



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:32 pm BST

PDB ID : 2JKT
Title : AP2 CLATHRIN ADAPTOR CORE with CD4 Dileucine peptide
RM(phosphoS) EIKRLLSE Q to E mutant
Authors : Owen, D.J.; McCoy, A.J.; Kelly, B.T.; Evans, P.R.
Deposited on : 2008-08-29
Resolution : 3.40 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
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

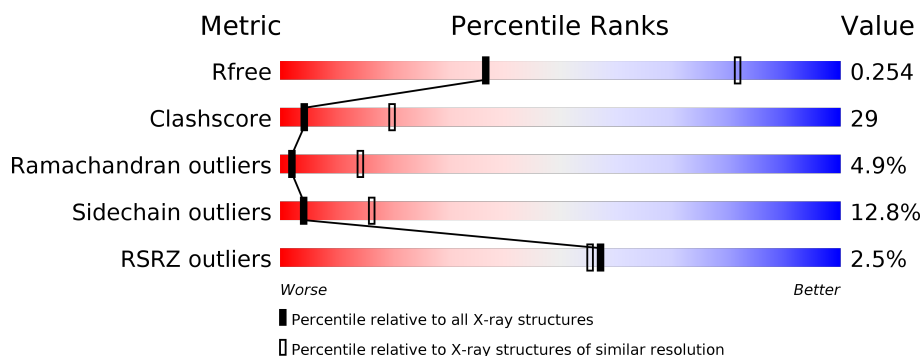
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	623	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>41%</div> <div>8%</div> <div>.</div> </div> </div>
1	L	623	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>41%</div> <div>9%</div> <div>.</div> </div> </div>
2	B	591	<div> <div>2%</div> <div> <div></div> <div>40%</div> <div>47%</div> <div>9%</div> <div>..</div> </div> </div>
2	E	591	<div> <div>4%</div> <div> <div></div> <div>38%</div> <div>48%</div> <div>10%</div> <div>..</div> </div> </div>
3	I	142	<div> <div></div> <div> <div>57%</div> <div>36%</div> <div>7%</div> </div> </div>
3	S	142	<div> <div></div> <div> <div>53%</div> <div>40%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	M	435	
4	U	435	
5	P	11	
5	Q	11	

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	SO4	A	1624	-	-	X	-
6	SO4	A	1627	-	-	X	-
6	SO4	A	1630	-	-	-	X
6	SO4	E	1586	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28120 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 AP-2 COMPLEX SUBUNIT ALPHA-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	0	0
			4885	3109	842	913	21			
1	L	621	Total	C	N	O	S	0	0	0
			4885	3109	842	913	21			

- Molecule 2 is a protein called AP-2 COMPLEX SUBUNIT BETA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	571	Total	C	N	O	S	0	0	0
			4527	2883	752	867	25			
2	E	571	Total	C	N	O	S	0	0	0
			4527	2883	752	867	25			

- Molecule 3 is a protein called AP-2 COMPLEX SUBUNIT SIGMA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	142	Total	C	N	O	S	0	0	0
			1200	778	200	215	7			
3	S	142	Total	C	N	O	S	0	0	0
			1200	778	200	215	7			

- Molecule 4 is a protein called AP-2 COMPLEX SUBUNIT MU-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	409	Total	C	N	O	S	0	0	0
			3288	2111	573	585	19			
4	U	409	Total	C	N	O	S	0	0	0
			3288	2111	573	585	19			

- Molecule 5 is a protein called CD4 PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	9	Total	C	N	O	S	0	0	0
			73	46	13	13	1			
5	Q	9	Total	C	N	O	S	0	0	0
			73	46	13	13	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	4	GLU	GLN	engineered mutation	UNP B0AZV7
Q	4	GLU	GLN	engineered mutation	UNP B0AZV7

- Molecule 6 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	U	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	U	1	Total	O	S	0	0
			5	4	1		
6	U	1	Total	O	S	0	0
			5	4	1		
6	U	1	Total	O	S	0	0
			5	4	1		

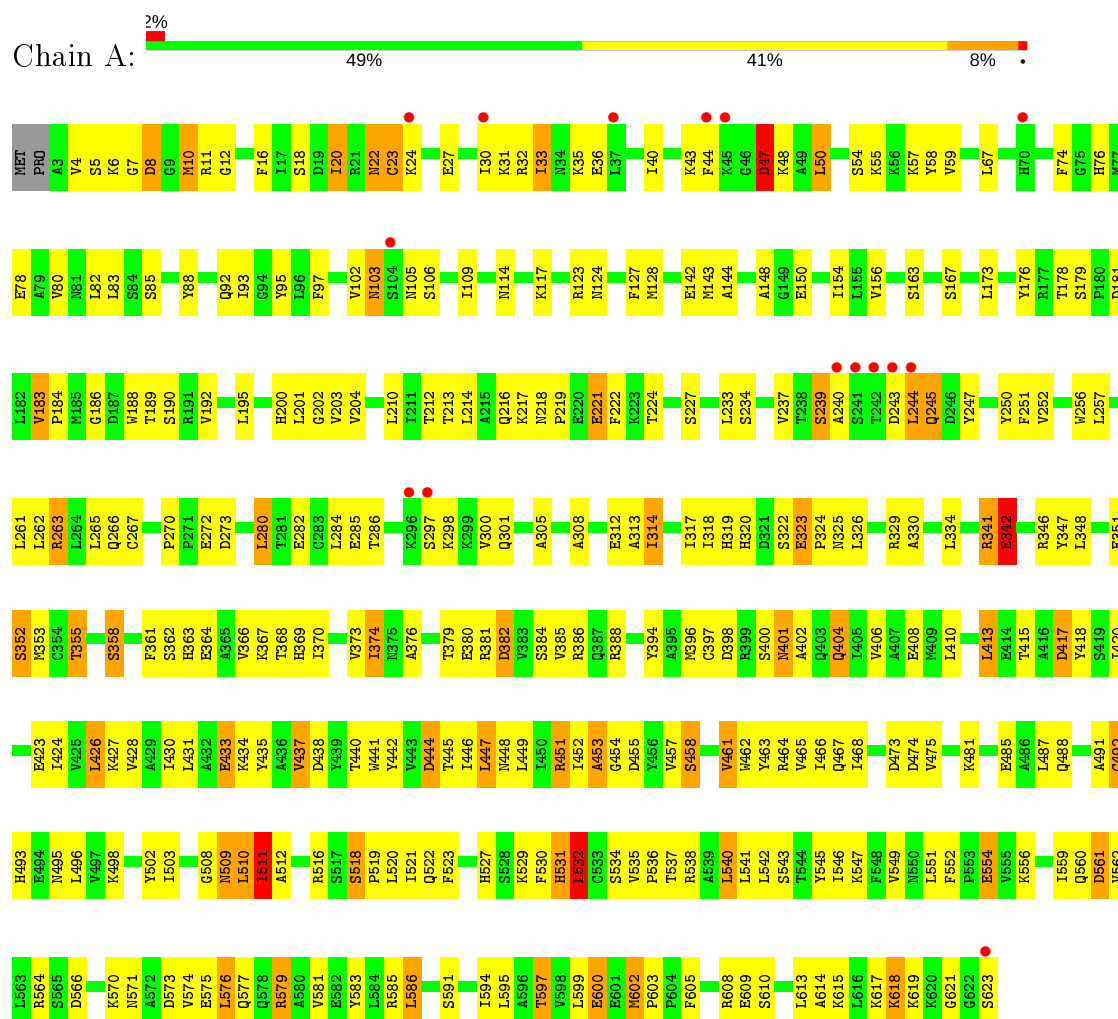
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	O	0	0
			2	2		
7	B	3	Total	O	0	0
			3	3		
7	E	3	Total	O	0	0
			3	3		
7	I	1	Total	O	0	0
			1	1		
7	L	2	Total	O	0	0
			2	2		
7	M	3	Total	O	0	0
			3	3		
7	Q	1	Total	O	0	0
			1	1		
7	S	3	Total	O	0	0
			3	3		
7	U	1	Total	O	0	0
			1	1		

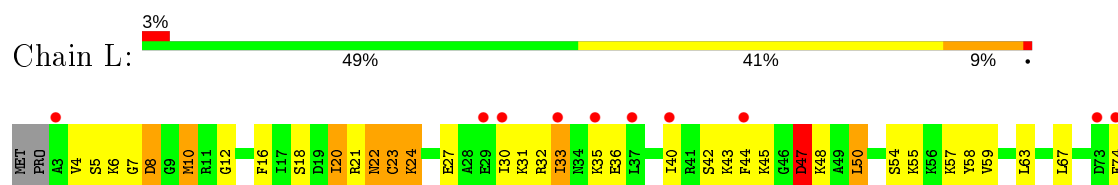
3 Residue-property plots [i](#)

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

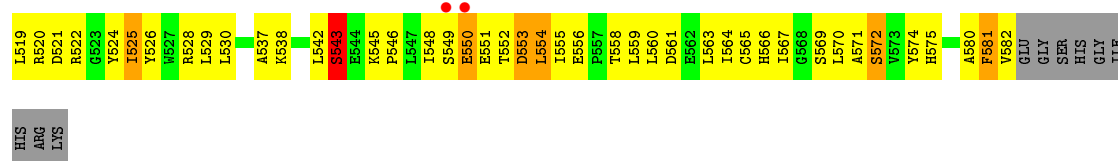
• Molecule 1: AP-2 COMPLEX SUBUNIT ALPHA-2



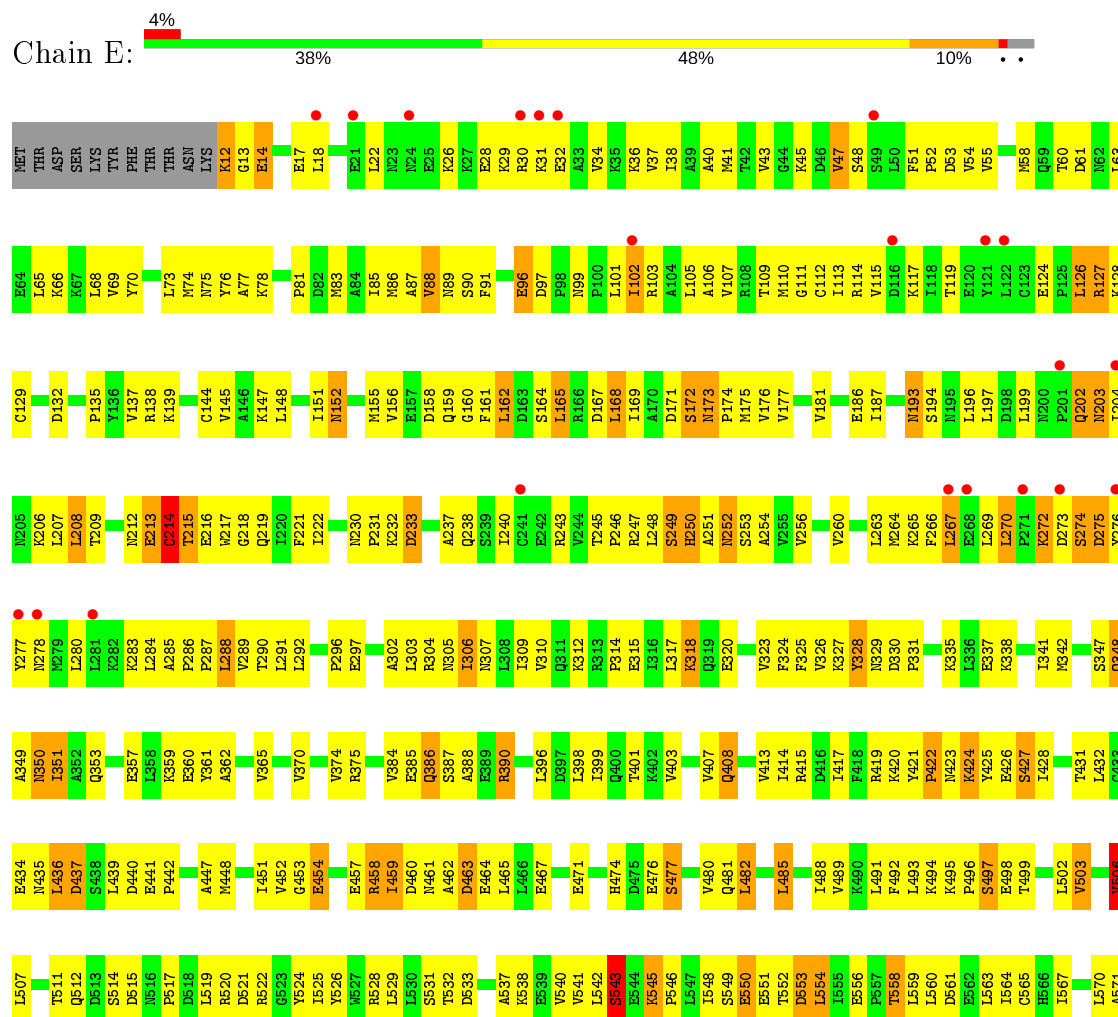
• Molecule 1: AP-2 COMPLEX SUBUNIT ALPHA-2



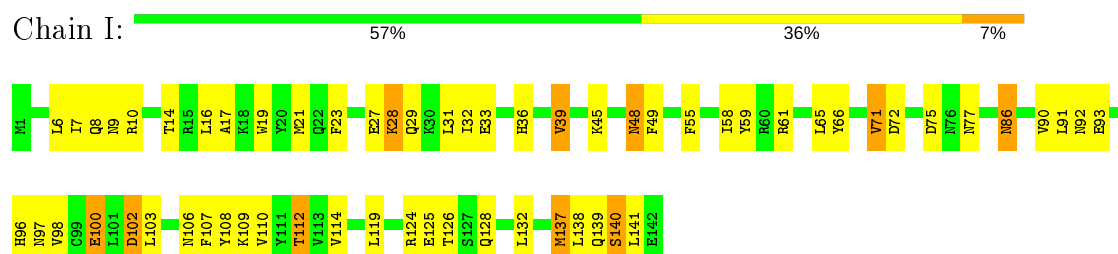




● Molecule 2: AP-2 COMPLEX SUBUNIT BETA-1

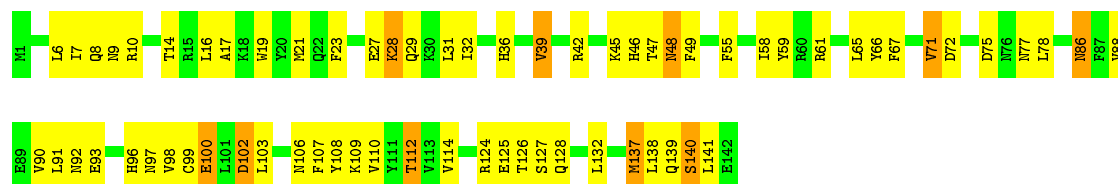


- Molecule 3: AP-2 COMPLEX SUBUNIT SIGMA-1



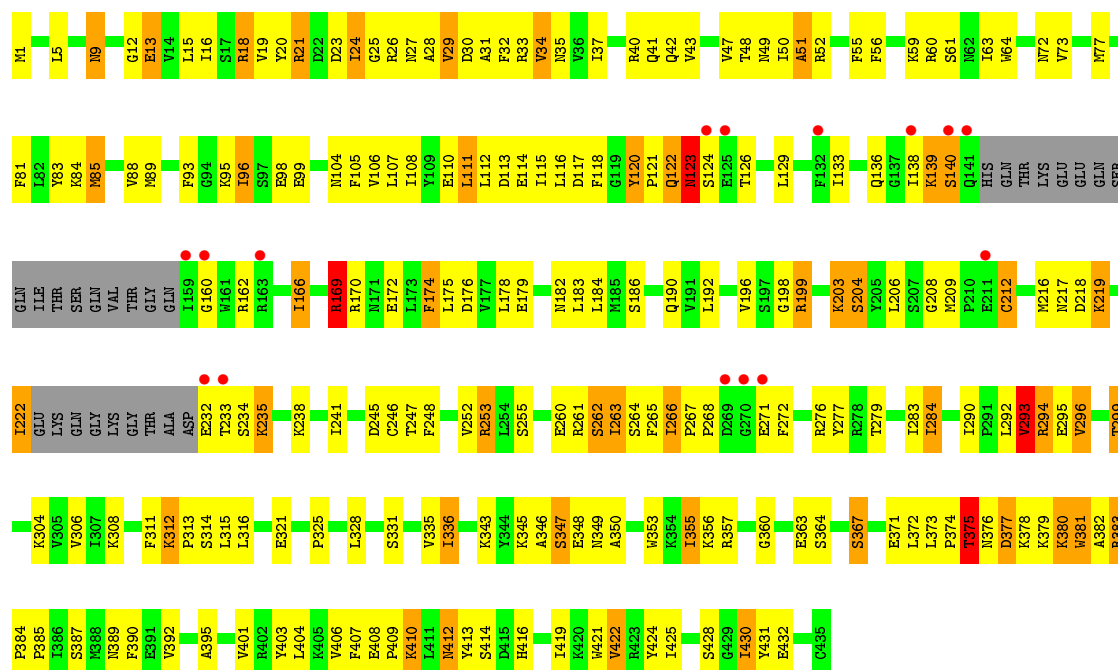
• Molecule 3: AP-2 COMPLEX SUBUNIT SIGMA-1

Chain S: 




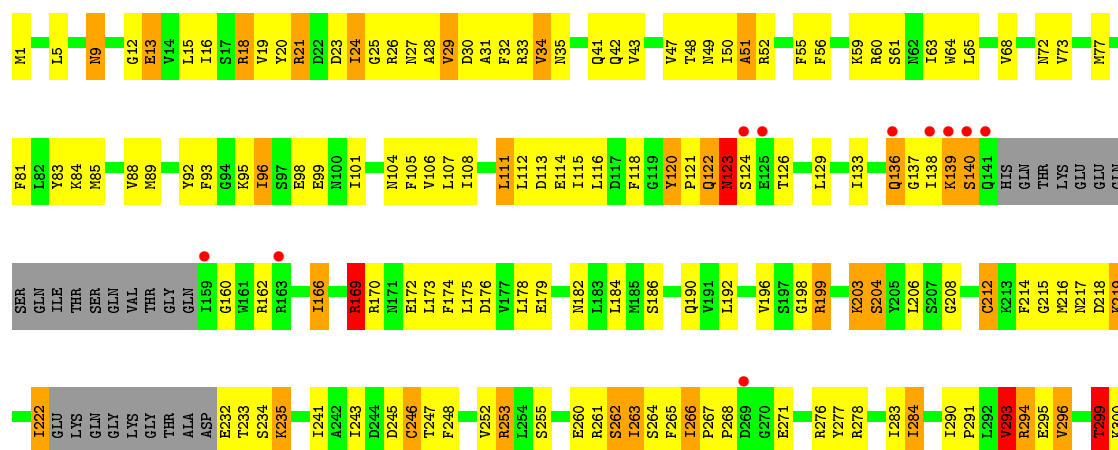
• Molecule 4: AP-2 COMPLEX SUBUNIT MU-1

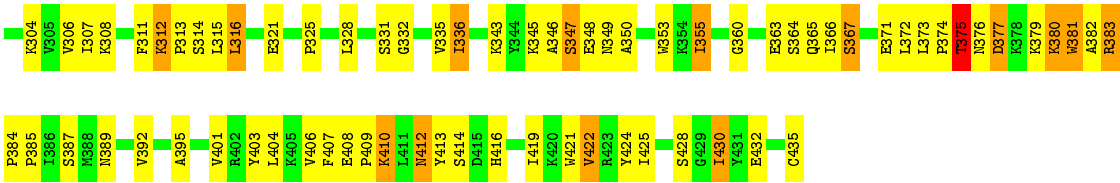
Chain M: 



• Molecule 4: AP-2 COMPLEX SUBUNIT MU-1

Chain U: 

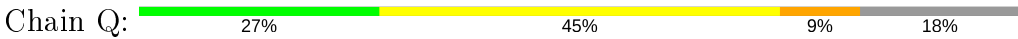




• Molecule 5: CD4 PEPTIDE



• Molecule 5: CD4 PEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	171.20 Å 171.20 Å 324.27 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.70 – 3.40 45.70 – 3.40	Depositor EDS
% Data completeness (in resolution range)	91.7 (45.70-3.40) 95.7 (45.70-3.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.40 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.202 , 0.256 0.201 , 0.254	Depositor DCC
R_{free} test set	3257 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28120	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: SO4, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.42	0/4970	0.61	0/6734
1	L	0.41	0/4970	0.61	0/6734
2	B	0.40	0/4597	0.61	0/6236
2	E	0.40	0/4597	0.61	0/6236
3	I	0.46	0/1224	0.63	0/1650
3	S	0.44	0/1224	0.64	0/1650
4	M	0.44	0/3353	0.62	0/4513
4	U	0.44	0/3353	0.63	0/4513
5	P	0.40	0/65	0.56	0/82
5	Q	0.40	0/65	0.62	0/82
All	All	0.42	0/28418	0.61	0/38430

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4885	0	4999	292	0
1	L	4885	0	4999	303	1
2	B	4527	0	4646	308	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	4527	0	4646	319	0
3	I	1200	0	1195	67	0
3	S	1200	0	1195	77	0
4	M	3288	0	3382	193	0
4	U	3288	0	3382	191	0
5	P	73	0	81	15	0
5	Q	73	0	81	14	0
6	A	35	0	0	5	0
6	B	25	0	0	0	0
6	E	20	0	0	5	0
6	L	40	0	0	0	0
6	M	15	0	0	1	0
6	U	20	0	0	1	0
7	A	2	0	0	0	0
7	B	3	0	0	1	0
7	E	3	0	0	1	0
7	I	1	0	0	0	0
7	L	2	0	0	0	1
7	M	3	0	0	0	0
7	Q	1	0	0	0	0
7	S	3	0	0	0	0
7	U	1	0	0	0	0
All	All	28120	0	28606	1654	1

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 29.

All (1654) 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)
3:I:92:ASN:HD22	3:I:98:VAL:HG12	1.18	1.07
4:M:115:ILE:HD13	4:M:124:SER:HB2	1.35	1.07
3:S:92:ASN:HD22	3:S:98:VAL:HG12	1.19	1.05
2:E:174:PRO:HB3	2:E:214:CYS:HA	1.39	1.05
1:L:20:ILE:HD11	1:L:33:ILE:HD11	1.40	1.04
4:U:115:ILE:HD13	4:U:124:SER:HB2	1.40	1.03
2:B:174:PRO:HB3	2:B:214:CYS:HA	1.41	1.02
1:A:20:ILE:HD11	1:A:33:ILE:HD11	1.46	0.98
1:L:402:ALA:O	1:L:406:VAL:HG23	1.66	0.95
2:E:390:ARG:HH11	2:E:390:ARG:HB3	1.33	0.93
2:B:390:ARG:HB3	2:B:390:ARG:HH11	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20:ILE:HD11	1:L:33:ILE:CD1	2.00	0.92
4:M:176:ASP:HB3	4:M:178:LEU:HD21	1.52	0.92
1:L:579:ARG:HG2	1:L:579:ARG:HH11	1.35	0.91
1:A:381:ARG:O	1:A:382:ASP:HB3	1.70	0.91
3:I:16:LEU:HD21	3:I:114:VAL:HG21	1.51	0.90
4:U:222:ILE:HD12	4:U:222:ILE:H	1.35	0.90
2:E:127:ARG:HH11	2:E:127:ARG:HG2	1.34	0.90
1:L:381:ARG:O	1:L:382:ASP:HB3	1.71	0.90
3:I:86:ASN:HB2	3:I:128:GLN:HE21	1.36	0.90
4:M:222:ILE:H	4:M:222:ILE:HD12	1.36	0.90
2:B:127:ARG:HG2	2:B:127:ARG:HH11	1.36	0.89
2:B:302:ALA:O	2:B:306:ILE:HG12	1.72	0.89
3:S:86:ASN:HB2	3:S:128:GLN:HE21	1.35	0.89
1:A:402:ALA:O	1:A:406:VAL:HG23	1.72	0.89
2:B:434:GLU:HG3	2:B:435:ASN:HD22	1.35	0.89
1:A:20:ILE:HD11	1:A:33:ILE:CD1	2.04	0.88
2:E:434:GLU:HG3	2:E:435:ASN:HD22	1.35	0.88
2:E:434:GLU:HG3	2:E:435:ASN:ND2	1.88	0.88
2:E:55:VAL:O	2:E:58:MET:HB2	1.73	0.87
1:L:487:LEU:HD23	1:L:496:LEU:HD23	1.57	0.87
2:B:55:VAL:O	2:B:58:MET:HB2	1.74	0.87
3:S:16:LEU:HD21	3:S:114:VAL:HG21	1.54	0.87
1:A:50:LEU:H	1:A:50:LEU:HD12	1.41	0.86
4:U:176:ASP:HB3	4:U:178:LEU:HD21	1.57	0.86
1:A:381:ARG:HD2	3:S:45:LYS:HD2	1.57	0.86
2:E:302:ALA:O	2:E:306:ILE:HG12	1.76	0.85
1:L:508:GLY:H	1:L:510:LEU:CD1	1.89	0.85
3:S:19:TRP:CZ2	3:S:28:LYS:HG3	2.12	0.85
1:A:487:LEU:HD23	1:A:496:LEU:HD23	1.59	0.85
3:I:19:TRP:CZ2	3:I:28:LYS:HG3	2.12	0.85
2:B:434:GLU:HG3	2:B:435:ASN:ND2	1.91	0.84
1:A:11:ARG:HB3	6:A:1625:SO4:O2	1.78	0.84
1:A:579:ARG:HG2	1:A:579:ARG:HH11	1.41	0.84
1:L:370:ILE:HG12	1:L:396:MET:HE1	1.60	0.83
1:A:44:PHE:CD1	1:A:78:GLU:HG2	2.13	0.83
1:L:540:LEU:HD12	1:L:540:LEU:O	1.78	0.83
2:E:482:LEU:HD23	1:L:575:GLU:OE1	1.79	0.83
1:L:50:LEU:H	1:L:50:LEU:HD12	1.44	0.82
1:A:609:GLU:OE1	1:L:610:SER:HB2	1.79	0.82
1:L:44:PHE:CD1	1:L:78:GLU:HG2	2.15	0.82
2:B:296:PRO:HB3	2:B:331:PRO:HG3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:615:LYS:H	1:L:623:SER:HB2	1.43	0.81
2:B:307:ASN:HD22	2:B:575:HIS:HE1	1.28	0.81
2:B:119:THR:HG21	2:B:152:ASN:HD22	1.44	0.81
4:U:186:SER:HB3	4:U:190:GLN:HB2	1.61	0.80
2:B:285:ALA:HB3	2:B:286:PRO:HD3	1.63	0.80
2:E:285:ALA:HB3	2:E:286:PRO:HD3	1.63	0.80
3:S:92:ASN:ND2	3:S:98:VAL:HG12	1.97	0.80
2:E:564:ILE:O	2:E:567:ILE:HG13	1.82	0.80
2:B:26:LYS:HD2	2:B:29:LYS:HD2	1.64	0.79
1:A:508:GLY:H	1:A:510:LEU:CD1	1.95	0.79
2:B:292:LEU:HD12	2:B:323:VAL:HG12	1.63	0.79
2:E:292:LEU:HD12	2:E:323:VAL:HG12	1.62	0.79
2:E:482:LEU:HD12	2:E:519:LEU:HD13	1.64	0.79
2:E:218:GLY:HA2	2:E:221:PHE:CD1	2.18	0.79
1:L:509:ASN:HB3	1:L:551:LEU:HD23	1.64	0.79
3:S:86:ASN:HB2	3:S:128:GLN:NE2	1.97	0.79
2:E:26:LYS:HD2	2:E:29:LYS:HD2	1.65	0.79
2:E:307:ASN:HD22	2:E:575:HIS:HE1	1.30	0.79
1:A:540:LEU:HD12	1:A:540:LEU:O	1.84	0.78
1:L:317:ILE:HD13	1:L:326:LEU:HB3	1.66	0.78
4:U:374:PRO:O	4:U:375:THR:HG22	1.83	0.78
4:M:9:ASN:HD22	4:M:9:ASN:C	1.87	0.78
2:E:495:LYS:O	2:E:499:THR:HG22	1.83	0.78
4:U:9:ASN:C	4:U:9:ASN:HD22	1.87	0.78
1:A:615:LYS:H	1:A:623:SER:HB2	1.48	0.78
2:E:216:GLU:HB3	2:E:250:HIS:HE1	1.48	0.77
3:I:86:ASN:HB2	3:I:128:GLN:NE2	2.00	0.77
4:U:172:GLU:HB3	4:U:419:ILE:HB	1.66	0.77
1:A:370:ILE:HG12	1:A:396:MET:HE3	1.66	0.77
2:B:495:LYS:O	2:B:499:THR:HG22	1.83	0.77
1:L:446:ILE:HG21	1:L:465:VAL:HG11	1.66	0.77
2:E:119:THR:HG21	2:E:152:ASN:HD22	1.49	0.77
4:M:186:SER:HB3	4:M:190:GLN:HB2	1.65	0.77
2:B:216:GLU:HB3	2:B:250:HIS:HE1	1.49	0.77
2:B:482:LEU:HD12	2:B:519:LEU:HD13	1.67	0.77
2:B:85:ILE:O	2:B:88:VAL:HG22	1.85	0.76
2:E:78:LYS:NZ	6:E:1586:SO4:O4	2.16	0.76
2:B:218:GLY:HA2	2:B:221:PHE:CD1	2.19	0.76
4:M:172:GLU:HB3	4:M:419:ILE:HB	1.66	0.76
2:E:40:ALA:HA	2:E:43:VAL:HG22	1.68	0.76
2:E:156:VAL:HG12	2:E:162:LEU:HD23	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:545:LYS:HG3	1:L:581:VAL:HG21	1.66	0.76
4:U:166:ILE:H	4:U:166:ILE:HD13	1.50	0.75
2:B:264:MET:HA	2:B:267:LEU:HD23	1.67	0.75
2:E:296:PRO:HB3	2:E:331:PRO:HG3	1.66	0.75
1:A:88:TYR:HB2	3:S:141:LEU:HD13	1.68	0.75
1:L:508:GLY:H	1:L:510:LEU:HD12	1.50	0.75
3:S:8:GLN:HE22	3:S:36:HIS:HB2	1.51	0.75
2:E:461:ASN:HB3	2:E:465:LEU:HG	1.66	0.75
2:E:78:LYS:HE3	2:E:112:CYS:SG	2.27	0.75
2:B:40:ALA:HA	2:B:43:VAL:HG22	1.69	0.74
1:A:380:GLU:O	1:A:386:ARG:HD2	1.87	0.74
2:E:263:LEU:HD22	2:E:280:LEU:HD11	1.68	0.74
1:A:509:ASN:HB3	1:A:551:LEU:HD23	1.67	0.74
2:B:570:LEU:HD22	2:B:574:TYR:CE2	2.21	0.74
1:L:614:ALA:HA	1:L:623:SER:CB	2.18	0.74
2:E:103:ARG:NH1	2:E:137:VAL:HG21	2.02	0.74
2:B:515:ASP:O	2:B:517:PRO:HD3	1.88	0.73
1:L:380:GLU:O	1:L:386:ARG:HD2	1.87	0.73
1:A:610:SER:HB2	1:L:609:GLU:OE1	1.89	0.73
1:A:200:HIS:HD2	1:A:203:VAL:H	1.34	0.73
2:B:156:VAL:HG12	2:B:162:LEU:HD23	1.69	0.73
1:L:200:HIS:HD2	1:L:203:VAL:H	1.36	0.73
2:E:482:LEU:HD21	1:L:579:ARG:HH21	1.54	0.73
2:B:286:PRO:O	2:B:290:THR:HG23	1.89	0.73
1:A:446:ILE:HG21	1:A:465:VAL:HG11	1.69	0.72
2:B:492:PHE:CD1	2:B:503:VAL:HG21	2.24	0.72
4:M:253:ARG:HB2	4:M:264:SER:O	1.89	0.72
4:U:31:ALA:O	4:U:35:ASN:HB2	1.89	0.72
1:A:575:GLU:OE1	2:B:482:LEU:HD23	1.89	0.72
2:E:327:LYS:HE2	2:E:330:ASP:OD2	1.89	0.72
2:B:488:ILE:HG21	2:B:506:VAL:HG21	1.72	0.72
2:B:312:LYS:HB2	2:B:560:LEU:HD21	1.70	0.72
3:I:92:ASN:ND2	3:I:98:VAL:HG12	1.99	0.72
2:E:85:ILE:HG12	2:E:113:ILE:HG21	1.71	0.72
4:U:26:ARG:HH22	4:U:33:ARG:HH21	1.36	0.72
1:A:358:SER:HB3	4:M:295:GLU:HB3	1.72	0.71
2:E:447:ALA:O	2:E:451:ILE:HG13	1.91	0.71
2:B:218:GLY:HA2	2:B:221:PHE:HD1	1.55	0.71
2:B:461:ASN:HB3	2:B:465:LEU:HG	1.69	0.71
2:E:515:ASP:O	2:E:517:PRO:HD3	1.89	0.71
4:M:26:ARG:HH22	4:M:33:ARG:HH21	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:HD13	1:A:355:THR:HG22	1.73	0.71
2:E:177:VAL:HB	2:E:214:CYS:SG	2.30	0.71
3:I:19:TRP:CE2	3:I:28:LYS:HG3	2.25	0.71
2:E:218:GLY:HA2	2:E:221:PHE:HD1	1.55	0.71
2:E:292:LEU:HD12	2:E:323:VAL:CG1	2.20	0.71
2:E:488:ILE:HG21	2:E:506:VAL:HG21	1.73	0.71
1:A:317:ILE:HD13	1:A:326:LEU:HB3	1.73	0.71
2:B:292:LEU:HD12	2:B:323:VAL:CG1	2.20	0.71
2:E:492:PHE:CD1	2:E:503:VAL:HG21	2.26	0.71
2:E:85:ILE:O	2:E:88:VAL:HG22	1.90	0.71
2:B:440:ASP:HB3	4:M:316:LEU:HD12	1.73	0.71
2:B:327:LYS:HE2	2:B:330:ASP:OD2	1.91	0.71
4:M:374:PRO:O	4:M:375:THR:HG22	1.90	0.71
3:S:19:TRP:CE2	3:S:28:LYS:HG3	2.25	0.71
2:E:264:MET:HA	2:E:267:LEU:HD23	1.71	0.71
2:E:422:PRO:HB2	2:E:424:LYS:HB2	1.73	0.71
1:L:617:LYS:O	1:L:619:LYS:N	2.21	0.71
2:B:85:ILE:HG12	2:B:113:ILE:HG21	1.72	0.71
1:L:250:TYR:CD2	1:L:301:GLN:HB2	2.26	0.71
4:U:182:ASN:ND2	4:U:430:ILE:H	1.87	0.71
4:U:293:VAL:HG22	4:U:294:ARG:H	1.56	0.71
2:E:489:VAL:O	2:E:493:LEU:HD12	1.91	0.70
2:E:97:ASP:OD2	2:E:102:ILE:HD11	1.90	0.70
1:A:510:LEU:H	1:A:510:LEU:HD12	1.56	0.70
3:I:16:LEU:HD21	3:I:114:VAL:CG2	2.21	0.70
5:P:4:GLU:HB3	3:S:100:GLU:HB3	1.72	0.70
1:L:334:LEU:HD11	1:L:352:SER:HB3	1.73	0.70
4:M:166:ILE:HD13	4:M:166:ILE:H	1.55	0.70
3:S:48:ASN:H	3:S:48:ASN:HD22	1.40	0.70
4:M:31:ALA:O	4:M:35:ASN:HB2	1.91	0.70
4:U:253:ARG:HB2	4:U:264:SER:O	1.91	0.70
1:A:272:GLU:CD	1:A:272:GLU:H	1.93	0.70
2:B:489:VAL:O	2:B:493:LEU:HD12	1.92	0.70
1:A:40:ILE:HG23	1:A:58:TYR:HB3	1.73	0.70
2:B:284:LEU:O	2:B:288:LEU:HD22	1.91	0.70
4:M:169:ARG:HH11	4:M:169:ARG:HB3	1.57	0.70
2:B:457:GLU:OE1	2:B:494:LYS:HE2	1.92	0.70
1:A:12:GLY:HA3	1:A:57:LYS:HE3	1.73	0.70
4:M:293:VAL:HG13	4:M:294:ARG:N	2.05	0.70
2:B:169:ILE:HD11	2:B:206:LYS:NZ	2.07	0.70
1:A:250:TYR:CD2	1:A:301:GLN:HB2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:LYS:O	1:A:619:LYS:N	2.24	0.69
2:E:174:PRO:HB3	2:E:214:CYS:CA	2.19	0.69
1:L:272:GLU:H	1:L:272:GLU:CD	1.94	0.69
4:U:81:PHE:HE1	4:U:115:ILE:HG13	1.57	0.69
1:L:12:GLY:HA3	1:L:57:LYS:HE3	1.72	0.69
2:B:177:VAL:HB	2:B:214:CYS:SG	2.33	0.69
2:B:28:GLU:O	2:B:32:GLU:HG2	1.93	0.69
2:E:28:GLU:O	2:E:32:GLU:HG2	1.93	0.69
1:L:31:LYS:O	1:L:35:LYS:HG3	1.93	0.69
2:B:78:LYS:HE3	2:B:112:CYS:SG	2.33	0.69
1:A:218:ASN:N	1:A:219:PRO:HD3	2.07	0.69
2:B:249:SER:O	2:B:251:ALA:N	2.25	0.69
1:L:178:THR:HG22	1:L:179:SER:OG	1.92	0.69
2:B:306:ILE:O	2:B:310:VAL:HG22	1.93	0.69
2:E:169:ILE:HD11	2:E:206:LYS:NZ	2.08	0.69
4:M:21:ARG:HH11	4:M:21:ARG:HB2	1.57	0.69
2:E:208:LEU:HD13	2:E:243:ARG:HE	1.58	0.68
1:L:546:ILE:HD13	1:L:583:TYR:HB3	1.74	0.68
2:B:422:PRO:HB2	2:B:424:LYS:HB2	1.75	0.68
2:E:286:PRO:O	2:E:290:THR:HG23	1.93	0.68
3:I:8:GLN:HE22	3:I:36:HIS:HB2	1.56	0.68
2:B:263:LEU:HD22	2:B:280:LEU:HD11	1.75	0.68
1:L:556:LYS:O	1:L:560:GLN:HB2	1.94	0.68
2:B:103:ARG:NH1	2:B:137:VAL:HG21	2.08	0.68
2:E:312:LYS:HB2	2:E:560:LEU:HD21	1.75	0.68
1:A:178:THR:HG22	1:A:179:SER:OG	1.93	0.68
3:I:61:ARG:HD2	3:I:66:TYR:CE1	2.29	0.68
1:L:218:ASN:N	1:L:219:PRO:HD3	2.09	0.68
1:L:47:ASP:OD2	1:L:48:LYS:HG3	1.93	0.68
1:L:615:LYS:N	1:L:623:SER:HB2	2.08	0.68
2:E:193:ASN:HD22	2:E:194:SER:H	1.39	0.68
1:L:464:ARG:O	1:L:468:ILE:HG13	1.94	0.68
2:B:447:ALA:O	2:B:451:ILE:HG13	1.93	0.68
2:B:423:ASN:O	2:B:425:TYR:N	2.27	0.67
2:E:457:GLU:OE1	2:E:494:LYS:HE2	1.94	0.67
1:L:358:SER:HB3	4:U:295:GLU:HB3	1.75	0.67
1:A:508:GLY:H	1:A:510:LEU:HD11	1.59	0.67
1:A:47:ASP:OD2	1:A:48:LYS:HG3	1.95	0.67
2:B:127:ARG:CG	2:B:127:ARG:HH11	2.07	0.67
2:B:564:ILE:O	2:B:567:ILE:HG13	1.95	0.67
2:E:284:LEU:O	2:E:288:LEU:HD22	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:423:ASN:O	2:E:425:TYR:N	2.25	0.67
4:U:198:GLY:O	4:U:199:ARG:HB2	1.94	0.67
2:B:174:PRO:HB3	2:B:214:CYS:CA	2.22	0.67
2:B:193:ASN:HD22	2:B:194:SER:H	1.41	0.67
2:B:208:LEU:HD13	2:B:243:ARG:HE	1.60	0.67
3:I:48:ASN:HD22	3:I:48:ASN:H	1.43	0.67
2:B:581:PHE:HA	4:M:52:ARG:HG2	1.77	0.67
1:L:508:GLY:H	1:L:510:LEU:HD11	1.60	0.67
2:E:312:LYS:HE2	2:E:561:ASP:OD1	1.95	0.67
2:B:97:ASP:OD2	2:B:102:ILE:HD11	1.95	0.66
2:E:215:THR:O	2:E:219:GLN:HG3	1.94	0.66
3:I:141:LEU:HD13	1:L:88:TYR:HB2	1.78	0.66
3:S:102:ASP:O	3:S:106:ASN:HB2	1.96	0.66
2:B:215:THR:O	2:B:219:GLN:HG3	1.96	0.66
4:M:21:ARG:HB2	4:M:21:ARG:NH1	2.10	0.66
1:A:54:SER:O	1:A:58:TYR:HD1	1.79	0.66
2:E:193:ASN:HD22	2:E:194:SER:N	1.93	0.66
4:U:21:ARG:HH11	4:U:21:ARG:HB2	1.60	0.66
1:A:381:ARG:O	1:A:382:ASP:CB	2.43	0.66
2:B:305:ASN:HD21	2:B:572:SER:HB3	1.60	0.66
2:E:464:GLU:HA	2:E:467:GLU:HB3	1.78	0.66
1:A:556:LYS:O	1:A:560:GLN:HB2	1.96	0.66
2:B:193:ASN:HD22	2:B:194:SER:N	1.94	0.66
2:B:78:LYS:HZ3	4:M:18:ARG:NH1	1.93	0.65
3:S:92:ASN:HD21	3:S:97:ASN:HA	1.60	0.65
4:U:169:ARG:HB3	4:U:169:ARG:HH11	1.61	0.65
2:B:326:VAL:CG1	2:B:335:LYS:HG2	2.27	0.65
1:L:318:ILE:HD13	1:L:355:THR:HG22	1.78	0.65
1:L:20:ILE:CD1	1:L:33:ILE:HD11	2.22	0.65
4:M:424:TYR:O	4:M:425:ILE:HD13	1.96	0.65
1:A:597:THR:HG21	1:L:324:PRO:HG3	1.79	0.65
2:E:103:ARG:HH11	2:E:137:VAL:HG21	1.60	0.65
4:U:379:LYS:C	4:U:381:TRP:H	2.00	0.65
1:A:324:PRO:HG3	1:L:597:THR:HG21	1.79	0.65
2:B:398:LEU:O	2:B:401:THR:HG23	1.96	0.65
2:E:115:VAL:HG12	2:E:117:LYS:H	1.62	0.65
1:A:546:ILE:HD13	1:A:583:TYR:HB3	1.78	0.65
1:L:54:SER:O	1:L:58:TYR:HD1	1.78	0.65
4:M:182:ASN:ND2	4:M:430:ILE:H	1.94	0.65
2:B:135:PRO:HG3	2:B:138:ARG:NH2	2.11	0.65
2:B:511:THR:HG23	2:B:524:TYR:CZ	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:GLU:OE2	4:M:118:PHE:HE2	1.79	0.65
4:M:32:PHE:HB2	4:M:55:PHE:CE2	2.31	0.65
1:L:40:ILE:HG23	1:L:58:TYR:HB3	1.78	0.65
1:L:614:ALA:HA	1:L:623:SER:HB3	1.79	0.65
4:U:216:MET:H	4:U:261:ARG:CB	2.10	0.65
2:B:115:VAL:HG12	2:B:117:LYS:H	1.63	0.65
2:B:324:PHE:O	2:B:338:LYS:HD2	1.97	0.65
1:L:508:GLY:N	1:L:510:LEU:HD12	2.12	0.65
4:U:343:LYS:HE2	4:U:345:LYS:HE3	1.79	0.65
3:S:138:LEU:O	3:S:139:GLN:HB3	1.97	0.64
4:U:21:ARG:HB2	4:U:21:ARG:NH1	2.12	0.64
2:E:375:ARG:HD3	6:E:1585:SO4:O4	1.96	0.64
3:I:102:ASP:O	3:I:106:ASN:HB2	1.96	0.64
3:I:138:LEU:O	3:I:139:GLN:HB3	1.96	0.64
1:L:618:LYS:O	1:L:619:LYS:HG2	1.97	0.64
3:S:61:ARG:HD2	3:S:66:TYR:CE1	2.33	0.64
1:A:250:TYR:CD2	1:A:301:GLN:CB	2.80	0.64
2:E:571:ALA:H	4:U:72:ASN:HD21	1.44	0.64
1:A:615:LYS:N	1:A:623:SER:HB2	2.13	0.64
2:B:464:GLU:HA	2:B:467:GLU:HB3	1.78	0.64
1:L:318:ILE:HG21	1:L:355:THR:HG22	1.78	0.64
5:P:2:MET:HE1	3:S:10:ARG:H	1.61	0.64
4:U:32:PHE:HB2	4:U:55:PHE:CE2	2.32	0.64
1:A:614:ALA:HA	1:A:623:SER:CB	2.27	0.64
2:B:312:LYS:HE2	2:B:561:ASP:OD1	1.96	0.64
2:B:365:VAL:HG22	4:M:422:VAL:CG1	2.28	0.64
2:B:554:LEU:H	2:B:554:LEU:HD12	1.61	0.64
1:L:173:LEU:HD11	1:L:213:THR:HB	1.80	0.64
1:L:510:LEU:H	1:L:510:LEU:HD12	1.62	0.64
4:M:343:LYS:HE2	4:M:345:LYS:HE3	1.79	0.64
3:S:16:LEU:HD21	3:S:114:VAL:CG2	2.26	0.64
2:B:318:LYS:HE3	2:B:318:LYS:O	1.97	0.64
2:E:306:ILE:O	2:E:310:VAL:HG22	1.98	0.64
4:M:81:PHE:HE1	4:M:115:ILE:HG13	1.62	0.64
5:P:4:GLU:HB3	3:S:100:GLU:CB	2.27	0.64
1:A:7:GLY:O	1:A:8:ASP:HB2	1.98	0.63
2:E:74:MET:SD	2:E:109:THR:HG22	2.37	0.63
2:E:581:PHE:HA	4:U:52:ARG:HG2	1.80	0.63
1:L:250:TYR:CD2	1:L:301:GLN:CB	2.81	0.63
2:E:390:ARG:HH11	2:E:390:ARG:CB	2.11	0.63
4:M:299:THR:O	4:M:372:LEU:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:VAL:HG12	2:B:69:VAL:HG13	1.79	0.63
2:E:570:LEU:HD22	2:E:574:TYR:CE2	2.33	0.63
3:S:14:THR:OG1	3:S:32:ILE:HD13	1.98	0.63
1:A:534:SER:OG	1:A:536:PRO:HD2	1.99	0.63
4:M:379:LYS:C	4:M:381:TRP:H	2.02	0.63
1:A:173:LEU:HD13	1:A:210:LEU:HA	1.81	0.63
1:A:31:LYS:O	1:A:35:LYS:HG3	1.98	0.63
1:L:7:GLY:O	1:L:8:ASP:HB2	1.99	0.63
2:B:571:ALA:H	4:M:72:ASN:HD21	1.45	0.63
4:U:50:ILE:O	4:U:51:ALA:HB3	1.97	0.63
1:A:342:GLU:O	1:A:346:ARG:HD3	1.98	0.63
2:B:284:LEU:O	2:B:287:PRO:HD2	1.99	0.63
4:M:343:LYS:HE2	4:M:345:LYS:CE	2.29	0.63
2:E:127:ARG:HH11	2:E:127:ARG:CG	2.07	0.62
2:E:413:VAL:O	2:E:417:ILE:HG13	1.99	0.62
4:M:410:LYS:H	4:M:410:LYS:HD3	1.64	0.62
1:A:20:ILE:CD1	1:A:33:ILE:HD11	2.27	0.62
1:A:602:MET:HE1	2:B:521:ASP:HA	1.81	0.62
1:A:263:ARG:HD3	1:A:312:GLU:OE2	1.97	0.62
2:B:103:ARG:HH11	2:B:137:VAL:HG21	1.64	0.62
2:E:318:LYS:O	2:E:318:LYS:HE3	1.99	0.62
4:U:162:ARG:HD2	4:U:267:PRO:O	1.99	0.62
4:U:299:THR:O	4:U:372:LEU:HB2	2.00	0.62
2:E:249:SER:O	2:E:251:ALA:N	2.28	0.62
1:L:109:ILE:HG21	1:L:142:GLU:HG2	1.81	0.62
4:M:385:PRO:HB2	4:M:432:GLU:HB3	1.80	0.62
4:M:59:LYS:HE3	4:M:64:TRP:CZ2	2.34	0.62
2:B:511:THR:HG23	2:B:524:TYR:CE1	2.34	0.62
2:B:493:LEU:HD22	2:B:538:LYS:HA	1.82	0.62
2:B:580:ALA:C	2:B:581:PHE:HD2	2.03	0.62
3:I:45:LYS:HD2	1:L:381:ARG:HD2	1.81	0.62
1:A:464:ARG:O	1:A:468:ILE:HG13	1.99	0.62
1:A:508:GLY:H	1:A:510:LEU:HD12	1.61	0.62
2:E:284:LEU:O	2:E:287:PRO:HD2	1.99	0.62
1:L:59:VAL:HG21	1:L:82:LEU:HD11	1.81	0.62
1:L:36:GLU:O	1:L:40:ILE:HG13	1.99	0.62
1:L:464:ARG:HH11	1:L:467:GLN:HE21	1.48	0.62
4:M:20:TYR:CZ	4:M:116:LEU:HD23	2.35	0.62
3:S:48:ASN:N	3:S:48:ASN:HD22	1.98	0.62
4:U:385:PRO:HB2	4:U:432:GLU:HB3	1.81	0.61
3:I:100:GLU:HB3	5:Q:4:GLU:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:579:ARG:NH1	1:L:579:ARG:HG2	2.03	0.61
4:U:410:LYS:HD3	4:U:410:LYS:H	1.65	0.61
2:B:476:GLU:OE1	2:B:480:VAL:HG21	2.00	0.61
2:E:305:ASN:HD21	2:E:572:SER:HB3	1.66	0.61
2:E:63:LEU:HD21	2:E:101:LEU:HD12	1.82	0.61
1:L:381:ARG:O	1:L:382:ASP:CB	2.46	0.61
4:U:20:TYR:CZ	4:U:116:LEU:HD23	2.35	0.61
4:U:217:ASN:HB2	6:U:1436:SO4:O1	2.01	0.61
4:U:59:LYS:HE3	4:U:64:TRP:CZ2	2.35	0.61
4:U:99:GLU:HA	4:U:99:GLU:OE2	2.00	0.61
2:E:326:VAL:CG1	2:E:335:LYS:HG2	2.31	0.61
2:E:365:VAL:CG1	4:U:401:VAL:HG12	2.31	0.61
1:L:449:LEU:H	1:L:449:LEU:HD12	1.64	0.61
2:B:73:LEU:HD13	2:B:91:PHE:CZ	2.36	0.61
2:E:106:ALA:O	2:E:110:MET:HB2	2.01	0.61
1:A:619:LYS:HD3	2:E:471:GLU:OE1	2.00	0.61
3:I:14:THR:OG1	3:I:32:ILE:HD13	2.00	0.61
1:L:318:ILE:HG21	1:L:355:THR:CG2	2.30	0.61
1:A:173:LEU:HD11	1:A:213:THR:HB	1.82	0.61
1:A:591:SER:HB2	1:A:594:ILE:H	1.65	0.61
3:S:86:ASN:CB	3:S:128:GLN:HE21	2.10	0.61
2:B:305:ASN:ND2	2:B:572:SER:HB3	2.15	0.61
2:E:435:ASN:C	2:E:437:ASP:H	2.05	0.61
4:M:293:VAL:HG22	4:M:294:ARG:H	1.65	0.61
2:B:326:VAL:HG13	2:B:335:LYS:HG2	1.83	0.60
2:E:216:GLU:HB3	2:E:250:HIS:CE1	2.33	0.60
2:E:511:THR:HG23	2:E:524:TYR:CZ	2.36	0.60
2:E:554:LEU:H	2:E:554:LEU:HD12	1.66	0.60
1:L:520:LEU:O	1:L:520:LEU:HG	2.00	0.60
4:U:343:LYS:HE2	4:U:345:LYS:CE	2.31	0.60
1:A:36:GLU:O	1:A:40:ILE:HG13	2.01	0.60
2:B:270:LEU:C	2:B:270:LEU:HD23	2.21	0.60
2:E:135:PRO:HG3	2:E:138:ARG:NH2	2.15	0.60
2:E:22:LEU:O	2:E:30:ARG:HG2	2.01	0.60
2:E:73:LEU:HD13	2:E:91:PHE:CZ	2.37	0.60
2:B:78:LYS:NZ	4:M:18:ARG:NH1	2.49	0.60
4:M:198:GLY:HA3	4:M:277:TYR:CE1	2.37	0.60
4:M:216:MET:H	4:M:261:ARG:CB	2.13	0.60
4:M:50:ILE:O	4:M:51:ALA:HB3	2.01	0.60
1:A:173:LEU:HD13	1:A:210:LEU:HD12	1.84	0.60
1:A:464:ARG:HH11	1:A:467:GLN:HE21	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ARG:NH1	1:A:579:ARG:HG2	2.09	0.60
2:B:307:ASN:HB2	7:B:2001:HOH:O	2.01	0.60
2:B:74:MET:SD	2:B:109:THR:HG22	2.41	0.60
2:E:493:LEU:HD22	2:E:538:LYS:HA	1.84	0.60
1:L:263:ARG:HD3	1:L:312:GLU:OE2	2.02	0.60
1:L:173:LEU:HD13	1:L:210:LEU:HA	1.84	0.60
2:B:272:LYS:NZ	2:B:278:ASN:HD21	2.00	0.60
2:B:51:PHE:O	2:B:55:VAL:HG23	2.02	0.60
2:E:148:LEU:HG	2:E:156:VAL:CG2	2.32	0.60
2:B:63:LEU:HD21	2:B:101:LEU:HD12	1.83	0.59
3:I:86:ASN:CB	3:I:128:GLN:HE21	2.13	0.59
2:E:520:ARG:HD3	1:L:605:PHE:CZ	2.37	0.59
2:E:87:ALA:HB3	2:E:91:PHE:HE2	1.67	0.59
3:I:92:ASN:HD21	3:I:97:ASN:HA	1.66	0.59
2:B:217:TRP:HE1	4:M:123:ASN:HA	1.67	0.59
4:M:252:VAL:HG13	4:M:263:ILE:HG23	1.83	0.59
2:B:106:ALA:O	2:B:110:MET:HB2	2.01	0.59
2:E:305:ASN:O	2:E:309:ILE:HG13	2.01	0.59
2:B:216:GLU:HB3	2:B:250:HIS:CE1	2.34	0.59
2:B:51:PHE:HB3	2:B:52:PRO:HD3	1.83	0.59
1:L:591:SER:HB2	1:L:594:ILE:H	1.66	0.59
4:M:40:ARG:HB2	6:M:1437:SO4:O4	2.01	0.59
2:E:272:LYS:NZ	2:E:278:ASN:HD21	2.01	0.59
4:M:162:ARG:HD2	4:M:267:PRO:O	2.02	0.59
2:B:491:LEU:HD11	2:B:495:LYS:HD2	1.83	0.59
2:E:297:GLU:HB2	4:U:83:TYR:OH	2.02	0.59
1:A:59:VAL:HG21	1:A:82:LEU:HD11	1.84	0.59
2:E:51:PHE:O	2:E:55:VAL:HG23	2.02	0.59
4:M:88:VAL:HG11	4:M:111:LEU:HD11	1.83	0.59
4:U:293:VAL:HG13	4:U:294:ARG:N	2.18	0.59
2:B:148:LEU:HG	2:B:156:VAL:CG2	2.33	0.59
1:L:523:PHE:CE1	1:L:559:ILE:HG12	2.38	0.59
1:A:334:LEU:HD11	1:A:352:SER:HB3	1.85	0.59
1:A:618:LYS:O	1:A:619:LYS:HG2	2.03	0.59
2:E:51:PHE:HB3	2:E:52:PRO:HD3	1.84	0.59
2:B:18:LEU:HD13	2:B:37:VAL:HG22	1.85	0.58
1:L:59:VAL:HG21	1:L:82:LEU:CD1	2.33	0.58
1:A:498:LYS:HE3	1:A:537:THR:OG1	2.02	0.58
2:B:169:ILE:HD11	2:B:206:LYS:HZ3	1.67	0.58
1:L:16:PHE:O	1:L:20:ILE:HB	2.03	0.58
2:E:324:PHE:O	2:E:338:LYS:HD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:471:GLU:OE1	1:L:619:LYS:HD3	2.03	0.58
4:M:99:GLU:OE2	4:M:99:GLU:HA	2.02	0.58
1:A:105:ASN:O	1:A:109:ILE:HD13	2.02	0.58
2:E:127:ARG:NH1	2:E:127:ARG:HG2	2.15	0.58
2:E:151:ILE:O	2:E:152:ASN:HB2	2.03	0.58
1:L:534:SER:OG	1:L:536:PRO:HD2	2.03	0.58
4:M:198:GLY:O	4:M:199:ARG:HB2	2.04	0.58
3:S:138:LEU:C	3:S:140:SER:H	2.06	0.58
2:B:151:ILE:O	2:B:152:ASN:HB2	2.03	0.58
2:B:574:TYR:CE1	4:M:49:ASN:HB2	2.39	0.58
1:L:4:VAL:HG12	1:L:5:SER:N	2.18	0.58
1:A:263:ARG:NH2	3:S:75:ASP:HA	2.19	0.58
1:A:449:LEU:H	1:A:449:LEU:HD12	1.67	0.58
2:E:511:THR:HG23	2:E:524:TYR:CE1	2.38	0.58
3:I:126:THR:HG21	1:L:256:TRP:HB2	1.85	0.58
4:U:312:LYS:HG3	4:U:313:PRO:CD	2.33	0.58
1:A:109:ILE:HG21	1:A:142:GLU:HG2	1.85	0.58
1:A:508:GLY:N	1:A:510:LEU:HD12	2.19	0.58
2:B:399:ILE:HG23	2:B:407:VAL:HG22	1.84	0.58
1:A:256:TRP:HB2	3:S:126:THR:HG21	1.85	0.58
2:B:435:ASN:C	2:B:437:ASP:H	2.07	0.58
2:E:362:ALA:HA	2:E:370:VAL:HG13	1.86	0.58
3:I:48:ASN:N	3:I:48:ASN:HD22	2.01	0.58
2:E:85:ILE:HD11	2:E:115:VAL:HB	1.86	0.58
4:M:179:GLU:CD	4:M:395:ALA:HB1	2.24	0.58
2:E:169:ILE:HD11	2:E:206:LYS:HZ2	1.68	0.58
2:E:514:SER:OG	2:E:519:LEU:HD23	2.04	0.58
1:L:614:ALA:HA	1:L:623:SER:HB2	1.84	0.58
2:B:362:ALA:HA	2:B:370:VAL:HG13	1.85	0.57
2:B:413:VAL:O	2:B:417:ILE:HG13	2.04	0.57
4:U:252:VAL:HG13	4:U:263:ILE:HG23	1.86	0.57
2:B:552:THR:O	2:B:553:ASP:HB2	2.04	0.57
4:U:424:TYR:O	4:U:425:ILE:HD13	2.05	0.57
1:A:433:GLU:HG3	1:A:433:GLU:O	2.04	0.57
1:A:579:ARG:HH21	2:B:482:LEU:HD21	1.68	0.57
2:B:554:LEU:N	2:B:554:LEU:HD12	2.19	0.57
2:E:256:VAL:O	2:E:260:VAL:HG23	2.04	0.57
3:S:6:LEU:HD21	3:S:32:ILE:HG12	1.85	0.57
2:B:22:LEU:O	2:B:30:ARG:HG2	2.04	0.57
2:B:408:GLN:HE22	2:B:440:ASP:H	1.50	0.57
2:E:217:TRP:HE1	4:U:123:ASN:HA	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:270:LEU:C	2:E:270:LEU:HD23	2.24	0.57
2:E:305:ASN:ND2	2:E:572:SER:HB3	2.19	0.57
4:M:216:MET:HG2	4:M:261:ARG:CB	2.34	0.57
4:U:81:PHE:CE1	4:U:115:ILE:HG13	2.39	0.57
1:A:318:ILE:HG21	1:A:355:THR:CG2	2.34	0.57
2:B:204:ILE:O	2:B:208:LEU:HB2	2.04	0.57
2:B:426:GLU:OE1	2:B:458:ARG:HG2	2.04	0.57
2:E:552:THR:O	2:E:553:ASP:HB2	2.05	0.57
1:A:200:HIS:HD2	1:A:203:VAL:N	2.01	0.57
1:A:605:PHE:CZ	2:B:520:ARG:HD3	2.40	0.57
1:L:103:ASN:O	1:L:109:ILE:HD11	2.04	0.57
4:M:293:VAL:O	4:M:294:ARG:HB2	2.04	0.57
2:B:273:ASP:O	2:B:274:SER:O	2.22	0.57
2:B:496:PRO:O	2:B:497:SER:CB	2.53	0.57
2:E:273:ASP:O	2:E:274:SER:O	2.21	0.57
2:E:532:THR:OG1	1:L:594:ILE:HD11	2.05	0.57
1:L:233:LEU:O	1:L:237:VAL:HG22	2.05	0.57
4:U:179:GLU:CD	4:U:395:ALA:HB1	2.24	0.57
1:A:603:PRO:O	2:B:520:ARG:NH2	2.38	0.57
1:A:577:GLN:HE21	2:B:546:PRO:HD2	1.68	0.57
2:E:408:GLN:HE22	2:E:440:ASP:H	1.51	0.57
1:L:342:GLU:O	1:L:346:ARG:HD3	2.05	0.57
3:S:27:GLU:O	3:S:31:LEU:HB2	2.04	0.57
4:U:266:ILE:N	4:U:266:ILE:HD12	2.20	0.57
2:E:31:LYS:HA	2:E:65:LEU:CD1	2.34	0.57
4:M:175:LEU:HD11	4:M:404:LEU:CD2	2.35	0.57
2:B:457:GLU:O	2:B:458:ARG:HD2	2.05	0.57
2:E:232:LYS:O	2:E:233:ASP:HB2	2.05	0.57
2:E:476:GLU:OE1	2:E:480:VAL:HG21	2.05	0.57
1:L:442:TYR:CE2	1:L:465:VAL:HG12	2.40	0.57
1:L:54:SER:O	1:L:58:TYR:CD1	2.57	0.57
1:A:367:LYS:NZ	1:A:398:ASP:HB3	2.20	0.56
2:E:54:VAL:HG12	2:E:69:VAL:HG13	1.86	0.56
2:B:390:ARG:HH11	2:B:390:ARG:CB	2.11	0.56
2:B:54:VAL:CG1	2:B:69:VAL:HG13	2.34	0.56
1:A:614:ALA:HA	1:A:623:SER:HB3	1.88	0.56
4:U:389:ASN:HA	4:U:428:SER:OG	2.05	0.56
2:E:580:ALA:C	2:E:581:PHE:HD2	2.09	0.56
4:U:175:LEU:HD11	4:U:404:LEU:CD2	2.35	0.56
1:L:492:CYS:SG	1:L:529:LYS:HE2	2.45	0.56
1:A:520:LEU:O	1:A:520:LEU:HG	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:ILE:HD11	2:B:115:VAL:HB	1.87	0.56
2:E:273:ASP:CG	2:E:274:SER:H	2.09	0.56
2:E:398:LEU:O	2:E:401:THR:HG23	2.05	0.56
2:E:520:ARG:NH2	1:L:603:PRO:O	2.38	0.56
3:I:27:GLU:O	3:I:31:LEU:HB2	2.05	0.56
4:M:408:GLU:O	4:M:412:ASN:HA	2.05	0.56
1:A:318:ILE:HG21	1:A:355:THR:HG22	1.86	0.56
2:E:18:LEU:HD13	2:E:37:VAL:HG22	1.87	0.56
3:I:6:LEU:HD21	3:I:32:ILE:HG12	1.87	0.56
2:E:421:TYR:O	2:E:422:PRO:O	2.24	0.56
1:L:239:SER:HB2	1:L:243:ASP:OD2	2.06	0.56
4:U:312:LYS:HG3	4:U:313:PRO:HD2	1.88	0.56
1:A:204:VAL:HG12	1:A:257:LEU:HD11	1.88	0.56
2:E:212:ASN:C	2:E:213:GLU:HG3	2.26	0.56
4:M:266:ILE:HD12	4:M:266:ILE:N	2.21	0.56
5:P:5:ILE:HD12	3:S:99:CYS:SG	2.45	0.56
1:L:200:HIS:HD2	1:L:203:VAL:N	2.01	0.56
1:L:250:TYR:O	1:L:251:PHE:HB2	2.05	0.56
1:L:341:ARG:CZ	1:L:341:ARG:O	2.54	0.56
2:B:256:VAL:O	2:B:260:VAL:HG23	2.05	0.56
1:L:462:TRP:CZ2	1:L:498:LYS:HD3	2.40	0.56
1:A:531:HIS:O	1:A:532:LEU:HB3	2.06	0.55
1:A:571:ASN:HD21	1:A:576:LEU:HD23	1.71	0.55
1:A:88:TYR:HB3	3:S:141:LEU:HB3	1.88	0.55
1:A:481:LYS:HG3	1:A:511:ILE:HD11	1.88	0.55
1:A:59:VAL:HG21	1:A:82:LEU:CD1	2.37	0.55
2:B:13:GLY:HA2	2:B:17:GLU:HG3	1.87	0.55
2:E:267:LEU:HD12	2:E:277:TYR:CE1	2.42	0.55
2:E:288:LEU:HA	2:E:291:LEU:HB2	1.86	0.55
1:L:379:THR:OG1	1:L:380:GLU:N	2.39	0.55
1:L:250:TYR:HD2	1:L:301:GLN:HB2	1.68	0.55
1:L:433:GLU:O	1:L:433:GLU:HG3	2.06	0.55
4:U:222:ILE:HD12	4:U:222:ILE:N	2.15	0.55
4:U:28:ALA:HA	4:U:31:ALA:HB3	1.88	0.55
3:I:138:LEU:C	3:I:140:SER:H	2.09	0.55
4:M:389:ASN:HA	4:M:428:SER:OG	2.07	0.55
4:U:371:GLU:O	4:U:372:LEU:HD23	2.07	0.55
1:A:547:LYS:O	1:A:551:LEU:HD13	2.06	0.55
2:B:421:TYR:O	2:B:422:PRO:O	2.25	0.55
2:E:31:LYS:HA	2:E:65:LEU:HD13	1.88	0.55
1:L:571:ASN:HD21	1:L:576:LEU:HD23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:308:LYS:HA	4:U:363:GLU:HG2	1.88	0.55
2:B:274:SER:O	2:B:276:TYR:N	2.40	0.55
4:U:212:CYS:HB3	4:U:406:VAL:HA	1.87	0.55
4:U:9:ASN:C	4:U:9:ASN:ND2	2.59	0.55
2:B:365:VAL:CG1	4:M:401:VAL:HG12	2.36	0.55
1:A:577:GLN:NE2	2:B:546:PRO:HD2	2.22	0.55
1:L:571:ASN:ND2	1:L:576:LEU:HB3	2.21	0.55
2:B:177:VAL:O	2:B:181:VAL:HG23	2.07	0.55
2:B:267:LEU:HD12	2:B:277:TYR:CE1	2.42	0.55
4:M:28:ALA:HA	4:M:31:ALA:HB3	1.89	0.55
4:U:293:VAL:O	4:U:294:ARG:HB2	2.06	0.55
4:M:308:LYS:HA	4:M:363:GLU:HG2	1.89	0.55
4:M:381:TRP:CE3	4:M:383:ARG:HB3	2.41	0.55
1:A:341:ARG:CZ	1:A:341:ARG:O	2.54	0.54
1:A:442:TYR:CE2	1:A:465:VAL:HG12	2.42	0.54
2:B:212:ASN:C	2:B:213:GLU:HG3	2.27	0.54
2:B:232:LYS:O	2:B:233:ASP:HB2	2.07	0.54
1:L:204:VAL:HG12	1:L:257:LEU:HD11	1.90	0.54
2:E:496:PRO:O	2:E:497:SER:CB	2.54	0.54
1:L:531:HIS:O	1:L:532:LEU:HB3	2.05	0.54
1:A:16:PHE:O	1:A:20:ILE:HB	2.08	0.54
1:L:233:LEU:HD21	1:L:262:LEU:HD21	1.88	0.54
1:L:574:VAL:HG23	1:L:575:GLU:N	2.22	0.54
1:A:233:LEU:HD21	1:A:262:LEU:HD21	1.87	0.54
1:A:27:GLU:HA	1:A:30:ILE:HG13	1.89	0.54
1:A:80:VAL:HA	1:A:83:LEU:HD12	1.88	0.54
2:B:365:VAL:HG22	4:M:422:VAL:HG11	1.88	0.54
1:A:250:TYR:O	1:A:251:PHE:HB2	2.08	0.54
1:A:581:VAL:O	1:A:585:ARG:HB2	2.08	0.54
4:M:24:ILE:HG22	4:M:25:GLY:N	2.23	0.54
1:A:571:ASN:ND2	1:A:576:LEU:HB3	2.21	0.54
2:E:274:SER:O	2:E:276:TYR:N	2.40	0.54
2:E:457:GLU:O	2:E:458:ARG:HD2	2.08	0.54
1:L:192:VAL:O	1:L:195:LEU:HB2	2.08	0.54
1:A:54:SER:O	1:A:58:TYR:CD1	2.58	0.54
2:B:488:ILE:HD13	2:B:506:VAL:CG2	2.37	0.54
2:E:426:GLU:OE1	2:E:458:ARG:HG2	2.08	0.54
4:U:175:LEU:HD11	4:U:404:LEU:HD22	1.90	0.54
2:B:31:LYS:HA	2:B:65:LEU:CD1	2.38	0.54
1:L:273:ASP:OD1	1:L:273:ASP:C	2.46	0.54
1:A:192:VAL:O	1:A:195:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PHE:CE1	1:A:78:GLU:HG2	2.43	0.54
2:B:99:ASN:O	2:B:102:ILE:HG12	2.08	0.54
2:E:36:LYS:HE2	1:L:24:LYS:HE2	1.90	0.54
2:E:522:ARG:NH2	1:L:582:GLU:OE1	2.39	0.54
4:M:63:ILE:HD11	4:M:98:GLU:HB2	1.90	0.54
4:M:89:MET:HG2	4:M:93:PHE:CZ	2.42	0.54
4:U:196:VAL:HG23	4:U:283:ILE:HG12	1.89	0.54
4:U:63:ILE:HD11	4:U:98:GLU:HB2	1.90	0.54
1:L:464:ARG:NH1	1:L:467:GLN:HE21	2.06	0.54
1:L:547:LYS:O	1:L:551:LEU:HD13	2.08	0.54
1:L:584:LEU:O	1:L:584:LEU:HD12	2.07	0.54
1:A:491:ALA:O	1:A:492:CYS:O	2.25	0.53
2:B:514:SER:OG	2:B:519:LEU:HD23	2.08	0.53
1:L:581:VAL:O	1:L:585:ARG:HB2	2.07	0.53
4:M:175:LEU:HD11	4:M:404:LEU:HD22	1.90	0.53
4:M:81:PHE:CE1	4:M:115:ILE:HG13	2.42	0.53
5:P:2:MET:CE	3:S:10:ARG:H	2.21	0.53
1:A:618:LYS:HE3	6:A:1627:SO4:O3	2.07	0.53
1:A:394:TYR:CE2	4:M:294:ARG:HD3	2.43	0.53
2:E:87:ALA:HB3	2:E:91:PHE:CE2	2.43	0.53
1:L:44:PHE:CG	1:L:78:GLU:HG2	2.41	0.53
4:M:162:ARG:NH2	4:M:206:LEU:O	2.41	0.53
4:M:312:LYS:HG3	4:M:313:PRO:CD	2.38	0.53
1:A:103:ASN:O	1:A:109:ILE:HD11	2.09	0.53
2:B:273:ASP:CG	2:B:274:SER:H	2.11	0.53
2:E:204:ILE:O	2:E:208:LEU:HB2	2.08	0.53
2:E:495:LYS:HD3	2:E:498:GLU:OE2	2.08	0.53
2:E:38:ILE:HD12	2:E:68:LEU:HD22	1.90	0.53
1:L:334:LEU:CD1	1:L:352:SER:HB3	2.38	0.53
5:P:4:GLU:O	3:S:100:GLU:HB2	2.08	0.53
2:E:13:GLY:HA2	2:E:17:GLU:HG3	1.90	0.53
1:L:173:LEU:HD13	1:L:210:LEU:HD12	1.90	0.53
4:M:1:MET:CE	4:M:121:PRO:HD2	2.39	0.53
2:B:428:ILE:O	2:B:431:THR:HB	2.09	0.53
4:M:410:LYS:N	4:M:410:LYS:HD3	2.22	0.53
4:U:1:MET:CE	4:U:121:PRO:HD2	2.39	0.53
1:A:218:ASN:N	1:A:219:PRO:CD	2.72	0.53
2:B:347:SER:C	2:B:349:ALA:H	2.11	0.53
1:L:5:SER:OG	1:L:6:LYS:N	2.42	0.53
4:M:32:PHE:HB2	4:M:55:PHE:CD2	2.44	0.53
4:U:216:MET:HG2	4:U:261:ARG:CB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:THR:HG22	1:A:475:VAL:HG12	1.90	0.53
3:S:16:LEU:HD12	3:S:17:ALA:H	1.73	0.53
1:A:233:LEU:O	1:A:237:VAL:HG22	2.08	0.53
1:A:523:PHE:HZ	1:A:562:VAL:HG21	1.74	0.53
1:A:574:VAL:HG23	1:A:575:GLU:N	2.23	0.53
2:E:197:LEU:HB3	2:E:199:LEU:HD22	1.90	0.53
2:E:213:GLU:O	2:E:215:THR:N	2.42	0.53
1:L:367:LYS:NZ	1:L:398:ASP:HB3	2.23	0.53
1:L:481:LYS:HG3	1:L:511:ILE:HD11	1.90	0.53
3:S:92:ASN:ND2	3:S:98:VAL:H	2.06	0.53
4:U:198:GLY:HA3	4:U:277:TYR:CE1	2.44	0.53
1:A:396:MET:O	1:A:396:MET:HG3	2.08	0.53
2:E:218:GLY:CA	2:E:221:PHE:CD1	2.90	0.53
2:E:511:THR:HG22	2:E:512:GLN:NE2	2.23	0.53
2:E:77:ALA:HB1	2:E:113:ILE:HG12	1.91	0.53
4:M:234:SER:O	4:M:235:LYS:C	2.47	0.53
4:M:59:LYS:HE3	4:M:64:TRP:CE2	2.43	0.53
4:U:32:PHE:HB2	4:U:55:PHE:CD2	2.44	0.53
1:A:297:SER:OG	1:A:298:LYS:N	2.41	0.53
1:A:44:PHE:CG	1:A:78:GLU:HG2	2.43	0.53
2:E:415:ARG:O	2:E:419:ARG:HG3	2.09	0.53
4:M:312:LYS:HG3	4:M:313:PRO:HD2	1.91	0.53
4:M:408:GLU:HG2	4:M:413:TYR:CE2	2.44	0.53
4:U:408:GLU:O	4:U:412:ASN:HA	2.09	0.53
1:A:252:VAL:HG21	1:A:305:ALA:HB3	1.89	0.52
2:B:581:PHE:CD2	2:B:581:PHE:N	2.76	0.52
2:E:511:THR:HG22	2:E:512:GLN:HE21	1.75	0.52
1:L:44:PHE:CE1	1:L:78:GLU:HG2	2.44	0.52
5:P:2:MET:HE1	3:S:10:ARG:N	2.24	0.52
3:S:90:VAL:CG2	3:S:128:GLN:HG2	2.39	0.52
1:A:273:ASP:C	1:A:273:ASP:OD1	2.47	0.52
1:A:4:VAL:HG12	1:A:5:SER:N	2.24	0.52
2:B:511:THR:HG22	2:B:512:GLN:HE21	1.74	0.52
2:E:326:VAL:HG13	2:E:335:LYS:HG2	1.91	0.52
4:M:1:MET:HE2	4:M:121:PRO:HD2	1.91	0.52
4:U:410:LYS:HD3	4:U:410:LYS:N	2.23	0.52
4:U:89:MET:HG2	4:U:93:PHE:CZ	2.43	0.52
1:A:200:HIS:CD2	1:A:202:GLY:H	2.28	0.52
1:A:239:SER:HB2	1:A:243:ASP:OD2	2.08	0.52
1:A:243:ASP:O	1:A:244:LEU:C	2.47	0.52
2:B:31:LYS:HA	2:B:65:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:ARG:O	2:B:419:ARG:HG3	2.10	0.52
4:M:261:ARG:O	4:M:263:ILE:HD13	2.09	0.52
4:U:381:TRP:CE3	4:U:383:ARG:HB3	2.43	0.52
2:B:246:PRO:C	2:B:248:LEU:H	2.11	0.52
2:E:305:ASN:ND2	2:E:567:ILE:O	2.42	0.52
2:E:347:SER:C	2:E:349:ALA:H	2.11	0.52
2:E:357:GLU:HG3	2:E:361:TYR:CZ	2.44	0.52
2:E:521:ASP:HA	1:L:602:MET:HE1	1.91	0.52
1:A:50:LEU:N	1:A:50:LEU:HD12	2.18	0.52
2:B:127:ARG:CG	2:B:127:ARG:NH1	2.71	0.52
2:B:581:PHE:O	2:B:582:VAL:HG23	2.09	0.52
2:E:139:LYS:N	2:E:176:VAL:HG22	2.24	0.52
4:M:241:ILE:HG12	3:S:31:LEU:HD13	1.91	0.52
2:E:365:VAL:HG13	4:U:401:VAL:HG12	1.91	0.52
1:A:492:CYS:SG	1:A:529:LYS:HE2	2.49	0.52
2:B:213:GLU:O	2:B:215:THR:N	2.42	0.52
2:E:127:ARG:NH1	2:E:127:ARG:CG	2.70	0.52
2:E:328:TYR:CE1	2:E:329:ASN:HB3	2.44	0.52
3:I:75:ASP:HA	1:L:263:ARG:NH2	2.24	0.52
1:L:374:ILE:HG23	1:L:408:GLU:HG2	1.91	0.52
4:M:42:GLN:HA	4:M:42:GLN:HE21	1.74	0.52
2:B:78:LYS:NZ	4:M:18:ARG:HH12	2.08	0.52
2:E:365:VAL:HG22	4:U:422:VAL:CG1	2.40	0.52
1:A:76:HIS:O	1:A:80:VAL:HG23	2.10	0.52
2:B:307:ASN:HD22	2:B:575:HIS:CE1	2.18	0.52
2:E:574:TYR:CE1	4:U:49:ASN:HB2	2.44	0.52
1:L:189:THR:HG21	1:L:221:GLU:HG3	1.90	0.52
1:L:243:ASP:O	1:L:244:LEU:C	2.48	0.52
4:M:196:VAL:HG23	4:M:283:ILE:HG12	1.90	0.52
4:M:162:ARG:HB3	4:M:209:MET:HE1	1.92	0.52
4:U:222:ILE:CD1	4:U:222:ILE:H	2.11	0.52
2:B:145:VAL:HG11	2:B:165:LEU:HD22	1.91	0.52
2:B:288:LEU:HA	2:B:291:LEU:HB2	1.90	0.52
2:E:581:PHE:O	2:E:582:VAL:HG23	2.09	0.52
4:U:296:VAL:HG22	4:U:296:VAL:O	2.08	0.52
4:U:312:LYS:O	4:U:360:GLY:HA3	2.10	0.52
2:B:328:TYR:CE1	2:B:329:ASN:HB3	2.45	0.52
2:B:387:SER:O	2:B:388:ALA:C	2.49	0.52
3:I:8:GLN:HE22	3:I:36:HIS:CB	2.23	0.52
1:L:80:VAL:HA	1:L:83:LEU:HD12	1.91	0.52
4:M:212:CYS:HB3	4:M:406:VAL:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:222:ILE:HD12	4:M:222:ILE:N	2.16	0.52
3:I:27:GLU:HG2	4:U:241:ILE:HB	1.91	0.52
1:A:401:ASN:O	1:A:404:GLN:HB2	2.10	0.51
2:B:511:THR:HG22	2:B:512:GLN:NE2	2.24	0.51
1:L:124:ASN:O	1:L:128:MET:HG3	2.10	0.51
2:E:246:PRO:C	2:E:248:LEU:H	2.14	0.51
4:M:61:SER:C	4:M:63:ILE:H	2.13	0.51
4:U:24:ILE:HG22	4:U:25:GLY:N	2.25	0.51
1:A:464:ARG:NH1	1:A:467:GLN:HE21	2.08	0.51
2:E:325:PHE:HA	2:E:342:MET:HE1	1.92	0.51
3:I:100:GLU:CB	5:Q:4:GLU:HB3	2.40	0.51
1:L:362:SER:O	1:L:363:HIS:HB2	2.10	0.51
4:M:26:ARG:HH22	4:M:33:ARG:NH2	2.05	0.51
4:U:26:ARG:HH22	4:U:33:ARG:NH2	2.06	0.51
4:U:59:LYS:HE3	4:U:64:TRP:CE2	2.45	0.51
1:A:250:TYR:HD2	1:A:301:GLN:HB2	1.72	0.51
1:A:379:THR:OG1	1:A:380:GLU:N	2.44	0.51
2:E:99:ASN:O	2:E:102:ILE:HG12	2.10	0.51
2:E:135:PRO:HB3	2:E:173:ASN:OD1	2.10	0.51
4:M:203:LYS:HG3	4:M:271:GLU:HB2	1.92	0.51
1:A:455:ASP:HA	1:A:493:HIS:CE1	2.46	0.51
1:A:615:LYS:HD3	1:A:617:LYS:HE2	1.92	0.51
2:B:325:PHE:HA	2:B:342:MET:HE1	1.91	0.51
2:E:177:VAL:O	2:E:181:VAL:HG23	2.11	0.51
2:E:485:LEU:HD22	2:E:526:TYR:CD1	2.45	0.51
1:L:369:HIS:O	1:L:373:VAL:HG13	2.10	0.51
2:B:330:ASP:OD1	2:B:338:LYS:NZ	2.44	0.51
2:B:77:ALA:HB1	2:B:113:ILE:HG12	1.92	0.51
2:E:81:PRO:HB2	2:E:115:VAL:HG23	1.93	0.51
1:A:263:ARG:HH21	3:S:75:ASP:HA	1.75	0.51
4:U:234:SER:O	4:U:235:LYS:C	2.49	0.51
1:A:614:ALA:HA	1:A:623:SER:HB2	1.92	0.51
1:L:55:LYS:O	1:L:59:VAL:HG23	2.11	0.51
4:M:371:GLU:O	4:M:372:LEU:HD23	2.11	0.51
3:S:48:ASN:N	3:S:48:ASN:ND2	2.59	0.51
2:B:81:PRO:HB2	2:B:115:VAL:HG23	1.93	0.51
2:B:365:VAL:HG22	4:M:422:VAL:HG12	1.93	0.51
2:B:38:ILE:HD12	2:B:68:LEU:HD22	1.92	0.51
4:M:18:ARG:HB3	4:M:20:TYR:CE1	2.46	0.51
2:B:139:LYS:N	2:B:176:VAL:HG22	2.26	0.51
2:B:197:LEU:HB3	2:B:199:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:LEU:HD22	2:B:526:TYR:CD1	2.45	0.51
2:E:139:LYS:NZ	4:U:122:GLN:HG3	2.26	0.51
2:E:307:ASN:HD22	2:E:575:HIS:CE1	2.20	0.51
4:U:88:VAL:HG11	4:U:111:LEU:HD11	1.91	0.51
1:A:167:SER:OG	3:S:124:ARG:NH2	2.44	0.51
1:A:270:PRO:HA	1:A:320:HIS:CE1	2.46	0.51
2:B:70:TYR:HD2	2:B:109:THR:HG21	1.75	0.51
2:E:440:ASP:HB3	4:U:316:LEU:HD12	1.93	0.51
2:E:550:GLU:HG2	2:E:551:GLU:N	2.26	0.51
2:E:554:LEU:HD12	2:E:554:LEU:N	2.26	0.51
4:M:123:ASN:ND2	4:M:123:ASN:O	2.44	0.51
4:U:18:ARG:HB3	4:U:20:TYR:CE1	2.46	0.51
2:B:550:GLU:HG2	2:B:551:GLU:N	2.26	0.50
3:I:65:LEU:HD12	5:Q:8:LEU:HD11	1.93	0.50
4:U:169:ARG:HG3	4:U:170:ARG:H	1.76	0.50
1:A:124:ASN:ND2	1:A:127:PHE:CE1	2.79	0.50
2:B:251:ALA:O	2:B:252:ASN:C	2.49	0.50
2:E:74:MET:HE3	6:E:1586:SO4:O4	2.12	0.50
2:E:491:LEU:HD11	2:E:495:LYS:HD2	1.92	0.50
1:L:218:ASN:N	1:L:219:PRO:CD	2.74	0.50
1:L:297:SER:OG	1:L:298:LYS:N	2.44	0.50
1:L:426:LEU:O	1:L:430:ILE:HD13	2.11	0.50
4:M:166:ILE:HD11	4:M:208:GLY:O	2.11	0.50
3:S:49:PHE:CE2	3:S:77:ASN:HB3	2.46	0.50
1:A:55:LYS:O	1:A:59:VAL:HG23	2.11	0.50
2:B:267:LEU:HD12	2:B:277:TYR:HE1	1.77	0.50
2:E:138:ARG:NH1	2:E:171:ASP:OD2	2.44	0.50
1:L:27:GLU:HA	1:L:30:ILE:HG13	1.94	0.50
4:M:261:ARG:O	4:M:263:ILE:N	2.44	0.50
3:S:93:GLU:HG3	3:S:132:LEU:HD11	1.93	0.50
1:A:426:LEU:O	1:A:430:ILE:HD13	2.11	0.50
2:B:436:LEU:CD1	2:B:465:LEU:HD22	2.41	0.50
2:B:85:ILE:HG22	2:B:85:ILE:O	2.11	0.50
2:E:507:LEU:O	2:E:511:THR:HB	2.12	0.50
3:I:19:TRP:CE2	3:I:28:LYS:CG	2.94	0.50
3:I:39:VAL:HG22	3:I:59:TYR:CD1	2.46	0.50
4:M:104:ASN:HD21	4:M:138:ILE:H	1.59	0.50
2:B:60:THR:HG23	2:B:61:ASP:N	2.26	0.50
2:E:581:PHE:N	2:E:581:PHE:CD2	2.80	0.50
3:I:48:ASN:N	3:I:48:ASN:ND2	2.60	0.50
1:L:143:MET:O	1:L:144:ALA:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:595:LEU:CD2	1:L:599:LEU:HD12	2.42	0.50
4:U:1:MET:HE1	4:U:121:PRO:HD2	1.92	0.50
2:E:428:ILE:O	2:E:431:THR:HB	2.12	0.50
1:L:105:ASN:O	1:L:109:ILE:HD13	2.12	0.50
1:L:445:THR:O	1:L:448:ASN:HB2	2.12	0.50
4:U:184:LEU:HG	4:U:192:LEU:HD12	1.94	0.50
1:A:18:SER:O	1:A:22:ASN:HB2	2.12	0.50
1:A:586:LEU:C	1:A:586:LEU:HD12	2.32	0.50
2:B:111:GLY:O	2:B:147:LYS:HG2	2.11	0.50
2:B:87:ALA:HB3	2:B:91:PHE:HE2	1.77	0.50
4:M:349:ASN:O	4:M:350:ALA:HB2	2.10	0.50
4:U:162:ARG:NH2	4:U:206:LEU:O	2.44	0.50
4:U:408:GLU:HG2	4:U:413:TYR:CE2	2.47	0.50
4:U:425:ILE:O	4:U:425:ILE:HG22	2.11	0.50
2:B:218:GLY:CA	2:B:221:PHE:CD1	2.93	0.50
2:B:420:LYS:NZ	2:B:550:GLU:OE2	2.45	0.50
2:B:307:ASN:ND2	2:B:575:HIS:HE1	2.03	0.50
1:L:434:LYS:HE2	1:L:435:TYR:CZ	2.47	0.50
4:M:204:SER:OG	4:M:204:SER:O	2.30	0.50
1:A:200:HIS:CD2	1:A:202:GLY:N	2.80	0.50
2:E:107:VAL:HG13	2:E:144:CYS:SG	2.51	0.49
2:B:127:ARG:HG2	2:B:127:ARG:NH1	2.16	0.49
2:B:495:LYS:HD3	2:B:498:GLU:OE2	2.12	0.49
2:E:399:ILE:HG23	2:E:407:VAL:HG22	1.94	0.49
4:U:267:PRO:C	4:U:268:PRO:O	2.50	0.49
1:A:189:THR:HG21	1:A:221:GLU:HG3	1.93	0.49
2:B:13:GLY:O	2:B:14:GLU:HB3	2.12	0.49
2:B:297:GLU:HB2	4:M:83:TYR:OH	2.12	0.49
2:E:423:ASN:C	2:E:425:TYR:H	2.14	0.49
3:I:90:VAL:CG2	3:I:128:GLN:HG2	2.42	0.49
1:L:18:SER:O	1:L:22:ASN:HB2	2.12	0.49
1:L:440:THR:HG22	1:L:475:VAL:HG12	1.93	0.49
4:M:409:PRO:HD2	4:M:410:LYS:HD3	1.94	0.49
4:M:425:ILE:O	4:M:425:ILE:HG22	2.11	0.49
1:A:440:THR:O	1:A:444:ASP:HB2	2.13	0.49
2:E:156:VAL:HG12	2:E:162:LEU:CD2	2.40	0.49
2:E:401:THR:C	2:E:403:VAL:H	2.16	0.49
4:U:9:ASN:ND2	4:U:12:GLY:H	2.10	0.49
4:U:166:ILE:HD11	4:U:208:GLY:O	2.12	0.49
1:A:535:VAL:HG11	1:A:573:ASP:OD1	2.12	0.49
2:E:212:ASN:O	2:E:213:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:ILE:HG22	2:E:85:ILE:O	2.12	0.49
1:L:396:MET:O	1:L:396:MET:HG3	2.12	0.49
4:U:376:ASN:O	4:U:377:ASP:HB3	2.13	0.49
1:A:325:ASN:O	1:A:329:ARG:HG2	2.11	0.49
2:E:41:MET:HG2	2:E:47:VAL:HG21	1.95	0.49
1:L:549:VAL:HG13	1:L:556:LYS:HG3	1.94	0.49
4:M:403:TYR:CD1	4:M:403:TYR:C	2.86	0.49
4:U:123:ASN:O	4:U:123:ASN:ND2	2.43	0.49
1:A:346:ARG:NH2	1:A:376:ALA:HA	2.27	0.49
2:B:169:ILE:HD11	2:B:206:LYS:HZ2	1.77	0.49
2:B:488:ILE:HD13	2:B:506:VAL:HG22	1.93	0.49
2:B:507:LEU:O	2:B:511:THR:HB	2.13	0.49
2:E:78:LYS:HZ2	4:U:18:ARG:NH1	2.11	0.49
3:S:138:LEU:O	3:S:139:GLN:CB	2.61	0.49
3:S:19:TRP:CE2	3:S:28:LYS:CG	2.94	0.49
2:E:267:LEU:HD12	2:E:277:TYR:HE1	1.76	0.49
3:I:55:PHE:HB3	3:I:71:VAL:O	2.13	0.49
1:L:200:HIS:CD2	1:L:202:GLY:H	2.30	0.49
4:M:139:LYS:O	4:M:140:SER:HB2	2.13	0.49
4:M:293:VAL:CG1	4:M:294:ARG:N	2.76	0.49
4:M:321:GLU:HB2	4:M:389:ASN:HB2	1.95	0.49
2:E:348:GLN:CB	2:E:386:GLN:HE22	2.26	0.49
3:I:16:LEU:HD12	3:I:17:ALA:H	1.78	0.49
3:I:72:ASP:HB2	3:I:75:ASP:OD2	2.13	0.49
1:L:124:ASN:ND2	1:L:127:PHE:CE1	2.81	0.49
1:L:491:ALA:O	1:L:492:CYS:O	2.30	0.49
1:A:250:TYR:CD2	1:A:301:GLN:HB3	2.48	0.49
2:E:54:VAL:CG1	2:E:69:VAL:HG13	2.42	0.49
3:S:8:GLN:HE22	3:S:36:HIS:CB	2.23	0.49
4:U:203:LYS:HG3	4:U:271:GLU:HB2	1.95	0.49
1:A:523:PHE:CE1	1:A:559:ILE:HG12	2.48	0.48
2:B:305:ASN:O	2:B:309:ILE:HG13	2.13	0.48
2:E:208:LEU:HD13	2:E:243:ARG:NE	2.28	0.48
2:E:212:ASN:O	2:E:213:GLU:CG	2.61	0.48
1:L:449:LEU:N	1:L:449:LEU:HD12	2.28	0.48
1:L:455:ASP:HA	1:L:493:HIS:CE1	2.48	0.48
4:M:174:PHE:N	4:M:174:PHE:CD1	2.81	0.48
4:M:21:ARG:HG2	4:M:23:ASP:OD2	2.11	0.48
4:M:376:ASN:O	4:M:377:ASP:HB3	2.13	0.48
4:U:29:VAL:HG13	4:U:30:ASP:H	1.77	0.48
4:U:321:GLU:HB2	4:U:389:ASN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:NH1	1:A:452:ILE:HG13	2.28	0.48
2:B:580:ALA:C	2:B:581:PHE:CD2	2.84	0.48
2:E:70:TYR:HD2	2:E:109:THR:HG21	1.77	0.48
2:E:103:ARG:HD3	2:E:128:LYS:NZ	2.27	0.48
2:E:13:GLY:O	2:E:14:GLU:HB3	2.13	0.48
2:E:47:VAL:O	2:E:48:SER:HB3	2.13	0.48
1:L:406:VAL:HG21	1:L:441:TRP:CZ2	2.48	0.48
4:U:261:ARG:O	4:U:262:SER:C	2.51	0.48
4:U:28:ALA:HB1	4:U:55:PHE:CZ	2.49	0.48
1:A:124:ASN:O	1:A:128:MET:HG3	2.14	0.48
1:A:595:LEU:CD2	1:A:599:LEU:HD12	2.43	0.48
2:B:12:LYS:CD	2:B:12:LYS:N	2.77	0.48
2:B:156:VAL:HG12	2:B:162:LEU:CD2	2.40	0.48
2:E:365:VAL:HG22	4:U:422:VAL:HG11	1.95	0.48
1:L:540:LEU:C	1:L:540:LEU:HD12	2.33	0.48
4:U:29:VAL:HG13	4:U:30:ASP:N	2.29	0.48
4:U:409:PRO:HD2	4:U:410:LYS:HD3	1.95	0.48
2:E:114:ARG:HA	2:E:151:ILE:HD13	1.94	0.48
2:E:326:VAL:HG11	2:E:335:LYS:HG2	1.96	0.48
2:E:435:ASN:C	2:E:437:ASP:N	2.67	0.48
1:L:233:LEU:HD13	1:L:261:LEU:HB2	1.95	0.48
2:E:540:VAL:HG21	1:L:586:LEU:HB3	1.96	0.48
1:A:212:THR:O	1:A:216:GLN:HG3	2.13	0.48
1:A:267:CYS:O	4:M:378:LYS:NZ	2.46	0.48
2:B:135:PRO:HB3	2:B:173:ASN:OD1	2.14	0.48
2:B:267:LEU:C	2:B:269:LEU:H	2.16	0.48
2:E:545:LYS:CG	1:L:581:VAL:HG21	2.42	0.48
4:U:111:LEU:HD22	4:U:133:ILE:CD1	2.43	0.48
2:B:139:LYS:NZ	4:M:122:GLN:HG3	2.28	0.48
2:E:12:LYS:N	2:E:12:LYS:CD	2.77	0.48
1:L:212:THR:O	1:L:216:GLN:HG3	2.13	0.48
4:M:169:ARG:HG3	4:M:170:ARG:H	1.79	0.48
4:U:104:ASN:O	4:U:105:PHE:C	2.51	0.48
1:A:462:TRP:CZ2	1:A:498:LYS:HD3	2.49	0.48
2:B:401:THR:C	2:B:403:VAL:H	2.16	0.48
1:L:103:ASN:HD22	1:L:103:ASN:C	2.17	0.48
1:L:615:LYS:HD3	1:L:617:LYS:HE2	1.94	0.48
4:U:61:SER:C	4:U:63:ILE:H	2.15	0.48
2:B:348:GLN:CB	2:B:386:GLN:HE22	2.27	0.48
2:B:542:LEU:O	2:B:543:SER:O	2.32	0.48
1:L:200:HIS:CD2	1:L:202:GLY:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:543:SER:HB2	1:L:585:ARG:HH21	1.77	0.48
1:L:74:PHE:C	1:L:74:PHE:CD1	2.87	0.48
1:A:143:MET:O	1:A:144:ALA:C	2.53	0.48
1:A:445:THR:O	1:A:448:ASN:HB2	2.14	0.48
2:B:138:ARG:NH1	2:B:171:ASP:OD2	2.47	0.48
2:B:348:GLN:HB2	2:B:386:GLN:NE2	2.29	0.48
2:B:477:SER:HB2	2:B:480:VAL:H	1.79	0.48
2:E:265:LYS:HE3	2:E:565:CYS:SG	2.53	0.48
2:E:349:ALA:O	2:E:350:ASN:HB3	2.14	0.48
3:I:93:GLU:HG3	3:I:132:LEU:HD11	1.95	0.48
1:L:595:LEU:HD21	1:L:599:LEU:HD12	1.96	0.48
4:M:115:ILE:O	4:M:115:ILE:HG13	2.12	0.48
1:A:189:THR:HG22	1:A:190:SER:N	2.28	0.48
1:A:31:LYS:HG2	1:A:35:LYS:HE2	1.95	0.48
1:A:434:LYS:HE2	1:A:435:TYR:CZ	2.49	0.48
2:B:103:ARG:HD3	2:B:128:LYS:NZ	2.28	0.48
2:B:423:ASN:C	2:B:425:TYR:H	2.16	0.48
2:E:126:LEU:HD23	2:E:161:PHE:CE2	2.49	0.48
2:E:387:SER:O	2:E:388:ALA:C	2.52	0.48
3:I:109:LYS:HA	3:I:112:THR:HG23	1.96	0.48
1:L:444:ASP:O	1:L:447:LEU:HD12	2.13	0.48
1:A:124:ASN:ND2	1:A:127:PHE:CD1	2.83	0.47
1:A:284:LEU:CD2	1:A:313:ALA:HB1	2.44	0.47
2:E:330:ASP:OD1	2:E:338:LYS:NZ	2.46	0.47
2:E:522:ARG:HH11	2:E:522:ARG:HG2	1.78	0.47
1:L:280:LEU:HG	1:L:280:LEU:O	2.13	0.47
1:L:334:LEU:HB3	1:L:353:MET:HE2	1.96	0.47
1:L:473:ASP:C	1:L:475:VAL:H	2.17	0.47
4:U:104:ASN:HD21	4:U:138:ILE:H	1.62	0.47
2:E:186:GLU:OE2	4:U:118:PHE:HE2	1.97	0.47
1:A:406:VAL:HG21	1:A:441:TRP:CZ2	2.48	0.47
1:A:374:ILE:HG23	1:A:408:GLU:HG2	1.95	0.47
2:B:87:ALA:HB3	2:B:91:PHE:CE2	2.49	0.47
1:A:319:HIS:CE1	4:M:380:LYS:HE3	2.49	0.47
1:A:465:VAL:HG23	1:A:466:ILE:N	2.28	0.47
1:A:457:VAL:HG13	1:A:495:ASN:HD22	1.79	0.47
1:A:540:LEU:HD12	1:A:540:LEU:C	2.34	0.47
3:I:141:LEU:HB3	1:L:88:TYR:HB3	1.95	0.47
4:M:122:GLN:HE21	4:M:122:GLN:CA	2.27	0.47
3:S:90:VAL:HG23	3:S:128:GLN:HG2	1.95	0.47
1:A:214:LEU:HB3	1:A:222:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LEU:HD12	1:A:449:LEU:N	2.29	0.47
2:B:324:PHE:CD2	2:B:341:ILE:HG21	2.50	0.47
2:B:442:PRO:HD3	4:M:316:LEU:HD21	1.94	0.47
2:B:522:ARG:HH11	2:B:522:ARG:HG2	1.78	0.47
2:E:348:GLN:HB2	2:E:386:GLN:NE2	2.29	0.47
3:I:137:MET:C	3:I:137:MET:SD	2.93	0.47
1:L:334:LEU:HB3	1:L:353:MET:CE	2.45	0.47
1:L:50:LEU:N	1:L:50:LEU:HD12	2.23	0.47
1:L:76:HIS:O	1:L:80:VAL:HG23	2.14	0.47
4:M:179:GLU:OE2	4:M:277:TYR:OH	2.24	0.47
2:E:74:MET:CE	6:E:1586:SO4:O4	2.63	0.47
2:E:570:LEU:HB2	4:U:72:ASN:HD22	1.80	0.47
1:L:270:PRO:HA	1:L:320:HIS:CE1	2.50	0.47
1:L:473:ASP:O	1:L:475:VAL:N	2.48	0.47
4:M:248:PHE:CD2	4:M:252:VAL:HG11	2.50	0.47
1:A:437:VAL:HG23	1:A:438:ASP:H	1.79	0.47
2:E:213:GLU:HB2	2:E:214:CYS:H	1.52	0.47
4:U:217:ASN:ND2	4:U:219:LYS:HD3	2.29	0.47
4:U:349:ASN:O	4:U:350:ALA:HB2	2.13	0.47
4:U:380:LYS:O	4:U:382:ALA:N	2.42	0.47
1:A:410:LEU:HA	1:A:410:LEU:HD23	1.79	0.47
1:A:473:ASP:C	1:A:475:VAL:H	2.18	0.47
2:E:251:ALA:O	2:E:252:ASN:C	2.53	0.47
1:L:124:ASN:ND2	1:L:127:PHE:CD1	2.83	0.47
1:L:239:SER:CB	1:L:243:ASP:OD2	2.62	0.47
1:L:367:LYS:O	1:L:370:ILE:HG13	2.14	0.47
4:U:186:SER:CB	4:U:190:GLN:HB2	2.38	0.47
1:A:322:SER:O	1:A:323:GLU:O	2.32	0.47
1:A:458:SER:O	1:A:461:VAL:HG23	2.15	0.47
2:E:436:LEU:CD1	2:E:465:LEU:HD22	2.44	0.47
2:E:60:THR:HG23	2:E:61:ASP:N	2.30	0.47
1:L:535:VAL:HG11	1:L:573:ASP:OD1	2.15	0.47
4:U:169:ARG:CG	4:U:170:ARG:H	2.28	0.47
4:U:263:ILE:HD12	4:U:263:ILE:HA	1.62	0.47
1:A:114:ASN:O	1:A:117:LYS:HB3	2.15	0.47
1:A:74:PHE:CD1	1:A:74:PHE:C	2.88	0.47
2:E:13:GLY:CA	2:E:17:GLU:HG3	2.45	0.47
2:E:520:ARG:HG2	2:E:520:ARG:NH1	2.30	0.47
1:L:454:GLY:O	1:L:457:VAL:HG12	2.15	0.47
3:S:58:ILE:HD13	3:S:58:ILE:N	2.29	0.47
1:A:265:LEU:HD13	1:A:280:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LYS:HZ3	1:A:398:ASP:HB3	1.79	0.47
1:A:454:GLY:O	1:A:457:VAL:HG12	2.15	0.47
2:B:197:LEU:HD13	2:B:199:LEU:HD21	1.96	0.47
2:B:326:VAL:HG11	2:B:335:LYS:HG2	1.96	0.47
2:E:420:LYS:NZ	2:E:550:GLU:OE2	2.48	0.47
2:E:477:SER:HB2	2:E:480:VAL:H	1.80	0.47
1:L:189:THR:HG21	1:L:221:GLU:CG	2.45	0.47
4:M:380:LYS:O	4:M:382:ALA:N	2.42	0.47
3:S:55:PHE:HB3	3:S:71:VAL:O	2.15	0.47
3:S:72:ASP:O	3:S:75:ASP:HB2	2.15	0.47
3:S:92:ASN:HD22	3:S:98:VAL:H	1.62	0.47
1:A:282:GLU:O	1:A:285:GLU:HB2	2.15	0.47
2:B:485:LEU:HD22	2:B:526:TYR:HD1	1.80	0.47
4:M:28:ALA:HB1	4:M:55:PHE:CZ	2.50	0.47
4:M:312:LYS:O	4:M:360:GLY:HA3	2.15	0.47
3:S:109:LYS:HA	3:S:112:THR:HG23	1.97	0.47
4:U:204:SER:OG	4:U:204:SER:O	2.33	0.47
4:U:261:ARG:O	4:U:263:ILE:N	2.48	0.47
1:A:266:GLN:O	4:M:380:LYS:HE3	2.15	0.46
1:A:597:THR:HA	1:A:600:GLU:HG3	1.97	0.46
2:B:317:LEU:HD23	2:B:317:LEU:HA	1.72	0.46
2:B:566:HIS:HB3	2:B:569:SER:OG	2.15	0.46
3:I:124:ARG:NH2	1:L:167:SER:OG	2.48	0.46
4:U:293:VAL:HG11	4:U:383:ARG:HH12	1.79	0.46
1:A:300:VAL:HG13	1:A:301:GLN:NE2	2.30	0.46
1:A:284:LEU:HD23	1:A:313:ALA:HB1	1.97	0.46
2:B:435:ASN:C	2:B:437:ASP:N	2.69	0.46
2:E:580:ALA:C	2:E:581:PHE:CD2	2.89	0.46
2:E:96:GLU:O	2:E:97:ASP:C	2.53	0.46
3:I:91:LEU:HD13	3:I:103:LEU:HD21	1.97	0.46
1:L:380:GLU:HG3	1:L:385:VAL:HG11	1.96	0.46
2:B:559:LEU:HG	2:B:559:LEU:O	2.15	0.46
3:I:112:THR:HG22	1:L:92:GLN:NE2	2.30	0.46
1:L:176:TYR:HA	1:L:183:VAL:HG21	1.97	0.46
1:L:446:ILE:HG21	1:L:465:VAL:CG1	2.40	0.46
2:E:533:ASP:HB2	1:L:594:ILE:HG12	1.96	0.46
1:L:595:LEU:HD23	1:L:595:LEU:C	2.36	0.46
1:L:80:VAL:HG13	1:L:83:LEU:HD12	1.97	0.46
4:M:296:VAL:HG22	4:M:296:VAL:O	2.13	0.46
1:A:363:HIS:O	1:A:364:GLU:HB2	2.14	0.46
1:A:369:HIS:O	1:A:373:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLU:HG2	1:A:554:GLU:H	1.36	0.46
2:B:274:SER:C	2:B:276:TYR:N	2.69	0.46
2:B:549:SER:O	2:B:550:GLU:O	2.33	0.46
2:B:582:VAL:O	2:B:582:VAL:HG12	2.15	0.46
2:E:442:PRO:HD3	4:U:316:LEU:HD21	1.98	0.46
2:E:307:ASN:ND2	2:E:575:HIS:HE1	2.07	0.46
1:L:401:ASN:O	1:L:404:GLN:HB2	2.14	0.46
3:S:7:ILE:CD1	3:S:16:LEU:HD23	2.46	0.46
4:U:9:ASN:HD21	4:U:13:GLU:H	1.63	0.46
2:B:41:MET:HG2	2:B:47:VAL:HG21	1.98	0.46
2:E:97:ASP:CG	2:E:102:ILE:HD11	2.36	0.46
4:M:88:VAL:HG21	4:M:124:SER:OG	2.15	0.46
3:S:65:LEU:HD11	3:S:100:GLU:HG2	1.96	0.46
4:U:118:PHE:HD2	4:U:120:TYR:CE2	2.33	0.46
1:A:176:TYR:HA	1:A:183:VAL:HG21	1.97	0.46
1:A:530:PHE:O	1:A:532:LEU:N	2.36	0.46
2:B:126:LEU:HD23	2:B:161:PHE:CE2	2.50	0.46
2:E:169:ILE:HD11	2:E:206:LYS:HZ3	1.78	0.46
3:I:90:VAL:HG23	3:I:128:GLN:HG2	1.97	0.46
1:L:214:LEU:HB3	1:L:222:PHE:CE1	2.51	0.46
1:L:59:VAL:HG13	1:L:97:PHE:CD1	2.50	0.46
4:U:88:VAL:HG21	4:U:124:SER:OG	2.15	0.46
4:U:42:GLN:HA	4:U:42:GLN:HE21	1.80	0.46
2:B:265:LYS:HA	2:B:265:LYS:HD3	1.68	0.46
2:E:197:LEU:HD13	2:E:199:LEU:HD21	1.97	0.46
2:E:325:PHE:HA	2:E:342:MET:CE	2.45	0.46
2:E:436:LEU:HD21	2:E:448:MET:SD	2.55	0.46
1:L:418:TYR:HD1	1:L:418:TYR:N	2.13	0.46
1:L:586:LEU:HD12	1:L:586:LEU:C	2.36	0.46
4:M:112:LEU:C	4:M:114:GLU:H	2.19	0.46
3:S:93:GLU:HA	3:S:93:GLU:OE2	2.16	0.46
1:A:346:ARG:HH21	1:A:376:ALA:HA	1.81	0.46
1:A:362:SER:O	1:A:363:HIS:HB2	2.15	0.46
2:B:419:ARG:CZ	2:B:548:ILE:HG21	2.45	0.46
2:E:66:LYS:HD2	2:E:102:ILE:HG21	1.97	0.46
4:M:107:LEU:O	4:M:111:LEU:HB2	2.16	0.46
4:M:261:ARG:O	4:M:262:SER:C	2.54	0.46
4:U:115:ILE:O	4:U:115:ILE:HG13	2.15	0.46
4:U:235:LYS:H	4:U:276:ARG:HH21	1.64	0.46
4:U:379:LYS:O	4:U:381:TRP:N	2.45	0.46
1:A:189:THR:HG21	1:A:221:GLU:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:VAL:O	1:A:538:ARG:N	2.49	0.46
1:A:59:VAL:HG13	1:A:97:PHE:CD1	2.51	0.46
2:B:285:ALA:HB3	2:B:286:PRO:CD	2.40	0.46
2:B:284:LEU:C	2:B:287:PRO:HD2	2.37	0.46
2:E:267:LEU:C	2:E:269:LEU:H	2.19	0.46
2:E:480:VAL:O	2:E:481:GLN:C	2.54	0.46
1:L:418:TYR:CD1	1:L:418:TYR:N	2.83	0.46
1:L:437:VAL:HG23	1:L:438:ASP:H	1.81	0.46
1:L:440:THR:O	1:L:444:ASP:HB2	2.16	0.46
1:L:498:LYS:HE3	1:L:537:THR:OG1	2.15	0.46
4:M:267:PRO:C	4:M:268:PRO:O	2.54	0.46
4:U:92:TYR:HE2	4:U:133:ILE:HG21	1.81	0.46
4:M:263:ILE:HD12	4:M:263:ILE:HA	1.57	0.46
4:U:120:TYR:N	4:U:120:TYR:CD2	2.84	0.46
4:U:336:ILE:HD12	4:U:367:SER:O	2.16	0.46
1:A:144:ALA:O	1:A:148:ALA:HB2	2.16	0.45
1:A:406:VAL:HG21	1:A:441:TRP:HZ2	1.80	0.45
1:A:5:SER:OG	1:A:6:LYS:N	2.49	0.45
2:B:208:LEU:HD13	2:B:243:ARG:NE	2.30	0.45
2:B:31:LYS:HG3	2:B:65:LEU:HD13	1.98	0.45
1:L:325:ASN:O	1:L:329:ARG:HG2	2.15	0.45
1:L:449:LEU:H	1:L:449:LEU:CD1	2.29	0.45
1:L:523:PHE:HZ	1:L:562:VAL:HG21	1.81	0.45
4:M:129:LEU:O	4:M:133:ILE:HG12	2.16	0.45
4:M:336:ILE:HD12	4:M:367:SER:O	2.17	0.45
3:S:39:VAL:HG22	3:S:59:TYR:CD1	2.51	0.45
4:U:120:TYR:N	4:U:120:TYR:HD2	2.15	0.45
2:B:66:LYS:HD2	2:B:102:ILE:HG21	1.98	0.45
2:B:436:LEU:HD11	2:B:465:LEU:HD22	1.98	0.45
3:I:7:ILE:CD1	3:I:16:LEU:HD23	2.47	0.45
1:L:451:ARG:NH1	1:L:452:ILE:HG13	2.31	0.45
2:E:254:ALA:HB2	4:U:77:MET:N	2.30	0.45
1:A:239:SER:CB	1:A:243:ASP:OD2	2.64	0.45
1:A:341:ARG:HD3	1:A:341:ARG:H	1.81	0.45
1:A:481:LYS:HA	1:A:511:ILE:HD12	1.97	0.45
2:B:231:PRO:HD3	2:B:266:PHE:CE2	2.50	0.45
2:B:465:LEU:HD23	2:B:465:LEU:HA	1.71	0.45
2:E:237:ALA:O	2:E:240:ILE:HG22	2.17	0.45
1:L:427:LYS:O	1:L:431:LEU:HG	2.17	0.45
1:A:20:ILE:C	1:A:22:ASN:N	2.70	0.45
2:E:485:LEU:HD22	2:E:526:TYR:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:250:TYR:CD2	1:L:301:GLN:HB3	2.51	0.45
1:L:509:ASN:HA	1:L:552:PHE:HZ	1.81	0.45
2:E:549:SER:H	1:L:570:LYS:HB3	1.81	0.45
2:B:143:VAL:HG21	4:M:117:ASP:OD2	2.16	0.45
4:M:212:CYS:SG	4:M:267:PRO:HG3	2.56	0.45
4:M:331:SER:HB3	4:M:373:LEU:HG	1.99	0.45
3:S:65:LEU:HD21	3:S:100:GLU:HG2	1.98	0.45
1:A:280:LEU:O	1:A:280:LEU:HG	2.14	0.45
1:A:334:LEU:HB3	1:A:353:MET:CE	2.47	0.45
1:A:367:LYS:O	1:A:370:ILE:HG13	2.17	0.45
1:A:510:LEU:HD12	1:A:510:LEU:N	2.24	0.45
1:A:546:ILE:HD12	1:A:549:VAL:HG21	1.98	0.45
2:E:169:ILE:O	2:E:177:VAL:HG13	2.17	0.45
2:E:274:SER:C	2:E:276:TYR:N	2.70	0.45
3:I:29:GLN:NE2	3:I:29:GLN:HA	2.31	0.45
1:L:233:LEU:CD2	1:L:262:LEU:HD21	2.46	0.45
1:L:265:LEU:HD13	1:L:280:LEU:HD13	1.98	0.45
4:M:169:ARG:CG	4:M:170:ARG:H	2.30	0.45
5:Q:5:ILE:O	5:Q:5:ILE:HG13	2.16	0.45
1:A:88:TYR:CB	3:S:141:LEU:HD13	2.42	0.45
1:A:512:ALA:HB1	1:A:519:PRO:HD3	1.98	0.45
2:B:208:LEU:HA	2:B:208:LEU:HD23	1.78	0.45
2:B:237:ALA:O	2:B:240:ILE:HG22	2.16	0.45
2:E:284:LEU:C	2:E:287:PRO:HD2	2.37	0.45
1:L:156:VAL:HG11	1:L:188:TRP:CB	2.47	0.45
1:L:252:VAL:HG21	1:L:305:ALA:HB3	1.99	0.45
4:M:430:ILE:O	4:M:430:ILE:CG1	2.64	0.45
4:U:335:VAL:O	4:U:336:ILE:HG13	2.17	0.45
1:A:549:VAL:HG13	1:A:556:LYS:HG3	1.97	0.45
2:B:70:TYR:CD2	2:B:105:LEU:HG	2.52	0.45
2:B:13:GLY:CA	2:B:17:GLU:HG3	2.47	0.45
2:B:193:ASN:H	2:B:193:ASN:ND2	2.15	0.45
2:B:492:PHE:HA	2:B:499:THR:HG21	1.99	0.45
2:E:559:LEU:HG	2:E:559:LEU:O	2.16	0.45
1:L:201:LEU:HD23	1:L:201:LEU:HA	1.83	0.45
1:L:406:VAL:HG21	1:L:441:TRP:HZ2	1.81	0.45
4:M:184:LEU:HG	4:M:192:LEU:HD12	1.99	0.45
4:U:328:LEU:HD13	4:U:349:ASN:HD21	1.82	0.45
4:U:328:LEU:HD13	4:U:349:ASN:ND2	2.32	0.45
4:U:430:ILE:CG1	4:U:430:ILE:O	2.63	0.45
1:A:314:ILE:CD1	1:A:330:ALA:HB1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LYS:O	1:A:431:LEU:HG	2.17	0.45
2:B:286:PRO:N	2:B:287:PRO:CD	2.80	0.45
2:B:305:ASN:ND2	2:B:567:ILE:O	2.50	0.45
3:I:72:ASP:O	3:I:75:ASP:HB2	2.16	0.45
1:L:282:GLU:O	1:L:285:GLU:HB2	2.16	0.45
5:P:5:ILE:O	5:P:5:ILE:HG13	2.17	0.45
1:A:449:LEU:H	1:A:449:LEU:CD1	2.30	0.45
1:A:521:ILE:HD13	1:A:521:ILE:HA	1.77	0.45
3:I:65:LEU:HD21	3:I:100:GLU:HG2	1.99	0.45
1:L:351:GLU:HA	1:L:388:ARG:HH21	1.82	0.45
4:M:379:LYS:C	4:M:381:TRP:N	2.70	0.45
4:M:42:GLN:HA	4:M:42:GLN:NE2	2.32	0.45
5:P:2:MET:CE	3:S:9:ASN:HB2	2.47	0.45
4:U:21:ARG:HG2	4:U:23:ASP:OD2	2.16	0.45
4:U:245:ASP:O	4:U:246:CYS:HB2	2.16	0.45
1:A:370:ILE:HG12	1:A:396:MET:CE	2.40	0.45
1:A:418:TYR:N	1:A:418:TYR:HD1	2.15	0.45
1:A:442:TYR:CZ	1:A:465:VAL:HG12	2.52	0.45
1:A:527:HIS:HD2	1:A:545:TYR:OH	1.99	0.45
2:B:147:LYS:HE2	2:B:147:LYS:HB2	1.67	0.45
2:B:497:SER:C	2:B:499:THR:H	2.20	0.45
2:E:285:ALA:HB3	2:E:286:PRO:CD	2.41	0.45
1:L:523:PHE:CD1	1:L:559:ILE:HG12	2.52	0.45
4:M:162:ARG:NH2	4:M:166:ILE:HG13	2.32	0.45
4:M:217:ASN:ND2	4:M:219:LYS:HD3	2.32	0.45
4:M:183:LEU:HD23	4:M:431:TYR:CE2	2.51	0.45
5:Q:2:MET:SD	5:Q:2:MET:N	2.90	0.45
2:B:213:GLU:HB2	2:B:214:CYS:H	1.51	0.44
2:B:306:ILE:H	2:B:306:ILE:HG12	1.68	0.44
2:E:31:LYS:HG3	2:E:65:LEU:HD13	2.00	0.44
3:I:75:ASP:HA	1:L:263:ARG:HH21	1.82	0.44
1:L:458:SER:O	1:L:461:VAL:HG23	2.17	0.44
4:M:111:LEU:HD22	4:M:133:ILE:CD1	2.47	0.44
4:M:9:ASN:HD21	4:M:13:GLU:H	1.65	0.44
3:S:107:PHE:CG	3:S:108:TYR:N	2.85	0.44
1:A:247:TYR:CE2	3:S:127:SER:HB2	2.53	0.44
3:S:16:LEU:HD12	3:S:17:ALA:N	2.32	0.44
4:U:50:ILE:O	4:U:51:ALA:CB	2.63	0.44
1:A:103:ASN:C	1:A:103:ASN:HD22	2.21	0.44
1:A:368:THR:HG22	1:A:368:THR:O	2.17	0.44
2:B:148:LEU:HG	2:B:156:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:GLN:NE2	2:B:439:LEU:HA	2.31	0.44
3:I:119:LEU:HB3	1:L:170:LEU:HD12	1.99	0.44
1:L:368:THR:O	1:L:368:THR:HG22	2.18	0.44
1:L:370:ILE:HG12	1:L:396:MET:CE	2.39	0.44
1:L:509:ASN:HA	1:L:552:PHE:CZ	2.53	0.44
5:P:2:MET:HG2	5:P:2:MET:O	2.17	0.44
3:I:10:ARG:H	5:Q:2:MET:HE1	1.81	0.44
1:A:442:TYR:CZ	1:A:468:ILE:HD12	2.51	0.44
2:E:314:PRO:HD2	2:E:315:GLU:OE2	2.18	0.44
2:E:414:ILE:HD13	2:E:414:ILE:HA	1.81	0.44
2:E:496:PRO:O	2:E:497:SER:OG	2.30	0.44
1:L:31:LYS:HG2	1:L:35:LYS:HE2	1.99	0.44
1:L:554:GLU:H	1:L:554:GLU:HG2	1.40	0.44
1:L:94:GLY:O	1:L:98:ILE:HG23	2.17	0.44
4:M:235:LYS:H	4:M:276:ARG:HH21	1.65	0.44
4:M:430:ILE:HG13	4:M:432:GLU:HG3	1.99	0.44
1:A:418:TYR:N	1:A:418:TYR:CD1	2.85	0.44
1:A:518:SER:O	1:A:522:GLN:HG3	2.18	0.44
1:A:509:ASN:HA	1:A:552:PHE:HZ	1.82	0.44
1:A:83:LEU:HD22	1:A:95:TYR:CE2	2.52	0.44
2:B:114:ARG:HA	2:B:151:ILE:HD13	1.98	0.44
2:E:365:VAL:HG13	2:E:365:VAL:O	2.17	0.44
1:L:22:ASN:HB3	1:L:23:CYS:H	1.41	0.44
1:L:527:HIS:HD2	1:L:545:TYR:OH	2.00	0.44
1:L:542:LEU:HD23	1:L:542:LEU:HA	1.69	0.44
4:M:120:TYR:N	4:M:120:TYR:HD2	2.16	0.44
4:U:179:GLU:OE2	4:U:277:TYR:OH	2.27	0.44
1:A:103:ASN:HD22	1:A:105:ASN:H	1.65	0.44
2:B:97:ASP:CG	2:B:102:ILE:HD11	2.38	0.44
2:B:520:ARG:NH1	2:B:520:ARG:HG2	2.33	0.44
2:E:365:VAL:HG13	4:U:401:VAL:CG1	2.47	0.44
2:E:492:PHE:HA	2:E:499:THR:HG21	1.99	0.44
1:A:361:PHE:CZ	2:E:531:SER:OG	2.70	0.44
1:L:346:ARG:NH2	1:L:376:ALA:HA	2.32	0.44
4:M:120:TYR:N	4:M:120:TYR:CD2	2.85	0.44
3:S:138:LEU:C	3:S:140:SER:N	2.70	0.44
1:L:394:TYR:CE2	4:U:294:ARG:HD3	2.52	0.44
1:A:334:LEU:HB3	1:A:353:MET:HE2	2.00	0.44
2:E:145:VAL:HG11	2:E:165:LEU:HD22	1.99	0.44
1:L:189:THR:HG22	1:L:190:SER:N	2.31	0.44
1:L:243:ASP:O	1:L:245:GLN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:614:ALA:O	4:U:332:GLY:HA2	2.18	0.44
4:U:139:LYS:O	4:U:140:SER:HB2	2.17	0.44
4:U:174:PHE:CD1	4:U:174:PHE:N	2.86	0.44
1:A:527:HIS:HE1	6:A:1624:SO4:O2	2.01	0.44
1:A:595:LEU:HD21	1:A:599:LEU:HD12	2.00	0.44
2:E:148:LEU:HG	2:E:156:VAL:HG23	2.00	0.44
2:E:193:ASN:ND2	2:E:193:ASN:H	2.16	0.44
3:I:107:PHE:HE1	1:L:63:LEU:HD23	1.83	0.44
1:L:40:ILE:O	1:L:43:LYS:HB2	2.17	0.44
1:L:521:ILE:HD13	1:L:521:ILE:HA	1.78	0.44
4:M:235:LYS:H	4:M:276:ARG:NH2	2.16	0.44
1:A:457:VAL:HG23	1:A:461:VAL:HB	1.99	0.44
2:B:289:VAL:HG12	2:B:290:THR:N	2.33	0.44
2:B:351:ILE:HD12	2:B:351:ILE:H	1.82	0.44
2:E:320:GLU:OE1	2:E:320:GLU:HA	2.18	0.44
2:E:488:ILE:HD13	2:E:506:VAL:CG2	2.47	0.44
1:L:341:ARG:HD3	1:L:341:ARG:H	1.83	0.44
4:M:222:ILE:H	4:M:222:ILE:CD1	2.12	0.44
4:M:34:VAL:HG13	4:M:34:VAL:O	2.18	0.44
4:U:278:ARG:O	4:U:278:ARG:HG3	2.18	0.44
4:U:353:TRP:CZ2	4:U:355:ILE:HD11	2.52	0.44
4:U:385:PRO:CB	4:U:432:GLU:HB3	2.47	0.44
1:A:467:GLN:HG3	1:A:605:PHE:CG	2.52	0.44
1:A:473:ASP:O	1:A:475:VAL:N	2.51	0.44
1:A:509:ASN:HA	1:A:552:PHE:CZ	2.53	0.44
2:B:414:ILE:HA	2:B:414:ILE:HD13	1.82	0.44
2:B:432:LEU:C	2:B:434:GLU:H	2.21	0.44
2:E:520:ARG:HG2	2:E:520:ARG:HH11	1.82	0.44
2:E:581:PHE:HA	4:U:52:ARG:CG	2.47	0.44
1:L:147:PHE:C	1:L:149:GLY:N	2.71	0.44
1:L:20:ILE:C	1:L:22:ASN:N	2.71	0.44
1:L:401:ASN:HD22	1:L:401:ASN:C	2.21	0.44
1:L:597:THR:HA	1:L:600:GLU:HG3	2.00	0.44
4:M:353:TRP:CZ2	4:M:355:ILE:HD11	2.52	0.44
3:S:23:PHE:HD2	3:S:27:GLU:OE1	2.01	0.44
3:S:72:ASP:HB2	3:S:75:ASP:OD2	2.18	0.44
2:E:436:LEU:HD11	2:E:465:LEU:HD22	2.00	0.43
2:E:419:ARG:CZ	2:E:548:ILE:HG21	2.47	0.43
3:I:137:MET:C	3:I:138:LEU:O	2.56	0.43
3:I:141:LEU:HA	3:I:141:LEU:HD23	1.70	0.43
3:I:49:PHE:CE2	3:I:77:ASN:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:300:VAL:HG13	1:L:301:GLN:NE2	2.33	0.43
1:L:410:LEU:HA	1:L:410:LEU:HD23	1.80	0.43
1:L:413:LEU:HD21	1:L:453:ALA:CB	2.48	0.43
4:U:129:LEU:O	4:U:133:ILE:HG12	2.17	0.43
4:U:248:PHE:HB3	4:U:252:VAL:HG21	2.00	0.43
4:U:41:GLN:HG2	4:U:284:ILE:CG2	2.48	0.43
1:A:351:GLU:HA	1:A:388:ARG:HH21	1.83	0.43
2:E:265:LYS:HD3	2:E:265:LYS:HA	1.68	0.43
2:E:365:VAL:CG1	4:U:401:VAL:CG1	2.96	0.43
4:U:101:ILE:HG23	4:U:108:ILE:CD1	2.49	0.43
1:A:243:ASP:O	1:A:245:GLN:N	2.51	0.43
1:A:347:TYR:CD2	1:A:347:TYR:C	2.92	0.43
2:E:452:VAL:HG13	2:E:459:ILE:HD12	2.00	0.43
2:E:529:LEU:HD21	2:E:537:ALA:HA	2.00	0.43
1:L:545:TYR:O	1:L:549:VAL:HG23	2.19	0.43
3:S:92:ASN:ND2	3:S:98:VAL:N	2.66	0.43
4:U:261:ARG:O	4:U:263:ILE:HD13	2.18	0.43
1:A:566:ASP:HB3	1:A:570:LYS:HD2	2.00	0.43
1:A:618:LYS:HD2	6:A:1627:SO4:O4	2.18	0.43
2:B:124:GLU:HG3	2:B:127:ARG:HH12	1.82	0.43
2:B:306:ILE:CG2	2:B:317:LEU:HD12	2.49	0.43
2:B:502:LEU:O	2:B:506:VAL:HG23	2.18	0.43
2:B:529:LEU:HD21	2:B:537:ALA:HA	2.01	0.43
2:E:218:GLY:O	2:E:222:ILE:HG13	2.19	0.43
2:E:231:PRO:HD3	2:E:266:PHE:CE2	2.53	0.43
2:E:540:VAL:CG2	1:L:586:LEU:HB3	2.48	0.43
2:E:70:TYR:CD2	2:E:105:LEU:HG	2.54	0.43
1:L:457:VAL:HG23	1:L:461:VAL:HB	2.00	0.43
1:L:487:LEU:CD2	1:L:496:LEU:HD23	2.38	0.43
1:L:535:VAL:O	1:L:538:ARG:N	2.50	0.43
4:U:379:LYS:C	4:U:381:TRP:N	2.69	0.43
1:A:40:ILE:O	1:A:43:LYS:HB2	2.18	0.43
2:B:365:VAL:HG13	2:B:365:VAL:O	2.18	0.43
2:E:453:GLY:C	2:E:454:GLU:O	2.54	0.43
2:E:517:PRO:HD2	1:L:463:TYR:CD2	2.53	0.43
2:E:549:SER:O	2:E:550:GLU:O	2.36	0.43
3:I:58:ILE:N	3:I:58:ILE:HD13	2.33	0.43
1:L:364:GLU:C	1:L:366:VAL:N	2.71	0.43
1:L:464:ARG:HH11	1:L:467:GLN:NE2	2.14	0.43
1:L:530:PHE:O	1:L:532:LEU:N	2.42	0.43
5:P:2:MET:O	5:P:3:SEP:C	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:91:LEU:HD13	3:S:103:LEU:HD21	2.00	0.43
4:U:252:VAL:HA	4:U:265:PHE:HB3	2.00	0.43
1:A:406:VAL:HG13	1:A:428:VAL:HG13	2.00	0.43
2:B:96:GLU:O	2:B:97:ASP:C	2.56	0.43
1:L:311:PHE:CZ	1:L:348:LEU:HB3	2.54	0.43
1:L:370:ILE:HA	1:L:396:MET:HE1	2.00	0.43
1:L:375:ASN:O	1:L:378:LYS:N	2.48	0.43
1:L:4:VAL:HG12	1:L:5:SER:H	1.83	0.43
1:L:507:PHE:HB3	1:L:510:LEU:HD11	2.01	0.43
4:M:9:ASN:C	4:M:9:ASN:ND2	2.60	0.43
5:P:2:MET:SD	5:P:2:MET:N	2.92	0.43
5:Q:2:MET:HG2	5:Q:2:MET:O	2.18	0.43
3:S:42:ARG:NH2	3:S:46:HIS:HB3	2.34	0.43
4:U:9:ASN:HD22	4:U:12:GLY:H	1.67	0.43
1:A:376:ALA:O	1:A:380:GLU:HB2	2.19	0.43
1:A:420:ILE:HG22	1:A:424:ILE:HG13	2.00	0.43
1:A:43:LYS:HB3	1:A:50:LEU:HD21	2.01	0.43
2:B:522:ARG:NH1	2:B:522:ARG:HG2	2.34	0.43
2:E:502:LEU:O	2:E:506:VAL:HG23	2.18	0.43
2:E:522:ARG:HD2	1:L:579:ARG:CZ	2.48	0.43
4:M:16:ILE:HD12	4:M:108:ILE:HG21	2.01	0.43
4:U:243:ILE:O	4:U:243:ILE:HD12	2.18	0.43
1:A:150:GLU:O	1:A:154:ILE:HG13	2.18	0.43
1:A:233:LEU:HD13	1:A:261:LEU:HB2	2.00	0.43
1:A:464:ARG:HH11	1:A:467:GLN:NE2	2.17	0.43
2:B:212:ASN:O	2:B:213:GLU:HG3	2.19	0.43
1:A:603:PRO:HG2	2:B:524:TYR:CE2	2.54	0.43
2:B:529:LEU:CD2	2:B:537:ALA:HA	2.49	0.43
2:E:124:GLU:HG3	2:E:127:ARG:HH12	1.83	0.43
2:E:263:LEU:O	2:E:267:LEU:HB3	2.18	0.43
2:E:522:ARG:NH1	2:E:522:ARG:HG2	2.34	0.43
1:L:105:ASN:OD1	1:L:108:LEU:HG	2.18	0.43
1:L:367:LYS:HZ3	1:L:398:ASP:HB3	1.81	0.43
4:M:29:VAL:HG13	4:M:30:ASP:N	2.34	0.43
4:M:335:VAL:O	4:M:336:ILE:HG13	2.19	0.43
1:A:217:LYS:C	1:A:219:PRO:HD3	2.39	0.43
1:A:341:ARG:N	1:A:341:ARG:HD3	2.33	0.43
2:B:476:GLU:HB3	2:B:480:VAL:HG22	2.01	0.43
1:L:108:LEU:HD23	1:L:111:LEU:HD12	2.00	0.43
1:L:406:VAL:HG13	1:L:428:VAL:HG13	2.00	0.43
1:L:606:PRO:O	1:L:608:ARG:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:56:PHE:CD1	4:M:56:PHE:N	2.87	0.43
4:U:331:SER:HB3	4:U:373:LEU:HG	2.01	0.43
4:U:403:TYR:C	4:U:403:TYR:CD1	2.91	0.43
1:A:446:ILE:CG2	1:A:465:VAL:HG11	2.45	0.43
2:B:351:ILE:HD12	2:B:351:ILE:N	2.33	0.43
2:E:34:VAL:O	2:E:38:ILE:HG13	2.19	0.43
1:L:222:PHE:C	1:L:224:THR:H	2.22	0.43
1:L:322:SER:O	1:L:323:GLU:O	2.37	0.43
4:M:104:ASN:O	4:M:105:PHE:C	2.56	0.43
4:M:252:VAL:HA	4:M:265:PHE:HB3	2.01	0.43
1:A:80:VAL:HG13	1:A:83:LEU:HD12	2.00	0.42
2:B:193:ASN:N	2:B:193:ASN:ND2	2.65	0.42
2:E:246:PRO:O	2:E:248:LEU:N	2.52	0.42
2:E:63:LEU:HD12	2:E:63:LEU:HA	1.84	0.42
3:I:9:ASN:HB2	5:Q:2:MET:CE	2.49	0.42
1:L:103:ASN:HD22	1:L:105:ASN:H	1.66	0.42
4:M:232:GLU:HG3	4:M:247:THR:OG1	2.18	0.42
1:A:124:ASN:C	1:A:124:ASN:OD1	2.57	0.42
1:A:370:ILE:HA	1:A:396:MET:HE3	2.01	0.42
1:A:594:ILE:HA	1:A:594:ILE:HD12	1.71	0.42
2:B:246:PRO:C	2:B:248:LEU:N	2.72	0.42
2:E:197:LEU:HB3	2:E:199:LEU:CD2	2.49	0.42
2:E:493:LEU:HD13	2:E:541:VAL:HG21	2.01	0.42
1:L:543:SER:HA	1:L:583:TYR:CE2	2.54	0.42
1:L:602:MET:HA	1:L:603:PRO:HD3	1.86	0.42
5:P:5:ILE:O	5:P:5:ILE:CG1	2.67	0.42
3:S:67:PHE:CE2	3:S:88:VAL:HG22	2.54	0.42
2:B:373:ALA:O	2:B:376:ALA:HB3	2.19	0.42
2:E:357:GLU:CG	2:E:361:TYR:OH	2.67	0.42
1:L:341:ARG:HD3	1:L:341:ARG:N	2.33	0.42
7:E:2002:HOH:O	1:L:574:VAL:CG2	2.67	0.42
4:M:379:LYS:O	4:M:381:TRP:N	2.46	0.42
4:M:98:GLU:HG2	4:M:98:GLU:O	2.19	0.42
3:I:9:ASN:HB2	5:Q:2:MET:HE2	2.01	0.42
3:S:141:LEU:HA	3:S:141:LEU:HD23	1.69	0.42
1:A:308:ALA:HB2	3:S:78:LEU:HB3	2.02	0.42
4:U:306:VAL:HG12	4:U:307:ILE:N	2.34	0.42
1:A:487:LEU:HD23	1:A:487:LEU:HA	1.87	0.42
1:A:549:VAL:H	1:A:549:VAL:HG23	1.61	0.42
2:B:480:VAL:O	2:B:481:GLN:C	2.57	0.42
2:B:81:PRO:O	2:B:84:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:PRO:CB	2:E:214:CYS:HA	2.29	0.42
1:L:534:SER:CB	1:L:536:PRO:HD2	2.50	0.42
2:B:78:LYS:HZ2	4:M:18:ARG:HH12	1.67	0.42
4:U:112:LEU:C	4:U:114:GLU:H	2.23	0.42
4:U:414:SER:C	4:U:416:HIS:N	2.71	0.42
2:B:129:CYS:HA	2:B:132:ASP:HB2	2.02	0.42
3:I:92:ASN:ND2	3:I:98:VAL:H	2.18	0.42
1:L:217:LYS:C	1:L:219:PRO:HD3	2.40	0.42
4:M:196:VAL:HB	4:M:279:THR:HG23	2.02	0.42
4:M:328:LEU:HD13	4:M:349:ASN:ND2	2.34	0.42
3:S:65:LEU:HD21	3:S:100:GLU:CG	2.50	0.42
4:U:248:PHE:CD2	4:U:252:VAL:HG11	2.54	0.42
1:A:364:GLU:C	1:A:366:VAL:N	2.73	0.42
1:A:413:LEU:HD21	1:A:453:ALA:CB	2.50	0.42
1:A:605:PHE:CE2	2:B:520:ARG:HD3	2.54	0.42
2:B:158:ASP:C	2:B:160:GLY:H	2.23	0.42
2:B:314:PRO:HD2	2:B:315:GLU:OE2	2.19	0.42
2:B:325:PHE:HA	2:B:342:MET:CE	2.49	0.42
2:B:436:LEU:HD21	2:B:448:MET:SD	2.60	0.42
2:E:129:CYS:HA	2:E:132:ASP:HB2	2.02	0.42
1:L:147:PHE:O	1:L:148:ALA:C	2.57	0.42
4:M:41:GLN:HG2	4:M:284:ILE:CG2	2.49	0.42
1:A:543:SER:HA	1:A:583:TYR:CE2	2.55	0.42
2:B:123:CYS:SG	2:B:159:GLN:HG3	2.60	0.42
2:B:172:SER:HB2	2:B:173:ASN:H	1.71	0.42
2:B:419:ARG:NH2	2:B:548:ILE:HG21	2.34	0.42
2:E:111:GLY:O	2:E:147:LYS:HG2	2.19	0.42
2:E:440:ASP:O	2:E:441:GLU:C	2.57	0.42
2:E:546:PRO:HD2	1:L:577:GLN:HE21	1.83	0.42
3:I:138:LEU:C	3:I:140:SER:N	2.73	0.42
1:L:156:VAL:HG11	1:L:188:TRP:HB2	2.01	0.42
1:L:257:LEU:O	1:L:261:LEU:HG	2.19	0.42
1:L:318:ILE:HD11	1:L:356:LEU:HD12	2.00	0.42
1:L:512:ALA:HB1	1:L:519:PRO:HD3	2.01	0.42
1:L:576:LEU:HA	1:L:576:LEU:HD12	1.82	0.42
4:M:390:PHE:CD1	4:M:390:PHE:C	2.93	0.42
5:P:2:MET:HE2	3:S:9:ASN:HB2	2.01	0.42
4:U:173:LEU:HD12	4:U:173:LEU:O	2.19	0.42
1:A:485:GLU:O	1:A:488:GLN:HB2	2.20	0.42
2:B:420:LYS:O	2:B:420:LYS:HG3	2.19	0.42
2:E:351:ILE:HG12	2:E:384:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:THR:CG2	1:L:324:PRO:HG3	2.49	0.42
1:L:50:LEU:CD1	1:L:50:LEU:H	2.23	0.42
4:M:15:LEU:HD11	4:M:98:GLU:HG3	2.02	0.42
4:M:18:ARG:HB3	4:M:20:TYR:HE1	1.85	0.42
4:M:1:MET:HE3	4:M:77:MET:CE	2.50	0.42
4:M:245:ASP:O	4:M:246:CYS:HB2	2.19	0.42
4:M:408:GLU:HA	4:M:409:PRO:HD3	1.71	0.42
5:P:9:LEU:HB3	5:P:10:SER:H	1.54	0.42
4:U:235:LYS:H	4:U:276:ARG:NH2	2.17	0.42
2:B:145:VAL:HG21	2:B:165:LEU:HD13	2.00	0.42
2:B:212:ASN:O	2:B:213:GLU:CG	2.68	0.42
2:B:265:LYS:HE3	2:B:565:CYS:SG	2.60	0.42
2:B:458:ARG:HD2	2:B:458:ARG:HA	1.87	0.42
2:E:303:LEU:HD13	2:E:337:GLU:HB2	2.01	0.42
2:E:463:ASP:HB2	2:E:464:GLU:H	1.72	0.42
1:L:144:ALA:O	1:L:148:ALA:HB2	2.20	0.42
1:L:442:TYR:CZ	1:L:465:VAL:HG12	2.55	0.42
1:L:467:GLN:HG3	1:L:605:PHE:CG	2.55	0.42
4:M:268:PRO:HD2	4:M:272:PHE:CE2	2.54	0.42
4:M:356:LYS:HA	4:M:356:LYS:HD2	1.74	0.42
5:Q:5:ILE:O	5:Q:5:ILE:CG1	2.67	0.42
4:U:84:LYS:HD3	4:U:124:SER:HB3	2.01	0.42
4:U:290:ILE:HA	4:U:291:PRO:HD3	1.85	0.42
1:A:33:ILE:HA	1:A:33:ILE:HD12	1.80	0.42
1:A:401:ASN:HD22	1:A:401:ASN:C	2.22	0.42
1:A:535:VAL:N	1:A:536:PRO:CD	2.83	0.42
2:B:47:VAL:O	2:B:48:SER:HB3	2.19	0.42
2:E:306:ILE:CG2	2:E:317:LEU:HD12	2.49	0.42
3:I:33:GLU:O	3:I:36:HIS:HB3	2.19	0.42
4:M:29:VAL:HG13	4:M:30:ASP:H	1.85	0.42
4:M:316:LEU:HD13	4:M:357:ARG:HB2	2.01	0.42
4:U:232:GLU:HG3	4:U:247:THR:OG1	2.20	0.42
1:A:233:LEU:CD2	1:A:262:LEU:HD21	2.50	0.41
1:A:380:GLU:HG3	1:A:385:VAL:HG11	2.01	0.41
1:A:442:TYR:CE2	1:A:468:ILE:HD12	2.54	0.41
2:B:461:ASN:O	2:B:462:ALA:C	2.58	0.41
2:E:101:LEU:O	2:E:105:LEU:HB2	2.19	0.41
2:E:173:ASN:HD21	2:E:175:MET:HE2	1.85	0.41
2:E:497:SER:C	2:E:499:THR:H	2.23	0.41
1:L:42:SER:HA	1:L:45:LYS:HB3	2.02	0.41
4:M:104:ASN:O	4:M:108:ILE:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:293:VAL:O	4:M:294:ARG:CB	2.66	0.41
5:Q:2:MET:O	5:Q:3:SEP:C	2.68	0.41
3:S:137:MET:C	3:S:138:LEU:O	2.54	0.41
4:U:214:PHE:HE2	4:U:401:VAL:HG13	1.85	0.41
1:A:22:ASN:HB3	1:A:23:CYS:H	1.43	0.41
2:B:149:HIS:NE2	2:B:187:ILE:HG23	2.36	0.41
2:B:18:LEU:HD23	2:B:18:LEU:HA	1.84	0.41
2:B:246:PRO:O	2:B:248:LEU:N	2.53	0.41
2:B:34:VAL:O	2:B:38:ILE:HG13	2.19	0.41
2:E:303:LEU:HD22	2:E:341:ILE:HD12	2.01	0.41
2:E:351:ILE:H	2:E:351:ILE:HD12	1.85	0.41
2:E:351:ILE:N	2:E:351:ILE:HD12	2.35	0.41
2:E:432:LEU:C	2:E:434:GLU:H	2.23	0.41
3:I:107:PHE:CG	3:I:108:TYR:N	2.88	0.41
1:L:124:ASN:OD1	1:L:124:ASN:C	2.58	0.41
1:L:362:SER:O	1:L:363:HIS:CB	2.68	0.41
1:L:386:ARG:HG2	1:L:386:ARG:NH1	2.35	0.41
4:M:118:PHE:HD2	4:M:120:TYR:CE2	2.38	0.41
4:U:325:PRO:CB	4:U:384:PRO:HG2	2.49	0.41
4:U:383:ARG:HG3	4:U:383:ARG:O	2.20	0.41
1:A:397:CYS:SG	1:A:431:LEU:HD13	2.61	0.41
2:B:101:LEU:O	2:B:105:LEU:HB2	2.20	0.41
2:B:347:SER:C	2:B:349:ALA:N	2.73	0.41
2:B:520:ARG:HH11	2:B:520:ARG:HG2	1.84	0.41
2:B:550:GLU:HG2	2:B:551:GLU:H	1.85	0.41
2:E:193:ASN:ND2	2:E:193:ASN:N	2.67	0.41
2:E:419:ARG:NH2	2:E:548:ILE:HG21	2.35	0.41
3:I:31:LEU:HD12	3:I:31:LEU:HA	1.86	0.41
1:L:457:VAL:HG13	1:L:495:ASN:HD22	1.86	0.41
1:L:481:LYS:HA	1:L:511:ILE:HD12	2.01	0.41
1:L:566:ASP:HB3	1:L:570:LYS:HD2	2.01	0.41
2:B:71:LEU:HD11	4:M:110:GLU:HB2	2.01	0.41
1:A:334:LEU:CD1	1:A:352:SER:HB3	2.48	0.41
2:B:387:SER:O	2:B:390:ARG:HG2	2.20	0.41
2:B:530:LEU:HD23	2:B:530:LEU:HA	1.78	0.41
2:E:175:MET:HE3	2:E:175:MET:HB3	1.90	0.41
2:E:317:LEU:HD23	2:E:317:LEU:HA	1.73	0.41
2:E:387:SER:O	2:E:390:ARG:HG2	2.19	0.41
2:E:435:ASN:O	2:E:437:ASP:N	2.53	0.41
2:E:488:ILE:HD13	2:E:506:VAL:HG22	2.02	0.41
3:I:10:ARG:H	5:Q:2:MET:CE	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:518:SER:O	1:L:522:GLN:HG3	2.21	0.41
1:A:426:LEU:HB3	4:M:292:LEU:HD11	2.02	0.41
4:U:107:LEU:O	4:U:111:LEU:HB2	2.20	0.41
4:U:16:ILE:HD12	4:U:108:ILE:HG21	2.02	0.41
4:U:296:VAL:CG1	4:U:300:LYS:HG3	2.50	0.41
4:U:384:PRO:O	4:U:435:CYS:SG	2.78	0.41
4:U:15:LEU:HD11	4:U:98:GLU:HG3	2.03	0.41
2:B:40:ALA:HA	2:B:43:VAL:CG2	2.46	0.41
2:E:286:PRO:N	2:E:287:PRO:CD	2.83	0.41
2:E:40:ALA:O	2:E:45:LYS:HB2	2.20	0.41
1:L:250:TYR:N	1:L:250:TYR:CD1	2.88	0.41
1:L:346:ARG:HH21	1:L:376:ALA:HA	1.86	0.41
4:M:9:ASN:ND2	4:M:12:GLY:H	2.19	0.41
4:U:136:GLN:HG2	4:U:136:GLN:H	1.63	0.41
4:U:55:PHE:CD2	4:U:68:VAL:HG22	2.56	0.41
2:B:272:LYS:HZ1	2:B:278:ASN:HD21	1.68	0.41
2:B:351:ILE:CD1	2:B:351:ILE:H	2.31	0.41
2:B:437:ASP:OD1	2:B:437:ASP:N	2.54	0.41
2:E:187:ILE:HG22	2:E:196:LEU:HD13	2.01	0.41
3:I:138:LEU:O	3:I:139:GLN:CB	2.61	0.41
1:L:541:LEU:HD12	1:L:541:LEU:HA	1.87	0.41
4:M:383:ARG:HA	4:M:384:PRO:HD2	1.74	0.41
4:M:414:SER:C	4:M:416:HIS:N	2.73	0.41
5:Q:6:LYS:HE3	5:Q:6:LYS:HB2	1.90	0.41
3:S:42:ARG:HH21	3:S:47:THR:H	1.67	0.41
1:A:156:VAL:HG11	1:A:188:TRP:CB	2.51	0.41
1:A:313:ALA:O	1:A:317:ILE:HG13	2.21	0.41
1:A:446:ILE:HG21	1:A:465:VAL:CG1	2.43	0.41
1:A:602:MET:HA	1:A:603:PRO:HD3	1.88	0.41
2:B:408:GLN:HE22	2:B:440:ASP:N	2.15	0.41
2:E:324:PHE:CD2	2:E:341:ILE:HG21	2.56	0.41
2:E:542:LEU:O	2:E:543:SER:O	2.39	0.41
1:L:114:ASN:O	1:L:117:LYS:HB3	2.20	0.41
1:L:150:GLU:O	1:L:154:ILE:HG13	2.20	0.41
1:L:250:TYR:HD1	1:L:250:TYR:N	2.19	0.41
4:M:325:PRO:CB	4:M:384:PRO:HG2	2.50	0.41
4:U:34:VAL:HG13	4:U:34:VAL:O	2.20	0.41
4:U:215:GLY:HA3	4:U:403:TYR:CZ	2.55	0.41
2:B:525:ILE:HG22	2:B:526:TYR:N	2.36	0.41
2:E:420:LYS:HG3	2:E:420:LYS:O	2.20	0.41
1:L:83:LEU:HD22	1:L:95:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:346:ALA:C	4:U:348:GLU:N	2.73	0.41
1:A:444:ASP:O	1:A:447:LEU:HD12	2.21	0.41
2:B:17:GLU:O	2:B:21:GLU:HG3	2.20	0.41
2:B:476:GLU:HB3	2:B:480:VAL:CG2	2.51	0.41
1:L:183:VAL:HA	1:L:184:PRO:HD3	1.87	0.41
1:L:430:ILE:O	1:L:434:LYS:HB3	2.21	0.41
4:M:84:LYS:HD3	4:M:124:SER:HB3	2.02	0.41
1:A:527:HIS:CE1	6:A:1624:SO4:O2	2.74	0.41
2:B:99:ASN:HB3	2:B:102:ILE:CD1	2.51	0.41
2:B:263:LEU:O	2:B:267:LEU:HB3	2.21	0.41
2:E:40:ALA:HA	2:E:43:VAL:CG2	2.46	0.41
2:E:550:GLU:HG2	2:E:551:GLU:H	1.85	0.41
2:E:83:MET:O	2:E:86:MET:HE2	2.21	0.41
1:L:43:LYS:HB3	1:L:50:LEU:HD21	2.03	0.41
4:M:346:ALA:C	4:M:348:GLU:N	2.74	0.41
1:A:341:ARG:H	1:A:341:ARG:CD	2.34	0.41
2:B:555:ILE:O	2:B:556:GLU:C	2.59	0.41
2:E:250:HIS:ND1	2:E:250:HIS:O	2.54	0.41
2:E:476:GLU:HB3	2:E:480:VAL:HG22	2.03	0.41
2:E:529:LEU:HG	2:E:537:ALA:HB2	2.03	0.41
2:E:543:SER:HB2	1:L:585:ARG:NH2	2.36	0.41
1:L:20:ILE:CG2	1:L:21:ARG:N	2.84	0.41
1:L:363:HIS:O	1:L:364:GLU:HB2	2.21	0.41
4:U:92:TYR:CE2	4:U:133:ILE:HG21	2.55	0.41
4:U:290:ILE:HB	4:U:306:VAL:HB	2.03	0.41
1:A:257:LEU:O	1:A:261:LEU:HG	2.21	0.40
1:A:364:GLU:O	1:A:366:VAL:N	2.53	0.40
1:A:382:ASP:O	1:A:384:SER:N	2.54	0.40
2:B:357:GLU:HG3	2:B:361:TYR:CZ	2.56	0.40
2:E:556:GLU:HG2	2:E:558:THR:H	1.84	0.40
2:E:582:VAL:O	2:E:582:VAL:HG12	2.21	0.40
3:I:93:GLU:HA	3:I:93:GLU:OE2	2.21	0.40
1:L:173:LEU:O	1:L:177:ARG:HG3	2.21	0.40
1:L:364:GLU:O	1:L:366:VAL:N	2.53	0.40
1:L:504:LEU:O	1:L:548:PHE:HE1	2.04	0.40
4:M:290:ILE:HB	4:M:306:VAL:HB	2.02	0.40
1:A:426:LEU:CB	4:M:292:LEU:HD11	2.52	0.40
1:A:319:HIS:HE1	4:M:380:LYS:HG3	1.86	0.40
4:U:84:LYS:HE2	4:U:84:LYS:HB2	1.90	0.40
1:A:250:TYR:CE2	1:A:301:GLN:HB2	2.56	0.40
1:A:4:VAL:HG12	1:A:5:SER:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:HD23	1:A:542:LEU:HA	1.78	0.40
1:A:570:LYS:O	1:A:571:ASN:C	2.59	0.40
2:B:103:ARG:HD3	2:B:128:LYS:HZ2	1.85	0.40
2:B:97:ASP:HB3	2:B:102:ILE:HG13	2.03	0.40
2:E:437:ASP:N	2:E:437:ASP:OD1	2.54	0.40
2:E:461:ASN:O	2:E:462:ALA:C	2.60	0.40
1:L:386:ARG:HG2	1:L:386:ARG:HH11	1.86	0.40
1:L:397:CYS:HA	1:L:401:ASN:HD21	1.85	0.40
1:L:446:ILE:CG2	1:L:465:VAL:HG11	2.42	0.40
4:M:186:SER:CB	4:M:190:GLN:HB2	2.44	0.40
3:S:29:GLN:HA	3:S:29:GLN:NE2	2.37	0.40
4:U:365:GLN:HG2	4:U:366:ILE:N	2.36	0.40
4:U:56:PHE:N	4:U:56:PHE:CD1	2.88	0.40
1:A:463:TYR:CD2	2:B:517:PRO:HD2	2.57	0.40
2:E:158:ASP:C	2:E:160:GLY:H	2.24	0.40
2:E:202:GLN:HG3	2:E:203:ASN:N	2.36	0.40
1:L:135:ILE:CG2	1:L:171:CYS:SG	3.10	0.40
1:L:222:PHE:C	1:L:224:THR:N	2.75	0.40
4:M:238:LYS:HE3	4:M:238:LYS:HB2	1.92	0.40
4:M:33:ARG:O	4:M:37:ILE:HB	2.21	0.40
4:M:85:MET:CE	4:M:112:LEU:HD21	2.52	0.40
3:S:137:MET:SD	3:S:137:MET:C	2.99	0.40
4:U:18:ARG:HB3	4:U:20:TYR:HE1	1.86	0.40
1:A:201:LEU:HB2	1:A:247:TYR:CE1	2.56	0.40
1:A:466:ILE:HD13	1:A:502:TYR:CD2	2.57	0.40
1:A:561:ASP:HB3	1:A:564:ARG:HE	1.87	0.40
2:B:351:ILE:HG12	2:B:384:VAL:HG11	2.02	0.40
2:B:83:MET:O	2:B:86:MET:HE2	2.22	0.40
2:E:162:LEU:HA	2:E:162:LEU:HD22	1.89	0.40
3:I:21:MET:HG3	3:I:23:PHE:CE1	2.56	0.40
1:L:250:TYR:CE2	1:L:301:GLN:HB2	2.57	0.40
5:Q:3:SEP:C	5:Q:5:ILE:H	2.35	0.40
4:U:136:GLN:HB2	4:U:137:GLY:H	1.66	0.40
4:U:162:ARG:NH2	4:U:166:ILE:HG13	2.37	0.40
4:U:65:LEU:N	4:U:65:LEU:HD23	2.37	0.40
2:B:26:LYS:H	2:B:26:LYS:HG3	1.71	0.40
6:E:1586:SO4:O1	4:U:118:PHE:N	2.42	0.40
2:E:408:GLN:NE2	2:E:439:LEU:HA	2.36	0.40
1:L:446:ILE:HD13	1:L:446:ILE:HA	1.84	0.40
4:M:241:ILE:N	4:M:241:ILE:HD12	2.35	0.40
4:M:328:LEU:HD13	4:M:349:ASN:HD21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:21:MET:HG3	3:S:23:PHE:CE1	2.57	0.40
4:M:241:ILE:HB	3:S:27:GLU:HG2	2.02	0.40
4:U:1:MET:N	4:U:21:ARG:NH2	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:437:VAL:CG2	7:L:2002:HOH:O[8_554]	2.16	0.04

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	619/623 (99%)	528 (85%)	63 (10%)	28 (4%)	2	16
1	L	619/623 (99%)	524 (85%)	69 (11%)	26 (4%)	3	18
2	B	569/591 (96%)	464 (82%)	78 (14%)	27 (5%)	2	15
2	E	569/591 (96%)	465 (82%)	73 (13%)	31 (5%)	2	13
3	I	140/142 (99%)	121 (86%)	18 (13%)	1 (1%)	22	55
3	S	140/142 (99%)	120 (86%)	19 (14%)	1 (1%)	22	55
4	M	403/435 (93%)	309 (77%)	67 (17%)	27 (7%)	1	8
4	U	403/435 (93%)	310 (77%)	64 (16%)	29 (7%)	1	7
5	P	6/11 (54%)	4 (67%)	2 (33%)	0	100	100
5	Q	6/11 (54%)	4 (67%)	2 (33%)	0	100	100
All	All	3474/3604 (96%)	2849 (82%)	455 (13%)	170 (5%)	2	14

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	ALA
1	A	382	ASP
1	A	453	ALA
1	A	492	CYS
1	A	532	LEU
1	A	600	GLU
1	A	618	LYS
2	B	47	VAL
2	B	152	ASN
2	B	214	CYS
2	B	250	HIS
2	B	274	SER
2	B	422	PRO
2	B	424	LYS
2	B	463	ASP
2	B	497	SER
2	B	550	GLU
2	E	47	VAL
2	E	152	ASN
2	E	214	CYS
2	E	250	HIS
2	E	274	SER
2	E	422	PRO
2	E	424	LYS
2	E	463	ASP
2	E	497	SER
2	E	550	GLU
1	L	240	ALA
1	L	382	ASP
1	L	453	ALA
1	L	492	CYS
1	L	532	LEU
1	L	600	GLU
1	L	618	LYS
4	M	24	ILE
4	M	27	ASN
4	M	29	VAL
4	M	136	GLN
4	M	218	ASP
4	M	262	SER
4	M	294	ARG
4	M	377	ASP
4	U	24	ILE

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Mol	Chain	Res	Type
4	U	27	ASN
4	U	29	VAL
4	U	123	ASN
4	U	136	GLN
4	U	218	ASP
4	U	294	ARG
4	U	377	ASP
4	U	381	TRP
1	A	22	ASN
1	A	23	CYS
1	A	186	GLY
1	A	602	MET
1	A	621	GLY
2	B	76	TYR
2	B	172	SER
2	B	215	THR
2	B	233	ASP
2	B	252	ASN
2	B	272	LYS
2	B	275	ASP
2	B	350	ASN
2	B	543	SER
2	B	553	ASP
2	E	76	TYR
2	E	172	SER
2	E	213	GLU
2	E	215	THR
2	E	233	ASP
2	E	247	ARG
2	E	252	ASN
2	E	272	LYS
2	E	275	ASP
2	E	350	ASN
2	E	436	LEU
2	E	553	ASP
3	I	96	HIS
1	L	23	CYS
1	L	85	SER
1	L	186	GLY
1	L	474	ASP
1	L	602	MET
1	L	621	GLY

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Mol	Chain	Res	Type
4	M	123	ASN
4	M	160	GLY
4	M	169	ARG
4	M	199	ARG
4	M	235	LYS
4	M	381	TRP
3	S	96	HIS
4	U	160	GLY
4	U	169	ARG
4	U	199	ARG
4	U	235	LYS
4	U	262	SER
4	U	347	SER
4	U	412	ASN
1	A	8	ASP
1	A	85	SER
1	A	123	ARG
1	A	184	PRO
1	A	244	LEU
1	A	323	GLU
1	A	417	ASP
1	A	474	ASP
2	B	14	GLU
2	B	213	GLU
2	B	270	LEU
2	B	436	LEU
2	B	437	ASP
2	E	14	GLU
2	E	159	GLN
2	E	270	LEU
2	E	437	ASP
2	E	543	SER
1	L	8	ASP
1	L	22	ASN
1	L	244	LEU
4	M	347	SER
4	M	412	ASN
4	U	113	ASP
4	U	260	GLU
1	A	10	MET
1	A	24	LYS
1	A	342	GLU

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Mol	Chain	Res	Type
2	B	159	GLN
1	L	10	MET
1	L	24	LYS
1	L	184	PRO
1	L	323	GLU
1	L	342	GLU
1	L	417	ASP
4	M	140	SER
4	M	260	GLU
4	M	293	VAL
4	M	380	LYS
4	U	140	SER
4	U	293	VAL
1	A	47	ASP
1	A	531	HIS
2	E	328	TYR
1	L	47	ASP
1	L	67	LEU
1	L	511	ILE
1	L	531	HIS
4	M	113	ASP
4	M	255	SER
4	M	375	THR
4	M	383	ARG
4	U	51	ALA
4	U	246	CYS
4	U	255	SER
4	U	299	THR
4	U	380	LYS
4	U	383	ARG
1	A	67	LEU
1	A	451	ARG
2	B	427	SER
2	E	168	LEU
2	E	427	SER
4	M	51	ALA
4	U	375	THR
1	A	511	ILE
4	M	96	ILE
4	U	336	ILE
2	E	506	VAL
4	U	96	ILE

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Mol	Chain	Res	Type
4	M	336	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	542/544 (100%)	480 (89%)	62 (11%)	5	21
1	L	542/544 (100%)	480 (89%)	62 (11%)	5	21
2	B	514/532 (97%)	444 (86%)	70 (14%)	3	14
2	E	514/532 (97%)	445 (87%)	69 (13%)	4	15
3	I	131/131 (100%)	119 (91%)	12 (9%)	9	31
3	S	131/131 (100%)	119 (91%)	12 (9%)	9	31
4	M	364/387 (94%)	309 (85%)	55 (15%)	3	12
4	U	364/387 (94%)	309 (85%)	55 (15%)	3	12
5	P	8/10 (80%)	7 (88%)	1 (12%)	4	17
5	Q	8/10 (80%)	7 (88%)	1 (12%)	4	17
All	All	3118/3208 (97%)	2719 (87%)	399 (13%)	4	16

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	20	ILE
1	A	32	ARG
1	A	33	ILE
1	A	47	ASP
1	A	50	LEU
1	A	92	GLN
1	A	93	ILE
1	A	102	VAL
1	A	103	ASN
1	A	106	SER
1	A	163	SER

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Mol	Chain	Res	Type
1	A	181	ASP
1	A	183	VAL
1	A	221	GLU
1	A	224	THR
1	A	227	SER
1	A	234	SER
1	A	239	SER
1	A	245	GLN
1	A	263	ARG
1	A	280	LEU
1	A	286	THR
1	A	314	ILE
1	A	341	ARG
1	A	342	GLU
1	A	348	LEU
1	A	352	SER
1	A	355	THR
1	A	358	SER
1	A	374	ILE
1	A	400	SER
1	A	401	ASN
1	A	404	GLN
1	A	413	LEU
1	A	415	THR
1	A	417	ASP
1	A	423	GLU
1	A	426	LEU
1	A	433	GLU
1	A	437	VAL
1	A	444	ASP
1	A	447	LEU
1	A	458	SER
1	A	461	VAL
1	A	503	ILE
1	A	509	ASN
1	A	510	LEU
1	A	511	ILE
1	A	516	ARG
1	A	518	SER
1	A	532	LEU
1	A	540	LEU
1	A	541	LEU

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Mol	Chain	Res	Type
1	A	554	GLU
1	A	561	ASP
1	A	576	LEU
1	A	579	ARG
1	A	586	LEU
1	A	597	THR
1	A	608	ARG
1	A	613	LEU
2	B	12	LYS
2	B	53	ASP
2	B	62	ASN
2	B	75	ASN
2	B	88	VAL
2	B	89	ASN
2	B	90	SER
2	B	96	GLU
2	B	102	ILE
2	B	126	LEU
2	B	127	ARG
2	B	133	GLU
2	B	155	MET
2	B	162	LEU
2	B	165	LEU
2	B	167	ASP
2	B	168	LEU
2	B	172	SER
2	B	173	ASN
2	B	193	ASN
2	B	199	LEU
2	B	202	GLN
2	B	203	ASN
2	B	207	LEU
2	B	208	LEU
2	B	209	THR
2	B	214	CYS
2	B	230	ASN
2	B	238	GLN
2	B	245	THR
2	B	249	SER
2	B	253	SER
2	B	267	LEU
2	B	275	ASP

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Mol	Chain	Res	Type
2	B	283	LYS
2	B	288	LEU
2	B	289	VAL
2	B	304	ARG
2	B	306	ILE
2	B	318	LYS
2	B	348	GLN
2	B	351	ILE
2	B	353	GLN
2	B	359	LYS
2	B	360	GLU
2	B	385	GLU
2	B	386	GLN
2	B	390	ARG
2	B	396	LEU
2	B	408	GLN
2	B	427	SER
2	B	454	GLU
2	B	458	ARG
2	B	459	ILE
2	B	460	ASP
2	B	474	HIS
2	B	477	SER
2	B	482	LEU
2	B	485	LEU
2	B	503	VAL
2	B	506	VAL
2	B	525	ILE
2	B	528	ARG
2	B	543	SER
2	B	545	LYS
2	B	554	LEU
2	B	558	THR
2	B	563	LEU
2	B	572	SER
2	B	581	PHE
2	E	12	LYS
2	E	53	ASP
2	E	75	ASN
2	E	88	VAL
2	E	89	ASN
2	E	90	SER

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Mol	Chain	Res	Type
2	E	96	GLU
2	E	102	ILE
2	E	126	LEU
2	E	127	ARG
2	E	155	MET
2	E	162	LEU
2	E	164	SER
2	E	165	LEU
2	E	167	ASP
2	E	168	LEU
2	E	172	SER
2	E	173	ASN
2	E	193	ASN
2	E	202	GLN
2	E	203	ASN
2	E	207	LEU
2	E	208	LEU
2	E	209	THR
2	E	214	CYS
2	E	230	ASN
2	E	238	GLN
2	E	245	THR
2	E	249	SER
2	E	253	SER
2	E	267	LEU
2	E	275	ASP
2	E	283	LYS
2	E	288	LEU
2	E	289	VAL
2	E	304	ARG
2	E	306	ILE
2	E	318	LYS
2	E	348	GLN
2	E	351	ILE
2	E	353	GLN
2	E	359	LYS
2	E	360	GLU
2	E	374	VAL
2	E	385	GLU
2	E	386	GLN
2	E	390	ARG
2	E	396	LEU

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Mol	Chain	Res	Type
2	E	408	GLN
2	E	427	SER
2	E	454	GLU
2	E	458	ARG
2	E	459	ILE
2	E	460	ASP
2	E	474	HIS
2	E	477	SER
2	E	482	LEU
2	E	485	LEU
2	E	503	VAL
2	E	506	VAL
2	E	525	ILE
2	E	528	ARG
2	E	543	SER
2	E	545	LYS
2	E	554	LEU
2	E	558	THR
2	E	563	LEU
2	E	572	SER
2	E	581	PHE
3	I	28	LYS
3	I	39	VAL
3	I	48	ASN
3	I	71	VAL
3	I	86	ASN
3	I	100	GLU
3	I	102	ASP
3	I	110	VAL
3	I	112	THR
3	I	125	GLU
3	I	137	MET
3	I	140	SER
1	L	10	MET
1	L	20	ILE
1	L	32	ARG
1	L	33	ILE
1	L	47	ASP
1	L	50	LEU
1	L	92	GLN
1	L	93	ILE
1	L	102	VAL

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Mol	Chain	Res	Type
1	L	103	ASN
1	L	163	SER
1	L	181	ASP
1	L	183	VAL
1	L	221	GLU
1	L	224	THR
1	L	227	SER
1	L	234	SER
1	L	239	SER
1	L	245	GLN
1	L	263	ARG
1	L	280	LEU
1	L	286	THR
1	L	309	VAL
1	L	341	ARG
1	L	342	GLU
1	L	348	LEU
1	L	352	SER
1	L	355	THR
1	L	358	SER
1	L	375	ASN
1	L	400	SER
1	L	401	ASN
1	L	404	GLN
1	L	413	LEU
1	L	415	THR
1	L	417	ASP
1	L	423	GLU
1	L	426	LEU
1	L	433	GLU
1	L	437	VAL
1	L	444	ASP
1	L	447	LEU
1	L	458	SER
1	L	461	VAL
1	L	503	ILE
1	L	509	ASN
1	L	510	LEU
1	L	511	ILE
1	L	516	ARG
1	L	518	SER
1	L	532	LEU

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Mol	Chain	Res	Type
1	L	540	LEU
1	L	541	LEU
1	L	554	GLU
1	L	561	ASP
1	L	576	LEU
1	L	579	ARG
1	L	586	LEU
1	L	597	THR
1	L	605	PHE
1	L	608	ARG
1	L	613	LEU
4	M	5	LEU
4	M	9	ASN
4	M	13	GLU
4	M	18	ARG
4	M	19	VAL
4	M	21	ARG
4	M	34	VAL
4	M	43	VAL
4	M	47	VAL
4	M	48	THR
4	M	60	ARG
4	M	73	VAL
4	M	85	MET
4	M	95	LYS
4	M	96	ILE
4	M	106	VAL
4	M	111	LEU
4	M	120	TYR
4	M	122	GLN
4	M	123	ASN
4	M	126	THR
4	M	139	LYS
4	M	166	ILE
4	M	169	ARG
4	M	174	PHE
4	M	203	LYS
4	M	204	SER
4	M	212	CYS
4	M	219	LYS
4	M	222	ILE
4	M	233	THR

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Mol	Chain	Res	Type
4	M	253	ARG
4	M	263	ILE
4	M	266	ILE
4	M	284	ILE
4	M	293	VAL
4	M	296	VAL
4	M	299	THR
4	M	304	LYS
4	M	311	PHE
4	M	312	LYS
4	M	314	SER
4	M	315	LEU
4	M	347	SER
4	M	355	ILE
4	M	364	SER
4	M	367	SER
4	M	375	THR
4	M	387	SER
4	M	392	VAL
4	M	407	PHE
4	M	410	LYS
4	M	421	TRP
4	M	422	VAL
4	M	430	ILE
5	P	2	MET
5	Q	2	MET
3	S	28	LYS
3	S	39	VAL
3	S	48	ASN
3	S	71	VAL
3	S	86	ASN
3	S	100	GLU
3	S	102	ASP
3	S	110	VAL
3	S	112	THR
3	S	125	GLU
3	S	137	MET
3	S	140	SER
4	U	5	LEU
4	U	9	ASN
4	U	13	GLU
4	U	18	ARG

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Mol	Chain	Res	Type
4	U	19	VAL
4	U	21	ARG
4	U	34	VAL
4	U	43	VAL
4	U	47	VAL
4	U	48	THR
4	U	60	ARG
4	U	73	VAL
4	U	85	MET
4	U	95	LYS
4	U	96	ILE
4	U	106	VAL
4	U	111	LEU
4	U	120	TYR
4	U	122	GLN
4	U	123	ASN
4	U	126	THR
4	U	139	LYS
4	U	166	ILE
4	U	169	ARG
4	U	203	LYS
4	U	204	SER
4	U	212	CYS
4	U	219	LYS
4	U	222	ILE
4	U	233	THR
4	U	253	ARG
4	U	263	ILE
4	U	266	ILE
4	U	284	ILE
4	U	293	VAL
4	U	296	VAL
4	U	299	THR
4	U	304	LYS
4	U	311	PHE
4	U	312	LYS
4	U	314	SER
4	U	315	LEU
4	U	316	LEU
4	U	347	SER
4	U	355	ILE
4	U	364	SER

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Mol	Chain	Res	Type
4	U	367	SER
4	U	375	THR
4	U	387	SER
4	U	392	VAL
4	U	407	PHE
4	U	410	LYS
4	U	421	TRP
4	U	422	VAL
4	U	430	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	103	ASN
1	A	200	HIS
1	A	301	GLN
1	A	319	HIS
1	A	320	HIS
1	A	401	ASN
1	A	467	GLN
1	A	488	GLN
1	A	509	ASN
1	A	527	HIS
1	A	550	ASN
2	B	62	ASN
2	B	152	ASN
2	B	173	ASN
2	B	179	ASN
2	B	191	HIS
2	B	193	ASN
2	B	228	ASN
2	B	278	ASN
2	B	299	GLN
2	B	305	ASN
2	B	311	GLN
2	B	319	GLN
2	B	348	GLN
2	B	353	GLN
2	B	386	GLN
2	B	408	GLN
2	B	435	ASN

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Mol	Chain	Res	Type
2	B	474	HIS
2	B	479	GLN
2	B	481	GLN
2	B	512	GLN
2	B	575	HIS
2	E	62	ASN
2	E	152	ASN
2	E	173	ASN
2	E	191	HIS
2	E	193	ASN
2	E	228	ASN
2	E	278	ASN
2	E	299	GLN
2	E	307	ASN
2	E	311	GLN
2	E	348	GLN
2	E	353	GLN
2	E	386	GLN
2	E	408	GLN
2	E	435	ASN
2	E	479	GLN
2	E	481	GLN
2	E	512	GLN
3	I	8	GLN
3	I	29	GLN
3	I	36	HIS
3	I	48	ASN
3	I	92	ASN
3	I	128	GLN
1	L	92	GLN
1	L	103	ASN
1	L	200	HIS
1	L	301	GLN
1	L	319	HIS
1	L	320	HIS
1	L	401	ASN
1	L	467	GLN
1	L	488	GLN
1	L	509	ASN
1	L	527	HIS
1	L	550	ASN
1	L	578	GLN

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Mol	Chain	Res	Type
4	M	9	ASN
4	M	35	ASN
4	M	42	GLN
4	M	72	ASN
4	M	100	ASN
4	M	104	ASN
4	M	122	GLN
4	M	135	GLN
4	M	141	GLN
4	M	182	ASN
4	M	349	ASN
3	S	8	GLN
3	S	29	GLN
3	S	36	HIS
3	S	48	ASN
3	S	92	ASN
3	S	128	GLN
4	U	9	ASN
4	U	42	GLN
4	U	72	ASN
4	U	100	ASN
4	U	104	ASN
4	U	135	GLN
4	U	141	GLN
4	U	182	ASN
4	U	349	ASN
4	U	365	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	SEP	P	3	5	4,5,10	0.51	0	0,5,14	0.00	-
5	SEP	Q	3	5	4,5,10	0.53	0	0,5,14	0.00	-

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	SEP	P	3	5	-	2/2/4/10	-
5	SEP	Q	3	5	-	2/2/4/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	P	3	SEP	N-CA-CB-OG
5	Q	3	SEP	N-CA-CB-OG
5	P	3	SEP	C-CA-CB-OG
5	Q	3	SEP	C-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	3	SEP	1	0
5	Q	3	SEP	2	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

31 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	E	1583	-	4,4,4	0.18	0	6,6,6	0.35	0
6	SO4	L	1626	-	4,4,4	0.14	0	6,6,6	0.28	0
6	SO4	M	1436	-	4,4,4	0.20	0	6,6,6	0.31	0
6	SO4	U	1437	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	A	1629	-	4,4,4	0.12	0	6,6,6	0.17	0
6	SO4	A	1627	-	4,4,4	0.19	0	6,6,6	0.16	0
6	SO4	L	1628	-	4,4,4	0.11	0	6,6,6	0.13	0
6	SO4	A	1626	-	4,4,4	0.12	0	6,6,6	0.25	0
6	SO4	E	1586	-	4,4,4	0.17	0	6,6,6	0.19	0
6	SO4	L	1631	-	4,4,4	0.15	0	6,6,6	0.12	0
6	SO4	A	1625	-	4,4,4	0.14	0	6,6,6	0.20	0
6	SO4	B	1583	-	4,4,4	0.13	0	6,6,6	0.11	0
6	SO4	L	1630	-	4,4,4	0.17	0	6,6,6	0.15	0
6	SO4	E	1584	-	4,4,4	0.17	0	6,6,6	0.14	0
6	SO4	L	1627	-	4,4,4	0.13	0	6,6,6	0.14	0
6	SO4	A	1628	-	4,4,4	0.14	0	6,6,6	0.15	0
6	SO4	M	1437	-	4,4,4	0.10	0	6,6,6	0.30	0
6	SO4	B	1586	-	4,4,4	0.20	0	6,6,6	0.17	0
6	SO4	M	1438	-	4,4,4	0.14	0	6,6,6	0.23	0
6	SO4	L	1629	-	4,4,4	0.17	0	6,6,6	0.11	0
6	SO4	B	1585	-	4,4,4	0.15	0	6,6,6	0.10	0
6	SO4	E	1585	-	4,4,4	0.18	0	6,6,6	0.24	0
6	SO4	L	1625	-	4,4,4	0.13	0	6,6,6	0.21	0
6	SO4	B	1584	-	4,4,4	0.17	0	6,6,6	0.12	0
6	SO4	U	1439	-	4,4,4	0.14	0	6,6,6	0.19	0
6	SO4	B	1587	-	4,4,4	0.17	0	6,6,6	0.19	0
6	SO4	A	1630	-	4,4,4	0.12	0	6,6,6	0.15	0
6	SO4	A	1624	-	4,4,4	0.16	0	6,6,6	0.29	0
6	SO4	L	1624	-	4,4,4	0.13	0	6,6,6	0.37	0
6	SO4	U	1438	-	4,4,4	0.17	0	6,6,6	0.28	0
6	SO4	U	1436	-	4,4,4	0.18	0	6,6,6	0.29	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1627	SO4	2	0
6	E	1586	SO4	4	0
6	A	1625	SO4	1	0
6	M	1437	SO4	1	0
6	E	1585	SO4	1	0
6	A	1624	SO4	2	0
6	U	1436	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	621/623 (99%)	-0.13	15 (2%) 59 57	37, 73, 130, 204	0
1	L	621/623 (99%)	-0.10	18 (2%) 51 50	35, 73, 129, 204	0
2	B	571/591 (96%)	-0.05	9 (1%) 72 70	41, 86, 150, 203	0
2	E	571/591 (96%)	0.03	22 (3%) 39 38	39, 85, 150, 204	0
3	I	142/142 (100%)	-0.40	0 100 100	41, 67, 115, 146	0
3	S	142/142 (100%)	-0.35	0 100 100	42, 67, 115, 147	0
4	M	409/435 (94%)	0.02	15 (3%) 41 40	42, 75, 148, 224	0
4	U	409/435 (94%)	0.00	10 (2%) 59 57	36, 75, 148, 223	0
5	P	8/11 (72%)	0.18	0 100 100	61, 100, 143, 145	0
5	Q	8/11 (72%)	0.11	0 100 100	61, 100, 143, 144	0
All	All	3502/3604 (97%)	-0.07	89 (2%) 57 55	35, 76, 142, 224	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	159	ILE	7.1
1	L	241	SER	6.7
1	L	240	ALA	6.5
1	A	241	SER	5.8
4	U	141	GLN	5.8
1	A	240	ALA	5.0
4	U	124	SER	5.0
4	U	163	ARG	4.5
4	U	159	ILE	4.5
1	A	242	THR	4.2
2	E	278	ASN	4.1
2	E	204	ILE	3.6
2	B	549	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	271	PRO	3.5
1	A	243	ASP	3.5
1	L	242	THR	3.4
2	E	277	TYR	3.3
4	U	125	GLU	3.2
2	B	550	GLU	3.0
4	U	140	SER	3.0
4	M	160	GLY	3.0
1	A	37	LEU	2.9
4	U	139	LYS	2.9
4	M	232	GLU	2.9
1	L	243	ASP	2.9
1	L	33	ILE	2.9
2	B	25	GLU	2.9
2	E	201	PRO	2.9
1	L	74	PHE	2.9
4	M	270	GLY	2.8
4	M	141	GLN	2.8
4	M	233	THR	2.8
1	L	29	GLU	2.7
2	B	196	LEU	2.7
2	E	122	LEU	2.7
4	U	138	ILE	2.7
2	E	21	GLU	2.7
1	L	623	SER	2.7
1	A	24	LYS	2.6
4	M	140	SER	2.6
2	E	273	ASP	2.6
1	L	239	SER	2.6
1	L	73	ASP	2.6
1	L	44	PHE	2.6
1	L	3	ALA	2.5
2	B	280	LEU	2.5
4	M	269	ASP	2.5
2	E	18	LEU	2.5
1	A	104	SER	2.4
4	M	132	PHE	2.4
2	E	121	TYR	2.4
2	E	31	LYS	2.4
4	M	138	ILE	2.4
2	B	273	ASP	2.3
1	L	298	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	102	ILE	2.3
1	A	244	LEU	2.3
4	M	163	ARG	2.3
1	L	37	LEU	2.3
1	A	44	PHE	2.3
1	A	45	LYS	2.3
1	L	40	ILE	2.3
1	A	296	LYS	2.3
1	A	70	HIS	2.2
2	E	49	SER	2.2
2	E	281	LEU	2.2
4	M	271	GLU	2.2
2	B	63	LEU	2.2
1	A	297	SER	2.2
2	E	268	GLU	2.2
2	E	32	GLU	2.2
2	E	241	CYS	2.2
1	A	623	SER	2.2
2	B	281	LEU	2.1
4	M	125	GLU	2.1
2	E	267	LEU	2.1
2	E	116	ASP	2.1
1	L	30	ILE	2.1
2	B	45	LYS	2.1
4	U	136	GLN	2.1
2	E	30	ARG	2.1
1	A	30	ILE	2.1
4	M	124	SER	2.1
4	M	211	GLU	2.0
4	U	269	ASP	2.0
1	L	297	SER	2.0
1	L	35	LYS	2.0
2	E	24	ASN	2.0
2	E	276	TYR	2.0

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

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(\AA^2)	Q<0.9
5	SEP	Q	3	6/11	0.88	0.18	92,110,121,128	0
5	SEP	P	3	6/11	0.92	0.15	88,109,121,129	0

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(\AA^2)	Q<0.9
6	SO4	A	1627	5/5	0.62	0.25	165,172,180,191	0
6	SO4	A	1630	5/5	0.73	0.45	180,181,183,183	0
6	SO4	L	1625	5/5	0.78	0.19	134,138,148,152	0
6	SO4	L	1628	5/5	0.80	0.32	141,146,156,159	0
6	SO4	E	1583	5/5	0.82	0.24	88,106,113,139	0
6	SO4	U	1437	5/5	0.84	0.24	142,156,162,164	0
6	SO4	L	1629	5/5	0.84	0.39	147,158,169,173	0
6	SO4	L	1630	5/5	0.85	0.17	124,130,140,147	0
6	SO4	A	1625	5/5	0.85	0.16	146,150,158,170	0
6	SO4	A	1626	5/5	0.86	0.36	105,121,140,141	0
6	SO4	E	1585	5/5	0.86	0.34	126,128,134,141	0
6	SO4	E	1584	5/5	0.87	0.26	135,144,147,158	0
6	SO4	B	1585	5/5	0.88	0.32	128,139,146,149	0
6	SO4	B	1584	5/5	0.89	0.35	134,140,152,161	0
6	SO4	L	1626	5/5	0.90	0.31	110,112,136,142	0
6	SO4	B	1586	5/5	0.90	0.32	120,135,142,144	0
6	SO4	A	1629	5/5	0.91	0.67	170,175,180,182	0
6	SO4	U	1438	5/5	0.91	0.17	104,108,115,122	0
6	SO4	U	1439	5/5	0.92	0.19	126,134,137,150	0
6	SO4	B	1583	5/5	0.92	0.16	109,128,133,136	0
6	SO4	L	1624	5/5	0.92	0.25	103,111,123,123	0
6	SO4	L	1627	5/5	0.92	0.24	116,134,136,143	0
6	SO4	L	1631	5/5	0.93	0.26	119,121,125,136	0
6	SO4	M	1437	5/5	0.94	0.18	100,114,121,131	0
6	SO4	B	1587	5/5	0.95	0.17	99,113,114,120	0
6	SO4	M	1438	5/5	0.95	0.16	99,103,106,106	0
6	SO4	A	1628	5/5	0.96	0.20	114,125,129,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	M	1436	5/5	0.96	0.21	48,58,69,88	0
6	SO4	E	1586	5/5	0.97	0.18	126,130,132,146	0
6	SO4	A	1624	5/5	0.98	0.17	80,82,85,97	0
6	SO4	U	1436	5/5	0.99	0.16	53,73,76,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.