76:VAL:CG2	2.45	0.47
3:G:165:PHE:CE2	3:G:179:GLU:HB2	2.49	0.47
2:X:90:GLU:HB2	2:X:111:SER:HB3	1.96	0.47
1:K:29:GLU:O	1:K:92:ARG:HB2	2.15	0.47
2:V:62:ILE:HD11	2:V:272:LEU:HD11	1.97	0.47
1:L:346:SER:HB3	2:M:260:ARG:HH22	1.80	0.47
2:E:135:GLU:OE2	2:E:433:ARG:HD3	2.15	0.47
2:N:187:VAL:HG13	2:N:232:VAL:HG23	1.96	0.46
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.97	0.46
1:A:38:ASP:HB3	1:A:286:LEU:HD22	1.96	0.46
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.97	0.46
1:K:382:VAL:HG11	1:K:440:THR:HG21	1.97	0.46
2:N:134:LEU:HD13	2:N:149:ARG:HG3	1.96	0.46
2:O:154:GLY:HA3	2:O:329:LEU:HD13	1.97	0.46
1:A:450:GLY:HA2	1:A:455:LEU:HD12	1.97	0.46
2:O:237:LEU:HD21	2:O:295:ARG:CB	2.43	0.46
2:N:32:ALA:O	2:N:35:ASN:HB2	2.16	0.46
1:K:354:LEU:HB3	1:K:366:ALA:HB3	1.97	0.46
4:Q:89:GLU:CB	5:R:21:ILE:HD11	2.44	0.46
3:G:182:ILE:HD12	3:G:214:LEU:HA	1.96	0.46
1:A:364:ARG:HA	1:A:365:PRO:C	2.34	0.46
1:T:269:VAL:HG12	1:T:271:ASP:HB2	1.97	0.46
2:N:237:LEU:HD21	2:N:295:ARG:HB2	1.96	0.46
2:O:37:LEU:HB2	2:O:48:LEU:HB2	1.96	0.46
2:W:97:ASN:OD1	2:W:97:ASN:C	2.54	0.46
5:R:19:GLN:NE2	5:R:38:SER:HB3	2.30	0.46
1:B:478:HIS:HB3	1:B:481:LEU:HG	1.96	0.46
1:C:300:VAL:HG22	1:C:300:VAL:O	2.15	0.46
1:A:397:ALA:CA	1:A:400:ARG:CZ	2.86	0.46
1:A:99:VAL:HG21	1:A:251:THR:HG23	1.97	0.46
1:B:453:GLY:C	1:B:455:LEU:H	2.18	0.46
1:K:204:VAL:O	1:K:268:ILE:HA	2.15	0.46
2:N:152:LYS:HE2	2:N:293:GLN:HB3	1.98	0.46
1:U:34:LEU:HG	1:U:44:PHE:HB2	1.98	0.46
1:C:456:ASP:OD1	1:C:456:ASP:N	2.47	0.46
1:C:215:VAL:O	1:C:219:VAL:HG13	2.16	0.46
2:V:163:LYS:HZ1	2:V:311:TYR:HA	1.80	0.46
1:U:50:GLN:HB3	2:V:69:GLY:HA2	1.97	0.46
1:K:109:VAL:HG13	1:K:233:ILE:HB	1.97	0.46
2:N:98:VAL:HG21	2:N:231:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:202:LYS:HZ2	2:V:209:LEU:HD21	1.80	0.46
2:E:240:ALA:HB1	2:E:251:VAL:HG11	1.97	0.46
1:K:344:VAL:HA	1:K:347:ILE:HD12	1.98	0.46
1:U:338:ALA:HB3	1:U:341:PRO:HG2	1.97	0.46
2:E:367:HIS:CD2	2:E:434:LEU:HD11	2.51	0.46
2:V:296:ILE:HG21	2:V:306:SER:HB3	1.97	0.46
2:O:384:LEU:HB3	2:O:388:ILE:HD11	1.97	0.46
1:S:99:VAL:HG23	1:S:100:PRO:HD2	1.96	0.46
1:C:28:ASN:HB3	1:C:48:ASN:HD22	1.80	0.46
2:E:177:ALA:HB1	2:E:433:ARG:HH12	1.81	0.46
2:F:181:PHE:HD2	2:F:243:PHE:CD1	2.34	0.46
1:J:143:SER:H	2:N:199:ARG:NH1	2.13	0.46
1:U:369:VAL:HG11	1:U:396:LEU:CB	2.45	0.46
1:A:203:CYS:O	1:A:231:SER:HA	2.16	0.46
2:N:168:GLN:NE2	2:N:200:GLU:O	2.47	0.46
1:A:302:TYR:CZ	1:A:306:ARG:HG3	2.51	0.46
1:A:395:PHE:HE2	1:A:423:GLY:HA2	1.81	0.46
1:T:140:PRO:HB3	1:T:318:GLU:HG3	1.98	0.46
2:X:389:ALA:O	3:Y:243:ASN:ND2	2.49	0.46
4:H:96:PHE:O	5:I:25:LEU:HA	2.16	0.46
2:M:26:GLU:H	2:M:29:GLU:HG2	1.81	0.46
1:K:138:ILE:HG13	2:O:191:THR:HG23	1.97	0.46
1:B:285:LEU:HD22	2:E:275:ILE:CG2	2.46	0.46
2:O:10:THR:HG21	2:O:75:LYS:HD3	1.98	0.46
2:F:325:THR:HG22	2:F:329:LEU:HD11	1.98	0.46
1:L:492:SER:H	1:L:495:LEU:HD12	1.81	0.46
1:C:440:THR:O	1:C:444:VAL:HG23	2.16	0.46
2:X:321:ALA:HB3	2:X:322:PRO:CD	2.46	0.46
3:G:96:ARG:NE	3:G:121:THR:HG21	2.09	0.46
1:A:396:LEU:O	1:A:400:ARG:CG	2.63	0.46
2:X:382:LYS:O	2:X:385:GLN:HG2	2.16	0.46
1:L:249:PRO:HB3	1:L:270:TYR:CD1	2.51	0.46
1:U:116:PRO:HG3	1:U:122:PRO:HA	1.98	0.46
2:F:417:PRO:HG2	2:F:430:LYS:HG3	1.97	0.46
1:J:211:LYS:HD3	2:M:328:HIS:HA	1.97	0.46
2:M:53:HIS:CD2	2:M:59:VAL:HG12	2.51	0.46
2:D:449:TYR:HD1	2:D:452:ILE:HD12	1.80	0.46
1:T:474:LEU:HD13	1:T:482:LEU:HD21	1.98	0.46
1:C:478:HIS:CE1	1:C:502:ALA:HB2	2.52	0.45
2:X:70:LEU:HD23	2:X:70:LEU:HA	1.83	0.45
2:X:147:TYR:CZ	2:X:153:ILE:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HD22	1:B:92:ARG:HG3	1.97	0.45
2:M:244:ARG:O	2:M:248:GLY:HA2	2.15	0.45
1:J:67:ILE:HD12	1:J:287:LEU:HD22	1.98	0.45
1:S:153:LYS:HG2	1:S:432:GLN:OE1	2.16	0.45
2:F:367:HIS:HD1	2:F:367:HIS:C	2.19	0.45
1:J:289:ARG:HH21	2:N:17:ILE:CG2	2.29	0.45
2:M:387:ILE:HG23	2:M:391:LEU:HD22	1.98	0.45
2:E:370:VAL:HG21	2:E:442:LYS:HB2	1.98	0.45
2:W:170:LEU:HD23	2:W:170:LEU:HA	1.87	0.45
2:F:335:LEU:HA	2:F:347:ALA:O	2.17	0.45
1:T:335:ASP:HB2	3:Y:257:ARG:NH1	2.31	0.45
2:W:152:LYS:HE3	2:W:296:ILE:HB	1.98	0.45
1:T:170:ILE:HG23	1:T:353:PHE:HA	1.98	0.45
2:X:406:ARG:NH2	2:X:450:ASP:OD2	2.50	0.45
1:J:187:ASN:O	1:J:190:ARG:HG3	2.16	0.45
2:E:221:GLN:NE2	2:E:224:GLU:OE2	2.49	0.45
2:N:45:LYS:HE3	2:N:99:ILE:HD12	1.96	0.45
1:K:179:ALA:HB2	6:K:600:ANP:H8	1.98	0.45
1:K:107:GLY:HA2	1:K:228:MET:O	2.17	0.45
1:B:484:GLU:O	1:B:488:LYS:HB2	2.17	0.45
4:Q:14:PHE:HA	4:Q:85:VAL:HB	1.99	0.45
1:L:241:ALA:HB1	1:L:243:PRO:HD2	1.99	0.45
2:N:281:TYR:OH	2:N:321:ALA:HB2	2.16	0.45
1:J:49:ILE:HA	1:J:92:ARG:HE	1.81	0.45
3:P:75:VAL:HA	3:P:108:VAL:O	2.17	0.45
4:H:48:THR:H	4:H:77:VAL:HB	1.81	0.45
2:V:7:THR:N	2:V:8:PRO:HD3	2.31	0.45
2:X:15:ALA:HB3	2:X:22:ASP:HB2	1.98	0.45
3:P:10:LEU:HD13	3:P:251:TYR:HB3	1.98	0.45
1:B:290:PRO:HA	1:B:291:PRO:HD2	1.90	0.45
1:K:30:THR:HB	2:X:464:GLU:OE2	2.16	0.45
2:E:99:ILE:HG13	2:E:101:GLU:HG3	1.98	0.45
1:J:428:GLN:HG2	1:J:463:ILE:HB	1.98	0.45
2:V:345:TYR:HA	2:V:346:PRO:C	2.36	0.45
2:V:34:LEU:HD22	2:V:118:HIS:CE1	2.52	0.45
1:L:284:SER:CB	1:L:297:PRO:HG3	2.46	0.45
1:S:272:ASP:HB2	1:S:328:VAL:O	2.17	0.45
2:D:256:ASP:HA	2:D:257:ASN:HA	1.66	0.45
1:K:155:VAL:HA	1:K:159:VAL:HG23	1.99	0.45
1:A:316:GLU:CD	1:A:316:GLU:H	2.20	0.45
2:V:33:ILE:HA	2:V:50:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:247:GLU:HB2	2:V:249:GLN:HG2	1.98	0.45
1:J:455:LEU:HD21	1:J:466:PHE:CE1	2.52	0.45
2:V:93:GLY:N	2:V:215:VAL:O	2.50	0.45
1:J:220:GLN:HG2	1:J:224:GLN:HE21	1.82	0.45
2:W:220:GLY:HA3	2:W:232:VAL:HG21	1.97	0.45
3:P:248:ILE:O	3:P:252:SER:HB2	2.17	0.45
1:K:503:THR:O	1:K:507:VAL:HG23	2.17	0.45
1:A:103:PRO:HD3	1:A:258:TRP:CH2	2.52	0.45
1:L:302:TYR:HA	1:L:305:SER:OG	2.17	0.45
2:D:95:ILE:CG2	2:D:103:ILE:HG13	2.47	0.45
1:L:168:LEU:HB2	1:L:348:THR:HG21	1.99	0.45
1:L:468:SER:HA	1:L:471:LEU:HD12	1.99	0.45
1:T:147:PRO:HB3	1:T:380:ALA:O	2.17	0.45
1:B:196:ASP:OD2	1:B:199:LYS:HG3	2.16	0.45
1:L:254:SER:OG	1:L:310:ARG:NH2	2.49	0.45
1:U:39:GLY:HA2	1:U:77:LEU:HD12	1.99	0.45
2:D:391:LEU:HD22	2:D:395:GLU:HG2	1.99	0.45
1:B:138:ILE:O	2:F:195:ASN:ND2	2.50	0.45
2:M:32:ALA:O	2:M:35:ASN:HB2	2.16	0.45
1:K:95:ASN:ND2	1:K:98:ASP:OD2	2.49	0.45
1:B:187:ASN:OD1	1:B:190:ARG:NH1	2.50	0.45
2:F:187:VAL:HG22	2:F:232:VAL:HG13	1.99	0.45
1:L:77:LEU:CD1	1:L:81:ASP:HB3	2.47	0.44
1:C:216:ALA:O	1:C:219:VAL:HG22	2.17	0.44
1:L:348:THR:O	2:M:190:ARG:NH2	2.45	0.44
2:W:185:THR:OG1	2:W:236:GLY:HA3	2.18	0.44
2:F:33:ILE:HG22	2:F:34:LEU:HG	1.99	0.44
2:O:321:ALA:HB3	2:O:322:PRO:CD	2.47	0.44
1:T:385:LEU:HG	1:T:444:VAL:HG12	1.99	0.44
1:K:103:PRO:HD2	1:K:126:ALA:HB2	1.99	0.44
2:X:252:LEU:HD23	2:X:305:THR:HB	1.97	0.44
2:V:256:ASP:HA	2:V:257:ASN:HA	1.72	0.44
5:I:46:GLN:HG3	5:I:47:TYR:H	1.81	0.44
1:K:93:THR:HG22	1:K:95:ASN:HB2	1.99	0.44
1:K:173:ARG:HG2	1:K:174:GLN:HG2	1.99	0.44
1:U:302:TYR:HA	1:U:305:SER:OG	2.16	0.44
2:M:256:ASP:HA	2:M:257:ASN:HA	1.76	0.44
1:S:117:ILE:O	2:V:124:PHE:HD2	2.00	0.44
2:O:90:GLU:HB2	2:O:111:SER:CB	2.47	0.44
1:K:110:VAL:CG2	1:K:234:VAL:HG22	2.47	0.44
2:E:410:ILE:HG23	2:E:441:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:364:ARG:HB3	6:J:600:ANP:N6	2.31	0.44
1:K:435:TYR:O	1:K:437:PRO:HD3	2.17	0.44
2:M:258:ILE:O	2:M:261:PHE:HB3	2.17	0.44
1:K:314:LEU:HB2	1:K:321:GLY:O	2.17	0.44
3:G:250:ARG:HA	3:G:253:ILE:HD12	2.00	0.44
3:P:208:ASP:HA	3:P:211:GLU:HB2	1.98	0.44
4:Q:70:ILE:HG22	4:Q:72:GLY:H	1.81	0.44
1:U:269:VAL:HG22	1:U:326:LEU:HD12	1.99	0.44
2:F:244:ARG:HD3	2:F:304:VAL:HG23	1.98	0.44
2:M:30:LEU:HD11	2:M:57:ASN:HA	1.99	0.44
1:J:185:ILE:HG23	1:J:203:CYS:SG	2.57	0.44
2:X:17:ILE:HG22	2:X:271:LEU:HD22	1.98	0.44
3:Y:230:ILE:HD13	3:Y:233:ARG:HH12	1.82	0.44
2:N:259:PHE:CE1	2:N:313:PRO:HG3	2.53	0.44
1:K:37:GLY:HA3	2:N:52:GLN:HG2	1.98	0.44
2:O:179:GLY:H	2:O:214:LYS:NZ	2.15	0.44
1:C:149:GLN:O	1:C:188:GLN:NE2	2.50	0.44
1:C:365:PRO:HB2	1:C:367:ILE:HG13	1.98	0.44
1:S:190:ARG:NH2	1:S:437:PRO:O	2.51	0.44
2:O:90:GLU:HB2	2:O:111:SER:HB3	1.99	0.44
1:B:156:ASP:O	1:B:385:LEU:HD13	2.18	0.44
3:G:274:ALA:C	3:G:276:SER:H	2.21	0.44
1:T:216:ALA:HA	2:W:124:PHE:CE1	2.52	0.44
1:S:46:LEU:O	1:S:49:ILE:HG22	2.18	0.44
1:J:36:VAL:HG21	1:J:84:VAL:HB	1.99	0.44
2:F:258:ILE:HD11	2:F:292:LEU:HD21	1.99	0.44
2:N:163:LYS:NZ	2:N:256:ASP:OD2	2.50	0.44
1:T:335:ASP:HB2	3:Y:257:ARG:HH11	1.83	0.44
1:L:258:TRP:O	1:L:262:ASN:ND2	2.50	0.44
2:M:458:TYR:O	2:M:460:VAL:HG13	2.18	0.44
2:W:168:GLN:NE2	2:W:204:THR:CG2	2.69	0.44
2:W:67:THR:HB	2:W:70:LEU:HD12	1.99	0.44
1:B:50:GLN:HB3	2:F:69:GLY:HA2	1.98	0.44
2:O:359:ASP:O	2:O:363:VAL:HG22	2.17	0.44
1:A:67:ILE:HD12	1:A:287:LEU:HD22	2.00	0.44
1:J:417:LYS:O	1:J:417:LYS:HG2	2.16	0.44
3:P:92:ALA:HB1	3:P:118:LEU:HD11	2.00	0.44
2:N:136:THR:HG21	2:N:141:VAL:HG11	2.00	0.44
1:K:269:VAL:HG22	1:K:326:LEU:HB2	1.99	0.44
4:Q:16:LEU:HB3	4:Q:17:PRO:HD2	2.00	0.44
2:N:260:ARG:HA	2:N:263:GLN:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:168:GLN:HG2	2:V:197:LEU:CD1	2.48	0.44
2:E:256:ASP:HA	2:E:257:ASN:HA	1.76	0.44
2:D:22:ASP:OD2	2:D:60:ARG:NH2	2.51	0.44
2:O:193:GLU:HA	2:O:196:ASP:HB2	2.00	0.44
1:A:146:GLU:CB	1:A:163:ARG:HG3	2.43	0.44
2:V:208:ASN:HB3	2:V:212:GLU:O	2.18	0.44
2:V:317:LEU:HD22	2:V:326:PHE:HE2	1.83	0.44
3:P:151:LEU:HD23	3:P:156:ALA:HB3	1.99	0.44
1:B:280:TYR:CD2	1:B:303:LEU:HD22	2.53	0.44
2:V:27:GLN:HA	2:V:57:ASN:HD21	1.83	0.44
1:B:111:ASP:OD1	1:B:111:ASP:C	2.56	0.44
1:T:289:ARG:NH1	1:T:289:ARG:CG	2.70	0.43
1:T:212:ARG:HG2	2:W:124:PHE:HA	2.00	0.43
2:F:345:TYR:HA	2:F:346:PRO:C	2.38	0.43
1:A:36:VAL:HG21	1:A:84:VAL:HB	1.99	0.43
1:A:51:ALA:O	1:A:52:GLU:HB2	2.18	0.43
2:M:139:LYS:HG3	2:M:432:VAL:HG21	1.99	0.43
1:S:190:ARG:HH12	1:S:439:ALA:HB2	1.77	0.43
1:U:167:GLU:O	1:U:327:PRO:HD2	2.18	0.43
3:G:80:ASP:OD1	3:G:111:GLY:HA2	2.18	0.43
2:D:16:VAL:HG21	2:D:70:LEU:HB3	2.00	0.43
2:E:335:LEU:HA	2:E:347:ALA:O	2.18	0.43
1:A:394:LEU:HD13	1:A:398:GLN:NE2	2.33	0.43
2:M:249:GLN:NE2	2:M:249:GLN:HA	2.26	0.43
2:M:452:ILE:HG23	2:M:453:PRO:HD2	2.00	0.43
5:I:29:LEU:HA	5:I:29:LEU:HD12	1.79	0.43
1:K:166:ARG:CD	1:K:308:LEU:O	2.64	0.43
2:D:49:GLU:CD	2:D:231:ARG:HE	2.21	0.43
1:S:108:ARG:NH1	1:S:123:ILE:HD13	2.33	0.43
2:W:220:GLY:HA3	2:W:232:VAL:HG11	2.00	0.43
1:S:506:PHE:O	1:S:509:THR:HG22	2.19	0.43
2:O:140:VAL:HA	2:O:414:LEU:HD22	2.00	0.43
2:D:84:SER:HB3	2:D:114:ARG:HB3	1.99	0.43
1:A:280:TYR:CE2	1:A:297:PRO:CG	3.01	0.43
1:S:81:ASP:OD1	1:S:81:ASP:N	2.52	0.43
1:A:480:GLU:CD	1:A:480:GLU:H	2.20	0.43
1:S:439:ALA:HB3	1:S:442:GLU:HG3	2.01	0.43
1:S:453:GLY:C	1:S:455:LEU:H	2.22	0.43
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.99	0.43
1:T:302:TYR:HA	1:T:305:SER:OG	2.18	0.43
3:G:90:GLN:HA	3:G:93:LYS:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:446:LEU:HD11	1:T:467:GLU:HG3	2.00	0.43
2:W:140:VAL:HG13	2:W:414:LEU:HB3	2.01	0.43
2:D:425:THR:HB	2:D:427:ILE:HD12	2.00	0.43
2:F:409:LYS:HE3	2:F:450:ASP:HA	2.01	0.43
1:S:273:LEU:HD22	1:S:304:HIS:CD2	2.54	0.43
1:T:166:ARG:HG2	1:T:311:ALA:HB3	2.00	0.43
1:J:446:LEU:HD11	1:J:471:LEU:HD11	2.00	0.43
3:P:77:ILE:HG21	3:P:222:MET:HA	2.00	0.43
3:Y:267:LEU:O	3:Y:271:ILE:HG12	2.18	0.43
2:E:186:GLY:HA3	2:E:219:PHE:CD1	2.53	0.43
2:E:321:ALA:HB3	2:E:322:PRO:HD3	2.00	0.43
1:J:289:ARG:HD3	1:J:290:PRO:CD	2.40	0.43
2:E:267:GLU:O	2:E:271:LEU:HG	2.19	0.43
2:M:187:VAL:HG22	2:M:232:VAL:HG13	2.00	0.43
3:P:17:GLU:HG3	3:P:248:ILE:HD12	2.01	0.43
1:A:271:ASP:HA	1:A:272:ASP:HA	1.77	0.43
1:A:156:ASP:HB3	1:A:385:LEU:HD21	1.99	0.43
2:N:280:GLY:HA2	3:P:267:LEU:CD2	2.48	0.43
2:F:15:ALA:HB3	2:F:22:ASP:CB	2.38	0.43
2:E:199:ARG:HB2	2:E:199:ARG:HE	1.50	0.43
1:J:174:GLN:O	1:J:174:GLN:HG3	2.18	0.43
2:E:32:ALA:O	2:E:35:ASN:HB2	2.19	0.43
2:X:258:ILE:HD11	2:X:292:LEU:HD21	1.99	0.43
2:E:168:GLN:HE21	2:E:201:MET:HG2	1.84	0.43
1:C:364:ARG:HB3	6:C:600:ANP:N6	2.34	0.43
1:U:167:GLU:HB3	1:U:326:LEU:HD23	2.01	0.43
1:C:280:TYR:CD2	1:C:297:PRO:HG2	2.53	0.43
1:L:181:ALA:HB1	1:L:269:VAL:HG21	2.01	0.43
2:N:140:VAL:HG22	2:N:414:LEU:HB3	2.00	0.43
1:T:208:VAL:HG21	1:T:249:PRO:HG3	2.01	0.43
1:S:269:VAL:HG22	1:S:326:LEU:HB2	2.01	0.43
2:X:144:LEU:O	2:X:358:LEU:HD22	2.19	0.43
2:M:226:PRO:HB2	2:M:268:VAL:HG13	2.00	0.43
1:L:67:ILE:HD12	1:L:287:LEU:HD22	2.01	0.43
2:W:228:ALA:O	2:W:232:VAL:HG22	2.18	0.43
1:B:103:PRO:HD2	1:B:126:ALA:HB2	2.01	0.43
3:G:83:LEU:HB3	3:G:237:MET:CE	2.49	0.43
1:K:36:VAL:HG23	1:K:40:ILE:O	2.19	0.43
2:E:7:THR:N	2:E:8:PRO:HD3	2.34	0.43
1:U:176:GLY:O	1:U:180:VAL:HG23	2.18	0.43
2:M:160:GLY:CA	6:M:600:ANP:HNB1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:427:ILE:HD13	2:F:459:MET:HG2	2.00	0.43
2:X:256:ASP:HA	2:X:257:ASN:HA	1.86	0.43
2:O:63:ALA:O	2:O:227:GLY:HA3	2.19	0.43
1:A:227:ALA:HA	1:A:230:TYR:CE2	2.54	0.43
3:G:18:LYS:O	3:G:22:THR:OG1	2.27	0.43
2:N:370:VAL:O	2:N:374:VAL:HG23	2.19	0.43
2:D:158:GLY:O	2:D:163:LYS:NZ	2.52	0.43
3:G:77:ILE:CD1	3:G:110:ILE:HD12	2.49	0.43
1:J:473:TYR:CZ	1:J:506:PHE:HB2	2.54	0.42
1:B:219:VAL:HG22	1:B:233:ILE:HG13	2.01	0.42
1:S:455:LEU:HD23	1:S:458:ILE:HD12	2.00	0.42
1:K:23:ASP:HB3	1:K:26:ASN:HD22	1.84	0.42
1:J:192:ASN:HA	1:J:200:LYS:HG2	2.01	0.42
1:U:106:LEU:HD22	1:U:230:TYR:HA	2.00	0.42
1:A:354:LEU:HA	1:A:366:ALA:O	2.19	0.42
1:U:103:PRO:HD3	1:U:258:TRP:CZ2	2.54	0.42
1:B:37:GLY:O	1:B:38:ASP:HB2	2.19	0.42
1:C:243:PRO:HA	1:C:246:TYR:HB3	2.01	0.42
3:G:19:ILE:HG22	3:G:23:MET:CE	2.46	0.42
2:F:220:GLY:HA3	2:F:232:VAL:HG11	2.00	0.42
1:S:161:ILE:HD13	1:S:326:LEU:HD21	2.00	0.42
3:P:124:ASN:HA	5:R:49:ASN:HA	2.00	0.42
2:X:247:GLU:O	2:X:249:GLN:HG3	2.19	0.42
1:K:140:PRO:HB3	1:K:318:GLU:HG3	2.01	0.42
4:H:57:VAL:HB	4:H:70:ILE:HD12	2.01	0.42
2:D:174:ILE:HG22	2:D:252:LEU:HD11	2.01	0.42
2:X:39:ILE:HD12	2:X:46:LEU:HD23	2.01	0.42
2:E:150:GLY:O	2:E:297:THR:HA	2.19	0.42
3:G:247:MET:HG2	3:G:250:ARG:NH2	2.35	0.42
1:C:159:VAL:HG11	1:C:372:SER:HB3	2.01	0.42
1:B:314:LEU:HB2	1:B:321:GLY:O	2.19	0.42
1:B:139:LEU:CD2	2:F:105:GLU:HB2	2.49	0.42
1:S:363:ILE:HA	1:S:431:LYS:HE2	2.01	0.42
3:P:139:THR:HG21	5:R:37:ARG:HA	2.02	0.42
2:M:299:THR:OG1	2:M:300:LYS:N	2.52	0.42
2:X:52:GLN:CG	2:X:60:ARG:HB3	2.49	0.42
1:K:27:LEU:CD2	1:K:30:THR:HG22	2.49	0.42
2:V:237:LEU:HD22	2:V:292:LEU:HD12	2.01	0.42
1:S:73:VAL:HG12	1:S:75:ILE:HG13	2.01	0.42
3:G:71:LYS:O	3:G:160:PRO:HD2	2.18	0.42
4:H:88:ILE:HD11	5:I:14:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:GLN:HA	6:C:600:ANP:N3B	2.33	0.42
1:S:455:LEU:HD22	1:S:458:ILE:HD12	2.02	0.42
1:A:82:ARG:HA	2:D:33:ILE:HB	2.02	0.42
2:M:41:THR:HB	2:M:42:PRO:CD	2.49	0.42
2:O:346:PRO:HG3	2:O:418:PHE:CZ	2.55	0.42
1:L:64:MET:H	1:L:75:ILE:HG23	1.85	0.42
1:S:492:SER:HB2	1:S:495:LEU:HB2	2.01	0.42
2:E:322:PRO:O	2:E:326:PHE:HD1	2.03	0.42
1:A:407:GLN:HB3	2:D:387:ILE:HD11	2.02	0.42
1:A:55:VAL:HG21	1:A:75:ILE:HD13	2.01	0.42
2:N:377:THR:HG22	2:N:407:ALA:HB2	2.01	0.42
2:F:95:ILE:HG22	2:F:103:ILE:HG13	2.01	0.42
1:J:426:LEU:O	1:J:430:LEU:HG	2.19	0.42
2:X:237:LEU:CD2	2:X:292:LEU:HD12	2.50	0.42
2:V:202:LYS:HZ3	2:V:209:LEU:HD21	1.85	0.42
1:S:146:GLU:CB	1:S:163:ARG:HG3	2.50	0.42
2:V:166:PHE:CE2	2:V:346:PRO:HB2	2.55	0.42
3:G:90:GLN:HA	3:G:93:LYS:CG	2.50	0.42
1:J:478:HIS:HB3	1:J:481:LEU:HG	2.02	0.42
1:K:398:GLN:HA	1:K:401:GLU:HG3	2.02	0.42
3:Y:32:SER:C	3:Y:34:ALA:H	2.22	0.42
2:X:197:LEU:O	2:X:201:MET:CG	2.60	0.42
2:X:237:LEU:HD21	2:X:295:ARG:HB2	2.00	0.42
1:T:413:ASP:CG	1:T:414:ALA:H	2.23	0.42
2:N:319:ASP:O	2:N:322:PRO:HD2	2.20	0.42
2:V:162:GLY:HA2	6:V:600:ANP:O1A	2.20	0.42
2:O:187:VAL:HG22	2:O:232:VAL:HG13	2.02	0.42
1:A:131:ALA:O	1:A:250:PHE:HB3	2.19	0.42
2:D:71:VAL:O	2:D:74:GLU:HB2	2.20	0.42
1:K:77:LEU:HD12	1:K:81:ASP:HA	2.02	0.42
1:U:253:ALA:O	1:U:257:GLU:HG3	2.19	0.42
2:O:460:VAL:HB	2:O:465:ASP:HB3	2.02	0.42
1:L:35:ALA:HB1	2:O:53:HIS:O	2.20	0.42
2:W:258:ILE:O	2:W:261:PHE:HB3	2.20	0.42
1:S:146:GLU:OE1	1:S:313:LYS:HE2	2.20	0.42
2:N:122:PRO:HB2	2:N:127:GLN:HE21	1.84	0.42
2:O:84:SER:HB3	2:O:114:ARG:HB3	2.02	0.42
2:N:169:GLU:HG2	2:N:418:PHE:CD1	2.55	0.42
1:B:145:HIS:CD2	1:B:146:GLU:HG3	2.55	0.42
2:F:185:THR:OG1	2:F:236:GLY:HA3	2.20	0.42
1:J:99:VAL:HG21	1:J:251:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:168:LEU:HB2	1:K:348:THR:HG21	2.02	0.42
1:J:415:SER:O	1:J:418:GLN:HB2	2.20	0.42
2:E:408:ARG:O	2:E:412:ARG:HD2	2.19	0.42
1:C:274:SER:O	1:C:278:VAL:HG23	2.20	0.42
2:F:50:VAL:CA	2:F:61:THR:HG22	2.41	0.42
1:B:348:THR:O	2:F:190:ARG:NH2	2.53	0.42
2:O:388:ILE:HD12	2:O:396:LEU:HD11	2.02	0.42
1:A:36:VAL:HG12	2:D:53:HIS:HB2	2.02	0.42
2:E:408:ARG:NH1	2:E:454:GLU:OE1	2.50	0.42
2:E:258:ILE:O	2:E:261:PHE:HB3	2.19	0.42
4:Q:45:HIS:O	4:Q:77:VAL:HG11	2.20	0.42
2:N:183:VAL:HG13	2:N:216:ALA:HB3	2.01	0.42
2:E:184:PHE:CD2	2:E:254:PHE:HB2	2.55	0.42
2:F:117:ILE:HG22	2:F:235:THR:HA	2.01	0.41
1:B:309:GLU:OE1	2:F:191:THR:OG1	2.38	0.41
2:E:204:THR:OG1	2:E:420:VAL:HB	2.20	0.41
1:C:146:GLU:CB	1:C:163:ARG:HD2	2.50	0.41
5:R:55:GLU:CB	5:R:56:PRO:HD3	2.50	0.41
1:C:109:VAL:HG12	1:C:117:ILE:HD11	2.01	0.41
1:T:305:SER:HB2	2:X:222:MET:HB2	2.02	0.41
2:W:43:GLN:NE2	2:W:45:LYS:O	2.53	0.41
1:C:349:ASP:O	1:C:375:ARG:HB2	2.20	0.41
1:J:68:LEU:HD23	1:J:73:VAL:HG13	2.02	0.41
2:X:422:GLU:HG3	2:X:427:ILE:O	2.20	0.41
2:E:386:ASP:OD1	2:E:386:ASP:N	2.52	0.41
1:A:163:ARG:O	1:A:313:LYS:HB2	2.20	0.41
2:N:380:THR:O	2:N:384:LEU:HG	2.21	0.41
1:B:142:ARG:HB3	1:B:313:LYS:HG3	2.02	0.41
2:D:311:TYR:CE2	2:D:313:PRO:HA	2.55	0.41
1:T:138:ILE:CD1	2:X:219:PHE:CD2	3.02	0.41
2:E:25:PHE:HB2	2:E:30:LEU:HD23	2.01	0.41
2:F:449:TYR:HD1	2:F:452:ILE:HD12	1.85	0.41
1:T:150:THR:HG21	1:T:155:VAL:HG11	2.02	0.41
2:F:197:LEU:O	2:F:201:MET:HG2	2.19	0.41
1:U:206:VAL:HG11	1:U:249:PRO:HA	2.01	0.41
1:K:135:ALA:HB3	2:O:223:ASN:HD22	1.85	0.41
1:U:28:ASN:HA	1:U:47:ASN:HB2	2.02	0.41
2:D:340:SER:HB3	2:D:347:ALA:HB2	2.00	0.41
2:W:385:GLN:HG2	2:W:385:GLN:H	1.71	0.41
1:B:347:ILE:O	2:F:190:ARG:NE	2.51	0.41
1:C:455:LEU:HD21	1:C:466:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.50	0.41
1:J:112:ALA:O	1:J:251:THR:HG21	2.20	0.41
1:B:98:ASP:HB2	1:B:129:SER:O	2.20	0.41
1:K:184:THR:O	1:K:188:GLN:HG2	2.20	0.41
1:B:270:TYR:HB2	1:B:327:PRO:HA	2.01	0.41
1:K:272:ASP:HB2	1:K:328:VAL:O	2.21	0.41
1:U:178:THR:HG23	1:U:271:ASP:OD2	2.19	0.41
3:G:118:LEU:HB3	3:G:126:ILE:HD11	2.02	0.41
3:P:25:ILE:HA	3:P:28:SER:OG	2.19	0.41
3:G:60:LEU:HD21	3:G:190:GLN:HB2	2.02	0.41
2:X:191:THR:HA	2:X:221:GLN:HG3	2.01	0.41
1:T:173:ARG:HB3	1:T:173:ARG:NH1	2.36	0.41
1:L:162:GLY:CA	1:L:380:ALA:HB1	2.51	0.41
1:B:408:PHE:CD2	1:B:411:ASP:HB3	2.56	0.41
1:B:421:VAL:O	1:B:425:ARG:HG2	2.21	0.41
1:C:152:LEU:HA	1:C:432:GLN:OE1	2.21	0.41
2:X:137:GLY:HA2	2:X:432:VAL:O	2.21	0.41
1:S:217:GLN:HA	2:V:129:THR:HG21	2.02	0.41
2:V:99:ILE:H	2:V:99:ILE:HG12	1.63	0.41
2:W:85:VAL:HG11	2:W:235:THR:CG2	2.39	0.41
2:V:296:ILE:HG23	2:V:304:VAL:HG12	2.01	0.41
3:Y:9:ARG:HD3	3:Y:251:TYR:HE1	1.82	0.41
1:S:243:PRO:CG	1:S:283:LEU:HD21	2.48	0.41
1:U:153:LYS:HA	1:U:443:GLN:OE1	2.20	0.41
1:J:309:GLU:CB	2:N:223:ASN:HB3	2.50	0.41
1:T:203:CYS:HB2	1:T:231:SER:HB3	2.01	0.41
1:U:468:SER:O	1:U:472:SER:HB2	2.21	0.41
1:A:165:GLN:O	1:A:324:THR:HG23	2.20	0.41
2:E:416:GLN:NE2	2:E:430:LYS:O	2.54	0.41
1:T:204:VAL:O	1:T:268:ILE:HA	2.19	0.41
2:N:443:ALA:HB1	2:N:449:TYR:HE2	1.85	0.41
2:N:275:ILE:HA	2:N:276:PRO:HD3	1.90	0.41
2:D:253:LEU:O	2:D:306:SER:HA	2.20	0.41
1:L:354:LEU:HA	1:L:366:ALA:O	2.21	0.41
1:B:285:LEU:HD22	2:E:275:ILE:HG21	2.03	0.41
1:S:55:VAL:HG21	1:S:75:ILE:HD13	2.01	0.41
1:L:383:LYS:HE3	1:L:386:LYS:HD3	2.02	0.41
1:U:184:THR:O	1:U:188:GLN:HG2	2.21	0.41
1:A:146:GLU:HA	1:A:147:PRO:HD3	1.94	0.41
1:U:168:LEU:CD2	1:U:345:ILE:HG13	2.51	0.41
2:W:133:ILE:HD13	2:W:357:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:191:TRP:HD1	1:K:199:LYS:HB3	1.85	0.41
2:V:52:GLN:NE2	2:V:60:ARG:HD2	2.35	0.41
1:J:182:LEU:HD21	1:J:435:TYR:HE1	1.86	0.41
1:T:387:GLN:HE22	1:T:491:LEU:H	1.68	0.41
1:K:96:ILE:O	1:K:97:VAL:C	2.59	0.41
3:G:169:PRO:HB3	3:G:228:ALA:HB2	2.03	0.41
2:F:85:VAL:HG11	2:F:235:THR:CG2	2.44	0.41
1:C:65:ALA:HA	1:C:75:ILE:HG12	2.02	0.41
1:T:30:THR:CG2	1:T:31:GLY:N	2.83	0.41
3:Y:253:ILE:HG22	3:Y:257:ARG:NH1	2.36	0.41
1:C:462:ARG:O	1:C:465:GLU:HG2	2.21	0.41
2:V:250:ASP:OD2	2:V:303:SER:HB3	2.21	0.41
2:M:269:SER:O	2:M:274:ARG:HB2	2.21	0.41
2:M:34:LEU:HD13	2:M:118:HIS:CG	2.56	0.41
2:V:148:ALA:O	2:V:150:GLY:N	2.53	0.41
2:X:405:GLU:O	2:X:409:LYS:HG3	2.20	0.41
3:G:115:LYS:O	3:G:119:LEU:HB2	2.21	0.41
1:S:158:LEU:HD22	1:S:393:LYS:HG2	2.03	0.41
1:B:271:ASP:HA	1:B:272:ASP:HA	1.68	0.41
3:G:50:LEU:CG	4:H:78:GLN:HE21	2.33	0.41
2:X:182:SER:O	2:X:215:VAL:HA	2.21	0.41
1:A:440:THR:O	1:A:444:VAL:HG13	2.20	0.41
2:X:33:ILE:HA	2:X:50:VAL:HG12	2.03	0.41
2:V:168:GLN:HG2	2:V:197:LEU:HD13	2.03	0.41
2:F:95:ILE:HD11	2:F:198:TYR:CG	2.55	0.41
1:T:138:ILE:O	2:X:195:ASN:ND2	2.53	0.41
1:B:311:ALA:HA	1:B:323:LEU:HB3	2.03	0.41
2:N:346:PRO:HB2	2:N:348:VAL:HG23	2.02	0.41
2:E:134:LEU:HB2	2:E:149:ARG:HB2	2.03	0.41
2:O:186:GLY:HA2	2:O:256:ASP:O	2.20	0.41
2:W:278:ALA:HA	3:Y:264:THR:HG23	2.02	0.41
4:H:71:SER:HB2	4:H:89:GLU:HB2	2.01	0.41
1:C:139:LEU:HD13	2:D:104:ASP:HA	2.02	0.41
1:U:136:PRO:HD2	1:U:310:ARG:HA	2.02	0.41
1:B:469:SER:HB3	1:B:506:PHE:HZ	1.86	0.41
1:L:455:LEU:HD21	1:L:466:PHE:CE1	2.56	0.41
1:T:340:ILE:N	1:T:341:PRO:CD	2.84	0.41
1:A:463:ILE:O	1:A:466:PHE:HB3	2.20	0.41
2:W:321:ALA:HB3	2:W:322:PRO:CD	2.50	0.41
1:J:254:SER:O	1:J:257:GLU:HB2	2.20	0.41
2:M:409:LYS:O	2:M:413:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:96:ILE:HB	2:E:218:VAL:HG22	2.03	0.41
2:M:9:ILE:HD12	2:M:9:ILE:H	1.85	0.41
1:C:455:LEU:HD21	1:C:466:PHE:CE1	2.55	0.41
1:T:444:VAL:HG22	1:T:445:PRO:HD3	2.03	0.41
2:M:154:GLY:HA3	2:M:329:LEU:HD13	2.03	0.41
1:A:237:THR:N	1:A:240:GLU:HG3	2.36	0.41
1:C:192:ASN:HA	1:C:200:LYS:HG2	2.02	0.41
2:N:142:ASP:HA	2:N:146:PRO:HB3	2.01	0.41
2:E:287:THR:O	2:E:291:LEU:HG	2.21	0.41
2:D:198:TYR:O	2:D:202:LYS:HG3	2.21	0.41
1:S:202:TYR:O	1:S:266:ALA:HA	2.21	0.41
2:M:263:GLN:O	2:M:266:SER:HB3	2.21	0.41
2:E:276:PRO:HD2	3:G:271:ILE:HG13	2.02	0.41
1:K:86:GLU:OE1	2:N:30:LEU:HD11	2.20	0.41
2:V:147:TYR:CD2	2:V:153:ILE:HD13	2.56	0.41
2:M:52:GLN:HE21	2:M:52:GLN:HB2	1.68	0.41
2:W:204:THR:HG22	2:W:206:VAL:H	1.86	0.40
1:B:369:VAL:HG13	1:B:393:LYS:HD2	2.03	0.40
2:F:258:ILE:HG22	2:F:310:VAL:HG22	2.02	0.40
2:E:67:THR:HB	2:E:70:LEU:HD12	2.02	0.40
1:B:166:ARG:HD2	1:B:308:LEU:O	2.21	0.40
1:T:444:VAL:N	1:T:445:PRO:CD	2.84	0.40
2:N:240:ALA:HB2	2:N:253:LEU:HD13	2.04	0.40
2:F:136:THR:HA	2:F:174:ILE:HD11	2.03	0.40
2:M:237:LEU:HD21	2:M:295:ARG:CB	2.49	0.40
3:P:108:VAL:HG21	3:P:150:LEU:HD11	2.04	0.40
1:A:506:PHE:O	1:A:509:THR:HG22	2.21	0.40
2:E:193:GLU:O	2:E:196:ASP:HB2	2.21	0.40
3:P:95:VAL:O	3:P:99:LEU:HB2	2.21	0.40
2:N:184:PHE:HA	2:N:254:PHE:HB2	2.03	0.40
1:C:271:ASP:HA	1:C:272:ASP:HA	1.79	0.40
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.91	0.40
1:T:158:LEU:HB3	1:T:393:LYS:HD3	2.04	0.40
2:X:189:GLU:O	2:X:222:MET:HG2	2.21	0.40
2:M:41:THR:HB	2:M:42:PRO:HD2	2.03	0.40
1:A:250:PHE:CE1	1:A:307:LEU:HB2	2.56	0.40
2:N:89:ARG:C	2:N:91:THR:H	2.22	0.40
1:L:36:VAL:HG21	1:L:84:VAL:HB	2.02	0.40
1:C:34:LEU:N	1:C:42:ARG:O	2.52	0.40
2:O:33:ILE:HG22	2:O:34:LEU:HG	2.03	0.40
2:F:224:GLU:HA	2:F:225:PRO:HD3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:111:ASP:OD1	1:U:111:ASP:C	2.60	0.40
1:T:187:ASN:OD1	1:T:437:PRO:HB2	2.21	0.40
1:L:340:ILE:HB	1:L:341:PRO:HD3	2.04	0.40
1:A:280:TYR:CE2	1:A:297:PRO:HG2	2.56	0.40
1:K:272:ASP:OD1	1:K:272:ASP:C	2.58	0.40
3:P:185:ALA:HB2	3:P:207:ARG:HA	2.02	0.40
2:W:109:ILE:HG22	2:W:111:SER:HB2	2.02	0.40
1:U:228:MET:HA	1:U:231:SER:HB2	2.04	0.40
2:O:141:VAL:HG22	2:O:333:THR:HG21	2.02	0.40
1:A:257:GLU:HG2	1:A:260:ARG:CZ	2.52	0.40
3:G:39:ILE:O	3:G:43:LYS:HB2	2.22	0.40
3:P:256:ASN:HA	3:P:259:ARG:HB3	2.02	0.40
1:J:289:ARG:HH21	2:N:17:ILE:HG21	1.87	0.40
1:J:44:PHE:C	1:J:44:PHE:CD2	2.95	0.40
2:N:98:VAL:HB	2:N:232:VAL:HG13	2.03	0.40
1:U:153:LYS:NZ	1:U:467:GLU:OE1	2.54	0.40
2:N:345:TYR:HA	2:N:346:PRO:C	2.41	0.40
1:L:165:GLN:HB2	1:L:376:VAL:HG21	2.03	0.40
1:C:488:LYS:C	1:C:490:GLU:H	2.25	0.40
2:F:442:LYS:O	2:F:446:GLU:HG3	2.22	0.40
1:A:211:LYS:HE3	1:A:213:SER:OG	2.21	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	483/510 (95%)	457 (95%)	25 (5%)	1 (0%)	52 88
1	B	484/510 (95%)	455 (94%)	25 (5%)	4 (1%)	24 69
1	C	482/510 (94%)	458 (95%)	23 (5%)	1 (0%)	52 88
1	J	478/510 (94%)	443 (93%)	32 (7%)	3 (1%)	30 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	479/510 (94%)	442 (92%)	37 (8%)	0	100	100
1	L	475/510 (93%)	442 (93%)	31 (6%)	2 (0%)	39	80
1	S	479/510 (94%)	458 (96%)	20 (4%)	1 (0%)	52	88
1	T	480/510 (94%)	454 (95%)	26 (5%)	0	100	100
1	U	483/510 (95%)	450 (93%)	31 (6%)	2 (0%)	39	80
2	D	468/484 (97%)	440 (94%)	26 (6%)	2 (0%)	39	80
2	E	467/484 (96%)	437 (94%)	28 (6%)	2 (0%)	39	80
2	F	467/484 (96%)	443 (95%)	24 (5%)	0	100	100
2	M	458/484 (95%)	421 (92%)	34 (7%)	3 (1%)	26	72
2	N	459/484 (95%)	422 (92%)	34 (7%)	3 (1%)	26	72
2	O	467/484 (96%)	433 (93%)	33 (7%)	1 (0%)	52	88
2	V	354/484 (73%)	318 (90%)	31 (9%)	5 (1%)	14	57
2	W	466/484 (96%)	435 (93%)	30 (6%)	1 (0%)	52	88
2	X	467/484 (96%)	430 (92%)	35 (8%)	2 (0%)	39	80
3	G	264/278 (95%)	249 (94%)	14 (5%)	1 (0%)	39	80
3	P	264/278 (95%)	243 (92%)	19 (7%)	2 (1%)	24	69
3	Y	109/278 (39%)	102 (94%)	7 (6%)	0	100	100
4	H	118/138 (86%)	98 (83%)	17 (14%)	3 (2%)	7	41
4	Q	91/138 (66%)	81 (89%)	10 (11%)	0	100	100
5	I	51/61 (84%)	44 (86%)	3 (6%)	4 (8%)	1	8
5	R	51/61 (84%)	43 (84%)	7 (14%)	1 (2%)	9	48
All	All	9344/10178 (92%)	8698 (93%)	602 (6%)	44 (0%)	34	78

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	99	GLU
5	I	55	GLU
2	M	27	GLN
5	R	58	PRO
4	H	33	PRO
5	I	13	TYR
2	M	279	VAL
3	P	170	VAL
1	S	97	VAL

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Mol	Chain	Res	Type
1	B	27	LEU
2	E	366	GLU
4	H	100	ASN
1	U	390	GLY
2	V	28	SER
1	B	390	GLY
1	B	415	SER
5	I	58	PRO
1	J	379	ALA
2	M	29	GLU
1	U	70	PRO
1	A	70	PRO
3	G	202	ASP
5	I	8	ILE
1	J	70	PRO
1	L	283	LEU
3	P	243	ASN
2	V	149	ARG
2	V	354	LYS
2	X	123	SER
1	B	367	ILE
2	N	221	GLN
1	C	489	GLY
2	D	188	GLY
2	V	279	VAL
2	D	279	VAL
2	E	279	VAL
2	O	108	PRO
2	N	279	VAL
1	J	97	VAL
1	L	122	PRO
2	N	87	VAL
2	W	279	VAL
2	V	44	GLY
2	X	279	VAL

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	391/412 (95%)	361 (92%)	30 (8%)	16 54
1	B	390/412 (95%)	369 (95%)	21 (5%)	27 68
1	C	390/412 (95%)	369 (95%)	21 (5%)	27 68
1	J	388/412 (94%)	367 (95%)	21 (5%)	27 68
1	K	366/412 (89%)	348 (95%)	18 (5%)	31 72
1	L	378/412 (92%)	359 (95%)	19 (5%)	30 71
1	S	382/412 (93%)	357 (94%)	25 (6%)	21 61
1	T	379/412 (92%)	353 (93%)	26 (7%)	19 59
1	U	348/412 (84%)	329 (94%)	19 (6%)	27 68
2	D	379/390 (97%)	362 (96%)	17 (4%)	34 74
2	E	371/390 (95%)	345 (93%)	26 (7%)	19 58
2	F	378/390 (97%)	358 (95%)	20 (5%)	28 69
2	M	363/390 (93%)	339 (93%)	24 (7%)	21 61
2	N	352/390 (90%)	330 (94%)	22 (6%)	22 63
2	O	357/390 (92%)	339 (95%)	18 (5%)	30 71
2	V	261/390 (67%)	246 (94%)	15 (6%)	25 67
2	W	361/390 (93%)	343 (95%)	18 (5%)	30 71
2	X	354/390 (91%)	342 (97%)	12 (3%)	44 80
3	G	226/236 (96%)	206 (91%)	20 (9%)	12 45
3	P	178/236 (75%)	160 (90%)	18 (10%)	9 36
3	Y	72/236 (30%)	64 (89%)	8 (11%)	8 32
4	H	71/112 (63%)	62 (87%)	9 (13%)	5 25
4	Q	46/112 (41%)	43 (94%)	3 (6%)	21 61
5	I	34/48 (71%)	27 (79%)	7 (21%)	1 7
5	R	28/48 (58%)	26 (93%)	2 (7%)	18 57
All	All	7243/8246 (88%)	6804 (94%)	439 (6%)	23 64

All (439) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	88	GLU

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Mol	Chain	Res	Type
1	A	142	ARG
1	A	156	ASP
1	A	163	ARG
1	A	166	ARG
1	A	173	ARG
1	A	211	LYS
1	A	274	SER
1	A	289	ARG
1	A	306	ARG
1	A	342	THR
1	A	357	GLU
1	A	378	SER
1	A	394	LEU
1	A	401	GLU
1	A	408	PHE
1	A	411	ASP
1	A	429	LEU
1	A	436	SER
1	A	444	VAL
1	A	465	GLU
1	A	468	SER
1	A	480	GLU
1	A	492	SER
1	A	495	LEU
1	A	498	SER
1	A	505	SER
1	A	509	THR
1	A	510	PHE
1	B	30	THR
1	B	40	ILE
1	B	72	GLN
1	B	89	LEU
1	B	99	VAL
1	B	106	LEU
1	B	195	SER
1	B	196	ASP
1	B	246	TYR
1	B	309	GLU
1	B	336	VAL
1	B	351	GLN
1	B	378	SER
1	B	391	SER

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Mol	Chain	Res	Type
1	B	399	TYR
1	B	408	PHE
1	B	434	GLN
1	B	444	VAL
1	B	463	ILE
1	B	472	SER
1	B	480	GLU
1	C	54	LEU
1	C	62	LYS
1	C	99	VAL
1	C	163	ARG
1	C	166	ARG
1	C	183	ASP
1	C	223	GLU
1	C	267	LEU
1	C	284	SER
1	C	293	ARG
1	C	364	ARG
1	C	373	VAL
1	C	394	LEU
1	C	417	LYS
1	C	418	GLN
1	C	424	GLU
1	C	440	THR
1	C	456	ASP
1	C	477	ASN
1	C	479	ASN
1	C	509	THR
2	D	7	THR
2	D	9	ILE
2	D	17	ILE
2	D	52	GLN
2	D	62	ILE
2	D	77	LEU
2	D	84	SER
2	D	132	GLU
2	D	149	ARG
2	D	176	LYS
2	D	185	THR
2	D	192	ARG
2	D	268	VAL
2	D	285	LEU

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Mol	Chain	Res	Type
2	D	289	MET
2	D	303	SER
2	D	388	ILE
2	E	10	THR
2	E	17	ILE
2	E	27	GLN
2	E	56	GLU
2	E	68	GLU
2	E	128	SER
2	E	136	THR
2	E	140	VAL
2	E	152	LYS
2	E	164	THR
2	E	204	THR
2	E	210	GLU
2	E	221	GLN
2	E	224	GLU
2	E	232	VAL
2	E	263	GLN
2	E	292	LEU
2	E	337	ARG
2	E	352	ASP
2	E	378	LEU
2	E	386	ASP
2	E	391	LEU
2	E	399	GLN
2	E	403	THR
2	E	412	ARG
2	E	433	ARG
2	F	12	LYS
2	F	17	ILE
2	F	28	SER
2	F	30	LEU
2	F	43	GLN
2	F	128	SER
2	F	130	SER
2	F	140	VAL
2	F	167	ILE
2	F	168	GLN
2	F	191	THR
2	F	208	ASN
2	F	274	ARG

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Mol	Chain	Res	Type
2	F	279	VAL
2	F	299	THR
2	F	306	SER
2	F	397	SER
2	F	403	THR
2	F	413	PHE
2	F	465	ASP
3	G	3	LEU
3	G	4	LYS
3	G	7	GLU
3	G	22	THR
3	G	48	GLU
3	G	53	LYS
3	G	102	GLN
3	G	118	LEU
3	G	136	ASP
3	G	143	SER
3	G	145	LEU
3	G	150	LEU
3	G	173	LEU
3	G	190	GLN
3	G	202	ASP
3	G	204	ASN
3	G	207	ARG
3	G	231	SER
3	G	254	LEU
3	G	275	SER
4	H	14	PHE
4	H	20	THR
4	H	28	THR
4	H	35	LYS
4	H	42	LEU
4	H	48	THR
4	H	60	MET
4	H	66	LYS
4	H	70	ILE
5	I	14	LEU
5	I	28	GLU
5	I	29	LEU
5	I	35	LEU
5	I	37	ARG
5	I	38	SER

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Mol	Chain	Res	Type
5	I	57	THR
1	J	27	LEU
1	J	44	PHE
1	J	54	LEU
1	J	58	SER
1	J	72	GLN
1	J	81	ASP
1	J	142	ARG
1	J	163	ARG
1	J	166	ARG
1	J	173	ARG
1	J	289	ARG
1	J	342	THR
1	J	369	VAL
1	J	375	ARG
1	J	407	GLN
1	J	411	ASP
1	J	419	THR
1	J	429	LEU
1	J	473	TYR
1	J	483	THR
1	J	509	THR
1	K	30	THR
1	K	52	GLU
1	K	59	SER
1	K	66	LEU
1	K	99	VAL
1	K	106	LEU
1	K	129	SER
1	K	178	THR
1	K	195	SER
1	K	218	LEU
1	K	246	TYR
1	K	283	LEU
1	K	351	GLN
1	K	378	SER
1	K	407	GLN
1	K	418	GLN
1	K	422	ARG
1	K	456	ASP
1	L	32	ARG
1	L	54	LEU

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Mol	Chain	Res	Type
1	L	66	LEU
1	L	72	GLN
1	L	89	LEU
1	L	99	VAL
1	L	166	ARG
1	L	173	ARG
1	L	214	THR
1	L	220	GLN
1	L	293	ARG
1	L	300	VAL
1	L	351	GLN
1	L	394	LEU
1	L	433	ASN
1	L	477	ASN
1	L	479	ASN
1	L	487	GLU
1	L	507	VAL
2	M	26	GLU
2	M	113	LEU
2	M	133	ILE
2	M	192	ARG
2	M	199	ARG
2	M	206	VAL
2	M	215	VAL
2	M	247	GLU
2	M	249	GLN
2	M	251	VAL
2	M	274	ARG
2	M	292	LEU
2	M	306	SER
2	M	315	ASP
2	M	336	SER
2	M	342	LEU
2	M	377	THR
2	M	394	ASP
2	M	413	PHE
2	M	422	GLU
2	M	431	LEU
2	M	455	HIS
2	M	464	GLU
2	M	465	ASP
2	N	10	THR

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Mol	Chain	Res	Type
2	N	56	GLU
2	N	57	ASN
2	N	68	GLU
2	N	103	ILE
2	N	113	LEU
2	N	189	GLU
2	N	196	ASP
2	N	210	GLU
2	N	232	VAL
2	N	251	VAL
2	N	275	ILE
2	N	298	THR
2	N	337	ARG
2	N	352	ASP
2	N	377	THR
2	N	386	ASP
2	N	405	GLU
2	N	423	VAL
2	N	436	ASP
2	N	437	THR
2	N	450	ASP
2	O	40	LYS
2	O	68	GLU
2	O	111	SER
2	O	140	VAL
2	O	172	ASN
2	O	176	LYS
2	O	206	VAL
2	O	208	ASN
2	O	224	GLU
2	O	274	ARG
2	O	277	SER
2	O	289	MET
2	O	300	LYS
2	O	359	ASP
2	O	377	THR
2	O	423	VAL
2	O	427	ILE
2	O	455	HIS
3	P	23	MET
3	P	29	THR
3	P	43	LYS

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Mol	Chain	Res	Type
3	P	44	MET
3	P	78	THR
3	P	112	ASP
3	P	117	GLN
3	P	150	LEU
3	P	158	THR
3	P	190	GLN
3	P	202	ASP
3	P	204	ASN
3	P	234	ARG
3	P	248	ILE
3	P	254	LEU
3	P	266	GLU
3	P	269	ASP
3	P	276	SER
4	Q	14	PHE
4	Q	51	GLN
4	Q	76	THR
5	R	4	ARG
5	R	5	LYS
1	S	36	VAL
1	S	81	ASP
1	S	124	ASP
1	S	129	SER
1	S	142	ARG
1	S	153	LYS
1	S	163	ARG
1	S	166	ARG
1	S	221	THR
1	S	251	THR
1	S	289	ARG
1	S	318	GLU
1	S	359	PHE
1	S	364	ARG
1	S	378	SER
1	S	393	LYS
1	S	394	LEU
1	S	395	PHE
1	S	413	ASP
1	S	444	VAL
1	S	465	GLU
1	S	468	SER

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Mol	Chain	Res	Type
1	S	495	LEU
1	S	501	SER
1	S	509	THR
1	T	36	VAL
1	T	59	SER
1	T	62	LYS
1	T	91	LYS
1	T	99	VAL
1	T	159	VAL
1	T	214	THR
1	T	246	TYR
1	T	274	SER
1	T	283	LEU
1	T	288	ARG
1	T	289	ARG
1	T	299	ASP
1	T	317	LYS
1	T	351	GLN
1	T	369	VAL
1	T	394	LEU
1	T	399	TYR
1	T	400	ARG
1	T	419	THR
1	T	422	ARG
1	T	460	LEU
1	T	465	GLU
1	T	472	SER
1	T	484	GLU
1	T	501	SER
1	U	27	LEU
1	U	30	THR
1	U	56	GLU
1	U	61	VAL
1	U	72	GLN
1	U	99	VAL
1	U	129	SER
1	U	159	VAL
1	U	213	SER
1	U	220	GLN
1	U	254	SER
1	U	290	PRO
1	U	346	SER

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Mol	Chain	Res	Type
1	U	357	GLU
1	U	376	VAL
1	U	418	GLN
1	U	424	GLU
1	U	472	SER
1	U	495	LEU
2	V	9	ILE
2	V	17	ILE
2	V	65	ASP
2	V	87	VAL
2	V	99	ILE
2	V	167	ILE
2	V	192	ARG
2	V	204	THR
2	V	269	SER
2	V	274	ARG
2	V	285	LEU
2	V	301	LYS
2	V	306	SER
2	V	315	ASP
2	V	369	ASP
2	W	22	ASP
2	W	74	GLU
2	W	113	LEU
2	W	136	THR
2	W	140	VAL
2	W	176	LYS
2	W	204	THR
2	W	221	GLN
2	W	232	VAL
2	W	337	ARG
2	W	352	ASP
2	W	366	GLU
2	W	380	THR
2	W	386	ASP
2	W	403	THR
2	W	406	ARG
2	W	423	VAL
2	W	434	LEU
2	X	68	GLU
2	X	140	VAL
2	X	167	ILE

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Mol	Chain	Res	Type
2	X	208	ASN
2	X	210	GLU
2	X	224	GLU
2	X	251	VAL
2	X	274	ARG
2	X	285	LEU
2	X	383	SER
2	X	403	THR
2	X	420	VAL
3	Y	2	THR
3	Y	3	LEU
3	Y	23	MET
3	Y	219	LEU
3	Y	220	THR
3	Y	239	ASN
3	Y	254	LEU
3	Y	275	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	GLN
1	B	50	GLN
1	B	115	ASN
1	C	48	ASN
1	C	95	ASN
1	C	174	GLN
1	C	454	HIS
2	D	52	GLN
2	D	195	ASN
2	E	168	GLN
2	E	221	GLN
2	F	27	GLN
2	F	208	ASN
3	G	102	GLN
3	G	122	HIS
3	G	216	ASN
3	G	217	GLN
4	H	13	GLN
4	H	82	GLN
5	I	36	ASN
5	I	49	ASN

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Mol	Chain	Res	Type
1	J	115	ASN
1	J	224	GLN
1	J	381	GLN
1	J	407	GLN
1	K	26	ASN
1	K	192	ASN
1	K	428	GLN
1	K	477	ASN
1	L	145	HIS
1	L	174	GLN
1	L	351	GLN
1	L	368	ASN
1	L	387	GLN
2	M	52	GLN
2	M	178	HIS
2	M	195	ASN
2	M	249	GLN
2	M	375	GLN
2	N	127	GLN
2	N	263	GLN
2	O	24	HIS
2	O	97	ASN
2	O	208	ASN
3	P	125	ASN
4	Q	45	HIS
5	R	15	ASN
1	S	145	HIS
1	S	220	GLN
1	S	351	GLN
1	S	407	GLN
1	S	477	ASN
1	T	387	GLN
1	U	418	GLN
2	V	52	GLN
2	V	249	GLN
2	V	367	HIS
2	W	168	GLN
2	W	367	HIS
2	W	411	GLN
2	X	52	GLN
2	X	208	ASN

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 30 ligands modelled in this entry, 15 are monoatomic - leaving 15 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	1.93	7 (25%)	30,52,52	2.28	8 (26%)
6	ANP	B	600	7	27,33,33	2.04	7 (25%)	30,52,52	2.21	8 (26%)
6	ANP	C	600	7	27,33,33	2.05	7 (25%)	30,52,52	2.40	8 (26%)
6	ANP	D	600	7	27,33,33	2.03	7 (25%)	30,52,52	2.13	8 (26%)
6	ANP	F	600	7	27,33,33	2.05	6 (22%)	30,52,52	2.02	7 (23%)
6	ANP	J	600	7	27,33,33	1.97	6 (22%)	30,52,52	2.41	8 (26%)
6	ANP	K	600	7	27,33,33	2.15	6 (22%)	30,52,52	2.16	8 (26%)
6	ANP	L	600	7	27,33,33	1.97	5 (18%)	30,52,52	2.27	8 (26%)
6	ANP	M	600	7	27,33,33	1.96	7 (25%)	30,52,52	2.55	8 (26%)
6	ANP	O	600	7	27,33,33	2.08	9 (33%)	30,52,52	2.20	8 (26%)
6	ANP	S	600	7	27,33,33	2.11	6 (22%)	30,52,52	2.34	6 (20%)
6	ANP	T	600	7	27,33,33	2.09	8 (29%)	30,52,52	2.25	7 (23%)
6	ANP	U	600	7	27,33,33	2.05	7 (25%)	30,52,52	2.23	7 (23%)
6	ANP	V	600	7	27,33,33	2.39	7 (25%)	30,52,52	2.39	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	ANP	X	600	7	27,33,33	1.79	6 (22%)	30,52,52	2.70	9 (30%)

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	-	1/12/38/38	0/3/3/3
6	ANP	B	600	7	-	1/12/38/38	0/3/3/3
6	ANP	C	600	7	-	2/12/38/38	0/3/3/3
6	ANP	D	600	7	-	0/12/38/38	0/3/3/3
6	ANP	F	600	7	-	0/12/38/38	0/3/3/3
6	ANP	J	600	7	-	2/12/38/38	0/3/3/3
6	ANP	K	600	7	-	1/12/38/38	0/3/3/3
6	ANP	L	600	7	-	0/12/38/38	0/3/3/3
6	ANP	M	600	7	-	1/12/38/38	0/3/3/3
6	ANP	O	600	7	-	0/12/38/38	0/3/3/3
6	ANP	S	600	7	-	0/12/38/38	0/3/3/3
6	ANP	T	600	7	-	1/12/38/38	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 (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	600	ANP	PG-O3G	-2.34	1.50	1.56
6	A	600	ANP	PG-O3G	-2.31	1.50	1.56
6	A	600	ANP	PG-O2G	-2.30	1.50	1.56
6	C	600	ANP	PG-O2G	-2.28	1.50	1.56
6	D	600	ANP	PG-O3G	-2.26	1.50	1.56
6	X	600	ANP	PG-O2G	-2.17	1.50	1.56
6	B	600	ANP	PG-O2G	-2.10	1.50	1.56
6	O	600	ANP	PG-O3G	-2.06	1.50	1.56
6	O	600	ANP	PG-O2G	-2.01	1.51	1.56
6	T	600	ANP	PB-O2B	-2.01	1.51	1.56
6	T	600	ANP	PG-O3G	-2.00	1.51	1.56
6	S	600	ANP	C2-N3	2.03	1.35	1.32
6	J	600	ANP	O4'-C1'	2.03	1.43	1.41
6	U	600	ANP	C2-N3	2.05	1.35	1.32
6	T	600	ANP	PB-O3A	2.07	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	600	ANP	O4'-C1'	2.09	1.43	1.41
6	M	600	ANP	PB-O3A	2.11	1.61	1.59
6	O	600	ANP	PB-O3A	2.15	1.61	1.59
6	C	600	ANP	C2-N3	2.22	1.36	1.32
6	O	600	ANP	O4'-C1'	2.24	1.44	1.41
6	V	600	ANP	O4'-C1'	2.38	1.44	1.41
6	K	600	ANP	O4'-C1'	2.44	1.44	1.41
6	B	600	ANP	PB-O3A	2.48	1.62	1.59
6	U	600	ANP	PB-O3A	2.57	1.62	1.59
6	F	600	ANP	PB-O3A	2.74	1.62	1.59
6	A	600	ANP	C5-C4	3.09	1.47	1.40
6	S	600	ANP	C5-C4	3.11	1.47	1.40
6	J	600	ANP	C5-C4	3.15	1.47	1.40
6	X	600	ANP	C5-C4	3.16	1.47	1.40
6	F	600	ANP	C5-C4	3.17	1.47	1.40
6	L	600	ANP	C5-C4	3.22	1.47	1.40
6	X	600	ANP	PB-O1B	3.25	1.49	1.46
6	D	600	ANP	C5-C4	3.25	1.47	1.40
6	V	600	ANP	C5-C4	3.27	1.47	1.40
6	U	600	ANP	C5-C4	3.33	1.48	1.40
6	M	600	ANP	C5-C4	3.38	1.48	1.40
6	B	600	ANP	C5-C4	3.38	1.48	1.40
6	V	600	ANP	PB-O3A	3.43	1.63	1.59
6	C	600	ANP	C5-C4	3.45	1.48	1.40
6	O	600	ANP	C5-C4	3.45	1.48	1.40
6	T	600	ANP	C5-C4	3.46	1.48	1.40
6	K	600	ANP	C5-C4	3.53	1.48	1.40
6	X	600	ANP	PG-O1G	3.61	1.50	1.46
6	J	600	ANP	PG-N3B	3.68	1.73	1.63
6	A	600	ANP	PG-N3B	3.69	1.73	1.63
6	X	600	ANP	PB-N3B	3.71	1.73	1.63
6	A	600	ANP	PB-N3B	3.75	1.73	1.63
6	M	600	ANP	PG-N3B	3.80	1.73	1.63
6	B	600	ANP	PB-O1B	3.80	1.50	1.46
6	X	600	ANP	PG-N3B	3.81	1.73	1.63
6	C	600	ANP	PB-N3B	3.87	1.73	1.63
6	C	600	ANP	PG-N3B	3.89	1.73	1.63
6	U	600	ANP	PG-N3B	3.91	1.73	1.63
6	L	600	ANP	PB-N3B	3.92	1.73	1.63
6	M	600	ANP	PG-O1G	3.94	1.50	1.46
6	B	600	ANP	PG-N3B	3.95	1.73	1.63
6	K	600	ANP	PG-N3B	3.95	1.73	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	600	ANP	PB-O1B	3.97	1.50	1.46
6	M	600	ANP	PB-N3B	4.00	1.73	1.63
6	J	600	ANP	PB-N3B	4.02	1.74	1.63
6	T	600	ANP	PG-N3B	4.04	1.74	1.63
6	A	600	ANP	PB-O1B	4.07	1.50	1.46
6	K	600	ANP	PB-N3B	4.07	1.74	1.63
6	O	600	ANP	PG-N3B	4.12	1.74	1.63
6	D	600	ANP	PB-O1B	4.12	1.50	1.46
6	L	600	ANP	PB-O1B	4.13	1.50	1.46
6	D	600	ANP	PG-N3B	4.14	1.74	1.63
6	B	600	ANP	PB-N3B	4.15	1.74	1.63
6	D	600	ANP	PB-N3B	4.18	1.74	1.63
6	U	600	ANP	PB-N3B	4.18	1.74	1.63
6	F	600	ANP	PB-O1B	4.21	1.50	1.46
6	O	600	ANP	PB-O1B	4.21	1.50	1.46
6	O	600	ANP	PG-O1G	4.23	1.51	1.46
6	M	600	ANP	PB-O1B	4.24	1.51	1.46
6	L	600	ANP	PG-N3B	4.25	1.74	1.63
6	F	600	ANP	PG-N3B	4.29	1.74	1.63
6	T	600	ANP	PB-N3B	4.33	1.74	1.63
6	F	600	ANP	PB-N3B	4.34	1.74	1.63
6	U	600	ANP	PB-O1B	4.34	1.51	1.46
6	S	600	ANP	PG-N3B	4.38	1.74	1.63
6	F	600	ANP	PG-O1G	4.46	1.51	1.46
6	L	600	ANP	PG-O1G	4.46	1.51	1.46
6	U	600	ANP	PG-O1G	4.47	1.51	1.46
6	S	600	ANP	PB-N3B	4.51	1.75	1.63
6	J	600	ANP	PG-O1G	4.53	1.51	1.46
6	T	600	ANP	PB-O1B	4.54	1.51	1.46
6	A	600	ANP	PG-O1G	4.55	1.51	1.46
6	S	600	ANP	PG-O1G	4.59	1.51	1.46
6	C	600	ANP	PB-O1B	4.61	1.51	1.46
6	O	600	ANP	PB-N3B	4.63	1.75	1.63
6	C	600	ANP	PG-O1G	4.64	1.51	1.46
6	K	600	ANP	PB-O1B	4.73	1.51	1.46
6	T	600	ANP	PG-O1G	4.74	1.51	1.46
6	S	600	ANP	PB-O1B	4.77	1.51	1.46
6	D	600	ANP	PG-O1G	4.80	1.51	1.46
6	B	600	ANP	PG-O1G	4.89	1.51	1.46
6	V	600	ANP	PB-O1B	5.04	1.51	1.46
6	V	600	ANP	PG-O1G	5.04	1.51	1.46
6	V	600	ANP	PB-N3B	5.27	1.77	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	600	ANP	PG-O1G	5.35	1.52	1.46
6	V	600	ANP	PG-N3B	5.44	1.77	1.63

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	600	ANP	N3-C2-N1	-7.78	122.93	128.89
6	J	600	ANP	N3-C2-N1	-7.72	122.98	128.89
6	X	600	ANP	N3-C2-N1	-7.57	123.10	128.89
6	A	600	ANP	N3-C2-N1	-7.36	123.25	128.89
6	U	600	ANP	N3-C2-N1	-7.32	123.29	128.89
6	B	600	ANP	N3-C2-N1	-7.30	123.30	128.89
6	T	600	ANP	N3-C2-N1	-7.08	123.47	128.89
6	V	600	ANP	N3-C2-N1	-7.02	123.52	128.89
6	O	600	ANP	N3-C2-N1	-7.01	123.53	128.89
6	K	600	ANP	N3-C2-N1	-6.84	123.66	128.89
6	D	600	ANP	N3-C2-N1	-6.78	123.70	128.89
6	S	600	ANP	N3-C2-N1	-6.72	123.75	128.89
6	S	600	ANP	O1G-PG-N3B	-6.53	101.89	111.90
6	F	600	ANP	N3-C2-N1	-6.45	123.96	128.89
6	C	600	ANP	N3-C2-N1	-6.38	124.01	128.89
6	L	600	ANP	N3-C2-N1	-6.33	124.04	128.89
6	V	600	ANP	O1G-PG-N3B	-6.25	102.31	111.90
6	X	600	ANP	O1B-PB-N3B	-6.13	102.50	111.90
6	T	600	ANP	O1G-PG-N3B	-6.08	102.57	111.90
6	X	600	ANP	O1G-PG-N3B	-5.97	102.75	111.90
6	O	600	ANP	O1G-PG-N3B	-5.27	103.81	111.90
6	L	600	ANP	O1G-PG-N3B	-4.95	104.31	111.90
6	C	600	ANP	C2'-C1'-N9	-4.94	106.75	114.29
6	M	600	ANP	C2'-C1'-N9	-4.92	106.77	114.29
6	M	600	ANP	O1B-PB-N3B	-4.83	104.49	111.90
6	K	600	ANP	O1G-PG-N3B	-4.67	104.73	111.90
6	C	600	ANP	O1G-PG-N3B	-4.59	104.86	111.90
6	M	600	ANP	O1G-PG-N3B	-4.56	104.90	111.90
6	V	600	ANP	C2'-C1'-N9	-4.50	107.42	114.29
6	J	600	ANP	O1G-PG-N3B	-4.47	105.04	111.90
6	B	600	ANP	O1G-PG-N3B	-4.40	105.15	111.90
6	D	600	ANP	O1B-PB-N3B	-4.37	105.20	111.90
6	F	600	ANP	O1G-PG-N3B	-4.31	105.29	111.90
6	B	600	ANP	O1B-PB-N3B	-4.24	105.39	111.90
6	U	600	ANP	O1B-PB-N3B	-4.07	105.65	111.90
6	U	600	ANP	O1G-PG-N3B	-4.04	105.70	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	600	ANP	C2'-C1'-N9	-4.02	108.15	114.29
6	C	600	ANP	PA-O3A-PB	-3.91	119.55	132.67
6	S	600	ANP	PA-O3A-PB	-3.87	119.68	132.67
6	X	600	ANP	C2'-C1'-N9	-3.76	108.55	114.29
6	L	600	ANP	PA-O3A-PB	-3.68	120.33	132.67
6	J	600	ANP	O1B-PB-N3B	-3.67	106.28	111.90
6	O	600	ANP	C2'-C1'-N9	-3.63	108.74	114.29
6	A	600	ANP	PA-O3A-PB	-3.60	120.59	132.67
6	M	600	ANP	C4-C5-N7	-3.58	106.18	109.48
6	A	600	ANP	O1G-PG-N3B	-3.56	106.44	111.90
6	S	600	ANP	C2'-C1'-N9	-3.56	108.86	114.29
6	A	600	ANP	O1B-PB-N3B	-3.52	106.50	111.90
6	T	600	ANP	C4-C5-N7	-3.46	106.30	109.48
6	U	600	ANP	PA-O3A-PB	-3.33	121.49	132.67
6	L	600	ANP	O1B-PB-N3B	-3.26	106.90	111.90
6	K	600	ANP	PA-O3A-PB	-3.24	121.81	132.67
6	C	600	ANP	C4-C5-N7	-3.22	106.51	109.48
6	T	600	ANP	PA-O3A-PB	-3.20	121.94	132.67
6	D	600	ANP	PA-O3A-PB	-3.19	121.98	132.67
6	D	600	ANP	O1G-PG-N3B	-3.15	107.06	111.90
6	K	600	ANP	C4-C5-N7	-3.12	106.61	109.48
6	V	600	ANP	O1B-PB-N3B	-3.09	107.16	111.90
6	X	600	ANP	PA-O3A-PB	-3.09	122.31	132.67
6	C	600	ANP	O1B-PB-N3B	-3.08	107.18	111.90
6	O	600	ANP	PA-O3A-PB	-2.94	122.81	132.67
6	A	600	ANP	C4-C5-N7	-2.92	106.79	109.48
6	L	600	ANP	C4-C5-N7	-2.90	106.81	109.48
6	D	600	ANP	C4-C5-N7	-2.88	106.83	109.48
6	K	600	ANP	O1B-PB-N3B	-2.82	107.58	111.90
6	J	600	ANP	PA-O3A-PB	-2.71	123.57	132.67
6	O	600	ANP	C4-C5-N7	-2.67	107.02	109.48
6	T	600	ANP	O1B-PB-N3B	-2.62	107.88	111.90
6	S	600	ANP	C4-C5-N7	-2.62	107.07	109.48
6	O	600	ANP	O1B-PB-N3B	-2.60	107.91	111.90
6	F	600	ANP	O1B-PB-N3B	-2.56	107.97	111.90
6	X	600	ANP	C4-C5-N7	-2.53	107.15	109.48
6	J	600	ANP	C4-C5-N7	-2.53	107.16	109.48
6	U	600	ANP	C4-C5-N7	-2.52	107.16	109.48
6	B	600	ANP	C4-C5-N7	-2.49	107.19	109.48
6	M	600	ANP	PA-O3A-PB	-2.46	124.42	132.67
6	F	600	ANP	C2'-C1'-N9	-2.43	110.57	114.29
6	L	600	ANP	C2'-C1'-N9	-2.43	110.58	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	V	600	ANP	C4-C5-N7	-2.33	107.33	109.48
6	F	600	ANP	C4-C5-N7	-2.22	107.43	109.48
6	B	600	ANP	C2'-C1'-N9	-2.14	111.03	114.29
6	D	600	ANP	O3G-PG-O2G	2.02	113.56	107.58
6	D	600	ANP	C4'-O4'-C1'	2.03	111.95	109.72
6	B	600	ANP	C2-N1-C6	2.06	122.46	118.77
6	K	600	ANP	O4'-C1'-N9	2.07	112.43	108.10
6	B	600	ANP	O3G-PG-O2G	2.07	113.72	107.58
6	X	600	ANP	C2-N1-C6	2.08	122.49	118.77
6	J	600	ANP	O3G-PG-O2G	2.14	113.92	107.58
6	O	600	ANP	O3G-PG-O2G	2.22	114.16	107.58
6	F	600	ANP	O3G-PG-O2G	2.23	114.19	107.58
6	L	600	ANP	O3G-PG-O2G	2.25	114.26	107.58
6	A	600	ANP	C2-N1-C6	2.25	122.79	118.77
6	K	600	ANP	O3G-PG-O2G	2.29	114.38	107.58
6	T	600	ANP	O3G-PG-O2G	2.33	114.49	107.58
6	C	600	ANP	O4'-C1'-N9	2.35	113.01	108.10
6	M	600	ANP	O3G-PG-O2G	2.52	115.04	107.58
6	A	600	ANP	O3G-PG-O2G	2.54	115.10	107.58
6	U	600	ANP	O3G-PG-O2G	2.70	115.60	107.58
6	X	600	ANP	O3G-PG-O2G	2.78	115.83	107.58
6	O	600	ANP	O2B-PB-O1B	3.57	117.45	110.00
6	T	600	ANP	O2B-PB-O1B	3.81	117.94	110.00
6	U	600	ANP	O2B-PB-O1B	4.05	118.45	110.00
6	V	600	ANP	O2B-PB-O1B	4.25	118.88	110.00
6	K	600	ANP	O2B-PB-O1B	4.37	119.11	110.00
6	F	600	ANP	O2B-PB-O1B	4.41	119.20	110.00
6	D	600	ANP	O2B-PB-O1B	4.53	119.45	110.00
6	S	600	ANP	O2B-PB-O1B	4.64	119.68	110.00
6	B	600	ANP	O2B-PB-O1B	4.68	119.78	110.00
6	M	600	ANP	O2B-PB-O1B	4.81	120.05	110.00
6	J	600	ANP	O2B-PB-O1B	4.87	120.16	110.00
6	A	600	ANP	O2B-PB-O1B	5.01	120.46	110.00
6	C	600	ANP	O2B-PB-O1B	5.41	121.29	110.00
6	X	600	ANP	O2B-PB-O1B	5.50	121.48	110.00
6	L	600	ANP	O2B-PB-O1B	5.51	121.49	110.00

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	600	ANP	O1G-PG-N3B-PB

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Mol	Chain	Res	Type	Atoms
6	M	600	ANP	O1G-PG-N3B-PB
6	C	600	ANP	O1G-PG-N3B-PB
6	C	600	ANP	O1B-PB-N3B-PG
6	T	600	ANP	O1B-PB-N3B-PG
6	J	600	ANP	O1G-PG-N3B-PB
6	J	600	ANP	O1B-PB-N3B-PG
6	B	600	ANP	O1B-PB-N3B-PG
6	A	600	ANP	O1G-PG-N3B-PB

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	600	ANP	2	0
6	C	600	ANP	3	0
6	D	600	ANP	2	0
6	F	600	ANP	3	0
6	J	600	ANP	3	0
6	K	600	ANP	1	0
6	M	600	ANP	3	0
6	T	600	ANP	2	0
6	V	600	ANP	2	0
6	X	600	ANP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	485/510 (95%)	-0.19	1 (0%) 95 94	49, 67, 102, 161	0
1	B	486/510 (95%)	0.08	13 (2%) 58 44	60, 94, 131, 172	0
1	C	484/510 (94%)	0.13	12 (2%) 61 47	62, 83, 134, 166	0
1	J	482/510 (94%)	0.18	20 (4%) 41 27	63, 91, 159, 179	0
1	K	483/510 (94%)	0.40	36 (7%) 17 9	78, 118, 163, 170	0
1	L	479/510 (93%)	0.15	17 (3%) 48 32	63, 88, 145, 168	0
1	S	483/510 (94%)	-0.04	7 (1%) 78 65	60, 84, 110, 171	0
1	T	484/510 (94%)	-0.03	4 (0%) 87 80	59, 84, 108, 143	0
1	U	485/510 (95%)	0.15	23 (4%) 35 22	81, 104, 132, 166	0
2	D	470/484 (97%)	0.04	9 (1%) 70 55	54, 80, 131, 155	0
2	E	469/484 (96%)	0.11	16 (3%) 49 34	56, 86, 126, 152	0
2	F	469/484 (96%)	0.11	9 (1%) 70 55	59, 89, 114, 134	0
2	M	460/484 (95%)	0.19	26 (5%) 27 15	63, 87, 146, 171	0
2	N	463/484 (95%)	0.46	46 (9%) 9 5	71, 115, 157, 166	0
2	O	469/484 (96%)	0.28	29 (6%) 24 13	78, 110, 159, 167	0
2	V	360/484 (74%)	0.43	27 (7%) 17 9	78, 109, 146, 178	0
2	W	468/484 (96%)	-0.14	4 (0%) 85 78	57, 72, 103, 143	0
2	X	469/484 (96%)	-0.03	4 (0%) 85 78	65, 91, 113, 132	0
3	G	268/278 (96%)	-0.01	1 (0%) 93 90	62, 92, 108, 115	0
3	P	268/278 (96%)	0.77	43 (16%) 3 2	82, 145, 165, 176	0
3	Y	115/278 (41%)	1.11	31 (26%) 1 0	73, 116, 148, 153	0
4	H	122/138 (88%)	0.00	0 100 100	76, 97, 150, 167	0
4	Q	101/138 (73%)	1.57	37 (36%) 0 0	138, 152, 169, 175	0
5	I	55/61 (90%)	0.03	1 (1%) 71 58	90, 111, 134, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
5	R	55/61 (90%)	0.78	5 (9%) 11 6	126, 146, 163, 167	0
All	All	9432/10178 (92%)	0.17	421 (4%) 37 23	49, 93, 152, 179	0

All (421) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	396	LEU	9.5
4	Q	71	SER	7.1
2	V	144	LEU	5.9
4	Q	12	LEU	5.9
4	Q	54	PRO	5.8
4	Q	72	GLY	5.7
4	Q	85	VAL	5.6
4	Q	14	PHE	5.6
3	P	31	LEU	5.4
1	K	503	THR	5.3
2	V	343	GLY	5.2
1	U	404	ALA	5.2
4	Q	15	ALA	5.2
2	N	463	ILE	5.2
2	O	393	MET	5.2
4	Q	21	LEU	5.0
1	J	406	ALA	5.0
3	Y	215	ALA	5.0
2	O	445	LEU	4.9
1	K	446	LEU	4.9
2	N	144	LEU	4.9
1	K	195	SER	4.9
2	V	172	ASN	4.9
3	Y	214	LEU	4.9
2	O	391	LEU	4.9
2	V	143	LEU	4.8
2	N	392	GLY	4.8
2	V	8	PRO	4.8
2	M	404	VAL	4.7
3	Y	15	ASN	4.7
1	C	470	PHE	4.6
3	P	107	ILE	4.6
2	N	446	GLU	4.6
1	J	507	VAL	4.6
3	Y	40	SER	4.5
2	N	403	THR	4.5

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Mol	Chain	Res	Type	RSRZ
4	Q	49	VAL	4.4
1	J	391	SER	4.4
1	J	405	PHE	4.4
4	Q	20	THR	4.4
2	N	467	VAL	4.3
2	N	470	ALA	4.3
3	P	34	ALA	4.3
1	S	410	SER	4.3
1	S	414	ALA	4.3
2	N	473	LEU	4.3
2	N	462	GLY	4.3
2	N	445	LEU	4.3
2	M	387	ILE	4.2
4	Q	59	VAL	4.2
1	J	407	GLN	4.2
1	K	447	ILE	4.2
3	Y	37	ALA	4.1
1	U	407	GLN	4.1
3	Y	216	ASN	4.1
1	K	466	PHE	4.0
2	O	392	GLY	4.0
3	Y	223	ALA	4.0
2	M	451	ASN	4.0
1	L	471	LEU	4.0
2	M	453	PRO	4.0
2	N	390	ILE	4.0
3	P	128	LEU	4.0
3	Y	34	ALA	4.0
2	M	457	PHE	3.9
2	M	403	THR	3.9
4	Q	76	THR	3.9
2	N	457	PHE	3.8
2	V	167	ILE	3.8
4	Q	33	PRO	3.8
2	O	400	ASP	3.8
2	M	384	LEU	3.8
2	O	453	PRO	3.8
2	N	474	ALA	3.7
1	C	478	HIS	3.7
2	M	445	LEU	3.7
1	J	508	ALA	3.7
2	N	458	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
4	Q	36	SER	3.6
1	B	499	LEU	3.6
2	N	398	GLU	3.6
1	J	491	LEU	3.6
1	J	485	ILE	3.6
3	Y	139	THR	3.6
2	M	395	GLU	3.5
3	Y	39	ILE	3.5
2	O	404	VAL	3.5
2	V	7	THR	3.5
1	K	414	ALA	3.5
2	D	470	ALA	3.5
2	F	463	ILE	3.5
1	U	454	HIS	3.5
2	V	214	LYS	3.5
2	N	466	VAL	3.5
4	Q	28	THR	3.5
3	P	26	VAL	3.5
1	K	504	GLU	3.5
3	P	29	THR	3.4
2	D	467	VAL	3.4
1	B	471	LEU	3.4
2	O	386	ASP	3.4
3	P	157	GLY	3.4
4	Q	13	GLN	3.4
1	L	461	SER	3.4
2	O	387	ILE	3.4
1	K	454	HIS	3.4
1	B	510	PHE	3.4
1	J	503	THR	3.4
1	L	447	ILE	3.4
2	E	453	PRO	3.4
3	Y	143	SER	3.4
2	M	432	VAL	3.4
2	E	445	LEU	3.3
2	N	391	LEU	3.3
4	Q	41	VAL	3.3
2	M	444	VAL	3.3
1	L	446	LEU	3.3
4	Q	79	PRO	3.3
1	K	507	VAL	3.3
2	F	444	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	448	TYR	3.3
2	V	27	GLN	3.3
1	U	123	ILE	3.3
4	Q	48	THR	3.3
1	U	414	ALA	3.2
2	O	213	SER	3.2
2	M	448	LYS	3.2
4	Q	58	GLU	3.2
1	U	408	PHE	3.2
3	P	237	MET	3.2
1	K	460	LEU	3.2
5	R	47	TYR	3.2
1	U	508	ALA	3.2
2	W	475	ALA	3.2
2	W	390	ILE	3.1
1	K	203	CYS	3.1
3	Y	32	SER	3.1
1	C	481	LEU	3.1
3	P	135	LYS	3.1
3	Y	138	PRO	3.1
3	Y	220	THR	3.1
2	E	398	GLU	3.1
2	N	388	ILE	3.1
1	U	507	VAL	3.1
2	N	113	LEU	3.1
2	N	404	VAL	3.1
3	P	60	LEU	3.1
2	D	453	PRO	3.1
3	Y	227	ALA	3.1
3	Y	22	THR	3.1
2	N	145	ALA	3.1
2	X	7	THR	3.0
2	O	388	ILE	3.0
2	N	387	ILE	3.0
2	N	8	PRO	3.0
2	M	463	ILE	3.0
2	V	212	GLU	3.0
4	Q	43	ALA	3.0
2	E	396	LEU	3.0
2	V	377	THR	3.0
1	S	406	ALA	3.0
3	P	182	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
5	R	56	PRO	2.9
2	V	381	TYR	2.9
1	B	491	LEU	2.9
2	O	390	ILE	2.9
2	N	10	THR	2.9
2	V	366	GLU	2.9
4	Q	57	VAL	2.9
1	K	459	GLU	2.9
2	E	393	MET	2.9
3	P	106	ASP	2.9
2	O	180	GLY	2.9
2	M	454	GLU	2.9
2	V	26	GLU	2.9
3	P	59	ASN	2.9
1	K	469	SER	2.9
3	Y	41	ALA	2.9
1	K	202	TYR	2.9
3	P	99	LEU	2.8
1	J	469	SER	2.8
1	K	461	SER	2.8
1	L	489	GLY	2.8
2	O	108	PRO	2.8
2	N	407	ALA	2.8
2	V	57	ASN	2.8
3	P	197	PHE	2.8
4	Q	30	VAL	2.8
1	S	482	LEU	2.8
2	X	113	LEU	2.8
1	U	409	GLY	2.8
2	V	380	THR	2.8
3	P	119	LEU	2.8
1	S	44	PHE	2.7
1	U	102	GLY	2.7
2	D	6	SER	2.7
2	E	473	LEU	2.7
3	P	22	THR	2.7
2	M	386	ASP	2.7
1	K	429	LEU	2.7
5	R	24	SER	2.7
1	L	450	GLY	2.7
2	E	462	GLY	2.7
1	C	499	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	O	143	LEU	2.7
1	K	196	ASP	2.6
1	J	401	GLU	2.6
2	M	464	GLU	2.6
2	N	389	ALA	2.6
1	K	470	PHE	2.6
2	V	170	LEU	2.6
2	M	405	GLU	2.6
1	U	448	TYR	2.6
1	C	503	THR	2.6
1	L	473	TYR	2.6
1	U	125	ALA	2.6
4	Q	26	GLU	2.6
3	Y	224	GLN	2.6
1	U	405	PHE	2.6
3	P	154	MET	2.6
1	U	510	PHE	2.6
4	Q	38	ARG	2.6
2	F	469	LYS	2.6
2	V	145	ALA	2.6
2	F	23	VAL	2.6
3	Y	213	THR	2.6
3	P	173	LEU	2.5
3	Y	145	LEU	2.5
4	Q	31	ASN	2.5
1	K	499	LEU	2.5
1	T	490	GLU	2.5
4	Q	55	GLY	2.5
1	B	25	ALA	2.5
3	P	105	ALA	2.5
2	N	46	LEU	2.5
2	N	453	PRO	2.5
1	K	413	ASP	2.5
2	E	441	PHE	2.5
3	P	72	GLU	2.5
2	M	407	ALA	2.5
1	L	491	LEU	2.5
2	O	406	ARG	2.5
4	Q	37	GLY	2.5
1	K	445	PRO	2.5
2	V	28	SER	2.5
1	J	460	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	386	ASP	2.5
1	B	407	GLN	2.5
3	Y	221	ALA	2.5
3	P	167	ASN	2.5
1	B	405	PHE	2.5
3	Y	20	THR	2.5
1	K	87	GLY	2.5
1	J	402	VAL	2.5
1	S	407	GLN	2.5
2	O	399	GLN	2.5
4	Q	40	GLY	2.5
3	Y	222	MET	2.5
1	U	406	ALA	2.5
1	J	454	HIS	2.5
2	M	450	ASP	2.5
3	P	77	ILE	2.4
2	N	402	LEU	2.4
4	Q	42	LEU	2.4
4	Q	69	PHE	2.4
1	K	415	SER	2.4
1	K	458	ILE	2.4
3	Y	13	ILE	2.4
1	C	469	SER	2.4
2	O	407	ALA	2.4
1	K	149	GLN	2.4
3	P	25	ILE	2.4
3	P	138	PRO	2.4
2	E	388	ILE	2.4
2	N	410	ILE	2.4
1	B	89	LEU	2.4
3	P	62	VAL	2.4
1	U	503	THR	2.4
2	M	452	ILE	2.4
1	J	395	PHE	2.4
3	Y	219	LEU	2.4
1	L	506	PHE	2.4
1	L	65	ALA	2.4
2	M	462	GLY	2.4
1	K	420	LEU	2.4
2	N	400	ASP	2.4
2	O	473	LEU	2.4
3	P	73	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	125	ASN	2.4
1	K	480	GLU	2.4
1	L	507	VAL	2.4
2	V	25	PHE	2.4
3	P	89	SER	2.3
2	V	166	PHE	2.3
3	P	136	ASP	2.3
1	B	484	GLU	2.3
1	U	410	SER	2.3
1	U	449	ALA	2.3
1	L	89	LEU	2.3
2	N	358	LEU	2.3
2	V	176	LYS	2.3
3	P	112	ASP	2.3
1	B	485	ILE	2.3
2	E	391	LEU	2.3
2	N	143	LEU	2.3
2	N	27	GLN	2.3
2	N	471	GLU	2.3
1	B	195	SER	2.3
1	K	492	SER	2.3
2	D	473	LEU	2.3
2	V	29	GLU	2.3
3	Y	142	GLU	2.3
3	P	27	ALA	2.3
2	O	209	LEU	2.3
2	E	399	GLN	2.3
3	Y	140	PHE	2.3
1	K	419	THR	2.3
1	B	460	LEU	2.3
2	V	344	ILE	2.3
1	K	424	GLU	2.3
2	O	454	GLU	2.3
2	M	27	GLN	2.3
2	M	390	ILE	2.3
2	W	474	ALA	2.3
1	K	201	LEU	2.3
1	K	441	GLU	2.2
2	N	454	GLU	2.2
1	L	460	LEU	2.2
3	P	175	PHE	2.2
2	N	432	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
4	Q	39	ILE	2.2
1	B	410	SER	2.2
4	Q	75	ALA	2.2
1	L	477	ASN	2.2
1	U	44	PHE	2.2
2	V	207	ILE	2.2
1	C	482	LEU	2.2
2	N	384	LEU	2.2
2	O	438	VAL	2.2
1	L	58	SER	2.2
4	Q	22	TYR	2.2
2	O	207	ILE	2.2
1	T	412	LEU	2.2
1	K	440	THR	2.2
1	L	458	ILE	2.2
4	Q	70	ILE	2.2
2	F	467	VAL	2.2
3	P	30	ARG	2.2
3	P	177	PRO	2.2
2	F	77	LEU	2.2
2	O	113	LEU	2.2
4	Q	18	HIS	2.2
3	Y	19	ILE	2.2
2	D	28	SER	2.2
2	V	77	LEU	2.2
1	J	501	SER	2.2
2	E	403	THR	2.2
1	T	385	LEU	2.2
2	O	109	ILE	2.2
3	P	196	LYS	2.2
1	C	474	LEU	2.2
1	C	496	LEU	2.2
5	R	20	ALA	2.2
1	J	414	ALA	2.1
1	T	491	LEU	2.1
2	N	383	SER	2.1
3	P	193	SER	2.1
1	K	232	ILE	2.1
2	X	53	HIS	2.1
2	E	452	ILE	2.1
1	U	456	ASP	2.1
2	O	441	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	P	51	PHE	2.1
2	O	403	THR	2.1
2	D	474	ALA	2.1
3	Y	36	LYS	2.1
2	N	447	GLY	2.1
5	R	15	ASN	2.1
3	P	248	ILE	2.1
2	D	441	PHE	2.1
2	N	401	LYS	2.1
3	Y	276	SER	2.1
1	J	404	ALA	2.1
1	U	509	THR	2.1
3	G	62	VAL	2.1
1	S	413	ASP	2.1
2	F	471	GLU	2.1
2	E	463	ILE	2.1
2	O	462	GLY	2.1
2	E	390	ILE	2.1
2	N	344	ILE	2.1
4	Q	44	ASN	2.1
1	J	502	ALA	2.1
1	U	388	VAL	2.1
3	Y	144	ALA	2.1
3	P	188	ILE	2.1
1	A	405	PHE	2.1
2	M	408	ARG	2.1
2	M	460	VAL	2.1
1	C	473	TYR	2.0
5	I	47	TYR	2.0
2	N	413	PHE	2.0
2	E	466	VAL	2.0
1	K	478	HIS	2.0
2	N	452	ILE	2.0
2	X	390	ILE	2.0
1	L	472	SER	2.0
1	C	485	ILE	2.0
2	D	406	ARG	2.0
2	N	385	GLN	2.0
2	O	30	LEU	2.0
3	P	116	MET	2.0
2	F	30	LEU	2.0
2	V	156	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	W	395	GLU	2.0
1	K	505	SER	2.0
1	U	425	ARG	2.0
2	F	470	ALA	2.0
3	P	47	ALA	2.0
3	P	162	ILE	2.0
1	C	491	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	MG	F	700	1/1	0.93	0.45	7.14	83,83,83,83	0
7	MG	M	700	1/1	0.96	0.43	6.74	80,80,80,80	0
7	MG	O	700	1/1	0.97	0.36	6.67	91,91,91,91	0
7	MG	X	700	1/1	0.98	0.43	5.94	80,80,80,80	0
7	MG	D	700	1/1	0.93	0.52	5.42	83,83,83,83	0
6	ANP	T	600	31/31	0.93	0.25	1.90	69,72,75,76	0
6	ANP	A	600	31/31	0.95	0.22	1.28	58,62,65,66	0
6	ANP	B	600	31/31	0.90	0.24	1.19	80,88,97,98	0
6	ANP	C	600	31/31	0.91	0.24	1.03	77,83,89,89	0
6	ANP	F	600	31/31	0.93	0.27	0.83	82,84,88,89	0
6	ANP	X	600	31/31	0.96	0.25	0.67	70,72,78,78	0
6	ANP	M	600	31/31	0.95	0.23	0.44	78,85,94,94	0
6	ANP	O	600	31/31	0.94	0.22	0.21	90,102,107,107	0
6	ANP	D	600	31/31	0.95	0.24	0.10	82,89,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	ANP	S	600	31/31	0.93	0.20	-0.08	83,85,86,86	0
6	ANP	J	600	31/31	0.93	0.20	-0.11	78,89,93,94	0
6	ANP	L	600	31/31	0.95	0.21	-0.17	83,86,87,88	0
6	ANP	U	600	31/31	0.95	0.20	-0.34	82,84,87,87	0
6	ANP	V	600	31/31	0.90	0.20	-0.55	114,116,117,118	0
6	ANP	K	600	31/31	0.88	0.18	-0.65	105,113,114,115	0
7	MG	B	700	1/1	0.93	0.48	-	82,82,82,82	0
7	MG	V	700	1/1	0.84	0.11	-	112,112,112,112	0
7	MG	A	700	1/1	0.95	0.44	-	66,66,66,66	0
7	MG	S	700	1/1	0.97	0.50	-	84,84,84,84	0
7	MG	T	700	1/1	0.96	0.64	-	76,76,76,76	0
7	MG	K	700	1/1	0.93	0.35	-	102,102,102,102	0
7	MG	U	700	1/1	0.95	0.46	-	83,83,83,83	0
7	MG	J	700	1/1	0.88	0.40	-	81,81,81,81	0
7	MG	L	700	1/1	0.93	0.40	-	86,86,86,86	0
7	MG	C	700	1/1	0.91	0.51	-	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.