Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM 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:

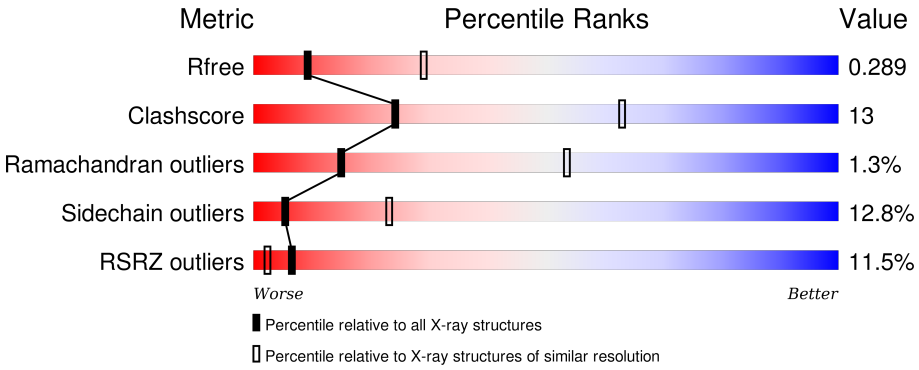
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.99 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	12% 71% 25%
1	B	524	11% 71% 24% 5%
1	C	524	10% 69% 27%
1	D	524	10% 69% 26%
1	E	524	13% 69% 26%

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Mol	Chain	Length	Quality of chain
1	F	524	14% 71% 24%
1	G	524	13% 69% 26% 5%
1	H	524	4% 63% 33%
1	I	524	2% 63% 31% 5%
1	J	524	6% 63% 33%
1	K	524	9% 63% 32% 5%
1	L	524	9% 62% 33% 5%
1	M	524	7% 62% 34%
1	N	524	7% 64% 32%
2	O	97	37% 64% 29% 7%
2	P	97	30% 64% 27% 9%
2	Q	97	33% 66% 27% 7%
2	R	97	26% 63% 29% 8%
2	S	97	30% 65% 28% 7%
2	T	97	29% 66% 26% 7%
2	U	97	76% 63% 30% 7%

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			

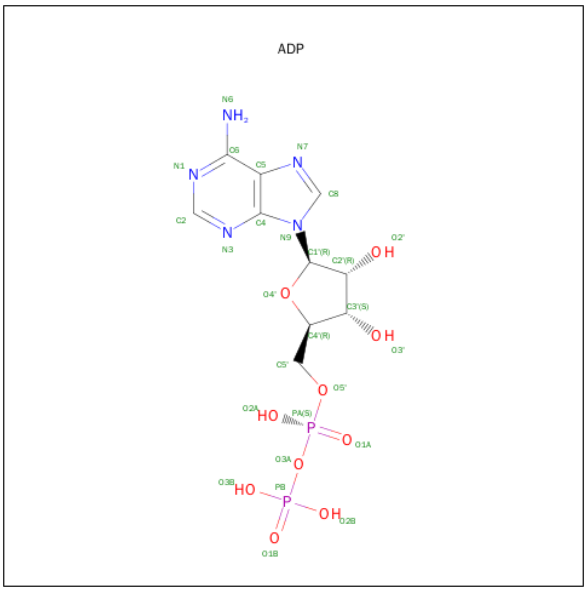
- Molecule 2 is a protein called groES protein.

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: $C_{10}H_{15}N_5O_{10}P_2$).



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		

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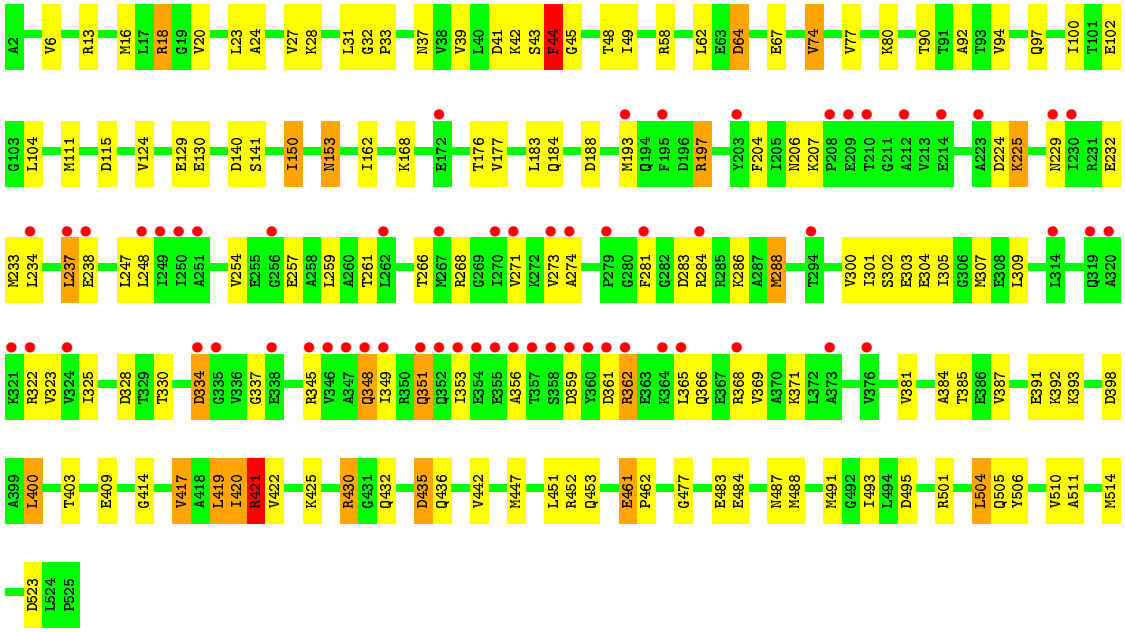
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total O 1 1	0	0
5	G	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

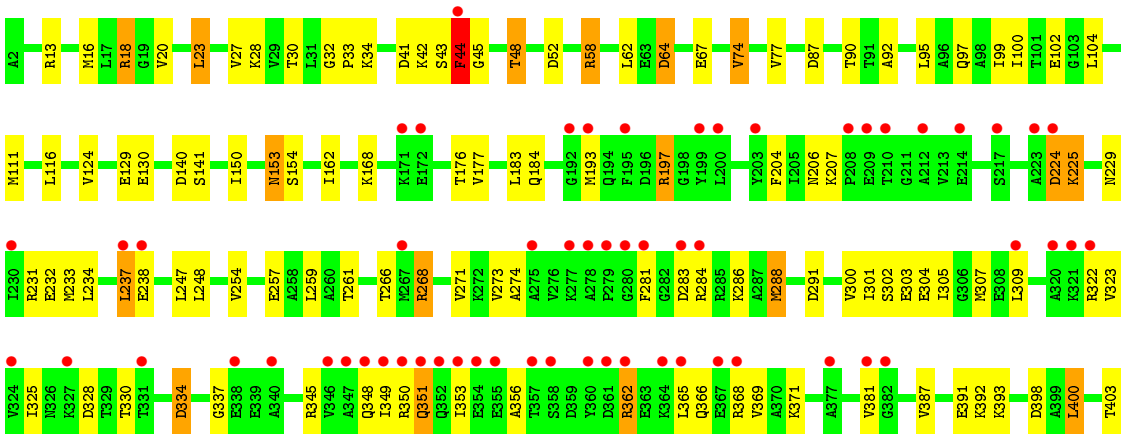
- Molecule 1: groEL protein

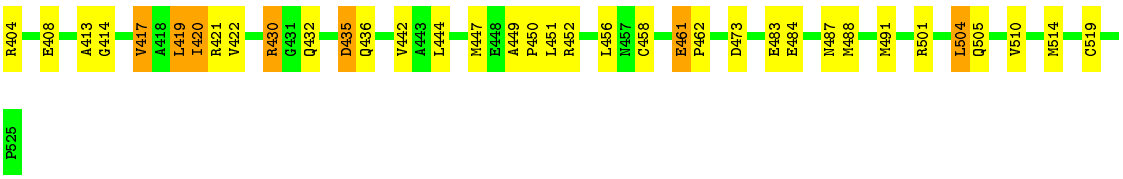
Chain A:



- Molecule 1: groEL protein

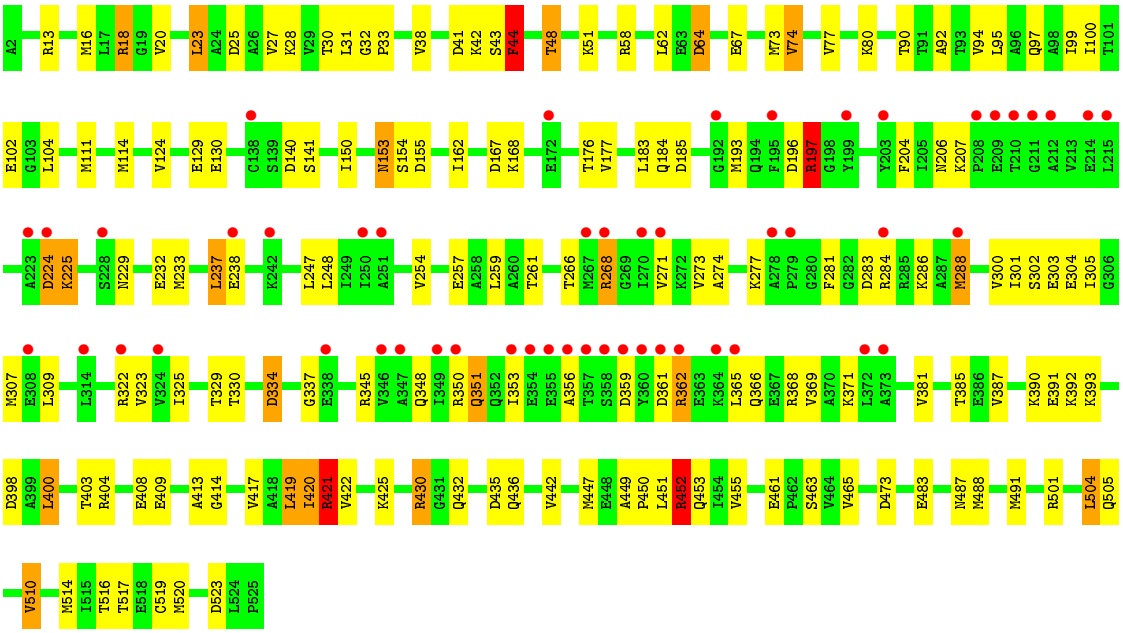
Chain B:





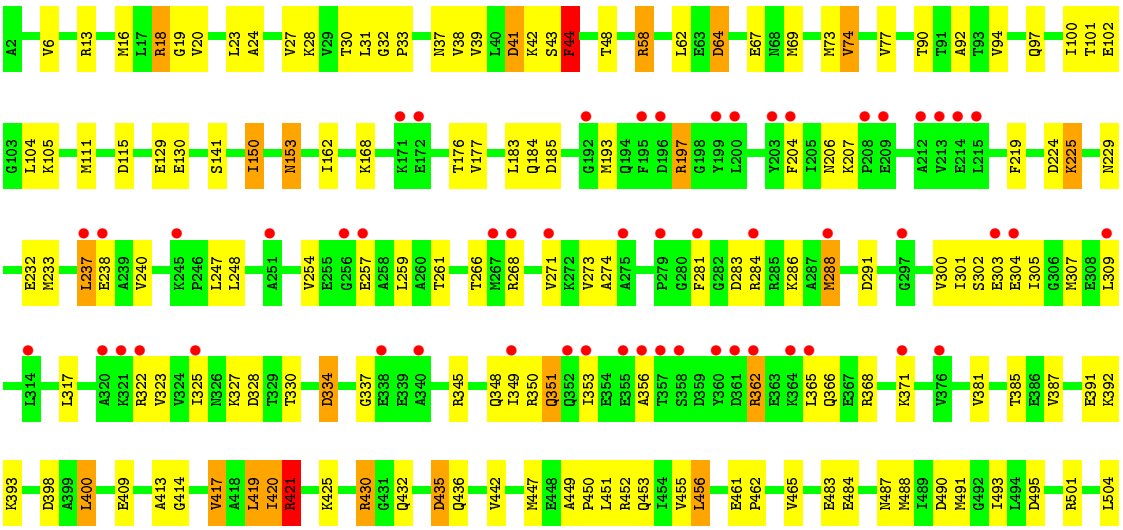
• Molecule 1: groEL protein

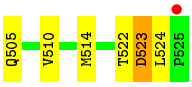
Chain C:



• Molecule 1: groEL protein

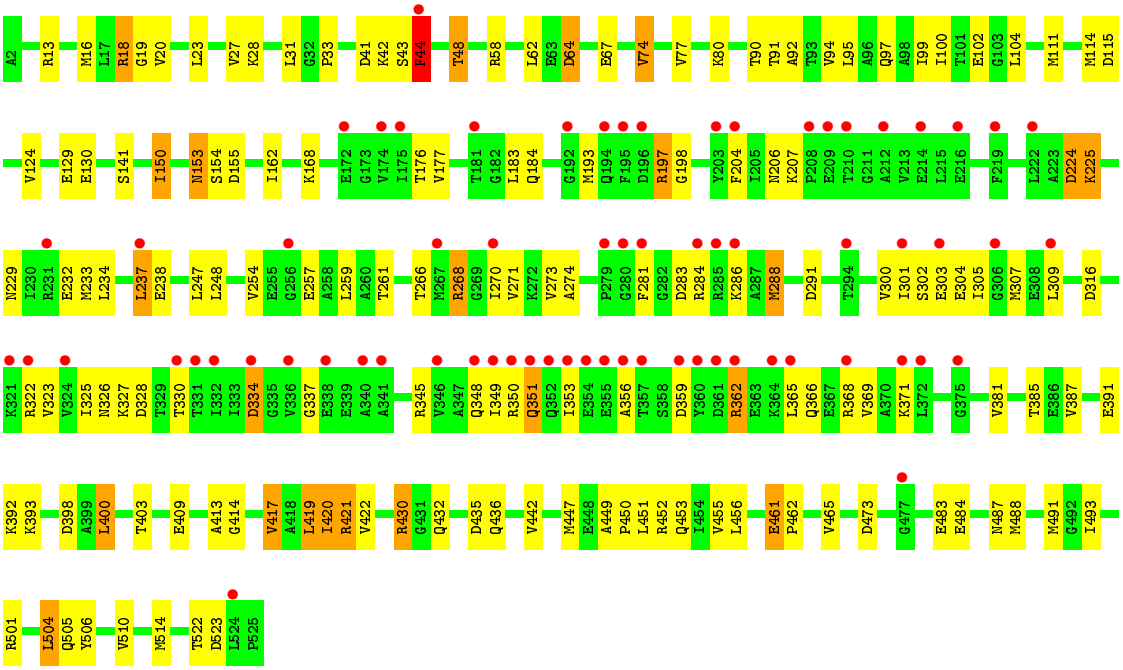
Chain D:





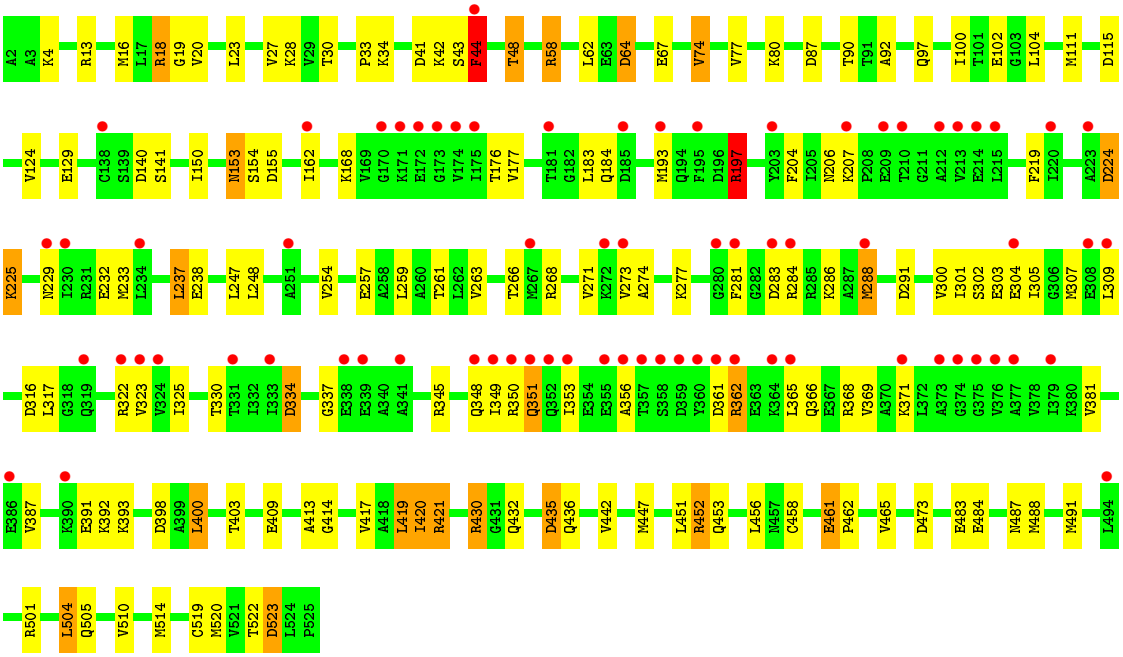
• Molecule 1: groEL protein

Chain E:



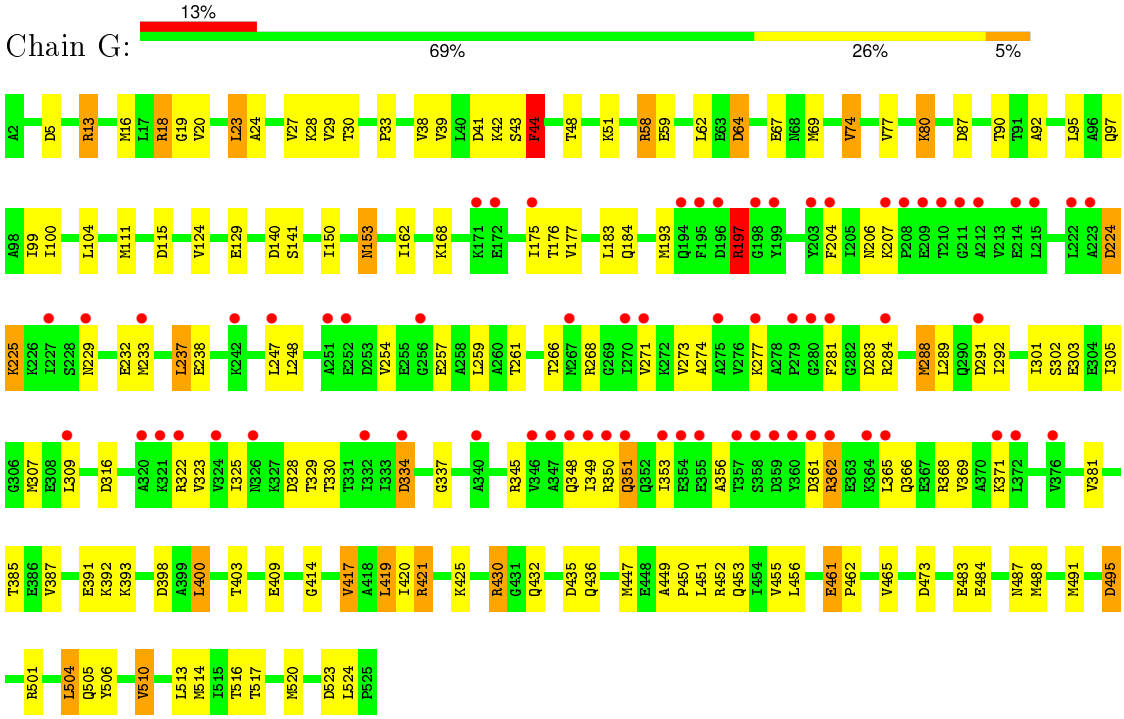
• Molecule 1: groEL protein

Chain F:



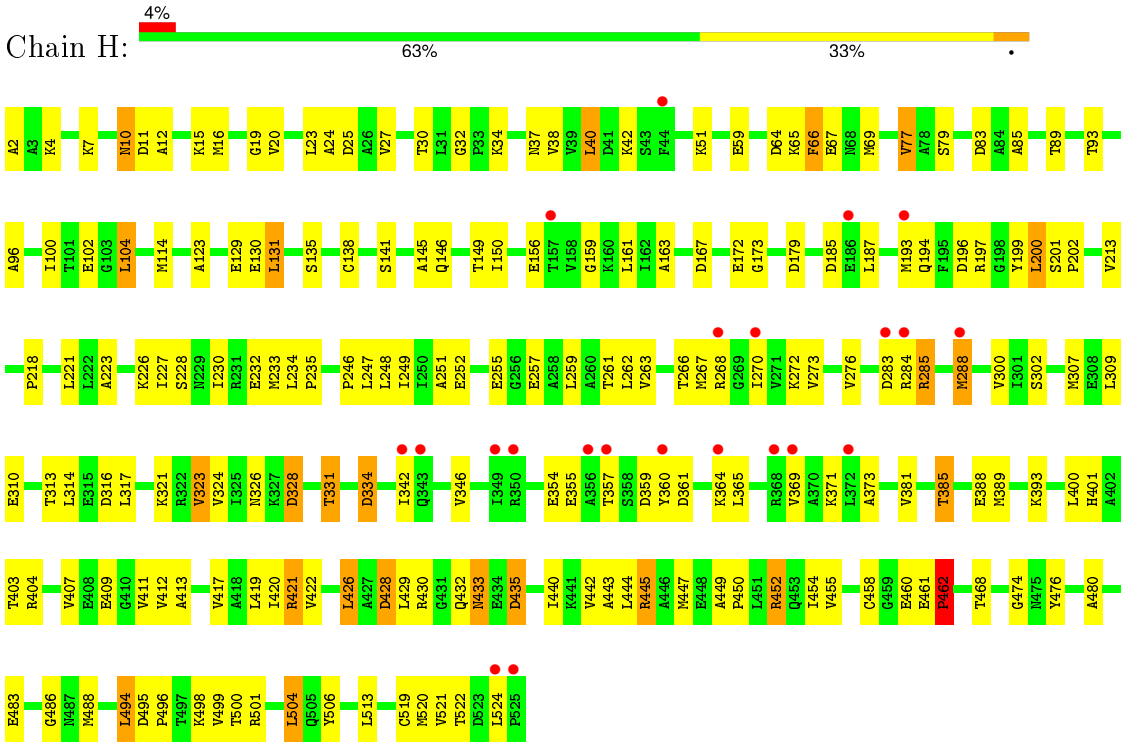
• Molecule 1: groEL protein

Chain G:



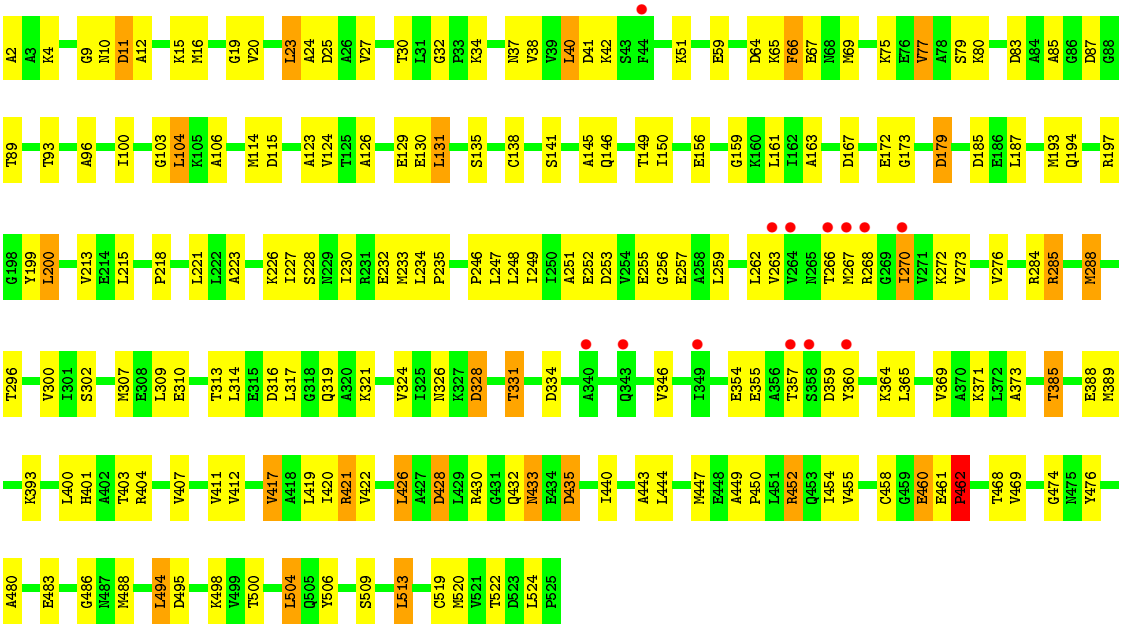
• Molecule 1: groEL protein

Chain H:



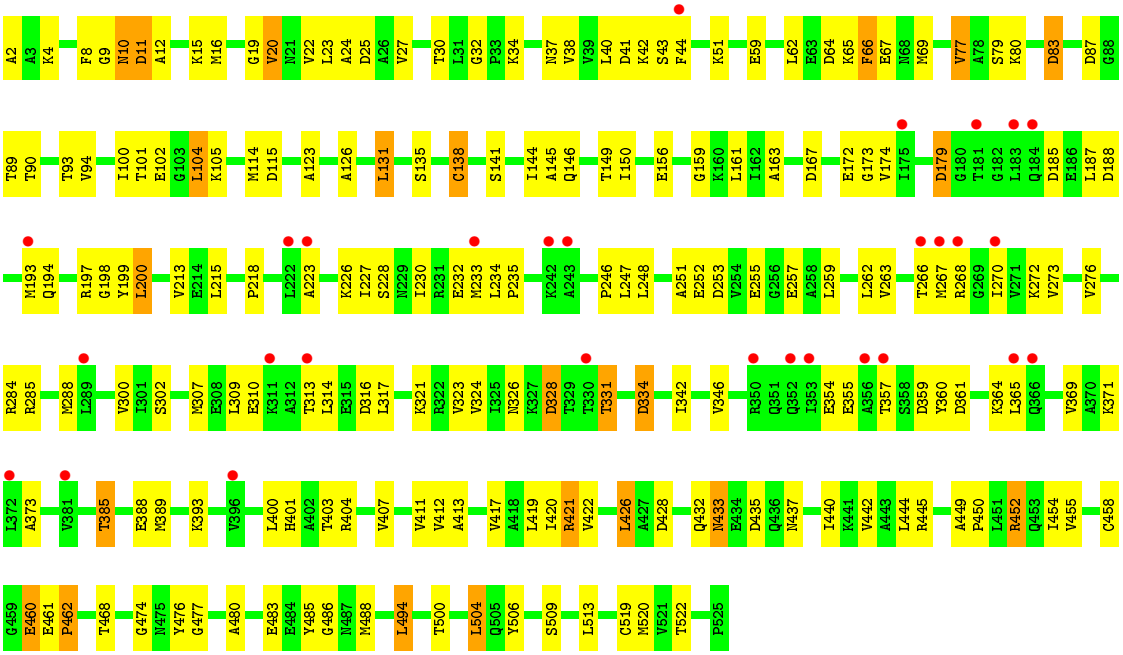
• Molecule 1: groEL protein

Chain I:



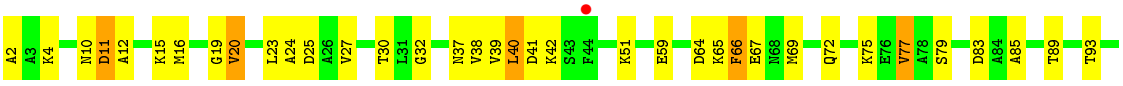
• Molecule 1: groEL protein

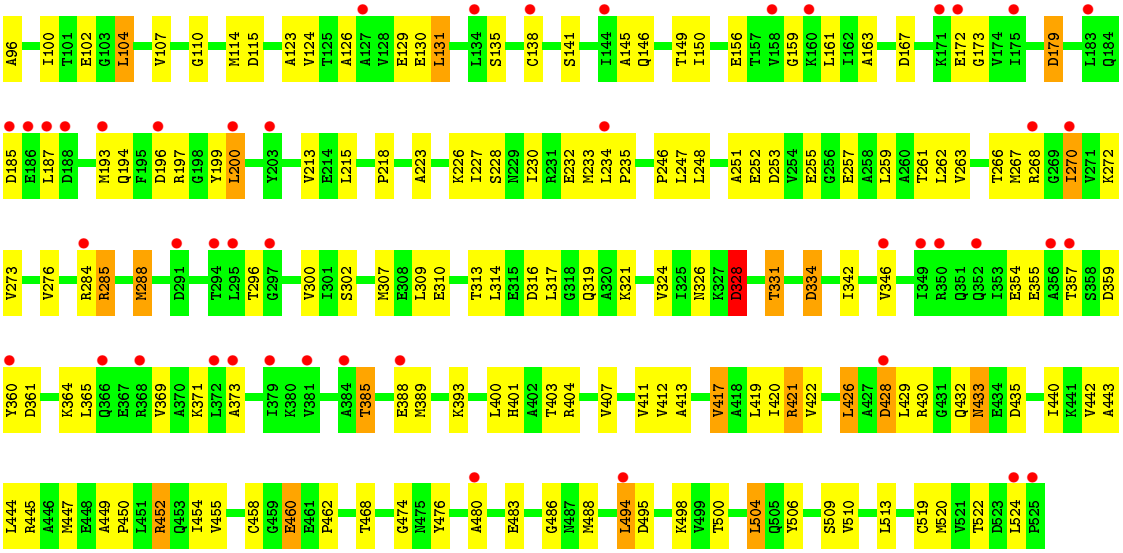
Chain J:



• Molecule 1: groEL protein

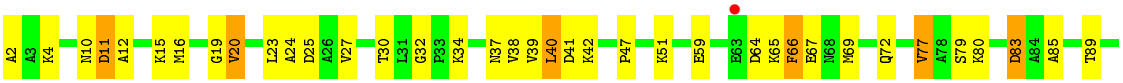
Chain K:

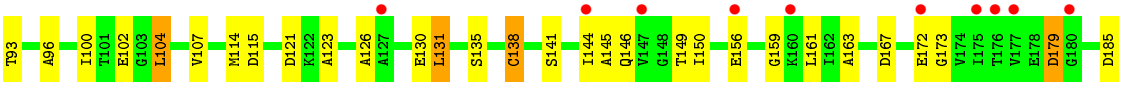


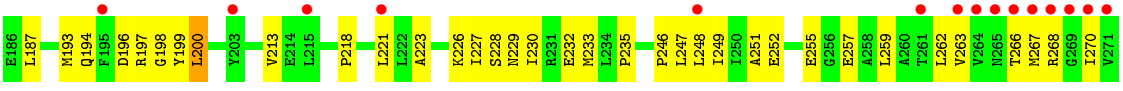


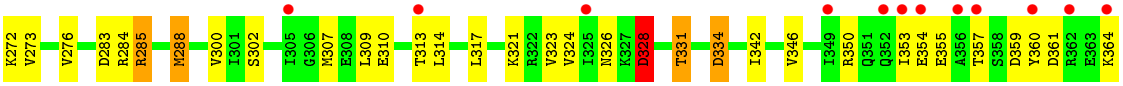
• Molecule 1: groEL protein

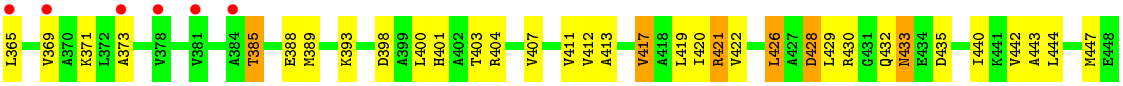
Chain L:

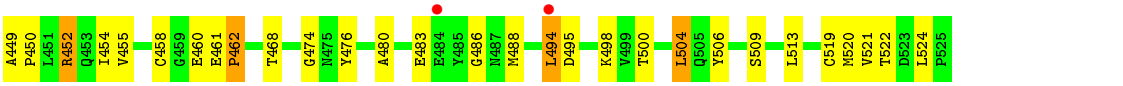






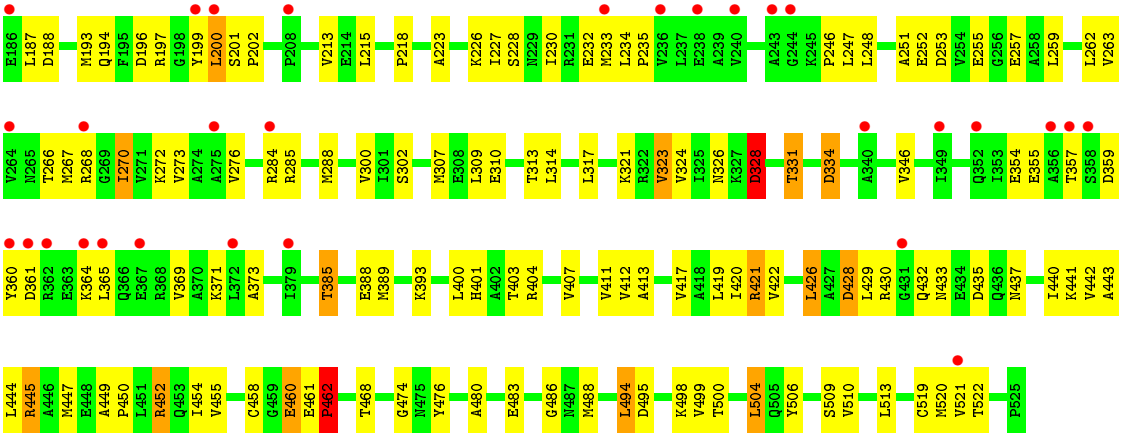






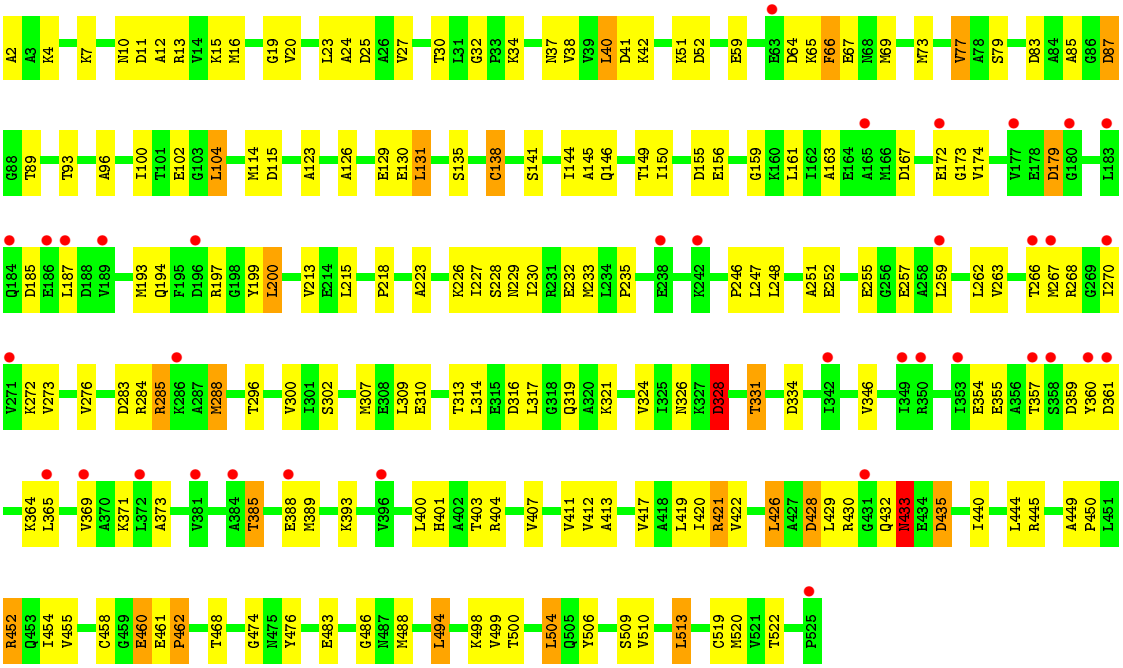
• Molecule 1: groEL protein

Chain M:



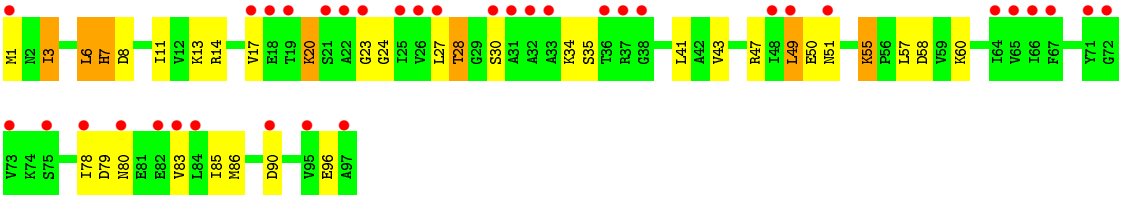
• Molecule 1: groEL protein

Chain N:



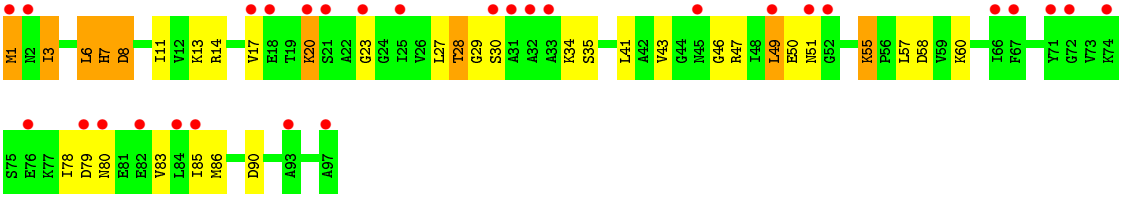
• Molecule 2: groES protein

Chain O:



• Molecule 2: groES protein

Chain P:

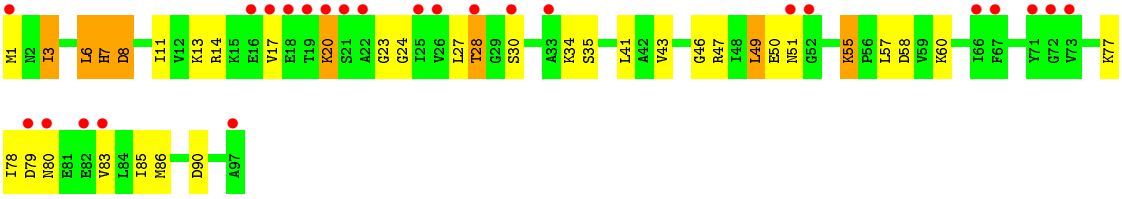


• Molecule 2: groES protein

Chain Q:

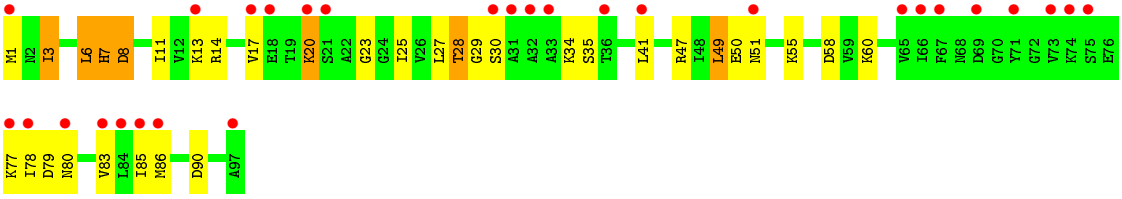
• Molecule 2: groES protein

Chain R:



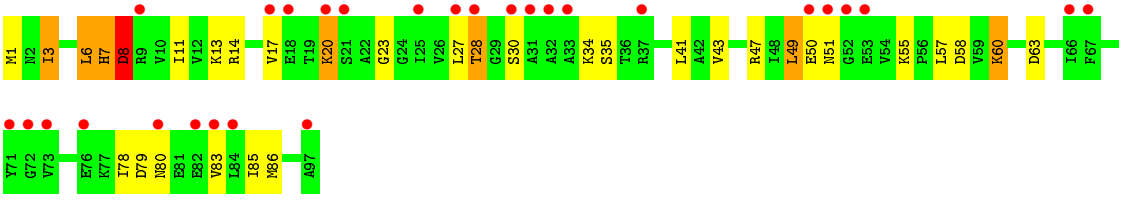
• Molecule 2: groES protein

Chain S:



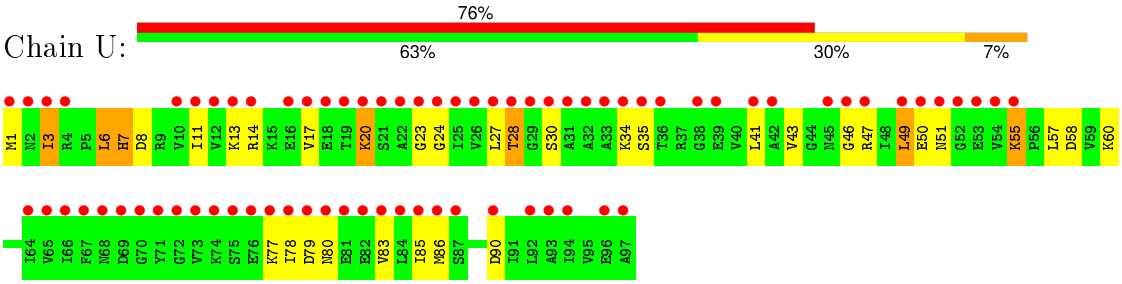
• Molecule 2: groES protein

Chain T:



• Molecule 2: groES protein

Chain U:


76%
63%
30%
7%
M1 N2 I3 R4 P5 L6 H7 D8 R9 V10 I11 V12 K13 R14 K15 E16 V17 E18 T19 K20 S21 A22 G23 G24 I25 V26 L27 T28 G29 S30 A31 A32 A33 K34 S35 T36 R37 G38 E39 V40 L41 A42 V43 G44 N45 G46 R47 I48 L49 E50 N51 G52 E53 V54 K55 P56 L57 D58 V59 K60
I64 V65 I66 F67 N68 D69 G70 Y71 G72 V73 K74 S75 E76 K77 I78 D79 N80 E81 E82 V83 L84 I85 N86 S87 D90 I91 L92 A93 I94 V95 E96 A97

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 58.3	EDS
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 242645 reflections	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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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:F:414:GLY:O	1:F:417:VAL:HG12	1.59	1.02
1:D:414:GLY:O	1:D:417:VAL:HG12	1.58	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:F:18:ARG:NH1	1:F:18:ARG:HG2	1.76	0.95
1:B:204:PHE:HE2	1:B:266:THR:HG21	1.32	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

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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:HH11	1:E:18:ARG:CG	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:G:18:ARG:NH1	1:G:18:ARG:HG2	1.81	0.91
1:E:432:GLN:HE21	1:E:436:GLN:HE22	0.96	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:H:65:LYS:O	1:H:66:PHE:HB2	1.66	0.91
1:A:44:PHE:H	1:A:44:PHE:HD1	1.07	0.91
1:L:69:MET:HE1	1:L:522:THR:HB	1.52	0.90
1:J:426:LEU:HD12	1:J:444:LEU:HD21	1.53	0.90
1:G:432:GLN:HE21	1:G:436:GLN:NE2	1.70	0.90
1:C:18:ARG:NH1	1:C:18:ARG:HG2	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:M:426:LEU:HD12	1:M:444:LEU:HD21	1.54	0.89
1:B:44:PHE:HD1	1:B:44:PHE:H	1.00	0.89
1:G:44:PHE:H	1:G:44:PHE:HD1	1.08	0.88
1:B:432:GLN:HE21	1:B:436:GLN:NE2	1.70	0.88
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.36	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:HG2	1:G:430:ARG:HH11	1.40	0.85
1:A:432:GLN:HE21	1:A:436:GLN:HE22	0.86	0.85

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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:H:69:MET:HE1	1:H:522:THR:HB	1.58	0.84
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.43	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:N	1:F:44:PHE:CD1	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:D:18:ARG:HG2	1:D:18:ARG:NH1	1.91	0.78
1:B:44:PHE:CD1	1:B:44:PHE:N	2.46	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: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:E:13:ARG:HD2	1:E:104:LEU:HD22	1.66	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:D:432:GLN:HE21	1:D:436:GLN:HE22	0.79	0.77
1:C:74:VAL:O	1:C:77:VAL:HG13	1.85	0.77
1:A:409:GLU:OE2	1:A:501:ARG:NH2	2.17	0.77
1:M:421:ARG:HD2	1:M:474:GLY:O	1.85	0.76
1:M:131:LEU:HD13	1:M:422:VAL:HG11	1.66	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.71	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:M:419:LEU:CD2	1:M:500:THR:HG23	2.20	0.72
1:J:232:GLU:HB3	1:J:309:LEU:HB2	1.70	0.72
1:N:421:ARG:HD2	1:N:474:GLY:O	1.89	0.72
1:H:421:ARG:HD2	1:H:474:GLY:O	1.89	0.72
1:H:100:ILE:O	1:H:104:LEU:HB2	1.90	0.72
1:N:100:ILE:O	1:N:104:LEU:HB2	1.90	0.72
1:K:149:THR:HG23	1:K:159:GLY:HA3	1.70	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:J:100:ILE:O	1:J:104:LEU:HB2	1.90	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:D:409:GLU:OE2	1:D:501:ARG:NH2	2.22	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:L:227:ILE:HD12	1:L:309:LEU:HD11	1.73	0.71
1:K:32:GLY:HA2	1:K:454:ILE:HD13	1.71	0.71
1:N:227:ILE:HD12	1:N:309:LEU:HD11	1.72	0.71
1:I:227:ILE:HD12	1:I:309:LEU:HD11	1.72	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: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: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:K:69:MET:CE	1:K:522:THR:HB	2.21	0.70
1:H:419:LEU:CD2	1:H:500:THR:CG2	2.69	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

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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:M:419:LEU:CD2	1:M:500:THR:CG2	2.69	0.69
1:H:27:VAL:HG11	1:H:93:THR:HG21	1.73	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:I:419:LEU:CD2	1:I:500:THR:HG23	2.23	0.69
1:F:33:PRO:HA	1:F:153:ASN:HD21	1.57	0.69
1:M:404:ARG:NH1	1:M:404:ARG:HG2	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:M:173:GLY:O	1:M:404:ARG:NH2	2.25	0.68
1:K:200:LEU:HD12	1:K:276:VAL:HA	1.74	0.68
1:M:32:GLY:HA2	1:M:454:ILE:HD13	1.75	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: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:K:65:LYS:O	1:K:66:PHE:CB	2.38	0.67
1:J:131:LEU:CD1	1:J:422:VAL:HG11	2.25	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:I:65:LYS:O	1:I:66:PHE:CB	2.40	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: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

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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:L:194:GLN:HB2	1:L:331:THR:HB	1.77	0.66
1:F:13:ARG:HD2	1:F:104:LEU:HD22	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:G:100:ILE:HD11	1:G:514:MET:HE1	1.78	0.66
1:L:419:LEU:CD2	1:L:500:THR:CG2	2.74	0.66
1:A:13:ARG:HD2	1:A:104:LEU:HD22	1.78	0.66
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.59	0.66
1:I:452:ARG:HH11	1:I:452:ARG:HG2	1.60	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:I:194:GLN:HB2	1:I:331:THR:HB	1.78	0.65
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.78	0.65
1:N:32:GLY:HA2	1:N:454:ILE:HD13	1.77	0.65
1:M:452:ARG:HG2	1:M:452:ARG:HH11	1.59	0.65
2:U:7:HIS:O	2:U:8:ASP:HB3	1.97	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
4:B:701:ADP:O3B	5:B:801:HOH:O	2.13	0.65
2:S:7:HIS:O	2:S:8:ASP:HB3	1.95	0.65
1:I:32:GLY:HA2	1:I:454:ILE:HD13	1.77	0.65
1:L:27:VAL:HG11	1:L:93:THR:HG21	1.78	0.65
1:H:65:LYS:O	1:H:66:PHE:CB	2.37	0.65
1:A:39:VAL:HG23	1:G:517:THR:HG23	1.78	0.65
1:M:385:THR:HG23	1:M:388:GLU:HB2	1.79	0.64
1:F:44:PHE:N	1:F:44:PHE:HD1	1.87	0.64
1:M:65:LYS:O	1:M:66:PHE:CB	2.34	0.64
1:C:430:ARG:NH1	1:C:430:ARG:HG2	2.10	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:L:131:LEU:CD1	1:L:422:VAL:HG11	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:MET:HG2	1:G:368:ARG:HD2	1.79	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: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:H:194:GLN:HB2	1:H:331:THR:HB	1.81	0.63
1:J:65:LYS:O	1:J:66:PHE:CB	2.40	0.63
1:I:30:THR:HB	1:I:51:LYS:O	1.99	0.63
1:H:96:ALA:O	1:H:100:ILE:HG13	1.98	0.62
1:D:18:ARG:CB	1:D:18:ARG:HH11	2.11	0.62
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.79	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:L:173:GLY:O	1:L:404:ARG:NH2	2.32	0.62
1:J:194:GLN:HB2	1:J:331:THR:HB	1.82	0.62
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.82	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
1:B:111:MET:HG2	1:B:435:ASP:OD1	1.99	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
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
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

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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:N:173:GLY:O	1:N:404:ARG:NH2	2.33	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:J:426:LEU:CD1	1:J:444:LEU:HD21	2.30	0.61
1:I:2:ALA:O	1:I:4:LYS:HE3	1.99	0.61
1:A:414:GLY:O	1:A:417:VAL:CG1	2.40	0.61
2:S:20:LYS:HB3	2:S:27:LEU:HG	1.83	0.61
2:P:20:LYS:HB3	2:P:27:LEU:HG	1.83	0.61
1:N:131:LEU:HD13	1:N:422:VAL:HG11	1.82	0.61
1:L:426:LEU:CD1	1:L:444:LEU:HD21	2.27	0.61
1:K:199:TYR:HA	1:K:276:VAL:HG12	1.83	0.61
1:F:409:GLU:OE2	1:F:501:ARG:NH2	2.31	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:K:419:LEU:HD21	1:K:500:THR:HG23	1.82	0.60
1:F:419:LEU:HG	1:F:447:MET:HG2	1.82	0.60
1:B:419:LEU:HG	1:B:447:MET:HG2	1.83	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: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:J:449:ALA:HB3	1:J:450:PRO:HD3	1.83	0.60
1:N:385:THR:HG23	1:N:388:GLU:HB2	1.83	0.60
1:G:33:PRO:HA	1:G:153:ASN:ND2	2.17	0.60
1:F:193:MET:HG3	1:F:371:LYS:HB3	1.84	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:L:404:ARG:HG2	1:L:404:ARG:NH1	2.11	0.60
1:G:302:SER:H	1:G:307:MET:HE3	1.66	0.60
1:L:24:ALA:HA	1:L:27:VAL:HG12	1.84	0.59
1:B:510:VAL:HG12	1:C:385:THR:HG21	1.84	0.59
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:325:ILE:HG12	1:F:330:THR:HG23	1.83	0.59
1:L:149:THR:CG2	1:L:159:GLY:HA3	2.32	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:G:325:ILE:HG12	1:G:330:THR:HG23	1.84	0.59
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.83	0.59
1:M:426:LEU:CD1	1:M:444:LEU:HD21	2.30	0.59
1:M:149:THR:CG2	1:M:159:GLY:HA3	2.31	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:C:520:MET:HG2	1:D:39:VAL:HB	1.84	0.58
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: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:I:411:VAL:HG21	1:I:494:LEU:HD12	1.86	0.58
1:A:325:ILE:HG12	1:A:330:THR:HG23	1.85	0.58
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.85	0.58
1:A:419:LEU:HG	1:A:447:MET:HG2	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: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:B:325:ILE:HG12	1:B:330:THR:HG23	1.86	0.58
1:L:64:ASP:HB3	1:L:67:GLU:HB2	1.85	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: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:L:39:VAL:HB	1:M:520:MET:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:426:LEU:CD1	1:N:444:LEU:HD21	2.31	0.57
1:D:325:ILE:HG12	1:D:330:THR:HG23	1.85	0.57
1:L:313:THR:HG22	1:L:314:LEU:H	1.69	0.57
1:J:199:TYR:HA	1:J:276:VAL:HG12	1.87	0.57
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.87	0.57
1:L:146:GLN:HE21	1:L:150:ILE:HD11	1.69	0.57
1:C:20:VAL:HG13	1:C:74:VAL:HG11	1.86	0.57
1:N:404:ARG:NH1	1:N:404:ARG:HG2	2.20	0.57
1:A:39:VAL:HB	1:G:520:MET:HG2	1.86	0.57
2:P:3:ILE:HD13	2:P:11:ILE:HG21	1.87	0.57
1:A:37:ASN:ND2	1:G:516:THR:OG1	2.31	0.57
1:A:33:PRO:HA	1:A:153:ASN:HD21	1.70	0.57
1:M:270:ILE:HA	1:N:257:GLU:OE2	2.04	0.57
1:B:193:MET:HG3	1:B:371:LYS:HB3	1.87	0.57
1:J:24:ALA:HA	1:J:27:VAL:HG12	1.86	0.57
1:E:419:LEU:HG	1:E:447:MET:HG2	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:K:426:LEU:CD1	1:K:444:LEU:HD21	2.33	0.57
1:K:385:THR:HG23	1:K:388:GLU:HB2	1.86	0.57
1:N:223:ALA:HB3	1:N:251:ALA:HB2	1.87	0.57
1:H:223:ALA:HB3	1:H:251:ALA:HB2	1.87	0.57
1:L:19:GLY:HA3	1:L:67:GLU:O	2.04	0.56
1:G:111:MET:HG2	1:G:435:ASP:OD1	2.05	0.56
1:H:16:MET:HG3	1:H:520:MET:SD	2.44	0.56
1:F:18:ARG:NH1	1:F:18:ARG:CG	2.45	0.56
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.15	0.56
1:J:145:ALA:O	1:J:149:THR:HG23	2.05	0.56
1:I:419:LEU:HD21	1:I:500:THR:HG23	1.87	0.56
1:G:419:LEU:HG	1:G:447:MET:HG2	1.88	0.56
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.87	0.56
1:J:313:THR:HG22	1:J:314:LEU:H	1.69	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:D:288:MET:HG2	1:D:368:ARG:HD2	1.86	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:N:19:GLY:HA3	1:N:67:GLU:O	2.05	0.56
1:E:430:ARG:NH1	1:E:430:ARG:HG2	2.13	0.56
1:K:96:ALA:O	1:K:100:ILE:HG13	2.05	0.56

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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:F:33:PRO:HA	1:F:153:ASN:ND2	2.21	0.56
1:F:64:ASP:HB3	1:F:67:GLU:HB2	1.88	0.56
1:L:199:TYR:HA	1:L:276:VAL:HG12	1.87	0.56
1:J:385:THR:HG23	1:J:388:GLU:HB2	1.86	0.56
1:H:313:THR:HG22	1:H:314:LEU:H	1.70	0.56
1:H:426:LEU:CD1	1:H:444:LEU:HD21	2.34	0.56
1:C:268:ARG:HD2	2:Q:27:LEU:CD2	2.34	0.56
1:N:146:GLN:HE21	1:N:150:ILE:HD11	1.69	0.56
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.87	0.56
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.86	0.56
1:J:123:ALA:HB2	1:J:440:ILE:HG23	1.88	0.56
1:M:69:MET:HE2	1:M:522:THR:HB	1.88	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:H:404:ARG:HG2	1:H:404:ARG:NH1	2.20	0.56
1:M:199:TYR:HA	1:M:276:VAL:HG12	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:A:111:MET:HG2	1:A:435:ASP:OD1	2.05	0.56
2:T:3:ILE:HD13	2:T:11:ILE:HG21	1.87	0.56
1:C:419:LEU:HG	1:C:447:MET:HG2	1.86	0.56
1:M:47:PRO:HG2	1:N:73:MET:HG3	1.88	0.56
1:H:199:TYR:HA	1:H:276:VAL:HG12	1.87	0.56
1:M:90:THR:O	1:M:94:VAL:HG23	2.05	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: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
2:O:3:ILE:HD13	2:O:11:ILE:HG21	1.88	0.55
1:K:2:ALA:O	1:K:4:LYS:HE3	2.05	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: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:H:146:GLN:HE21	1:H:150:ILE:HD11	1.70	0.55
1:M:413:ALA:HB1	1:M:417:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:VAL:HG13	1:F:504:LEU:HD13	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:N:77:VAL:HG22	1:N:506:TYR:HD1	1.71	0.55
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.88	0.55
1:F:74:VAL:HG13	1:F:514:MET:HE3	1.88	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:I:426:LEU:CD1	1:I:444:LEU:HD21	2.31	0.55
1:M:346:VAL:HG21	1:M:373:ALA:HB2	1.89	0.55
1:K:313:THR:HG22	1:K:314:LEU:H	1.72	0.55
1:G:238:GLU:HA	1:G:238:GLU:OE2	2.07	0.55
1:N:452:ARG:NH1	1:N:452:ARG:HG2	2.22	0.55
1:N:419:LEU:HD21	1:N:500:THR:HG23	1.89	0.55
1:D:409:GLU:CD	1:D:501:ARG:HH21	2.07	0.55
1:N:149:THR:CG2	1:N:159:GLY:HA3	2.36	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:A:238:GLU:OE2	1:A:238:GLU:HA	2.07	0.55
1:H:24:ALA:HA	1:H:27:VAL:HG12	1.88	0.54
2:R:13:LYS:HB3	2:R:41:LEU:HD11	1.89	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
1:E:64:ASP:HB3	1:E:67:GLU:HB2	1.90	0.54
1:M:419:LEU:HD21	1:M:500:THR:HG23	1.89	0.54
1:I:27:VAL:HG11	1:I:93:THR:HG21	1.88	0.54
1:D:487:ASN:O	1:D:491:MET:HG3	2.08	0.54
2:Q:3:ILE:HD13	2:Q:11:ILE:HG21	1.88	0.54
1:C:238:GLU:HA	1:C:238:GLU:OE2	2.07	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: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:N:419:LEU:HD11	1:N:504:LEU:HG	1.89	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:510:VAL:HG23	1:D:514:MET:CE	2.38	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:H:449:ALA:HB3	1:H:450:PRO:HD3	1.89	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: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:D:353:ILE:HG12	1:D:365:LEU:HB3	1.89	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:J:419:LEU:HD11	1:J:504:LEU:HG	1.89	0.53
1:J:16:MET:O	1:J:20:VAL:HG12	2.08	0.53
2:Q:13:LYS:HB3	2:Q:41:LEU:HD11	1.90	0.53
1:J:223:ALA:HB3	1:J:251:ALA:HB2	1.90	0.53
1:D:452:ARG:HH11	1:D:452:ARG:HG2	1.73	0.53
1:H:130:GLU:HG3	1:H:426:LEU:HD23	1.91	0.53
1:G:510:VAL:CG2	1:G:514:MET:HE2	2.38	0.53
1:I:313:THR:HG22	1:I:314:LEU:H	1.74	0.53
1:D:150:ILE:HD13	1:D:493:ILE:HA	1.90	0.53
1:L:218:PRO:HB3	1:L:246:PRO:HB2	1.91	0.53
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.89	0.53
1:B:238:GLU:HA	1:B:238:GLU:OE2	2.09	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:510:VAL:HG23	1:G:514:MET:HE2	1.89	0.53
1:J:149:THR:CG2	1:J:156:GLU:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLU:OE1	2:O:24:GLY:HA3	2.09	0.53
1:K:403:THR:O	1:K:407:VAL:HG23	2.09	0.53
1:G:162:ILE:HG21	1:G:403:THR:HG21	1.90	0.53
1:J:419:LEU:HD21	1:J:500:THR:HG23	1.90	0.53
1:C:27:VAL:HG12	1:C:90: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:C:18:ARG:NH1	1:C:18:ARG:CG	2.46	0.53
1:E:20:VAL:HG13	1:E:74:VAL:HG11	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:B:302:SER:H	1:B:307:MET:HE3	1.74	0.53
1:L:161:LEU:HD21	1:L:185:ASP:HB3	1.90	0.53
1:D:302:SER:H	1:D:307:MET:HE3	1.73	0.53
1:J:161:LEU:HD21	1:J:185:ASP:HB3	1.91	0.53
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:N:123:ALA:HB2	1:N:440:ILE:HG23	1.91	0.52
1:K:161:LEU:HD21	1:K:185:ASP:HB3	1.90	0.52
1:D:162:ILE:HG12	1:D:400:LEU:HD23	1.90	0.52
1:B:18:ARG:CB	1:B:18:ARG:HH11	2.20	0.52
1:K:419:LEU:HD11	1:K:504:LEU:HG	1.92	0.52
1:I:145:ALA:O	1:I:149:THR:HG23	2.09	0.52
1:I:149:THR:CG2	1:I:156:GLU:HA	2.38	0.52
2:Q:47:ARG:HD2	2:Q:49:LEU:HB2	1.91	0.52
1:C:409:GLU:OE2	1:C:501:ARG:NH2	2.33	0.52
1:H:123:ALA:HB2	1:H:440:ILE:HG23	1.92	0.52
1:E:238:GLU:HA	1:E:238:GLU:OE2	2.09	0.52
1:N:66:PHE:H	1:N:69:MET:HG3	1.75	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: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:L:145:ALA:O	1:L:149:THR:HG23	2.09	0.52
1:K:145:ALA:O	1:K:149:THR:HG23	2.10	0.52
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.92	0.52
1:F:77:VAL:HG23	1:F:92:ALA:HB1	1.91	0.52
2:O:23:GLY:H	2:P:80:ASN:HD21	1.58	0.52
1:M:326:ASN:ND2	1:M:328:ASP:H	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HG12	1:B:400:LEU:HD23	1.91	0.52
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.90	0.52
2:Q:23:GLY:H	2:R: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
1:A:74:VAL:HG13	1:A:514:MET:HE1	1.91	0.52
1:A:224:ASP:HB3	1:A:302:SER:HA	1.91	0.52
1:L:326:ASN:ND2	1:L:328:ASP:H	2.08	0.52
1:F:487:ASN:O	1:F:491:MET:HG3	2.09	0.52
1:L:123:ALA:HB2	1:L:440:ILE:HG23	1.92	0.52
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.92	0.52
1:F:452:ARG:HG2	1:F:452:ARG:HH11	1.74	0.52
1:E:77:VAL:HG23	1:E:92:ALA:HB1	1.92	0.52
1:E:268:ARG:HH21	2:S:27:LEU:HD23	1.75	0.52
1:H:443:ALA:O	1:H:447:MET:HG3	2.10	0.52
1:H:161:LEU:HD21	1:H:185:ASP:HB3	1.92	0.52
2:T:47:ARG:HD2	2:T:49:LEU:HB2	1.92	0.52
1:F:238:GLU:HA	1:F:238:GLU:OE2	2.08	0.52
1:N:411:VAL:HG21	1:N:494:LEU:HD12	1.92	0.52
1:K:19:GLY:HA3	1:K:67:GLU:O	2.09	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
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:M:145:ALA:O	1:M:149:THR:HG23	2.10	0.51
1:N:131:LEU:CD1	1:N:422:VAL:HG11	2.40	0.51
1:C:501:ARG:HD3	1:C:505:GLN:OE1	2.11	0.51
1:C:381:VAL:CG1	1:C:392:LYS:HG2	2.40	0.51
1:K:346:VAL:HG21	1:K:373:ALA:HB2	1.91	0.51
1:M:161:LEU:HD21	1:M:185:ASP:HB3	1.91	0.51
2:P:23:GLY:H	2:Q:80:ASN:HD21	1.58	0.51
1:M:2:ALA:O	1:M:4:LYS:HE3	2.11	0.51
1:E:162:ILE:HG12	1:E:400:LEU:HD23	1.91	0.51
1:D:6:VAL:HG23	1:D:6:VAL:O	2.11	0.51
1:D:32:GLY:HA2	4:D:703:ADP:H5'1	1.91	0.51
1:C:302:SER:H	1:C:307:MET:HE3	1.75	0.51
1:A:487:ASN:O	1:A:491:MET:HG3	2.10	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:M:64:ASP:HB3	1:M:67:GLU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:149:THR:CG2	1:K:156:GLU:HA	2.41	0.51
1:J:16:MET:O	1:J:20:VAL:CG1	2.59	0.51
2:T:47:ARG:HD3	2:T:49:LEU:HD12	1.93	0.51
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.92	0.51
1:C:452:ARG:HG2	1:C:452:ARG:HH11	1.74	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:J:452:ARG:HG2	1:J:452:ARG:NH1	2.26	0.51
1:H:38:VAL:HG22	1:I:519:CYS:HB3	1.91	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:N:419:LEU:HD22	1:N:500:THR:CG2	2.41	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:M:123:ALA:HB2	1:M:440:ILE:HG23	1.93	0.51
1:L:346:VAL:HG21	1:L:373:ALA:HB2	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:E:224:ASP:HB3	1:E:302:SER:HA	1.92	0.51
1:L:77:VAL:HG22	1:L:506:TYR:HD1	1.75	0.51
1:F:18:ARG:HH11	1:F:18:ARG:CB	2.21	0.51
1:E:153:ASN:O	1:E:154:SER:HB2	2.11	0.51
2:U:11:ILE:HG12	2:U:85:ILE:HG12	1.93	0.51
1:N:476:TYR:HA	1:N:486:GLY:O	2.10	0.51
1:J:218:PRO:HB3	1:J:246:PRO:HB2	1.93	0.51
1:I:161:LEU:HD21	1:I:185:ASP:HB3	1.92	0.51
1:D:510:VAL:HG12	1:E:385:THR:HG21	1.93	0.51
1:I:38:VAL:HG12	1:I:40:LEU:HD13	1.92	0.51
1:I:218:PRO:HB3	1:I:246:PRO:HB2	1.93	0.51
1:L:458:CYS:SG	1:L:480:ALA:HB1	2.51	0.51
1:I:146:GLN:HE21	1:I:150:ILE:HD11	1.74	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: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:B:420:ILE:HD13	1:B:451:LEU:HD13	1.93	0.50
1:A:28:LYS:HD2	1:A:453:GLN:CD	2.31	0.50
1:D:238:GLU:HA	1:D:238:GLU:OE2	2.11	0.50
1:N:135:SER:HA	1:N:412:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:259:LEU:O	1:N:263:VAL:HG23	2.11	0.50
2:O:13:LYS:HB3	2:O:41:LEU:HD11	1.93	0.50
1:L:228:SER:O	1:L:257:GLU:HB3	2.11	0.50
1:J:66:PHE:H	1:J:69:MET:HG3	1.77	0.50
1:A:409:GLU:CD	1:A:501:ARG:HH21	2.10	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:B:381:VAL:HG21	1:B:393:LYS:HA	1.93	0.50
1:D:204:PHE:HE1	1:D:274:ALA:HB2	1.77	0.50
1:K:102:GLU:OE2	1:K:445:ARG:NH1	2.44	0.50
2:P:47:ARG:HD2	2:P:49:LEU:HB2	1.94	0.50
2:O:50:GLU:HA	2:U:50:GLU:OE1	2.11	0.50
1:A:300:VAL:O	1:A:307:MET:HE3	2.11	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:C:42:LYS:HE2	1:C:48:THR:OG1	2.11	0.50
1:N:145:ALA:O	1:N:149:THR:HG23	2.11	0.50
1:L:96:ALA:O	1:L:100:ILE:HG13	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:H:417:VAL:HG21	1:H:488:MET:HG3	1.92	0.50
1:B:237:LEU:HD21	1:B:271:VAL:HG21	1.93	0.50
1:N:2:ALA:O	1:N:4:LYS:HE3	2.11	0.50
2:T:6:LEU:O	2:T:7:HIS:O	2.29	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
2:O:47:ARG:HD2	2:O:49:LEU:HB2	1.94	0.50
1:J:413:ALA:HB1	1:J:417:VAL:HB	1.92	0.50
1:N:193:MET:HG3	1:N:371:LYS:HB3	1.93	0.50
1:K:218:PRO:HB3	1:K:246:PRO:HB2	1.93	0.50
1:F:356:ALA:HB3	1:F:362:ARG:HG3	1.94	0.50
1:J:135:SER:HA	1:J:412:VAL:HG12	1.94	0.50
1:I:346:VAL:HG21	1:I:373:ALA:HB2	1.93	0.50
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.94	0.50
1:C:28:LYS:HD2	1:C:453:GLN:CD	2.32	0.50
1:B:452:ARG:HG2	1:B:452:ARG:HH11	1.75	0.50
1:B:224:ASP:HB3	1:B:302:SER:HA	1.93	0.50
2:U:47:ARG:HD3	2:U:49:LEU:HD12	1.94	0.50
1:D:28:LYS:HD2	1:D:453:GLN:CD	2.32	0.50
1:I:193:MET:HG3	1:I:371:LYS:HB3	1.92	0.50

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:VAL:HG22	1:H:506:TYR:HD1	1.76	0.49
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
1:C:224:ASP:HB3	1:C:302:SER:HA	1.94	0.49
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.94	0.49
1:K:193:MET:HG3	1:K:371:LYS:HB3	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:J:193:MET:HG3	1:J:371:LYS:HB3	1.93	0.49
1:H:179:ASP:OD1	1:H:393:LYS:HD2	2.12	0.49
1:H:321:LYS:HB2	1:H:334:ASP:HB3	1.95	0.49
1:M:135:SER:HA	1:M:412:VAL:HG12	1.95	0.49
2:O:80:ASN:ND2	2:U:23:GLY:H	2.09	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
1:G:28:LYS:C	1:G:30:THR:N	2.66	0.49
2:T:11:ILE:HG12	2:T:85:ILE:HG12	1.95	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
1:G:414:GLY:O	1:G:417:VAL:CG1	2.45	0.48
1:E:204:PHE:HE1	1:E:274:ALA:HB2	1.77	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:237:LEU:HD21	1:A:271:VAL:HG21	1.95	0.48
1:G:356:ALA:HB3	1:G:362:ARG:HG3	1.95	0.48
1:E:18:ARG:HH11	1:E:18:ARG:CB	2.25	0.48
1:A:18:ARG:HB2	1:A:67:GLU:HG2	1.95	0.48
1:I:66:PHE:H	1:I:69:MET:HG3	1.78	0.48
1:H:419:LEU:HD21	1:H:500:THR:CG2	2.40	0.48
1:H:452:ARG:NH1	1:H:452:ARG:HG2	2.27	0.48
1:L:411:VAL:HG21	1:L:494:LEU:HD12	1.94	0.48
1:C:95:LEU:O	1:C:99:ILE:HG13	2.12	0.48
1:B:356:ALA:HB3	1:B:362:ARG:HG3	1.95	0.48
1:J:38:VAL:HG22	1:K:519:CYS:HB3	1.94	0.48
1:N:15:LYS:HB3	1:N:66:PHE:HB3	1.95	0.48
1:C:517:THR:HG23	1:D:39:VAL:HG23	1.95	0.48
1:C:247:LEU:HB3	1:C:273:VAL:HG12	1.94	0.48
1:M:130:GLU:HG3	1:M:426:LEU:HD23	1.94	0.48
2:O:47:ARG:HD3	2:O:49:LEU:HD12	1.95	0.48
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.95	0.48
1:H:403:THR:O	1:H:407:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:443:ALA:O	1:M:447:MET:HG3	2.13	0.48
1:N:266:THR:CG2	1:N:273:VAL:H	2.26	0.48
1:I:179:ASP:OD1	1:I:393:LYS:HD2	2.13	0.48
1:K:413:ALA:HB1	1:K:417:VAL:HB	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:N:130:GLU:HG3	1:N:426:LEU:CD2	2.44	0.48
2:P:11:ILE:HG12	2:P:85:ILE:HG12	1.94	0.48
2:O:11:ILE:HG12	2:O:85:ILE:HG12	1.95	0.48
1:L:428:ASP:O	1:L:430:ARG:HG2	2.13	0.48
1:I:80:LYS:HA	1:I:83:ASP:HB2	1.94	0.48
1:C:204:PHE:HE1	1:C:274:ALA:HB2	1.77	0.48
1:M:130:GLU:HG3	1:M:426:LEU:CD2	2.43	0.48
1:D:356:ALA:HB3	1:D:362:ARG:HG3	1.95	0.48
1:A:257:GLU:O	1:A:261:THR:HG23	2.13	0.48
1:N:455:VAL:HG13	1:N:460:GLU:HB2	1.95	0.48
1:H:193:MET:HG3	1:H:371:LYS:HB3	1.94	0.48
1:D:420:ILE:HD13	1:D:451:LEU:HD13	1.95	0.48
1:E:18:ARG:CG	1:E:18:ARG:NH1	2.51	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:G:162:ILE:HG12	1:G:400:LEU:HD23	1.95	0.48
1:B:381:VAL:CG1	1:B:392:LYS:CG	2.91	0.48
1:K:30:THR:HB	1:K:51:LYS:O	2.13	0.48
1:J:102:GLU:HB3	1:J:442:VAL:HG22	1.96	0.48
1:D:102:GLU:HB3	1:D:442:VAL:HG22	1.96	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:J:321:LYS:HB2	1:J:334:ASP:HB3	1.96	0.48
1:E:95:LEU:O	1:E:99:ILE:HG13	2.13	0.48
1:I:15:LYS:HB3	1:I:66:PHE:HB3	1.96	0.48
1:K:102:GLU:HB3	1:K:442:VAL:HG22	1.96	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:I:77:VAL:HG22	1:I:506:TYR:HD1	1.78	0.48
2:R:34:LYS:HG3	2:R:35:SER:H	1.79	0.48
1:H:519:CYS:HB3	1:N:38:VAL:HG22	1.96	0.48
1:L:179:ASP:OD1	1:L:393:LYS:HD2	2.14	0.48
1:I:34:LYS:HB2	1:I:458:CYS:SG	2.54	0.48
1:D:237:LEU:HD21	1:D:271:VAL:HG21	1.96	0.48
1:K:135:SER:HA	1:K:412:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:85:ALA:HA	1:L:498:LYS:HD3	1.96	0.48
1:C:356:ALA:HB3	1:C:362:ARG:HG3	1.95	0.48
1:K:123:ALA:HB2	1:K:440:ILE:HG23	1.96	0.48
1:E:247:LEU:HB3	1:E:273:VAL:HG12	1.96	0.48
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:A:510:VAL:HG23	1:A:514:MET:HE2	1.96	0.47
1:D:20:VAL:HG13	1:D:74:VAL:HG11	1.95	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:N:11:ASP:O	1:N:12:ALA:C	2.50	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:B:257:GLU:O	1:B:261:THR: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:K:259:LEU:O	1:K:263:VAL:HG23	2.14	0.47
1:K:16:MET:HG3	1:K:520:MET:SD	2.54	0.47
1:H:226:LYS:HG3	1:H:252:GLU:HB3	1.96	0.47
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.96	0.47
1:F:204:PHE:HE1	1:F:274:ALA:HB2	1.79	0.47
1:F:197:ARG:HD3	1:F:197:ARG:HA	1.62	0.47
2:S:47:ARG:HD3	2:S:49:LEU:HD12	1.95	0.47
1:I:259:LEU:O	1:I:263:VAL:HG23	2.14	0.47
1:I:163:ALA:O	1:I:167:ASP:HB2	2.14	0.47
1:H:455:VAL:HG11	1:H:461:GLU:O	2.13	0.47
1:J:266:THR:CG2	1:J:273:VAL:H	2.27	0.47
1:A:204:PHE:HE1	1:A:274:ALA:HB2	1.78	0.47
1:N:69:MET:HE2	1:N:522:THR:HB	1.93	0.47
1:C:74:VAL:HG13	1:C:514:MET:HE1	1.95	0.47
2:P:47:ARG:HD3	2:P:49:LEU:HD12	1.95	0.47
1:J:417:VAL:HG21	1:J:488:MET:HG3	1.96	0.47
1:I:103:GLY:O	1:I:106:ALA:HB3	2.14	0.47
1:B:232:GLU:HB3	1:B:309:LEU:HB3	1.96	0.47
1:F:461:GLU:HA	1:F:462:PRO:HD3	1.79	0.47
1:J:138:CYS:SG	1:J:144:ILE:HD13	2.54	0.47
1:I:266:THR:CG2	1:I:273:VAL:H	2.27	0.47
1:A:80:LYS:HD2	1:A:506:TYR:CE1	2.50	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:H:135:SER:HA	1:H:412:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:163:ALA:O	1:N:167:ASP:HB2	2.14	0.47
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.96	0.47
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.97	0.47
1:J:179:ASP:OD1	1:J:393:LYS:HD2	2.15	0.47
1:G:42:LYS:HG2	1:G:44:PHE:CE2	2.50	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:M:193:MET:HG3	1:M:371:LYS:HB3	1.96	0.47
1:F:432:GLN:NE2	1:F:436:GLN:NE2	2.41	0.47
1:N:15:LYS:HD3	1:N:15:LYS:HA	1.70	0.47
1:G:510:VAL:CG2	1:G:514:MET:CE	2.92	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:E:381:VAL:CG1	1:E:392:LYS:HG2	2.45	0.47
1:F:300:VAL:O	1:F:307:MET:HE3	2.14	0.47
2:R:47:ARG:HD3	2:R:49:LEU:HD12	1.95	0.47
1:F:381:VAL:CG1	1:F:392:LYS:HG2	2.45	0.47
1:G:455:VAL:HG21	1:G:465:VAL:HG11	1.96	0.47
1:I:123:ALA:HB2	1:I:440:ILE:HG23	1.97	0.47
2:O:78:ILE:HD13	2:O:83:VAL:HG21	1.96	0.47
1:G:18:ARG:CB	1:G:18:ARG:HH11	2.26	0.47
1:L:130:GLU:HG3	1:L:426:LEU:CD2	2.44	0.47
1:J:15:LYS:HB3	1:J:66:PHE:HB3	1.97	0.47
1:E:510:VAL:HG23	1:E:514:MET:CE	2.45	0.47
1:B:268:ARG:HH21	2:P:27:LEU:CD2	2.27	0.47
1:L:413:ALA:HB1	1:L:417:VAL:HB	1.97	0.47
1:B:234:LEU:HD22	2:P:23:GLY:HA3	1.96	0.47
1:K:443:ALA:O	1:K:447:MET:HG3	2.14	0.47
1:G:232:GLU:HB3	1:G:309:LEU:HB3	1.97	0.47
1:L:360:TYR:O	1:L:364:LYS:HB2	2.15	0.47
1:K:179:ASP:OD1	1:K:393:LYS:HD2	2.14	0.47
1:G:247:LEU:HB3	1:G:273:VAL:HG12	1.97	0.47
1:E:232:GLU:HB3	1:E:309:LEU:HB3	1.96	0.47
1:F:232:GLU:HB3	1:F:309:LEU:HB3	1.96	0.47
1:J:228:SER:O	1:J:257:GLU:HB3	2.15	0.47
1:I:365:LEU:O	1:I:369:VAL:HG23	2.15	0.47
1:F:18:ARG:HB2	1:F:67:GLU:HG2	1.96	0.47
1:I:130:GLU:HG3	1:I:426:LEU:HD23	1.97	0.47
1:M:444:LEU:HD23	1:M:444:LEU:HA	1.72	0.47
1:L:38:VAL:HG12	1:L:40:LEU:HD13	1.97	0.47

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:38:VAL:HG12	1:M:40:LEU:HD13	1.96	0.46
1:B:32:GLY:HA2	4:B:701:ADP:H5'1	1.98	0.46
2:T:78:ILE:HD13	2:T:83:VAL:HG21	1.98	0.46
1:C:206:ASN:O	1:C:207:LYS:HG2	2.16	0.46
1:F:28:LYS:HD2	1:F:453:GLN:CD	2.36	0.46
1:E:124:VAL:HG13	1:E:504:LEU:HD13	1.96	0.46
1:D:254:VAL:HG12	1:D:259:LEU:HB2	1.97	0.46
1:K:426:LEU:O	1:K:444:LEU:HD11	2.16	0.45
1:G:501:ARG:HD3	1:G:505:GLN:OE1	2.15	0.45
1:A:381:VAL:CG1	1:A:392:LYS:CG	2.94	0.45
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.56	0.45
1:B:351:GLN:O	1:B:351:GLN:HG2	2.16	0.45
1:A:501:ARG:HD3	1:A:505:GLN:OE1	2.16	0.45
1:G:225:LYS:HG2	1:G:303:GLU:HB2	1.99	0.45
1:L:433:ASN:OD1	1:L:435:ASP:HB2	2.17	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:G:381:VAL:HG21	1:G:393:LYS:HA	1.98	0.45
1:F:351:GLN:O	1:F:351:GLN:HG2	2.16	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: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:I:270:ILE:HA	1:J:257:GLU:OE2	2.16	0.45
1:A:49:ILE:HD13	1:G:513:LEU:HB3	1.97	0.45
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.97	0.45
1:D:381:VAL:CG1	1:D:392:LYS:HG2	2.47	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: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:I:104:LEU:HA	1:I:104:LEU:HD12	1.75	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:85:ALA:HA	1:I:498:LYS:HD3	1.98	0.45
1:D:225:LYS:HG2	1:D:303:GLU:HB2	1.98	0.45
2:R:78:ILE:HD13	2:R:83:VAL:HG21	1.98	0.45
1:A:384:ALA:O	1:G:506:TYR:HE1	1.99	0.45
1:M:179:ASP:OD1	1:M:393:LYS:HD2	2.17	0.45
1:K:270:ILE:HG23	1:L:229:ASN:HD21	1.82	0.45

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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:M:321:LYS:HB2	1:M:334:ASP:HB3	1.99	0.45
1:C:23:LEU:CD1	1:C:23:LEU:C	2.84	0.45
1:M:138:CYS:SG	1:M:144:ILE:HD13	2.56	0.45
1:A:77:VAL:HG23	1:A:92:ALA:HB1	1.99	0.45
1:N:228:SER:O	1:N:257:GLU:HB3	2.17	0.45
1:B:300:VAL:O	1:B:307:MET:HE3	2.17	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
2:S:23:GLY:H	2:T:80:ASN:HD21	1.64	0.45
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.57	0.45
1:L:444:LEU:HD23	1:L:444:LEU:HA	1.74	0.45
1:G:197:ARG:HG2	1:G:277:LYS:O	2.17	0.45
1:M:270:ILE:HG23	1:N:229:ASN:ND2	2.32	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:L:433:ASN:HD22	1:L:433:ASN:HA	1.59	0.45
1:L:365:LEU:O	1:L:369:VAL:HG23	2.16	0.45
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.57	0.45
1:F:413:ALA:CB	1:F:417:VAL:HG13	2.47	0.45
1:M:16:MET:HG3	1:M:520:MET:SD	2.57	0.45
1:A:28:LYS:HD2	1:A:453:GLN:NE2	2.31	0.45
1:F:233:MET:HB3	1:F:237:LEU:HD12	1.98	0.45
1:I:417:VAL:HG21	1:I:488:MET:HG3	1.98	0.45
1:D:105:LYS:HB2	1:D:105:LYS:HE3	1.74	0.45
1:C:257:GLU:O	1:C:261:THR:HG23	2.17	0.45
1:E:351:GLN:HG2	1:E:351:GLN:O	2.16	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:L:16:MET:O	1:L:20:VAL:HG12	2.17	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:D:351:GLN:O	1:D:351:GLN:HG2	2.16	0.45
1:J:64:ASP:OD1	1:J:65:LYS:O	2.34	0.44
2:Q:11:ILE:HG12	2:Q:85:ILE:HG12	1.98	0.44
1:L:259:LEU:O	1:L:263:VAL:HG23	2.18	0.44
1:J:365:LEU:O	1:J:369:VAL:HG23	2.17	0.44
1:H:15:LYS:HB3	1:H:66:PHE:HB3	1.99	0.44
1:K:444:LEU:HA	1:K:444:LEU:HD23	1.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:GLY:HA2	4:C:702:ADP:H5'1	1.98	0.44
1:N:429:LEU:HB3	1:N:440:ILE:HG21	2.00	0.44
1:D:28:LYS:C	1:D:30:THR:H	2.21	0.44
1:N:262:LEU:O	1:N:266:THR:HG23	2.17	0.44
1:I:213:VAL:O	1:I:324:VAL:HA	2.17	0.44
2:P:34:LYS:HG3	2:P:35:SER:H	1.82	0.44
1:F:510:VAL:HG23	1:F:514:MET:CE	2.47	0.44
1:B:153:ASN:O	1:B:154:SER:HB2	2.17	0.44
1:M:417:VAL:HG21	1:M:488:MET:HG3	1.99	0.44
1:K:16:MET:O	1:K:20:VAL:HG12	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: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:M:458:CYS:SG	1:M:480:ALA:HB1	2.57	0.44
1:B:18:ARG:HB2	1:B:67:GLU:HG2	1.99	0.44
1:N:77:VAL:HG11	1:N:510:VAL:HB	1.99	0.44
1:F:254:VAL:HG12	1:F:259:LEU:HB2	2.00	0.44
2:Q:43:VAL:HG13	2:Q:57:LEU:HD12	2.00	0.44
1:N:16:MET:HG3	1:N:520:MET:SD	2.57	0.44
1:C:420:ILE:HD13	1:C:451:LEU:HD13	1.99	0.44
1:J:163:ALA:O	1:J:167:ASP:HB2	2.17	0.44
1:G:18:ARG:HB2	1:G:67:GLU:HG2	1.99	0.44
1:J:69:MET:HE2	1:J:522:THR:HB	1.95	0.44
1:H:15:LYS:HD3	1:H:15:LYS:HA	1.72	0.44
1:J:444:LEU:HA	1:J:444:LEU:HD23	1.71	0.44
1:K:126:ALA:HB1	1:K:426:LEU:HD22	2.00	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: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:K:38:VAL:HG12	1:K:40:LEU:HD13	1.98	0.44
1:M:419:LEU:HD21	1:M:500:THR:CG2	2.42	0.44
1:L:342:ILE:O	1:L:346:VAL:HG23	2.17	0.44
1:G:24:ALA:O	1:G:28:LYS:HG3	2.17	0.44
1:E:233:MET:HB3	1:E:237:LEU:HD12	1.98	0.44
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.58	0.44
1:L:226:LYS:HG3	1:L:252:GLU:HB3	1.99	0.44
1:A:461:GLU:HA	1:A:462:PRO:HD3	1.89	0.44
1:C:413:ALA:CB	1:C:417:VAL:HG13	2.47	0.44
4:G:706:ADP:O3B	5:G:806:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:PRO:HG3	4:F:705:ADP:C6	2.53	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:J:90:THR:O	1:J:94:VAL:HG23	2.17	0.44
1:E:150:ILE:HD13	1:E:493:ILE:HA	1.99	0.44
1:N:513:LEU:HD12	1:N:513:LEU:HA	1.90	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:A:233:MET:HB3	1:A:237:LEU:HD12	2.00	0.44
1:H:34:LYS:HB2	1:H:458:CYS:SG	2.58	0.44
1:E:31:LEU:HD23	1:E:453:GLN:HB3	2.00	0.44
1:C:225:LYS:HG2	1:C:303:GLU:HB2	2.00	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:D:42:LYS:HG2	1:D:44:PHE:CE2	2.52	0.44
1:J:126:ALA:HB1	1:J:426:LEU:HD22	2.00	0.44
1:D:100:ILE:HD11	1:D:514:MET:CE	2.46	0.44
1:G:495:ASP:CG	4:G:706:ADP:HO2'	2.21	0.44
1:D:300:VAL:O	1:D:307:MET:HE3	2.18	0.44
1:F:162:ILE:HG21	1:F:403:THR:HG21	2.00	0.44
1:K:270:ILE:HG23	1:L:229:ASN:ND2	2.33	0.44
1:G:451:LEU:HD21	1:G:465:VAL:HG12	1.99	0.44
1:D:301:ILE:O	1:D:301:ILE:HG22	2.18	0.44
1:G:80:LYS:HD2	1:G:506:TYR:CE1	2.53	0.44
1:A:130:GLU:HB3	1:A:422:VAL:HB	1.99	0.44
1:M:85:ALA:HA	1:M:498:LYS:HD3	2.00	0.44
1:M:15:LYS:HB3	1:M:66:PHE:HB3	2.00	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:I:228:SER:O	1:I:257:GLU:HB3	2.18	0.44
1:M:15:LYS:HD3	1:M:15:LYS:HA	1.73	0.43
1:J:64:ASP:C	1:J:65:LYS:O	2.55	0.43
1:I:326:ASN:HD22	1:I:328:ASP:H	1.65	0.43
1:D:28:LYS:C	1:D:30:THR:N	2.68	0.43
1:G:28:LYS:HD2	1:G:453:GLN:NE2	2.32	0.43
1:M:262:LEU:O	1:M:266:THR:HG23	2.17	0.43
1:F:451:LEU:HD21	1:F:465:VAL:HG12	1.98	0.43
1:I:296:THR:HB	1:I:319:GLN:H	1.82	0.43
1:I:285:ARG:HA	1:I:288:MET:HB2	1.99	0.43
1:A:254:VAL:HG12	1:A:259:LEU:HB2	2.00	0.43
1:L:455:VAL:HG11	1:L:461:GLU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:LYS:HG3	1:G:59:GLU:O	2.18	0.43
1:F:225:LYS:HG2	1:F:303:GLU:HB2	2.00	0.43
2:T:43:VAL:HG13	2:T:57:LEU:HD12	2.00	0.43
1:D:327:LYS:HG2	1:D:327:LYS:O	2.18	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:J:104:LEU:HA	1:J:104:LEU:HD12	1.66	0.43
1:A:361:ASP:O	1:A:365:LEU:HD23	2.18	0.43
1:A:349:ILE:HG23	1:A:365:LEU:HD12	2.00	0.43
1:N:38:VAL:HG12	1:N:40:LEU:HD13	1.99	0.43
1:E:234:LEU:HD22	2:S:23:GLY:HA3	1.99	0.43
2:O:96:GLU:O	2:P:1:MET:HB2	2.18	0.43
1:M:87:ASP:HB3	1:M:499:VAL:HG21	2.00	0.43
1:B:413:ALA:CB	1:B:417:VAL:HG13	2.48	0.43
1:D:414:GLY:O	1:D:417:VAL:CG1	2.48	0.43
1:A:381:VAL:HG11	1:A:392:LYS:HG3	2.01	0.43
2:T:34:LYS:HG3	2:T:35:SER:H	1.82	0.43
1:C:254:VAL:HG12	1:C:259:LEU:HB2	2.00	0.43
1:A:102:GLU:HB3	1:A:442:VAL:HG22	2.01	0.43
1:B:519:CYS:HB3	1:C:38:VAL:HG22	2.01	0.43
1:I:476:TYR:HA	1:I:486:GLY:O	2.18	0.43
1:D:18:ARG:HH11	1:D:18:ARG:HB3	1.83	0.43
1:N:104:LEU:HD12	1:N:104:LEU:HA	1.71	0.43
1:K:452:ARG:HG2	1:K:452:ARG:NH1	2.32	0.43
1:D:6:VAL:CG2	1:D:6:VAL:O	2.66	0.43
2:O:50:GLU:OE1	2:P:50:GLU:HA	2.18	0.43
1:J:461:GLU:HA	1:J:462:PRO:HD3	1.90	0.43
1:N:102:GLU:OE2	1:N:445:ARG:NH1	2.50	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:A:421:ARG:HA	1:A:421:ARG:HD3	1.68	0.43
1:K:130:GLU:HG3	1:K:426:LEU:HD23	1.99	0.43
1:G:175:ILE:HG21	1:G:400:LEU:HD21	2.01	0.43
1:N:213:VAL:O	1:N:324:VAL:HA	2.18	0.43
1:J:80:LYS:HA	1:J:83:ASP:HB2	2.00	0.43
1:K:77:VAL:HG11	1:K:510:VAL:HB	1.98	0.43
1:K:77:VAL:HG22	1:K:506:TYR:HD1	1.82	0.43
1:K:226:LYS:HG3	1:K:252:GLU:HB3	2.00	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:F:197:ARG:HG2	1:F:277:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:77:VAL:HG22	1:N:506:TYR:CD1	2.53	0.43
1:C:300:VAL:O	1:C:307:MET:HE3	2.19	0.43
1:L:102:GLU:HB3	1:L:442:VAL:HG22	2.01	0.43
1:B:225:LYS:HG2	1:B:303:GLU:HB2	2.01	0.43
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.52	0.43
1:C:510:VAL:HG23	1:C:514:MET:CE	2.49	0.43
2:P:50:GLU:OE1	2:Q:50:GLU:HA	2.19	0.43
1:D:257:GLU:O	1:D:261:THR:HG23	2.18	0.43
2:Q:34:LYS:HG3	2:Q:35:SER:H	1.83	0.43
1:H:409:GLU:OE2	1:H:501:ARG:NH2	2.47	0.43
2:T:23:GLY:H	2:U:80:ASN:HD21	1.66	0.43
1:N:34:LYS:HB2	1:N:458:CYS:SG	2.58	0.43
1:I:443:ALA:O	1:I:447:MET:HG3	2.19	0.43
1:N:126:ALA:HB1	1:N:426:LEU:HD22	2.00	0.43
1:D:452:ARG:NH1	1:D:452:ARG:HG2	2.33	0.43
1:G:254:VAL:HG12	1:G:259:LEU:HB2	2.00	0.43
2:R:46:GLY:HA3	2:R:55:LYS:O	2.19	0.43
1:E:248:LEU:HD22	1:E:323:VAL:HG11	2.00	0.43
1:K:524:LEU:HD23	1:K:524:LEU:HA	1.87	0.43
1:G:421:ARG:HD3	1:G:421:ARG:HA	1.69	0.43
1:K:66:PHE:H	1:K:69:MET:HG3	1.83	0.43
1:N:69:MET:CE	1:N:522:THR:CB	2.93	0.43
1:L:34:LYS:HB2	1:L:458:CYS:SG	2.58	0.43
1:G:381:VAL:CG1	1:G:392:LYS:CG	2.97	0.43
1:M:80:LYS:HA	1:M:83:ASP:HB2	2.00	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:524:LEU:HA	1:G:524:LEU:HD23	1.84	0.43
1:L:72:GLN:HA	1:L:72:GLN:NE2	2.33	0.43
1:G:19:GLY:HA3	1:G:67:GLU:O	2.19	0.43
1:E:42:LYS:HG2	1:E:44:PHE:CE2	2.53	0.43
1:N:7:LYS:HD2	1:N:66:PHE:CE2	2.54	0.43
1:H:7:LYS:HD2	1:H:66:PHE:CE2	2.54	0.43
1:G:77:VAL:HG23	1:G:92:ALA:HB1	2.01	0.43
1:M:419:LEU:HD22	1:M:500:THR:CG2	2.47	0.43
1:G:28:LYS:HD2	1:G:453:GLN:CD	2.39	0.43
1:J:262:LEU:O	1:J:266:THR:HG23	2.18	0.43
1:E:409:GLU:OE2	1:E:501:ARG:NH2	2.42	0.43
1:B:130:GLU:HB3	1:B:422:VAL:HB	2.01	0.43
1:F:248:LEU:HD22	1:F:323:VAL:HG11	1.99	0.43
1:H:433:ASN:OD1	1:H:435:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:64:ASP:C	1:M:65:LYS:O	2.56	0.42
1:K:64:ASP:OD1	1:K:65:LYS:O	2.37	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: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:M:365:LEU:O	1:M:369:VAL:HG23	2.19	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:432:GLN:NE2	1:B:436:GLN:NE2	2.39	0.42
1:K:285:ARG:HA	1:K:288:MET:HB2	2.01	0.42
1:B:102:GLU:HB3	1:B:442:VAL:HG22	2.01	0.42
1:J:226:LYS:HG3	1:J:252:GLU:HB3	2.01	0.42
1:F:520:MET:HG2	1:G:39:VAL:HB	2.00	0.42
1:A:477:GLY:HA3	1:A:488:MET:SD	2.59	0.42
1:A:365:LEU:O	1:A:369:VAL:HG13	2.19	0.42
1:G:349:ILE:HG23	1:G:365:LEU:HD12	2.01	0.42
1:D:349:ILE:HG23	1:D:365:LEU:HD12	2.01	0.42
1:K:429:LEU:HB3	1:K:440:ILE:HG21	2.01	0.42
1:G:455:VAL:HG11	1:G:462:PRO:HA	2.02	0.42
2:U:43:VAL:HG13	2:U:57:LEU:HD12	2.01	0.42
2:U:34:LYS:HG3	2:U:35:SER:H	1.84	0.42
1:D:421:ARG:HA	1:D:421:ARG:HD3	1.73	0.42
1:M:426:LEU:H	1:M:426:LEU:HG	1.67	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:J:32:GLY:HA2	1:J:454:ILE:CD1	2.46	0.42
1:G:288:MET:O	1:G:291:ASP:HB2	2.19	0.42
1:J:77:VAL:HG22	1:J:506:TYR:CD1	2.54	0.42
1:N:215:LEU:HB3	1:N:218:PRO:HG3	2.01	0.42
1:D:451:LEU:HD21	1:D:465:VAL:HG12	2.01	0.42
1:D:105:LYS:HD3	1:K:110:GLY:O	2.19	0.42
1:J:477:GLY:O	1:J:485:TYR:HA	2.19	0.42
1:M:441:LYS:O	1:M:442:VAL:C	2.58	0.42
1:A:286:LYS:HE2	1:A:304:GLU:OE1	2.19	0.42
1:D:248:LEU:HD22	1:D:323:VAL:HG11	2.01	0.42
1:N:285:ARG:HA	1:N:288:MET:HB2	2.01	0.42
1:L:524:LEU:HD23	1:L:524:LEU:HA	1.82	0.42
1:I:15:LYS:HD3	1:I:15:LYS:HA	1.73	0.42
1:D:77:VAL:HG23	1:D:92:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:22:VAL:HG11	1:M:62:LEU:HD21	2.02	0.42
1:E:80:LYS:HD2	1:E:506:TYR:CE1	2.54	0.42
1:F:42:LYS:HG2	1:F:44:PHE:CE2	2.54	0.42
1:B:510:VAL:HG23	1:B:514:MET:CE	2.49	0.42
1:A:90:THR:O	1:A:94:VAL:HG23	2.19	0.42
1:D:28:LYS:O	1:D:30:THR:N	2.52	0.42
1:A:381:VAL:CG1	1:A:392:LYS:HG2	2.49	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:K:15:LYS:HD3	1:K:15:LYS:HA	1.74	0.42
1:H:419:LEU:HD22	1:H:500:THR:CG2	2.47	0.42
1:L:213:VAL:O	1:L:324:VAL:HA	2.20	0.42
1:L:138:CYS:SG	1:L:144:ILE:HD13	2.60	0.42
1:L:126:ALA:HB1	1:L:426:LEU:HD22	2.02	0.42
1:D:430:ARG:CG	1:D:430:ARG:NH1	2.75	0.42
1:M:104:LEU:HD12	1:M:104:LEU:HA	1.72	0.42
1:J:419:LEU:HD22	1:J:500:THR:CG2	2.47	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:M:413:ALA:CB	1:M:417:VAL:HB	2.50	0.42
1:A:301:ILE:HG21	1:A:309:LEU:HD12	2.02	0.42
1:I:262:LEU:O	1:I:266:THR:HG23	2.19	0.42
1:N:87:ASP:HB3	1:N:499:VAL:HG21	2.02	0.42
1:J:8:PHE:O	1:J:9:GLY:C	2.57	0.42
1:F:34:LYS:HD2	1:F:458:CYS:SG	2.60	0.42
1:D:41:ASP:O	1:D:42:LYS:HG3	2.20	0.42
1:F:204:PHE:CG	1:F:204:PHE:O	2.73	0.42
1:I:130:GLU:HG3	1:I:426:LEU:CD2	2.49	0.42
1:B:42:LYS:HG2	1:B:44:PHE:CE2	2.55	0.42
1:N:444:LEU:HD23	1:N:444:LEU:HA	1.68	0.42
1:D:33:PRO:HG3	4:D:703:ADP:C6	2.55	0.42
1:M:215:LEU:HB3	1:M:218:PRO:HG3	2.01	0.42
1:J:215:LEU:HB3	1:J:218:PRO:HG3	2.02	0.42
1:B:381:VAL:HG11	1:B:392:LYS:HG3	2.02	0.42
1:M:234:LEU:N	1:M:235:PRO:HD2	2.34	0.42
1:A:150:ILE:HD13	1:A:493:ILE:HA	2.02	0.42
1:K:213:VAL:O	1:K:324:VAL:HA	2.20	0.42
1:E:286:LYS:HE2	1:E:304:GLU:OE1	2.20	0.42
1:H:285:ARG:HA	1:H:288:MET:HB2	2.01	0.42
1:C:455:VAL:HG21	1:C:465:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:15:LYS:HB3	1:L:66:PHE:HB3	2.02	0.42
1:A:288:MET:CG	1:A:368:ARG:HD2	2.50	0.42
1:F:501:ARG:HD3	1:F:505:GLN:OE1	2.19	0.42
1:K:342:ILE:O	1:K:346:VAL:HG23	2.20	0.42
1:F:301:ILE:HG22	1:F:301:ILE:O	2.20	0.42
1:E:455:VAL:HG21	1:E:465:VAL:HG11	2.02	0.42
1:M:455:VAL:HG13	1:M:460:GLU:HB2	2.01	0.42
1:K:11:ASP:O	1:K:12:ALA:C	2.59	0.42
1:L:80:LYS:HA	1:L:83:ASP:HB2	2.02	0.42
1:F:219:PHE:HB3	1:F:317:LEU:HD13	2.01	0.42
1:F:413:ALA:HB3	1:F:417:VAL:HG13	2.02	0.41
1:L:15:LYS:HA	1:L:15:LYS:HD3	1.76	0.41
1:N:149:THR:HG22	1:N:156:GLU:HA	2.02	0.41
1:H:234:LEU:N	1:H:235:PRO:HD2	2.35	0.41
1:B:381:VAL:HG12	1:B:392:LYS:HG2	2.02	0.41
1:G:28:LYS:C	1:G:30:THR:H	2.22	0.41
1:M:39:VAL:HB	1:N:520:MET:HG2	2.02	0.41
1:L:443:ALA:O	1:L:447:MET:HG3	2.20	0.41
1:L:285:ARG:HA	1:L:288:MET:HB2	2.02	0.41
1:J:213:VAL:O	1:J:324:VAL:HA	2.19	0.41
1:B:23:LEU:C	1:B:23:LEU:CD1	2.88	0.41
1:N:64:ASP:OD1	1:N:65:LYS:O	2.37	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:G:301:ILE:HG21	1:G:309:LEU:HD12	2.02	0.41
1:A:381:VAL:CG1	1:A:392:LYS:HG3	2.50	0.41
1:N:85:ALA:HA	1:N:498:LYS:HD3	2.02	0.41
1:C:130:GLU:HB3	1:C:422:VAL:HB	2.03	0.41
2:S:34:LYS:HG3	2:S:35:SER:H	1.84	0.41
1:K:296:THR:HB	1:K:319:GLN:H	1.84	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:H:342:ILE:O	1:H:346:VAL:HG23	2.20	0.41
1:A:24:ALA:O	1:A:28:LYS:HG3	2.20	0.41
1:K:428:ASP:O	1:K:429:LEU:C	2.58	0.41
1:K:39:VAL:HB	1:L:520:MET:HG2	2.02	0.41
1:F:28:LYS:O	1:F:30:THR:N	2.53	0.41
1:B:286:LYS:HE2	1:B:304:GLU:OE1	2.20	0.41
1:J:2:ALA:O	1:J:4:LYS:HE3	2.20	0.41
1:M:476:TYR:HA	1:M:486:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:GLU:HB3	1:E:422:VAL:HB	2.01	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:M:226:LYS:HG3	1:M:252:GLU:HB3	2.01	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:H:104:LEU:HD12	1:H:104:LEU:HA	1.74	0.41
1:N:100:ILE:HG23	1:N:104:LEU:HD22	2.01	0.41
1:D:28:LYS:HD2	1:D:453:GLN:NE2	2.36	0.41
1:K:16:MET:O	1:K:20:VAL:CG1	2.69	0.41
1:E:102:GLU:HB3	1:E:442:VAL:HG22	2.03	0.41
2:T:60:LYS:HG2	2:T:63:ASP:OD2	2.20	0.41
1:C:286:LYS:HE2	1:C:304:GLU:OE1	2.21	0.41
1:B:501:ARG:HD3	1:B:505:GLN:OE1	2.20	0.41
1:E:270:ILE:HG23	2:S:25:ILE:HG22	2.03	0.41
1:C:114:MET:HE3	1:C:114:MET:O	2.20	0.41
1:C:204:PHE:CG	1:C:204:PHE:O	2.73	0.41
1:C:197:ARG:H	1:C:329:THR:HA	1.84	0.41
1:N:13:ARG:HD2	1:N:104:LEU:HD11	2.03	0.41
1:F:349:ILE:HG23	1:F:365:LEU:HD12	2.01	0.41
1:D:238:GLU:OE1	2:R:24:GLY:HA3	2.20	0.41
1:L:16:MET:O	1:L:20:VAL:CG1	2.69	0.41
1:H:428:ASP:O	1:H:429:LEU:C	2.58	0.41
1:E:150:ILE:CD1	1:E:493:ILE:HA	2.50	0.41
1:D:69:MET:O	1:D:73:MET:HG3	2.21	0.41
1:G:289:LEU:HA	1:G:292:ILE:HD12	2.02	0.41
1:F:421:ARG:HA	1:F:421:ARG:HD3	1.74	0.41
1:M:66:PHE:HD1	1:M:520:MET:HE2	1.85	0.41
1:E:365:LEU:O	1:E:369:VAL:HG13	2.20	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:K:215:LEU:HB3	1:K:218:PRO:HG3	2.02	0.41
1:B:261:THR:HG22	2:P:29:GLY:HA3	2.01	0.41
1:F:301:ILE:HG21	1:F:309:LEU:HD12	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:H:69:MET:HE2	1:H:522:THR:HB	2.00	0.41
1:G:16:MET:HE1	1:G:514:MET:HB3	2.03	0.41
1:E:288:MET:CG	1:E:368:ARG:HD2	2.49	0.41
1:J:437:ASN:HA	1:J:440:ILE:HD12	2.01	0.41
1:H:10:ASN:O	1:H:11:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:LYS:C	1:F:30:THR:N	2.73	0.41
1:A:248:LEU:HD22	1:A:323:VAL:HG11	2.02	0.41
1:N:296:THR:HB	1:N:319:GLN:H	1.85	0.41
1:G:248:LEU:HD22	1:G:323:VAL:HG11	2.02	0.41
1:J:101:THR:HG22	1:J:105:LYS:HE3	2.02	0.41
1:B:95:LEU:O	1:B:99:ILE:HG13	2.21	0.41
1:M:461:GLU:HA	1:M:462:PRO:HD3	1.89	0.41
1:I:11:ASP:O	1:I:12:ALA:C	2.58	0.41
1:C:421:ARG:HD3	1:C:421:ARG:HA	1.74	0.41
1:A:204:PHE:O	1:A:204:PHE:CG	2.74	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:M:270:ILE:HG23	1:N:229:ASN:HD21	1.86	0.41
1:L:198:GLY:HA3	1:L:328:ASP:HA	2.03	0.41
1:C:452:ARG:HH12	1:C:463:SER:HB3	1.85	0.41
1:C:162:ILE:HG21	1:C:403:THR:HG21	2.03	0.41
1:D:240:VAL:HG11	1:D:247:LEU:HB2	2.03	0.41
1:E:451:LEU:HD21	1:E:465:VAL:HG12	2.02	0.41
1:H:433:ASN:HA	1:H:433:ASN:HD22	1.54	0.41
1:B:248:LEU:HD22	1:B:323:VAL:HG11	2.01	0.41
1:I:221:LEU:HD12	1:I:249:ILE:HG23	2.02	0.41
1:E:198:GLY:HA2	1:E:326:ASN:O	2.21	0.41
1:C:30:THR:HB	1:C:51:LYS:HG2	2.03	0.41
1:D:524:LEU:HA	1:D:524:LEU:HD23	1.99	0.41
1:D:456:LEU:HD13	1:D:462:PRO:CG	2.51	0.41
1:D:413:ALA:CB	1:D:417:VAL:HG13	2.51	0.41
1:D:19:GLY:HA3	1:D:67:GLU:O	2.20	0.41
1:K:15:LYS:HB3	1:K:66:PHE:HB3	2.03	0.41
1:A:510:VAL:O	1:A:511:ALA:C	2.57	0.41
1:B:16:MET:HE1	1:B:514:MET:HB3	2.03	0.41
1:I:421:ARG:NH2	1:I:469:VAL:O	2.51	0.41
1:E:16:MET:HE1	1:E:514:MET:HB3	2.03	0.41
1:H:200:LEU:CD1	1:H:276:VAL:HA	2.49	0.41
1:M:452:ARG:HG2	1:M:452:ARG:NH1	2.29	0.41
1:A:39:VAL:HG12	1:G:69:MET:CE	2.51	0.41
1:E:288:MET:O	1:E:291:ASP:HB2	2.21	0.41
1:F:288:MET:CG	1:F:368:ARG:HD2	2.49	0.41
1:B:444:LEU:O	1:B:447:MET:HB2	2.20	0.41
1:F:361:ASP:O	1:F:365:LEU:HD23	2.21	0.41
1:D:288:MET:O	1:D:291:ASP:HB2	2.21	0.41
1:B:365:LEU:O	1:B:369:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:GLU:OE1	2:Q:24:GLY:HA3	2.21	0.41
1:J:342:ILE:O	1:J:346:VAL:HG23	2.21	0.41
1:D:150:ILE:CD1	1:D:493:ILE:HA	2.51	0.41
1:J:234:LEU:N	1:J:235:PRO:HD2	2.36	0.41
1:K:234:LEU:N	1:K:235:PRO:HD2	2.36	0.41
1:L:266:THR:HG22	1:L:273:VAL:H	1.85	0.41
1:B:247:LEU:O	1:B:273:VAL:HA	2.21	0.41
1:F:259:LEU:O	1:F:263:VAL:HG23	2.21	0.41
1:J:43:SER:HB2	1:J:44:PHE:CD1	2.55	0.41
1:N:138:CYS:SG	1:N:144:ILE:HD13	2.61	0.41
1:K:455:VAL:HG13	1:K:460:GLU:HB2	2.02	0.41
1:D:286:LYS:HE2	1:D:304:GLU:OE1	2.20	0.41
1:F:519:CYS:HB3	1:G:38:VAL:HG22	2.03	0.41
1:A:6:VAL:HG23	1:A:6:VAL:O	2.20	0.41
1:M:213:VAL:O	1:M:324:VAL:HA	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:F:102:GLU:HB3	1:F:442:VAL:HG22	2.03	0.41
1:A:348:GLN:HE21	1:A:348:GLN:HB3	1.68	0.41
1:E:19:GLY:HA3	1:E:67:GLU:O	2.21	0.41
1:I:100:ILE:HG23	1:I:104:LEU:HD22	2.02	0.41
1:C:288:MET:CG	1:C:368:ARG:HD2	2.49	0.41
1:J:34:LYS:HB2	1:J:458:CYS:SG	2.61	0.41
1:G:95:LEU:O	1:G:99:ILE:HG13	2.21	0.41
1:J:22:VAL:HG11	1:J:62:LEU:HD21	2.02	0.41
1:N:461:GLU:HA	1:N:462:PRO:HD3	1.93	0.41
1:L:221:LEU:HD12	1:L:249:ILE:HG23	2.02	0.41
1:I:513:LEU:HA	1:I:513:LEU:HD12	1.94	0.41
1:F:19:GLY:HA3	1:F:67:GLU:O	2.21	0.40
1:B:204:PHE:CG	1:B:204:PHE:O	2.74	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:F:288:MET:O	1:F:291:ASP:HB2	2.21	0.40
1:E:349:ILE:HG23	1:E:365:LEU:HD12	2.01	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
1:H:381:VAL:HG21	1:H:393:LYS:HA	2.03	0.40
2:U:46:GLY:HA3	2:U:55:LYS:O	2.21	0.40
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.92	0.40
1:F:42:LYS:HE2	1:F:48:THR:OG1	2.22	0.40
1:L:419:LEU:HD22	1:L:500:THR:CG2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ASP:O	1:C:365:LEU:HD23	2.21	0.40
1:H:521:VAL:HB	1:N:40:LEU:HD12	2.04	0.40
1:G:461:GLU:HA	1:G:462:PRO:HD3	1.84	0.40
1:J:11:ASP:O	1:J:12:ALA:C	2.59	0.40
1:C:404:ARG:O	1:C:408:GLU:HG2	2.21	0.40
2:R:43:VAL:HG13	2:R:57:LEU:HD12	2.04	0.40
1:C:301:ILE:HG22	1:C:301:ILE:O	2.22	0.40
1:J:433:ASN:HA	1:J:433:ASN:HD22	1.57	0.40
1:E:327:LYS:O	1:E:327:LYS:HG2	2.20	0.40
1:C:413:ALA:HB3	1:C:417:VAL:HG13	2.02	0.40
1:B:16:MET:CE	1:B:514:MET:HB3	2.51	0.40
1:G:288:MET:CG	1:G:368:ARG:HD2	2.48	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:L:429:LEU:HB3	1:L:440:ILE:HG21	2.04	0.40
1:H:38:VAL:HG12	1:H:40:LEU:HD13	2.03	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:E:301:ILE:HG21	1:E:309:LEU:HD12	2.04	0.40
1:D:301:ILE:HG21	1:D:309:LEU:HD12	2.04	0.40
1:H:496:PRO:HB2	1:H:499:VAL:HG13	2.04	0.40
1:L:350:ARG:HA	1:L:353:ILE:HD12	2.04	0.40
1:I:433:ASN:OD1	1:I:435:ASP:HB2	2.22	0.40
1:B:461:GLU:HA	1:B:462:PRO:HD3	1.83	0.40
1:M:201:SER:HA	1:M:202:PRO:HD3	1.95	0.40
1:A:452:ARG:HH11	1:A:452:ARG:HG2	1.86	0.40
1:D:204:PHE:O	1:D:204:PHE:CG	2.74	0.40
1:E:33:PRO:HG3	4:E:704:ADP:C6	2.56	0.40
1:N:32:GLY:CA	1:N:454:ILE:HG23	2.52	0.40
1:A:301:ILE:O	1:A:301:ILE:HG22	2.21	0.40
1:E:247:LEU:O	1:E:273:VAL:HA	2.21	0.40
1:M:266:THR:HG22	1:M:273:VAL:H	1.86	0.40
1:G:381:VAL:CG1	1:G:392:LYS:HG3	2.52	0.40
1:D:219:PHE:HB3	1:D:317:LEU:HD13	2.02	0.40
1:F:286:LYS:HE2	1:F:304:GLU:OE1	2.22	0.40
1:H:201:SER:HA	1:H:202:PRO:HD3	1.95	0.40
2:O:55:LYS:H	2:O:55:LYS:HE2	1.87	0.40
1:E:452:ARG:HG2	1:E:452:ARG:HH11	1.86	0.40
1:E:413:ALA:HB3	1:E:417:VAL:HG13	2.04	0.40
1:G:197:ARG:H	1:G:329:THR:HA	1.87	0.40
1:D:90:THR:O	1:D:94:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:THR:HG22	1:H:156:GLU:HA	2.04	0.40
1:E:90:THR:O	1:E:94:VAL:HG23	2.21	0.40
1:J:198:GLY:HA3	1:J:328:ASP:HA	2.03	0.40
1:G:28:LYS:O	1:G:29:VAL:C	2.59	0.40
1:H:461:GLU:HA	1:H:462:PRO:HD3	1.90	0.40
1:B:301:ILE:HG21	1:B:309:LEU:HD12	2.04	0.40
2:P:46:GLY:HA3	2:P:55:LYS:O	2.22	0.40
1:D:449:ALA:HB3	1:D:450:PRO:HD3	2.04	0.40
1:B:404:ARG:O	1:B:408:GLU:HG2	2.21	0.40
1:K:72:GLN:HE22	1:K:75:LYS:NZ	2.20	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%)	24	66
1	B	522/524 (100%)	484 (93%)	33 (6%)	5 (1%)	19	61
1	C	522/524 (100%)	484 (93%)	34 (6%)	4 (1%)	24	66
1	D	522/524 (100%)	485 (93%)	32 (6%)	5 (1%)	19	61
1	E	522/524 (100%)	489 (94%)	29 (6%)	4 (1%)	24	66
1	F	522/524 (100%)	490 (94%)	27 (5%)	5 (1%)	19	61
1	G	522/524 (100%)	481 (92%)	36 (7%)	5 (1%)	19	61
1	H	522/524 (100%)	481 (92%)	36 (7%)	5 (1%)	19	61
1	I	522/524 (100%)	483 (92%)	32 (6%)	7 (1%)	15	53
1	J	522/524 (100%)	480 (92%)	38 (7%)	4 (1%)	24	66
1	K	522/524 (100%)	479 (92%)	38 (7%)	5 (1%)	19	61
1	L	522/524 (100%)	483 (92%)	34 (6%)	5 (1%)	19	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	522/524 (100%)	480 (92%)	37 (7%)	5 (1%)	19 61
1	N	522/524 (100%)	483 (92%)	35 (7%)	4 (1%)	24 66
2	O	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2 14
2	P	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2 14
2	Q	95/97 (98%)	76 (80%)	13 (14%)	6 (6%)	2 9
2	R	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2 14
2	S	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2 14
2	T	95/97 (98%)	76 (80%)	13 (14%)	6 (6%)	2 9
2	U	95/97 (98%)	76 (80%)	14 (15%)	5 (5%)	2 14
All	All	7973/8015 (100%)	7303 (92%)	566 (7%)	104 (1%)	15 53

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

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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

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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 (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/404 (100%)	359 (89%)	45 (11%)	8	29
1	B	404/404 (100%)	358 (89%)	46 (11%)	7	28
1	C	404/404 (100%)	356 (88%)	48 (12%)	6	26
1	D	404/404 (100%)	357 (88%)	47 (12%)	7	27
1	E	404/404 (100%)	358 (89%)	46 (11%)	7	28
1	F	404/404 (100%)	357 (88%)	47 (12%)	7	27
1	G	404/404 (100%)	354 (88%)	50 (12%)	6	24
1	H	404/404 (100%)	347 (86%)	57 (14%)	4	19
1	I	404/404 (100%)	349 (86%)	55 (14%)	5	20
1	J	404/404 (100%)	349 (86%)	55 (14%)	5	20
1	K	404/404 (100%)	347 (86%)	57 (14%)	4	19
1	L	404/404 (100%)	348 (86%)	56 (14%)	4	19
1	M	404/404 (100%)	347 (86%)	57 (14%)	4	19
1	N	404/404 (100%)	349 (86%)	55 (14%)	5	20
2	O	80/80 (100%)	70 (88%)	10 (12%)	6	24
2	P	80/80 (100%)	70 (88%)	10 (12%)	6	24
2	Q	80/80 (100%)	70 (88%)	10 (12%)	6	24
2	R	80/80 (100%)	69 (86%)	11 (14%)	4	20
2	S	80/80 (100%)	69 (86%)	11 (14%)	4	20
2	T	80/80 (100%)	70 (88%)	10 (12%)	6	24
2	U	80/80 (100%)	69 (86%)	11 (14%)	4	20
All	All	6216/6216 (100%)	5422 (87%)	794 (13%)	5	23

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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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	22,29,29	1.23	3 (13%)	27,45,45	3.17	10 (37%)
4	ADP	B	701	3	22,29,29	1.35	2 (9%)	27,45,45	2.97	7 (25%)
4	ADP	C	702	3	22,29,29	1.17	2 (9%)	27,45,45	3.15	11 (40%)
4	ADP	D	703	3	22,29,29	1.45	4 (18%)	27,45,45	3.27	8 (29%)
4	ADP	E	704	3	22,29,29	1.24	2 (9%)	27,45,45	2.96	7 (25%)
4	ADP	F	705	3	22,29,29	1.13	2 (9%)	27,45,45	2.91	6 (22%)
4	ADP	G	706	3	22,29,29	1.20	1 (4%)	27,45,45	3.02	9 (33%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	703	ADP	O4'-C1'	-3.03	1.37	1.41
4	A	700	ADP	O4'-C4'	-2.26	1.39	1.45
4	D	703	ADP	O4'-C4'	-2.13	1.40	1.45
4	A	700	ADP	C2-N1	2.25	1.38	1.33
4	E	704	ADP	C2-N1	2.50	1.38	1.33
4	F	705	ADP	C2-N1	2.53	1.38	1.33
4	C	702	ADP	C2-N1	2.63	1.38	1.33
4	D	703	ADP	C2-N1	2.97	1.39	1.33
4	B	701	ADP	C2-N1	3.07	1.39	1.33
4	F	705	ADP	C2-N3	3.13	1.37	1.32
4	C	702	ADP	C2-N3	3.17	1.37	1.32
4	E	704	ADP	C2-N3	3.36	1.38	1.32
4	A	700	ADP	C2-N3	3.38	1.38	1.32
4	D	703	ADP	C2-N3	3.48	1.38	1.32
4	B	701	ADP	C2-N3	3.74	1.38	1.32
4	G	706	ADP	C2-N3	3.99	1.39	1.32

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	703	ADP	N3-C2-N1	-13.37	118.65	128.89
4	A	700	ADP	N3-C2-N1	-12.61	119.24	128.89
4	F	705	ADP	N3-C2-N1	-12.02	119.69	128.89
4	C	702	ADP	N3-C2-N1	-11.63	119.99	128.89
4	E	704	ADP	N3-C2-N1	-11.59	120.02	128.89
4	B	701	ADP	N3-C2-N1	-11.43	120.14	128.89
4	G	706	ADP	N3-C2-N1	-11.07	120.42	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	702	ADP	PA-O3A-PB	-4.93	116.14	132.67
4	E	704	ADP	PA-O3A-PB	-4.82	116.52	132.67
4	G	706	ADP	PA-O3A-PB	-4.76	116.71	132.67
4	F	705	ADP	PA-O3A-PB	-4.68	116.96	132.67
4	A	700	ADP	PA-O3A-PB	-4.67	117.00	132.67
4	D	703	ADP	PA-O3A-PB	-4.67	117.01	132.67
4	B	701	ADP	PA-O3A-PB	-4.53	117.47	132.67
4	A	700	ADP	C1'-N9-C4	-4.50	120.16	126.94
4	E	704	ADP	C1'-N9-C4	-4.47	120.20	126.94
4	C	702	ADP	O3'-C3'-C4'	-4.41	97.82	111.05
4	B	701	ADP	C1'-N9-C4	-4.36	120.37	126.94
4	G	706	ADP	C4-C5-N7	-4.24	105.58	109.48
4	D	703	ADP	C1'-N9-C4	-4.18	120.64	126.94
4	B	701	ADP	C4-C5-N7	-4.11	105.70	109.48
4	G	706	ADP	O3'-C3'-C4'	-3.99	99.09	111.05
4	B	701	ADP	O3'-C3'-C4'	-3.91	99.31	111.05
4	C	702	ADP	C4-C5-N7	-3.86	105.93	109.48
4	C	702	ADP	C1'-N9-C4	-3.71	121.35	126.94
4	E	704	ADP	C4-C5-N7	-3.66	106.11	109.48
4	F	705	ADP	C1'-N9-C4	-3.51	121.65	126.94
4	G	706	ADP	C1'-N9-C4	-3.43	121.76	126.94
4	A	700	ADP	C4-C5-N7	-3.38	106.37	109.48
4	D	703	ADP	O3'-C3'-C4'	-3.27	101.23	111.05
4	F	705	ADP	C4-C5-N7	-3.18	106.55	109.48
4	A	700	ADP	O3'-C3'-C4'	-2.93	102.27	111.05
4	D	703	ADP	C4-C5-N7	-2.79	106.91	109.48
4	F	705	ADP	O3'-C3'-C4'	-2.66	103.07	111.05
4	E	704	ADP	O3'-C3'-C4'	-2.51	103.51	111.05
4	C	702	ADP	O3A-PA-O5'	-2.30	96.84	102.94
4	G	706	ADP	O3'-C3'-C2'	-2.28	104.43	111.83
4	A	700	ADP	N6-C6-N1	-2.24	114.40	119.20
4	A	700	ADP	O3'-C3'-C2'	-2.06	105.11	111.83
4	B	701	ADP	C2'-C3'-C4'	2.05	106.83	102.61
4	E	704	ADP	C2'-C3'-C4'	2.09	106.90	102.61
4	C	702	ADP	O3B-PB-O3A	2.25	115.28	105.09
4	C	702	ADP	O2B-PB-O1B	2.28	117.93	110.58
4	C	702	ADP	C2'-C3'-C4'	2.29	107.33	102.61
4	D	703	ADP	O2B-PB-O1B	2.37	118.21	110.58
4	A	700	ADP	C2'-C3'-C4'	2.42	107.59	102.61
4	G	706	ADP	O5'-C5'-C4'	2.61	118.75	109.12
4	A	700	ADP	C4'-O4'-C1'	2.67	112.65	109.72
4	C	702	ADP	O5'-C5'-C4'	2.68	119.00	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	700	ADP	O5'-C5'-C4'	2.71	119.11	109.12
4	D	703	ADP	C4'-O4'-C1'	2.76	112.75	109.72
4	G	706	ADP	C2'-C3'-C4'	2.76	108.29	102.61
4	B	701	ADP	O5'-C5'-C4'	2.78	119.36	109.12
4	F	705	ADP	O5'-C5'-C4'	2.82	119.50	109.12
4	D	703	ADP	O5'-C5'-C4'	2.89	119.78	109.12
4	E	704	ADP	O5'-C5'-C4'	3.05	120.35	109.12
4	C	702	ADP	C4'-O4'-C1'	3.11	113.14	109.72
4	G	706	ADP	C4'-O4'-C1'	3.37	113.43	109.72

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	524/524 (100%)	0.62	61 (11%) 6 2	5, 7, 9, 10	0
1	B	524/524 (100%)	0.72	60 (11%) 6 2	5, 7, 9, 10	0
1	C	524/524 (100%)	0.51	51 (9%) 10 4	5, 7, 9, 10	0
1	D	524/524 (100%)	0.54	55 (10%) 8 3	5, 7, 9, 10	0
1	E	524/524 (100%)	0.82	69 (13%) 4 2	5, 7, 9, 10	0
1	F	524/524 (100%)	0.88	73 (13%) 4 1	5, 7, 9, 10	0
1	G	524/524 (100%)	0.71	67 (12%) 5 2	5, 7, 9, 10	0
1	H	524/524 (100%)	0.35	22 (4%) 40 16	6, 7, 9, 10	0
1	I	524/524 (100%)	0.31	13 (2%) 61 30	5, 7, 9, 10	0
1	J	524/524 (100%)	0.44	29 (5%) 29 11	5, 7, 9, 10	0
1	K	524/524 (100%)	0.60	47 (8%) 12 4	5, 7, 9, 10	0
1	L	524/524 (100%)	0.65	46 (8%) 12 4	5, 7, 9, 10	0
1	M	524/524 (100%)	0.50	38 (7%) 18 6	5, 7, 9, 10	0
1	N	524/524 (100%)	0.54	36 (6%) 20 7	5, 7, 9, 10	0
2	O	97/97 (100%)	1.76	36 (37%) 0 0	7, 7, 8, 8	0
2	P	97/97 (100%)	1.65	29 (29%) 1 0	7, 7, 8, 8	0
2	Q	97/97 (100%)	1.44	32 (32%) 0 0	7, 7, 8, 8	0
2	R	97/97 (100%)	1.53	25 (25%) 1 1	7, 7, 8, 8	0
2	S	97/97 (100%)	1.76	29 (29%) 1 0	7, 7, 8, 8	0
2	T	97/97 (100%)	1.60	28 (28%) 1 0	7, 7, 8, 8	0
2	U	97/97 (100%)	3.23	74 (76%) 0 0	7, 7, 8, 8	0
All	All	8015/8015 (100%)	0.69	920 (11%) 6 2	5, 7, 9, 10	0

All (920) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	361	ASP	17.3
1	F	361	ASP	11.0
1	E	361	ASP	10.4
1	A	361	ASP	10.2
1	G	199	TYR	9.2
1	G	361	ASP	9.2
1	G	208	PRO	8.8
1	E	353	ILE	8.7
1	A	353	ILE	8.3
2	U	32	ALA	8.3
1	B	361	ASP	8.3
1	F	357	THR	8.0
1	D	361	ASP	7.8
1	L	357	THR	7.6
1	B	353	ILE	7.5
1	D	212	ALA	7.5
1	A	357	THR	7.4
2	S	32	ALA	7.3
1	B	355	GLU	7.3
1	F	355	GLU	7.3
1	A	321	LYS	7.3
1	E	281	PHE	7.2
1	F	353	ILE	7.2
1	L	264	VAL	7.2
2	P	32	ALA	7.1
2	T	97	ALA	7.0
1	C	212	ALA	7.0
2	U	33	ALA	7.0
1	B	365	LEU	6.9
1	C	357	THR	6.9
1	I	264	VAL	6.9
2	O	97	ALA	6.8
2	P	23	GLY	6.8
2	U	30	SER	6.8
1	A	208	PRO	6.8
1	D	357	THR	6.8
2	T	18	GLU	6.7
2	O	25	ILE	6.7
1	D	365	LEU	6.6
1	B	357	THR	6.6
2	U	17	VAL	6.6
1	F	210	THR	6.6
1	A	365	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
1	G	357	THR	6.5
2	R	17	VAL	6.5
1	F	172	GLU	6.5
2	U	31	ALA	6.4
1	F	349	ILE	6.4
1	I	268	ARG	6.3
2	S	31	ALA	6.3
1	C	353	ILE	6.3
1	G	353	ILE	6.2
2	P	18	GLU	6.1
1	K	356	ALA	6.1
1	G	362	ARG	6.1
1	A	349	ILE	6.0
1	A	360	TYR	6.0
1	G	251	ALA	6.0
2	R	18	GLU	6.0
2	U	22	ALA	6.0
2	U	18	GLU	6.0
1	E	357	THR	6.0
2	U	51	ASN	5.9
1	E	280	GLY	5.9
2	S	51	ASN	5.9
2	Q	18	GLU	5.9
1	G	214	GLU	5.8
1	E	365	LEU	5.8
1	C	270	ILE	5.8
1	M	358	SER	5.8
2	T	25	ILE	5.8
1	E	338	GLU	5.8
1	D	353	ILE	5.8
2	S	33	ALA	5.7
1	C	267	MET	5.7
2	O	72	GLY	5.7
2	R	51	ASN	5.7
1	C	360	TYR	5.6
1	K	360	TYR	5.6
1	E	340	ALA	5.6
1	M	360	TYR	5.5
2	U	97	ALA	5.5
1	F	171	LYS	5.5
2	U	28	THR	5.5
2	T	52	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	N	183	LEU	5.4
2	R	25	ILE	5.4
1	M	357	THR	5.4
1	G	212	ALA	5.4
1	E	364	LYS	5.4
1	H	360	TYR	5.4
1	B	349	ILE	5.4
1	E	354	GLU	5.3
1	K	186	GLU	5.3
1	B	348	GLN	5.3
2	U	71	TYR	5.3
2	Q	25	ILE	5.3
1	E	279	PRO	5.2
2	P	1	MET	5.2
1	G	195	PHE	5.2
1	B	279	PRO	5.2
2	U	19	THR	5.2
1	F	212	ALA	5.1
1	C	210	THR	5.1
2	S	18	GLU	5.1
1	B	284	ARG	5.1
2	R	80	ASN	5.1
2	O	83	VAL	5.0
1	C	199	TYR	5.0
1	G	210	THR	5.0
1	A	203	TYR	5.0
2	O	17	VAL	5.0
1	F	375	GLY	5.0
2	U	1	MET	5.0
1	B	364	LYS	5.0
1	E	355	GLU	5.0
1	A	284	ARG	5.0
1	D	349	ILE	4.9
2	O	1	MET	4.9
1	G	349	ILE	4.9
1	D	209	GLU	4.9
2	U	21	SER	4.9
1	L	353	ILE	4.9
2	S	17	VAL	4.9
1	F	267	MET	4.9
2	U	25	ILE	4.9
2	P	51	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
2	S	30	SER	4.9
1	E	321	LYS	4.9
1	G	256	GLY	4.8
2	S	80	ASN	4.8
2	S	97	ALA	4.8
1	D	284	ARG	4.8
1	L	177	VAL	4.8
2	U	26	VAL	4.8
1	J	365	LEU	4.7
2	S	1	MET	4.7
1	A	355	GLU	4.7
1	E	360	TYR	4.7
1	F	331	THR	4.7
2	U	69	ASP	4.7
1	N	360	TYR	4.7
1	E	209	GLU	4.7
1	B	192	GLY	4.7
1	E	284	ARG	4.7
1	L	268	ARG	4.7
1	D	199	TYR	4.6
1	J	353	ILE	4.6
2	T	82	GLU	4.6
2	U	23	GLY	4.6
1	F	352	GLN	4.6
2	P	31	ALA	4.6
1	B	346	VAL	4.6
2	U	78	ILE	4.6
1	G	360	TYR	4.6
2	Q	32	ALA	4.6
2	R	1	MET	4.6
1	E	210	THR	4.6
1	G	354	GLU	4.6
1	N	266	THR	4.5
1	K	188	ASP	4.5
2	P	49	LEU	4.5
1	I	357	THR	4.5
1	N	357	THR	4.5
1	A	364	LYS	4.5
2	U	16	GLU	4.5
2	Q	71	TYR	4.5
2	P	33	ALA	4.4
1	G	350	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	365	LEU	4.4
1	L	349	ILE	4.4
1	D	268	ARG	4.4
1	B	352	GLN	4.4
2	P	20	LYS	4.4
1	D	321	LYS	4.4
1	F	364	LYS	4.3
2	P	67	PHE	4.3
2	Q	27	LEU	4.3
1	D	338	GLU	4.3
1	D	360	TYR	4.3
2	U	20	LYS	4.3
1	F	374	GLY	4.3
1	E	341	ALA	4.3
1	B	354	GLU	4.3
2	O	21	SER	4.2
1	M	264	VAL	4.2
2	S	83	VAL	4.2
2	S	21	SER	4.2
2	U	80	ASN	4.2
2	U	65	VAL	4.2
2	T	17	VAL	4.2
2	R	79	ASP	4.2
2	U	52	GLY	4.2
2	U	27	LEU	4.2
1	C	362	ARG	4.1
1	G	279	PRO	4.1
2	Q	78	ILE	4.1
1	B	351	GLN	4.1
1	B	350	ARG	4.1
1	C	251	ALA	4.1
2	R	20	LYS	4.1
1	M	284	ARG	4.1
2	S	66	ILE	4.1
2	U	79	ASP	4.1
2	O	31	ALA	4.1
1	C	349	ILE	4.1
2	P	71	TYR	4.1
2	U	35	SER	4.1
1	E	346	VAL	4.1
1	F	251	ALA	4.1
1	E	349	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
2	P	25	ILE	4.0
2	R	21	SER	4.0
2	U	72	GLY	4.0
1	K	187	LEU	4.0
2	T	71	TYR	4.0
2	S	36	THR	4.0
1	J	356	ALA	4.0
1	E	352	GLN	4.0
2	P	85	ILE	4.0
2	U	83	VAL	4.0
1	F	350	ARG	4.0
2	O	22	ALA	4.0
1	C	271	VAL	4.0
2	O	66	ILE	4.0
2	R	83	VAL	4.0
1	G	198	GLY	4.0
1	K	295	LEU	4.0
1	M	268	ARG	4.0
2	U	75	SER	3.9
2	R	30	SER	3.9
1	E	195	PHE	3.9
2	O	36	THR	3.9
2	U	49	LEU	3.9
1	D	172	GLU	3.9
2	T	80	ASN	3.9
1	F	273	VAL	3.9
1	G	222	LEU	3.9
2	U	38	GLY	3.9
2	O	32	ALA	3.9
1	A	238	GLU	3.9
1	A	338	GLU	3.9
1	J	181	THR	3.9
2	T	72	GLY	3.8
1	I	360	TYR	3.8
1	L	362	ARG	3.8
2	O	80	ASN	3.8
1	B	360	TYR	3.8
1	F	360	TYR	3.8
2	T	33	ALA	3.8
1	B	208	PRO	3.8
2	T	51	ASN	3.8
1	A	320	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	365	LEU	3.7
1	B	224	ASP	3.7
1	I	270	ILE	3.7
2	Q	80	ASN	3.7
1	F	203	TYR	3.7
1	F	214	GLU	3.7
1	C	279	PRO	3.7
1	E	334	ASP	3.7
1	K	349	ILE	3.7
2	U	53	GLU	3.7
2	O	51	ASN	3.7
1	C	365	LEU	3.7
1	G	364	LYS	3.7
2	T	32	ALA	3.7
2	U	2	ASN	3.7
2	P	97	ALA	3.7
1	A	281	PHE	3.6
2	U	84	LEU	3.6
1	C	350	ARG	3.6
1	A	352	GLN	3.6
2	P	21	SER	3.6
1	E	371	LYS	3.6
1	J	366	GLN	3.6
1	F	377	ALA	3.6
1	E	256	GLY	3.6
2	U	67	PHE	3.6
1	N	186	GLU	3.6
2	O	18	GLU	3.6
1	J	330	THR	3.6
2	R	97	ALA	3.6
2	U	82	GLU	3.6
2	P	30	SER	3.6
2	S	67	PHE	3.6
1	J	372	LEU	3.5
2	P	17	VAL	3.5
1	M	349	ILE	3.5
1	C	358	SER	3.5
1	J	267	MET	3.5
1	C	284	ARG	3.5
2	T	53	GLU	3.5
2	O	82	GLU	3.5
1	G	203	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	174	VAL	3.5
1	F	323	VAL	3.5
1	J	223	ALA	3.4
1	B	203	TYR	3.4
1	G	209	GLU	3.4
1	L	270	ILE	3.4
2	U	10	VAL	3.4
1	A	230	ILE	3.4
1	H	356	ALA	3.4
1	K	185	ASP	3.4
1	N	350	ARG	3.4
1	K	372	LEU	3.4
1	L	267	MET	3.4
1	L	356	ALA	3.4
1	A	193	MET	3.4
2	Q	26	VAL	3.4
1	F	283	ASP	3.4
1	G	229	ASN	3.4
1	G	284	ARG	3.4
1	D	195	PHE	3.4
1	E	270	ILE	3.4
1	D	251	ALA	3.4
1	E	332	ILE	3.3
1	E	368	ARG	3.3
1	G	376	VAL	3.3
1	J	268	ARG	3.3
2	T	83	VAL	3.3
1	L	352	GLN	3.3
1	N	184	GLN	3.3
1	A	358	SER	3.3
2	Q	82	GLU	3.3
2	T	27	LEU	3.3
1	F	230	ILE	3.3
1	E	362	ARG	3.3
2	R	82	GLU	3.3
1	B	238	GLU	3.3
2	O	67	PHE	3.3
2	T	67	PHE	3.3
2	U	96	GLU	3.3
1	B	199	TYR	3.3
1	G	207	LYS	3.3
2	O	27	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	355	GLU	3.2
2	U	93	ALA	3.2
2	P	80	ASN	3.2
1	E	196	ASP	3.2
2	O	30	SER	3.2
1	F	356	ALA	3.2
2	O	38	GLY	3.2
2	R	22	ALA	3.2
2	Q	20	LYS	3.2
1	K	352	GLN	3.2
2	U	36	THR	3.2
1	J	396	VAL	3.2
2	S	71	TYR	3.2
2	Q	13	LYS	3.2
1	F	376	VAL	3.2
1	G	371	LYS	3.2
1	A	322	ARG	3.2
1	G	267	MET	3.2
2	R	33	ALA	3.2
2	P	84	LEU	3.2
2	P	52	GLY	3.2
1	G	281	PHE	3.2
2	S	74	LYS	3.2
1	B	367	GLU	3.1
2	U	66	ILE	3.1
2	U	85	ILE	3.1
1	D	362	ARG	3.1
1	G	172	GLU	3.1
1	G	321	LYS	3.1
1	A	271	VAL	3.1
1	D	203	TYR	3.1
2	U	92	LEU	3.1
1	F	281	PHE	3.1
1	A	172	GLU	3.1
1	A	376	VAL	3.1
1	F	213	VAL	3.1
1	K	384	ALA	3.1
1	D	309	LEU	3.1
1	G	271	VAL	3.1
1	C	242	LYS	3.1
2	S	20	LYS	3.1
1	G	332	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	3.1
2	U	39	GLU	3.1
2	U	29	GLY	3.1
1	F	170	GLY	3.1
1	G	211	GLY	3.1
1	F	288	MET	3.1
1	B	278	ALA	3.1
1	F	209	GLU	3.1
1	F	351	GLN	3.1
1	H	342	ILE	3.1
2	Q	66	ILE	3.1
1	J	193	MET	3.1
1	M	233	MET	3.1
1	E	350	ARG	3.1
1	N	525	PRO	3.1
1	I	267	MET	3.0
1	A	210	THR	3.0
2	T	28	THR	3.0
2	U	41	LEU	3.0
1	B	44	PHE	3.0
1	F	284	ARG	3.0
1	B	267	MET	3.0
1	M	186	GLU	3.0
1	F	358	SER	3.0
1	A	209	GLU	3.0
1	C	214	GLU	3.0
1	A	279	PRO	3.0
2	U	81	GLU	3.0
1	H	186	GLU	3.0
1	M	208	PRO	3.0
2	Q	65	VAL	3.0
1	E	44	PHE	3.0
1	B	223	ALA	3.0
2	U	12	VAL	3.0
1	F	338	GLU	3.0
1	M	372	LEU	3.0
1	B	212	ALA	3.0
1	G	359	ASP	3.0
1	D	352	GLN	3.0
1	G	280	GLY	3.0
2	R	72	GLY	3.0
1	G	309	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	347	ALA	3.0
1	D	279	PRO	3.0
2	U	68	ASN	3.0
1	D	314	LEU	3.0
2	R	52	GLY	2.9
1	B	193	MET	2.9
2	U	13	LYS	2.9
1	B	214	GLU	2.9
1	L	360	TYR	2.9
1	M	243	ALA	2.9
1	N	242	LYS	2.9
2	R	73	VAL	2.9
2	S	73	VAL	2.9
1	F	195	PHE	2.9
1	A	256	GLY	2.9
2	O	26	VAL	2.9
1	M	176	THR	2.9
1	G	322	ARG	2.9
1	K	44	PHE	2.9
1	L	354	GLU	2.9
2	U	24	GLY	2.9
1	K	144	ILE	2.9
1	C	223	ALA	2.9
1	L	271	VAL	2.9
2	Q	12	VAL	2.9
1	L	180	GLY	2.9
1	N	369	VAL	2.9
1	M	361	ASP	2.9
1	E	172	GLU	2.9
1	L	215	LEU	2.9
1	D	267	MET	2.9
2	O	23	GLY	2.9
1	C	172	GLU	2.9
1	M	185	ASP	2.9
1	A	251	ALA	2.9
1	N	361	ASP	2.8
2	S	85	ILE	2.8
1	H	44	PHE	2.8
1	G	340	ALA	2.8
2	U	76	GLU	2.8
1	C	203	TYR	2.8
1	E	203	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	S	13	LYS	2.8
1	N	267	MET	2.8
2	O	33	ALA	2.8
2	U	34	LYS	2.8
1	E	303	GLU	2.8
1	E	336	VAL	2.8
1	E	331	THR	2.8
1	J	357	THR	2.8
1	D	192	GLY	2.8
1	K	268	ARG	2.8
2	O	37	ARG	2.8
2	T	30	SER	2.8
1	B	362	ARG	2.8
2	U	70	GLY	2.8
1	B	209	GLU	2.8
1	B	338	GLU	2.8
2	U	77	LYS	2.8
1	A	373	ALA	2.8
1	K	193	MET	2.8
1	G	346	VAL	2.8
1	F	44	PHE	2.8
1	G	277	LYS	2.8
1	A	195	PHE	2.8
1	D	257	GLU	2.8
2	U	3	ILE	2.8
1	N	165	ALA	2.8
1	C	288	MET	2.8
2	S	65	VAL	2.8
1	A	214	GLU	2.8
1	M	175	ILE	2.8
2	S	69	ASP	2.8
1	K	294	THR	2.8
1	E	216	GLU	2.7
1	A	270	ILE	2.7
1	D	204	PHE	2.7
1	G	247	LEU	2.7
1	H	372	LEU	2.7
2	S	78	ILE	2.7
1	K	350	ARG	2.7
1	J	352	GLN	2.7
1	C	211	GLY	2.7
1	C	195	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	364	LYS	2.7
1	C	209	GLU	2.7
1	D	214	GLU	2.7
1	M	244	GLY	2.7
1	F	373	ALA	2.7
1	N	238	GLU	2.7
1	N	342	ILE	2.7
2	Q	49	LEU	2.7
2	Q	50	GLU	2.7
1	K	346	VAL	2.7
1	D	208	PRO	2.7
2	O	19	THR	2.7
1	D	237	LEU	2.7
1	F	333	ILE	2.7
1	G	215	LEU	2.7
1	L	221	LEU	2.7
1	M	138	CYS	2.7
2	T	21	SER	2.7
1	E	322	ARG	2.7
1	A	229	ASN	2.7
1	B	277	LYS	2.7
1	B	382	GLY	2.7
1	E	324	VAL	2.7
2	O	95	VAL	2.7
1	H	193	MET	2.7
1	I	44	PHE	2.7
1	A	345	ARG	2.7
1	B	230	ILE	2.7
1	F	304	GLU	2.7
2	Q	73	VAL	2.7
1	L	305	ILE	2.7
1	E	286	LYS	2.7
1	K	171	LYS	2.7
2	T	20	LYS	2.7
1	J	44	PHE	2.7
1	L	156	GLU	2.7
1	C	278	ALA	2.7
2	Q	33	ALA	2.7
2	P	2	ASN	2.6
1	F	386	GLU	2.6
1	K	196	ASP	2.6
1	C	364	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	338	GLU	2.6
2	U	50	GLU	2.6
1	B	237	LEU	2.6
2	O	71	TYR	2.6
2	S	41	LEU	2.6
2	S	84	LEU	2.6
2	U	86	MET	2.6
1	K	381	VAL	2.6
2	R	66	ILE	2.6
1	A	356	ALA	2.6
1	B	283	ASP	2.6
1	D	364	LYS	2.6
1	K	291	ASP	2.6
2	Q	55	LYS	2.6
1	B	322	ARG	2.6
1	E	231	ARG	2.6
1	B	321	LYS	2.6
1	B	327	LYS	2.6
1	F	319	GLN	2.6
2	P	72	GLY	2.6
1	B	368	ARG	2.6
1	G	171	LYS	2.6
1	I	349	ILE	2.6
2	R	28	THR	2.6
1	J	183	LEU	2.6
2	O	78	ILE	2.6
1	G	347	ALA	2.6
1	G	351	GLN	2.6
1	H	525	PRO	2.6
1	F	272	LYS	2.6
1	M	44	PHE	2.6
1	C	355	GLU	2.6
1	C	138	CYS	2.6
1	J	381	VAL	2.6
2	T	73	VAL	2.6
2	Q	67	PHE	2.6
1	J	266	THR	2.6
1	F	173	GLY	2.6
1	B	320	ALA	2.6
1	B	340	ALA	2.6
1	F	341	ALA	2.6
1	G	320	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	P	93	ALA	2.6
1	A	346	VAL	2.6
1	D	376	VAL	2.6
1	C	268	ARG	2.5
1	G	355	GLU	2.5
1	M	365	LEU	2.5
1	H	357	THR	2.5
1	J	311	LYS	2.5
1	K	368	ARG	2.5
1	B	171	LYS	2.5
1	B	331	THR	2.5
1	E	359	ASP	2.5
1	N	189	VAL	2.5
2	Q	17	VAL	2.5
2	U	54	VAL	2.5
2	U	73	VAL	2.5
1	F	181	THR	2.5
1	G	334	ASP	2.5
1	J	233	MET	2.5
1	C	208	PRO	2.5
1	N	180	GLY	2.5
1	N	365	LEU	2.5
1	F	322	ARG	2.5
1	C	347	ALA	2.5
1	K	270	ILE	2.5
1	E	214	GLU	2.5
1	N	396	VAL	2.5
1	A	368	ARG	2.5
1	E	309	LEU	2.5
1	H	368	ARG	2.5
2	Q	38	GLY	2.5
1	A	212	ALA	2.5
1	C	356	ALA	2.5
1	F	193	MET	2.5
2	T	76	GLU	2.5
1	D	358	SER	2.5
1	M	161	LEU	2.5
2	Q	84	LEU	2.5
1	F	359	ASP	2.5
1	B	358	SER	2.5
1	L	266	THR	2.5
1	B	309	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	R	16	GLU	2.5
1	D	196	ASP	2.5
1	K	158	VAL	2.5
1	L	195	PHE	2.5
2	R	26	VAL	2.5
2	U	74	LYS	2.5
1	D	322	ARG	2.5
1	A	359	ASP	2.5
1	L	484	GLU	2.4
1	A	223	ALA	2.4
2	S	77	LYS	2.4
1	B	280	GLY	2.4
1	L	269	GLY	2.4
1	F	362	ARG	2.4
1	F	138	CYS	2.4
1	L	63	GLU	2.4
1	N	187	LEU	2.4
1	A	348	GLN	2.4
2	P	74	LYS	2.4
1	K	373	ALA	2.4
1	K	379	ILE	2.4
1	G	291	ASP	2.4
1	K	297	GLY	2.4
1	A	324	VAL	2.4
1	H	268	ARG	2.4
1	D	171	LYS	2.4
1	H	364	LYS	2.4
2	O	75	SER	2.4
2	O	65	VAL	2.4
2	U	90	ASP	2.4
1	D	238	GLU	2.4
1	E	372	LEU	2.4
1	N	372	LEU	2.4
1	B	275	ALA	2.4
1	J	175	ILE	2.4
1	L	313	THR	2.4
2	Q	85	ILE	2.4
2	R	71	TYR	2.4
1	C	354	GLU	2.4
1	F	309	LEU	2.4
2	O	49	LEU	2.4
1	F	162	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	349	ILE	2.4
2	U	55	LYS	2.4
1	C	308	GLU	2.4
1	G	252	GLU	2.4
1	E	174	VAL	2.4
1	G	196	ASP	2.4
2	O	73	VAL	2.4
1	E	194	GLN	2.4
1	A	250	ILE	2.4
1	G	270	ILE	2.4
1	L	160	LYS	2.4
1	D	256	GLY	2.4
1	E	219	PHE	2.4
1	E	285	ARG	2.4
1	K	494	LEU	2.4
1	G	223	ALA	2.4
1	E	175	ILE	2.4
1	L	263	VAL	2.4
1	L	381	VAL	2.4
1	K	183	LEU	2.4
1	F	348	GLN	2.4
1	A	362	ARG	2.4
1	D	297	GLY	2.4
1	F	280	GLY	2.4
2	U	4	ARG	2.4
1	A	334	ASP	2.4
1	C	224	ASP	2.4
1	E	524	LEU	2.3
1	N	270	ILE	2.3
1	H	283	ASP	2.3
1	D	320	ALA	2.3
1	E	267	MET	2.3
1	M	275	ALA	2.3
1	M	340	ALA	2.3
1	G	227	ILE	2.3
2	U	46	GLY	2.3
1	G	324	VAL	2.3
1	M	236	VAL	2.3
1	A	274	ALA	2.3
1	I	266	THR	2.3
1	I	340	ALA	2.3
2	T	31	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	494	LEU	2.3
1	K	366	GLN	2.3
1	K	127	ALA	2.3
2	Q	19	THR	2.3
2	U	11	ILE	2.3
1	F	339	GLU	2.3
1	N	381	VAL	2.3
1	C	359	ASP	2.3
1	D	245	LYS	2.3
1	F	185	ASP	2.3
1	G	194	GLN	2.3
2	U	45	ASN	2.3
1	M	152	ALA	2.3
1	A	267	MET	2.3
1	G	204	PHE	2.3
1	H	369	VAL	2.3
1	N	172	GLU	2.3
1	A	237	LEU	2.3
1	E	477	GLY	2.3
1	A	248	LEU	2.3
1	F	215	LEU	2.3
1	D	340	ALA	2.3
2	Q	97	ALA	2.3
1	M	364	LYS	2.3
2	O	48	ILE	2.3
1	J	289	LEU	2.3
1	F	390	LYS	2.3
2	R	67	PHE	2.3
1	L	369	VAL	2.3
1	C	192	GLY	2.3
1	E	348	GLN	2.3
1	H	524	LEU	2.3
1	K	203	TYR	2.2
1	M	199	TYR	2.2
1	M	367	GLU	2.2
1	E	330	THR	2.2
1	K	480	ALA	2.2
1	M	362	ARG	2.2
2	P	82	GLU	2.2
2	U	47	ARG	2.2
1	G	358	SER	2.2
2	S	75	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	127	ALA	2.2
1	F	175	ILE	2.2
1	G	326	ASN	2.2
1	G	348	GLN	2.2
1	G	372	LEU	2.2
1	J	184	GLN	2.2
1	K	234	LEU	2.2
1	K	524	LEU	2.2
2	T	50	GLU	2.2
1	L	384	ALA	2.2
1	D	325	ILE	2.2
1	C	324	VAL	2.2
1	A	351	GLN	2.2
1	L	248	LEU	2.2
1	B	377	ALA	2.2
1	B	195	PHE	2.2
1	C	238	GLU	2.2
1	J	313	THR	2.2
1	D	371	LYS	2.2
1	E	192	GLY	2.2
1	D	200	LEU	2.2
1	F	234	LEU	2.2
2	U	14	ARG	2.2
1	E	301	ILE	2.2
1	K	175	ILE	2.2
1	E	375	GLY	2.2
1	N	431	GLY	2.2
1	F	229	ASN	2.2
1	L	494	LEU	2.2
1	B	217	SER	2.2
2	T	9	ARG	2.2
1	B	281	PHE	2.2
1	K	138	CYS	2.2
1	A	354	GLU	2.2
1	F	308	GLU	2.2
1	L	325	ILE	2.2
1	L	261	THR	2.2
1	D	288	MET	2.2
1	I	263	VAL	2.2
1	C	373	ALA	2.2
1	M	356	ALA	2.2
1	G	175	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	431	GLY	2.1
1	A	273	VAL	2.1
1	B	381	VAL	2.1
1	D	213	VAL	2.1
1	K	134	LEU	2.1
1	L	378	VAL	2.1
1	J	242	LYS	2.1
1	N	384	ALA	2.1
1	L	172	GLU	2.1
1	F	220	ILE	2.1
1	H	270	ILE	2.1
1	K	284	ARG	2.1
1	M	379	ILE	2.1
1	C	346	VAL	2.1
1	H	343	GLN	2.1
1	C	372	LEU	2.1
2	S	86	MET	2.1
1	L	265	ASN	2.1
1	M	238	GLU	2.1
2	P	79	ASP	2.1
1	A	249	ILE	2.1
1	L	175	ILE	2.1
1	I	343	GLN	2.1
1	L	176	THR	2.1
1	L	373	ALA	2.1
1	E	204	PHE	2.1
2	T	37	ARG	2.1
1	C	228	SER	2.1
2	O	64	ILE	2.1
2	P	66	ILE	2.1
2	T	66	ILE	2.1
1	D	525	PRO	2.1
1	E	237	LEU	2.1
1	L	365	LEU	2.1
1	A	347	ALA	2.1
1	D	275	ALA	2.1
1	K	388	GLU	2.1
1	F	371	LYS	2.1
1	H	350	ARG	2.1
1	J	350	ARG	2.1
1	A	314	LEU	2.1
1	B	324	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	172	GLU	2.1
1	K	357	THR	2.1
2	Q	79	ASP	2.1
1	C	322	ARG	2.1
1	H	284	ARG	2.1
1	K	525	PRO	2.1
1	N	177	VAL	2.1
1	N	271	VAL	2.1
2	Q	74	LYS	2.1
1	E	356	ALA	2.1
1	E	181	THR	2.1
1	K	428	ASP	2.1
1	C	250	ILE	2.1
1	F	379	ILE	2.1
1	M	168	LYS	2.1
2	Q	75	SER	2.1
1	A	262	LEU	2.1
1	K	200	LEU	2.1
1	M	240	VAL	2.1
1	D	356	ALA	2.1
1	E	212	ALA	2.1
2	U	42	ALA	2.1
2	O	90	ASP	2.1
1	B	172	GLU	2.1
1	N	63	GLU	2.1
1	E	351	GLN	2.1
1	I	358	SER	2.1
1	C	215	LEU	2.1
1	J	222	LEU	2.1
2	Q	83	VAL	2.1
1	D	303	GLU	2.0
1	D	304	GLU	2.0
1	N	353	ILE	2.0
1	N	388	GLU	2.0
2	U	64	ILE	2.0
2	U	94	ILE	2.0
1	A	234	LEU	2.0
1	F	324	VAL	2.0
1	N	259	LEU	2.0
2	O	84	LEU	2.0
1	F	207	LYS	2.0
1	G	233	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	242	LYS	2.0
1	K	160	LYS	2.0
1	N	196	ASP	2.0
1	A	319	GLN	2.0
1	H	157	THR	2.0
1	M	352	GLN	2.0
1	D	271	VAL	2.0
1	E	222	LEU	2.0
1	M	200	LEU	2.0
1	F	223	ALA	2.0
1	J	243	ALA	2.0
1	A	335	GLY	2.0
1	N	286	LYS	2.0
2	Q	22	ALA	2.0
2	U	87	SER	2.0
1	H	288	MET	2.0
1	H	349	ILE	2.0
1	J	270	ILE	2.0
1	L	144	ILE	2.0
1	A	294	THR	2.0
1	B	210	THR	2.0
1	L	203	TYR	2.0
1	C	314	LEU	2.0
1	D	215	LEU	2.0
1	M	521	VAL	2.0
2	P	45	ASN	2.0
2	T	84	LEU	2.0
1	G	275	ALA	2.0
1	E	208	PRO	2.0
2	P	76	GLU	2.0
2	Q	1	MET	2.0
1	E	294	THR	2.0
1	L	147	VAL	2.0
1	E	306	GLY	2.0
2	R	19	THR	2.0
1	D	281	PHE	2.0
1	N	358	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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	-1.22	6,8,9,10	0
4	ADP	C	702	27/27	0.95	0.13	-2.33	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.