



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:43 am GMT

PDB ID : 1PF9
Title : GroEL-GroES-ADP
Authors : Chaudhry, C.; Farr, G.W.; Todd, M.J.; Rye, H.S.; Brunger, A.T.; Adams, P.D.; Horwich, A.L.; Sigler, P.B.
Deposited on : 2003-05-24
Resolution : 2.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

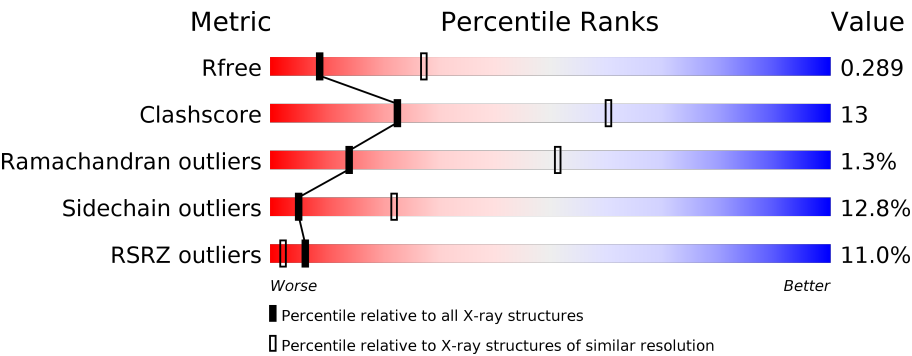
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.99 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	524	<div><div>11%</div><div><div></div><div>71%</div><div>25%</div><div>.</div></div></div>
1	B	524	<div><div>11%</div><div><div></div><div>71%</div><div>24%</div><div>5%</div></div></div>
1	C	524	<div><div>10%</div><div><div></div><div>69%</div><div>27%</div><div>.</div><div>.</div></div></div>
1	D	524	<div><div>10%</div><div><div></div><div>69%</div><div>26%</div><div>.</div></div></div>
1	E	524	<div><div>12%</div><div><div></div><div>69%</div><div>26%</div><div>.</div></div></div>
1	F	524	<div><div>14%</div><div><div></div><div>71%</div><div>24%</div><div>.</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	524	
1	H	524	
1	I	524	
1	J	524	
1	K	524	
1	L	524	
1	M	524	
1	N	524	
2	O	97	
2	P	97	
2	Q	97	
2	R	97	
2	S	97	
2	T	97	
2	U	97	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 59283 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 groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	B	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	C	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	D	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	E	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	F	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	G	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	H	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	I	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	J	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	K	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	L	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	M	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	N	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			

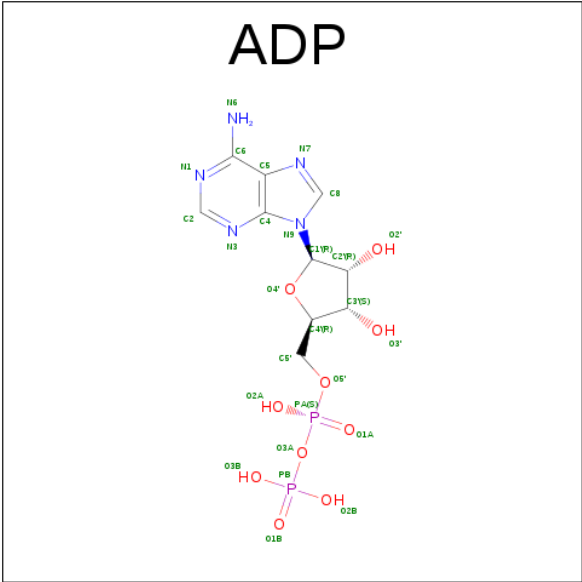
- Molecule 2 is a protein called groES protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	P	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	Q	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	R	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	S	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	T	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	U	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		
5	E	1	Total	O	0	0
			1	1		

Continued on next page...

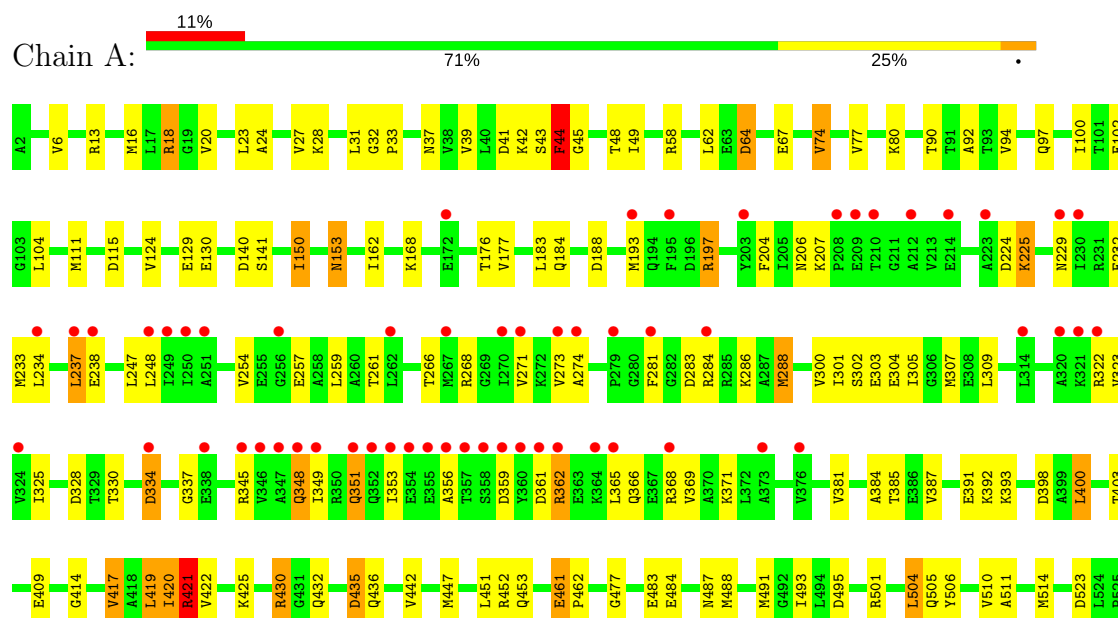
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	O	0	0
			1	1		
5	G	1	Total	O	0	0
			1	1		

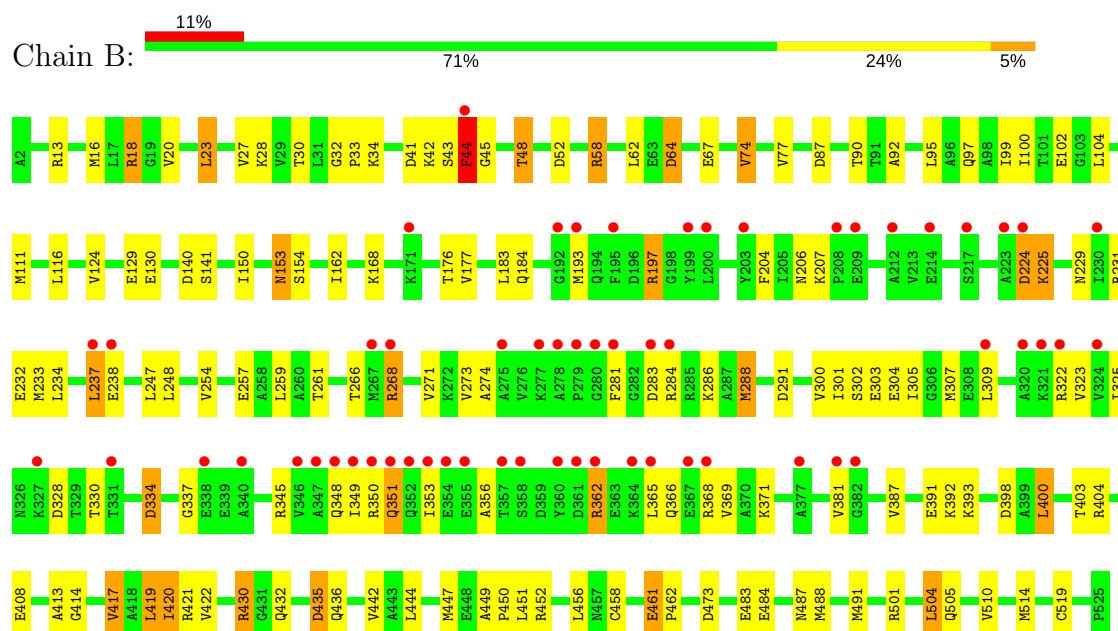
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

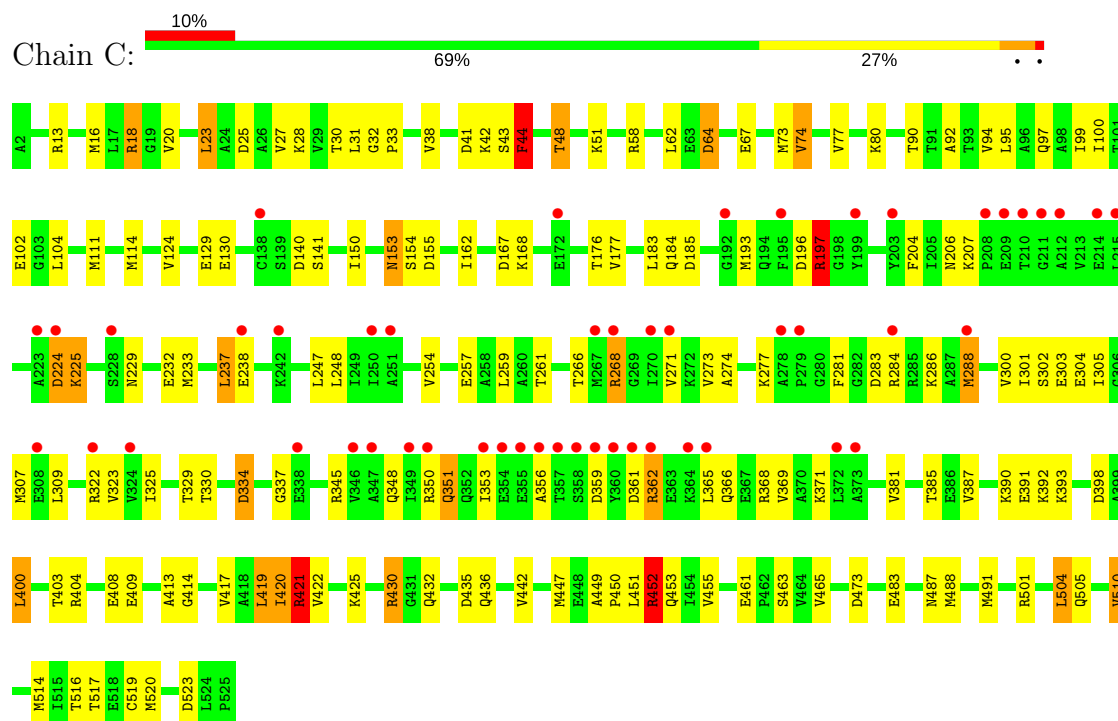
• Molecule 1: groEL protein



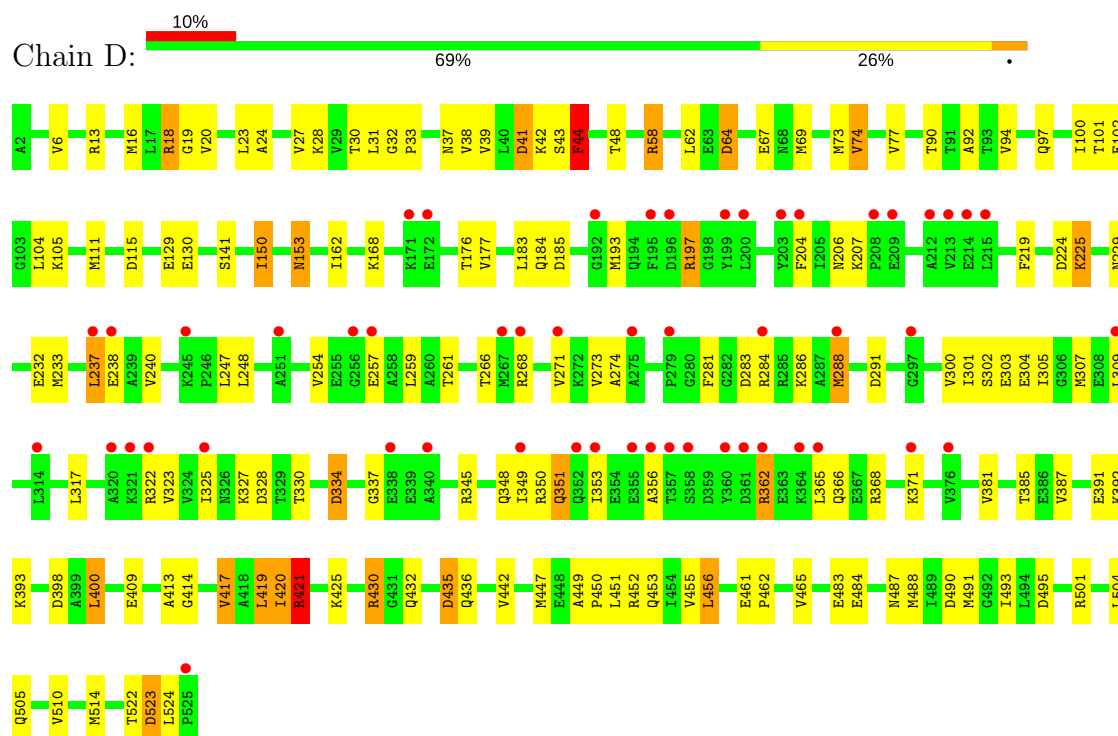
• Molecule 1: groEL protein



- Molecule 1: groEL protein

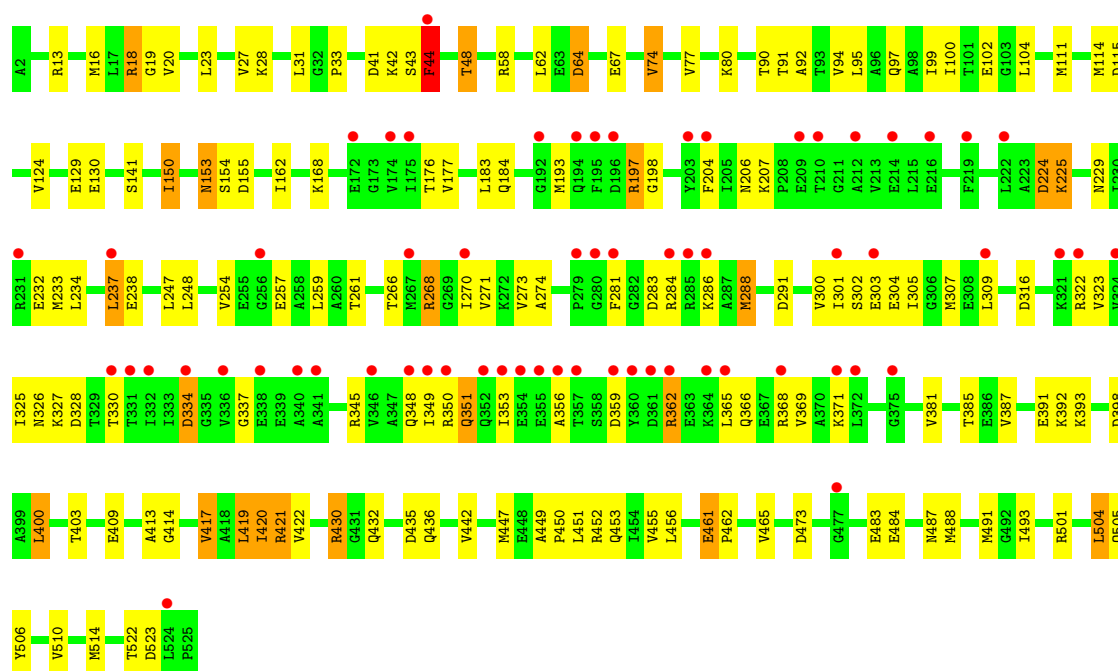


- Molecule 1: groEL protein

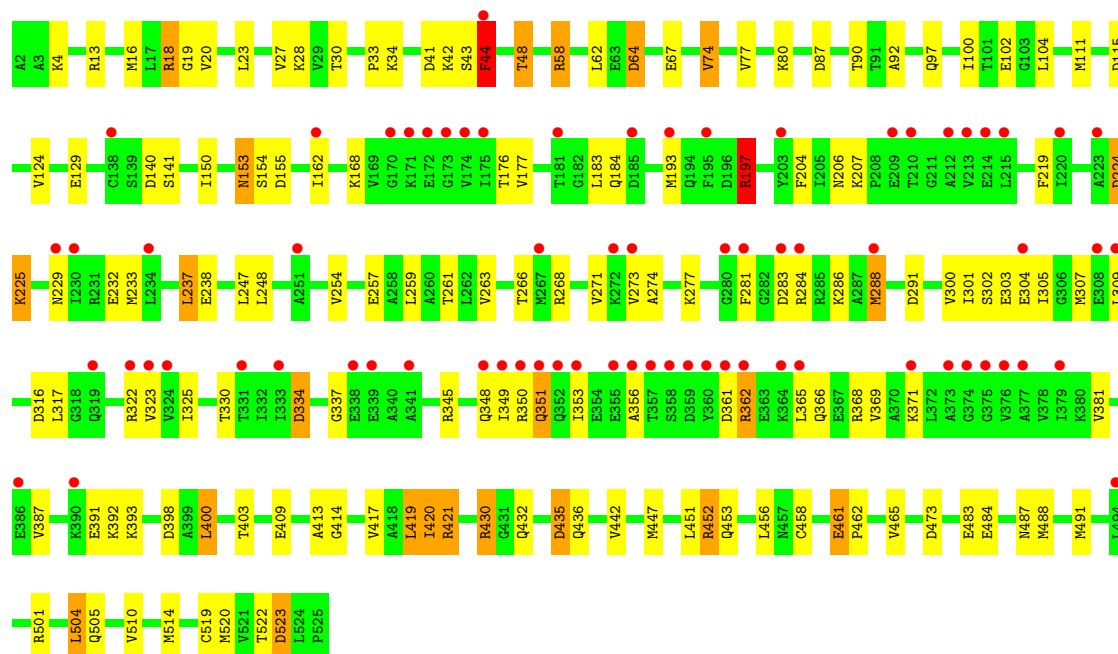


- Molecule 1: groEL protein

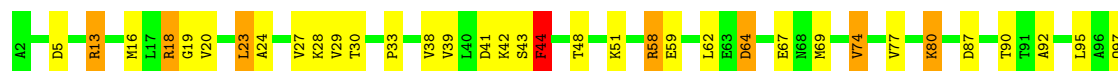


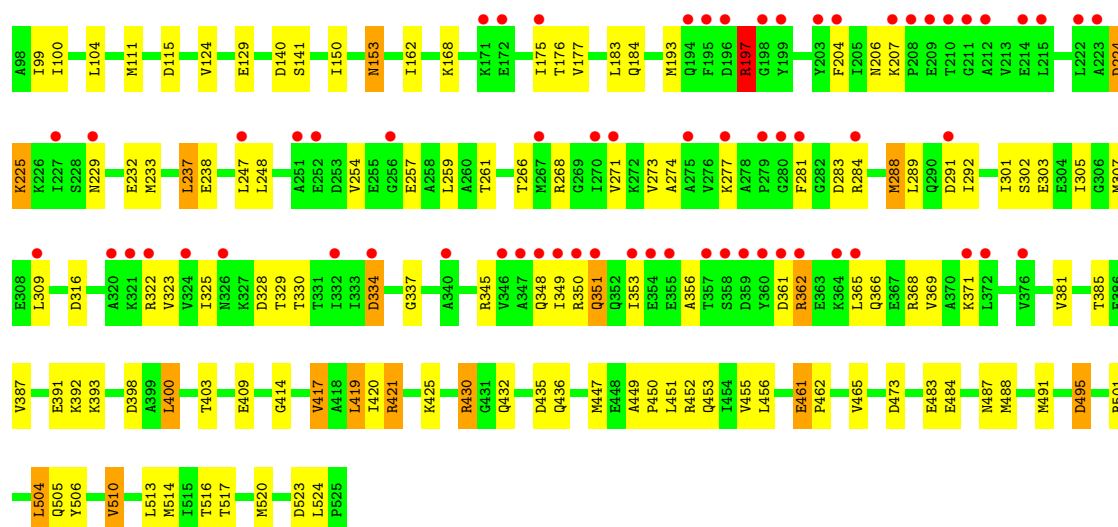


- Molecule 1: groEL protein

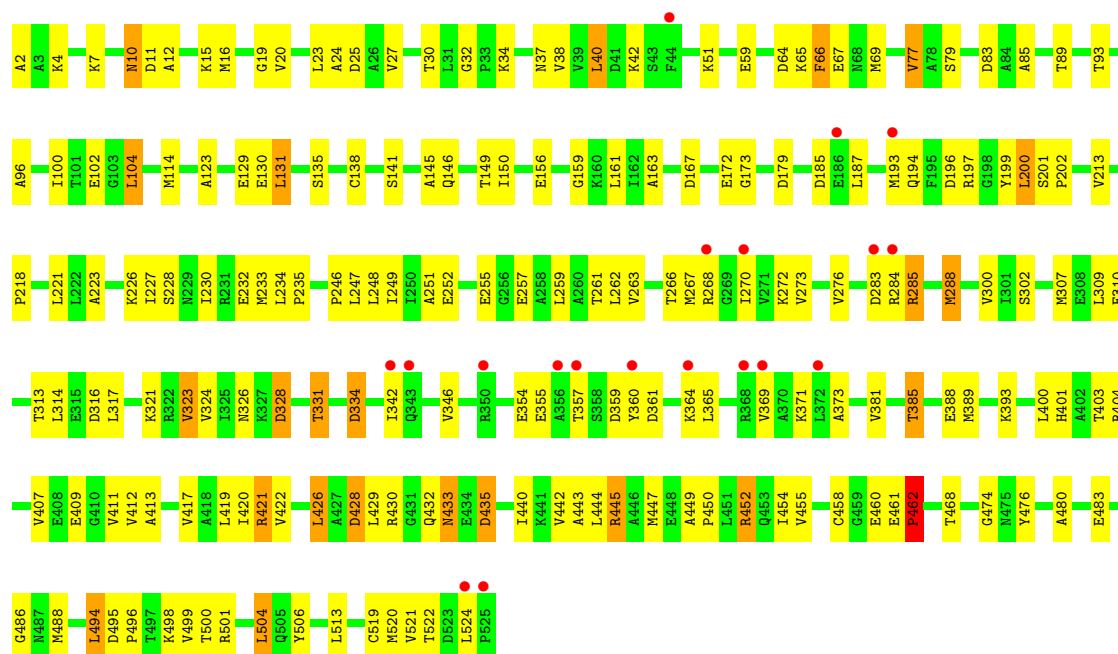


- Molecule 1: groEL protein

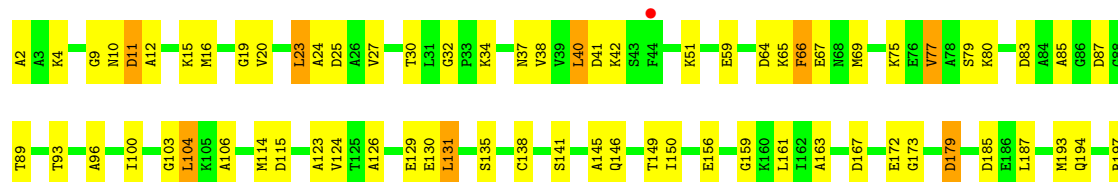


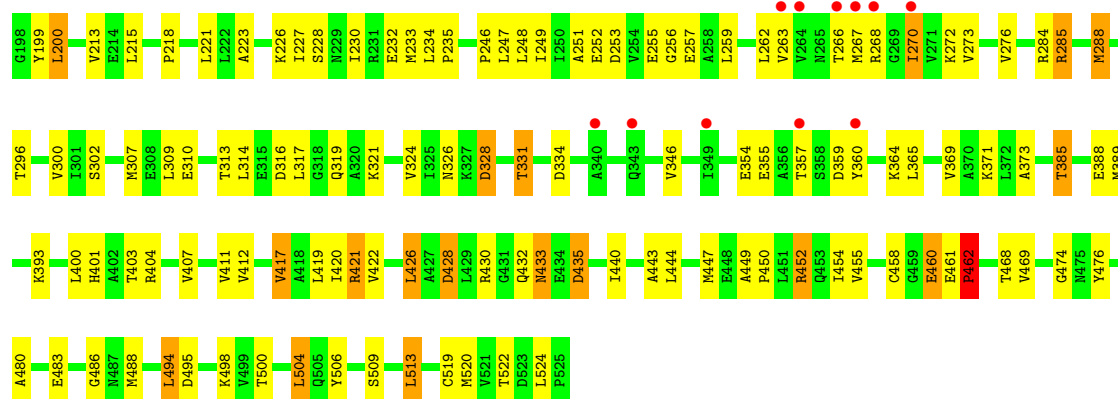


• Molecule 1: groEL protein

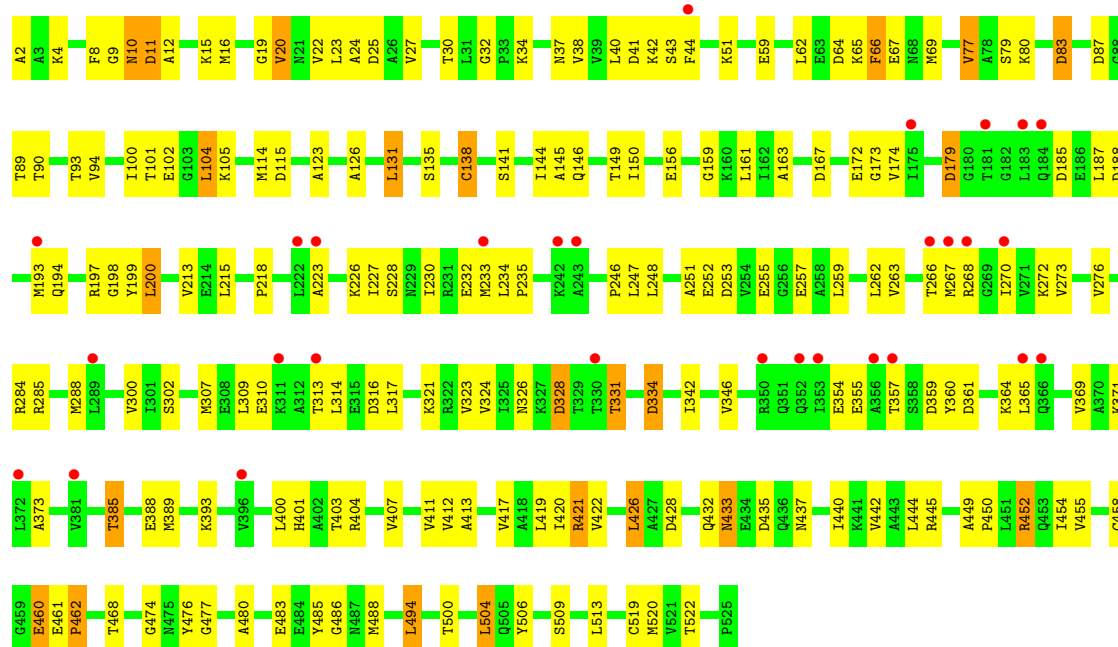


• Molecule 1: groEL protein

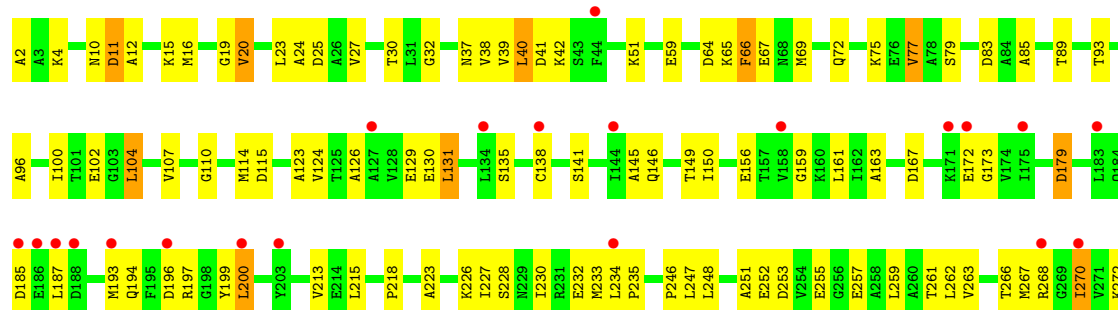


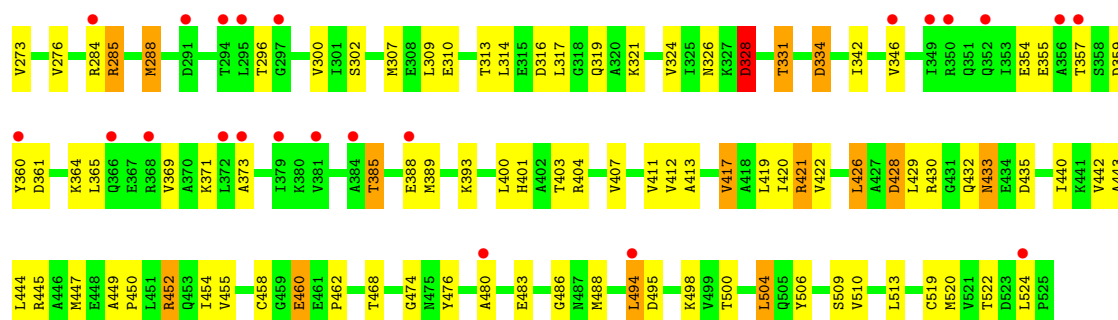


• Molecule 1: groEL protein

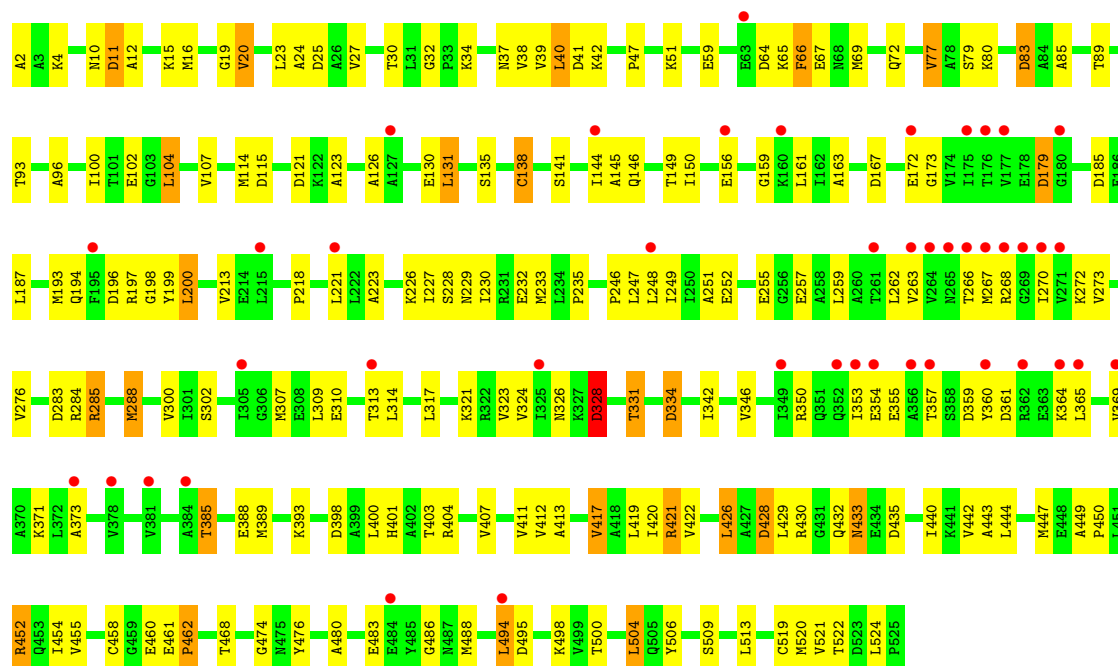


• Molecule 1: groEL protein

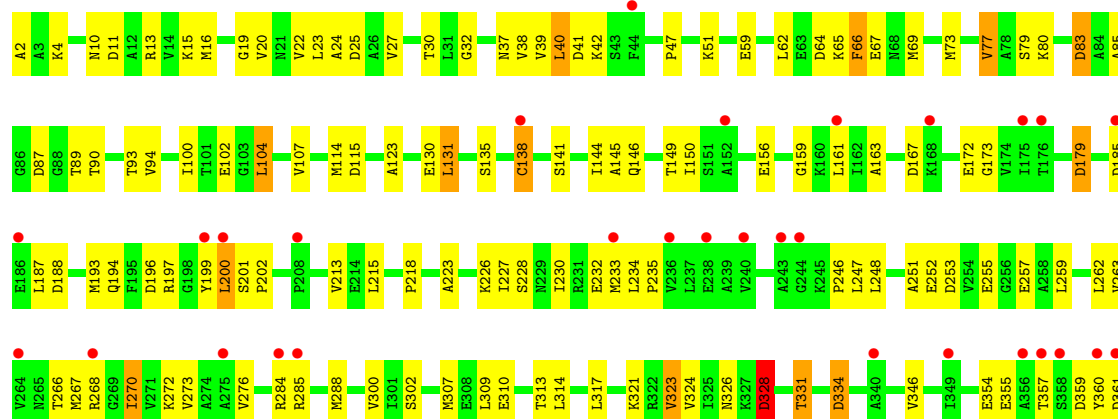


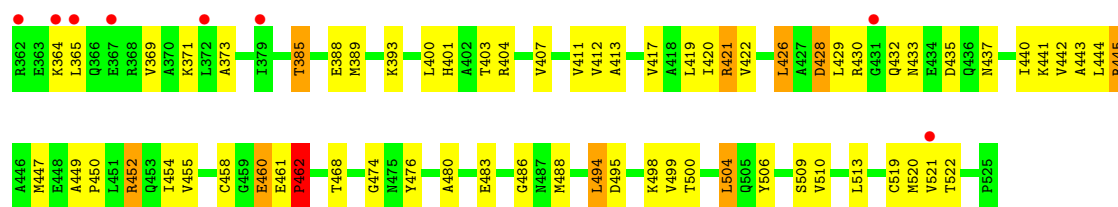


• Molecule 1: groEL protein

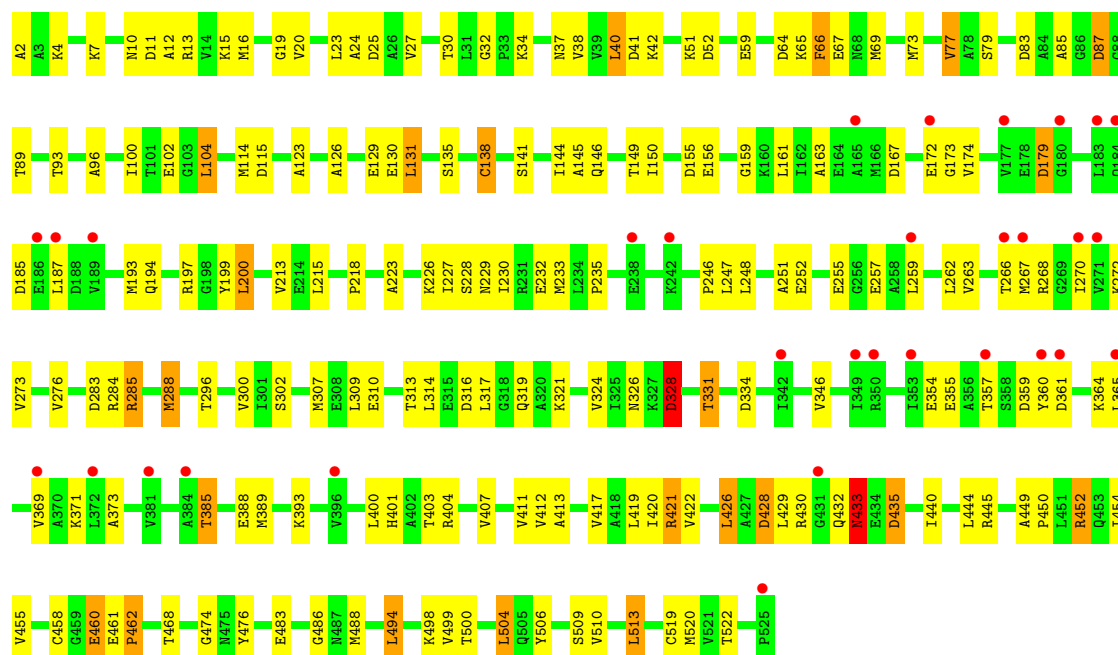


• Molecule 1: groEL protein

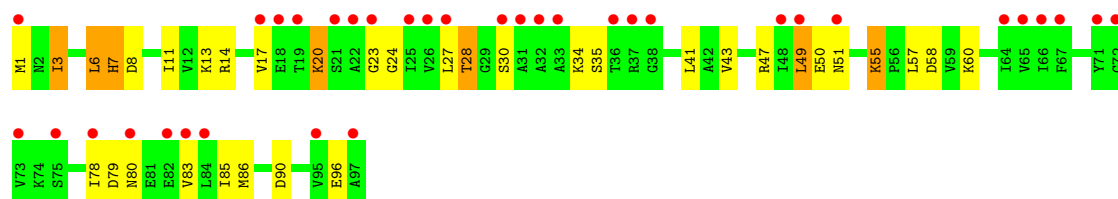




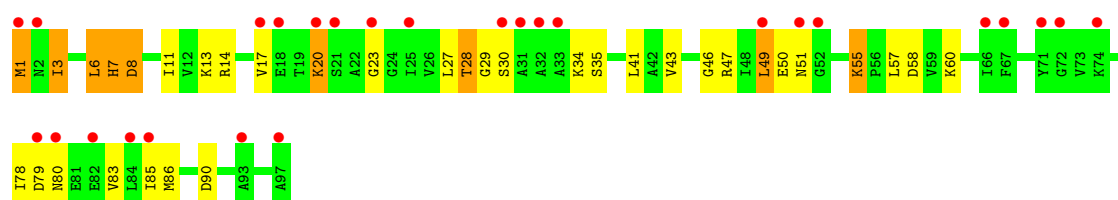
• Molecule 1: groEL protein



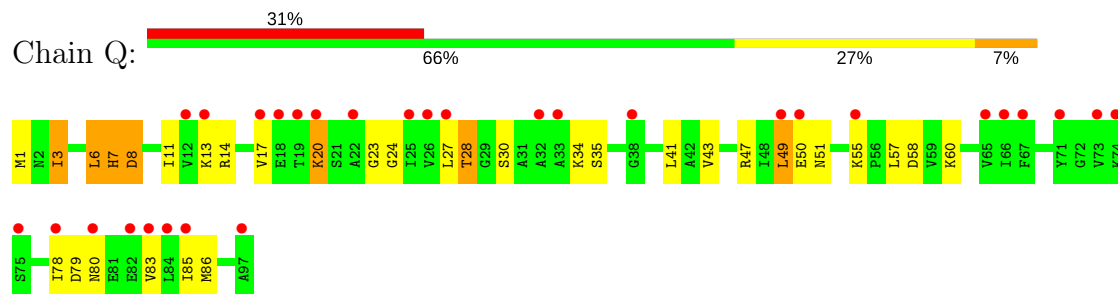
• Molecule 2: groES protein



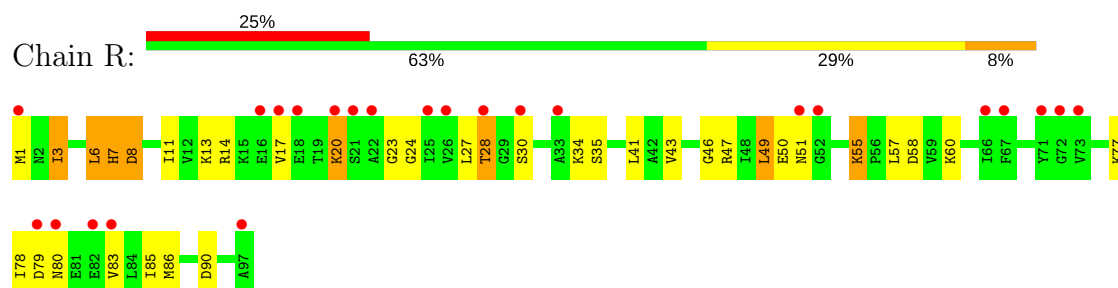
• Molecule 2: groES protein



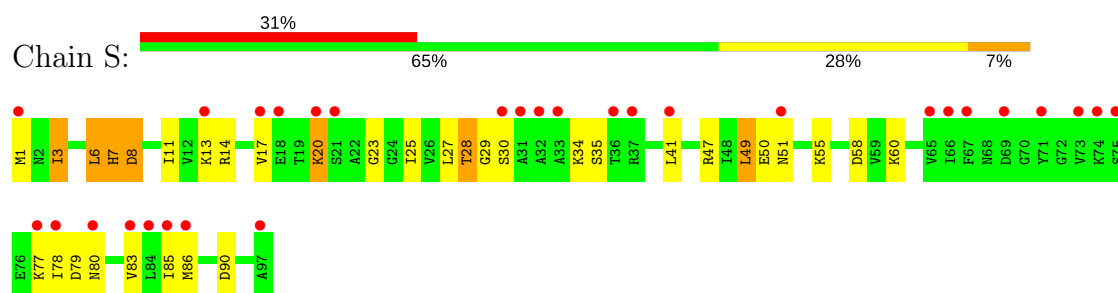
- Molecule 2: groES protein



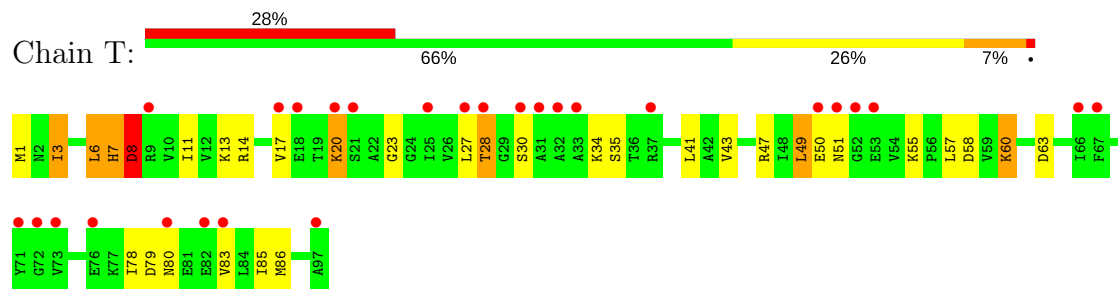
- Molecule 2: groES protein



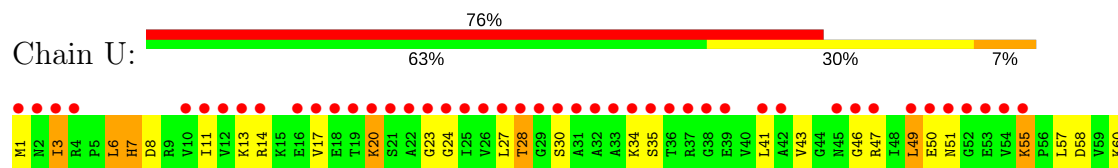
- Molecule 2: groES protein

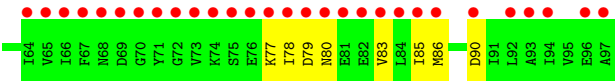


- Molecule 2: groES protein



- Molecule 2: groES protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	255.26Å 265.25Å 184.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.16 – 2.99 40.07 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.16-2.99) 96.7 (40.07-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.269 , 0.287 0.272 , 0.289	Depositor DCC
R_{free} test set	12081 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	59283	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.67	0/3884	0.90	18/5243 (0.3%)
1	B	0.60	0/3884	0.95	18/5243 (0.3%)
1	C	0.64	0/3884	0.91	20/5243 (0.4%)
1	D	0.66	1/3884 (0.0%)	0.90	17/5243 (0.3%)
1	E	0.57	0/3884	0.86	15/5243 (0.3%)
1	F	0.55	0/3884	0.86	17/5243 (0.3%)
1	G	0.64	0/3884	0.91	20/5243 (0.4%)
1	H	0.59	0/3884	0.85	14/5243 (0.3%)
1	I	0.64	0/3884	0.86	15/5243 (0.3%)
1	J	0.61	0/3884	0.87	18/5243 (0.3%)
1	K	0.54	0/3884	0.83	17/5243 (0.3%)
1	L	0.51	0/3884	0.87	20/5243 (0.4%)
1	M	0.59	0/3884	0.90	20/5243 (0.4%)
1	N	0.59	0/3884	0.85	17/5243 (0.3%)
2	O	0.37	0/732	0.73	3/983 (0.3%)
2	P	0.37	0/732	0.73	4/983 (0.4%)
2	Q	0.38	0/732	0.73	2/983 (0.2%)
2	R	0.41	0/732	0.74	4/983 (0.4%)
2	S	0.39	0/732	0.74	4/983 (0.4%)
2	T	0.39	0/732	0.74	3/983 (0.3%)
2	U	0.38	0/732	0.72	3/983 (0.3%)
All	All	0.59	1/59500 (0.0%)	0.87	269/80283 (0.3%)

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	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	130	GLU	CD-OE1	5.35	1.31	1.25

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ARG	NE-CZ-NH1	-19.37	110.61	120.30
1	B	231	ARG	NE-CZ-NH2	18.28	129.44	120.30
1	L	268	ARG	NE-CZ-NH2	14.85	127.72	120.30
1	M	268	ARG	NE-CZ-NH2	14.77	127.68	120.30
1	M	268	ARG	NE-CZ-NH1	-14.67	112.97	120.30
1	L	268	ARG	NE-CZ-NH1	-14.62	112.99	120.30
1	G	268	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	D	268	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	A	268	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	A	268	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	D	268	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	G	268	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	G	197	ARG	NE-CZ-NH1	-10.53	115.03	120.30
1	F	197	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	C	197	ARG	NE-CZ-NH1	-10.17	115.22	120.30
1	G	197	ARG	NE-CZ-NH2	9.95	125.28	120.30
1	C	197	ARG	NE-CZ-NH2	9.68	125.14	120.30
1	F	197	ARG	NE-CZ-NH2	9.57	125.08	120.30
1	C	268	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	B	268	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	E	268	ARG	NE-CZ-NH2	9.47	125.04	120.30
1	C	268	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	B	268	ARG	NE-CZ-NH1	-9.26	115.67	120.30
1	B	231	ARG	CD-NE-CZ	9.20	136.48	123.60
1	E	268	ARG	NE-CZ-NH1	-9.19	115.70	120.30
1	F	268	ARG	NE-CZ-NH1	-9.17	115.72	120.30
1	F	268	ARG	NE-CZ-NH2	9.14	124.87	120.30
1	J	25	ASP	CB-CG-OD2	9.01	126.41	118.30
1	E	197	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	B	197	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	K	25	ASP	CB-CG-OD2	7.63	125.16	118.30
1	A	197	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	N	25	ASP	CB-CG-OD2	7.51	125.06	118.30
1	H	25	ASP	CB-CG-OD2	7.47	125.03	118.30
1	L	25	ASP	CB-CG-OD2	7.22	124.80	118.30
1	L	268	ARG	CD-NE-CZ	7.21	133.69	123.60
1	N	83	ASP	CB-CG-OD2	7.18	124.76	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	268	ARG	CD-NE-CZ	7.12	133.57	123.60
1	E	64	ASP	CB-CG-OD2	7.12	124.70	118.30
1	E	197	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	D	495	ASP	CB-CG-OD2	7.05	124.64	118.30
1	D	197	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	D	64	ASP	CB-CG-OD2	6.88	124.49	118.30
1	M	41	ASP	CB-CG-OD2	6.82	124.44	118.30
1	M	25	ASP	CB-CG-OD2	6.82	124.43	118.30
1	J	428	ASP	CB-CG-OD2	6.79	124.41	118.30
1	B	197	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	K	41	ASP	CB-CG-OD2	6.64	124.28	118.30
1	K	428	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	197	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	M	115	ASP	CB-CG-OD2	6.58	124.23	118.30
1	G	64	ASP	CB-CG-OD2	6.57	124.22	118.30
1	A	421	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	B	435	ASP	CB-CG-OD2	6.53	124.18	118.30
1	K	83	ASP	CB-CG-OD2	6.50	124.15	118.30
1	D	197	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	K	268	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	C	25	ASP	CB-CG-OD2	6.39	124.05	118.30
1	L	83	ASP	CB-CG-OD2	6.39	124.05	118.30
1	N	41	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	334	ASP	CB-CG-OD2	6.33	123.99	118.30
1	M	11	ASP	CB-CG-OD2	6.32	123.99	118.30
1	H	268	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	G	140	ASP	CB-CG-OD2	6.30	123.97	118.30
1	E	41	ASP	CB-CG-OD2	6.30	123.97	118.30
1	C	334	ASP	CB-CG-OD2	6.28	123.95	118.30
1	J	83	ASP	CB-CG-OD2	6.27	123.94	118.30
1	I	268	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	F	334	ASP	CB-CG-OD2	6.19	123.87	118.30
1	L	428	ASP	CB-CG-OD2	6.19	123.87	118.30
1	G	334	ASP	CB-CG-OD2	6.18	123.87	118.30
1	K	268	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	87	ASP	CB-CG-OD2	6.16	123.85	118.30
1	D	334	ASP	CB-CG-OD2	6.16	123.84	118.30
1	L	115	ASP	CB-CG-OD2	6.15	123.84	118.30
1	E	334	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	435	ASP	CB-CG-OD2	6.12	123.81	118.30
1	J	268	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	334	ASP	CB-CG-OD2	6.11	123.80	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASP	CB-CG-OD2	6.09	123.78	118.30
1	J	41	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	140	ASP	CB-CG-OD2	6.05	123.74	118.30
1	D	421	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	I	41	ASP	CB-CG-OD2	6.03	123.72	118.30
1	M	428	ASP	CB-CG-OD2	6.03	123.72	118.30
1	D	41	ASP	CB-CG-OD2	6.02	123.72	118.30
1	L	11	ASP	CB-CG-OD2	6.01	123.70	118.30
1	I	25	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	283	ASP	CB-CG-OD2	5.96	123.66	118.30
1	D	435	ASP	CB-CG-OD2	5.94	123.64	118.30
1	F	64	ASP	CB-CG-OD2	5.94	123.64	118.30
1	J	115	ASP	CB-CG-OD2	5.94	123.64	118.30
1	H	334	ASP	CB-CG-OD2	5.93	123.64	118.30
1	J	11	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	64	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	523	ASP	CB-CG-OD2	5.91	123.62	118.30
1	C	140	ASP	CB-CG-OD2	5.91	123.62	118.30
1	N	268	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	F	283	ASP	CB-CG-OD2	5.89	123.60	118.30
1	I	268	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	I	428	ASP	CB-CG-OD2	5.87	123.58	118.30
1	N	268	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	115	ASP	CB-CG-OD2	5.86	123.57	118.30
2	R	8	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	283	ASP	CB-CG-OD2	5.85	123.57	118.30
2	Q	58	ASP	CB-CG-OD2	5.85	123.57	118.30
1	J	435	ASP	CB-CG-OD2	5.84	123.56	118.30
1	H	268	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	P	58	ASP	CB-CG-OD2	5.83	123.55	118.30
1	F	41	ASP	CB-CG-OD2	5.83	123.55	118.30
1	D	523	ASP	CB-CG-OD2	5.80	123.52	118.30
1	H	428	ASP	CB-CG-OD2	5.79	123.51	118.30
1	H	495	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	41	ASP	CB-CG-OD2	5.77	123.49	118.30
1	D	268	ARG	CD-NE-CZ	5.77	131.67	123.60
1	I	495	ASP	CB-CG-OD2	5.76	123.48	118.30
1	M	83	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	268	ARG	CD-NE-CZ	5.75	131.66	123.60
2	T	58	ASP	CB-CG-OD2	5.75	123.47	118.30
1	N	428	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	41	ASP	CB-CG-OD2	5.72	123.44	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	435	ASP	CB-CG-OD2	5.69	123.42	118.30
1	I	115	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	283	ASP	CB-CG-OD2	5.68	123.41	118.30
1	I	435	ASP	CB-CG-OD2	5.68	123.41	118.30
1	J	334	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	473	ASP	CB-CG-OD2	5.66	123.39	118.30
2	R	58	ASP	CB-CG-OD2	5.66	123.39	118.30
1	F	140	ASP	CB-CG-OD2	5.66	123.39	118.30
1	M	328	ASP	CB-CG-OD2	5.65	123.39	118.30
1	G	495	ASP	CB-CG-OD2	5.65	123.38	118.30
2	O	58	ASP	CB-CG-OD2	5.65	123.38	118.30
1	G	13	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	G	268	ARG	CD-NE-CZ	5.62	131.47	123.60
1	G	283	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	495	ASP	CB-CG-OD2	5.61	123.35	118.30
1	N	87	ASP	CB-CG-OD2	5.60	123.34	118.30
1	E	283	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	283	ASP	CB-CG-OD2	5.58	123.32	118.30
1	J	268	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	224	ASP	CB-CG-OD2	5.55	123.29	118.30
2	P	8	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	473	ASP	CB-CG-OD2	5.53	123.28	118.30
1	M	334	ASP	CB-CG-OD2	5.51	123.26	118.30
1	M	179	ASP	CB-CG-OD2	5.48	123.24	118.30
1	G	87	ASP	CB-CG-OD2	5.48	123.23	118.30
1	K	115	ASP	CB-CG-OD2	5.48	123.23	118.30
1	E	155	ASP	CB-CG-OD2	5.48	123.23	118.30
1	G	523	ASP	CB-CG-OD2	5.48	123.23	118.30
1	F	523	ASP	CB-CG-OD2	5.47	123.22	118.30
1	H	83	ASP	CB-CG-OD2	5.47	123.23	118.30
2	U	90	ASP	CB-CG-OD2	5.47	123.22	118.30
1	L	334	ASP	CB-CG-OD2	5.47	123.22	118.30
1	G	473	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	523	ASP	CB-CG-OD2	5.46	123.21	118.30
1	H	359	ASP	CB-CG-OD2	5.45	123.20	118.30
1	H	196	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	64	ASP	CB-CG-OD2	5.44	123.19	118.30
1	L	359	ASP	CB-CG-OD2	5.44	123.19	118.30
1	G	224	ASP	CB-CG-OD2	5.43	123.19	118.30
1	K	196	ASP	CB-CG-OD2	5.42	123.18	118.30
1	J	316	ASP	CB-CG-OD2	5.42	123.18	118.30
1	J	179	ASP	CB-CG-OD2	5.41	123.17	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	316	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	115	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	155	ASP	CB-CG-OD2	5.37	123.13	118.30
2	T	79	ASP	CB-CG-OD2	5.37	123.13	118.30
1	K	179	ASP	CB-CG-OD2	5.36	123.12	118.30
1	M	253	ASP	CB-CG-OD2	5.34	123.11	118.30
1	F	155	ASP	CB-CG-OD2	5.34	123.10	118.30
1	N	179	ASP	CB-CG-OD2	5.33	123.10	118.30
1	L	121	ASP	CB-CG-OD2	5.33	123.10	118.30
1	F	473	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	140	ASP	CB-CG-OD2	5.33	123.09	118.30
2	Q	79	ASP	CB-CG-OD2	5.32	123.09	118.30
1	J	253	ASP	CB-CG-OD2	5.31	123.08	118.30
1	L	462	PRO	N-CD-CG	-5.31	95.23	103.20
1	E	473	ASP	CB-CG-OD2	5.31	123.08	118.30
1	G	5	ASP	CB-CG-OD2	5.30	123.07	118.30
1	I	87	ASP	CB-CG-OD2	5.30	123.07	118.30
1	K	359	ASP	CB-CG-OD2	5.30	123.07	118.30
1	K	495	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	188	ASP	CB-CG-OD2	5.29	123.06	118.30
1	I	359	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	64	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	185	ASP	CB-CG-OD2	5.29	123.06	118.30
1	J	359	ASP	CB-CG-OD2	5.29	123.06	118.30
1	M	361	ASP	CB-CG-OD2	5.29	123.06	118.30
1	M	435	ASP	CB-CG-OD2	5.28	123.06	118.30
1	K	316	ASP	CB-CG-OD2	5.28	123.05	118.30
1	H	283	ASP	CB-CG-OD2	5.27	123.05	118.30
2	P	79	ASP	CB-CG-OD2	5.27	123.05	118.30
1	F	87	ASP	CB-CG-OD2	5.27	123.04	118.30
1	M	359	ASP	CB-CG-OD2	5.26	123.04	118.30
1	C	452	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	L	495	ASP	CB-CG-OD2	5.25	123.03	118.30
1	L	41	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	115	ASP	CB-CG-OD2	5.25	123.03	118.30
1	L	179	ASP	CB-CG-OD2	5.25	123.03	118.30
1	E	328	ASP	CB-CG-OD2	5.25	123.02	118.30
1	L	196	ASP	CB-CG-OD2	5.25	123.02	118.30
1	N	328	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	185	ASP	CB-CG-OD2	5.24	123.02	118.30
2	O	90	ASP	CB-CG-OD2	5.24	123.02	118.30
1	F	224	ASP	CB-CG-OD2	5.24	123.02	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	495	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	115	ASP	CB-CG-OD2	5.22	123.00	118.30
1	L	361	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	224	ASP	CB-CG-OD2	5.22	123.00	118.30
2	O	79	ASP	CB-CG-OD2	5.22	123.00	118.30
1	H	361	ASP	CB-CG-OD2	5.21	122.99	118.30
1	N	435	ASP	CB-CG-OD2	5.21	122.99	118.30
1	L	328	ASP	CB-CG-OD2	5.20	122.98	118.30
1	M	462	PRO	N-CD-CG	-5.20	95.40	103.20
1	I	253	ASP	CB-CG-OD2	5.20	122.98	118.30
1	K	334	ASP	CB-CG-OD2	5.20	122.98	118.30
1	G	41	ASP	CB-CG-OD2	5.20	122.98	118.30
1	I	316	ASP	CB-CG-OD2	5.19	122.97	118.30
2	R	79	ASP	CB-CG-OD2	5.19	122.97	118.30
1	J	361	ASP	CB-CG-OD2	5.19	122.97	118.30
1	H	435	ASP	CB-CG-OD2	5.19	122.97	118.30
1	J	188	ASP	CB-CG-OD2	5.19	122.97	118.30
2	U	58	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	490	ASP	CB-CG-OD2	5.18	122.97	118.30
1	C	421	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	I	11	ASP	CB-CG-OD2	5.16	122.95	118.30
1	N	155	ASP	CB-CG-OD2	5.16	122.94	118.30
1	N	115	ASP	CB-CG-OD2	5.15	122.94	118.30
1	G	316	ASP	CB-CG-OD2	5.15	122.93	118.30
1	H	316	ASP	CB-CG-OD2	5.15	122.93	118.30
1	I	179	ASP	CB-CG-OD2	5.14	122.93	118.30
1	M	196	ASP	CB-CG-OD2	5.14	122.93	118.30
1	L	398	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	196	ASP	CB-CG-OD2	5.14	122.92	118.30
2	S	79	ASP	CB-CG-OD2	5.13	122.92	118.30
1	N	52	ASP	CB-CG-OD2	5.13	122.91	118.30
1	E	316	ASP	CB-CG-OD2	5.12	122.91	118.30
1	N	359	ASP	CB-CG-OD2	5.12	122.90	118.30
1	H	462	PRO	N-CD-CG	-5.11	95.53	103.20
1	K	253	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	167	ASP	CB-CG-OD2	5.11	122.90	118.30
1	K	328	ASP	CB-CG-OD2	5.11	122.90	118.30
2	S	8	ASP	CB-CG-OD2	5.11	122.90	118.30
2	S	90	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	224	ASP	CB-CG-OD2	5.10	122.89	118.30
1	K	361	ASP	CB-CG-OD2	5.09	122.89	118.30
2	U	79	ASP	CB-CG-OD2	5.09	122.88	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	90	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	328	ASP	CB-CG-OD2	5.08	122.87	118.30
1	N	361	ASP	CB-CG-OD2	5.08	122.87	118.30
1	G	115	ASP	CB-CG-OD2	5.07	122.86	118.30
2	R	90	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	328	ASP	CB-CG-OD2	5.06	122.86	118.30
2	S	58	ASP	CB-CG-OD2	5.06	122.86	118.30
1	L	283	ASP	CB-CG-OD2	5.06	122.86	118.30
1	I	462	PRO	N-CD-CG	-5.06	95.61	103.20
1	A	328	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	316	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	359	ASP	CB-CG-OD2	5.04	122.84	118.30
1	M	188	ASP	CB-CG-OD2	5.04	122.84	118.30
1	G	328	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	52	ASP	CB-CG-OD2	5.02	122.82	118.30
2	T	8	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	359	ASP	CB-CG-OD2	5.02	122.82	118.30
1	J	87	ASP	CB-CG-OD2	5.02	122.81	118.30
1	J	328	ASP	CB-CG-OD2	5.01	122.81	118.30
1	N	283	ASP	CB-CG-OD2	5.01	122.81	118.30
1	K	11	ASP	CB-CG-OD2	5.01	122.81	118.30
1	E	359	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	433	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3856	0	3976	105	0
1	B	3856	0	3976	99	0
1	C	3856	0	3976	109	0
1	D	3856	0	3976	115	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3856	0	3976	104	0
1	F	3856	0	3976	99	0
1	G	3856	0	3976	113	0
1	H	3856	0	3976	107	0
1	I	3856	0	3976	104	0
1	J	3856	0	3976	106	0
1	K	3856	0	3976	110	0
1	L	3856	0	3976	112	0
1	M	3856	0	3976	115	0
1	N	3856	0	3976	111	0
2	O	728	0	762	20	0
2	P	728	0	762	21	0
2	Q	728	0	762	18	0
2	R	728	0	762	17	0
2	S	728	0	762	19	0
2	T	728	0	762	15	0
2	U	728	0	762	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	27	0	12	2	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	3	0
4	E	27	0	12	1	0
4	F	27	0	12	1	0
4	G	27	0	12	3	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
5	C	1	0	0	1	0
5	D	1	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	1	0
All	All	59283	0	61082	1567	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 13.

All (1567) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:MET:CE	1:E:114:MET:SD	2.05	1.45
1:C:73:MET:SD	1:C:73:MET:CE	2.05	1.42
1:C:18:ARG:HG2	1:C:18:ARG:HH11	1.07	1.19
1:G:18:ARG:HH11	1:G:18:ARG:HG2	1.07	1.17
1:D:432:GLN:NE2	1:D:436:GLN:HE22	1.47	1.13
1:F:18:ARG:HH11	1:F:18:ARG:HG2	1.03	1.11
1:E:18:ARG:HH11	1:E:18:ARG:HG2	1.11	1.11
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.14	1.11
1:B:18:ARG:HH11	1:B:18:ARG:HG2	1.00	1.10
1:B:414:GLY:O	1:B:417:VAL:HG12	1.52	1.09
1:A:432:GLN:NE2	1:A:436:GLN:HE22	1.51	1.09
1:G:432:GLN:NE2	1:G:436:GLN:HE22	1.52	1.07
1:A:414:GLY:O	1:A:417:VAL:HG12	1.51	1.07
1:G:414:GLY:O	1:G:417:VAL:HG12	1.54	1.06
1:C:432:GLN:NE2	1:C:436:GLN:HE22	1.53	1.05
1:B:18:ARG:CG	1:B:18:ARG:HH11	1.71	1.03
1:B:432:GLN:NE2	1:B:436:GLN:HE22	1.56	1.02
1:D:414:GLY:O	1:D:417:VAL:HG12	1.58	1.02
1:F:414:GLY:O	1:F:417:VAL:HG12	1.59	1.02
1:C:414:GLY:O	1:C:417:VAL:HG12	1.57	1.02
1:E:432:GLN:NE2	1:E:436:GLN:HE22	1.57	1.02
1:F:432:GLN:NE2	1:F:436:GLN:HE22	1.58	1.01
1:D:18:ARG:HH11	1:D:18:ARG:HG2	1.24	1.01
1:D:432:GLN:HE21	1:D:436:GLN:NE2	1.58	1.00
1:F:18:ARG:CG	1:F:18:ARG:HH11	1.73	1.00
1:E:414:GLY:O	1:E:417:VAL:HG12	1.62	0.99
1:M:65:LYS:O	1:M:66:PHE:HB2	1.61	0.99
1:D:44:PHE:HD1	1:D:44:PHE:H	1.03	0.98
1:G:18:ARG:CG	1:G:18:ARG:HH11	1.77	0.97
1:C:18:ARG:CG	1:C:18:ARG:HH11	1.76	0.97
1:L:426:LEU:HD12	1:L:444:LEU:HD21	1.48	0.95
1:E:44:PHE:H	1:E:44:PHE:HD1	1.06	0.95
1:B:204:PHE:HE2	1:B:266:THR:HG21	1.32	0.95
1:F:18:ARG:NH1	1:F:18:ARG:HG2	1.76	0.95
1:B:18:ARG:NH1	1:B:18:ARG:HG2	1.72	0.95
1:A:204:PHE:HE2	1:A:266:THR:HG21	1.31	0.94
1:C:432:GLN:HE21	1:C:436:GLN:HE22	0.96	0.94
1:G:204:PHE:HE2	1:G:266:THR:HG21	1.32	0.94
1:A:432:GLN:HE21	1:A:436:GLN:NE2	1.64	0.94
1:D:18:ARG:CG	1:D:18:ARG:HH11	1.81	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:PHE:HE2	1:D:266:THR:HG21	1.33	0.93
1:E:204:PHE:HE2	1:E:266:THR:HG21	1.31	0.93
1:E:18:ARG:CG	1:E:18:ARG:HH11	1.80	0.93
1:K:65:LYS:O	1:K:66:PHE:HB2	1.66	0.93
1:F:204:PHE:HE2	1:F:266:THR:HG21	1.30	0.93
1:N:65:LYS:O	1:N:66:PHE:HB2	1.64	0.93
1:B:432:GLN:HE21	1:B:436:GLN:HE22	0.96	0.93
1:C:44:PHE:HD1	1:C:44:PHE:H	0.99	0.93
1:I:404:ARG:HH11	1:I:404:ARG:HG2	1.34	0.93
1:J:65:LYS:O	1:J:66:PHE:HB2	1.68	0.93
1:C:204:PHE:HE2	1:C:266:THR:HG21	1.32	0.92
1:F:44:PHE:HD1	1:F:44:PHE:H	1.11	0.92
1:A:18:ARG:CG	1:A:18:ARG:HH11	1.81	0.92
1:C:432:GLN:HE21	1:C:436:GLN:NE2	1.66	0.92
1:G:432:GLN:HE21	1:G:436:GLN:HE22	0.94	0.92
1:E:432:GLN:HE21	1:E:436:GLN:HE22	0.96	0.91
1:G:18:ARG:NH1	1:G:18:ARG:HG2	1.81	0.91
1:D:430:ARG:HH11	1:D:430:ARG:HG2	1.32	0.91
1:I:65:LYS:O	1:I:66:PHE:HB2	1.70	0.91
1:L:65:LYS:O	1:L:66:PHE:HB2	1.71	0.91
1:A:44:PHE:H	1:A:44:PHE:HD1	1.07	0.91
1:H:65:LYS:O	1:H:66:PHE:HB2	1.66	0.91
1:J:426:LEU:HD12	1:J:444:LEU:HD21	1.53	0.90
1:L:69:MET:HE1	1:L:522:THR:HB	1.52	0.90
1:G:432:GLN:HE21	1:G:436:GLN:NE2	1.70	0.90
1:C:18:ARG:HG2	1:C:18:ARG:NH1	1.77	0.89
1:I:426:LEU:HD12	1:I:444:LEU:HD21	1.53	0.89
1:E:432:GLN:HE21	1:E:436:GLN:NE2	1.69	0.89
1:B:44:PHE:HD1	1:B:44:PHE:H	1.00	0.89
1:M:426:LEU:HD12	1:M:444:LEU:HD21	1.54	0.89
1:G:44:PHE:H	1:G:44:PHE:HD1	1.08	0.88
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.36	0.88
1:B:432:GLN:HE21	1:B:436:GLN:NE2	1.70	0.88
1:F:432:GLN:HE21	1:F:436:GLN:NE2	1.70	0.88
1:N:426:LEU:HD12	1:N:444:LEU:HD21	1.53	0.88
1:E:18:ARG:HG2	1:E:18:ARG:NH1	1.82	0.88
1:F:432:GLN:HE21	1:F:436:GLN:HE22	0.95	0.87
1:I:69:MET:HE1	1:I:522:THR:HB	1.56	0.87
1:K:426:LEU:HD12	1:K:444:LEU:HD21	1.55	0.86
1:G:430:ARG:HH11	1:G:430:ARG:HG2	1.40	0.85
1:A:432:GLN:HE21	1:A:436:GLN:HE22	0.86	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:426:LEU:HD12	1:H:444:LEU:HD21	1.57	0.85
1:K:69:MET:HE1	1:K:522:THR:HB	1.57	0.84
1:A:74:VAL:O	1:A:77:VAL:HG13	1.78	0.84
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.43	0.84
1:H:69:MET:HE1	1:H:522:THR:HB	1.58	0.84
1:A:18:ARG:HG2	1:A:18:ARG:NH1	1.83	0.83
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.43	0.83
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.43	0.83
1:E:44:PHE:N	1:E:44:PHE:CD1	2.47	0.83
1:D:74:VAL:O	1:D:77:VAL:HG13	1.79	0.82
1:E:430:ARG:HH11	1:E:430:ARG:HG2	1.43	0.82
1:C:100:ILE:HD11	1:C:514:MET:HE1	1.60	0.82
1:F:44:PHE:CD1	1:F:44:PHE:N	2.48	0.81
1:D:44:PHE:N	1:D:44:PHE:CD1	2.48	0.81
1:F:204:PHE:CE2	1:F:266:THR:HG21	2.16	0.81
1:N:69:MET:HE1	1:N:522:THR:HB	1.62	0.81
1:A:204:PHE:CE2	1:A:266:THR:HG21	2.16	0.81
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.46	0.81
1:C:204:PHE:CE2	1:C:266:THR:HG21	2.17	0.80
1:F:430:ARG:HH11	1:F:430:ARG:HG2	1.45	0.79
1:E:204:PHE:CE2	1:E:266:THR:HG21	2.17	0.79
1:J:69:MET:HE1	1:J:522:THR:HB	1.62	0.79
1:B:204:PHE:CE2	1:B:266:THR:HG21	2.17	0.79
1:J:131:LEU:HD13	1:J:422:VAL:HG11	1.63	0.78
1:K:419:LEU:CD2	1:K:500:THR:HG23	2.13	0.78
1:B:44:PHE:CD1	1:B:44:PHE:N	2.46	0.78
1:D:18:ARG:HG2	1:D:18:ARG:NH1	1.91	0.78
1:G:204:PHE:CE2	1:G:266:THR:HG21	2.18	0.78
1:G:44:PHE:N	1:G:44:PHE:CD1	2.48	0.78
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.66	0.77
1:H:419:LEU:CD2	1:H:500:THR:HG23	2.14	0.77
1:I:131:LEU:HD13	1:I:422:VAL:HG11	1.65	0.77
1:N:69:MET:CE	1:N:522:THR:HB	2.15	0.77
1:C:44:PHE:CD1	1:C:44:PHE:N	2.46	0.77
1:C:74:VAL:O	1:C:77:VAL:HG13	1.85	0.77
1:D:432:GLN:HE21	1:D:436:GLN:HE22	0.79	0.77
1:A:409:GLU:OE2	1:A:501:ARG:NH2	2.17	0.77
1:M:131:LEU:HD13	1:M:422:VAL:HG11	1.66	0.76
1:M:421:ARG:HD2	1:M:474:GLY:O	1.85	0.76
1:F:197:ARG:HD2	1:F:277:LYS:HB2	1.68	0.76
1:G:197:ARG:HD2	1:G:277:LYS:HB2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:PRO:HA	1:E:153:ASN:HD21	1.50	0.76
1:L:38:VAL:HG22	1:M:519:CYS:HB3	1.67	0.76
1:B:74:VAL:O	1:B:77:VAL:HG13	1.85	0.76
1:C:197:ARG:HD2	1:C:277:LYS:HB2	1.66	0.76
1:J:69:MET:CE	1:J:522:THR:HB	2.15	0.76
1:K:100:ILE:O	1:K:104:LEU:HB2	1.86	0.75
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.51	0.75
1:A:44:PHE:CD1	1:A:44:PHE:N	2.46	0.75
1:H:69:MET:CE	1:H:522:THR:HB	2.16	0.75
1:C:33:PRO:HA	1:C:153:ASN:HD21	1.51	0.75
1:C:44:PHE:HD1	1:C:44:PHE:N	1.81	0.75
1:D:204:PHE:CE2	1:D:266:THR:HG21	2.18	0.75
1:L:149:THR:HG23	1:L:159:GLY:HA3	1.67	0.75
1:G:74:VAL:O	1:G:77:VAL:HG13	1.85	0.75
1:N:452:ARG:HH11	1:N:452:ARG:HG2	1.52	0.75
1:J:149:THR:HG23	1:J:159:GLY:HA3	1.68	0.75
1:J:404:ARG:HH11	1:J:404:ARG:HG2	1.52	0.74
1:K:232:GLU:HB3	1:K:309:LEU:HB2	1.68	0.74
1:N:232:GLU:HB3	1:N:309:LEU:HB2	1.69	0.74
1:L:232:GLU:HB3	1:L:309:LEU:HB2	1.69	0.74
1:L:69:MET:CE	1:L:522:THR:HB	2.17	0.74
1:M:69:MET:CE	1:M:522:THR:HB	2.17	0.74
1:I:421:ARG:HD2	1:I:474:GLY:O	1.86	0.74
1:K:419:LEU:CD2	1:K:500:THR:CG2	2.65	0.74
1:A:100:ILE:HD11	1:A:514:MET:HE1	1.70	0.74
1:B:44:PHE:HD1	1:B:44:PHE:N	1.82	0.74
1:N:65:LYS:O	1:N:66:PHE:CB	2.36	0.74
1:A:385:THR:HG21	1:G:510:VAL:HG12	1.71	0.73
1:M:100:ILE:O	1:M:104:LEU:HB2	1.88	0.73
1:N:419:LEU:CD2	1:N:500:THR:HG23	2.18	0.73
1:I:149:THR:HG23	1:I:159:GLY:HA3	1.70	0.73
1:J:421:ARG:HD2	1:J:474:GLY:O	1.87	0.73
1:H:131:LEU:HD13	1:H:422:VAL:HG11	1.70	0.73
1:J:419:LEU:CD2	1:J:500:THR:CG2	2.66	0.73
1:E:44:PHE:N	1:E:44:PHE:HD1	1.85	0.73
1:H:32:GLY:HA2	1:H:454:ILE:HD13	1.70	0.73
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.70	0.73
1:E:74:VAL:O	1:E:77:VAL:HG13	1.88	0.73
1:H:149:THR:HG23	1:H:159:GLY:HA3	1.71	0.73
1:M:232:GLU:HB3	1:M:309:LEU:HB2	1.71	0.73
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:232:GLU:HB3	1:H:309:LEU:HB2	1.69	0.72
1:K:38:VAL:HG22	1:L:519:CYS:HB3	1.70	0.72
1:J:32:GLY:HA2	1:J:454:ILE:HD13	1.70	0.72
1:G:33:PRO:HA	1:G:153:ASN:HD21	1.53	0.72
1:G:417:VAL:HG11	1:G:488:MET:HG3	1.72	0.72
1:H:421:ARG:HD2	1:H:474:GLY:O	1.89	0.72
1:J:232:GLU:HB3	1:J:309:LEU:HB2	1.70	0.72
1:M:419:LEU:CD2	1:M:500:THR:HG23	2.20	0.72
1:N:421:ARG:HD2	1:N:474:GLY:O	1.89	0.72
1:H:100:ILE:O	1:H:104:LEU:HB2	1.90	0.72
1:K:149:THR:HG23	1:K:159:GLY:HA3	1.70	0.72
1:N:100:ILE:O	1:N:104:LEU:HB2	1.90	0.72
1:D:100:ILE:HD11	1:D:514:MET:HE1	1.72	0.72
1:L:32:GLY:HA2	1:L:454:ILE:HD13	1.71	0.72
1:I:131:LEU:CD1	1:I:422:VAL:HG11	2.20	0.72
1:D:409:GLU:OE2	1:D:501:ARG:NH2	2.22	0.71
1:F:74:VAL:O	1:F:77:VAL:HG13	1.90	0.71
1:I:232:GLU:HB3	1:I:309:LEU:HB2	1.71	0.71
1:J:100:ILE:O	1:J:104:LEU:HB2	1.90	0.71
1:G:44:PHE:N	1:G:44:PHE:HD1	1.86	0.71
1:H:227:ILE:HD12	1:H:309:LEU:HD11	1.72	0.71
1:L:421:ARG:HD2	1:L:474:GLY:O	1.90	0.71
1:K:32:GLY:HA2	1:K:454:ILE:HD13	1.71	0.71
1:L:227:ILE:HD12	1:L:309:LEU:HD11	1.73	0.71
1:I:227:ILE:HD12	1:I:309:LEU:HD11	1.72	0.71
1:K:131:LEU:HD13	1:K:422:VAL:HG11	1.70	0.71
1:L:131:LEU:HD13	1:L:422:VAL:HG11	1.71	0.71
1:M:149:THR:HG23	1:M:159:GLY:HA3	1.71	0.71
1:N:149:THR:HG23	1:N:159:GLY:HA3	1.73	0.71
1:N:227:ILE:HD12	1:N:309:LEU:HD11	1.72	0.71
1:M:69:MET:HE1	1:M:522:THR:HB	1.72	0.71
1:I:404:ARG:HG2	1:I:404:ARG:NH1	2.05	0.71
1:K:227:ILE:HD12	1:K:309:LEU:HD11	1.72	0.70
1:M:227:ILE:HD12	1:M:309:LEU:HD11	1.72	0.70
1:A:417:VAL:HG11	1:A:488:MET:HG3	1.73	0.70
1:K:421:ARG:HD2	1:K:474:GLY:O	1.90	0.70
1:H:419:LEU:CD2	1:H:500:THR:CG2	2.69	0.70
1:K:69:MET:CE	1:K:522:THR:HB	2.21	0.70
1:B:33:PRO:HA	1:B:153:ASN:HD21	1.55	0.70
1:I:69:MET:CE	1:I:522:THR:HB	2.22	0.70
1:J:227:ILE:HD12	1:J:309:LEU:HD11	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:100:ILE:O	1:L:104:LEU:HB2	1.92	0.70
1:A:430:ARG:NH1	1:A:430:ARG:HG2	2.07	0.70
1:I:419:LEU:CD2	1:I:500:THR:CG2	2.69	0.70
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.73	0.70
1:A:20:VAL:HG13	1:A:74:VAL:HG11	1.73	0.69
1:H:27:VAL:HG11	1:H:93:THR:HG21	1.73	0.69
1:M:419:LEU:CD2	1:M:500:THR:CG2	2.69	0.69
1:C:64:ASP:HB3	1:C:67:GLU:HB2	1.74	0.69
1:M:27:VAL:HG11	1:M:93:THR:HG21	1.73	0.69
1:L:419:LEU:CD2	1:L:500:THR:HG23	2.23	0.69
1:I:173:GLY:O	1:I:404:ARG:NH2	2.24	0.69
1:J:419:LEU:CD2	1:J:500:THR:HG23	2.22	0.69
1:K:27:VAL:HG11	1:K:93:THR:HG21	1.75	0.69
1:F:33:PRO:HA	1:F:153:ASN:HD21	1.57	0.69
1:I:419:LEU:CD2	1:I:500:THR:HG23	2.23	0.69
1:M:404:ARG:HG2	1:M:404:ARG:NH1	2.08	0.69
1:J:200:LEU:HD12	1:J:276:VAL:HA	1.75	0.69
1:D:44:PHE:N	1:D:44:PHE:HD1	1.84	0.68
1:A:44:PHE:HD1	1:A:44:PHE:N	1.85	0.68
1:K:200:LEU:HD12	1:K:276:VAL:HA	1.74	0.68
1:M:173:GLY:O	1:M:404:ARG:NH2	2.25	0.68
1:H:200:LEU:HD12	1:H:276:VAL:HA	1.75	0.68
1:H:452:ARG:HH11	1:H:452:ARG:HG2	1.58	0.68
1:M:32:GLY:HA2	1:M:454:ILE:HD13	1.75	0.68
1:G:430:ARG:HG2	1:G:430:ARG:NH1	2.08	0.68
1:C:417:VAL:HG11	1:C:488:MET:HG3	1.75	0.68
1:M:194:GLN:HB2	1:M:331:THR:HB	1.74	0.68
2:T:7:HIS:O	2:T:8:ASP:HB3	1.94	0.68
1:N:404:ARG:HH11	1:N:404:ARG:HG2	1.58	0.67
2:Q:7:HIS:O	2:Q:8:ASP:HB3	1.94	0.67
1:N:200:LEU:HD12	1:N:276:VAL:HA	1.75	0.67
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.57	0.67
1:J:131:LEU:CD1	1:J:422:VAL:HG11	2.25	0.67
1:K:65:LYS:O	1:K:66:PHE:CB	2.38	0.67
1:M:131:LEU:CD1	1:M:422:VAL:HG11	2.23	0.67
1:D:430:ARG:NH1	1:D:430:ARG:HG2	2.05	0.67
1:B:430:ARG:HG2	1:B:430:ARG:NH1	2.10	0.67
1:C:487:ASN:O	1:C:491:MET:HG3	1.94	0.67
1:I:65:LYS:O	1:I:66:PHE:CB	2.40	0.67
1:L:200:LEU:HD12	1:L:276:VAL:HA	1.76	0.67
1:I:200:LEU:HD12	1:I:276:VAL:HA	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:MET:O	1:C:20:VAL:HG23	1.95	0.66
2:P:7:HIS:O	2:P:8:ASP:HB3	1.95	0.66
1:F:100:ILE:HD11	1:F:514:MET:HE3	1.77	0.66
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.77	0.66
1:L:194:GLN:HB2	1:L:331:THR:HB	1.77	0.66
4:C:702:ADP:O3B	5:C:802:HOH:O	2.12	0.66
1:G:487:ASN:O	1:G:491:MET:HG3	1.95	0.66
1:I:100:ILE:O	1:I:104:LEU:HB2	1.95	0.66
1:C:510:VAL:HG12	1:D:385:THR:HG21	1.77	0.66
1:M:200:LEU:HD12	1:M:276:VAL:HA	1.76	0.66
1:D:417:VAL:HG11	1:D:488:MET:HG3	1.77	0.66
1:A:13:ARG:HD2	1:A:104:LEU:HD22	1.78	0.66
1:G:100:ILE:HD11	1:G:514:MET:HE1	1.78	0.66
1:I:452:ARG:HH11	1:I:452:ARG:HG2	1.60	0.66
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.59	0.66
1:L:419:LEU:CD2	1:L:500:THR:CG2	2.74	0.66
1:B:74:VAL:HG13	1:B:514:MET:HE3	1.78	0.66
1:M:38:VAL:HG22	1:N:519:CYS:HB3	1.77	0.66
2:O:7:HIS:O	2:O:8:ASP:HB3	1.96	0.66
1:E:74:VAL:HG13	1:E:514:MET:HE1	1.78	0.65
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.78	0.65
1:I:194:GLN:HB2	1:I:331:THR:HB	1.78	0.65
1:M:452:ARG:HG2	1:M:452:ARG:HH11	1.59	0.65
1:N:32:GLY:HA2	1:N:454:ILE:HD13	1.77	0.65
2:U:7:HIS:O	2:U:8:ASP:HB3	1.97	0.65
4:B:701:ADP:O3B	5:B:801:HOH:O	2.13	0.65
1:C:33:PRO:HA	1:C:153:ASN:ND2	2.11	0.65
1:E:100:ILE:HD11	1:E:514:MET:HE1	1.77	0.65
1:I:32:GLY:HA2	1:I:454:ILE:HD13	1.77	0.65
2:S:7:HIS:O	2:S:8:ASP:HB3	1.95	0.65
1:L:27:VAL:HG11	1:L:93:THR:HG21	1.78	0.65
1:A:39:VAL:HG23	1:G:517:THR:HG23	1.78	0.65
1:H:65:LYS:O	1:H:66:PHE:CB	2.37	0.65
1:M:385:THR:HG23	1:M:388:GLU:HB2	1.79	0.64
1:F:44:PHE:HD1	1:F:44:PHE:N	1.87	0.64
1:C:430:ARG:NH1	1:C:430:ARG:HG2	2.10	0.64
1:M:65:LYS:O	1:M:66:PHE:CB	2.34	0.64
1:C:516:THR:OG1	1:D:37:ASN:ND2	2.29	0.64
1:K:452:ARG:HH11	1:K:452:ARG:HG2	1.62	0.64
1:E:417:VAL:HG11	1:E:488:MET:HG3	1.79	0.64
1:G:288:MET:HG2	1:G:368:ARG:HD2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:LEU:CD1	1:L:422:VAL:HG11	2.28	0.64
1:J:173:GLY:O	1:J:404:ARG:NH2	2.30	0.64
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.79	0.64
1:K:194:GLN:HB2	1:K:331:THR:HB	1.80	0.64
1:F:111:MET:HG2	1:F:435:ASP:OD1	1.98	0.63
1:N:194:GLN:HB2	1:N:331:THR:HB	1.80	0.63
1:A:288:MET:HG2	1:A:368:ARG:HD2	1.80	0.63
2:O:20:LYS:HB3	2:O:27:LEU:HG	1.81	0.63
1:B:288:MET:HG2	1:B:368:ARG:HD2	1.80	0.63
1:N:419:LEU:CD2	1:N:500:THR:CG2	2.75	0.63
1:F:417:VAL:HG11	1:F:488:MET:HG3	1.79	0.63
1:H:194:GLN:HB2	1:H:331:THR:HB	1.81	0.63
1:H:173:GLY:O	1:H:404:ARG:NH2	2.31	0.63
1:J:27:VAL:HG11	1:J:93:THR:HG21	1.81	0.63
1:I:30:THR:HB	1:I:51:LYS:O	1.99	0.63
1:J:65:LYS:O	1:J:66:PHE:CB	2.40	0.63
1:H:96:ALA:O	1:H:100:ILE:HG13	1.98	0.62
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.79	0.62
1:D:18:ARG:CB	1:D:18:ARG:HH11	2.11	0.62
1:L:47:PRO:HG2	1:M:73:MET:HG3	1.80	0.62
1:E:288:MET:HG2	1:E:368:ARG:HD2	1.80	0.62
1:B:100:ILE:HD11	1:B:514:MET:HE3	1.80	0.62
1:G:409:GLU:OE2	1:G:501:ARG:NH2	2.29	0.62
2:T:20:LYS:HB3	2:T:27:LEU:HG	1.82	0.62
1:F:430:ARG:NH1	1:F:430:ARG:HG2	2.12	0.62
1:B:64:ASP:HB3	1:B:67:GLU:HB2	1.81	0.62
1:J:194:GLN:HB2	1:J:331:THR:HB	1.82	0.62
1:L:173:GLY:O	1:L:404:ARG:NH2	2.32	0.62
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.82	0.62
1:B:111:MET:HG2	1:B:435:ASP:OD1	1.99	0.62
1:K:131:LEU:CD1	1:K:422:VAL:HG11	2.30	0.62
2:R:20:LYS:HB3	2:R:27:LEU:HG	1.81	0.62
2:R:7:HIS:O	2:R:8:ASP:HB3	1.98	0.62
2:U:20:LYS:HB3	2:U:27:LEU:HG	1.82	0.62
1:H:419:LEU:HD21	1:H:500:THR:HG23	1.82	0.61
1:J:149:THR:CG2	1:J:159:GLY:HA3	2.29	0.61
2:Q:20:LYS:HB3	2:Q:27:LEU:HG	1.81	0.61
4:A:700:ADP:O3B	5:A:800:HOH:O	2.16	0.61
1:G:193:MET:HG3	1:G:371:LYS:HB3	1.82	0.61
1:G:510:VAL:HG23	1:G:514:MET:CE	2.30	0.61
1:H:131:LEU:CD1	1:H:422:VAL:HG11	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ASP:HB3	1:D:67:GLU:HB2	1.83	0.61
1:F:288:MET:HG2	1:F:368:ARG:HD2	1.81	0.61
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.81	0.61
1:N:173:GLY:O	1:N:404:ARG:NH2	2.33	0.61
1:I:2:ALA:O	1:I:4:LYS:HE3	1.99	0.61
1:J:426:LEU:CD1	1:J:444:LEU:HD21	2.30	0.61
1:A:414:GLY:O	1:A:417:VAL:CG1	2.40	0.61
2:P:20:LYS:HB3	2:P:27:LEU:HG	1.83	0.61
2:S:20:LYS:HB3	2:S:27:LEU:HG	1.83	0.61
1:N:131:LEU:HD13	1:N:422:VAL:HG11	1.82	0.61
1:F:409:GLU:OE2	1:F:501:ARG:NH2	2.31	0.61
1:K:199:TYR:HA	1:K:276:VAL:HG12	1.83	0.61
1:L:426:LEU:CD1	1:L:444:LEU:HD21	2.27	0.61
1:A:234:LEU:HD22	2:O:23:GLY:HA3	1.81	0.61
1:C:288:MET:HG2	1:C:368:ARG:HD2	1.81	0.61
1:H:385:THR:HG23	1:H:388:GLU:HB2	1.81	0.61
1:B:419:LEU:HG	1:B:447:MET:HG2	1.83	0.60
1:F:419:LEU:HG	1:F:447:MET:HG2	1.82	0.60
1:K:419:LEU:HD21	1:K:500:THR:HG23	1.82	0.60
1:B:417:VAL:HG11	1:B:488:MET:HG3	1.82	0.60
1:I:149:THR:CG2	1:I:159:GLY:HA3	2.30	0.60
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.83	0.60
1:K:149:THR:CG2	1:K:159:GLY:HA3	2.31	0.60
1:N:174:VAL:HG21	1:N:194:GLN:HB3	1.84	0.60
1:N:385:THR:HG23	1:N:388:GLU:HB2	1.83	0.60
1:F:193:MET:HG3	1:F:371:LYS:HB3	1.84	0.60
1:G:33:PRO:HA	1:G:153:ASN:ND2	2.17	0.60
1:L:452:ARG:HG2	1:L:452:ARG:HH11	1.66	0.60
1:E:33:PRO:HA	1:E:153:ASN:ND2	2.16	0.60
1:E:193:MET:HG3	1:E:371:LYS:HB3	1.84	0.60
1:G:302:SER:H	1:G:307:MET:HE3	1.66	0.60
1:L:404:ARG:HG2	1:L:404:ARG:NH1	2.11	0.60
1:L:24:ALA:HA	1:L:27:VAL:HG12	1.84	0.59
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.83	0.59
1:B:510:VAL:HG12	1:C:385:THR:HG21	1.84	0.59
1:C:325:ILE:HG12	1:C:330:THR:HG23	1.84	0.59
1:I:385:THR:HG23	1:I:388:GLU:HB2	1.82	0.59
1:H:2:ALA:O	1:H:4:LYS:HE3	2.02	0.59
1:L:385:THR:HG23	1:L:388:GLU:HB2	1.83	0.59
1:B:16:MET:O	1:B:20:VAL:HG23	2.03	0.59
1:D:193:MET:HG3	1:D:371:LYS:HB3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:ILE:HG12	1:F:330:THR:HG23	1.83	0.59
1:K:173:GLY:O	1:K:404:ARG:NH2	2.35	0.59
1:M:411:VAL:HG21	1:M:494:LEU:HD12	1.83	0.59
2:R:23:GLY:H	2:S:80:ASN:ND2	2.00	0.59
1:A:420:ILE:HD13	1:A:451:LEU:HD13	1.83	0.59
1:B:487:ASN:O	1:B:491:MET:HG3	2.03	0.59
1:L:149:THR:CG2	1:L:159:GLY:HA3	2.32	0.59
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.83	0.59
1:G:325:ILE:HG12	1:G:330:THR:HG23	1.84	0.59
1:M:149:THR:CG2	1:M:159:GLY:HA3	2.31	0.59
1:M:426:LEU:CD1	1:M:444:LEU:HD21	2.30	0.59
1:M:146:GLN:HE21	1:M:150:ILE:HD11	1.68	0.59
1:N:27:VAL:HG11	1:N:93:THR:HG21	1.85	0.59
1:A:193:MET:HG3	1:A:371:LYS:HB3	1.85	0.58
1:C:111:MET:HG2	1:C:435:ASP:OD1	2.03	0.58
1:C:520:MET:HG2	1:D:39:VAL:HB	1.84	0.58
1:A:432:GLN:NE2	1:A:436:GLN:NE2	2.35	0.58
1:K:146:GLN:HE21	1:K:150:ILE:HD11	1.67	0.58
1:A:325:ILE:HG12	1:A:330:THR:HG23	1.85	0.58
1:A:419:LEU:HG	1:A:447:MET:HG2	1.85	0.58
1:I:411:VAL:HG21	1:I:494:LEU:HD12	1.86	0.58
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.85	0.58
1:G:64:ASP:HB3	1:G:67:GLU:HB2	1.86	0.58
1:J:146:GLN:HE21	1:J:150:ILE:HD11	1.68	0.58
1:B:325:ILE:HG12	1:B:330:THR:HG23	1.86	0.58
1:B:33:PRO:HA	1:B:153:ASN:ND2	2.18	0.58
1:J:174:VAL:HG21	1:J:194:GLN:HB3	1.86	0.58
1:E:268:ARG:HH21	2:S:27:LEU:CD2	2.16	0.58
1:L:223:ALA:HB3	1:L:251:ALA:HB2	1.86	0.58
1:L:64:ASP:HB3	1:L:67:GLU:HB2	1.85	0.58
1:F:510:VAL:HG12	1:G:385:THR:HG21	1.85	0.58
1:M:30:THR:HB	1:M:51:LYS:O	2.04	0.58
1:I:199:TYR:HA	1:I:276:VAL:HG12	1.86	0.58
1:N:313:THR:HG22	1:N:314:LEU:H	1.69	0.58
1:C:432:GLN:NE2	1:C:436:GLN:NE2	2.34	0.57
1:H:149:THR:CG2	1:H:159:GLY:HA3	2.33	0.57
1:A:162:ILE:HG12	1:A:400:LEU:HD23	1.86	0.57
1:C:102:GLU:HB3	1:C:442:VAL:HG22	1.86	0.57
1:D:33:PRO:HA	1:D:153:ASN:HD21	1.68	0.57
1:K:223:ALA:HB3	1:K:251:ALA:HB2	1.87	0.57
1:D:325:ILE:HG12	1:D:330:THR:HG23	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:313:THR:HG22	1:L:314:LEU:H	1.69	0.57
1:L:39:VAL:HB	1:M:520:MET:HG2	1.86	0.57
1:N:426:LEU:CD1	1:N:444:LEU:HD21	2.31	0.57
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.87	0.57
1:J:199:TYR:HA	1:J:276:VAL:HG12	1.87	0.57
1:L:146:GLN:HE21	1:L:150:ILE:HD11	1.69	0.57
1:A:39:VAL:HB	1:G:520:MET:HG2	1.86	0.57
1:C:20:VAL:HG13	1:C:74:VAL:HG11	1.86	0.57
1:N:404:ARG:HG2	1:N:404:ARG:NH1	2.20	0.57
1:A:33:PRO:HA	1:A:153:ASN:HD21	1.70	0.57
1:B:193:MET:HG3	1:B:371:LYS:HB3	1.87	0.57
1:A:37:ASN:ND2	1:G:516:THR:OG1	2.31	0.57
1:M:270:ILE:HA	1:N:257:GLU:OE2	2.04	0.57
2:P:3:ILE:HD13	2:P:11:ILE:HG21	1.87	0.57
1:E:419:LEU:HG	1:E:447:MET:HG2	1.86	0.57
1:J:24:ALA:HA	1:J:27:VAL:HG12	1.86	0.57
1:B:18:ARG:CG	1:B:18:ARG:NH1	2.43	0.57
1:C:193:MET:HG3	1:C:371:LYS:HB3	1.87	0.57
1:G:432:GLN:NE2	1:G:436:GLN:NE2	2.36	0.57
1:H:223:ALA:HB3	1:H:251:ALA:HB2	1.87	0.57
1:K:385:THR:HG23	1:K:388:GLU:HB2	1.86	0.57
1:K:426:LEU:CD1	1:K:444:LEU:HD21	2.33	0.57
1:N:223:ALA:HB3	1:N:251:ALA:HB2	1.87	0.57
1:G:111:MET:HG2	1:G:435:ASP:OD1	2.05	0.56
1:L:19:GLY:HA3	1:L:67:GLU:O	2.04	0.56
1:H:16:MET:HG3	1:H:520:MET:SD	2.44	0.56
1:G:419:LEU:HG	1:G:447:MET:HG2	1.88	0.56
1:I:419:LEU:HD21	1:I:500:THR:HG23	1.87	0.56
1:J:145:ALA:O	1:J:149:THR:HG23	2.05	0.56
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.87	0.56
1:F:18:ARG:NH1	1:F:18:ARG:CG	2.45	0.56
1:J:313:THR:HG22	1:J:314:LEU:H	1.69	0.56
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.15	0.56
1:D:288:MET:HG2	1:D:368:ARG:HD2	1.86	0.56
1:I:64:ASP:HB3	1:I:67:GLU:HB2	1.87	0.56
1:N:24:ALA:HA	1:N:27:VAL:HG12	1.87	0.56
1:N:403:THR:O	1:N:407:VAL:HG23	2.06	0.56
1:A:64:ASP:HB3	1:A:67:GLU:HB2	1.88	0.56
1:E:430:ARG:NH1	1:E:430:ARG:HG2	2.13	0.56
1:F:33:PRO:HA	1:F:153:ASN:ND2	2.21	0.56
1:K:96:ALA:O	1:K:100:ILE:HG13	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:24:ALA:HA	1:M:27:VAL:HG12	1.88	0.56
1:N:19:GLY:HA3	1:N:67:GLU:O	2.05	0.56
1:F:64:ASP:HB3	1:F:67:GLU:HB2	1.88	0.56
1:H:313:THR:HG22	1:H:314:LEU:H	1.70	0.56
1:J:385:THR:HG23	1:J:388:GLU:HB2	1.86	0.56
1:L:199:TYR:HA	1:L:276:VAL:HG12	1.87	0.56
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.86	0.56
1:C:268:ARG:HD2	2:Q:27:LEU:CD2	2.34	0.56
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.87	0.56
1:H:426:LEU:CD1	1:H:444:LEU:HD21	2.34	0.56
1:N:146:GLN:HE21	1:N:150:ILE:HD11	1.69	0.56
1:J:123:ALA:HB2	1:J:440:ILE:HG23	1.88	0.56
1:A:111:MET:HG2	1:A:435:ASP:OD1	2.05	0.56
1:C:419:LEU:HG	1:C:447:MET:HG2	1.86	0.56
1:C:519:CYS:HB3	1:D:38:VAL:HG22	1.88	0.56
1:E:353:ILE:HG12	1:E:365:LEU:HB3	1.88	0.56
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.20	0.56
1:J:64:ASP:HB3	1:J:67:GLU:HB2	1.88	0.56
1:L:65:LYS:O	1:L:66:PHE:CB	2.43	0.56
1:M:199:TYR:HA	1:M:276:VAL:HG12	1.86	0.56
1:M:69:MET:HE2	1:M:522:THR:HB	1.88	0.56
1:M:47:PRO:HG2	1:N:73:MET:HG3	1.88	0.56
2:T:3:ILE:HD13	2:T:11:ILE:HG21	1.87	0.56
1:H:199:TYR:HA	1:H:276:VAL:HG12	1.87	0.56
1:I:326:ASN:ND2	1:I:328:ASP:H	2.03	0.56
1:J:403:THR:O	1:J:407:VAL:HG23	2.06	0.56
1:M:90:THR:O	1:M:94:VAL:HG23	2.05	0.56
1:D:432:GLN:NE2	1:D:436:GLN:NE2	2.30	0.55
1:J:419:LEU:HD21	1:J:500:THR:CG2	2.36	0.55
1:K:2:ALA:O	1:K:4:LYS:HE3	2.05	0.55
2:O:3:ILE:HD13	2:O:11:ILE:HG21	1.88	0.55
1:A:16:MET:O	1:A:20:VAL:HG23	2.05	0.55
1:E:487:ASN:O	1:E:491:MET:HG3	2.05	0.55
1:G:353:ILE:HG12	1:G:365:LEU:HB3	1.88	0.55
1:L:417:VAL:HG21	1:L:488:MET:HG3	1.87	0.55
1:K:24:ALA:HA	1:K:27:VAL:HG12	1.88	0.55
2:R:3:ILE:HD13	2:R:11:ILE:HG21	1.87	0.55
1:H:146:GLN:HE21	1:H:150:ILE:HD11	1.70	0.55
1:I:419:LEU:HD21	1:I:500:THR:CG2	2.36	0.55
1:N:326:ASN:ND2	1:N:328:ASP:H	2.03	0.55
1:F:124:VAL:HG13	1:F:504:LEU:HD13	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:413:ALA:HB1	1:M:417:VAL:HB	1.88	0.55
1:C:100:ILE:CD1	1:C:514:MET:HE1	2.33	0.55
1:G:20:VAL:HG13	1:G:74:VAL:HG11	1.87	0.55
1:I:24:ALA:HA	1:I:27:VAL:HG12	1.87	0.55
1:C:18:ARG:CB	1:C:18:ARG:HH11	2.18	0.55
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.88	0.55
1:N:77:VAL:HG22	1:N:506:TYR:HD1	1.71	0.55
1:B:353:ILE:HG12	1:B:365:LEU:HB3	1.88	0.55
1:D:111:MET:HG2	1:D:435:ASP:OD1	2.06	0.55
1:F:74:VAL:HG13	1:F:514:MET:HE3	1.88	0.55
1:G:238:GLU:HA	1:G:238:GLU:OE2	2.07	0.55
1:I:426:LEU:CD1	1:I:444:LEU:HD21	2.31	0.55
1:K:313:THR:HG22	1:K:314:LEU:H	1.72	0.55
1:M:346:VAL:HG21	1:M:373:ALA:HB2	1.89	0.55
1:A:238:GLU:OE2	1:A:238:GLU:HA	2.07	0.55
1:D:409:GLU:CD	1:D:501:ARG:HH21	2.07	0.55
1:J:326:ASN:ND2	1:J:328:ASP:H	2.04	0.55
1:L:193:MET:HG3	1:L:371:LYS:HB3	1.89	0.55
1:N:149:THR:CG2	1:N:159:GLY:HA3	2.36	0.55
1:N:419:LEU:HD21	1:N:500:THR:HG23	1.89	0.55
1:N:452:ARG:NH1	1:N:452:ARG:HG2	2.22	0.55
1:H:24:ALA:HA	1:H:27:VAL:HG12	1.88	0.54
1:I:223:ALA:HB3	1:I:251:ALA:HB2	1.88	0.54
1:M:313:THR:HG22	1:M:314:LEU:H	1.71	0.54
2:R:13:LYS:HB3	2:R:41:LEU:HD11	1.89	0.54
1:C:238:GLU:HA	1:C:238:GLU:OE2	2.07	0.54
1:D:487:ASN:O	1:D:491:MET:HG3	2.08	0.54
1:E:64:ASP:HB3	1:E:67:GLU:HB2	1.90	0.54
1:I:27:VAL:HG11	1:I:93:THR:HG21	1.88	0.54
1:K:417:VAL:HG21	1:K:488:MET:HG3	1.88	0.54
1:M:403:THR:O	1:M:407:VAL:HG23	2.07	0.54
1:M:419:LEU:HD21	1:M:500:THR:HG23	1.89	0.54
2:Q:3:ILE:HD13	2:Q:11:ILE:HG21	1.88	0.54
1:G:18:ARG:NH1	1:G:18:ARG:CG	2.49	0.54
1:J:404:ARG:NH1	1:J:404:ARG:HG2	2.16	0.54
1:N:199:TYR:HA	1:N:276:VAL:HG12	1.88	0.54
1:J:476:TYR:HA	1:J:486:GLY:O	2.08	0.54
1:N:433:ASN:OD1	1:N:435:ASP:HB2	2.07	0.54
1:H:346:VAL:HG21	1:H:373:ALA:HB2	1.90	0.54
1:K:326:ASN:ND2	1:K:328:ASP:H	2.06	0.54
1:N:419:LEU:HD11	1:N:504:LEU:HG	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:3:ILE:HD13	2:S:11:ILE:HG21	1.89	0.54
2:T:13:LYS:HB3	2:T:41:LEU:HD11	1.89	0.54
1:D:510:VAL:HG23	1:D:514:MET:CE	2.38	0.54
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.89	0.54
1:N:96:ALA:O	1:N:100:ILE:HG13	2.07	0.54
1:N:149:THR:CG2	1:N:156:GLU:HA	2.37	0.54
1:A:510:VAL:HG23	1:A:514:MET:CE	2.38	0.54
1:E:16:MET:O	1:E:20:VAL:HG23	2.08	0.54
2:U:3:ILE:HD13	2:U:11:ILE:HG21	1.89	0.54
1:E:302:SER:H	1:E:307:MET:HE3	1.73	0.54
1:D:353:ILE:HG12	1:D:365:LEU:HB3	1.89	0.54
1:H:149:THR:CG2	1:H:156:GLU:HA	2.38	0.54
2:O:6:LEU:O	2:O:7:HIS:O	2.26	0.54
2:R:23:GLY:H	2:S:80:ASN:HD21	1.56	0.54
1:C:153:ASN:O	1:C:154:SER:HB2	2.07	0.54
1:J:346:VAL:HG21	1:J:373:ALA:HB2	1.88	0.54
1:J:77:VAL:HG22	1:J:506:TYR:HD1	1.73	0.54
1:A:18:ARG:CB	1:A:18:ARG:HH11	2.21	0.53
1:D:452:ARG:HH11	1:D:452:ARG:HG2	1.73	0.53
1:J:16:MET:O	1:J:20:VAL:HG12	2.08	0.53
1:J:223:ALA:HB3	1:J:251:ALA:HB2	1.90	0.53
1:J:419:LEU:HD11	1:J:504:LEU:HG	1.89	0.53
2:Q:13:LYS:HB3	2:Q:41:LEU:HD11	1.90	0.53
1:D:150:ILE:HD13	1:D:493:ILE:HA	1.90	0.53
1:G:510:VAL:CG2	1:G:514:MET:HE2	2.38	0.53
1:H:130:GLU:HG3	1:H:426:LEU:HD23	1.91	0.53
1:I:313:THR:HG22	1:I:314:LEU:H	1.74	0.53
1:L:218:PRO:HB3	1:L:246:PRO:HB2	1.91	0.53
1:B:238:GLU:HA	1:B:238:GLU:OE2	2.09	0.53
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.89	0.53
1:G:124:VAL:HG13	1:G:504:LEU:HD13	1.91	0.53
1:H:64:ASP:HB3	1:H:67:GLU:HB2	1.89	0.53
1:J:30:THR:HB	1:J:51:LYS:O	2.07	0.53
1:D:74:VAL:HG13	1:D:514:MET:HE1	1.90	0.53
4:D:703:ADP:O3B	5:D:803:HOH:O	2.19	0.53
1:N:346:VAL:HG21	1:N:373:ALA:HB2	1.90	0.53
1:B:42:LYS:HE2	1:B:48:THR:OG1	2.08	0.53
1:M:223:ALA:HB3	1:M:251:ALA:HB2	1.90	0.53
1:M:218:PRO:HB3	1:M:246:PRO:HB2	1.91	0.53
1:G:162:ILE:HG21	1:G:403:THR:HG21	1.90	0.53
1:G:510:VAL:HG23	1:G:514:MET:HE2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:149:THR:CG2	1:J:156:GLU:HA	2.38	0.53
1:K:403:THR:O	1:K:407:VAL:HG23	2.09	0.53
1:A:238:GLU:OE1	2:O:24:GLY:HA3	2.09	0.53
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.90	0.53
1:J:419:LEU:HD21	1:J:500:THR:HG23	1.90	0.53
1:D:16:MET:O	1:D:20:VAL:HG23	2.08	0.53
1:D:419:LEU:HG	1:D:447:MET:HG2	1.89	0.53
1:G:452:ARG:HH11	1:G:452:ARG:HG2	1.73	0.53
1:B:302:SER:H	1:B:307:MET:HE3	1.74	0.53
1:C:18:ARG:NH1	1:C:18:ARG:CG	2.46	0.53
1:D:302:SER:H	1:D:307:MET:HE3	1.73	0.53
1:E:20:VAL:HG13	1:E:74:VAL:HG11	1.90	0.53
1:J:161:LEU:HD21	1:J:185:ASP:HB3	1.91	0.53
1:L:161:LEU:HD21	1:L:185:ASP:HB3	1.90	0.53
1:L:419:LEU:HD21	1:L:500:THR:HG23	1.91	0.53
2:U:6:LEU:O	2:U:7:HIS:O	2.27	0.53
1:D:162:ILE:HG12	1:D:400:LEU:HD23	1.90	0.52
1:E:42:LYS:HE2	1:E:48:THR:OG1	2.09	0.52
1:J:16:MET:HG3	1:J:520:MET:SD	2.49	0.52
1:K:161:LEU:HD21	1:K:185:ASP:HB3	1.90	0.52
1:N:123:ALA:HB2	1:N:440:ILE:HG23	1.91	0.52
1:B:18:ARG:CB	1:B:18:ARG:HH11	2.20	0.52
1:C:409:GLU:OE2	1:C:501:ARG:NH2	2.33	0.52
1:E:238:GLU:HA	1:E:238:GLU:OE2	2.09	0.52
1:H:123:ALA:HB2	1:H:440:ILE:HG23	1.92	0.52
1:I:149:THR:CG2	1:I:156:GLU:HA	2.38	0.52
1:I:145:ALA:O	1:I:149:THR:HG23	2.09	0.52
1:K:419:LEU:HD11	1:K:504:LEU:HG	1.92	0.52
2:Q:47:ARG:HD2	2:Q:49:LEU:HB2	1.91	0.52
1:A:162:ILE:HG21	1:A:403:THR:HG21	1.90	0.52
1:L:403:THR:O	1:L:407:VAL:HG23	2.08	0.52
1:N:66:PHE:H	1:N:69:MET:HG3	1.75	0.52
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.52	0.52
1:I:16:MET:HG3	1:I:520:MET:SD	2.49	0.52
1:B:20:VAL:HG13	1:B:74:VAL:HG11	1.92	0.52
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.92	0.52
1:K:145:ALA:O	1:K:149:THR:HG23	2.10	0.52
1:L:145:ALA:O	1:L:149:THR:HG23	2.09	0.52
1:B:162:ILE:HG12	1:B:400:LEU:HD23	1.91	0.52
1:F:77:VAL:HG23	1:F:92:ALA:HB1	1.91	0.52
1:M:326:ASN:ND2	1:M:328:ASP:H	2.07	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.90	0.52
2:O:23:GLY:H	2:P:80:ASN:HD21	1.58	0.52
1:H:218:PRO:HB3	1:H:246:PRO:HB2	1.92	0.52
2:O:80:ASN:HD21	2:U:23:GLY:H	1.58	0.52
2:Q:23:GLY:H	2:R:80:ASN:HD21	1.58	0.52
1:A:224:ASP:HB3	1:A:302:SER:HA	1.91	0.52
1:A:74:VAL:HG13	1:A:514:MET:HE1	1.91	0.52
1:F:452:ARG:HG2	1:F:452:ARG:HH11	1.74	0.52
1:F:487:ASN:O	1:F:491:MET:HG3	2.09	0.52
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.92	0.52
1:L:326:ASN:ND2	1:L:328:ASP:H	2.08	0.52
1:L:123:ALA:HB2	1:L:440:ILE:HG23	1.92	0.52
1:E:77:VAL:HG23	1:E:92:ALA:HB1	1.92	0.52
1:F:238:GLU:HA	1:F:238:GLU:OE2	2.08	0.52
1:H:161:LEU:HD21	1:H:185:ASP:HB3	1.92	0.52
1:H:443:ALA:O	1:H:447:MET:HG3	2.10	0.52
1:N:411:VAL:HG21	1:N:494:LEU:HD12	1.92	0.52
1:E:268:ARG:HH21	2:S:27:LEU:HD23	1.75	0.52
2:T:47:ARG:HD2	2:T:49:LEU:HB2	1.92	0.52
1:H:130:GLU:HG3	1:H:426:LEU:CD2	2.40	0.52
1:H:102:GLU:OE2	1:H:445:ARG:NH1	2.43	0.52
1:K:19:GLY:HA3	1:K:67:GLU:O	2.09	0.52
2:S:47:ARG:HD2	2:S:49:LEU:HB2	1.92	0.52
1:G:33:PRO:HG3	4:G:706:ADP:C6	2.45	0.51
2:P:6:LEU:O	2:P:7:HIS:O	2.28	0.51
1:C:381:VAL:CG1	1:C:392:LYS:HG2	2.40	0.51
1:C:501:ARG:HD3	1:C:505:GLN:OE1	2.11	0.51
1:D:6:VAL:HG23	1:D:6:VAL:O	2.11	0.51
1:E:162:ILE:HG12	1:E:400:LEU:HD23	1.91	0.51
1:K:346:VAL:HG21	1:K:373:ALA:HB2	1.91	0.51
1:M:145:ALA:O	1:M:149:THR:HG23	2.10	0.51
1:M:161:LEU:HD21	1:M:185:ASP:HB3	1.91	0.51
1:M:2:ALA:O	1:M:4:LYS:HE3	2.11	0.51
1:N:131:LEU:CD1	1:N:422:VAL:HG11	2.40	0.51
2:P:23:GLY:H	2:Q:80:ASN:HD21	1.58	0.51
1:A:487:ASN:O	1:A:491:MET:HG3	2.10	0.51
1:C:302:SER:H	1:C:307:MET:HE3	1.75	0.51
1:D:32:GLY:HA2	4:D:703:ADP:H5'1	1.91	0.51
1:D:510:VAL:HG23	1:D:514:MET:HE2	1.92	0.51
2:P:13:LYS:HB3	2:P:41:LEU:HD11	1.92	0.51
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:ARG:HG2	1:C:452:ARG:HH11	1.74	0.51
1:G:510:VAL:HG23	1:G:514:MET:HE3	1.93	0.51
1:H:145:ALA:O	1:H:149:THR:HG23	2.09	0.51
1:J:16:MET:O	1:J:20:VAL:CG1	2.59	0.51
1:K:149:THR:CG2	1:K:156:GLU:HA	2.41	0.51
1:M:64:ASP:HB3	1:M:67:GLU:HB2	1.91	0.51
2:T:47:ARG:HD3	2:T:49:LEU:HD12	1.93	0.51
1:E:432:GLN:NE2	1:E:436:GLN:NE2	2.39	0.51
1:H:66:PHE:H	1:H:69:MET:HG3	1.76	0.51
1:H:38:VAL:HG22	1:I:519:CYS:HB3	1.91	0.51
1:J:452:ARG:HG2	1:J:452:ARG:NH1	2.26	0.51
1:C:268:ARG:HH21	2:Q:27:LEU:HD23	1.74	0.51
1:F:162:ILE:HG12	1:F:400:LEU:HD23	1.92	0.51
1:I:126:ALA:HB1	1:I:426:LEU:HD22	1.92	0.51
1:L:149:THR:CG2	1:L:156:GLU:HA	2.41	0.51
1:L:346:VAL:HG21	1:L:373:ALA:HB2	1.92	0.51
1:M:123:ALA:HB2	1:M:440:ILE:HG23	1.93	0.51
1:N:419:LEU:HD22	1:N:500:THR:CG2	2.41	0.51
1:E:224:ASP:HB3	1:E:302:SER:HA	1.92	0.51
1:J:19:GLY:HA3	1:J:67:GLU:O	2.09	0.51
1:K:419:LEU:HD21	1:K:500:THR:CG2	2.37	0.51
1:L:77:VAL:HG22	1:L:506:TYR:HD1	1.75	0.51
1:E:153:ASN:O	1:E:154:SER:HB2	2.11	0.51
1:F:18:ARG:HH11	1:F:18:ARG:CB	2.21	0.51
1:I:161:LEU:HD21	1:I:185:ASP:HB3	1.92	0.51
1:J:218:PRO:HB3	1:J:246:PRO:HB2	1.93	0.51
1:N:476:TYR:HA	1:N:486:GLY:O	2.10	0.51
2:U:11:ILE:HG12	2:U:85:ILE:HG12	1.93	0.51
1:D:510:VAL:HG12	1:E:385:THR:HG21	1.93	0.51
1:I:146:GLN:HE21	1:I:150:ILE:HD11	1.74	0.51
1:I:218:PRO:HB3	1:I:246:PRO:HB2	1.93	0.51
1:I:38:VAL:HG12	1:I:40:LEU:HD13	1.92	0.51
1:L:458:CYS:SG	1:L:480:ALA:HB1	2.51	0.51
2:U:13:LYS:HB3	2:U:41:LEU:HD11	1.91	0.51
2:U:47:ARG:HD2	2:U:49:LEU:HB2	1.93	0.51
1:A:28:LYS:HD2	1:A:453:GLN:CD	2.31	0.50
1:B:420:ILE:HD13	1:B:451:LEU:HD13	1.93	0.50
1:D:238:GLU:HA	1:D:238:GLU:OE2	2.11	0.50
1:L:64:ASP:C	1:L:65:LYS:O	2.46	0.50
1:G:238:GLU:OE1	2:U:24:GLY:HA3	2.11	0.50
1:L:228:SER:O	1:L:257:GLU:HB3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:259:LEU:O	1:N:263:VAL:HG23	2.11	0.50
1:N:135:SER:HA	1:N:412:VAL:HG12	1.94	0.50
2:O:13:LYS:HB3	2:O:41:LEU:HD11	1.93	0.50
1:A:409:GLU:CD	1:A:501:ARG:HH21	2.10	0.50
1:B:381:VAL:HG21	1:B:393:LYS:HA	1.93	0.50
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.92	0.50
1:H:163:ALA:O	1:H:167:ASP:HB2	2.11	0.50
1:J:66:PHE:H	1:J:69:MET:HG3	1.77	0.50
1:A:300:VAL:O	1:A:307:MET:HE3	2.11	0.50
1:C:42:LYS:HE2	1:C:48:THR:OG1	2.11	0.50
1:D:204:PHE:HE1	1:D:274:ALA:HB2	1.77	0.50
1:H:11:ASP:O	1:H:12:ALA:C	2.50	0.50
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.94	0.50
1:K:102:GLU:OE2	1:K:445:ARG:NH1	2.44	0.50
2:O:50:GLU:HA	2:U:50:GLU:OE1	2.11	0.50
2:P:47:ARG:HD2	2:P:49:LEU:HB2	1.94	0.50
1:B:237:LEU:HD21	1:B:271:VAL:HG21	1.93	0.50
1:H:417:VAL:HG21	1:H:488:MET:HG3	1.92	0.50
1:L:96:ALA:O	1:L:100:ILE:HG13	2.11	0.50
1:N:145:ALA:O	1:N:149:THR:HG23	2.11	0.50
1:N:2:ALA:O	1:N:4:LYS:HE3	2.11	0.50
2:R:6:LEU:O	2:R:7:HIS:O	2.29	0.50
2:R:11:ILE:HG12	2:R:85:ILE:HG12	1.92	0.50
2:U:78:ILE:HD13	2:U:83:VAL:HG21	1.94	0.50
1:B:268:ARG:HH21	2:P:27:LEU:HD23	1.77	0.50
1:H:19:GLY:HA3	1:H:67:GLU:O	2.11	0.50
1:J:413:ALA:HB1	1:J:417:VAL:HB	1.92	0.50
1:K:218:PRO:HB3	1:K:246:PRO:HB2	1.93	0.50
1:N:193:MET:HG3	1:N:371:LYS:HB3	1.93	0.50
2:O:47:ARG:HD2	2:O:49:LEU:HB2	1.94	0.50
2:T:6:LEU:O	2:T:7:HIS:O	2.29	0.50
1:B:452:ARG:HG2	1:B:452:ARG:HH11	1.75	0.50
1:C:28:LYS:HD2	1:C:453:GLN:CD	2.32	0.50
1:F:356:ALA:HB3	1:F:362:ARG:HG3	1.94	0.50
1:I:346:VAL:HG21	1:I:373:ALA:HB2	1.93	0.50
1:J:135:SER:HA	1:J:412:VAL:HG12	1.94	0.50
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.94	0.50
1:A:356:ALA:HB3	1:A:362:ARG:HG3	1.94	0.50
1:B:224:ASP:HB3	1:B:302:SER:HA	1.93	0.50
1:D:28:LYS:HD2	1:D:453:GLN:CD	2.32	0.50
1:E:381:VAL:HG21	1:E:393:LYS:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ASP:HB3	1:F:302:SER:HA	1.93	0.50
1:I:193:MET:HG3	1:I:371:LYS:HB3	1.92	0.50
1:M:102:GLU:OE2	1:M:445:ARG:NH1	2.45	0.50
1:N:161:LEU:HD21	1:N:185:ASP:HB3	1.93	0.50
1:N:30:THR:HB	1:N:51:LYS:O	2.12	0.50
2:U:47:ARG:HD3	2:U:49:LEU:HD12	1.94	0.50
1:A:124:VAL:HG13	1:A:504:LEU:HD13	1.94	0.50
1:B:34:LYS:HD2	1:B:458:CYS:SG	2.52	0.50
1:B:381:VAL:CG1	1:B:392:LYS:HG2	2.42	0.50
1:C:162:ILE:HG12	1:C:400:LEU:HD23	1.93	0.50
1:C:381:VAL:HG21	1:C:393:LYS:HA	1.93	0.50
1:C:77:VAL:HG23	1:C:92:ALA:HB1	1.93	0.50
1:E:111:MET:HG2	1:E:435:ASP:OD1	2.12	0.50
1:I:19:GLY:HA3	1:I:67:GLU:O	2.11	0.50
1:M:149:THR:CG2	1:M:156:GLU:HA	2.42	0.50
1:C:237:LEU:HD21	1:C:271:VAL:HG21	1.93	0.49
1:D:501:ARG:HD3	1:D:505:GLN:OE1	2.12	0.49
1:H:419:LEU:HD11	1:H:504:LEU:HG	1.94	0.49
1:M:19:GLY:HA3	1:M:67:GLU:O	2.12	0.49
1:A:42:LYS:HG2	1:A:44:PHE:CE2	2.47	0.49
1:D:224:ASP:HB3	1:D:302:SER:HA	1.93	0.49
1:F:20:VAL:HG13	1:F:74:VAL:HG11	1.93	0.49
1:F:16:MET:O	1:F:20:VAL:HG23	2.12	0.49
1:G:224:ASP:HB3	1:G:302:SER:HA	1.93	0.49
1:G:237:LEU:HD21	1:G:271:VAL:HG21	1.93	0.49
1:C:124:VAL:HG13	1:C:504:LEU:HD13	1.93	0.49
1:E:356:ALA:HB3	1:E:362:ARG:HG3	1.94	0.49
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.94	0.49
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.94	0.49
2:R:47:ARG:HD2	2:R:49:LEU:HB2	1.94	0.49
1:K:228:SER:O	1:K:257:GLU:HB3	2.12	0.49
1:K:419:LEU:HD22	1:K:500:THR:CG2	2.42	0.49
1:M:419:LEU:HD11	1:M:504:LEU:HG	1.93	0.49
1:N:417:VAL:HG21	1:N:488:MET:HG3	1.93	0.49
1:D:522:THR:OG1	1:D:523:ASP:N	2.46	0.49
1:F:237:LEU:HD21	1:F:271:VAL:HG21	1.93	0.49
1:H:259:LEU:O	1:H:263:VAL:HG23	2.13	0.49
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.94	0.49
1:N:218:PRO:HB3	1:N:246:PRO:HB2	1.95	0.49
1:G:74:VAL:HG13	1:G:514:MET:HE1	1.95	0.49
1:H:77:VAL:HG22	1:H:506:TYR:HD1	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:163:ALA:O	1:L:167:ASP:HB2	2.12	0.49
1:L:2:ALA:O	1:L:4:LYS:HE3	2.13	0.49
2:Q:47:ARG:HD3	2:Q:49:LEU:HD12	1.94	0.49
1:C:224:ASP:HB3	1:C:302:SER:HA	1.94	0.49
1:K:193:MET:HG3	1:K:371:LYS:HB3	1.94	0.49
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.94	0.49
1:M:360:TYR:O	1:M:364:LYS:HB2	2.12	0.49
2:S:13:LYS:HB3	2:S:41:LEU:HD11	1.93	0.49
1:H:321:LYS:HB2	1:H:334:ASP:HB3	1.95	0.49
1:H:179:ASP:OD1	1:H:393:LYS:HD2	2.12	0.49
1:J:193:MET:HG3	1:J:371:LYS:HB3	1.93	0.49
1:M:135:SER:HA	1:M:412:VAL:HG12	1.95	0.49
1:G:28:LYS:C	1:G:30:THR:N	2.66	0.49
1:L:321:LYS:HB2	1:L:334:ASP:HB3	1.95	0.49
1:N:179:ASP:OD1	1:N:393:LYS:HD2	2.13	0.49
2:O:80:ASN:ND2	2:U:23:GLY:H	2.09	0.49
1:H:360:TYR:O	1:H:364:LYS:HB2	2.12	0.49
1:J:360:TYR:O	1:J:364:LYS:HB2	2.13	0.49
2:T:11:ILE:HG12	2:T:85:ILE:HG12	1.95	0.49
1:A:237:LEU:HD21	1:A:271:VAL:HG21	1.95	0.48
1:E:204:PHE:HE1	1:E:274:ALA:HB2	1.77	0.48
1:G:356:ALA:HB3	1:G:362:ARG:HG3	1.95	0.48
1:G:414:GLY:O	1:G:417:VAL:CG1	2.45	0.48
1:N:64:ASP:HB3	1:N:67:GLU:HB2	1.94	0.48
2:Q:6:LEU:O	2:Q:7:HIS:O	2.31	0.48
1:A:18:ARG:HB2	1:A:67:GLU:HG2	1.95	0.48
1:B:356:ALA:HB3	1:B:362:ARG:HG3	1.95	0.48
1:C:95:LEU:O	1:C:99:ILE:HG13	2.12	0.48
1:E:18:ARG:HH11	1:E:18:ARG:CB	2.25	0.48
1:H:452:ARG:NH1	1:H:452:ARG:HG2	2.27	0.48
1:H:419:LEU:HD21	1:H:500:THR:CG2	2.40	0.48
1:I:66:PHE:H	1:I:69:MET:HG3	1.78	0.48
1:J:38:VAL:HG22	1:K:519:CYS:HB3	1.94	0.48
1:L:411:VAL:HG21	1:L:494:LEU:HD12	1.94	0.48
1:C:247:LEU:HB3	1:C:273:VAL:HG12	1.94	0.48
1:C:517:THR:HG23	1:D:39:VAL:HG23	1.95	0.48
1:N:15:LYS:HB3	1:N:66:PHE:HB3	1.95	0.48
1:H:403:THR:O	1:H:407:VAL:HG23	2.13	0.48
1:I:179:ASP:OD1	1:I:393:LYS:HD2	2.13	0.48
1:M:130:GLU:HG3	1:M:426:LEU:HD23	1.94	0.48
1:M:443:ALA:O	1:M:447:MET:HG3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.95	0.48
1:N:266:THR:CG2	1:N:273:VAL:H	2.26	0.48
2:O:47:ARG:HD3	2:O:49:LEU:HD12	1.95	0.48
1:F:247:LEU:HB3	1:F:273:VAL:HG12	1.95	0.48
1:G:23:LEU:CD1	1:G:23:LEU:C	2.81	0.48
1:K:413:ALA:HB1	1:K:417:VAL:HB	1.95	0.48
1:I:80:LYS:HA	1:I:83:ASP:HB2	1.94	0.48
1:L:428:ASP:O	1:L:430:ARG:HG2	2.13	0.48
1:N:130:GLU:HG3	1:N:426:LEU:CD2	2.44	0.48
2:O:11:ILE:HG12	2:O:85:ILE:HG12	1.95	0.48
2:P:11:ILE:HG12	2:P:85:ILE:HG12	1.94	0.48
1:A:257:GLU:O	1:A:261:THR:HG23	2.13	0.48
1:C:204:PHE:HE1	1:C:274:ALA:HB2	1.77	0.48
1:D:356:ALA:HB3	1:D:362:ARG:HG3	1.95	0.48
1:D:420:ILE:HD13	1:D:451:LEU:HD13	1.95	0.48
1:H:193:MET:HG3	1:H:371:LYS:HB3	1.94	0.48
1:M:130:GLU:HG3	1:M:426:LEU:CD2	2.43	0.48
1:N:455:VAL:HG13	1:N:460:GLU:HB2	1.95	0.48
1:B:381:VAL:CG1	1:B:392:LYS:CG	2.91	0.48
1:D:102:GLU:HB3	1:D:442:VAL:HG22	1.96	0.48
1:E:18:ARG:CG	1:E:18:ARG:NH1	2.51	0.48
1:E:95:LEU:O	1:E:99:ILE:HG13	2.13	0.48
1:G:162:ILE:HG12	1:G:400:LEU:HD23	1.95	0.48
1:I:124:VAL:HG13	1:I:504:LEU:HD13	1.96	0.48
1:I:419:LEU:HD11	1:I:504:LEU:HG	1.94	0.48
1:J:102:GLU:HB3	1:J:442:VAL:HG22	1.96	0.48
1:J:321:LYS:HB2	1:J:334:ASP:HB3	1.96	0.48
1:K:30:THR:HB	1:K:51:LYS:O	2.13	0.48
1:M:163:ALA:O	1:M:167:ASP:HB2	2.14	0.48
1:N:428:ASP:O	1:N:430:ARG:HG2	2.14	0.48
1:A:232:GLU:HB3	1:A:309:LEU:HB3	1.96	0.48
1:E:237:LEU:HD21	1:E:271:VAL:HG21	1.95	0.48
1:H:519:CYS:HB3	1:N:38:VAL:HG22	1.96	0.48
1:I:15:LYS:HB3	1:I:66:PHE:HB3	1.96	0.48
1:I:34:LYS:HB2	1:I:458:CYS:SG	2.54	0.48
1:I:77:VAL:HG22	1:I:506:TYR:HD1	1.78	0.48
1:K:102:GLU:HB3	1:K:442:VAL:HG22	1.96	0.48
1:L:179:ASP:OD1	1:L:393:LYS:HD2	2.14	0.48
2:R:34:LYS:HG3	2:R:35:SER:H	1.79	0.48
1:C:356:ALA:HB3	1:C:362:ARG:HG3	1.95	0.48
1:D:237:LEU:HD21	1:D:271:VAL:HG21	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:LEU:HB3	1:E:273:VAL:HG12	1.96	0.48
1:K:135:SER:HA	1:K:412:VAL:HG12	1.96	0.48
1:K:123:ALA:HB2	1:K:440:ILE:HG23	1.96	0.48
1:L:85:ALA:HA	1:L:498:LYS:HD3	1.96	0.48
1:A:510:VAL:HG23	1:A:514:MET:HE2	1.96	0.47
1:A:32:GLY:HA2	4:A:700:ADP:H5'1	1.96	0.47
1:B:206:ASN:O	1:B:207:LYS:HG2	2.14	0.47
1:B:257:GLU:O	1:B:261:THR:HG23	2.14	0.47
1:D:20:VAL:HG13	1:D:74:VAL:HG11	1.95	0.47
1:E:413:ALA:CB	1:E:417:VAL:HG13	2.44	0.47
1:G:204:PHE:HE1	1:G:274:ALA:HB2	1.78	0.47
1:H:266:THR:CG2	1:H:273:VAL:H	2.27	0.47
1:K:163:ALA:O	1:K:167:ASP:HB2	2.13	0.47
1:N:11:ASP:O	1:N:12:ALA:C	2.50	0.47
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.96	0.47
1:H:226:LYS:HG3	1:H:252:GLU:HB3	1.96	0.47
1:K:16:MET:HG3	1:K:520:MET:SD	2.54	0.47
1:K:259:LEU:O	1:K:263:VAL:HG23	2.14	0.47
1:L:130:GLU:HG3	1:L:426:LEU:HD23	1.94	0.47
1:M:428:ASP:O	1:M:430:ARG:HG2	2.14	0.47
1:F:197:ARG:HD3	1:F:197:ARG:HA	1.62	0.47
1:F:204:PHE:HE1	1:F:274:ALA:HB2	1.79	0.47
1:H:455:VAL:HG11	1:H:461:GLU:O	2.13	0.47
1:I:163:ALA:O	1:I:167:ASP:HB2	2.14	0.47
1:I:259:LEU:O	1:I:263:VAL:HG23	2.14	0.47
1:J:266:THR:CG2	1:J:273:VAL:H	2.27	0.47
2:S:47:ARG:HD3	2:S:49:LEU:HD12	1.95	0.47
1:A:204:PHE:HE1	1:A:274:ALA:HB2	1.78	0.47
1:A:80:LYS:HD2	1:A:506:TYR:CE1	2.50	0.47
1:B:232:GLU:HB3	1:B:309:LEU:HB3	1.96	0.47
1:C:74:VAL:HG13	1:C:514:MET:HE1	1.95	0.47
1:F:461:GLU:HA	1:F:462:PRO:HD3	1.79	0.47
1:I:103:GLY:O	1:I:106:ALA:HB3	2.14	0.47
1:I:266:THR:CG2	1:I:273:VAL:H	2.27	0.47
1:J:138:CYS:SG	1:J:144:ILE:HD13	2.54	0.47
1:J:417:VAL:HG21	1:J:488:MET:HG3	1.96	0.47
1:N:69:MET:HE2	1:N:522:THR:HB	1.93	0.47
2:P:47:ARG:HD3	2:P:49:LEU:HD12	1.95	0.47
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.97	0.47
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.96	0.47
1:H:135:SER:HA	1:H:412:VAL:HG12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:ASP:OD1	1:J:393:LYS:HD2	2.15	0.47
1:K:124:VAL:HG13	1:K:504:LEU:HD13	1.96	0.47
1:K:360:TYR:O	1:K:364:LYS:HB2	2.14	0.47
1:N:163:ALA:O	1:N:167:ASP:HB2	2.14	0.47
1:D:510:VAL:CG2	1:D:514:MET:HE2	2.44	0.47
1:E:206:ASN:O	1:E:207:LYS:HG2	2.15	0.47
1:E:522:THR:OG1	1:E:523:ASP:N	2.48	0.47
1:G:42:LYS:HG2	1:G:44:PHE:CE2	2.50	0.47
1:M:193:MET:HG3	1:M:371:LYS:HB3	1.96	0.47
1:E:381:VAL:CG1	1:E:392:LYS:HG2	2.45	0.47
1:F:381:VAL:CG1	1:F:392:LYS:HG2	2.45	0.47
1:F:432:GLN:NE2	1:F:436:GLN:NE2	2.41	0.47
1:G:455:VAL:HG21	1:G:465:VAL:HG11	1.96	0.47
2:R:47:ARG:HD3	2:R:49:LEU:HD12	1.95	0.47
2:S:11:ILE:HG12	2:S:85:ILE:HG12	1.95	0.47
1:B:233:MET:HB3	1:B:237:LEU:HD12	1.97	0.47
1:F:300:VAL:O	1:F:307:MET:HE3	2.14	0.47
1:G:510:VAL:CG2	1:G:514:MET:CE	2.92	0.47
1:I:123:ALA:HB2	1:I:440:ILE:HG23	1.97	0.47
1:N:15:LYS:HD3	1:N:15:LYS:HA	1.70	0.47
2:O:78:ILE:HD13	2:O:83:VAL:HG21	1.96	0.47
1:E:232:GLU:HB3	1:E:309:LEU:HB3	1.96	0.47
1:E:510:VAL:HG23	1:E:514:MET:CE	2.45	0.47
1:F:232:GLU:HB3	1:F:309:LEU:HB3	1.96	0.47
1:G:18:ARG:CB	1:G:18:ARG:HH11	2.26	0.47
1:G:232:GLU:HB3	1:G:309:LEU:HB3	1.97	0.47
1:G:247:LEU:HB3	1:G:273:VAL:HG12	1.97	0.47
1:I:365:LEU:O	1:I:369:VAL:HG23	2.15	0.47
1:J:15:LYS:HB3	1:J:66:PHE:HB3	1.97	0.47
1:J:228:SER:O	1:J:257:GLU:HB3	2.15	0.47
1:K:179:ASP:OD1	1:K:393:LYS:HD2	2.14	0.47
1:K:443:ALA:O	1:K:447:MET:HG3	2.14	0.47
1:L:360:TYR:O	1:L:364:LYS:HB2	2.15	0.47
1:L:413:ALA:HB1	1:L:417:VAL:HB	1.97	0.47
1:L:130:GLU:HG3	1:L:426:LEU:CD2	2.44	0.47
1:B:234:LEU:HD22	2:P:23:GLY:HA3	1.96	0.47
1:B:268:ARG:HH21	2:P:27:LEU:CD2	2.27	0.47
1:A:247:LEU:HB3	1:A:273:VAL:HG12	1.96	0.47
1:C:90:THR:O	1:C:94:VAL:HG23	2.15	0.47
1:E:162:ILE:HG21	1:E:403:THR:HG21	1.97	0.47
1:F:18:ARG:HB2	1:F:67:GLU:HG2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.96	0.47
1:I:130:GLU:HG3	1:I:426:LEU:HD23	1.97	0.47
1:I:360:TYR:O	1:I:364:LYS:HB2	2.15	0.47
1:L:266:THR:CG2	1:L:273:VAL:H	2.27	0.47
1:L:38:VAL:HG12	1:L:40:LEU:HD13	1.97	0.47
1:L:40:LEU:HD12	1:M:521:VAL:HB	1.96	0.47
1:L:30:THR:HB	1:L:51:LYS:O	2.14	0.47
1:M:444:LEU:HD23	1:M:444:LEU:HA	1.72	0.47
2:Q:50:GLU:OE1	2:R:50:GLU:HA	2.15	0.47
1:D:233:MET:HB3	1:D:237:LEU:HD12	1.96	0.47
1:G:206:ASN:O	1:G:207:LYS:HG2	2.15	0.47
1:I:321:LYS:HB2	1:I:334:ASP:HB3	1.97	0.47
1:I:135:SER:HA	1:I:412:VAL:HG12	1.96	0.47
1:K:411:VAL:HG21	1:K:494:LEU:HD12	1.97	0.47
1:M:66:PHE:H	1:M:69:MET:HG3	1.80	0.47
2:S:6:LEU:O	2:S:7:HIS:O	2.32	0.47
1:B:247:LEU:HB3	1:B:273:VAL:HG12	1.96	0.46
1:C:73:MET:CG	1:C:73:MET:CE	2.92	0.46
1:D:247:LEU:HB3	1:D:273:VAL:HG12	1.97	0.46
1:G:257:GLU:O	1:G:261:THR:HG23	2.15	0.46
1:H:228:SER:O	1:H:257:GLU:HB3	2.15	0.46
1:H:326:ASN:ND2	1:H:328:ASP:H	2.12	0.46
1:I:428:ASP:O	1:I:430:ARG:HG2	2.14	0.46
1:L:11:ASP:O	1:L:12:ALA:C	2.51	0.46
1:M:77:VAL:HG11	1:M:510:VAL:HB	1.97	0.46
1:N:360:TYR:O	1:N:364:LYS:HB2	2.15	0.46
1:B:414:GLY:O	1:B:417:VAL:CG1	2.43	0.46
1:J:259:LEU:O	1:J:263:VAL:HG23	2.15	0.46
1:L:476:TYR:HA	1:L:486:GLY:O	2.15	0.46
1:L:16:MET:HG3	1:L:520:MET:SD	2.56	0.46
1:M:266:THR:CG2	1:M:273:VAL:H	2.28	0.46
1:A:206:ASN:O	1:A:207:LYS:HG2	2.15	0.46
1:C:233:MET:HB3	1:C:237:LEU:HD12	1.96	0.46
1:E:420:ILE:HD13	1:E:451:LEU:HD13	1.97	0.46
1:E:18:ARG:HB2	1:E:67:GLU:HG2	1.97	0.46
1:F:302:SER:H	1:F:307:MET:HE3	1.79	0.46
1:G:351:GLN:HG2	1:G:351:GLN:O	2.15	0.46
1:K:262:LEU:O	1:K:266:THR:HG23	2.15	0.46
1:K:433:ASN:OD1	1:K:435:ASP:HB2	2.16	0.46
1:K:40:LEU:HD12	1:L:521:VAL:HB	1.96	0.46
1:M:13:ARG:HD2	1:M:104:LEU:HD11	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HG21	1:B:403:THR:HG21	1.96	0.46
1:C:232:GLU:HB3	1:C:309:LEU:HB3	1.98	0.46
1:C:351:GLN:O	1:C:351:GLN:HG2	2.16	0.46
1:C:31:LEU:HD23	1:C:453:GLN:HB3	1.98	0.46
1:D:232:GLU:HB3	1:D:309:LEU:HB3	1.98	0.46
1:G:233:MET:HB3	1:G:237:LEU:HD12	1.98	0.46
1:B:254:VAL:HG12	1:B:259:LEU:HB2	1.97	0.46
1:J:100:ILE:HG23	1:J:104:LEU:HD22	1.97	0.46
1:L:135:SER:HA	1:L:412:VAL:HG12	1.98	0.46
1:A:430:ARG:CG	1:A:430:ARG:NH1	2.78	0.46
1:A:31:LEU:HD23	1:A:453:GLN:HB3	1.98	0.46
1:A:510:VAL:CG2	1:A:514:MET:HE2	2.45	0.46
1:B:204:PHE:HE1	1:B:274:ALA:HB2	1.80	0.46
1:E:461:GLU:HA	1:E:462:PRO:HD3	1.82	0.46
1:H:85:ALA:HA	1:H:498:LYS:HD3	1.98	0.46
1:I:403:THR:O	1:I:407:VAL:HG23	2.15	0.46
1:M:259:LEU:O	1:M:263:VAL:HG23	2.15	0.46
1:M:77:VAL:HG22	1:M:506:TYR:HD1	1.81	0.46
1:N:321:LYS:HB2	1:N:334:ASP:HB3	1.98	0.46
1:N:413:ALA:HB1	1:N:417:VAL:HB	1.98	0.46
1:C:248:LEU:HD22	1:C:323:VAL:HG11	1.97	0.46
1:C:381:VAL:CG1	1:C:392:LYS:CG	2.93	0.46
1:D:24:ALA:O	1:D:28:LYS:HG3	2.15	0.46
1:D:455:VAL:HG21	1:D:465:VAL:HG11	1.98	0.46
1:E:381:VAL:CG1	1:E:392:LYS:CG	2.94	0.46
1:F:381:VAL:CG1	1:F:392:LYS:CG	2.94	0.46
1:H:428:ASP:O	1:H:430:ARG:HG2	2.16	0.46
1:H:411:VAL:HG21	1:H:494:LEU:HD12	1.98	0.46
1:A:351:GLN:HG2	1:A:351:GLN:O	2.15	0.46
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.98	0.46
1:E:501:ARG:HD3	1:E:505:GLN:OE1	2.16	0.46
1:G:28:LYS:O	1:G:30:THR:N	2.48	0.46
1:H:262:LEU:O	1:H:266:THR:HG23	2.16	0.46
1:K:85:ALA:HA	1:K:498:LYS:HD3	1.98	0.46
1:A:225:LYS:HG2	1:A:303:GLU:HB2	1.98	0.46
1:D:206:ASN:O	1:D:207:LYS:HG2	2.16	0.46
1:E:91:THR:O	1:E:92:ALA:C	2.53	0.46
1:F:206:ASN:O	1:F:207:LYS:HG2	2.16	0.46
1:H:476:TYR:HA	1:H:486:GLY:O	2.16	0.46
1:J:411:VAL:HG21	1:J:494:LEU:HD12	1.97	0.46
1:N:130:GLU:HG3	1:N:426:LEU:HD23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLY:HA2	4:B:701:ADP:H5'1	1.98	0.46
1:C:206:ASN:O	1:C:207:LYS:HG2	2.16	0.46
1:D:254:VAL:HG12	1:D:259:LEU:HB2	1.97	0.46
1:E:124:VAL:HG13	1:E:504:LEU:HD13	1.96	0.46
1:F:28:LYS:HD2	1:F:453:GLN:CD	2.36	0.46
1:M:38:VAL:HG12	1:M:40:LEU:HD13	1.96	0.46
2:T:78:ILE:HD13	2:T:83:VAL:HG21	1.98	0.46
1:A:381:VAL:CG1	1:A:392:LYS:CG	2.94	0.45
1:B:351:GLN:O	1:B:351:GLN:HG2	2.16	0.45
1:G:501:ARG:HD3	1:G:505:GLN:OE1	2.15	0.45
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.56	0.45
1:K:426:LEU:O	1:K:444:LEU:HD11	2.16	0.45
1:A:501:ARG:HD3	1:A:505:GLN:OE1	2.16	0.45
1:F:351:GLN:HG2	1:F:351:GLN:O	2.16	0.45
1:G:225:LYS:HG2	1:G:303:GLU:HB2	1.99	0.45
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.98	0.45
1:I:23:LEU:HD11	1:I:75:LYS:HG3	1.97	0.45
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.99	0.45
1:L:433:ASN:OD1	1:L:435:ASP:HB2	2.17	0.45
1:I:226:LYS:HG3	1:I:252:GLU:HB3	1.98	0.45
1:K:321:LYS:HB2	1:K:334:ASP:HB3	1.98	0.45
1:K:428:ASP:O	1:K:430:ARG:HG2	2.16	0.45
1:L:262:LEU:O	1:L:266:THR:HG23	2.16	0.45
2:Q:78:ILE:HD13	2:Q:83:VAL:HG21	1.98	0.45
1:A:49:ILE:HD13	1:G:513:LEU:HB3	1.97	0.45
1:D:381:VAL:CG1	1:D:392:LYS:HG2	2.47	0.45
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.97	0.45
1:I:270:ILE:HA	1:J:257:GLU:OE2	2.16	0.45
1:E:261:THR:HG22	2:S:29:GLY:HA3	1.97	0.45
2:S:78:ILE:HD13	2:S:83:VAL:HG21	1.99	0.45
1:A:384:ALA:O	1:G:506:TYR:HE1	1.99	0.45
1:B:77:VAL:HG23	1:B:92:ALA:HB1	1.98	0.45
1:C:197:ARG:HG2	1:C:277:LYS:O	2.16	0.45
1:D:225:LYS:HG2	1:D:303:GLU:HB2	1.98	0.45
1:E:300:VAL:O	1:E:307:MET:HE3	2.17	0.45
1:F:522:THR:OG1	1:F:523:ASP:N	2.50	0.45
1:I:104:LEU:HA	1:I:104:LEU:HD12	1.75	0.45
1:I:85:ALA:HA	1:I:498:LYS:HD3	1.98	0.45
1:M:179:ASP:OD1	1:M:393:LYS:HD2	2.17	0.45
2:R:78:ILE:HD13	2:R:83:VAL:HG21	1.98	0.45
1:C:23:LEU:CD1	1:C:23:LEU:C	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:413:ALA:HB1	1:H:417:VAL:HB	1.99	0.45
1:K:266:THR:CG2	1:K:273:VAL:H	2.29	0.45
1:K:270:ILE:HG23	1:L:229:ASN:HD21	1.82	0.45
1:M:138:CYS:SG	1:M:144:ILE:HD13	2.56	0.45
1:M:321:LYS:HB2	1:M:334:ASP:HB3	1.99	0.45
1:A:77:VAL:HG23	1:A:92:ALA:HB1	1.99	0.45
1:B:300:VAL:O	1:B:307:MET:HE3	2.17	0.45
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.57	0.45
1:K:365:LEU:O	1:K:369:VAL:HG23	2.17	0.45
1:K:476:TYR:HA	1:K:486:GLY:O	2.17	0.45
1:N:228:SER:O	1:N:257:GLU:HB3	2.17	0.45
2:S:23:GLY:H	2:T:80:ASN:HD21	1.64	0.45
1:C:409:GLU:CD	1:C:501:ARG:HH21	2.19	0.45
1:F:28:LYS:HD2	1:F:453:GLN:NE2	2.32	0.45
1:G:197:ARG:HG2	1:G:277:LYS:O	2.17	0.45
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.57	0.45
1:L:365:LEU:O	1:L:369:VAL:HG23	2.16	0.45
1:L:433:ASN:HD22	1:L:433:ASN:HA	1.59	0.45
1:L:444:LEU:HD23	1:L:444:LEU:HA	1.74	0.45
1:M:270:ILE:HG23	1:N:229:ASN:ND2	2.32	0.45
1:A:28:LYS:HD2	1:A:453:GLN:NE2	2.31	0.45
1:C:257:GLU:O	1:C:261:THR:HG23	2.17	0.45
1:D:105:LYS:HB2	1:D:105:LYS:HE3	1.74	0.45
1:E:351:GLN:HG2	1:E:351:GLN:O	2.16	0.45
1:F:233:MET:HB3	1:F:237:LEU:HD12	1.98	0.45
1:F:413:ALA:CB	1:F:417:VAL:HG13	2.47	0.45
1:I:417:VAL:HG21	1:I:488:MET:HG3	1.98	0.45
1:M:16:MET:HG3	1:M:520:MET:SD	2.57	0.45
1:D:351:GLN:O	1:D:351:GLN:HG2	2.16	0.45
1:D:381:VAL:CG1	1:D:392:LYS:CG	2.95	0.45
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.99	0.45
1:F:420:ILE:HD13	1:F:451:LEU:HD13	1.98	0.45
1:L:16:MET:O	1:L:20:VAL:HG12	2.17	0.45
1:L:419:LEU:HD11	1:L:504:LEU:HG	1.99	0.45
1:L:47:PRO:CG	1:M:73:MET:HG3	2.44	0.45
1:J:365:LEU:O	1:J:369:VAL:HG23	2.17	0.44
1:J:64:ASP:OD1	1:J:65:LYS:O	2.34	0.44
1:L:259:LEU:O	1:L:263:VAL:HG23	2.18	0.44
2:Q:11:ILE:HG12	2:Q:85:ILE:HG12	1.98	0.44
1:C:32:GLY:HA2	4:C:702:ADP:H5'1	1.98	0.44
1:D:28:LYS:C	1:D:30:THR:H	2.21	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:LYS:HB3	1:H:66:PHE:HB3	1.99	0.44
1:I:213:VAL:O	1:I:324:VAL:HA	2.17	0.44
1:K:444:LEU:HA	1:K:444:LEU:HD23	1.69	0.44
1:N:262:LEU:O	1:N:266:THR:HG23	2.17	0.44
1:N:429:LEU:HB3	1:N:440:ILE:HG21	2.00	0.44
2:P:34:LYS:HG3	2:P:35:SER:H	1.82	0.44
1:B:153:ASN:O	1:B:154:SER:HB2	2.17	0.44
1:E:257:GLU:O	1:E:261:THR:HG23	2.17	0.44
1:E:28:LYS:HD2	1:E:453:GLN:CD	2.38	0.44
1:F:510:VAL:HG23	1:F:514:MET:CE	2.47	0.44
1:K:16:MET:O	1:K:20:VAL:HG12	2.17	0.44
1:M:417:VAL:HG21	1:M:488:MET:HG3	1.99	0.44
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.57	0.44
1:N:226:LYS:HG3	1:N:252:GLU:HB3	1.98	0.44
2:P:78:ILE:HD13	2:P:83:VAL:HG21	1.99	0.44
1:B:18:ARG:HB2	1:B:67:GLU:HG2	1.99	0.44
1:C:420:ILE:HD13	1:C:451:LEU:HD13	1.99	0.44
1:F:254:VAL:HG12	1:F:259:LEU:HB2	2.00	0.44
1:J:163:ALA:O	1:J:167:ASP:HB2	2.17	0.44
1:N:77:VAL:HG11	1:N:510:VAL:HB	1.99	0.44
1:N:16:MET:HG3	1:N:520:MET:SD	2.57	0.44
2:Q:43:VAL:HG13	2:Q:57:LEU:HD12	2.00	0.44
1:A:461:GLU:HA	1:A:462:PRO:HD3	1.89	0.44
1:C:100:ILE:HD11	1:C:514:MET:CE	2.38	0.44
1:C:510:VAL:CG2	1:C:514:MET:HE2	2.48	0.44
1:E:233:MET:HB3	1:E:237:LEU:HD12	1.98	0.44
1:G:18:ARG:HB2	1:G:67:GLU:HG2	1.99	0.44
1:G:197:ARG:HA	1:G:197:ARG:HD3	1.64	0.44
1:G:16:MET:O	1:G:20:VAL:HG23	2.18	0.44
1:G:24:ALA:O	1:G:28:LYS:HG3	2.17	0.44
1:H:15:LYS:HD3	1:H:15:LYS:HA	1.72	0.44
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.58	0.44
1:J:444:LEU:HA	1:J:444:LEU:HD23	1.71	0.44
1:J:69:MET:HE2	1:J:522:THR:HB	1.95	0.44
1:K:38:VAL:HG12	1:K:40:LEU:HD13	1.98	0.44
1:K:126:ALA:HB1	1:K:426:LEU:HD22	2.00	0.44
1:L:226:LYS:HG3	1:L:252:GLU:HB3	1.99	0.44
1:L:342:ILE:O	1:L:346:VAL:HG23	2.17	0.44
1:M:419:LEU:HD21	1:M:500:THR:CG2	2.42	0.44
1:C:413:ALA:CB	1:C:417:VAL:HG13	2.47	0.44
1:E:150:ILE:HD13	1:E:493:ILE:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:PRO:HG3	4:F:705:ADP:C6	2.53	0.44
4:G:706:ADP:O3B	5:G:806:HOH:O	2.21	0.44
1:J:90:THR:O	1:J:94:VAL:HG23	2.17	0.44
1:N:513:LEU:HD12	1:N:513:LEU:HA	1.90	0.44
2:O:43:VAL:HG13	2:O:57:LEU:HD12	2.00	0.44
2:P:43:VAL:HG13	2:P:57:LEU:HD12	2.00	0.44
1:A:233:MET:HB3	1:A:237:LEU:HD12	2.00	0.44
1:C:225:LYS:HG2	1:C:303:GLU:HB2	2.00	0.44
1:C:365:LEU:O	1:C:369:VAL:HG13	2.18	0.44
1:C:28:LYS:HD2	1:C:453:GLN:NE2	2.33	0.44
1:E:225:LYS:HG2	1:E:303:GLU:HB2	1.99	0.44
1:E:421:ARG:HD3	1:E:421:ARG:HA	1.72	0.44
1:E:31:LEU:HD23	1:E:453:GLN:HB3	2.00	0.44
1:H:34:LYS:HB2	1:H:458:CYS:SG	2.58	0.44
1:A:130:GLU:HB3	1:A:422:VAL:HB	1.99	0.44
1:D:100:ILE:HD11	1:D:514:MET:CE	2.46	0.44
1:D:301:ILE:O	1:D:301:ILE:HG22	2.18	0.44
1:D:300:VAL:O	1:D:307:MET:HE3	2.18	0.44
1:D:42:LYS:HG2	1:D:44:PHE:CE2	2.52	0.44
1:F:162:ILE:HG21	1:F:403:THR:HG21	2.00	0.44
1:G:451:LEU:HD21	1:G:465:VAL:HG12	1.99	0.44
1:G:80:LYS:HD2	1:G:506:TYR:CE1	2.53	0.44
1:G:495:ASP:CG	4:G:706:ADP:HO2'	2.21	0.44
1:J:126:ALA:HB1	1:J:426:LEU:HD22	2.00	0.44
1:K:270:ILE:HG23	1:L:229:ASN:ND2	2.33	0.44
1:M:85:ALA:HA	1:M:498:LYS:HD3	2.00	0.44
1:I:228:SER:O	1:I:257:GLU:HB3	2.18	0.44
1:K:64:ASP:HB3	1:K:67:GLU:HB2	1.98	0.44
1:L:419:LEU:HD21	1:L:500:THR:CG2	2.45	0.44
1:M:15:LYS:HB3	1:M:66:PHE:HB3	2.00	0.44
1:A:254:VAL:HG12	1:A:259:LEU:HB2	2.00	0.43
1:D:28:LYS:C	1:D:30:THR:N	2.68	0.43
1:D:327:LYS:HG2	1:D:327:LYS:O	2.18	0.43
1:F:225:LYS:HG2	1:F:303:GLU:HB2	2.00	0.43
1:F:451:LEU:HD21	1:F:465:VAL:HG12	1.98	0.43
1:F:4:LYS:HG3	1:G:59:GLU:O	2.18	0.43
1:G:28:LYS:HD2	1:G:453:GLN:NE2	2.32	0.43
1:I:285:ARG:HA	1:I:288:MET:HB2	1.99	0.43
1:I:296:THR:HB	1:I:319:GLN:H	1.82	0.43
1:I:326:ASN:HD22	1:I:328:ASP:H	1.65	0.43
1:J:64:ASP:C	1:J:65:LYS:O	2.55	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:455:VAL:HG11	1:L:461:GLU:O	2.17	0.43
1:M:15:LYS:HD3	1:M:15:LYS:HA	1.73	0.43
1:M:262:LEU:O	1:M:266:THR:HG23	2.17	0.43
2:T:43:VAL:HG13	2:T:57:LEU:HD12	2.00	0.43
1:A:349:ILE:HG23	1:A:365:LEU:HD12	2.00	0.43
1:A:361:ASP:O	1:A:365:LEU:HD23	2.18	0.43
1:J:104:LEU:HD12	1:J:104:LEU:HA	1.66	0.43
1:K:130:GLU:HG3	1:K:426:LEU:CD2	2.48	0.43
1:M:227:ILE:CD1	1:M:309:LEU:HD11	2.47	0.43
1:M:87:ASP:HB3	1:M:499:VAL:HG21	2.00	0.43
1:N:38:VAL:HG12	1:N:40:LEU:HD13	1.99	0.43
2:O:96:GLU:O	2:P:1:MET:HB2	2.18	0.43
1:E:234:LEU:HD22	2:S:23:GLY:HA3	1.99	0.43
1:A:102:GLU:HB3	1:A:442:VAL:HG22	2.01	0.43
1:A:381:VAL:HG11	1:A:392:LYS:HG3	2.01	0.43
1:B:413:ALA:CB	1:B:417:VAL:HG13	2.48	0.43
1:B:519:CYS:HB3	1:C:38:VAL:HG22	2.01	0.43
1:C:254:VAL:HG12	1:C:259:LEU:HB2	2.00	0.43
1:D:414:GLY:O	1:D:417:VAL:CG1	2.48	0.43
1:I:476:TYR:HA	1:I:486:GLY:O	2.18	0.43
2:T:34:LYS:HG3	2:T:35:SER:H	1.82	0.43
1:A:421:ARG:HA	1:A:421:ARG:HD3	1.68	0.43
1:D:18:ARG:HH11	1:D:18:ARG:HB3	1.83	0.43
1:D:6:VAL:CG2	1:D:6:VAL:O	2.66	0.43
1:H:365:LEU:O	1:H:369:VAL:HG23	2.19	0.43
1:H:30:THR:HB	1:H:51:LYS:O	2.18	0.43
1:J:461:GLU:HA	1:J:462:PRO:HD3	1.90	0.43
1:K:452:ARG:HG2	1:K:452:ARG:NH1	2.32	0.43
1:N:102:GLU:OE2	1:N:445:ARG:NH1	2.50	0.43
1:N:104:LEU:HD12	1:N:104:LEU:HA	1.71	0.43
2:O:50:GLU:OE1	2:P:50:GLU:HA	2.18	0.43
1:G:175:ILE:HG21	1:G:400:LEU:HD21	2.01	0.43
1:J:80:LYS:HA	1:J:83:ASP:HB2	2.00	0.43
1:K:130:GLU:HG3	1:K:426:LEU:HD23	1.99	0.43
1:K:226:LYS:HG3	1:K:252:GLU:HB3	2.00	0.43
1:K:77:VAL:HG22	1:K:506:TYR:HD1	1.82	0.43
1:K:77:VAL:HG11	1:K:510:VAL:HB	1.98	0.43
1:N:213:VAL:O	1:N:324:VAL:HA	2.18	0.43
2:O:34:LYS:HG3	2:O:35:SER:H	1.83	0.43
1:A:44:PHE:HB2	1:A:45:GLY:H	1.72	0.43
1:B:225:LYS:HG2	1:B:303:GLU:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:VAL:O	1:C:307:MET:HE3	2.19	0.43
1:F:197:ARG:HG2	1:F:277:LYS:O	2.18	0.43
1:L:102:GLU:HB3	1:L:442:VAL:HG22	2.01	0.43
1:N:77:VAL:HG22	1:N:506:TYR:CD1	2.53	0.43
1:C:510:VAL:HG23	1:C:514:MET:CE	2.49	0.43
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.52	0.43
1:D:257:GLU:O	1:D:261:THR:HG23	2.18	0.43
1:H:409:GLU:OE2	1:H:501:ARG:NH2	2.47	0.43
1:I:443:ALA:O	1:I:447:MET:HG3	2.19	0.43
1:N:34:LYS:HB2	1:N:458:CYS:SG	2.58	0.43
2:P:50:GLU:OE1	2:Q:50:GLU:HA	2.19	0.43
2:Q:34:LYS:HG3	2:Q:35:SER:H	1.83	0.43
2:T:23:GLY:H	2:U:80:ASN:HD21	1.66	0.43
1:D:452:ARG:NH1	1:D:452:ARG:HG2	2.33	0.43
1:E:248:LEU:HD22	1:E:323:VAL:HG11	2.00	0.43
1:G:254:VAL:HG12	1:G:259:LEU:HB2	2.00	0.43
1:G:421:ARG:HD3	1:G:421:ARG:HA	1.69	0.43
1:K:524:LEU:HD23	1:K:524:LEU:HA	1.87	0.43
1:N:126:ALA:HB1	1:N:426:LEU:HD22	2.00	0.43
2:R:46:GLY:HA3	2:R:55:LYS:O	2.19	0.43
1:B:28:LYS:C	1:B:30:THR:N	2.72	0.43
1:B:449:ALA:HB3	1:B:450:PRO:HD3	2.00	0.43
1:G:381:VAL:CG1	1:G:392:LYS:CG	2.97	0.43
1:G:524:LEU:HA	1:G:524:LEU:HD23	1.84	0.43
1:K:66:PHE:H	1:K:69:MET:HG3	1.83	0.43
1:L:34:LYS:HB2	1:L:458:CYS:SG	2.58	0.43
1:L:72:GLN:HA	1:L:72:GLN:NE2	2.33	0.43
1:M:80:LYS:HA	1:M:83:ASP:HB2	2.00	0.43
1:N:69:MET:CE	1:N:522:THR:CB	2.93	0.43
1:B:130:GLU:HB3	1:B:422:VAL:HB	2.01	0.43
1:E:409:GLU:OE2	1:E:501:ARG:NH2	2.42	0.43
1:E:42:LYS:HG2	1:E:44:PHE:CE2	2.53	0.43
1:F:248:LEU:HD22	1:F:323:VAL:HG11	1.99	0.43
1:G:19:GLY:HA3	1:G:67:GLU:O	2.19	0.43
1:G:28:LYS:HD2	1:G:453:GLN:CD	2.39	0.43
1:G:77:VAL:HG23	1:G:92:ALA:HB1	2.01	0.43
1:H:433:ASN:OD1	1:H:435:ASP:HB2	2.18	0.43
1:H:7:LYS:HD2	1:H:66:PHE:CE2	2.54	0.43
1:J:262:LEU:O	1:J:266:THR:HG23	2.18	0.43
1:M:419:LEU:HD22	1:M:500:THR:CG2	2.47	0.43
1:N:7:LYS:HD2	1:N:66:PHE:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ILE:HG22	1:B:301:ILE:O	2.19	0.42
1:F:257:GLU:O	1:F:261:THR:HG23	2.19	0.42
1:H:444:LEU:HA	1:H:444:LEU:HD23	1.72	0.42
1:I:96:ALA:O	1:I:100:ILE:HG13	2.18	0.42
1:K:270:ILE:HA	1:L:257:GLU:OE2	2.19	0.42
1:K:64:ASP:OD1	1:K:65:LYS:O	2.37	0.42
1:M:365:LEU:O	1:M:369:VAL:HG23	2.19	0.42
1:M:64:ASP:C	1:M:65:LYS:O	2.56	0.42
1:N:365:LEU:O	1:N:369:VAL:HG23	2.19	0.42
2:S:50:GLU:OE1	2:T:50:GLU:HA	2.19	0.42
1:B:102:GLU:HB3	1:B:442:VAL:HG22	2.01	0.42
1:B:432:GLN:NE2	1:B:436:GLN:NE2	2.39	0.42
1:F:520:MET:HG2	1:G:39:VAL:HB	2.00	0.42
1:J:226:LYS:HG3	1:J:252:GLU:HB3	2.01	0.42
1:K:285:ARG:HA	1:K:288:MET:HB2	2.01	0.42
1:A:365:LEU:O	1:A:369:VAL:HG13	2.19	0.42
1:A:477:GLY:HA3	1:A:488:MET:SD	2.59	0.42
1:D:349:ILE:HG23	1:D:365:LEU:HD12	2.01	0.42
1:D:421:ARG:HA	1:D:421:ARG:HD3	1.73	0.42
1:G:349:ILE:HG23	1:G:365:LEU:HD12	2.01	0.42
1:G:455:VAL:HG11	1:G:462:PRO:HA	2.02	0.42
1:K:429:LEU:HB3	1:K:440:ILE:HG21	2.01	0.42
2:U:34:LYS:HG3	2:U:35:SER:H	1.84	0.42
2:U:43:VAL:HG13	2:U:57:LEU:HD12	2.01	0.42
1:A:286:LYS:HE2	1:A:304:GLU:OE1	2.19	0.42
1:A:510:VAL:HG23	1:A:514:MET:HE3	2.02	0.42
1:D:100:ILE:O	1:D:101:THR:C	2.56	0.42
1:D:248:LEU:HD22	1:D:323:VAL:HG11	2.01	0.42
1:D:451:LEU:HD21	1:D:465:VAL:HG12	2.01	0.42
1:G:288:MET:O	1:G:291:ASP:HB2	2.19	0.42
1:J:32:GLY:HA2	1:J:454:ILE:CD1	2.46	0.42
1:J:477:GLY:O	1:J:485:TYR:HA	2.19	0.42
1:J:77:VAL:HG22	1:J:506:TYR:CD1	2.54	0.42
1:D:105:LYS:HD3	1:K:110:GLY:O	2.19	0.42
1:L:524:LEU:HD23	1:L:524:LEU:HA	1.82	0.42
1:M:426:LEU:H	1:M:426:LEU:HG	1.67	0.42
1:M:441:LYS:O	1:M:442:VAL:C	2.58	0.42
1:N:215:LEU:HB3	1:N:218:PRO:HG3	2.01	0.42
1:N:285:ARG:HA	1:N:288:MET:HB2	2.01	0.42
1:D:77:VAL:HG23	1:D:92:ALA:HB1	2.01	0.42
1:E:80:LYS:HD2	1:E:506:TYR:CE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:LYS:HD3	1:I:15:LYS:HA	1.73	0.42
1:M:22:VAL:HG11	1:M:62:LEU:HD21	2.02	0.42
1:A:381:VAL:CG1	1:A:392:LYS:HG2	2.49	0.42
1:A:90:THR:O	1:A:94:VAL:HG23	2.19	0.42
1:B:510:VAL:HG23	1:B:514:MET:CE	2.49	0.42
1:D:28:LYS:O	1:D:30:THR:N	2.52	0.42
1:F:42:LYS:HG2	1:F:44:PHE:CE2	2.54	0.42
1:I:461:GLU:HA	1:I:462:PRO:HD3	1.90	0.42
1:M:228:SER:O	1:M:257:GLU:HB3	2.20	0.42
1:D:18:ARG:HB2	1:D:67:GLU:HG2	2.00	0.42
1:H:419:LEU:HD22	1:H:500:THR:CG2	2.47	0.42
1:K:15:LYS:HD3	1:K:15:LYS:HA	1.74	0.42
1:L:138:CYS:SG	1:L:144:ILE:HD13	2.60	0.42
1:L:213:VAL:O	1:L:324:VAL:HA	2.20	0.42
1:A:301:ILE:HG21	1:A:309:LEU:HD12	2.02	0.42
1:D:430:ARG:NH1	1:D:430:ARG:CG	2.75	0.42
1:F:34:LYS:HD2	1:F:458:CYS:SG	2.60	0.42
1:G:361:ASP:O	1:G:365:LEU:HD23	2.19	0.42
1:G:365:LEU:O	1:G:369:VAL:HG13	2.19	0.42
1:I:262:LEU:O	1:I:266:THR:HG23	2.19	0.42
1:J:419:LEU:HD22	1:J:500:THR:CG2	2.47	0.42
1:J:8:PHE:O	1:J:9:GLY:C	2.57	0.42
1:L:126:ALA:HB1	1:L:426:LEU:HD22	2.02	0.42
1:M:104:LEU:HA	1:M:104:LEU:HD12	1.72	0.42
1:M:413:ALA:CB	1:M:417:VAL:HB	2.50	0.42
1:N:87:ASP:HB3	1:N:499:VAL:HG21	2.02	0.42
1:A:150:ILE:HD13	1:A:493:ILE:HA	2.02	0.42
1:B:381:VAL:HG11	1:B:392:LYS:HG3	2.02	0.42
1:B:42:LYS:HG2	1:B:44:PHE:CE2	2.55	0.42
1:C:455:VAL:HG21	1:C:465:VAL:HG11	2.01	0.42
1:D:41:ASP:O	1:D:42:LYS:HG3	2.20	0.42
1:D:33:PRO:HG3	4:D:703:ADP:C6	2.55	0.42
1:E:286:LYS:HE2	1:E:304:GLU:OE1	2.20	0.42
1:F:204:PHE:CG	1:F:204:PHE:O	2.73	0.42
1:H:285:ARG:HA	1:H:288:MET:HB2	2.01	0.42
1:I:130:GLU:HG3	1:I:426:LEU:CD2	2.49	0.42
1:J:215:LEU:HB3	1:J:218:PRO:HG3	2.02	0.42
1:K:213:VAL:O	1:K:324:VAL:HA	2.20	0.42
1:M:215:LEU:HB3	1:M:218:PRO:HG3	2.01	0.42
1:M:234:LEU:N	1:M:235:PRO:HD2	2.34	0.42
1:N:444:LEU:HD23	1:N:444:LEU:HA	1.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:MET:CG	1:A:368:ARG:HD2	2.50	0.42
1:E:455:VAL:HG21	1:E:465:VAL:HG11	2.02	0.42
1:F:301:ILE:HG22	1:F:301:ILE:O	2.20	0.42
1:F:219:PHE:HB3	1:F:317:LEU:HD13	2.01	0.42
1:F:501:ARG:HD3	1:F:505:GLN:OE1	2.19	0.42
1:K:11:ASP:O	1:K:12:ALA:C	2.59	0.42
1:K:342:ILE:O	1:K:346:VAL:HG23	2.20	0.42
1:L:15:LYS:HB3	1:L:66:PHE:HB3	2.02	0.42
1:L:80:LYS:HA	1:L:83:ASP:HB2	2.02	0.42
1:M:455:VAL:HG13	1:M:460:GLU:HB2	2.01	0.42
1:B:23:LEU:C	1:B:23:LEU:CD1	2.88	0.41
1:B:381:VAL:HG12	1:B:392:LYS:HG2	2.02	0.41
1:F:413:ALA:HB3	1:F:417:VAL:HG13	2.02	0.41
1:G:28:LYS:C	1:G:30:THR:H	2.22	0.41
1:H:234:LEU:N	1:H:235:PRO:HD2	2.35	0.41
1:J:213:VAL:O	1:J:324:VAL:HA	2.19	0.41
1:L:15:LYS:HA	1:L:15:LYS:HD3	1.76	0.41
1:L:285:ARG:HA	1:L:288:MET:HB2	2.02	0.41
1:L:443:ALA:O	1:L:447:MET:HG3	2.20	0.41
1:N:149:THR:HG22	1:N:156:GLU:HA	2.02	0.41
1:M:39:VAL:HB	1:N:520:MET:HG2	2.02	0.41
1:A:381:VAL:CG1	1:A:392:LYS:HG3	2.50	0.41
1:C:130:GLU:HB3	1:C:422:VAL:HB	2.03	0.41
1:G:301:ILE:HG21	1:G:309:LEU:HD12	2.02	0.41
1:K:296:THR:HB	1:K:319:GLN:H	1.84	0.41
1:L:104:LEU:HA	1:L:104:LEU:HD12	1.74	0.41
1:L:428:ASP:O	1:L:429:LEU:C	2.59	0.41
1:M:429:LEU:HB3	1:M:440:ILE:HG21	2.03	0.41
1:N:64:ASP:OD1	1:N:65:LYS:O	2.37	0.41
1:N:85:ALA:HA	1:N:498:LYS:HD3	2.02	0.41
2:S:34:LYS:HG3	2:S:35:SER:H	1.84	0.41
1:A:24:ALA:O	1:A:28:LYS:HG3	2.20	0.41
1:B:286:LYS:HE2	1:B:304:GLU:OE1	2.20	0.41
1:B:44:PHE:HB2	1:B:45:GLY:H	1.76	0.41
1:C:197:ARG:HD3	1:C:197:ARG:HA	1.66	0.41
1:E:130:GLU:HB3	1:E:422:VAL:HB	2.01	0.41
1:F:28:LYS:O	1:F:30:THR:N	2.53	0.41
1:H:342:ILE:O	1:H:346:VAL:HG23	2.20	0.41
1:H:524:LEU:HA	1:H:524:LEU:HD23	1.84	0.41
1:I:524:LEU:HD23	1:I:524:LEU:HA	1.85	0.41
1:J:2:ALA:O	1:J:4:LYS:HE3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:VAL:HB	1:L:520:MET:HG2	2.02	0.41
1:K:428:ASP:O	1:K:429:LEU:C	2.58	0.41
1:M:226:LYS:HG3	1:M:252:GLU:HB3	2.01	0.41
1:M:476:TYR:HA	1:M:486:GLY:O	2.20	0.41
1:B:501:ARG:HD3	1:B:505:GLN:OE1	2.20	0.41
1:C:114:MET:HE3	1:C:114:MET:O	2.20	0.41
1:C:286:LYS:HE2	1:C:304:GLU:OE1	2.21	0.41
1:D:28:LYS:HD2	1:D:453:GLN:NE2	2.36	0.41
1:E:102:GLU:HB3	1:E:442:VAL:HG22	2.03	0.41
1:H:104:LEU:HA	1:H:104:LEU:HD12	1.74	0.41
1:I:64:ASP:C	1:I:65:LYS:O	2.58	0.41
1:K:104:LEU:HA	1:K:104:LEU:HD12	1.80	0.41
1:K:16:MET:O	1:K:20:VAL:CG1	2.69	0.41
1:N:100:ILE:HG23	1:N:104:LEU:HD22	2.01	0.41
1:E:270:ILE:HG23	2:S:25:ILE:HG22	2.03	0.41
2:T:60:LYS:HG2	2:T:63:ASP:OD2	2.20	0.41
1:C:197:ARG:H	1:C:329:THR:HA	1.84	0.41
1:C:204:PHE:CG	1:C:204:PHE:O	2.73	0.41
1:D:238:GLU:OE1	2:R:24:GLY:HA3	2.20	0.41
1:D:69:MET:O	1:D:73:MET:HG3	2.21	0.41
1:E:150:ILE:CD1	1:E:493:ILE:HA	2.50	0.41
1:F:349:ILE:HG23	1:F:365:LEU:HD12	2.01	0.41
1:F:421:ARG:HA	1:F:421:ARG:HD3	1.74	0.41
1:G:289:LEU:HA	1:G:292:ILE:HD12	2.02	0.41
1:H:428:ASP:O	1:H:429:LEU:C	2.58	0.41
1:L:16:MET:O	1:L:20:VAL:CG1	2.69	0.41
1:N:13:ARG:HD2	1:N:104:LEU:HD11	2.03	0.41
1:B:261:THR:HG22	2:P:29:GLY:HA3	2.01	0.41
1:E:365:LEU:O	1:E:369:VAL:HG13	2.20	0.41
1:F:301:ILE:HG21	1:F:309:LEU:HD12	2.03	0.41
1:H:102:GLU:HB3	1:H:442:VAL:HG22	2.02	0.41
1:I:215:LEU:HB3	1:I:218:PRO:HG3	2.03	0.41
1:I:455:VAL:HG13	1:I:460:GLU:HB2	2.02	0.41
1:J:10:ASN:O	1:J:11:ASP:C	2.59	0.41
1:K:215:LEU:HB3	1:K:218:PRO:HG3	2.02	0.41
1:M:66:PHE:HD1	1:M:520:MET:HE2	1.85	0.41
1:A:248:LEU:HD22	1:A:323:VAL:HG11	2.02	0.41
1:B:95:LEU:O	1:B:99:ILE:HG13	2.21	0.41
1:C:421:ARG:HD3	1:C:421:ARG:HA	1.74	0.41
1:E:288:MET:CG	1:E:368:ARG:HD2	2.49	0.41
1:F:28:LYS:C	1:F:30:THR:N	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:MET:HE1	1:G:514:MET:HB3	2.03	0.41
1:G:248:LEU:HD22	1:G:323:VAL:HG11	2.02	0.41
1:H:10:ASN:O	1:H:11:ASP:C	2.59	0.41
1:H:69:MET:HE2	1:H:522:THR:HB	2.00	0.41
1:I:11:ASP:O	1:I:12:ALA:C	2.58	0.41
1:J:101:THR:HG22	1:J:105:LYS:HE3	2.02	0.41
1:J:437:ASN:HA	1:J:440:ILE:HD12	2.01	0.41
1:M:461:GLU:HA	1:M:462:PRO:HD3	1.89	0.41
1:N:296:THR:HB	1:N:319:GLN:H	1.85	0.41
1:A:204:PHE:O	1:A:204:PHE:CG	2.74	0.41
1:B:248:LEU:HD22	1:B:323:VAL:HG11	2.01	0.41
1:C:30:THR:HB	1:C:51:LYS:HG2	2.03	0.41
1:C:162:ILE:HG21	1:C:403:THR:HG21	2.03	0.41
1:C:452:ARG:HH12	1:C:463:SER:HB3	1.85	0.41
1:D:240:VAL:HG11	1:D:247:LEU:HB2	2.03	0.41
1:D:456:LEU:HD13	1:D:462:PRO:CG	2.51	0.41
1:D:524:LEU:HA	1:D:524:LEU:HD23	1.99	0.41
1:E:198:GLY:HA2	1:E:326:ASN:O	2.21	0.41
1:E:451:LEU:HD21	1:E:465:VAL:HG12	2.02	0.41
1:F:153:ASN:O	1:F:154:SER:HB2	2.21	0.41
1:F:365:LEU:O	1:F:369:VAL:HG13	2.20	0.41
1:H:433:ASN:HA	1:H:433:ASN:HD22	1.54	0.41
1:I:221:LEU:HD12	1:I:249:ILE:HG23	2.02	0.41
1:L:198:GLY:HA3	1:L:328:ASP:HA	2.03	0.41
1:M:270:ILE:HG23	1:N:229:ASN:HD21	1.86	0.41
1:A:39:VAL:HG12	1:G:69:MET:CE	2.51	0.41
1:A:510:VAL:O	1:A:511:ALA:C	2.57	0.41
1:A:6:VAL:HG23	1:A:6:VAL:O	2.20	0.41
1:B:16:MET:HE1	1:B:514:MET:HB3	2.03	0.41
1:B:247:LEU:O	1:B:273:VAL:HA	2.21	0.41
1:D:150:ILE:CD1	1:D:493:ILE:HA	2.51	0.41
1:D:286:LYS:HE2	1:D:304:GLU:OE1	2.20	0.41
1:D:413:ALA:CB	1:D:417:VAL:HG13	2.51	0.41
1:F:259:LEU:O	1:F:263:VAL:HG23	2.21	0.41
1:F:288:MET:CG	1:F:368:ARG:HD2	2.49	0.41
1:F:519:CYS:HB3	1:G:38:VAL:HG22	2.03	0.41
1:H:200:LEU:CD1	1:H:276:VAL:HA	2.49	0.41
1:I:421:ARG:NH2	1:I:469:VAL:O	2.51	0.41
1:J:43:SER:HB2	1:J:44:PHE:CD1	2.55	0.41
1:K:455:VAL:HG13	1:K:460:GLU:HB2	2.02	0.41
1:M:452:ARG:HG2	1:M:452:ARG:NH1	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:138:CYS:SG	1:N:144:ILE:HD13	2.61	0.41
1:A:348:GLN:HE21	1:A:348:GLN:HB3	1.68	0.41
1:B:365:LEU:O	1:B:369:VAL:HG13	2.21	0.41
1:B:444:LEU:O	1:B:447:MET:HB2	2.20	0.41
1:C:238:GLU:OE1	2:Q:24:GLY:HA3	2.21	0.41
1:D:288:MET:O	1:D:291:ASP:HB2	2.21	0.41
1:D:19:GLY:HA3	1:D:67:GLU:O	2.20	0.41
1:E:16:MET:HE1	1:E:514:MET:HB3	2.03	0.41
1:E:288:MET:O	1:E:291:ASP:HB2	2.21	0.41
1:F:102:GLU:HB3	1:F:442:VAL:HG22	2.03	0.41
1:F:361:ASP:O	1:F:365:LEU:HD23	2.21	0.41
1:H:213:VAL:O	1:H:324:VAL:HA	2.20	0.41
1:H:221:LEU:HD12	1:H:249:ILE:HG23	2.02	0.41
1:J:234:LEU:N	1:J:235:PRO:HD2	2.36	0.41
1:J:342:ILE:O	1:J:346:VAL:HG23	2.21	0.41
1:K:234:LEU:N	1:K:235:PRO:HD2	2.36	0.41
1:K:15:LYS:HB3	1:K:66:PHE:HB3	2.03	0.41
1:L:266:THR:HG22	1:L:273:VAL:H	1.85	0.41
1:M:213:VAL:O	1:M:324:VAL:HA	2.21	0.41
1:C:288:MET:CG	1:C:368:ARG:HD2	2.49	0.41
1:E:19:GLY:HA3	1:E:67:GLU:O	2.21	0.41
1:G:95:LEU:O	1:G:99:ILE:HG13	2.21	0.41
1:I:100:ILE:HG23	1:I:104:LEU:HD22	2.02	0.41
1:I:513:LEU:HA	1:I:513:LEU:HD12	1.94	0.41
1:J:22:VAL:HG11	1:J:62:LEU:HD21	2.02	0.41
1:J:34:LYS:HB2	1:J:458:CYS:SG	2.61	0.41
1:L:221:LEU:HD12	1:L:249:ILE:HG23	2.02	0.41
1:N:461:GLU:HA	1:N:462:PRO:HD3	1.93	0.41
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.92	0.40
1:B:204:PHE:CG	1:B:204:PHE:O	2.74	0.40
1:E:349:ILE:HG23	1:E:365:LEU:HD12	2.01	0.40
1:F:19:GLY:HA3	1:F:67:GLU:O	2.21	0.40
1:F:288:MET:O	1:F:291:ASP:HB2	2.21	0.40
1:H:381:VAL:HG21	1:H:393:LYS:HA	2.03	0.40
1:I:444:LEU:HD23	1:I:444:LEU:HA	1.67	0.40
1:I:452:ARG:NH1	1:I:452:ARG:HG2	2.31	0.40
1:M:428:ASP:O	1:M:429:LEU:C	2.59	0.40
1:M:437:ASN:HA	1:M:440:ILE:HD12	2.03	0.40
2:U:46:GLY:HA3	2:U:55:LYS:O	2.21	0.40
1:C:301:ILE:HG22	1:C:301:ILE:O	2.22	0.40
1:C:361:ASP:O	1:C:365:LEU:HD23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ARG:O	1:C:408:GLU:HG2	2.21	0.40
1:E:327:LYS:O	1:E:327:LYS:HG2	2.20	0.40
1:F:42:LYS:HE2	1:F:48:THR:OG1	2.22	0.40
1:G:461:GLU:HA	1:G:462:PRO:HD3	1.84	0.40
1:H:521:VAL:HB	1:N:40:LEU:HD12	2.04	0.40
1:J:11:ASP:O	1:J:12:ALA:C	2.59	0.40
1:J:433:ASN:HA	1:J:433:ASN:HD22	1.57	0.40
1:L:419:LEU:HD22	1:L:500:THR:CG2	2.50	0.40
2:R:43:VAL:HG13	2:R:57:LEU:HD12	2.04	0.40
1:A:452:ARG:HH11	1:A:452:ARG:HG2	1.86	0.40
1:B:288:MET:O	1:B:291:ASP:HB2	2.22	0.40
1:B:349:ILE:HG23	1:B:365:LEU:HD12	2.02	0.40
1:B:461:GLU:HA	1:B:462:PRO:HD3	1.83	0.40
1:B:16:MET:CE	1:B:514:MET:HB3	2.51	0.40
1:C:413:ALA:HB3	1:C:417:VAL:HG13	2.02	0.40
1:D:301:ILE:HG21	1:D:309:LEU:HD12	2.04	0.40
1:E:301:ILE:HG21	1:E:309:LEU:HD12	2.04	0.40
1:G:288:MET:CG	1:G:368:ARG:HD2	2.48	0.40
1:H:38:VAL:HG12	1:H:40:LEU:HD13	2.03	0.40
1:H:496:PRO:HB2	1:H:499:VAL:HG13	2.04	0.40
1:I:234:LEU:N	1:I:235:PRO:HD2	2.36	0.40
1:I:266:THR:HG22	1:I:273:VAL:H	1.85	0.40
1:I:433:ASN:OD1	1:I:435:ASP:HB2	2.22	0.40
1:L:350:ARG:HA	1:L:353:ILE:HD12	2.04	0.40
1:L:429:LEU:HB3	1:L:440:ILE:HG21	2.04	0.40
1:M:201:SER:HA	1:M:202:PRO:HD3	1.95	0.40
1:A:301:ILE:O	1:A:301:ILE:HG22	2.21	0.40
1:D:204:PHE:O	1:D:204:PHE:CG	2.74	0.40
1:D:219:PHE:HB3	1:D:317:LEU:HD13	2.02	0.40
1:E:247:LEU:O	1:E:273:VAL:HA	2.21	0.40
1:E:33:PRO:HG3	4:E:704:ADP:C6	2.56	0.40
1:E:452:ARG:HG2	1:E:452:ARG:HH11	1.86	0.40
1:F:286:LYS:HE2	1:F:304:GLU:OE1	2.22	0.40
1:G:381:VAL:CG1	1:G:392:LYS:HG3	2.52	0.40
1:H:201:SER:HA	1:H:202:PRO:HD3	1.95	0.40
1:M:266:THR:HG22	1:M:273:VAL:H	1.86	0.40
1:N:32:GLY:CA	1:N:454:ILE:HG23	2.52	0.40
2:O:55:LYS:H	2:O:55:LYS:HE2	1.87	0.40
1:B:301:ILE:HG21	1:B:309:LEU:HD12	2.04	0.40
1:B:404:ARG:O	1:B:408:GLU:HG2	2.21	0.40
1:D:449:ALA:HB3	1:D:450:PRO:HD3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:THR:O	1:D:94:VAL:HG23	2.21	0.40
1:E:413:ALA:HB3	1:E:417:VAL:HG13	2.04	0.40
1:E:90:THR:O	1:E:94:VAL:HG23	2.21	0.40
1:G:197:ARG:H	1:G:329:THR:HA	1.87	0.40
1:G:28:LYS:O	1:G:29:VAL:C	2.59	0.40
1:H:149:THR:HG22	1:H:156:GLU:HA	2.04	0.40
1:H:461:GLU:HA	1:H:462:PRO:HD3	1.90	0.40
1:J:198:GLY:HA3	1:J:328:ASP:HA	2.03	0.40
1:K:72:GLN:HE22	1:K:75:LYS:NZ	2.20	0.40
2:P:46:GLY:HA3	2:P:55:LYS:O	2.22	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	522/524 (100%)	485 (93%)	33 (6%)	4 (1%)	22	64
1	B	522/524 (100%)	484 (93%)	33 (6%)	5 (1%)	18	59
1	C	522/524 (100%)	484 (93%)	34 (6%)	4 (1%)	22	64
1	D	522/524 (100%)	485 (93%)	32 (6%)	5 (1%)	18	59
1	E	522/524 (100%)	489 (94%)	29 (6%)	4 (1%)	22	64
1	F	522/524 (100%)	490 (94%)	27 (5%)	5 (1%)	18	59
1	G	522/524 (100%)	481 (92%)	36 (7%)	5 (1%)	18	59
1	H	522/524 (100%)	481 (92%)	36 (7%)	5 (1%)	18	59
1	I	522/524 (100%)	483 (92%)	32 (6%)	7 (1%)	14	51
1	J	522/524 (100%)	480 (92%)	38 (7%)	4 (1%)	22	64
1	K	522/524 (100%)	479 (92%)	38 (7%)	5 (1%)	18	59
1	L	522/524 (100%)	483 (92%)	34 (6%)	5 (1%)	18	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	522/524 (100%)	480 (92%)	37 (7%)	5 (1%)	18	59
1	N	522/524 (100%)	483 (92%)	35 (7%)	4 (1%)	22	64
2	O	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	13
2	P	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	13
2	Q	95/97 (98%)	76 (80%)	13 (14%)	6 (6%)	1	9
2	R	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	13
2	S	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	13
2	T	95/97 (98%)	76 (80%)	13 (14%)	6 (6%)	1	9
2	U	95/97 (98%)	76 (80%)	14 (15%)	5 (5%)	2	13
All	All	7973/8015 (100%)	7303 (92%)	566 (7%)	104 (1%)	14	51

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	B	44	PHE
1	C	44	PHE
1	D	44	PHE
1	E	44	PHE
1	F	44	PHE
1	G	44	PHE
2	O	7	HIS
2	P	7	HIS
2	Q	7	HIS
2	R	7	HIS
2	S	7	HIS
2	T	7	HIS
2	U	7	HIS
1	A	337	GLY
1	B	337	GLY
1	C	337	GLY
1	D	337	GLY
1	E	337	GLY
1	F	337	GLY
1	G	337	GLY
1	H	66	PHE
1	H	270	ILE
1	I	66	PHE
1	I	270	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	270	ILE
1	K	270	ILE
1	L	270	ILE
1	M	66	PHE
1	M	270	ILE
1	N	66	PHE
1	N	270	ILE
2	O	28	THR
2	P	28	THR
2	Q	28	THR
2	R	28	THR
2	S	28	THR
2	T	28	THR
2	U	28	THR
1	A	334	ASP
1	C	334	ASP
1	D	58	ARG
1	F	58	ARG
1	G	58	ARG
1	H	267	MET
1	H	462	PRO
1	I	267	MET
1	I	462	PRO
1	J	66	PHE
1	J	267	MET
1	K	66	PHE
1	K	267	MET
1	K	462	PRO
1	L	462	PRO
1	M	267	MET
1	M	462	PRO
1	N	267	MET
1	N	462	PRO
2	O	51	ASN
2	P	51	ASN
2	Q	49	LEU
2	Q	51	ASN
2	R	51	ASN
2	S	51	ASN
2	T	51	ASN
2	U	49	LEU
2	U	51	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	58	ARG
1	B	334	ASP
1	D	334	ASP
1	E	334	ASP
1	F	334	ASP
1	G	334	ASP
1	J	462	PRO
1	L	66	PHE
1	L	267	MET
2	O	49	LEU
2	P	49	LEU
2	R	49	LEU
2	S	49	LEU
2	T	49	LEU
1	I	417	VAL
1	L	417	VAL
2	Q	8	ASP
2	T	8	ASP
2	R	17	VAL
1	C	305	ILE
1	G	305	ILE
2	O	17	VAL
2	S	17	VAL
1	A	305	ILE
1	B	305	ILE
1	D	305	ILE
1	E	305	ILE
1	F	305	ILE
1	H	323	VAL
1	I	9	GLY
1	M	323	VAL
2	P	17	VAL
2	Q	17	VAL
2	T	17	VAL
2	U	17	VAL
1	I	256	GLY
1	K	417	VAL

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/404 (100%)	359 (89%)	45 (11%)	7	28
1	B	404/404 (100%)	358 (89%)	46 (11%)	7	27
1	C	404/404 (100%)	356 (88%)	48 (12%)	6	25
1	D	404/404 (100%)	357 (88%)	47 (12%)	6	26
1	E	404/404 (100%)	358 (89%)	46 (11%)	7	27
1	F	404/404 (100%)	357 (88%)	47 (12%)	6	26
1	G	404/404 (100%)	354 (88%)	50 (12%)	5	23
1	H	404/404 (100%)	347 (86%)	57 (14%)	4	18
1	I	404/404 (100%)	349 (86%)	55 (14%)	4	19
1	J	404/404 (100%)	349 (86%)	55 (14%)	4	19
1	K	404/404 (100%)	347 (86%)	57 (14%)	4	18
1	L	404/404 (100%)	348 (86%)	56 (14%)	4	18
1	M	404/404 (100%)	347 (86%)	57 (14%)	4	18
1	N	404/404 (100%)	349 (86%)	55 (14%)	4	19
2	O	80/80 (100%)	70 (88%)	10 (12%)	5	23
2	P	80/80 (100%)	70 (88%)	10 (12%)	5	23
2	Q	80/80 (100%)	70 (88%)	10 (12%)	5	23
2	R	80/80 (100%)	69 (86%)	11 (14%)	4	19
2	S	80/80 (100%)	69 (86%)	11 (14%)	4	19
2	T	80/80 (100%)	70 (88%)	10 (12%)	5	23
2	U	80/80 (100%)	69 (86%)	11 (14%)	4	19
All	All	6216/6216 (100%)	5422 (87%)	794 (13%)	5	22

All (794) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	23	LEU
1	A	43	SER
1	A	44	PHE
1	A	48	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	58	ARG
1	A	62	LEU
1	A	74	VAL
1	A	97	GLN
1	A	129	GLU
1	A	141	SER
1	A	150	ILE
1	A	153	ASN
1	A	168	LYS
1	A	176	THR
1	A	177	VAL
1	A	183	LEU
1	A	184	GLN
1	A	197	ARG
1	A	225	LYS
1	A	229	ASN
1	A	237	LEU
1	A	281	PHE
1	A	284	ARG
1	A	288	MET
1	A	322	ARG
1	A	345	ARG
1	A	348	GLN
1	A	351	GLN
1	A	362	ARG
1	A	366	GLN
1	A	387	VAL
1	A	391	GLU
1	A	398	ASP
1	A	400	LEU
1	A	417	VAL
1	A	419	LEU
1	A	420	ILE
1	A	421	ARG
1	A	425	LYS
1	A	430	ARG
1	A	461	GLU
1	A	483	GLU
1	A	484	GLU
1	A	504	LEU
1	B	18	ARG
1	B	23	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	43	SER
1	B	44	PHE
1	B	48	THR
1	B	58	ARG
1	B	62	LEU
1	B	74	VAL
1	B	97	GLN
1	B	129	GLU
1	B	141	SER
1	B	150	ILE
1	B	153	ASN
1	B	168	LYS
1	B	176	THR
1	B	177	VAL
1	B	183	LEU
1	B	184	GLN
1	B	197	ARG
1	B	225	LYS
1	B	229	ASN
1	B	237	LEU
1	B	281	PHE
1	B	284	ARG
1	B	288	MET
1	B	322	ARG
1	B	345	ARG
1	B	348	GLN
1	B	350	ARG
1	B	351	GLN
1	B	362	ARG
1	B	366	GLN
1	B	387	VAL
1	B	391	GLU
1	B	398	ASP
1	B	400	LEU
1	B	417	VAL
1	B	419	LEU
1	B	420	ILE
1	B	421	ARG
1	B	430	ARG
1	B	456	LEU
1	B	461	GLU
1	B	483	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	484	GLU
1	B	504	LEU
1	C	18	ARG
1	C	23	LEU
1	C	43	SER
1	C	44	PHE
1	C	48	THR
1	C	58	ARG
1	C	62	LEU
1	C	74	VAL
1	C	80	LYS
1	C	97	GLN
1	C	129	GLU
1	C	141	SER
1	C	150	ILE
1	C	153	ASN
1	C	168	LYS
1	C	176	THR
1	C	177	VAL
1	C	183	LEU
1	C	184	GLN
1	C	197	ARG
1	C	225	LYS
1	C	229	ASN
1	C	237	LEU
1	C	281	PHE
1	C	284	ARG
1	C	288	MET
1	C	322	ARG
1	C	345	ARG
1	C	348	GLN
1	C	350	ARG
1	C	351	GLN
1	C	362	ARG
1	C	366	GLN
1	C	387	VAL
1	C	390	LYS
1	C	391	GLU
1	C	398	ASP
1	C	400	LEU
1	C	419	LEU
1	C	420	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	421	ARG
1	C	425	LYS
1	C	430	ARG
1	C	452	ARG
1	C	461	GLU
1	C	483	GLU
1	C	504	LEU
1	C	510	VAL
1	D	18	ARG
1	D	23	LEU
1	D	43	SER
1	D	44	PHE
1	D	48	THR
1	D	58	ARG
1	D	62	LEU
1	D	74	VAL
1	D	97	GLN
1	D	129	GLU
1	D	141	SER
1	D	150	ILE
1	D	153	ASN
1	D	168	LYS
1	D	176	THR
1	D	177	VAL
1	D	183	LEU
1	D	184	GLN
1	D	197	ARG
1	D	225	LYS
1	D	229	ASN
1	D	237	LEU
1	D	281	PHE
1	D	284	ARG
1	D	288	MET
1	D	322	ARG
1	D	345	ARG
1	D	348	GLN
1	D	350	ARG
1	D	351	GLN
1	D	362	ARG
1	D	366	GLN
1	D	387	VAL
1	D	391	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	398	ASP
1	D	400	LEU
1	D	417	VAL
1	D	419	LEU
1	D	420	ILE
1	D	421	ARG
1	D	425	LYS
1	D	430	ARG
1	D	456	LEU
1	D	461	GLU
1	D	483	GLU
1	D	484	GLU
1	D	504	LEU
1	E	18	ARG
1	E	23	LEU
1	E	43	SER
1	E	44	PHE
1	E	48	THR
1	E	58	ARG
1	E	62	LEU
1	E	74	VAL
1	E	97	GLN
1	E	129	GLU
1	E	141	SER
1	E	150	ILE
1	E	153	ASN
1	E	168	LYS
1	E	176	THR
1	E	177	VAL
1	E	183	LEU
1	E	184	GLN
1	E	197	ARG
1	E	225	LYS
1	E	229	ASN
1	E	237	LEU
1	E	281	PHE
1	E	284	ARG
1	E	288	MET
1	E	322	ARG
1	E	345	ARG
1	E	348	GLN
1	E	350	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	351	GLN
1	E	362	ARG
1	E	366	GLN
1	E	387	VAL
1	E	391	GLU
1	E	398	ASP
1	E	400	LEU
1	E	417	VAL
1	E	419	LEU
1	E	420	ILE
1	E	421	ARG
1	E	430	ARG
1	E	456	LEU
1	E	461	GLU
1	E	483	GLU
1	E	484	GLU
1	E	504	LEU
1	F	18	ARG
1	F	23	LEU
1	F	43	SER
1	F	44	PHE
1	F	48	THR
1	F	58	ARG
1	F	62	LEU
1	F	74	VAL
1	F	80	LYS
1	F	97	GLN
1	F	129	GLU
1	F	141	SER
1	F	150	ILE
1	F	153	ASN
1	F	168	LYS
1	F	176	THR
1	F	177	VAL
1	F	183	LEU
1	F	184	GLN
1	F	197	ARG
1	F	225	LYS
1	F	229	ASN
1	F	237	LEU
1	F	281	PHE
1	F	284	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	288	MET
1	F	322	ARG
1	F	345	ARG
1	F	348	GLN
1	F	350	ARG
1	F	351	GLN
1	F	362	ARG
1	F	366	GLN
1	F	387	VAL
1	F	391	GLU
1	F	398	ASP
1	F	400	LEU
1	F	419	LEU
1	F	420	ILE
1	F	421	ARG
1	F	430	ARG
1	F	452	ARG
1	F	456	LEU
1	F	461	GLU
1	F	483	GLU
1	F	484	GLU
1	F	504	LEU
1	G	18	ARG
1	G	23	LEU
1	G	43	SER
1	G	44	PHE
1	G	48	THR
1	G	51	LYS
1	G	58	ARG
1	G	62	LEU
1	G	74	VAL
1	G	80	LYS
1	G	97	GLN
1	G	129	GLU
1	G	141	SER
1	G	150	ILE
1	G	153	ASN
1	G	168	LYS
1	G	176	THR
1	G	177	VAL
1	G	183	LEU
1	G	184	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	197	ARG
1	G	225	LYS
1	G	229	ASN
1	G	237	LEU
1	G	281	PHE
1	G	284	ARG
1	G	288	MET
1	G	322	ARG
1	G	345	ARG
1	G	348	GLN
1	G	350	ARG
1	G	351	GLN
1	G	362	ARG
1	G	366	GLN
1	G	387	VAL
1	G	391	GLU
1	G	398	ASP
1	G	400	LEU
1	G	417	VAL
1	G	419	LEU
1	G	420	ILE
1	G	421	ARG
1	G	425	LYS
1	G	430	ARG
1	G	456	LEU
1	G	461	GLU
1	G	483	GLU
1	G	484	GLU
1	G	504	LEU
1	G	510	VAL
1	H	10	ASN
1	H	20	VAL
1	H	23	LEU
1	H	37	ASN
1	H	40	LEU
1	H	42	LYS
1	H	59	GLU
1	H	77	VAL
1	H	79	SER
1	H	89	THR
1	H	104	LEU
1	H	114	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	129	GLU
1	H	131	LEU
1	H	138	CYS
1	H	141	SER
1	H	172	GLU
1	H	187	LEU
1	H	197	ARG
1	H	200	LEU
1	H	230	ILE
1	H	233	MET
1	H	247	LEU
1	H	248	LEU
1	H	255	GLU
1	H	261	THR
1	H	272	LYS
1	H	284	ARG
1	H	285	ARG
1	H	288	MET
1	H	300	VAL
1	H	302	SER
1	H	307	MET
1	H	317	LEU
1	H	323	VAL
1	H	328	ASP
1	H	331	THR
1	H	354	GLU
1	H	355	GLU
1	H	357	THR
1	H	385	THR
1	H	389	MET
1	H	400	LEU
1	H	401	HIS
1	H	420	ILE
1	H	421	ARG
1	H	426	LEU
1	H	432	GLN
1	H	433	ASN
1	H	445	ARG
1	H	452	ARG
1	H	460	GLU
1	H	468	THR
1	H	483	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	494	LEU
1	H	504	LEU
1	H	513	LEU
1	I	10	ASN
1	I	20	VAL
1	I	23	LEU
1	I	37	ASN
1	I	40	LEU
1	I	42	LYS
1	I	59	GLU
1	I	77	VAL
1	I	79	SER
1	I	89	THR
1	I	104	LEU
1	I	114	MET
1	I	129	GLU
1	I	131	LEU
1	I	138	CYS
1	I	141	SER
1	I	172	GLU
1	I	187	LEU
1	I	197	ARG
1	I	200	LEU
1	I	230	ILE
1	I	233	MET
1	I	247	LEU
1	I	248	LEU
1	I	255	GLU
1	I	272	LYS
1	I	284	ARG
1	I	285	ARG
1	I	288	MET
1	I	300	VAL
1	I	302	SER
1	I	307	MET
1	I	317	LEU
1	I	328	ASP
1	I	331	THR
1	I	354	GLU
1	I	355	GLU
1	I	357	THR
1	I	385	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	389	MET
1	I	400	LEU
1	I	401	HIS
1	I	420	ILE
1	I	421	ARG
1	I	426	LEU
1	I	432	GLN
1	I	433	ASN
1	I	452	ARG
1	I	460	GLU
1	I	468	THR
1	I	483	GLU
1	I	494	LEU
1	I	504	LEU
1	I	509	SER
1	I	513	LEU
1	J	10	ASN
1	J	20	VAL
1	J	23	LEU
1	J	37	ASN
1	J	40	LEU
1	J	42	LYS
1	J	59	GLU
1	J	77	VAL
1	J	79	SER
1	J	89	THR
1	J	104	LEU
1	J	114	MET
1	J	131	LEU
1	J	138	CYS
1	J	141	SER
1	J	172	GLU
1	J	187	LEU
1	J	197	ARG
1	J	200	LEU
1	J	230	ILE
1	J	233	MET
1	J	247	LEU
1	J	248	LEU
1	J	255	GLU
1	J	272	LYS
1	J	284	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	285	ARG
1	J	288	MET
1	J	300	VAL
1	J	302	SER
1	J	307	MET
1	J	317	LEU
1	J	323	VAL
1	J	331	THR
1	J	354	GLU
1	J	355	GLU
1	J	357	THR
1	J	385	THR
1	J	389	MET
1	J	400	LEU
1	J	401	HIS
1	J	420	ILE
1	J	421	ARG
1	J	426	LEU
1	J	432	GLN
1	J	433	ASN
1	J	445	ARG
1	J	452	ARG
1	J	460	GLU
1	J	468	THR
1	J	483	GLU
1	J	494	LEU
1	J	504	LEU
1	J	509	SER
1	J	513	LEU
1	K	10	ASN
1	K	20	VAL
1	K	23	LEU
1	K	37	ASN
1	K	40	LEU
1	K	42	LYS
1	K	59	GLU
1	K	77	VAL
1	K	79	SER
1	K	89	THR
1	K	104	LEU
1	K	107	VAL
1	K	114	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	129	GLU
1	K	131	LEU
1	K	138	CYS
1	K	141	SER
1	K	172	GLU
1	K	187	LEU
1	K	197	ARG
1	K	200	LEU
1	K	230	ILE
1	K	233	MET
1	K	247	LEU
1	K	248	LEU
1	K	255	GLU
1	K	261	THR
1	K	272	LYS
1	K	284	ARG
1	K	285	ARG
1	K	288	MET
1	K	300	VAL
1	K	302	SER
1	K	307	MET
1	K	317	LEU
1	K	328	ASP
1	K	331	THR
1	K	354	GLU
1	K	355	GLU
1	K	357	THR
1	K	385	THR
1	K	389	MET
1	K	400	LEU
1	K	401	HIS
1	K	420	ILE
1	K	421	ARG
1	K	426	LEU
1	K	432	GLN
1	K	433	ASN
1	K	452	ARG
1	K	460	GLU
1	K	468	THR
1	K	483	GLU
1	K	494	LEU
1	K	504	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	509	SER
1	K	513	LEU
1	L	10	ASN
1	L	20	VAL
1	L	23	LEU
1	L	37	ASN
1	L	40	LEU
1	L	42	LYS
1	L	59	GLU
1	L	77	VAL
1	L	79	SER
1	L	89	THR
1	L	104	LEU
1	L	107	VAL
1	L	114	MET
1	L	131	LEU
1	L	138	CYS
1	L	141	SER
1	L	172	GLU
1	L	187	LEU
1	L	197	ARG
1	L	200	LEU
1	L	230	ILE
1	L	233	MET
1	L	247	LEU
1	L	248	LEU
1	L	255	GLU
1	L	272	LYS
1	L	284	ARG
1	L	285	ARG
1	L	288	MET
1	L	300	VAL
1	L	302	SER
1	L	307	MET
1	L	317	LEU
1	L	323	VAL
1	L	328	ASP
1	L	331	THR
1	L	354	GLU
1	L	355	GLU
1	L	357	THR
1	L	385	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	389	MET
1	L	400	LEU
1	L	401	HIS
1	L	420	ILE
1	L	421	ARG
1	L	426	LEU
1	L	432	GLN
1	L	433	ASN
1	L	452	ARG
1	L	460	GLU
1	L	468	THR
1	L	483	GLU
1	L	494	LEU
1	L	504	LEU
1	L	509	SER
1	L	513	LEU
1	M	10	ASN
1	M	20	VAL
1	M	23	LEU
1	M	37	ASN
1	M	40	LEU
1	M	42	LYS
1	M	59	GLU
1	M	77	VAL
1	M	79	SER
1	M	89	THR
1	M	104	LEU
1	M	107	VAL
1	M	114	MET
1	M	131	LEU
1	M	138	CYS
1	M	141	SER
1	M	172	GLU
1	M	187	LEU
1	M	197	ARG
1	M	200	LEU
1	M	230	ILE
1	M	233	MET
1	M	247	LEU
1	M	248	LEU
1	M	255	GLU
1	M	272	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	284	ARG
1	M	285	ARG
1	M	288	MET
1	M	300	VAL
1	M	302	SER
1	M	307	MET
1	M	317	LEU
1	M	323	VAL
1	M	328	ASP
1	M	331	THR
1	M	354	GLU
1	M	355	GLU
1	M	357	THR
1	M	385	THR
1	M	389	MET
1	M	400	LEU
1	M	401	HIS
1	M	420	ILE
1	M	421	ARG
1	M	426	LEU
1	M	432	GLN
1	M	433	ASN
1	M	445	ARG
1	M	452	ARG
1	M	460	GLU
1	M	468	THR
1	M	483	GLU
1	M	494	LEU
1	M	504	LEU
1	M	509	SER
1	M	513	LEU
1	N	10	ASN
1	N	20	VAL
1	N	23	LEU
1	N	37	ASN
1	N	40	LEU
1	N	42	LYS
1	N	59	GLU
1	N	77	VAL
1	N	79	SER
1	N	89	THR
1	N	104	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	114	MET
1	N	129	GLU
1	N	131	LEU
1	N	138	CYS
1	N	141	SER
1	N	172	GLU
1	N	187	LEU
1	N	197	ARG
1	N	200	LEU
1	N	230	ILE
1	N	233	MET
1	N	247	LEU
1	N	248	LEU
1	N	255	GLU
1	N	272	LYS
1	N	284	ARG
1	N	285	ARG
1	N	288	MET
1	N	300	VAL
1	N	302	SER
1	N	307	MET
1	N	317	LEU
1	N	328	ASP
1	N	331	THR
1	N	354	GLU
1	N	355	GLU
1	N	357	THR
1	N	385	THR
1	N	389	MET
1	N	400	LEU
1	N	401	HIS
1	N	420	ILE
1	N	421	ARG
1	N	426	LEU
1	N	432	GLN
1	N	433	ASN
1	N	452	ARG
1	N	460	GLU
1	N	468	THR
1	N	483	GLU
1	N	494	LEU
1	N	504	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	509	SER
1	N	513	LEU
2	O	1	MET
2	O	3	ILE
2	O	6	LEU
2	O	14	ARG
2	O	20	LYS
2	O	28	THR
2	O	30	SER
2	O	55	LYS
2	O	60	LYS
2	O	86	MET
2	P	1	MET
2	P	3	ILE
2	P	6	LEU
2	P	14	ARG
2	P	20	LYS
2	P	28	THR
2	P	30	SER
2	P	55	LYS
2	P	60	LYS
2	P	86	MET
2	Q	1	MET
2	Q	3	ILE
2	Q	6	LEU
2	Q	14	ARG
2	Q	20	LYS
2	Q	28	THR
2	Q	30	SER
2	Q	55	LYS
2	Q	60	LYS
2	Q	86	MET
2	R	1	MET
2	R	3	ILE
2	R	6	LEU
2	R	14	ARG
2	R	20	LYS
2	R	28	THR
2	R	30	SER
2	R	55	LYS
2	R	60	LYS
2	R	77	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	86	MET
2	S	1	MET
2	S	3	ILE
2	S	6	LEU
2	S	14	ARG
2	S	20	LYS
2	S	28	THR
2	S	30	SER
2	S	55	LYS
2	S	60	LYS
2	S	77	LYS
2	S	86	MET
2	T	1	MET
2	T	3	ILE
2	T	6	LEU
2	T	14	ARG
2	T	20	LYS
2	T	28	THR
2	T	30	SER
2	T	55	LYS
2	T	60	LYS
2	T	86	MET
2	U	1	MET
2	U	3	ILE
2	U	6	LEU
2	U	14	ARG
2	U	20	LYS
2	U	28	THR
2	U	30	SER
2	U	55	LYS
2	U	60	LYS
2	U	77	LYS
2	U	86	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	37	ASN
1	A	97	GLN
1	A	146	GLN
1	A	153	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	348	GLN
1	A	432	GLN
1	A	453	GLN
1	A	457	ASN
1	A	475	ASN
1	B	21	ASN
1	B	97	GLN
1	B	146	GLN
1	B	153	ASN
1	B	348	GLN
1	B	432	GLN
1	B	453	GLN
1	B	457	ASN
1	B	475	ASN
1	C	21	ASN
1	C	97	GLN
1	C	146	GLN
1	C	153	ASN
1	C	265	ASN
1	C	348	GLN
1	C	432	GLN
1	C	453	GLN
1	C	457	ASN
1	C	475	ASN
1	D	21	ASN
1	D	37	ASN
1	D	146	GLN
1	D	153	ASN
1	D	265	ASN
1	D	348	GLN
1	D	432	GLN
1	D	453	GLN
1	D	457	ASN
1	D	475	ASN
1	E	21	ASN
1	E	146	GLN
1	E	153	ASN
1	E	348	GLN
1	E	432	GLN
1	E	453	GLN
1	E	457	ASN
1	E	475	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	21	ASN
1	F	82	ASN
1	F	97	GLN
1	F	146	GLN
1	F	153	ASN
1	F	265	ASN
1	F	348	GLN
1	F	432	GLN
1	F	453	GLN
1	F	457	ASN
1	F	475	ASN
1	G	21	ASN
1	G	97	GLN
1	G	146	GLN
1	G	153	ASN
1	G	265	ASN
1	G	348	GLN
1	G	432	GLN
1	G	453	GLN
1	G	457	ASN
1	G	475	ASN
1	H	21	ASN
1	H	72	GLN
1	H	97	GLN
1	H	146	GLN
1	H	326	ASN
1	H	348	GLN
1	H	433	ASN
1	H	436	GLN
1	I	21	ASN
1	I	72	GLN
1	I	97	GLN
1	I	146	GLN
1	I	153	ASN
1	I	326	ASN
1	I	348	GLN
1	I	433	ASN
1	J	21	ASN
1	J	72	GLN
1	J	97	GLN
1	J	146	GLN
1	J	326	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	348	GLN
1	J	433	ASN
1	J	436	GLN
1	K	21	ASN
1	K	72	GLN
1	K	97	GLN
1	K	146	GLN
1	K	326	ASN
1	K	348	GLN
1	K	433	ASN
1	L	21	ASN
1	L	37	ASN
1	L	72	GLN
1	L	97	GLN
1	L	146	GLN
1	L	326	ASN
1	L	348	GLN
1	L	433	ASN
1	M	21	ASN
1	M	37	ASN
1	M	72	GLN
1	M	97	GLN
1	M	146	GLN
1	M	326	ASN
1	M	348	GLN
1	M	433	ASN
1	N	21	ASN
1	N	72	GLN
1	N	97	GLN
1	N	146	GLN
1	N	326	ASN
1	N	348	GLN
1	N	433	ASN
1	N	436	GLN
2	O	80	ASN
2	P	68	ASN
2	P	80	ASN
2	Q	68	ASN
2	Q	80	ASN
2	R	68	ASN
2	R	80	ASN
2	S	68	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	80	ASN
2	T	80	ASN
2	U	68	ASN
2	U	80	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	$\# Z > 2$
4	ADP	A	700	3	25,29,29	1.28	3 (12%)	24,45,45	2.92	10 (41%)
4	ADP	B	701	3	25,29,29	1.38	4 (16%)	24,45,45	2.74	7 (29%)
4	ADP	C	702	3	25,29,29	1.20	2 (8%)	24,45,45	2.91	8 (33%)
4	ADP	D	703	3	25,29,29	1.47	5 (20%)	24,45,45	3.01	8 (33%)
4	ADP	E	704	3	25,29,29	1.26	2 (8%)	24,45,45	2.69	7 (29%)
4	ADP	F	705	3	25,29,29	1.11	2 (8%)	24,45,45	2.62	5 (20%)
4	ADP	G	706	3	25,29,29	1.22	1 (4%)	24,45,45	2.82	9 (37%)

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
4	ADP	A	700	3	-	0/12/32/32	0/3/3/3
4	ADP	B	701	3	-	0/12/32/32	0/3/3/3
4	ADP	C	702	3	-	0/12/32/32	0/3/3/3
4	ADP	D	703	3	-	0/12/32/32	0/3/3/3
4	ADP	E	704	3	-	0/12/32/32	0/3/3/3
4	ADP	F	705	3	-	0/12/32/32	0/3/3/3
4	ADP	G	706	3	-	0/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	703	ADP	O4'-C1'	-2.81	1.37	1.41
4	D	703	ADP	C2'-C1'	-2.70	1.49	1.53
4	A	700	ADP	O4'-C4'	-2.30	1.39	1.45
4	B	701	ADP	C2'-C1'	-2.23	1.50	1.53
4	D	703	ADP	O4'-C4'	-2.17	1.40	1.45
4	B	701	ADP	O4'-C4'	-2.01	1.40	1.45
4	A	700	ADP	C2-N1	2.28	1.38	1.33
4	E	704	ADP	C2-N1	2.53	1.38	1.33
4	F	705	ADP	C2-N1	2.56	1.38	1.33
4	C	702	ADP	C2-N1	2.66	1.38	1.33
4	D	703	ADP	C2-N1	3.00	1.39	1.33
4	B	701	ADP	C2-N1	3.11	1.39	1.33
4	F	705	ADP	C2-N3	3.33	1.37	1.32
4	C	702	ADP	C2-N3	3.38	1.37	1.32
4	E	704	ADP	C2-N3	3.57	1.38	1.32
4	A	700	ADP	C2-N3	3.60	1.38	1.32
4	D	703	ADP	C2-N3	3.71	1.38	1.32
4	B	701	ADP	C2-N3	3.98	1.38	1.32
4	G	706	ADP	C2-N3	4.24	1.39	1.32

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	ADP	N3-C2-N1	-11.72	118.65	128.86
4	A	700	ADP	N3-C2-N1	-11.05	119.24	128.86
4	F	705	ADP	N3-C2-N1	-10.53	119.69	128.86
4	C	702	ADP	N3-C2-N1	-10.18	119.99	128.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	704	ADP	N3-C2-N1	-10.15	120.02	128.86
4	B	701	ADP	N3-C2-N1	-10.01	120.14	128.86
4	G	706	ADP	N3-C2-N1	-9.69	120.42	128.86
4	C	702	ADP	O3'-C3'-C4'	-4.54	97.82	111.09
4	G	706	ADP	O3'-C3'-C4'	-4.11	99.09	111.09
4	B	701	ADP	O3'-C3'-C4'	-4.03	99.31	111.09
4	G	706	ADP	C4-C5-N7	-3.96	105.58	109.41
4	B	701	ADP	C4-C5-N7	-3.84	105.70	109.41
4	A	700	ADP	C1'-N9-C4	-3.75	120.16	126.64
4	E	704	ADP	C1'-N9-C4	-3.72	120.20	126.64
4	B	701	ADP	C1'-N9-C4	-3.63	120.37	126.64
4	C	702	ADP	C4-C5-N7	-3.61	105.93	109.41
4	D	703	ADP	C1'-N9-C4	-3.47	120.64	126.64
4	E	704	ADP	C4-C5-N7	-3.41	106.11	109.41
4	D	703	ADP	O3'-C3'-C4'	-3.37	101.23	111.09
4	A	700	ADP	C4-C5-N7	-3.14	106.37	109.41
4	D	703	ADP	O2'-C2'-C1'	-3.14	101.80	111.61
4	C	702	ADP	C1'-N9-C4	-3.06	121.35	126.64
4	A	700	ADP	O3'-C3'-C4'	-3.02	102.27	111.09
4	C	702	ADP	O2'-C2'-C1'	-2.99	102.25	111.61
4	F	705	ADP	C4-C5-N7	-2.96	106.55	109.41
4	F	705	ADP	C1'-N9-C4	-2.88	121.65	126.64
4	G	706	ADP	C1'-N9-C4	-2.82	121.76	126.64
4	E	704	ADP	O2'-C2'-C1'	-2.76	102.98	111.61
4	F	705	ADP	O3'-C3'-C4'	-2.74	103.07	111.09
4	E	704	ADP	O3'-C3'-C4'	-2.59	103.51	111.09
4	D	703	ADP	C4-C5-N7	-2.58	106.91	109.41
4	G	706	ADP	O2'-C2'-C1'	-2.52	103.74	111.61
4	B	701	ADP	O2'-C2'-C1'	-2.44	104.00	111.61
4	G	706	ADP	O3'-C3'-C2'	-2.31	104.43	111.83
4	A	700	ADP	O2'-C2'-C1'	-2.21	104.70	111.61
4	A	700	ADP	N6-C6-N1	-2.20	114.40	118.77
4	A	700	ADP	O3'-C3'-C2'	-2.10	105.11	111.83
4	D	703	ADP	C2'-C3'-C4'	2.02	106.56	102.62
4	B	701	ADP	C2'-C3'-C4'	2.16	106.83	102.62
4	E	704	ADP	C2'-C3'-C4'	2.20	106.90	102.62
4	C	702	ADP	C2'-C3'-C4'	2.42	107.33	102.62
4	A	700	ADP	C2'-C3'-C4'	2.55	107.59	102.62
4	A	700	ADP	C4'-O4'-C1'	2.71	112.65	109.77
4	G	706	ADP	O5'-C5'-C4'	2.75	118.75	109.00
4	D	703	ADP	C4'-O4'-C1'	2.80	112.75	109.77
4	C	702	ADP	O5'-C5'-C4'	2.82	119.00	109.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	ADP	O5'-C5'-C4'	2.85	119.11	109.00
4	G	706	ADP	C2'-C3'-C4'	2.91	108.29	102.62
4	B	701	ADP	O5'-C5'-C4'	2.92	119.36	109.00
4	F	705	ADP	O5'-C5'-C4'	2.96	119.50	109.00
4	D	703	ADP	O5'-C5'-C4'	3.04	119.78	109.00
4	C	702	ADP	C4'-O4'-C1'	3.17	113.14	109.77
4	E	704	ADP	O5'-C5'-C4'	3.20	120.35	109.00
4	G	706	ADP	C4'-O4'-C1'	3.44	113.43	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	ADP	2	0
4	B	701	ADP	2	0
4	C	702	ADP	2	0
4	D	703	ADP	3	0
4	E	704	ADP	1	0
4	F	705	ADP	1	0
4	G	706	ADP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	524/524 (100%)	0.61	58 (11%) 6 2	5, 7, 9, 10	0
1	B	524/524 (100%)	0.71	59 (11%) 6 2	5, 7, 9, 10	0
1	C	524/524 (100%)	0.49	50 (9%) 9 3	5, 7, 9, 10	0
1	D	524/524 (100%)	0.53	52 (9%) 8 3	5, 7, 9, 10	0
1	E	524/524 (100%)	0.79	64 (12%) 5 2	5, 7, 9, 10	0
1	F	524/524 (100%)	0.85	72 (13%) 3 1	5, 7, 9, 10	0
1	G	524/524 (100%)	0.69	65 (12%) 4 2	5, 7, 9, 10	0
1	H	524/524 (100%)	0.34	19 (3%) 43 18	6, 7, 9, 10	0
1	I	524/524 (100%)	0.30	12 (2%) 61 31	5, 7, 9, 10	0
1	J	524/524 (100%)	0.42	29 (5%) 26 10	5, 7, 9, 10	0
1	K	524/524 (100%)	0.59	44 (8%) 12 4	5, 7, 9, 10	0
1	L	524/524 (100%)	0.63	44 (8%) 12 4	5, 7, 9, 10	0
1	M	524/524 (100%)	0.48	38 (7%) 16 6	5, 7, 9, 10	0
1	N	524/524 (100%)	0.53	31 (5%) 23 9	5, 7, 9, 10	0
2	O	97/97 (100%)	1.73	35 (36%) 0 0	7, 7, 8, 8	0
2	P	97/97 (100%)	1.62	27 (27%) 1 0	7, 7, 8, 8	0
2	Q	97/97 (100%)	1.41	30 (30%) 0 0	7, 7, 8, 8	0
2	R	97/97 (100%)	1.50	24 (24%) 1 0	7, 7, 8, 8	0
2	S	97/97 (100%)	1.73	30 (30%) 0 0	7, 7, 8, 8	0
2	T	97/97 (100%)	1.57	27 (27%) 1 0	7, 7, 8, 8	0
2	U	97/97 (100%)	3.19	74 (76%) 0 0	7, 7, 8, 8	0
All	All	8015/8015 (100%)	0.67	884 (11%) 6 2	5, 7, 9, 10	0

All (884) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	361	ASP	16.9
1	F	361	ASP	10.7
1	E	361	ASP	10.1
1	A	361	ASP	9.9
1	G	199	TYR	9.0
1	G	361	ASP	8.9
1	E	353	ILE	8.6
1	G	208	PRO	8.5
2	U	32	ALA	8.3
1	A	353	ILE	8.2
1	B	361	ASP	8.0
1	F	357	THR	7.8
1	D	361	ASP	7.6
1	D	212	ALA	7.6
1	L	357	THR	7.4
1	B	353	ILE	7.4
2	S	32	ALA	7.3
1	A	357	THR	7.2
1	F	355	GLU	7.2
1	A	321	LYS	7.2
1	B	355	GLU	7.2
1	L	264	VAL	7.1
2	P	32	ALA	7.1
2	T	97	ALA	7.1
1	E	281	PHE	7.1
1	C	212	ALA	7.1
1	F	353	ILE	7.0
2	U	33	ALA	7.0
2	O	97	ALA	6.9
1	I	264	VAL	6.9
1	B	365	LEU	6.8
1	C	357	THR	6.8
2	P	23	GLY	6.7
2	U	30	SER	6.6
2	O	25	ILE	6.6
2	T	18	GLU	6.6
1	D	357	THR	6.6
1	I	268	ARG	6.6
1	A	208	PRO	6.5
1	D	365	LEU	6.5
2	U	17	VAL	6.5
2	R	17	VAL	6.5
1	B	357	THR	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	U	31	ALA	6.5
1	A	365	LEU	6.4
2	S	31	ALA	6.4
1	F	210	THR	6.4
1	G	357	THR	6.3
1	F	172	GLU	6.3
1	G	362	ARG	6.3
1	F	349	ILE	6.3
1	C	353	ILE	6.2
1	K	356	ALA	6.1
1	G	251	ALA	6.1
1	G	353	ILE	6.1
2	U	22	ALA	6.0
2	P	18	GLU	6.0
1	A	349	ILE	5.9
1	A	360	TYR	5.9
1	E	280	GLY	5.9
2	R	18	GLU	5.9
2	U	18	GLU	5.9
1	E	357	THR	5.8
2	S	33	ALA	5.8
2	U	51	ASN	5.8
2	S	51	ASN	5.8
2	Q	18	GLU	5.7
1	C	270	ILE	5.7
1	E	365	LEU	5.7
1	G	214	GLU	5.7
2	T	25	ILE	5.7
1	M	358	SER	5.7
1	D	353	ILE	5.7
1	E	338	GLU	5.7
2	O	72	GLY	5.7
1	E	340	ALA	5.6
1	C	267	MET	5.6
2	U	97	ALA	5.6
2	R	51	ASN	5.5
1	K	360	TYR	5.5
1	C	360	TYR	5.5
1	G	212	ALA	5.4
1	M	360	TYR	5.4
1	F	171	LYS	5.4
2	T	52	GLY	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	U	28	THR	5.4
2	R	25	ILE	5.3
1	N	183	LEU	5.3
1	E	364	LYS	5.3
1	M	357	THR	5.3
1	B	284	ARG	5.2
1	B	349	ILE	5.2
1	H	360	TYR	5.2
1	E	354	GLU	5.2
1	K	186	GLU	5.2
1	F	212	ALA	5.2
2	Q	25	ILE	5.2
1	A	284	ARG	5.2
2	U	71	TYR	5.1
1	B	348	GLN	5.1
1	G	195	PHE	5.1
2	P	1	MET	5.1
1	E	279	PRO	5.0
2	U	19	THR	5.0
1	D	284	ARG	5.0
1	B	279	PRO	5.0
2	S	18	GLU	5.0
2	O	17	VAL	5.0
2	O	83	VAL	5.0
1	C	210	THR	5.0
1	F	375	GLY	4.9
2	R	80	ASN	4.9
1	B	364	LYS	4.9
1	C	199	TYR	4.9
2	S	17	VAL	4.9
1	A	203	TYR	4.9
1	D	349	ILE	4.9
2	U	1	MET	4.9
1	E	355	GLU	4.9
1	G	210	THR	4.9
2	S	97	ALA	4.9
1	L	268	ARG	4.8
1	G	349	ILE	4.8
1	L	353	ILE	4.8
1	E	284	ARG	4.8
2	O	1	MET	4.8
2	U	21	SER	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	209	GLU	4.8
2	U	25	ILE	4.8
1	F	267	MET	4.8
2	U	26	VAL	4.8
1	G	256	GLY	4.8
1	L	177	VAL	4.8
2	S	30	SER	4.8
1	E	321	LYS	4.8
2	P	51	ASN	4.7
2	P	31	ALA	4.7
2	S	80	ASN	4.7
1	J	365	LEU	4.7
2	Q	32	ALA	4.6
1	G	350	ARG	4.6
1	A	355	GLU	4.6
1	B	192	GLY	4.6
2	S	1	MET	4.6
1	E	360	TYR	4.6
1	F	331	THR	4.6
1	N	360	TYR	4.6
1	B	346	VAL	4.6
1	J	353	ILE	4.6
1	E	209	GLU	4.6
2	U	23	GLY	4.6
1	D	268	ARG	4.6
2	U	69	ASP	4.6
1	D	199	TYR	4.5
2	U	78	ILE	4.5
2	T	82	GLU	4.5
2	P	33	ALA	4.5
1	F	352	GLN	4.5
2	R	1	MET	4.5
1	G	360	TYR	4.5
1	E	210	THR	4.5
1	G	354	GLU	4.4
2	P	49	LEU	4.4
1	N	266	THR	4.4
1	K	188	ASP	4.4
1	A	364	LYS	4.4
1	N	357	THR	4.4
1	G	365	LEU	4.4
2	U	16	GLU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	349	ILE	4.4
1	I	357	THR	4.4
2	Q	71	TYR	4.3
1	C	362	ARG	4.3
2	P	20	LYS	4.3
1	E	341	ALA	4.3
1	M	284	ARG	4.3
1	B	352	GLN	4.3
1	B	350	ARG	4.3
1	D	321	LYS	4.3
1	F	364	LYS	4.3
2	P	67	PHE	4.2
2	Q	27	LEU	4.2
1	M	264	VAL	4.2
2	S	83	VAL	4.2
1	F	374	GLY	4.2
2	U	20	LYS	4.2
1	D	338	GLU	4.2
2	U	65	VAL	4.2
1	D	360	TYR	4.2
1	B	354	GLU	4.2
2	O	21	SER	4.1
2	T	17	VAL	4.1
2	U	52	GLY	4.1
1	F	350	ARG	4.1
1	C	251	ALA	4.1
2	O	31	ALA	4.1
2	S	21	SER	4.1
1	M	268	ARG	4.1
2	U	80	ASN	4.1
2	U	27	LEU	4.1
1	F	251	ALA	4.1
2	Q	78	ILE	4.1
1	J	356	ALA	4.1
2	R	79	ASP	4.0
2	S	66	ILE	4.0
1	E	346	VAL	4.0
2	R	20	LYS	4.0
2	O	22	ALA	4.0
1	C	349	ILE	4.0
1	E	349	ILE	4.0
2	U	72	GLY	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	279	PRO	4.0
2	U	35	SER	4.0
1	K	187	LEU	4.0
2	U	79	ASP	4.0
2	P	25	ILE	4.0
1	B	351	GLN	4.0
2	P	71	TYR	4.0
1	C	271	VAL	4.0
2	U	83	VAL	4.0
2	R	21	SER	4.0
1	L	362	ARG	4.0
2	R	83	VAL	3.9
2	P	85	ILE	3.9
2	O	32	ALA	3.9
2	T	71	TYR	3.9
2	O	66	ILE	3.9
2	S	36	THR	3.9
1	G	198	GLY	3.9
1	K	295	LEU	3.9
1	E	352	GLN	3.9
1	F	273	VAL	3.9
2	R	30	SER	3.9
2	U	75	SER	3.9
2	U	38	GLY	3.8
1	E	195	PHE	3.8
1	G	222	LEU	3.8
2	U	49	LEU	3.8
1	D	172	GLU	3.8
2	T	33	ALA	3.8
1	A	238	GLU	3.8
1	A	338	GLU	3.8
2	O	36	THR	3.8
2	T	80	ASN	3.8
2	T	72	GLY	3.8
1	C	350	ARG	3.8
1	J	181	THR	3.8
1	A	320	ALA	3.8
1	I	360	TYR	3.7
1	B	360	TYR	3.7
2	P	97	ALA	3.7
2	T	32	ALA	3.7
1	F	365	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	284	ARG	3.7
1	F	360	TYR	3.7
1	I	270	ILE	3.7
2	O	80	ASN	3.7
2	T	51	ASN	3.6
1	B	208	PRO	3.6
1	K	349	ILE	3.6
1	B	224	ASP	3.6
1	C	365	LEU	3.6
1	F	214	GLU	3.6
1	F	377	ALA	3.6
2	U	84	LEU	3.6
2	U	53	GLU	3.6
1	G	364	LYS	3.6
1	A	281	PHE	3.6
2	R	97	ALA	3.6
2	Q	80	ASN	3.6
1	E	334	ASP	3.6
1	F	203	TYR	3.6
1	C	279	PRO	3.6
2	O	51	ASN	3.6
1	N	350	ARG	3.6
2	U	2	ASN	3.6
1	E	371	LYS	3.5
1	E	256	GLY	3.5
2	U	67	PHE	3.5
2	P	21	SER	3.5
2	P	17	VAL	3.5
1	G	284	ARG	3.5
1	A	352	GLN	3.5
1	J	372	LEU	3.5
1	M	349	ILE	3.5
1	J	366	GLN	3.5
2	O	18	GLU	3.5
2	S	67	PHE	3.5
1	N	186	GLU	3.5
2	U	82	GLU	3.5
1	J	330	THR	3.5
1	J	223	ALA	3.5
1	E	368	ARG	3.5
2	P	30	SER	3.5
1	H	356	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	358	SER	3.4
1	J	268	ARG	3.4
1	F	323	VAL	3.4
1	J	267	MET	3.4
1	L	356	ALA	3.4
1	E	362	ARG	3.4
1	F	174	VAL	3.4
2	T	53	GLU	3.4
1	G	203	TYR	3.4
2	U	10	VAL	3.4
2	O	82	GLU	3.4
1	A	230	ILE	3.4
1	D	251	ALA	3.4
1	L	270	ILE	3.4
1	K	372	LEU	3.4
1	G	209	GLU	3.4
2	Q	26	VAL	3.4
1	B	203	TYR	3.4
1	A	193	MET	3.3
1	A	322	ARG	3.3
1	D	195	PHE	3.3
1	L	267	MET	3.3
1	E	270	ILE	3.3
1	E	332	ILE	3.3
1	G	376	VAL	3.3
2	T	83	VAL	3.3
1	F	283	ASP	3.3
1	K	185	ASP	3.3
1	D	362	ARG	3.3
2	T	27	LEU	3.3
1	G	229	ASN	3.3
1	F	356	ALA	3.3
2	U	93	ALA	3.3
1	F	230	ILE	3.2
2	T	67	PHE	3.2
2	R	22	ALA	3.2
2	R	82	GLU	3.2
1	A	358	SER	3.2
2	O	67	PHE	3.2
1	N	184	GLN	3.2
2	Q	82	GLU	3.2
1	L	352	GLN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	33	ALA	3.2
2	U	96	GLU	3.2
1	G	207	LYS	3.2
1	B	199	TYR	3.2
1	B	238	GLU	3.2
2	O	38	GLY	3.2
2	O	27	LEU	3.2
1	F	376	VAL	3.2
1	J	396	VAL	3.2
1	E	350	ARG	3.2
1	F	284	ARG	3.2
1	K	384	ALA	3.1
2	Q	13	LYS	3.1
2	Q	20	LYS	3.1
2	O	30	SER	3.1
1	D	355	GLU	3.1
2	P	52	GLY	3.1
2	P	80	ASN	3.1
2	S	71	TYR	3.1
1	G	371	LYS	3.1
2	P	84	LEU	3.1
1	E	196	ASP	3.1
1	A	271	VAL	3.1
1	K	352	GLN	3.1
2	U	36	THR	3.1
1	G	281	PHE	3.1
2	U	66	ILE	3.1
2	U	85	ILE	3.1
1	B	278	ALA	3.1
1	G	267	MET	3.1
1	A	376	VAL	3.1
1	F	213	VAL	3.1
1	G	271	VAL	3.1
2	S	74	LYS	3.1
2	U	92	LEU	3.1
1	D	309	LEU	3.1
1	F	281	PHE	3.1
1	G	321	LYS	3.1
1	G	332	ILE	3.1
1	B	367	GLU	3.1
2	U	29	GLY	3.1
1	D	203	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	170	GLY	3.1
1	B	200	LEU	3.0
1	G	172	GLU	3.0
1	G	211	GLY	3.0
2	Q	66	ILE	3.0
1	C	242	LYS	3.0
2	S	20	LYS	3.0
1	A	172	GLU	3.0
1	H	342	ILE	3.0
1	G	322	ARG	3.0
1	B	212	ALA	3.0
2	U	39	GLU	3.0
1	B	223	ALA	3.0
2	U	41	LEU	3.0
1	F	288	MET	3.0
1	B	44	PHE	3.0
1	J	193	MET	3.0
1	M	233	MET	3.0
1	B	347	ALA	3.0
1	F	209	GLU	3.0
1	B	267	MET	3.0
2	Q	65	VAL	3.0
2	U	12	VAL	3.0
1	F	358	SER	3.0
2	T	28	THR	3.0
1	A	209	GLU	3.0
1	I	267	MET	3.0
1	M	243	ALA	2.9
1	N	525	PRO	2.9
1	G	280	GLY	2.9
1	A	210	THR	2.9
1	C	214	GLU	2.9
1	F	351	GLN	2.9
1	M	186	GLU	2.9
1	E	44	PHE	2.9
1	M	372	LEU	2.9
2	U	81	GLU	2.9
2	O	37	ARG	2.9
1	G	309	LEU	2.9
2	R	72	GLY	2.9
1	H	186	GLU	2.9
1	K	268	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	223	ALA	2.9
1	D	314	LEU	2.9
2	R	52	GLY	2.9
2	O	26	VAL	2.9
2	R	73	VAL	2.9
2	S	73	VAL	2.9
1	A	279	PRO	2.9
1	F	338	GLU	2.9
1	M	208	PRO	2.9
1	B	362	ARG	2.9
2	U	13	LYS	2.9
1	D	352	GLN	2.9
2	U	68	ASN	2.9
1	B	214	GLU	2.9
1	K	44	PHE	2.9
1	L	271	VAL	2.9
1	N	369	VAL	2.9
2	Q	12	VAL	2.9
2	U	24	GLY	2.9
1	A	251	ALA	2.9
1	G	340	ALA	2.9
1	D	279	PRO	2.9
1	K	144	ILE	2.9
1	L	360	TYR	2.9
1	G	359	ASP	2.9
1	A	256	GLY	2.9
1	F	195	PHE	2.9
1	K	350	ARG	2.9
2	O	33	ALA	2.9
1	N	242	LYS	2.8
1	L	180	GLY	2.8
1	B	193	MET	2.8
1	L	215	LEU	2.8
1	L	354	GLU	2.8
1	M	176	THR	2.8
2	S	85	ILE	2.8
1	E	322	ARG	2.8
2	O	23	GLY	2.8
1	A	373	ALA	2.8
1	D	267	MET	2.8
1	H	44	PHE	2.8
1	E	336	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	345	ARG	2.8
1	N	165	ALA	2.8
1	C	172	GLU	2.8
1	E	172	GLU	2.8
2	S	13	LYS	2.8
1	D	192	GLY	2.8
1	M	361	ASP	2.8
2	U	76	GLU	2.8
2	U	70	GLY	2.8
2	U	34	LYS	2.8
1	G	346	VAL	2.8
1	C	203	TYR	2.8
1	E	203	TYR	2.8
1	N	267	MET	2.7
1	M	185	ASP	2.7
1	N	361	ASP	2.7
2	S	65	VAL	2.7
2	T	30	SER	2.7
1	F	373	ALA	2.7
1	A	195	PHE	2.7
1	E	303	GLU	2.7
1	F	44	PHE	2.7
2	U	3	ILE	2.7
1	E	331	THR	2.7
2	U	77	LYS	2.7
1	B	338	GLU	2.7
1	B	209	GLU	2.7
1	J	357	THR	2.7
1	K	193	MET	2.7
1	A	270	ILE	2.7
1	M	175	ILE	2.7
2	S	78	ILE	2.7
1	G	247	LEU	2.7
1	G	277	LYS	2.7
1	H	372	LEU	2.7
1	B	368	ARG	2.7
1	E	231	ARG	2.7
1	D	257	GLU	2.7
1	B	322	ARG	2.7
1	A	214	GLU	2.7
1	C	211	GLY	2.7
1	M	244	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	204	PHE	2.7
1	N	342	ILE	2.7
1	K	346	VAL	2.7
2	Q	49	LEU	2.7
1	C	278	ALA	2.7
2	Q	33	ALA	2.7
1	C	195	PHE	2.7
1	C	288	MET	2.7
1	F	333	ILE	2.7
1	K	294	THR	2.7
1	D	237	LEU	2.7
1	E	324	VAL	2.7
2	O	95	VAL	2.7
1	C	268	ARG	2.7
1	C	209	GLU	2.7
1	E	216	GLU	2.7
2	Q	73	VAL	2.7
2	S	69	ASP	2.7
1	L	364	LYS	2.7
1	K	368	ARG	2.7
1	B	230	ILE	2.6
1	N	238	GLU	2.6
1	G	215	LEU	2.6
1	J	352	GLN	2.6
1	L	221	LEU	2.6
1	B	382	GLY	2.6
1	I	44	PHE	2.6
1	D	214	GLU	2.6
1	L	305	ILE	2.6
1	A	356	ALA	2.6
2	Q	50	GLU	2.6
2	T	21	SER	2.6
2	O	19	THR	2.6
1	B	277	LYS	2.6
1	K	171	LYS	2.6
2	T	20	LYS	2.6
1	J	44	PHE	2.6
1	H	193	MET	2.6
1	F	322	ARG	2.6
1	K	381	VAL	2.6
1	D	208	PRO	2.6
1	F	304	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	368	ARG	2.6
1	H	368	ARG	2.6
1	B	237	LEU	2.6
2	S	84	LEU	2.6
1	E	286	LYS	2.6
1	A	229	ASN	2.6
1	B	320	ALA	2.6
1	B	340	ALA	2.6
1	G	347	ALA	2.6
2	R	66	ILE	2.6
2	P	72	GLY	2.6
2	S	41	LEU	2.6
2	O	71	TYR	2.6
1	M	138	CYS	2.6
1	G	320	ALA	2.6
1	F	386	GLU	2.6
1	L	156	GLU	2.6
2	P	2	ASN	2.6
2	P	93	ALA	2.6
1	C	364	LYS	2.6
1	D	364	LYS	2.6
1	I	349	ILE	2.6
2	U	86	MET	2.6
1	C	338	GLU	2.6
2	U	50	GLU	2.6
1	K	196	ASP	2.6
1	B	321	LYS	2.6
1	D	322	ARG	2.6
1	F	341	ALA	2.6
2	Q	55	LYS	2.6
2	O	78	ILE	2.5
1	J	381	VAL	2.5
2	T	73	VAL	2.5
1	J	183	LEU	2.5
1	B	327	LYS	2.5
1	A	346	VAL	2.5
1	D	376	VAL	2.5
1	H	268	ARG	2.5
1	C	347	ALA	2.5
1	M	44	PHE	2.5
1	F	319	GLN	2.5
1	G	171	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	362	ARG	2.5
1	N	189	VAL	2.5
2	Q	17	VAL	2.5
2	R	28	THR	2.5
2	U	73	VAL	2.5
1	B	283	ASP	2.5
1	K	291	ASP	2.5
2	Q	67	PHE	2.5
1	A	212	ALA	2.5
1	C	356	ALA	2.5
1	F	173	GLY	2.5
1	M	365	LEU	2.5
2	U	54	VAL	2.5
1	F	272	LYS	2.5
1	C	355	GLU	2.5
1	G	351	GLN	2.5
1	N	180	GLY	2.5
1	H	525	PRO	2.5
1	J	311	LYS	2.5
1	N	396	VAL	2.5
1	J	266	THR	2.5
1	K	270	ILE	2.5
1	B	171	LYS	2.5
1	N	365	LEU	2.5
1	C	138	CYS	2.5
1	G	355	GLU	2.5
1	A	223	ALA	2.5
1	B	331	THR	2.5
1	H	357	THR	2.5
1	K	373	ALA	2.5
2	Q	38	GLY	2.5
1	E	309	LEU	2.5
2	Q	84	LEU	2.5
1	A	362	ARG	2.5
1	E	285	ARG	2.5
1	M	161	LEU	2.5
2	U	4	ARG	2.4
1	K	158	VAL	2.4
2	R	26	VAL	2.4
1	B	309	LEU	2.4
1	J	233	MET	2.4
1	B	275	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	214	GLU	2.4
1	F	181	THR	2.4
2	T	76	GLU	2.4
1	C	208	PRO	2.4
1	A	324	VAL	2.4
1	D	358	SER	2.4
1	L	195	PHE	2.4
1	B	280	GLY	2.4
1	E	359	ASP	2.4
1	F	193	MET	2.4
1	G	334	ASP	2.4
1	K	379	ILE	2.4
2	U	74	LYS	2.4
1	B	358	SER	2.4
1	N	187	LEU	2.4
1	L	266	THR	2.4
2	O	65	VAL	2.4
1	K	297	GLY	2.4
1	L	269	GLY	2.4
2	R	16	GLU	2.4
1	G	223	ALA	2.4
1	E	372	LEU	2.4
2	Q	85	ILE	2.4
1	J	175	ILE	2.4
1	N	372	LEU	2.4
1	E	174	VAL	2.4
1	H	364	LYS	2.4
2	P	74	LYS	2.4
2	S	77	LYS	2.4
1	L	63	GLU	2.4
1	F	359	ASP	2.4
1	M	275	ALA	2.4
1	F	162	ILE	2.4
1	F	309	LEU	2.4
1	N	349	ILE	2.4
2	O	49	LEU	2.4
1	D	171	LYS	2.4
1	L	484	GLU	2.4
2	O	73	VAL	2.4
1	A	359	ASP	2.4
1	D	196	ASP	2.4
1	D	320	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	340	ALA	2.4
1	M	340	ALA	2.4
2	O	75	SER	2.4
2	T	31	ALA	2.4
1	A	250	ILE	2.4
1	G	270	ILE	2.4
1	K	494	LEU	2.4
1	D	256	GLY	2.3
1	L	263	VAL	2.3
2	R	71	TYR	2.3
1	F	138	CYS	2.3
1	L	313	THR	2.3
2	U	55	LYS	2.3
1	E	175	ILE	2.3
1	D	238	GLU	2.3
1	D	297	GLY	2.3
1	E	219	PHE	2.3
1	A	348	GLN	2.3
1	L	381	VAL	2.3
1	M	362	ARG	2.3
2	U	47	ARG	2.3
1	A	274	ALA	2.3
1	K	183	LEU	2.3
1	F	280	GLY	2.3
1	L	160	LYS	2.3
1	G	291	ASP	2.3
2	U	90	ASP	2.3
1	K	127	ALA	2.3
1	M	152	ALA	2.3
1	C	354	GLU	2.3
1	E	524	LEU	2.3
1	G	252	GLU	2.3
2	U	46	GLY	2.3
1	E	194	GLN	2.3
1	G	324	VAL	2.3
1	C	308	GLU	2.3
1	G	227	ILE	2.3
1	M	236	VAL	2.3
1	G	196	ASP	2.3
1	D	340	ALA	2.3
1	N	270	ILE	2.3
1	F	494	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	U	11	ILE	2.3
1	F	348	GLN	2.3
1	H	369	VAL	2.3
1	N	381	VAL	2.3
1	C	224	ASP	2.3
1	E	267	MET	2.3
2	Q	97	ALA	2.3
2	U	14	ARG	2.3
1	A	334	ASP	2.3
2	T	9	ARG	2.3
1	A	237	LEU	2.3
1	E	477	GLY	2.3
1	K	480	ALA	2.3
2	O	48	ILE	2.3
1	G	204	PHE	2.3
1	I	266	THR	2.2
2	Q	19	THR	2.2
1	F	215	LEU	2.2
1	L	127	ALA	2.2
1	L	369	VAL	2.2
1	D	245	LYS	2.2
1	H	283	ASP	2.2
1	A	248	LEU	2.2
1	J	289	LEU	2.2
1	A	267	MET	2.2
1	F	339	GLU	2.2
1	G	194	GLN	2.2
1	K	366	GLN	2.2
1	B	377	ALA	2.2
1	H	524	LEU	2.2
1	L	384	ALA	2.2
1	N	172	GLU	2.2
1	K	284	ARG	2.2
1	M	364	LYS	2.2
2	U	45	ASN	2.2
1	C	192	GLY	2.2
1	C	359	ASP	2.2
2	R	67	PHE	2.2
1	F	390	LYS	2.2
1	F	185	ASP	2.2
1	D	325	ILE	2.2
1	F	175	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	37	ARG	2.2
1	K	203	TYR	2.2
1	C	324	VAL	2.2
1	G	372	LEU	2.2
1	H	350	ARG	2.2
1	K	234	LEU	2.2
1	K	524	LEU	2.2
1	M	199	TYR	2.2
1	M	367	GLU	2.2
1	J	350	ARG	2.2
1	L	248	LEU	2.2
1	C	373	ALA	2.2
1	E	330	THR	2.2
2	S	75	SER	2.2
2	P	82	GLU	2.2
1	C	322	ARG	2.2
1	H	284	ARG	2.2
1	B	195	PHE	2.2
1	F	234	LEU	2.2
1	M	356	ALA	2.2
1	E	348	GLN	2.2
1	G	358	SER	2.2
1	E	192	GLY	2.1
1	D	200	LEU	2.1
1	E	301	ILE	2.1
1	K	175	ILE	2.1
1	N	384	ALA	2.1
2	T	50	GLU	2.1
1	D	213	VAL	2.1
1	E	375	GLY	2.1
1	N	431	GLY	2.1
1	L	494	LEU	2.1
1	D	371	LYS	2.1
1	G	175	ILE	2.1
1	G	326	ASN	2.1
1	L	325	ILE	2.1
1	A	273	VAL	2.1
1	B	381	VAL	2.1
1	I	263	VAL	2.1
1	L	378	VAL	2.1
1	B	281	PHE	2.1
1	A	347	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	238	GLU	2.1
1	D	275	ALA	2.1
1	F	220	ILE	2.1
1	G	348	GLN	2.1
1	J	184	GLN	2.1
1	L	373	ALA	2.1
1	M	431	GLY	2.1
1	J	313	THR	2.1
1	K	134	LEU	2.1
1	A	351	GLN	2.1
1	H	270	ILE	2.1
1	M	379	ILE	2.1
1	D	288	MET	2.1
1	C	346	VAL	2.1
1	C	372	LEU	2.1
1	A	249	ILE	2.1
1	E	356	ALA	2.1
1	L	175	ILE	2.1
2	P	66	ILE	2.1
1	B	217	SER	2.1
1	F	308	GLU	2.1
1	L	261	THR	2.1
1	E	212	ALA	2.1
2	O	64	ILE	2.1
2	T	66	ILE	2.1
2	U	42	ALA	2.1
1	F	229	ASN	2.1
1	B	324	VAL	2.1
1	N	271	VAL	2.1
2	S	86	MET	2.1
1	E	204	PHE	2.1
1	E	237	LEU	2.1
1	J	242	LYS	2.1
1	D	356	ALA	2.1
1	A	354	GLU	2.1
1	L	172	GLU	2.1
1	N	177	VAL	2.1
1	A	314	LEU	2.1
1	L	365	LEU	2.1
1	K	138	CYS	2.1
1	F	379	ILE	2.1
1	L	176	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	285	ARG	2.1
1	M	240	VAL	2.1
1	A	262	LEU	2.0
1	C	228	SER	2.0
1	H	343	GLN	2.0
1	K	200	LEU	2.0
1	B	268	ARG	2.0
1	C	250	ILE	2.0
1	F	223	ALA	2.0
1	G	275	ALA	2.0
1	J	243	ALA	2.0
1	F	371	LYS	2.0
1	M	238	GLU	2.0
2	Q	83	VAL	2.0
1	I	343	GLN	2.0
2	U	37	ARG	2.0
2	Q	22	ALA	2.0
2	U	64	ILE	2.0
1	K	388	GLU	2.0
1	D	525	PRO	2.0
1	C	215	LEU	2.0
1	J	222	LEU	2.0
1	L	265	ASN	2.0
1	N	259	LEU	2.0
2	P	79	ASP	2.0
2	Q	74	LYS	2.0
2	U	94	ILE	2.0
1	K	172	GLU	2.0
1	K	357	THR	2.0
1	D	271	VAL	2.0
1	F	324	VAL	2.0
1	A	234	LEU	2.0
1	E	222	LEU	2.0
2	O	84	LEU	2.0
2	S	37	ARG	2.0
1	M	168	LYS	2.0
1	J	270	ILE	2.0
1	L	144	ILE	2.0
1	N	353	ILE	2.0
2	Q	75	SER	2.0
1	M	521	VAL	2.0
1	D	215	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	200	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ADP	A	700	27/27	0.92	0.18	-0.05	6,8,9,11	0
4	ADP	B	701	27/27	0.90	0.20	-0.19	6,8,9,10	0
4	ADP	F	705	27/27	0.91	0.21	-0.36	6,8,9,10	0
4	ADP	E	704	27/27	0.89	0.19	-0.62	6,8,9,10	0
4	ADP	D	703	27/27	0.93	0.17	-0.81	6,8,9,10	0
4	ADP	G	706	27/27	0.94	0.15	-1.19	6,8,9,10	0
4	ADP	C	702	27/27	0.95	0.13	-2.34	6,8,9,10	0
3	MG	D	604	1/1	0.97	0.32	-	2,2,2,2	0
3	MG	G	607	1/1	0.98	0.20	-	2,2,2,2	0
3	MG	F	606	1/1	0.96	0.27	-	2,2,2,2	0
3	MG	C	603	1/1	0.95	0.18	-	2,2,2,2	0
3	MG	E	605	1/1	0.97	0.18	-	2,2,2,2	0
3	MG	A	601	1/1	0.96	0.28	-	2,2,2,2	0
3	MG	B	602	1/1	0.94	0.21	-	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.