Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:37 AM GMT

PDB ID	:	2HLD
Title	:	Crystal structure of yeast mitochondrial F1-ATPase
Authors	:	Kabaleeswaran, V.; Puri, N.; Walker, J.E.; Leslie, A.G.; Mueller, D.M.
Deposited on	:	2006-07-06
Resolution	:	2.80 Å(reported)

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

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

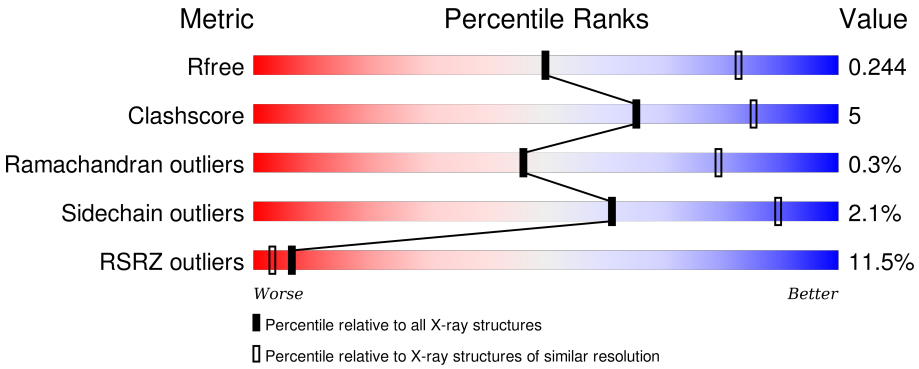
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	510	3% 83% 11% 5%
1	B	510	6% 81% 12% • 5%
1	C	510	6% 82% 12% • 5%
1	J	510	7% 85% 9% • 6%
1	K	510	9% 80% 14% • 5%

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Mol	Chain	Length	Quality of chain
1	L	510	5% 79% 14% • 5%
1	S	510	8% 83% 11% • 6%
1	T	510	18% 82% 12% • 6%
1	U	510	20% 83% 10% • 6%
2	D	478	6% 87% 11% • •
2	E	478	9% 84% 14% •
2	F	478	5% 84% 13% • •
2	M	478	5% 83% 15% • •
2	N	478	13% 87% 10% • •
2	O	478	7% 87% 10% • •
2	V	478	17% 85% 12% • •
2	W	478	17% 85% 13% •
2	X	478	14% 80% 17% •
3	G	278	10% 73% 21% • 5%
3	P	278	22% 65% 19% • 13%
3	Y	278	20% 55% 17% 28%
4	H	138	32% 78% 8% • 13%
4	Q	138	20% 56% 5% 39%
4	Z	138	7% 12% 88%
5	1	61	18% 38% 7% 56%
5	I	61	13% 69% 8% • 21%
5	R	61	16% 52% • 44%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 72841 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 alpha chain, mitochondrial.

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
			3674	2319	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
			3684	2326	652	703	3			
1	L	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	S	480	Total	C	N	O	S	0	0	0
			3651	2307	645	696	3			
1	T	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			
1	U	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			

- Molecule 2 is a protein called ATP synthase beta chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	E	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	F	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			
2	M	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	N	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	468	Total	C	N	O	S	0	0	0
			3538	2244	602	686	6			
2	V	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	W	467	Total	C	N	O	S	0	0	0
			3531	2240	601	684	6			
2	X	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			

- Molecule 3 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	265	Total	C	N	O	S	0	0	0
			2031	1277	355	389	10			
3	P	243	Total	C	N	O	S	0	0	0
			1851	1165	322	355	9			
3	Y	200	Total	C	N	O	S	0	0	0
			1517	944	273	291	9			

- Molecule 4 is a protein called ATP synthase delta chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	120	Total	C	N	O	S	0	0	0
			758	475	134	147	2			
4	Q	84	Total	C	N	O		0	0	0
			436	262	87	87				
4	Z	17	Total	C	N	O		0	0	0
			85	51	17	17				

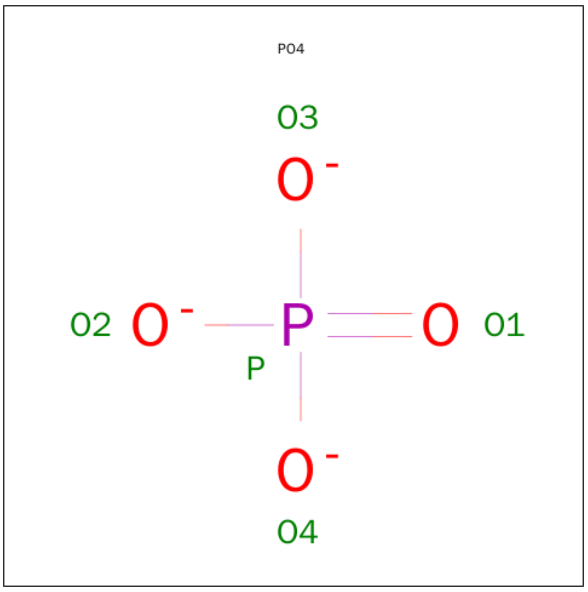
- Molecule 5 is a protein called ATP synthase epsilon chain, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	48	Total	C	N	O	0	0	0
			324	201	56	67			
5	R	34	Total	C	N	O	0	0	0
			170	102	34	34			
5	1	27	Total	C	N	O	0	0	0
			135	81	27	27			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

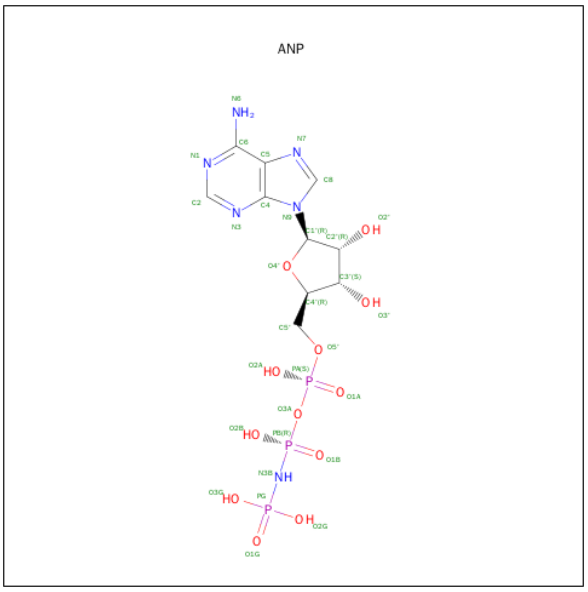
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	K	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	V	1	Total Mg 1 1	0	0
6	A	1	Total Mg 1 1	0	0
6	T	1	Total Mg 1 1	0	0
6	U	1	Total Mg 1 1	0	0
6	X	1	Total Mg 1 1	0	0
6	O	1	Total Mg 1 1	0	0
6	L	1	Total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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	26	Total	O	0	0
			26	26		
9	B	18	Total	O	0	0
			18	18		
9	C	13	Total	O	0	0
			13	13		
9	D	20	Total	O	0	0
			20	20		
9	E	13	Total	O	0	0
			13	13		
9	F	11	Total	O	0	0
			11	11		

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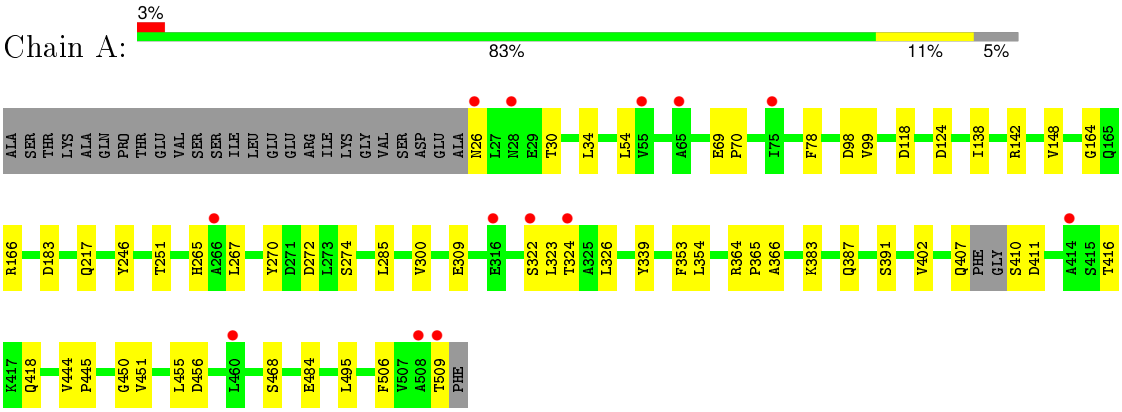
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	3	Total O 3 3	0	0
9	J	17	Total O 17 17	0	0
9	K	4	Total O 4 4	0	0
9	L	19	Total O 19 19	0	0
9	M	9	Total O 9 9	0	0
9	N	8	Total O 8 8	0	0
9	O	7	Total O 7 7	0	0
9	P	2	Total O 2 2	0	0
9	Q	1	Total O 1 1	0	0
9	S	6	Total O 6 6	0	0
9	T	1	Total O 1 1	0	0
9	U	3	Total O 3 3	0	0
9	X	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

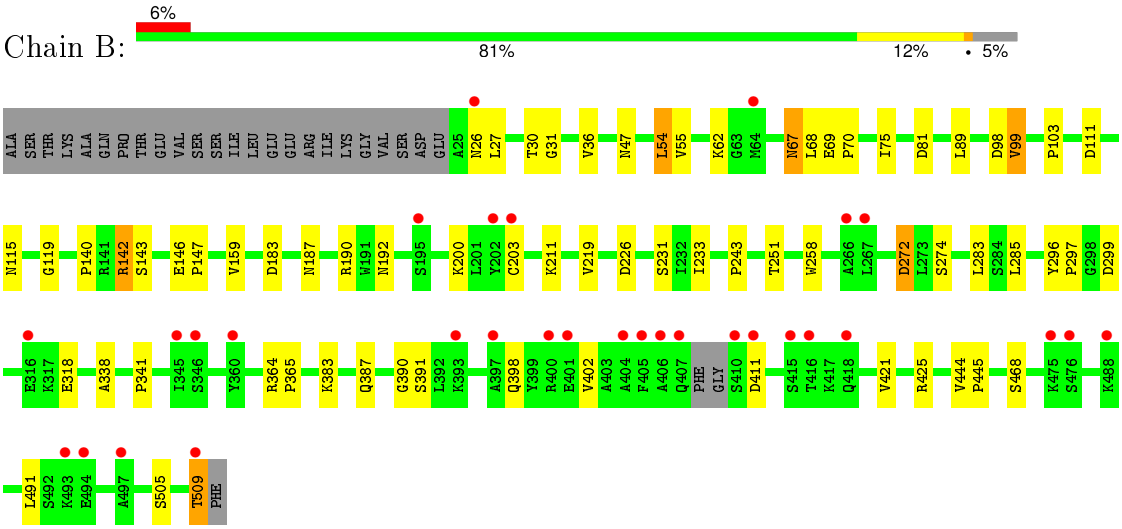
- Molecule 1: ATP synthase alpha chain, mitochondrial

Chain A:



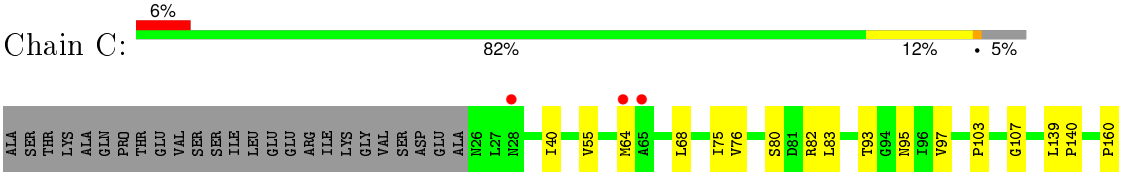
- Molecule 1: ATP synthase alpha chain, mitochondrial

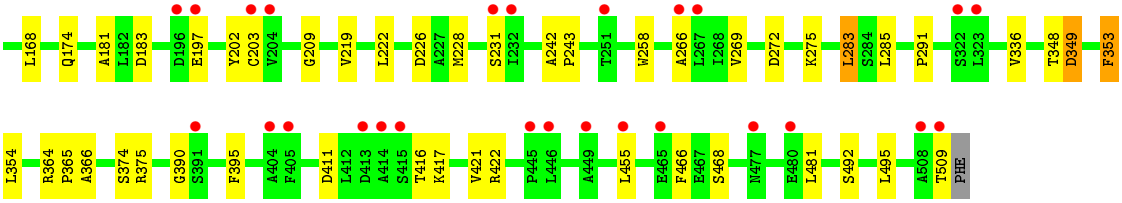
Chain B:



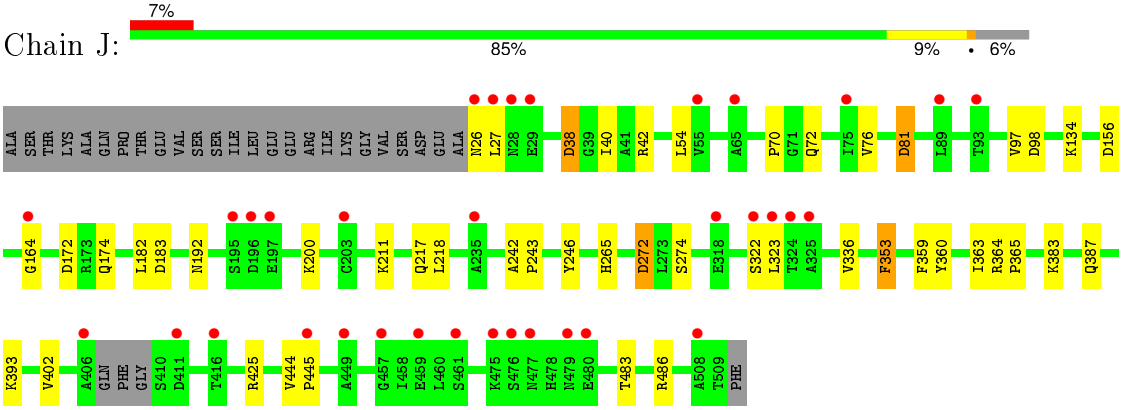
- Molecule 1: ATP synthase alpha chain, mitochondrial

Chain C:

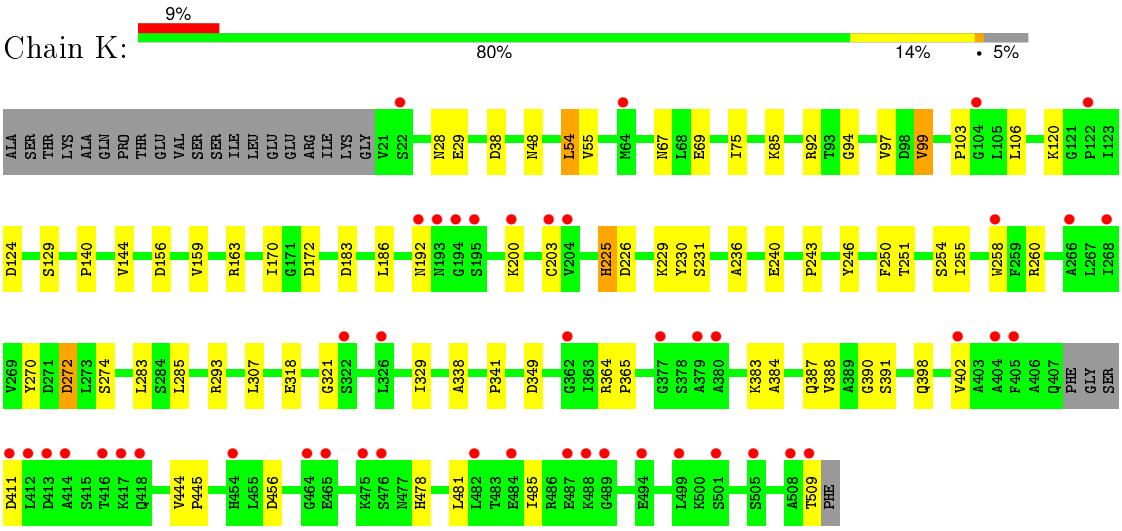




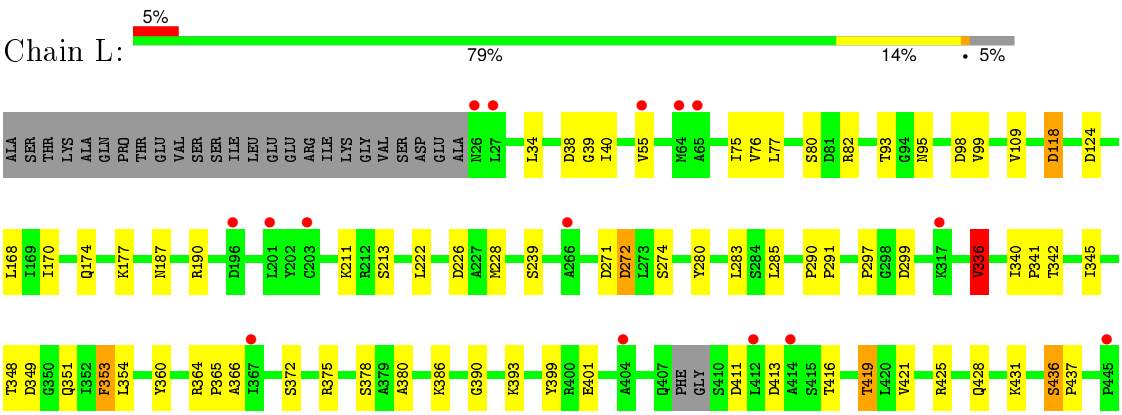
• Molecule 1: ATP synthase alpha chain, mitochondrial

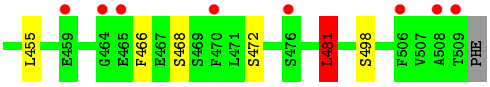


• Molecule 1: ATP synthase alpha chain, mitochondrial



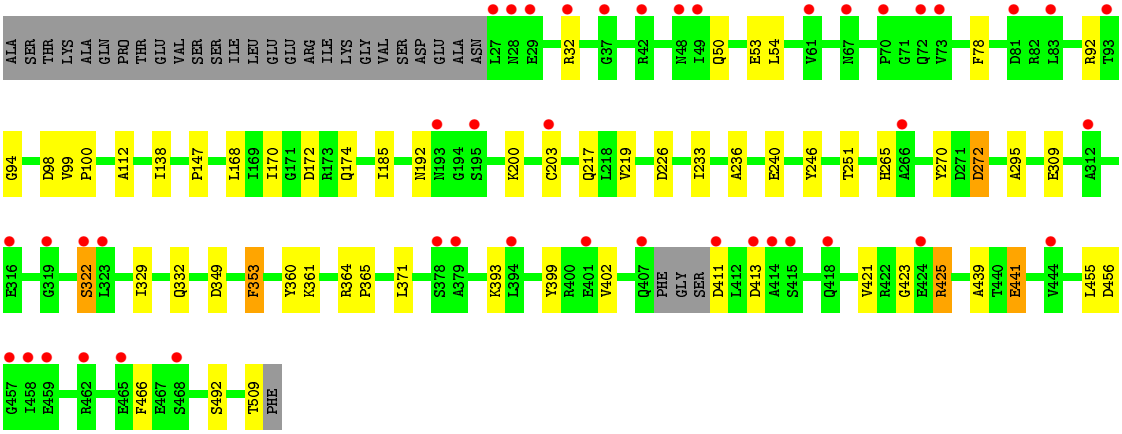
• Molecule 1: ATP synthase alpha chain, mitochondrial





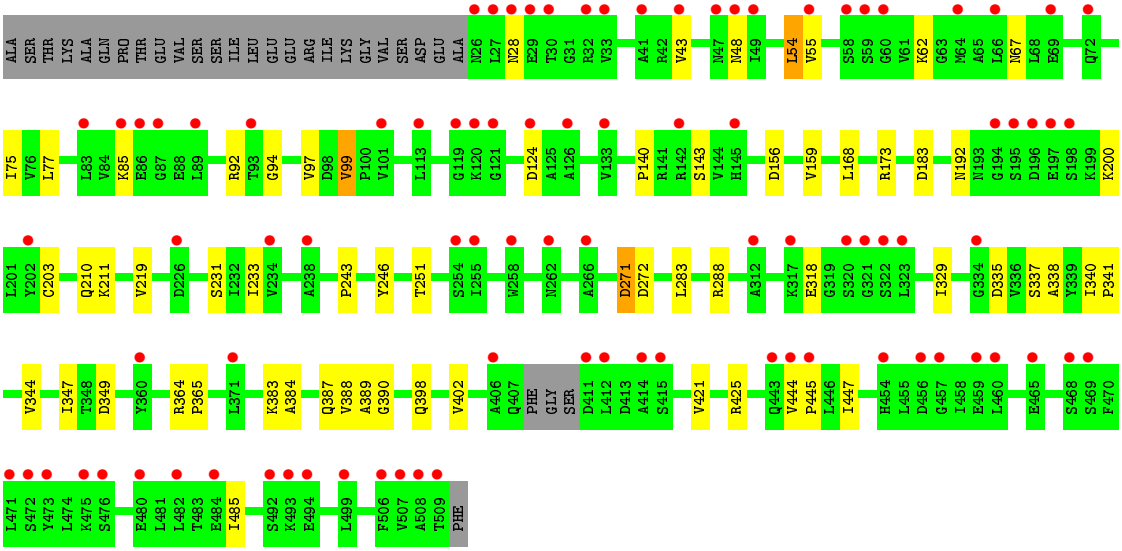
• Molecule 1: ATP synthase alpha chain, mitochondrial

Chain S:



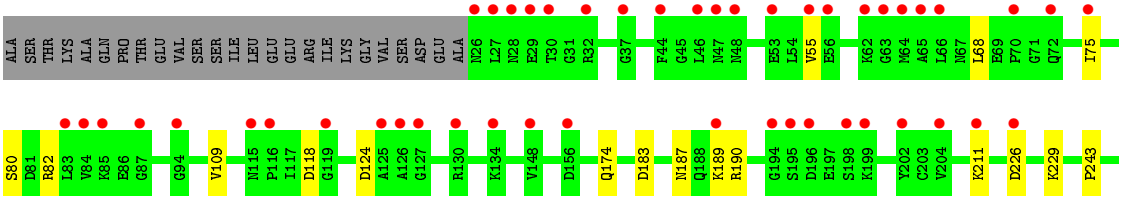
• Molecule 1: ATP synthase alpha chain, mitochondrial

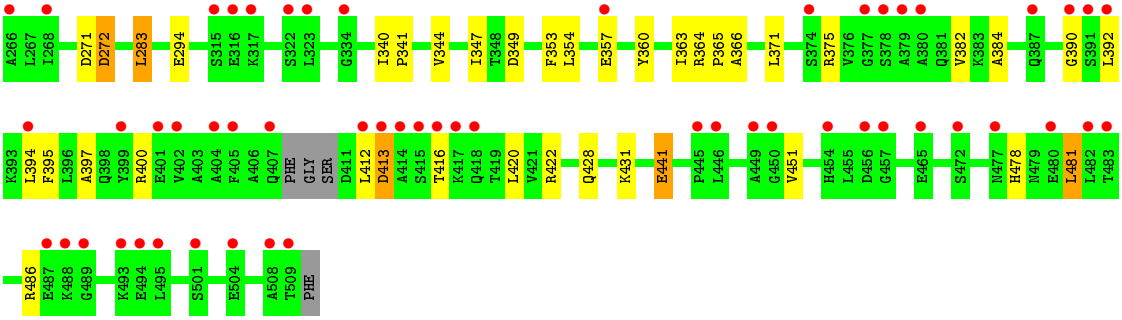
Chain T:



• Molecule 1: ATP synthase alpha chain, mitochondrial

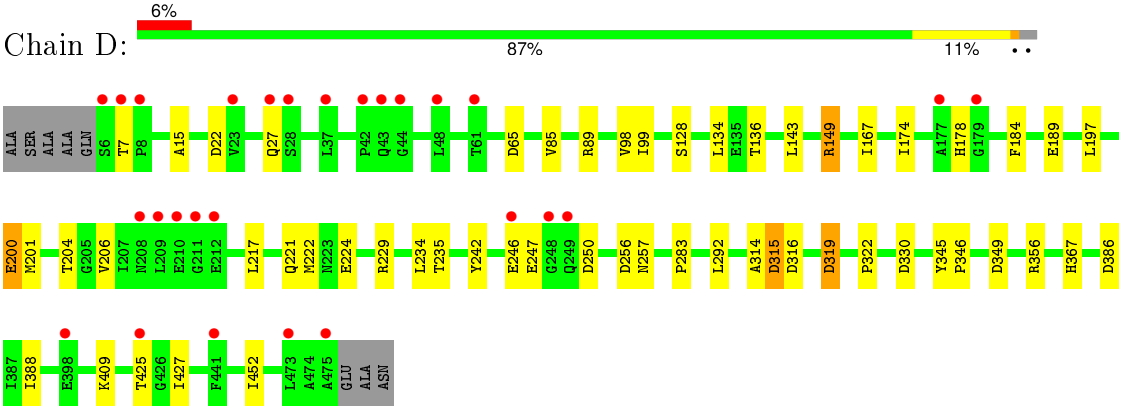
Chain U:





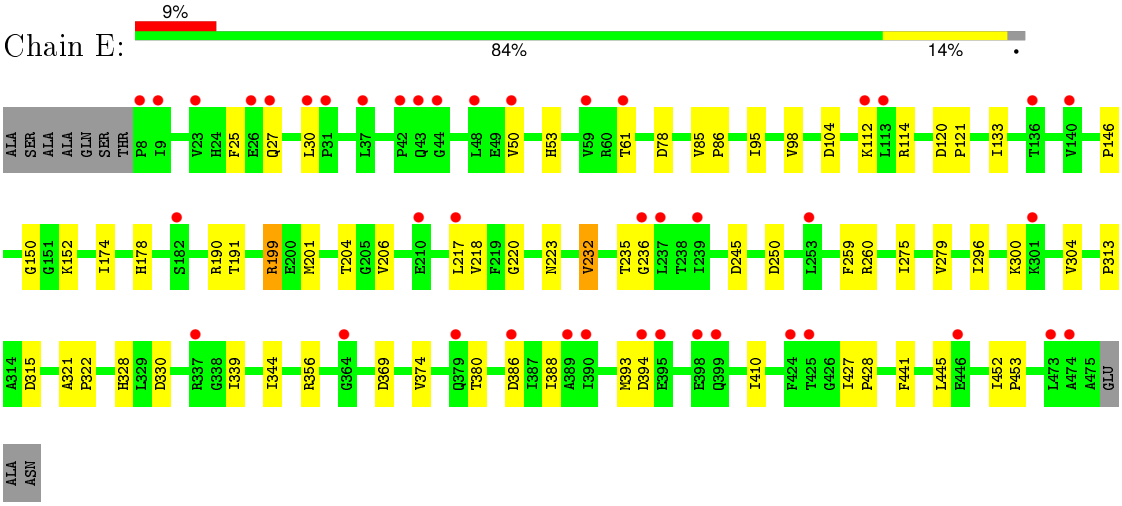
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain D:



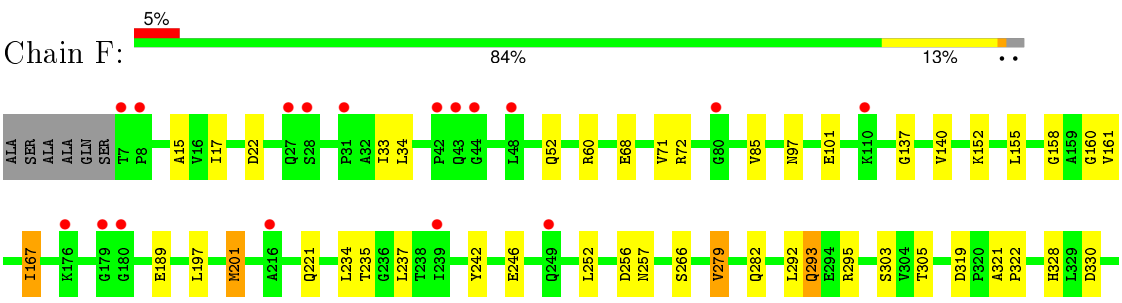
• Molecule 2: ATP synthase beta chain, mitochondrial

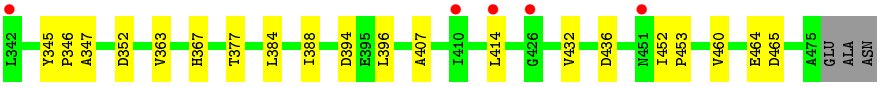
Chain E:



• Molecule 2: ATP synthase beta chain, mitochondrial

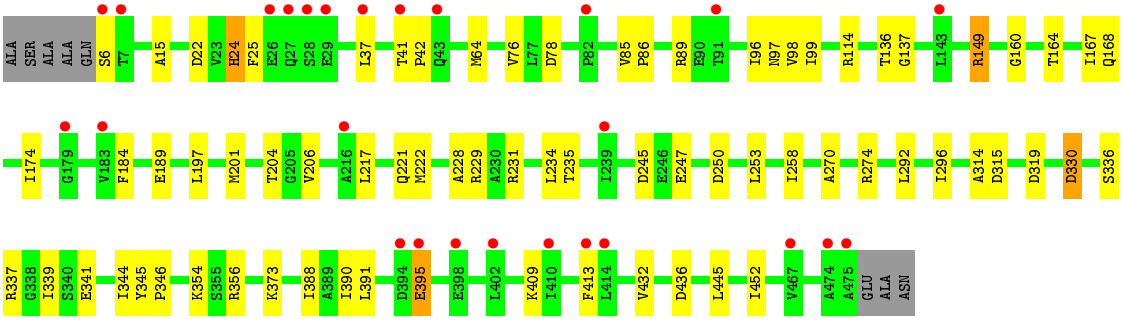
Chain F:





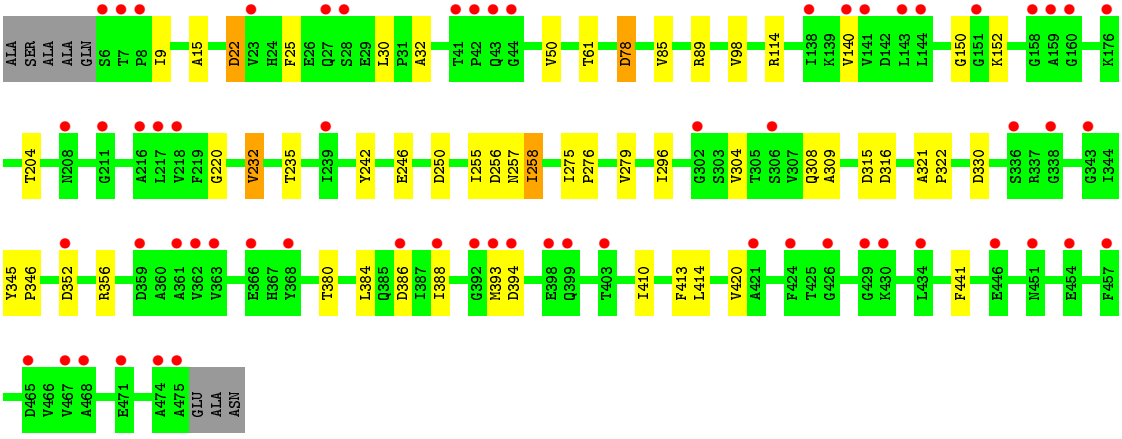
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain M:



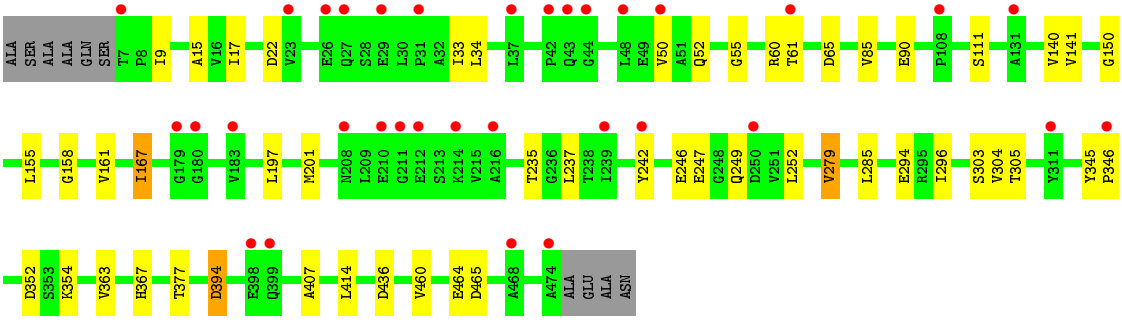
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain N:



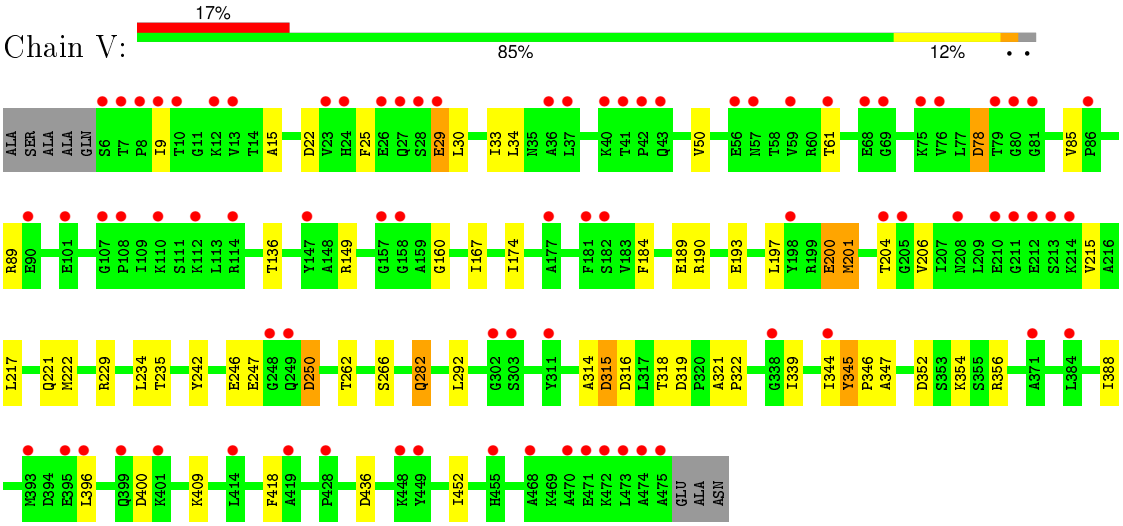
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain O:



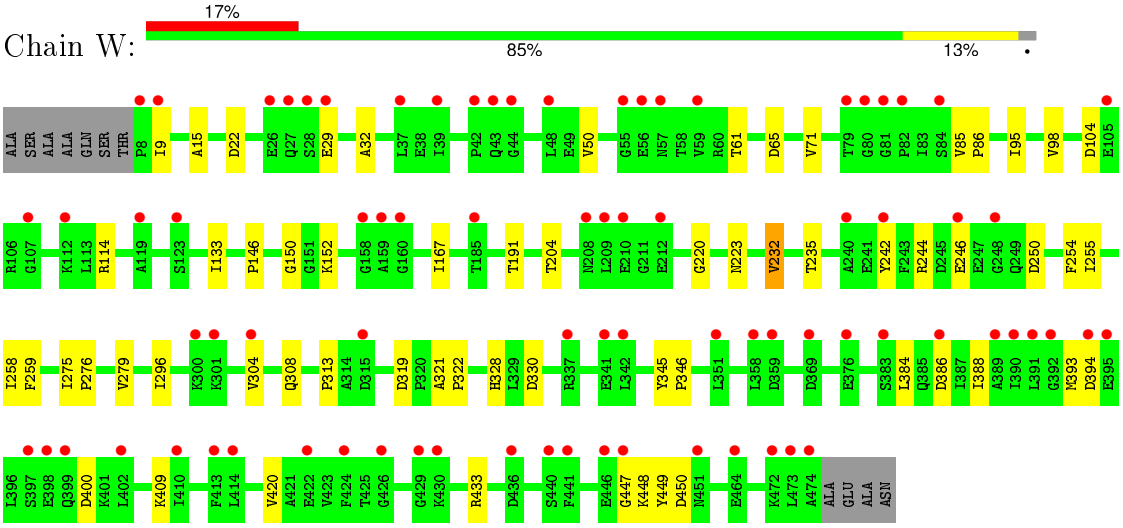
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain V:



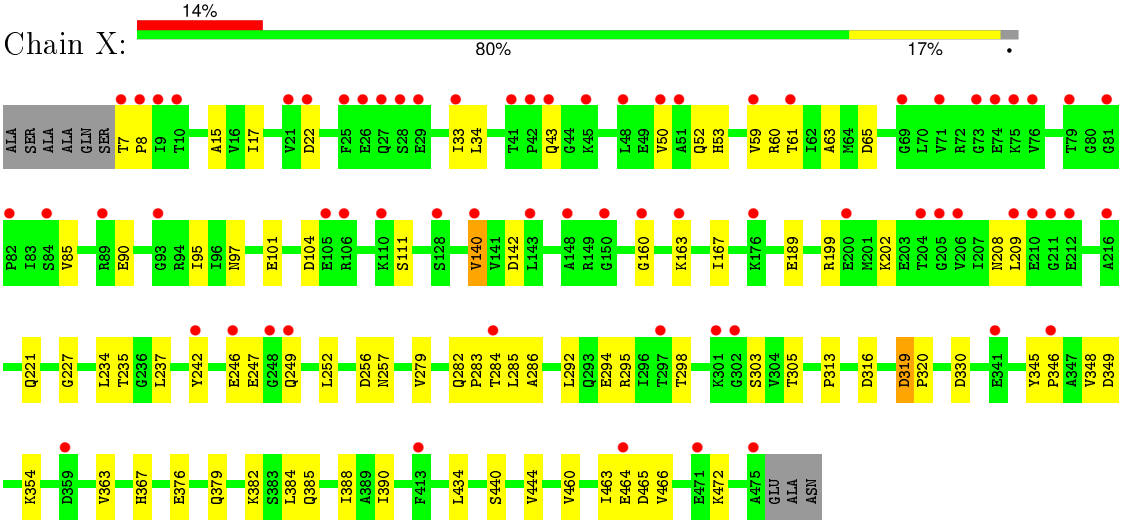
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain W:

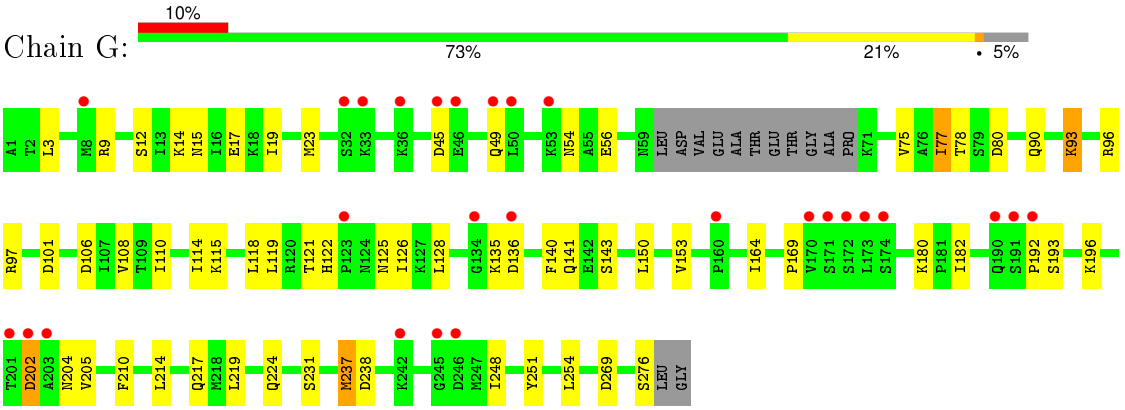


• Molecule 2: ATP synthase beta chain, mitochondrial

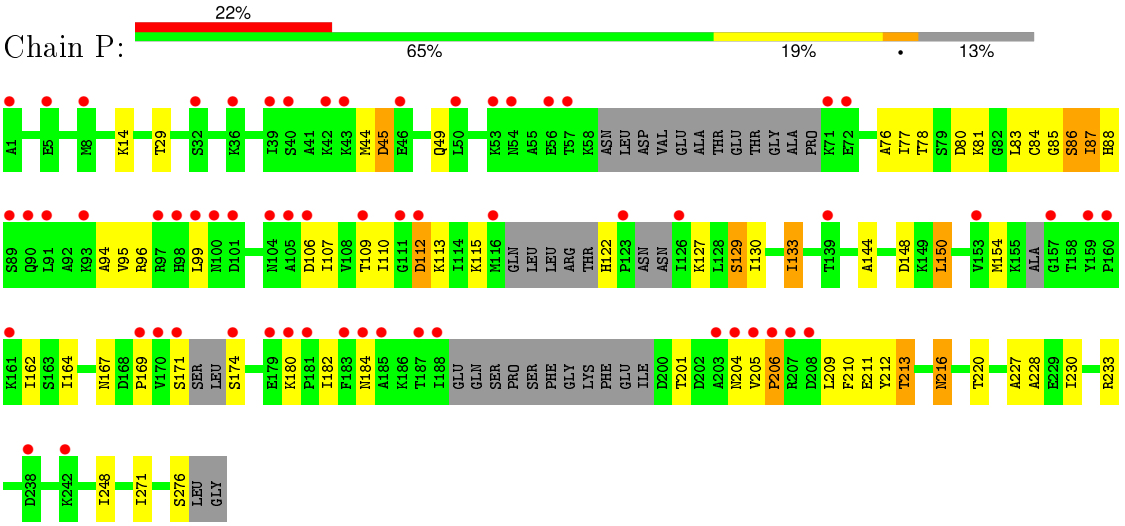
Chain X:



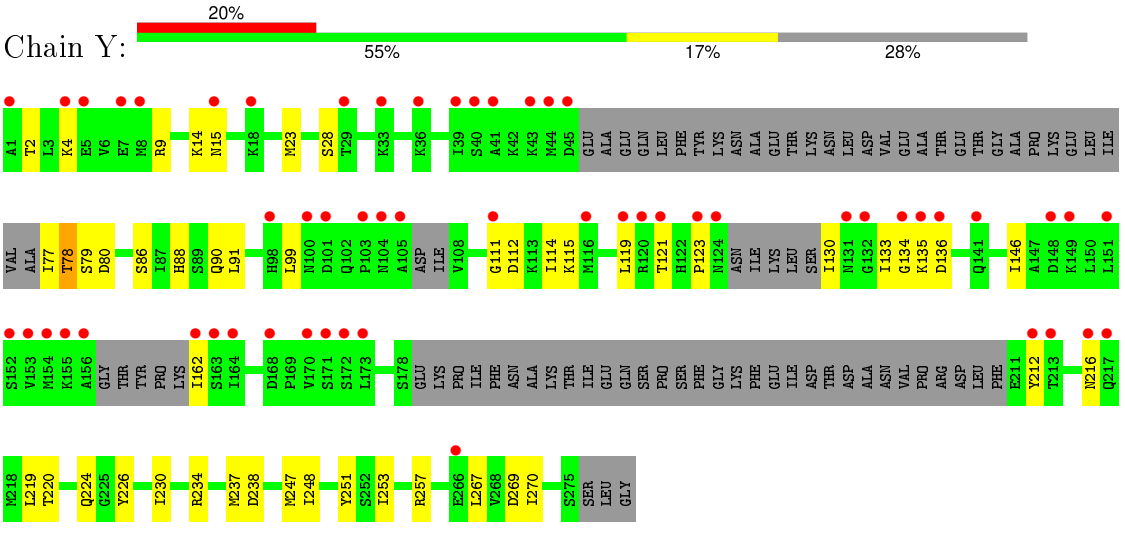
• Molecule 3: ATP synthase gamma chain, mitochondrial



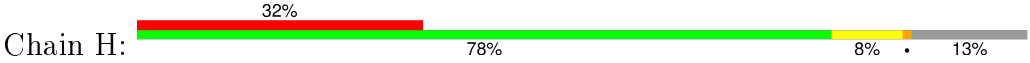
• Molecule 3: ATP synthase gamma chain, mitochondrial

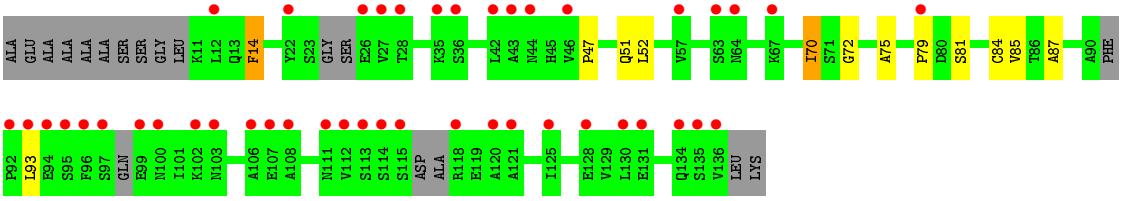


• Molecule 3: ATP synthase gamma chain, mitochondrial



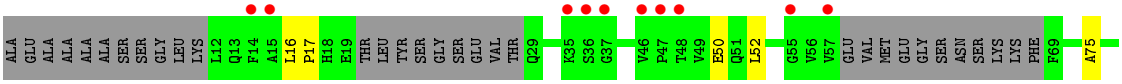
• Molecule 4: ATP synthase delta chain, mitochondrial

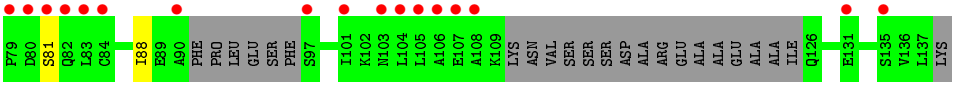




• Molecule 4: ATP synthase delta chain, mitochondrial

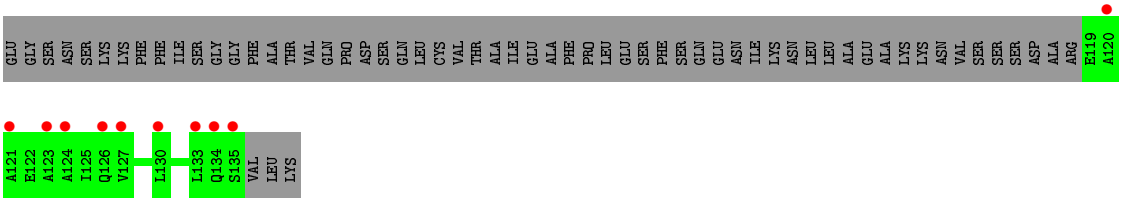
Chain Q:





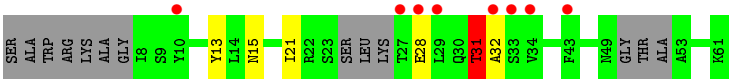
• Molecule 4: ATP synthase delta chain, mitochondrial

Chain Z:



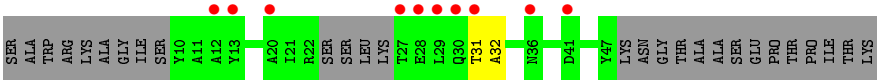
• Molecule 5: ATP synthase epsilon chain, mitochondrial

Chain I:



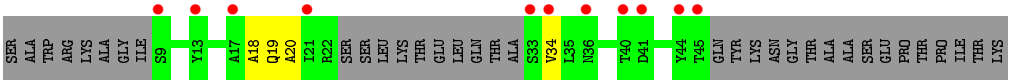
• Molecule 5: ATP synthase epsilon chain, mitochondrial

Chain R:



• Molecule 5: ATP synthase epsilon chain, mitochondrial

Chain 1:


SER
ALA
TRP
ARG
LYS
ALA
GLY
ILE
S9
Y13
A17
A18
Q19
A20
I21
R22
SER
SER
LEU
LYS
THR
GLU
LEU
GLN
THR
ALA
S33
V34
L35
N36
T40
D41
Y44
T45
GLN
TYR
LYS
ASN
GLY
THR
ALA
ALA
SER
GLU
PRO
THR
PRO
ILE
THR
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.52Å 294.13Å 190.43Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.80) 99.9 (19.99-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.244 0.211 , 0.244	Depositor DCC
R_{free} test set	5938 reflections (2.07%)	DCC
Wilson B-factor (Å^2)	72.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 80.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 292845 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	72841	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.64	0/3718	0.79	6/5032 (0.1%)
1	B	0.57	0/3723	0.76	6/5039 (0.1%)
1	C	0.57	0/3729	0.76	5/5048 (0.1%)
1	J	0.55	0/3709	0.74	7/5020 (0.1%)
1	K	0.46	0/3738	0.69	9/5060 (0.2%)
1	L	0.62	1/3718 (0.0%)	0.81	13/5032 (0.3%)
1	S	0.47	0/3705	0.72	8/5014 (0.2%)
1	T	0.38	0/3713	0.64	5/5025 (0.1%)
1	U	0.41	0/3713	0.68	6/5025 (0.1%)
2	D	0.57	0/3605	0.81	9/4889 (0.2%)
2	E	0.56	0/3592	0.76	10/4870 (0.2%)
2	F	0.54	0/3599	0.78	5/4881 (0.1%)
2	M	0.55	0/3605	0.80	5/4889 (0.1%)
2	N	0.48	0/3605	0.74	7/4889 (0.1%)
2	O	0.50	0/3594	0.75	4/4874 (0.1%)
2	V	0.43	0/3605	0.75	8/4889 (0.2%)
2	W	0.40	0/3587	0.69	6/4863 (0.1%)
2	X	0.42	0/3599	0.70	5/4881 (0.1%)
3	G	0.48	0/2056	0.74	6/2767 (0.2%)
3	P	0.47	0/1868	0.70	2/2508 (0.1%)
3	Y	0.37	0/1527	0.63	2/2048 (0.1%)
4	H	0.47	0/766	0.64	0/1051
4	Q	0.41	0/434	0.55	0/595
4	Z	0.42	0/84	0.51	0/116
5	1	0.38	0/133	0.44	0/183
5	I	0.55	0/326	0.69	0/445
5	R	0.45	0/168	0.51	0/232
All	All	0.51	1/73219 (0.0%)	0.74	134/99165 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	1
2	D	0	1
2	V	0	1
2	W	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	353	PHE	CB-CG	-5.87	1.41	1.51

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	345	TYR	C-N-CD	-13.32	91.28	120.60
2	D	22	ASP	CB-CG-OD2	10.23	127.51	118.30
2	F	436	ASP	CB-CG-OD2	7.85	125.37	118.30
1	C	283	LEU	CA-CB-CG	7.74	133.09	115.30
2	M	319	ASP	CB-CG-OD2	7.57	125.11	118.30
2	D	319	ASP	CB-CG-OD2	7.38	124.94	118.30
1	L	283	LEU	CA-CB-CG	7.33	132.15	115.30
1	L	124	ASP	CB-CG-OD2	6.89	124.50	118.30
1	K	38	ASP	CB-CG-OD2	6.85	124.47	118.30
1	C	272	ASP	CB-CG-OD2	6.65	124.29	118.30
1	C	183	ASP	CB-CG-OD2	6.65	124.28	118.30
1	L	353	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	L	38	ASP	CB-CG-OD2	6.57	124.22	118.30
2	E	199	ARG	NE-CZ-NH1	-6.45	117.07	120.30
1	J	38	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	81	ASP	CB-CG-OD2	6.30	123.97	118.30
2	F	330	ASP	CB-CG-OD2	6.29	123.97	118.30
2	X	319	ASP	CB-CG-OD2	6.28	123.95	118.30
1	U	183	ASP	CB-CG-OD2	6.20	123.88	118.30
2	X	349	ASP	CB-CG-OD2	6.12	123.81	118.30
2	V	319	ASP	CB-CG-OD2	6.09	123.79	118.30
1	C	226	ASP	CB-CG-OD2	6.04	123.73	118.30
2	O	65	ASP	CB-CG-OD2	6.01	123.71	118.30
3	P	148	ASP	CB-CG-OD1	5.98	123.68	118.30
1	T	272	ASP	CB-CG-OD2	5.94	123.64	118.30
1	B	272	ASP	CB-CG-OD2	5.94	123.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	118	ASP	CB-CG-OD2	5.90	123.61	118.30
1	S	349	ASP	CB-CG-OD2	5.88	123.60	118.30
2	V	352	ASP	CB-CG-OD2	5.88	123.59	118.30
1	L	336	VAL	CB-CA-C	-5.88	100.23	111.40
2	F	352	ASP	CB-CG-OD2	5.86	123.57	118.30
2	N	250	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	118	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	98	ASP	CB-CG-OD2	5.77	123.50	118.30
1	U	283	LEU	CA-CB-CG	5.77	128.57	115.30
2	F	394	ASP	CB-CG-OD2	5.77	123.49	118.30
2	O	436	ASP	CB-CG-OD2	5.75	123.48	118.30
3	G	238	ASP	CB-CG-OD2	5.75	123.47	118.30
2	M	245	ASP	CB-CG-OD2	5.72	123.45	118.30
1	L	226	ASP	CB-CG-OD2	5.68	123.41	118.30
1	J	98	ASP	CB-CG-OD2	5.66	123.40	118.30
1	B	299	ASP	CB-CG-OD2	5.66	123.39	118.30
2	N	330	ASP	CB-CG-OD2	5.64	123.38	118.30
1	S	172	ASP	CB-CG-OD2	5.64	123.38	118.30
3	G	136	ASP	CB-CG-OD2	5.64	123.37	118.30
1	L	299	ASP	CB-CG-OD2	5.63	123.37	118.30
1	S	411	ASP	CB-CG-OD2	5.62	123.36	118.30
1	S	272	ASP	CB-CG-OD2	5.61	123.35	118.30
1	T	349	ASP	CB-CG-OD2	5.60	123.34	118.30
1	J	156	ASP	CB-CG-OD2	5.60	123.34	118.30
2	M	330	ASP	CB-CG-OD2	5.60	123.34	118.30
2	E	250	ASP	CB-CG-OD2	5.59	123.33	118.30
2	D	349	ASP	CB-CG-OD2	5.59	123.33	118.30
1	U	272	ASP	CB-CG-OD2	5.59	123.33	118.30
1	L	272	ASP	CB-CG-OD2	5.58	123.32	118.30
3	G	80	ASP	CB-CG-OD2	5.58	123.32	118.30
2	O	394	ASP	CB-CG-OD2	5.53	123.28	118.30
2	E	245	ASP	CB-CG-OD2	5.53	123.28	118.30
3	P	45	ASP	CB-CG-OD2	5.52	123.27	118.30
1	K	272	ASP	CB-CG-OD2	5.51	123.26	118.30
1	S	413	ASP	CB-CG-OD2	5.51	123.26	118.30
2	D	315	ASP	CB-CG-OD2	5.50	123.25	118.30
2	N	386	ASP	CB-CG-OD2	5.50	123.25	118.30
1	T	271	ASP	CB-CG-OD2	5.50	123.25	118.30
1	L	98	ASP	CB-CG-OD2	5.50	123.25	118.30
2	D	386	ASP	CB-CG-OD2	5.49	123.25	118.30
2	E	330	ASP	CB-CG-OD2	5.49	123.24	118.30
2	W	330	ASP	CB-CG-OD2	5.49	123.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	349	ASP	CB-CG-OD2	5.49	123.24	118.30
3	Y	238	ASP	CB-CG-OD2	5.49	123.24	118.30
2	O	352	ASP	CB-CG-OD2	5.48	123.23	118.30
2	X	330	ASP	CB-CG-OD2	5.47	123.23	118.30
2	F	319	ASP	CB-CG-OD2	5.46	123.21	118.30
2	W	319	ASP	CB-CG-OD2	5.45	123.21	118.30
1	K	156	ASP	CB-CG-OD2	5.45	123.20	118.30
2	N	316	ASP	CB-CG-OD2	5.44	123.20	118.30
2	X	65	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	183	ASP	CB-CG-OD2	5.43	123.19	118.30
2	V	78	ASP	CB-CG-OD2	5.42	123.18	118.30
1	L	271	ASP	CB-CG-OD2	5.38	123.15	118.30
1	K	411	ASP	CB-CG-OD2	5.38	123.14	118.30
2	E	386	ASP	CB-CG-OD2	5.38	123.14	118.30
1	S	456	ASP	CB-CG-OD2	5.38	123.14	118.30
2	E	199	ARG	NE-CZ-NH2	5.37	122.99	120.30
2	E	315	ASP	CB-CG-OD2	5.37	123.13	118.30
1	S	226	ASP	CB-CG-OD2	5.36	123.13	118.30
2	D	22	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	U	349	ASP	CB-CG-OD2	5.35	123.12	118.30
2	W	400	ASP	CB-CG-OD2	5.35	123.11	118.30
2	E	78	ASP	CB-CG-OD2	5.34	123.11	118.30
1	K	456	ASP	CB-CG-OD2	5.33	123.09	118.30
1	L	481	LEU	CA-CB-CG	5.31	127.52	115.30
2	W	65	ASP	CB-CG-OD2	5.29	123.06	118.30
2	E	104	ASP	CB-CG-OD2	5.29	123.06	118.30
2	D	330	ASP	CB-CG-OD2	5.28	123.05	118.30
3	G	106	ASP	CB-CG-OD2	5.28	123.05	118.30
1	J	272	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	98	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	456	ASP	CB-CG-OD2	5.25	123.02	118.30
1	U	124	ASP	CB-CG-OD2	5.24	123.02	118.30
3	G	101	ASP	CB-CG-OD2	5.22	123.00	118.30
2	W	386	ASP	CB-CG-OD2	5.21	122.99	118.30
2	M	78	ASP	CB-CG-OD2	5.21	122.98	118.30
1	L	411	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	226	ASP	CB-CG-OD2	5.19	122.97	118.30
1	K	226	ASP	CB-CG-OD2	5.18	122.96	118.30
3	Y	136	ASP	CB-CG-OD2	5.17	122.96	118.30
2	X	316	ASP	CB-CG-OD2	5.16	122.94	118.30
1	T	156	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	411	ASP	CB-CG-OD2	5.15	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	316	ASP	CB-CG-OD2	5.12	122.91	118.30
1	J	183	ASP	CB-CG-OD2	5.12	122.91	118.30
1	K	349	ASP	CB-CG-OD2	5.12	122.91	118.30
2	M	436	ASP	CB-CG-OD2	5.12	122.90	118.30
1	J	172	ASP	CB-CG-OD2	5.11	122.90	118.30
2	V	316	ASP	CB-CG-OD2	5.10	122.89	118.30
2	N	315	ASP	CB-CG-OD2	5.09	122.89	118.30
1	S	98	ASP	CB-CG-OD2	5.09	122.89	118.30
2	V	250	ASP	CB-CG-OD2	5.09	122.88	118.30
1	U	413	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	124	ASP	CB-CG-OD2	5.07	122.87	118.30
2	V	436	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	411	ASP	CB-CG-OD2	5.07	122.86	118.30
2	N	78	ASP	CB-CG-OD2	5.07	122.86	118.30
1	K	172	ASP	CB-CG-OD2	5.06	122.86	118.30
3	G	269	ASP	CB-CG-OD2	5.06	122.86	118.30
1	K	124	ASP	CB-CG-OD2	5.04	122.83	118.30
1	T	124	ASP	CB-CG-OD2	5.04	122.83	118.30
1	J	81	ASP	CB-CG-OD2	5.03	122.83	118.30
2	E	369	ASP	CB-CG-OD2	5.02	122.82	118.30
2	W	250	ASP	CB-CG-OD2	5.02	122.82	118.30
2	D	65	ASP	CB-CG-OD2	5.02	122.81	118.30
2	V	315	ASP	CB-CG-OD2	5.01	122.81	118.30
2	N	22	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	7	THR	Peptide
1	S	147	PRO	Peptide
2	V	345	TYR	Peptide
2	W	447	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3748	27	0
1	B	3669	0	3752	40	0
1	C	3674	0	3756	39	0
1	J	3655	0	3739	31	0
1	K	3684	0	3758	43	0
1	L	3664	0	3747	45	0
1	S	3651	0	3740	35	0
1	T	3659	0	3745	35	0
1	U	3659	0	3745	29	0
2	D	3549	0	3620	29	0
2	E	3536	0	3610	39	0
2	F	3543	0	3615	40	0
2	M	3549	0	3620	52	0
2	N	3549	0	3621	33	0
2	O	3538	0	3610	31	0
2	V	3549	0	3620	38	0
2	W	3531	0	3605	37	0
2	X	3543	0	3615	49	0
3	G	2031	0	2084	31	0
3	P	1851	0	1893	39	0
3	Y	1517	0	1561	28	0
4	H	758	0	602	9	0
4	Q	436	0	215	3	0
4	Z	85	0	45	0	0
5	1	135	0	70	1	0
5	I	324	0	249	2	0
5	R	170	0	87	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	O	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
6	U	1	0	0	0	0
6	V	1	0	0	0	0
6	X	1	0	0	0	0
7	N	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	31	0	13	0	0
8	B	31	0	13	0	0
8	C	31	0	13	1	0
8	D	31	0	13	0	0
8	F	31	0	13	2	0
8	J	31	0	13	0	0
8	K	31	0	13	1	0
8	L	31	0	13	1	0
8	M	31	0	13	6	0
8	O	31	0	13	0	0
8	S	31	0	13	1	0
8	T	31	0	13	0	0
8	U	31	0	13	0	0
8	V	31	0	13	3	0
8	X	31	0	13	4	0
9	A	26	0	0	2	0
9	B	18	0	0	0	0
9	C	13	0	0	0	0
9	D	20	0	0	0	0
9	E	13	0	0	1	0
9	F	11	0	0	0	0
9	G	3	0	0	0	0
9	J	17	0	0	0	0
9	K	4	0	0	0	0
9	L	19	0	0	0	0
9	M	9	0	0	0	0
9	N	8	0	0	0	0
9	O	7	0	0	0	0
9	P	2	0	0	0	0
9	Q	1	0	0	2	0
9	S	6	0	0	0	0
9	T	1	0	0	0	0
9	U	3	0	0	0	0
9	X	2	0	0	0	0
All	All	72841	0	73267	728	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 5.

All (728) 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:V:85:VAL:HG11	2:V:235:THR:HG23	1.26	1.16
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.27	1.12
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.28	1.11
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.25	1.11
3:G:96:ARG:HE	3:G:121:THR:HG21	1.10	1.09
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.19	1.09
1:B:26:ASN:O	1:B:30:THR:HB	1.55	1.06
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.38	1.02
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.39	1.00
4:H:14:PHE:HZ	4:H:70:ILE:HD11	1.28	0.99
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.45	0.98
1:C:336:VAL:HG11	1:C:353:PHE:CZ	1.99	0.97
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.44	0.97
1:J:336:VAL:HG11	1:J:353:PHE:HZ	1.27	0.95
2:M:149:ARG:HH11	2:M:149:ARG:HG2	1.32	0.95
2:D:85:VAL:HG11	2:D:235:THR:CG2	1.99	0.93
2:M:160:GLY:H	8:M:600:ANP:HNB1	1.14	0.91
1:K:99:VAL:HG11	1:K:251:THR:HB	1.50	0.91
2:V:160:GLY:H	8:V:600:ANP:HNB1	1.10	0.91
3:P:88:HIS:HD2	3:P:113:LYS:HB2	1.34	0.90
3:P:88:HIS:CD2	3:P:113:LYS:HB2	2.09	0.88
1:C:336:VAL:HG11	1:C:353:PHE:CE1	2.09	0.87
1:J:336:VAL:HG11	1:J:353:PHE:CZ	2.10	0.87
2:M:85:VAL:HG11	2:M:235:THR:CG2	2.05	0.84
3:P:112:ASP:O	3:P:115:LYS:HB3	1.77	0.84
1:C:242:ALA:HB3	1:C:243:PRO:HD3	1.58	0.83
2:D:85:VAL:CG1	2:D:235:THR:HG23	2.08	0.82
1:B:67:ASN:HB2	2:F:17:ILE:HG12	1.61	0.82
2:X:160:GLY:H	8:X:600:ANP:HNB1	1.28	0.82
2:F:52:GLN:HE21	2:F:60:ARG:HD2	1.44	0.81
2:N:242:TYR:CE1	2:N:246:GLU:HG3	2.16	0.81
3:G:96:ARG:NE	3:G:121:THR:HG21	1.95	0.81
2:M:149:ARG:HH11	2:M:149:ARG:CG	1.95	0.79
1:S:265:HIS:ND1	1:S:322:SER:HB2	1.98	0.78
1:U:68:LEU:O	2:V:15:ALA:HA	1.85	0.77
4:H:14:PHE:CZ	4:H:70:ILE:HD11	2.19	0.76
3:G:45:ASP:O	3:G:49:GLN:HB2	1.86	0.75
4:Q:75:ALA:HB2	9:Q:802:HOH:O	1.87	0.74
1:S:112:ALA:O	1:S:251:THR:HG21	1.87	0.74
1:K:67:ASN:HB2	2:O:17:ILE:HG12	1.67	0.74
1:K:236:ALA:HA	1:K:240:GLU:OE1	1.87	0.74
3:P:76:ALA:O	3:P:109:THR:HA	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:234:LEU:HD23	2:M:292:LEU:HD13	1.69	0.73
1:L:170:ILE:HG23	1:L:353:PHE:HD1	1.53	0.73
2:V:346:PRO:HG3	2:V:418:PHE:CZ	2.24	0.73
1:S:425:ARG:CG	1:S:425:ARG:HH11	2.01	0.73
1:C:336:VAL:HG11	1:C:353:PHE:HZ	1.51	0.72
2:W:220:GLY:HA3	2:W:232:VAL:HG11	1.71	0.72
3:Y:133:ILE:HD12	3:Y:134:GLY:H	1.54	0.72
1:B:243:PRO:HG3	1:B:283:LEU:HD21	1.72	0.72
3:G:122:HIS:HB3	3:G:125:ASN:HD22	1.56	0.71
2:M:189:GLU:O	2:M:221:GLN:HB3	1.91	0.71
1:L:174:GLN:HA	8:L:600:ANP:HNB1	1.56	0.70
2:W:242:TYR:CE1	2:W:246:GLU:HG3	2.27	0.70
1:T:99:VAL:HG11	1:T:251:THR:HB	1.73	0.70
2:E:85:VAL:HG11	2:E:235:THR:CG2	2.17	0.69
2:M:85:VAL:CG1	2:M:235:THR:HG23	2.10	0.69
1:K:106:LEU:HD23	1:K:230:TYR:HA	1.73	0.69
2:D:234:LEU:HD23	2:D:292:LEU:HD13	1.75	0.68
1:A:272:ASP:OD1	1:A:274:SER:HB2	1.93	0.68
3:P:205:VAL:N	3:P:206:PRO:HD3	2.08	0.68
9:A:825:HOH:O	2:E:260:ARG:HD3	1.94	0.68
1:J:336:VAL:CG1	1:J:353:PHE:HZ	2.04	0.68
1:K:54:LEU:HD12	1:K:97:VAL:HA	1.76	0.68
3:G:96:ARG:HE	3:G:121:THR:CG2	1.99	0.67
2:V:346:PRO:O	2:V:347:ALA:HB3	1.93	0.67
4:H:14:PHE:HZ	4:H:70:ILE:CD1	2.04	0.67
1:S:425:ARG:HG3	1:S:425:ARG:HH11	1.58	0.67
1:A:506:PHE:O	1:A:509:THR:HG22	1.95	0.67
1:C:40:ILE:CD1	1:C:76:VAL:HG12	2.25	0.67
3:P:184:ASN:HA	3:P:210:PHE:CE1	2.30	0.67
3:P:88:HIS:HD2	3:P:113:LYS:CB	2.07	0.66
2:X:252:LEU:HD23	2:X:305:THR:HB	1.77	0.66
1:S:217:GLN:OE1	2:V:356:ARG:NH2	2.29	0.66
2:N:98:VAL:HB	2:N:232:VAL:HG13	1.76	0.66
1:J:265:HIS:ND1	1:J:322:SER:HB2	2.11	0.65
2:D:197:LEU:O	2:D:201:MET:HG2	1.95	0.65
1:A:265:HIS:ND1	1:A:322:SER:HB3	2.11	0.65
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.79	0.65
2:V:85:VAL:CG1	2:V:235:THR:HG23	2.17	0.65
1:K:243:PRO:HG3	1:K:283:LEU:HD21	1.79	0.65
3:P:110:ILE:HG22	3:P:133:ILE:HD13	1.78	0.65
3:Y:2:THR:HG22	3:Y:4:LYS:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:14:LYS:HA	3:Y:248:ILE:HD11	1.79	0.64
2:M:89:ARG:NH1	2:M:247:GLU:OE2	2.30	0.64
1:B:285:LEU:HD22	2:E:275:ILE:HG22	1.80	0.64
1:T:243:PRO:HG3	1:T:283:LEU:HD21	1.79	0.64
2:N:85:VAL:CG1	2:N:235:THR:HG23	2.17	0.64
1:C:174:GLN:HA	8:C:600:ANP:HNB1	1.62	0.64
2:N:85:VAL:HG11	2:N:235:THR:CG2	2.17	0.64
2:M:160:GLY:N	8:M:600:ANP:HNB1	1.92	0.64
1:B:99:VAL:HG11	1:B:251:THR:HB	1.80	0.64
3:P:45:ASP:O	3:P:49:GLN:HB2	1.97	0.64
1:U:55:VAL:HG21	1:U:75:ILE:HD13	1.78	0.63
2:D:409:LYS:NZ	2:D:452:ILE:O	2.31	0.63
1:J:425:ARG:HG3	1:J:425:ARG:HH11	1.63	0.63
1:S:455:LEU:HD21	1:S:466:PHE:CE2	2.33	0.63
2:N:150:GLY:HA2	2:N:304:VAL:O	1.98	0.63
1:K:390:GLY:O	1:K:391:SER:HB2	1.98	0.63
1:K:444:VAL:HG23	1:K:445:PRO:HD3	1.81	0.63
2:X:463:ILE:O	2:X:466:VAL:HB	1.99	0.63
2:W:50:VAL:HA	2:W:61:THR:HG22	1.81	0.62
2:X:52:GLN:HE21	2:X:60:ARG:HD2	1.63	0.62
1:L:372:SER:O	1:L:393:LYS:NZ	2.26	0.62
1:K:186:LEU:HD13	1:K:225:HIS:HD2	1.63	0.62
2:E:85:VAL:CG1	2:E:235:THR:HG23	2.18	0.62
3:G:193:SER:HB3	3:G:196:LYS:HG3	1.81	0.62
2:W:388:ILE:HD12	2:W:393:MET:HG2	1.81	0.61
2:X:7:THR:HB	2:X:8:PRO:HD2	1.82	0.61
3:Y:77:ILE:N	3:Y:114:ILE:HG21	2.15	0.61
2:O:50:VAL:HA	2:O:61:THR:HG22	1.81	0.61
2:V:234:LEU:HD23	2:V:292:LEU:HD13	1.82	0.61
1:S:425:ARG:HG3	1:S:425:ARG:NH1	2.15	0.61
1:K:444:VAL:CG2	1:K:445:PRO:HD3	2.31	0.61
1:U:80:SER:OG	1:U:82:ARG:HG3	2.01	0.60
3:G:205:VAL:HG22	4:H:51:GLN:HE22	1.66	0.60
1:B:67:ASN:HB2	2:F:17:ILE:CG1	2.30	0.60
3:Y:121:THR:O	3:Y:123:PRO:HD3	2.01	0.60
1:K:186:LEU:HD13	1:K:225:HIS:CD2	2.37	0.60
1:S:439:ALA:HB1	1:S:441:GLU:OE2	2.02	0.60
1:B:140:PRO:HB3	1:B:318:GLU:HG3	1.83	0.60
1:B:55:VAL:HG21	1:B:75:ILE:HD13	1.84	0.60
2:N:388:ILE:HD12	2:N:393:MET:HG2	1.82	0.59
3:P:205:VAL:N	3:P:206:PRO:CD	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:152:LYS:HE3	2:N:296:ILE:HB	1.84	0.59
2:E:86:PRO:HD3	2:E:114:ARG:NH1	2.16	0.59
1:T:28:ASN:HD22	1:T:48:ASN:CG	2.05	0.59
1:L:80:SER:OG	1:L:82:ARG:HG3	2.02	0.59
1:L:170:ILE:HG23	1:L:353:PHE:CD1	2.37	0.59
1:A:164:GLY:HA2	1:A:323:LEU:O	2.03	0.59
2:F:252:LEU:HD23	2:F:305:THR:HB	1.84	0.59
4:H:52:LEU:HD11	4:H:85:VAL:HG13	1.84	0.58
1:U:441:GLU:HG2	1:U:486:ARG:HB2	1.83	0.58
1:K:272:ASP:OD1	1:K:274:SER:HB2	2.03	0.58
2:X:237:LEU:HD21	2:X:295:ARG:HB2	1.85	0.58
3:P:96:ARG:HA	3:P:122:HIS:HE1	1.68	0.58
2:W:86:PRO:HD3	2:W:114:ARG:NH1	2.17	0.58
1:U:397:ALA:HA	1:U:400:ARG:NH2	2.18	0.58
1:U:375:ARG:NH1	8:V:600:ANP:O3G	2.37	0.58
3:Y:133:ILE:HD12	3:Y:134:GLY:N	2.17	0.58
2:F:152:LYS:NZ	2:F:293:GLN:HG3	2.19	0.58
1:L:336:VAL:HG13	1:L:353:PHE:CZ	2.39	0.58
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.85	0.57
1:S:170:ILE:HG23	1:S:353:PHE:CD1	2.38	0.57
3:P:167:ASN:HB2	3:P:228:ALA:CB	2.34	0.57
2:N:50:VAL:HA	2:N:61:THR:HG22	1.85	0.57
3:G:75:VAL:HB	3:G:164:ILE:HD13	1.86	0.57
2:W:220:GLY:CA	2:W:232:VAL:HG11	2.34	0.57
2:N:276:PRO:HD2	3:P:271:ILE:HD11	1.87	0.57
1:L:428:GLN:NE2	1:L:431:LYS:HD2	2.18	0.57
3:G:115:LYS:O	3:G:119:LEU:HB2	2.04	0.57
2:F:363:VAL:HB	2:F:367:HIS:ND1	2.19	0.57
1:S:364:ARG:HA	1:S:365:PRO:C	2.25	0.57
2:F:388:ILE:HD11	2:F:396:LEU:HD21	1.87	0.57
1:A:383:LYS:O	1:A:387:GLN:HG3	2.04	0.57
2:D:184:PHE:HB3	2:D:217:LEU:HD23	1.87	0.57
1:L:336:VAL:CG1	1:L:353:PHE:CZ	2.88	0.56
2:E:388:ILE:HD12	2:E:393:MET:HG2	1.87	0.56
1:L:336:VAL:CG1	1:L:353:PHE:CE1	2.88	0.56
2:X:284:THR:O	2:X:285:LEU:C	2.44	0.56
2:V:160:GLY:N	8:V:600:ANP:HNB1	1.91	0.56
1:J:192:ASN:HA	1:J:200:LYS:HG2	1.88	0.56
2:M:234:LEU:CD2	2:M:292:LEU:HD13	2.35	0.56
2:M:390:ILE:HG22	2:M:391:LEU:HG	1.87	0.55
2:D:204:THR:HB	2:D:206:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:265:HIS:ND1	1:J:322:SER:CB	2.70	0.55
2:E:86:PRO:HD3	2:E:114:ARG:HH12	1.72	0.55
2:X:384:LEU:O	2:X:388:ILE:HG12	2.05	0.55
1:K:192:ASN:HA	1:K:200:LYS:HG2	1.89	0.55
1:A:364:ARG:HA	1:A:365:PRO:C	2.27	0.55
3:G:108:VAL:HG22	3:G:128:LEU:HB3	1.89	0.55
2:V:321:ALA:HB3	2:V:322:PRO:CD	2.37	0.55
1:T:55:VAL:HG21	1:T:75:ILE:HD13	1.88	0.55
1:B:364:ARG:HA	1:B:365:PRO:C	2.27	0.55
3:Y:23:MET:CE	3:Y:23:MET:HA	2.36	0.55
2:V:197:LEU:O	2:V:201:MET:HG3	2.07	0.55
1:A:285:LEU:HD12	2:D:283:PRO:HB3	1.89	0.54
2:V:222:MET:HA	2:V:229:ARG:HD2	1.89	0.54
1:B:54:LEU:HD21	1:B:62:LYS:HD3	1.89	0.54
2:O:52:GLN:NE2	2:O:60:ARG:HD2	2.22	0.54
3:G:9:ARG:HG2	3:G:251:TYR:CE1	2.43	0.54
2:F:293:GLN:HG2	2:F:328:HIS:CG	2.43	0.54
2:V:346:PRO:O	2:V:347:ALA:CB	2.56	0.54
3:Y:79:SER:HB3	3:Y:88:HIS:HE1	1.73	0.54
2:V:409:LYS:NZ	2:V:452:ILE:O	2.28	0.54
2:E:152:LYS:HE3	2:E:296:ILE:HB	1.89	0.54
1:L:285:LEU:HD21	1:L:291:PRO:HB3	1.89	0.54
1:T:444:VAL:CG2	1:T:445:PRO:HD3	2.38	0.54
1:C:364:ARG:HA	1:C:365:PRO:C	2.27	0.54
3:P:171:SER:HG	3:P:174:SER:N	2.06	0.54
1:T:67:ASN:HB2	2:X:17:ILE:HG12	1.90	0.54
1:J:383:LYS:O	1:J:387:GLN:HG3	2.08	0.53
2:O:252:LEU:HD23	2:O:305:THR:HB	1.89	0.53
1:L:109:VAL:HB	1:L:118:ASP:HB3	1.90	0.53
1:U:294:GLU:N	3:Y:269:ASP:OD2	2.37	0.53
2:X:234:LEU:HD23	2:X:292:LEU:HD13	1.90	0.53
2:W:242:TYR:CZ	2:W:246:GLU:HG3	2.43	0.53
3:P:95:VAL:O	3:P:99:LEU:HB2	2.09	0.53
2:F:97:ASN:HB2	2:F:101:GLU:H	1.73	0.53
1:K:29:GLU:HA	1:K:92:ARG:HD3	1.90	0.53
2:W:86:PRO:HD3	2:W:114:ARG:HH12	1.73	0.53
2:E:25:PHE:HB2	2:E:30:LEU:HD23	1.91	0.53
2:O:15:ALA:HB3	2:O:22:ASP:HB2	1.91	0.52
1:B:192:ASN:HA	1:B:200:LYS:HG2	1.91	0.52
2:E:98:VAL:HB	2:E:232:VAL:HG13	1.91	0.52
2:N:220:GLY:HA3	2:N:232:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:200:GLU:OE1	2:V:200:GLU:HA	2.09	0.52
1:A:54:LEU:HD11	1:A:78:PHE:HE2	1.73	0.52
2:V:204:THR:HB	2:V:206:VAL:HG23	1.92	0.52
1:T:288:ARG:HH12	2:W:275:ILE:HD11	1.74	0.52
3:Y:79:SER:OG	3:Y:80:ASP:N	2.37	0.52
1:K:364:ARG:HA	1:K:365:PRO:C	2.30	0.52
2:E:50:VAL:HA	2:E:61:THR:HG22	1.92	0.52
2:V:25:PHE:HB2	2:V:30:LEU:HD23	1.92	0.52
1:A:402:VAL:HG12	1:A:402:VAL:O	2.09	0.52
1:T:192:ASN:HA	1:T:200:LYS:HG2	1.91	0.52
1:B:111:ASP:OD2	1:B:115:ASN:HB2	2.09	0.52
1:U:441:GLU:CG	1:U:486:ARG:HB2	2.40	0.52
3:P:106:ASP:HB3	3:P:127:LYS:HG3	1.91	0.52
2:E:339:ILE:HG22	2:E:344:ILE:HB	1.92	0.51
2:D:134:LEU:HD13	2:D:149:ARG:HH11	1.75	0.51
1:J:272:ASP:OD1	1:J:274:SER:HB2	2.10	0.51
2:X:7:THR:HB	2:X:8:PRO:CD	2.39	0.51
2:E:300:LYS:HG3	9:E:814:HOH:O	2.10	0.51
2:O:279:VAL:HG12	2:O:279:VAL:O	2.10	0.51
3:G:14:LYS:HA	3:G:248:ILE:HD11	1.92	0.51
2:M:391:LEU:HD22	3:P:83:LEU:HD13	1.92	0.51
2:X:460:VAL:HB	2:X:465:ASP:HB3	1.92	0.51
2:O:242:TYR:CE1	2:O:246:GLU:HG3	2.45	0.51
1:T:203:CYS:HB2	1:T:231:SER:HB3	1.92	0.51
1:K:398:GLN:O	1:K:402:VAL:HG23	2.11	0.51
2:F:293:GLN:HG2	2:F:328:HIS:CB	2.41	0.51
1:S:399:TYR:CD1	1:S:423:GLY:HA3	2.45	0.51
1:C:68:LEU:O	2:D:15:ALA:HA	2.11	0.51
1:K:144:VAL:HG12	1:K:163:ARG:O	2.11	0.51
2:M:86:PRO:HD3	2:M:114:ARG:NH1	2.26	0.51
2:V:266:SER:HB2	2:V:282:GLN:HE21	1.75	0.51
3:Y:226:TYR:O	3:Y:230:ILE:HG12	2.10	0.51
1:C:395:PHE:CZ	1:C:422:ARG:HB3	2.45	0.51
1:C:336:VAL:HG11	1:C:353:PHE:HE1	1.72	0.51
1:T:444:VAL:HG23	1:T:445:PRO:HD3	1.93	0.51
3:P:212:TYR:O	3:P:216:ASN:HB2	2.11	0.51
1:B:338:ALA:HB3	1:B:341:PRO:HG2	1.92	0.51
3:G:141:GLN:HG3	5:I:15:ASN:HD21	1.75	0.51
1:A:217:GLN:OE1	2:D:356:ARG:NH2	2.44	0.51
2:M:391:LEU:CD2	3:P:83:LEU:CD1	2.90	0.51
2:W:15:ALA:HB3	2:W:22:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:75:ALA:HA	4:H:84:CYS:O	2.09	0.51
2:V:184:PHE:HB3	2:V:217:LEU:HD23	1.92	0.51
1:K:55:VAL:HG21	1:K:75:ILE:HD13	1.93	0.50
1:T:389:ALA:HB2	1:T:447:ILE:HG21	1.92	0.50
3:G:118:LEU:HB3	3:G:126:ILE:HD11	1.94	0.50
3:P:77:ILE:HG23	3:P:110:ILE:HB	1.93	0.50
1:J:360:TYR:HE1	2:M:354:LYS:HZ1	1.58	0.50
1:B:272:ASP:OD1	1:B:274:SER:HB2	2.10	0.50
1:B:187:ASN:OD1	1:B:190:ARG:NH1	2.43	0.50
1:A:444:VAL:HG22	1:A:445:PRO:HD3	1.92	0.50
2:X:284:THR:O	2:X:286:ALA:N	2.44	0.50
3:G:15:ASN:O	3:G:19:ILE:HG12	2.10	0.50
3:P:81:LYS:HB3	3:P:233:ARG:NH2	2.26	0.50
1:S:92:ARG:HH21	1:S:94:GLY:HA2	1.76	0.50
2:X:390:ILE:HD11	3:Y:247:MET:SD	2.51	0.50
1:C:168:LEU:HB2	1:C:348:THR:HG21	1.93	0.50
1:J:364:ARG:HA	1:J:365:PRO:C	2.31	0.50
1:C:55:VAL:HG21	1:C:75:ILE:HD13	1.93	0.50
1:K:285:LEU:HD22	2:N:275:ILE:HG22	1.93	0.50
2:F:345:TYR:HA	2:F:346:PRO:C	2.31	0.50
1:L:187:ASN:O	1:L:190:ARG:HG3	2.11	0.50
2:M:391:LEU:HD22	3:P:83:LEU:CD1	2.41	0.50
1:C:395:PHE:HZ	1:C:422:ARG:HB3	1.76	0.50
3:P:164:ILE:HD11	3:P:182:ILE:HG12	1.93	0.50
2:W:150:GLY:HA2	2:W:304:VAL:O	2.12	0.50
1:C:336:VAL:CG1	1:C:353:PHE:CZ	2.86	0.50
3:G:23:MET:HG3	3:G:237:MET:HG2	1.93	0.50
3:Y:23:MET:HB3	3:Y:237:MET:HG3	1.93	0.50
2:X:15:ALA:HB3	2:X:22:ASP:HB2	1.94	0.50
2:M:314:ALA:O	2:M:315:ASP:HB2	2.12	0.50
1:B:30:THR:CG2	1:B:31:GLY:N	2.75	0.49
8:M:600:ANP:O5'	8:M:600:ANP:H8	2.11	0.49
2:M:222:MET:HA	2:M:229:ARG:HD2	1.93	0.49
2:W:152:LYS:HE3	2:W:296:ILE:HB	1.93	0.49
1:J:70:PRO:HD3	2:N:15:ALA:HB2	1.93	0.49
2:F:140:VAL:HG12	2:F:414:LEU:HB3	1.95	0.49
2:X:63:ALA:O	2:X:227:GLY:HA3	2.12	0.49
3:G:182:ILE:HG21	3:G:214:LEU:HD13	1.93	0.49
2:W:255:ILE:HB	2:W:308:GLN:HG2	1.94	0.49
3:Y:115:LYS:O	3:Y:119:LEU:HB2	2.11	0.49
1:J:336:VAL:CG1	1:J:353:PHE:CZ	2.87	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:349:ASP:HA	1:L:375:ARG:HD2	1.94	0.49
2:X:163:LYS:HG3	8:X:600:ANP:O1B	2.12	0.49
2:O:140:VAL:HG12	2:O:414:LEU:HD22	1.94	0.49
2:D:136:THR:HA	2:D:174:ILE:HD11	1.94	0.49
1:B:444:VAL:HG23	1:B:445:PRO:HD3	1.95	0.49
1:B:444:VAL:CG2	1:B:445:PRO:HD3	2.42	0.49
1:C:349:ASP:O	1:C:375:ARG:HB2	2.11	0.49
1:C:80:SER:OG	1:C:82:ARG:HG2	2.11	0.49
2:O:247:GLU:O	2:O:249:GLN:HG2	2.12	0.49
3:Y:78:THR:HG23	3:Y:91:LEU:HD22	1.94	0.49
8:M:600:ANP:O2G	8:M:600:ANP:O2B	2.31	0.49
2:W:98:VAL:HB	2:W:232:VAL:HG13	1.94	0.49
2:M:336:SER:HB3	2:M:339:ILE:HG12	1.94	0.49
1:B:390:GLY:O	1:B:391:SER:HB2	2.11	0.49
3:G:78:THR:OG1	3:G:114:ILE:HB	2.12	0.49
2:O:460:VAL:HB	2:O:465:ASP:HB3	1.93	0.49
2:D:149:ARG:HG3	2:D:149:ARG:HH11	1.78	0.49
4:Q:16:LEU:CB	4:Q:17:PRO:HD2	2.43	0.49
2:X:345:TYR:HA	2:X:346:PRO:C	2.33	0.49
1:J:425:ARG:HG3	1:J:425:ARG:NH1	2.28	0.49
3:P:162:ILE:HB	3:P:182:ILE:O	2.12	0.49
1:J:164:GLY:HA2	1:J:323:LEU:O	2.13	0.49
2:D:319:ASP:O	2:D:322:PRO:HD2	2.13	0.49
3:P:150:LEU:O	3:P:154:MET:HB2	2.13	0.49
3:P:109:THR:O	3:P:129:SER:HA	2.12	0.49
2:V:15:ALA:HB3	2:V:22:ASP:HB2	1.94	0.49
2:F:33:ILE:O	2:F:34:LEU:HB2	2.12	0.49
1:T:364:ARG:HA	1:T:365:PRO:C	2.33	0.49
1:T:211:LYS:HD2	2:W:328:HIS:HA	1.95	0.49
1:C:203:CYS:O	1:C:231:SER:HA	2.13	0.49
2:F:137:GLY:HA2	2:F:432:VAL:O	2.13	0.49
1:B:387:GLN:OE1	1:B:491:LEU:HB2	2.12	0.49
1:C:336:VAL:CG1	1:C:353:PHE:HZ	2.24	0.48
1:J:174:GLN:OE1	2:M:354:LYS:HD2	2.13	0.48
2:V:9:ILE:HB	2:V:78:ASP:HB3	1.95	0.48
2:M:149:ARG:HG2	2:M:149:ARG:NH1	2.10	0.48
1:L:375:ARG:NH1	8:M:600:ANP:O2A	2.46	0.48
2:X:298:THR:HG23	2:X:303:SER:HA	1.94	0.48
2:W:204:THR:OG1	2:W:420:VAL:HB	2.14	0.48
2:O:9:ILE:HD12	2:O:9:ILE:H	1.78	0.48
2:V:242:TYR:CE1	2:V:246:GLU:HG3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:182:LEU:HD13	1:J:218:LEU:HD11	1.94	0.48
2:F:279:VAL:HG12	2:F:279:VAL:O	2.13	0.48
3:P:115:LYS:HB2	3:P:129:SER:OG	2.14	0.48
1:K:383:LYS:O	1:K:387:GLN:HG3	2.13	0.48
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.96	0.48
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.96	0.48
1:A:484:GLU:HG2	1:A:495:LEU:HD11	1.94	0.48
1:J:444:VAL:CG2	1:J:445:PRO:HD3	2.43	0.48
1:B:119:GLY:O	2:N:89:ARG:NH2	2.47	0.48
1:A:418:GLN:HG3	9:A:814:HOH:O	2.12	0.48
1:J:26:ASN:O	1:J:27:LEU:HB2	2.13	0.48
2:W:321:ALA:HB3	2:W:322:PRO:CD	2.44	0.48
1:J:217:GLN:OE1	2:M:356:ARG:NH2	2.47	0.48
2:V:89:ARG:NH1	2:V:247:GLU:OE2	2.46	0.48
2:D:242:TYR:CE1	2:D:246:GLU:HG3	2.48	0.48
1:J:359:PHE:CE1	1:J:364:ARG:NH2	2.82	0.48
2:O:150:GLY:HA2	2:O:304:VAL:O	2.14	0.48
1:T:219:VAL:HG22	1:T:233:ILE:HG13	1.95	0.48
1:T:54:LEU:HD21	1:T:62:LYS:HD3	1.96	0.48
1:J:54:LEU:HD13	1:J:97:VAL:HG22	1.94	0.48
2:X:363:VAL:HB	2:X:367:HIS:ND1	2.28	0.48
1:K:28:ASN:HB3	1:K:48:ASN:ND2	2.29	0.48
1:S:138:ILE:HD13	2:W:191:THR:HG23	1.95	0.47
3:Y:220:THR:O	3:Y:224:GLN:HG3	2.13	0.47
3:G:54:ASN:C	3:G:56:GLU:H	2.17	0.47
2:X:319:ASP:OD1	2:X:320:PRO:HD2	2.14	0.47
3:Y:130:ILE:HD13	3:Y:146:ILE:HG12	1.96	0.47
1:L:413:ASP:O	1:L:416:THR:HG22	2.14	0.47
1:T:344:VAL:HA	1:T:347:ILE:HD12	1.95	0.47
2:M:409:LYS:NZ	2:M:452:ILE:O	2.46	0.47
1:C:103:PRO:HD3	1:C:258:TRP:CH2	2.49	0.47
1:C:222:LEU:HB2	1:C:228:MET:HE2	1.97	0.47
1:U:395:PHE:CE2	1:U:422:ARG:HD2	2.50	0.47
3:G:93:LYS:HE2	3:G:97:ARG:HH22	1.79	0.47
1:L:345:ILE:HG12	1:L:351:GLN:HG2	1.97	0.47
2:N:321:ALA:HB3	2:N:322:PRO:CD	2.45	0.47
1:L:39:GLY:HA2	1:L:77:LEU:HD12	1.96	0.47
3:P:86:SER:O	3:P:87:ILE:C	2.51	0.47
2:X:97:ASN:HD22	2:X:101:GLU:HB2	1.79	0.47
3:G:75:VAL:HB	3:G:164:ILE:CD1	2.44	0.47
1:C:64:MET:HG3	1:C:97:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLN:O	1:B:402:VAL:HG23	2.15	0.47
2:F:293:GLN:HG2	2:F:328:HIS:HB3	1.96	0.47
1:K:92:ARG:HH21	1:K:94:GLY:HA2	1.78	0.47
1:B:142:ARG:HG2	1:B:143:SER:N	2.30	0.47
1:A:354:LEU:HA	1:A:366:ALA:O	2.15	0.47
2:D:314:ALA:O	2:D:315:ASP:HB2	2.15	0.47
3:G:169:PRO:HD3	3:G:224:GLN:O	2.14	0.47
2:N:255:ILE:HB	2:N:308:GLN:HG2	1.97	0.47
2:O:197:LEU:O	2:O:201:MET:HG2	2.15	0.47
1:L:290:PRO:HB2	2:M:270:ALA:HB1	1.97	0.47
2:V:136:THR:HA	2:V:174:ILE:HD11	1.97	0.47
2:D:222:MET:HA	2:D:229:ARG:HD2	1.96	0.47
1:K:140:PRO:HB3	1:K:318:GLU:HG3	1.97	0.47
1:B:36:VAL:CG1	2:E:53:HIS:HB2	2.45	0.47
1:S:270:TYR:O	1:S:272:ASP:HA	2.14	0.47
1:K:260:ARG:O	1:K:321:GLY:HA3	2.14	0.47
2:W:85:VAL:CG1	2:W:235:THR:HG23	2.28	0.47
2:N:220:GLY:CA	2:N:232:VAL:HG11	2.45	0.47
2:M:391:LEU:CD2	3:P:83:LEU:HD13	2.45	0.47
2:N:15:ALA:HB3	2:N:22:ASP:HB2	1.97	0.47
2:D:189:GLU:O	2:D:221:GLN:HB3	2.15	0.47
1:S:50:GLN:HG2	2:W:71:VAL:HG22	1.96	0.47
1:T:398:GLN:O	1:T:402:VAL:HG23	2.15	0.47
2:M:136:THR:HA	2:M:174:ILE:HD11	1.97	0.47
1:K:99:VAL:CG1	1:K:251:THR:HB	2.34	0.46
1:S:192:ASN:HA	1:S:200:LYS:HG2	1.97	0.46
1:S:353:PHE:HD2	1:S:371:LEU:HB3	1.80	0.46
3:P:180:LYS:NZ	3:P:220:THR:HB	2.29	0.46
1:K:384:ALA:O	1:K:388:VAL:HG13	2.15	0.46
2:E:201:MET:SD	2:E:217:LEU:HD21	2.55	0.46
1:L:360:TYR:OH	2:O:354:LYS:NZ	2.23	0.46
2:E:374:VAL:HG23	2:E:445:LEU:HD11	1.97	0.46
1:L:272:ASP:OD1	1:L:274:SER:HB2	2.16	0.46
2:F:460:VAL:HB	2:F:465:ASP:HB3	1.97	0.46
1:L:481:LEU:HD21	1:L:498:SER:HB3	1.96	0.46
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.46	0.46
1:S:50:GLN:HB2	1:S:53:GLU:HB2	1.97	0.46
1:J:211:LYS:NZ	2:M:330:ASP:OD1	2.44	0.46
2:E:112:LYS:HD2	1:K:120:LYS:HG2	1.98	0.46
3:Y:9:ARG:HG2	3:Y:251:TYR:CE1	2.50	0.46
2:M:197:LEU:O	2:M:201:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:392:LEU:HD13	1:U:451:VAL:HG22	1.97	0.46
1:K:106:LEU:HD23	1:K:229:LYS:O	2.15	0.46
1:C:209:GLY:HA3	1:C:275:LYS:HD3	1.97	0.46
1:A:99:VAL:HG21	1:A:251:THR:HG23	1.98	0.46
3:P:14:LYS:HA	3:P:248:ILE:HD11	1.97	0.46
2:E:410:ILE:HG23	2:E:441:PHE:HE2	1.81	0.46
2:D:224:GLU:O	2:D:229:ARG:HD3	2.14	0.46
2:V:190:ARG:HD2	2:V:193:GLU:OE2	2.16	0.46
2:N:345:TYR:HA	2:N:346:PRO:C	2.36	0.46
1:A:270:TYR:O	1:A:272:ASP:HA	2.16	0.46
2:W:384:LEU:O	2:W:388:ILE:HG12	2.16	0.46
2:V:50:VAL:HA	2:V:61:THR:HG22	1.98	0.46
2:O:33:ILE:O	2:O:34:LEU:HB2	2.16	0.46
1:J:444:VAL:HG22	1:J:445:PRO:HD3	1.98	0.46
1:T:421:VAL:O	1:T:425:ARG:HG2	2.16	0.46
3:P:227:ALA:HA	3:P:230:ILE:HG22	1.98	0.46
2:V:339:ILE:HG22	2:V:344:ILE:HB	1.97	0.46
8:F:600:ANP:O5'	8:F:600:ANP:H8	2.15	0.46
1:C:202:TYR:O	1:C:266:ALA:HA	2.16	0.45
2:O:377:THR:HG22	2:O:407:ALA:HB2	1.99	0.45
2:F:197:LEU:O	2:F:201:MET:HG2	2.16	0.45
2:D:200:GLU:HA	2:D:200:GLU:OE1	2.16	0.45
2:F:242:TYR:CE1	2:F:246:GLU:HG3	2.51	0.45
1:A:407:GLN:O	1:A:410:SER:N	2.49	0.45
1:T:140:PRO:HB3	1:T:318:GLU:HG3	1.98	0.45
2:F:155:LEU:HD12	2:F:167:ILE:HG13	1.99	0.45
1:C:417:LYS:O	1:C:421:VAL:HG23	2.15	0.45
2:N:242:TYR:CZ	2:N:246:GLU:HG3	2.50	0.45
1:L:280:TYR:CD2	1:L:297:PRO:HG2	2.51	0.45
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.98	0.45
1:T:54:LEU:HD12	1:T:97:VAL:HG22	1.98	0.45
1:J:402:VAL:O	1:J:402:VAL:HG12	2.14	0.45
1:B:203:CYS:HB2	1:B:231:SER:HB3	1.98	0.45
1:B:36:VAL:HG13	2:E:53:HIS:HB2	1.98	0.45
1:T:92:ARG:HH21	1:T:94:GLY:HA2	1.81	0.45
2:D:89:ARG:NH1	2:D:247:GLU:OE2	2.49	0.45
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.51	0.45
1:B:68:LEU:HB3	2:F:72:ARG:HD3	1.98	0.45
5:I:31:THR:OG1	5:I:32:ALA:N	2.50	0.45
1:T:77:LEU:O	1:T:243:PRO:HG2	2.16	0.45
3:Y:28:SER:OG	3:Y:234:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:338:ALA:HB3	1:T:341:PRO:HG2	1.99	0.45
2:D:345:TYR:HA	2:D:346:PRO:C	2.36	0.45
3:G:77:ILE:HD13	3:G:110:ILE:HD12	1.99	0.45
1:K:444:VAL:HG21	1:K:485:ILE:HG21	1.97	0.45
2:M:339:ILE:HG22	2:M:344:ILE:HB	1.99	0.45
1:A:391:SER:OG	1:A:451:VAL:HG11	2.17	0.45
1:T:384:ALA:O	1:T:388:VAL:HG22	2.16	0.45
1:A:148:VAL:HG21	1:A:324:THR:HG21	1.98	0.45
2:M:24:HIS:CE1	2:M:25:PHE:O	2.70	0.45
1:K:203:CYS:HB2	1:K:231:SER:HB3	1.99	0.45
2:D:134:LEU:HD13	2:D:149:ARG:NH1	2.32	0.45
2:X:313:PRO:HG2	2:X:319:ASP:OD2	2.16	0.45
1:S:174:GLN:HA	8:S:600:ANP:HNB1	1.80	0.45
1:S:332:GLN:HB3	2:V:318:THR:HB	1.98	0.45
1:S:402:VAL:O	1:S:402:VAL:HG12	2.16	0.45
4:Q:52:LEU:CB	9:Q:802:HOH:O	2.64	0.45
1:S:99:VAL:CG2	1:S:100:PRO:HD2	2.47	0.45
3:Y:253:ILE:CG2	3:Y:257:ARG:HH22	2.30	0.45
1:K:250:PHE:CE1	1:K:307:LEU:HB2	2.52	0.45
2:X:95:ILE:HD12	2:X:104:ASP:HB3	1.98	0.45
3:P:88:HIS:CD2	3:P:113:LYS:CB	2.89	0.44
3:P:205:VAL:H	3:P:206:PRO:HD3	1.83	0.44
1:T:43:VAL:HG21	1:T:75:ILE:HD12	1.99	0.44
2:N:321:ALA:N	2:N:322:PRO:HD2	2.32	0.44
1:L:436:SER:N	1:L:437:PRO:HD3	2.31	0.44
2:M:149:ARG:NH1	2:M:149:ARG:CG	2.65	0.44
1:S:309:GLU:HG3	2:W:223:ASN:HB3	1.99	0.44
2:X:189:GLU:O	2:X:221:GLN:HB3	2.17	0.44
2:M:395:GLU:HA	2:M:395:GLU:OE1	2.17	0.44
1:T:85:LYS:HE2	2:W:32:ALA:HB2	1.99	0.44
2:F:189:GLU:O	2:F:221:GLN:HB3	2.16	0.44
1:S:219:VAL:HG22	1:S:233:ILE:HG13	1.99	0.44
1:B:30:THR:HG21	1:B:89:LEU:HD11	2.00	0.44
2:W:244:ARG:HD3	2:W:304:VAL:HG23	2.00	0.44
1:C:103:PRO:HD3	1:C:258:TRP:CZ2	2.53	0.44
2:N:25:PHE:HB2	2:N:30:LEU:HD23	1.99	0.44
2:M:231:ARG:HA	2:M:231:ARG:HD3	1.81	0.44
1:A:69:GLU:HB3	1:A:70:PRO:HD2	1.99	0.44
2:W:167:ILE:HG23	2:W:254:PHE:CE2	2.53	0.44
2:F:52:GLN:HG3	2:F:60:ARG:HB3	1.99	0.44
3:G:90:GLN:HA	3:G:93:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:455:LEU:HD21	1:L:466:PHE:CE1	2.53	0.44
1:U:382:VAL:HG12	1:U:384:ALA:H	1.82	0.44
1:B:103:PRO:HD3	1:B:258:TRP:CZ2	2.53	0.44
1:C:455:LEU:HD21	1:C:466:PHE:CE1	2.53	0.44
3:Y:121:THR:C	3:Y:123:PRO:HD3	2.38	0.44
1:J:40:ILE:CD1	1:J:76:VAL:HG12	2.46	0.44
1:C:93:THR:HG22	1:C:95:ASN:OD1	2.17	0.44
1:L:222:LEU:HB2	1:L:228:MET:HE2	2.00	0.44
3:P:94:ALA:C	3:P:96:ARG:N	2.71	0.44
2:V:262:THR:O	2:V:282:GLN:NE2	2.50	0.44
2:V:396:LEU:HD12	2:V:400:ASP:HB3	2.00	0.44
2:V:189:GLU:O	2:V:221:GLN:HB3	2.18	0.44
2:X:160:GLY:N	8:X:600:ANP:HNB1	2.07	0.44
1:B:444:VAL:N	1:B:445:PRO:CD	2.81	0.44
2:F:33:ILE:HG22	2:F:34:LEU:HG	1.99	0.44
2:F:160:GLY:HA2	8:F:600:ANP:HNB1	1.82	0.44
1:L:378:SER:HB2	1:L:386:LYS:HG3	2.00	0.44
2:O:345:TYR:HA	2:O:346:PRO:C	2.38	0.44
2:W:409:LYS:NZ	2:W:450:ASP:O	2.50	0.44
2:V:29:GLU:HG3	2:V:29:GLU:O	2.18	0.44
1:B:383:LYS:O	1:B:387:GLN:HG3	2.18	0.44
4:H:79:PRO:C	4:H:81:SER:H	2.20	0.44
2:O:158:GLY:O	2:O:161:VAL:HG22	2.17	0.44
1:K:251:THR:O	1:K:255:ILE:HG13	2.16	0.43
1:L:416:THR:O	1:L:419:THR:HG22	2.17	0.43
4:H:72:GLY:O	4:H:87:ALA:HA	2.17	0.43
1:C:285:LEU:HD21	1:C:291:PRO:HB3	2.00	0.43
2:O:90:GLU:HG3	2:O:111:SER:HA	2.00	0.43
2:M:184:PHE:HB3	2:M:217:LEU:HD23	1.99	0.43
1:L:239:SER:HB3	2:O:294:GLU:HG3	1.99	0.43
2:W:448:LYS:O	2:W:449:TYR:HB2	2.18	0.43
1:S:509:THR:HG22	1:S:509:THR:O	2.18	0.43
8:K:600:ANP:H5'1	8:K:600:ANP:H8	2.00	0.43
2:N:384:LEU:O	2:N:388:ILE:HG12	2.17	0.43
1:U:416:THR:O	1:U:420:LEU:HB2	2.16	0.43
1:B:27:LEU:O	1:B:47:ASN:ND2	2.51	0.43
2:X:90:GLU:HG3	2:X:111:SER:HA	2.00	0.43
2:E:174:ILE:HD12	2:E:178:HIS:HD2	1.82	0.43
1:T:288:ARG:NH1	2:W:275:ILE:HD11	2.33	0.43
1:U:428:GLN:NE2	1:U:431:LYS:HD2	2.34	0.43
2:O:52:GLN:HE21	2:O:60:ARG:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:321:ALA:HB3	2:N:322:PRO:HD3	1.99	0.43
1:S:295:ALA:HB2	3:Y:270:ILE:HD13	2.01	0.43
2:V:321:ALA:HB3	2:V:322:PRO:HD3	2.00	0.43
3:G:77:ILE:CD1	3:G:110:ILE:HD12	2.49	0.43
1:B:421:VAL:O	1:B:425:ARG:HG2	2.19	0.43
1:U:174:GLN:HB3	2:X:354:LYS:HD3	1.99	0.43
1:U:187:ASN:OD1	1:U:190:ARG:NH1	2.51	0.43
1:C:354:LEU:HA	1:C:366:ALA:O	2.18	0.43
1:L:177:LYS:HE2	1:L:177:LYS:HB2	1.84	0.43
2:F:293:GLN:HA	2:F:293:GLN:OE1	2.19	0.43
1:C:219:VAL:HG12	1:C:228:MET:HE1	2.01	0.43
2:X:33:ILE:O	2:X:34:LEU:HB2	2.18	0.43
1:B:505:SER:O	1:B:509:THR:HG22	2.19	0.43
1:K:478:HIS:HB3	1:K:481:LEU:HG	1.99	0.43
2:V:314:ALA:O	2:V:315:ASP:HB2	2.19	0.43
2:D:425:THR:HB	2:D:427:ILE:HD12	2.01	0.43
1:C:242:ALA:N	1:C:243:PRO:CD	2.81	0.43
1:K:270:TYR:O	1:K:272:ASP:HA	2.18	0.43
1:U:189:LYS:HE3	1:U:226:ASP:HB3	2.00	0.43
1:A:309:GLU:HG3	2:E:223:ASN:HB3	2.00	0.43
3:G:118:LEU:HA	3:G:121:THR:HG22	2.00	0.43
3:Y:133:ILE:O	3:Y:135:LYS:N	2.48	0.43
1:L:211:LYS:HE3	1:L:213:SER:OG	2.18	0.43
1:B:146:GLU:HA	1:B:147:PRO:HD3	1.88	0.43
2:N:256:ASP:HA	2:N:257:ASN:HA	1.77	0.43
2:O:363:VAL:HB	2:O:367:HIS:ND1	2.33	0.43
1:L:168:LEU:HB2	1:L:348:THR:HG21	2.01	0.43
2:X:440:SER:O	2:X:444:VAL:HG23	2.19	0.43
2:V:33:ILE:O	2:V:34:LEU:HB2	2.18	0.43
2:X:202:LYS:HE3	2:X:209:LEU:HD11	2.01	0.43
2:D:143:LEU:O	2:D:367:HIS:HE1	2.02	0.43
1:K:85:LYS:HE2	2:N:32:ALA:HB2	2.01	0.43
1:U:353:PHE:CE2	1:U:371:LEU:O	2.72	0.43
1:T:383:LYS:O	1:T:387:GLN:HG3	2.18	0.43
1:U:478:HIS:O	1:U:481:LEU:HB2	2.19	0.43
2:F:256:ASP:HA	2:F:257:ASN:HA	1.88	0.43
2:N:204:THR:OG1	2:N:420:VAL:HB	2.19	0.43
2:X:345:TYR:HB3	8:X:600:ANP:C6	2.49	0.42
1:B:285:LEU:HD22	2:E:275:ILE:CG2	2.47	0.42
1:L:378:SER:C	1:L:380:ALA:H	2.23	0.42
1:C:492:SER:H	1:C:495:LEU:HD12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:50:VAL:HA	2:X:61:THR:HG22	2.00	0.42
2:M:204:THR:HB	2:M:206:VAL:HG23	2.01	0.42
1:U:243:PRO:HA	1:U:283:LEU:HD11	2.01	0.42
1:S:168:LEU:HD11	1:S:329:ILE:HB	2.01	0.42
3:Y:78:THR:HG23	3:Y:91:LEU:CD2	2.49	0.42
1:L:378:SER:C	1:L:380:ALA:N	2.73	0.42
1:J:483:THR:HG23	1:J:486:ARG:NH2	2.34	0.42
2:F:237:LEU:HD21	2:F:295:ARG:HB2	2.01	0.42
1:B:69:GLU:HB3	1:B:70:PRO:HD2	2.01	0.42
2:E:190:ARG:HG3	2:E:190:ARG:HH11	1.84	0.42
2:V:201:MET:SD	2:V:215:VAL:HG11	2.59	0.42
2:M:345:TYR:HA	2:M:346:PRO:C	2.38	0.42
2:F:452:ILE:HA	2:F:453:PRO:HD3	1.90	0.42
2:O:237:LEU:HD13	2:O:296:ILE:HG12	2.01	0.42
2:O:155:LEU:HD12	2:O:167:ILE:HG13	2.00	0.42
2:W:9:ILE:HG23	2:W:29:GLU:HG2	2.01	0.42
2:N:275:ILE:HA	2:N:276:PRO:HD3	1.81	0.42
3:Y:80:ASP:OD2	3:Y:111:GLY:HA2	2.19	0.42
1:L:364:ARG:HA	1:L:365:PRO:C	2.40	0.42
2:M:373:LYS:HB3	2:M:445:LEU:HD13	2.02	0.42
1:S:185:ILE:HG23	1:S:203:CYS:SG	2.60	0.42
1:A:26:ASN:HB3	1:A:30:THR:OG1	2.19	0.42
1:K:129:SER:HB2	1:K:254:SER:HB3	2.01	0.42
2:F:234:LEU:HD23	2:F:292:LEU:HD13	2.02	0.42
1:U:354:LEU:HA	1:U:366:ALA:O	2.19	0.42
2:D:256:ASP:HA	2:D:257:ASN:HA	1.88	0.42
1:B:296:TYR:HB3	1:B:297:PRO:HD2	2.01	0.42
1:L:34:LEU:O	2:O:55:GLY:HA2	2.20	0.42
1:J:38:ASP:OD1	2:M:274:ARG:NH2	2.47	0.42
3:G:3:LEU:HD23	3:G:3:LEU:C	2.40	0.42
1:T:444:VAL:HG21	1:T:485:ILE:HG21	2.01	0.42
1:T:340:ILE:HB	1:T:341:PRO:HD3	2.02	0.42
2:N:258:ILE:HG22	2:N:309:ALA:O	2.20	0.42
5:1:18:ALA:C	5:1:20:ALA:H	2.23	0.42
2:X:140:VAL:HG21	2:X:348:VAL:HB	2.01	0.42
2:E:150:GLY:HA2	2:E:304:VAL:O	2.20	0.42
2:M:64:MET:HE3	2:M:228:ALA:HA	2.01	0.42
2:X:464:GLU:O	2:X:464:GLU:HG3	2.20	0.42
1:C:242:ALA:HB3	1:C:243:PRO:CD	2.41	0.42
2:M:391:LEU:CD2	3:P:83:LEU:HD11	2.49	0.42
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:140:VAL:HG23	2:O:141:VAL:N	2.35	0.42
2:W:345:TYR:HA	2:W:346:PRO:C	2.39	0.42
1:L:93:THR:HG22	1:L:95:ASN:OD1	2.19	0.42
2:N:356:ARG:NH1	2:N:356:ARG:HB3	2.35	0.42
1:L:375:ARG:HA	8:M:600:ANP:O3'	2.20	0.42
2:X:282:GLN:HA	2:X:283:PRO:HD3	1.94	0.42
1:U:271:ASP:HA	1:U:272:ASP:HA	1.80	0.42
2:W:275:ILE:HA	2:W:276:PRO:HD3	1.88	0.42
3:G:140:PHE:HA	3:G:219:LEU:HD12	2.01	0.42
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.49	0.42
1:S:360:TYR:HE1	2:V:354:LYS:HZ1	1.66	0.42
1:J:42:ARG:HE	1:J:72:GLN:HE22	1.66	0.42
1:S:99:VAL:HG21	1:S:251:THR:CG2	2.49	0.41
2:V:282:GLN:HG3	2:V:282:GLN:H	1.50	0.41
2:F:71:VAL:HG12	2:F:72:ARG:O	2.20	0.41
2:E:452:ILE:HA	2:E:453:PRO:HD2	1.93	0.41
1:B:219:VAL:HG22	1:B:233:ILE:HG13	2.02	0.41
1:U:364:ARG:HA	1:U:365:PRO:C	2.40	0.41
2:O:285:LEU:C	2:O:285:LEU:HD23	2.40	0.41
2:N:140:VAL:HG13	2:N:414:LEU:HD22	2.02	0.41
1:U:357:GLU:HG3	2:X:379:GLN:NE2	2.35	0.41
2:E:95:ILE:HG12	2:E:217:LEU:HD12	2.02	0.41
1:L:211:LYS:HB2	2:O:294:GLU:OE2	2.20	0.41
2:M:64:MET:CE	2:M:228:ALA:HA	2.51	0.41
1:C:139:LEU:N	1:C:140:PRO:HD2	2.35	0.41
1:S:425:ARG:HD3	1:S:455:LEU:O	2.20	0.41
1:S:236:ALA:HA	1:S:240:GLU:OE1	2.19	0.41
1:T:335:ASP:OD1	1:T:337:SER:HB2	2.19	0.41
2:E:120:ASP:HA	2:E:121:PRO:HD3	1.90	0.41
2:E:27:GLN:HG3	2:E:27:GLN:H	1.64	0.41
1:A:267:LEU:HD11	1:A:326:LEU:HG	2.02	0.41
1:U:340:ILE:N	1:U:341:PRO:CD	2.83	0.41
2:D:98:VAL:HG13	2:D:99:ILE:HG23	2.03	0.41
1:C:160:PRO:O	1:C:374:SER:OG	2.26	0.41
2:M:15:ALA:HB3	2:M:22:ASP:HB2	2.03	0.41
2:E:218:VAL:HG21	2:E:236:GLY:HA2	2.03	0.41
2:X:247:GLU:O	2:X:249:GLN:HG2	2.21	0.41
1:C:83:LEU:HA	1:C:83:LEU:HD23	1.91	0.41
3:Y:86:SER:O	3:Y:90:GLN:HB2	2.20	0.41
2:M:137:GLY:HA2	2:M:432:VAL:O	2.20	0.41
1:U:344:VAL:HA	1:U:347:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:421:VAL:HG13	1:L:425:ARG:NH1	2.35	0.41
2:F:52:GLN:NE2	2:F:60:ARG:HD2	2.24	0.41
2:M:258:ILE:HD11	2:M:292:LEU:HD21	2.03	0.41
1:S:421:VAL:HG13	1:S:425:ARG:NH2	2.36	0.41
1:A:450:GLY:HA2	1:A:455:LEU:HD12	2.03	0.41
2:W:259:PHE:CE1	2:W:313:PRO:HG3	2.56	0.41
1:C:181:ALA:HB1	1:C:269:VAL:HG21	2.02	0.41
2:M:37:LEU:HB3	2:M:76:VAL:HG12	2.03	0.41
2:N:9:ILE:HB	2:N:78:ASP:HB3	2.03	0.41
1:T:444:VAL:N	1:T:445:PRO:CD	2.84	0.41
1:K:92:ARG:HB3	1:K:92:ARG:HE	1.74	0.41
3:P:164:ILE:HG12	3:P:180:LYS:O	2.20	0.41
1:L:280:TYR:CE2	1:L:297:PRO:HG2	2.56	0.41
1:T:210:GLN:NE2	1:T:271:ASP:O	2.51	0.41
1:K:338:ALA:HB3	1:K:341:PRO:HG2	2.03	0.41
1:J:134:LYS:HD3	1:J:134:LYS:HA	1.83	0.41
2:M:98:VAL:HG13	2:M:99:ILE:HG23	2.03	0.41
1:T:168:LEU:HD11	1:T:329:ILE:HB	2.03	0.41
2:M:164:THR:O	2:M:168:GLN:HG3	2.21	0.41
2:X:242:TYR:CE1	2:X:246:GLU:HG3	2.55	0.41
2:W:133:ILE:HD12	2:W:146:PRO:HB2	2.03	0.41
1:A:34:LEU:HA	1:A:34:LEU:HD23	1.89	0.41
3:G:202:ASP:N	3:G:202:ASP:OD1	2.50	0.41
2:X:256:ASP:HA	2:X:257:ASN:HA	1.85	0.41
2:F:97:ASN:HD22	2:F:101:GLU:HB2	1.86	0.41
2:W:276:PRO:HG2	3:Y:267:LEU:HD21	2.03	0.41
2:X:97:ASN:HB2	2:X:101:GLU:H	1.86	0.41
1:L:378:SER:O	1:L:380:ALA:N	2.54	0.41
1:A:138:ILE:HD13	2:E:191:THR:HG23	2.03	0.41
1:L:354:LEU:HA	1:L:366:ALA:O	2.21	0.41
2:X:142:ASP:HB3	2:X:434:LEU:HD12	2.02	0.41
1:C:243:PRO:HA	1:C:283:LEU:HD11	2.03	0.40
1:K:444:VAL:HG23	1:K:445:PRO:CD	2.49	0.40
1:U:340:ILE:HB	1:U:341:PRO:HD3	2.03	0.40
1:L:340:ILE:HB	1:L:341:PRO:HD3	2.03	0.40
1:U:211:LYS:HA	2:X:294:GLU:OE2	2.21	0.40
2:X:382:LYS:O	2:X:385:GLN:HG2	2.20	0.40
3:G:180:LYS:HE3	3:G:217:GLN:HB3	2.03	0.40
2:E:427:ILE:HA	2:E:428:PRO:HD2	1.94	0.40
2:M:96:ILE:HG22	2:M:97:ASN:O	2.21	0.40
1:K:103:PRO:HD3	1:K:258:TRP:CZ2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:103:PRO:O	1:K:106:LEU:HD13	2.21	0.40
2:W:321:ALA:HB3	2:W:322:PRO:HD3	2.03	0.40
2:X:382:LYS:HA	2:X:385:GLN:HE21	1.87	0.40
2:F:158:GLY:O	2:F:161:VAL:HG22	2.21	0.40
2:M:337:ARG:O	2:M:341:GLU:HG3	2.21	0.40
2:F:266:SER:HB3	2:F:282:GLN:OE1	2.21	0.40
1:L:40:ILE:CD1	1:L:76:VAL:HG12	2.51	0.40
2:E:204:THR:HG23	2:E:206:VAL:H	1.87	0.40
1:S:54:LEU:HD11	1:S:78:PHE:HE2	1.86	0.40
1:S:99:VAL:HG23	1:S:100:PRO:HD2	2.03	0.40
2:F:384:LEU:O	2:F:388:ILE:HG12	2.20	0.40
1:C:107:GLY:HA2	1:C:228:MET:O	2.20	0.40
1:B:211:LYS:HD2	2:E:328:HIS:HA	2.03	0.40
1:J:242:ALA:N	1:J:243:PRO:CD	2.84	0.40
1:U:360:TYR:O	2:X:376:GLU:HA	2.20	0.40
1:K:170:ILE:HG13	1:K:329:ILE:HG22	2.03	0.40
3:G:205:VAL:HG22	4:H:51:GLN:NE2	2.34	0.40
1:U:109:VAL:HB	1:U:118:ASP:HB3	2.03	0.40
1:T:143:SER:H	2:X:199:ARG:HH22	1.68	0.40
2:N:410:ILE:HG23	2:N:441:PHE:HE2	1.85	0.40
1:A:300:VAL:CG1	1:A:339:TYR:HE2	2.35	0.40
2:W:95:ILE:HD12	2:W:104:ASP:HB3	2.04	0.40
2:M:41:THR:HB	2:M:42:PRO:HD2	2.03	0.40
2:M:253:LEU:HD23	2:M:296:ILE:HG23	2.03	0.40
2:D:178:HIS:NE2	2:D:250:ASP:HB3	2.37	0.40
1:K:67:ASN:HB2	2:O:17:ILE:CG1	2.44	0.40
3:P:209:LEU:O	3:P:213:THR:OG1	2.39	0.40
2:X:53:HIS:CD2	2:X:59:VAL:HG12	2.57	0.40
3:Y:212:TYR:O	3:Y:216:ASN:HB2	2.21	0.40
2:O:394:ASP:CB	3:P:85:GLY:HA2	2.52	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%)	465 (97%)	13 (3%)	0	100	100
1	B	479/510 (94%)	462 (96%)	17 (4%)	0	100	100
1	C	482/510 (94%)	469 (97%)	12 (2%)	1 (0%)	52	84
1	J	477/510 (94%)	466 (98%)	11 (2%)	0	100	100
1	K	482/510 (94%)	469 (97%)	13 (3%)	0	100	100
1	L	478/510 (94%)	458 (96%)	19 (4%)	1 (0%)	52	84
1	S	476/510 (93%)	461 (97%)	15 (3%)	0	100	100
1	T	477/510 (94%)	466 (98%)	10 (2%)	1 (0%)	52	84
1	U	477/510 (94%)	462 (97%)	14 (3%)	1 (0%)	52	84
2	D	468/478 (98%)	452 (97%)	16 (3%)	0	100	100
2	E	466/478 (98%)	446 (96%)	19 (4%)	1 (0%)	52	84
2	F	467/478 (98%)	445 (95%)	19 (4%)	3 (1%)	30	65
2	M	468/478 (98%)	449 (96%)	19 (4%)	0	100	100
2	N	468/478 (98%)	454 (97%)	13 (3%)	1 (0%)	52	84
2	O	466/478 (98%)	446 (96%)	19 (4%)	1 (0%)	52	84
2	V	468/478 (98%)	448 (96%)	20 (4%)	0	100	100
2	W	465/478 (97%)	450 (97%)	14 (3%)	1 (0%)	52	84
2	X	467/478 (98%)	448 (96%)	18 (4%)	1 (0%)	52	84
3	G	261/278 (94%)	235 (90%)	23 (9%)	3 (1%)	17	50
3	P	229/278 (82%)	201 (88%)	21 (9%)	7 (3%)	5	17
3	Y	188/278 (68%)	172 (92%)	16 (8%)	0	100	100
4	H	110/138 (80%)	98 (89%)	10 (9%)	2 (2%)	11	34
4	Q	74/138 (54%)	59 (80%)	12 (16%)	3 (4%)	3	11
4	Z	15/138 (11%)	13 (87%)	2 (13%)	0	100	100
5	1	23/61 (38%)	20 (87%)	1 (4%)	2 (9%)	1	2
5	I	42/61 (69%)	35 (83%)	5 (12%)	2 (5%)	3	9
5	R	30/61 (49%)	23 (77%)	5 (17%)	2 (7%)	1	4
All	All	9481/10323 (92%)	9072 (96%)	376 (4%)	33 (0%)	46	79

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	135	LYS
5	I	31	THR
5	R	31	THR
5	R	32	ALA
3	G	204	ASN
4	H	93	LEU
1	L	390	GLY
3	P	204	ASN
3	P	211	GLU
4	Q	88	ILE
1	T	390	GLY
5	1	34	VAL
1	C	390	GLY
5	I	21	ILE
3	P	201	THR
3	P	206	PRO
2	F	68	GLU
3	P	144	ALA
3	P	169	PRO
5	1	19	GLN
2	F	279	VAL
4	Q	50	GLU
2	F	347	ALA
3	G	192	PRO
4	Q	81	SER
1	U	390	GLY
2	E	279	VAL
2	N	279	VAL
4	H	47	PRO
2	O	279	VAL
3	P	87	ILE
2	W	279	VAL
2	X	279	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	388/412 (94%)	382 (98%)	6 (2%)	72 93
1	B	388/412 (94%)	380 (98%)	8 (2%)	61 90
1	C	389/412 (94%)	382 (98%)	7 (2%)	66 91
1	J	387/412 (94%)	382 (99%)	5 (1%)	76 94
1	K	388/412 (94%)	379 (98%)	9 (2%)	58 88
1	L	388/412 (94%)	378 (97%)	10 (3%)	54 86
1	S	387/412 (94%)	378 (98%)	9 (2%)	58 88
1	T	388/412 (94%)	382 (98%)	6 (2%)	72 93
1	U	388/412 (94%)	381 (98%)	7 (2%)	66 91
2	D	380/384 (99%)	374 (98%)	6 (2%)	70 93
2	E	378/384 (98%)	373 (99%)	5 (1%)	76 94
2	F	379/384 (99%)	374 (99%)	5 (1%)	76 94
2	M	380/384 (99%)	372 (98%)	8 (2%)	61 90
2	N	380/384 (99%)	373 (98%)	7 (2%)	66 91
2	O	379/384 (99%)	376 (99%)	3 (1%)	86 97
2	V	380/384 (99%)	372 (98%)	8 (2%)	61 90
2	W	378/384 (98%)	374 (99%)	4 (1%)	80 95
2	X	379/384 (99%)	374 (99%)	5 (1%)	76 94
3	G	219/236 (93%)	206 (94%)	13 (6%)	24 57
3	P	198/236 (84%)	183 (92%)	15 (8%)	16 42
3	Y	163/236 (69%)	157 (96%)	6 (4%)	41 76
4	H	54/112 (48%)	52 (96%)	2 (4%)	41 76
4	Q	5/112 (4%)	5 (100%)	0	100 100
5	I	23/48 (48%)	20 (87%)	3 (13%)	5 15
All	All	7566/8144 (93%)	7409 (98%)	157 (2%)	61 90

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ARG
1	A	166	ARG
1	A	246	TYR
1	A	353	PHE
1	A	416	THR
1	A	468	SER

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Mol	Chain	Res	Type
1	B	54	LEU
1	B	67	ASN
1	B	99	VAL
1	B	142	ARG
1	B	159	VAL
1	B	183	ASP
1	B	468	SER
1	B	509	THR
1	C	197	GLU
1	C	353	PHE
1	C	411	ASP
1	C	416	THR
1	C	468	SER
1	C	481	LEU
1	C	509	THR
2	D	27	GLN
2	D	128	SER
2	D	149	ARG
2	D	167	ILE
2	D	200	GLU
2	D	388	ILE
2	E	199	ARG
2	E	232	VAL
2	E	356	ARG
2	E	380	THR
2	E	394	ASP
2	F	167	ILE
2	F	201	MET
2	F	293	GLN
2	F	303	SER
2	F	464	GLU
3	G	12	SER
3	G	17	GLU
3	G	77	ILE
3	G	93	LYS
3	G	143	SER
3	G	150	LEU
3	G	153	VAL
3	G	202	ASP
3	G	210	PHE
3	G	231	SER
3	G	237	MET

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Mol	Chain	Res	Type
3	G	254	LEU
3	G	276	SER
4	H	14	PHE
4	H	70	ILE
5	I	13	TYR
5	I	28	GLU
5	I	31	THR
1	J	81	ASP
1	J	246	TYR
1	J	353	PHE
1	J	363	ILE
1	J	393	LYS
1	K	54	LEU
1	K	69	GLU
1	K	99	VAL
1	K	159	VAL
1	K	183	ASP
1	K	225	HIS
1	K	246	TYR
1	K	293	ARG
1	K	509	THR
1	L	99	VAL
1	L	336	VAL
1	L	342	THR
1	L	399	TYR
1	L	401	GLU
1	L	419	THR
1	L	436	SER
1	L	468	SER
1	L	472	SER
1	L	481	LEU
2	M	6	SER
2	M	24	HIS
2	M	149	ARG
2	M	167	ILE
2	M	250	ASP
2	M	388	ILE
2	M	395	GLU
2	M	413	PHE
2	N	114	ARG
2	N	232	VAL
2	N	258	ILE

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Mol	Chain	Res	Type
2	N	352	ASP
2	N	380	THR
2	N	394	ASP
2	N	413	PHE
2	O	167	ILE
2	O	303	SER
2	O	464	GLU
3	P	29	THR
3	P	44	MET
3	P	78	THR
3	P	80	ASP
3	P	84	CYS
3	P	86	SER
3	P	107	ILE
3	P	112	ASP
3	P	129	SER
3	P	130	ILE
3	P	133	ILE
3	P	150	LEU
3	P	213	THR
3	P	216	ASN
3	P	276	SER
1	S	32	ARG
1	S	246	TYR
1	S	322	SER
1	S	353	PHE
1	S	361	LYS
1	S	393	LYS
1	S	425	ARG
1	S	441	GLU
1	S	492	SER
1	T	54	LEU
1	T	99	VAL
1	T	159	VAL
1	T	173	ARG
1	T	183	ASP
1	T	246	TYR
1	U	229	LYS
1	U	363	ILE
1	U	394	LEU
1	U	412	LEU
1	U	413	ASP

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Mol	Chain	Res	Type
1	U	441	GLU
1	U	481	LEU
2	V	29	GLU
2	V	149	ARG
2	V	167	ILE
2	V	200	GLU
2	V	201	MET
2	V	250	ASP
2	V	282	GLN
2	V	388	ILE
2	W	232	VAL
2	W	258	ILE
2	W	394	ASP
2	W	433	ARG
2	X	43	GLN
2	X	140	VAL
2	X	167	ILE
2	X	208	ASN
2	X	472	LYS
3	Y	15	ASN
3	Y	78	THR
3	Y	99	LEU
3	Y	112	ASP
3	Y	162	ILE
3	Y	219	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	GLN
2	D	52	GLN
2	D	195	ASN
2	D	367	HIS
2	F	52	GLN
3	G	125	ASN
3	G	190	GLN
4	H	18	HIS
4	H	45	HIS
5	I	15	ASN
1	K	26	ASN
1	L	174	GLN
1	L	220	GLN

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Mol	Chain	Res	Type
1	L	351	GLN
1	L	398	GLN
2	O	52	GLN
2	O	328	HIS
3	P	88	HIS
3	P	122	HIS
3	P	216	ASN
1	S	351	GLN
1	S	407	GLN
1	T	28	ASN
1	U	224	GLN
1	U	452	ASN
2	V	195	ASN
2	V	282	GLN
2	X	43	GLN
2	X	52	GLN
2	X	379	GLN
2	X	385	GLN
3	Y	117	GLN
3	Y	141	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 15 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
8	ANP	A	600	6	27,33,33	2.27	9 (33%)	30,52,52	2.23	8 (26%)
8	ANP	B	600	6	27,33,33	1.96	6 (22%)	30,52,52	2.30	7 (23%)
8	ANP	C	600	6	27,33,33	1.91	8 (29%)	30,52,52	2.47	8 (26%)
8	ANP	D	600	6	27,33,33	1.76	8 (29%)	30,52,52	2.27	9 (30%)
8	ANP	F	600	6	27,33,33	1.87	7 (25%)	30,52,52	2.56	7 (23%)
8	ANP	J	600	6	27,33,33	1.98	8 (29%)	30,52,52	2.59	6 (20%)
8	ANP	K	600	6	27,33,33	1.94	6 (22%)	30,52,52	2.42	7 (23%)
8	ANP	L	600	6	27,33,33	2.05	7 (25%)	30,52,52	2.53	9 (30%)
8	ANP	M	600	6	27,33,33	1.93	7 (25%)	30,52,52	2.65	8 (26%)
7	PO4	N	800	-	4,4,4	0.45	0	6,6,6	0.29	0
8	ANP	O	600	6	27,33,33	2.02	7 (25%)	30,52,52	2.30	10 (33%)
8	ANP	S	600	6	27,33,33	2.19	5 (18%)	30,52,52	2.67	12 (40%)
8	ANP	T	600	6	27,33,33	2.22	7 (25%)	30,52,52	2.21	6 (20%)
8	ANP	U	600	6	27,33,33	2.01	7 (25%)	30,52,52	2.06	7 (23%)
8	ANP	V	600	6	27,33,33	2.09	7 (25%)	30,52,52	2.30	7 (23%)
8	ANP	X	600	6	27,33,33	1.90	5 (18%)	30,52,52	2.75	9 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ANP	A	600	6	-	2/12/38/38	0/3/3/3
8	ANP	B	600	6	-	1/12/38/38	0/3/3/3
8	ANP	C	600	6	-	2/12/38/38	0/3/3/3
8	ANP	D	600	6	-	1/12/38/38	0/3/3/3
8	ANP	F	600	6	-	0/12/38/38	0/3/3/3
8	ANP	J	600	6	-	1/12/38/38	0/3/3/3
8	ANP	K	600	6	-	2/12/38/38	0/3/3/3
8	ANP	L	600	6	-	2/12/38/38	0/3/3/3
8	ANP	M	600	6	-	0/12/38/38	0/3/3/3
7	PO4	N	800	-	-	0/0/0/0	0/0/0/0
8	ANP	O	600	6	-	0/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ANP	S	600	6	-	1/12/38/38	0/3/3/3
8	ANP	T	600	6	-	1/12/38/38	0/3/3/3
8	ANP	U	600	6	-	0/12/38/38	0/3/3/3
8	ANP	V	600	6	-	0/12/38/38	0/3/3/3
8	ANP	X	600	6	-	0/12/38/38	0/3/3/3

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	600	ANP	PB-O2B	-2.93	1.48	1.56
8	C	600	ANP	PG-O2G	-2.83	1.48	1.56
8	A	600	ANP	PG-O2G	-2.67	1.49	1.56
8	J	600	ANP	PG-O2G	-2.59	1.49	1.56
8	L	600	ANP	PB-O2B	-2.50	1.49	1.56
8	L	600	ANP	PG-O2G	-2.49	1.49	1.56
8	O	600	ANP	PB-O2B	-2.43	1.49	1.56
8	D	600	ANP	PG-O3G	-2.38	1.50	1.56
8	F	600	ANP	PB-O2B	-2.24	1.50	1.56
8	T	600	ANP	PG-O3G	-2.23	1.50	1.56
8	M	600	ANP	PG-O3G	-2.18	1.50	1.56
8	V	600	ANP	PG-O3G	-2.16	1.50	1.56
8	D	600	ANP	PB-O2B	-2.14	1.50	1.56
8	O	600	ANP	PG-O2G	-2.12	1.50	1.56
8	D	600	ANP	PG-O2G	-2.06	1.51	1.56
8	F	600	ANP	PG-O3G	-2.03	1.51	1.56
8	K	600	ANP	PB-O3A	2.03	1.61	1.59
8	B	600	ANP	PB-O3A	2.10	1.61	1.59
8	J	600	ANP	O4'-C1'	2.11	1.43	1.41
8	C	600	ANP	PB-O3A	2.15	1.61	1.59
8	V	600	ANP	C2-N3	2.32	1.36	1.32
8	T	600	ANP	O4'-C1'	2.36	1.44	1.41
8	A	600	ANP	PB-O3A	2.44	1.62	1.59
8	A	600	ANP	O4'-C1'	2.44	1.44	1.41
8	M	600	ANP	PB-O3A	2.55	1.62	1.59
8	C	600	ANP	O4'-C1'	2.58	1.44	1.41
8	U	600	ANP	C2-N3	2.62	1.36	1.32
8	J	600	ANP	C5-C4	2.63	1.46	1.40
8	S	600	ANP	PB-O1B	2.75	1.49	1.46
8	D	600	ANP	C5-C4	2.80	1.46	1.40
8	O	600	ANP	PB-O1B	2.88	1.49	1.46
8	F	600	ANP	C5-C4	2.89	1.47	1.40
8	M	600	ANP	PG-N3B	2.92	1.71	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	600	ANP	PB-N3B	2.94	1.71	1.63
8	M	600	ANP	C5-C4	2.95	1.47	1.40
8	D	600	ANP	PB-O1B	2.99	1.49	1.46
8	U	600	ANP	PB-O3A	3.02	1.62	1.59
8	B	600	ANP	C5-C4	3.06	1.47	1.40
8	C	600	ANP	C5-C4	3.07	1.47	1.40
8	B	600	ANP	PB-N3B	3.19	1.71	1.63
8	A	600	ANP	C5-C4	3.20	1.47	1.40
8	O	600	ANP	C5-C4	3.22	1.47	1.40
8	V	600	ANP	C5-C4	3.23	1.47	1.40
8	D	600	ANP	PG-O1G	3.27	1.49	1.46
8	J	600	ANP	PB-N3B	3.32	1.72	1.63
8	K	600	ANP	C5-C4	3.32	1.48	1.40
8	S	600	ANP	C5-C4	3.34	1.48	1.40
8	J	600	ANP	PB-O3A	3.35	1.63	1.59
8	T	600	ANP	C5-C4	3.36	1.48	1.40
8	X	600	ANP	C5-C4	3.38	1.48	1.40
8	B	600	ANP	PG-N3B	3.47	1.72	1.63
8	L	600	ANP	PB-N3B	3.48	1.72	1.63
8	F	600	ANP	PB-O1B	3.52	1.50	1.46
8	C	600	ANP	PG-N3B	3.56	1.72	1.63
8	U	600	ANP	C5-C4	3.56	1.48	1.40
8	U	600	ANP	PG-N3B	3.60	1.72	1.63
8	C	600	ANP	PB-O1B	3.61	1.50	1.46
8	L	600	ANP	PG-O1G	3.61	1.50	1.46
8	U	600	ANP	PG-O1G	3.62	1.50	1.46
8	M	600	ANP	PB-N3B	3.68	1.73	1.63
8	V	600	ANP	PG-N3B	3.70	1.73	1.63
8	L	600	ANP	C5-C4	3.70	1.48	1.40
8	L	600	ANP	PG-N3B	3.72	1.73	1.63
8	F	600	ANP	PG-N3B	3.73	1.73	1.63
8	J	600	ANP	PG-N3B	3.75	1.73	1.63
8	X	600	ANP	PG-N3B	3.83	1.73	1.63
8	K	600	ANP	PB-O1B	3.84	1.50	1.46
8	D	600	ANP	PG-N3B	3.89	1.73	1.63
8	B	600	ANP	PG-O1G	3.90	1.50	1.46
8	X	600	ANP	PG-O1G	3.95	1.50	1.46
8	A	600	ANP	PG-N3B	3.98	1.73	1.63
8	F	600	ANP	PB-N3B	4.02	1.74	1.63
8	K	600	ANP	PG-O1G	4.02	1.50	1.46
8	J	600	ANP	PB-O1B	4.02	1.50	1.46
8	D	600	ANP	PB-N3B	4.05	1.74	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	600	ANP	PG-N3B	4.12	1.74	1.63
8	U	600	ANP	PB-O1B	4.12	1.50	1.46
8	X	600	ANP	PB-N3B	4.17	1.74	1.63
8	K	600	ANP	PB-N3B	4.18	1.74	1.63
8	F	600	ANP	PG-O1G	4.23	1.51	1.46
8	O	600	ANP	PB-N3B	4.23	1.74	1.63
8	X	600	ANP	PB-O1B	4.24	1.51	1.46
8	A	600	ANP	PB-N3B	4.24	1.74	1.63
8	V	600	ANP	PB-N3B	4.35	1.74	1.63
8	T	600	ANP	PG-N3B	4.35	1.74	1.63
8	S	600	ANP	PB-N3B	4.37	1.74	1.63
8	U	600	ANP	PB-N3B	4.37	1.74	1.63
8	M	600	ANP	PB-O1B	4.40	1.51	1.46
8	O	600	ANP	PG-N3B	4.43	1.75	1.63
8	T	600	ANP	PB-N3B	4.43	1.75	1.63
8	J	600	ANP	PG-O1G	4.50	1.51	1.46
8	V	600	ANP	PB-O1B	4.60	1.51	1.46
8	S	600	ANP	PG-N3B	4.67	1.75	1.63
8	C	600	ANP	PG-O1G	4.68	1.51	1.46
8	M	600	ANP	PG-O1G	4.79	1.51	1.46
8	T	600	ANP	PB-O1B	4.97	1.51	1.46
8	A	600	ANP	PB-O1B	5.09	1.51	1.46
8	O	600	ANP	PG-O1G	5.11	1.52	1.46
8	V	600	ANP	PG-O1G	5.22	1.52	1.46
8	L	600	ANP	PB-O1B	5.30	1.52	1.46
8	A	600	ANP	PG-O1G	5.31	1.52	1.46
8	T	600	ANP	PG-O1G	5.50	1.52	1.46
8	B	600	ANP	PB-O1B	5.73	1.52	1.46
8	S	600	ANP	PG-O1G	6.91	1.54	1.46

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	600	ANP	N3-C2-N1	-9.66	121.50	128.89
8	X	600	ANP	N3-C2-N1	-8.94	122.05	128.89
8	S	600	ANP	N3-C2-N1	-8.77	122.18	128.89
8	J	600	ANP	O1G-PG-N3B	-8.65	98.62	111.90
8	M	600	ANP	N3-C2-N1	-8.27	122.56	128.89
8	K	600	ANP	N3-C2-N1	-8.16	122.65	128.89
8	C	600	ANP	N3-C2-N1	-7.84	122.89	128.89
8	O	600	ANP	N3-C2-N1	-7.76	122.96	128.89
8	J	600	ANP	N3-C2-N1	-7.61	123.07	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	600	ANP	N3-C2-N1	-7.54	123.12	128.89
8	L	600	ANP	N3-C2-N1	-7.45	123.19	128.89
8	B	600	ANP	O1G-PG-N3B	-7.00	101.17	111.90
8	C	600	ANP	O1G-PG-N3B	-6.90	101.31	111.90
8	T	600	ANP	N3-C2-N1	-6.83	123.67	128.89
8	A	600	ANP	N3-C2-N1	-6.83	123.67	128.89
8	L	600	ANP	O1G-PG-N3B	-6.76	101.54	111.90
8	V	600	ANP	N3-C2-N1	-6.42	123.98	128.89
8	M	600	ANP	O1G-PG-N3B	-6.26	102.30	111.90
8	B	600	ANP	N3-C2-N1	-6.14	124.19	128.89
8	X	600	ANP	O1G-PG-N3B	-6.09	102.56	111.90
8	U	600	ANP	N3-C2-N1	-5.88	124.39	128.89
8	A	600	ANP	O1G-PG-N3B	-5.84	102.94	111.90
8	K	600	ANP	O1G-PG-N3B	-5.83	102.96	111.90
8	F	600	ANP	O1G-PG-N3B	-5.75	103.09	111.90
8	M	600	ANP	C2'-C1'-N9	-5.07	106.54	114.29
8	X	600	ANP	O1B-PB-N3B	-4.94	104.32	111.90
8	D	600	ANP	O1B-PB-N3B	-4.92	104.35	111.90
8	U	600	ANP	O1G-PG-N3B	-4.64	104.78	111.90
8	V	600	ANP	C2'-C1'-N9	-4.46	107.48	114.29
8	T	600	ANP	O1G-PG-N3B	-4.42	105.11	111.90
8	T	600	ANP	PA-O3A-PB	-4.42	117.84	132.67
8	V	600	ANP	PA-O3A-PB	-4.36	118.03	132.67
8	V	600	ANP	O1B-PB-N3B	-4.27	105.35	111.90
8	O	600	ANP	O1G-PG-N3B	-4.10	105.62	111.90
8	S	600	ANP	C2'-C1'-N9	-4.09	108.04	114.29
8	S	600	ANP	O1G-PG-N3B	-4.09	105.63	111.90
8	X	600	ANP	PA-O3A-PB	-3.92	119.52	132.67
8	M	600	ANP	O1B-PB-N3B	-3.65	106.30	111.90
8	X	600	ANP	C2'-C1'-N9	-3.61	108.78	114.29
8	A	600	ANP	C2'-C1'-N9	-3.59	108.80	114.29
8	O	600	ANP	C2'-C1'-N9	-3.57	108.84	114.29
8	B	600	ANP	C4-C5-N7	-3.52	106.24	109.48
8	S	600	ANP	C1'-N9-C4	-3.51	121.65	126.94
8	V	600	ANP	C4-C5-N7	-3.47	106.29	109.48
8	U	600	ANP	C4-C5-N7	-3.44	106.31	109.48
8	D	600	ANP	C2'-C1'-N9	-3.35	109.18	114.29
8	T	600	ANP	C4-C5-N7	-3.32	106.42	109.48
8	O	600	ANP	O1B-PB-N3B	-3.31	106.82	111.90
8	D	600	ANP	PA-O3A-PB	-3.28	121.67	132.67
8	K	600	ANP	PA-O3A-PB	-3.27	121.71	132.67
8	S	600	ANP	PA-O3A-PB	-3.25	121.76	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	600	ANP	C4-C5-N7	-3.23	106.51	109.48
8	L	600	ANP	O1B-PB-N3B	-3.22	106.96	111.90
8	D	600	ANP	O1G-PG-N3B	-3.15	107.07	111.90
8	J	600	ANP	C2'-C1'-N9	-3.06	109.62	114.29
8	U	600	ANP	O1B-PB-N3B	-3.05	107.22	111.90
8	J	600	ANP	C4-C5-N7	-2.99	106.73	109.48
8	S	600	ANP	C4-C5-N7	-2.91	106.81	109.48
8	K	600	ANP	C4-C5-N7	-2.87	106.84	109.48
8	L	600	ANP	C2'-C1'-N9	-2.86	109.92	114.29
8	S	600	ANP	O2G-PG-O1G	-2.77	106.13	113.49
8	O	600	ANP	PA-O3A-PB	-2.76	123.41	132.67
8	C	600	ANP	C4-C5-N7	-2.62	107.07	109.48
8	L	600	ANP	O3A-PA-O5'	-2.61	96.01	102.94
8	B	600	ANP	O3A-PB-N3B	-2.59	99.30	106.44
8	A	600	ANP	O3A-PB-N3B	-2.50	99.55	106.44
8	T	600	ANP	C2'-C1'-N9	-2.42	110.59	114.29
8	F	600	ANP	C2'-C1'-N9	-2.34	110.71	114.29
8	O	600	ANP	C4-C5-N7	-2.32	107.34	109.48
8	F	600	ANP	PA-O3A-PB	-2.29	125.00	132.67
8	X	600	ANP	C4-C5-N7	-2.16	107.49	109.48
8	A	600	ANP	C4-C5-N7	-2.14	107.51	109.48
8	M	600	ANP	PA-O3A-PB	-2.14	125.50	132.67
8	C	600	ANP	PA-O3A-PB	-2.08	125.71	132.67
8	B	600	ANP	PA-O3A-PB	-2.06	125.77	132.67
8	D	600	ANP	C4-C5-N7	-2.04	107.60	109.48
8	B	600	ANP	O1B-PB-N3B	-2.00	108.83	111.90
8	C	600	ANP	O3G-PG-O2G	2.11	113.83	107.58
8	F	600	ANP	O3G-PG-O2G	2.13	113.89	107.58
8	M	600	ANP	C4'-O4'-C1'	2.15	112.08	109.72
8	D	600	ANP	C2-N1-C6	2.15	122.61	118.77
8	L	600	ANP	O3G-PG-O2G	2.15	113.96	107.58
8	K	600	ANP	C2-N1-C6	2.16	122.63	118.77
8	L	600	ANP	O2G-PG-O1G	2.17	119.28	113.49
8	U	600	ANP	C4'-O4'-C1'	2.23	112.17	109.72
8	A	600	ANP	O2B-PB-O3A	2.26	115.36	105.09
8	C	600	ANP	O2B-PB-O3A	2.33	115.67	105.09
8	O	600	ANP	O3G-PG-O2G	2.33	114.50	107.58
8	C	600	ANP	C2-N1-C6	2.40	123.05	118.77
8	O	600	ANP	C2-N1-C6	2.43	123.11	118.77
8	V	600	ANP	C4'-O4'-C1'	2.49	112.45	109.72
8	A	600	ANP	O3G-PG-O1G	2.51	120.16	113.49
8	S	600	ANP	C2-N1-C6	2.52	123.28	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	O	600	ANP	C4'-O4'-C1'	2.62	112.59	109.72
8	X	600	ANP	O3G-PG-O2G	2.73	115.67	107.58
8	S	600	ANP	O3G-PG-O2G	2.76	115.75	107.58
8	J	600	ANP	O3G-PG-O1G	2.82	120.99	113.49
8	U	600	ANP	O3G-PG-O2G	2.86	116.06	107.58
8	L	600	ANP	C2-N1-C6	2.99	124.10	118.77
8	D	600	ANP	O2B-PB-O1B	3.01	116.27	110.00
8	S	600	ANP	O2B-PB-O1B	3.02	116.30	110.00
8	F	600	ANP	C2-N1-C6	3.06	124.23	118.77
8	X	600	ANP	C2-N1-C6	3.08	124.27	118.77
8	S	600	ANP	O3G-PG-O1G	3.15	121.87	113.49
8	A	600	ANP	O3G-PG-O2G	3.22	117.13	107.58
8	K	600	ANP	O3G-PG-O2G	3.30	117.36	107.58
8	S	600	ANP	O4'-C1'-N9	3.40	115.22	108.10
8	D	600	ANP	O3G-PG-O2G	3.55	118.10	107.58
8	J	600	ANP	O2B-PB-O1B	3.83	118.00	110.00
8	K	600	ANP	O2B-PB-O1B	3.88	118.10	110.00
8	O	600	ANP	O2B-PB-O1B	3.90	118.15	110.00
8	X	600	ANP	O2B-PB-O1B	3.97	118.28	110.00
8	U	600	ANP	O2B-PB-O1B	4.03	118.41	110.00
8	F	600	ANP	O2B-PB-O1B	4.21	118.78	110.00
8	L	600	ANP	O2B-PB-O1B	4.24	118.86	110.00
8	B	600	ANP	O2B-PB-O1B	4.45	119.28	110.00
8	V	600	ANP	O2B-PB-O1B	4.53	119.46	110.00
8	T	600	ANP	O2B-PB-O1B	4.85	120.13	110.00
8	M	600	ANP	O2B-PB-O1B	5.13	120.70	110.00
8	C	600	ANP	O2B-PB-O1B	5.23	120.92	110.00

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	600	ANP	O1G-PG-N3B-PB
8	J	600	ANP	O1B-PB-N3B-PG
8	A	600	ANP	O1G-PG-N3B-PB
8	B	600	ANP	O1B-PB-N3B-PG
8	A	600	ANP	O1B-PB-N3B-PG
8	S	600	ANP	O1G-PG-N3B-PB
8	D	600	ANP	O1B-PB-N3B-PG
8	L	600	ANP	O1B-PB-N3B-PG
8	K	600	ANP	O1G-PG-N3B-PB
8	T	600	ANP	O1B-PB-N3B-PG

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Mol	Chain	Res	Type	Atoms
8	C	600	ANP	O1G-PG-N3B-PB
8	K	600	ANP	O1B-PB-N3B-PG
8	C	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	600	ANP	1	0
8	F	600	ANP	2	0
8	K	600	ANP	1	0
8	L	600	ANP	1	0
8	M	600	ANP	6	0
8	S	600	ANP	1	0
8	V	600	ANP	3	0
8	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	482/510 (94%)	0.28	13 (2%) 58 45	41, 64, 77, 93	0
1	B	483/510 (94%)	0.56	31 (6%) 23 14	49, 69, 89, 110	0
1	C	484/510 (94%)	0.44	29 (5%) 25 15	48, 66, 86, 108	0
1	J	481/510 (94%)	0.50	34 (7%) 19 10	50, 65, 82, 103	0
1	K	486/510 (95%)	0.65	46 (9%) 10 5	55, 72, 84, 107	0
1	L	482/510 (94%)	0.37	23 (4%) 34 23	49, 66, 82, 100	0
1	S	480/510 (94%)	0.61	43 (8%) 12 6	59, 71, 84, 99	0
1	T	481/510 (94%)	1.07	91 (18%) 2 1	54, 68, 84, 123	0
1	U	481/510 (94%)	1.09	102 (21%) 1 1	51, 67, 86, 111	0
2	D	470/478 (98%)	0.43	27 (5%) 27 17	45, 67, 93, 107	0
2	E	468/478 (97%)	0.56	42 (8%) 12 6	44, 68, 87, 100	0
2	F	469/478 (98%)	0.41	22 (4%) 35 24	51, 67, 83, 104	0
2	M	470/478 (98%)	0.50	26 (5%) 29 18	46, 66, 90, 112	0
2	N	470/478 (98%)	0.72	62 (13%) 4 2	53, 69, 88, 115	0
2	O	468/478 (97%)	0.48	33 (7%) 19 10	50, 68, 85, 102	0
2	V	470/478 (98%)	1.03	80 (17%) 2 1	57, 74, 94, 135	0
2	W	467/478 (97%)	0.94	80 (17%) 2 1	54, 67, 85, 108	0
2	X	469/478 (98%)	0.97	68 (14%) 3 2	54, 72, 90, 124	0
3	G	265/278 (95%)	0.26	27 (10%) 9 4	21, 64, 90, 97	0
3	P	243/278 (87%)	1.10	61 (25%) 1 0	28, 93, 121, 127	0
3	Y	200/278 (71%)	1.25	56 (28%) 1 0	64, 107, 127, 132	0
4	H	120/138 (86%)	1.54	44 (36%) 0 0	60, 91, 129, 131	0
4	Q	84/138 (60%)	1.59	27 (32%) 1 0	88, 107, 134, 137	0
4	Z	17/138 (12%)	2.48	10 (58%) 0 0	132, 134, 140, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
5	1	27/61 (44%)	2.03	11 (40%) 0 0	107, 111, 115, 115	0
5	I	48/61 (78%)	0.88	8 (16%) 2 1	71, 84, 93, 94	0
5	R	34/61 (55%)	1.33	10 (29%) 1 0	95, 103, 112, 115	0
All	All	9599/10323 (92%)	0.69	1106 (11%) 6 3	21, 69, 99, 140	0

All (1106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	398	GLU	13.2
3	P	126	ILE	10.1
2	X	28	SER	7.8
1	U	509	THR	7.7
2	X	29	GLU	7.7
1	U	394	LEU	7.7
1	B	397	ALA	7.6
2	V	10	THR	7.6
2	V	8	PRO	7.6
2	V	43	GLN	7.5
2	X	249	GLN	7.2
2	V	7	THR	7.0
2	W	27	GLN	6.9
1	B	411	ASP	6.8
2	X	7	THR	6.8
4	Q	15	ALA	6.8
3	Y	163	SER	6.7
2	W	390	ILE	6.7
2	V	6	SER	6.4
2	X	248	GLY	6.4
1	K	465	GLU	6.4
4	Q	36	SER	6.4
1	U	418	GLN	6.4
2	W	44	GLY	6.2
1	K	195	SER	6.2
2	D	208	ASN	6.0
3	P	39	ILE	6.0
2	V	473	LEU	6.0
2	W	8	PRO	6.0
2	X	43	GLN	6.0
2	X	8	PRO	5.9
2	X	211	GLY	5.9
2	V	474	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
3	G	173	LEU	5.8
2	V	210	GLU	5.8
2	V	57	ASN	5.8
3	P	187	THR	5.8
1	U	26	ASN	5.7
2	X	284	THR	5.7
1	T	415	SER	5.7
2	N	474	ALA	5.7
3	P	53	LYS	5.7
2	N	394	ASP	5.7
2	V	42	PRO	5.7
1	U	126	ALA	5.6
1	T	48	ASN	5.6
1	T	406	ALA	5.6
2	W	389	ALA	5.6
2	V	37	LEU	5.6
2	V	393	MET	5.5
1	K	379	ALA	5.5
1	U	494	GLU	5.5
1	J	416	THR	5.5
1	S	415	SER	5.5
4	Z	121	ALA	5.5
1	T	87	GLY	5.5
1	U	456	ASP	5.4
2	N	7	THR	5.4
1	T	509	THR	5.3
2	E	473	LEU	5.3
2	V	80	GLY	5.3
2	V	27	GLN	5.3
2	X	82	PRO	5.3
1	U	495	LEU	5.2
1	U	85	LYS	5.2
2	V	28	SER	5.2
1	U	317	LYS	5.2
1	T	457	GLY	5.1
2	W	342	LEU	5.1
1	K	194	GLY	5.1
2	O	7	THR	5.1
2	V	41	THR	5.1
2	M	6	SER	5.1
2	V	9	ILE	5.0
2	N	398	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	T	43	VAL	5.0
3	P	71	LYS	5.0
1	T	414	ALA	5.0
2	W	414	LEU	5.0
1	U	390	GLY	5.0
1	B	26	ASN	5.0
2	V	110	LYS	5.0
2	X	42	PRO	4.9
4	Q	79	PRO	4.9
3	Y	18	LYS	4.9
1	T	411	ASP	4.9
3	Y	39	ILE	4.9
2	W	159	ALA	4.9
2	X	212	GLU	4.9
2	D	6	SER	4.8
2	O	212	GLU	4.8
2	E	389	ALA	4.8
1	U	28	ASN	4.8
1	U	55	VAL	4.7
3	P	54	ASN	4.7
2	D	7	THR	4.7
1	K	411	ASP	4.7
2	D	473	LEU	4.7
2	V	177	ALA	4.7
2	D	248	GLY	4.7
1	U	405	PHE	4.7
1	B	404	ALA	4.7
3	P	36	LYS	4.6
2	W	301	LYS	4.6
2	W	474	ALA	4.6
2	M	7	THR	4.6
1	U	315	SER	4.6
2	E	210	GLU	4.6
2	X	110	LYS	4.6
1	T	28	ASN	4.6
1	B	407	GLN	4.6
1	U	65	ALA	4.6
1	U	508	ALA	4.6
2	E	27	GLN	4.5
3	P	204	ASN	4.5
3	Y	45	ASP	4.5
1	T	29	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	S	27	LEU	4.5
2	W	473	LEU	4.5
4	H	95	SER	4.5
1	U	493	LYS	4.5
2	N	467	VAL	4.5
2	V	108	PRO	4.5
3	Y	104	ASN	4.5
2	W	472	LYS	4.5
4	Q	80	ASP	4.5
3	Y	119	LEU	4.5
2	W	42	PRO	4.5
3	Y	173	LEU	4.5
4	Z	126	GLN	4.5
1	T	472	SER	4.4
1	K	509	THR	4.4
1	U	63	GLY	4.4
2	V	428	PRO	4.4
3	P	206	PRO	4.4
1	T	59	SER	4.4
2	M	28	SER	4.4
4	H	63	SER	4.4
1	T	412	LEU	4.4
4	Q	81	SER	4.4
2	W	391	LEU	4.4
1	B	405	PHE	4.4
5	I	33	SER	4.4
5	1	33	SER	4.4
4	Q	37	GLY	4.4
1	K	414	ALA	4.4
3	P	32	SER	4.4
4	H	135	SER	4.4
4	H	106	ALA	4.4
2	M	29	GLU	4.3
5	I	29	LEU	4.3
1	U	412	LEU	4.3
1	U	387	GLN	4.3
2	N	465	ASP	4.3
5	R	27	THR	4.3
1	U	198	SER	4.3
1	U	487	GLU	4.3
2	F	179	GLY	4.3
2	X	210	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	414	ALA	4.3
2	W	392	GLY	4.2
1	T	468	SER	4.2
1	U	56	GLU	4.2
4	H	97	SER	4.2
2	N	475	ALA	4.2
1	S	459	GLU	4.2
1	J	26	ASN	4.2
4	H	100	ASN	4.2
2	V	302	GLY	4.2
1	J	459	GLU	4.2
1	S	401	GLU	4.2
2	W	105	GLU	4.2
4	Q	131	GLU	4.2
2	V	79	THR	4.1
4	Z	135	SER	4.1
2	N	27	GLN	4.1
2	V	107	GLY	4.1
2	O	210	GLU	4.1
1	T	30	THR	4.1
2	W	447	GLY	4.1
1	B	400	ARG	4.1
1	U	399	TYR	4.1
2	W	210	GLU	4.1
1	J	89	LEU	4.1
4	Q	90	ALA	4.1
3	Y	8	MET	4.1
1	T	508	ALA	4.1
1	U	83	LEU	4.1
1	U	401	GLU	4.1
2	D	43	GLN	4.0
3	P	111	GLY	4.0
1	S	378	SER	4.0
2	M	27	GLN	4.0
2	W	55	GLY	4.0
2	V	449	TYR	4.0
1	U	62	LYS	4.0
4	Q	103	ASN	4.0
2	X	9	ILE	4.0
3	Y	43	LYS	4.0
2	O	26	GLU	4.0
2	X	26	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	U	417	LYS	3.9
1	J	195	SER	3.9
2	N	28	SER	3.9
2	F	7	THR	3.9
2	D	246	GLU	3.9
1	B	476	SER	3.9
1	U	29	GLU	3.9
2	X	341	GLU	3.9
1	U	407	GLN	3.9
2	W	386	ASP	3.9
1	U	94	GLY	3.9
4	Q	135	SER	3.9
1	S	48	ASN	3.9
1	U	125	ALA	3.9
2	W	37	LEU	3.9
2	V	455	HIS	3.9
2	O	43	GLN	3.9
1	U	413	ASP	3.9
1	S	319	GLY	3.9
1	T	476	SER	3.9
4	H	99	GLU	3.8
3	P	100	ASN	3.8
1	C	203	CYS	3.8
4	H	107	GLU	3.8
2	N	6	SER	3.8
3	Y	40	SER	3.8
1	T	480	GLU	3.8
2	E	474	ALA	3.8
1	S	418	GLN	3.8
1	L	509	THR	3.8
1	T	26	ASN	3.8
1	T	454	HIS	3.8
2	M	398	GLU	3.8
2	V	112	LYS	3.8
4	H	36	SER	3.8
4	Z	120	ALA	3.7
3	G	50	LEU	3.7
1	T	72	GLN	3.7
2	N	176	LYS	3.7
5	1	41	ASP	3.7
2	V	101	GLU	3.7
4	H	103	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	U	489	GLY	3.7
1	S	195	SER	3.7
2	V	249	GLN	3.7
3	G	46	GLU	3.7
2	N	468	ALA	3.7
2	V	396	LEU	3.7
2	V	212	GLU	3.7
2	W	399	GLN	3.7
4	Z	134	GLN	3.7
2	E	395	GLU	3.7
2	W	81	GLY	3.7
1	U	380	ALA	3.7
1	B	195	SER	3.6
1	S	49	ILE	3.6
2	N	158	GLY	3.6
2	N	366	GLU	3.6
1	T	27	LEU	3.6
2	E	44	GLY	3.6
1	U	457	GLY	3.6
2	X	61	THR	3.6
4	H	113	SER	3.6
5	R	28	GLU	3.6
1	S	37	GLY	3.6
1	T	323	LEU	3.6
2	V	75	LYS	3.6
3	Y	15	ASN	3.6
1	J	476	SER	3.6
3	Y	123	PRO	3.6
3	Y	100	ASN	3.6
1	B	203	CYS	3.6
1	T	322	SER	3.6
1	J	27	LEU	3.6
5	1	13	TYR	3.6
1	T	93	THR	3.6
1	K	377	GLY	3.6
4	H	22	TYR	3.5
4	H	134	GLN	3.5
1	U	379	ALA	3.5
4	H	121	ALA	3.5
1	U	134	LYS	3.5
2	M	41	THR	3.5
1	K	508	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	393	LYS	3.5
4	H	111	ASN	3.5
4	H	42	LEU	3.5
1	T	55	VAL	3.5
2	N	399	GLN	3.5
1	T	32	ARG	3.5
2	W	212	GLU	3.5
3	Y	7	GLU	3.5
1	T	202	TYR	3.5
3	P	50	LEU	3.5
4	H	114	SER	3.5
3	P	97	ARG	3.5
2	M	394	ASP	3.5
2	E	8	PRO	3.5
1	U	27	LEU	3.5
2	V	214	LYS	3.5
3	G	170	VAL	3.5
2	O	211	GLY	3.5
2	X	73	GLY	3.5
3	G	201	THR	3.5
1	T	445	PRO	3.5
2	X	89	ARG	3.5
2	W	358	LEU	3.5
2	D	27	GLN	3.5
2	W	56	GLU	3.5
2	X	27	GLN	3.5
2	F	451	ASN	3.5
1	C	449	ALA	3.5
1	T	493	LYS	3.5
3	P	184	ASN	3.4
2	M	395	GLU	3.4
3	P	170	VAL	3.4
1	K	192	ASN	3.4
2	N	159	ALA	3.4
2	W	82	PRO	3.4
2	N	338	GLY	3.4
1	T	195	SER	3.4
1	T	101	VAL	3.4
1	U	48	ASN	3.4
1	T	258	TRP	3.4
1	T	371	LEU	3.4
4	H	92	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
4	H	125	ILE	3.4
1	L	464	GLY	3.4
3	Y	171	SER	3.4
1	C	65	ALA	3.4
5	1	17	ALA	3.4
2	W	57	ASN	3.4
1	T	121	GLY	3.4
1	J	322	SER	3.4
2	X	59	VAL	3.4
2	W	410	ILE	3.4
3	Y	212	TYR	3.4
1	A	65	ALA	3.4
1	C	414	ALA	3.4
1	S	266	ALA	3.4
2	W	209	LEU	3.3
3	Y	124	ASN	3.3
3	Y	44	MET	3.3
2	X	242	TYR	3.3
1	U	127	GLY	3.3
2	W	43	GLN	3.3
1	B	346	SER	3.3
1	U	415	SER	3.3
4	Q	47	PRO	3.3
1	K	418	GLN	3.3
1	L	27	LEU	3.3
1	U	32	ARG	3.3
3	Y	105	ALA	3.3
1	T	197	GLU	3.3
2	W	397	SER	3.3
1	K	417	LYS	3.3
3	P	160	PRO	3.3
1	J	55	VAL	3.3
1	S	42	ARG	3.3
1	U	504	GLU	3.3
2	F	216	ALA	3.3
1	L	203	CYS	3.3
1	U	445	PRO	3.3
3	P	101	ASP	3.3
3	Y	172	SER	3.3
5	1	9	SER	3.3
3	Y	120	ARG	3.3
4	H	26	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
4	H	136	VAL	3.3
3	Y	41	ALA	3.3
5	I	27	THR	3.3
2	W	28	SER	3.3
2	N	43	GLN	3.2
2	V	26	GLU	3.2
2	V	471	GLU	3.2
3	P	171	SER	3.2
1	U	66	LEU	3.2
1	C	391	SER	3.2
1	K	22	SER	3.2
4	Q	97	SER	3.2
1	T	266	ALA	3.2
1	J	93	THR	3.2
2	E	425	THR	3.2
2	W	359	ASP	3.2
1	L	445	PRO	3.2
1	C	204	VAL	3.2
1	T	320	SER	3.2
1	K	405	PHE	3.2
2	M	26	GLU	3.2
1	U	472	SER	3.2
1	T	49	ILE	3.2
1	B	416	THR	3.2
1	C	413	ASP	3.2
1	U	450	GLY	3.2
3	G	192	PRO	3.2
1	T	360	TYR	3.2
1	U	414	ALA	3.2
1	K	489	GLY	3.2
2	M	179	GLY	3.2
3	Y	36	LYS	3.2
2	W	436	ASP	3.2
3	P	1	ALA	3.1
1	B	345	ILE	3.1
2	W	9	ILE	3.1
1	B	410	SER	3.1
3	G	191	SER	3.1
3	Y	98	HIS	3.1
1	K	412	LEU	3.1
2	F	176	LYS	3.1
4	H	46	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	454	HIS	3.1
3	P	181	PRO	3.1
1	K	416	THR	3.1
1	B	494	GLU	3.1
1	S	414	ALA	3.1
1	U	199	LYS	3.1
3	P	157	GLY	3.1
2	W	430	LYS	3.1
3	Y	111	GLY	3.1
1	U	44	PHE	3.1
2	N	388	ILE	3.1
3	P	123	PRO	3.1
3	P	43	LYS	3.1
4	Q	108	ALA	3.1
2	N	143	LEU	3.1
3	G	123	PRO	3.1
1	S	32	ARG	3.0
1	T	484	GLU	3.0
2	N	218	VAL	3.0
2	N	138	ILE	3.0
2	N	217	LEU	3.0
1	J	324	THR	3.0
3	G	171	SER	3.0
3	Y	152	SER	3.0
2	O	27	GLN	3.0
5	1	40	THR	3.0
1	T	60	GLY	3.0
2	N	42	PRO	3.0
3	Y	103	PRO	3.0
2	E	26	GLU	3.0
2	W	300	LYS	3.0
4	H	67	LYS	3.0
1	S	457	GLY	3.0
1	T	119	GLY	3.0
1	T	142	ARG	3.0
2	W	395	GLU	3.0
3	P	72	GLU	3.0
2	E	50	VAL	3.0
2	M	474	ALA	3.0
2	M	475	ALA	3.0
3	P	203	ALA	3.0
2	E	9	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	G	174	SER	3.0
1	U	30	THR	3.0
3	Y	4	LYS	3.0
2	D	398	GLU	3.0
2	W	451	ASN	3.0
2	D	210	GLU	3.0
2	X	200	GLU	3.0
3	Y	213	THR	3.0
2	V	475	ALA	3.0
3	Y	149	LYS	3.0
1	U	194	GLY	3.0
2	F	80	GLY	3.0
1	U	316	GLU	3.0
2	N	424	PHE	3.0
1	U	488	LYS	3.0
1	T	124	ASP	3.0
1	S	72	GLN	3.0
2	F	426	GLY	3.0
2	X	150	GLY	3.0
1	T	494	GLU	3.0
1	C	323	LEU	3.0
1	K	505	SER	3.0
1	J	235	ALA	3.0
1	U	226	ASP	3.0
1	S	28	ASN	3.0
3	Y	116	MET	3.0
2	F	110	LYS	3.0
3	G	136	ASP	2.9
2	N	451	ASN	2.9
2	D	37	LEU	2.9
2	M	413	PHE	2.9
2	O	216	ALA	2.9
1	U	483	THR	2.9
2	E	43	GLN	2.9
2	W	112	LYS	2.9
1	L	26	ASN	2.9
1	S	83	LEU	2.9
1	C	508	ALA	2.9
1	U	196	ASP	2.9
2	X	41	THR	2.9
4	H	79	PRO	2.9
1	S	316	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	T	465	GLU	2.9
1	U	72	GLN	2.9
2	W	208	ASN	2.9
2	D	44	GLY	2.9
4	H	120	ALA	2.9
3	G	190	GLN	2.9
3	Y	141	GLN	2.9
1	J	197	GLU	2.9
1	S	67	ASN	2.9
2	V	12	LYS	2.9
4	H	64	ASN	2.9
1	S	203	CYS	2.9
2	V	211	GLY	2.9
4	H	43	ALA	2.9
2	V	76	VAL	2.9
1	U	501	SER	2.9
3	Y	148	ASP	2.9
2	W	341	GLU	2.9
2	X	209	LEU	2.9
1	U	454	HIS	2.9
2	V	208	ASN	2.9
2	M	43	GLN	2.9
1	T	58	SER	2.9
1	C	445	PRO	2.9
2	E	31	PRO	2.9
2	E	398	GLU	2.9
2	O	31	PRO	2.9
1	A	509	THR	2.9
1	J	28	ASN	2.9
1	K	464	GLY	2.9
1	U	404	ALA	2.9
5	I	32	ALA	2.9
1	B	418	GLN	2.9
2	V	29	GLU	2.9
1	T	255	ILE	2.9
2	N	144	LEU	2.9
2	X	204	THR	2.9
2	V	419	ALA	2.9
2	O	399	GLN	2.8
4	Z	123	ALA	2.8
1	L	465	GLU	2.8
1	T	473	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
3	Y	101	ASP	2.8
1	T	492	SER	2.8
2	V	248	GLY	2.8
2	V	59	VAL	2.8
2	W	29	GLU	2.8
2	W	185	THR	2.8
3	Y	29	THR	2.8
1	S	411	ASP	2.8
1	K	362	GLY	2.8
1	U	87	GLY	2.8
1	K	476	SER	2.8
1	J	406	ALA	2.8
2	X	148	ALA	2.8
2	X	475	ALA	2.8
1	U	204	VAL	2.8
2	N	446	GLU	2.8
3	P	153	VAL	2.8
1	K	203	CYS	2.8
1	T	469	SER	2.8
3	G	203	ALA	2.8
4	H	44	ASN	2.8
2	W	351	LEU	2.8
3	Y	33	LYS	2.8
3	G	49	GLN	2.8
3	G	36	LYS	2.8
4	H	12	LEU	2.8
4	H	102	LYS	2.8
1	L	459	GLU	2.8
2	W	246	GLU	2.8
2	W	446	GLU	2.8
2	F	8	PRO	2.8
1	U	119	GLY	2.8
1	C	446	LEU	2.8
1	S	193	ASN	2.8
2	M	414	LEU	2.8
2	X	79	THR	2.8
1	U	130	ARG	2.8
1	U	449	ALA	2.8
1	U	84	VAL	2.8
2	W	440	SER	2.7
5	I	28	GLU	2.7
1	L	196	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	M	37	LEU	2.7
2	W	441	PHE	2.7
3	G	202	ASP	2.7
3	Y	136	ASP	2.7
2	M	91	THR	2.7
2	X	51	ALA	2.7
5	1	44	TYR	2.7
1	U	377	GLY	2.7
1	L	266	ALA	2.7
3	Y	154	MET	2.7
4	H	128	GLU	2.7
4	Z	130	LEU	2.7
1	S	73	VAL	2.7
4	H	35	LYS	2.7
2	M	410	ILE	2.7
3	P	40	SER	2.7
2	F	27	GLN	2.7
3	P	56	GLU	2.7
1	T	33	VAL	2.7
2	F	42	PRO	2.7
2	V	472	LYS	2.7
2	X	163	LYS	2.7
1	T	226	ASP	2.7
1	C	465	GLU	2.7
2	O	183	VAL	2.7
1	J	318	GLU	2.7
2	X	246	GLU	2.7
1	J	475	LYS	2.7
1	K	193	ASN	2.7
1	T	321	GLY	2.7
1	T	334	GLY	2.7
2	N	363	VAL	2.7
2	V	81	GLY	2.7
4	Q	55	GLY	2.7
2	O	108	PRO	2.7
2	W	79	THR	2.7
1	J	480	GLU	2.7
3	P	238	ASP	2.7
2	D	177	ALA	2.7
2	D	211	GLY	2.7
1	T	234	VAL	2.7
1	T	444	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
5	R	13	TYR	2.7
2	N	471	GLU	2.7
3	P	161	LYS	2.7
1	T	196	ASP	2.7
1	B	415	SER	2.7
1	S	61	VAL	2.7
5	1	36	ASN	2.6
1	U	465	GLU	2.6
2	E	37	LEU	2.6
2	M	402	LEU	2.6
2	N	359	ASP	2.6
3	Y	1	ALA	2.6
2	N	343	GLY	2.6
1	K	484	GLU	2.6
2	E	424	PHE	2.6
2	O	44	GLY	2.6
2	V	205	GLY	2.6
2	X	81	GLY	2.6
1	U	148	VAL	2.6
2	F	28	SER	2.6
2	E	386	ASP	2.6
2	O	179	GLY	2.6
2	V	40	LYS	2.6
2	W	80	GLY	2.6
2	M	183	VAL	2.6
2	X	76	VAL	2.6
1	A	26	ASN	2.6
3	Y	131	ASN	2.6
1	T	86	GLU	2.6
2	F	48	LEU	2.6
1	B	493	LYS	2.6
2	O	61	THR	2.6
1	T	254	SER	2.6
2	D	28	SER	2.6
2	X	48	LEU	2.6
1	T	194	GLY	2.6
2	V	36	ALA	2.6
2	X	22	ASP	2.6
4	H	118	ARG	2.6
5	R	12	ALA	2.6
1	L	506	PHE	2.6
3	P	91	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	497	ALA	2.6
2	N	352	ASP	2.6
4	Q	84	CYS	2.6
2	E	140	VAL	2.6
3	P	205	VAL	2.6
3	P	139	THR	2.6
1	K	487	GLU	2.6
1	U	378	SER	2.6
2	E	239	ILE	2.6
2	E	390	ILE	2.6
3	P	179	GLU	2.6
2	V	470	ALA	2.6
2	O	50	VAL	2.6
4	H	96	PHE	2.5
2	X	176	LYS	2.5
3	P	180	LYS	2.5
1	L	404	ALA	2.5
1	U	391	SER	2.5
2	X	128	SER	2.5
3	G	172	SER	2.5
3	Y	162	ILE	2.5
4	H	115	SER	2.5
2	D	42	PRO	2.5
2	O	398	GLU	2.5
2	N	393	MET	2.5
2	V	303	SER	2.5
2	X	216	ALA	2.5
3	Y	156	ALA	2.5
3	P	106	ASP	2.5
2	M	216	ALA	2.5
4	Q	48	THR	2.5
1	C	231	SER	2.5
1	J	196	ASP	2.5
3	P	174	SER	2.5
2	X	301	LYS	2.5
2	V	414	LEU	2.5
2	W	248	GLY	2.5
2	V	114	ARG	2.5
1	C	404	ALA	2.5
4	Z	124	ALA	2.5
1	T	64	MET	2.5
2	N	454	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	X	71	VAL	2.5
2	F	414	LEU	2.5
2	X	93	GLY	2.5
2	D	475	ALA	2.5
3	Y	164	ILE	2.5
1	U	446	LEU	2.5
3	P	98	HIS	2.5
2	V	23	VAL	2.5
2	N	302	GLY	2.5
3	P	104	ASN	2.5
3	P	188	ILE	2.5
4	H	131	GLU	2.5
1	T	85	LYS	2.5
1	C	509	THR	2.5
2	N	403	THR	2.5
1	S	379	ALA	2.5
2	F	43	GLN	2.5
2	V	399	GLN	2.5
5	R	30	GLN	2.5
1	K	200	LYS	2.5
1	C	405	PHE	2.5
4	Q	46	VAL	2.5
1	U	374	SER	2.4
3	G	160	PRO	2.4
3	P	57	THR	2.4
4	H	130	LEU	2.4
4	Q	83	LEU	2.4
1	T	47	ASN	2.4
1	K	404	ALA	2.4
1	S	458	ILE	2.4
4	Q	101	ILE	2.4
1	S	413	ASP	2.4
2	N	426	GLY	2.4
1	A	322	SER	2.4
1	K	499	LEU	2.4
2	W	123	SER	2.4
1	C	28	ASN	2.4
2	E	236	GLY	2.4
2	V	158	GLY	2.4
3	G	245	GLY	2.4
1	K	402	VAL	2.4
1	B	316	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	401	GLU	2.4
1	K	494	GLU	2.4
1	U	482	LEU	2.4
2	D	212	GLU	2.4
1	C	415	SER	2.4
2	O	42	PRO	2.4
2	V	182	SER	2.4
5	1	45	THR	2.4
1	U	334	GLY	2.4
2	X	160	GLY	2.4
2	N	23	VAL	2.4
2	O	29	GLU	2.4
1	U	46	LEU	2.4
1	T	443	GLN	2.4
1	U	116	PRO	2.4
3	P	207	ARG	2.4
1	T	317	LYS	2.4
2	E	301	LYS	2.4
2	W	424	PHE	2.4
1	A	316	GLU	2.4
3	P	8	MET	2.4
1	B	266	ALA	2.4
1	J	325	ALA	2.4
2	X	106	ARG	2.4
3	P	105	ALA	2.4
4	Q	106	ALA	2.4
3	P	183	PHE	2.4
3	G	45	ASP	2.4
2	D	249	GLN	2.4
1	T	120	LYS	2.4
2	M	239	ILE	2.4
3	Y	155	LYS	2.4
1	U	195	SER	2.4
2	N	306	SER	2.4
1	S	465	GLU	2.4
2	N	368	TYR	2.4
2	W	422	GLU	2.4
4	H	94	GLU	2.4
4	Z	133	LEU	2.4
5	R	29	LEU	2.4
1	K	380	ALA	2.4
1	K	122	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	W	26	GLU	2.4
2	X	464	GLU	2.4
4	Q	107	GLU	2.4
2	N	457	PHE	2.4
2	V	147	TYR	2.4
1	S	93	THR	2.4
2	W	315	ASP	2.4
1	K	488	LYS	2.4
3	Y	135	LYS	2.4
2	N	44	GLY	2.4
2	X	105	GLU	2.4
1	T	198	SER	2.4
1	T	145	HIS	2.4
1	U	323	LEU	2.3
2	E	113	LEU	2.3
2	N	434	LEU	2.3
1	U	64	MET	2.3
1	A	508	ALA	2.3
1	K	266	ALA	2.3
2	W	107	GLY	2.3
1	B	475	LYS	2.3
2	X	25	PHE	2.3
3	G	242	LYS	2.3
1	K	204	VAL	2.3
3	Y	168	ASP	2.3
5	R	36	ASN	2.3
1	J	323	LEU	2.3
1	S	323	LEU	2.3
1	T	482	LEU	2.3
1	T	499	LEU	2.3
2	E	253	LEU	2.3
2	W	48	LEU	2.3
5	R	31	THR	2.3
1	T	475	LYS	2.3
2	M	82	PRO	2.3
1	S	468	SER	2.3
1	U	156	ASP	2.3
2	E	182	SER	2.3
2	O	23	VAL	2.3
2	X	359	ASP	2.3
4	Z	127	VAL	2.3
1	A	324	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	266	ALA	2.3
2	D	61	THR	2.3
3	Y	5	GLU	2.3
2	V	344	ILE	2.3
1	J	445	PRO	2.3
2	X	21	VAL	2.3
1	B	267	LEU	2.3
1	C	197	GLU	2.3
1	T	69	GLU	2.3
2	E	394	ASP	2.3
2	V	24	HIS	2.3
1	B	406	ALA	2.3
1	U	416	THR	2.3
2	E	61	THR	2.3
2	N	392	GLY	2.3
1	S	70	PRO	2.3
2	E	23	VAL	2.3
2	W	376	GLU	2.3
3	G	33	LYS	2.3
4	H	57	VAL	2.3
1	T	471	LEU	2.3
2	M	143	LEU	2.3
3	Y	151	LEU	2.3
1	U	115	ASN	2.3
2	O	242	TYR	2.3
2	N	429	GLY	2.3
2	O	239	ILE	2.3
1	B	488	LYS	2.3
2	O	346	PRO	2.3
5	1	34	VAL	2.3
2	E	399	GLN	2.3
2	W	369	ASP	2.3
1	B	202	TYR	2.3
2	X	33	ILE	2.3
2	D	425	THR	2.3
2	V	395	GLU	2.3
1	T	133	VAL	2.3
1	T	83	LEU	2.3
2	E	48	LEU	2.3
2	W	402	LEU	2.3
4	Q	104	LEU	2.3
2	V	371	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	X	84	SER	2.3
3	P	42	LYS	2.3
1	J	75	ILE	2.3
1	B	509	THR	2.3
1	S	424	GLU	2.3
3	P	46	GLU	2.3
5	I	34	VAL	2.3
1	C	196	ASP	2.3
2	D	48	LEU	2.3
2	E	364	GLY	2.3
2	W	426	GLY	2.3
1	L	508	ALA	2.3
2	N	216	ALA	2.3
2	N	430	LYS	2.3
2	X	45	LYS	2.3
2	X	75	LYS	2.3
1	C	477	ASN	2.3
1	K	501	SER	2.3
2	O	208	ASN	2.3
1	T	507	VAL	2.3
2	X	10	THR	2.3
2	N	211	GLY	2.3
2	O	37	LEU	2.3
2	O	180	GLY	2.3
2	V	401	LYS	2.3
2	X	205	GLY	2.3
3	P	99	LEU	2.3
3	Y	132	GLY	2.3
1	J	461	SER	2.2
2	N	336	SER	2.2
2	X	297	THR	2.2
4	H	27	VAL	2.2
1	U	70	PRO	2.2
5	R	41	ASP	2.2
4	H	108	ALA	2.2
2	V	56	GLU	2.2
1	U	477	ASN	2.2
3	P	89	SER	2.2
2	N	41	THR	2.2
1	S	312	ALA	2.2
1	U	266	ALA	2.2
2	F	239	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	P	159	TYR	2.2
2	D	23	VAL	2.2
2	W	158	GLY	2.2
2	W	429	GLY	2.2
4	Q	57	VAL	2.2
2	X	143	LEU	2.2
2	E	112	LYS	2.2
2	N	8	PRO	2.2
2	O	468	ALA	2.2
1	K	268	ILE	2.2
1	S	394	LEU	2.2
1	T	89	LEU	2.2
1	T	459	GLU	2.2
1	K	413	ASP	2.2
2	N	386	ASP	2.2
3	P	169	PRO	2.2
2	F	44	GLY	2.2
2	F	180	GLY	2.2
2	O	311	TYR	2.2
2	V	157	GLY	2.2
2	X	302	GLY	2.2
1	C	267	LEU	2.2
3	P	93	LYS	2.2
2	W	240	ALA	2.2
3	Y	121	THR	2.2
1	L	64	MET	2.2
2	E	446	GLU	2.2
1	A	28	ASN	2.2
1	S	322	SER	2.2
2	N	141	VAL	2.2
3	Y	153	VAL	2.2
1	S	81	ASP	2.2
1	T	41	ALA	2.2
1	T	312	ALA	2.2
2	O	250	ASP	2.2
3	P	112	ASP	2.2
2	E	42	PRO	2.2
2	X	346	PRO	2.2
1	A	75	ILE	2.2
2	V	61	THR	2.2
1	U	37	GLY	2.2
2	X	74	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	140	VAL	2.2
2	E	30	LEU	2.2
2	N	208	ASN	2.2
1	A	266	ALA	2.2
1	J	449	ALA	2.2
2	V	213	SER	2.2
2	V	468	ALA	2.2
2	X	413	PHE	2.2
5	I	43	PHE	2.2
1	C	480	GLU	2.2
1	U	75	ILE	2.2
1	B	360	TYR	2.2
1	K	326	LEU	2.2
4	H	112	VAL	2.2
1	C	322	SER	2.1
1	L	414	ALA	2.2
1	T	262	ASN	2.2
1	U	47	ASN	2.2
3	Y	216	ASN	2.2
2	W	84	SER	2.1
2	W	383	SER	2.1
2	W	394	ASP	2.1
4	Q	35	LYS	2.1
3	P	5	GLU	2.1
2	X	69	GLY	2.1
1	K	482	LEU	2.1
2	F	249	GLN	2.1
4	Q	105	LEU	2.1
1	J	65	ALA	2.1
2	N	361	ALA	2.1
5	R	20	ALA	2.1
1	J	411	ASP	2.1
1	U	480	GLU	2.1
2	N	151	GLY	2.1
1	C	64	MET	2.1
1	L	55	VAL	2.1
3	P	90	GLN	2.1
1	T	126	ALA	2.1
2	V	90	GLU	2.1
1	K	322	SER	2.1
1	L	476	SER	2.1
2	W	337	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	V	448	LYS	2.1
1	T	66	LEU	2.1
2	E	59	VAL	2.1
2	X	206	VAL	2.1
1	J	508	ALA	2.1
2	X	471	GLU	2.1
2	D	179	GLY	2.1
2	N	160	GLY	2.1
1	S	407	GLN	2.1
2	V	13	VAL	2.1
3	Y	217	GLN	2.1
1	U	392	LEU	2.1
4	H	93	LEU	2.1
1	S	29	GLU	2.1
3	G	8	MET	2.1
3	Y	266	GLU	2.1
1	K	104	GLY	2.1
1	U	202	TYR	2.1
2	W	39	ILE	2.1
2	V	86	PRO	2.1
1	J	29	GLU	2.1
2	M	467	VAL	2.1
1	K	475	LYS	2.1
1	T	238	ALA	2.1
2	N	421	ALA	2.1
2	W	119	ALA	2.1
3	P	116	MET	2.1
1	L	470	PHE	2.1
1	J	457	GLY	2.1
1	J	479	ASN	2.1
3	G	32	SER	2.1
1	A	55	VAL	2.1
2	F	31	PRO	2.1
2	V	68	GLU	2.1
1	J	203	CYS	2.1
1	U	189	LYS	2.1
2	W	59	VAL	2.1
2	X	140	VAL	2.1
1	B	64	MET	2.1
2	D	441	PHE	2.1
2	E	136	THR	2.1
3	P	109	THR	2.1

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Mol	Chain	Res	Type	RSRZ
4	H	28	THR	2.1
1	U	268	ILE	2.1
1	U	211	LYS	2.1
2	E	379	GLN	2.1
2	W	464	GLU	2.1
1	A	460	LEU	2.1
1	L	412	LEU	2.1
2	D	8	PRO	2.1
2	V	384	LEU	2.1
1	K	64	MET	2.1
2	E	337	ARG	2.1
2	V	69	GLY	2.1
3	G	134	GLY	2.1
3	G	246	ASP	2.1
2	N	239	ILE	2.1
5	I	10	TYR	2.1
1	C	455	LEU	2.1
1	S	444	VAL	2.1
1	U	322	SER	2.1
1	T	113	LEU	2.1
2	N	362	VAL	2.1
3	Y	134	GLY	2.0
2	O	214	LYS	2.0
2	V	198	TYR	2.0
1	J	477	ASN	2.0
1	U	402	VAL	2.0
2	D	209	LEU	2.0
2	E	217	LEU	2.0
2	E	237	LEU	2.0
2	X	50	VAL	2.0
1	K	258	TRP	2.0
2	W	160	GLY	2.0
3	G	53	LYS	2.0
1	U	53	GLU	2.0
5	1	21	ILE	2.0
1	S	462	ARG	2.0
2	V	204	THR	2.0
2	V	311	TYR	2.0
1	L	201	LEU	2.0
2	W	304	VAL	2.0
3	Y	170	VAL	2.0
2	O	131	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	P	185	ALA	2.0
2	V	181	PHE	2.0
2	V	338	GLY	2.0
1	T	456	ASP	2.0
1	C	232	ILE	2.0
4	Q	82	GLN	2.0
1	C	251	THR	2.0
2	F	342	LEU	2.0
1	J	164	GLY	2.0
1	T	506	PHE	2.0
4	Q	14	PHE	2.0
3	P	208	ASP	2.0
1	L	367	ILE	2.0
2	F	410	ILE	2.0
1	L	317	LYS	2.0
3	P	242	LYS	2.0
1	T	460	LEU	2.0
2	O	48	LEU	2.0
2	W	242	TYR	2.0
1	L	65	ALA	2.0
2	O	474	ALA	2.0
1	U	357	GLU	2.0
2	W	413	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	PO4	N	800	5/5	0.93	0.26	1.42	78,80,84,85	0
6	MG	F	700	1/1	0.98	0.26	0.31	44,44,44,44	0
8	ANP	T	600	31/31	0.95	0.27	0.29	66,89,91,97	0
8	ANP	K	600	31/31	0.97	0.23	-0.24	49,62,70,74	0
8	ANP	J	600	31/31	0.98	0.19	-0.55	23,46,52,53	0
8	ANP	U	600	31/31	0.94	0.20	-0.73	42,57,69,70	0
8	ANP	C	600	31/31	0.97	0.14	-1.30	25,41,50,60	0
8	ANP	L	600	31/31	0.97	0.15	-1.34	17,33,44,48	0
8	ANP	S	600	31/31	0.97	0.16	-1.45	37,52,58,63	0
8	ANP	F	600	31/31	0.96	0.14	-1.52	36,52,60,61	0
8	ANP	B	600	31/31	0.97	0.17	-1.57	29,37,41,44	0
6	MG	D	700	1/1	0.88	0.16	-2.03	46,46,46,46	0
8	ANP	X	600	31/31	0.95	0.15	-2.07	50,61,79,81	0
8	ANP	V	600	31/31	0.94	0.15	-2.09	61,74,81,90	0
8	ANP	A	600	31/31	0.98	0.13	-2.15	14,35,42,43	0
6	MG	V	700	1/1	0.81	0.14	-2.19	69,69,69,69	0
8	ANP	D	600	31/31	0.97	0.10	-2.31	37,51,57,64	0
8	ANP	O	600	31/31	0.97	0.10	-2.74	49,68,71,74	0
6	MG	O	700	1/1	0.80	0.12	-2.92	48,48,48,48	0
8	ANP	M	600	31/31	0.97	0.10	-3.04	31,52,59,65	0
6	MG	M	700	1/1	0.96	0.07	-3.10	52,52,52,52	0
6	MG	X	700	1/1	0.86	0.08	-5.79	67,67,67,67	0
6	MG	S	700	1/1	0.95	0.12	-	40,40,40,40	0
6	MG	B	700	1/1	0.95	0.08	-	43,43,43,43	0
6	MG	C	700	1/1	0.95	0.10	-	43,43,43,43	0
6	MG	U	700	1/1	0.95	0.12	-	78,78,78,78	0
6	MG	A	700	1/1	0.99	0.17	-	34,34,34,34	0
6	MG	L	700	1/1	0.97	0.14	-	49,49,49,49	0
6	MG	K	700	1/1	0.88	0.15	-	52,52,52,52	0
6	MG	T	700	1/1	0.86	0.22	-	70,70,70,70	0
6	MG	J	700	1/1	0.94	0.07	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.