



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:22 AM GMT

PDB ID : 3OEH
Title : Structure of four mutant forms of yeast F1 ATPase: beta-V279F
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.
Deposited on : 2010-08-12
Resolution : 3.00 Å(reported)

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

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

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

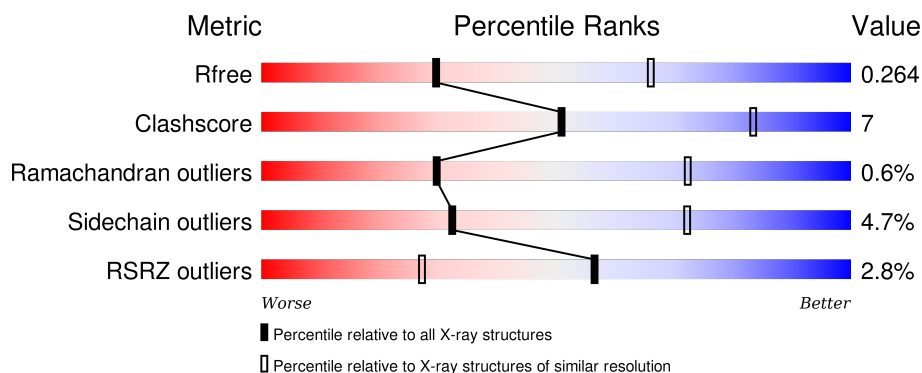
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.






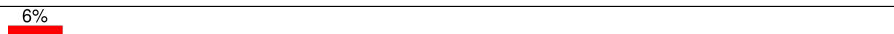
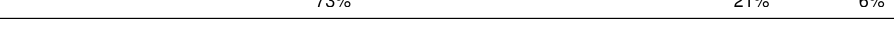
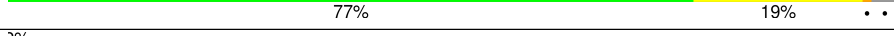



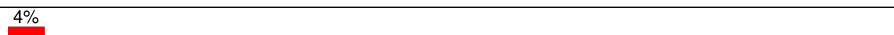
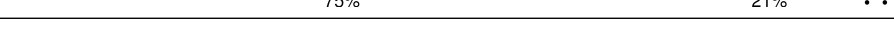




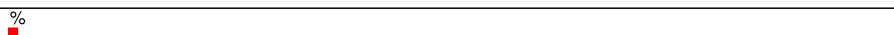






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	510	<div> <div></div> <div>78% 15% • 5%</div> </div>
1	B	510	<div> <div>3%</div> <div>75% 18% • 5%</div> </div>
1	C	510	<div> <div></div> <div>80% 14% • 5%</div> </div>
1	J	510	<div> <div></div> <div>79% 15% 6%</div> </div>
1	K	510	<div> <div>3%</div> <div>74% 21% • 5%</div> </div>

Continued on next page...

Continued from previous page...

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MG	D	700	-	-	-	X
7	MG	F	700	-	-	-	X
7	MG	M	700	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 72707 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	B	483	Total	C	N	O	S	0	0	0
			3669	2317	649	700	3			
1	C	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	J	481	Total	C	N	O	S	0	0	0
			3655	2309	646	697	3			
1	K	486	Total	C	N	O	S	0	0	0
			3688	2327	652	706	3			
1	L	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	S	478	Total	C	N	O	S	0	0	0
			3635	2297	643	692	3			
1	T	479	Total	C	N	O	S	0	0	0
			3642	2302	644	693	3			
1	U	481	Total	C	N	O	S	0	0	0
			3655	2308	646	698	3			

- 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
			3549	2252	603	688	6			
2	E	468	Total	C	N	O	S	0	0	0
			3508	2227	598	677	6			
2	F	469	Total	C	N	O	S	0	0	0
			3531	2242	602	681	6			
2	M	470	Total	C	N	O	S	0	0	0
			3543	2249	600	688	6			
2	N	470	Total	C	N	O	S	0	0	0
			3545	2249	602	688	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	468	Total	C	N	O	S	0	0	0
			3538	2246	602	684	6			
2	V	470	Total	C	N	O	S	0	0	0
			3550	2251	604	689	6			
2	W	467	Total	C	N	O	S	0	0	0
			3535	2244	601	684	6			
2	X	469	Total	C	N	O	S	0	0	0
			3547	2251	603	687	6			

There are 81 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
D	279	PHE	VAL	ENGINEERED MUTATION	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
E	279	PHE	VAL	ENGINEERED MUTATION	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
F	1	HIS	-	EXPRESSION TAG	UNP P00830
F	2	HIS	-	EXPRESSION TAG	UNP P00830
F	279	PHE	VAL	ENGINEERED MUTATION	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
M	279	PHE	VAL	ENGINEERED MUTATION	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
N	279	PHE	VAL	ENGINEERED MUTATION	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
O	279	PHE	VAL	ENGINEERED MUTATION	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
V	279	PHE	VAL	ENGINEERED MUTATION	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
W	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830
X	-5	ALA	-	EXPRESSION TAG	UNP P00830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
X	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	266	Total	C	N	O	S	0	0	0
			2059	1293	359	397	10			
3	P	246	Total	C	N	O	S	0	0	0
			1872	1175	327	361	9			
3	Y	201	Total	C	N	O	S	0	0	0
			1523	947	274	293	9			

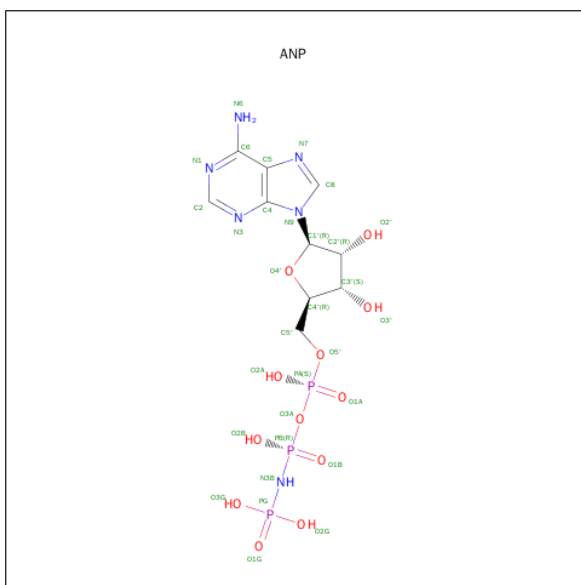
- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	116	Total	C	N	O	S	0	0	0
			763	477	132	152	2			
4	Q	84	Total	C	N	O		0	0	0
			454	277	89	88				
4	Z	17	Total	C	N	O		0	0	0
			85	51	17	17				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	49	Total	C	N	O		0	0	0
			339	212	57	70				
5	R	34	Total	C	N	O		0	0	0
			189	116	34	39				
5	1	27	Total	C	N	O		0	0	0
			145	86	31	28				

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



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

Continued on next page...

Continued from previous page...

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

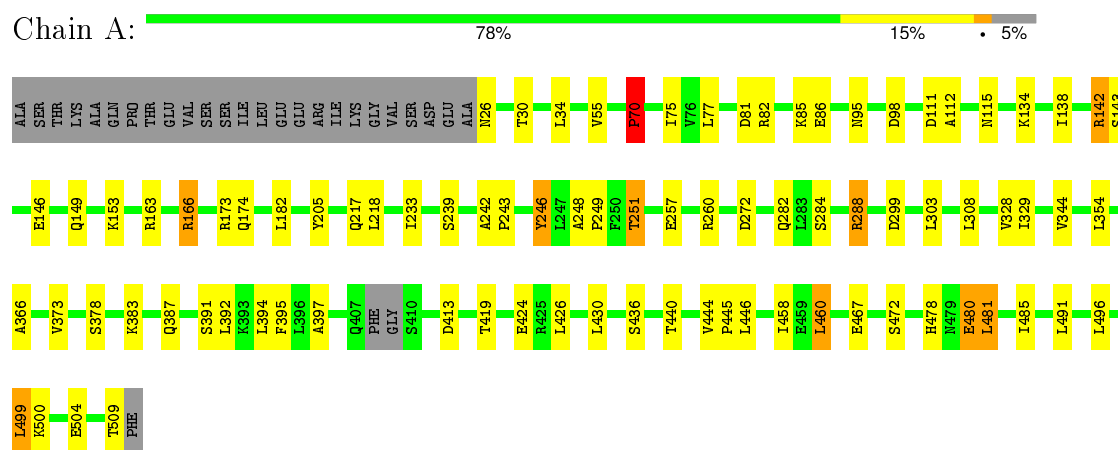
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		

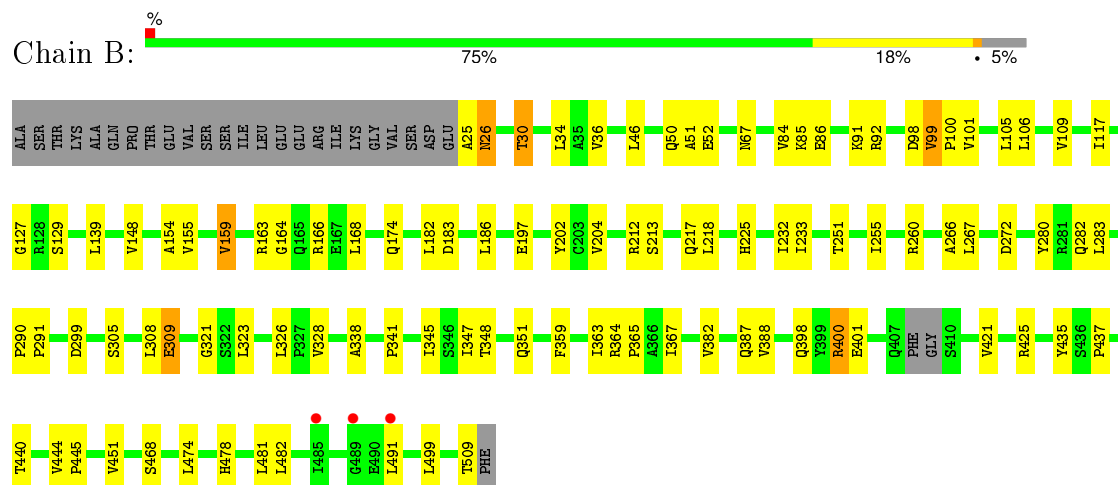
3 Residue-property plots

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.

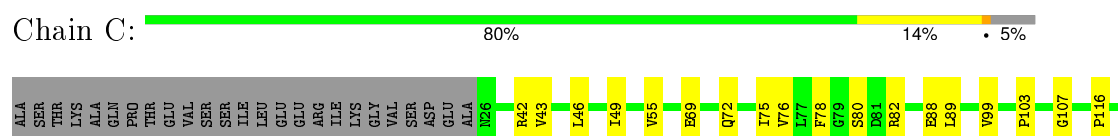
- Molecule 1: ATP synthase subunit alpha

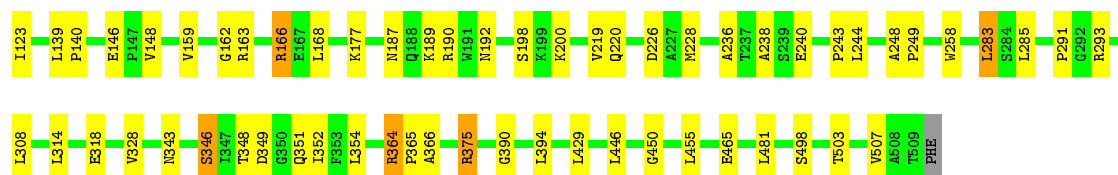


- Molecule 1: ATP synthase subunit alpha



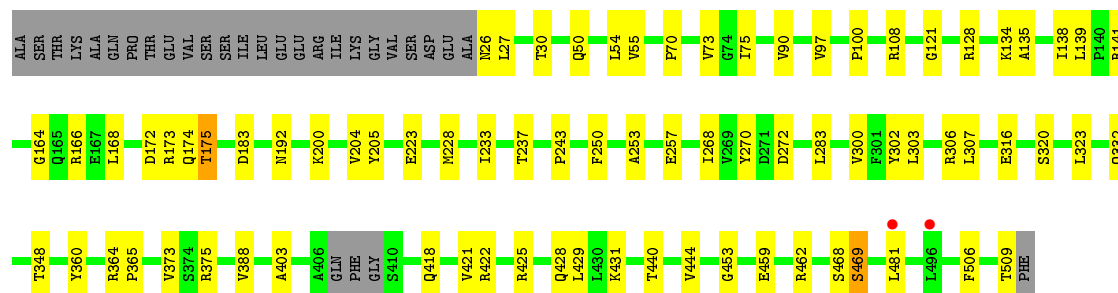
- Molecule 1: ATP synthase subunit alpha





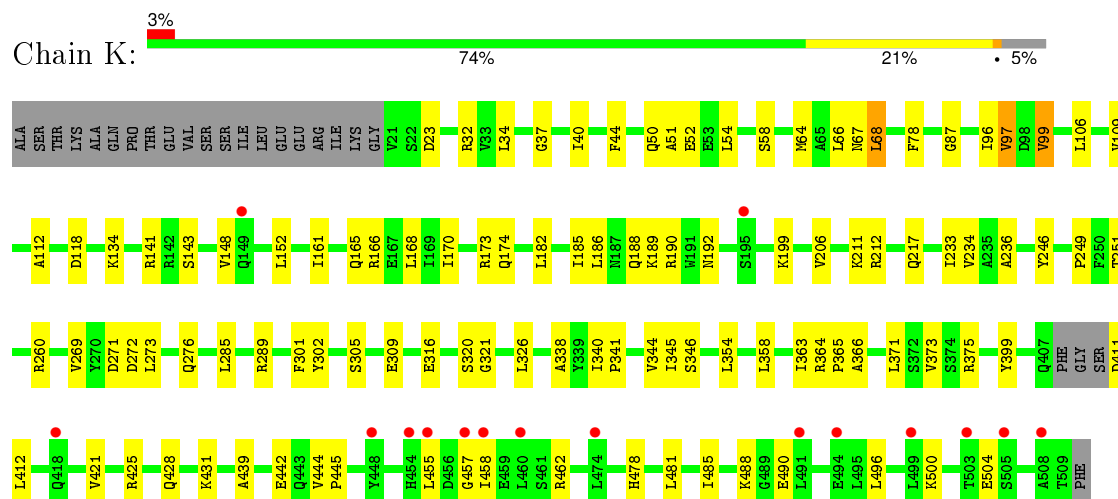
• Molecule 1: ATP synthase subunit alpha

Chain J:



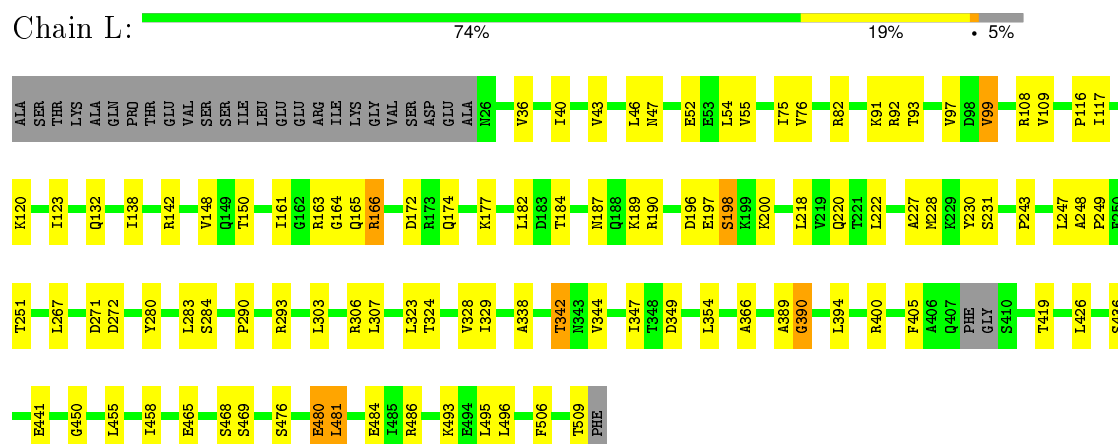
• Molecule 1: ATP synthase subunit alpha

Chain K:

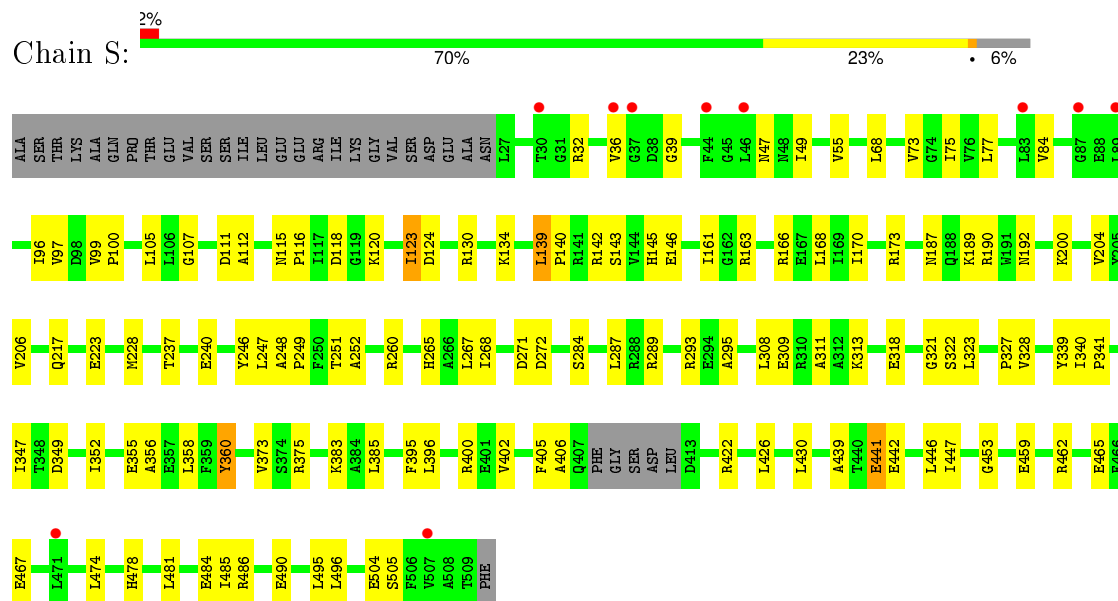


• Molecule 1: ATP synthase subunit alpha

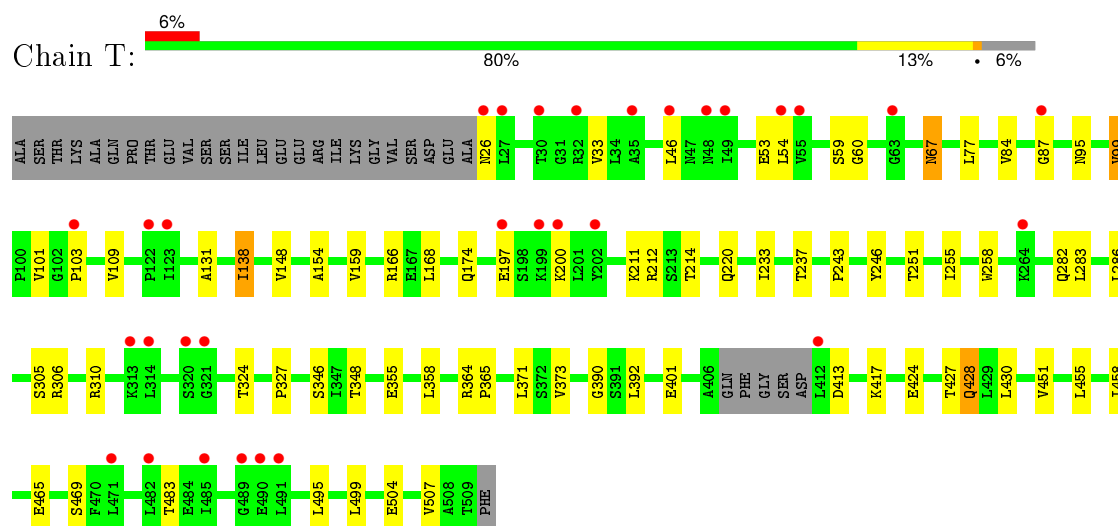
Chain L:



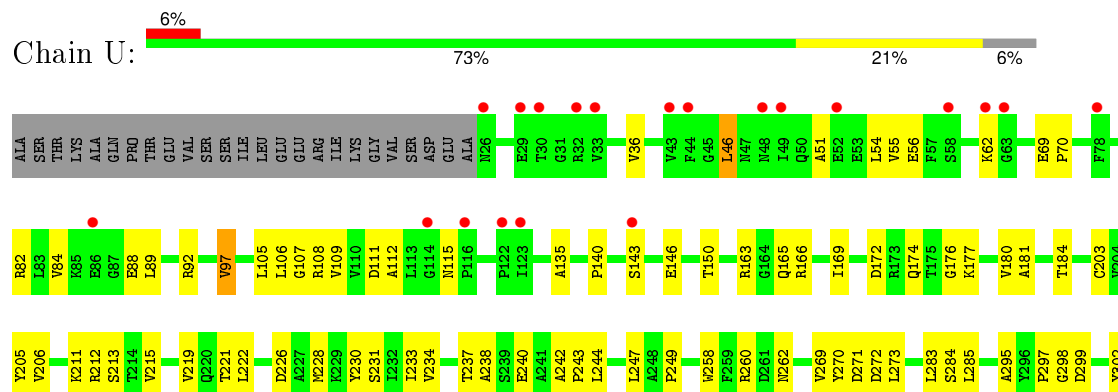
- Molecule 1: ATP synthase subunit alpha

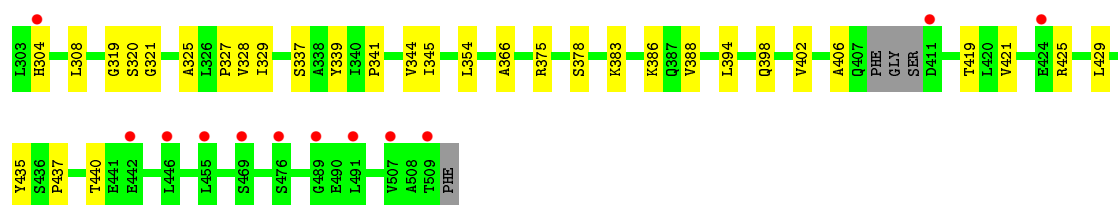


- Molecule 1: ATP synthase subunit alpha



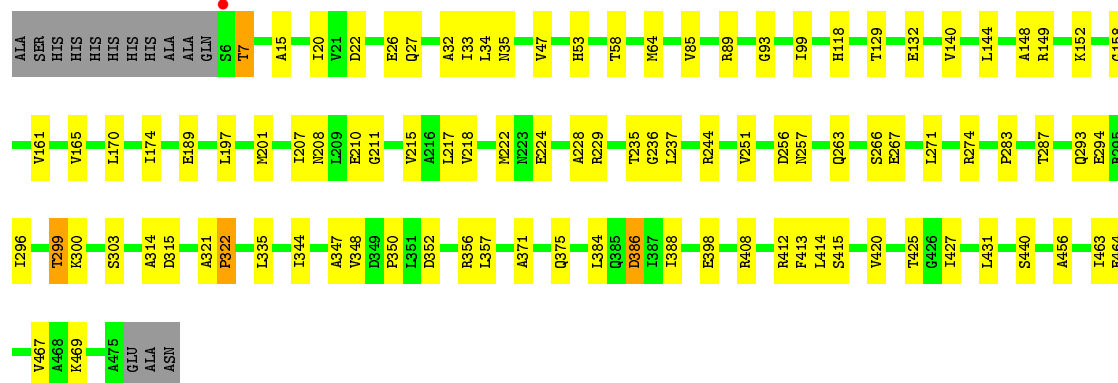
- Molecule 1: ATP synthase subunit alpha





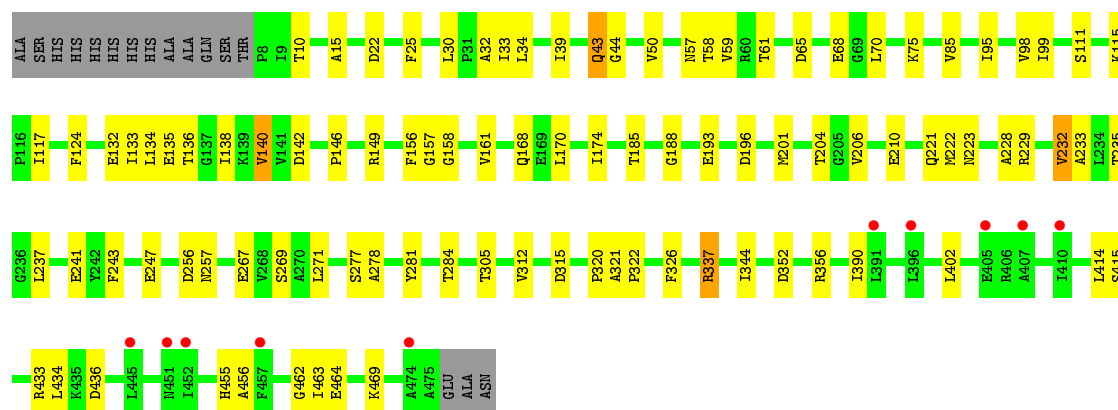
• Molecule 2: ATP synthase subunit beta

Chain D: 77% 19%



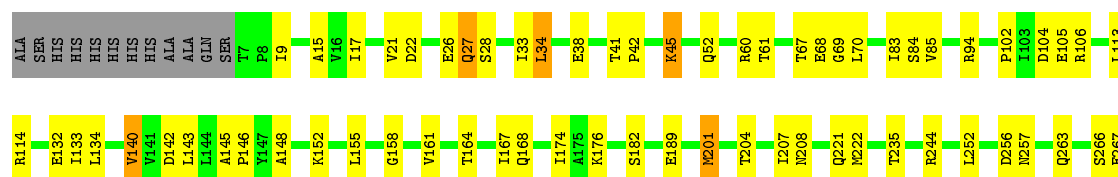
• Molecule 2: ATP synthase subunit beta

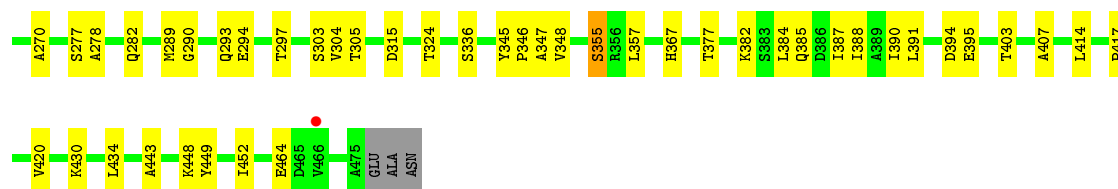
Chain E: 2% 76% 19%



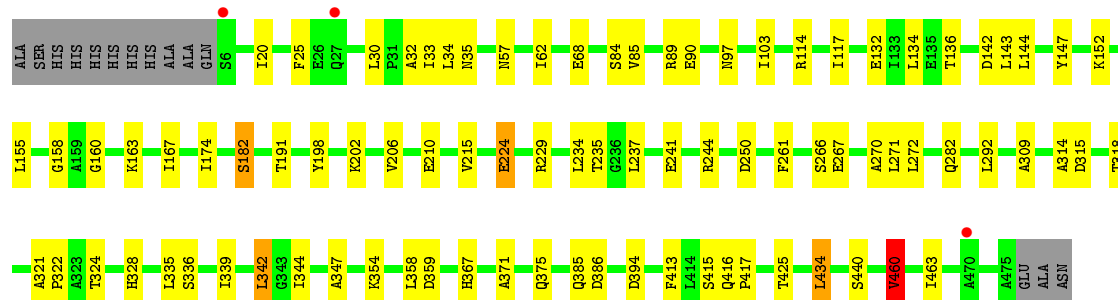
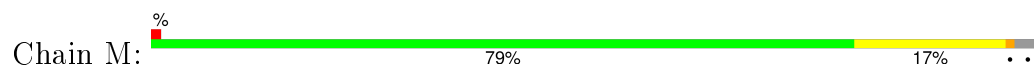
• Molecule 2: ATP synthase subunit beta

Chain F: 74% 21%

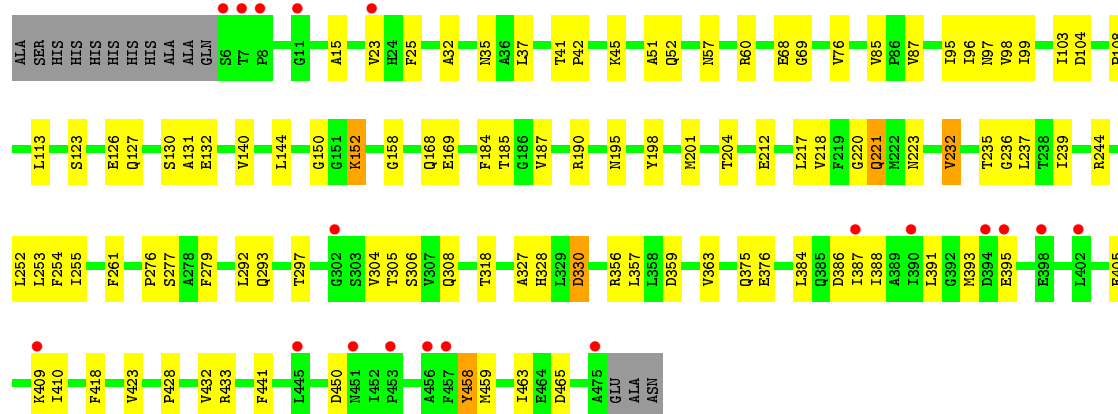
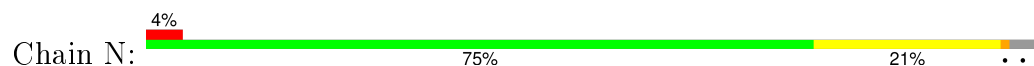




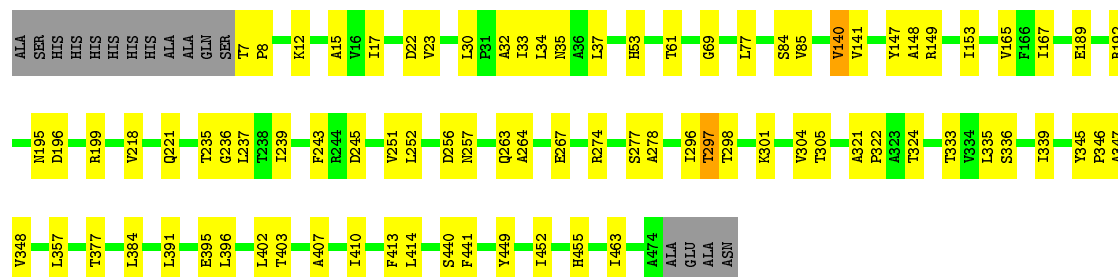
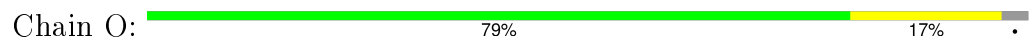
• Molecule 2: ATP synthase subunit beta



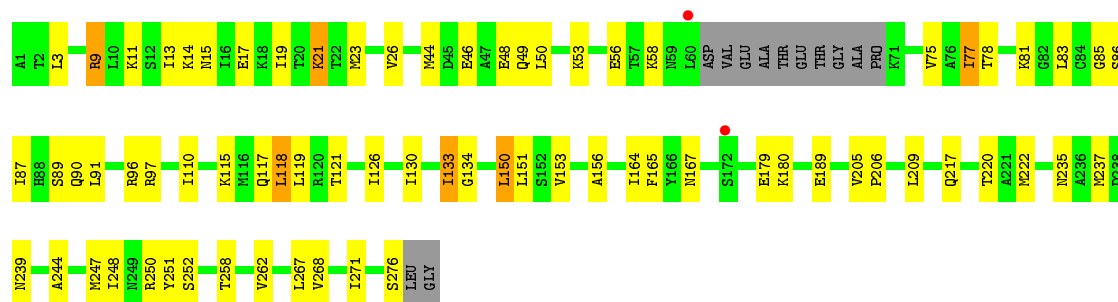
• Molecule 2: ATP synthase subunit beta



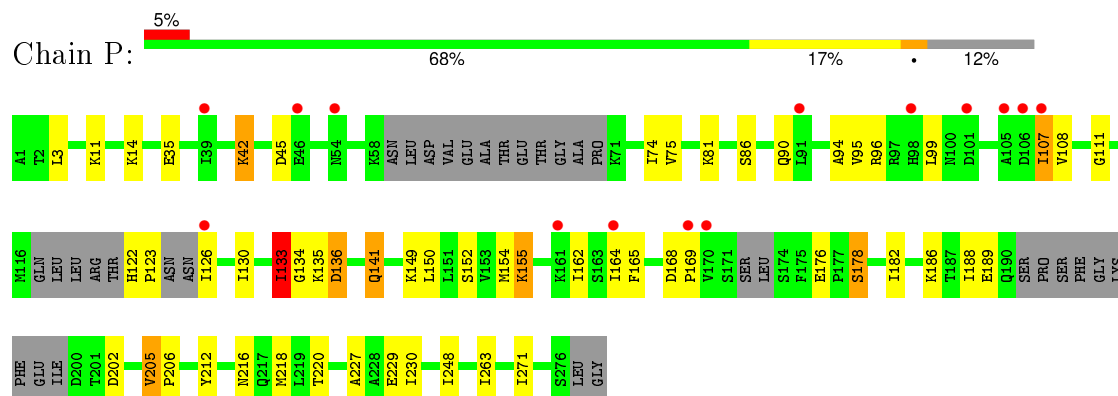
• Molecule 2: ATP synthase subunit beta



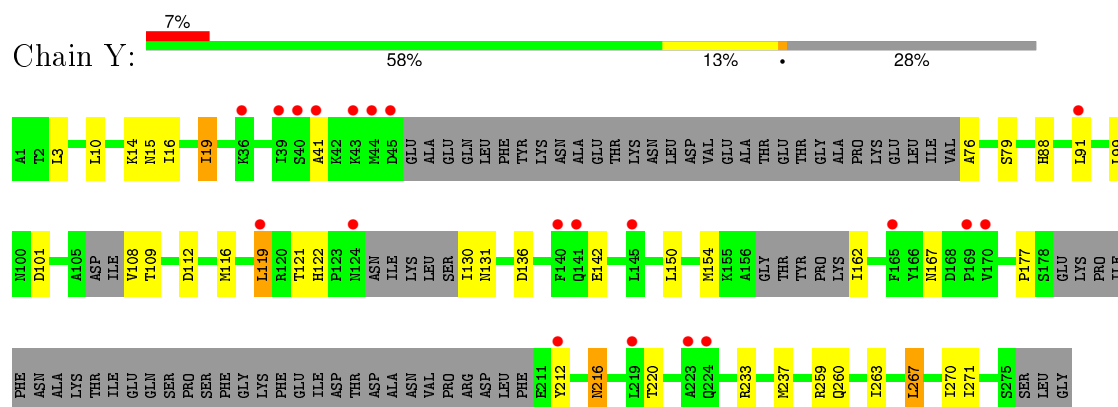
• Molecule 2: ATP synthase subunit beta



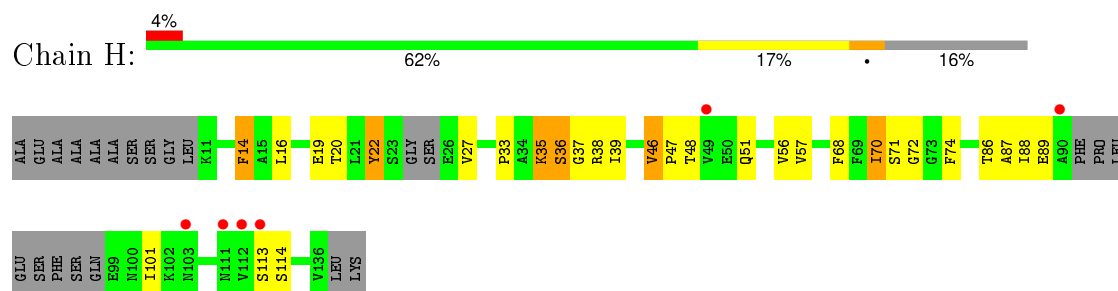
• Molecule 3: ATP synthase subunit gamma



• Molecule 3: ATP synthase subunit gamma

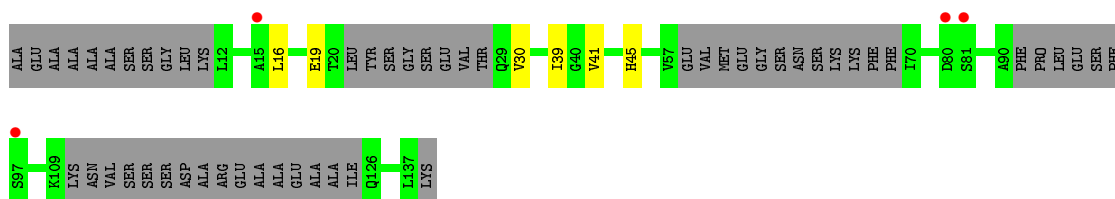


• Molecule 4: ATP synthase subunit delta

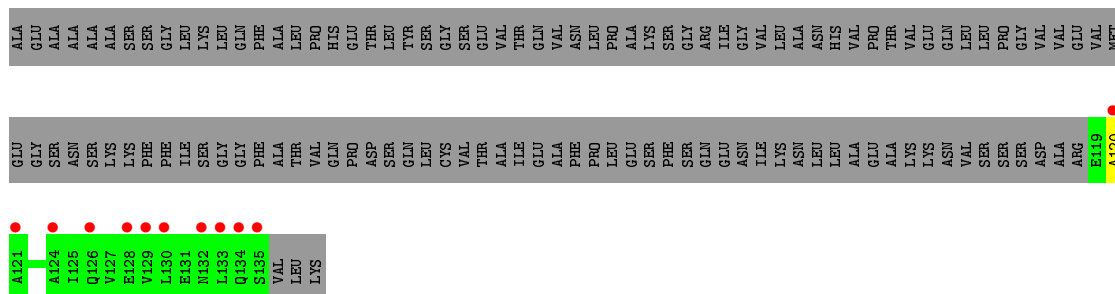


• Molecule 4: ATP synthase subunit delta

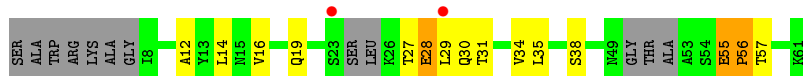




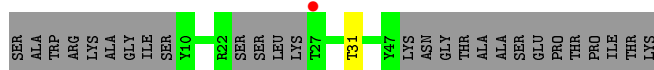
- Molecule 4: ATP synthase subunit delta



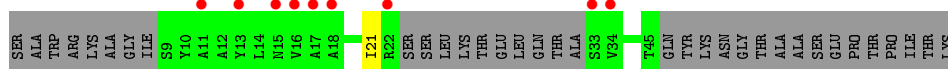
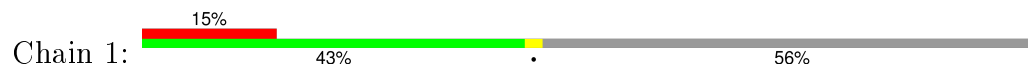
- Molecule 5: ATP synthase subunit epsilon



- Molecule 5: ATP synthase subunit epsilon



- Molecule 5: ATP synthase subunit epsilon



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.93Å 291.90Å 188.76Å 90.00° 101.91° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 49.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-3.00) 88.6 (49.39-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.209 , 0.270 0.206 , 0.264	Depositor DCC
R_{free} test set	4154 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	82.8	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 207723 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	72707	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	0/3718	0.65	0/5032
1	B	0.39	0/3723	0.59	0/5039
1	C	0.42	0/3736	0.62	1/5057 (0.0%)
1	J	0.36	0/3709	0.56	0/5020
1	K	0.35	0/3742	0.54	0/5065
1	L	0.43	0/3718	0.61	1/5032 (0.0%)
1	S	0.37	0/3689	0.54	0/4992
1	T	0.34	0/3696	0.50	0/5002
1	U	0.35	0/3709	0.54	0/5021
2	D	0.47	0/3606	0.61	0/4890
2	E	0.42	0/3565	0.58	0/4840
2	F	0.40	0/3588	0.58	0/4868
2	M	0.39	0/3600	0.58	0/4883
2	N	0.37	0/3602	0.53	1/4886 (0.0%)
2	O	0.37	0/3595	0.56	0/4875
2	V	0.37	0/3607	0.53	0/4891
2	W	0.36	0/3592	0.52	0/4869
2	X	0.36	0/3604	0.53	0/4887
3	G	0.39	0/2084	0.53	0/2803
3	P	0.36	0/1889	0.53	0/2537
3	Y	0.34	0/1533	0.51	0/2056
4	H	0.39	0/772	0.59	0/1058
4	Q	0.36	0/453	0.51	0/621
4	Z	0.35	0/84	0.45	0/116
5	1	0.30	0/143	0.42	0/195
5	I	0.42	0/343	0.59	0/470
5	R	0.39	0/189	0.50	0/261
All	All	0.39	0/73289	0.56	3/99266 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	283	LEU	CA-CB-CG	5.70	128.40	115.30
2	N	37	LEU	CA-CB-CG	5.34	127.57	115.30
1	C	283	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3747	59	0
1	B	3669	0	3752	59	0
1	C	3680	0	3763	40	0
1	J	3655	0	3739	43	0
1	K	3688	0	3763	63	0
1	L	3664	0	3747	54	0
1	S	3635	0	3724	70	0
1	T	3642	0	3733	36	0
1	U	3655	0	3734	62	0
2	D	3549	0	3614	59	0
2	E	3508	0	3550	51	0
2	F	3531	0	3592	58	0
2	M	3543	0	3603	49	0
2	N	3545	0	3604	63	0
2	O	3538	0	3606	47	0
2	V	3550	0	3611	64	0
2	W	3535	0	3605	47	0
2	X	3547	0	3615	39	0
3	G	2059	0	2127	43	0
3	P	1872	0	1917	34	0
3	Y	1523	0	1569	16	0
4	H	763	0	653	21	0
4	Q	454	0	259	2	0
4	Z	85	0	45	0	0
5	1	145	0	87	0	0
5	I	339	0	280	8	0
5	R	189	0	114	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	31	0	13	1	0
6	B	31	0	13	4	0
6	C	31	0	13	0	0
6	D	31	0	13	0	0
6	F	31	0	13	1	0
6	J	31	0	13	1	0
6	K	31	0	13	3	0
6	L	31	0	13	1	0
6	M	31	0	13	4	0
6	O	31	0	13	3	0
6	S	31	0	13	0	0
6	T	31	0	13	1	0
6	U	31	0	13	1	0
6	V	31	0	13	1	0
6	X	31	0	13	4	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	72707	0	73348	1008	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 7.

All (1008) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.30	1.12
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.15	1.09
1:A:395:PHE:HZ	1:A:419:THR:HA	1.15	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.38	1.01
1:B:174:GLN:HA	6:B:600:ANP:HNB1	1.28	0.97
1:A:395:PHE:CZ	1:A:419:THR:HA	2.00	0.96
1:A:77:LEU:HD12	1:A:81:ASP:HB3	1.49	0.95
3:P:205:VAL:H	3:P:206:PRO:HD2	1.30	0.94
2:M:160:GLY:H	6:M:600:ANP:HNB1	1.03	0.93
1:A:182:LEU:HD13	1:A:218:LEU:HD11	1.50	0.92
1:S:293:ARG:HD3	1:S:339:TYR:HD1	1.36	0.91
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.51	0.91
1:K:67:ASN:HB3	2:O:17:ILE:HD13	1.55	0.89
1:L:182:LEU:HD13	1:L:218:LEU:HD11	1.55	0.87
2:M:142:ASP:HB3	2:M:434:LEU:HD12	1.55	0.86
5:I:55:GLU:CB	5:I:56:PRO:HD3	2.06	0.86
2:V:85:VAL:HG11	2:V:235:THR:HG23	1.56	0.86
2:D:85:VAL:CG1	2:D:235:THR:HG23	2.04	0.85
1:S:293:ARG:HD3	1:S:339:TYR:CD1	2.11	0.84
3:P:122:HIS:N	3:P:123:PRO:HD3	1.93	0.84
1:S:146:GLU:OE1	1:S:313:LYS:HE2	1.77	0.83
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.60	0.82
1:T:99:VAL:HG11	1:T:251:THR:HB	1.62	0.82
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.61	0.81
2:M:182:SER:HB2	2:M:215:VAL:HG23	1.61	0.81
3:P:205:VAL:N	3:P:206:PRO:HD2	1.97	0.80
1:C:192:ASN:HA	1:C:200:LYS:HG2	1.65	0.79
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.64	0.78
3:G:23:MET:HG3	3:G:237:MET:HG3	1.66	0.78
1:S:112:ALA:O	1:S:251:THR:HG21	1.85	0.77
2:V:7:THR:HB	2:V:8:PRO:HD2	1.66	0.77
1:K:444:VAL:HG23	1:K:445:PRO:HD3	1.67	0.77
1:B:174:GLN:HA	6:B:600:ANP:N3B	2.00	0.76
2:D:371:ALA:O	2:D:375:GLN:HG3	1.86	0.75
1:U:166:ARG:HD3	1:U:308:LEU:O	1.87	0.75
1:J:469:SER:HB3	1:J:506:PHE:HZ	1.51	0.74
2:N:391:LEU:HB3	2:N:395:GLU:HG3	1.68	0.73
3:P:107:ILE:HG13	3:P:126:ILE:HA	1.71	0.73
1:T:346:SER:HA	6:X:600:ANP:O1G	1.89	0.73
3:G:89:SER:HA	3:G:117:GLN:HE21	1.53	0.73
1:K:364:ARG:HD3	6:K:600:ANP:C2	2.18	0.73
1:K:375:ARG:NH1	6:O:600:ANP:O2A	2.23	0.71
1:S:116:PRO:HB3	1:S:123:ILE:HD11	1.71	0.71
3:P:205:VAL:H	3:P:206:PRO:CD	2.03	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:14:LYS:HA	3:G:248:ILE:HD11	1.73	0.70
1:C:236:ALA:HA	1:C:240:GLU:OE2	1.91	0.70
2:E:140:VAL:HG13	2:E:414:LEU:HB3	1.73	0.70
3:P:155:LYS:HG2	3:P:155:LYS:O	1.89	0.70
2:V:154:GLY:HA3	2:V:329:LEU:HD13	1.71	0.70
1:C:343:ASN:O	1:C:346:SER:HB2	1.91	0.70
1:S:441:GLU:HG2	1:S:486:ARG:HB2	1.74	0.70
1:U:146:GLU:HB3	1:U:163:ARG:HD2	1.74	0.69
1:L:40:ILE:CD1	1:L:76:VAL:HG12	2.23	0.69
2:W:244:ARG:HD3	2:W:304:VAL:HG23	1.75	0.69
3:P:212:TYR:O	3:P:216:ASN:HB2	1.93	0.69
2:E:168:GLN:HE21	2:E:201:MET:HG3	1.58	0.69
1:L:52:GLU:OE1	2:M:68:GLU:HB3	1.92	0.69
2:V:440:SER:O	2:V:444:VAL:HG23	1.93	0.69
1:J:139:LEU:HD13	2:N:104:ASP:HA	1.75	0.68
2:O:391:LEU:HB3	2:O:395:GLU:HG3	1.74	0.68
3:G:23:MET:HA	3:G:26:VAL:HB	1.75	0.68
1:A:149:GLN:OE1	1:A:440:THR:OG1	2.10	0.68
1:B:398:GLN:HA	1:B:401:GLU:HG2	1.75	0.68
1:A:174:GLN:HA	6:A:600:ANP:HNB1	1.59	0.68
3:G:89:SER:HA	3:G:117:GLN:NE2	2.08	0.68
2:N:237:LEU:HD22	2:N:292:LEU:HD12	1.74	0.68
2:N:41:THR:HB	2:N:42:PRO:HD2	1.76	0.68
2:X:163:LYS:N	6:X:600:ANP:O1B	2.27	0.68
3:G:77:ILE:HG21	3:G:222:MET:HG2	1.75	0.68
2:D:7:THR:HG23	2:D:7:THR:O	1.94	0.67
2:N:279:PHE:HE1	3:P:263:ILE:HD12	1.59	0.67
2:O:377:THR:HG22	2:O:407:ALA:HB2	1.76	0.67
1:B:272:ASP:HB2	1:B:328:VAL:O	1.95	0.67
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.76	0.67
2:N:279:PHE:CE1	3:P:263:ILE:HD12	2.30	0.67
2:F:346:PRO:HB2	2:F:348:VAL:HG23	1.77	0.67
2:V:97:ASN:HD21	2:V:101:GLU:HB2	1.60	0.67
1:B:36:VAL:HG11	1:B:84:VAL:O	1.94	0.67
1:T:33:VAL:HB	1:T:87:GLY:H	1.60	0.66
2:X:128:SER:HB2	2:X:300:LYS:HG3	1.78	0.66
1:U:135:ALA:HB3	2:V:223:ASN:HD22	1.60	0.66
1:J:192:ASN:HA	1:J:200:LYS:HG2	1.77	0.65
2:D:26:GLU:OE2	2:D:26:GLU:HA	1.96	0.65
1:S:73:VAL:HG22	2:W:72:ARG:HH12	1.60	0.65
1:B:109:VAL:HG22	1:B:233:ILE:HB	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:358:LEU:HB2	1:K:366:ALA:HB1	1.79	0.65
1:S:349:ASP:O	1:S:375:ARG:HB2	1.96	0.65
1:K:99:VAL:HG11	1:K:251:THR:HB	1.79	0.65
1:B:166:ARG:HD3	1:B:308:LEU:O	1.96	0.65
1:S:107:GLY:HA2	1:S:228:MET:O	1.96	0.65
1:C:168:LEU:HB2	1:C:348:THR:HG21	1.79	0.64
1:A:112:ALA:O	1:A:251:THR:HG21	1.97	0.64
1:L:164:GLY:HA2	1:L:323:LEU:O	1.96	0.64
1:T:101:VAL:HG12	1:T:255:ILE:HA	1.79	0.64
1:J:70:PRO:HD3	2:N:15:ALA:HB2	1.78	0.64
2:O:264:ALA:HA	2:O:267:GLU:HG3	1.79	0.64
1:A:173:ARG:NH2	2:D:352:ASP:OD1	2.30	0.64
2:N:405:GLU:HG2	2:N:409:LYS:HE2	1.80	0.64
2:E:98:VAL:HB	2:E:232:VAL:HG13	1.79	0.64
2:E:158:GLY:O	2:E:161:VAL:HG22	1.98	0.64
1:A:329:ILE:HD11	1:A:344:VAL:HG21	1.80	0.64
3:G:15:ASN:O	3:G:19:ILE:HG12	1.98	0.64
1:L:290:PRO:HB2	2:M:270:ALA:HB1	1.79	0.64
1:U:111:ASP:OD1	1:U:115:ASN:HB2	1.98	0.64
2:F:41:THR:HB	2:F:42:PRO:HD2	1.79	0.63
2:O:252:LEU:HD23	2:O:305:THR:HB	1.80	0.63
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.81	0.63
1:J:375:ARG:HH22	2:N:190:ARG:NE	1.97	0.63
1:L:99:VAL:HG11	1:L:251:THR:HB	1.81	0.63
2:F:33:ILE:O	2:F:34:LEU:HB2	1.99	0.63
3:P:42:LYS:HD3	3:P:42:LYS:O	1.99	0.63
1:T:504:GLU:HA	1:T:507:VAL:HB	1.81	0.63
1:J:223:GLU:HG3	1:J:228:MET:HG3	1.79	0.63
1:U:176:GLY:O	1:U:180:VAL:HG23	1.98	0.63
2:E:157:GLY:HA2	2:E:337:ARG:HH22	1.64	0.63
2:V:84:SER:HB3	2:V:114:ARG:HE	1.62	0.63
2:V:189:GLU:O	2:V:222:MET:HG2	1.99	0.62
2:M:224:GLU:O	2:M:229:ARG:HD3	1.99	0.62
1:S:223:GLU:HG3	1:S:228:MET:HG3	1.81	0.62
3:P:122:HIS:N	3:P:123:PRO:CD	2.63	0.62
2:W:133:ILE:HD12	2:W:146:PRO:HB2	1.82	0.62
4:H:35:LYS:HD3	4:H:35:LYS:H	1.64	0.62
1:T:392:LEU:HD13	1:T:451:VAL:HG22	1.82	0.62
2:M:160:GLY:N	6:M:600:ANP:HNB1	1.87	0.61
1:U:212:ARG:HG2	1:U:237:THR:HG21	1.80	0.61
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:160:GLY:H	6:X:600:ANP:HNB1	1.46	0.61
2:F:345:TYR:HA	2:F:346:PRO:C	2.18	0.61
2:F:148:ALA:HB2	2:F:357:LEU:HD11	1.82	0.61
2:N:244:ARG:HD3	2:N:304:VAL:HG23	1.81	0.61
1:J:302:TYR:O	1:J:306:ARG:HB2	2.00	0.61
1:B:99:VAL:HG11	1:B:251:THR:HB	1.81	0.61
2:D:197:LEU:O	2:D:201:MET:HG2	2.01	0.61
1:J:469:SER:HB3	1:J:506:PHE:CZ	2.35	0.61
2:E:39:ILE:HD13	2:E:70:LEU:HD21	1.83	0.61
2:E:43:GLN:HG2	2:E:44:GLY:N	2.15	0.61
1:B:148:VAL:HG23	1:B:163:ARG:HG2	1.83	0.61
1:K:173:ARG:HH12	2:N:327:ALA:HA	1.66	0.61
2:N:458:TYR:HD2	2:N:459:MET:HG2	1.66	0.61
1:B:387:GLN:OE1	1:B:491:LEU:HB2	2.01	0.61
1:J:306:ARG:HA	2:N:223:ASN:HB2	1.83	0.60
2:V:252:LEU:HD23	2:V:305:THR:HB	1.83	0.60
2:X:386:ASP:O	2:X:390:ILE:HG12	2.01	0.60
2:W:15:ALA:HB3	2:W:22:ASP:HB2	1.83	0.60
6:F:600:ANP:O5'	6:F:600:ANP:H8	2.01	0.60
1:K:211:LYS:HD2	2:N:328:HIS:HA	1.83	0.60
1:U:97:VAL:HG11	1:U:247:LEU:HD11	1.83	0.60
2:N:255:ILE:HB	2:N:308:GLN:HG2	1.81	0.60
2:V:204:THR:HB	2:V:206:VAL:HG23	1.84	0.60
3:G:115:LYS:O	3:G:119:LEU:HB2	2.01	0.60
1:S:145:HIS:H	1:S:313:LYS:HZ3	1.50	0.60
1:L:116:PRO:HG3	1:L:123:ILE:HG12	1.84	0.60
3:G:49:GLN:HE21	3:G:217:GLN:NE2	1.99	0.60
3:G:205:VAL:O	3:G:209:LEU:HB2	2.02	0.59
1:K:346:SER:HA	6:O:600:ANP:O3G	2.02	0.59
1:T:220:GLN:HB2	2:W:129:THR:HB	1.84	0.59
3:P:81:LYS:HE3	3:P:135:LYS:HD2	1.84	0.59
1:J:173:ARG:HD2	1:J:174:GLN:HE21	1.66	0.59
1:C:116:PRO:HG3	1:C:123:ILE:HG12	1.85	0.59
2:N:23:VAL:HG11	2:N:76:VAL:HG21	1.84	0.59
1:L:248:ALA:HB3	1:L:249:PRO:HD3	1.85	0.59
1:A:77:LEU:CD1	1:A:81:ASP:HB3	2.29	0.59
2:D:208:ASN:ND2	2:D:211:GLY:HA3	2.18	0.59
2:V:94:ARG:NH2	2:V:106:ARG:HB2	2.18	0.59
2:M:234:LEU:CD2	2:M:292:LEU:HD13	2.33	0.59
2:M:371:ALA:O	2:M:375:GLN:HG3	2.03	0.59
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:64:MET:CE	2:V:99:ILE:HG22	2.33	0.58
1:K:34:LEU:HD21	1:K:44:PHE:HB2	1.85	0.58
1:L:493:LYS:HA	1:L:496:LEU:HD12	1.85	0.58
3:P:168:ASP:HB2	3:P:178:SER:OG	2.03	0.58
5:I:12:ALA:O	5:I:16:VAL:HG23	2.03	0.58
1:U:206:VAL:HG13	1:U:234:VAL:HB	1.84	0.58
1:A:239:SER:HB3	2:D:294:GLU:HG3	1.86	0.58
2:F:146:PRO:O	2:F:355:SER:OG	2.21	0.58
1:S:309:GLU:HG3	2:W:223:ASN:HB3	1.86	0.58
2:X:384:LEU:O	2:X:388:ILE:HG12	2.04	0.58
2:V:164:THR:O	2:V:167:ILE:HG22	2.04	0.58
1:K:364:ARG:HA	1:K:365:PRO:C	2.24	0.58
1:B:98:ASP:HB2	1:B:129:SER:O	2.04	0.58
1:L:148:VAL:HG21	1:L:324:THR:HG21	1.85	0.58
1:K:260:ARG:O	1:K:321:GLY:HA3	2.04	0.58
2:O:449:TYR:HB3	2:O:452:ILE:HD12	1.86	0.58
3:P:169:PRO:HG3	3:P:227:ALA:HB3	1.84	0.58
3:Y:16:ILE:HA	3:Y:19:ILE:HG22	1.86	0.58
2:V:182:SER:O	2:V:215:VAL:HA	2.04	0.57
1:K:186:LEU:O	1:K:189:LYS:HE3	2.03	0.57
2:X:178:HIS:HE2	2:X:250:ASP:HB3	1.69	0.57
1:T:67:ASN:HB3	2:X:17:ILE:HG23	1.86	0.57
1:S:439:ALA:HB3	1:S:442:GLU:HG3	1.85	0.57
1:S:217:GLN:HG2	2:V:356:ARG:HH21	1.68	0.57
1:A:146:GLU:HB2	1:A:163:ARG:HG3	1.87	0.57
2:D:263:GLN:O	2:D:266:SER:HB3	2.05	0.57
1:B:26:ASN:O	1:B:30:THR:HB	2.05	0.57
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.87	0.57
1:S:166:ARG:HD3	1:S:308:LEU:O	2.05	0.57
1:U:243:PRO:HA	1:U:283:LEU:HD11	1.87	0.57
2:V:339:ILE:HG22	2:V:344:ILE:HB	1.86	0.57
2:F:189:GLU:O	2:F:221:GLN:HB3	2.04	0.57
2:F:26:GLU:OE1	2:F:26:GLU:HA	2.04	0.57
1:A:182:LEU:CD1	1:A:218:LEU:HD11	2.31	0.56
2:V:345:TYR:HA	2:V:346:PRO:C	2.25	0.56
2:V:162:GLY:HA2	6:V:600:ANP:H8	1.86	0.56
2:O:345:TYR:HA	2:O:346:PRO:C	2.24	0.56
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.86	0.56
2:E:277:SER:OG	2:E:278:ALA:N	2.38	0.56
2:O:237:LEU:HD13	2:O:296:ILE:HG12	1.87	0.56
2:W:319:ASP:HA	3:Y:260:GLN:HE22	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:LYS:O	1:A:387:GLN:HG3	2.06	0.56
4:H:14:PHE:CB	4:H:22:TYR:HB2	2.35	0.56
2:N:96:ILE:HB	2:N:218:VAL:HG22	1.87	0.56
1:S:284:SER:O	1:S:289:ARG:HB2	2.06	0.56
1:S:192:ASN:HA	1:S:200:LYS:HG2	1.88	0.56
1:S:163:ARG:O	1:S:313:LYS:HE3	2.06	0.56
1:S:265:HIS:ND1	1:S:322:SER:HB2	2.21	0.56
2:M:229:ARG:NH2	2:M:267:GLU:OE1	2.37	0.56
4:H:14:PHE:CZ	4:H:70:ILE:HD11	2.40	0.56
2:V:346:PRO:O	2:V:347:ALA:HB3	2.04	0.56
1:A:55:VAL:HG21	1:A:75:ILE:HD13	1.87	0.56
1:J:364:ARG:HA	1:J:365:PRO:C	2.26	0.56
5:I:55:GLU:CB	5:I:56:PRO:CD	2.83	0.56
1:K:444:VAL:CG2	1:K:445:PRO:HD3	2.36	0.56
2:O:140:VAL:HG13	2:O:414:LEU:HB3	1.88	0.56
2:N:51:ALA:O	2:N:52:GLN:HG3	2.06	0.56
1:U:378:SER:HB3	1:U:386:LYS:HE2	1.88	0.56
4:H:14:PHE:HB3	4:H:22:TYR:HB2	1.88	0.55
1:C:450:GLY:HA2	1:C:455:LEU:HD12	1.87	0.55
1:U:237:THR:H	1:U:240:GLU:HG3	1.71	0.55
2:V:46:LEU:HD22	2:V:70:LEU:HD21	1.88	0.55
1:K:488:LYS:HE3	1:K:490:GLU:HB2	1.88	0.55
3:Y:108:VAL:HG12	3:Y:130:ILE:HG13	1.88	0.55
1:S:36:VAL:HG21	1:S:84:VAL:HB	1.88	0.55
3:G:46:GLU:O	3:G:50:LEU:HB2	2.05	0.55
1:S:484:GLU:HG2	1:S:495:LEU:HD11	1.87	0.55
1:U:169:ILE:HB	1:U:328:VAL:HG22	1.88	0.55
1:B:260:ARG:O	1:B:321:GLY:HA3	2.06	0.55
2:O:377:THR:HG23	2:O:403:THR:HG23	1.88	0.55
1:L:344:VAL:HA	1:L:347:ILE:HD12	1.89	0.55
2:V:9:ILE:HB	2:V:78:ASP:HB3	1.89	0.55
3:G:247:MET:HG3	3:G:250:ARG:HH21	1.71	0.55
1:B:105:LEU:O	1:B:232:ILE:HG12	2.07	0.55
2:V:192:ARG:NH1	2:V:193:GLU:HG2	2.22	0.55
2:D:144:LEU:HD22	2:D:375:GLN:HE21	1.72	0.55
3:P:111:GLY:HA2	3:P:133:ILE:HD11	1.88	0.55
2:N:220:GLY:HA3	2:N:232:VAL:HG11	1.89	0.55
1:L:306:ARG:HG2	1:L:307:LEU:N	2.21	0.55
1:A:500:LYS:O	1:A:504:GLU:HG3	2.06	0.55
4:H:72:GLY:O	4:H:87:ALA:HA	2.07	0.55
2:V:15:ALA:HB3	2:V:22:ASP:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:67:ASN:HB2	2:X:17:ILE:HG12	1.89	0.55
2:F:52:GLN:HG2	2:F:60:ARG:HB3	1.89	0.55
2:O:324:THR:O	2:O:324:THR:HG22	2.07	0.55
1:C:503:THR:O	1:C:507:VAL:HG23	2.07	0.54
1:B:444:VAL:HG22	1:B:445:PRO:HD3	1.88	0.54
2:X:167:ILE:HD12	2:X:309:ALA:HB2	1.89	0.54
2:V:346:PRO:O	2:V:347:ALA:CB	2.55	0.54
2:M:440:SER:OG	2:M:463:ILE:HG12	2.07	0.54
2:X:258:ILE:HD13	2:X:308:GLN:OE1	2.07	0.54
1:L:222:LEU:HD12	1:L:228:MET:HE2	1.90	0.54
1:B:359:PHE:HZ	6:B:600:ANP:O4'	1.90	0.54
1:S:311:ALA:HA	1:S:323:LEU:HB3	1.90	0.54
1:S:55:VAL:HG21	1:S:75:ILE:HD13	1.89	0.54
1:T:282:GLN:O	1:T:286:LEU:HG	2.08	0.54
1:L:196:ASP:OD1	1:L:198:SER:OG	2.23	0.54
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.37	0.54
3:P:205:VAL:N	3:P:206:PRO:CD	2.66	0.54
1:L:174:GLN:HA	6:L:600:ANP:HNB1	1.73	0.54
2:N:169:GLU:HG2	2:N:418:PHE:CD1	2.42	0.54
3:P:229:GLU:HG3	3:P:230:ILE:N	2.23	0.54
2:D:299:THR:OG1	2:D:300:LYS:N	2.41	0.54
1:U:165:GLN:HG2	1:U:166:ARG:H	1.73	0.54
5:I:19:GLN:HE22	5:I:38:SER:HB3	1.73	0.54
3:G:118:LEU:HB3	3:G:126:ILE:HD11	1.90	0.54
1:J:332:GLN:HB3	2:M:318:THR:HB	1.89	0.54
1:U:56:GLU:HG2	1:U:62:LYS:HG2	1.90	0.54
3:Y:91:LEU:HD12	3:Y:177:PRO:HB3	1.89	0.54
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.90	0.54
2:W:388:ILE:HD12	2:W:393:MET:HG2	1.90	0.54
1:C:429:LEU:HD11	1:C:446:LEU:HB3	1.90	0.54
1:A:111:ASP:OD2	1:A:115:ASN:HB2	2.08	0.54
2:X:237:LEU:HD13	2:X:296:ILE:HG12	1.89	0.53
1:S:462:ARG:HH11	1:S:465:GLU:HG3	1.73	0.53
3:P:86:SER:HB2	3:P:90:GLN:HG3	1.90	0.53
2:X:345:TYR:HA	2:X:346:PRO:C	2.29	0.53
2:M:321:ALA:HB3	2:M:322:PRO:CD	2.38	0.53
1:S:402:VAL:HA	1:S:405:PHE:HD1	1.73	0.53
2:E:344:ILE:HG23	2:E:415:SER:HB3	1.89	0.53
1:T:305:SER:HB2	2:X:222:MET:HB2	1.90	0.53
1:K:217:GLN:NE2	2:N:131:ALA:HB2	2.24	0.53
2:N:131:ALA:HB1	2:N:357:LEU:HD11	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:237:LEU:HD13	2:V:296:ILE:HG12	1.91	0.53
3:G:87:ILE:HG23	3:G:167:ASN:ND2	2.24	0.53
2:V:346:PRO:HD3	2:V:416:GLN:H	1.74	0.53
1:S:187:ASN:O	1:S:190:ARG:HG3	2.08	0.53
2:O:15:ALA:HB3	2:O:22:ASP:HB2	1.91	0.53
1:U:249:PRO:HB3	1:U:270:TYR:HD1	1.73	0.53
1:J:253:ALA:O	1:J:257:GLU:HG3	2.08	0.53
2:W:170:LEU:O	2:W:174:ILE:HG12	2.09	0.53
2:D:33:ILE:O	2:D:34:LEU:HB2	2.08	0.53
3:G:77:ILE:HD13	3:G:110:ILE:HD12	1.90	0.53
2:V:321:ALA:HB3	2:V:322:PRO:CD	2.39	0.53
4:H:57:VAL:CG2	4:H:70:ILE:HD12	2.38	0.53
2:M:425:THR:CG2	6:M:600:ANP:H2	2.39	0.53
2:E:228:ALA:O	2:E:232:VAL:HG22	2.09	0.53
1:K:301:PHE:CB	2:O:263:GLN:HE22	2.21	0.53
2:V:189:GLU:O	2:V:221:GLN:HB3	2.09	0.52
1:A:257:GLU:HG2	1:A:260:ARG:CZ	2.39	0.52
1:J:108:ARG:NH2	1:J:121:GLY:O	2.37	0.52
1:U:354:LEU:HA	1:U:366:ALA:O	2.08	0.52
1:U:54:LEU:HD21	1:U:97:VAL:HG13	1.90	0.52
3:P:133:ILE:O	3:P:135:LYS:N	2.35	0.52
1:K:148:VAL:HB	1:K:161:ILE:HB	1.91	0.52
1:S:118:ASP:OD1	1:S:120:LYS:HD2	2.09	0.52
2:M:336:SER:HB3	2:M:339:ILE:HG13	1.91	0.52
1:L:54:LEU:O	1:L:93:THR:HB	2.10	0.52
3:Y:79:SER:HB3	3:Y:88:HIS:HE1	1.73	0.52
2:N:384:LEU:O	2:N:388:ILE:HG12	2.08	0.52
2:V:192:ARG:HH11	2:V:193:GLU:HG2	1.74	0.52
1:C:43:VAL:HG21	1:C:75:ILE:HD12	1.90	0.52
2:O:221:GLN:OE1	2:O:221:GLN:HA	2.10	0.52
2:D:158:GLY:O	2:D:161:VAL:HG22	2.09	0.52
3:G:49:GLN:HE21	3:G:217:GLN:HE22	1.57	0.52
2:D:244:ARG:HD2	2:D:299:THR:HG22	1.91	0.52
1:C:189:LYS:HE3	1:C:226:ASP:HB3	1.91	0.52
1:A:478:HIS:HB3	1:A:481:LEU:HD21	1.91	0.52
2:N:98:VAL:HG13	2:N:99:ILE:HG23	1.90	0.52
2:N:184:PHE:HB3	2:N:217:LEU:HD23	1.90	0.52
2:N:152:LYS:HE2	2:N:293:GLN:O	2.10	0.52
1:S:311:ALA:HB1	1:S:323:LEU:O	2.10	0.52
3:P:168:ASP:N	3:P:176:GLU:O	2.40	0.51
1:U:249:PRO:HB3	1:U:270:TYR:CD1	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:PRO:HD3	1:C:258:TRP:CH2	2.45	0.51
1:J:421:VAL:O	1:J:425:ARG:HD2	2.10	0.51
2:E:136:THR:HG23	2:E:138:ILE:H	1.75	0.51
1:J:135:ALA:HB3	2:N:223:ASN:ND2	2.25	0.51
2:W:370:VAL:O	2:W:374:VAL:HG23	2.10	0.51
1:U:211:LYS:HE3	1:U:213:SER:HB2	1.92	0.51
1:L:481:LEU:HD13	1:L:495:LEU:HD22	1.91	0.51
1:T:77:LEU:O	1:T:243:PRO:HG2	2.11	0.51
1:U:150:THR:HA	1:U:184:THR:HG23	1.91	0.51
1:A:77:LEU:HD12	1:A:81:ASP:CB	2.33	0.51
1:K:269:VAL:HG22	1:K:326:LEU:HB2	1.91	0.51
1:L:187:ASN:O	1:L:190:ARG:HG3	2.09	0.51
2:F:176:LYS:HE2	2:F:204:THR:HB	1.93	0.51
4:H:33:PRO:HB3	4:H:38:ARG:NH1	2.26	0.51
1:K:354:LEU:HA	1:K:366:ALA:O	2.11	0.51
1:J:174:GLN:HA	6:J:600:ANP:HNB1	1.74	0.51
1:L:222:LEU:HD12	1:L:228:MET:CE	2.40	0.51
1:K:66:LEU:HD21	1:K:289:ARG:HH22	1.75	0.51
1:U:258:TRP:O	1:U:262:ASN:ND2	2.44	0.51
2:V:133:ILE:HD11	2:V:434:LEU:HD13	1.92	0.51
1:S:99:VAL:HG21	1:S:251:THR:HG23	1.92	0.51
1:S:422:ARG:HH21	1:S:453:GLY:HA3	1.75	0.51
2:E:50:VAL:HA	2:E:61:THR:HG22	1.91	0.51
2:O:37:LEU:HD12	2:O:61:THR:HG21	1.91	0.51
1:A:142:ARG:HD3	1:A:143:SER:O	2.11	0.51
1:A:153:LYS:NZ	1:A:467:GLU:OE1	2.42	0.51
2:M:425:THR:HG23	6:M:600:ANP:H2	1.93	0.51
3:G:110:ILE:HA	3:G:130:ILE:HB	1.93	0.51
2:D:7:THR:CG2	2:D:7:THR:O	2.59	0.51
1:S:422:ARG:HE	1:S:453:GLY:HA2	1.76	0.51
1:J:243:PRO:HD3	1:J:283:LEU:HD21	1.93	0.51
1:C:159:VAL:HG21	1:C:352:ILE:HG12	1.92	0.51
2:M:62:ILE:HD11	2:M:272:LEU:HD11	1.93	0.51
1:A:391:SER:O	1:A:394:LEU:HB2	2.10	0.51
3:G:165:PHE:CE2	3:G:179:GLU:HB2	2.46	0.51
2:W:220:GLY:HA3	2:W:232:VAL:HG11	1.92	0.51
2:D:64:MET:CE	2:D:228:ALA:HA	2.41	0.50
1:J:50:GLN:HB3	2:N:69:GLY:HA2	1.92	0.50
1:J:375:ARG:HH22	2:N:190:ARG:CZ	2.25	0.50
2:V:298:THR:HG23	2:V:303:SER:HA	1.93	0.50
2:V:82:PRO:HB3	2:V:118:HIS:HD2	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:168:GLN:HE21	2:N:201:MET:HG2	1.77	0.50
2:D:408:ARG:O	2:D:412:ARG:HD2	2.11	0.50
2:W:140:VAL:HG22	2:W:414:LEU:O	2.12	0.50
1:K:421:VAL:O	1:K:425:ARG:HG2	2.11	0.50
1:K:174:GLN:HA	6:K:600:ANP:N3B	2.27	0.50
1:A:444:VAL:HG22	1:A:445:PRO:HD3	1.92	0.50
1:K:32:ARG:HD2	1:K:87:GLY:O	2.11	0.50
2:D:20:ILE:HG13	2:D:271:LEU:HB3	1.93	0.50
2:D:148:ALA:HA	2:D:357:LEU:HD11	1.93	0.50
1:S:481:LEU:O	1:S:485:ILE:HG13	2.12	0.50
2:X:321:ALA:HB3	2:X:322:PRO:CD	2.42	0.50
4:H:57:VAL:HG21	4:H:70:ILE:HD12	1.93	0.50
1:C:107:GLY:HA2	1:C:228:MET:O	2.11	0.50
1:B:421:VAL:O	1:B:425:ARG:HG2	2.12	0.50
2:E:243:PHE:O	2:E:247:GLU:HB2	2.12	0.50
3:G:205:VAL:HB	3:G:206:PRO:HD3	1.93	0.50
2:M:20:ILE:HG13	2:M:271:LEU:HB3	1.94	0.50
1:A:282:GLN:HG3	2:D:283:PRO:O	2.11	0.50
1:S:248:ALA:HB3	1:S:249:PRO:HD3	1.92	0.50
2:W:284:THR:HB	2:W:288:ASP:OD1	2.12	0.50
2:W:242:TYR:CE1	2:W:246:GLU:HG3	2.47	0.50
1:S:287:LEU:HB2	1:S:289:ARG:HD2	1.94	0.49
1:C:219:VAL:HB	1:C:228:MET:HE3	1.94	0.49
3:Y:150:LEU:HA	3:Y:154:MET:HB2	1.93	0.49
3:P:162:ILE:HB	3:P:182:ILE:HB	1.94	0.49
4:H:14:PHE:HZ	4:H:70:ILE:HD11	1.76	0.49
3:Y:263:ILE:O	3:Y:267:LEU:HB3	2.13	0.49
2:V:33:ILE:O	2:V:34:LEU:HB2	2.12	0.49
2:D:218:VAL:HG21	2:D:236:GLY:HA2	1.94	0.49
1:B:168:LEU:HB2	1:B:348:THR:HG21	1.94	0.49
1:L:197:GLU:HA	1:L:200:LYS:HD2	1.95	0.49
2:W:419:ALA:HA	2:W:429:GLY:HA3	1.92	0.49
3:G:118:LEU:HA	3:G:121:THR:HG22	1.94	0.49
1:K:273:LEU:HD22	1:K:276:GLN:OE1	2.13	0.49
1:K:109:VAL:HG22	1:K:233:ILE:HB	1.93	0.49
2:N:253:LEU:O	2:N:306:SER:HA	2.13	0.49
2:D:201:MET:HE2	2:D:217:LEU:HD21	1.93	0.49
1:T:138:ILE:HD13	2:X:95:ILE:HG21	1.93	0.49
2:X:178:HIS:NE2	2:X:250:ASP:HB3	2.27	0.49
2:N:359:ASP:O	2:N:363:VAL:HG22	2.12	0.49
2:D:201:MET:HE1	2:D:215:VAL:HG11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:166:ARG:HH21	1:L:349:ASP:CG	2.16	0.49
2:F:140:VAL:HG12	2:F:414:LEU:HD22	1.94	0.49
2:N:410:ILE:HG23	2:N:441:PHE:HE2	1.77	0.49
1:B:117:ILE:HD12	2:E:124:PHE:HB3	1.95	0.49
2:N:220:GLY:CA	2:N:232:VAL:HG11	2.42	0.49
1:L:338:ALA:O	1:L:342:THR:OG1	2.31	0.49
2:M:152:LYS:HD3	2:M:328:HIS:O	2.12	0.49
1:L:484:GLU:HB3	1:L:495:LEU:HD11	1.95	0.49
1:L:441:GLU:OE2	1:L:486:ARG:HD3	2.13	0.49
1:J:428:GLN:HA	1:J:431:LYS:HD2	1.94	0.49
2:W:33:ILE:O	2:W:34:LEU:HB2	2.12	0.49
1:T:103:PRO:HD3	1:T:258:TRP:CZ2	2.48	0.49
3:P:150:LEU:HA	3:P:154:MET:HB2	1.95	0.49
1:U:242:ALA:HB3	1:U:243:PRO:HD3	1.95	0.48
2:E:33:ILE:O	2:E:34:LEU:HB2	2.13	0.48
1:U:285:LEU:HD11	1:U:295:ALA:HB1	1.95	0.48
5:I:28:GLU:O	5:I:30:GLN:N	2.42	0.48
1:S:441:GLU:CG	1:S:486:ARG:HB2	2.41	0.48
1:S:39:GLY:HA2	1:S:77:LEU:HD12	1.94	0.48
2:F:84:SER:HB2	2:F:114:ARG:HH11	1.78	0.48
1:U:166:ARG:HG2	1:U:325:ALA:HB3	1.95	0.48
1:J:173:ARG:HH11	1:J:174:GLN:HE21	1.60	0.48
2:M:234:LEU:HD22	2:M:292:LEU:HD13	1.96	0.48
1:B:445:PRO:HB3	1:B:499:LEU:HD11	1.95	0.48
1:L:161:ILE:HA	1:L:165:GLN:OE1	2.13	0.48
3:G:75:VAL:HB	3:G:164:ILE:HD13	1.95	0.48
2:O:346:PRO:HB2	2:O:348:VAL:HG23	1.95	0.48
2:D:34:LEU:HD22	2:D:118:HIS:CE1	2.49	0.48
1:S:340:ILE:HB	1:S:341:PRO:HD3	1.95	0.48
2:F:9:ILE:HG23	2:F:27:GLN:NE2	2.28	0.48
2:E:456:ALA:HA	2:E:469:LYS:HD3	1.96	0.48
2:D:384:LEU:O	2:D:388:ILE:HG12	2.13	0.48
2:M:335:LEU:HA	2:M:347:ALA:O	2.13	0.48
3:G:17:GLU:O	3:G:21:LYS:HB2	2.14	0.48
3:G:267:LEU:O	3:G:271:ILE:HG12	2.14	0.48
2:O:165:VAL:HG23	6:O:600:ANP:O1A	2.13	0.48
1:A:394:LEU:O	1:A:397:ALA:HB3	2.13	0.48
1:C:88:GLU:HG3	1:C:89:LEU:N	2.28	0.48
1:K:51:ALA:O	1:K:52:GLU:HB2	2.13	0.48
2:X:85:VAL:CG1	2:X:235:THR:HG23	2.44	0.48
1:C:481:LEU:HD21	1:C:498:SER:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:478:HIS:HB3	1:K:481:LEU:HG	1.96	0.48
2:N:252:LEU:HA	2:N:305:THR:O	2.14	0.48
2:E:10:THR:HG21	2:E:75:LYS:HE2	1.96	0.48
2:D:386:ASP:OD1	2:D:386:ASP:N	2.46	0.48
1:K:152:LEU:HD22	1:K:365:PRO:HG3	1.96	0.48
2:V:190:ARG:HB2	2:V:193:GLU:HG3	1.96	0.48
4:H:88:ILE:HD11	5:I:14:LEU:HB3	1.95	0.48
1:A:134:LYS:HE2	2:E:65:ASP:OD1	2.13	0.48
1:S:47:ASN:HA	2:W:72:ARG:HH21	1.79	0.48
2:M:143:LEU:O	2:M:367:HIS:HE1	1.97	0.48
1:L:172:ASP:O	1:L:177:LYS:NZ	2.47	0.48
1:B:345:ILE:HG12	1:B:351:GLN:HG2	1.94	0.48
1:S:395:PHE:HE1	1:S:422:ARG:HH11	1.61	0.48
2:D:47:VAL:HG21	2:D:99:ILE:HG21	1.95	0.48
2:N:330:ASP:O	2:N:356:ARG:HD3	2.14	0.48
2:E:221:GLN:HB2	2:E:223:ASN:OD1	2.14	0.48
1:A:395:PHE:HZ	1:A:419:THR:CA	2.06	0.47
2:X:190:ARG:NH1	6:X:600:ANP:O3G	2.45	0.47
4:H:88:ILE:CD1	5:I:14:LEU:HB3	2.44	0.47
1:B:291:PRO:HG2	3:G:268:VAL:HG22	1.96	0.47
1:A:272:ASP:HB2	1:A:328:VAL:O	2.14	0.47
1:K:428:GLN:O	1:K:431:LYS:HB2	2.14	0.47
1:S:260:ARG:O	1:S:321:GLY:HA3	2.13	0.47
1:T:355:GLU:HB3	1:T:358:LEU:HD12	1.97	0.47
1:L:108:ARG:NH2	1:L:120:LYS:HB2	2.28	0.47
2:F:67:THR:HB	2:F:70:LEU:HD12	1.96	0.47
1:B:46:LEU:HD22	1:B:92:ARG:HG3	1.96	0.47
1:B:26:ASN:ND2	1:B:26:ASN:H	2.13	0.47
1:J:100:PRO:HD3	1:J:128:ARG:NH1	2.30	0.47
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.96	0.47
2:N:184:PHE:HA	2:N:254:PHE:HB2	1.96	0.47
2:V:397:SER:HB3	2:V:400:ASP:HB2	1.95	0.47
1:T:413:ASP:O	1:T:417:LYS:HB2	2.15	0.47
2:M:167:ILE:HD12	2:M:309:ALA:HB2	1.96	0.47
1:S:142:ARG:HG2	1:S:143:SER:N	2.29	0.47
1:L:506:PHE:O	1:L:509:THR:HA	2.15	0.47
2:F:263:GLN:O	2:F:267:GLU:HG3	2.15	0.47
1:C:80:SER:OG	1:C:82:ARG:HG2	2.13	0.47
1:B:213:SER:O	1:B:217:GLN:HG3	2.15	0.47
1:J:388:VAL:HG21	1:J:444:VAL:HB	1.96	0.47
2:N:127:GLN:HE22	2:N:297:THR:HG21	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:136:ASP:N	3:P:136:ASP:OD2	2.48	0.47
2:M:416:GLN:HA	2:M:417:PRO:HD2	1.78	0.47
1:K:271:ASP:HA	1:K:272:ASP:HA	1.62	0.47
1:S:309:GLU:OE1	2:W:191:THR:OG1	2.26	0.47
2:V:330:ASP:O	2:V:356:ARG:HG2	2.14	0.47
2:W:220:GLY:CA	2:W:232:VAL:HG11	2.45	0.47
1:L:280:TYR:CD2	1:L:303:LEU:HD22	2.50	0.47
3:Y:116:MET:HA	3:Y:119:LEU:HB2	1.95	0.47
5:I:31:THR:HG22	5:I:34:VAL:HG23	1.97	0.47
1:C:364:ARG:HA	1:C:365:PRO:C	2.34	0.47
2:F:346:PRO:C	2:F:348:VAL:H	2.18	0.47
1:J:205:TYR:HB3	1:J:233:ILE:HD13	1.97	0.47
1:A:354:LEU:HA	1:A:366:ALA:O	2.15	0.47
2:W:98:VAL:HG13	2:W:99:ILE:HG23	1.95	0.47
1:U:46:LEU:HD22	1:U:92:ARG:HG3	1.97	0.47
2:F:164:THR:O	2:F:168:GLN:HG3	2.15	0.47
2:M:158:GLY:O	2:M:163:LYS:NZ	2.48	0.47
1:S:168:LEU:HD12	1:S:327:PRO:O	2.15	0.47
2:D:189:GLU:O	2:D:222:MET:HG2	2.14	0.47
1:B:202:TYR:O	1:B:266:ALA:HA	2.15	0.47
3:G:81:LYS:HD2	3:G:134:GLY:O	2.14	0.47
1:C:187:ASN:O	1:C:190:ARG:HG3	2.14	0.47
1:A:82:ARG:O	1:A:82:ARG:HG2	2.14	0.47
1:S:168:LEU:HD21	1:S:170:ILE:HD12	1.96	0.46
2:F:289:MET:SD	2:F:324:THR:HG22	2.55	0.46
2:V:315:ASP:OD2	2:V:337:ARG:NE	2.33	0.46
2:V:136:THR:HG21	2:V:147:TYR:CD2	2.49	0.46
2:F:394:ASP:HB3	3:G:85:GLY:O	2.15	0.46
2:V:373:LYS:HG2	2:V:445:LEU:HD22	1.97	0.46
2:E:136:THR:HG22	2:E:142:ASP:CG	2.36	0.46
1:C:42:ARG:HE	1:C:72:GLN:HE22	1.61	0.46
1:J:164:GLY:HA2	1:J:323:LEU:O	2.15	0.46
2:E:188:GLY:O	2:E:222:MET:HG3	2.16	0.46
1:J:459:GLU:HG3	1:J:462:ARG:HG3	1.97	0.46
3:G:56:GLU:O	3:G:58:LYS:HD3	2.15	0.46
1:S:272:ASP:HB2	1:S:328:VAL:O	2.15	0.46
3:G:180:LYS:HZ1	3:G:220:THR:HB	1.80	0.46
1:J:270:TYR:O	1:J:272:ASP:HA	2.15	0.46
1:B:51:ALA:O	1:B:52:GLU:HB2	2.16	0.46
1:A:445:PRO:HB3	1:A:499:LEU:HD11	1.98	0.46
1:C:349:ASP:O	1:C:375:ARG:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:338:ALA:HB3	1:K:341:PRO:HG2	1.98	0.46
2:O:245:ASP:OD1	2:O:301:LYS:HD3	2.15	0.46
1:S:206:VAL:HG22	1:S:252:ALA:CB	2.46	0.46
2:V:96:ILE:HB	2:V:218:VAL:HG22	1.96	0.46
1:T:166:ARG:HH22	2:X:190:ARG:CD	2.28	0.46
1:A:70:PRO:HD3	2:E:15:ALA:HB2	1.97	0.46
2:N:52:GLN:HB2	2:N:60:ARG:HB3	1.97	0.46
1:A:391:SER:O	1:A:394:LEU:N	2.49	0.46
1:U:106:LEU:HD22	1:U:230:TYR:HA	1.96	0.46
4:H:56:VAL:HA	4:H:68:PHE:O	2.15	0.46
2:D:256:ASP:OD1	2:D:257:ASN:HB2	2.15	0.46
2:V:222:MET:HA	2:V:229:ARG:HD2	1.97	0.46
1:B:364:ARG:HA	1:B:365:PRO:C	2.35	0.46
2:M:84:SER:HB2	2:M:114:ARG:HH21	1.80	0.46
4:Q:16:LEU:HB2	4:Q:19:GLU:HB2	1.96	0.46
2:O:336:SER:HB3	2:O:339:ILE:HD12	1.97	0.46
2:F:152:LYS:HZ1	2:F:293:GLN:HB3	1.81	0.46
2:N:187:VAL:HG11	2:N:261:PHE:HB2	1.97	0.46
2:V:417:PRO:HG2	2:V:430:LYS:HB2	1.98	0.46
3:G:13:ILE:HG22	3:G:248:ILE:HG13	1.98	0.46
2:V:99:ILE:HD11	2:V:101:GLU:CD	2.36	0.46
2:M:32:ALA:O	2:M:35:ASN:HB2	2.16	0.46
2:F:382:LYS:HA	2:F:385:GLN:HG2	1.97	0.46
1:K:64:MET:HB2	1:K:78:PHE:CE2	2.51	0.46
2:N:96:ILE:HG22	2:N:97:ASN:N	2.31	0.45
1:U:177:LYS:HG2	1:U:354:LEU:HD12	1.98	0.45
1:U:112:ALA:HB3	1:U:244:LEU:HD22	1.97	0.45
2:E:30:LEU:HD11	2:E:57:ASN:HA	1.98	0.45
1:T:154:ALA:HB2	1:T:430:LEU:HB3	1.98	0.45
1:U:421:VAL:O	1:U:425:ARG:HD2	2.16	0.45
2:X:252:LEU:HD23	2:X:305:THR:HB	1.99	0.45
1:J:30:THR:HA	1:J:90:VAL:O	2.15	0.45
4:H:113:SER:N	4:H:114:SER:HA	2.30	0.45
1:J:139:LEU:O	1:J:141:ARG:N	2.44	0.45
1:J:141:ARG:HB2	2:N:195:ASN:ND2	2.31	0.45
2:X:36:ALA:HB2	2:X:83:ILE:HG12	1.97	0.45
1:T:424:GLU:O	1:T:428:GLN:HB2	2.16	0.45
2:N:276:PRO:HD2	3:P:271:ILE:HD11	1.98	0.45
2:E:134:LEU:HD22	2:E:305:THR:HG21	1.97	0.45
1:S:396:LEU:O	1:S:400:ARG:HG3	2.17	0.45
2:O:7:THR:HA	2:O:8:PRO:HD3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:O	1:C:159:VAL:HG23	2.16	0.45
2:W:53:HIS:O	2:W:55:GLY:N	2.49	0.45
1:B:155:VAL:HA	1:B:159:VAL:HG23	1.98	0.45
2:N:23:VAL:CG1	2:N:76:VAL:HG21	2.46	0.45
1:K:182:LEU:HA	1:K:185:ILE:HD12	1.99	0.45
1:B:67:ASN:HB2	2:F:17:ILE:HG13	1.98	0.45
1:S:146:GLU:H	1:S:313:LYS:NZ	2.14	0.45
1:T:77:LEU:HD21	1:T:84:VAL:HG21	1.99	0.45
2:O:384:LEU:HD22	2:O:396:LEU:HD21	1.99	0.45
1:K:188:GLN:HB3	1:K:192:ASN:ND2	2.31	0.45
1:L:455:LEU:HA	1:L:458:ILE:HD12	1.99	0.45
1:U:205:TYR:HB3	1:U:233:ILE:HD13	1.99	0.45
2:N:144:LEU:HD22	2:N:375:GLN:HG3	1.98	0.45
1:U:181:ALA:HB1	1:U:269:VAL:HG21	1.97	0.45
1:L:227:ALA:HA	1:L:230:TYR:CE2	2.51	0.45
3:Y:212:TYR:O	3:Y:216:ASN:HB2	2.15	0.45
1:L:97:VAL:HG11	1:L:247:LEU:HD21	1.98	0.45
1:A:446:LEU:CD2	1:A:467:GLU:HG3	2.47	0.45
1:A:217:GLN:HG2	2:D:356:ARG:HH21	1.82	0.45
1:B:435:TYR:C	1:B:437:PRO:HD3	2.37	0.45
3:Y:76:ALA:HB1	3:Y:109:THR:HG22	1.99	0.45
1:L:243:PRO:O	1:L:247:LEU:HB2	2.16	0.45
4:H:71:SER:HB3	4:H:89:GLU:HB2	1.99	0.45
1:T:148:VAL:HG21	1:T:324:THR:HG21	1.97	0.45
2:F:143:LEU:O	2:F:367:HIS:HE1	2.00	0.45
2:X:284:THR:O	2:X:288:ASP:HB2	2.16	0.45
2:F:384:LEU:O	2:F:388:ILE:HG12	2.17	0.45
2:O:251:VAL:HB	2:O:304:VAL:HG22	1.99	0.45
2:F:390:ILE:HD12	3:G:244:ALA:HA	1.99	0.45
1:C:166:ARG:HD2	1:C:308:LEU:O	2.17	0.45
2:W:256:ASP:HA	2:W:257:ASN:HA	1.66	0.45
2:O:189:GLU:O	2:O:221:GLN:HB3	2.17	0.45
1:T:243:PRO:HG3	1:T:283:LEU:HD21	1.99	0.45
1:A:424:GLU:HB3	1:A:460:LEU:HD21	1.98	0.45
1:A:446:LEU:HD22	1:A:467:GLU:HG3	1.99	0.45
2:E:170:LEU:O	2:E:174:ILE:HG12	2.17	0.45
2:M:144:LEU:O	2:M:358:LEU:HD22	2.17	0.45
1:C:78:PHE:HB3	1:C:244:LEU:HD21	1.98	0.45
1:S:161:ILE:HD11	1:S:352:ILE:HD11	1.98	0.45
1:B:474:LEU:HB3	1:B:482:LEU:HD11	2.00	0.45
2:F:33:ILE:O	2:F:34:LEU:CB	2.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:96:ILE:HG22	2:N:97:ASN:O	2.18	0.44
1:K:109:VAL:HB	1:K:118:ASP:HB3	1.98	0.44
2:F:21:VAL:O	2:F:61:THR:OG1	2.30	0.44
2:F:277:SER:OG	2:F:278:ALA:N	2.50	0.44
1:J:360:TYR:OH	2:M:354:LYS:HE2	2.16	0.44
2:O:196:ASP:OD1	2:O:199:ARG:NH2	2.49	0.44
2:M:33:ILE:O	2:M:34:LEU:HB2	2.17	0.44
2:D:425:THR:HB	2:D:427:ILE:HD12	1.99	0.44
2:O:277:SER:OG	2:O:278:ALA:N	2.50	0.44
2:O:32:ALA:O	2:O:35:ASN:HB2	2.17	0.44
2:D:229:ARG:NH2	2:D:267:GLU:OE1	2.48	0.44
2:D:456:ALA:HA	2:D:469:LYS:HD3	1.99	0.44
1:A:205:TYR:HB3	1:A:233:ILE:HD13	1.99	0.44
2:W:168:GLN:HA	2:W:171:ILE:HD12	1.99	0.44
1:B:290:PRO:HG2	2:F:270:ALA:HB2	1.98	0.44
1:U:341:PRO:O	1:U:345:ILE:HG13	2.16	0.44
1:A:288:ARG:HG2	1:A:288:ARG:HH11	1.83	0.44
1:S:146:GLU:H	1:S:313:LYS:HZ3	1.65	0.44
2:E:142:ASP:HB3	2:E:434:LEU:HD12	1.99	0.44
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.49	0.44
2:W:185:THR:OG1	2:W:236:GLY:HA3	2.17	0.44
2:D:152:LYS:NZ	2:D:293:GLN:HB3	2.32	0.44
2:W:95:ILE:HB	2:W:104:ASP:HB3	1.98	0.44
1:S:385:LEU:HD11	1:S:447:ILE:HD12	1.98	0.44
2:W:102:PRO:HG3	2:W:109:ILE:HG13	2.00	0.44
2:F:94:ARG:NH2	2:F:102:PRO:HB2	2.32	0.44
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.48	0.44
2:W:410:ILE:HG23	2:W:441:PHE:HE2	1.82	0.44
2:E:256:ASP:HA	2:E:257:ASN:HA	1.76	0.44
2:O:33:ILE:HG22	2:O:34:LEU:HG	1.99	0.44
2:W:188:GLY:HA3	2:W:260:ARG:HD2	2.00	0.44
6:U:600:ANP:N3B	6:U:600:ANP:O2A	2.48	0.44
1:L:40:ILE:HD11	1:L:76:VAL:HG12	2.00	0.44
1:B:25:ALA:HB1	1:B:30:THR:HG21	1.99	0.44
1:C:55:VAL:HG21	1:C:75:ILE:HD13	1.99	0.44
1:U:211:LYS:O	1:U:215:VAL:HG23	2.16	0.44
1:T:168:LEU:HD12	1:T:327:PRO:O	2.17	0.44
1:U:219:VAL:HA	1:U:222:LEU:HD12	2.00	0.44
2:X:234:LEU:HD23	2:X:292:LEU:HD13	1.99	0.44
1:B:50:GLN:HB3	2:F:69:GLY:HA2	1.99	0.44
3:G:9:ARG:HD2	3:G:251:TYR:HE2	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:45:LYS:O	2:N:45:LYS:HG3	2.18	0.44
2:E:117:ILE:HG22	2:E:235:THR:HA	1.99	0.44
3:P:42:LYS:HA	3:P:45:ASP:HB2	1.99	0.44
4:H:35:LYS:HE2	4:H:37:GLY:H	1.83	0.44
1:L:187:ASN:OD1	1:L:190:ARG:NH1	2.47	0.44
1:B:117:ILE:HD12	2:E:124:PHE:CB	2.48	0.44
1:T:306:ARG:O	1:T:310:ARG:HD3	2.18	0.44
2:F:182:SER:HA	2:F:252:LEU:O	2.17	0.44
1:L:426:LEU:HD21	1:L:450:GLY:HA3	1.99	0.44
2:F:104:ASP:C	2:F:106:ARG:H	2.21	0.44
2:X:141:VAL:HG22	2:X:333:THR:HG21	1.99	0.44
2:W:320:PRO:O	2:W:324:THR:OG1	2.28	0.44
2:M:314:ALA:O	2:M:315:ASP:HB2	2.18	0.44
1:U:89:LEU:N	1:U:89:LEU:HD12	2.33	0.44
1:B:166:ARG:CD	1:B:308:LEU:O	2.65	0.44
2:V:138:ILE:HA	2:V:416:GLN:OE1	2.18	0.44
1:L:150:THR:HA	1:L:184:THR:HG23	2.00	0.44
1:K:112:ALA:HB2	1:K:236:ALA:HB2	1.98	0.44
2:D:314:ALA:O	2:D:315:ASP:HB2	2.18	0.44
2:N:150:GLY:HA2	2:N:304:VAL:O	2.18	0.44
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.99	0.44
3:Y:41:ALA:HB1	3:Y:220:THR:HA	2.00	0.44
2:V:97:ASN:HD22	2:V:103:ILE:HG23	1.83	0.44
1:U:375:ARG:NH1	2:V:190:ARG:NH2	2.66	0.44
2:X:333:THR:HA	2:X:353:SER:HB3	2.00	0.44
2:F:158:GLY:O	2:F:161:VAL:HG22	2.18	0.44
1:B:182:LEU:HD13	1:B:218:LEU:HD11	2.00	0.44
1:L:271:ASP:HA	1:L:272:ASP:HA	1.76	0.44
1:A:426:LEU:O	1:A:430:LEU:HG	2.18	0.44
1:J:300:VAL:O	1:J:303:LEU:HB3	2.18	0.44
3:P:94:ALA:C	3:P:96:ARG:H	2.21	0.44
2:E:237:LEU:O	2:E:241:GLU:HG3	2.18	0.44
2:M:198:TYR:CZ	2:M:202:LYS:HE2	2.52	0.44
1:B:34:LEU:O	1:B:86:GLU:HG3	2.18	0.44
1:B:164:GLY:HA2	1:B:323:LEU:O	2.18	0.44
2:O:218:VAL:HG21	2:O:236:GLY:HA2	2.00	0.44
3:G:133:ILE:HD13	3:G:133:ILE:HA	1.70	0.44
1:T:131:ALA:HB2	1:T:251:THR:HG22	2.00	0.43
2:D:224:GLU:O	2:D:229:ARG:NH1	2.44	0.43
1:U:107:GLY:HA2	1:U:228:MET:HG3	1.98	0.43
1:U:299:ASP:HB2	1:U:302:TYR:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:329:ILE:HD11	1:U:344:VAL:HG21	2.00	0.43
1:B:338:ALA:HB3	1:B:341:PRO:HG2	2.01	0.43
2:W:37:LEU:HD13	2:W:76:VAL:HG11	2.00	0.43
2:F:201:MET:HB2	2:F:207:ILE:HD12	2.00	0.43
2:W:258:ILE:HG22	2:W:309:ALA:O	2.18	0.43
1:K:364:ARG:HD3	6:K:600:ANP:N1	2.31	0.43
1:K:173:ARG:HH22	2:N:327:ALA:HB2	1.83	0.43
1:K:37:GLY:HA3	2:N:52:GLN:HG2	2.00	0.43
3:G:87:ILE:HG23	3:G:167:ASN:HD22	1.84	0.43
1:L:177:LYS:HD2	1:L:328:VAL:HG13	2.00	0.43
1:K:455:LEU:HD23	1:K:458:ILE:HD12	1.99	0.43
1:T:495:LEU:O	1:T:499:LEU:HD13	2.18	0.43
1:B:400:ARG:HE	1:B:400:ARG:HB3	1.46	0.43
1:L:480:GLU:H	1:L:480:GLU:HG3	1.67	0.43
1:A:77:LEU:CD1	1:A:81:ASP:CB	2.96	0.43
2:E:98:VAL:HG13	2:E:99:ILE:HG23	1.99	0.43
2:M:136:THR:HG21	2:M:147:TYR:CD2	2.53	0.43
2:M:342:LEU:HD13	2:M:344:ILE:HD12	2.01	0.43
4:H:51:GLN:HG2	4:H:74:PHE:CZ	2.53	0.43
1:A:480:GLU:H	1:A:480:GLU:HG3	1.38	0.43
1:U:271:ASP:HA	1:U:272:ASP:HA	1.68	0.43
1:K:301:PHE:HB3	2:O:263:GLN:NE2	2.33	0.43
2:E:25:PHE:O	2:E:57:ASN:HB3	2.19	0.43
1:A:392:LEU:HD13	1:A:426:LEU:HD22	2.00	0.43
2:F:387:ILE:HG23	2:F:391:LEU:HD12	1.99	0.43
1:L:389:ALA:O	1:L:390:GLY:C	2.55	0.43
1:C:354:LEU:HA	1:C:366:ALA:O	2.18	0.43
1:L:99:VAL:CG1	1:L:251:THR:HB	2.49	0.43
2:D:64:MET:HE3	2:D:228:ALA:HA	2.00	0.43
1:B:100:PRO:HA	1:B:127:GLY:O	2.19	0.43
1:A:246:TYR:CE1	1:A:303:LEU:HD11	2.53	0.43
1:C:46:LEU:O	1:C:49:ILE:HG22	2.18	0.43
1:A:217:GLN:OE1	2:D:129:THR:HB	2.19	0.43
1:J:55:VAL:HG21	1:J:75:ILE:HD13	2.01	0.43
2:F:38:GLU:HG2	2:F:45:LYS:HG2	2.00	0.43
1:C:238:ALA:O	2:F:290:GLY:HA3	2.18	0.43
1:L:109:VAL:HG12	1:L:117:ILE:HD11	2.00	0.43
1:U:435:TYR:C	1:U:437:PRO:HD3	2.39	0.43
1:K:285:LEU:HD13	2:N:277:SER:HB3	2.00	0.43
1:J:422:ARG:HE	1:J:453:GLY:HA2	1.83	0.43
2:F:395:GLU:HG3	3:G:83:LEU:HD23	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:ARG:HG2	2:D:149:ARG:HH11	1.83	0.43
1:K:444:VAL:HG21	1:K:485:ILE:HG21	2.01	0.43
2:E:22:ASP:HA	2:E:59:VAL:O	2.18	0.43
1:U:211:LYS:HB3	1:U:211:LYS:HE2	1.77	0.43
1:L:36:VAL:HG12	2:O:53:HIS:HB2	2.01	0.43
2:O:141:VAL:HG22	2:O:333:THR:HG21	2.01	0.43
2:O:239:ILE:HG22	2:O:243:PHE:HE2	1.83	0.43
2:W:87:VAL:HG12	2:W:239:ILE:HA	2.00	0.43
1:S:474:LEU:HD23	1:S:478:HIS:HB2	2.01	0.43
2:E:312:VAL:HG12	2:E:315:ASP:HA	2.01	0.43
2:W:164:THR:HA	2:W:167:ILE:HB	2.01	0.43
3:G:151:LEU:HD23	3:G:156:ALA:HB3	2.00	0.43
2:F:142:ASP:HB3	2:F:434:LEU:HD12	2.01	0.43
1:C:146:GLU:O	1:C:162:GLY:HA2	2.19	0.43
1:B:388:VAL:O	1:B:451:VAL:HG21	2.18	0.43
2:F:148:ALA:CB	2:F:357:LEU:HD11	2.49	0.43
2:F:377:THR:HG22	2:F:407:ALA:HB2	2.01	0.43
1:L:91:LYS:HG3	1:L:92:ARG:O	2.19	0.43
1:S:142:ARG:HG2	1:S:143:SER:H	1.84	0.43
2:X:256:ASP:HA	2:X:257:ASN:HA	1.79	0.43
2:F:155:LEU:CD1	2:F:167:ILE:HG12	2.48	0.43
1:S:246:TYR:CD2	1:S:247:LEU:HG	2.54	0.43
2:M:241:GLU:HG2	2:M:244:ARG:NH2	2.33	0.43
1:A:85:LYS:HG2	2:D:53:HIS:HE1	1.84	0.43
1:S:446:LEU:HD21	1:S:467:GLU:HA	2.01	0.43
3:G:44:MET:HE2	4:H:86:THR:HB	2.00	0.43
2:O:12:LYS:O	2:O:23:VAL:HA	2.19	0.43
2:W:135:GLU:HG3	2:W:434:LEU:HB2	2.01	0.43
1:S:295:ALA:HB2	3:Y:270:ILE:HD13	2.01	0.43
2:W:349:ASP:HA	2:W:350:PRO:HD3	1.86	0.43
1:U:238:ALA:HB1	2:X:328:HIS:HE1	1.84	0.43
1:L:394:LEU:HD11	2:M:425:THR:HG22	2.01	0.42
3:P:74:ILE:HG23	3:P:165:PHE:HD2	1.84	0.42
2:N:97:ASN:HB3	2:N:103:ILE:HD13	2.01	0.42
2:V:30:LEU:HA	2:V:31:PRO:HD3	1.87	0.42
1:A:34:LEU:O	1:A:86:GLU:HG3	2.19	0.42
1:C:148:VAL:HG22	1:C:163:ARG:HG3	2.00	0.42
2:E:132:GLU:OE2	2:E:149:ARG:NH1	2.52	0.42
4:H:46:VAL:HA	4:H:47:PRO:HD3	1.94	0.42
2:X:189:GLU:O	2:X:221:GLN:HB3	2.19	0.42
1:J:172:ASP:O	1:J:175:THR:OG1	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:150:LEU:HA	3:G:150:LEU:HD12	1.93	0.42
1:U:429:LEU:HG	1:U:429:LEU:O	2.18	0.42
3:Y:99:LEU:HD23	3:Y:122:HIS:CE1	2.54	0.42
1:U:143:SER:OG	2:V:199:ARG:NH2	2.52	0.42
2:D:201:MET:H	2:D:201:MET:HG2	1.66	0.42
2:W:96:ILE:O	2:W:218:VAL:HA	2.19	0.42
2:W:37:LEU:HD12	2:W:61:THR:HG21	2.01	0.42
2:W:37:LEU:HB2	2:W:48:LEU:HB2	2.02	0.42
2:X:339:ILE:HG22	2:X:344:ILE:HB	2.00	0.42
2:X:275:ILE:O	2:X:283:PRO:HG3	2.19	0.42
1:U:319:GLY:O	1:U:320:SER:HB2	2.19	0.42
1:C:139:LEU:HB3	1:C:140:PRO:HD3	2.01	0.42
2:N:432:VAL:HG12	2:N:433:ARG:H	1.83	0.42
1:U:284:SER:HB2	1:U:297:PRO:HG3	2.00	0.42
2:F:145:ALA:HA	2:F:355:SER:HB2	2.01	0.42
2:M:155:LEU:HD12	2:M:167:ILE:HG13	2.01	0.42
2:F:244:ARG:HD3	2:F:304:VAL:HG23	2.00	0.42
4:H:35:LYS:N	4:H:35:LYS:HD3	2.33	0.42
2:O:140:VAL:CG1	2:O:414:LEU:HB3	2.49	0.42
3:P:164:ILE:HD11	3:P:182:ILE:HG13	2.01	0.42
1:L:43:VAL:HG21	1:L:75:ILE:HD12	2.00	0.42
1:K:170:ILE:HD11	1:K:341:PRO:HB3	2.01	0.42
2:D:256:ASP:HA	2:D:257:ASN:HA	1.88	0.42
2:N:432:VAL:HG12	2:N:433:ARG:N	2.34	0.42
2:O:256:ASP:HA	2:O:257:ASN:HA	1.71	0.42
1:K:96:ILE:O	1:K:97:VAL:C	2.58	0.42
1:U:273:LEU:HD11	1:U:327:PRO:HB3	2.01	0.42
1:K:442:GLU:C	1:K:445:PRO:HD2	2.39	0.42
2:O:239:ILE:HG22	2:O:243:PHE:CE2	2.55	0.42
2:F:256:ASP:HA	2:F:257:ASN:HA	1.78	0.42
2:D:170:LEU:O	2:D:174:ILE:HG12	2.19	0.42
2:N:95:ILE:HD11	2:N:198:TYR:CG	2.55	0.42
2:F:443:ALA:O	2:F:448:LYS:HG3	2.19	0.42
2:E:281:TYR:CD2	2:E:320:PRO:HG2	2.55	0.42
1:J:204:VAL:O	1:J:268:ILE:HA	2.19	0.42
1:K:496:LEU:O	1:K:500:LYS:HB2	2.19	0.42
1:B:305:SER:HB2	2:F:222:MET:HB2	2.02	0.42
1:U:105:LEU:O	1:U:108:ARG:HB2	2.19	0.42
3:G:189:GLU:HG2	3:G:206:PRO:HG2	2.02	0.42
1:U:272:ASP:HB3	1:U:328:VAL:HG12	2.01	0.42
1:K:363:ILE:HA	1:K:431:LYS:HE2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ARG:NE	1:C:72:GLN:HE22	2.17	0.42
1:K:340:ILE:HB	1:K:341:PRO:HD3	2.01	0.42
1:U:222:LEU:HB2	1:U:228:MET:HE1	2.02	0.42
1:U:221:THR:HG21	1:U:435:TYR:CE1	2.53	0.42
1:J:54:LEU:HD13	1:J:97:VAL:HG22	2.00	0.42
2:N:87:VAL:HG12	2:N:239:ILE:HA	2.02	0.42
1:U:203:CYS:O	1:U:231:SER:HA	2.20	0.42
2:M:25:PHE:HB2	2:M:30:LEU:CD2	2.49	0.42
4:H:16:LEU:HB2	4:H:19:GLU:O	2.19	0.42
1:B:478:HIS:HB3	1:B:481:LEU:HG	2.01	0.42
2:V:85:VAL:CG1	2:V:235:THR:HG23	2.39	0.42
2:V:15:ALA:O	2:V:21:VAL:HA	2.19	0.42
1:C:103:PRO:HD3	1:C:258:TRP:CZ2	2.54	0.42
1:U:55:VAL:HG12	1:U:92:ARG:HA	2.02	0.42
1:U:109:VAL:HG22	1:U:233:ILE:HB	2.01	0.42
1:C:76:VAL:HB	1:C:243:PRO:HG2	2.01	0.42
2:X:49:GLU:O	2:X:61:THR:HA	2.20	0.42
1:T:455:LEU:HA	1:T:458:ILE:HD13	2.02	0.42
1:B:280:TYR:OH	1:B:299:ASP:OD2	2.32	0.42
1:A:485:ILE:HG12	1:A:491:LEU:HD21	2.01	0.42
1:K:51:ALA:HB2	1:K:68:LEU:HD11	2.01	0.42
2:W:50:VAL:HA	2:W:61:THR:HG22	2.02	0.42
1:A:26:ASN:HB3	1:A:30:THR:OG1	2.20	0.42
2:E:135:GLU:OE2	2:E:433:ARG:HD3	2.20	0.42
1:A:242:ALA:N	1:A:243:PRO:CD	2.83	0.42
1:B:174:GLN:CA	6:B:600:ANP:HNB1	2.14	0.42
1:K:341:PRO:O	1:K:345:ILE:HG13	2.19	0.42
2:X:37:LEU:HD23	2:X:78:ASP:HA	2.02	0.42
1:L:354:LEU:HA	1:L:366:ALA:O	2.20	0.42
3:Y:10:LEU:HG	3:Y:14:LYS:HE2	2.02	0.42
1:C:314:LEU:HB3	1:C:318:GLU:HB2	2.01	0.42
2:F:417:PRO:HG2	2:F:430:LYS:H	1.85	0.42
1:T:364:ARG:HA	1:T:365:PRO:C	2.40	0.42
1:T:197:GLU:HG3	1:T:200:LYS:HD2	2.00	0.42
2:F:134:LEU:HD11	2:F:174:ILE:HG21	2.02	0.42
1:J:250:PHE:CE1	1:J:307:LEU:HB2	2.55	0.42
2:E:156:PHE:HZ	2:E:326:PHE:CZ	2.38	0.42
2:M:344:ILE:HG23	2:M:415:SER:HB3	2.02	0.41
2:V:384:LEU:O	2:V:388:ILE:HG12	2.20	0.41
1:B:85:LYS:HE2	2:E:32:ALA:HB2	2.02	0.41
2:O:321:ALA:HB3	2:O:322:PRO:CD	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LYS:HD2	1:C:328:VAL:HG13	2.02	0.41
2:O:335:LEU:HA	2:O:347:ALA:O	2.19	0.41
2:O:147:TYR:CE2	2:O:153:ILE:HG21	2.55	0.41
2:D:140:VAL:HA	2:D:414:LEU:HD22	2.01	0.41
1:S:204:VAL:O	1:S:268:ILE:HA	2.20	0.41
1:S:145:HIS:H	1:S:313:LYS:NZ	2.16	0.41
1:C:168:LEU:HD23	1:C:351:GLN:HG2	2.03	0.41
2:M:237:LEU:HD23	2:M:292:LEU:HD12	2.02	0.41
2:F:290:GLY:O	2:F:294:GLU:HB2	2.20	0.41
1:C:285:LEU:HD21	1:C:291:PRO:HB3	2.02	0.41
2:M:97:ASN:HD22	2:M:103:ILE:HG23	1.86	0.41
3:P:188:ILE:O	3:P:188:ILE:HG22	2.21	0.41
2:M:324:THR:O	2:M:324:THR:HG22	2.20	0.41
2:W:262:THR:HG21	2:W:321:ALA:HB2	2.01	0.41
2:D:32:ALA:O	2:D:35:ASN:HB2	2.19	0.41
1:T:212:ARG:HA	1:T:237:THR:HG21	2.02	0.41
3:Y:233:ARG:O	3:Y:237:MET:HG2	2.21	0.41
2:M:417:PRO:HD2	2:M:460:VAL:O	2.20	0.41
4:Q:30:VAL:H	4:Q:41:VAL:HG12	1.85	0.41
2:O:297:THR:OG1	2:O:298:THR:N	2.54	0.41
3:G:258:THR:O	3:G:262:VAL:HG23	2.20	0.41
1:K:302:TYR:HA	1:K:305:SER:OG	2.20	0.41
1:B:154:ALA:HB3	1:B:367:ILE:HD12	2.03	0.41
2:O:148:ALA:HB2	2:O:357:LEU:HD11	2.02	0.41
2:V:16:VAL:HG12	2:V:21:VAL:HG22	2.02	0.41
2:X:255:ILE:HB	2:X:308:GLN:HG2	2.02	0.41
2:D:64:MET:HE1	2:D:228:ALA:HA	2.02	0.41
1:C:219:VAL:HB	1:C:228:MET:CE	2.50	0.41
1:J:73:VAL:HG12	1:J:75:ILE:HG13	2.02	0.41
2:X:275:ILE:HA	2:X:276:PRO:HD3	1.95	0.41
2:F:134:LEU:CD2	2:F:305:THR:HG21	2.50	0.41
1:A:138:ILE:HG21	2:E:95:ILE:HD13	2.02	0.41
1:S:173:ARG:NH2	2:V:317:LEU:HD13	2.36	0.41
1:U:36:VAL:HG21	1:U:84:VAL:HB	2.03	0.41
3:P:141:GLN:HE21	3:P:141:GLN:HA	1.85	0.41
1:U:375:ARG:HH12	2:V:190:ARG:NH2	2.19	0.41
2:D:152:LYS:HZ3	2:D:293:GLN:HB3	1.84	0.41
1:K:54:LEU:HG	1:K:97:VAL:HA	2.03	0.41
3:Y:3:LEU:HD11	3:Y:259:ARG:HD3	2.03	0.41
2:F:266:SER:HB3	2:F:282:GLN:OE1	2.21	0.41
1:S:356:ALA:HB1	1:S:360:TYR:OH	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:64:MET:O	2:X:65:ASP:HB2	2.21	0.41
1:B:267:LEU:HD11	1:B:326:LEU:HG	2.02	0.41
1:B:186:LEU:HD22	1:B:225:HIS:CB	2.50	0.41
2:W:156:PHE:HB2	2:W:334:VAL:HG22	2.02	0.41
2:D:335:LEU:HA	2:D:347:ALA:O	2.21	0.41
2:V:372:SER:O	2:V:376:GLU:HG3	2.20	0.41
2:N:201:MET:HA	2:N:204:THR:HG22	2.03	0.41
1:A:246:TYR:HE1	1:A:303:LEU:HD11	1.84	0.41
1:A:299:ASP:HB3	2:E:271:LEU:HD21	2.02	0.41
1:B:101:VAL:HG12	1:B:255:ILE:HA	2.03	0.41
1:A:166:ARG:HD2	1:A:308:LEU:O	2.21	0.41
2:M:266:SER:HB3	2:M:282:GLN:OE1	2.20	0.41
1:S:139:LEU:N	1:S:140:PRO:CD	2.84	0.41
1:S:139:LEU:N	1:S:140:PRO:HD2	2.36	0.41
3:P:14:LYS:HA	3:P:248:ILE:HD11	2.03	0.41
1:S:99:VAL:HG22	1:S:100:PRO:HD2	2.02	0.41
1:T:166:ARG:HH22	2:X:190:ARG:HD3	1.86	0.41
3:G:14:LYS:HA	3:G:248:ILE:CD1	2.48	0.41
2:X:346:PRO:HB2	2:X:348:VAL:HG23	2.03	0.41
2:F:134:LEU:HD22	2:F:305:THR:HG21	2.03	0.41
1:U:398:GLN:O	1:U:402:VAL:HG23	2.21	0.41
1:U:51:ALA:HB3	2:V:67:THR:O	2.20	0.41
1:K:190:ARG:NE	1:K:439:ALA:HB2	2.35	0.41
2:W:237:LEU:HD21	2:W:295:ARG:HB2	2.03	0.41
1:L:46:LEU:O	1:L:47:ASN:C	2.58	0.41
3:P:149:LYS:HA	3:P:152:SER:HB2	2.03	0.41
2:D:165:VAL:HG13	2:D:420:VAL:HG12	2.03	0.41
2:V:153:ILE:C	2:V:329:LEU:HD22	2.41	0.41
2:W:244:ARG:HG3	2:W:303:SER:N	2.36	0.41
1:J:138:ILE:HG22	1:J:139:LEU:HD12	2.02	0.41
1:B:308:LEU:HB2	1:B:347:ILE:HG21	2.03	0.41
1:S:271:ASP:HA	1:S:272:ASP:HA	1.84	0.41
2:W:185:THR:HA	2:W:218:VAL:O	2.21	0.41
1:T:168:LEU:HB2	1:T:348:THR:HG21	2.02	0.41
1:L:389:ALA:O	1:L:390:GLY:O	2.39	0.41
1:B:309:GLU:HG3	2:F:222:MET:HG3	2.02	0.41
2:E:193:GLU:HA	2:E:196:ASP:HB2	2.03	0.41
1:C:248:ALA:HB3	1:C:249:PRO:HD3	2.03	0.41
1:S:426:LEU:O	1:S:430:LEU:HG	2.21	0.41
2:N:185:THR:OG1	2:N:236:GLY:HA3	2.21	0.41
1:S:355:GLU:HB2	1:S:358:LEU:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:440:SER:OG	2:O:463:ILE:HB	2.21	0.41
1:L:138:ILE:HD12	2:M:191:THR:HG23	2.02	0.41
1:A:98:ASP:C	1:A:98:ASP:OD1	2.58	0.41
2:V:97:ASN:ND2	2:V:101:GLU:HB2	2.34	0.41
2:D:201:MET:CE	2:D:215:VAL:HG11	2.50	0.41
1:K:161:ILE:HD13	1:K:326:LEU:HD21	2.03	0.41
1:A:142:ARG:HG3	1:A:142:ARG:HH11	1.86	0.41
2:E:462:GLY:O	2:E:464:GLU:N	2.54	0.41
2:M:134:LEU:HD11	2:M:174:ILE:HD12	2.03	0.41
2:V:377:THR:HG22	2:V:407:ALA:HB2	2.03	0.41
1:J:316:GLU:HA	1:J:320:SER:OG	2.21	0.41
2:N:25:PHE:O	2:N:57:ASN:HB3	2.21	0.41
2:V:132:GLU:HB3	2:V:149:ARG:HB2	2.03	0.41
1:K:168:LEU:HD13	1:K:344:VAL:HG11	2.02	0.41
1:T:211:LYS:HB2	1:T:214:THR:OG1	2.20	0.41
1:B:99:VAL:CG1	1:B:251:THR:HB	2.51	0.40
2:M:117:ILE:HD12	2:M:234:LEU:HB2	2.03	0.40
1:L:82:ARG:HG2	2:O:34:LEU:HD12	2.03	0.40
1:K:141:ARG:HB2	2:O:195:ASN:ND2	2.36	0.40
1:K:206:VAL:HG13	1:K:234:VAL:HB	2.02	0.40
3:G:86:SER:O	3:G:90:GLN:HG2	2.21	0.40
2:E:201:MET:HG2	2:E:206:VAL:CG2	2.51	0.40
1:L:329:ILE:HD11	1:L:344:VAL:HG21	2.03	0.40
2:N:168:GLN:HE21	2:N:201:MET:CG	2.35	0.40
1:K:249:PRO:HG2	1:K:276:GLN:NE2	2.36	0.40
2:D:222:MET:HA	2:D:229:ARG:HD2	2.03	0.40
2:X:37:LEU:HD12	2:X:61:THR:HG21	2.02	0.40
1:T:174:GLN:HA	6:T:600:ANP:HNB1	1.86	0.40
1:S:96:ILE:HB	1:S:130:ARG:HD2	2.02	0.40
2:E:185:THR:HG21	2:E:233:ALA:HA	2.03	0.40
3:P:74:ILE:O	3:P:107:ILE:HA	2.21	0.40
3:G:96:ARG:HE	3:G:121:THR:HG21	1.85	0.40
1:K:161:ILE:HA	1:K:165:GLN:OE1	2.21	0.40
1:A:491:LEU:HD13	1:A:496:LEU:HD23	2.03	0.40
2:D:440:SER:OG	2:D:463:ILE:HB	2.22	0.40
3:P:75:VAL:HG22	3:P:108:VAL:HB	2.03	0.40
1:T:109:VAL:HG13	1:T:233:ILE:HB	2.02	0.40
2:D:93:GLY:HA2	2:D:207:ILE:HG12	2.03	0.40
2:O:410:ILE:HG23	2:O:441:PHE:HE2	1.86	0.40
1:K:212:ARG:NH1	2:N:123:SER:HA	2.36	0.40
1:S:347:ILE:HA	2:W:222:MET:SD	2.62	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:168:LEU:HB2	1:J:348:THR:HG21	2.03	0.40
1:T:53:GLU:HG2	1:T:54:LEU:H	1.87	0.40
2:V:324:THR:HG22	2:V:324:THR:O	2.22	0.40
4:H:14:PHE:HB2	4:H:22:TYR:HB2	2.02	0.40
3:G:78:THR:HG23	3:G:91:LEU:HD23	2.03	0.40
1:K:50:GLN:NE2	2:O:69:GLY:HA2	2.37	0.40
1:S:237:THR:N	1:S:240:GLU:OE1	2.55	0.40
2:F:449:TYR:HB3	2:F:452:ILE:HD12	2.02	0.40
1:U:337:SER:HB3	2:V:314:ALA:HB1	2.02	0.40
2:N:32:ALA:O	2:N:35:ASN:HB2	2.22	0.40
2:V:239:ILE:O	2:V:243:PHE:HD2	2.05	0.40
1:B:382:VAL:HG11	1:B:440:THR:HG21	2.03	0.40
1:B:139:LEU:HA	1:B:139:LEU:HD12	1.83	0.40
2:M:237:LEU:CD2	2:M:292:LEU:HD12	2.51	0.40
2:W:183:VAL:HG11	2:W:236:GLY:O	2.21	0.40
1:U:69:GLU:HB3	1:U:70:PRO:HD2	2.03	0.40
1:U:260:ARG:O	1:U:321:GLY:HA3	2.22	0.40
2:D:348:VAL:O	2:D:350:PRO:HD3	2.21	0.40
1:S:49:ILE:HG23	1:S:68:LEU:HD22	2.04	0.40
1:B:282:GLN:OE1	2:E:284:THR:HA	2.21	0.40
2:V:258:ILE:HG13	2:V:258:ILE:O	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	478/510 (94%)	454 (95%)	23 (5%)	1 (0%)	52	88
1	B	479/510 (94%)	448 (94%)	30 (6%)	1 (0%)	52	88
1	C	482/510 (94%)	453 (94%)	28 (6%)	1 (0%)	52	88
1	J	477/510 (94%)	460 (96%)	16 (3%)	1 (0%)	52	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	482/510 (94%)	442 (92%)	35 (7%)	5 (1%)	19	61
1	L	478/510 (94%)	450 (94%)	27 (6%)	1 (0%)	52	88
1	S	474/510 (93%)	447 (94%)	25 (5%)	2 (0%)	39	80
1	T	475/510 (93%)	438 (92%)	33 (7%)	4 (1%)	24	66
1	U	477/510 (94%)	432 (91%)	39 (8%)	6 (1%)	15	53
2	D	468/484 (97%)	439 (94%)	28 (6%)	1 (0%)	52	88
2	E	466/484 (96%)	436 (94%)	28 (6%)	2 (0%)	39	80
2	F	467/484 (96%)	435 (93%)	27 (6%)	5 (1%)	17	58
2	M	468/484 (97%)	437 (93%)	30 (6%)	1 (0%)	52	88
2	N	468/484 (97%)	431 (92%)	33 (7%)	4 (1%)	21	64
2	O	466/484 (96%)	442 (95%)	24 (5%)	0	100	100
2	V	468/484 (97%)	423 (90%)	38 (8%)	7 (2%)	13	50
2	W	465/484 (96%)	432 (93%)	30 (6%)	3 (1%)	30	72
2	X	467/484 (96%)	432 (92%)	33 (7%)	2 (0%)	39	80
3	G	262/278 (94%)	245 (94%)	17 (6%)	0	100	100
3	P	234/278 (84%)	210 (90%)	19 (8%)	5 (2%)	9	40
3	Y	189/278 (68%)	176 (93%)	13 (7%)	0	100	100
4	H	110/138 (80%)	89 (81%)	19 (17%)	2 (2%)	11	45
4	Q	74/138 (54%)	61 (82%)	13 (18%)	0	100	100
4	Z	15/138 (11%)	11 (73%)	3 (20%)	1 (7%)	1	8
5	1	23/61 (38%)	19 (83%)	3 (13%)	1 (4%)	3	19
5	I	43/61 (70%)	33 (77%)	6 (14%)	4 (9%)	1	4
5	R	30/61 (49%)	25 (83%)	5 (17%)	0	100	100
All	All	9485/10377 (91%)	8800 (93%)	625 (7%)	60 (1%)	30	72

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	101	ILE
5	I	55	GLU
1	L	390	GLY
2	N	221	GLN
2	V	347	ALA
2	W	54	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	390	GLY
2	D	27	GLN
2	E	463	ILE
1	K	412	LEU
3	P	134	GLY
1	T	46	LEU
1	U	97	VAL
1	U	298	GLY
2	V	27	GLN
2	V	68	GLU
2	F	315	ASP
5	I	29	LEU
1	J	403	ALA
1	K	316	GLU
1	K	373	VAL
3	P	202	ASP
1	S	406	ALA
2	W	28	SER
1	B	363	ILE
2	F	34	LEU
2	F	83	ILE
2	F	105	GLU
1	K	457	GLY
1	T	59	SER
1	T	60	GLY
1	U	226	ASP
1	U	406	ALA
2	X	390	ILE
4	Z	120	ALA
2	E	455	HIS
4	H	36	SER
1	K	97	VAL
2	M	460	VAL
3	P	205	VAL
1	U	46	LEU
2	V	28	SER
2	V	34	LEU
2	W	158	GLY
1	A	70	PRO
2	F	347	ALA
5	I	28	GLU
1	U	140	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	X	18	GLY
2	N	108	PRO
3	P	133	ILE
5	I	56	PRO
3	P	95	VAL
2	V	346	PRO
5	1	21	ILE
1	T	390	GLY
2	N	158	GLY
1	S	97	VAL
2	V	82	PRO
2	N	428	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/412 (94%)	369 (95%)	19 (5%)	31	71
1	B	388/412 (94%)	373 (96%)	15 (4%)	39	77
1	C	390/412 (95%)	378 (97%)	12 (3%)	47	83
1	J	387/412 (94%)	372 (96%)	15 (4%)	39	77
1	K	390/412 (95%)	372 (95%)	18 (5%)	33	73
1	L	388/412 (94%)	365 (94%)	23 (6%)	24	63
1	S	385/412 (93%)	365 (95%)	20 (5%)	29	68
1	T	386/412 (94%)	371 (96%)	15 (4%)	39	77
1	U	387/412 (94%)	376 (97%)	11 (3%)	51	84
2	D	379/390 (97%)	362 (96%)	17 (4%)	34	74
2	E	370/390 (95%)	354 (96%)	16 (4%)	35	75
2	F	375/390 (96%)	358 (96%)	17 (4%)	34	74
2	M	378/390 (97%)	360 (95%)	18 (5%)	31	71
2	N	378/390 (97%)	357 (94%)	21 (6%)	26	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	378/390 (97%)	366 (97%)	12 (3%)	46	82
2	V	379/390 (97%)	364 (96%)	15 (4%)	38	77
2	W	378/390 (97%)	360 (95%)	18 (5%)	31	71
2	X	379/390 (97%)	364 (96%)	15 (4%)	38	77
3	G	226/236 (96%)	210 (93%)	16 (7%)	18	54
3	P	200/236 (85%)	184 (92%)	16 (8%)	15	47
3	Y	164/236 (70%)	150 (92%)	14 (8%)	13	45
4	H	64/112 (57%)	54 (84%)	10 (16%)	3	16
4	Q	11/112 (10%)	9 (82%)	2 (18%)	2	11
5	1	2/48 (4%)	2 (100%)	0	100	100
5	I	28/48 (58%)	25 (89%)	3 (11%)	8	31
5	R	5/48 (10%)	4 (80%)	1 (20%)	1	8
All	All	7583/8294 (91%)	7224 (95%)	359 (5%)	32	72

All (359) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
1	A	95	ASN
1	A	142	ARG
1	A	166	ARG
1	A	246	TYR
1	A	251	THR
1	A	284	SER
1	A	288	ARG
1	A	373	VAL
1	A	378	SER
1	A	413	ASP
1	A	436	SER
1	A	458	ILE
1	A	460	LEU
1	A	472	SER
1	A	480	GLU
1	A	481	LEU
1	A	499	LEU
1	A	509	THR
1	B	26	ASN
1	B	30	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	91	LYS
1	B	99	VAL
1	B	106	LEU
1	B	159	VAL
1	B	183	ASP
1	B	197	GLU
1	B	204	VAL
1	B	212	ARG
1	B	283	LEU
1	B	309	GLU
1	B	400	ARG
1	B	468	SER
1	B	509	THR
1	C	69	GLU
1	C	99	VAL
1	C	166	ARG
1	C	198	SER
1	C	220	GLN
1	C	283	LEU
1	C	293	ARG
1	C	346	SER
1	C	364	ARG
1	C	375	ARG
1	C	394	LEU
1	C	465	GLU
2	D	7	THR
2	D	58	THR
2	D	89	ARG
2	D	132	GLU
2	D	210	GLU
2	D	251	VAL
2	D	274	ARG
2	D	287	THR
2	D	299	THR
2	D	303	SER
2	D	322	PRO
2	D	386	ASP
2	D	398	GLU
2	D	413	PHE
2	D	431	LEU
2	D	464	GLU
2	D	467	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	43	GLN
2	E	58	THR
2	E	68	GLU
2	E	111	SER
2	E	115	LYS
2	E	140	VAL
2	E	204	THR
2	E	210	GLU
2	E	232	VAL
2	E	269	SER
2	E	337	ARG
2	E	352	ASP
2	E	356	ARG
2	E	390	ILE
2	E	402	LEU
2	E	436	ASP
2	F	27	GLN
2	F	28	SER
2	F	45	LYS
2	F	68	GLU
2	F	113	LEU
2	F	132	GLU
2	F	133	ILE
2	F	140	VAL
2	F	201	MET
2	F	208	ASN
2	F	297	THR
2	F	303	SER
2	F	336	SER
2	F	355	SER
2	F	403	THR
2	F	420	VAL
2	F	464	GLU
3	G	3	LEU
3	G	9	ARG
3	G	11	LYS
3	G	21	LYS
3	G	48	GLU
3	G	53	LYS
3	G	77	ILE
3	G	97	ARG
3	G	118	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	133	ILE
3	G	150	LEU
3	G	153	VAL
3	G	235	ASN
3	G	239	ASN
3	G	252	SER
3	G	276	SER
4	H	14	PHE
4	H	20	THR
4	H	22	TYR
4	H	27	VAL
4	H	35	LYS
4	H	36	SER
4	H	39	ILE
4	H	46	VAL
4	H	48	THR
4	H	70	ILE
5	I	27	THR
5	I	35	LEU
5	I	57	THR
1	J	26	ASN
1	J	27	LEU
1	J	134	LYS
1	J	166	ARG
1	J	175	THR
1	J	183	ASP
1	J	237	THR
1	J	373	VAL
1	J	418	GLN
1	J	429	LEU
1	J	440	THR
1	J	468	SER
1	J	469	SER
1	J	481	LEU
1	J	509	THR
1	K	23	ASP
1	K	40	ILE
1	K	58	SER
1	K	68	LEU
1	K	99	VAL
1	K	106	LEU
1	K	134	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	143	SER
1	K	166	ARG
1	K	199	LYS
1	K	246	TYR
1	K	309	GLU
1	K	320	SER
1	K	371	LEU
1	K	399	TYR
1	K	411	ASP
1	K	462	ARG
1	K	504	GLU
1	L	99	VAL
1	L	132	GLN
1	L	142	ARG
1	L	163	ARG
1	L	166	ARG
1	L	189	LYS
1	L	198	SER
1	L	220	GLN
1	L	231	SER
1	L	267	LEU
1	L	284	SER
1	L	293	ARG
1	L	342	THR
1	L	400	ARG
1	L	405	PHE
1	L	419	THR
1	L	436	SER
1	L	465	GLU
1	L	468	SER
1	L	469	SER
1	L	476	SER
1	L	480	GLU
1	L	481	LEU
2	M	57	ASN
2	M	89	ARG
2	M	90	GLU
2	M	132	GLU
2	M	182	SER
2	M	206	VAL
2	M	210	GLU
2	M	224	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	250	ASP
2	M	261	PHE
2	M	342	LEU
2	M	359	ASP
2	M	385	GLN
2	M	386	ASP
2	M	394	ASP
2	M	413	PHE
2	M	434	LEU
2	M	460	VAL
2	N	68	GLU
2	N	113	LEU
2	N	126	GLU
2	N	130	SER
2	N	132	GLU
2	N	140	VAL
2	N	152	LYS
2	N	212	GLU
2	N	221	GLN
2	N	232	VAL
2	N	318	THR
2	N	330	ASP
2	N	376	GLU
2	N	386	ASP
2	N	387	ILE
2	N	393	MET
2	N	423	VAL
2	N	450	ASP
2	N	458	TYR
2	N	463	ILE
2	N	465	ASP
2	O	30	LEU
2	O	77	LEU
2	O	84	SER
2	O	140	VAL
2	O	149	ARG
2	O	167	ILE
2	O	192	ARG
2	O	274	ARG
2	O	297	THR
2	O	402	LEU
2	O	413	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	455	HIS
3	P	3	LEU
3	P	11	LYS
3	P	35	GLU
3	P	42	LYS
3	P	99	LEU
3	P	107	ILE
3	P	130	ILE
3	P	133	ILE
3	P	136	ASP
3	P	141	GLN
3	P	155	LYS
3	P	178	SER
3	P	186	LYS
3	P	189	GLU
3	P	218	MET
3	P	220	THR
4	Q	39	ILE
4	Q	45	HIS
5	R	31	THR
1	S	32	ARG
1	S	105	LEU
1	S	111	ASP
1	S	115	ASN
1	S	123	ILE
1	S	124	ASP
1	S	134	LYS
1	S	139	LEU
1	S	189	LYS
1	S	267	LEU
1	S	318	GLU
1	S	360	TYR
1	S	373	VAL
1	S	383	LYS
1	S	441	GLU
1	S	459	GLU
1	S	490	GLU
1	S	496	LEU
1	S	504	GLU
1	S	505	SER
1	T	26	ASN
1	T	67	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	95	ASN
1	T	99	VAL
1	T	138	ILE
1	T	159	VAL
1	T	246	TYR
1	T	371	LEU
1	T	373	VAL
1	T	401	GLU
1	T	427	THR
1	T	428	GLN
1	T	465	GLU
1	T	469	SER
1	T	483	THR
1	U	82	ARG
1	U	88	GLU
1	U	172	ASP
1	U	174	GLN
1	U	304	HIS
1	U	339	TYR
1	U	383	LYS
1	U	388	VAL
1	U	394	LEU
1	U	419	THR
1	U	440	THR
2	V	46	LEU
2	V	133	ILE
2	V	149	ARG
2	V	192	ARG
2	V	204	THR
2	V	250	ASP
2	V	268	VAL
2	V	354	LYS
2	V	357	LEU
2	V	386	ASP
2	V	387	ILE
2	V	413	PHE
2	V	423	VAL
2	V	425	THR
2	V	460	VAL
2	W	27	GLN
2	W	65	ASP
2	W	106	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	W	109	ILE
2	W	140	VAL
2	W	204	THR
2	W	210	GLU
2	W	232	VAL
2	W	257	ASN
2	W	284	THR
2	W	324	THR
2	W	352	ASP
2	W	373	LYS
2	W	386	ASP
2	W	387	ILE
2	W	393	MET
2	W	433	ARG
2	W	448	LYS
2	X	14	THR
2	X	22	ASP
2	X	27	GLN
2	X	29	GLU
2	X	46	LEU
2	X	84	SER
2	X	155	LEU
2	X	167	ILE
2	X	208	ASN
2	X	250	ASP
2	X	274	ARG
2	X	336	SER
2	X	356	ARG
2	X	427	ILE
2	X	454	GLU
3	Y	15	ASN
3	Y	19	ILE
3	Y	101	ASP
3	Y	112	ASP
3	Y	119	LEU
3	Y	121	THR
3	Y	131	ASN
3	Y	136	ASP
3	Y	142	GLU
3	Y	162	ILE
3	Y	167	ASN
3	Y	216	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Y	267	LEU
3	Y	271	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	418	GLN
1	B	26	ASN
1	B	428	GLN
1	C	72	GLN
1	C	174	GLN
1	C	210	GLN
1	C	418	GLN
2	D	178	HIS
2	D	208	ASN
2	D	375	GLN
2	E	168	GLN
2	F	27	GLN
2	F	208	ASN
3	G	49	GLN
3	G	59	ASN
3	G	102	GLN
3	G	117	GLN
3	G	216	ASN
3	G	235	ASN
4	H	45	HIS
4	H	51	GLN
1	J	26	ASN
1	J	174	GLN
1	J	262	ASN
1	J	351	GLN
1	J	479	ASN
1	K	50	GLN
1	K	217	GLN
1	K	265	HIS
1	K	428	GLN
1	L	132	GLN
1	L	174	GLN
1	L	217	GLN
1	L	220	GLN
1	L	398	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	195	ASN
2	M	367	HIS
2	M	375	GLN
2	N	168	GLN
2	O	27	GLN
2	O	208	ASN
2	O	328	HIS
3	P	88	HIS
3	P	141	GLN
4	Q	51	GLN
1	T	67	ASN
1	T	145	HIS
1	T	149	GLN
1	T	217	GLN
1	T	304	HIS
1	T	387	GLN
1	U	225	HIS
1	U	262	ASN
1	U	387	GLN
1	U	479	ASN
2	V	118	HIS
2	V	168	GLN
2	W	27	GLN
2	W	385	GLN
2	X	27	GLN
2	X	43	GLN
2	X	118	HIS
2	X	263	GLN
2	X	328	HIS
2	X	365	GLN
3	Y	100	ASN
3	Y	122	HIS
3	Y	260	GLN
3	Y	265	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	2.15	8 (29%)	30,52,52	2.19	5 (16%)
6	ANP	B	600	7	27,33,33	2.01	7 (25%)	30,52,52	2.38	7 (23%)
6	ANP	C	600	7	27,33,33	2.08	6 (22%)	30,52,52	2.33	7 (23%)
6	ANP	D	600	7	27,33,33	1.90	6 (22%)	30,52,52	2.20	8 (26%)
6	ANP	F	600	7	27,33,33	2.01	6 (22%)	30,52,52	2.33	7 (23%)
6	ANP	J	600	7	27,33,33	1.97	6 (22%)	30,52,52	2.31	6 (20%)
6	ANP	K	600	7	27,33,33	2.06	6 (22%)	30,52,52	2.35	8 (26%)
6	ANP	L	600	7	27,33,33	2.15	8 (29%)	30,52,52	2.26	9 (30%)
6	ANP	M	600	7	27,33,33	1.95	5 (18%)	30,52,52	2.50	6 (20%)
6	ANP	O	600	7	27,33,33	1.96	6 (22%)	30,52,52	2.30	7 (23%)
6	ANP	S	600	7	27,33,33	2.13	7 (25%)	30,52,52	2.25	7 (23%)
6	ANP	T	600	7	27,33,33	2.18	6 (22%)	30,52,52	2.31	7 (23%)
6	ANP	U	600	7	27,33,33	2.06	6 (22%)	30,52,52	2.48	8 (26%)
6	ANP	V	600	7	27,33,33	1.97	6 (22%)	30,52,52	2.43	9 (30%)
6	ANP	X	600	7	27,33,33	1.97	6 (22%)	30,52,52	2.45	8 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	A	600	7	-	2/12/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	B	600	7	-	2/12/38/38	0/3/3/3
6	ANP	C	600	7	-	1/12/38/38	0/3/3/3
6	ANP	D	600	7	-	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	-	0/12/38/38	0/3/3/3
6	ANP	L	600	7	-	2/12/38/38	0/3/3/3
6	ANP	M	600	7	-	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 (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	600	ANP	PG-O2G	-2.54	1.49	1.56
6	A	600	ANP	PG-O2G	-2.49	1.49	1.56
6	L	600	ANP	PG-O3G	-2.16	1.50	1.56
6	D	600	ANP	PB-O2B	-2.13	1.50	1.56
6	V	600	ANP	C2-N3	2.05	1.35	1.32
6	B	600	ANP	O4'-C1'	2.06	1.43	1.41
6	S	600	ANP	C2-N3	2.12	1.35	1.32
6	C	600	ANP	O4'-C1'	2.13	1.43	1.41
6	X	600	ANP	PB-O3A	2.16	1.61	1.59
6	B	600	ANP	PB-O3A	2.17	1.61	1.59
6	T	600	ANP	PB-O3A	2.27	1.61	1.59
6	A	600	ANP	O4'-C1'	2.31	1.44	1.41
6	U	600	ANP	PB-O3A	2.56	1.62	1.59
6	S	600	ANP	PB-O3A	2.60	1.62	1.59
6	J	600	ANP	PB-O3A	2.76	1.62	1.59
6	M	600	ANP	C5-C4	2.77	1.46	1.40
6	F	600	ANP	PB-O3A	2.79	1.62	1.59
6	A	600	ANP	C5-C4	2.85	1.46	1.40
6	A	600	ANP	PB-O3A	2.99	1.62	1.59
6	S	600	ANP	C5-C4	3.03	1.47	1.40
6	O	600	ANP	PB-O3A	3.03	1.62	1.59
6	C	600	ANP	C5-C4	3.03	1.47	1.40
6	L	600	ANP	PB-O3A	3.04	1.62	1.59
6	U	600	ANP	C5-C4	3.10	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	600	ANP	C5-C4	3.11	1.47	1.40
6	V	600	ANP	C5-C4	3.12	1.47	1.40
6	J	600	ANP	C5-C4	3.14	1.47	1.40
6	O	600	ANP	C5-C4	3.15	1.47	1.40
6	F	600	ANP	C5-C4	3.19	1.47	1.40
6	T	600	ANP	C5-C4	3.26	1.47	1.40
6	L	600	ANP	C5-C4	3.27	1.47	1.40
6	B	600	ANP	C5-C4	3.36	1.48	1.40
6	M	600	ANP	PG-N3B	3.42	1.72	1.63
6	X	600	ANP	C5-C4	3.43	1.48	1.40
6	D	600	ANP	PB-O1B	3.44	1.50	1.46
6	K	600	ANP	C5-C4	3.45	1.48	1.40
6	K	600	ANP	PB-O3A	3.50	1.63	1.59
6	K	600	ANP	PG-N3B	3.58	1.72	1.63
6	O	600	ANP	PB-O1B	3.66	1.50	1.46
6	J	600	ANP	PB-O1B	3.81	1.50	1.46
6	M	600	ANP	PB-N3B	3.84	1.73	1.63
6	V	600	ANP	PB-N3B	3.84	1.73	1.63
6	K	600	ANP	PB-N3B	3.85	1.73	1.63
6	O	600	ANP	PG-N3B	3.89	1.73	1.63
6	B	600	ANP	PB-O1B	3.90	1.50	1.46
6	O	600	ANP	PB-N3B	3.91	1.73	1.63
6	U	600	ANP	PG-N3B	3.98	1.73	1.63
6	A	600	ANP	PB-N3B	3.99	1.73	1.63
6	J	600	ANP	PG-N3B	4.00	1.73	1.63
6	X	600	ANP	PG-O1G	4.00	1.50	1.46
6	B	600	ANP	PB-N3B	4.03	1.74	1.63
6	D	600	ANP	PB-N3B	4.08	1.74	1.63
6	F	600	ANP	PB-N3B	4.08	1.74	1.63
6	F	600	ANP	PG-N3B	4.09	1.74	1.63
6	D	600	ANP	PG-N3B	4.11	1.74	1.63
6	V	600	ANP	PG-N3B	4.12	1.74	1.63
6	B	600	ANP	PG-N3B	4.14	1.74	1.63
6	L	600	ANP	PG-O1G	4.16	1.50	1.46
6	J	600	ANP	PB-N3B	4.16	1.74	1.63
6	X	600	ANP	PG-N3B	4.17	1.74	1.63
6	S	600	ANP	PB-O1B	4.18	1.50	1.46
6	F	600	ANP	PB-O1B	4.19	1.50	1.46
6	X	600	ANP	PB-O1B	4.26	1.51	1.46
6	L	600	ANP	PB-N3B	4.29	1.74	1.63
6	U	600	ANP	PB-N3B	4.32	1.74	1.63
6	C	600	ANP	PG-N3B	4.33	1.74	1.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	600	ANP	PB-O1B	4.34	1.51	1.46
6	C	600	ANP	PB-N3B	4.36	1.74	1.63
6	U	600	ANP	PB-O1B	4.37	1.51	1.46
6	V	600	ANP	PG-O1G	4.37	1.51	1.46
6	F	600	ANP	PG-O1G	4.40	1.51	1.46
6	S	600	ANP	PB-N3B	4.41	1.75	1.63
6	A	600	ANP	PG-N3B	4.42	1.75	1.63
6	O	600	ANP	PG-O1G	4.44	1.51	1.46
6	D	600	ANP	PG-O1G	4.44	1.51	1.46
6	X	600	ANP	PB-N3B	4.46	1.75	1.63
6	C	600	ANP	PG-O1G	4.49	1.51	1.46
6	T	600	ANP	PB-N3B	4.50	1.75	1.63
6	J	600	ANP	PG-O1G	4.50	1.51	1.46
6	K	600	ANP	PB-O1B	4.55	1.51	1.46
6	T	600	ANP	PB-O1B	4.58	1.51	1.46
6	V	600	ANP	PB-O1B	4.58	1.51	1.46
6	T	600	ANP	PG-N3B	4.59	1.75	1.63
6	C	600	ANP	PB-O1B	4.60	1.51	1.46
6	K	600	ANP	PG-O1G	4.63	1.51	1.46
6	B	600	ANP	PG-O1G	4.66	1.51	1.46
6	M	600	ANP	PG-O1G	4.66	1.51	1.46
6	L	600	ANP	PG-N3B	4.74	1.75	1.63
6	S	600	ANP	PG-N3B	4.75	1.75	1.63
6	A	600	ANP	PG-O1G	4.81	1.51	1.46
6	M	600	ANP	PB-O1B	4.82	1.51	1.46
6	U	600	ANP	PG-O1G	4.83	1.51	1.46
6	S	600	ANP	PG-O1G	4.84	1.51	1.46
6	A	600	ANP	PB-O1B	5.05	1.51	1.46
6	T	600	ANP	PG-O1G	5.57	1.52	1.46

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	ANP	N3-C2-N1	-7.82	122.91	128.89
6	D	600	ANP	N3-C2-N1	-7.64	123.05	128.89
6	U	600	ANP	N3-C2-N1	-7.50	123.15	128.89
6	M	600	ANP	O1G-PG-N3B	-7.43	100.51	111.90
6	T	600	ANP	N3-C2-N1	-7.39	123.23	128.89
6	C	600	ANP	N3-C2-N1	-7.23	123.36	128.89
6	S	600	ANP	N3-C2-N1	-7.21	123.37	128.89
6	J	600	ANP	N3-C2-N1	-7.20	123.38	128.89
6	F	600	ANP	N3-C2-N1	-7.15	123.42	128.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	600	ANP	N3-C2-N1	-7.13	123.44	128.89
6	V	600	ANP	N3-C2-N1	-7.00	123.53	128.89
6	X	600	ANP	N3-C2-N1	-6.97	123.56	128.89
6	K	600	ANP	N3-C2-N1	-6.95	123.57	128.89
6	O	600	ANP	N3-C2-N1	-6.94	123.58	128.89
6	A	600	ANP	N3-C2-N1	-6.82	123.67	128.89
6	K	600	ANP	O1G-PG-N3B	-6.33	102.20	111.90
6	J	600	ANP	O1G-PG-N3B	-6.32	102.21	111.90
6	A	600	ANP	O1G-PG-N3B	-6.14	102.47	111.90
6	X	600	ANP	O1G-PG-N3B	-6.10	102.54	111.90
6	M	600	ANP	N3-C2-N1	-6.02	124.28	128.89
6	V	600	ANP	O1G-PG-N3B	-5.96	102.76	111.90
6	B	600	ANP	O1G-PG-N3B	-5.94	102.79	111.90
6	F	600	ANP	O1G-PG-N3B	-5.63	103.26	111.90
6	T	600	ANP	O1G-PG-N3B	-5.63	103.26	111.90
6	U	600	ANP	O1G-PG-N3B	-5.55	103.39	111.90
6	C	600	ANP	O1G-PG-N3B	-5.15	103.99	111.90
6	O	600	ANP	O1G-PG-N3B	-5.03	104.18	111.90
6	O	600	ANP	O1B-PB-N3B	-4.58	104.88	111.90
6	S	600	ANP	O1G-PG-N3B	-4.44	105.09	111.90
6	L	600	ANP	O1G-PG-N3B	-4.39	105.16	111.90
6	U	600	ANP	O1B-PB-N3B	-4.33	105.26	111.90
6	X	600	ANP	O1B-PB-N3B	-4.24	105.40	111.90
6	D	600	ANP	O1G-PG-N3B	-4.04	105.69	111.90
6	T	600	ANP	O1B-PB-N3B	-4.02	105.73	111.90
6	X	600	ANP	PA-O3A-PB	-4.01	119.22	132.67
6	M	600	ANP	C2'-C1'-N9	-3.88	108.36	114.29
6	L	600	ANP	O1B-PB-N3B	-3.85	105.99	111.90
6	F	600	ANP	C2'-C1'-N9	-3.80	108.48	114.29
6	S	600	ANP	PA-O3A-PB	-3.80	119.92	132.67
6	O	600	ANP	C2'-C1'-N9	-3.63	108.74	114.29
6	K	600	ANP	O1B-PB-N3B	-3.48	106.56	111.90
6	V	600	ANP	PA-O3A-PB	-3.39	121.30	132.67
6	F	600	ANP	O1B-PB-N3B	-3.37	106.73	111.90
6	V	600	ANP	O1B-PB-N3B	-3.34	106.78	111.90
6	V	600	ANP	C4-C5-N7	-3.34	106.41	109.48
6	M	600	ANP	O1B-PB-N3B	-3.27	106.89	111.90
6	S	600	ANP	O1B-PB-N3B	-3.26	106.90	111.90
6	U	600	ANP	C4-C5-N7	-3.23	106.51	109.48
6	T	600	ANP	PA-O3A-PB	-3.23	121.84	132.67
6	J	600	ANP	C4-C5-N7	-3.19	106.55	109.48
6	D	600	ANP	C2'-C1'-N9	-3.18	109.43	114.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	600	ANP	C4-C5-N7	-3.15	106.58	109.48
6	M	600	ANP	C4-C5-N7	-3.14	106.59	109.48
6	U	600	ANP	PA-O3A-PB	-3.10	122.26	132.67
6	O	600	ANP	C4-C5-N7	-2.98	106.74	109.48
6	D	600	ANP	PA-O3A-PB	-2.95	122.78	132.67
6	A	600	ANP	C4-C5-N7	-2.94	106.78	109.48
6	L	600	ANP	C4-C5-N7	-2.93	106.79	109.48
6	B	600	ANP	C4-C5-N7	-2.88	106.83	109.48
6	C	600	ANP	PA-O3A-PB	-2.85	123.13	132.67
6	K	600	ANP	PA-O3A-PB	-2.83	123.19	132.67
6	X	600	ANP	C4-C5-N7	-2.78	106.92	109.48
6	V	600	ANP	C2'-C1'-N9	-2.74	110.10	114.29
6	B	600	ANP	PA-O3A-PB	-2.72	123.56	132.67
6	C	600	ANP	C4-C5-N7	-2.71	106.98	109.48
6	T	600	ANP	C4-C5-N7	-2.68	107.02	109.48
6	S	600	ANP	C4-C5-N7	-2.61	107.08	109.48
6	D	600	ANP	C4-C5-N7	-2.57	107.12	109.48
6	J	600	ANP	PA-O3A-PB	-2.42	124.56	132.67
6	U	600	ANP	C2'-C1'-N9	-2.38	110.66	114.29
6	F	600	ANP	PA-O3A-PB	-2.35	124.79	132.67
6	C	600	ANP	O1B-PB-N3B	-2.28	108.40	111.90
6	A	600	ANP	O1B-PB-N3B	-2.21	108.52	111.90
6	L	600	ANP	C2'-C1'-N9	-2.17	110.98	114.29
6	O	600	ANP	PA-O3A-PB	-2.08	125.69	132.67
6	D	600	ANP	C2-N1-C6	2.01	122.35	118.77
6	J	600	ANP	O3G-PG-O2G	2.09	113.77	107.58
6	K	600	ANP	O2B-PB-O3A	2.10	114.61	105.09
6	L	600	ANP	O3G-PG-O2G	2.11	113.84	107.58
6	L	600	ANP	O4'-C1'-N9	2.13	112.55	108.10
6	L	600	ANP	O3A-PB-N3B	2.17	112.42	106.44
6	T	600	ANP	O3G-PG-O2G	2.24	114.23	107.58
6	K	600	ANP	O3G-PG-O2G	2.26	114.27	107.58
6	V	600	ANP	O3G-PG-O2G	2.44	114.80	107.58
6	U	600	ANP	O3G-PG-O2G	2.50	115.00	107.58
6	C	600	ANP	O3G-PG-O2G	2.53	115.08	107.58
6	V	600	ANP	O4'-C1'-N9	2.57	113.48	108.10
6	B	600	ANP	O3G-PG-O2G	2.60	115.29	107.58
6	F	600	ANP	O3G-PG-O2G	2.61	115.30	107.58
6	X	600	ANP	O3G-PG-O2G	2.65	115.43	107.58
6	X	600	ANP	C4'-O4'-C1'	2.75	112.74	109.72
6	S	600	ANP	O3G-PG-O2G	2.86	116.06	107.58
6	B	600	ANP	O4'-C1'-N9	3.13	114.64	108.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	600	ANP	O3G-PG-O2G	3.20	117.06	107.58
6	D	600	ANP	O2B-PB-O1B	3.58	117.48	110.00
6	K	600	ANP	O2B-PB-O1B	3.68	117.69	110.00
6	S	600	ANP	O2B-PB-O1B	3.77	117.86	110.00
6	T	600	ANP	O2B-PB-O1B	3.93	118.20	110.00
6	O	600	ANP	O2B-PB-O1B	4.08	118.53	110.00
6	A	600	ANP	O2B-PB-O1B	4.33	119.04	110.00
6	B	600	ANP	O2B-PB-O1B	4.45	119.30	110.00
6	X	600	ANP	O2B-PB-O1B	4.46	119.30	110.00
6	J	600	ANP	O2B-PB-O1B	4.50	119.38	110.00
6	F	600	ANP	O2B-PB-O1B	4.54	119.47	110.00
6	V	600	ANP	O2B-PB-O1B	4.65	119.72	110.00
6	L	600	ANP	O2B-PB-O1B	4.77	119.96	110.00
6	U	600	ANP	O2B-PB-O1B	5.26	120.98	110.00
6	M	600	ANP	O2B-PB-O1B	5.80	122.10	110.00
6	C	600	ANP	O2B-PB-O1B	5.97	122.45	110.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	600	ANP	1	0
6	B	600	ANP	4	0
6	F	600	ANP	1	0
6	J	600	ANP	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	600	ANP	3	0
6	L	600	ANP	1	0
6	M	600	ANP	4	0
6	O	600	ANP	3	0
6	T	600	ANP	1	0
6	U	600	ANP	1	0
6	V	600	ANP	1	0
6	X	600	ANP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	482/510 (94%)	-0.48	0 100 100	41, 63, 99, 156	0
1	B	483/510 (94%)	-0.21	3 (0%) 90 73	48, 92, 148, 188	0
1	C	484/510 (94%)	-0.39	0 100 100	43, 73, 129, 177	0
1	J	481/510 (94%)	-0.24	2 (0%) 93 80	60, 100, 149, 206	0
1	K	486/510 (95%)	-0.04	16 (3%) 50 22	78, 126, 187, 217	0
1	L	482/510 (94%)	-0.39	0 100 100	47, 68, 137, 194	0
1	S	478/510 (93%)	-0.19	10 (2%) 67 36	77, 109, 153, 179	0
1	T	479/510 (93%)	0.24	31 (6%) 22 8	103, 151, 186, 202	0
1	U	481/510 (94%)	0.22	32 (6%) 21 7	104, 150, 181, 217	0
2	D	470/484 (97%)	-0.42	1 (0%) 95 87	42, 70, 123, 181	0
2	E	468/484 (96%)	-0.21	10 (2%) 67 36	46, 86, 161, 211	0
2	F	469/484 (96%)	-0.29	1 (0%) 95 87	48, 89, 129, 169	0
2	M	470/484 (97%)	-0.30	3 (0%) 90 73	55, 86, 134, 180	0
2	N	470/484 (97%)	0.09	19 (4%) 42 17	71, 133, 199, 229	0
2	O	468/484 (96%)	-0.29	0 100 100	54, 94, 141, 175	0
2	V	470/484 (97%)	0.13	28 (5%) 25 9	93, 138, 180, 210	0
2	W	467/484 (96%)	-0.05	18 (3%) 43 18	89, 117, 164, 189	0
2	X	469/484 (96%)	0.08	21 (4%) 37 15	93, 134, 185, 234	0
3	G	266/278 (95%)	-0.23	2 (0%) 87 67	63, 103, 140, 167	0
3	P	246/278 (88%)	0.25	14 (5%) 27 10	69, 131, 195, 237	0
3	Y	201/278 (72%)	0.46	20 (9%) 9 4	107, 146, 192, 232	0
4	H	116/138 (84%)	-0.03	6 (5%) 31 12	82, 127, 216, 236	0
4	Q	84/138 (60%)	0.03	4 (4%) 34 14	109, 150, 208, 214	0
4	Z	17/138 (12%)	2.27	11 (64%) 0 0	190, 210, 236, 245	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	1	27/61 (44%)	1.60	9 (33%) 0 0	159, 168, 187, 210	0
5	I	49/61 (80%)	-0.06	2 (4%) 41 16	97, 127, 178, 217	0
5	R	34/61 (55%)	-0.32	1 (2%) 55 26	108, 122, 187, 200	0
All	All	9597/10377 (92%)	-0.12	264 (2%) 56 27	41, 108, 176, 245	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	26	ASN	6.4
1	T	491	LEU	5.5
2	X	7	THR	5.3
5	1	33	SER	5.1
2	X	90	GLU	4.9
3	P	170	VAL	4.8
3	Y	140	PHE	4.8
1	U	63	GLY	4.6
2	W	474	ALA	4.5
2	N	387	ILE	4.5
1	U	62	LYS	4.4
3	Y	170	VAL	4.4
2	V	214	LYS	4.4
2	D	6	SER	4.4
2	X	30	LEU	4.3
1	T	27	LEU	4.2
4	Z	121	ALA	4.2
2	N	457	PHE	4.1
1	T	485	ILE	4.1
2	X	28	SER	4.0
1	T	35	ALA	4.0
2	V	213	SER	4.0
2	X	9	ILE	4.0
3	P	54	ASN	4.0
2	N	453	PRO	3.9
1	T	46	LEU	3.9
2	X	55	GLY	3.9
1	U	43	VAL	3.9
1	K	494	GLU	3.8
1	K	503	THR	3.8
2	N	6	SER	3.7
1	S	87	GLY	3.7
4	H	90	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	491	LEU	3.6
3	Y	41	ALA	3.6
2	X	8	PRO	3.6
3	P	169	PRO	3.6
1	T	202	TYR	3.6
2	V	110	LYS	3.6
2	N	475	ALA	3.5
2	V	57	ASN	3.5
2	E	457	PHE	3.5
2	N	23	VAL	3.5
2	V	28	SER	3.4
4	Q	81	SER	3.4
2	X	76	VAL	3.4
1	U	122	PRO	3.3
1	T	32	ARG	3.3
1	T	54	LEU	3.3
4	Z	135	SER	3.3
1	K	457	GLY	3.3
1	K	195	SER	3.2
2	X	249	GLN	3.2
5	1	11	ALA	3.2
2	E	391	LEU	3.2
2	V	9	ILE	3.2
1	U	489	GLY	3.2
1	U	446	LEU	3.2
3	Y	91	LEU	3.1
1	T	55	VAL	3.1
4	H	111	ASN	3.1
1	K	454	HIS	3.1
1	T	26	ASN	3.1
5	1	22	ARG	3.1
4	Z	128	GLU	3.1
1	U	52	GLU	3.1
1	S	89	LEU	3.1
1	T	30	THR	3.1
2	V	108	PRO	3.1
2	X	31	PRO	3.1
1	T	314	LEU	3.1
1	U	30	THR	3.0
4	Z	129	VAL	3.0
1	S	37	GLY	3.0
2	W	470	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	114	GLY	3.0
2	X	77	LEU	3.0
4	H	103	ASN	3.0
2	X	11	GLY	3.0
3	Y	45	ASP	3.0
1	U	491	LEU	3.0
1	U	455	LEU	2.9
2	V	27	GLN	2.9
3	P	105	ALA	2.9
2	V	210	GLU	2.9
2	W	437	THR	2.9
4	Z	124	ALA	2.9
2	M	6	SER	2.9
2	N	8	PRO	2.9
5	1	18	ALA	2.9
2	X	10	THR	2.9
2	V	102	PRO	2.8
2	V	71	VAL	2.8
2	X	75	LYS	2.8
1	B	485	ILE	2.8
3	P	106	ASP	2.8
1	S	30	THR	2.8
1	T	320	SER	2.8
4	Z	132	ASN	2.8
1	T	63	GLY	2.8
2	X	32	ALA	2.8
1	K	474	LEU	2.7
2	W	390	ILE	2.7
2	W	463	ILE	2.7
1	K	505	SER	2.7
1	T	49	ILE	2.7
2	W	394	ASP	2.7
1	U	123	ILE	2.7
5	1	15	ASN	2.7
2	N	7	THR	2.7
2	N	409	LYS	2.7
4	H	113	SER	2.7
1	T	199	LYS	2.7
2	N	302	GLY	2.7
2	W	473	LEU	2.7
4	Z	130	LEU	2.7
2	V	475	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	W	453	PRO	2.7
1	T	321	GLY	2.6
5	I	23	SER	2.6
4	Z	134	GLN	2.6
1	U	442	GLU	2.6
1	T	489	GLY	2.6
1	U	509	THR	2.6
3	P	161	LYS	2.6
2	N	445	LEU	2.6
2	W	395	GLU	2.6
1	T	313	LYS	2.6
1	T	412	LEU	2.6
1	U	507	VAL	2.6
3	Y	165	PHE	2.6
3	Y	223	ALA	2.5
2	V	31	PRO	2.5
4	H	112	VAL	2.5
3	Y	219	LEU	2.5
1	U	143	SER	2.5
2	W	387	ILE	2.5
3	P	39	ILE	2.5
2	N	451	ASN	2.5
3	Y	124	ASN	2.5
3	P	46	GLU	2.5
2	E	474	ALA	2.5
3	Y	141	GLN	2.5
2	N	402	LEU	2.5
3	Y	119	LEU	2.4
2	V	29	GLU	2.4
3	G	172	SER	2.4
5	R	27	THR	2.4
1	T	200	LYS	2.4
4	Q	80	ASP	2.4
1	T	197	GLU	2.4
3	P	164	ILE	2.4
1	J	481	LEU	2.4
3	G	60	LEU	2.4
1	U	424	GLU	2.4
4	Z	126	GLN	2.4
2	E	451	ASN	2.4
1	U	44	PHE	2.4
2	N	456	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	S	507	VAL	2.3
2	E	410	ILE	2.3
2	V	467	VAL	2.3
2	E	405	GLU	2.3
1	B	489	GLY	2.3
2	V	302	GLY	2.3
1	K	499	LEU	2.3
1	T	122	PRO	2.3
3	Y	169	PRO	2.3
1	K	491	LEU	2.3
2	V	212	GLU	2.3
4	H	49	VAL	2.3
5	1	13	TYR	2.3
1	U	58	SER	2.3
3	Y	39	ILE	2.3
1	U	411	ASP	2.3
1	U	476	SER	2.3
1	S	36	VAL	2.3
2	V	8	PRO	2.3
1	T	482	LEU	2.3
1	U	469	SER	2.3
2	V	23	VAL	2.3
2	E	407	ALA	2.2
1	U	48	ASN	2.2
2	V	90	GLU	2.2
2	X	248	GLY	2.2
5	1	16	VAL	2.2
3	Y	40	SER	2.2
1	U	29	GLU	2.2
2	E	445	LEU	2.2
1	U	304	HIS	2.2
2	N	395	GLU	2.2
3	P	91	LEU	2.2
1	K	418	GLN	2.2
1	U	116	PRO	2.2
3	Y	212	TYR	2.2
1	U	33	VAL	2.2
2	V	427	ILE	2.2
1	T	264	LYS	2.2
1	K	149	GLN	2.2
1	U	86	GLU	2.2
4	Z	133	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	390	ILE	2.2
1	T	490	GLU	2.2
5	1	17	ALA	2.2
1	T	103	PRO	2.2
2	X	42	PRO	2.2
2	W	72	ARG	2.2
2	W	58	THR	2.2
1	K	460	LEU	2.2
1	S	44	PHE	2.2
1	K	448	TYR	2.2
2	V	26	GLU	2.2
1	K	508	ALA	2.2
4	Q	97	SER	2.2
2	V	211	GLY	2.2
1	T	123	ILE	2.2
2	V	109	ILE	2.2
3	P	101	ASP	2.2
2	X	112	LYS	2.1
3	Y	44	MET	2.1
2	W	391	LEU	2.1
2	E	452	ILE	2.1
3	P	126	ILE	2.1
2	V	45	LYS	2.1
4	Z	120	ALA	2.1
5	1	34	VAL	2.1
2	N	11	GLY	2.1
1	K	458	ILE	2.1
1	T	48	ASN	2.1
1	J	496	LEU	2.1
2	W	457	PHE	2.1
2	V	25	PHE	2.1
3	Y	145	LEU	2.1
2	M	27	GLN	2.1
1	K	455	LEU	2.1
2	X	12	LYS	2.1
2	N	394	ASP	2.1
2	X	25	PHE	2.1
3	Y	36	LYS	2.1
2	V	14	THR	2.1
1	U	49	ILE	2.1
3	Y	224	GLN	2.1
1	S	83	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	78	PHE	2.1
2	W	393	MET	2.1
3	P	107	ILE	2.1
1	U	32	ARG	2.1
2	V	449	TYR	2.1
2	F	466	VAL	2.1
4	Q	15	ALA	2.1
1	S	46	LEU	2.0
2	N	398	GLU	2.0
1	S	471	LEU	2.0
2	W	402	LEU	2.0
2	W	462	GLY	2.0
2	E	396	LEU	2.0
3	P	98	HIS	2.0
5	I	29	LEU	2.0
2	X	87	VAL	2.0
2	M	470	ALA	2.0
2	W	384	LEU	2.0
1	T	87	GLY	2.0
3	Y	43	LYS	2.0
1	T	471	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	MG	F	700	1/1	0.97	0.33	5.27	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MG	M	700	1/1	0.92	0.35	5.03	53,53,53,53	0
7	MG	D	700	1/1	0.94	0.29	4.72	48,48,48,48	0
6	ANP	C	600	31/31	0.96	0.20	0.54	57,68,75,75	0
6	ANP	D	600	31/31	0.98	0.19	0.34	55,65,68,69	0
6	ANP	M	600	31/31	0.98	0.20	0.19	60,70,73,74	0
6	ANP	A	600	31/31	0.98	0.19	0.16	44,57,61,63	0
6	ANP	L	600	31/31	0.96	0.19	0.00	49,62,70,70	0
6	ANP	K	600	31/31	0.91	0.19	-0.06	79,96,100,101	0
6	ANP	F	600	31/31	0.96	0.20	-0.23	65,79,84,85	0
6	ANP	J	600	31/31	0.94	0.17	-0.24	60,74,82,83	0
6	ANP	V	600	31/31	0.95	0.20	-0.42	80,100,102,102	0
7	MG	V	700	1/1	0.97	0.21	-0.48	61,61,61,61	0
6	ANP	U	600	31/31	0.89	0.20	-0.48	73,79,82,82	0
6	ANP	T	600	31/31	0.92	0.17	-0.52	81,102,107,108	0
6	ANP	B	600	31/31	0.95	0.16	-0.71	66,79,81,82	0
6	ANP	O	600	31/31	0.97	0.18	-0.75	69,79,81,82	0
6	ANP	S	600	31/31	0.96	0.14	-0.89	64,78,80,80	0
6	ANP	X	600	31/31	0.96	0.17	-1.15	83,95,97,97	0
7	MG	O	700	1/1	0.95	0.11	-3.73	61,61,61,61	0
7	MG	X	700	1/1	0.98	0.15	-5.66	70,70,70,70	0
7	MG	K	700	1/1	0.97	0.19	-	66,66,66,66	0
7	MG	L	700	1/1	0.95	0.33	-	48,48,48,48	0
7	MG	S	700	1/1	0.96	0.27	-	53,53,53,53	0
7	MG	C	700	1/1	0.97	0.37	-	52,52,52,52	0
7	MG	A	700	1/1	0.98	0.32	-	41,41,41,41	0
7	MG	B	700	1/1	0.98	0.32	-	57,57,57,57	0
7	MG	U	700	1/1	0.99	0.30	-	61,61,61,61	0
7	MG	J	700	1/1	0.88	0.24	-	51,51,51,51	0
7	MG	T	700	1/1	0.93	0.28	-	62,62,62,62	0

6.5 Other polymers

There are no such residues in this entry.