



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:37 am BST

PDB ID : 1SVT
Title : Crystal structure of GroEL14-GroES7-(ADP-AlFx)7
Authors : Chaudhry, C.; Horwich, A.L.; Brunger, A.T.; Adams, P.D.
Deposited on : 2004-03-29
Resolution : 2.81 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

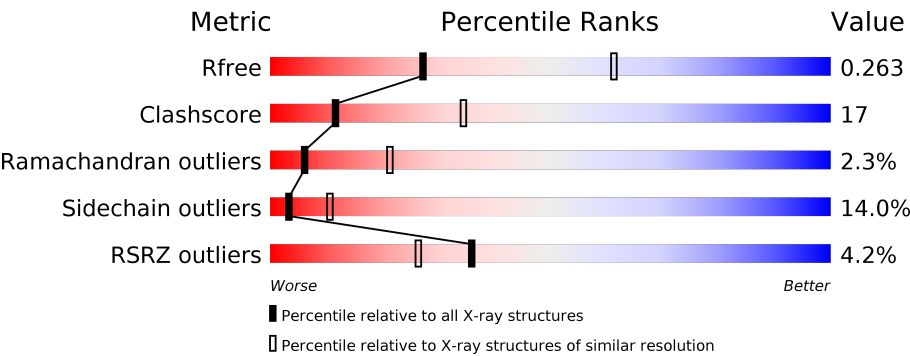
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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.





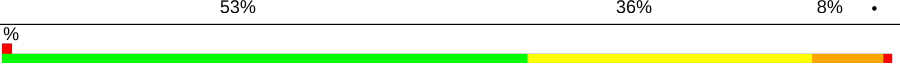
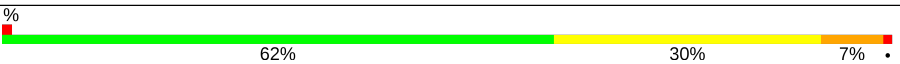





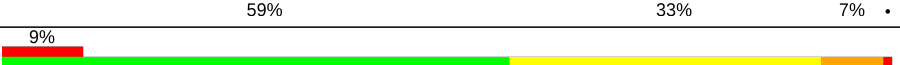

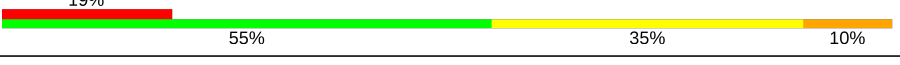


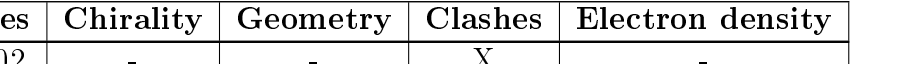
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	524	<div><div>4%</div><div><div></div><div>57%</div><div>35%</div><div>6%</div></div><div></div></div>
1	B	524	<div><div>6%</div><div><div></div><div>62%</div><div>31%</div><div>6%</div></div><div></div></div>
1	C	524	<div><div>5%</div><div><div></div><div>59%</div><div>34%</div><div>6%</div></div><div></div></div>
1	D	524	<div><div>5%</div><div><div></div><div>60%</div><div>33%</div><div>6%</div></div><div></div></div>
1	E	524	<div><div>7%</div><div><div></div><div>64%</div><div>31%</div><div></div></div><div></div></div>
1	F	524	<div><div>8%</div><div><div></div><div>65%</div><div>30%</div><div></div></div><div></div></div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AF3	A	602	-	-	X	-
6	AF3	D	602	-	-	X	-
6	AF3	F	602	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 59498 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
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	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 POTASSIUM ION (three-letter code: K) (formula: K).

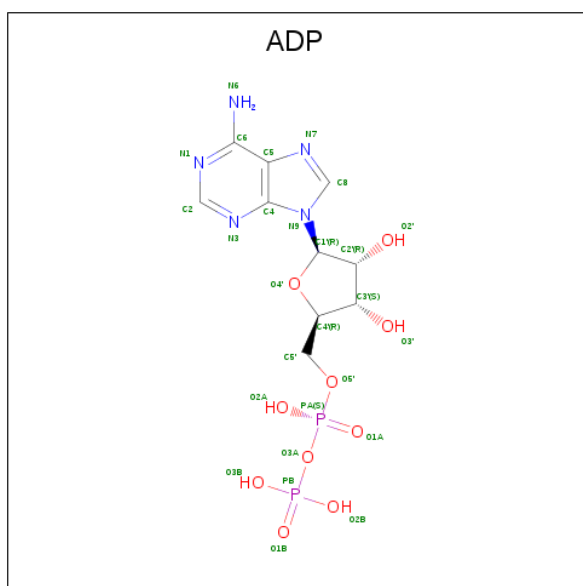
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		

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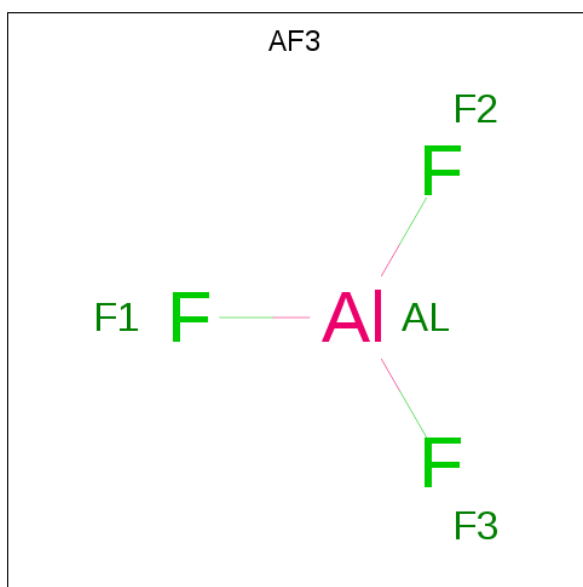
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	F	1	Total	K	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 6 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	Al 1	F 3	0	0
6	B	1	Total 4	Al 1	F 3	0	0
6	C	1	Total 4	Al 1	F 3	0	0
6	D	1	Total 4	Al 1	F 3	0	0
6	E	1	Total 4	Al 1	F 3	0	0
6	F	1	Total 4	Al 1	F 3	0	0
6	G	1	Total 4	Al 1	F 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	19	Total 19	O 19	0	0
7	B	10	Total 10	O 10	0	0
7	C	21	Total 21	O 21	0	0
7	D	14	Total 14	O 14	0	0
7	E	12	Total 12	O 12	0	0

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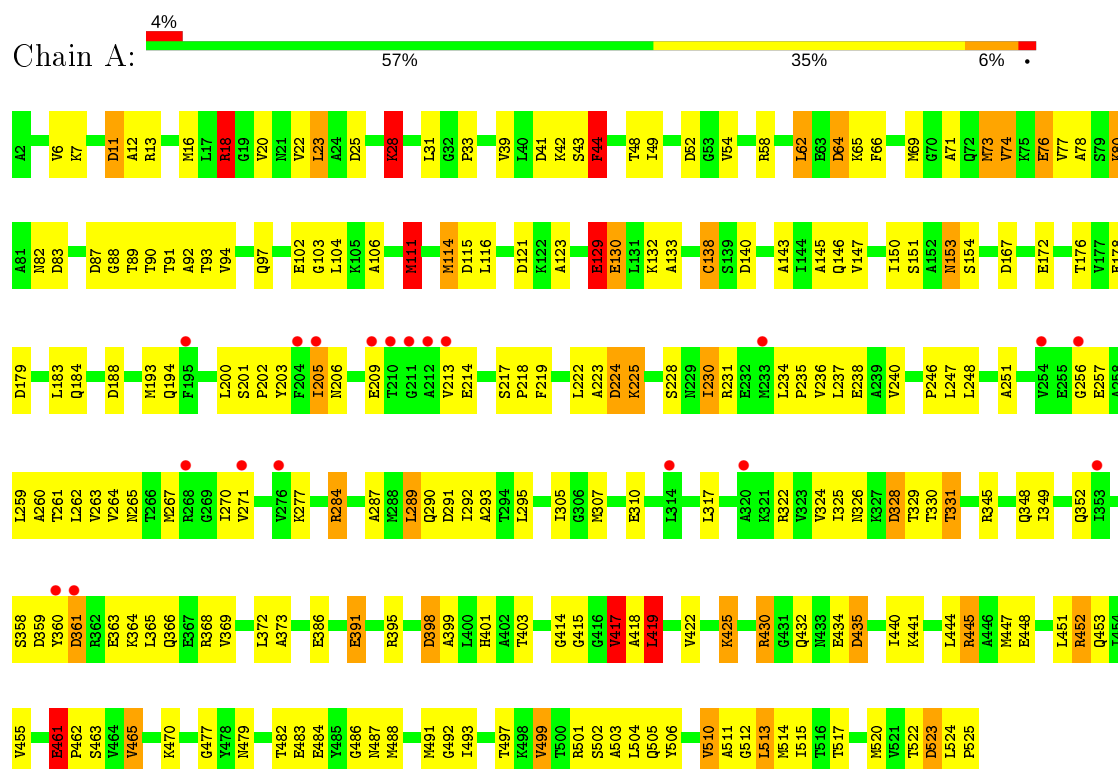
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	11	Total 11	O 11	0	0
7	G	20	Total 20	O 20	0	0
7	H	11	Total 11	O 11	0	0
7	I	17	Total 17	O 17	0	0
7	J	12	Total 12	O 12	0	0
7	K	14	Total 14	O 14	0	0
7	L	13	Total 13	O 13	0	0
7	M	10	Total 10	O 10	0	0
7	N	10	Total 10	O 10	0	0

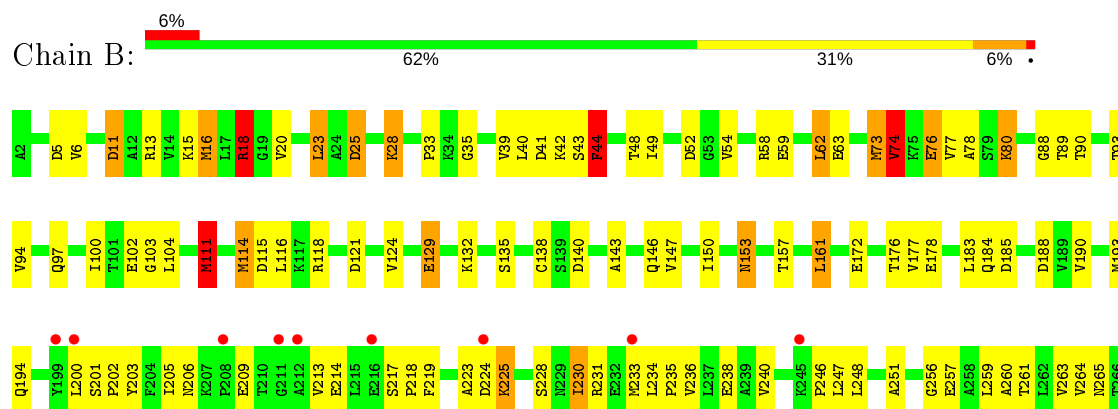
3 Residue-property plots

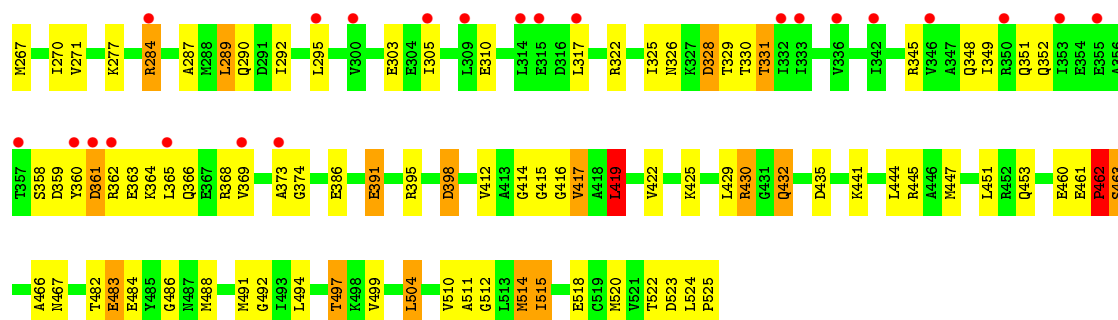
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: groEL protein

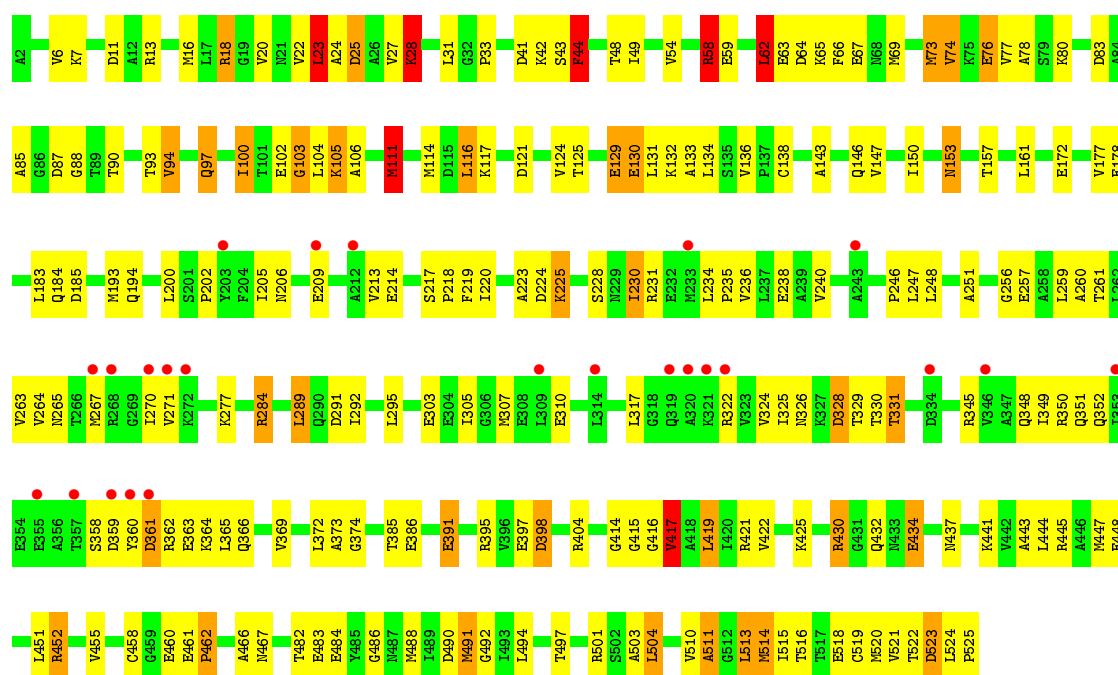


• Molecule 1: groEL protein

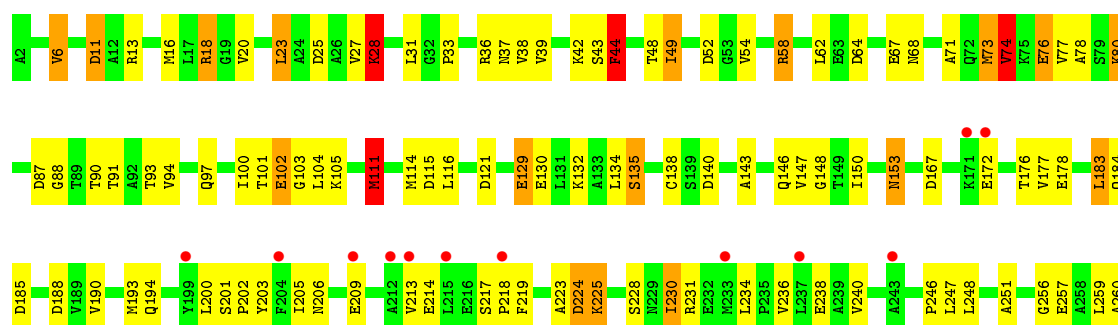


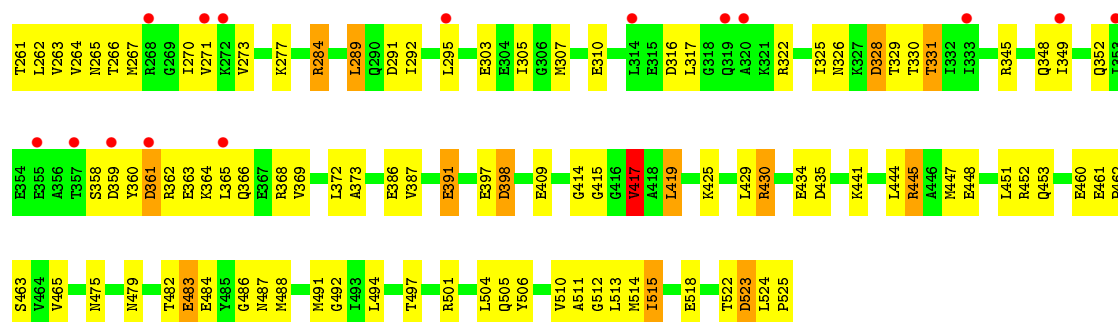


• Molecule 1: groEL protein

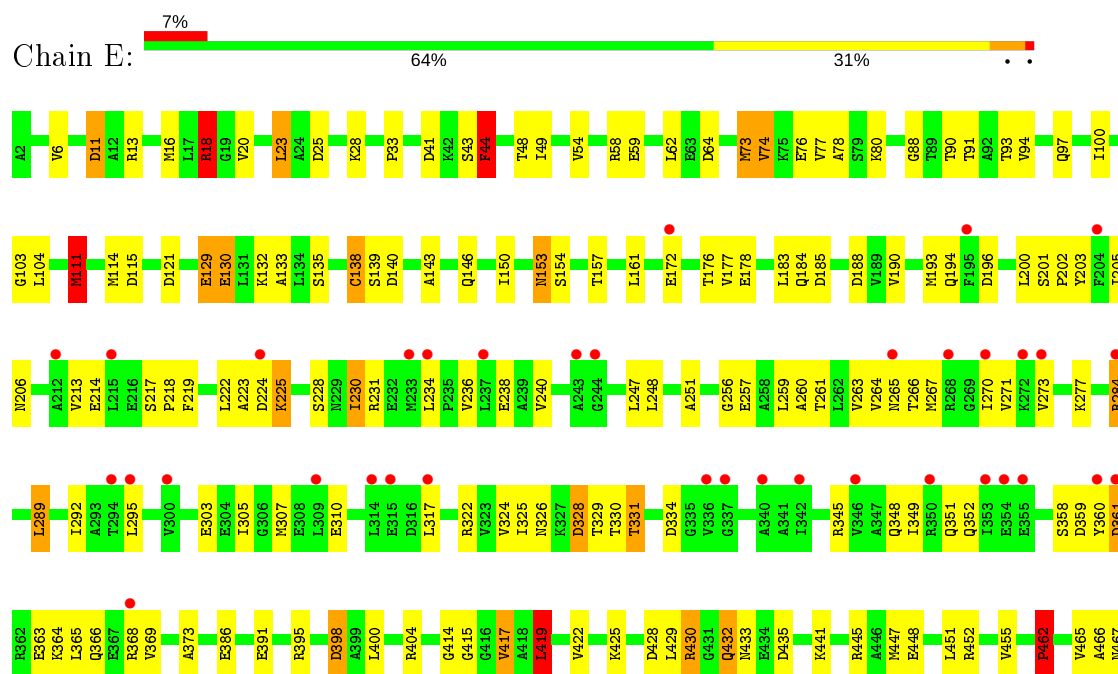


• Molecule 1: groEL protein

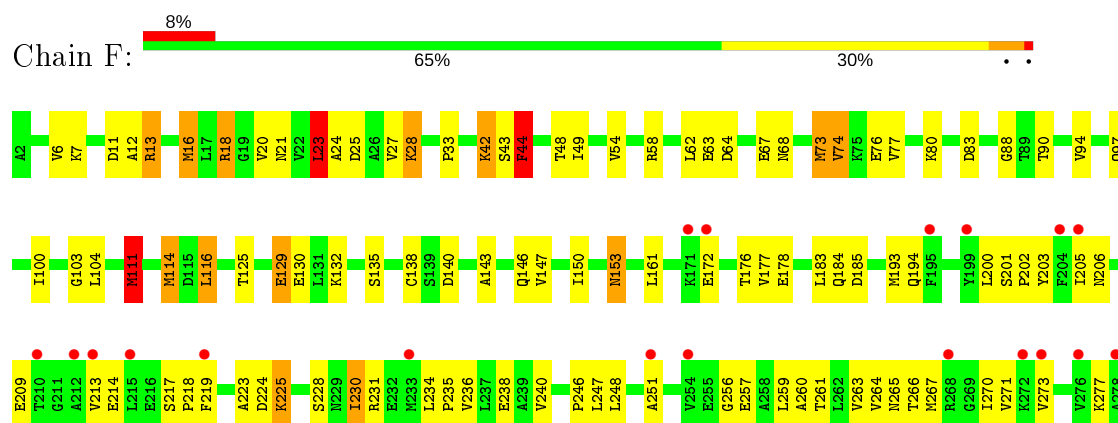


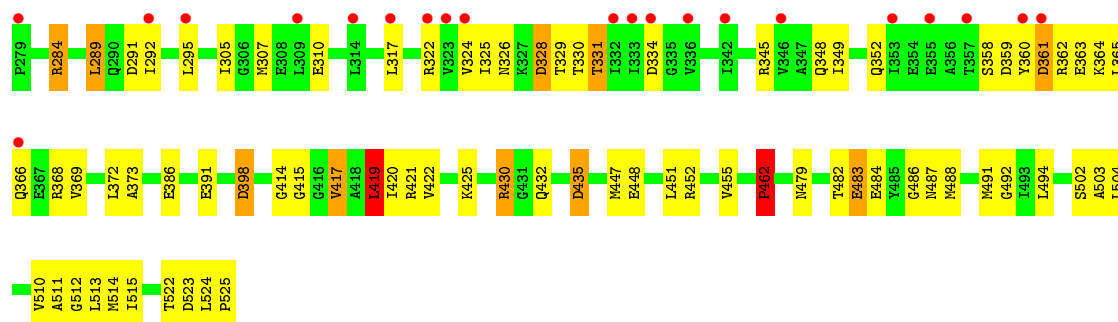


• Molecule 1: groEL protein

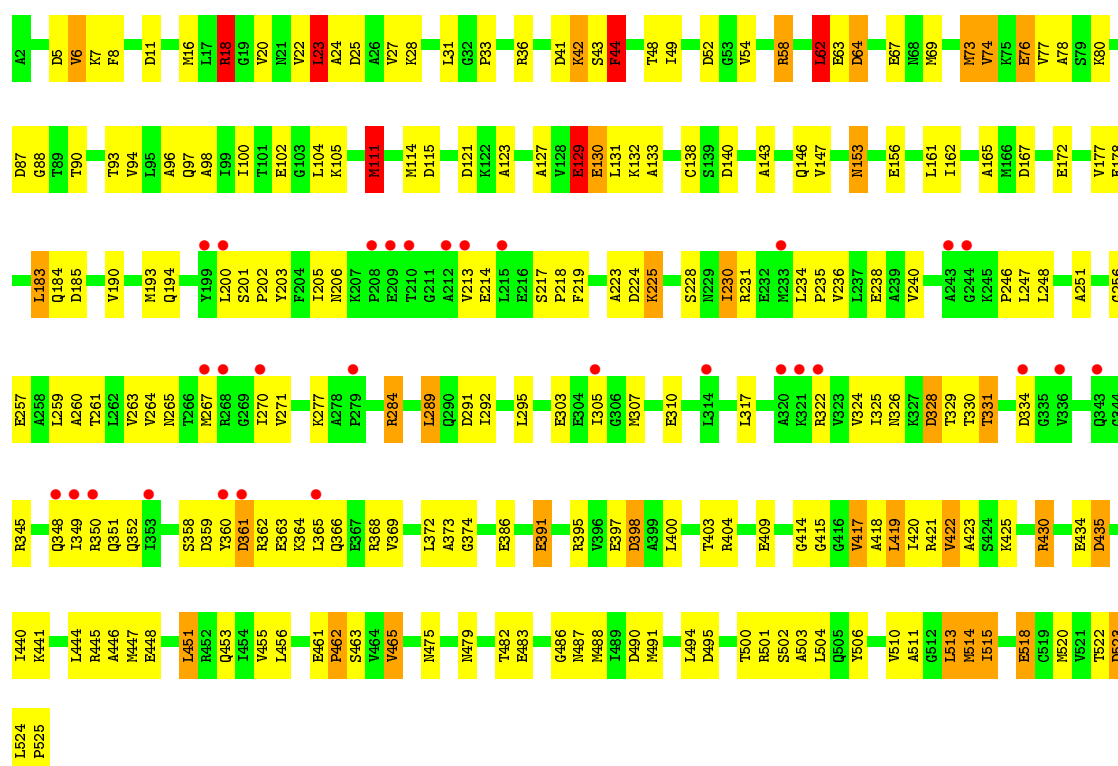


• Molecule 1: groEL protein

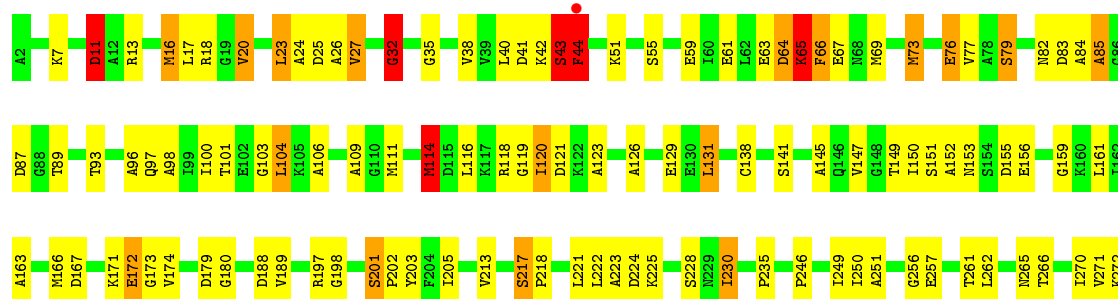


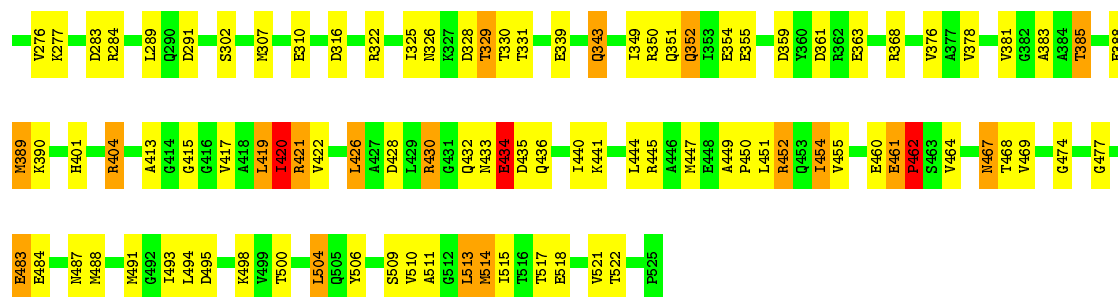


• Molecule 1: groEL protein



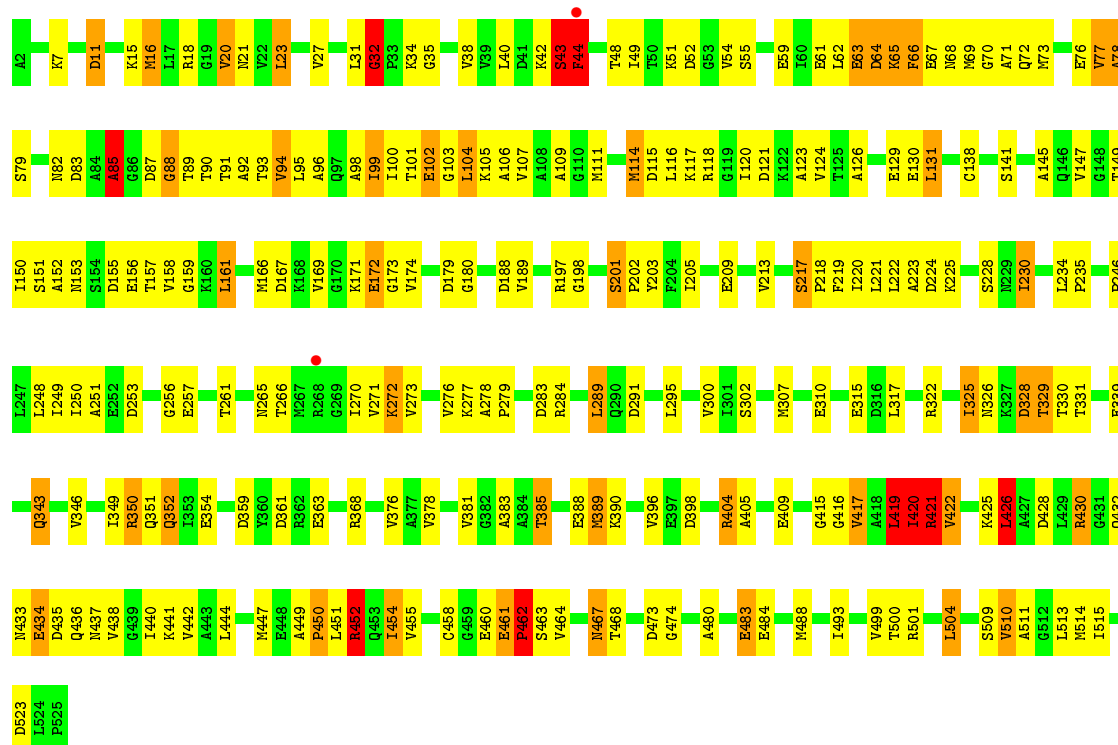
• Molecule 1: groEL protein





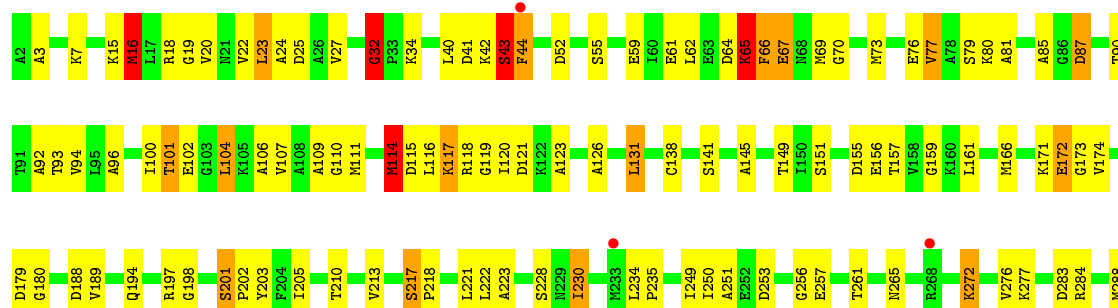
• Molecule 1: groEL protein

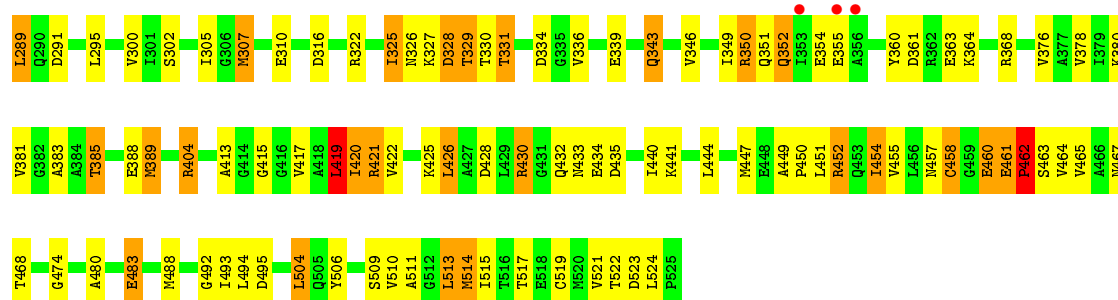
Chain I: 53% 36% 8%



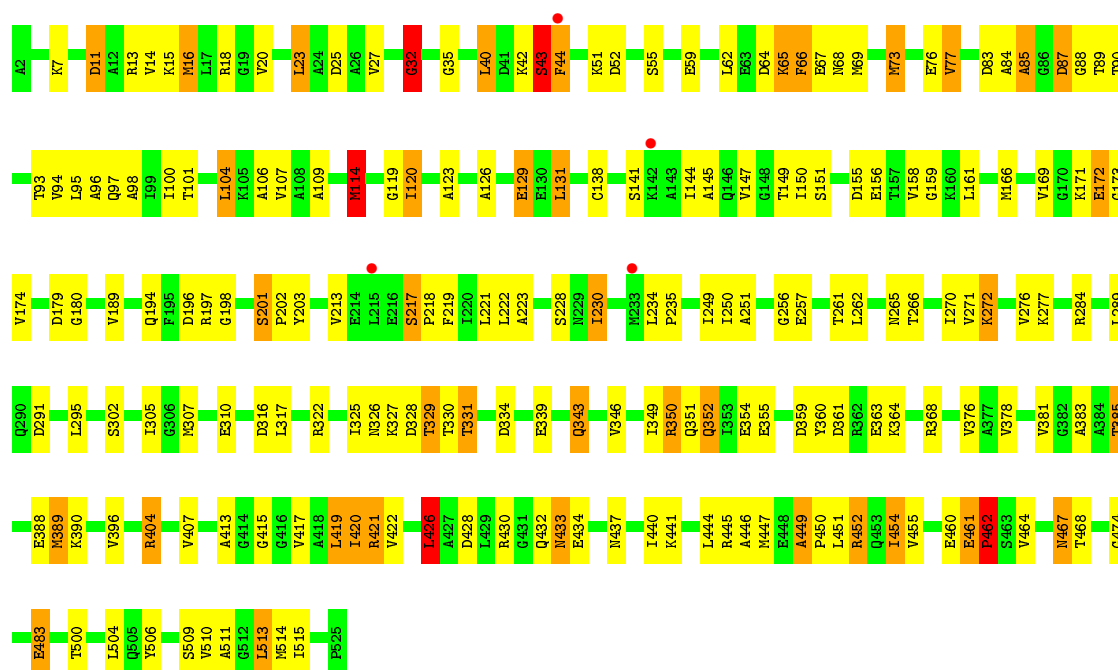
• Molecule 1: groEL protein

Chain J: 59% 32% 8%

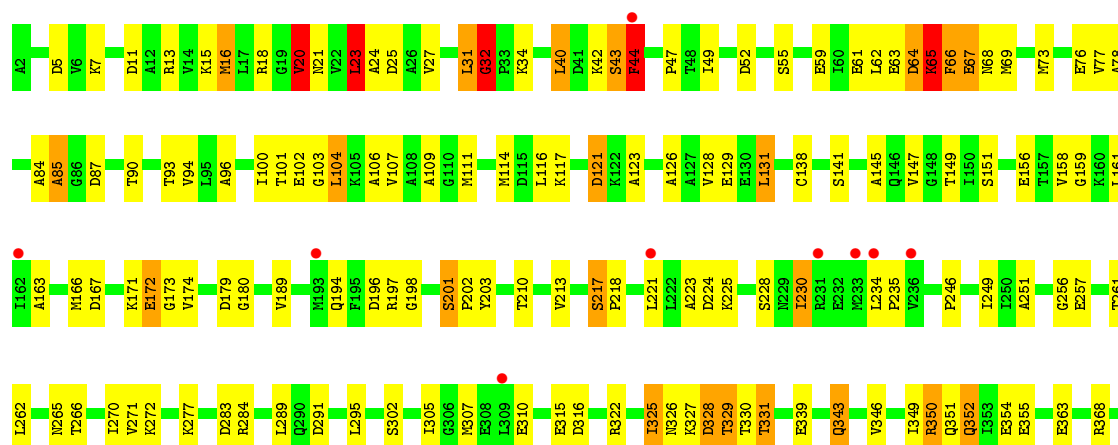


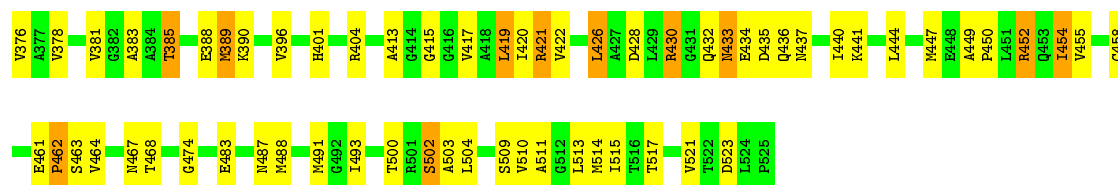


• Molecule 1: groEL protein

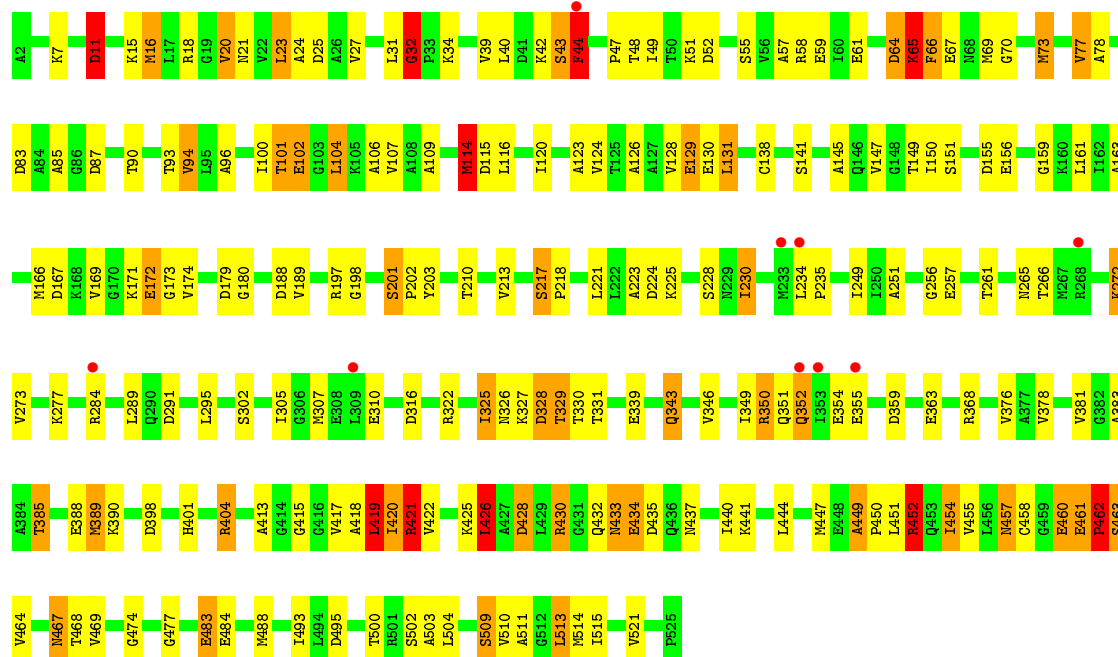


• Molecule 1: groEL protein

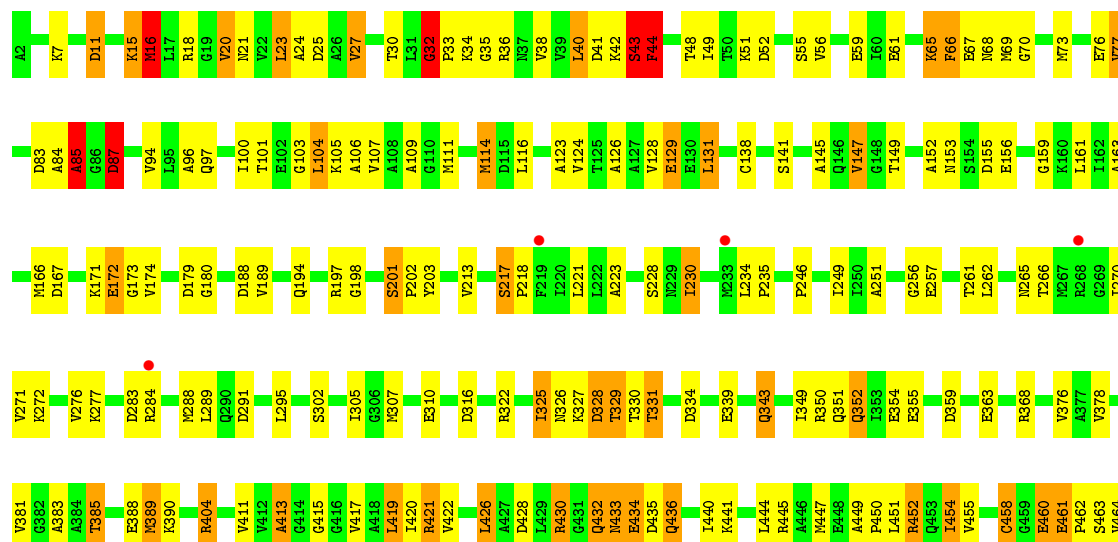


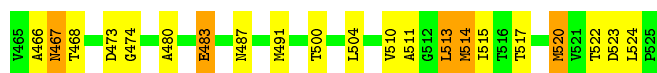


• Molecule 1: groEL protein

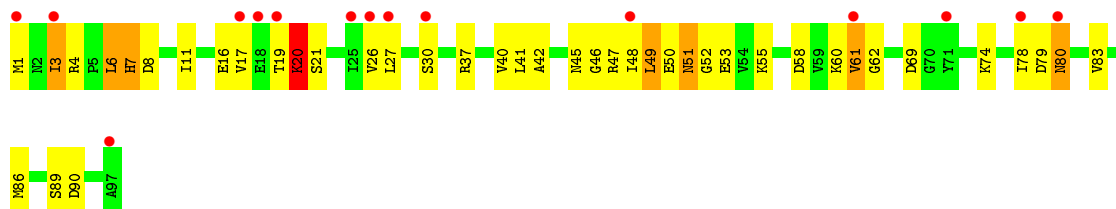


• Molecule 1: groEL protein

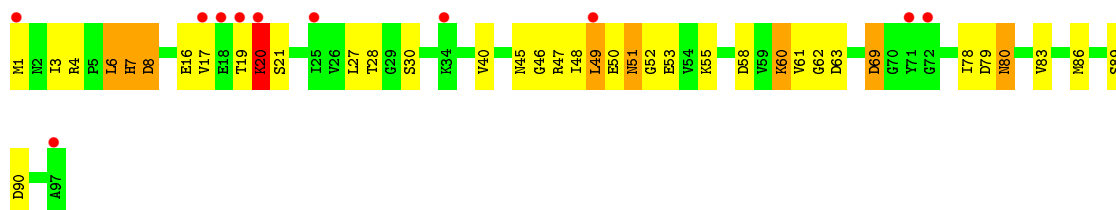




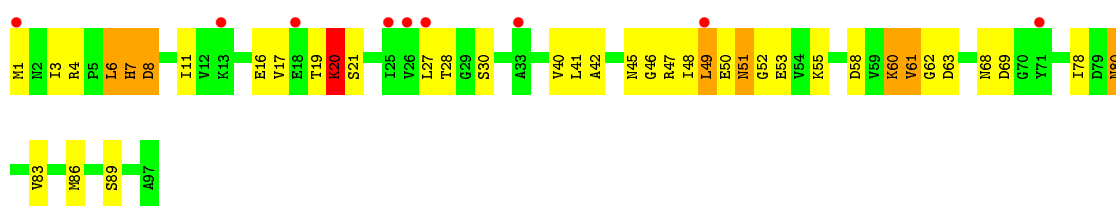
- Molecule 2: groES protein



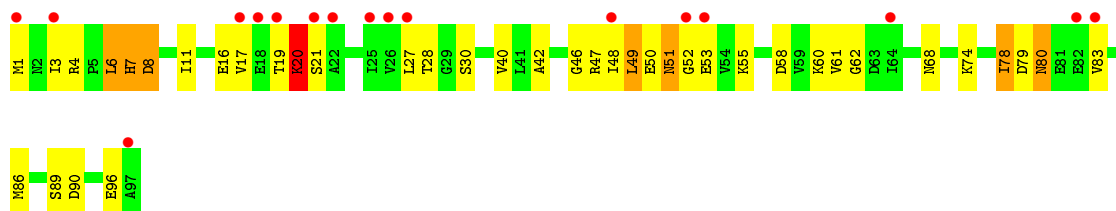
- Molecule 2: groES protein



- Molecule 2: groES protein

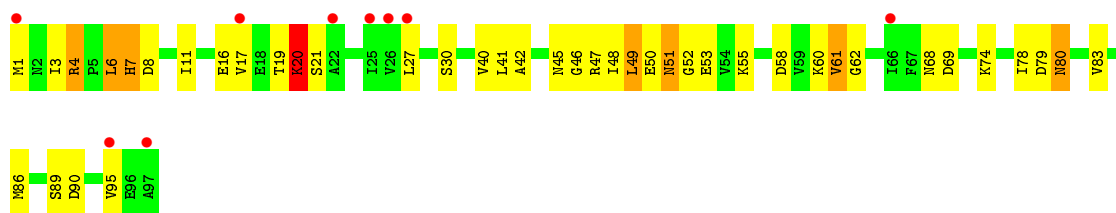


- Molecule 2: groES protein

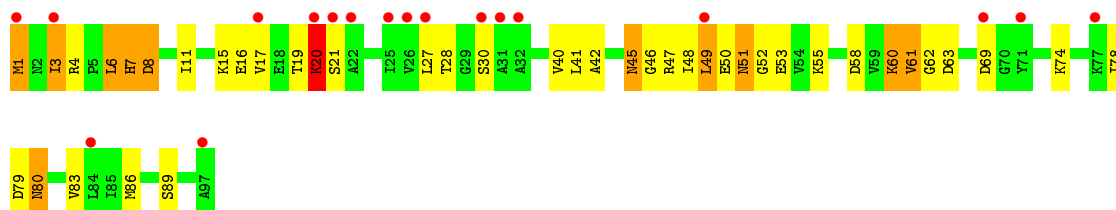


- Molecule 2: groES protein

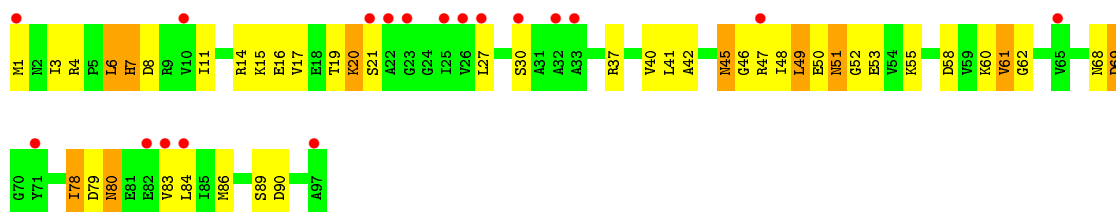




● Molecule 2: groES protein



● Molecule 2: groES protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	255.55Å 266.86Å 187.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.81 49.44 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.39-2.81) 60.7 (49.44-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.32Å)	Xtriage
Refinement program	REFMAC refmac _5.1.19	Depositor
R, R_{free}	0.247 , 0.274 0.244 , 0.263	Depositor DCC
R_{free} test set	6710 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.958	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	59498	wwPDB-VP
Average B, all atoms (Å ²)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, ADP, AF3

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	1.36	34/3883 (0.9%)	1.20	32/5243 (0.6%)
1	B	1.23	24/3883 (0.6%)	1.13	25/5243 (0.5%)
1	C	1.39	43/3883 (1.1%)	1.21	27/5243 (0.5%)
1	D	1.33	32/3883 (0.8%)	1.17	25/5243 (0.5%)
1	E	1.07	8/3883 (0.2%)	1.08	22/5243 (0.4%)
1	F	1.07	12/3883 (0.3%)	1.06	16/5243 (0.3%)
1	G	1.27	26/3883 (0.7%)	1.18	37/5243 (0.7%)
1	H	1.24	30/3884 (0.8%)	1.12	23/5243 (0.4%)
1	I	1.41	35/3884 (0.9%)	1.24	31/5243 (0.6%)
1	J	1.23	17/3884 (0.4%)	1.13	24/5243 (0.5%)
1	K	1.08	13/3884 (0.3%)	1.06	15/5243 (0.3%)
1	L	1.00	10/3884 (0.3%)	1.03	16/5243 (0.3%)
1	M	1.26	26/3884 (0.7%)	1.16	27/5243 (0.5%)
1	N	1.22	24/3884 (0.6%)	1.14	26/5243 (0.5%)
2	O	0.60	0/732	0.81	4/983 (0.4%)
2	P	0.59	0/732	0.83	6/983 (0.6%)
2	Q	0.57	0/732	0.83	4/983 (0.4%)
2	R	0.58	0/732	0.82	4/983 (0.4%)
2	S	0.55	0/732	0.82	4/983 (0.4%)
2	T	0.54	0/732	0.82	5/983 (0.5%)
2	U	0.58	0/732	0.82	4/983 (0.4%)
All	All	1.19	334/59493 (0.6%)	1.11	377/80283 (0.5%)

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	A	0	1
1	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	8

All (334) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	461	GLU	CD-OE2	12.41	1.39	1.25
1	C	76	GLU	CD-OE1	11.87	1.38	1.25
1	I	483	GLU	CD-OE2	11.28	1.38	1.25
1	M	461	GLU	CD-OE2	11.22	1.38	1.25
1	G	76	GLU	CD-OE2	10.55	1.37	1.25
1	A	76	GLU	CD-OE1	10.40	1.37	1.25
1	N	483	GLU	CD-OE2	10.36	1.37	1.25
1	D	130	GLU	CD-OE1	10.35	1.37	1.25
1	A	76	GLU	CD-OE2	10.34	1.37	1.25
1	C	73	MET	SD-CE	9.78	2.32	1.77
1	I	434	GLU	CD-OE1	9.72	1.36	1.25
1	C	102	GLU	CG-CD	9.66	1.66	1.51
1	H	76	GLU	CD-OE1	9.63	1.36	1.25
1	M	461	GLU	CD-OE1	9.50	1.36	1.25
1	I	461	GLU	CD-OE1	9.47	1.36	1.25
1	N	76	GLU	CD-OE1	9.13	1.35	1.25
1	B	483	GLU	CD-OE1	8.92	1.35	1.25
1	M	483	GLU	CD-OE2	8.91	1.35	1.25
1	J	461	GLU	CD-OE2	8.87	1.35	1.25
1	H	434	GLU	CD-OE1	8.87	1.35	1.25
1	I	102	GLU	CG-CD	8.84	1.65	1.51
1	A	73	MET	SD-CE	8.81	2.27	1.77
1	F	73	MET	SD-CE	8.80	2.27	1.77
1	I	85	ALA	CA-CB	8.80	1.71	1.52
1	G	76	GLU	CD-OE1	8.59	1.35	1.25
1	C	94	VAL	C-O	8.57	1.39	1.23
1	A	129	GLU	CD-OE2	8.41	1.34	1.25
1	E	484	GLU	CD-OE2	8.38	1.34	1.25
1	N	514	MET	SD-CE	8.36	2.24	1.77
1	I	422	VAL	CB-CG2	-8.31	1.35	1.52
1	J	483	GLU	CD-OE2	8.27	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	102	GLU	C-O	8.26	1.39	1.23
1	F	76	GLU	CD-OE1	8.24	1.34	1.25
1	C	398	ASP	CB-CG	8.20	1.69	1.51
1	C	83	ASP	C-O	8.20	1.39	1.23
1	D	76	GLU	CD-OE1	8.15	1.34	1.25
1	B	76	GLU	CD-OE1	8.11	1.34	1.25
1	A	129	GLU	CD-OE1	8.11	1.34	1.25
1	H	114	MET	SD-CE	8.08	2.23	1.77
1	J	76	GLU	CD-OE1	8.04	1.34	1.25
1	G	102	GLU	CD-OE1	8.03	1.34	1.25
1	H	61	GLU	CD-OE2	7.84	1.34	1.25
1	G	73	MET	SD-CE	7.80	2.21	1.77
1	A	484	GLU	CD-OE2	7.80	1.34	1.25
1	M	102	GLU	CD-OE2	7.73	1.34	1.25
1	B	514	MET	SD-CE	7.73	2.21	1.77
1	A	130	GLU	CD-OE1	7.67	1.34	1.25
1	N	16	MET	SD-CE	7.65	2.20	1.77
1	N	76	GLU	CD-OE2	7.63	1.34	1.25
1	M	434	GLU	CD-OE1	7.62	1.34	1.25
1	A	129	GLU	CG-CD	7.61	1.63	1.51
1	C	117	LYS	CB-CG	-7.53	1.32	1.52
1	F	76	GLU	CD-OE2	7.52	1.33	1.25
1	J	114	MET	SD-CE	7.50	2.19	1.77
1	I	61	GLU	CD-OE2	7.49	1.33	1.25
1	C	102	GLU	CD-OE1	7.47	1.33	1.25
1	F	67	GLU	CD-OE1	7.45	1.33	1.25
1	E	73	MET	SD-CE	7.43	2.19	1.77
1	D	391	GLU	CD-OE1	7.40	1.33	1.25
1	C	129	GLU	CG-CD	7.37	1.63	1.51
1	C	97	GLN	CB-CG	-7.29	1.32	1.52
1	E	111	MET	SD-CE	7.25	2.18	1.77
1	C	129	GLU	CD-OE1	7.21	1.33	1.25
1	M	484	GLU	CD-OE2	7.13	1.33	1.25
1	D	102	GLU	CG-CD	7.11	1.62	1.51
1	A	506	TYR	CG-CD1	-7.10	1.29	1.39
1	K	18	ARG	NE-CZ	7.10	1.42	1.33
1	D	130	GLU	CD-OE2	7.09	1.33	1.25
1	J	461	GLU	CD-OE1	7.09	1.33	1.25
1	D	102	GLU	CD-OE1	7.07	1.33	1.25
1	K	76	GLU	CD-OE1	7.04	1.33	1.25
1	D	73	MET	SD-CE	7.03	2.17	1.77
1	N	129	GLU	CD-OE2	6.97	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	85	ALA	CA-CB	6.96	1.67	1.52
1	I	63	GLU	CD-OE2	6.93	1.33	1.25
1	C	458	CYS	CB-SG	-6.92	1.70	1.82
1	A	434	GLU	CG-CD	6.92	1.62	1.51
1	M	94	VAL	C-O	6.86	1.36	1.23
1	D	398	ASP	CB-CG	6.82	1.66	1.51
1	H	44	PHE	CG-CD1	6.78	1.49	1.38
1	N	129	GLU	CD-OE1	6.77	1.33	1.25
1	H	514	MET	SD-CE	6.76	2.15	1.77
1	N	461	GLU	CD-OE2	6.76	1.33	1.25
1	H	44	PHE	CE2-CZ	6.75	1.50	1.37
1	A	434	GLU	CD-OE1	6.71	1.33	1.25
1	A	391	GLU	CD-OE1	6.69	1.33	1.25
1	C	511	ALA	CA-CB	6.68	1.66	1.52
1	I	417	VAL	CA-CB	-6.67	1.40	1.54
1	I	484	GLU	CD-OE2	6.66	1.32	1.25
1	G	130	GLU	CD-OE1	6.65	1.32	1.25
1	B	391	GLU	CD-OE1	6.64	1.32	1.25
1	I	452	ARG	NE-CZ	6.63	1.41	1.33
1	M	73	MET	CG-SD	6.63	1.98	1.81
1	I	18	ARG	CZ-NH2	6.61	1.41	1.33
1	G	461	GLU	CD-OE1	6.61	1.32	1.25
1	H	61	GLU	CD-OE1	6.59	1.32	1.25
1	D	44	PHE	CE1-CZ	6.58	1.49	1.37
1	B	111	MET	SD-CE	6.57	2.14	1.77
1	C	105	LYS	CD-CE	6.56	1.67	1.51
1	D	417	VAL	CB-CG1	-6.54	1.39	1.52
1	A	510	VAL	CB-CG1	-6.54	1.39	1.52
1	D	397	GLU	CD-OE2	6.51	1.32	1.25
1	I	480	ALA	CA-CB	-6.50	1.38	1.52
1	B	484	GLU	CD-OE2	6.46	1.32	1.25
1	J	92	ALA	CA-CB	-6.45	1.38	1.52
1	L	76	GLU	CD-OE1	6.45	1.32	1.25
1	D	129	GLU	CG-CD	6.44	1.61	1.51
1	C	391	GLU	CD-OE1	6.43	1.32	1.25
1	F	111	MET	SD-CE	6.42	2.13	1.77
1	I	409	GLU	CD-OE1	6.39	1.32	1.25
1	D	111	MET	SD-CE	6.38	2.13	1.77
1	B	102	GLU	CG-CD	6.38	1.61	1.51
1	C	514	MET	SD-CE	6.36	2.13	1.77
1	I	20	VAL	CB-CG1	-6.36	1.39	1.52
1	J	61	GLU	CD-OE2	6.35	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	MET	SD-CE	6.34	2.13	1.77
1	C	397	GLU	CD-OE2	6.34	1.32	1.25
1	J	514	MET	SD-CE	6.33	2.13	1.77
1	H	76	GLU	CD-OE2	6.32	1.32	1.25
1	M	114	MET	SD-CE	6.32	2.13	1.77
1	I	44	PHE	CE2-CZ	6.31	1.49	1.37
1	L	61	GLU	CD-OE2	6.31	1.32	1.25
1	H	461	GLU	CD-OE2	6.30	1.32	1.25
1	I	76	GLU	CD-OE1	6.30	1.32	1.25
1	D	121	ASP	CG-OD1	6.29	1.39	1.25
1	H	79	SER	CB-OG	-6.28	1.34	1.42
1	F	42	LYS	CD-CE	6.25	1.66	1.51
1	G	395	ARG	NE-CZ	6.23	1.41	1.33
1	B	129	GLU	CG-CD	6.23	1.61	1.51
1	H	461	GLU	CD-OE1	6.23	1.32	1.25
1	D	102	GLU	CD-OE2	6.22	1.32	1.25
1	I	78	ALA	CA-C	6.21	1.69	1.52
1	D	74	VAL	CB-CG1	-6.21	1.39	1.52
1	F	44	PHE	CE1-CZ	6.18	1.49	1.37
1	K	449	ALA	CA-CB	-6.16	1.39	1.52
1	C	432	GLN	CG-CD	6.13	1.65	1.51
1	G	67	GLU	CD-OE1	6.08	1.32	1.25
1	E	59	GLU	CD-OE2	6.06	1.32	1.25
1	H	18	ARG	NE-CZ	6.02	1.40	1.33
1	M	452	ARG	CB-CG	-6.02	1.36	1.52
1	N	461	GLU	CD-OE1	6.02	1.32	1.25
1	H	506	TYR	CB-CG	-6.01	1.42	1.51
1	D	115	ASP	CB-CG	6.01	1.64	1.51
1	C	105	LYS	C-O	6.01	1.34	1.23
1	H	73	MET	CG-SD	6.01	1.96	1.81
1	A	44	PHE	CE1-CZ	6.01	1.48	1.37
1	C	398	ASP	CG-OD1	6.01	1.39	1.25
1	C	129	GLU	CD-OE2	6.00	1.32	1.25
1	N	114	MET	SD-CE	5.99	2.11	1.77
1	J	506	TYR	CB-CG	-5.97	1.42	1.51
1	H	38	VAL	CB-CG1	-5.97	1.40	1.52
1	C	434	GLU	CD-OE1	5.96	1.32	1.25
1	A	102	GLU	CD-OE2	5.95	1.32	1.25
1	B	102	GLU	CD-OE1	5.94	1.32	1.25
1	J	67	GLU	CD-OE1	5.93	1.32	1.25
1	F	484	GLU	CD-OE2	5.93	1.32	1.25
1	B	412	VAL	CB-CG2	-5.92	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	130	GLU	CD-OE2	5.91	1.32	1.25
1	J	480	ALA	CA-CB	-5.90	1.40	1.52
1	G	42	LYS	CD-CE	5.90	1.66	1.51
1	C	460	GLU	CD-OE1	5.89	1.32	1.25
1	A	121	ASP	CB-CG	5.87	1.64	1.51
1	J	465	VAL	CB-CG2	-5.86	1.40	1.52
1	B	73	MET	SD-CE	5.84	2.10	1.77
1	G	130	GLU	CD-OE2	5.83	1.32	1.25
1	N	87	ASP	CB-CG	5.80	1.64	1.51
1	A	417	VAL	CB-CG1	-5.80	1.40	1.52
1	F	483	GLU	CD-OE1	5.79	1.32	1.25
1	D	460	GLU	CD-OE2	5.79	1.32	1.25
1	L	76	GLU	CD-OE2	5.79	1.32	1.25
1	A	121	ASP	CG-OD1	5.76	1.38	1.25
1	B	44	PHE	CE1-CZ	5.73	1.48	1.37
1	J	87	ASP	CB-CG	5.73	1.63	1.51
1	F	73	MET	CG-SD	5.72	1.96	1.81
1	C	452	ARG	NE-CZ	5.70	1.40	1.33
1	A	434	GLU	CD-OE2	5.70	1.31	1.25
1	C	130	GLU	CD-OE1	5.69	1.31	1.25
1	C	484	GLU	CD-OE2	5.69	1.31	1.25
1	C	501	ARG	CB-CG	-5.68	1.37	1.52
1	M	51	LYS	CE-NZ	5.68	1.63	1.49
1	J	16	MET	SD-CE	5.67	2.09	1.77
1	B	483	GLU	CD-OE2	5.66	1.31	1.25
1	G	501	ARG	CG-CD	-5.66	1.37	1.51
1	I	114	MET	SD-CE	5.66	2.09	1.77
1	D	129	GLU	CD-OE2	5.65	1.31	1.25
1	N	27	VAL	CB-CG2	-5.65	1.41	1.52
1	I	442	VAL	CB-CG1	-5.64	1.41	1.52
1	A	102	GLU	CD-OE1	5.63	1.31	1.25
1	B	35	GLY	C-O	5.63	1.32	1.23
1	B	432	GLN	CG-CD	5.62	1.64	1.51
1	B	461	GLU	CD-OE1	5.62	1.31	1.25
1	M	484	GLU	CD-OE1	5.62	1.31	1.25
1	D	484	GLU	CD-OE2	5.62	1.31	1.25
1	B	76	GLU	CD-OE2	5.61	1.31	1.25
1	H	44	PHE	CE1-CZ	5.61	1.48	1.37
1	M	129	GLU	CD-OE1	5.60	1.31	1.25
1	N	18	ARG	CG-CD	5.60	1.66	1.51
1	B	74	VAL	CB-CG1	-5.60	1.41	1.52
1	C	434	GLU	CG-CD	5.60	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	121	ASP	CB-CG	5.60	1.63	1.51
1	E	121	ASP	CB-CG	5.59	1.63	1.51
1	M	130	GLU	CD-OE2	5.59	1.31	1.25
1	D	121	ASP	CB-CG	5.59	1.63	1.51
1	A	18	ARG	NE-CZ	5.59	1.40	1.33
1	C	59	GLU	CD-OE2	5.58	1.31	1.25
1	G	465	VAL	CB-CG1	-5.58	1.41	1.52
1	N	61	GLU	CD-OE2	5.58	1.31	1.25
1	C	452	ARG	C-O	5.58	1.33	1.23
1	H	445	ARG	CZ-NH1	5.58	1.40	1.33
1	D	71	ALA	CA-CB	-5.58	1.40	1.52
1	N	44	PHE	CE1-CZ	5.57	1.48	1.37
1	A	499	VAL	CB-CG1	-5.57	1.41	1.52
1	I	510	VAL	CA-C	-5.57	1.38	1.52
1	I	409	GLU	CD-OE2	5.57	1.31	1.25
1	E	130	GLU	CD-OE1	5.56	1.31	1.25
1	M	61	GLU	CD-OE2	5.56	1.31	1.25
1	K	461	GLU	CD-OE2	5.55	1.31	1.25
1	G	44	PHE	CE1-CZ	5.54	1.47	1.37
1	K	73	MET	CG-SD	5.53	1.95	1.81
1	A	71	ALA	CA-CB	-5.51	1.40	1.52
1	C	395	ARG	CG-CD	5.51	1.65	1.51
1	N	445	ARG	NE-CZ	5.51	1.40	1.33
1	L	67	GLU	CD-OE1	5.50	1.31	1.25
1	K	87	ASP	CB-CG	5.50	1.63	1.51
1	I	118	ARG	CG-CD	5.49	1.65	1.51
1	G	44	PHE	CD2-CE2	5.47	1.50	1.39
1	A	465	VAL	CB-CG2	-5.47	1.41	1.52
1	H	27	VAL	CB-CG2	-5.47	1.41	1.52
1	A	145	ALA	CA-CB	-5.47	1.41	1.52
1	C	461	GLU	CD-OE2	5.46	1.31	1.25
1	A	391	GLU	CG-CD	5.45	1.60	1.51
1	B	44	PHE	CE2-CZ	5.44	1.47	1.37
1	M	452	ARG	NE-CZ	5.44	1.40	1.33
1	A	130	GLU	CD-OE2	5.43	1.31	1.25
1	H	518	GLU	CD-OE2	5.43	1.31	1.25
1	N	27	VAL	CB-CG1	-5.42	1.41	1.52
1	M	44	PHE	CG-CD1	5.42	1.46	1.38
1	M	463	SER	CB-OG	5.42	1.49	1.42
1	C	121	ASP	CG-OD1	5.42	1.37	1.25
1	L	20	VAL	CB-CG1	-5.42	1.41	1.52
1	N	105	LYS	CD-CE	5.42	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	118	ARG	CG-CD	5.42	1.65	1.51
1	M	18	ARG	NE-CZ	5.41	1.40	1.33
1	B	460	GLU	CD-OE2	5.40	1.31	1.25
1	I	434	GLU	CD-OE2	5.40	1.31	1.25
1	N	56	VAL	CB-CG2	-5.40	1.41	1.52
1	K	506	TYR	CB-CG	-5.39	1.43	1.51
1	C	503	ALA	CA-CB	-5.38	1.41	1.52
1	D	434	GLU	CD-OE1	5.38	1.31	1.25
1	C	76	GLU	CD-OE2	5.38	1.31	1.25
1	H	118	ARG	NE-CZ	5.38	1.40	1.33
1	D	483	GLU	CD-OE2	5.37	1.31	1.25
1	M	31	LEU	CG-CD1	5.36	1.71	1.51
1	D	28	LYS	CD-CE	5.36	1.64	1.51
1	I	54	VAL	CA-CB	-5.36	1.43	1.54
1	M	44	PHE	CG-CD2	5.34	1.46	1.38
1	C	491	MET	CG-SD	-5.34	1.67	1.81
1	G	129	GLU	CD-OE2	5.34	1.31	1.25
1	H	483	GLU	CD-OE2	5.33	1.31	1.25
1	I	94	VAL	CB-CG2	-5.32	1.41	1.52
1	I	88	GLY	C-O	5.32	1.32	1.23
1	G	446	ALA	CA-CB	-5.31	1.41	1.52
1	F	130	GLU	CD-OE1	5.30	1.31	1.25
1	L	102	GLU	CG-CD	5.30	1.59	1.51
1	E	18	ARG	NE-CZ	5.30	1.40	1.33
1	L	18	ARG	NE-CZ	5.29	1.40	1.33
1	N	480	ALA	CA-CB	-5.29	1.41	1.52
1	K	114	MET	SD-CE	5.28	2.07	1.77
1	I	118	ARG	NE-CZ	5.28	1.40	1.33
1	K	129	GLU	CD-OE2	5.28	1.31	1.25
1	M	460	GLU	CD-OE1	5.26	1.31	1.25
1	G	397	GLU	CD-OE2	5.26	1.31	1.25
1	C	130	GLU	CD-OE2	5.25	1.31	1.25
1	G	111	MET	SD-CE	5.24	2.07	1.77
1	F	16	MET	SD-CE	5.23	2.07	1.77
1	G	506	TYR	CG-CD1	-5.23	1.32	1.39
1	B	111	MET	CG-SD	5.23	1.94	1.81
1	G	8	PHE	CB-CG	-5.23	1.42	1.51
1	D	105	LYS	CD-CE	5.22	1.64	1.51
1	C	417	VAL	CB-CG1	-5.21	1.41	1.52
1	N	460	GLU	CD-OE2	5.21	1.31	1.25
1	G	67	GLU	CD-OE2	5.21	1.31	1.25
1	L	502	SER	CB-OG	-5.20	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	484	GLU	CD-OE2	5.20	1.31	1.25
1	M	32	GLY	CA-C	5.19	1.60	1.51
1	G	434	GLU	CG-CD	5.19	1.59	1.51
1	K	445	ARG	NE-CZ	5.19	1.39	1.33
1	N	24	ALA	CA-CB	-5.18	1.41	1.52
1	D	465	VAL	CB-CG2	-5.17	1.42	1.52
1	H	98	ALA	C-O	5.17	1.33	1.23
1	K	76	GLU	CD-OE2	5.16	1.31	1.25
1	I	44	PHE	CG-CD2	5.16	1.46	1.38
1	J	521	VAL	CB-CG2	-5.16	1.42	1.52
1	C	443	ALA	CA-CB	-5.15	1.41	1.52
1	H	506	TYR	CD2-CE2	5.15	1.47	1.39
1	J	18	ARG	NE-CZ	5.12	1.39	1.33
1	D	506	TYR	CZ-OH	5.12	1.46	1.37
1	G	156	GLU	CD-OE2	5.12	1.31	1.25
1	L	44	PHE	CE2-CZ	5.11	1.47	1.37
1	C	521	VAL	CB-CG2	-5.11	1.42	1.52
1	A	470	LYS	CD-CE	5.11	1.64	1.51
1	B	18	ARG	NE-CZ	5.10	1.39	1.33
1	I	78	ALA	C-O	-5.10	1.13	1.23
1	A	465	VAL	CB-CG1	-5.10	1.42	1.52
1	A	461	GLU	CD-OE1	5.09	1.31	1.25
1	C	460	GLU	CD-OE2	5.09	1.31	1.25
1	C	111	MET	SD-CE	5.08	2.06	1.77
1	H	24	ALA	CA-CB	-5.08	1.41	1.52
1	K	114	MET	CG-SD	5.08	1.94	1.81
1	E	76	GLU	CD-OE1	5.07	1.31	1.25
1	I	129	GLU	CG-CD	5.07	1.59	1.51
1	A	425	LYS	CE-NZ	5.07	1.61	1.49
1	G	105	LYS	CD-CE	5.07	1.64	1.51
1	B	39	VAL	CB-CG1	-5.06	1.42	1.52
1	L	63	GLU	CD-OE1	5.06	1.31	1.25
1	D	434	GLU	CG-CD	5.05	1.59	1.51
1	J	460	GLU	CD-OE2	5.05	1.31	1.25
1	G	404	ARG	NE-CZ	5.05	1.39	1.33
1	K	483	GLU	CD-OE2	5.05	1.31	1.25
1	M	44	PHE	CE2-CZ	5.05	1.47	1.37
1	A	102	GLU	CG-CD	5.04	1.59	1.51
1	C	67	GLU	CD-OE1	5.04	1.31	1.25
1	D	76	GLU	CD-OE2	5.04	1.31	1.25
1	H	26	ALA	CA-CB	-5.04	1.41	1.52
1	G	391	GLU	CG-CD	5.04	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	465	VAL	CA-CB	-5.04	1.44	1.54
1	A	18	ARG	CZ-NH2	5.03	1.39	1.33
1	B	460	GLU	CD-OE1	5.03	1.31	1.25
1	H	63	GLU	CD-OE2	5.03	1.31	1.25
1	I	405	ALA	CA-CB	-5.02	1.41	1.52
1	D	44	PHE	CE2-CZ	5.02	1.46	1.37
1	M	509	SER	C-O	5.01	1.32	1.23
1	M	449	ALA	CA-CB	-5.01	1.42	1.52
1	N	38	VAL	CB-CG1	-5.00	1.42	1.52

All (377) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	25	ASP	CB-CG-OD2	11.00	128.20	118.30
1	M	25	ASP	CB-CG-OD2	10.63	127.87	118.30
1	I	428	ASP	CB-CG-OD2	10.62	127.86	118.30
1	D	121	ASP	CB-CG-OD1	10.19	127.47	118.30
1	N	428	ASP	CB-CG-OD2	9.83	127.15	118.30
1	C	398	ASP	CB-CG-OD1	9.82	127.14	118.30
1	I	452	ARG	NE-CZ-NH2	9.76	125.18	120.30
1	J	25	ASP	CB-CG-OD2	9.73	127.06	118.30
1	J	428	ASP	CB-CG-OD2	9.71	127.04	118.30
1	A	64	ASP	CB-CG-OD2	9.37	126.73	118.30
1	K	428	ASP	CB-CG-OD2	9.35	126.72	118.30
1	C	121	ASP	CB-CG-OD1	9.28	126.65	118.30
1	L	428	ASP	CB-CG-OD2	9.25	126.63	118.30
1	K	25	ASP	CB-CG-OD2	9.25	126.62	118.30
1	A	523	ASP	CB-CG-OD2	9.11	126.50	118.30
1	B	115	ASP	CB-CG-OD2	8.70	126.13	118.30
1	E	41	ASP	CB-CG-OD2	8.63	126.06	118.30
1	B	11	ASP	CB-CG-OD1	-8.45	110.70	118.30
1	B	62	LEU	CB-CG-CD2	-8.36	96.78	111.00
1	E	398	ASP	CB-CG-OD1	8.34	125.81	118.30
1	G	462	PRO	N-CD-CG	-8.30	90.74	103.20
1	H	428	ASP	CB-CG-OD2	8.24	125.72	118.30
1	F	398	ASP	CB-CG-OD1	8.24	125.71	118.30
1	L	25	ASP	CB-CG-OD2	8.08	125.57	118.30
1	D	523	ASP	CB-CG-OD2	8.00	125.50	118.30
1	N	25	ASP	CB-CG-OD1	-7.99	111.11	118.30
1	M	25	ASP	CB-CG-OD1	-7.98	111.12	118.30
1	E	121	ASP	CB-CG-OD1	7.95	125.46	118.30
1	A	115	ASP	CB-CG-OD2	7.94	125.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	395	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	M	428	ASP	CB-CG-OD2	7.86	125.38	118.30
1	A	398	ASP	CB-CG-OD1	7.86	125.37	118.30
1	F	64	ASP	CB-CG-OD2	7.83	125.35	118.30
1	D	121	ASP	CB-CG-OD2	-7.82	111.27	118.30
1	C	131	LEU	CB-CG-CD2	-7.78	97.78	111.00
1	E	64	ASP	CB-CG-OD2	7.77	125.29	118.30
1	I	473	ASP	CB-CG-OD2	7.71	125.24	118.30
1	E	395	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	M	115	ASP	CB-CG-OD2	7.70	125.23	118.30
1	A	121	ASP	CB-CG-OD1	7.70	125.23	118.30
1	K	83	ASP	CB-CG-OD2	7.64	125.18	118.30
1	G	115	ASP	CB-CG-OD2	7.63	125.17	118.30
1	E	11	ASP	CB-CG-OD1	-7.63	111.44	118.30
1	F	49	ILE	CG1-CB-CG2	-7.62	94.62	111.40
1	N	435	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	452	ARG	NE-CZ-NH1	-7.57	116.51	120.30
1	N	23	LEU	CB-CG-CD1	-7.55	98.16	111.00
1	G	52	ASP	CB-CG-OD1	7.53	125.08	118.30
1	C	62	LEU	CB-CG-CD2	-7.49	98.27	111.00
1	A	11	ASP	CB-CG-OD2	7.47	125.02	118.30
1	D	11	ASP	CB-CG-OD2	7.46	125.02	118.30
1	C	514	MET	CG-SD-CE	-7.42	88.32	100.20
1	C	523	ASP	CB-CG-OD2	7.40	124.96	118.30
1	G	18	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	I	435	ASP	CB-CG-OD2	7.38	124.95	118.30
1	N	428	ASP	CB-CG-OD1	-7.38	111.66	118.30
1	C	87	ASP	CB-CG-OD1	7.37	124.93	118.30
1	D	188	ASP	CB-CG-OD2	7.32	124.89	118.30
1	G	121	ASP	CB-CG-OD1	7.30	124.87	118.30
1	I	421	ARG	NE-CZ-NH1	-7.29	116.65	120.30
1	M	179	ASP	CB-CG-OD2	7.23	124.81	118.30
1	J	188	ASP	CB-CG-OD2	7.23	124.80	118.30
1	A	87	ASP	CB-CG-OD1	7.19	124.77	118.30
1	B	419	LEU	CB-CG-CD2	-7.17	98.80	111.00
1	G	49	ILE	CG1-CB-CG2	-7.13	95.72	111.40
1	D	11	ASP	CB-CG-OD1	-7.12	111.89	118.30
1	G	398	ASP	CB-CG-OD1	7.10	124.69	118.30
1	G	501	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	M	328	ASP	CB-CG-OD2	7.01	124.61	118.30
1	M	11	ASP	CB-CG-OD2	6.97	124.57	118.30
1	N	458	CYS	CA-CB-SG	-6.96	101.46	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	ASP	CB-CG-OD2	6.96	124.56	118.30
1	C	513	LEU	CA-CB-CG	-6.96	99.30	115.30
1	L	5	ASP	CB-CG-OD2	6.96	124.56	118.30
1	H	25	ASP	CB-CG-OD2	6.96	124.56	118.30
1	C	41	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	49	ILE	CG1-CB-CG2	-6.89	96.25	111.40
1	D	435	ASP	CB-CG-OD2	6.85	124.47	118.30
1	I	83	ASP	CB-CG-OD2	6.85	124.46	118.30
1	J	435	ASP	CB-CG-OD2	6.84	124.45	118.30
1	G	41	ASP	CB-CG-OD2	6.76	124.38	118.30
1	J	428	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	B	435	ASP	CB-CG-OD2	6.75	124.37	118.30
1	C	100	ILE	CG1-CB-CG2	-6.72	96.61	111.40
1	A	444	LEU	CB-CG-CD1	-6.71	99.60	111.00
1	C	64	ASP	CB-CG-OD2	6.70	124.33	118.30
1	J	328	ASP	CB-CG-OD2	6.70	124.33	118.30
1	H	495	ASP	CB-CG-OD2	6.69	124.32	118.30
1	F	83	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	435	ASP	CB-CG-OD2	6.68	124.31	118.30
1	B	25	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	K	426	LEU	CB-CG-CD1	-6.67	99.65	111.00
1	G	421	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	N	52	ASP	CB-CG-OD1	6.66	124.30	118.30
1	I	115	ASP	CB-CG-OD2	6.64	124.28	118.30
1	F	435	ASP	CB-CG-OD2	6.61	124.25	118.30
1	C	49	ILE	CG1-CB-CG2	-6.60	96.88	111.40
1	N	83	ASP	CB-CG-OD2	6.59	124.23	118.30
1	I	328	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	188	ASP	CB-CG-OD2	6.56	124.20	118.30
1	H	435	ASP	CB-CG-OD2	6.55	124.20	118.30
1	N	328	ASP	CB-CG-OD2	6.55	124.20	118.30
1	M	461	GLU	OE1-CD-OE2	6.54	131.15	123.30
1	G	513	LEU	CB-CG-CD2	-6.54	99.89	111.00
1	G	64	ASP	CB-CG-OD2	6.53	124.18	118.30
1	H	462	PRO	N-CD-CG	-6.53	93.41	103.20
1	G	523	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	116	LEU	CB-CG-CD1	-6.48	99.98	111.00
1	N	41	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	328	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	328	ASP	CB-CG-OD2	6.46	124.12	118.30
1	J	316	ASP	CB-CG-OD2	6.43	124.09	118.30
1	H	179	ASP	CB-CG-OD2	6.43	124.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	179	ASP	CB-CG-OD2	6.39	124.06	118.30
1	H	83	ASP	CB-CG-OD2	6.38	124.04	118.30
1	L	196	ASP	CB-CG-OD2	6.38	124.04	118.30
1	G	328	ASP	CB-CG-OD2	6.37	124.03	118.30
1	L	179	ASP	CB-CG-OD2	6.34	124.00	118.30
1	C	501	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	J	420	ILE	CG1-CB-CG2	-6.32	97.49	111.40
1	G	62	LEU	CB-CG-CD2	-6.30	100.29	111.00
1	C	134	LEU	CB-CG-CD2	-6.29	100.30	111.00
1	L	121	ASP	CB-CG-OD2	6.28	123.95	118.30
1	D	64	ASP	CB-CG-OD2	6.27	123.94	118.30
1	N	188	ASP	CB-CG-OD2	6.24	123.92	118.30
2	S	90	ASP	CB-CG-OD2	6.22	123.90	118.30
1	E	419	LEU	CB-CG-CD2	-6.22	100.43	111.00
1	J	462	PRO	N-CD-CG	-6.21	93.88	103.20
1	B	118	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	K	428	ASP	CB-CG-OD1	-6.16	112.75	118.30
1	F	421	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	Q	69	ASP	CB-CG-OD2	6.14	123.83	118.30
1	I	461	GLU	OE1-CD-OE2	6.14	130.67	123.30
2	Q	58	ASP	CB-CG-OD2	6.14	123.83	118.30
1	K	462	PRO	N-CD-CG	-6.12	94.02	103.20
1	I	419	LEU	CB-CG-CD1	-6.10	100.64	111.00
1	N	283	ASP	CB-CG-OD2	6.09	123.78	118.30
1	I	420	ILE	CG1-CB-CG2	-6.08	98.02	111.40
1	A	65	LYS	CD-CE-NZ	-6.08	97.72	111.70
1	H	155	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	490	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	398	ASP	CB-CG-OD1	6.07	123.77	118.30
1	I	48	THR	OG1-CB-CG2	-6.07	96.05	110.00
1	M	462	PRO	N-CD-CG	-6.05	94.13	103.20
1	B	140	ASP	CB-CG-OD2	6.04	123.74	118.30
1	H	420	ILE	CG1-CB-CG2	-6.04	98.11	111.40
1	M	398	ASP	CB-CG-OD2	6.04	123.73	118.30
1	N	473	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	419	LEU	CB-CG-CD2	-6.02	100.76	111.00
1	I	99	ILE	CG1-CB-CG2	6.02	124.64	111.40
1	L	435	ASP	CB-CG-OD2	6.01	123.71	118.30
1	I	114	MET	CG-SD-CE	6.00	109.81	100.20
1	B	49	ILE	CG1-CB-CG2	-6.00	98.20	111.40
1	J	253	ASP	CB-CG-OD2	5.99	123.69	118.30
1	E	404	ARG	NE-CZ-NH1	5.99	123.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	11	ASP	CB-CG-OD2	5.98	123.68	118.30
1	G	490	ASP	CB-CG-OD2	5.95	123.66	118.30
1	L	23	LEU	CB-CG-CD1	-5.94	100.91	111.00
1	G	518	GLU	OE1-CD-OE2	-5.93	116.18	123.30
1	E	295	LEU	CA-CB-CG	5.92	128.92	115.30
1	D	513	LEU	CA-CB-CG	-5.91	101.71	115.30
1	B	25	ASP	CB-CG-OD2	5.91	123.61	118.30
1	J	334	ASP	CB-CG-OD2	5.90	123.61	118.30
1	H	316	ASP	CB-CG-OD2	5.90	123.61	118.30
2	P	79	ASP	CB-CG-OD2	5.89	123.60	118.30
1	M	419	LEU	CB-CG-CD2	5.88	120.99	111.00
1	E	328	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	52	ASP	CB-CG-OD1	5.85	123.57	118.30
1	B	5	ASP	CB-CG-OD2	5.84	123.55	118.30
1	G	167	ASP	CB-CG-OD2	5.83	123.55	118.30
1	J	23	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	D	87	ASP	CB-CG-OD1	5.82	123.54	118.30
1	J	458	CYS	CA-CB-SG	-5.81	103.54	114.00
1	A	361	ASP	CB-CG-OD2	5.81	123.53	118.30
1	M	188	ASP	CB-CG-OD2	5.80	123.52	118.30
2	O	58	ASP	CB-CG-OD2	5.80	123.52	118.30
2	S	79	ASP	CB-CG-OD2	5.80	123.52	118.30
1	E	428	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	295	LEU	CA-CB-CG	5.79	128.61	115.30
1	E	361	ASP	CB-CG-OD2	5.78	123.51	118.30
1	J	495	ASP	CB-CG-OD2	5.78	123.50	118.30
1	F	361	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	36	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	462	PRO	N-CD-CG	-5.77	94.54	103.20
2	Q	8	ASP	CB-CG-OD2	5.77	123.49	118.30
1	C	295	LEU	CA-CB-CG	5.76	128.56	115.30
1	C	361	ASP	CB-CG-OD2	5.76	123.48	118.30
1	G	5	ASP	CB-CG-OD2	5.76	123.48	118.30
1	M	435	ASP	CB-CG-OD2	5.75	123.48	118.30
1	M	426	LEU	CB-CG-CD1	-5.75	101.23	111.00
1	B	295	LEU	CA-CB-CG	5.74	128.51	115.30
1	A	167	ASP	CB-CG-OD2	5.74	123.46	118.30
1	C	25	ASP	CB-CG-OD2	5.74	123.46	118.30
1	G	73	MET	CG-SD-CE	5.73	109.36	100.20
2	R	8	ASP	CB-CG-OD2	5.73	123.45	118.30
1	B	361	ASP	CB-CG-OD2	5.71	123.44	118.30
1	I	398	ASP	CB-CG-OD2	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	513	LEU	CA-CB-CG	-5.71	102.18	115.30
2	T	58	ASP	CB-CG-OD2	5.71	123.44	118.30
1	I	523	ASP	CB-CG-OD2	5.70	123.43	118.30
1	F	328	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	140	ASP	CB-CG-OD2	5.69	123.42	118.30
1	N	48	THR	OG1-CB-CG2	-5.69	96.91	110.00
1	B	41	ASP	CB-CG-OD2	5.68	123.41	118.30
1	G	295	LEU	CA-CB-CG	5.67	128.34	115.30
1	C	395	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	H	64	ASP	CB-CG-OD1	5.67	123.40	118.30
1	J	419	LEU	CB-CG-CD1	-5.66	101.37	111.00
2	T	63	ASP	CB-CG-OD2	5.66	123.40	118.30
1	M	83	ASP	CB-CG-OD2	5.66	123.39	118.30
2	O	90	ASP	CB-CG-OD2	5.64	123.37	118.30
1	C	58	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	I	78	ALA	CB-CA-C	5.63	118.55	110.10
1	H	17	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	G	361	ASP	CB-CG-OD2	5.62	123.36	118.30
1	H	514	MET	CG-SD-CE	-5.62	91.21	100.20
1	L	283	ASP	CB-CG-OD2	5.62	123.36	118.30
1	L	316	ASP	CB-CG-OD2	5.61	123.35	118.30
1	N	36	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	328	ASP	CB-CG-OD2	5.59	123.33	118.30
1	H	23	LEU	CB-CG-CD1	-5.59	101.50	111.00
1	H	188	ASP	CB-CG-OD2	5.58	123.32	118.30
1	L	523	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	395	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	N	430	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	404	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	H	517	THR	OG1-CB-CG2	-5.55	97.23	110.00
1	G	87	ASP	CB-CG-OD1	5.55	123.29	118.30
1	M	495	ASP	CB-CG-OD2	5.55	123.29	118.30
1	K	316	ASP	CB-CG-OD2	5.54	123.29	118.30
1	G	11	ASP	CB-CG-OD2	5.54	123.29	118.30
1	I	179	ASP	CB-CG-OD2	5.54	123.29	118.30
2	Q	63	ASP	CB-CG-OD2	5.54	123.29	118.30
1	J	117	LYS	CD-CE-NZ	-5.54	98.97	111.70
1	C	421	ARG	NE-CZ-NH1	5.53	123.07	120.30
2	U	58	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	73	MET	CG-SD-CE	5.53	109.04	100.20
2	O	79	ASP	CB-CG-OD2	5.53	123.27	118.30
2	P	58	ASP	CB-CG-OD2	5.53	123.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	361	ASP	CB-CG-OD2	5.52	123.27	118.30
1	M	316	ASP	CB-CG-OD2	5.52	123.27	118.30
1	J	179	ASP	CB-CG-OD2	5.51	123.26	118.30
1	F	462	PRO	N-CD-CG	-5.51	94.93	103.20
1	A	23	LEU	CA-CB-CG	5.50	127.94	115.30
1	E	49	ILE	CG1-CB-CG2	-5.49	99.31	111.40
1	G	36	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	H	283	ASP	CB-CG-OD2	5.49	123.24	118.30
1	M	421	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	I	462	PRO	N-CD-CG	-5.49	94.97	103.20
1	I	361	ASP	CB-CG-OD2	5.47	123.22	118.30
1	E	435	ASP	CB-CG-OD2	5.47	123.22	118.30
1	N	23	LEU	CB-CG-CD2	5.46	120.29	111.00
1	G	500	THR	OG1-CB-CG2	-5.46	97.45	110.00
1	I	426	LEU	CB-CG-CD1	-5.45	101.73	111.00
2	O	69	ASP	CB-CG-OD2	5.45	123.21	118.30
1	I	155	ASP	CB-CG-OD2	5.45	123.20	118.30
1	E	115	ASP	CB-CG-OD2	5.44	123.20	118.30
1	L	64	ASP	CB-CG-OD1	5.44	123.20	118.30
2	R	79	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	116	LEU	CB-CG-CD1	-5.44	101.76	111.00
1	H	522	THR	OG1-CB-CG2	-5.44	97.49	110.00
1	B	188	ASP	CB-CG-OD2	5.44	123.19	118.30
1	N	334	ASP	CB-CG-OD2	5.43	123.19	118.30
1	K	334	ASP	CB-CG-OD2	5.43	123.19	118.30
1	G	58	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	E	462	PRO	N-CD-CG	-5.42	95.08	103.20
1	E	513	LEU	CA-CB-CG	-5.42	102.84	115.30
1	D	183	LEU	CA-CB-CG	5.42	127.75	115.30
1	J	514	MET	CG-SD-CE	-5.41	91.55	100.20
1	D	87	ASP	CB-CG-OD2	5.41	123.17	118.30
1	N	155	ASP	CB-CG-OD2	5.40	123.16	118.30
1	M	31	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	I	64	ASP	CB-CG-OD1	5.40	123.16	118.30
1	K	359	ASP	CB-CG-OD2	5.40	123.16	118.30
1	G	23	LEU	CA-CB-CG	5.39	127.70	115.30
1	M	155	ASP	CB-CG-OD2	5.38	123.14	118.30
2	T	79	ASP	CB-CG-OD2	5.38	123.14	118.30
1	L	328	ASP	CB-CG-OD2	5.37	123.13	118.30
1	K	23	LEU	CB-CG-CD1	-5.37	101.88	111.00
2	P	8	ASP	CB-CG-OD2	5.37	123.13	118.30
1	M	18	ARG	NE-CZ-NH2	5.36	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	102	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	C	31	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	D	91	THR	OG1-CB-CG2	-5.34	97.71	110.00
1	I	253	ASP	CB-CG-OD2	5.34	123.11	118.30
2	P	90	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	16	MET	CG-SD-CE	-5.34	91.66	100.20
1	F	419	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	A	179	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	295	LEU	CA-CB-CG	5.30	127.50	115.30
1	E	188	ASP	CB-CG-OD2	5.30	123.08	118.30
1	D	87	ASP	OD1-CG-OD2	-5.30	113.22	123.30
1	D	316	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	140	ASP	CB-CG-OD2	5.29	123.07	118.30
1	G	140	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	361	ASP	CB-CG-OD2	5.29	123.06	118.30
1	I	501	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	J	115	ASP	CB-CG-OD2	5.29	123.06	118.30
2	U	79	ASP	CB-CG-OD2	5.27	123.05	118.30
1	M	419	LEU	CB-CG-CD1	-5.26	102.05	111.00
1	F	13	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	I	450	PRO	N-CD-CG	-5.25	95.32	103.20
1	F	23	LEU	CA-CB-CG	5.25	127.38	115.30
1	D	328	ASP	CB-CG-OD2	5.24	123.02	118.30
2	R	90	ASP	CB-CG-OD2	5.24	123.02	118.30
1	M	23	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	J	283	ASP	CB-CG-OD2	5.23	123.01	118.30
1	J	41	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	121	ASP	CB-CG-OD1	5.23	123.00	118.30
1	E	91	THR	OG1-CB-CG2	-5.22	97.99	110.00
1	F	295	LEU	CA-CB-CG	5.22	127.31	115.30
1	M	420	ILE	CG1-CB-CG2	-5.22	99.92	111.40
1	G	183	LEU	CA-CB-CG	5.21	127.29	115.30
1	E	334	ASP	CB-CG-OD2	5.21	122.99	118.30
1	I	188	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	138	CYS	CA-CB-SG	5.20	123.36	114.00
1	N	520	MET	CG-SD-CE	5.19	108.51	100.20
1	I	23	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	E	140	ASP	CB-CG-OD2	5.19	122.97	118.30
1	J	155	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	510	VAL	CG1-CB-CG2	-5.17	102.62	110.90
2	U	69	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	497	THR	CA-CB-CG2	-5.16	105.17	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	VAL	CG1-CB-CG2	5.16	119.15	110.90
1	F	116	LEU	CB-CG-CD1	-5.16	102.23	111.00
2	T	8	ASP	CB-CG-OD2	5.15	122.94	118.30
1	N	179	ASP	CB-CG-OD2	5.14	122.93	118.30
1	F	334	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	41	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	87	ASP	OD1-CG-OD2	-5.14	113.54	123.30
2	T	69	ASP	CB-CG-OD2	5.13	122.92	118.30
1	H	504	LEU	CB-CG-CD2	5.13	119.72	111.00
1	N	359	ASP	CB-CG-OD2	5.12	122.91	118.30
1	N	11	ASP	CB-CG-OD2	5.12	122.91	118.30
1	N	517	THR	OG1-CB-CG2	-5.11	98.25	110.00
1	D	167	ASP	CB-CG-OD2	5.11	122.89	118.30
1	N	316	ASP	CB-CG-OD2	5.10	122.89	118.30
1	J	517	THR	OG1-CB-CG2	-5.09	98.28	110.00
2	P	63	ASP	CB-CG-OD2	5.09	122.89	118.30
1	L	517	THR	OG1-CB-CG2	-5.09	98.30	110.00
2	S	69	ASP	CB-CG-OD2	5.09	122.88	118.30
1	K	196	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	134	LEU	CB-CA-C	-5.07	100.56	110.20
1	L	31	LEU	CB-CG-CD2	-5.07	102.38	111.00
2	R	58	ASP	CB-CG-OD2	5.07	122.86	118.30
2	S	58	ASP	CB-CG-OD2	5.07	122.86	118.30
1	K	11	ASP	CB-CG-OD2	5.07	122.86	118.30
1	G	11	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	I	161	LEU	CB-CG-CD2	-5.06	102.40	111.00
1	I	283	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	52	ASP	CB-CG-OD1	5.06	122.85	118.30
1	G	435	ASP	CB-CG-OD2	5.05	122.85	118.30
1	H	11	ASP	CB-CG-OD2	5.05	122.85	118.30
2	P	69	ASP	CB-CG-OD2	5.05	122.85	118.30
2	U	90	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	52	ASP	CB-CG-OD2	5.05	122.85	118.30
1	G	501	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	A	224	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	11	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	F	140	ASP	CB-CG-OD2	5.04	122.84	118.30
1	H	13	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	49	ILE	CG1-CB-CG2	-5.04	100.31	111.40
1	M	64	ASP	CB-CG-OD2	5.04	122.83	118.30
1	M	48	THR	OG1-CB-CG2	-5.04	98.42	110.00
1	G	456	LEU	CB-CG-CD1	5.03	119.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	361	ASP	CB-CG-OD2	5.03	122.83	118.30
1	K	155	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	83	ASP	CB-CG-OD2	5.03	122.83	118.30
1	H	361	ASP	CB-CG-OD2	5.03	122.83	118.30
1	G	334	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	28	LYS	CD-CE-NZ	-5.03	100.14	111.70
1	L	13	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	C	458	CYS	CA-CB-SG	-5.01	104.99	114.00
1	D	224	ASP	CB-CG-OD2	5.01	122.81	118.30
1	M	32	GLY	N-CA-C	5.00	125.61	113.10
1	G	451	LEU	CA-CB-CG	5.00	126.81	115.30
1	H	41	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	SER	Peptide
1	H	32	GLY	Peptide
1	I	32	GLY	Peptide
1	J	32	GLY	Peptide
1	K	32	GLY	Peptide
1	L	32	GLY	Peptide
1	M	32	GLY	Peptide
1	N	32	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3974	158	0
1	B	3855	0	3976	151	0
1	C	3855	0	3975	155	0
1	D	3855	0	3976	145	0
1	E	3855	0	3975	122	0
1	F	3855	0	3976	133	0
1	G	3855	0	3974	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3856	0	3976	129	0
1	I	3856	0	3976	174	0
1	J	3856	0	3976	143	0
1	K	3856	0	3976	130	0
1	L	3856	0	3976	135	0
1	M	3856	0	3976	144	0
1	N	3856	0	3976	143	0
2	O	728	0	762	26	0
2	P	728	0	762	22	0
2	Q	728	0	762	23	0
2	R	728	0	762	21	0
2	S	728	0	762	23	0
2	T	728	0	762	27	0
2	U	728	0	762	25	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	27	0	12	1	0
5	B	27	0	12	1	0
5	C	27	0	12	2	0
5	D	27	0	12	3	0
5	E	27	0	12	1	0
5	F	27	0	12	2	0
5	G	27	0	12	1	0
6	A	4	0	0	2	0
6	B	4	0	0	0	0
6	C	4	0	0	1	0
6	D	4	0	0	2	0
6	E	4	0	0	1	0
6	F	4	0	0	2	0
6	G	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	19	0	0	2	0
7	B	10	0	0	1	0
7	C	21	0	0	5	0
7	D	14	0	0	4	0
7	E	12	0	0	3	0
7	F	11	0	0	3	0
7	G	20	0	0	2	0
7	H	11	0	0	3	0
7	I	17	0	0	4	0
7	J	12	0	0	1	0
7	K	14	0	0	2	0
7	L	13	0	0	3	0
7	M	10	0	0	6	0
7	N	10	0	0	5	0
All	All	59498	0	61076	2099	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 17.

All (2099) 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:N:288:MET:SD	1:N:288:MET:CE	2.01	1.46
1:F:114:MET:CE	1:F:114:MET:SD	2.02	1.46
1:I:447:MET:SD	1:I:447:MET:CE	2.05	1.45
1:K:16:MET:SD	1:K:16:MET:CE	2.05	1.45
1:J:288:MET:SD	1:J:288:MET:CE	2.04	1.45
1:B:114:MET:SD	1:B:114:MET:CE	2.04	1.45
1:B:16:MET:CE	1:B:16:MET:SD	2.05	1.44
1:M:514:MET:CE	1:M:514:MET:SD	2.04	1.44
1:I:16:MET:CE	1:I:16:MET:SD	2.05	1.44
1:M:16:MET:SD	1:M:16:MET:CE	2.04	1.44
1:L:114:MET:CE	1:L:114:MET:SD	2.04	1.44
1:A:114:MET:SD	1:A:114:MET:CE	2.02	1.44
1:C:111:MET:CE	1:C:111:MET:SD	2.06	1.43
1:G:111:MET:CE	1:G:111:MET:SD	2.07	1.43
1:F:16:MET:CE	1:F:16:MET:SD	2.07	1.42
1:K:114:MET:CE	1:K:114:MET:SD	2.07	1.41
1:I:114:MET:CE	1:I:114:MET:SD	2.09	1.39
1:J:16:MET:CE	1:J:16:MET:SD	2.09	1.39
1:B:73:MET:SD	1:B:73:MET:CE	2.10	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:114:MET:CE	1:N:114:MET:SD	2.11	1.39
1:A:111:MET:SD	1:A:111:MET:CE	2.13	1.37
1:F:111:MET:CE	1:F:111:MET:SD	2.13	1.36
1:J:514:MET:CE	1:J:514:MET:SD	2.13	1.36
1:B:111:MET:CE	1:B:111:MET:SD	2.14	1.35
1:C:514:MET:SD	1:C:514:MET:CE	2.13	1.35
1:D:111:MET:SD	1:D:111:MET:CE	2.13	1.35
1:H:514:MET:SD	1:H:514:MET:CE	2.15	1.34
1:M:114:MET:CE	1:M:114:MET:SD	2.13	1.34
1:D:73:MET:SD	1:D:73:MET:CE	2.17	1.33
1:E:111:MET:SD	1:E:111:MET:CE	2.18	1.31
1:E:73:MET:SD	1:E:73:MET:CE	2.19	1.30
1:J:114:MET:SD	1:J:114:MET:CE	2.19	1.30
1:N:16:MET:SD	1:N:16:MET:CE	2.20	1.29
1:G:73:MET:SD	1:G:73:MET:CE	2.21	1.28
1:B:514:MET:CE	1:B:514:MET:SD	2.21	1.28
1:H:114:MET:CE	1:H:114:MET:SD	2.23	1.26
1:N:514:MET:CE	1:N:514:MET:SD	2.24	1.26
1:C:18:ARG:CB	1:C:18:ARG:HH11	1.52	1.23
1:A:73:MET:CE	1:A:73:MET:SD	2.27	1.23
1:F:73:MET:CE	1:F:73:MET:SD	2.27	1.22
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.06	1.17
1:C:73:MET:SD	1:C:73:MET:CE	2.32	1.16
1:G:430:ARG:HG2	1:G:430:ARG:HH11	1.10	1.16
1:C:18:ARG:NH1	1:C:18:ARG:HB3	1.60	1.15
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.05	1.14
1:I:77:VAL:HG21	1:I:510:VAL:HB	1.22	1.14
1:B:18:ARG:CB	1:B:18:ARG:HH11	1.61	1.13
1:F:430:ARG:HH11	1:F:430:ARG:HG2	1.04	1.13
1:B:18:ARG:HB3	1:B:18:ARG:NH1	1.64	1.11
1:G:90:THR:O	1:G:94:VAL:HG23	1.47	1.11
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.00	1.10
1:J:404:ARG:HH11	1:J:404:ARG:HG2	1.11	1.10
1:C:18:ARG:CG	1:C:18:ARG:HH11	1.65	1.10
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.11	1.09
1:D:430:ARG:HH11	1:D:430:ARG:HG2	1.16	1.09
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.05	1.07
1:L:444:LEU:HA	1:L:447:MET:HE3	1.33	1.06
1:F:18:ARG:HH11	1:F:18:ARG:CB	1.68	1.06
1:H:326:ASN:HD22	1:H:329:THR:HB	1.20	1.06
1:I:404:ARG:HH11	1:I:404:ARG:HG2	1.11	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:ARG:HH11	1:E:430:ARG:HG2	0.89	1.05
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.19	1.05
1:A:452:ARG:NH1	7:A:614:HOH:O	1.88	1.04
1:I:425:LYS:NZ	7:I:540:HOH:O	1.90	1.04
1:N:404:ARG:HH11	1:N:404:ARG:HG2	1.21	1.04
1:I:444:LEU:HD23	1:I:447:MET:CE	1.87	1.04
1:C:90:THR:O	1:C:94:VAL:HG23	1.56	1.03
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.40	1.03
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.41	1.02
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.42	1.01
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.42	1.00
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.43	1.00
1:D:18:ARG:CG	1:D:18:ARG:HH11	1.73	1.00
1:I:326:ASN:HD22	1:I:329:THR:HB	1.25	1.00
1:E:18:ARG:HH11	1:E:18:ARG:CB	1.74	1.00
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.26	1.00
1:A:18:ARG:CG	1:A:18:ARG:HH11	1.74	0.99
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.41	0.99
1:J:326:ASN:HD22	1:J:329:THR:HB	1.26	0.98
1:E:18:ARG:CG	1:E:18:ARG:HH11	1.76	0.98
1:A:18:ARG:CB	1:A:18:ARG:HH11	1.76	0.98
1:N:326:ASN:HD22	1:N:329:THR:HB	1.23	0.98
1:L:326:ASN:HD22	1:L:329:THR:HB	1.26	0.98
1:E:430:ARG:NH1	1:E:430:ARG:HG2	1.65	0.97
1:G:18:ARG:CB	1:G:18:ARG:HH11	1.76	0.97
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.44	0.97
1:F:18:ARG:NH1	1:F:18:ARG:HB3	1.79	0.97
2:T:50:GLU:HG2	2:U:51:ASN:HB2	1.47	0.97
1:A:430:ARG:NH1	1:A:430:ARG:HG2	1.72	0.97
1:E:138:CYS:HA	7:E:611:HOH:O	1.63	0.96
1:M:326:ASN:HD22	1:M:329:THR:HB	1.27	0.96
1:J:444:LEU:HA	1:J:447:MET:HE3	1.47	0.96
1:K:326:ASN:HD22	1:K:329:THR:HB	1.29	0.96
2:P:50:GLU:HG2	2:Q:51:ASN:HB2	1.47	0.95
1:E:430:ARG:CG	1:E:430:ARG:HH11	1.79	0.95
1:G:18:ARG:NH1	1:G:18:ARG:HB3	1.82	0.95
1:N:444:LEU:HA	1:N:447:MET:HE3	1.46	0.94
1:B:430:ARG:NH1	1:B:430:ARG:HG2	1.76	0.94
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.50	0.93
1:D:18:ARG:CB	1:D:18:ARG:HH11	1.81	0.93
1:F:18:ARG:CG	1:F:18:ARG:HH11	1.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:444:LEU:HD23	1:I:447:MET:HE1	1.50	0.92
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.51	0.92
1:F:18:ARG:HB3	1:F:18:ARG:HH11	1.35	0.91
1:F:430:ARG:NH1	1:F:430:ARG:HG2	1.76	0.91
1:B:18:ARG:CG	1:B:18:ARG:HH11	1.83	0.91
1:C:430:ARG:NH1	1:C:430:ARG:HG2	1.77	0.91
2:S:50:GLU:HG2	2:T:51:ASN:HB2	1.53	0.91
1:K:65:LYS:O	1:K:66:PHE:HB2	1.68	0.90
1:D:18:ARG:HG2	1:D:18:ARG:HH11	1.34	0.90
1:N:65:LYS:O	1:N:66:PHE:HB2	1.71	0.89
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.54	0.89
1:A:18:ARG:HB3	1:A:18:ARG:NH1	1.87	0.89
1:D:18:ARG:HB3	1:D:18:ARG:NH1	1.88	0.89
1:M:404:ARG:NH1	1:M:404:ARG:HG2	1.86	0.88
1:M:425:LYS:NZ	7:M:532:HOH:O	2.06	0.88
1:C:510:VAL:CG1	1:C:514:MET:HE1	2.02	0.88
1:K:123:ALA:HB2	1:K:440:ILE:HG23	1.56	0.88
1:G:430:ARG:HG2	1:G:430:ARG:NH1	1.81	0.88
2:Q:50:GLU:HG2	2:R:51:ASN:HB2	1.55	0.87
1:B:90:THR:O	1:B:94:VAL:HG23	1.73	0.87
1:C:18:ARG:NH1	1:C:18:ARG:CB	2.23	0.86
1:C:349:ILE:HA	1:C:352:GLN:CG	2.05	0.86
1:C:414:GLY:O	1:C:417:VAL:HG12	1.75	0.86
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.57	0.86
1:B:349:ILE:HA	1:B:352:GLN:CG	2.05	0.86
1:M:444:LEU:HA	1:M:447:MET:HE3	1.54	0.86
1:I:106:ALA:O	1:I:109:ALA:HB3	1.76	0.86
1:E:18:ARG:NH1	1:E:18:ARG:HB3	1.90	0.86
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.56	0.86
1:I:444:LEU:HA	1:I:447:MET:HE3	1.58	0.86
1:A:414:GLY:O	1:A:417:VAL:HG12	1.76	0.85
1:G:349:ILE:HA	1:G:352:GLN:CG	2.05	0.85
1:F:90:THR:O	1:F:94:VAL:HG23	1.76	0.84
1:G:409:GLU:OE1	7:G:619:HOH:O	1.95	0.84
1:D:349:ILE:HA	1:D:352:GLN:CG	2.07	0.84
1:H:326:ASN:HD22	1:H:329:THR:CB	1.89	0.84
1:H:444:LEU:HD23	1:H:447:MET:CE	2.07	0.84
1:C:18:ARG:NH1	1:C:18:ARG:CG	2.38	0.84
1:K:444:LEU:HD23	1:K:447:MET:CE	2.08	0.84
1:B:18:ARG:HB3	1:B:18:ARG:HH11	1.23	0.84
1:I:404:ARG:HG2	1:I:404:ARG:NH1	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.39	0.83
1:K:444:LEU:HA	1:K:447:MET:HE3	1.59	0.83
1:B:351:GLN:HE22	1:C:209:GLU:HB3	1.43	0.83
1:G:18:ARG:HH11	1:G:18:ARG:HB3	1.39	0.83
1:J:404:ARG:HG2	1:J:404:ARG:NH1	1.90	0.83
1:L:444:LEU:HD23	1:L:447:MET:CE	2.08	0.83
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.61	0.83
1:H:444:LEU:HA	1:H:447:MET:HE3	1.61	0.83
1:N:106:ALA:O	1:N:109:ALA:HB3	1.78	0.83
1:H:65:LYS:O	1:H:66:PHE:HB2	1.77	0.83
1:E:18:ARG:HH11	1:E:18:ARG:HG2	1.40	0.83
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.60	0.83
1:E:349:ILE:HA	1:E:352:GLN:CG	2.08	0.83
1:A:18:ARG:CB	1:A:18:ARG:NH1	2.41	0.82
1:A:349:ILE:HA	1:A:352:GLN:CG	2.09	0.82
1:C:514:MET:HB2	1:C:514:MET:HE3	1.61	0.82
1:I:65:LYS:O	1:I:66:PHE:HB2	1.76	0.82
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.62	0.82
1:G:414:GLY:O	1:G:417:VAL:HG12	1.80	0.82
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.60	0.82
1:M:404:ARG:CG	1:M:404:ARG:HH11	1.90	0.82
1:K:131:LEU:HD12	1:K:422:VAL:HG11	1.62	0.82
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.62	0.81
1:D:462:PRO:HD2	7:D:608:HOH:O	1.81	0.81
1:A:510:VAL:HG12	1:A:514:MET:HE3	1.63	0.81
1:J:65:LYS:O	1:J:66:PHE:HB2	1.79	0.81
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.61	0.81
1:I:349:ILE:HA	1:I:352:GLN:HG3	1.62	0.81
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.63	0.81
2:O:50:GLU:HG2	2:P:51:ASN:HB2	1.61	0.81
1:C:206:ASN:HD21	1:C:214:GLU:H	1.29	0.81
1:E:18:ARG:NH1	1:E:18:ARG:CB	2.43	0.81
1:C:514:MET:HB2	1:C:514:MET:CE	2.12	0.80
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.61	0.80
1:D:18:ARG:CB	1:D:18:ARG:NH1	2.43	0.80
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.61	0.80
1:C:510:VAL:CG1	1:C:514:MET:CE	2.60	0.80
1:I:326:ASN:HD22	1:I:329:THR:CB	1.94	0.80
1:J:291:ASP:OD2	1:J:368:ARG:HD2	1.81	0.80
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.63	0.79
1:A:90:THR:O	1:A:94:VAL:HG23	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.64	0.79
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.62	0.79
1:F:414:GLY:O	1:F:417:VAL:HG12	1.82	0.79
1:B:514:MET:CE	1:B:514:MET:HB2	2.12	0.79
1:C:18:ARG:HG2	1:C:18:ARG:HH11	1.47	0.79
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.64	0.79
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.65	0.79
1:L:131:LEU:HD12	1:L:422:VAL:HG11	1.64	0.79
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.63	0.79
1:M:131:LEU:HD12	1:M:422:VAL:HG11	1.64	0.79
1:F:305:ILE:HG23	1:G:267:MET:HG2	1.64	0.78
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.65	0.78
1:A:234:LEU:O	1:A:238:GLU:HG3	1.83	0.78
1:D:430:ARG:NH1	1:D:430:ARG:HG2	1.84	0.78
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.64	0.78
1:F:349:ILE:HA	1:F:352:GLN:CG	2.13	0.78
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.66	0.78
1:N:444:LEU:HD23	1:N:447:MET:CE	2.13	0.78
1:B:206:ASN:HD21	1:B:214:GLU:H	1.32	0.78
1:J:415:GLY:H	1:J:417:VAL:HG23	1.49	0.78
1:J:326:ASN:HD22	1:J:329:THR:CB	1.97	0.78
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.66	0.77
1:D:234:LEU:O	1:D:238:GLU:HG3	1.83	0.77
1:G:18:ARG:CG	1:G:18:ARG:HH11	1.97	0.77
1:I:444:LEU:HA	1:I:447:MET:CE	2.13	0.77
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.64	0.77
1:L:326:ASN:HD22	1:L:329:THR:CB	1.97	0.77
1:H:404:ARG:CG	1:H:404:ARG:HH11	1.94	0.77
1:L:455:VAL:HG11	1:L:462:PRO:HA	1.63	0.77
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.65	0.77
1:N:326:ASN:HD22	1:N:329:THR:CB	1.96	0.77
1:B:18:ARG:CB	1:B:18:ARG:NH1	2.33	0.77
1:I:131:LEU:HD12	1:I:422:VAL:HG11	1.66	0.77
1:B:259:LEU:O	1:B:263:VAL:HG23	1.85	0.77
1:C:325:ILE:HG22	1:C:330:THR:HG23	1.65	0.77
1:G:234:LEU:O	1:G:238:GLU:HG3	1.85	0.77
1:N:415:GLY:H	1:N:417:VAL:HG23	1.47	0.77
1:B:414:GLY:O	1:B:417:VAL:HG12	1.85	0.77
1:I:404:ARG:HH11	1:I:404:ARG:CG	1.92	0.77
1:E:414:GLY:O	1:E:417:VAL:HG12	1.85	0.76
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:PRO:HD2	7:A:613:HOH:O	1.86	0.76
1:L:32:GLY:HA2	1:L:454:ILE:HG23	1.68	0.76
1:A:430:ARG:CG	1:A:430:ARG:HH11	1.90	0.76
1:B:510:VAL:CG1	1:B:514:MET:CE	2.63	0.76
1:H:166:MET:HE3	1:H:171:LYS:HA	1.68	0.76
1:L:444:LEU:HD23	1:L:447:MET:HE3	1.67	0.76
1:M:32:GLY:HA2	1:M:454:ILE:HG23	1.68	0.76
1:B:510:VAL:CG1	1:B:514:MET:HE1	2.16	0.76
1:I:32:GLY:HA2	1:I:454:ILE:HG23	1.67	0.76
2:O:51:ASN:HB2	2:U:50:GLU:HG2	1.68	0.76
1:D:452:ARG:NH1	7:D:609:HOH:O	2.18	0.76
1:E:430:ARG:NH1	1:E:430:ARG:CG	2.42	0.76
1:I:455:VAL:HG11	1:I:462:PRO:HA	1.67	0.76
1:G:510:VAL:HG12	1:G:514:MET:HE3	1.68	0.76
1:H:415:GLY:H	1:H:417:VAL:HG23	1.49	0.76
1:A:510:VAL:HG12	1:A:514:MET:CE	2.16	0.75
1:E:206:ASN:HD21	1:E:214:GLU:H	1.35	0.75
1:N:166:MET:HE3	1:N:171:LYS:HA	1.67	0.75
1:N:131:LEU:HD12	1:N:422:VAL:HG11	1.68	0.75
1:A:325:ILE:HG22	1:A:330:THR:HG23	1.69	0.75
1:B:325:ILE:HG22	1:B:330:THR:HG23	1.68	0.75
1:M:213:VAL:HB	1:M:325:ILE:HG12	1.69	0.75
1:N:444:LEU:HD23	1:N:447:MET:HE3	1.67	0.75
1:A:206:ASN:HD21	1:A:214:GLU:H	1.33	0.75
1:E:259:LEU:O	1:E:263:VAL:HG23	1.86	0.75
1:A:419:LEU:HG	1:A:447:MET:HG2	1.67	0.75
1:B:514:MET:HB2	1:B:514:MET:HE3	1.68	0.74
1:C:510:VAL:HG13	1:C:514:MET:HE1	1.69	0.74
1:J:404:ARG:HH11	1:J:404:ARG:CG	1.95	0.74
1:K:444:LEU:HD23	1:K:447:MET:HE3	1.68	0.74
1:M:326:ASN:HD22	1:M:329:THR:CB	1.99	0.74
1:E:260:ALA:O	1:E:264:VAL:HG23	1.86	0.74
1:J:425:LYS:NZ	7:J:537:HOH:O	2.21	0.74
1:A:209:GLU:HB3	1:G:351:GLN:HE22	1.52	0.74
1:C:205:ILE:HA	1:C:213:VAL:HG22	1.70	0.74
1:E:325:ILE:HG22	1:E:330:THR:HG23	1.69	0.74
1:N:96:ALA:O	1:N:100:ILE:HG13	1.88	0.74
1:N:213:VAL:HB	1:N:325:ILE:HG12	1.70	0.74
1:G:205:ILE:HA	1:G:213:VAL:HG22	1.70	0.74
1:I:16:MET:CE	1:I:16:MET:HB2	2.18	0.74
1:I:415:GLY:H	1:I:417:VAL:HG23	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:213:VAL:HB	1:L:325:ILE:HG12	1.69	0.74
1:J:444:LEU:HD23	1:J:447:MET:CE	2.18	0.74
1:D:90:THR:O	1:D:94:VAL:HG23	1.89	0.73
1:F:325:ILE:HG22	1:F:330:THR:HG23	1.69	0.73
1:N:65:LYS:O	1:N:66:PHE:CB	2.34	0.73
1:D:259:LEU:O	1:D:263:VAL:HG23	1.88	0.73
1:H:444:LEU:HD23	1:H:447:MET:HE3	1.69	0.73
1:H:123:ALA:HB2	1:H:440:ILE:HG23	1.69	0.73
1:K:455:VAL:HG11	1:K:462:PRO:HA	1.68	0.73
1:I:166:MET:HE3	1:I:171:LYS:HA	1.70	0.73
1:C:100:ILE:HG13	1:C:511:ALA:HB1	1.70	0.73
1:L:65:LYS:O	1:L:66:PHE:HB2	1.86	0.73
1:G:260:ALA:O	1:G:264:VAL:HG23	1.88	0.73
1:L:123:ALA:HB2	1:L:440:ILE:HG23	1.71	0.73
1:I:213:VAL:HB	1:I:325:ILE:HG12	1.71	0.73
1:K:166:MET:HE3	1:K:171:LYS:HA	1.71	0.73
1:K:326:ASN:HD22	1:K:329:THR:CB	2.02	0.73
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.70	0.73
1:I:166:MET:CE	1:I:171:LYS:HA	2.19	0.72
1:F:260:ALA:O	1:F:264:VAL:HG23	1.89	0.72
1:L:511:ALA:O	1:L:515:ILE:HD12	1.88	0.72
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.69	0.72
1:M:444:LEU:HD23	1:M:447:MET:CE	2.20	0.72
1:M:383:ALA:HB3	1:M:389:MET:HB2	1.72	0.72
1:H:32:GLY:HA2	1:H:454:ILE:HG23	1.72	0.72
1:C:510:VAL:HG13	1:C:514:MET:CE	2.20	0.72
1:K:32:GLY:HA2	1:K:454:ILE:HG23	1.72	0.72
1:F:366:GLN:O	1:F:369:VAL:HG22	1.90	0.72
1:K:96:ALA:O	1:K:100:ILE:HG13	1.89	0.72
1:M:428:ASP:HB2	7:M:534:HOH:O	1.90	0.72
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.71	0.71
1:H:455:VAL:HG11	1:H:462:PRO:HA	1.72	0.71
1:G:325:ILE:HG22	1:G:330:THR:HG23	1.70	0.71
1:H:213:VAL:HB	1:H:325:ILE:HG12	1.71	0.71
1:J:131:LEU:HD12	1:J:422:VAL:HG11	1.70	0.71
1:G:206:ASN:HD21	1:G:214:GLU:H	1.37	0.71
1:J:149:THR:HG21	1:J:156:GLU:HA	1.73	0.71
1:K:213:VAL:HB	1:K:325:ILE:HG12	1.70	0.71
1:L:415:GLY:H	1:L:417:VAL:HG23	1.54	0.71
2:R:50:GLU:HG2	2:S:51:ASN:HB2	1.71	0.71
1:J:213:VAL:HB	1:J:325:ILE:HG12	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:65:LYS:O	1:M:66:PHE:HB2	1.90	0.71
1:N:166:MET:CE	1:N:171:LYS:HA	2.21	0.71
1:D:366:GLN:O	1:D:369:VAL:HG22	1.90	0.71
1:I:149:THR:HG21	1:I:156:GLU:HA	1.73	0.71
1:L:126:ALA:HB1	1:L:426:LEU:HD22	1.71	0.71
1:N:123:ALA:HB2	1:N:440:ILE:HG23	1.70	0.71
1:A:510:VAL:CG1	1:A:514:MET:HE1	2.21	0.71
1:E:234:LEU:O	1:E:238:GLU:HG3	1.91	0.71
1:F:486:GLY:HA3	1:F:491:MET:HE2	1.73	0.71
1:D:206:ASN:HD21	1:D:214:GLU:H	1.36	0.71
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.72	0.71
1:C:260:ALA:O	1:C:264:VAL:HG23	1.91	0.71
1:D:18:ARG:HG2	1:D:18:ARG:NH1	2.06	0.71
1:H:404:ARG:HG2	1:H:404:ARG:NH1	1.91	0.71
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.73	0.71
1:D:44:PHE:H	1:D:44:PHE:HD1	1.38	0.70
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.71	0.70
1:B:44:PHE:HD1	1:B:44:PHE:H	1.39	0.70
1:E:90:THR:O	1:E:94:VAL:HG23	1.90	0.70
1:B:260:ALA:O	1:B:264:VAL:HG23	1.92	0.70
1:F:234:LEU:O	1:F:238:GLU:HG3	1.91	0.70
1:G:270:ILE:HD13	2:U:27:LEU:HB3	1.74	0.70
1:M:149:THR:HG21	1:M:156:GLU:HA	1.73	0.70
1:N:291:ASP:OD2	1:N:368:ARG:HD2	1.92	0.70
1:J:166:MET:HE3	1:J:171:LYS:HA	1.74	0.70
1:A:260:ALA:O	1:A:264:VAL:HG23	1.91	0.70
1:B:234:LEU:O	1:B:238:GLU:HG3	1.91	0.70
1:N:404:ARG:HH11	1:N:404:ARG:CG	2.01	0.70
1:C:270:ILE:HD13	2:Q:27:LEU:HB3	1.72	0.70
1:C:366:GLN:O	1:C:369:VAL:HG22	1.92	0.69
1:C:524:LEU:CD2	1:C:525:PRO:HD2	2.23	0.69
1:F:259:LEU:O	1:F:263:VAL:HG23	1.91	0.69
1:G:42:LYS:HG2	1:G:44:PHE:CE2	2.26	0.69
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.73	0.69
1:J:32:GLY:HA2	1:J:454:ILE:HG23	1.74	0.69
1:K:404:ARG:HG2	1:K:404:ARG:NH1	1.96	0.69
1:I:444:LEU:HD23	1:I:447:MET:HE3	1.74	0.69
1:A:259:LEU:O	1:A:263:VAL:HG23	1.93	0.69
1:B:366:GLN:O	1:B:369:VAL:HG22	1.92	0.69
1:C:44:PHE:HD1	1:C:44:PHE:H	1.37	0.69
1:I:16:MET:CE	1:I:16:MET:CB	2.70	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:385:THR:HG23	1:I:388:GLU:HB2	1.74	0.69
1:D:325:ILE:HG22	1:D:330:THR:HG23	1.74	0.69
1:C:430:ARG:NH1	1:C:430:ARG:CG	2.56	0.69
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.75	0.69
1:D:260:ALA:O	1:D:264:VAL:HG23	1.92	0.69
1:F:18:ARG:HH11	1:F:18:ARG:HG2	1.57	0.69
1:J:96:ALA:O	1:J:100:ILE:HG13	1.93	0.69
1:J:123:ALA:HB2	1:J:440:ILE:HG23	1.75	0.69
1:M:172:GLU:HA	1:M:172:GLU:OE1	1.93	0.69
1:N:349:ILE:HA	1:N:352:GLN:HG3	1.75	0.69
1:A:74:VAL:O	1:A:77:VAL:HG13	1.93	0.68
1:C:234:LEU:O	1:C:238:GLU:HG3	1.92	0.68
1:I:65:LYS:O	1:I:66:PHE:CB	2.41	0.68
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.74	0.68
1:B:205:ILE:HA	1:B:213:VAL:HG22	1.76	0.68
1:L:166:MET:HE3	1:L:171:LYS:HA	1.76	0.68
1:L:383:ALA:HB3	1:L:389:MET:HB2	1.75	0.68
1:F:486:GLY:HA3	1:F:491:MET:CE	2.23	0.68
1:I:123:ALA:HB2	1:I:440:ILE:HG23	1.74	0.68
1:C:16:MET:O	1:C:20:VAL:HG23	1.94	0.68
1:G:430:ARG:NH1	1:G:430:ARG:CG	2.57	0.68
1:K:65:LYS:O	1:K:66:PHE:CB	2.38	0.68
1:N:326:ASN:ND2	1:N:329:THR:HB	2.05	0.68
1:A:430:ARG:CG	1:A:430:ARG:NH1	2.50	0.68
1:C:259:LEU:O	1:C:263:VAL:HG23	1.94	0.68
1:B:16:MET:HG3	1:B:520:MET:HE3	1.76	0.68
1:C:414:GLY:O	1:C:417:VAL:CG1	2.42	0.68
1:L:149:THR:HG21	1:L:156:GLU:HA	1.76	0.68
1:A:510:VAL:CG1	1:A:514:MET:CE	2.71	0.67
1:F:510:VAL:HG12	1:F:514:MET:HE3	1.76	0.67
1:H:421:ARG:HD2	1:H:474:GLY:O	1.94	0.67
1:B:419:LEU:HG	1:B:447:MET:HG2	1.75	0.67
1:C:65:LYS:HG2	7:C:606:HOH:O	1.94	0.67
1:D:414:GLY:O	1:D:417:VAL:HG12	1.94	0.67
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.74	0.67
1:B:524:LEU:CD2	1:B:525:PRO:HD2	2.24	0.67
1:E:129:GLU:OE2	1:E:129:GLU:HA	1.93	0.67
1:M:96:ALA:O	1:M:100:ILE:HG13	1.95	0.67
1:C:125:THR:O	7:C:609:HOH:O	2.12	0.67
1:E:88:GLY:HA2	5:E:600:ADP:O2B	1.95	0.67
1:F:510:VAL:CG1	1:F:514:MET:CE	2.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:126:ALA:HB1	1:N:426:LEU:HD22	1.77	0.67
1:N:452:ARG:HH11	1:N:452:ARG:HG2	1.58	0.67
2:U:7:HIS:O	2:U:8:ASP:HB3	1.94	0.67
1:E:486:GLY:HA3	1:E:491:MET:HE2	1.76	0.67
1:J:106:ALA:O	1:J:109:ALA:HB3	1.94	0.67
1:M:385:THR:HG23	1:M:388:GLU:HB2	1.76	0.67
1:M:166:MET:HE3	1:M:171:LYS:HA	1.77	0.67
1:A:365:LEU:O	1:A:369:VAL:HG13	1.95	0.66
1:E:18:ARG:HG2	1:E:18:ARG:NH1	2.05	0.66
1:F:430:ARG:CG	1:F:430:ARG:NH1	2.53	0.66
1:F:44:PHE:HD1	1:F:44:PHE:H	1.41	0.66
1:K:149:THR:HG21	1:K:156:GLU:HA	1.77	0.66
1:N:404:ARG:HG2	1:N:404:ARG:NH1	2.02	0.66
1:I:173:GLY:O	1:I:404:ARG:NH2	2.27	0.66
1:M:272:LYS:NZ	1:N:228:SER:HB3	2.10	0.66
1:C:44:PHE:CD1	1:C:44:PHE:N	2.62	0.66
1:H:434:GLU:N	7:H:536:HOH:O	1.93	0.66
1:E:486:GLY:HA3	1:E:491:MET:CE	2.25	0.66
2:R:7:HIS:O	2:R:8:ASP:HB3	1.95	0.66
1:C:417:VAL:HG11	1:C:488:MET:HG3	1.76	0.66
1:D:25:ASP:HA	1:D:28:LYS:HE2	1.77	0.66
1:G:270:ILE:CD1	2:U:27:LEU:HB3	2.26	0.66
1:C:365:LEU:O	1:C:369:VAL:HG13	1.96	0.66
1:H:131:LEU:HD12	1:H:422:VAL:HG11	1.78	0.66
1:I:77:VAL:HG12	1:I:78:ALA:N	2.09	0.66
1:J:166:MET:CE	1:J:171:LYS:HA	2.26	0.66
1:L:291:ASP:OD2	1:L:368:ARG:HD2	1.96	0.66
2:T:50:GLU:HG2	2:U:51:ASN:CB	2.23	0.66
1:D:510:VAL:HG12	1:D:514:MET:HE3	1.78	0.66
1:J:415:GLY:N	1:J:417:VAL:HG23	2.11	0.66
1:M:419:LEU:HD12	1:M:447:MET:HB3	1.76	0.66
1:M:428:ASP:N	7:M:534:HOH:O	2.20	0.66
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.77	0.66
1:K:16:MET:O	1:K:20:VAL:HG12	1.96	0.65
1:M:123:ALA:HB2	1:M:440:ILE:HG23	1.78	0.65
1:F:205:ILE:HA	1:F:213:VAL:HG22	1.78	0.65
1:F:419:LEU:HG	1:F:447:MET:HG2	1.78	0.65
1:M:421:ARG:HD2	1:M:474:GLY:O	1.95	0.65
1:N:173:GLY:O	1:N:404:ARG:NH2	2.29	0.65
1:E:366:GLN:O	1:E:369:VAL:HG22	1.96	0.65
1:I:149:THR:CG2	1:I:156:GLU:HA	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:172:GLU:HA	1:J:172:GLU:OE1	1.94	0.65
1:J:217:SER:N	1:J:218:PRO:HD3	2.12	0.65
2:P:7:HIS:NE2	2:P:48:ILE:HD11	2.12	0.65
1:C:448:GLU:O	1:C:452:ARG:HG3	1.95	0.65
1:C:524:LEU:HD23	1:C:525:PRO:HD2	1.77	0.65
1:D:44:PHE:N	1:D:44:PHE:CD1	2.65	0.65
1:G:44:PHE:H	1:G:44:PHE:HD1	1.41	0.65
1:G:415:GLY:O	1:G:451:LEU:HD23	1.96	0.65
2:S:7:HIS:O	2:S:8:ASP:HB3	1.97	0.65
1:B:360:TYR:HA	1:B:363:GLU:HG2	1.78	0.65
1:B:44:PHE:CD1	1:B:44:PHE:N	2.65	0.65
1:B:74:VAL:O	1:B:77:VAL:HG13	1.95	0.65
1:E:54:VAL:O	1:E:58:ARG:HG3	1.96	0.65
1:F:206:ASN:HD21	1:F:214:GLU:H	1.43	0.65
1:F:524:LEU:CD2	1:F:525:PRO:HD2	2.27	0.65
1:G:18:ARG:NH1	1:G:18:ARG:CB	2.46	0.65
1:L:444:LEU:HD23	1:L:447:MET:HE1	1.78	0.65
1:A:415:GLY:O	1:A:451:LEU:HD23	1.97	0.65
1:L:452:ARG:HG2	1:L:452:ARG:HH11	1.60	0.65
1:G:366:GLN:O	1:G:369:VAL:HG22	1.95	0.65
1:A:345:ARG:HA	1:A:348:GLN:HE21	1.60	0.65
1:B:88:GLY:HA2	5:B:600:ADP:O2B	1.95	0.65
1:C:351:GLN:HE22	1:D:209:GLU:HB3	1.61	0.65
2:P:50:GLU:HG2	2:Q:51:ASN:CB	2.23	0.65
1:C:73:MET:SD	1:D:49:ILE:HD11	2.38	0.64
1:G:259:LEU:O	1:G:263:VAL:HG23	1.96	0.64
2:T:50:GLU:CG	2:U:51:ASN:HB2	2.24	0.64
2:T:7:HIS:O	2:T:8:ASP:HB3	1.97	0.64
1:B:510:VAL:HG12	1:B:514:MET:HE3	1.80	0.64
1:D:441:LYS:HB3	1:D:445:ARG:HH21	1.62	0.64
1:K:421:ARG:HD2	1:K:474:GLY:O	1.96	0.64
1:M:415:GLY:H	1:M:417:VAL:HG23	1.63	0.64
1:F:111:MET:HG2	1:F:116:LEU:HD21	1.78	0.64
1:I:16:MET:O	1:I:20:VAL:HG12	1.97	0.64
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.80	0.64
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.79	0.64
2:P:7:HIS:O	2:P:8:ASP:HB3	1.96	0.64
1:B:486:GLY:HA3	1:B:491:MET:HE2	1.79	0.64
1:I:172:GLU:HA	1:I:172:GLU:OE1	1.98	0.64
1:I:416:GLY:HA2	7:I:538:HOH:O	1.97	0.64
1:I:461:GLU:OE1	1:I:461:GLU:HA	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:455:VAL:HG11	1:J:462:PRO:HA	1.79	0.64
1:N:415:GLY:N	1:N:417:VAL:HG23	2.12	0.64
1:B:190:VAL:HG11	1:B:194:GLN:NE2	2.12	0.64
1:D:111:MET:HG2	1:D:116:LEU:HD21	1.80	0.64
1:E:360:TYR:HA	1:E:363:GLU:HG2	1.78	0.64
1:J:173:GLY:O	1:J:404:ARG:NH2	2.31	0.64
1:L:126:ALA:CB	1:L:426:LEU:HD22	2.28	0.64
1:B:18:ARG:HH11	1:B:18:ARG:HG2	1.62	0.64
1:E:18:ARG:CG	1:E:18:ARG:NH1	2.46	0.64
1:F:125:THR:HG22	7:F:607:HOH:O	1.98	0.64
2:T:7:HIS:HB2	2:T:46:GLY:O	1.98	0.64
1:B:430:ARG:NH1	1:B:430:ARG:CG	2.55	0.64
1:E:365:LEU:O	1:E:369:VAL:HG13	1.97	0.64
1:H:174:VAL:HB	1:H:376:VAL:HG22	1.80	0.64
1:H:66:PHE:HA	1:H:69:MET:HE3	1.80	0.64
1:I:217:SER:N	1:I:218:PRO:HD3	2.12	0.64
1:M:511:ALA:O	1:M:515:ILE:HD12	1.98	0.64
1:N:16:MET:HB2	1:N:16:MET:CE	2.28	0.64
1:H:415:GLY:N	1:H:417:VAL:HG23	2.13	0.63
1:J:149:THR:CG2	1:J:156:GLU:HA	2.28	0.63
1:D:74:VAL:O	1:D:77:VAL:HG13	1.98	0.63
1:I:272:LYS:NZ	1:J:228:SER:HB3	2.13	0.63
1:J:421:ARG:HD2	1:J:474:GLY:O	1.98	0.63
1:N:223:ALA:O	1:N:251:ALA:HA	1.98	0.63
2:O:50:GLU:HG3	2:O:50:GLU:O	1.99	0.63
1:A:486:GLY:HA3	1:A:491:MET:CE	2.29	0.63
1:B:486:GLY:HA3	1:B:491:MET:CE	2.28	0.63
1:H:106:ALA:O	1:H:109:ALA:HB3	1.99	0.63
1:H:149:THR:HG21	1:H:156:GLU:HA	1.81	0.63
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.79	0.63
1:J:16:MET:O	1:J:20:VAL:HG12	1.98	0.63
1:L:421:ARG:NH2	7:L:537:HOH:O	2.10	0.63
2:U:7:HIS:HB2	2:U:46:GLY:O	1.98	0.63
1:D:518:GLU:O	1:D:518:GLU:HG3	1.99	0.63
1:H:65:LYS:O	1:H:66:PHE:CB	2.44	0.63
1:M:444:LEU:HD23	1:M:447:MET:HE3	1.79	0.63
1:G:365:LEU:O	1:G:369:VAL:HG13	1.98	0.63
1:J:444:LEU:HD23	1:J:447:MET:HE3	1.80	0.63
1:F:510:VAL:CG1	1:F:514:MET:HE1	2.28	0.63
1:H:326:ASN:ND2	1:H:329:THR:HB	2.02	0.63
1:A:366:GLN:O	1:A:369:VAL:HG22	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:444:LEU:HD23	1:H:447:MET:HE1	1.80	0.63
1:I:488:MET:HE3	1:I:493:ILE:HG21	1.81	0.63
1:M:173:GLY:O	1:M:404:ARG:NH2	2.32	0.63
1:E:16:MET:O	1:E:20:VAL:HG23	1.99	0.62
1:G:345:ARG:HA	1:G:348:GLN:HE21	1.63	0.62
1:I:421:ARG:HD2	1:I:474:GLY:O	1.98	0.62
1:M:27:VAL:HG11	1:M:93:THR:HG21	1.81	0.62
1:F:360:TYR:HA	1:F:363:GLU:HG2	1.80	0.62
1:I:415:GLY:N	1:I:417:VAL:HG23	2.14	0.62
1:F:365:LEU:O	1:F:369:VAL:HG13	1.99	0.62
1:I:221:LEU:HD23	1:I:249:ILE:HG23	1.82	0.62
1:I:174:VAL:HB	1:I:376:VAL:HG22	1.80	0.62
1:C:206:ASN:ND2	1:C:214:GLU:H	1.95	0.62
1:E:419:LEU:HG	1:E:447:MET:HG2	1.81	0.62
1:G:33:PRO:HA	1:G:153:ASN:HD21	1.64	0.62
1:J:126:ALA:HB1	1:J:426:LEU:HD22	1.80	0.62
1:K:149:THR:CG2	1:K:156:GLU:HA	2.29	0.62
2:U:50:GLU:HG3	2:U:50:GLU:O	1.99	0.62
1:C:416:GLY:HA2	7:C:623:HOH:O	1.98	0.62
1:E:150:ILE:CD1	1:E:492:GLY:O	2.47	0.62
1:G:360:TYR:HA	1:G:363:GLU:HG2	1.82	0.62
1:H:217:SER:N	1:H:218:PRO:HD3	2.14	0.62
1:L:217:SER:N	1:L:218:PRO:HD3	2.14	0.62
1:L:415:GLY:N	1:L:417:VAL:HG23	2.13	0.62
1:N:172:GLU:OE1	1:N:172:GLU:HA	2.00	0.62
1:N:174:VAL:HB	1:N:376:VAL:HG22	1.82	0.62
1:H:16:MET:O	1:H:20:VAL:HG12	2.00	0.62
1:M:455:VAL:HG11	1:M:462:PRO:HA	1.80	0.62
2:Q:7:HIS:O	2:Q:8:ASP:HB3	1.99	0.62
1:D:448:GLU:HB3	1:D:452:ARG:HD2	1.81	0.62
1:E:359:ASP:O	1:E:363:GLU:OE2	2.18	0.62
2:Q:50:GLU:HG3	2:Q:50:GLU:O	2.00	0.62
2:U:7:HIS:NE2	2:U:48:ILE:HD11	2.15	0.62
1:F:44:PHE:CD1	1:F:44:PHE:N	2.67	0.62
2:P:50:GLU:HG3	2:P:50:GLU:O	2.00	0.62
1:C:18:ARG:HG2	1:C:18:ARG:NH1	2.11	0.62
1:C:284:ARG:HH11	1:C:364:LYS:HD2	1.64	0.62
1:C:518:GLU:HG3	1:C:518:GLU:O	2.00	0.62
2:O:74:LYS:HD2	2:U:68:ASN:ND2	2.15	0.62
1:C:270:ILE:CD1	2:Q:27:LEU:HB3	2.29	0.62
1:A:414:GLY:O	1:A:417:VAL:CG1	2.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:444:LEU:HD23	1:J:447:MET:HE1	1.81	0.61
1:A:206:ASN:ND2	1:A:214:GLU:H	1.98	0.61
1:E:150:ILE:HD11	1:E:492:GLY:O	2.00	0.61
1:F:74:VAL:O	1:F:77:VAL:HG13	2.00	0.61
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.66	0.61
1:C:444:LEU:O	1:C:447:MET:HB2	1.99	0.61
1:K:16:MET:CE	1:K:16:MET:HB2	2.30	0.61
1:L:149:THR:HG23	1:L:159:GLY:HA3	1.80	0.61
1:M:426:LEU:CD1	1:M:444:LEU:HD21	2.30	0.61
1:A:270:ILE:HD13	2:O:27:LEU:HB3	1.82	0.61
1:B:359:ASP:O	1:B:363:GLU:OE2	2.18	0.61
1:C:111:MET:HG2	1:C:116:LEU:HD21	1.82	0.61
2:T:7:HIS:NE2	2:T:48:ILE:HD11	2.15	0.61
1:B:28:LYS:HD2	1:B:453:GLN:NE2	2.16	0.61
1:L:77:VAL:HG12	1:L:78:ALA:N	2.14	0.61
2:Q:7:HIS:HB2	2:Q:46:GLY:O	2.00	0.61
1:A:103:GLY:HA3	1:A:515:ILE:HG21	1.83	0.61
1:F:486:GLY:CA	1:F:491:MET:HE2	2.31	0.61
1:G:44:PHE:N	1:G:44:PHE:CD1	2.67	0.61
1:I:149:THR:CG2	1:I:159:GLY:HA3	2.30	0.61
1:N:32:GLY:HA2	1:N:454:ILE:HG23	1.82	0.61
1:C:360:TYR:HA	1:C:363:GLU:HG2	1.82	0.61
1:F:18:ARG:NH1	1:F:18:ARG:CB	2.41	0.61
1:I:291:ASP:OD2	1:I:368:ARG:HD2	2.01	0.61
1:L:404:ARG:HG2	1:L:404:ARG:NH1	2.01	0.61
1:A:18:ARG:HG2	1:A:18:ARG:NH1	2.07	0.61
1:A:44:PHE:CD1	1:A:44:PHE:N	2.68	0.61
1:C:441:LYS:HB3	1:C:445:ARG:HH21	1.65	0.61
1:C:514:MET:CG	1:C:514:MET:CE	2.79	0.61
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.83	0.61
1:I:426:LEU:CD1	1:I:444:LEU:HD21	2.31	0.61
1:J:326:ASN:ND2	1:J:329:THR:HB	2.08	0.61
1:L:326:ASN:ND2	1:L:329:THR:HB	2.08	0.61
1:D:510:VAL:CG1	1:D:514:MET:CE	2.78	0.60
1:K:106:ALA:O	1:K:109:ALA:HB3	2.01	0.60
1:L:149:THR:CG2	1:L:156:GLU:HA	2.31	0.60
1:C:415:GLY:O	1:C:451:LEU:HD23	2.01	0.60
1:G:420:ILE:HD13	1:G:448:GLU:HG2	1.83	0.60
1:H:413:ALA:HB1	1:H:417:VAL:HB	1.83	0.60
2:O:7:HIS:NE2	2:O:48:ILE:HD11	2.16	0.60
1:J:145:ALA:O	1:J:149:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:385:THR:HG23	1:H:388:GLU:HB2	1.83	0.60
1:M:145:ALA:O	1:M:149:THR:HG23	2.01	0.60
1:M:149:THR:CG2	1:M:156:GLU:HA	2.31	0.60
2:S:50:GLU:O	2:S:50:GLU:HG3	2.01	0.60
1:C:54:VAL:O	1:C:58:ARG:HG3	2.02	0.60
1:D:16:MET:O	1:D:20:VAL:HG23	2.01	0.60
1:D:365:LEU:O	1:D:369:VAL:HG13	2.00	0.60
1:F:359:ASP:O	1:F:363:GLU:OE2	2.20	0.60
1:I:107:VAL:HG11	1:I:515:ILE:HG23	1.84	0.60
1:M:326:ASN:ND2	1:M:329:THR:HB	2.09	0.60
1:N:413:ALA:HB1	1:N:417:VAL:HB	1.83	0.60
1:B:217:SER:N	1:B:218:PRO:HD3	2.17	0.60
1:G:284:ARG:HH11	1:G:364:LYS:HD2	1.66	0.60
1:N:149:THR:HG21	1:N:156:GLU:HA	1.84	0.60
1:B:16:MET:CG	1:B:520:MET:HE3	2.32	0.60
1:D:360:TYR:HA	1:D:363:GLU:HG2	1.83	0.60
1:M:73:MET:HE1	1:M:514:MET:HG2	1.83	0.60
2:O:6:LEU:O	2:O:7:HIS:O	2.19	0.60
1:A:486:GLY:HA3	1:A:491:MET:HE1	1.84	0.60
1:N:217:SER:N	1:N:218:PRO:HD3	2.17	0.60
1:A:236:VAL:O	1:A:240:VAL:HG23	2.02	0.59
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.84	0.59
1:G:90:THR:O	1:G:94:VAL:CG2	2.38	0.59
1:I:326:ASN:ND2	1:I:329:THR:HB	2.07	0.59
1:L:107:VAL:HG11	1:L:515:ILE:HG23	1.83	0.59
2:T:50:GLU:O	2:T:50:GLU:HG3	2.00	0.59
1:A:16:MET:HG3	1:A:520:MET:HE3	1.84	0.59
1:A:441:LYS:HB3	1:A:445:ARG:HH21	1.67	0.59
1:A:44:PHE:H	1:A:44:PHE:HD1	1.47	0.59
1:C:359:ASP:O	1:C:363:GLU:OE2	2.20	0.59
1:N:426:LEU:CD1	1:N:444:LEU:HD21	2.32	0.59
1:M:47:PRO:HG2	1:N:73:MET:HG3	1.83	0.59
1:B:16:MET:CG	1:B:16:MET:CE	2.80	0.59
1:B:510:VAL:HG13	1:B:514:MET:CE	2.32	0.59
1:B:510:VAL:CG1	1:B:514:MET:HE3	2.30	0.59
1:D:345:ARG:HA	1:D:348:GLN:HE21	1.67	0.59
2:S:6:LEU:O	2:S:7:HIS:O	2.20	0.59
1:E:522:THR:OG1	1:E:523:ASP:N	2.35	0.59
1:E:524:LEU:CD2	1:E:525:PRO:HD2	2.33	0.59
1:M:444:LEU:HA	1:M:447:MET:CE	2.30	0.59
1:A:217:SER:N	1:A:218:PRO:HD3	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:CG	1:B:18:ARG:NH1	2.55	0.59
1:K:444:LEU:HD23	1:K:447:MET:HE1	1.83	0.59
1:L:65:LYS:O	1:L:66:PHE:CB	2.49	0.59
1:M:217:SER:N	1:M:218:PRO:HD3	2.17	0.59
1:M:461:GLU:HA	1:M:461:GLU:OE1	2.01	0.59
1:N:455:VAL:HG13	1:N:460:GLU:HB2	1.83	0.59
1:B:305:ILE:HG23	1:C:267:MET:HG2	1.83	0.59
1:I:149:THR:HG23	1:I:159:GLY:HA3	1.84	0.59
1:N:421:ARG:HD2	1:N:474:GLY:O	2.03	0.59
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.83	0.59
2:P:50:GLU:CG	2:Q:51:ASN:HB2	2.28	0.59
1:A:360:TYR:HA	1:A:363:GLU:HG2	1.85	0.59
1:D:284:ARG:HH11	1:D:364:LYS:HD2	1.68	0.59
1:D:512:GLY:O	1:D:515:ILE:HG13	2.02	0.59
1:D:6:VAL:CG2	1:D:6:VAL:O	2.50	0.59
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.82	0.59
1:A:267:MET:HG2	1:G:305:ILE:HG23	1.85	0.59
1:D:135:SER:HB2	1:D:497:THR:OG1	2.02	0.59
1:E:345:ARG:HA	1:E:348:GLN:HE21	1.68	0.59
1:E:510:VAL:CG1	1:E:514:MET:CE	2.81	0.59
1:M:166:MET:CE	1:M:171:LYS:HA	2.33	0.59
1:N:126:ALA:CB	1:N:426:LEU:HD22	2.33	0.59
1:B:206:ASN:ND2	1:B:214:GLU:H	1.98	0.59
1:E:217:SER:N	1:E:218:PRO:HD3	2.17	0.59
1:K:16:MET:CE	1:K:16:MET:CB	2.81	0.59
1:K:217:SER:N	1:K:218:PRO:HD3	2.17	0.59
2:O:7:HIS:O	2:O:8:ASP:HB3	2.02	0.59
1:B:345:ARG:HA	1:B:348:GLN:HE21	1.68	0.59
1:G:511:ALA:O	1:G:515:ILE:HG12	2.02	0.59
1:G:510:VAL:CG1	1:G:514:MET:CE	2.81	0.59
1:M:149:THR:HG22	1:M:159:GLY:HA3	1.85	0.59
1:M:65:LYS:O	1:M:66:PHE:CB	2.51	0.59
2:P:7:HIS:HB2	2:P:46:GLY:O	2.01	0.59
2:R:50:GLU:O	2:R:50:GLU:HG3	2.03	0.58
1:D:461:GLU:OE2	1:J:452:ARG:NH2	2.35	0.58
1:L:145:ALA:O	1:L:149:THR:HG23	2.04	0.58
1:M:339:GLU:O	1:M:343:GLN:HB2	2.03	0.58
1:N:455:VAL:HG11	1:N:462:PRO:HA	1.84	0.58
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.85	0.58
1:I:126:ALA:HB1	1:I:426:LEU:HD22	1.86	0.58
2:T:6:LEU:O	2:T:7:HIS:O	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:173:GLY:O	1:H:404:ARG:NH2	2.36	0.58
1:C:100:ILE:HG13	1:C:511:ALA:CB	2.33	0.58
1:E:44:PHE:H	1:E:44:PHE:HD1	1.50	0.58
1:D:88:GLY:N	6:D:602:AF3:F2	2.26	0.58
1:K:65:LYS:HA	7:K:528:HOH:O	2.02	0.58
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.45	0.58
1:A:284:ARG:HH11	1:A:364:LYS:HD2	1.69	0.58
1:B:265:ASN:HA	1:B:270:ILE:HD12	1.84	0.58
1:I:11:ASP:OD1	1:I:11:ASP:N	2.35	0.58
1:J:404:ARG:CG	1:J:404:ARG:NH1	2.60	0.58
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.86	0.58
1:L:172:GLU:HA	1:L:172:GLU:OE1	2.03	0.58
1:M:101:THR:HG22	1:M:102:GLU:OE1	2.03	0.58
1:C:520:MET:HG2	1:D:39:VAL:HB	1.86	0.58
1:E:206:ASN:ND2	1:E:214:GLU:H	2.00	0.58
1:F:88:GLY:HA2	5:F:600:ADP:O2B	2.04	0.58
1:L:62:LEU:N	1:L:68:ASN:OD1	2.33	0.58
1:M:404:ARG:NH1	1:M:404:ARG:CG	2.57	0.58
1:B:42:LYS:HG2	1:B:44:PHE:CE2	2.39	0.58
1:B:365:LEU:O	1:B:369:VAL:HG13	2.04	0.57
1:B:414:GLY:O	1:B:417:VAL:CG1	2.52	0.57
1:D:444:LEU:O	1:D:447:MET:HB2	2.04	0.57
1:E:415:GLY:O	1:E:451:LEU:HD23	2.04	0.57
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.86	0.57
1:N:385:THR:HG23	1:N:388:GLU:HB2	1.85	0.57
1:N:451:LEU:O	1:N:452:ARG:C	2.39	0.57
1:E:351:GLN:HE22	1:F:209:GLU:HB3	1.68	0.57
1:F:217:SER:N	1:F:218:PRO:HD3	2.20	0.57
1:M:223:ALA:O	1:M:251:ALA:HA	2.03	0.57
1:C:33:PRO:HA	1:C:153:ASN:HD21	1.67	0.57
1:D:415:GLY:O	1:D:451:LEU:HD23	2.04	0.57
1:G:359:ASP:O	1:G:363:GLU:OE2	2.21	0.57
1:G:417:VAL:HG11	1:G:488:MET:HG3	1.86	0.57
2:S:7:HIS:NE2	2:S:48:ILE:HD11	2.19	0.57
1:B:33:PRO:HA	1:B:153:ASN:HD21	1.69	0.57
1:H:172:GLU:OE1	1:H:172:GLU:HA	2.04	0.57
1:I:444:LEU:CD2	1:I:447:MET:HE1	2.28	0.57
1:L:149:THR:CG2	1:L:159:GLY:HA3	2.33	0.57
1:B:284:ARG:HH11	1:B:364:LYS:HD2	1.69	0.57
1:D:419:LEU:HG	1:D:447:MET:HG2	1.87	0.57
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:326:ASN:HB2	1:H:329:THR:H	1.70	0.57
1:N:87:ASP:OD2	7:N:530:HOH:O	2.17	0.57
1:B:351:GLN:NE2	1:C:209:GLU:HB3	2.17	0.57
1:D:417:VAL:HG11	1:D:488:MET:HG3	1.85	0.57
1:G:510:VAL:HG12	1:G:514:MET:CE	2.33	0.57
1:H:145:ALA:O	1:H:149:THR:HG23	2.04	0.57
1:I:339:GLU:O	1:I:343:GLN:HB2	2.05	0.57
1:L:166:MET:CE	1:L:171:LYS:HA	2.34	0.57
2:O:7:HIS:HB2	2:O:46:GLY:O	2.03	0.57
2:R:7:HIS:NE2	2:R:48:ILE:HD11	2.20	0.57
1:A:143:ALA:HA	1:A:146:GLN:HE21	1.70	0.57
1:D:206:ASN:ND2	1:D:214:GLU:H	2.02	0.57
1:E:190:VAL:HG11	1:E:194:GLN:NE2	2.19	0.57
1:F:345:ARG:HA	1:F:348:GLN:HE21	1.69	0.57
1:H:149:THR:CG2	1:H:156:GLU:HA	2.35	0.57
1:I:27:VAL:HG11	1:I:93:THR:HG21	1.85	0.57
1:K:339:GLU:O	1:K:343:GLN:HB2	2.05	0.57
1:L:173:GLY:O	1:L:404:ARG:NH2	2.36	0.57
1:D:510:VAL:CG1	1:D:514:MET:HE1	2.35	0.57
1:L:201:SER:C	1:L:203:TYR:H	2.08	0.57
1:M:149:THR:CG2	1:M:159:GLY:HA3	2.34	0.57
1:M:201:SER:C	1:M:203:TYR:H	2.08	0.57
1:N:145:ALA:O	1:N:149:THR:HG23	2.05	0.57
1:A:143:ALA:HA	1:A:146:GLN:NE2	2.20	0.57
1:C:74:VAL:O	1:C:77:VAL:HG13	2.05	0.57
1:H:291:ASP:OD2	1:H:368:ARG:HD2	2.04	0.57
1:N:66:PHE:H	1:N:69:MET:HG3	1.69	0.57
2:Q:6:LEU:O	2:Q:7:HIS:O	2.22	0.57
2:S:7:HIS:HB2	2:S:46:GLY:O	2.05	0.57
1:B:524:LEU:HD22	1:B:525:PRO:HD2	1.86	0.57
1:K:173:GLY:O	1:K:404:ARG:NH2	2.36	0.57
2:Q:7:HIS:NE2	2:Q:48:ILE:HD11	2.19	0.57
1:E:289:LEU:HA	1:E:292:ILE:HD12	1.87	0.56
1:G:486:GLY:HA3	1:G:491:MET:CE	2.34	0.56
1:L:90:THR:O	1:L:94:VAL:HG23	2.05	0.56
2:R:6:LEU:O	2:R:7:HIS:O	2.23	0.56
1:D:217:SER:N	1:D:218:PRO:HD3	2.19	0.56
1:E:284:ARG:HH11	1:E:364:LYS:HD2	1.70	0.56
1:F:150:ILE:HD11	1:F:492:GLY:O	2.04	0.56
1:F:510:VAL:CG1	1:F:514:MET:HE3	2.35	0.56
1:F:522:THR:OG1	1:F:523:ASP:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:444:LEU:CD2	1:I:447:MET:CE	2.75	0.56
1:J:493:ILE:O	1:J:493:ILE:HG22	2.04	0.56
1:N:149:THR:CG2	1:N:156:GLU:HA	2.35	0.56
2:P:6:LEU:O	2:P:7:HIS:O	2.22	0.56
1:A:54:VAL:O	1:A:58:ARG:HG3	2.05	0.56
1:G:143:ALA:HA	1:G:146:GLN:NE2	2.20	0.56
1:I:447:MET:CE	1:I:447:MET:CG	2.83	0.56
1:B:194:GLN:HG3	1:B:331:THR:HB	1.87	0.56
1:K:166:MET:CE	1:K:171:LYS:HA	2.35	0.56
2:U:6:LEU:O	2:U:7:HIS:O	2.23	0.56
1:E:33:PRO:HA	1:E:153:ASN:HD21	1.70	0.56
1:G:486:GLY:HA3	1:G:491:MET:HE2	1.87	0.56
1:H:426:LEU:CD1	1:H:444:LEU:HD21	2.36	0.56
1:K:201:SER:C	1:K:203:TYR:H	2.09	0.56
1:L:213:VAL:HB	1:L:325:ILE:CG1	2.36	0.56
1:B:417:VAL:HG11	1:B:488:MET:HG3	1.88	0.56
1:H:27:VAL:HG11	1:H:93:THR:HG21	1.86	0.56
1:K:172:GLU:OE1	1:K:172:GLU:HA	2.06	0.56
1:F:236:VAL:O	1:F:240:VAL:HG23	2.05	0.56
1:I:325:ILE:HG22	1:I:330:THR:HG23	1.88	0.56
1:L:16:MET:O	1:L:20:VAL:HG12	2.05	0.56
1:M:100:ILE:HG22	1:M:104:LEU:HD22	1.88	0.56
1:M:11:ASP:OD1	1:M:11:ASP:N	2.37	0.56
1:M:197:ARG:HD2	1:M:277:LYS:HB2	1.88	0.56
1:M:16:MET:O	1:M:20:VAL:HG12	2.06	0.56
1:N:16:MET:O	1:N:20:VAL:HG12	2.05	0.56
1:I:65:LYS:HA	7:I:529:HOH:O	2.06	0.56
1:L:106:ALA:O	1:L:109:ALA:HB3	2.06	0.56
1:N:107:VAL:HG11	1:N:515:ILE:HG23	1.87	0.56
1:C:217:SER:N	1:C:218:PRO:HD3	2.20	0.56
1:F:486:GLY:C	1:F:491:MET:HE2	2.27	0.56
1:I:96:ALA:O	1:I:100:ILE:HG13	2.06	0.56
1:F:63:GLU:O	1:F:63:GLU:HG2	2.06	0.55
1:H:426:LEU:HD12	1:H:444:LEU:HD21	1.88	0.55
1:J:34:LYS:HB2	1:J:458:CYS:SG	2.46	0.55
1:N:16:MET:CB	1:N:16:MET:CE	2.85	0.55
2:U:40:VAL:HB	2:U:62:GLY:H	1.71	0.55
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.86	0.55
1:I:426:LEU:HD12	1:I:444:LEU:HD21	1.86	0.55
1:K:351:GLN:HA	1:K:354:GLU:HG2	1.88	0.55
1:N:434:GLU:CB	7:N:529:HOH:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:HG2	1:A:44:PHE:CE2	2.41	0.55
1:B:430:ARG:NH2	7:B:609:HOH:O	2.24	0.55
1:D:524:LEU:CD2	1:D:525:PRO:HD2	2.37	0.55
1:F:417:VAL:HG11	1:F:488:MET:HG3	1.88	0.55
1:G:265:ASN:HA	1:G:270:ILE:HD12	1.88	0.55
1:J:223:ALA:O	1:J:251:ALA:HA	2.07	0.55
1:K:223:ALA:O	1:K:251:ALA:HA	2.06	0.55
1:N:433:ASN:HB3	1:N:436:GLN:H	1.71	0.55
1:N:444:LEU:HD23	1:N:447:MET:HE1	1.87	0.55
1:E:44:PHE:N	1:E:44:PHE:CD1	2.74	0.55
1:E:510:VAL:HG12	1:E:514:MET:HE3	1.89	0.55
1:G:54:VAL:O	1:G:58:ARG:HG3	2.07	0.55
1:L:27:VAL:HG11	1:L:93:THR:HG21	1.87	0.55
1:M:291:ASP:OD2	1:M:368:ARG:HD2	2.07	0.55
2:R:96:GLU:OE1	2:S:4:ARG:HD3	2.07	0.55
1:C:25:ASP:HA	1:C:28:LYS:HE2	1.87	0.55
1:C:419:LEU:HG	1:C:447:MET:HG2	1.88	0.55
1:C:510:VAL:HG12	1:C:514:MET:CE	2.35	0.55
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.89	0.55
1:J:339:GLU:O	1:J:343:GLN:HB2	2.07	0.55
1:H:511:ALA:O	1:H:515:ILE:HD12	2.07	0.55
1:I:34:LYS:HB2	1:I:458:CYS:SG	2.47	0.55
1:B:486:GLY:CA	1:B:491:MET:HE2	2.37	0.55
1:B:510:VAL:HG12	1:B:514:MET:CE	2.34	0.55
1:B:305:ILE:HG12	1:C:267:MET:CE	2.37	0.55
1:C:510:VAL:CG1	1:C:514:MET:HE3	2.36	0.55
1:G:18:ARG:HH11	1:G:18:ARG:HG2	1.71	0.55
1:G:441:LYS:HB3	1:G:445:ARG:HH21	1.71	0.55
1:M:106:ALA:O	1:M:109:ALA:HB3	2.06	0.55
1:N:201:SER:C	1:N:203:TYR:H	2.10	0.55
1:A:477:GLY:HA3	1:A:488:MET:SD	2.46	0.55
1:C:147:VAL:HG12	1:C:494:LEU:HB2	1.88	0.55
1:D:430:ARG:CG	1:D:430:ARG:NH1	2.61	0.55
1:E:74:VAL:O	1:E:77:VAL:HG13	2.06	0.55
1:H:351:GLN:HA	1:H:354:GLU:HG2	1.89	0.55
1:L:444:LEU:HA	1:L:447:MET:CE	2.23	0.55
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.89	0.55
1:C:514:MET:CB	1:C:514:MET:CE	2.84	0.55
1:G:129:GLU:HA	1:G:129:GLU:OE2	2.05	0.55
1:H:201:SER:C	1:H:203:TYR:H	2.10	0.55
1:J:488:MET:HE3	1:J:493:ILE:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:426:LEU:CD1	1:K:444:LEU:HD21	2.37	0.55
1:B:524:LEU:HD23	1:B:525:PRO:HD2	1.89	0.55
1:M:426:LEU:HD12	1:M:444:LEU:HD21	1.88	0.55
1:M:449:ALA:HB3	1:M:450:PRO:CD	2.36	0.55
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.88	0.54
1:C:270:ILE:HG22	1:C:271:VAL:HG23	1.88	0.54
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.87	0.54
1:H:96:ALA:O	1:H:100:ILE:HG13	2.07	0.54
1:H:166:MET:CE	1:H:171:LYS:HA	2.35	0.54
1:K:213:VAL:HB	1:K:325:ILE:CG1	2.37	0.54
1:M:413:ALA:HB1	1:M:417:VAL:HB	1.89	0.54
1:N:221:LEU:HD23	1:N:249:ILE:HG23	1.87	0.54
1:D:236:VAL:O	1:D:240:VAL:HG23	2.07	0.54
1:D:326:ASN:HD22	1:D:329:THR:HB	1.71	0.54
1:E:510:VAL:CG1	1:E:514:MET:HE1	2.37	0.54
1:I:197:ARG:HD2	1:I:277:LYS:HB2	1.88	0.54
1:K:404:ARG:NH1	1:K:404:ARG:CG	2.67	0.54
1:M:272:LYS:HZ1	1:N:228:SER:HB3	1.72	0.54
2:P:47:ARG:HD3	2:P:49:LEU:HD12	1.88	0.54
1:C:466:ALA:O	1:C:467:ASN:C	2.44	0.54
1:F:18:ARG:NH1	1:F:18:ARG:CG	2.54	0.54
1:F:486:GLY:CA	1:F:491:MET:CE	2.85	0.54
1:I:100:ILE:HG22	1:I:104:LEU:HD22	1.89	0.54
1:J:201:SER:C	1:J:203:TYR:H	2.09	0.54
1:L:106:ALA:O	1:L:111:MET:HE3	2.07	0.54
1:L:415:GLY:CA	1:L:417:VAL:HG23	2.37	0.54
1:D:143:ALA:HA	1:D:146:GLN:NE2	2.23	0.54
1:K:326:ASN:ND2	1:K:329:THR:HB	2.11	0.54
1:K:413:ALA:HB1	1:K:417:VAL:HB	1.90	0.54
1:L:163:ALA:O	1:L:167:ASP:HB2	2.08	0.54
1:M:16:MET:HG2	1:M:70:GLY:HA2	1.87	0.54
1:N:33:PRO:CA	7:N:535:HOH:O	2.55	0.54
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.89	0.54
1:C:65:LYS:CG	7:C:606:HOH:O	2.53	0.54
1:G:217:SER:N	1:G:218:PRO:HD3	2.23	0.54
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.88	0.54
1:K:325:ILE:HG22	1:K:330:THR:HG23	1.90	0.54
1:H:149:THR:CG2	1:H:159:GLY:HA3	2.38	0.54
1:I:85:ALA:HB1	1:I:499:VAL:HB	1.88	0.54
1:J:514:MET:CG	1:J:514:MET:CE	2.85	0.54
1:N:325:ILE:HG22	1:N:330:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ASN:HD22	1:B:329:THR:HB	1.71	0.54
1:G:289:LEU:HA	1:G:292:ILE:HD12	1.89	0.54
1:A:13:ARG:HD2	1:A:104:LEU:HD22	1.89	0.54
1:B:305:ILE:O	1:B:305:ILE:HG22	2.07	0.54
1:E:228:SER:O	1:E:257:GLU:HB3	2.07	0.54
1:E:486:GLY:CA	1:E:491:MET:HE2	2.38	0.54
1:L:47:PRO:HG2	1:M:73:MET:HG3	1.90	0.54
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.90	0.54
1:D:510:VAL:CG1	1:D:514:MET:HE3	2.38	0.54
1:E:25:ASP:HA	1:E:28:LYS:HE2	1.89	0.54
1:G:414:GLY:O	1:G:417:VAL:CG1	2.52	0.54
2:T:40:VAL:HB	2:T:62:GLY:H	1.73	0.54
1:A:22:VAL:HG11	1:A:62:LEU:HD11	1.90	0.54
1:G:206:ASN:ND2	1:G:214:GLU:H	2.04	0.54
1:H:383:ALA:HB3	1:H:389:MET:HB2	1.89	0.54
1:H:432:GLN:H	1:H:436:GLN:NE2	2.06	0.54
1:L:421:ARG:HD2	1:L:474:GLY:O	2.07	0.54
1:M:514:MET:CG	1:M:514:MET:CE	2.84	0.54
1:E:236:VAL:O	1:E:240:VAL:HG23	2.07	0.53
1:F:147:VAL:HG12	1:F:494:LEU:HB2	1.90	0.53
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.89	0.53
1:I:16:MET:HE2	1:I:16:MET:HB2	1.88	0.53
1:I:451:LEU:O	1:I:452:ARG:C	2.46	0.53
1:A:448:GLU:HB3	1:A:452:ARG:HD2	1.90	0.53
1:D:78:ALA:HB2	1:D:93:THR:OG1	2.09	0.53
1:F:16:MET:O	1:F:20:VAL:HG23	2.08	0.53
1:J:90:THR:O	1:J:94:VAL:HG23	2.08	0.53
1:K:145:ALA:O	1:K:149:THR:HG23	2.08	0.53
1:K:511:ALA:O	1:K:515:ILE:HD12	2.07	0.53
1:K:62:LEU:N	1:K:68:ASN:OD1	2.33	0.53
2:Q:40:VAL:HB	2:Q:62:GLY:H	1.74	0.53
1:A:172:GLU:HA	1:A:172:GLU:OE1	2.08	0.53
1:B:522:THR:OG1	1:B:523:ASP:N	2.40	0.53
1:B:54:VAL:O	1:B:58:ARG:HG3	2.08	0.53
1:L:66:PHE:O	1:L:67:GLU:C	2.47	0.53
1:J:325:ILE:HG22	1:J:330:THR:HG23	1.91	0.53
1:L:223:ALA:O	1:L:251:ALA:HA	2.09	0.53
1:A:305:ILE:HD12	1:A:307:MET:HE2	1.91	0.53
1:F:18:ARG:NH1	1:F:18:ARG:HG2	2.23	0.53
2:R:7:HIS:HB2	2:R:46:GLY:O	2.08	0.53
1:C:482:THR:O	1:C:483:GLU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:198:GLY:HA3	1:K:327:LYS:O	2.08	0.53
1:G:444:LEU:O	1:G:447:MET:HB2	2.08	0.53
1:I:201:SER:C	1:I:203:TYR:H	2.12	0.53
1:J:149:THR:HG23	1:J:159:GLY:HA3	1.91	0.53
1:K:27:VAL:HG11	1:K:93:THR:HG21	1.91	0.53
1:N:197:ARG:HD2	1:N:277:LYS:HB2	1.91	0.53
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.90	0.53
1:G:22:VAL:HG11	1:G:62:LEU:HD11	1.91	0.53
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.91	0.53
1:K:149:THR:CG2	1:K:159:GLY:HA3	2.39	0.53
1:M:16:MET:CE	1:M:16:MET:HB2	2.39	0.53
2:O:50:GLU:CG	2:P:51:ASN:HB2	2.34	0.53
2:U:78:ILE:HD13	2:U:83:VAL:HG21	1.91	0.53
1:C:265:ASN:HA	1:C:270:ILE:HD12	1.90	0.53
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.90	0.53
1:F:289:LEU:HA	1:F:292:ILE:HD12	1.92	0.53
1:K:221:LEU:HD23	1:K:249:ILE:HG23	1.90	0.53
1:M:437:ASN:HA	1:M:440:ILE:HD12	1.92	0.53
1:N:339:GLU:O	1:N:343:GLN:HB2	2.08	0.53
1:B:16:MET:HB3	1:B:16:MET:CE	2.38	0.52
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.89	0.52
1:F:510:VAL:HG13	1:F:514:MET:CE	2.40	0.52
1:H:213:VAL:HB	1:H:325:ILE:CG1	2.39	0.52
1:M:444:LEU:HD23	1:M:447:MET:HE1	1.90	0.52
1:E:265:ASN:HA	1:E:270:ILE:HD12	1.90	0.52
1:I:223:ALA:O	1:I:251:ALA:HA	2.09	0.52
1:J:16:MET:CE	1:J:16:MET:HB2	2.39	0.52
1:J:351:GLN:HA	1:J:354:GLU:HG2	1.92	0.52
1:M:461:GLU:HB3	1:M:464:VAL:HB	1.91	0.52
1:A:359:ASP:O	1:A:363:GLU:OE2	2.26	0.52
1:E:230:ILE:CD1	1:E:261:THR:HG21	2.38	0.52
1:F:482:THR:O	1:F:483:GLU:HB2	2.09	0.52
1:G:172:GLU:OE1	1:G:172:GLU:HA	2.09	0.52
1:G:510:VAL:CG1	1:G:514:MET:HE3	2.38	0.52
1:H:494:LEU:O	1:H:494:LEU:HD12	2.09	0.52
1:L:201:SER:O	1:L:203:TYR:N	2.43	0.52
1:H:149:THR:HG23	1:H:159:GLY:HA3	1.92	0.52
1:H:444:LEU:HA	1:H:447:MET:CE	2.35	0.52
1:B:150:ILE:CD1	1:B:492:GLY:O	2.58	0.52
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.45	0.52
1:E:510:VAL:CG1	1:E:514:MET:HE3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:339:GLU:O	1:L:343:GLN:HB2	2.10	0.52
1:A:153:ASN:O	1:A:154:SER:HB2	2.09	0.52
1:C:305:ILE:HG12	1:D:267:MET:CE	2.39	0.52
1:E:466:ALA:O	1:E:467:ASN:C	2.47	0.52
1:F:54:VAL:O	1:F:58:ARG:HG3	2.09	0.52
1:K:97:GLN:O	1:K:97:GLN:HG2	2.09	0.52
1:L:106:ALA:CA	1:L:111:MET:HE3	2.40	0.52
1:L:351:GLN:HA	1:L:354:GLU:HG2	1.91	0.52
1:A:228:SER:O	1:A:257:GLU:HB3	2.09	0.52
1:G:28:LYS:HD2	1:G:453:GLN:NE2	2.25	0.52
1:H:180:GLY:HA3	1:H:381:VAL:O	2.09	0.52
1:J:66:PHE:O	1:J:67:GLU:C	2.48	0.52
1:A:76:GLU:O	1:A:76:GLU:HG2	2.09	0.52
1:H:451:LEU:O	1:H:452:ARG:C	2.46	0.52
1:I:120:ILE:O	1:I:124:VAL:HG23	2.10	0.52
1:J:419:LEU:HD12	1:J:447:MET:HB3	1.90	0.52
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.92	0.52
1:L:49:ILE:HD12	1:M:513:LEU:HD23	1.92	0.52
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.92	0.52
5:A:600:ADP:PB	6:A:602:AF3:F2	2.58	0.52
1:C:345:ARG:HA	1:C:348:GLN:HE21	1.73	0.52
1:D:265:ASN:HA	1:D:270:ILE:HD12	1.92	0.52
1:C:305:ILE:HG12	1:D:267:MET:HE3	1.92	0.52
1:D:359:ASP:O	1:D:363:GLU:OE2	2.28	0.52
1:D:54:VAL:O	1:D:58:ARG:HG3	2.09	0.52
1:F:305:ILE:HG12	1:G:267:MET:HE3	1.92	0.52
1:G:100:ILE:HG13	1:G:511:ALA:HB1	1.91	0.52
1:G:510:VAL:CG1	1:G:514:MET:HE1	2.39	0.52
1:H:452:ARG:HH11	1:H:452:ARG:HG2	1.74	0.52
1:M:107:VAL:HG11	1:M:515:ILE:HG23	1.92	0.52
1:B:150:ILE:HD11	1:B:492:GLY:O	2.10	0.52
1:C:42:LYS:HG2	1:C:44:PHE:CE2	2.45	0.52
1:I:419:LEU:HD12	1:I:447:MET:HB3	1.92	0.52
1:J:197:ARG:HD2	1:J:277:LYS:HB2	1.91	0.52
1:J:415:GLY:CA	1:J:417:VAL:HG23	2.40	0.52
1:N:33:PRO:HA	7:N:535:HOH:O	2.08	0.52
1:A:524:LEU:CD2	1:A:525:PRO:HD2	2.40	0.51
1:C:510:VAL:HG12	1:C:514:MET:HE3	1.91	0.51
1:D:486:GLY:C	1:D:491:MET:HE2	2.31	0.51
1:H:514:MET:CG	1:H:514:MET:CE	2.87	0.51
1:J:426:LEU:CD1	1:J:444:LEU:HD21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:511:ALA:O	1:J:515:ILE:HD12	2.09	0.51
2:U:16:GLU:HB2	2:U:19:THR:OG1	2.11	0.51
1:A:33:PRO:HA	1:A:153:ASN:HD21	1.75	0.51
1:B:289:LEU:HA	1:B:292:ILE:HD12	1.92	0.51
1:C:219:PHE:HB3	1:C:317:LEU:HD23	1.91	0.51
1:G:228:SER:O	1:G:257:GLU:HB3	2.10	0.51
1:I:44:PHE:HD1	1:I:44:PHE:H	1.58	0.51
2:T:16:GLU:HB2	2:T:19:THR:OG1	2.10	0.51
1:C:194:GLN:HG3	1:C:331:THR:HB	1.92	0.51
1:D:6:VAL:HG23	1:D:6:VAL:O	2.09	0.51
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.93	0.51
1:E:512:GLY:O	1:E:515:ILE:HG13	2.10	0.51
1:J:413:ALA:HB1	1:J:417:VAL:HB	1.92	0.51
1:K:44:PHE:HD1	1:K:44:PHE:H	1.59	0.51
1:L:103:GLY:O	1:L:106:ALA:HB3	2.11	0.51
1:L:413:ALA:HB1	1:L:417:VAL:HB	1.91	0.51
1:M:120:ILE:O	1:M:124:VAL:HG23	2.10	0.51
1:N:149:THR:HG23	1:N:159:GLY:HA3	1.92	0.51
2:O:50:GLU:O	2:O:51:ASN:HB3	2.10	0.51
1:A:194:GLN:HG3	1:A:331:THR:HB	1.92	0.51
1:C:305:ILE:HG23	1:D:267:MET:HG2	1.92	0.51
1:H:221:LEU:HD23	1:H:249:ILE:HG23	1.92	0.51
1:H:461:GLU:HB3	1:H:464:VAL:HB	1.93	0.51
1:M:421:ARG:CD	1:M:474:GLY:O	2.58	0.51
1:M:66:PHE:H	1:M:69:MET:HG3	1.75	0.51
1:N:44:PHE:HD1	1:N:44:PHE:H	1.58	0.51
2:R:50:GLU:O	2:R:51:ASN:HB3	2.11	0.51
1:A:25:ASP:HA	1:A:28:LYS:HE2	1.93	0.51
1:C:230:ILE:CD1	1:C:261:THR:HG21	2.34	0.51
1:H:11:ASP:N	1:H:11:ASP:OD1	2.44	0.51
1:H:326:ASN:HD22	1:H:329:THR:CG2	2.24	0.51
1:I:198:GLY:O	1:I:276:VAL:HG12	2.10	0.51
1:I:452:ARG:HH11	1:I:452:ARG:HG2	1.75	0.51
1:K:180:GLY:HA3	1:K:381:VAL:O	2.11	0.51
1:A:326:ASN:HD22	1:A:329:THR:HB	1.75	0.51
1:B:228:SER:O	1:B:257:GLU:HB3	2.11	0.51
1:B:466:ALA:O	1:B:467:ASN:C	2.48	0.51
1:B:76:GLU:O	1:B:76:GLU:HG2	2.11	0.51
1:C:522:THR:OG1	1:C:523:ASP:N	2.41	0.51
1:E:130:GLU:O	1:E:133:ALA:HB3	2.11	0.51
1:I:62:LEU:N	1:I:68:ASN:OD1	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:197:ARG:HG3	1:J:277:LYS:O	2.11	0.51
1:A:16:MET:CG	1:A:520:MET:HE3	2.41	0.51
1:A:487:ASN:O	1:A:491:MET:HG3	2.10	0.51
1:B:486:GLY:CA	1:B:491:MET:CE	2.89	0.51
1:D:284:ARG:NH1	1:D:364:LYS:HD2	2.26	0.51
1:F:33:PRO:HA	1:F:153:ASN:HD21	1.75	0.51
1:F:23:LEU:O	1:F:24:ALA:C	2.49	0.51
1:I:415:GLY:CA	1:I:417:VAL:HG23	2.41	0.51
1:A:16:MET:O	1:A:20:VAL:HG23	2.11	0.51
1:C:103:GLY:O	1:C:106:ALA:N	2.41	0.51
1:C:486:GLY:HA3	1:C:491:MET:CE	2.41	0.51
1:G:172:GLU:OE2	1:G:350:ARG:CZ	2.59	0.51
1:K:228:SER:O	1:K:257:GLU:HB3	2.10	0.51
1:M:419:LEU:HD22	1:M:500:THR:CG2	2.41	0.51
2:T:47:ARG:HD3	2:T:49:LEU:HD12	1.93	0.51
1:I:82:ASN:HB2	1:I:89:THR:OG1	2.11	0.51
1:J:106:ALA:CA	1:J:111:MET:HE3	2.41	0.51
1:L:65:LYS:HA	7:L:529:HOH:O	2.11	0.51
2:Q:47:ARG:HD3	2:Q:49:LEU:HD12	1.91	0.51
5:C:600:ADP:PB	6:C:602:AF3:F2	2.59	0.51
1:D:150:ILE:HD11	1:D:492:GLY:O	2.11	0.51
1:F:512:GLY:O	1:F:515:ILE:HG13	2.10	0.51
1:G:305:ILE:HD12	1:G:307:MET:HE2	1.93	0.51
1:J:172:GLU:OE1	1:J:172:GLU:CA	2.58	0.51
1:J:174:VAL:HB	1:J:376:VAL:HG22	1.93	0.51
1:K:415:GLY:H	1:K:417:VAL:HG23	1.76	0.51
1:L:64:ASP:O	1:L:65:LYS:O	2.29	0.51
1:M:90:THR:O	1:M:94:VAL:HG23	2.11	0.51
1:N:149:THR:CG2	1:N:159:GLY:HA3	2.40	0.51
1:M:39:VAL:HB	1:N:520:MET:HG2	1.92	0.51
2:U:47:ARG:HD3	2:U:49:LEU:HD12	1.93	0.51
1:B:25:ASP:HA	1:B:28:LYS:HE2	1.93	0.50
1:D:461:GLU:OE1	1:J:463:SER:HB3	2.12	0.50
1:G:25:ASP:HA	1:G:28:LYS:HE2	1.92	0.50
1:H:197:ARG:HD2	1:H:277:LYS:HB2	1.92	0.50
1:J:65:LYS:O	1:J:66:PHE:CB	2.44	0.50
1:N:351:GLN:HA	1:N:354:GLU:HG2	1.93	0.50
1:A:417:VAL:HG11	1:A:488:MET:HG3	1.92	0.50
1:B:16:MET:O	1:B:20:VAL:HG23	2.11	0.50
1:B:415:GLY:O	1:B:451:LEU:HD23	2.12	0.50
1:D:100:ILE:HG13	1:D:511:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:GLN:HG3	1:D:331:THR:HB	1.93	0.50
1:G:6:VAL:O	1:G:6:VAL:CG2	2.57	0.50
1:H:201:SER:O	1:H:203:TYR:N	2.44	0.50
1:L:106:ALA:HA	1:L:111:MET:CE	2.41	0.50
1:M:100:ILE:CG2	1:M:104:LEU:HD22	2.40	0.50
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.92	0.50
1:C:88:GLY:HA2	5:C:600:ADP:O2B	2.12	0.50
1:F:206:ASN:ND2	1:F:214:GLU:H	2.08	0.50
1:F:111:MET:HG3	1:F:435:ASP:OD1	2.11	0.50
1:I:106:ALA:HA	1:I:111:MET:CE	2.41	0.50
1:K:444:LEU:HA	1:K:447:MET:CE	2.36	0.50
1:L:325:ILE:HG22	1:L:330:THR:HG23	1.93	0.50
1:A:365:LEU:CD2	1:A:368:ARG:HH21	2.25	0.50
1:D:228:SER:O	1:D:257:GLU:HB3	2.11	0.50
1:F:524:LEU:HD23	1:F:525:PRO:HD2	1.92	0.50
1:I:106:ALA:HA	1:I:111:MET:HE3	1.92	0.50
1:A:345:ARG:O	1:A:348:GLN:HB2	2.12	0.50
1:A:486:GLY:C	1:A:491:MET:HE2	2.32	0.50
1:A:486:GLY:CA	1:A:491:MET:CE	2.89	0.50
1:F:414:GLY:O	1:F:417:VAL:CG1	2.58	0.50
1:F:305:ILE:HG12	1:G:267:MET:CE	2.41	0.50
1:G:414:GLY:HA2	1:G:495:ASP:OD2	2.11	0.50
1:I:272:LYS:HZ1	1:J:228:SER:HB3	1.75	0.50
1:K:291:ASP:OD2	1:K:368:ARG:HD2	2.11	0.50
1:K:385:THR:HG23	1:K:388:GLU:HB2	1.93	0.50
1:L:404:ARG:CG	1:L:404:ARG:NH1	2.72	0.50
1:N:228:SER:O	1:N:257:GLU:HB3	2.11	0.50
2:P:78:ILE:HD13	2:P:83:VAL:HG21	1.93	0.50
1:D:270:ILE:HD13	2:R:27:LEU:HB3	1.94	0.50
1:E:417:VAL:HG11	1:E:488:MET:HG3	1.94	0.50
1:E:414:GLY:HA2	1:E:495:ASP:OD2	2.12	0.50
1:F:265:ASN:HA	1:F:270:ILE:HD12	1.92	0.50
1:H:325:ILE:HG22	1:H:330:THR:HG23	1.93	0.50
1:I:158:VAL:HG13	1:I:396:VAL:HG22	1.93	0.50
1:J:66:PHE:H	1:J:69:MET:HG3	1.76	0.50
1:M:213:VAL:HB	1:M:325:ILE:CG1	2.39	0.50
1:M:44:PHE:HD1	1:M:44:PHE:H	1.59	0.50
2:P:50:GLU:O	2:P:51:ASN:HB3	2.12	0.50
1:D:511:ALA:O	1:D:515:ILE:HG12	2.11	0.50
1:N:66:PHE:O	1:N:67:GLU:C	2.49	0.50
1:C:326:ASN:HD22	1:C:329:THR:HB	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:524:LEU:HD22	1:E:525:PRO:HD2	1.93	0.50
1:I:16:MET:CE	1:I:16:MET:CG	2.90	0.50
1:I:461:GLU:HB3	1:I:464:VAL:HB	1.94	0.50
2:R:40:VAL:HB	2:R:62:GLY:H	1.76	0.50
2:S:11:ILE:HD12	2:S:42:ALA:HB3	1.94	0.50
1:A:482:THR:O	1:A:483:GLU:HB2	2.11	0.50
1:C:236:VAL:O	1:C:240:VAL:HG23	2.12	0.50
1:F:524:LEU:HD22	1:F:525:PRO:HD2	1.92	0.50
1:G:284:ARG:NH1	1:G:364:LYS:HD2	2.27	0.50
1:H:326:ASN:HB2	1:H:329:THR:HB	1.93	0.50
1:I:106:ALA:CA	1:I:111:MET:HE3	2.42	0.50
1:K:149:THR:HG23	1:K:159:GLY:HA3	1.93	0.50
1:L:426:LEU:CD1	1:L:444:LEU:HD21	2.42	0.50
1:E:326:ASN:HD22	1:E:329:THR:HB	1.76	0.49
1:J:106:ALA:HA	1:J:111:MET:CE	2.42	0.49
1:J:106:ALA:HA	1:J:111:MET:HE3	1.93	0.49
1:J:385:THR:HG23	1:J:388:GLU:HB2	1.94	0.49
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.94	0.49
1:C:284:ARG:NH1	1:C:364:LYS:HD2	2.25	0.49
1:G:305:ILE:O	1:G:305:ILE:HG22	2.12	0.49
1:A:39:VAL:HB	1:G:520:MET:HG2	1.93	0.49
1:I:217:SER:N	1:I:218:PRO:CD	2.75	0.49
1:K:64:ASP:OD1	1:K:65:LYS:O	2.29	0.49
1:K:66:PHE:H	1:K:69:MET:HG3	1.78	0.49
1:M:351:GLN:HA	1:M:354:GLU:HG2	1.93	0.49
1:C:22:VAL:HG11	1:C:62:LEU:HD11	1.93	0.49
1:D:510:VAL:HG12	1:D:514:MET:CE	2.40	0.49
5:D:600:ADP:O1B	6:D:602:AF3:F2	2.19	0.49
1:E:487:ASN:O	1:E:491:MET:HG3	2.12	0.49
1:J:44:PHE:H	1:J:44:PHE:HD1	1.59	0.49
1:L:385:THR:HG23	1:L:388:GLU:HB2	1.94	0.49
1:M:201:SER:O	1:M:203:TYR:N	2.44	0.49
1:M:452:ARG:HG2	1:M:452:ARG:HH11	1.77	0.49
1:B:111:MET:HG2	1:B:116:LEU:HD21	1.93	0.49
1:F:143:ALA:HA	1:F:146:GLN:NE2	2.28	0.49
1:G:147:VAL:HG12	1:G:494:LEU:HB2	1.94	0.49
1:H:339:GLU:O	1:H:343:GLN:HB2	2.12	0.49
1:M:221:LEU:HD23	1:M:249:ILE:HG23	1.93	0.49
2:U:7:HIS:HB3	2:U:45:ASN:HD22	1.77	0.49
1:H:73:MET:HE1	1:H:514:MET:HG2	1.94	0.49
1:H:82:ASN:ND2	1:H:89:THR:OG1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:426:LEU:HD12	1:K:444:LEU:HD21	1.94	0.49
1:L:44:PHE:HD1	1:L:44:PHE:H	1.60	0.49
1:N:326:ASN:HB2	1:N:329:THR:HB	1.94	0.49
1:D:305:ILE:HG23	1:E:267:MET:HG2	1.94	0.49
1:K:461:GLU:HA	1:K:461:GLU:OE1	2.13	0.49
1:N:106:ALA:CA	1:N:111:MET:HE3	2.42	0.49
1:N:461:GLU:HB3	1:N:464:VAL:HB	1.94	0.49
1:D:501:ARG:HD3	1:D:505:GLN:OE1	2.13	0.49
1:I:455:VAL:CG1	1:I:462:PRO:HA	2.41	0.49
1:K:201:SER:O	1:K:203:TYR:N	2.44	0.49
1:M:15:LYS:NZ	1:M:64:ASP:OD2	2.46	0.49
2:P:16:GLU:HB2	2:P:19:THR:OG1	2.13	0.49
2:Q:16:GLU:HB2	2:Q:19:THR:OG1	2.12	0.49
2:S:40:VAL:HB	2:S:62:GLY:H	1.77	0.49
1:B:365:LEU:CD2	1:B:368:ARG:HH21	2.25	0.49
1:B:147:VAL:HG12	1:B:494:LEU:HB2	1.94	0.49
1:D:524:LEU:HD23	1:D:525:PRO:HD2	1.93	0.49
1:E:486:GLY:CA	1:E:491:MET:CE	2.90	0.49
1:F:326:ASN:HD22	1:F:329:THR:HB	1.76	0.49
1:I:213:VAL:HB	1:I:325:ILE:CG1	2.41	0.49
1:J:149:THR:CG2	1:J:159:GLY:HA3	2.43	0.49
1:K:197:ARG:HD2	1:K:277:LYS:HB2	1.94	0.49
1:L:64:ASP:OD1	1:L:65:LYS:O	2.31	0.49
2:U:50:GLU:O	2:U:51:ASN:HB3	2.13	0.49
1:B:11:ASP:N	1:B:11:ASP:OD1	2.45	0.49
1:B:224:ASP:O	1:B:225:LYS:HB3	2.13	0.49
1:B:236:VAL:O	1:B:240:VAL:HG23	2.13	0.49
1:G:236:VAL:O	1:G:240:VAL:HG23	2.13	0.49
1:H:223:ALA:O	1:H:251:ALA:HA	2.13	0.49
1:K:107:VAL:HG11	1:K:515:ILE:HG23	1.94	0.49
1:N:35:GLY:O	1:N:51:LYS:HE3	2.12	0.49
1:C:305:ILE:O	1:C:305:ILE:HG22	2.13	0.49
1:C:63:GLU:HG2	1:C:63:GLU:O	2.13	0.49
1:E:305:ILE:HD12	1:E:307:MET:HE2	1.95	0.49
1:E:455:VAL:HG21	1:E:465:VAL:HG11	1.95	0.49
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.94	0.49
1:G:172:GLU:OE2	1:G:350:ARG:NH2	2.45	0.49
1:L:228:SER:O	1:L:257:GLU:HB3	2.12	0.49
1:B:482:THR:O	1:B:483:GLU:HB2	2.12	0.48
1:C:228:SER:O	1:C:257:GLU:HB3	2.13	0.48
1:D:441:LYS:HE2	7:D:615:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:MET:SD	1:G:514:MET:HG3	2.53	0.48
1:H:420:ILE:HD13	1:H:420:ILE:HG23	1.64	0.48
1:J:213:VAL:HB	1:J:325:ILE:CG1	2.40	0.48
1:L:106:ALA:HA	1:L:111:MET:HE3	1.94	0.48
1:M:224:ASP:O	1:M:225:LYS:HB3	2.13	0.48
1:N:194:GLN:HB2	1:N:331:THR:HB	1.95	0.48
2:O:16:GLU:HB2	2:O:19:THR:OG1	2.13	0.48
2:O:50:GLU:HG2	2:P:51:ASN:CB	2.38	0.48
2:T:50:GLU:O	2:T:51:ASN:HB3	2.12	0.48
1:A:111:MET:HG3	1:A:435:ASP:OD1	2.13	0.48
1:A:261:THR:O	1:A:262:LEU:C	2.51	0.48
1:E:441:LYS:HB3	1:E:445:ARG:HH21	1.79	0.48
1:H:76:GLU:O	1:H:76:GLU:HG2	2.13	0.48
1:J:16:MET:CE	1:J:16:MET:CB	2.91	0.48
1:M:415:GLY:N	1:M:417:VAL:HG23	2.27	0.48
1:M:461:GLU:CA	1:M:461:GLU:OE1	2.60	0.48
2:O:7:HIS:HB3	2:O:45:ASN:HD22	1.78	0.48
1:A:265:ASN:HA	1:A:270:ILE:HD12	1.95	0.48
1:C:524:LEU:HD22	1:C:525:PRO:HD2	1.95	0.48
1:D:247:LEU:HD12	1:D:248:LEU:N	2.28	0.48
1:F:16:MET:CG	1:F:16:MET:CE	2.91	0.48
1:I:145:ALA:O	1:I:149:THR:HG23	2.13	0.48
1:K:100:ILE:CG2	1:K:104:LEU:HD22	2.43	0.48
1:K:174:VAL:HB	1:K:376:VAL:HG22	1.95	0.48
1:K:451:LEU:O	1:K:452:ARG:C	2.51	0.48
1:B:486:GLY:C	1:B:491:MET:HE2	2.33	0.48
1:G:111:MET:HG3	1:G:435:ASP:OD1	2.13	0.48
1:H:404:ARG:CG	1:H:404:ARG:NH1	2.60	0.48
1:N:106:ALA:HA	1:N:111:MET:HE3	1.94	0.48
1:N:305:ILE:HD12	1:N:307:MET:HE2	1.94	0.48
2:O:47:ARG:HD3	2:O:49:LEU:HD12	1.95	0.48
2:O:40:VAL:HB	2:O:62:GLY:H	1.78	0.48
2:P:40:VAL:HB	2:P:62:GLY:H	1.77	0.48
2:U:7:HIS:CE1	2:U:48:ILE:HD11	2.48	0.48
1:B:16:MET:CB	1:B:16:MET:CE	2.90	0.48
1:B:444:LEU:O	1:B:447:MET:HB2	2.14	0.48
1:I:100:ILE:CG2	1:I:104:LEU:HD22	2.42	0.48
1:I:152:ALA:O	1:I:153:ASN:HB3	2.13	0.48
1:I:326:ASN:HB2	1:I:329:THR:HB	1.95	0.48
1:M:467:ASN:C	1:M:467:ASN:ND2	2.67	0.48
2:S:50:GLU:O	2:S:51:ASN:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:7:HIS:HB3	2:T:45:ASN:HD22	1.78	0.48
1:B:100:ILE:HG13	1:B:511:ALA:HB1	1.96	0.48
1:C:289:LEU:HA	1:C:292:ILE:HD12	1.96	0.48
1:E:365:LEU:CD2	1:E:368:ARG:HH21	2.26	0.48
1:F:305:ILE:HG22	1:F:305:ILE:O	2.13	0.48
1:F:150:ILE:CD1	1:F:492:GLY:O	2.61	0.48
1:F:104:LEU:HD23	1:F:515:ILE:HG22	1.94	0.48
1:H:218:PRO:HB3	1:H:246:PRO:HG2	1.96	0.48
1:H:44:PHE:H	1:H:44:PHE:HD1	1.61	0.48
1:J:106:ALA:O	1:J:111:MET:HE3	2.14	0.48
1:K:126:ALA:HB1	1:K:426:LEU:HD22	1.95	0.48
1:M:24:ALA:HA	1:M:27:VAL:HG12	1.95	0.48
1:A:511:ALA:O	1:A:515:ILE:HG12	2.14	0.48
1:F:448:GLU:O	1:F:452:ARG:HG3	2.13	0.48
1:H:126:ALA:HB1	1:H:426:LEU:HD22	1.96	0.48
1:H:469:VAL:HG13	1:H:477:GLY:HA2	1.95	0.48
1:J:180:GLY:HA3	1:J:381:VAL:O	2.14	0.48
1:K:455:VAL:HG13	1:K:460:GLU:HB2	1.95	0.48
1:N:326:ASN:HB2	1:N:329:THR:H	1.78	0.48
2:Q:78:ILE:HD13	2:Q:83:VAL:HG21	1.95	0.48
2:R:47:ARG:HD3	2:R:49:LEU:HD12	1.94	0.48
2:R:78:ILE:HD13	2:R:83:VAL:HG21	1.96	0.48
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.94	0.48
1:K:461:GLU:HB3	1:K:464:VAL:HB	1.96	0.48
2:R:11:ILE:HD12	2:R:42:ALA:HB3	1.96	0.48
1:A:358:SER:HB3	1:A:361:ASP:OD1	2.14	0.48
1:B:219:PHE:HB3	1:B:317:LEU:HD23	1.95	0.48
1:B:305:ILE:HG12	1:C:267:MET:HE3	1.96	0.48
1:D:305:ILE:O	1:D:305:ILE:HG22	2.14	0.48
1:D:486:GLY:HA3	1:D:491:MET:HE2	1.96	0.48
1:I:180:GLY:HA3	1:I:381:VAL:O	2.13	0.48
1:L:452:ARG:HG2	1:L:452:ARG:NH1	2.29	0.48
2:R:16:GLU:HB2	2:R:19:THR:OG1	2.14	0.48
1:E:143:ALA:HA	1:E:146:GLN:NE2	2.29	0.48
1:F:362:ARG:HG2	1:F:366:GLN:NE2	2.29	0.48
1:I:461:GLU:CA	1:I:461:GLU:OE1	2.58	0.48
1:J:194:GLN:HB2	1:J:331:THR:HB	1.96	0.48
1:J:221:LEU:HD23	1:J:249:ILE:HG23	1.96	0.48
1:L:218:PRO:HB3	1:L:246:PRO:HG2	1.96	0.48
1:M:172:GLU:CA	1:M:172:GLU:OE1	2.61	0.48
2:S:16:GLU:HB2	2:S:19:THR:OG1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:47:ARG:HD3	2:S:49:LEU:HD12	1.95	0.48
2:S:78:ILE:HD13	2:S:83:VAL:HG21	1.96	0.48
1:A:230:ILE:CD1	1:A:261:THR:HG21	2.39	0.47
1:E:524:LEU:HD23	1:E:525:PRO:HD2	1.96	0.47
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.96	0.47
1:F:365:LEU:CD2	1:F:368:ARG:HH21	2.27	0.47
1:G:94:VAL:O	1:G:98:ALA:HB2	2.14	0.47
1:I:116:LEU:HD23	1:I:116:LEU:HA	1.80	0.47
1:K:16:MET:HE2	1:K:16:MET:HB2	1.96	0.47
1:M:34:LYS:HB2	1:M:458:CYS:SG	2.54	0.47
1:H:521:VAL:HB	1:N:40:LEU:HD12	1.95	0.47
2:Q:7:HIS:HB3	2:Q:45:ASN:HD22	1.79	0.47
1:B:284:ARG:NH1	1:B:364:LYS:HD2	2.28	0.47
1:B:518:GLU:HG3	1:B:518:GLU:O	2.14	0.47
1:C:223:ALA:O	1:C:251:ALA:HA	2.15	0.47
1:G:143:ALA:HA	1:G:146:GLN:HE21	1.77	0.47
1:I:126:ALA:CB	1:I:426:LEU:HD22	2.44	0.47
1:I:234:LEU:N	1:I:235:PRO:HD2	2.29	0.47
1:I:326:ASN:HD22	1:I:329:THR:CG2	2.26	0.47
1:J:201:SER:O	1:J:203:TYR:N	2.47	0.47
1:J:488:MET:CE	1:J:493:ILE:HG21	2.43	0.47
2:S:68:ASN:ND2	2:T:74:LYS:HD2	2.29	0.47
1:D:289:LEU:HA	1:D:292:ILE:HD12	1.96	0.47
1:E:486:GLY:C	1:E:491:MET:HE2	2.34	0.47
1:F:415:GLY:O	1:F:451:LEU:HD23	2.13	0.47
1:G:74:VAL:O	1:G:77:VAL:HG13	2.14	0.47
1:I:91:THR:O	1:I:92:ALA:C	2.52	0.47
1:L:100:ILE:CG2	1:L:104:LEU:HD22	2.45	0.47
1:M:428:ASP:CA	7:M:534:HOH:O	2.58	0.47
2:P:7:HIS:CE1	2:P:48:ILE:HD11	2.50	0.47
1:B:15:LYS:O	1:B:16:MET:C	2.53	0.47
1:F:228:SER:O	1:F:257:GLU:HB3	2.13	0.47
1:G:486:GLY:C	1:G:491:MET:HE2	2.34	0.47
1:H:198:GLY:O	1:H:276:VAL:HG12	2.15	0.47
1:K:452:ARG:HH11	1:K:452:ARG:HG2	1.80	0.47
1:L:221:LEU:HD23	1:L:249:ILE:HG23	1.95	0.47
1:L:305:ILE:HD12	1:L:307:MET:HE2	1.97	0.47
1:L:174:VAL:HB	1:L:376:VAL:HG22	1.95	0.47
1:C:76:GLU:OE1	1:D:387:VAL:HG13	2.15	0.47
1:F:305:ILE:HD12	1:F:307:MET:HE2	1.97	0.47
1:A:267:MET:HE2	1:G:305:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:419:LEU:HG	1:G:447:MET:HG2	1.95	0.47
1:I:103:GLY:O	1:I:106:ALA:HB3	2.13	0.47
1:I:351:GLN:HA	1:I:354:GLU:HG2	1.97	0.47
1:I:419:LEU:CD2	1:I:500:THR:CG2	2.93	0.47
1:J:198:GLY:O	1:J:276:VAL:HG12	2.14	0.47
1:J:27:VAL:HG11	1:J:93:THR:HG21	1.96	0.47
1:J:419:LEU:HA	1:J:419:LEU:HD13	1.61	0.47
1:J:461:GLU:HB3	1:J:464:VAL:HB	1.96	0.47
1:K:198:GLY:O	1:K:276:VAL:HG12	2.14	0.47
1:K:73:MET:HE1	1:K:514:MET:HG2	1.95	0.47
1:M:64:ASP:OD1	1:M:65:LYS:O	2.33	0.47
2:P:7:HIS:HB3	2:P:45:ASN:HD22	1.79	0.47
1:A:224:ASP:O	1:A:225:LYS:HB3	2.15	0.47
1:A:486:GLY:CA	1:A:491:MET:HE1	2.45	0.47
1:C:247:LEU:HD12	1:C:248:LEU:N	2.29	0.47
1:I:220:ILE:HG12	1:I:248:LEU:HD23	1.97	0.47
1:I:66:PHE:H	1:I:69:MET:HG3	1.79	0.47
1:M:326:ASN:HB2	1:M:329:THR:H	1.79	0.47
1:M:126:ALA:HB1	1:M:426:LEU:HD22	1.97	0.47
1:N:426:LEU:HD12	1:N:444:LEU:HD21	1.96	0.47
2:Q:41:LEU:O	2:Q:61:VAL:HG13	2.14	0.47
1:A:78:ALA:HB2	1:A:93:THR:OG1	2.14	0.47
1:G:417:VAL:O	1:G:418:ALA:C	2.52	0.47
1:H:419:LEU:HD22	1:H:500:THR:CG2	2.45	0.47
1:N:201:SER:O	1:N:203:TYR:N	2.47	0.47
1:A:28:LYS:HD2	1:A:453:GLN:NE2	2.29	0.47
1:D:486:GLY:HA3	1:D:491:MET:CE	2.44	0.47
1:F:284:ARG:HH11	1:F:364:LYS:HD2	1.80	0.47
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.96	0.47
1:F:358:SER:HB3	1:F:361:ASP:HB2	1.97	0.47
1:F:455:VAL:HG11	1:F:462:PRO:HA	1.96	0.47
1:L:126:ALA:HB1	1:L:426:LEU:CD2	2.43	0.47
1:L:34:LYS:HB2	1:L:458:CYS:SG	2.55	0.47
1:C:143:ALA:HA	1:C:146:GLN:HE21	1.80	0.47
1:D:310:GLU:OE1	1:D:310:GLU:N	2.47	0.47
1:F:487:ASN:O	1:F:491:MET:HG3	2.15	0.47
1:A:267:MET:CE	1:G:305:ILE:HG12	2.44	0.47
1:G:365:LEU:CD2	1:G:368:ARG:HH21	2.27	0.47
1:G:486:GLY:CA	1:G:491:MET:HE2	2.45	0.47
1:H:467:ASN:ND2	1:H:467:ASN:C	2.68	0.47
1:J:126:ALA:CB	1:J:426:LEU:HD22	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:326:ASN:HB2	1:J:329:THR:HB	1.97	0.47
1:K:35:GLY:O	1:K:51:LYS:HE3	2.14	0.47
1:L:326:ASN:HB2	1:L:329:THR:HB	1.96	0.47
1:M:428:ASP:CB	7:M:534:HOH:O	2.58	0.47
1:N:103:GLY:O	1:N:106:ALA:HB3	2.15	0.47
1:N:234:LEU:N	1:N:235:PRO:HD2	2.30	0.47
1:N:15:LYS:HB3	1:N:66:PHE:HB3	1.96	0.47
1:B:270:ILE:HD13	2:P:27:LEU:HB3	1.97	0.47
1:C:455:VAL:HG11	1:C:462:PRO:HA	1.97	0.47
1:D:143:ALA:HA	1:D:146:GLN:HE21	1.79	0.47
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.97	0.47
1:E:305:ILE:HG23	1:F:267:MET:HG2	1.95	0.47
1:E:103:GLY:HA3	1:E:515:ILE:HG21	1.97	0.47
1:G:77:VAL:HG22	1:G:78:ALA:N	2.30	0.47
1:I:224:ASP:O	1:I:225:LYS:HB3	2.14	0.47
1:K:419:LEU:HD13	1:K:419:LEU:HA	1.72	0.47
1:N:106:ALA:HA	1:N:111:MET:CE	2.44	0.47
1:A:129:GLU:HA	1:A:129:GLU:OE2	2.15	0.47
1:A:223:ALA:O	1:A:251:ALA:HA	2.14	0.47
1:A:479:ASN:OD1	1:A:479:ASN:C	2.53	0.47
1:E:284:ARG:NH1	1:E:364:LYS:HD2	2.30	0.47
1:F:510:VAL:HG13	1:F:514:MET:HE1	1.95	0.47
1:G:349:ILE:HA	1:G:352:GLN:HG2	1.95	0.47
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.96	0.47
1:J:228:SER:O	1:J:257:GLU:HB3	2.14	0.47
1:K:100:ILE:O	1:K:104:LEU:HB2	2.14	0.47
1:L:197:ARG:HD2	1:L:277:LYS:HB2	1.97	0.47
1:L:23:LEU:HD22	1:L:23:LEU:O	2.15	0.47
2:Q:50:GLU:O	2:Q:51:ASN:HB3	2.15	0.47
1:A:358:SER:HB3	1:A:361:ASP:HB2	1.98	0.46
1:D:429:LEU:HA	1:D:429:LEU:HD12	1.71	0.46
1:C:105:LYS:HD3	1:J:110:GLY:O	2.15	0.46
1:K:90:THR:O	1:K:94:VAL:HG23	2.15	0.46
2:R:68:ASN:HD22	2:S:74:LYS:HD2	1.80	0.46
1:D:365:LEU:CD2	1:D:368:ARG:HH21	2.27	0.46
1:E:247:LEU:HD12	1:E:248:LEU:N	2.29	0.46
1:I:419:LEU:HA	1:I:419:LEU:HD13	1.65	0.46
1:K:16:MET:CG	1:K:16:MET:CE	2.93	0.46
1:L:262:LEU:O	1:L:266:THR:HG23	2.15	0.46
1:L:64:ASP:C	1:L:65:LYS:O	2.52	0.46
1:N:16:MET:HG2	1:N:70:GLY:HA2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:7:HIS:HB3	2:S:45:ASN:HD22	1.80	0.46
1:A:310:GLU:N	1:A:310:GLU:OE1	2.48	0.46
1:B:247:LEU:HD12	1:B:248:LEU:N	2.31	0.46
1:C:172:GLU:OE1	1:C:172:GLU:HA	2.15	0.46
1:D:33:PRO:HA	1:D:153:ASN:HD21	1.81	0.46
1:G:162:ILE:O	1:G:165:ALA:HB3	2.15	0.46
1:G:326:ASN:HD22	1:G:329:THR:HB	1.79	0.46
1:C:150:ILE:HD11	1:C:492:GLY:O	2.15	0.46
1:E:194:GLN:HG3	1:E:331:THR:HB	1.97	0.46
1:F:223:ALA:O	1:F:251:ALA:HA	2.16	0.46
1:I:106:ALA:O	1:I:111:MET:HE3	2.16	0.46
1:K:126:ALA:CB	1:K:426:LEU:HD22	2.45	0.46
1:M:198:GLY:HA3	1:M:327:LYS:O	2.16	0.46
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.97	0.46
1:D:190:VAL:HG11	1:D:194:GLN:NE2	2.30	0.46
1:F:172:GLU:OE1	1:F:172:GLU:HA	2.15	0.46
1:F:194:GLN:HG3	1:F:331:THR:HB	1.97	0.46
1:L:502:SER:O	1:L:503:ALA:C	2.54	0.46
1:N:413:ALA:CB	1:N:417:VAL:HB	2.44	0.46
1:C:20:VAL:HG13	1:C:74:VAL:HG11	1.98	0.46
1:C:519:CYS:HB3	1:D:38:VAL:HG22	1.97	0.46
1:F:42:LYS:HG2	1:F:44:PHE:CE2	2.51	0.46
1:G:310:GLU:OE1	1:G:310:GLU:N	2.49	0.46
1:N:419:LEU:HD22	1:N:500:THR:CG2	2.45	0.46
1:N:94:VAL:O	1:N:94:VAL:HG12	2.16	0.46
1:A:270:ILE:CD1	2:O:27:LEU:HB3	2.46	0.46
1:G:230:ILE:CD1	1:G:261:THR:HG21	2.38	0.46
1:H:449:ALA:N	1:H:450:PRO:CD	2.79	0.46
1:J:305:ILE:HD12	1:J:307:MET:HE2	1.96	0.46
1:K:467:ASN:ND2	1:K:467:ASN:C	2.68	0.46
1:L:488:MET:HE1	1:L:493:ILE:HG21	1.98	0.46
1:M:116:LEU:HD23	1:M:116:LEU:HA	1.84	0.46
1:N:452:ARG:NH1	1:N:452:ARG:HG2	2.27	0.46
1:N:514:MET:CE	1:N:514:MET:CG	2.93	0.46
1:A:130:GLU:O	1:A:133:ALA:HB3	2.15	0.46
1:A:291:ASP:HB3	1:A:372:LEU:HD11	1.98	0.46
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.71	0.46
1:B:429:LEU:O	1:B:430:ARG:NH1	2.49	0.46
1:E:153:ASN:O	1:E:154:SER:HB2	2.16	0.46
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.97	0.46
1:G:194:GLN:HG3	1:G:331:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:444:LEU:HA	1:H:444:LEU:HD23	1.69	0.46
1:J:180:GLY:HA2	1:J:380:LYS:HB3	1.97	0.46
1:N:43:SER:HB2	1:N:44:PHE:H	1.67	0.46
1:A:284:ARG:NH1	1:A:364:LYS:HD2	2.29	0.46
1:A:289:LEU:HA	1:A:292:ILE:HD12	1.98	0.46
1:A:6:VAL:CG2	1:A:6:VAL:O	2.61	0.46
1:C:172:GLU:OE2	1:C:350:ARG:NH2	2.48	0.46
1:F:224:ASP:O	1:F:225:LYS:HB3	2.15	0.46
1:G:224:ASP:O	1:G:225:LYS:HB3	2.16	0.46
1:N:197:ARG:HG3	1:N:277:LYS:O	2.16	0.46
1:N:444:LEU:HD23	1:N:444:LEU:HA	1.75	0.46
1:B:230:ILE:CD1	1:B:261:THR:HG21	2.41	0.46
1:D:486:GLY:CA	1:D:491:MET:HE2	2.46	0.46
1:F:230:ILE:CD1	1:F:261:THR:HG21	2.41	0.46
1:G:455:VAL:HG11	1:G:462:PRO:HA	1.97	0.46
1:H:224:ASP:O	1:H:225:LYS:HB3	2.15	0.46
1:H:415:GLY:CA	1:H:417:VAL:HG23	2.46	0.46
1:I:346:VAL:O	1:I:350:ARG:HB2	2.14	0.46
1:M:21:ASN:HD22	1:M:21:ASN:HA	1.46	0.46
1:N:511:ALA:O	1:N:515:ILE:HD12	2.16	0.46
2:O:78:ILE:HD13	2:O:83:VAL:HG21	1.98	0.46
1:A:452:ARG:NH2	1:A:463:SER:HA	2.31	0.45
1:D:305:ILE:HD12	1:D:307:MET:HE2	1.99	0.45
1:D:482:THR:O	1:D:483:GLU:HB2	2.16	0.45
1:H:100:ILE:O	1:H:104:LEU:HB2	2.16	0.45
1:H:106:ALA:HA	1:H:111:MET:HE3	1.98	0.45
1:I:326:ASN:HB2	1:I:329:THR:H	1.80	0.45
1:I:436:GLN:O	1:I:440:ILE:HG13	2.16	0.45
1:I:49:ILE:HD12	1:J:513:LEU:HD23	1.97	0.45
1:L:326:ASN:HB2	1:L:329:THR:H	1.81	0.45
1:L:426:LEU:HD12	1:L:444:LEU:HD21	1.96	0.45
1:N:147:VAL:HG21	1:N:411:VAL:HG11	1.98	0.45
2:Q:68:ASN:ND2	2:R:74:LYS:HD2	2.31	0.45
1:D:224:ASP:O	1:D:225:LYS:HB3	2.16	0.45
1:G:240:VAL:HG21	1:G:247:LEU:HD22	1.98	0.45
1:G:345:ARG:O	1:G:348:GLN:HB2	2.16	0.45
1:I:209:GLU:OE1	1:I:209:GLU:N	2.49	0.45
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.99	0.45
1:I:404:ARG:NH1	1:I:404:ARG:CG	2.60	0.45
1:J:119:GLY:O	1:J:120:ILE:C	2.54	0.45
1:N:180:GLY:HA3	1:N:381:VAL:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:466:ALA:O	1:N:467:ASN:C	2.52	0.45
1:A:205:ILE:CA	1:A:213:VAL:HG22	2.43	0.45
1:C:143:ALA:HA	1:C:146:GLN:NE2	2.31	0.45
1:C:310:GLU:N	1:C:310:GLU:OE1	2.48	0.45
1:F:310:GLU:OE1	1:F:310:GLU:N	2.50	0.45
1:G:358:SER:HB3	1:G:361:ASP:HB2	1.98	0.45
1:N:116:LEU:HA	1:N:116:LEU:HD23	1.87	0.45
1:N:65:LYS:HG3	1:N:65:LYS:H	1.27	0.45
1:A:305:ILE:HG22	1:A:305:ILE:O	2.17	0.45
1:B:441:LYS:HB3	1:B:445:ARG:HH21	1.82	0.45
1:D:67:GLU:O	1:D:68:ASN:C	2.53	0.45
1:H:35:GLY:O	1:H:51:LYS:HE3	2.17	0.45
1:I:511:ALA:O	1:I:515:ILE:HD12	2.16	0.45
1:I:63:GLU:HA	1:J:3:ALA:CB	2.47	0.45
1:K:234:LEU:N	1:K:235:PRO:HD2	2.32	0.45
1:M:64:ASP:C	1:M:65:LYS:O	2.53	0.45
1:N:419:LEU:HA	1:N:419:LEU:HD13	1.60	0.45
1:B:218:PRO:HB3	1:B:246:PRO:HG2	1.99	0.45
1:B:414:GLY:C	1:B:416:GLY:N	2.69	0.45
1:E:225:LYS:HD3	1:E:303:GLU:CD	2.36	0.45
1:E:310:GLU:OE1	1:E:310:GLU:N	2.50	0.45
1:E:345:ARG:O	1:E:348:GLN:HB2	2.16	0.45
1:F:11:ASP:O	1:F:12:ALA:C	2.55	0.45
1:G:482:THR:O	1:G:483:GLU:HB2	2.16	0.45
1:I:149:THR:HG22	1:I:159:GLY:HA3	1.99	0.45
1:J:117:LYS:O	1:J:118:ARG:C	2.54	0.45
1:K:419:LEU:CD2	1:K:500:THR:HG23	2.47	0.45
1:L:430:ARG:HA	1:L:430:ARG:HD3	1.76	0.45
1:L:461:GLU:HB3	1:L:464:VAL:HB	1.99	0.45
1:M:100:ILE:O	1:M:104:LEU:HB2	2.16	0.45
1:M:326:ASN:HB2	1:M:329:THR:HB	1.97	0.45
7:M:529:HOH:O	1:N:68:ASN:HB3	2.16	0.45
2:O:20:LYS:HB3	2:O:27:LEU:HG	1.98	0.45
1:B:514:MET:CE	1:B:514:MET:CB	2.92	0.45
1:D:172:GLU:OE1	1:D:172:GLU:HA	2.16	0.45
1:E:23:LEU:CD1	1:E:23:LEU:C	2.84	0.45
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.98	0.45
1:F:349:ILE:HA	1:F:352:GLN:HG2	1.97	0.45
1:G:502:SER:O	1:G:503:ALA:C	2.53	0.45
1:G:88:GLY:N	6:G:602:AF3:F2	2.40	0.45
2:T:3:ILE:H	2:T:3:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD23	1:A:453:GLN:HB3	1.98	0.45
1:H:228:SER:O	1:H:257:GLU:HB3	2.16	0.45
1:J:217:SER:N	1:J:218:PRO:CD	2.76	0.45
1:J:24:ALA:HA	1:J:27:VAL:HG12	1.97	0.45
1:J:492:GLY:O	1:J:493:ILE:HD13	2.17	0.45
1:K:104:LEU:HA	1:K:104:LEU:HD12	1.46	0.45
1:K:326:ASN:HB2	1:K:329:THR:HB	1.99	0.45
2:T:78:ILE:HD13	2:T:83:VAL:HG21	1.99	0.45
1:A:329:THR:O	1:A:329:THR:HG22	2.16	0.45
1:A:91:THR:O	1:A:92:ALA:C	2.54	0.45
1:C:78:ALA:HB2	1:C:93:THR:OG1	2.17	0.45
1:E:486:GLY:HA3	1:E:491:MET:HE1	1.98	0.45
1:F:129:GLU:HA	1:F:129:GLU:OE2	2.17	0.45
1:G:223:ALA:O	1:G:251:ALA:HA	2.17	0.45
1:G:487:ASN:O	1:G:491:MET:HG3	2.17	0.45
1:G:76:GLU:O	1:G:76:GLU:HG2	2.16	0.45
1:J:524:LEU:HD23	1:J:524:LEU:HA	1.78	0.45
1:L:270:ILE:HG22	1:L:271:VAL:HG23	1.98	0.45
2:S:95:VAL:HG11	2:T:1:MET:CE	2.47	0.45
1:A:452:ARG:HH22	1:A:463:SER:HB3	1.82	0.45
1:B:225:LYS:HD3	1:B:303:GLU:CD	2.38	0.45
1:B:78:ALA:HB2	1:B:93:THR:OG1	2.16	0.45
1:C:448:GLU:HB3	1:C:452:ARG:HD2	1.99	0.45
1:I:228:SER:O	1:I:257:GLU:HB3	2.17	0.45
1:K:222:LEU:HD23	1:K:250:ILE:HB	1.99	0.45
1:M:325:ILE:HG22	1:M:330:THR:HG23	1.98	0.45
1:A:486:GLY:HA3	1:A:491:MET:HE2	1.99	0.45
1:B:349:ILE:HA	1:B:352:GLN:HG2	1.92	0.45
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.98	0.45
1:C:358:SER:HB3	1:C:361:ASP:OD1	2.17	0.45
1:E:305:ILE:HG22	1:E:305:ILE:O	2.17	0.45
1:G:190:VAL:HG11	1:G:194:GLN:NE2	2.32	0.45
1:G:218:PRO:HB3	1:G:246:PRO:HG2	1.99	0.45
1:H:262:LEU:O	1:H:266:THR:HG23	2.17	0.45
1:J:467:ASN:ND2	1:J:467:ASN:C	2.69	0.45
1:J:22:VAL:HG11	1:J:62:LEU:HD21	1.99	0.45
1:L:73:MET:HE1	1:L:514:MET:HG2	1.98	0.45
1:M:47:PRO:CG	1:N:73:MET:HG3	2.46	0.45
1:N:34:LYS:HB2	1:N:458:CYS:SG	2.57	0.45
1:A:461:GLU:OE1	1:N:463:SER:HB3	2.17	0.45
1:B:23:LEU:C	1:B:23:LEU:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ASP:O	1:C:225:LYS:HB3	2.17	0.44
1:D:76:GLU:O	1:D:80:LYS:HB2	2.17	0.44
1:F:247:LEU:HD12	1:F:248:LEU:N	2.31	0.44
1:G:518:GLU:HG3	1:G:518:GLU:O	2.17	0.44
1:I:90:THR:O	1:I:94:VAL:HG23	2.17	0.44
1:I:99:ILE:O	1:I:102:GLU:N	2.46	0.44
1:J:100:ILE:O	1:J:104:LEU:HB2	2.16	0.44
1:N:522:THR:OG1	1:N:523:ASP:N	2.50	0.44
1:N:84:ALA:O	1:N:85:ALA:HB2	2.17	0.44
1:C:362:ARG:HG2	1:C:366:GLN:NE2	2.32	0.44
1:D:305:ILE:HG12	1:E:267:MET:CE	2.47	0.44
1:E:219:PHE:HB3	1:E:317:LEU:HD23	1.98	0.44
1:E:224:ASP:O	1:E:225:LYS:HB3	2.17	0.44
1:E:510:VAL:HG13	1:E:514:MET:CE	2.47	0.44
1:H:163:ALA:O	1:H:167:ASP:HB2	2.17	0.44
1:J:198:GLY:HA3	1:J:327:LYS:O	2.16	0.44
1:K:119:GLY:O	1:K:120:ILE:C	2.54	0.44
1:K:430:ARG:HD3	1:K:430:ARG:HA	1.63	0.44
1:L:198:GLY:HA3	1:L:327:LYS:O	2.17	0.44
1:M:169:VAL:HG13	1:M:173:GLY:HA3	2.00	0.44
1:A:486:GLY:CA	1:A:491:MET:HE2	2.48	0.44
1:D:291:ASP:HB3	1:D:372:LEU:HD11	1.99	0.44
1:G:247:LEU:HD12	1:G:248:LEU:N	2.32	0.44
1:H:498:LYS:NZ	7:H:532:HOH:O	2.40	0.44
1:K:326:ASN:HB2	1:K:329:THR:H	1.81	0.44
2:U:14:ARG:NH2	2:U:84:LEU:HD21	2.33	0.44
1:C:291:ASP:HB3	1:C:372:LEU:HD11	1.99	0.44
1:F:234:LEU:HB2	1:F:235:PRO:CD	2.47	0.44
1:F:486:GLY:HA3	1:F:491:MET:HE1	1.98	0.44
1:H:152:ALA:O	1:H:153:ASN:HB3	2.17	0.44
1:H:65:LYS:HG3	1:H:65:LYS:H	1.35	0.44
1:I:430:ARG:HD3	1:I:430:ARG:HA	1.59	0.44
1:K:144:ILE:CD1	1:K:407:VAL:HG22	2.48	0.44
1:K:13:ARG:HA	1:K:16:MET:CE	2.47	0.44
1:K:262:LEU:O	1:K:266:THR:HG23	2.17	0.44
1:L:77:VAL:CG1	1:L:78:ALA:N	2.81	0.44
1:M:305:ILE:HD12	1:M:307:MET:HE2	1.98	0.44
1:M:502:SER:O	1:M:503:ALA:C	2.55	0.44
1:C:206:ASN:HD21	1:C:214:GLU:N	2.06	0.44
1:C:358:SER:HB3	1:C:361:ASP:HB2	1.99	0.44
1:C:66:PHE:O	1:C:69:MET:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:THR:OG1	1:D:37:ASN:ND2	2.50	0.44
1:F:420:ILE:HD13	1:F:448:GLU:HG2	1.97	0.44
1:F:88:GLY:N	6:F:602:AF3:F2	2.40	0.44
1:G:16:MET:O	1:G:20:VAL:HG23	2.17	0.44
1:G:362:ARG:HG2	1:G:366:GLN:NE2	2.33	0.44
1:J:101:THR:HG22	1:J:102:GLU:OE1	2.17	0.44
1:L:437:ASN:HA	1:L:440:ILE:HD12	2.00	0.44
1:N:288:MET:CG	1:N:288:MET:CE	2.90	0.44
1:N:487:ASN:O	1:N:491:MET:HG3	2.17	0.44
1:B:345:ARG:O	1:B:348:GLN:HB2	2.17	0.44
1:E:139:SER:N	7:E:611:HOH:O	2.37	0.44
1:E:324:VAL:HB	1:E:331:THR:HG23	2.00	0.44
1:H:217:SER:N	1:H:218:PRO:CD	2.80	0.44
1:J:16:MET:HG2	1:J:70:GLY:HA2	1.98	0.44
1:J:451:LEU:O	1:J:452:ARG:C	2.54	0.44
1:K:305:ILE:HD12	1:K:307:MET:HE2	1.99	0.44
1:K:346:VAL:O	1:K:350:ARG:HB2	2.18	0.44
1:N:100:ILE:O	1:N:104:LEU:HB2	2.18	0.44
1:A:88:GLY:N	6:A:602:AF3:F2	2.40	0.44
1:B:20:VAL:H	1:B:20:VAL:HG23	1.62	0.44
1:C:486:GLY:HA3	1:C:491:MET:HE2	1.99	0.44
1:F:146:GLN:HB2	1:F:146:GLN:HE21	1.64	0.44
2:S:68:ASN:HD22	2:T:74:LYS:HD2	1.82	0.44
2:T:60:LYS:HG2	2:T:60:LYS:H	1.66	0.44
1:A:147:VAL:CG2	1:A:403:THR:HG22	2.48	0.44
1:A:502:SER:O	1:A:503:ALA:C	2.54	0.44
1:B:172:GLU:HA	1:B:172:GLU:OE1	2.17	0.44
1:C:486:GLY:C	1:C:491:MET:HE2	2.38	0.44
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.99	0.44
1:G:423:ALA:O	7:G:607:HOH:O	2.21	0.44
1:H:413:ALA:CB	1:H:417:VAL:HB	2.46	0.44
1:I:21:ASN:HD22	1:I:21:ASN:HA	1.44	0.44
1:L:104:LEU:HA	1:L:104:LEU:HD12	1.64	0.44
1:L:487:ASN:O	1:L:491:MET:HG3	2.18	0.44
1:M:430:ARG:HA	1:M:430:ARG:HD3	1.69	0.44
1:L:40:LEU:HD12	1:M:521:VAL:HB	1.98	0.44
2:S:95:VAL:HG11	2:T:1:MET:HE1	1.99	0.44
1:A:103:GLY:O	1:A:106:ALA:N	2.50	0.44
1:A:218:PRO:HB3	1:A:246:PRO:HG2	2.00	0.44
1:B:157:THR:O	1:B:161:LEU:HB2	2.18	0.44
1:D:23:LEU:C	1:D:23:LEU:CD1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ARG:O	1:D:348:GLN:HB2	2.18	0.44
1:G:130:GLU:O	1:G:133:ALA:HB3	2.18	0.44
1:G:23:LEU:O	1:G:24:ALA:C	2.56	0.44
1:I:16:MET:HG2	1:I:70:GLY:HA2	2.00	0.44
1:I:222:LEU:HD23	1:I:250:ILE:HB	2.00	0.44
1:I:73:MET:HE1	1:I:514:MET:HG2	2.00	0.44
1:J:234:LEU:N	1:J:235:PRO:HD2	2.33	0.44
1:K:95:LEU:HD23	1:K:446:ALA:O	2.18	0.44
1:M:228:SER:O	1:M:257:GLU:HB3	2.18	0.44
1:M:234:LEU:N	1:M:235:PRO:HD2	2.32	0.44
2:O:11:ILE:HD12	2:O:42:ALA:HB3	1.98	0.44
2:R:68:ASN:ND2	2:S:74:LYS:HD2	2.32	0.44
1:B:124:VAL:HG22	1:B:504:LEU:HD11	2.00	0.43
1:B:512:GLY:O	1:B:515:ILE:HG13	2.17	0.43
1:C:324:VAL:HB	1:C:331:THR:HG23	2.00	0.43
1:D:223:ALA:O	1:D:251:ALA:HA	2.18	0.43
1:D:522:THR:OG1	1:D:523:ASP:N	2.52	0.43
1:H:270:ILE:HG22	1:H:271:VAL:HG23	1.99	0.43
1:I:43:SER:HB2	1:I:44:PHE:H	1.72	0.43
1:A:270:ILE:HD11	2:O:27:LEU:HD13	2.00	0.43
1:A:349:ILE:HA	1:A:352:GLN:HG2	1.97	0.43
1:A:524:LEU:HD23	1:A:525:PRO:HD2	2.00	0.43
1:A:76:GLU:O	1:A:80:LYS:HB2	2.18	0.43
1:C:513:LEU:HA	1:C:513:LEU:HD23	1.78	0.43
1:D:18:ARG:HB3	1:D:18:ARG:CZ	2.48	0.43
1:F:479:ASN:C	1:F:479:ASN:OD1	2.56	0.43
1:F:513:LEU:HA	1:F:513:LEU:HD23	1.79	0.43
1:G:358:SER:HB3	1:G:361:ASP:OD1	2.18	0.43
1:H:126:ALA:CB	1:H:426:LEU:HD22	2.47	0.43
1:I:219:PHE:HB3	1:I:317:LEU:HD23	2.00	0.43
1:I:66:PHE:O	1:I:67:GLU:C	2.56	0.43
1:K:100:ILE:HG22	1:K:104:LEU:HD22	1.99	0.43
1:K:437:ASN:HA	1:K:440:ILE:HD12	2.00	0.43
1:D:409:GLU:CD	1:D:501:ARG:HH21	2.22	0.43
1:E:11:ASP:OD1	1:E:11:ASP:N	2.51	0.43
1:E:223:ALA:O	1:E:251:ALA:HA	2.17	0.43
1:H:66:PHE:O	1:H:67:GLU:C	2.55	0.43
1:I:218:PRO:HB3	1:I:246:PRO:HG2	2.00	0.43
1:K:444:LEU:HD23	1:K:444:LEU:HA	1.71	0.43
1:N:15:LYS:HD2	1:N:15:LYS:HA	1.82	0.43
1:A:82:ASN:HB2	1:A:89:THR:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:ALA:HA	1:E:146:GLN:HE21	1.82	0.43
1:G:104:LEU:HD23	1:G:515:ILE:HG22	1.99	0.43
1:H:455:VAL:HG13	1:H:460:GLU:HB2	1.99	0.43
1:I:172:GLU:CA	1:I:172:GLU:OE1	2.64	0.43
1:I:88:GLY:O	1:I:91:THR:N	2.52	0.43
1:J:117:LYS:HG2	1:J:121:ASP:OD2	2.19	0.43
1:K:66:PHE:O	1:K:67:GLU:C	2.56	0.43
1:L:66:PHE:HA	1:L:69:MET:HE3	1.99	0.43
2:O:3:ILE:CD1	2:O:3:ILE:H	2.31	0.43
2:U:11:ILE:HD12	2:U:42:ALA:HB3	2.00	0.43
1:B:240:VAL:HG21	1:B:247:LEU:HD22	2.00	0.43
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.99	0.43
1:B:305:ILE:HG12	1:C:267:MET:HE2	1.99	0.43
1:F:103:GLY:HA3	1:F:515:ILE:HG21	1.99	0.43
1:G:475:ASN:HD22	1:G:475:ASN:HA	1.56	0.43
1:H:222:LEU:HD23	1:H:250:ILE:HB	1.99	0.43
1:H:487:ASN:O	1:H:491:MET:HG3	2.18	0.43
1:H:65:LYS:HA	7:H:528:HOH:O	2.19	0.43
1:I:35:GLY:O	1:I:51:LYS:HE3	2.18	0.43
1:I:65:LYS:HB3	7:I:529:HOH:O	2.17	0.43
1:J:15:LYS:NZ	1:J:64:ASP:OD2	2.52	0.43
1:L:65:LYS:HG3	1:L:65:LYS:H	1.27	0.43
2:T:7:HIS:CE1	2:T:48:ILE:HD11	2.54	0.43
2:U:15:LYS:HB3	2:U:16:GLU:H	1.65	0.43
1:A:247:LEU:HD12	1:A:248:LEU:N	2.33	0.43
1:A:305:ILE:HG23	1:B:267:MET:HG2	2.00	0.43
1:B:143:ALA:HA	1:B:146:GLN:HE21	1.84	0.43
1:D:11:ASP:OD1	1:D:11:ASP:N	2.51	0.43
1:E:213:VAL:HB	1:E:325:ILE:HG12	2.00	0.43
1:F:324:VAL:HB	1:F:331:THR:HG23	2.00	0.43
1:G:42:LYS:HG2	1:G:44:PHE:CD2	2.53	0.43
1:J:346:VAL:O	1:J:350:ARG:HB2	2.19	0.43
1:L:217:SER:N	1:L:218:PRO:CD	2.80	0.43
1:M:163:ALA:O	1:M:167:ASP:HB2	2.18	0.43
1:M:385:THR:O	1:M:388:GLU:HB3	2.18	0.43
1:M:65:LYS:H	1:M:65:LYS:HG3	1.25	0.43
1:N:218:PRO:HB3	1:N:246:PRO:HG2	2.00	0.43
2:O:3:ILE:HD12	2:O:3:ILE:H	1.83	0.43
1:C:130:GLU:O	1:C:133:ALA:HB3	2.18	0.43
1:C:434:GLU:O	1:C:437:ASN:HB2	2.18	0.43
1:D:362:ARG:HG2	1:D:366:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:GLY:O	1:H:106:ALA:HB3	2.18	0.43
1:H:461:GLU:HA	1:H:461:GLU:OE1	2.18	0.43
1:I:169:VAL:O	1:I:169:VAL:HG22	2.19	0.43
1:K:65:LYS:HG3	1:K:65:LYS:H	1.30	0.43
1:L:158:VAL:HG13	1:L:396:VAL:HG22	2.01	0.43
1:L:21:ASN:HD22	1:L:21:ASN:HA	1.55	0.43
1:L:234:LEU:N	1:L:235:PRO:HD2	2.34	0.43
1:M:104:LEU:HD12	1:M:104:LEU:HA	1.82	0.43
1:M:451:LEU:O	1:M:452:ARG:C	2.57	0.43
1:C:305:ILE:HD12	1:C:307:MET:HE2	2.01	0.43
1:D:103:GLY:HA3	1:D:515:ILE:HG21	2.00	0.43
1:F:448:GLU:HB3	1:F:452:ARG:HD2	2.00	0.43
1:G:147:VAL:HG23	1:G:403:THR:HG22	2.01	0.43
1:I:504:LEU:HD23	1:I:504:LEU:HA	1.79	0.43
1:K:272:LYS:NZ	1:L:228:SER:HB3	2.34	0.43
1:K:88:GLY:O	1:K:89:THR:C	2.57	0.43
1:M:16:MET:CE	1:M:16:MET:CB	2.96	0.43
1:M:217:SER:N	1:M:218:PRO:CD	2.82	0.43
1:A:150:ILE:HD11	1:A:492:GLY:O	2.19	0.43
1:B:524:LEU:HD23	1:B:524:LEU:HA	1.69	0.43
1:C:172:GLU:OE2	1:C:350:ARG:CZ	2.66	0.43
1:G:234:LEU:HB2	1:G:235:PRO:CD	2.49	0.43
1:G:486:GLY:CA	1:G:491:MET:CE	2.97	0.43
1:H:106:ALA:CA	1:H:111:MET:HE3	2.49	0.43
1:I:104:LEU:HA	1:I:104:LEU:HD12	1.76	0.43
1:I:105:LYS:HE3	1:I:105:LYS:HB2	1.85	0.43
1:I:31:LEU:O	1:I:32:GLY:O	2.37	0.43
1:M:180:GLY:HA3	1:M:381:VAL:O	2.18	0.43
1:N:524:LEU:HA	1:N:524:LEU:HD23	1.81	0.43
1:C:349:ILE:HA	1:C:352:GLN:HG2	1.94	0.43
1:D:147:VAL:HG12	1:D:494:LEU:HB2	2.01	0.43
1:E:150:ILE:HD13	1:E:492:GLY:O	2.19	0.43
1:I:117:LYS:HG2	1:I:121:ASP:OD2	2.19	0.43
1:I:201:SER:O	1:I:203:TYR:N	2.52	0.43
1:I:64:ASP:C	1:I:65:LYS:O	2.54	0.43
1:L:194:GLN:HB2	1:L:331:THR:HB	2.01	0.43
1:D:100:ILE:O	1:D:101:THR:C	2.56	0.42
1:D:218:PRO:HB3	1:D:246:PRO:HG2	2.01	0.42
1:I:71:ALA:O	1:I:72:GLN:C	2.56	0.42
1:J:444:LEU:HA	1:J:444:LEU:HD23	1.63	0.42
1:J:522:THR:OG1	1:J:523:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:419:LEU:HD22	1:K:500:THR:CG2	2.48	0.42
1:M:57:ALA:O	1:M:58:ARG:C	2.57	0.42
1:N:455:VAL:CG1	1:N:462:PRO:HA	2.49	0.42
1:E:100:ILE:HG13	1:E:511:ALA:HB1	2.00	0.42
1:F:240:VAL:HG21	1:F:247:LEU:HD22	2.01	0.42
1:F:345:ARG:O	1:F:348:GLN:HB2	2.18	0.42
1:I:385:THR:O	1:I:388:GLU:HB3	2.19	0.42
1:M:433:ASN:HD22	1:M:433:ASN:HA	1.54	0.42
1:B:358:SER:HB3	1:B:361:ASP:HB2	2.02	0.42
1:D:510:VAL:HG13	1:D:514:MET:CE	2.48	0.42
1:D:524:LEU:HA	1:D:524:LEU:HD23	1.93	0.42
1:E:266:THR:CG2	1:E:273:VAL:HB	2.49	0.42
1:G:78:ALA:HB2	1:G:93:THR:OG1	2.19	0.42
1:J:289:LEU:HD22	1:J:300:VAL:HG13	2.01	0.42
1:K:13:ARG:O	1:K:14:VAL:C	2.55	0.42
2:O:41:LEU:O	2:O:61:VAL:HG13	2.20	0.42
2:O:74:LYS:HD2	2:U:68:ASN:HD22	1.82	0.42
1:A:234:LEU:HB2	1:A:235:PRO:CD	2.49	0.42
1:B:13:ARG:HD2	1:B:104:LEU:HD22	2.01	0.42
1:B:362:ARG:HG2	1:B:366:GLN:NE2	2.34	0.42
1:C:511:ALA:O	1:C:515:ILE:HG12	2.19	0.42
1:E:172:GLU:OE1	1:E:172:GLU:HA	2.18	0.42
1:E:222:LEU:HB3	1:E:289:LEU:CD2	2.49	0.42
1:H:106:ALA:O	1:H:111:MET:HE3	2.19	0.42
1:J:455:VAL:CG1	1:J:462:PRO:HA	2.47	0.42
1:K:270:ILE:HG22	1:K:271:VAL:HG23	2.00	0.42
1:K:513:LEU:HD12	1:K:513:LEU:HA	1.80	0.42
1:N:434:GLU:HB2	7:N:529:HOH:O	2.18	0.42
2:T:11:ILE:HD12	2:T:42:ALA:HB3	2.00	0.42
1:A:11:ASP:O	1:A:12:ALA:C	2.57	0.42
1:A:146:GLN:HB2	1:A:146:GLN:HE21	1.61	0.42
1:C:33:PRO:HA	1:C:153:ASN:ND2	2.32	0.42
1:E:78:ALA:HB2	1:E:93:THR:OG1	2.20	0.42
1:F:68:ASN:HB3	7:F:612:HOH:O	2.19	0.42
1:I:169:VAL:HG13	1:I:173:GLY:HA3	2.02	0.42
1:I:421:ARG:CD	1:I:474:GLY:O	2.66	0.42
1:L:117:LYS:HG2	1:L:121:ASP:OD2	2.19	0.42
1:M:124:VAL:O	1:M:128:VAL:HG23	2.20	0.42
1:N:124:VAL:O	1:N:128:VAL:HG23	2.20	0.42
1:A:324:VAL:HB	1:A:331:THR:HG23	2.02	0.42
1:B:462:PRO:O	1:B:463:SER:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LEU:CD1	1:C:23:LEU:C	2.87	0.42
1:F:25:ASP:HA	1:F:28:LYS:HE2	2.00	0.42
1:I:106:ALA:O	1:I:109:ALA:CB	2.57	0.42
1:I:417:VAL:HG23	1:I:417:VAL:H	1.48	0.42
1:I:62:LEU:HA	1:I:62:LEU:HD23	1.78	0.42
1:L:224:ASP:O	1:L:225:LYS:HB3	2.20	0.42
1:L:433:ASN:HB3	1:L:436:GLN:H	1.83	0.42
1:L:444:LEU:HA	1:L:444:LEU:HD23	1.76	0.42
1:N:217:SER:N	1:N:218:PRO:CD	2.82	0.42
1:N:433:ASN:HD22	1:N:433:ASN:HA	1.57	0.42
2:T:15:LYS:HB3	2:T:16:GLU:H	1.68	0.42
2:T:20:LYS:HB3	2:T:27:LEU:HG	2.01	0.42
1:B:124:VAL:HG22	1:B:504:LEU:CD1	2.50	0.42
1:B:310:GLU:N	1:B:310:GLU:OE1	2.52	0.42
1:B:103:GLY:HA3	1:B:515:ILE:HG21	2.00	0.42
1:C:124:VAL:HG22	1:C:504:LEU:CD1	2.49	0.42
1:C:23:LEU:O	1:C:24:ALA:C	2.55	0.42
1:D:147:VAL:HG23	1:D:148:GLY:N	2.34	0.42
1:D:42:LYS:HG2	1:D:44:PHE:CE2	2.55	0.42
1:E:146:GLN:HE21	1:E:146:GLN:HB2	1.66	0.42
1:G:147:VAL:CG2	1:G:403:THR:HG22	2.49	0.42
1:G:455:VAL:HG21	1:G:465:VAL:HG11	2.02	0.42
1:H:104:LEU:HD12	1:H:104:LEU:HA	1.45	0.42
1:I:270:ILE:HG22	1:I:271:VAL:HG23	2.01	0.42
1:I:444:LEU:HD23	1:I:444:LEU:HA	1.73	0.42
1:I:44:PHE:N	1:I:44:PHE:CD1	2.88	0.42
1:J:116:LEU:HD23	1:J:116:LEU:HA	1.92	0.42
1:K:360:TYR:CZ	1:K:364:LYS:HE3	2.55	0.42
1:K:158:VAL:HG13	1:K:396:VAL:HG22	2.00	0.42
1:M:66:PHE:O	1:M:67:GLU:C	2.56	0.42
1:B:223:ALA:O	1:B:251:ALA:HA	2.19	0.42
1:E:157:THR:O	1:E:161:LEU:HB2	2.20	0.42
1:M:488:MET:HE3	1:M:493:ILE:HG21	2.00	0.42
1:E:201:SER:C	1:E:203:TYR:H	2.23	0.42
1:E:497:THR:N	7:E:604:HOH:O	2.52	0.42
1:G:400:LEU:HD13	1:G:400:LEU:O	2.19	0.42
1:I:289:LEU:HD22	1:I:300:VAL:HG13	2.01	0.42
1:J:104:LEU:HD12	1:J:104:LEU:HA	1.51	0.42
1:J:426:LEU:HD12	1:J:444:LEU:HD21	2.02	0.42
1:L:417:VAL:HG21	1:L:488:MET:HG3	2.02	0.42
1:M:346:VAL:O	1:M:350:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:11:ILE:HD12	2:Q:42:ALA:HB3	2.02	0.42
2:U:41:LEU:O	2:U:61:VAL:HG13	2.20	0.42
1:A:267:MET:HG2	1:G:305:ILE:CG2	2.49	0.42
1:A:39:VAL:HG11	1:G:69:MET:HE2	2.01	0.42
1:A:501:ARG:HD3	1:A:505:GLN:OE1	2.20	0.42
1:B:143:ALA:HA	1:B:146:GLN:NE2	2.34	0.42
1:C:157:THR:O	1:C:161:LEU:HB2	2.20	0.42
1:C:65:LYS:CB	7:C:606:HOH:O	2.68	0.42
1:F:13:ARG:NH2	7:F:608:HOH:O	2.37	0.42
1:G:513:LEU:HD23	1:G:513:LEU:HA	1.78	0.42
1:H:16:MET:HE2	1:H:16:MET:HB2	1.92	0.42
1:H:205:ILE:HA	1:H:213:VAL:HG22	2.01	0.42
1:H:44:PHE:CD1	1:H:44:PHE:N	2.88	0.42
1:I:444:LEU:CD2	1:I:447:MET:HE3	2.45	0.42
1:I:95:LEU:O	1:I:98:ALA:N	2.49	0.42
1:J:430:ARG:HA	1:J:430:ARG:HD3	1.72	0.42
1:J:73:MET:HE1	1:J:514:MET:HG2	2.02	0.42
1:K:40:LEU:HD12	1:L:521:VAL:HB	2.02	0.42
1:L:84:ALA:O	1:L:85:ALA:HB2	2.19	0.42
1:M:444:LEU:HD23	1:M:444:LEU:HA	1.86	0.42
1:M:77:VAL:HG12	1:M:78:ALA:N	2.35	0.42
2:P:7:HIS:O	2:P:8:ASP:CB	2.65	0.42
2:R:7:HIS:CE1	2:R:48:ILE:HD11	2.55	0.42
1:A:287:ALA:O	1:A:290:GLN:HB3	2.20	0.41
1:A:419:LEU:HD12	1:A:419:LEU:HA	1.82	0.41
1:B:429:LEU:HA	1:B:429:LEU:HD12	1.67	0.41
1:B:486:GLY:HA3	1:B:491:MET:HE1	2.01	0.41
1:D:486:GLY:CA	1:D:491:MET:CE	2.98	0.41
1:D:76:GLU:HG2	1:D:76:GLU:O	2.19	0.41
1:F:358:SER:HB3	1:F:361:ASP:OD1	2.19	0.41
1:H:430:ARG:HD3	1:H:430:ARG:HA	1.57	0.41
1:H:417:VAL:HG21	1:H:488:MET:HG3	2.00	0.41
1:L:315:GLU:HG2	1:L:315:GLU:O	2.19	0.41
1:N:163:ALA:O	1:N:167:ASP:HB2	2.20	0.41
1:N:21:ASN:HA	1:N:21:ASN:HD22	1.51	0.41
1:A:417:VAL:O	1:A:418:ALA:C	2.58	0.41
1:F:502:SER:O	1:F:503:ALA:C	2.56	0.41
1:G:213:VAL:HB	1:G:325:ILE:HG12	2.02	0.41
1:H:64:ASP:OD1	1:H:65:LYS:O	2.38	0.41
1:I:205:ILE:HA	1:I:213:VAL:HG22	2.01	0.41
1:J:326:ASN:HB2	1:J:329:THR:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:449:ALA:HB3	1:L:450:PRO:HD3	2.01	0.41
1:D:266:THR:CG2	1:D:273:VAL:HB	2.51	0.41
1:D:88:GLY:HA2	5:D:600:ADP:O2B	2.20	0.41
1:G:18:ARG:NH1	1:G:18:ARG:CG	2.65	0.41
1:G:88:GLY:HA2	5:G:600:ADP:O2B	2.21	0.41
1:G:63:GLU:O	1:G:63:GLU:HG2	2.19	0.41
1:I:16:MET:CB	1:I:16:MET:HE3	2.47	0.41
1:I:437:ASN:O	1:I:438:VAL:C	2.57	0.41
1:J:513:LEU:HD12	1:J:513:LEU:HA	1.73	0.41
1:K:43:SER:HB2	1:K:44:PHE:H	1.76	0.41
1:K:98:ALA:HB3	1:K:446:ALA:HB1	2.03	0.41
1:M:413:ALA:CB	1:M:417:VAL:HB	2.49	0.41
1:N:174:VAL:HG23	1:N:174:VAL:H	1.66	0.41
1:N:198:GLY:HA3	1:N:327:LYS:O	2.20	0.41
1:N:415:GLY:CA	1:N:417:VAL:HG23	2.51	0.41
2:S:41:LEU:O	2:S:61:VAL:HG13	2.20	0.41
2:T:3:ILE:CD1	2:T:3:ILE:H	2.31	0.41
1:A:206:ASN:HD21	1:A:214:GLU:N	2.10	0.41
1:A:522:THR:OG1	1:A:523:ASP:N	2.53	0.41
1:B:16:MET:HG3	1:B:520:MET:CE	2.48	0.41
1:B:201:SER:C	1:B:203:TYR:H	2.24	0.41
1:B:345:ARG:HE	1:B:349:ILE:HD11	1.85	0.41
1:C:136:VAL:HG23	1:C:136:VAL:O	2.20	0.41
1:D:358:SER:HB3	1:D:361:ASP:HB2	2.02	0.41
1:D:358:SER:HB3	1:D:361:ASP:OD1	2.21	0.41
1:D:487:ASN:O	1:D:491:MET:HG3	2.20	0.41
1:H:488:MET:HE3	1:H:493:ILE:HG21	2.02	0.41
1:H:513:LEU:HA	1:H:513:LEU:HD12	1.50	0.41
1:J:107:VAL:HG11	1:J:515:ILE:HG23	2.02	0.41
1:J:222:LEU:HD23	1:J:250:ILE:HB	2.03	0.41
1:J:43:SER:HB2	1:J:44:PHE:H	1.68	0.41
1:K:65:LYS:CA	7:K:528:HOH:O	2.64	0.41
1:L:413:ALA:CB	1:L:417:VAL:HB	2.49	0.41
1:L:15:LYS:NZ	1:L:64:ASP:OD2	2.53	0.41
1:N:198:GLY:O	1:N:276:VAL:HG12	2.21	0.41
1:A:237:LEU:HB3	2:O:26:VAL:HG21	2.02	0.41
2:P:60:LYS:H	2:P:60:LYS:HG2	1.74	0.41
2:R:20:LYS:HB3	2:R:27:LEU:HG	2.03	0.41
1:A:213:VAL:HB	1:A:325:ILE:HG12	2.03	0.41
1:A:20:VAL:HG13	1:A:74:VAL:HG11	2.01	0.41
1:B:16:MET:SD	1:B:514:MET:HG3	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:SER:C	1:D:203:TYR:H	2.24	0.41
1:E:358:SER:HB3	1:E:361:ASP:HB2	2.03	0.41
1:E:88:GLY:N	6:E:602:AF3:F2	2.44	0.41
1:I:450:PRO:O	1:I:454:ILE:HG12	2.21	0.41
1:I:88:GLY:O	1:I:92:ALA:N	2.53	0.41
1:J:336:VAL:HG12	1:J:336:VAL:O	2.21	0.41
1:J:80:LYS:O	1:J:81:ALA:C	2.58	0.41
1:K:201:SER:C	1:K:203:TYR:N	2.74	0.41
1:K:217:SER:N	1:K:218:PRO:CD	2.81	0.41
1:K:194:GLN:HB2	1:K:331:THR:HB	2.03	0.41
1:M:469:VAL:HG13	1:M:477:GLY:HA2	2.03	0.41
1:N:430:ARG:HA	1:N:430:ARG:HD3	1.61	0.41
1:A:451:LEU:HD13	1:A:451:LEU:C	2.41	0.41
1:A:512:GLY:O	1:A:515:ILE:HG13	2.21	0.41
1:B:234:LEU:HB2	1:B:235:PRO:CD	2.51	0.41
1:B:63:GLU:O	1:B:63:GLU:HG2	2.19	0.41
1:D:225:LYS:HD3	1:D:303:GLU:CD	2.41	0.41
1:G:225:LYS:HD3	1:G:303:GLU:CD	2.41	0.41
1:G:291:ASP:HB3	1:G:372:LEU:HD11	2.02	0.41
1:G:96:ALA:C	1:G:98:ALA:H	2.24	0.41
1:I:467:ASN:ND2	1:I:467:ASN:C	2.70	0.41
1:I:66:PHE:O	1:I:69:MET:N	2.52	0.41
1:J:64:ASP:OD1	1:J:65:LYS:O	2.38	0.41
1:M:126:ALA:CB	1:M:426:LEU:HD22	2.49	0.41
1:N:262:LEU:O	1:N:266:THR:HG23	2.21	0.41
1:N:97:GLN:O	1:N:97:GLN:HG2	2.21	0.41
2:S:20:LYS:HB3	2:S:27:LEU:HG	2.02	0.41
1:A:222:LEU:HB3	1:A:289:LEU:CD2	2.50	0.41
1:D:230:ILE:CD1	1:D:261:THR:HG21	2.43	0.41
1:D:479:ASN:OD1	1:D:479:ASN:C	2.58	0.41
1:F:266:THR:CG2	1:F:273:VAL:HB	2.50	0.41
1:G:324:VAL:HB	1:G:331:THR:HG23	2.03	0.41
1:G:524:LEU:CD2	1:G:525:PRO:HD2	2.50	0.41
1:H:116:LEU:HD23	1:H:116:LEU:HA	1.99	0.41
1:H:351:GLN:HB3	1:H:351:GLN:HE21	1.65	0.41
1:H:84:ALA:O	1:H:85:ALA:HB2	2.21	0.41
1:J:272:LYS:HZ1	1:K:228:SER:HB3	1.84	0.41
1:L:180:GLY:HA3	1:L:381:VAL:O	2.21	0.41
1:M:174:VAL:HB	1:M:376:VAL:HG22	2.01	0.41
1:N:432:GLN:H	1:N:436:GLN:NE2	2.19	0.41
2:Q:60:LYS:H	2:Q:60:LYS:HG2	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ALA:O	1:B:290:GLN:HB3	2.20	0.41
1:B:511:ALA:O	1:B:515:ILE:HG12	2.21	0.41
1:C:219:PHE:C	1:C:220:ILE:HG13	2.41	0.41
1:E:400:LEU:O	1:E:400:LEU:HD13	2.20	0.41
1:H:43:SER:HB2	1:H:44:PHE:CD1	2.55	0.41
1:I:351:GLN:HE21	1:I:351:GLN:HB3	1.68	0.41
1:K:420:ILE:HG23	1:K:420:ILE:HD13	1.89	0.41
1:L:455:VAL:CG1	1:L:462:PRO:HA	2.42	0.41
1:M:272:LYS:HZ3	1:N:228:SER:HB3	1.83	0.41
1:A:234:LEU:N	1:A:235:PRO:HD2	2.36	0.41
1:A:455:VAL:HG21	1:A:465:VAL:HG11	2.03	0.41
1:C:16:MET:CG	1:C:520:MET:HE3	2.51	0.41
1:B:510:VAL:HG23	1:C:385:THR:HG21	2.02	0.41
1:F:100:ILE:HG13	1:F:511:ALA:HB1	2.03	0.41
1:F:201:SER:C	1:F:203:TYR:H	2.24	0.41
1:G:131:LEU:HD23	1:G:131:LEU:HA	1.93	0.41
1:H:64:ASP:C	1:H:65:LYS:O	2.59	0.41
1:I:278:ALA:HB1	1:I:279:PRO:HD2	2.02	0.41
1:I:420:ILE:HD13	1:I:420:ILE:HG23	1.65	0.41
1:L:116:LEU:HD23	1:L:116:LEU:HA	1.85	0.41
1:L:44:PHE:N	1:L:44:PHE:CD1	2.88	0.41
1:N:270:ILE:HG22	1:N:271:VAL:HG23	2.02	0.41
2:T:41:LEU:O	2:T:61:VAL:HG13	2.21	0.41
1:A:201:SER:C	1:A:203:TYR:H	2.24	0.41
1:B:76:GLU:O	1:B:80:LYS:HB2	2.21	0.41
1:C:234:LEU:HB2	1:C:235:PRO:CD	2.51	0.41
1:C:524:LEU:HA	1:C:524:LEU:HD23	1.84	0.41
1:G:365:LEU:HD23	1:G:368:ARG:HH21	1.86	0.41
1:H:97:GLN:HE21	1:H:97:GLN:HB3	1.70	0.41
1:K:169:VAL:HG13	1:K:173:GLY:HA3	2.02	0.41
1:L:128:VAL:HB	7:L:531:HOH:O	2.19	0.41
1:L:326:ASN:HD22	1:L:329:THR:CG2	2.34	0.41
2:Q:20:LYS:HB3	2:Q:27:LEU:HG	2.03	0.41
2:Q:68:ASN:HD22	2:R:74:LYS:HD2	1.86	0.41
1:A:66:PHE:O	1:A:69:MET:HB2	2.21	0.41
1:B:114:MET:CG	1:B:114:MET:CE	2.95	0.41
1:B:40:LEU:HD22	1:B:59:GLU:HG3	2.02	0.41
1:C:240:VAL:HG21	1:C:247:LEU:HD22	2.02	0.41
1:D:462:PRO:CD	7:D:608:HOH:O	2.51	0.41
1:D:33:PRO:HD3	5:D:600:ADP:C8	2.56	0.41
1:E:455:VAL:HG11	1:E:462:PRO:HA	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:PHE:HA	1:I:69:MET:HE3	2.03	0.41
1:K:219:PHE:HB3	1:K:317:LEU:HD23	2.03	0.41
1:L:201:SER:C	1:L:203:TYR:N	2.74	0.41
1:L:31:LEU:O	1:L:32:GLY:O	2.38	0.41
1:L:96:ALA:O	1:L:100:ILE:HG13	2.21	0.41
1:N:106:ALA:HB3	1:N:116:LEU:HD13	2.03	0.41
1:N:152:ALA:O	1:N:153:ASN:HB3	2.20	0.41
1:A:123:ALA:HB2	1:A:440:ILE:HG23	2.03	0.40
1:E:429:LEU:HD12	1:E:429:LEU:HA	1.84	0.40
5:F:600:ADP:O3B	6:F:602:AF3:F2	2.29	0.40
1:G:31:LEU:HD23	1:G:453:GLN:HB3	2.03	0.40
1:G:522:THR:OG1	1:G:523:ASP:N	2.55	0.40
1:I:64:ASP:O	1:I:65:LYS:O	2.39	0.40
1:J:360:TYR:CZ	1:J:364:LYS:HE3	2.56	0.40
1:K:84:ALA:O	1:K:85:ALA:HB2	2.21	0.40
1:L:20:VAL:O	1:L:21:ASN:C	2.59	0.40
1:L:419:LEU:HD22	1:L:500:THR:CG2	2.51	0.40
2:P:20:LYS:HB3	2:P:27:LEU:HG	2.03	0.40
1:G:270:ILE:HD11	2:U:27:LEU:HB3	2.03	0.40
1:C:225:LYS:HD3	1:C:303:GLU:CD	2.42	0.40
1:C:213:VAL:HB	1:C:325:ILE:HG12	2.02	0.40
1:F:63:GLU:CG	1:F:63:GLU:O	2.70	0.40
1:G:6:VAL:O	1:G:6:VAL:HG23	2.18	0.40
1:I:15:LYS:HA	1:I:15:LYS:HD2	1.83	0.40
1:J:504:LEU:HD23	1:J:504:LEU:HA	1.84	0.40
1:J:65:LYS:H	1:J:65:LYS:HG3	1.31	0.40
1:M:266:THR:HG21	1:M:273:VAL:O	2.22	0.40
1:N:30:THR:HB	1:N:51:LYS:O	2.22	0.40
1:N:421:ARG:HH11	1:N:421:ARG:HD2	1.69	0.40
1:A:151:SER:OG	1:A:399:ALA:HA	2.20	0.40
1:D:240:VAL:HG21	1:D:247:LEU:HD22	2.03	0.40
1:F:114:MET:CE	1:F:114:MET:CG	2.98	0.40
1:F:21:ASN:HA	1:F:21:ASN:HD22	1.73	0.40
1:F:291:ASP:HB3	1:F:372:LEU:HD11	2.03	0.40
1:G:146:GLN:HB2	1:G:146:GLN:HE21	1.56	0.40
1:G:127:ALA:HB1	1:G:422:VAL:HG21	2.02	0.40
1:G:479:ASN:C	1:G:479:ASN:OD1	2.59	0.40
1:H:452:ARG:NH1	1:H:452:ARG:HG2	2.37	0.40
1:J:19:GLY:HA3	1:J:67:GLU:O	2.20	0.40
1:K:272:LYS:HZ1	1:L:228:SER:HB3	1.87	0.40
1:K:433:ASN:HD22	1:K:433:ASN:HA	1.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:346:VAL:O	1:L:350:ARG:HB2	2.20	0.40
1:N:106:ALA:O	1:N:109:ALA:CB	2.62	0.40
1:A:493:ILE:O	1:A:493:ILE:HG22	2.21	0.40
1:E:289:LEU:O	1:E:292:ILE:HB	2.21	0.40
1:E:448:GLU:HB3	1:E:452:ARG:HD2	2.03	0.40
1:G:123:ALA:HB2	1:G:440:ILE:HG23	2.03	0.40
1:G:54:VAL:HG22	1:G:54:VAL:O	2.20	0.40
1:H:119:GLY:O	1:H:120:ILE:C	2.59	0.40
1:H:419:LEU:HA	1:H:419:LEU:HD13	1.53	0.40
1:I:266:THR:HG21	1:I:273:VAL:O	2.20	0.40
1:J:205:ILE:HA	1:J:213:VAL:HG22	2.02	0.40
1:J:272:LYS:NZ	1:K:228:SER:HB3	2.36	0.40
1:M:417:VAL:O	1:M:418:ALA:C	2.60	0.40
1:M:32:GLY:H	1:M:457:ASN:HD22	1.69	0.40
1:M:49:ILE:HD12	1:N:513:LEU:HD23	2.04	0.40
1:A:290:GLN:O	1:A:293:ALA:HB3	2.22	0.40
1:B:233:MET:O	1:B:234:LEU:C	2.59	0.40
1:B:358:SER:HB3	1:B:361:ASP:OD1	2.22	0.40
1:D:261:THR:O	1:D:262:LEU:C	2.58	0.40
1:D:475:ASN:HD22	1:D:475:ASN:HA	1.55	0.40
1:E:432:GLN:O	1:E:433:ASN:HB3	2.21	0.40
1:G:100:ILE:HG13	1:G:511:ALA:CB	2.52	0.40
1:G:201:SER:C	1:G:203:TYR:H	2.25	0.40
1:G:74:VAL:C	1:G:76:GLU:N	2.73	0.40
1:I:315:GLU:O	1:I:315:GLU:HG2	2.20	0.40
1:J:360:TYR:CE1	1:J:364:LYS:HE3	2.57	0.40
1:K:413:ALA:CB	1:K:417:VAL:HB	2.51	0.40
1:L:24:ALA:HA	1:L:27:VAL:HG12	2.02	0.40
1:M:44:PHE:N	1:M:44:PHE:CD1	2.89	0.40
1:M:49:ILE:HD13	1:N:73:MET:HE3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	472 (90%)	44 (8%)	6 (1%)	14	41
1	B	522/524 (100%)	476 (91%)	39 (8%)	7 (1%)	12	36
1	C	522/524 (100%)	473 (91%)	37 (7%)	12 (2%)	6	21
1	D	522/524 (100%)	475 (91%)	41 (8%)	6 (1%)	14	41
1	E	522/524 (100%)	474 (91%)	42 (8%)	6 (1%)	14	41
1	F	522/524 (100%)	478 (92%)	38 (7%)	6 (1%)	14	41
1	G	522/524 (100%)	479 (92%)	37 (7%)	6 (1%)	14	41
1	H	522/524 (100%)	477 (91%)	36 (7%)	9 (2%)	9	29
1	I	522/524 (100%)	471 (90%)	43 (8%)	8 (2%)	10	33
1	J	522/524 (100%)	473 (91%)	40 (8%)	9 (2%)	9	29
1	K	522/524 (100%)	473 (91%)	41 (8%)	8 (2%)	10	33
1	L	522/524 (100%)	479 (92%)	34 (6%)	9 (2%)	9	29
1	M	522/524 (100%)	477 (91%)	35 (7%)	10 (2%)	8	26
1	N	522/524 (100%)	471 (90%)	44 (8%)	7 (1%)	12	36
2	O	95/97 (98%)	68 (72%)	17 (18%)	10 (10%)	0	1
2	P	95/97 (98%)	68 (72%)	16 (17%)	11 (12%)	0	1
2	Q	95/97 (98%)	68 (72%)	17 (18%)	10 (10%)	0	1
2	R	95/97 (98%)	68 (72%)	17 (18%)	10 (10%)	0	1
2	S	95/97 (98%)	70 (74%)	15 (16%)	10 (10%)	0	1
2	T	95/97 (98%)	69 (73%)	15 (16%)	11 (12%)	0	1
2	U	95/97 (98%)	68 (72%)	15 (16%)	12 (13%)	0	1
All	All	7973/8015 (100%)	7127 (89%)	663 (8%)	183 (2%)	6	21

All (183) 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

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Mol	Chain	Res	Type
1	H	85	ALA
1	I	85	ALA
1	J	85	ALA
1	K	85	ALA
1	L	43	SER
1	L	85	ALA
1	M	32	GLY
1	M	85	ALA
1	M	463	SER
1	N	85	ALA
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	225	LYS
1	C	58	ARG
1	C	256	GLY
1	D	256	GLY
1	D	373	ALA
1	F	225	LYS
1	G	256	GLY
1	G	373	ALA
1	H	32	GLY
1	H	256	GLY
1	I	32	GLY
1	I	43	SER
1	I	66	PHE
1	I	256	GLY
1	J	32	GLY
1	J	43	SER
1	J	65	LYS
1	J	256	GLY
1	J	457	ASN
1	K	32	GLY
1	K	66	PHE
1	K	256	GLY
1	L	32	GLY
1	L	256	GLY
1	M	256	GLY

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Mol	Chain	Res	Type
1	M	457	ASN
1	M	462	PRO
1	N	32	GLY
1	N	43	SER
1	N	66	PHE
1	N	256	GLY
2	O	20	LYS
2	O	21	SER
2	O	52	GLY
2	P	20	LYS
2	P	21	SER
2	P	52	GLY
2	Q	20	LYS
2	Q	21	SER
2	Q	52	GLY
2	Q	61	VAL
2	R	20	LYS
2	R	21	SER
2	R	52	GLY
2	S	20	LYS
2	S	21	SER
2	S	52	GLY
2	T	20	LYS
2	T	21	SER
2	T	52	GLY
2	U	20	LYS
2	U	21	SER
2	U	49	LEU
2	U	52	GLY
2	U	61	VAL
1	A	373	ALA
1	B	225	LYS
1	B	373	ALA
1	C	28	LYS
1	C	225	LYS
1	C	373	ALA
1	D	225	LYS
1	E	225	LYS
1	E	256	GLY
1	E	373	ALA
1	F	373	ALA
1	G	225	LYS

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Mol	Chain	Res	Type
1	H	66	PHE
1	I	463	SER
1	J	66	PHE
1	L	65	LYS
1	L	66	PHE
1	M	43	SER
1	M	66	PHE
2	O	49	LEU
2	O	53	GLU
2	P	17	VAL
2	P	49	LEU
2	P	53	GLU
2	Q	49	LEU
2	Q	53	GLU
2	Q	80	ASN
2	R	49	LEU
2	R	53	GLU
2	R	61	VAL
2	S	49	LEU
2	S	53	GLU
2	S	61	VAL
2	T	49	LEU
2	T	53	GLU
2	T	61	VAL
2	U	53	GLU
1	A	256	GLY
1	B	202	PRO
1	B	256	GLY
1	C	85	ALA
1	D	58	ARG
1	D	202	PRO
1	F	256	GLY
1	H	43	SER
1	H	202	PRO
1	H	462	PRO
1	J	202	PRO
1	K	43	SER
1	K	202	PRO
1	L	202	PRO
1	M	202	PRO
1	N	202	PRO
2	O	17	VAL

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Mol	Chain	Res	Type
2	O	61	VAL
2	P	61	VAL
2	P	80	ASN
2	R	80	ASN
2	S	80	ASN
2	T	80	ASN
1	A	202	PRO
1	B	462	PRO
1	C	23	LEU
1	E	202	PRO
1	F	202	PRO
1	G	202	PRO
1	H	65	LYS
1	I	202	PRO
1	I	462	PRO
1	J	462	PRO
1	K	462	PRO
1	L	462	PRO
1	L	463	SER
1	M	65	LYS
2	O	51	ASN
2	P	51	ASN
2	Q	17	VAL
2	Q	51	ASN
2	R	17	VAL
2	R	51	ASN
2	S	51	ASN
2	T	17	VAL
2	T	45	ASN
2	T	51	ASN
2	U	51	ASN
2	U	69	ASP
2	U	80	ASN
1	C	202	PRO
1	C	374	GLY
1	E	462	PRO
1	N	413	ALA
2	O	80	ASN
2	P	69	ASP
2	U	17	VAL
2	U	45	ASN
1	B	374	GLY

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Mol	Chain	Res	Type
1	G	374	GLY
2	S	17	VAL
1	A	205	ILE
1	C	462	PRO
1	F	462	PRO
1	C	103	GLY
1	H	120	ILE
1	K	120	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/404 (100%)	358 (89%)	46 (11%)	5	18
1	B	404/404 (100%)	356 (88%)	48 (12%)	5	16
1	C	404/404 (100%)	363 (90%)	41 (10%)	7	22
1	D	404/404 (100%)	360 (89%)	44 (11%)	6	19
1	E	404/404 (100%)	361 (89%)	43 (11%)	6	20
1	F	404/404 (100%)	360 (89%)	44 (11%)	6	19
1	G	404/404 (100%)	360 (89%)	44 (11%)	6	19
1	H	404/404 (100%)	336 (83%)	68 (17%)	2	6
1	I	404/404 (100%)	334 (83%)	70 (17%)	2	6
1	J	404/404 (100%)	337 (83%)	67 (17%)	2	7
1	K	404/404 (100%)	337 (83%)	67 (17%)	2	7
1	L	404/404 (100%)	337 (83%)	67 (17%)	2	7
1	M	404/404 (100%)	332 (82%)	72 (18%)	2	5
1	N	404/404 (100%)	337 (83%)	67 (17%)	2	7
2	O	80/80 (100%)	68 (85%)	12 (15%)	3	9
2	P	80/80 (100%)	68 (85%)	12 (15%)	3	9
2	Q	80/80 (100%)	68 (85%)	12 (15%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	80/80 (100%)	67 (84%)	13 (16%)	2	7
2	S	80/80 (100%)	69 (86%)	11 (14%)	3	11
2	T	80/80 (100%)	68 (85%)	12 (15%)	3	9
2	U	80/80 (100%)	67 (84%)	13 (16%)	2	7
All	All	6216/6216 (100%)	5343 (86%)	873 (14%)	3	11

All (873) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	18	ARG
1	A	23	LEU
1	A	28	LYS
1	A	44	PHE
1	A	48	THR
1	A	62	LEU
1	A	64	ASP
1	A	74	VAL
1	A	80	LYS
1	A	97	GLN
1	A	111	MET
1	A	114	MET
1	A	129	GLU
1	A	132	LYS
1	A	138	CYS
1	A	153	ASN
1	A	176	THR
1	A	178	GLU
1	A	183	LEU
1	A	184	GLN
1	A	193	MET
1	A	230	ILE
1	A	231	ARG
1	A	284	ARG
1	A	289	LEU
1	A	322	ARG
1	A	328	ASP
1	A	331	THR
1	A	386	GLU
1	A	391	GLU
1	A	395	ARG

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Mol	Chain	Res	Type
1	A	398	ASP
1	A	401	HIS
1	A	417	VAL
1	A	419	LEU
1	A	422	VAL
1	A	425	LYS
1	A	430	ARG
1	A	432	GLN
1	A	445	ARG
1	A	461	GLU
1	A	497	THR
1	A	499	VAL
1	A	504	LEU
1	A	517	THR
1	B	6	VAL
1	B	18	ARG
1	B	23	LEU
1	B	28	LYS
1	B	43	SER
1	B	44	PHE
1	B	48	THR
1	B	62	LEU
1	B	74	VAL
1	B	80	LYS
1	B	89	THR
1	B	97	GLN
1	B	111	MET
1	B	114	MET
1	B	129	GLU
1	B	132	LYS
1	B	135	SER
1	B	138	CYS
1	B	153	ASN
1	B	161	LEU
1	B	176	THR
1	B	177	VAL
1	B	178	GLU
1	B	183	LEU
1	B	184	GLN
1	B	185	ASP
1	B	193	MET
1	B	209	GLU

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Mol	Chain	Res	Type
1	B	230	ILE
1	B	231	ARG
1	B	284	ARG
1	B	289	LEU
1	B	322	ARG
1	B	328	ASP
1	B	331	THR
1	B	386	GLU
1	B	391	GLU
1	B	398	ASP
1	B	417	VAL
1	B	419	LEU
1	B	422	VAL
1	B	425	LYS
1	B	430	ARG
1	B	432	GLN
1	B	463	SER
1	B	497	THR
1	B	504	LEU
1	B	515	ILE
1	C	6	VAL
1	C	7	LYS
1	C	18	ARG
1	C	23	LEU
1	C	28	LYS
1	C	43	SER
1	C	44	PHE
1	C	48	THR
1	C	62	LEU
1	C	74	VAL
1	C	80	LYS
1	C	97	GLN
1	C	111	MET
1	C	114	MET
1	C	129	GLU
1	C	132	LYS
1	C	138	CYS
1	C	153	ASN
1	C	177	VAL
1	C	178	GLU
1	C	183	LEU
1	C	184	GLN

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Mol	Chain	Res	Type
1	C	185	ASP
1	C	193	MET
1	C	230	ILE
1	C	231	ARG
1	C	284	ARG
1	C	289	LEU
1	C	322	ARG
1	C	328	ASP
1	C	331	THR
1	C	386	GLU
1	C	391	GLU
1	C	398	ASP
1	C	417	VAL
1	C	419	LEU
1	C	422	VAL
1	C	425	LYS
1	C	430	ARG
1	C	497	THR
1	C	504	LEU
1	D	6	VAL
1	D	18	ARG
1	D	23	LEU
1	D	28	LYS
1	D	43	SER
1	D	44	PHE
1	D	48	THR
1	D	62	LEU
1	D	74	VAL
1	D	80	LYS
1	D	97	GLN
1	D	102	GLU
1	D	111	MET
1	D	114	MET
1	D	129	GLU
1	D	132	LYS
1	D	135	SER
1	D	138	CYS
1	D	153	ASN
1	D	176	THR
1	D	177	VAL
1	D	178	GLU
1	D	183	LEU

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Mol	Chain	Res	Type
1	D	184	GLN
1	D	185	ASP
1	D	193	MET
1	D	230	ILE
1	D	231	ARG
1	D	284	ARG
1	D	289	LEU
1	D	322	ARG
1	D	328	ASP
1	D	331	THR
1	D	386	GLU
1	D	391	GLU
1	D	398	ASP
1	D	417	VAL
1	D	419	LEU
1	D	425	LYS
1	D	430	ARG
1	D	445	ARG
1	D	463	SER
1	D	504	LEU
1	D	515	ILE
1	E	6	VAL
1	E	18	ARG
1	E	23	LEU
1	E	43	SER
1	E	44	PHE
1	E	48	THR
1	E	62	LEU
1	E	74	VAL
1	E	80	LYS
1	E	97	GLN
1	E	111	MET
1	E	114	MET
1	E	129	GLU
1	E	132	LYS
1	E	135	SER
1	E	138	CYS
1	E	153	ASN
1	E	176	THR
1	E	177	VAL
1	E	178	GLU
1	E	183	LEU

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Mol	Chain	Res	Type
1	E	184	GLN
1	E	185	ASP
1	E	193	MET
1	E	196	ASP
1	E	230	ILE
1	E	231	ARG
1	E	284	ARG
1	E	289	LEU
1	E	322	ARG
1	E	328	ASP
1	E	331	THR
1	E	386	GLU
1	E	391	GLU
1	E	398	ASP
1	E	417	VAL
1	E	419	LEU
1	E	422	VAL
1	E	425	LYS
1	E	430	ARG
1	E	432	GLN
1	E	504	LEU
1	E	515	ILE
1	F	6	VAL
1	F	7	LYS
1	F	18	ARG
1	F	23	LEU
1	F	28	LYS
1	F	43	SER
1	F	44	PHE
1	F	48	THR
1	F	62	LEU
1	F	74	VAL
1	F	80	LYS
1	F	97	GLN
1	F	111	MET
1	F	114	MET
1	F	129	GLU
1	F	132	LYS
1	F	135	SER
1	F	138	CYS
1	F	153	ASN
1	F	161	LEU

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Mol	Chain	Res	Type
1	F	176	THR
1	F	177	VAL
1	F	178	GLU
1	F	183	LEU
1	F	184	GLN
1	F	185	ASP
1	F	193	MET
1	F	230	ILE
1	F	231	ARG
1	F	284	ARG
1	F	289	LEU
1	F	322	ARG
1	F	328	ASP
1	F	331	THR
1	F	386	GLU
1	F	391	GLU
1	F	398	ASP
1	F	417	VAL
1	F	419	LEU
1	F	422	VAL
1	F	425	LYS
1	F	430	ARG
1	F	432	GLN
1	F	504	LEU
1	G	6	VAL
1	G	7	LYS
1	G	18	ARG
1	G	23	LEU
1	G	43	SER
1	G	44	PHE
1	G	48	THR
1	G	62	LEU
1	G	64	ASP
1	G	74	VAL
1	G	80	LYS
1	G	97	GLN
1	G	111	MET
1	G	114	MET
1	G	129	GLU
1	G	132	LYS
1	G	138	CYS
1	G	153	ASN

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Mol	Chain	Res	Type
1	G	161	LEU
1	G	177	VAL
1	G	178	GLU
1	G	183	LEU
1	G	184	GLN
1	G	185	ASP
1	G	193	MET
1	G	230	ILE
1	G	231	ARG
1	G	284	ARG
1	G	289	LEU
1	G	322	ARG
1	G	328	ASP
1	G	331	THR
1	G	386	GLU
1	G	391	GLU
1	G	398	ASP
1	G	417	VAL
1	G	419	LEU
1	G	422	VAL
1	G	425	LYS
1	G	430	ARG
1	G	463	SER
1	G	504	LEU
1	G	514	MET
1	G	515	ILE
1	H	7	LYS
1	H	11	ASP
1	H	16	MET
1	H	20	VAL
1	H	23	LEU
1	H	40	LEU
1	H	42	LYS
1	H	43	SER
1	H	44	PHE
1	H	55	SER
1	H	59	GLU
1	H	65	LYS
1	H	79	SER
1	H	87	ASP
1	H	101	THR
1	H	104	LEU

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Mol	Chain	Res	Type
1	H	114	MET
1	H	129	GLU
1	H	131	LEU
1	H	138	CYS
1	H	141	SER
1	H	147	VAL
1	H	150	ILE
1	H	151	SER
1	H	161	LEU
1	H	172	GLU
1	H	189	VAL
1	H	201	SER
1	H	217	SER
1	H	230	ILE
1	H	265	ASN
1	H	272	LYS
1	H	284	ARG
1	H	289	LEU
1	H	302	SER
1	H	307	MET
1	H	322	ARG
1	H	328	ASP
1	H	329	THR
1	H	331	THR
1	H	343	GLN
1	H	350	ARG
1	H	352	GLN
1	H	355	GLU
1	H	359	ASP
1	H	363	GLU
1	H	378	VAL
1	H	385	THR
1	H	389	MET
1	H	390	LYS
1	H	401	HIS
1	H	404	ARG
1	H	419	LEU
1	H	420	ILE
1	H	421	ARG
1	H	426	LEU
1	H	430	ARG
1	H	433	ASN

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Mol	Chain	Res	Type
1	H	434	GLU
1	H	441	LYS
1	H	452	ARG
1	H	454	ILE
1	H	467	ASN
1	H	468	THR
1	H	483	GLU
1	H	504	LEU
1	H	509	SER
1	H	513	LEU
1	I	7	LYS
1	I	11	ASP
1	I	16	MET
1	I	23	LEU
1	I	40	LEU
1	I	42	LYS
1	I	43	SER
1	I	44	PHE
1	I	52	ASP
1	I	55	SER
1	I	59	GLU
1	I	65	LYS
1	I	77	VAL
1	I	79	SER
1	I	87	ASP
1	I	101	THR
1	I	104	LEU
1	I	131	LEU
1	I	138	CYS
1	I	141	SER
1	I	147	VAL
1	I	150	ILE
1	I	151	SER
1	I	157	THR
1	I	161	LEU
1	I	167	ASP
1	I	172	GLU
1	I	189	VAL
1	I	201	SER
1	I	217	SER
1	I	230	ILE
1	I	265	ASN

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Mol	Chain	Res	Type
1	I	272	LYS
1	I	284	ARG
1	I	289	LEU
1	I	295	LEU
1	I	302	SER
1	I	307	MET
1	I	322	ARG
1	I	325	ILE
1	I	328	ASP
1	I	329	THR
1	I	331	THR
1	I	343	GLN
1	I	350	ARG
1	I	352	GLN
1	I	359	ASP
1	I	363	GLU
1	I	378	VAL
1	I	385	THR
1	I	389	MET
1	I	390	LYS
1	I	404	ARG
1	I	419	LEU
1	I	420	ILE
1	I	421	ARG
1	I	426	LEU
1	I	430	ARG
1	I	432	GLN
1	I	433	ASN
1	I	434	GLU
1	I	441	LYS
1	I	452	ARG
1	I	454	ILE
1	I	467	ASN
1	I	468	THR
1	I	483	GLU
1	I	504	LEU
1	I	509	SER
1	I	513	LEU
1	J	7	LYS
1	J	16	MET
1	J	23	LEU
1	J	40	LEU

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Mol	Chain	Res	Type
1	J	42	LYS
1	J	43	SER
1	J	44	PHE
1	J	52	ASP
1	J	55	SER
1	J	59	GLU
1	J	65	LYS
1	J	77	VAL
1	J	79	SER
1	J	87	ASP
1	J	101	THR
1	J	104	LEU
1	J	114	MET
1	J	131	LEU
1	J	138	CYS
1	J	141	SER
1	J	151	SER
1	J	157	THR
1	J	161	LEU
1	J	172	GLU
1	J	189	VAL
1	J	201	SER
1	J	210	THR
1	J	217	SER
1	J	230	ILE
1	J	265	ASN
1	J	272	LYS
1	J	284	ARG
1	J	289	LEU
1	J	295	LEU
1	J	302	SER
1	J	307	MET
1	J	322	ARG
1	J	325	ILE
1	J	328	ASP
1	J	329	THR
1	J	331	THR
1	J	343	GLN
1	J	350	ARG
1	J	352	GLN
1	J	355	GLU
1	J	363	GLU

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Mol	Chain	Res	Type
1	J	378	VAL
1	J	385	THR
1	J	389	MET
1	J	404	ARG
1	J	419	LEU
1	J	420	ILE
1	J	421	ARG
1	J	426	LEU
1	J	430	ARG
1	J	432	GLN
1	J	433	ASN
1	J	434	GLU
1	J	441	LYS
1	J	452	ARG
1	J	454	ILE
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	7	LYS
1	K	11	ASP
1	K	15	LYS
1	K	16	MET
1	K	23	LEU
1	K	40	LEU
1	K	42	LYS
1	K	43	SER
1	K	44	PHE
1	K	52	ASP
1	K	55	SER
1	K	59	GLU
1	K	65	LYS
1	K	77	VAL
1	K	87	ASP
1	K	101	THR
1	K	104	LEU
1	K	114	MET
1	K	129	GLU
1	K	131	LEU
1	K	138	CYS

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Mol	Chain	Res	Type
1	K	141	SER
1	K	147	VAL
1	K	150	ILE
1	K	151	SER
1	K	161	LEU
1	K	172	GLU
1	K	189	VAL
1	K	201	SER
1	K	217	SER
1	K	230	ILE
1	K	265	ASN
1	K	272	LYS
1	K	284	ARG
1	K	289	LEU
1	K	295	LEU
1	K	302	SER
1	K	322	ARG
1	K	328	ASP
1	K	329	THR
1	K	331	THR
1	K	343	GLN
1	K	350	ARG
1	K	352	GLN
1	K	355	GLU
1	K	363	GLU
1	K	378	VAL
1	K	385	THR
1	K	389	MET
1	K	390	LYS
1	K	404	ARG
1	K	419	LEU
1	K	420	ILE
1	K	421	ARG
1	K	426	LEU
1	K	432	GLN
1	K	433	ASN
1	K	434	GLU
1	K	441	LYS
1	K	452	ARG
1	K	454	ILE
1	K	467	ASN
1	K	468	THR

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Mol	Chain	Res	Type
1	K	483	GLU
1	K	504	LEU
1	K	509	SER
1	K	513	LEU
1	L	7	LYS
1	L	11	ASP
1	L	16	MET
1	L	20	VAL
1	L	23	LEU
1	L	40	LEU
1	L	42	LYS
1	L	43	SER
1	L	44	PHE
1	L	52	ASP
1	L	55	SER
1	L	59	GLU
1	L	65	LYS
1	L	87	ASP
1	L	101	THR
1	L	104	LEU
1	L	129	GLU
1	L	131	LEU
1	L	138	CYS
1	L	141	SER
1	L	147	VAL
1	L	151	SER
1	L	161	LEU
1	L	172	GLU
1	L	189	VAL
1	L	201	SER
1	L	210	THR
1	L	217	SER
1	L	230	ILE
1	L	265	ASN
1	L	272	LYS
1	L	284	ARG
1	L	289	LEU
1	L	295	LEU
1	L	302	SER
1	L	322	ARG
1	L	325	ILE
1	L	328	ASP

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Mol	Chain	Res	Type
1	L	329	THR
1	L	331	THR
1	L	343	GLN
1	L	350	ARG
1	L	352	GLN
1	L	355	GLU
1	L	363	GLU
1	L	378	VAL
1	L	385	THR
1	L	389	MET
1	L	390	LYS
1	L	401	HIS
1	L	419	LEU
1	L	420	ILE
1	L	421	ARG
1	L	426	LEU
1	L	430	ARG
1	L	432	GLN
1	L	433	ASN
1	L	434	GLU
1	L	441	LYS
1	L	452	ARG
1	L	454	ILE
1	L	467	ASN
1	L	468	THR
1	L	483	GLU
1	L	504	LEU
1	L	509	SER
1	L	513	LEU
1	M	7	LYS
1	M	11	ASP
1	M	16	MET
1	M	20	VAL
1	M	23	LEU
1	M	40	LEU
1	M	42	LYS
1	M	43	SER
1	M	44	PHE
1	M	52	ASP
1	M	55	SER
1	M	59	GLU
1	M	65	LYS

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Mol	Chain	Res	Type
1	M	77	VAL
1	M	87	ASP
1	M	101	THR
1	M	104	LEU
1	M	114	MET
1	M	129	GLU
1	M	131	LEU
1	M	138	CYS
1	M	141	SER
1	M	147	VAL
1	M	150	ILE
1	M	151	SER
1	M	161	LEU
1	M	172	GLU
1	M	189	VAL
1	M	201	SER
1	M	210	THR
1	M	217	SER
1	M	230	ILE
1	M	265	ASN
1	M	272	LYS
1	M	284	ARG
1	M	289	LEU
1	M	295	LEU
1	M	302	SER
1	M	322	ARG
1	M	325	ILE
1	M	328	ASP
1	M	329	THR
1	M	331	THR
1	M	343	GLN
1	M	350	ARG
1	M	352	GLN
1	M	355	GLU
1	M	359	ASP
1	M	363	GLU
1	M	378	VAL
1	M	385	THR
1	M	389	MET
1	M	390	LYS
1	M	401	HIS
1	M	404	ARG

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Mol	Chain	Res	Type
1	M	419	LEU
1	M	420	ILE
1	M	421	ARG
1	M	426	LEU
1	M	430	ARG
1	M	432	GLN
1	M	433	ASN
1	M	434	GLU
1	M	441	LYS
1	M	452	ARG
1	M	454	ILE
1	M	467	ASN
1	M	468	THR
1	M	483	GLU
1	M	504	LEU
1	M	509	SER
1	M	513	LEU
1	N	7	LYS
1	N	11	ASP
1	N	15	LYS
1	N	16	MET
1	N	20	VAL
1	N	23	LEU
1	N	27	VAL
1	N	40	LEU
1	N	42	LYS
1	N	43	SER
1	N	44	PHE
1	N	49	ILE
1	N	55	SER
1	N	59	GLU
1	N	65	LYS
1	N	77	VAL
1	N	87	ASP
1	N	101	THR
1	N	104	LEU
1	N	129	GLU
1	N	131	LEU
1	N	138	CYS
1	N	141	SER
1	N	147	VAL
1	N	161	LEU

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Mol	Chain	Res	Type
1	N	172	GLU
1	N	189	VAL
1	N	201	SER
1	N	217	SER
1	N	230	ILE
1	N	265	ASN
1	N	272	LYS
1	N	284	ARG
1	N	289	LEU
1	N	295	LEU
1	N	302	SER
1	N	322	ARG
1	N	325	ILE
1	N	328	ASP
1	N	329	THR
1	N	331	THR
1	N	343	GLN
1	N	350	ARG
1	N	352	GLN
1	N	355	GLU
1	N	363	GLU
1	N	378	VAL
1	N	385	THR
1	N	389	MET
1	N	390	LYS
1	N	404	ARG
1	N	419	LEU
1	N	420	ILE
1	N	421	ARG
1	N	426	LEU
1	N	432	GLN
1	N	433	ASN
1	N	434	GLU
1	N	436	GLN
1	N	441	LYS
1	N	452	ARG
1	N	454	ILE
1	N	467	ASN
1	N	468	THR
1	N	483	GLU
1	N	504	LEU
1	N	513	LEU

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Mol	Chain	Res	Type
2	O	1	MET
2	O	3	ILE
2	O	4	ARG
2	O	6	LEU
2	O	20	LYS
2	O	30	SER
2	O	37	ARG
2	O	55	LYS
2	O	60	LYS
2	O	80	ASN
2	O	86	MET
2	O	89	SER
2	P	1	MET
2	P	3	ILE
2	P	4	ARG
2	P	6	LEU
2	P	20	LYS
2	P	28	THR
2	P	30	SER
2	P	55	LYS
2	P	60	LYS
2	P	80	ASN
2	P	86	MET
2	P	89	SER
2	Q	1	MET
2	Q	3	ILE
2	Q	4	ARG
2	Q	6	LEU
2	Q	20	LYS
2	Q	28	THR
2	Q	30	SER
2	Q	55	LYS
2	Q	60	LYS
2	Q	80	ASN
2	Q	86	MET
2	Q	89	SER
2	R	1	MET
2	R	3	ILE
2	R	4	ARG
2	R	6	LEU
2	R	20	LYS
2	R	28	THR

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Mol	Chain	Res	Type
2	R	30	SER
2	R	55	LYS
2	R	60	LYS
2	R	78	ILE
2	R	80	ASN
2	R	86	MET
2	R	89	SER
2	S	1	MET
2	S	3	ILE
2	S	4	ARG
2	S	6	LEU
2	S	20	LYS
2	S	30	SER
2	S	55	LYS
2	S	60	LYS
2	S	80	ASN
2	S	86	MET
2	S	89	SER
2	T	1	MET
2	T	3	ILE
2	T	4	ARG
2	T	6	LEU
2	T	20	LYS
2	T	28	THR
2	T	30	SER
2	T	55	LYS
2	T	60	LYS
2	T	80	ASN
2	T	86	MET
2	T	89	SER
2	U	1	MET
2	U	3	ILE
2	U	4	ARG
2	U	6	LEU
2	U	20	LYS
2	U	30	SER
2	U	37	ARG
2	U	55	LYS
2	U	60	LYS
2	U	78	ILE
2	U	80	ASN
2	U	86	MET

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Mol	Chain	Res	Type
2	U	89	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	97	GLN
1	A	146	GLN
1	A	153	ASN
1	A	206	ASN
1	A	326	ASN
1	A	348	GLN
1	A	351	GLN
1	A	453	GLN
1	A	457	ASN
1	A	475	ASN
1	B	21	ASN
1	B	37	ASN
1	B	97	GLN
1	B	146	GLN
1	B	153	ASN
1	B	194	GLN
1	B	206	ASN
1	B	326	ASN
1	B	348	GLN
1	B	351	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	206	ASN
1	C	265	ASN
1	C	326	ASN
1	C	348	GLN
1	C	351	GLN
1	C	453	GLN
1	C	457	ASN
1	C	475	ASN
1	D	10	ASN

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Mol	Chain	Res	Type
1	D	21	ASN
1	D	97	GLN
1	D	146	GLN
1	D	153	ASN
1	D	194	GLN
1	D	206	ASN
1	D	326	ASN
1	D	348	GLN
1	D	351	GLN
1	D	457	ASN
1	D	475	ASN
1	E	21	ASN
1	E	97	GLN
1	E	146	GLN
1	E	153	ASN
1	E	194	GLN
1	E	206	ASN
1	E	326	ASN
1	E	348	GLN
1	E	351	GLN
1	E	457	ASN
1	E	475	ASN
1	F	21	ASN
1	F	97	GLN
1	F	146	GLN
1	F	153	ASN
1	F	206	ASN
1	F	265	ASN
1	F	326	ASN
1	F	348	GLN
1	F	351	GLN
1	F	366	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	194	GLN
1	G	206	ASN
1	G	265	ASN
1	G	326	ASN

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Mol	Chain	Res	Type
1	G	348	GLN
1	G	351	GLN
1	G	453	GLN
1	G	457	ASN
1	G	475	ASN
1	H	21	ASN
1	H	72	GLN
1	H	82	ASN
1	H	97	GLN
1	H	153	ASN
1	H	265	ASN
1	H	326	ASN
1	H	351	GLN
1	H	366	GLN
1	H	433	ASN
1	H	436	GLN
1	H	467	ASN
1	I	21	ASN
1	I	72	GLN
1	I	97	GLN
1	I	265	ASN
1	I	326	ASN
1	I	351	GLN
1	I	366	GLN
1	I	433	ASN
1	I	436	GLN
1	I	467	ASN
1	J	21	ASN
1	J	72	GLN
1	J	97	GLN
1	J	153	ASN
1	J	265	ASN
1	J	326	ASN
1	J	351	GLN
1	J	366	GLN
1	J	433	ASN
1	J	436	GLN
1	J	467	ASN
1	K	21	ASN
1	K	72	GLN
1	K	97	GLN
1	K	265	ASN

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Mol	Chain	Res	Type
1	K	326	ASN
1	K	351	GLN
1	K	366	GLN
1	K	433	ASN
1	K	467	ASN
1	L	21	ASN
1	L	72	GLN
1	L	82	ASN
1	L	97	GLN
1	L	265	ASN
1	L	326	ASN
1	L	351	GLN
1	L	366	GLN
1	L	433	ASN
1	L	467	ASN
1	M	21	ASN
1	M	37	ASN
1	M	72	GLN
1	M	82	ASN
1	M	97	GLN
1	M	265	ASN
1	M	326	ASN
1	M	351	GLN
1	M	366	GLN
1	M	433	ASN
1	M	436	GLN
1	M	467	ASN
1	N	21	ASN
1	N	72	GLN
1	N	97	GLN
1	N	153	ASN
1	N	265	ASN
1	N	326	ASN
1	N	351	GLN
1	N	366	GLN
1	N	433	ASN
1	N	436	GLN
1	N	467	ASN
2	O	45	ASN
2	O	68	ASN
2	O	80	ASN
2	P	45	ASN

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Mol	Chain	Res	Type
2	P	68	ASN
2	Q	45	ASN
2	Q	68	ASN
2	R	45	ASN
2	R	68	ASN
2	R	80	ASN
2	S	45	ASN
2	S	68	ASN
2	S	80	ASN
2	T	45	ASN
2	T	68	ASN
2	U	45	ASN
2	U	68	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 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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	$\# Z > 2$
5	ADP	E	600	3,4,6	24,29,29	1.40	3 (12%)	29,45,45	2.19	13 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	AF3	B	602	1,3,5,4	0,3,3	0.00	-	-		
5	ADP	B	600	3,4,6	24,29,29	1.45	2 (8%)	29,45,45	2.21	13 (44%)
5	ADP	A	600	3,4,6	24,29,29	1.27	5 (20%)	29,45,45	1.78	7 (24%)
6	AF3	A	602	1,3,5,4	0,3,3	0.00	-	-		
5	ADP	C	600	3,4,6	24,29,29	1.33	4 (16%)	29,45,45	1.83	8 (27%)
6	AF3	G	602	1,3,5,4,7	0,3,3	0.00	-	-		
6	AF3	D	602	1,3,5,4	0,3,3	0.00	-	-		
6	AF3	E	602	1,3,5,4	0,3,3	0.00	-	-		
5	ADP	G	600	3,4,6	24,29,29	1.45	5 (20%)	29,45,45	1.83	8 (27%)
5	ADP	D	600	3,4,6	24,29,29	1.40	3 (12%)	29,45,45	1.77	6 (20%)
6	AF3	F	602	1,3,5,4	0,3,3	0.00	-	-		
6	AF3	C	602	1,3,5,4	0,3,3	0.00	-	-		
5	ADP	F	600	3,4,6	24,29,29	1.36	4 (16%)	29,45,45	1.89	7 (24%)

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
5	ADP	B	600	3,4,6	-	5/12/32/32	0/3/3/3
5	ADP	A	600	3,4,6	-	4/12/32/32	0/3/3/3
5	ADP	D	600	3,4,6	-	5/12/32/32	0/3/3/3
5	ADP	C	600	3,4,6	-	4/12/32/32	0/3/3/3
5	ADP	F	600	3,4,6	-	4/12/32/32	0/3/3/3
5	ADP	E	600	3,4,6	-	4/12/32/32	0/3/3/3
5	ADP	G	600	3,4,6	-	4/12/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	ADP	O4'-C1'	-3.74	1.35	1.41
5	G	600	ADP	C2'-C1'	-3.32	1.48	1.53
5	G	600	ADP	O4'-C4'	-3.23	1.37	1.45
5	C	600	ADP	C4-N3	-3.18	1.31	1.35
5	F	600	ADP	C2-N3	3.15	1.37	1.32
5	B	600	ADP	C2'-C1'	-3.09	1.49	1.53
5	D	600	ADP	C2'-C1'	-3.07	1.49	1.53
5	E	600	ADP	C4-N3	-2.86	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	600	ADP	O4'-C1'	-2.80	1.37	1.41
5	A	600	ADP	C4-N3	-2.77	1.31	1.35
5	D	600	ADP	O4'-C4'	-2.75	1.38	1.45
5	F	600	ADP	C4-N3	-2.67	1.32	1.35
5	G	600	ADP	C4-N3	-2.64	1.32	1.35
5	E	600	ADP	C2-N3	2.63	1.36	1.32
5	D	600	ADP	C4-N3	-2.56	1.32	1.35
5	A	600	ADP	C2-N3	2.52	1.36	1.32
5	F	600	ADP	C2-N1	2.48	1.38	1.33
5	G	600	ADP	C6-C5	-2.41	1.34	1.43
5	C	600	ADP	C2'-C1'	-2.39	1.50	1.53
5	C	600	ADP	O4'-C4'	-2.37	1.39	1.45
5	A	600	ADP	C2-N1	2.20	1.38	1.33
5	F	600	ADP	C5-N7	-2.19	1.31	1.39
5	A	600	ADP	C2'-C1'	-2.16	1.50	1.53
5	C	600	ADP	C2-N3	2.08	1.35	1.32
5	A	600	ADP	O2'-C2'	-2.07	1.38	1.43
5	G	600	ADP	C5-C4	-2.02	1.35	1.40

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	ADP	N3-C2-N1	-6.15	119.07	128.68
5	D	600	ADP	N3-C2-N1	-5.08	120.75	128.68
5	E	600	ADP	N3-C2-N1	-4.72	121.30	128.68
5	F	600	ADP	N3-C2-N1	-4.53	121.61	128.68
5	D	600	ADP	PA-O3A-PB	-4.29	118.10	132.83
5	A	600	ADP	N3-C2-N1	-4.19	122.12	128.68
5	C	600	ADP	N3-C2-N1	-4.11	122.25	128.68
5	E	600	ADP	C4-C5-N7	-4.02	105.21	109.40
5	A	600	ADP	C5-C6-N6	4.00	126.43	120.35
5	F	600	ADP	PA-O3A-PB	-3.99	119.15	132.83
5	F	600	ADP	O3B-PB-O2B	-3.94	92.58	107.64
5	G	600	ADP	N3-C2-N1	-3.91	122.56	128.68
5	B	600	ADP	PA-O3A-PB	-3.84	119.65	132.83
5	E	600	ADP	O3'-C3'-C4'	-3.78	100.12	111.05
5	E	600	ADP	C5-C6-N6	3.73	126.02	120.35
5	A	600	ADP	PA-O3A-PB	-3.72	120.05	132.83
5	G	600	ADP	O3B-PB-O2B	-3.72	93.42	107.64
5	C	600	ADP	C4-C5-N7	-3.67	105.57	109.40
5	C	600	ADP	C5-C6-N6	3.57	125.77	120.35
5	B	600	ADP	O4'-C1'-C2'	-3.23	102.21	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	600	ADP	C4-C5-N7	-3.07	106.20	109.40
5	E	600	ADP	PA-O3A-PB	-3.02	122.48	132.83
5	C	600	ADP	O3B-PB-O2B	-3.01	96.14	107.64
5	G	600	ADP	C1'-N9-C4	-2.98	121.41	126.64
5	G	600	ADP	C2'-C3'-C4'	2.92	108.33	102.64
5	A	600	ADP	O2A-PA-O1A	2.91	126.64	112.24
5	B	600	ADP	C5'-C4'-C3'	-2.87	104.42	115.18
5	B	600	ADP	O3B-PB-O1B	2.87	121.91	110.68
5	E	600	ADP	O4'-C1'-C2'	-2.80	102.83	106.93
5	B	600	ADP	C5-C6-N6	2.79	124.59	120.35
5	B	600	ADP	C4-C5-N7	-2.71	106.57	109.40
5	B	600	ADP	O3'-C3'-C4'	-2.71	103.21	111.05
5	E	600	ADP	C1'-N9-C4	-2.69	121.91	126.64
5	F	600	ADP	O2B-PB-O3A	2.66	113.57	104.64
5	E	600	ADP	O3B-PB-O2B	-2.59	97.74	107.64
5	G	600	ADP	C3'-C2'-C1'	-2.56	97.13	100.98
5	F	600	ADP	O3'-C3'-C4'	-2.55	103.68	111.05
5	D	600	ADP	O2'-C2'-C1'	-2.53	101.52	110.85
5	C	600	ADP	PA-O3A-PB	-2.52	124.17	132.83
5	B	600	ADP	O3B-PB-O2B	-2.51	98.06	107.64
5	B	600	ADP	C1'-N9-C4	-2.49	122.26	126.64
5	B	600	ADP	O2'-C2'-C3'	-2.41	104.02	111.82
5	E	600	ADP	O2B-PB-O3A	2.34	112.49	104.64
5	E	600	ADP	C5'-C4'-C3'	-2.32	106.47	115.18
5	G	600	ADP	PA-O3A-PB	-2.32	124.87	132.83
5	F	600	ADP	O5'-PA-O1A	-2.28	100.17	109.07
5	E	600	ADP	O2'-C2'-C3'	-2.27	104.48	111.82
5	A	600	ADP	C1'-N9-C4	-2.25	122.68	126.64
5	E	600	ADP	O2A-PA-O1A	2.23	123.27	112.24
5	A	600	ADP	N6-C6-N1	-2.23	113.95	118.57
5	D	600	ADP	C5-C6-N6	2.21	123.71	120.35
5	C	600	ADP	O2A-PA-O1A	2.19	123.07	112.24
5	C	600	ADP	O3'-C3'-C4'	-2.16	104.79	111.05
5	A	600	ADP	O3B-PB-O2B	-2.16	99.39	107.64
5	B	600	ADP	O2'-C2'-C1'	-2.14	102.95	110.85
5	G	600	ADP	O2B-PB-O1B	2.12	119.00	110.68
5	G	600	ADP	O2B-PB-O3A	2.10	111.66	104.64
5	E	600	ADP	O3B-PB-O1B	2.08	118.82	110.68
5	D	600	ADP	O4'-C1'-C2'	-2.03	103.96	106.93
5	B	600	ADP	O5'-PA-O1A	-2.02	101.16	109.07
5	F	600	ADP	O4'-C1'-C2'	-2.02	103.97	106.93
5	C	600	ADP	C2'-C3'-C4'	2.00	106.54	102.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	600	ADP	PA-O3A-PB-O2B
5	D	600	ADP	PA-O3A-PB-O2B
5	C	600	ADP	PA-O3A-PB-O2B
5	F	600	ADP	PA-O3A-PB-O2B
5	E	600	ADP	PA-O3A-PB-O1B
5	G	600	ADP	PA-O3A-PB-O1B
5	F	600	ADP	PA-O3A-PB-O1B
5	E	600	ADP	PA-O3A-PB-O2B
5	G	600	ADP	PA-O3A-PB-O3B
5	B	600	ADP	PA-O3A-PB-O2B
5	C	600	ADP	PB-O3A-PA-O1A
5	D	600	ADP	PB-O3A-PA-O1A
5	D	600	ADP	PB-O3A-PA-O2A
5	C	600	ADP	PB-O3A-PA-O2A
5	B	600	ADP	PB-O3A-PA-O1A
5	B	600	ADP	PB-O3A-PA-O2A
5	A	600	ADP	PA-O3A-PB-O1B
5	A	600	ADP	PB-O3A-PA-O2A
5	D	600	ADP	PA-O3A-PB-O1B
5	E	600	ADP	PA-O3A-PB-O3B
5	D	600	ADP	PA-O3A-PB-O3B
5	C	600	ADP	PA-O3A-PB-O3B
5	F	600	ADP	PA-O3A-PB-O3B
5	B	600	ADP	PA-O3A-PB-O3B
5	A	600	ADP	PA-O3A-PB-O2B
5	A	600	ADP	PA-O3A-PB-O3B
5	E	600	ADP	PB-O3A-PA-O2A
5	G	600	ADP	PB-O3A-PA-O2A
5	F	600	ADP	PB-O3A-PA-O2A
5	B	600	ADP	PA-O3A-PB-O1B

There are no ring outliers.

13 monomers are involved in 16 short contacts:

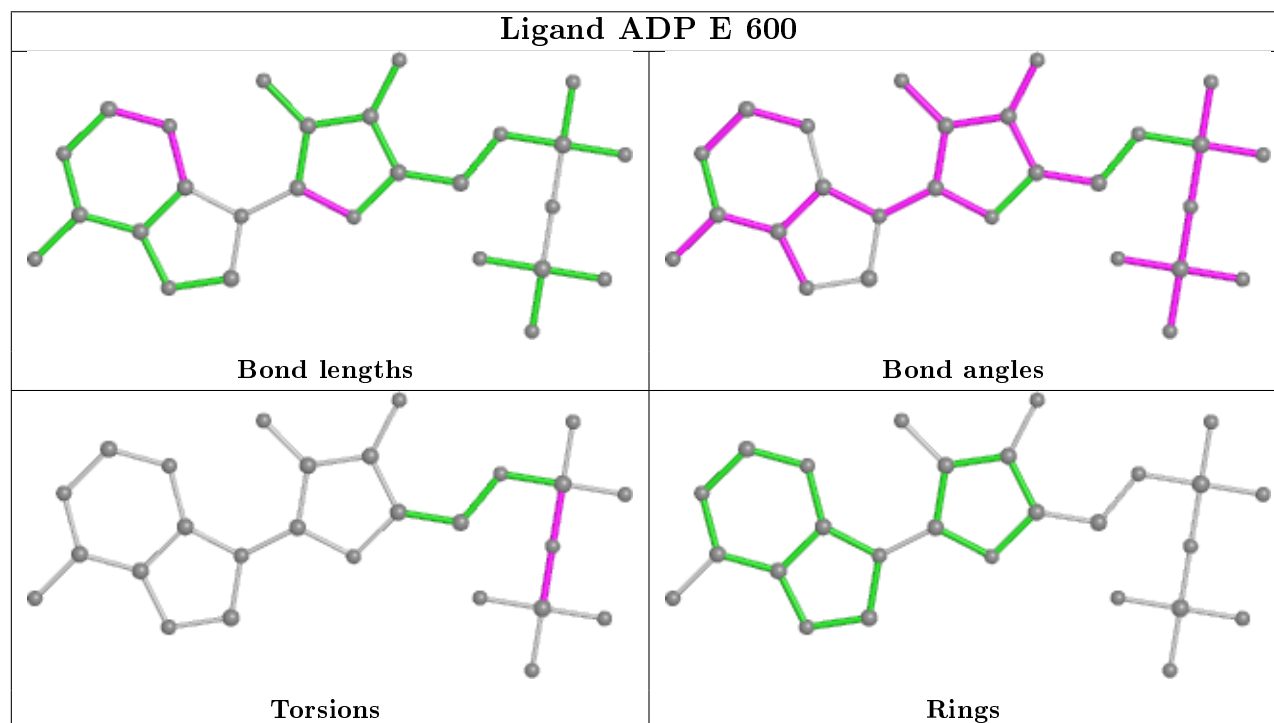
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	600	ADP	1	0
5	B	600	ADP	1	0
5	A	600	ADP	1	0
6	A	602	AF3	2	0
5	C	600	ADP	2	0

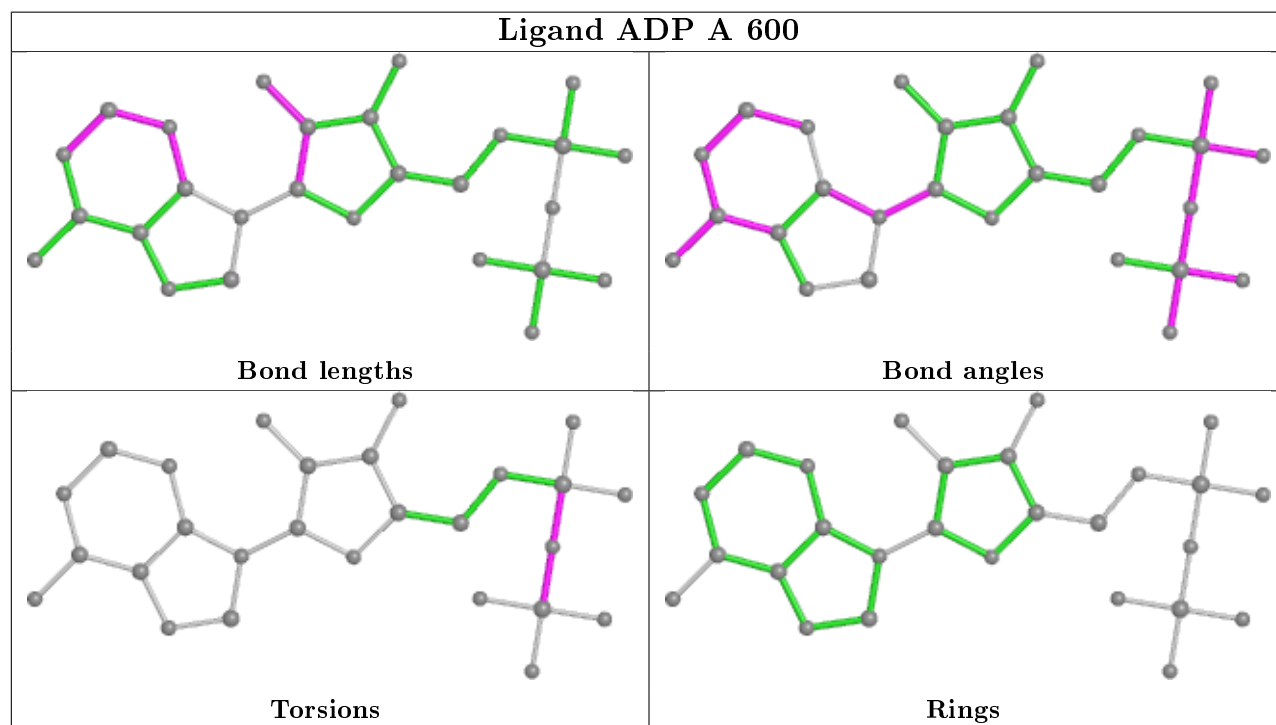
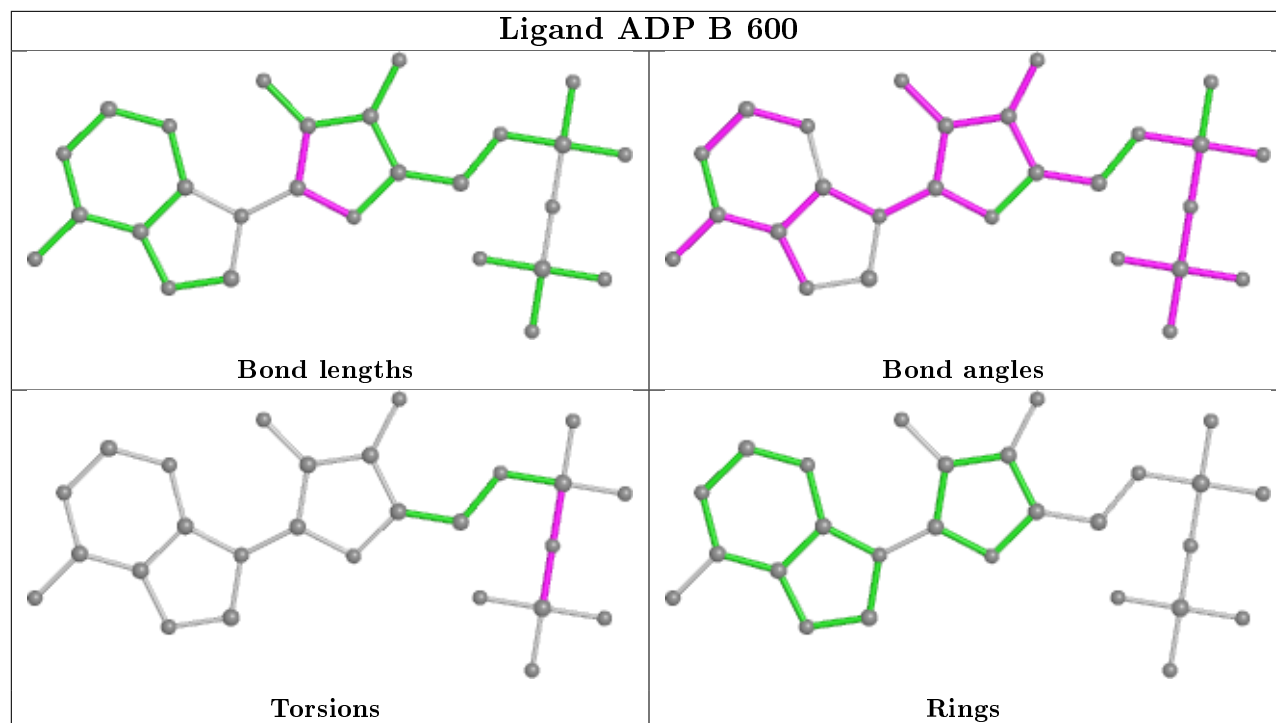
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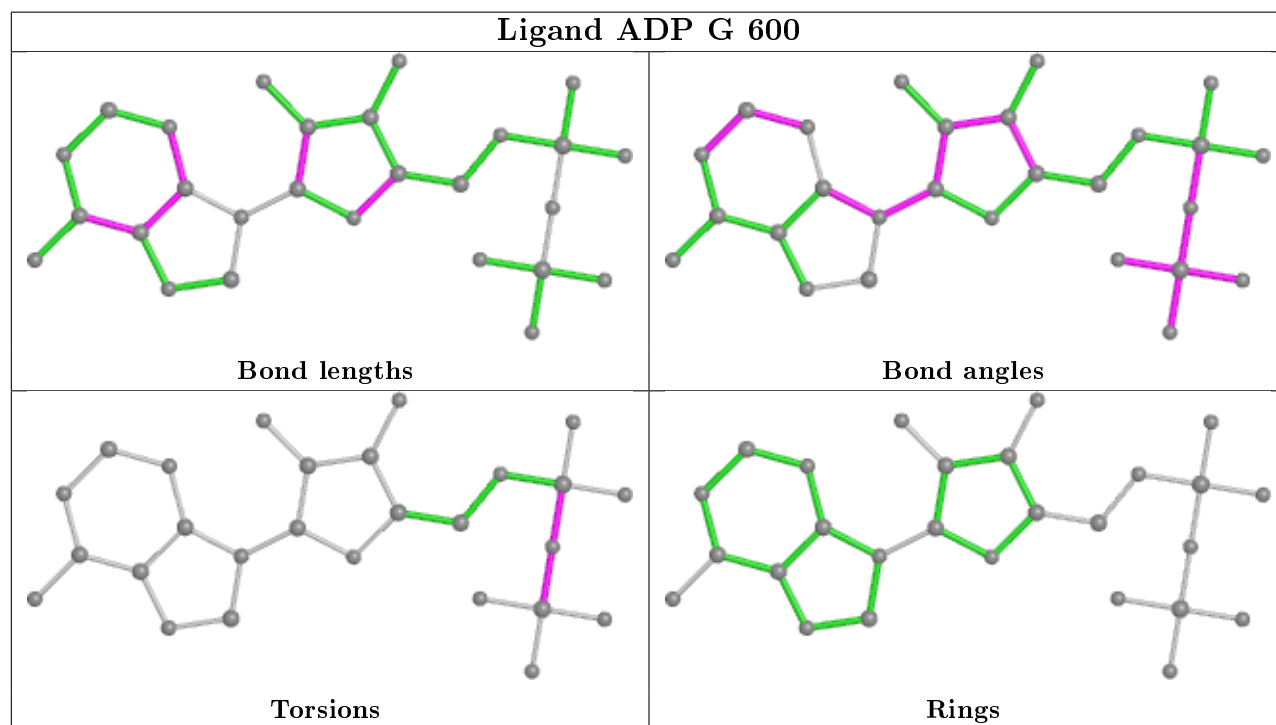
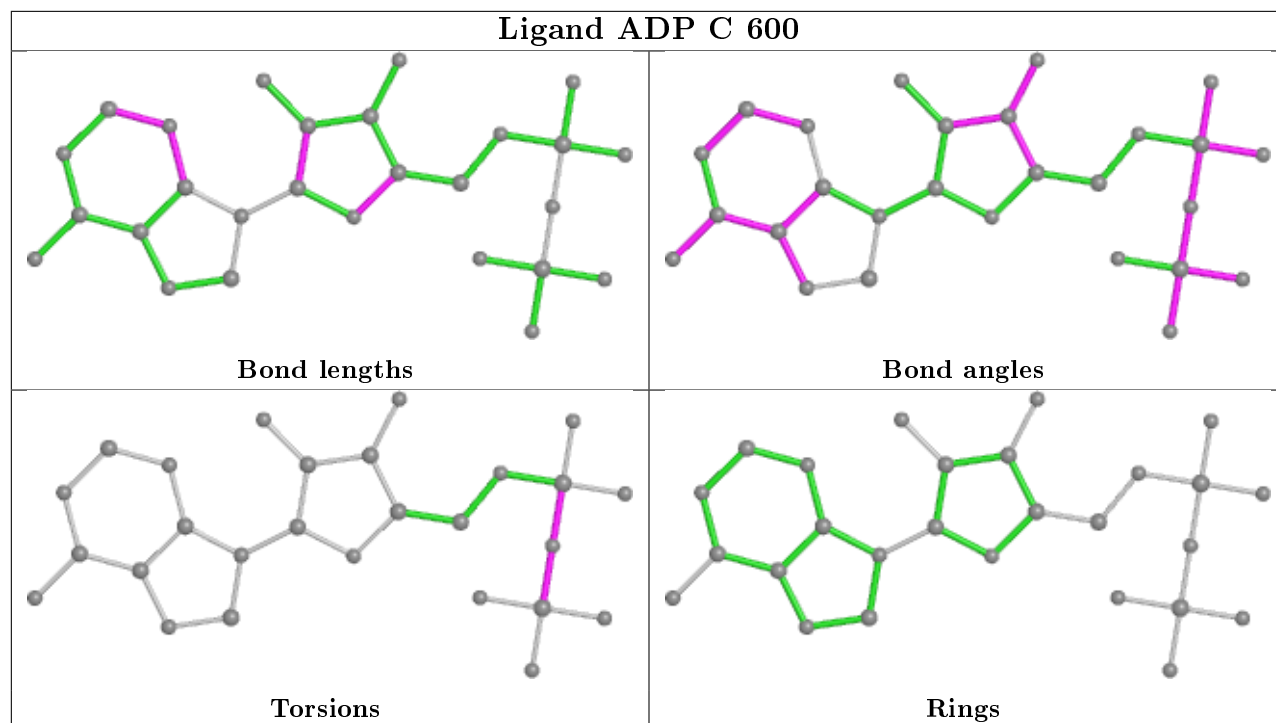
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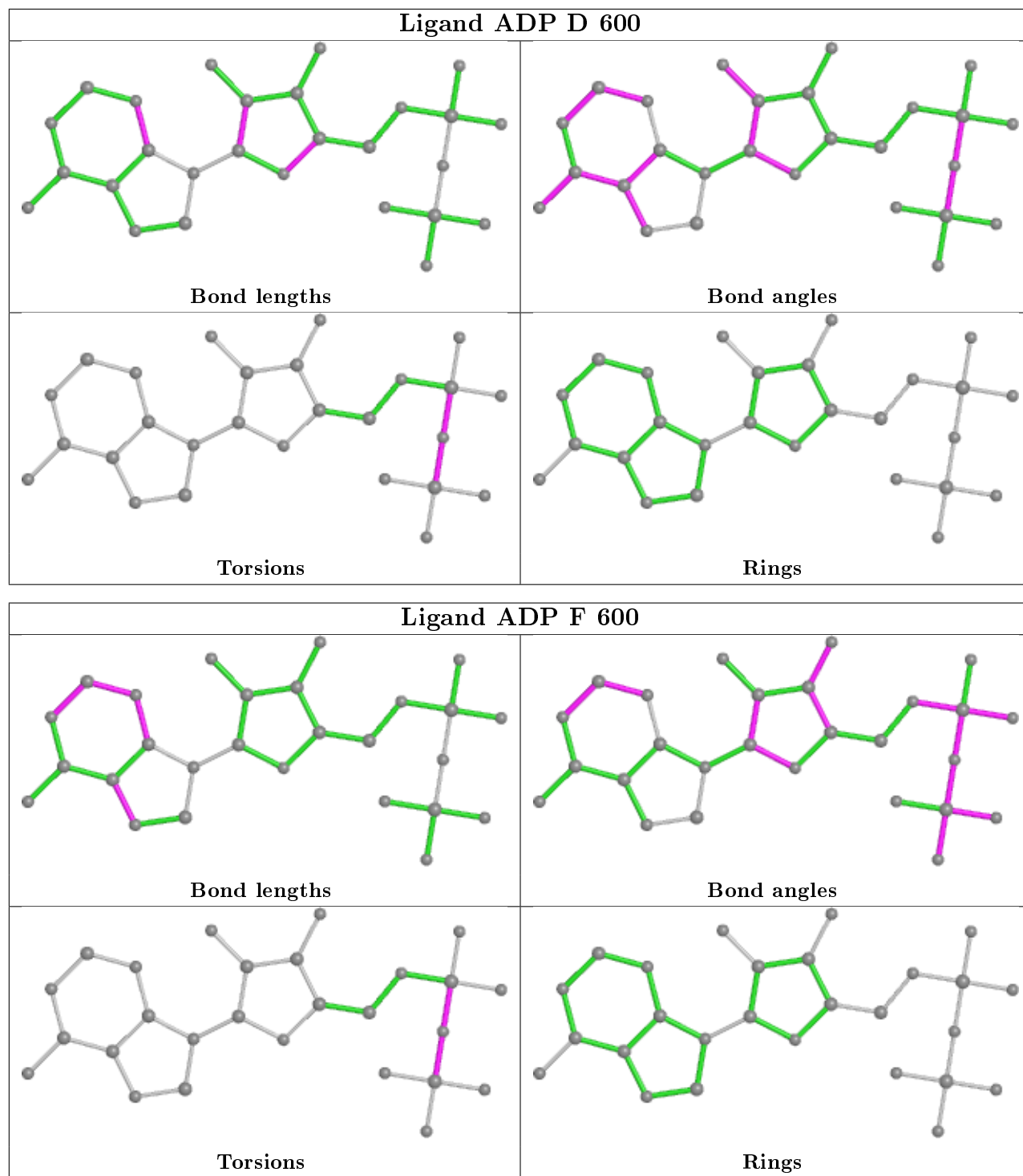
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	602	AF3	1	0
6	D	602	AF3	2	0
6	E	602	AF3	1	0
5	G	600	ADP	1	0
5	D	600	ADP	3	0
6	F	602	AF3	2	0
6	C	602	AF3	1	0
5	F	600	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	524/524 (100%)	-0.12	19 (3%) 42 32	2, 2, 4, 5	0
1	B	524/524 (100%)	-0.02	32 (6%) 21 13	2, 2, 4, 5	0
1	C	524/524 (100%)	-0.09	24 (4%) 32 22	2, 2, 4, 5	0
1	D	524/524 (100%)	-0.13	27 (5%) 27 18	2, 2, 4, 5	0
1	E	524/524 (100%)	0.00	36 (6%) 16 10	2, 2, 4, 5	0
1	F	524/524 (100%)	0.09	40 (7%) 13 7	2, 2, 4, 5	0
1	G	524/524 (100%)	-0.02	30 (5%) 23 15	2, 2, 4, 5	0
1	H	524/524 (100%)	-0.40	1 (0%) 95 94	2, 2, 4, 5	0
1	I	524/524 (100%)	-0.39	2 (0%) 92 91	2, 2, 4, 5	0
1	J	524/524 (100%)	-0.38	6 (1%) 80 75	2, 2, 4, 5	0
1	K	524/524 (100%)	-0.32	4 (0%) 86 81	2, 2, 4, 5	0
1	L	524/524 (100%)	-0.16	9 (1%) 70 63	2, 2, 3, 5	0
1	M	524/524 (100%)	-0.33	9 (1%) 70 63	2, 2, 4, 5	0
1	N	524/524 (100%)	-0.32	4 (0%) 86 81	2, 2, 4, 5	0
2	O	97/97 (100%)	0.80	15 (15%) 2 1	2, 2, 2, 2	0
2	P	97/97 (100%)	0.51	11 (11%) 5 3	2, 2, 2, 2	0
2	Q	97/97 (100%)	0.51	9 (9%) 8 4	2, 2, 2, 2	0
2	R	97/97 (100%)	0.87	17 (17%) 1 1	2, 2, 2, 2	0
2	S	97/97 (100%)	0.65	9 (9%) 8 4	2, 2, 2, 2	0
2	T	97/97 (100%)	0.85	18 (18%) 1 1	2, 2, 2, 2	0
2	U	97/97 (100%)	0.79	18 (18%) 1 1	2, 2, 2, 2	0
All	All	8015/8015 (100%)	-0.11	340 (4%) 36 26	2, 2, 4, 5	0

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	1	MET	8.7
2	T	22	ALA	7.7
1	B	314	LEU	7.5
2	T	25	ILE	7.2
1	F	215	LEU	7.1
1	E	361	ASP	7.0
2	O	1	MET	7.0
2	O	17	VAL	7.0
2	Q	25	ILE	6.6
1	C	361	ASP	5.9
1	N	233	MET	5.7
1	G	336	VAL	5.7
1	F	199	TYR	5.6
2	U	22	ALA	5.6
1	B	361	ASP	5.5
1	E	336	VAL	5.4
1	G	361	ASP	5.4
1	C	271	VAL	5.4
1	A	212	ALA	5.4
2	R	25	ILE	5.4
2	U	25	ILE	5.3
2	S	27	LEU	5.0
2	S	97	ALA	5.0
2	R	22	ALA	4.9
1	A	204	PHE	4.8
1	B	309	LEU	4.8
2	R	17	VAL	4.7
2	T	17	VAL	4.6
2	R	97	ALA	4.6
2	U	97	ALA	4.6
1	B	355	GLU	4.6
2	O	30	SER	4.6
1	F	332	ILE	4.5
1	G	270	ILE	4.5
1	C	212	ALA	4.5
2	Q	71	TYR	4.5
1	F	213	VAL	4.4
1	J	233	MET	4.4
2	T	27	LEU	4.4
1	F	314	LEU	4.3
1	I	44	PHE	4.3
1	G	353	ILE	4.2
2	O	3	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	322	ARG	4.1
1	B	357	THR	4.1
1	G	314	LEU	4.1
2	P	17	VAL	4.1
2	P	25	ILE	4.1
1	G	321	LYS	4.1
1	F	272	LYS	4.0
2	R	26	VAL	4.0
2	R	82	GLU	4.0
1	F	355	GLU	3.9
1	E	270	ILE	3.9
1	D	320	ALA	3.9
1	E	268	ARG	3.9
1	G	322	ARG	3.9
1	B	333	ILE	3.9
1	E	350	ARG	3.9
2	S	22	ALA	3.9
2	S	17	VAL	3.9
1	D	212	ALA	3.9
1	A	361	ASP	3.8
1	G	365	LEU	3.8
1	A	360	TYR	3.7
2	T	26	VAL	3.7
1	M	309	LEU	3.7
2	U	32	ALA	3.7
2	O	18	GLU	3.7
2	R	18	GLU	3.7
1	E	314	LEU	3.7
1	F	171	LYS	3.6
2	U	84	LEU	3.6
1	B	362	ARG	3.6
1	B	350	ARG	3.6
1	B	336	VAL	3.6
1	G	210	THR	3.6
1	A	211	GLY	3.5
2	S	25	ILE	3.5
1	D	243	ALA	3.5
1	B	353	ILE	3.5
1	H	44	PHE	3.5
2	O	80	ASN	3.5
1	E	346	VAL	3.5
1	D	209	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	R	83	VAL	3.5
1	F	295	LEU	3.5
1	A	353	ILE	3.5
1	F	273	VAL	3.5
2	U	23	GLY	3.4
1	B	208	PRO	3.4
1	D	172	GLU	3.4
1	G	350	ARG	3.4
2	R	21	SER	3.4
1	G	209	GLU	3.4
1	C	360	TYR	3.4
1	A	314	LEU	3.4
1	B	200	LEU	3.4
1	C	346	VAL	3.4
1	J	353	ILE	3.3
2	O	27	LEU	3.3
2	R	1	MET	3.3
1	D	215	LEU	3.3
1	E	353	ILE	3.3
1	G	279	PRO	3.3
1	C	243	ALA	3.3
1	F	279	PRO	3.3
2	Q	26	VAL	3.3
2	U	1	MET	3.3
2	T	71	TYR	3.2
1	B	212	ALA	3.2
2	T	77	LYS	3.2
2	P	97	ALA	3.2
2	O	48	ILE	3.2
2	R	3	ILE	3.2
1	E	212	ALA	3.2
2	P	18	GLU	3.2
1	F	357	THR	3.2
2	P	49	LEU	3.2
1	E	342	ILE	3.1
1	B	224	ASP	3.1
1	E	243	ALA	3.1
1	L	44	PHE	3.1
1	E	368	ARG	3.1
1	G	349	ILE	3.1
1	G	215	LEU	3.1
1	G	268	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	S	26	VAL	3.0
1	B	245	LYS	3.0
1	F	323	VAL	3.0
1	D	199	TYR	3.0
1	C	320	ALA	2.9
1	F	361	ASP	2.9
2	O	19	THR	2.9
1	F	336	VAL	2.9
2	Q	27	LEU	2.9
2	T	97	ALA	2.9
1	F	353	ILE	2.9
1	A	233	MET	2.9
1	F	212	ALA	2.9
1	K	44	PHE	2.9
1	C	314	LEU	2.9
1	F	360	TYR	2.9
1	A	213	VAL	2.9
1	G	320	ALA	2.9
1	E	295	LEU	2.9
1	J	355	GLU	2.8
1	N	268	ARG	2.8
1	D	213	VAL	2.8
1	D	314	LEU	2.8
1	E	354	GLU	2.8
1	D	333	ILE	2.8
1	E	237	LEU	2.8
1	A	256	GLY	2.8
1	E	360	TYR	2.8
2	T	49	LEU	2.8
1	E	273	VAL	2.8
1	D	272	LYS	2.8
2	T	69	ASP	2.8
1	D	319	GLN	2.8
2	U	83	VAL	2.8
1	D	171	LYS	2.7
2	O	78	ILE	2.7
1	G	208	PRO	2.7
2	Q	49	LEU	2.7
1	G	199	TYR	2.7
1	B	300	VAL	2.7
1	F	366	GLN	2.7
1	G	267	MET	2.7

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Mol	Chain	Res	Type	RSRZ
2	P	20	LYS	2.7
1	F	317	LEU	2.7
1	F	210	THR	2.7
2	U	26	VAL	2.7
1	D	237	LEU	2.7
1	F	334	ASP	2.6
1	M	268	ARG	2.6
1	F	219	PHE	2.6
1	B	295	LEU	2.6
1	G	212	ALA	2.6
1	J	356	ALA	2.6
1	A	205	ILE	2.6
1	C	357	THR	2.6
2	U	33	ALA	2.6
1	C	355	GLU	2.6
1	C	233	MET	2.6
1	M	234	LEU	2.6
1	L	233	MET	2.6
1	D	271	VAL	2.6
2	O	71	TYR	2.6
2	R	52	GLY	2.5
2	T	84	LEU	2.5
1	C	203	TYR	2.5
1	F	278	ALA	2.5
1	M	352	GLN	2.5
1	C	319	GLN	2.5
1	D	355	GLU	2.5
1	E	284	ARG	2.5
1	L	309	LEU	2.5
1	C	272	LYS	2.5
2	P	72	GLY	2.5
2	U	47	ARG	2.5
1	B	365	LEU	2.5
1	F	172	GLU	2.5
1	F	309	LEU	2.5
1	E	204	PHE	2.5
1	F	195	PHE	2.5
1	F	292	ILE	2.5
1	F	333	ILE	2.5
2	U	71	TYR	2.5
2	R	27	LEU	2.5
1	B	360	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	U	27	LEU	2.5
1	F	254	VAL	2.4
2	O	26	VAL	2.4
1	C	334	ASP	2.4
1	D	365	LEU	2.4
1	F	204	PHE	2.4
2	Q	1	MET	2.4
1	C	268	ARG	2.4
1	M	353	ILE	2.4
2	T	1	MET	2.4
2	T	31	ALA	2.4
1	E	309	LEU	2.4
2	T	3	ILE	2.4
1	B	346	VAL	2.4
2	P	71	TYR	2.4
1	F	233	MET	2.4
1	B	342	ILE	2.4
1	G	244	GLY	2.4
1	E	317	LEU	2.4
1	C	267	MET	2.3
1	G	243	ALA	2.3
1	E	215	LEU	2.3
1	D	233	MET	2.3
1	A	210	THR	2.3
1	F	342	ILE	2.3
1	M	44	PHE	2.3
1	A	276	VAL	2.3
1	E	355	GLU	2.3
2	O	25	ILE	2.3
1	G	360	TYR	2.3
1	K	233	MET	2.3
1	C	353	ILE	2.3
2	U	21	SER	2.3
1	D	361	ASP	2.3
1	I	268	ARG	2.3
2	R	19	THR	2.3
2	T	21	SER	2.3
2	T	30	SER	2.3
1	M	284	ARG	2.3
1	E	233	MET	2.3
1	E	244	GLY	2.3
1	M	233	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	321	LYS	2.3
1	E	172	GLU	2.3
1	L	236	VAL	2.2
1	C	322	ARG	2.2
1	D	268	ARG	2.2
1	D	295	LEU	2.2
2	O	97	ALA	2.2
1	A	268	ARG	2.2
2	Q	13	LYS	2.2
1	G	200	LEU	2.2
2	Q	33	ALA	2.2
1	L	193	MET	2.2
1	C	209	GLU	2.2
2	Q	18	GLU	2.2
2	R	53	GLU	2.2
1	E	300	VAL	2.2
1	G	334	ASP	2.2
1	B	315	GLU	2.2
1	L	231	ARG	2.2
1	E	224	ASP	2.2
1	D	359	ASP	2.2
1	C	270	ILE	2.2
1	D	349	ILE	2.2
1	F	276	VAL	2.2
1	F	268	ARG	2.2
2	P	34	LYS	2.2
1	G	348	GLN	2.2
2	O	61	VAL	2.2
1	E	337	GLY	2.2
1	L	234	LEU	2.2
2	S	66	ILE	2.2
1	F	346	VAL	2.2
1	D	218	PRO	2.2
1	N	284	ARG	2.2
2	U	10	VAL	2.2
1	N	219	PHE	2.1
1	E	272	LYS	2.1
2	U	30	SER	2.1
1	K	142	LYS	2.1
1	J	44	PHE	2.1
1	L	221	LEU	2.1
1	B	284	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	355	GLU	2.1
1	D	357	THR	2.1
1	J	268	ARG	2.1
2	R	64	ILE	2.1
2	T	32	ALA	2.1
1	E	265	ASN	2.1
1	F	324	VAL	2.1
1	G	213	VAL	2.1
1	E	294	THR	2.1
1	A	320	ALA	2.1
1	C	309	LEU	2.1
1	D	204	PHE	2.1
1	C	359	ASP	2.1
1	B	332	ILE	2.1
1	B	369	VAL	2.1
1	E	234	LEU	2.1
1	A	254	VAL	2.1
1	E	315	GLU	2.1
2	S	95	VAL	2.1
1	A	195	PHE	2.1
1	D	353	ILE	2.1
1	K	215	LEU	2.0
1	B	233	MET	2.0
2	P	1	MET	2.0
1	B	373	ALA	2.0
1	F	205	ILE	2.0
1	L	162	ILE	2.0
1	A	209	GLU	2.0
1	B	216	GLU	2.0
2	P	19	THR	2.0
2	T	20	LYS	2.0
1	A	271	VAL	2.0
1	E	195	PHE	2.0
1	B	305	ILE	2.0
1	G	305	ILE	2.0
2	R	48	ILE	2.0
1	E	340	ALA	2.0
1	F	251	ALA	2.0
1	B	199	TYR	2.0
1	G	233	MET	2.0
1	B	317	LEU	2.0
1	B	211	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	U	82	GLU	2.0
2	U	65	VAL	2.0
1	G	343	GLN	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

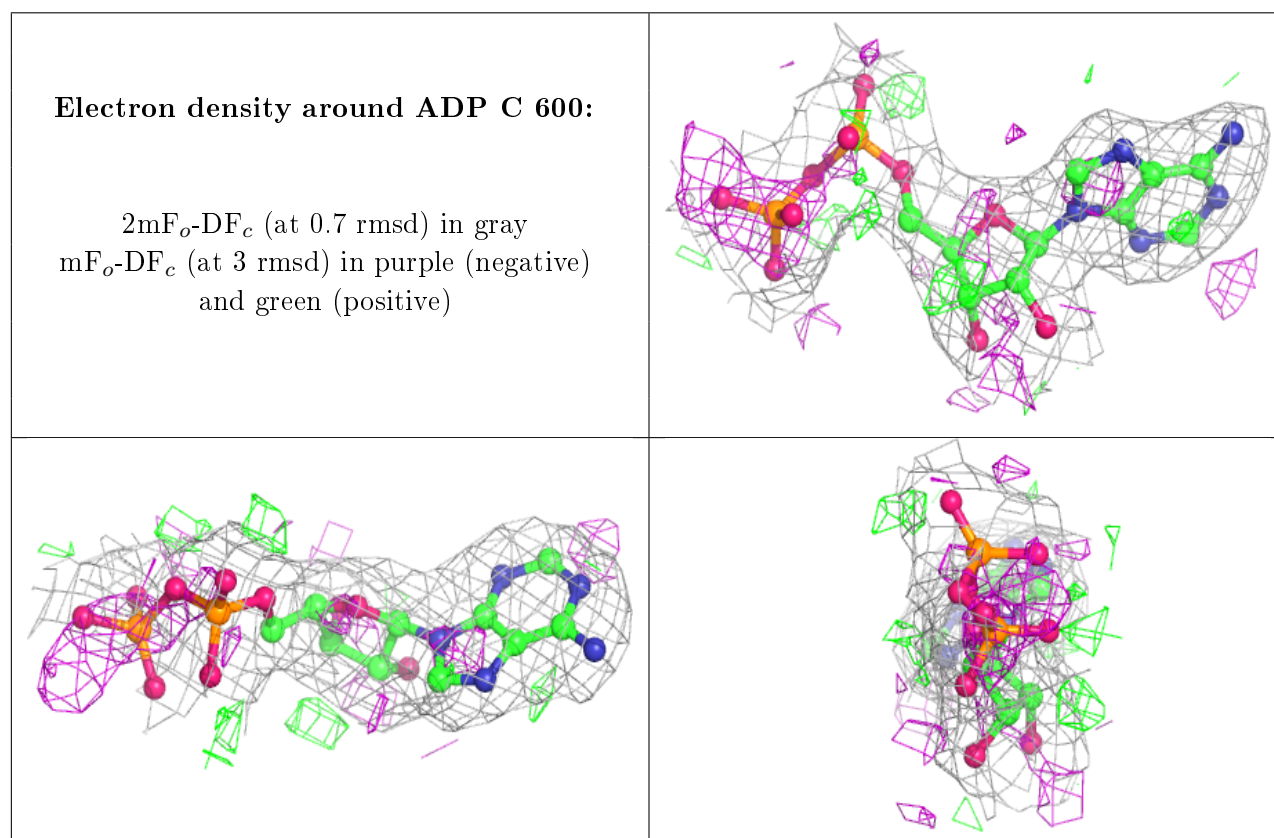
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	AF3	E	602	4/4	0.87	0.15	2,2,8,9	0
6	AF3	D	602	4/4	0.88	0.14	2,2,8,10	0
4	K	E	603	1/1	0.88	0.10	16,16,16,16	0
6	AF3	F	602	4/4	0.89	0.13	2,2,8,9	0
4	K	G	603	1/1	0.90	0.07	16,16,16,16	0
6	AF3	B	602	4/4	0.91	0.18	2,2,7,10	0
6	AF3	G	602	4/4	0.91	0.15	2,2,7,9	0
6	AF3	A	602	4/4	0.92	0.16	2,2,7,10	0
6	AF3	C	602	4/4	0.93	0.16	2,2,8,10	0
4	K	A	603	1/1	0.94	0.10	16,16,16,16	0
4	K	F	603	1/1	0.95	0.08	15,15,15,15	0
4	K	D	603	1/1	0.96	0.07	16,16,16,16	0
5	ADP	C	600	27/27	0.97	0.13	2,2,2,3	0
5	ADP	F	600	27/27	0.97	0.13	2,2,2,3	0
5	ADP	G	600	27/27	0.97	0.15	2,2,2,3	0
5	ADP	E	600	27/27	0.97	0.14	2,2,2,3	0
5	ADP	D	600	27/27	0.97	0.14	2,2,2,3	0
5	ADP	B	600	27/27	0.97	0.13	2,2,3,3	0
3	MG	E	601	1/1	0.98	0.20	2,2,2,2	0
4	K	B	603	1/1	0.98	0.06	16,16,16,16	0

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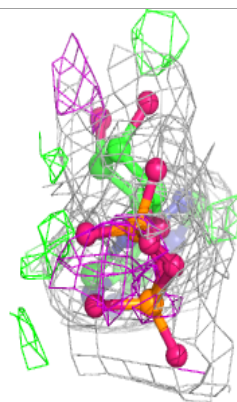
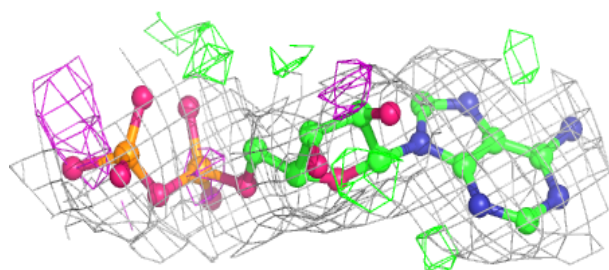
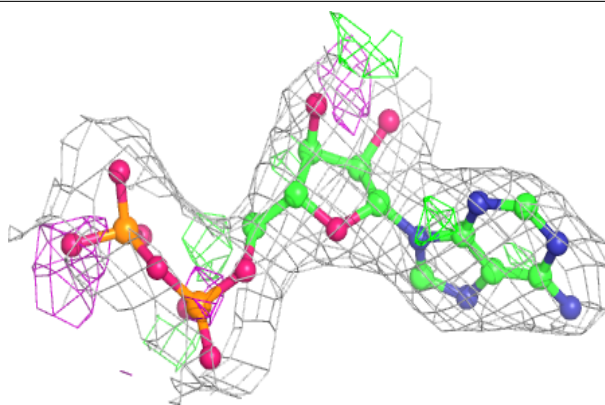
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ADP	A	600	27/27	0.98	0.14	2,2,2,3	0
4	K	C	603	1/1	0.98	0.05	15,15,15,15	0
3	MG	C	601	1/1	0.98	0.22	2,2,2,2	0
3	MG	D	601	1/1	0.99	0.20	2,2,2,2	0
3	MG	F	601	1/1	0.99	0.23	2,2,2,2	0
3	MG	G	601	1/1	0.99	0.21	2,2,2,2	0
3	MG	A	601	1/1	0.99	0.22	2,2,2,2	0
3	MG	B	601	1/1	0.99	0.22	2,2,2,2	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

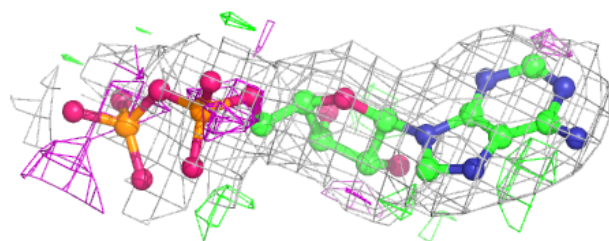
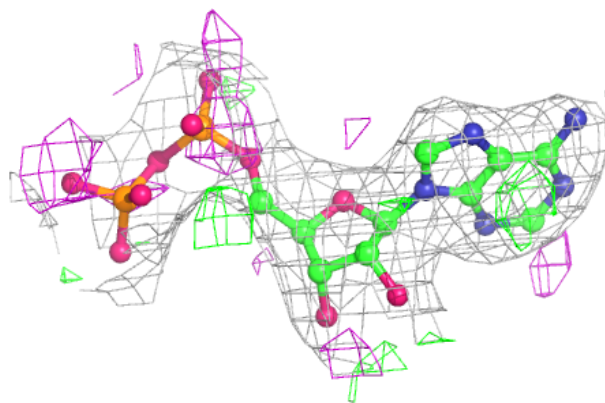


Electron density around ADP F 600:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

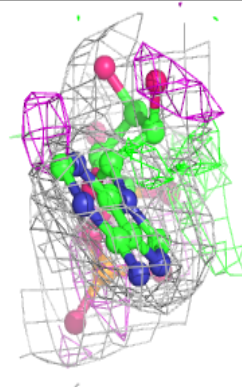
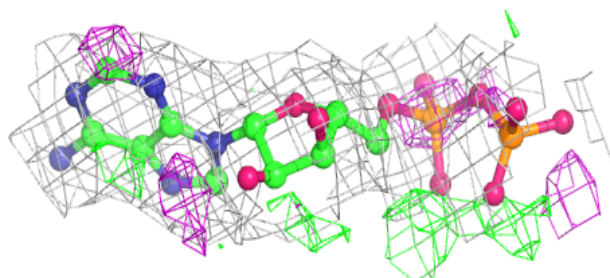
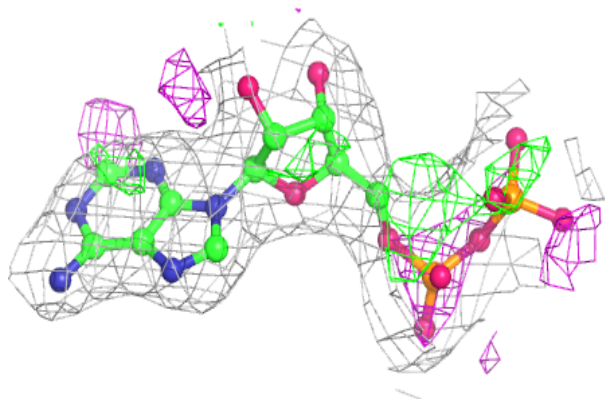
**Electron density around ADP G 600:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

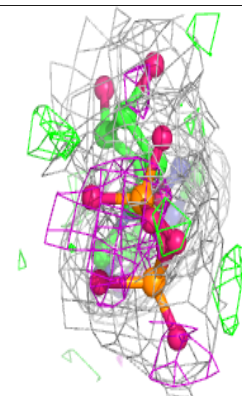
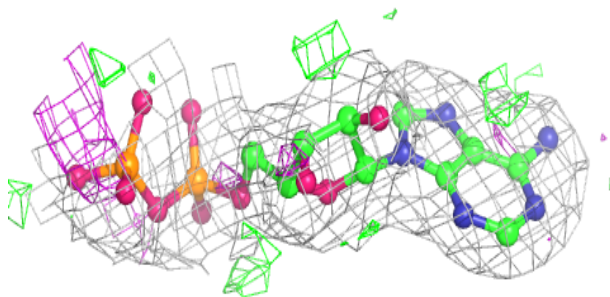
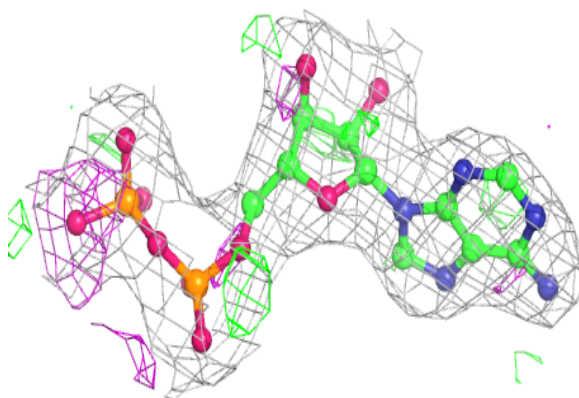


Electron density around ADP E 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

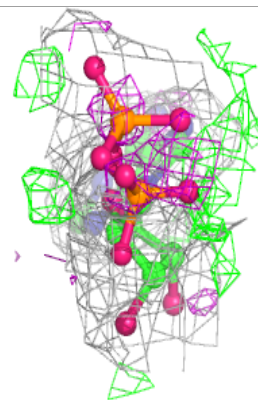
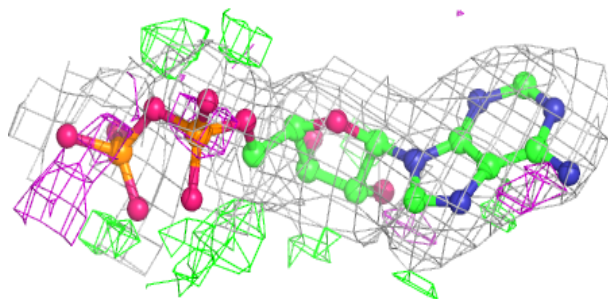
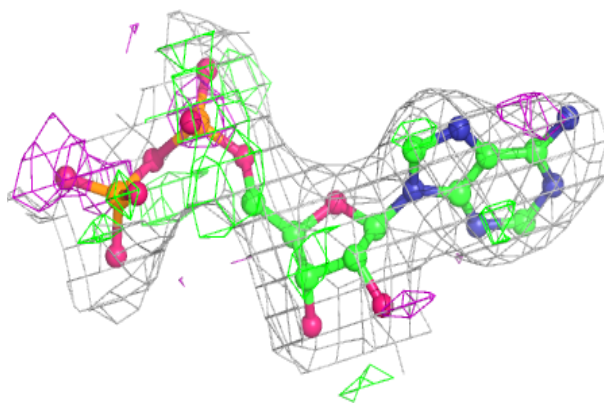
**Electron density around ADP D 600:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

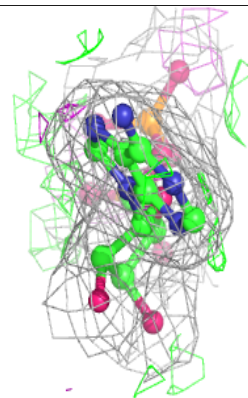
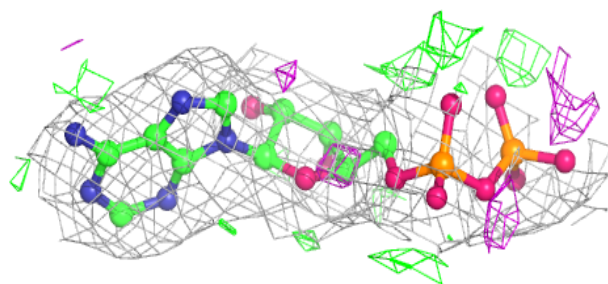
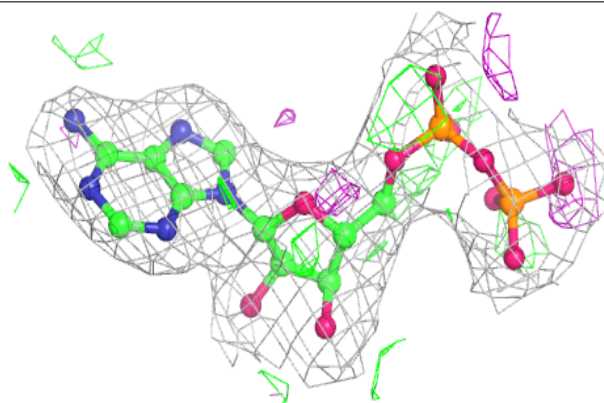


Electron density around ADP B 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP A 600:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.