Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 04:55 PM EDT

PDB ID	:	3E2P
Title	:	Catalytic subunit of M. Jannaschii aspartate transcarbamoylase in an orthorhombic crystal form
Authors	:	Vitali, J.; Colaneri, M.J.
Deposited on	:	2008-08-06
Resolution	:	3.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

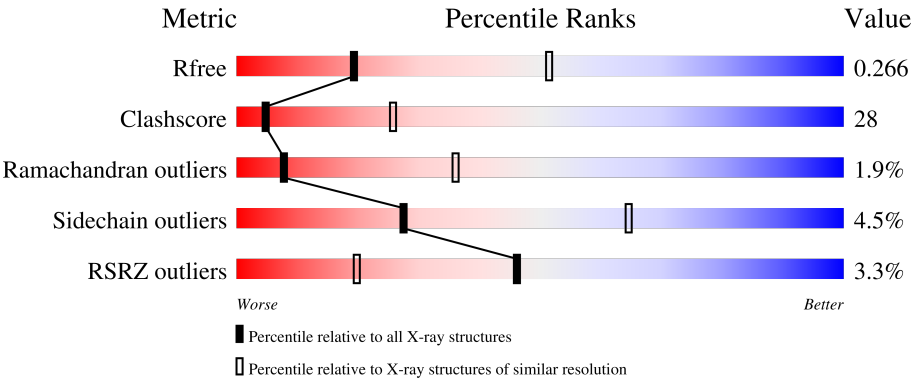
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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 <=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	306	2% 60% 36%
1	B	306	% 59% 37%
1	C	306	3% 58% 37% 5%
1	D	306	3% 56% 38% 6%
1	E	306	% 58% 38%

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Mol	Chain	Length	Quality of chain
1	F	306	2% 56% 38% 6%
1	I	306	8% 57% 37% 5%
1	J	306	3% 57% 38%
1	K	306	3% 55% 40% 5%
1	L	306	6% 58% 38%
1	M	306	6% 59% 36%
1	N	306	2% 57% 37% 6%

2 Entry composition (i)

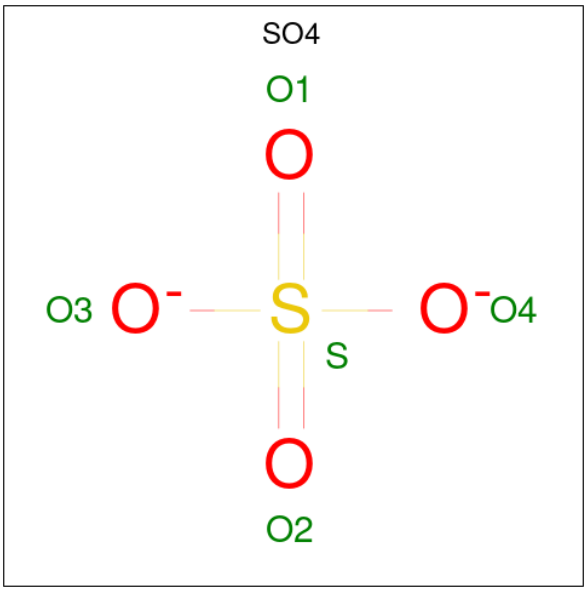
There are 3 unique types of molecules in this entry. The entry contains 30122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2474	1584	409	472	9			
1	B	304	Total	C	N	O	S	0	0	0
			2460	1577	407	467	9			
1	C	306	Total	C	N	O	S	0	0	0
			2474	1584	409	472	9			
1	D	306	Total	C	N	O	S	0	0	0
			2474	1584	409	472	9			
1	E	306	Total	C	N	O	S	0	0	0
			2474	1584	409	472	9			
1	F	306	Total	C	N	O	S	0	0	0
			2474	1584	409	472	9			
1	I	304	Total	C	N	O	S	0	0	0
			2460	1577	407	467	9			
1	J	304	Total	C	N	O	S	0	0	0
			2460	1577	407	467	9			
1	K	305	Total	C	N	O	S	0	0	0
			2464	1579	408	468	9			
1	L	305	Total	C	N	O	S	0	0	0
			2464	1579	408	468	9			
1	M	305	Total	C	N	O	S	0	0	0
			2464	1579	408	468	9			
1	N	304	Total	C	N	O	S	0	0	0
			2460	1577	407	467	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	61	Total O 61 61	0	0
3	B	59	Total O 59 59	0	0
3	C	51	Total O 51 51	0	0
3	D	62	Total O 62 62	0	0
3	E	60	Total O 60 60	0	0
3	F	36	Total O 36 36	0	0
3	I	24	Total O 24 24	0	0
3	J	25	Total O 25 25	0	0

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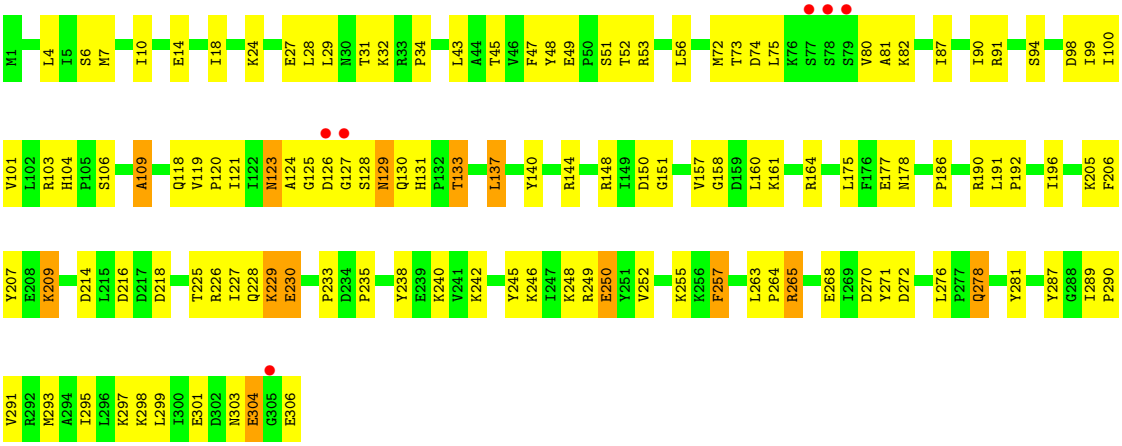
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	29	Total O 29 29	0	0
3	L	25	Total O 25 25	0	0
3	M	30	Total O 30 30	0	0
3	N	38	Total O 38 38	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

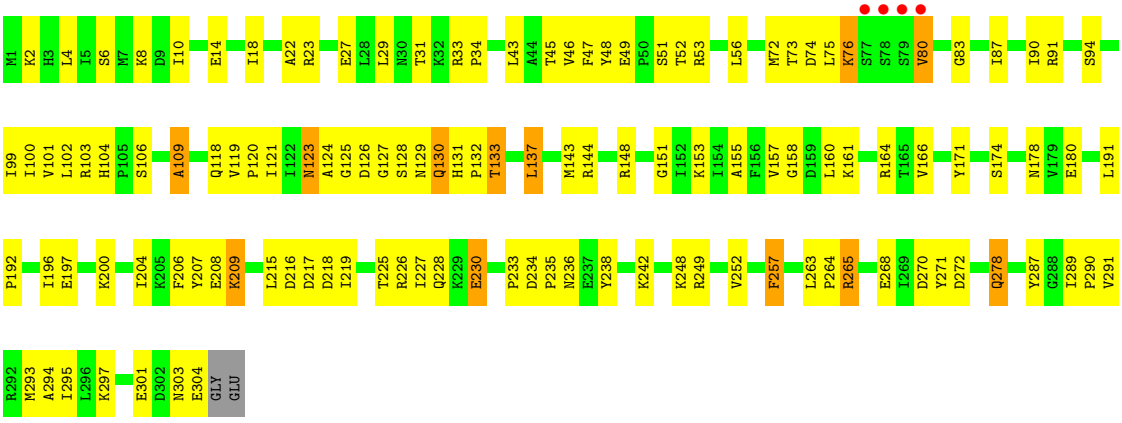
• Molecule 1: Aspartate carbamoyltransferase

Chain A:



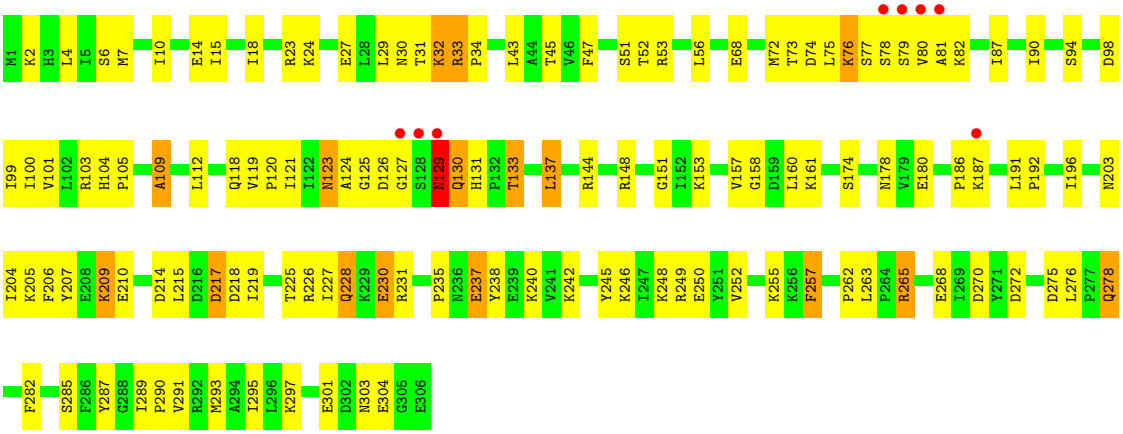
• Molecule 1: Aspartate carbamoyltransferase

Chain B:

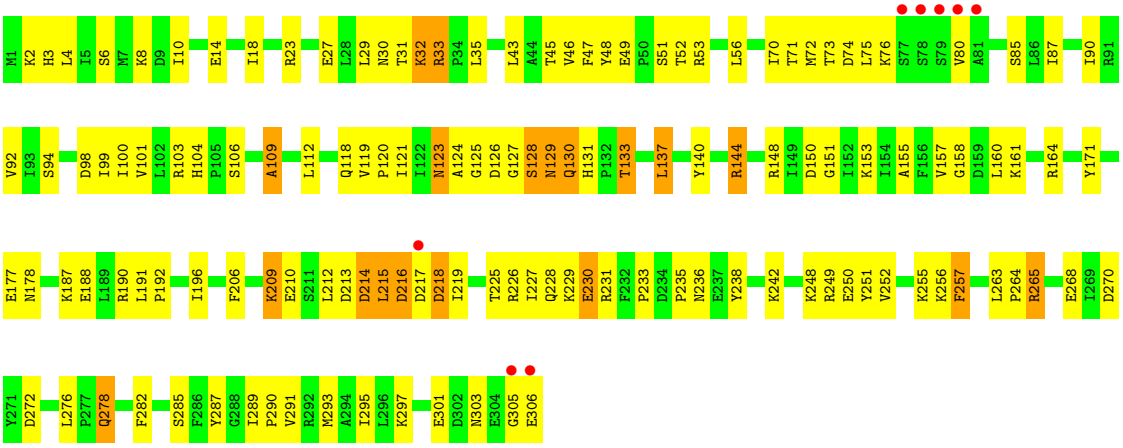


• Molecule 1: Aspartate carbamoyltransferase

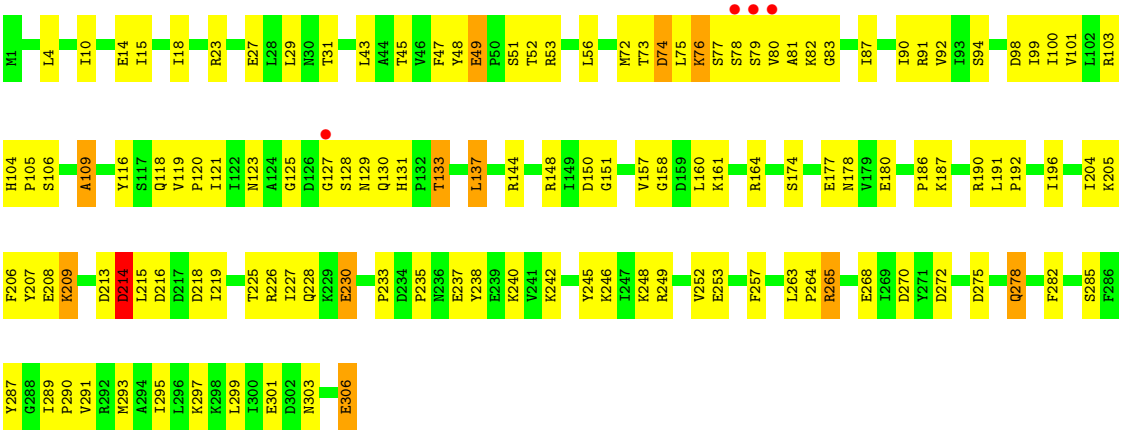
Chain C:



• Molecule 1: Aspartate carbamoyltransferase

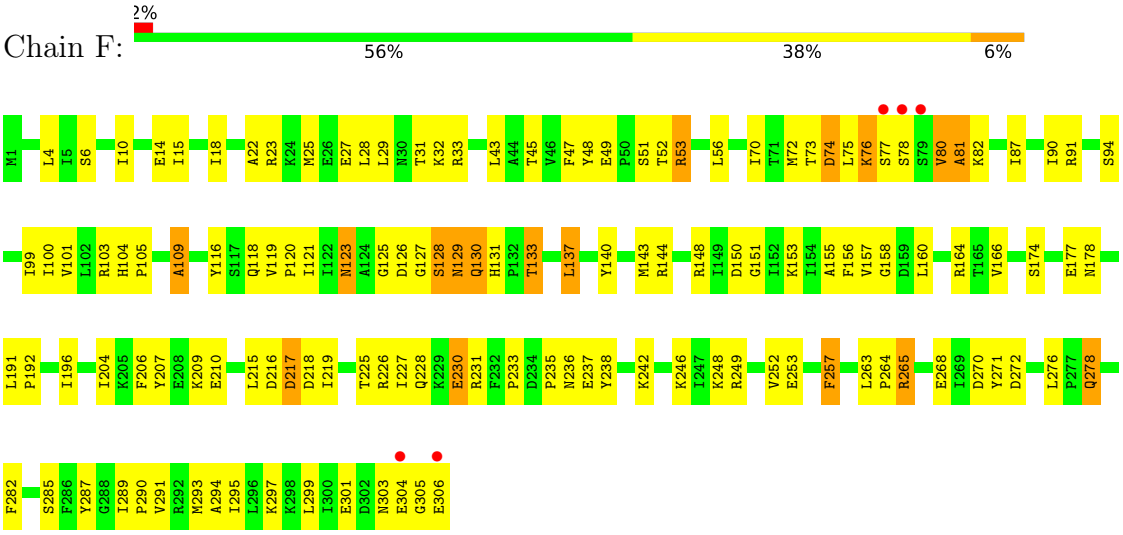


• Molecule 1: Aspartate carbamoyltransferase



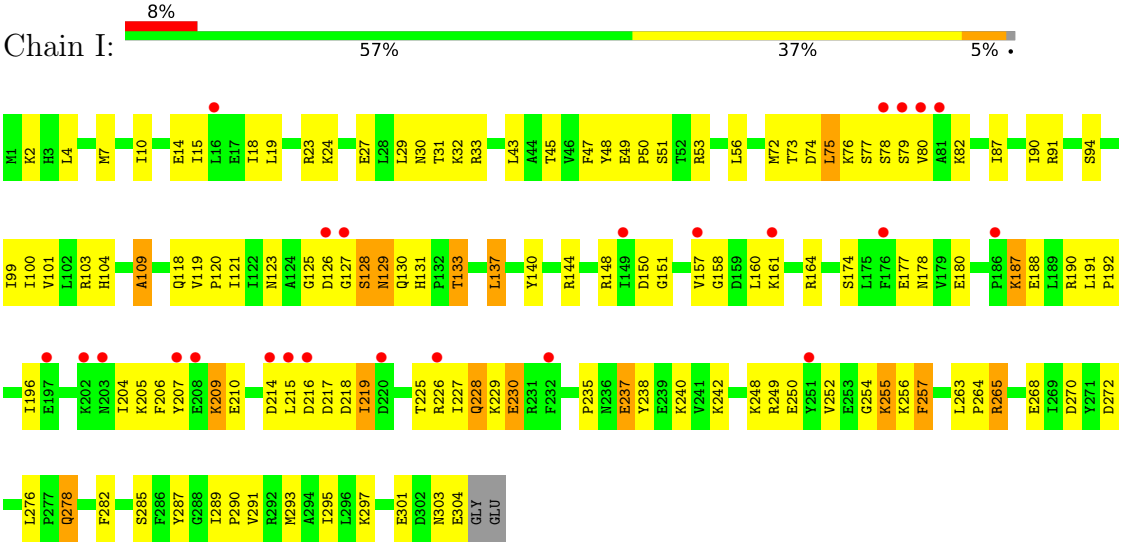
• Molecule 1: Aspartate carbamoyltransferase

Chain F:



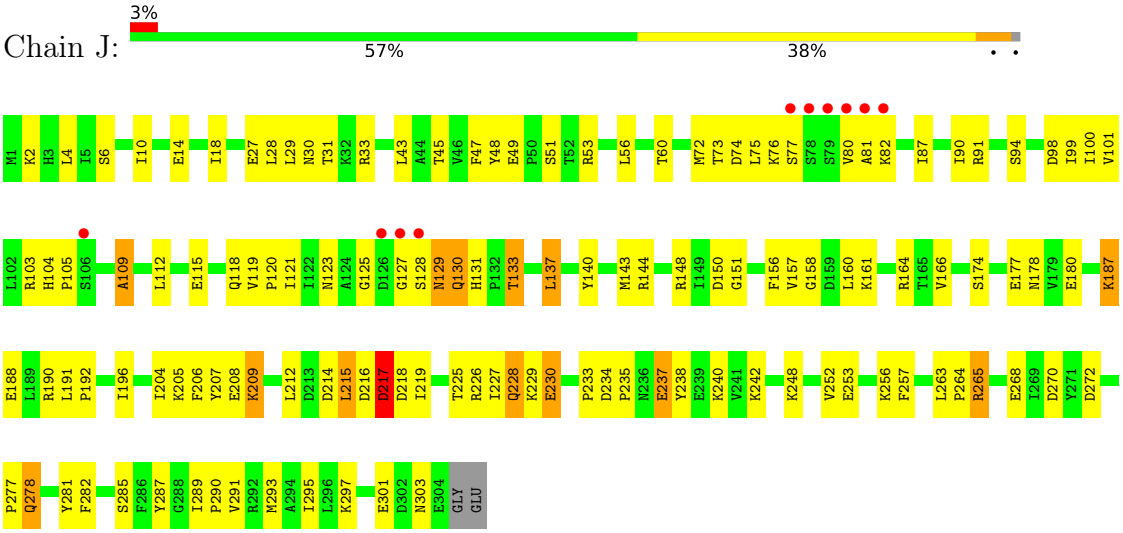
• Molecule 1: Aspartate carbamoyltransferase

Chain I:



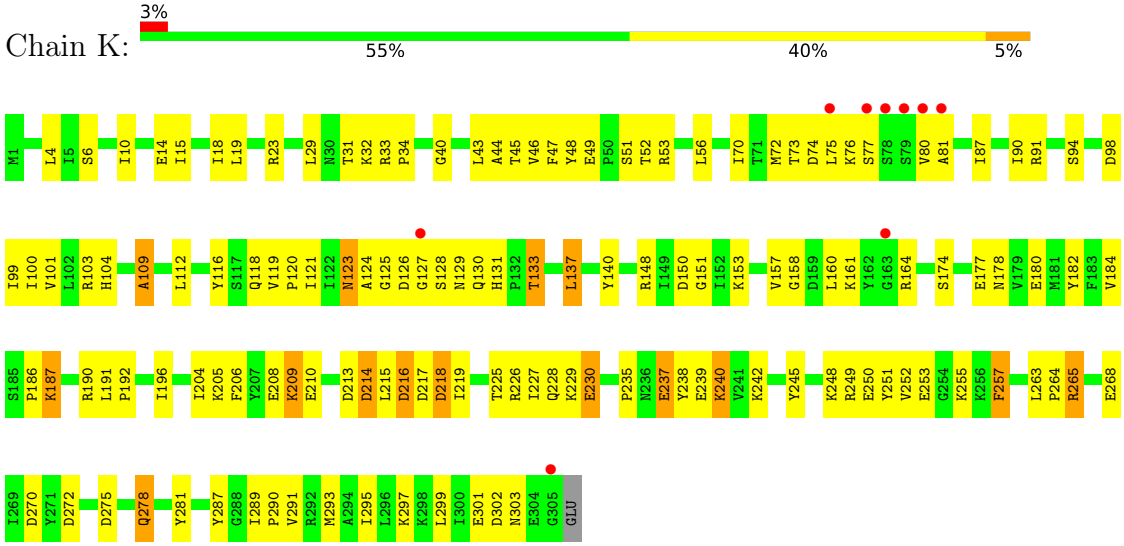
• Molecule 1: Aspartate carbamoyltransferase

Chain J:



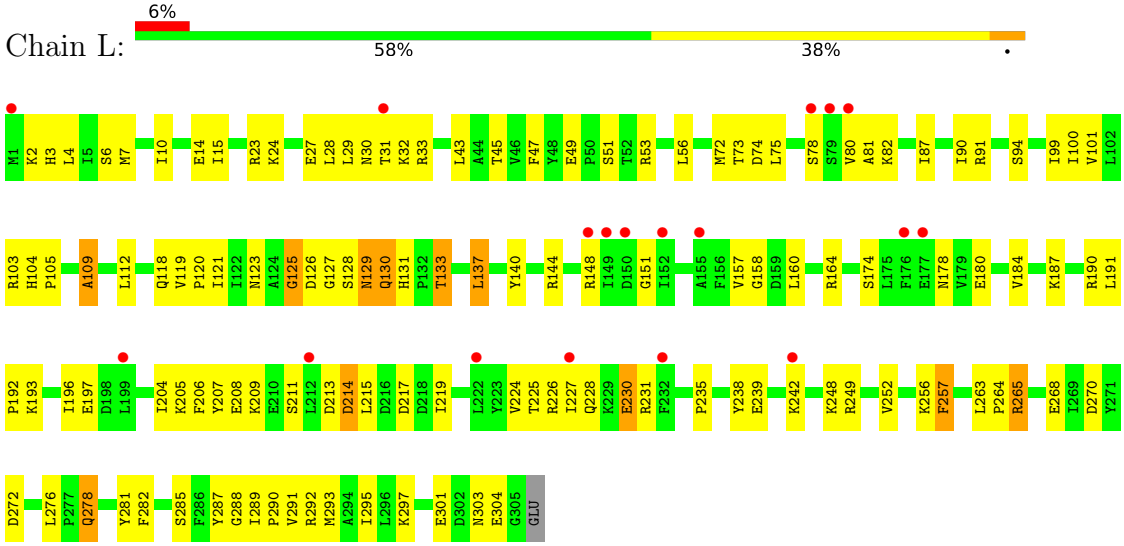
• Molecule 1: Aspartate carbamoyltransferase

Chain K:



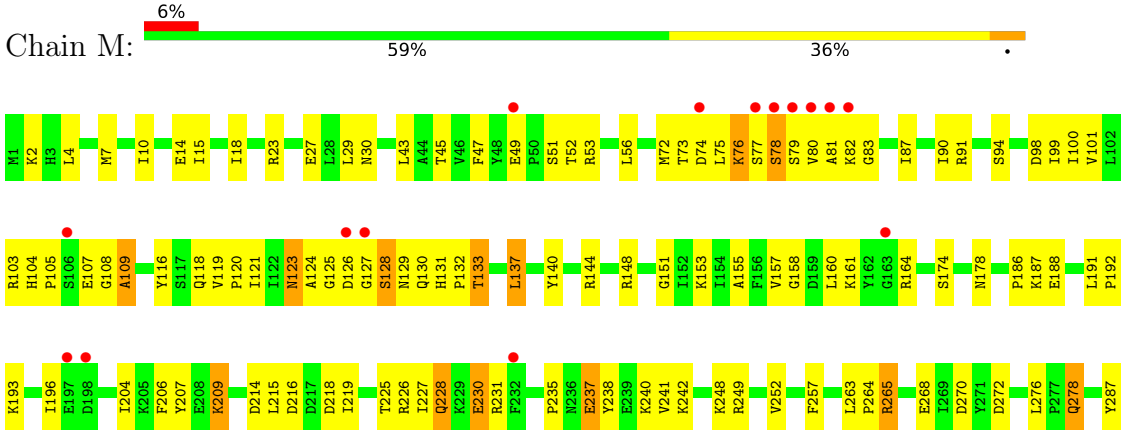
• Molecule 1: Aspartate carbamoyltransferase

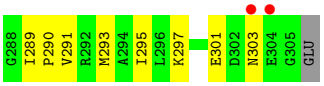
Chain L:



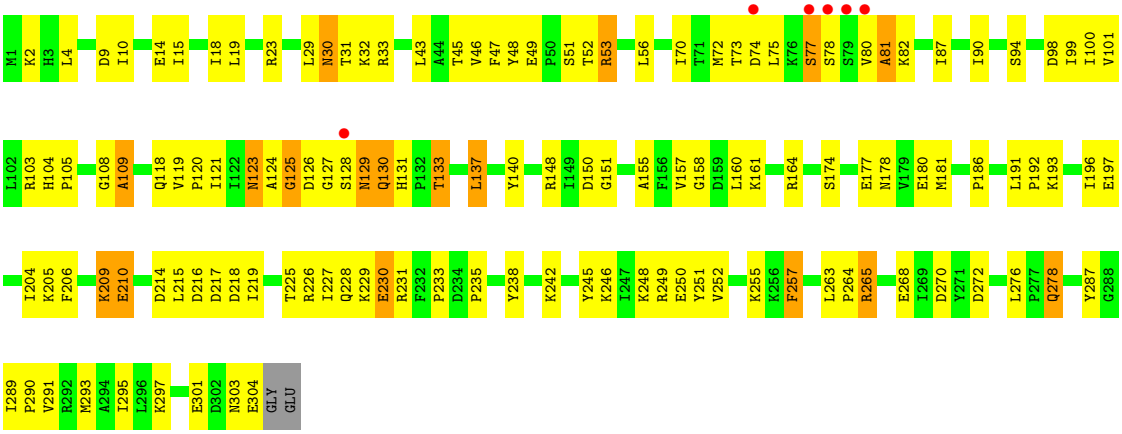
• Molecule 1: Aspartate carbamoyltransferase

Chain M:





• Molecule 1: Aspartate carbamoyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.13Å 167.93Å 319.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.09 – 3.02	Depositor EDS
% Data completeness (in resolution range)	93.9 (40.00-3.00) 93.0 (40.09-3.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.269 0.214 , 0.266	Depositor DCC
R_{free} test set	9209 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.4	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 89.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	30122	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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

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	0/2516	0.63	0/3385
1	B	0.44	0/2502	0.65	0/3368
1	C	0.39	0/2516	0.63	0/3385
1	D	0.43	0/2516	0.65	0/3385
1	E	0.41	0/2516	0.62	0/3385
1	F	0.41	0/2516	0.64	0/3385
1	I	0.32	0/2502	0.59	0/3368
1	J	0.37	0/2502	0.61	0/3368
1	K	0.34	0/2506	0.60	0/3373
1	L	0.32	0/2506	0.59	0/3373
1	M	0.36	0/2506	0.60	0/3373
1	N	0.35	0/2502	0.60	0/3368
All	All	0.38	0/30106	0.62	0/40516

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	2474	0	2538	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2460	0	2529	151	0
1	C	2474	0	2538	142	0
1	D	2474	0	2538	165	0
1	E	2474	0	2538	118	0
1	F	2474	0	2538	145	0
1	I	2460	0	2529	166	0
1	J	2460	0	2529	144	0
1	K	2464	0	2532	154	0
1	L	2464	0	2532	153	0
1	M	2464	0	2532	134	0
1	N	2460	0	2529	146	0
2	A	5	0	0	0	0
2	D	5	0	0	0	0
2	I	5	0	0	0	0
2	L	5	0	0	0	0
3	A	61	0	0	10	0
3	B	59	0	0	7	0
3	C	51	0	0	2	0
3	D	62	0	0	3	0
3	E	60	0	0	4	0
3	F	36	0	0	1	0
3	I	24	0	0	9	0
3	J	25	0	0	2	0
3	K	29	0	0	3	0
3	L	25	0	0	1	0
3	M	30	0	0	4	0
3	N	38	0	0	6	0
All	All	30122	0	30402	1667	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (1667) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:87:ILE:HD12	1:N:235:PRO:HD2	1.23	1.17
1:B:235:PRO:HD2	1:D:87:ILE:HD12	1.27	1.14
1:C:87:ILE:HD12	1:F:235:PRO:HD2	1.28	1.13
1:K:126:ASP:HB2	1:K:129:ASN:HD21	1.13	1.09
1:A:229:LYS:HE3	1:A:229:LYS:H	1.02	1.09
1:L:75:LEU:HD23	1:L:80:VAL:HG12	1.29	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:235:PRO:HD2	1:L:87:ILE:HD12	1.07	1.05
1:B:128:SER:HB3	1:B:164:ARG:HG3	1.32	1.05
1:E:187:LYS:HG3	1:E:190:ARG:HH22	1.15	1.04
1:N:2:LYS:HA	1:N:303:ASN:HD21	1.17	1.04
1:K:187:LYS:H	1:K:187:LYS:HD2	1.17	1.04
1:D:33:ARG:HH11	1:D:33:ARG:HB2	1.17	1.03
1:C:76:LYS:HE2	1:C:76:LYS:HA	1.39	1.00
1:M:249:ARG:HG2	1:M:276:LEU:HD11	1.39	1.00
1:N:31:THR:HG22	1:N:33:ARG:HG2	1.45	0.98
1:I:27:GLU:HA	1:I:30:ASN:HD22	1.27	0.98
1:J:235:PRO:CD	1:L:87:ILE:HD12	1.95	0.96
1:D:48:TYR:HB3	1:D:76:LYS:HG2	1.48	0.96
1:J:128:SER:HB3	1:J:164:ARG:HG3	1.45	0.95
1:L:128:SER:HB3	1:L:164:ARG:HG3	1.46	0.95
1:F:76:LYS:HA	1:F:76:LYS:HE2	1.49	0.94
1:M:53:ARG:HH22	1:N:82:LYS:HB2	1.30	0.94
1:D:187:LYS:HD2	1:D:190:ARG:HH22	1.32	0.94
1:I:187:LYS:HA	1:I:190:ARG:HH22	1.32	0.93
1:K:87:ILE:HD12	1:N:235:PRO:CD	1.99	0.92
1:A:229:LYS:HE3	1:A:229:LYS:N	1.84	0.91
1:A:229:LYS:H	1:A:229:LYS:CE	1.83	0.91
1:A:126:ASP:HB2	1:A:129:ASN:HD21	1.33	0.91
1:F:53:ARG:HD3	3:F:401:HOH:O	1.70	0.91
1:D:249:ARG:HG2	1:D:276:LEU:HD11	1.49	0.91
1:A:73:THR:HG22	1:A:74:ASP:H	1.33	0.91
1:M:51:SER:HB2	1:M:103:ARG:HH12	1.35	0.90
1:I:128:SER:HB3	1:I:164:ARG:HG3	1.52	0.90
1:F:75:LEU:HA	1:F:80:VAL:O	1.71	0.89
1:L:23:ARG:HH12	1:L:27:GLU:HB3	1.35	0.89
1:A:238:TYR:CE2	1:A:242:LYS:HD2	2.07	0.88
1:M:72:MET:HG2	1:M:75:LEU:HD11	1.53	0.88
1:A:51:SER:HB2	1:A:103:ARG:HH12	1.39	0.88
1:D:187:LYS:HD2	1:D:190:ARG:NH2	1.87	0.88
1:F:51:SER:HB2	1:F:103:ARG:HH12	1.38	0.88
1:E:238:TYR:CE2	1:E:242:LYS:HD2	2.09	0.88
1:A:306:GLU:HA	1:C:32:LYS:HG3	1.56	0.87
1:E:51:SER:HB2	1:E:103:ARG:HH12	1.37	0.87
1:N:125:GLY:HA2	1:N:130:GLN:O	1.74	0.87
1:J:87:ILE:HD12	1:L:235:PRO:HD2	1.57	0.86
1:A:24:LYS:O	1:A:27:GLU:HG2	1.76	0.86
1:K:238:TYR:CE2	1:K:242:LYS:HD2	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:SER:HB2	1:B:103:ARG:HH12	1.39	0.86
1:E:76:LYS:HE2	1:E:76:LYS:HA	1.57	0.86
1:D:51:SER:HB2	1:D:103:ARG:HH12	1.39	0.86
1:N:233:PRO:HA	3:N:415:HOH:O	1.74	0.85
1:N:51:SER:HB2	1:N:103:ARG:HH12	1.41	0.85
1:I:238:TYR:CE2	1:I:242:LYS:HD2	2.11	0.85
1:D:73:THR:HG22	1:D:74:ASP:H	1.40	0.85
1:M:238:TYR:CE2	1:M:242:LYS:HD2	2.12	0.85
1:F:238:TYR:CE2	1:F:242:LYS:HD2	2.12	0.85
1:I:76:LYS:HE2	1:I:76:LYS:HA	1.58	0.84
1:L:24:LYS:O	1:L:27:GLU:HG2	1.77	0.84
1:K:51:SER:HB2	1:K:103:ARG:HH12	1.40	0.84
1:C:238:TYR:CE2	1:C:242:LYS:HD2	2.12	0.84
1:J:238:TYR:CE2	1:J:242:LYS:HD2	2.12	0.84
1:C:87:ILE:HD12	1:F:235:PRO:CD	2.07	0.84
1:A:235:PRO:HD2	1:E:87:ILE:HD12	1.60	0.84
1:L:31:THR:HG22	1:L:33:ARG:H	1.42	0.84
1:J:51:SER:HB2	1:J:103:ARG:HH12	1.41	0.83
1:J:226:ARG:HG2	1:J:268:GLU:OE1	1.78	0.83
1:D:33:ARG:HB2	1:D:33:ARG:NH1	1.92	0.83
1:L:238:TYR:CE2	1:L:242:LYS:HD2	2.12	0.83
1:E:187:LYS:HG3	1:E:190:ARG:NH2	1.92	0.83
1:L:53:ARG:HG3	1:L:53:ARG:HH11	1.43	0.83
1:I:126:ASP:HB2	1:I:129:ASN:HD21	1.44	0.83
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.44	0.82
1:K:187:LYS:HD2	1:K:187:LYS:N	1.93	0.82
1:C:51:SER:HB2	1:C:103:ARG:HH12	1.43	0.82
1:B:87:ILE:HD12	1:D:235:PRO:HD2	1.60	0.82
1:N:103:ARG:HH11	1:N:103:ARG:HG2	1.45	0.82
1:I:103:ARG:HH11	1:I:103:ARG:HG2	1.44	0.82
1:N:238:TYR:CE2	1:N:242:LYS:HD2	2.15	0.81
1:J:125:GLY:HA2	1:J:130:GLN:O	1.81	0.81
1:A:73:THR:HG22	1:A:74:ASP:N	1.95	0.81
1:C:249:ARG:HG3	1:C:249:ARG:HH11	1.45	0.81
1:D:238:TYR:CE2	1:D:242:LYS:HD2	2.15	0.81
1:L:51:SER:HB2	1:L:103:ARG:HH12	1.45	0.81
1:A:301:GLU:HG2	3:A:453:HOH:O	1.80	0.81
1:M:53:ARG:NH2	1:N:82:LYS:HB2	1.96	0.81
1:B:29:LEU:HD11	1:B:293:MET:HE1	1.63	0.81
1:I:235:PRO:HD2	1:M:87:ILE:HD12	1.64	0.80
1:L:249:ARG:HG3	1:L:276:LEU:HD11	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:TYR:CE2	1:B:242:LYS:HD2	2.17	0.80
1:D:29:LEU:HD11	1:D:293:MET:HE1	1.60	0.80
1:J:103:ARG:HG2	1:J:103:ARG:HH11	1.45	0.80
1:J:187:LYS:H	1:J:187:LYS:CE	1.94	0.80
1:I:51:SER:HB2	1:I:103:ARG:HH12	1.44	0.80
1:A:250:GLU:CD	1:A:250:GLU:H	1.85	0.80
1:D:126:ASP:HB2	1:D:129:ASN:HD21	1.46	0.80
1:J:187:LYS:H	1:J:187:LYS:HE2	1.46	0.80
1:D:73:THR:HG22	1:D:74:ASP:N	1.97	0.79
1:M:75:LEU:HA	1:M:80:VAL:HB	1.64	0.79
1:C:103:ARG:HG2	1:C:103:ARG:HH11	1.46	0.79
1:L:103:ARG:HG2	1:L:103:ARG:HH11	1.46	0.79
1:K:187:LYS:H	1:K:187:LYS:CD	1.90	0.79
1:F:301:GLU:HA	1:F:304:GLU:HG3	1.64	0.79
1:M:103:ARG:HG2	1:M:103:ARG:HH11	1.48	0.79
1:C:249:ARG:HH12	1:C:276:LEU:HD21	1.45	0.79
1:K:128:SER:HB3	1:K:164:ARG:HG3	1.65	0.79
1:L:23:ARG:NH1	1:L:27:GLU:HB3	1.97	0.79
1:M:75:LEU:HG	1:M:80:VAL:HG12	1.65	0.79
1:B:103:ARG:HG2	1:B:103:ARG:HH11	1.47	0.78
1:J:125:GLY:C	1:J:127:GLY:H	1.87	0.78
1:L:73:THR:HG22	1:L:74:ASP:N	1.98	0.78
1:B:215:LEU:HD22	1:B:219:ILE:HD11	1.64	0.78
1:J:31:THR:HG22	1:J:33:ARG:HB2	1.63	0.78
1:M:240:LYS:HD3	1:M:241:VAL:N	1.98	0.78
1:A:82:LYS:HD3	1:C:53:ARG:HH12	1.48	0.78
1:I:31:THR:CG2	1:I:33:ARG:HD3	2.14	0.78
1:K:226:ARG:HG2	1:K:268:GLU:OE1	1.83	0.78
1:J:187:LYS:H	1:J:187:LYS:CD	1.95	0.78
1:B:49:GLU:OE2	1:B:127:GLY:HA2	1.84	0.78
1:F:103:ARG:HG2	1:F:103:ARG:HH11	1.47	0.78
1:M:29:LEU:HD11	1:M:293:MET:HE1	1.66	0.78
1:D:103:ARG:HH11	1:D:103:ARG:HG2	1.48	0.78
1:B:106:SER:HB3	1:D:233:PRO:HG3	1.65	0.77
1:K:103:ARG:HH11	1:K:103:ARG:HG2	1.47	0.77
1:L:184:VAL:HG21	1:L:215:LEU:HD11	1.65	0.77
1:B:128:SER:CB	1:B:164:ARG:HG3	2.11	0.77
1:I:87:ILE:HD12	1:M:235:PRO:HD2	1.64	0.77
1:N:215:LEU:HD22	1:N:219:ILE:HD12	1.66	0.77
1:N:73:THR:HG22	1:N:74:ASP:H	1.49	0.77
1:E:103:ARG:HG2	1:E:103:ARG:HH11	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:GLY:HA2	1:E:178:ASN:O	1.84	0.77
1:A:226:ARG:HG2	1:A:268:GLU:OE1	1.83	0.76
1:A:289:ILE:HB	1:A:290:PRO:HD3	1.67	0.76
1:C:235:PRO:HD2	1:F:87:ILE:HD12	1.66	0.76
1:E:49:GLU:HG2	1:E:105:PRO:HG3	1.67	0.76
1:J:212:LEU:O	1:J:215:LEU:HD12	1.85	0.76
1:A:304:GLU:HG3	1:A:306:GLU:HG2	1.67	0.76
1:A:144:ARG:HG2	1:A:287:TYR:CZ	2.20	0.76
1:M:73:THR:HG22	1:M:74:ASP:H	1.51	0.76
1:M:226:ARG:HG2	1:M:268:GLU:OE1	1.85	0.76
1:M:215:LEU:HD22	1:M:219:ILE:HD11	1.68	0.76
1:F:123:ASN:ND2	1:F:125:GLY:H	1.84	0.76
1:L:187:LYS:HD2	1:L:190:ARG:HH21	1.51	0.76
1:M:230:GLU:CD	1:M:230:GLU:H	1.90	0.75
1:N:289:ILE:HB	1:N:290:PRO:HD3	1.67	0.75
1:D:126:ASP:HB2	1:D:129:ASN:ND2	2.01	0.75
1:N:73:THR:HG22	1:N:74:ASP:N	2.01	0.75
1:K:31:THR:HG22	1:K:33:ARG:HB2	1.69	0.75
1:K:209:LYS:CG	1:K:214:ASP:HB2	2.17	0.75
1:J:28:LEU:O	1:J:31:THR:HB	1.85	0.75
1:K:180:GLU:HG3	1:K:205:LYS:HG3	1.68	0.75
1:E:29:LEU:HD11	1:E:293:MET:HE1	1.68	0.75
1:M:131:HIS:CD2	1:M:133:THR:HG23	2.22	0.75
1:L:29:LEU:HD11	1:L:293:MET:HE1	1.68	0.74
1:D:49:GLU:OE2	1:D:127:GLY:HA2	1.87	0.74
1:N:48:TYR:CE1	1:N:75:LEU:HD13	2.22	0.74
1:A:230:GLU:CD	1:A:230:GLU:H	1.90	0.74
1:K:131:HIS:CD2	1:K:133:THR:HG23	2.21	0.74
1:M:209:LYS:CG	1:M:214:ASP:HB3	2.17	0.74
1:N:75:LEU:HA	1:N:80:VAL:HG12	1.67	0.74
1:I:31:THR:HG22	1:I:33:ARG:HD3	1.69	0.74
1:B:155:ALA:HB2	1:B:219:ILE:HD13	1.70	0.74
1:F:51:SER:HB2	1:F:103:ARG:NH1	2.03	0.74
1:I:187:LYS:HA	1:I:190:ARG:NH2	2.03	0.74
1:M:51:SER:HB2	1:M:103:ARG:NH1	2.02	0.74
1:B:226:ARG:HG2	1:B:268:GLU:OE1	1.87	0.73
1:D:72:MET:HB2	1:F:56:LEU:HD11	1.70	0.73
1:D:249:ARG:HB2	1:D:272:ASP:OD2	1.88	0.73
1:C:226:ARG:HG2	1:C:268:GLU:OE1	1.87	0.73
1:D:289:ILE:HB	1:D:290:PRO:HD3	1.70	0.73
1:L:226:ARG:HG2	1:L:268:GLU:OE1	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:289:ILE:HB	1:K:290:PRO:HD3	1.70	0.73
1:M:187:LYS:NZ	1:M:187:LYS:H	1.87	0.73
1:M:151:GLY:HA2	1:M:178:ASN:O	1.88	0.73
1:F:29:LEU:HD11	1:F:293:MET:HE1	1.69	0.73
1:L:73:THR:HG22	1:L:74:ASP:H	1.54	0.73
1:I:75:LEU:HG	1:I:80:VAL:HG12	1.71	0.73
1:I:209:LYS:HG2	1:I:214:ASP:HB2	1.71	0.73
1:J:289:ILE:HB	1:J:290:PRO:HD3	1.70	0.73
1:M:72:MET:SD	1:M:75:LEU:HD21	2.29	0.73
1:M:73:THR:HG22	1:M:74:ASP:N	2.03	0.73
1:J:187:LYS:HG2	1:J:188:GLU:OE2	1.88	0.72
1:D:75:LEU:HD23	1:D:80:VAL:HG12	1.72	0.72
1:E:289:ILE:HB	1:E:290:PRO:HD3	1.70	0.72
1:D:151:GLY:HA2	1:D:178:ASN:O	1.89	0.72
1:E:290:PRO:HA	1:E:293:MET:HE2	1.72	0.72
1:B:235:PRO:CD	1:D:87:ILE:HD12	2.13	0.72
1:F:151:GLY:HA2	1:F:178:ASN:O	1.89	0.72
1:I:50:PRO:HB3	3:I:418:HOH:O	1.88	0.72
1:A:75:LEU:O	1:A:81:ALA:HB2	1.90	0.72
1:B:215:LEU:HD22	1:B:219:ILE:CD1	2.20	0.72
1:J:151:GLY:HA2	1:J:178:ASN:O	1.90	0.72
1:M:289:ILE:HB	1:M:290:PRO:HD3	1.70	0.72
1:A:82:LYS:HD3	1:C:53:ARG:NH1	2.05	0.71
1:F:226:ARG:HG2	1:F:268:GLU:OE1	1.90	0.71
1:C:230:GLU:CD	1:C:230:GLU:H	1.91	0.71
1:C:289:ILE:HB	1:C:290:PRO:HD3	1.72	0.71
1:I:226:ARG:HG2	1:I:268:GLU:OE1	1.89	0.71
1:E:226:ARG:HG2	1:E:268:GLU:OE1	1.88	0.71
1:I:151:GLY:HA2	1:I:178:ASN:O	1.91	0.71
1:K:126:ASP:HB2	1:K:129:ASN:ND2	1.98	0.71
1:M:216:ASP:HB2	1:M:218:ASP:OD1	1.91	0.71
1:N:29:LEU:HD11	1:N:293:MET:HE1	1.71	0.71
1:C:151:GLY:HA2	1:C:178:ASN:O	1.90	0.71
1:E:51:SER:HB2	1:E:103:ARG:NH1	2.05	0.71
1:K:29:LEU:HD11	1:K:293:MET:HE1	1.73	0.71
1:K:290:PRO:HA	1:K:293:MET:HE2	1.73	0.71
1:L:151:GLY:HA2	1:L:178:ASN:O	1.91	0.71
1:A:51:SER:HB2	1:A:103:ARG:NH1	2.05	0.71
1:B:51:SER:HB2	1:B:103:ARG:NH1	2.05	0.71
1:E:215:LEU:HD22	1:E:219:ILE:HD11	1.72	0.71
1:F:289:ILE:HB	1:F:290:PRO:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:151:GLY:HA2	1:K:178:ASN:O	1.89	0.71
1:B:144:ARG:HG3	1:B:144:ARG:HH11	1.55	0.70
1:J:230:GLU:CD	1:J:230:GLU:H	1.94	0.70
1:K:51:SER:HB2	1:K:103:ARG:NH1	2.06	0.70
1:B:301:GLU:O	1:B:304:GLU:HG2	1.91	0.70
1:D:51:SER:HB2	1:D:103:ARG:NH1	2.05	0.70
1:I:304:GLU:OE2	1:K:32:LYS:HD2	1.89	0.70
1:M:29:LEU:HD11	1:M:293:MET:CE	2.22	0.70
1:C:29:LEU:HD11	1:C:293:MET:HE1	1.71	0.70
1:L:289:ILE:HB	1:L:290:PRO:HD3	1.73	0.70
1:L:301:GLU:O	1:L:304:GLU:HG3	1.90	0.70
1:C:237:GLU:O	1:C:240:LYS:HB3	1.91	0.70
1:E:131:HIS:CD2	1:E:133:THR:HG23	2.26	0.70
1:F:23:ARG:O	1:F:27:GLU:HG3	1.91	0.69
1:I:49:GLU:OE2	1:I:127:GLY:HA2	1.92	0.69
1:I:289:ILE:HB	1:I:290:PRO:HD3	1.73	0.69
1:J:2:LYS:HA	1:J:303:ASN:HD21	1.57	0.69
1:L:7:MET:H	1:L:130:GLN:NE2	1.90	0.69
1:F:74:ASP:C	1:F:75:LEU:HD12	2.13	0.69
1:K:49:GLU:OE2	1:K:127:GLY:HA2	1.92	0.69
1:E:53:ARG:HH22	1:F:82:LYS:HB2	1.57	0.69
1:J:51:SER:HB2	1:J:103:ARG:NH1	2.07	0.69
1:A:240:LYS:HE2	3:A:454:HOH:O	1.90	0.69
1:M:155:ALA:HB2	1:M:219:ILE:HD13	1.72	0.69
1:D:305:GLY:O	1:D:306:GLU:HB3	1.92	0.69
1:E:287:TYR:O	1:E:291:VAL:HG13	1.92	0.69
1:B:230:GLU:CD	1:B:230:GLU:H	1.96	0.69
1:F:249:ARG:O	1:F:253:GLU:HG3	1.93	0.69
1:C:219:ILE:HG22	1:C:257:PHE:HB3	1.72	0.69
1:D:128:SER:HB3	1:D:164:ARG:HG3	1.74	0.69
1:E:230:GLU:CD	1:E:230:GLU:H	1.94	0.69
1:K:73:THR:HG22	1:K:74:ASP:N	2.08	0.69
1:N:31:THR:HG22	1:N:33:ARG:CG	2.21	0.69
1:D:31:THR:HB	1:D:33:ARG:HG2	1.73	0.69
1:F:131:HIS:CD2	1:F:133:THR:HG23	2.28	0.69
1:L:103:ARG:HG2	1:L:103:ARG:NH1	2.08	0.69
1:N:129:ASN:O	1:N:130:GLN:HB2	1.93	0.69
1:A:151:GLY:HA2	1:A:178:ASN:O	1.93	0.68
1:B:228:GLN:HB3	1:B:230:GLU:OE1	1.93	0.68
1:C:131:HIS:CD2	1:C:133:THR:HG23	2.28	0.68
1:E:205:LYS:HE2	1:E:207:TYR:OH	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:126:ASP:HB2	1:L:129:ASN:HD21	1.56	0.68
1:N:51:SER:HB2	1:N:103:ARG:NH1	2.06	0.68
1:N:226:ARG:HG2	1:N:268:GLU:OE1	1.92	0.68
1:B:289:ILE:HB	1:B:290:PRO:HD3	1.76	0.68
1:F:90:ILE:O	1:F:94:SER:HB2	1.92	0.68
1:J:103:ARG:HG2	1:J:103:ARG:NH1	2.08	0.68
1:A:73:THR:CG2	1:A:74:ASP:H	2.06	0.68
1:D:228:GLN:HB3	1:D:230:GLU:OE1	1.92	0.68
1:L:7:MET:HB2	1:L:130:GLN:HE22	1.59	0.68
1:A:216:ASP:HB2	1:A:218:ASP:OD1	1.94	0.68
1:B:151:GLY:HA2	1:B:178:ASN:O	1.93	0.68
1:K:73:THR:HG22	1:K:74:ASP:H	1.58	0.68
1:M:209:LYS:HG3	1:M:214:ASP:HB3	1.76	0.68
1:E:125:GLY:C	1:E:127:GLY:H	1.96	0.68
1:K:103:ARG:HG2	1:K:103:ARG:NH1	2.08	0.68
1:F:29:LEU:HD11	1:F:293:MET:CE	2.23	0.68
1:K:31:THR:CG2	1:K:33:ARG:HB2	2.23	0.68
1:N:131:HIS:CD2	1:N:133:THR:HG23	2.29	0.68
1:I:27:GLU:HA	1:I:30:ASN:ND2	2.07	0.68
1:E:90:ILE:O	1:E:94:SER:HB2	1.93	0.68
1:K:40:GLY:HA2	3:K:425:HOH:O	1.94	0.68
1:L:72:MET:HB2	1:N:56:LEU:HD11	1.74	0.68
1:N:151:GLY:HA2	1:N:178:ASN:O	1.93	0.68
1:A:49:GLU:OE2	1:A:127:GLY:HA2	1.94	0.68
1:F:153:LYS:HD2	1:F:218:ASP:O	1.94	0.67
1:A:131:HIS:CD2	1:A:133:THR:HG23	2.29	0.67
1:L:73:THR:O	1:L:80:VAL:HG11	1.94	0.67
1:D:226:ARG:HG2	1:D:268:GLU:OE1	1.93	0.67
1:I:51:SER:HB2	1:I:103:ARG:NH1	2.08	0.67
1:F:49:GLU:OE2	1:F:127:GLY:HA2	1.95	0.67
1:K:235:PRO:HD2	1:N:87:ILE:HD12	1.76	0.67
1:L:99:ILE:HA	1:L:119:VAL:CG1	2.25	0.67
1:A:126:ASP:HB2	1:A:129:ASN:ND2	2.09	0.67
1:C:51:SER:HB2	1:C:103:ARG:NH1	2.09	0.67
1:J:99:ILE:HA	1:J:119:VAL:CG1	2.25	0.67
1:N:180:GLU:HG3	1:N:205:LYS:HG3	1.77	0.67
1:A:119:VAL:HG13	1:A:120:PRO:HD2	1.77	0.67
1:B:56:LEU:HD11	1:C:72:MET:HB2	1.77	0.67
1:B:103:ARG:HG2	1:B:103:ARG:NH1	2.09	0.67
1:I:131:HIS:CD2	1:I:133:THR:HG23	2.30	0.67
1:L:51:SER:HB2	1:L:103:ARG:NH1	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:56:LEU:HD11	1:J:72:MET:HB2	1.76	0.66
1:M:103:ARG:HG2	1:M:103:ARG:NH1	2.09	0.66
1:D:209:LYS:HG2	1:D:214:ASP:O	1.95	0.66
1:J:290:PRO:HA	1:J:293:MET:HE2	1.78	0.66
1:B:73:THR:HG22	1:B:74:ASP:N	2.10	0.66
1:I:7:MET:H	1:I:130:GLN:NE2	1.93	0.66
1:J:119:VAL:HG13	1:J:120:PRO:HD2	1.78	0.66
1:K:229:LYS:HG2	1:K:238:TYR:CE2	2.30	0.66
1:E:119:VAL:HG13	1:E:120:PRO:HD2	1.78	0.66
1:J:75:LEU:O	1:J:81:ALA:HB2	1.96	0.66
1:L:72:MET:CG	1:L:75:LEU:HD21	2.24	0.66
1:L:290:PRO:HA	1:L:293:MET:HE2	1.78	0.66
1:K:48:TYR:CE1	1:K:75:LEU:HD13	2.30	0.66
1:K:209:LYS:HG3	1:K:214:ASP:HB2	1.77	0.66
1:B:166:VAL:HG23	3:B:405:HOH:O	1.93	0.66
1:D:99:ILE:HA	1:D:119:VAL:CG1	2.26	0.66
1:L:29:LEU:HD11	1:L:293:MET:CE	2.24	0.66
1:N:103:ARG:HG2	1:N:103:ARG:NH1	2.07	0.66
1:M:144:ARG:HD2	3:M:408:HOH:O	1.96	0.66
1:C:99:ILE:HA	1:C:119:VAL:CG1	2.26	0.66
1:M:99:ILE:HA	1:M:119:VAL:CG1	2.26	0.66
1:N:99:ILE:HA	1:N:119:VAL:CG1	2.25	0.66
1:B:287:TYR:O	1:B:291:VAL:HG13	1.96	0.65
1:C:125:GLY:C	1:C:127:GLY:H	1.99	0.65
1:F:103:ARG:HG2	1:F:103:ARG:NH1	2.09	0.65
1:A:29:LEU:HD11	1:A:293:MET:HE1	1.78	0.65
1:A:90:ILE:O	1:A:94:SER:HB2	1.95	0.65
1:B:290:PRO:HA	1:B:293:MET:HE2	1.78	0.65
1:N:180:GLU:OE2	1:N:205:LYS:HD2	1.96	0.65
1:D:218:ASP:OD2	1:D:219:ILE:N	2.29	0.65
1:K:99:ILE:HA	1:K:119:VAL:CG1	2.27	0.65
1:E:99:ILE:HA	1:E:119:VAL:CG1	2.27	0.65
1:A:48:TYR:CZ	1:A:75:LEU:HD13	2.32	0.65
1:C:90:ILE:O	1:C:94:SER:HB2	1.97	0.65
1:C:129:ASN:HD22	1:C:130:GLN:N	1.94	0.65
1:J:49:GLU:CG	1:J:105:PRO:HG3	2.26	0.65
1:A:56:LEU:HD11	1:B:72:MET:HB2	1.78	0.65
1:I:24:LYS:O	1:I:27:GLU:HG2	1.95	0.65
1:I:72:MET:SD	1:I:75:LEU:HD11	2.37	0.65
1:B:200:LYS:HE2	1:J:253:GLU:OE1	1.97	0.65
1:D:230:GLU:H	1:D:230:GLU:CD	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:HB3	1:D:236:ASN:OD1	1.97	0.64
1:C:249:ARG:NH2	1:C:272:ASP:HB2	2.11	0.64
1:D:23:ARG:O	1:D:27:GLU:HG3	1.97	0.64
1:E:48:TYR:HB3	1:E:76:LYS:HG2	1.79	0.64
1:I:99:ILE:HA	1:I:119:VAL:CG1	2.28	0.64
1:D:103:ARG:HG2	1:D:103:ARG:NH1	2.10	0.64
1:B:94:SER:OG	1:B:118:GLN:HG2	1.98	0.64
1:I:103:ARG:HG2	1:I:103:ARG:NH1	2.07	0.64
1:K:90:ILE:O	1:K:94:SER:HB2	1.96	0.64
1:M:76:LYS:HA	1:M:76:LYS:CE	2.28	0.64
1:M:94:SER:OG	1:M:118:GLN:HG2	1.98	0.64
1:F:99:ILE:HA	1:F:119:VAL:CG1	2.27	0.64
1:D:131:HIS:CD2	1:D:133:THR:HG23	2.33	0.64
1:L:53:ARG:HG3	1:L:53:ARG:NH1	2.12	0.64
1:B:52:THR:OG1	1:C:80:VAL:HG13	1.98	0.64
1:E:103:ARG:HG2	1:E:103:ARG:NH1	2.09	0.64
1:K:29:LEU:HD11	1:K:293:MET:CE	2.28	0.64
1:L:230:GLU:CD	1:L:230:GLU:H	1.98	0.64
1:M:56:LEU:HD11	1:N:72:MET:HB2	1.78	0.64
1:C:290:PRO:HA	1:C:293:MET:HE2	1.80	0.64
1:C:301:GLU:HA	1:C:304:GLU:HG2	1.79	0.64
1:C:31:THR:O	1:C:32:LYS:C	2.35	0.64
1:J:27:GLU:HA	1:J:30:ASN:ND2	2.13	0.64
1:L:90:ILE:O	1:L:94:SER:HB2	1.97	0.64
1:M:43:LEU:HD11	1:M:101:VAL:HG23	1.80	0.64
1:N:290:PRO:HA	1:N:293:MET:HE2	1.78	0.64
1:J:94:SER:OG	1:J:118:GLN:HG2	1.98	0.63
1:M:228:GLN:HB3	1:M:230:GLU:OE1	1.98	0.63
1:A:103:ARG:HG2	1:A:103:ARG:NH1	2.06	0.63
1:L:73:THR:CG2	1:L:74:ASP:H	2.11	0.63
1:E:125:GLY:HA2	1:E:130:GLN:O	1.98	0.63
1:J:31:THR:CG2	1:J:33:ARG:HB2	2.28	0.63
1:J:73:THR:HG22	1:J:74:ASP:N	2.13	0.63
1:L:287:TYR:O	1:L:291:VAL:HG13	1.99	0.63
1:B:99:ILE:HA	1:B:119:VAL:CG1	2.28	0.63
1:C:29:LEU:HD11	1:C:293:MET:CE	2.29	0.63
1:M:107:GLU:HG3	3:M:411:HOH:O	1.98	0.63
1:C:129:ASN:O	1:C:130:GLN:HB2	1.98	0.63
1:J:131:HIS:CD2	1:J:133:THR:HG23	2.33	0.63
1:M:126:ASP:C	1:M:128:SER:H	2.02	0.63
1:N:90:ILE:O	1:N:94:SER:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:THR:CG2	1:D:74:ASP:H	2.12	0.63
1:M:187:LYS:H	1:M:187:LYS:CE	2.12	0.63
1:N:2:LYS:HA	1:N:303:ASN:ND2	2.01	0.63
1:J:228:GLN:HB3	1:J:230:GLU:OE1	1.99	0.63
1:C:270:ASP:HB3	1:C:272:ASP:OD1	1.98	0.62
1:E:94:SER:OG	1:E:118:GLN:HG2	1.99	0.62
1:I:4:LEU:HD11	1:I:10:ILE:HD11	1.81	0.62
1:M:119:VAL:HG13	1:M:120:PRO:HD2	1.80	0.62
1:B:53:ARG:NH1	1:C:82:LYS:HD3	2.14	0.62
1:D:217:ASP:HB2	1:D:255:LYS:CD	2.29	0.62
1:D:306:GLU:OXT	1:D:306:GLU:HG2	1.98	0.62
1:F:75:LEU:HD12	1:F:75:LEU:N	2.14	0.62
1:D:90:ILE:O	1:D:94:SER:HB2	1.99	0.62
1:F:228:GLN:HB3	1:F:230:GLU:OE1	1.98	0.62
1:I:73:THR:HG22	1:I:74:ASP:N	2.14	0.62
1:K:228:GLN:HB3	1:K:230:GLU:OE1	2.00	0.62
1:C:287:TYR:O	1:C:291:VAL:HG13	1.99	0.62
1:D:270:ASP:HB3	1:D:272:ASP:OD1	1.99	0.62
1:F:290:PRO:HA	1:F:293:MET:HE2	1.80	0.62
1:I:209:LYS:CG	1:I:214:ASP:HB2	2.28	0.62
1:M:209:LYS:HG2	1:M:214:ASP:HB3	1.81	0.62
1:E:237:GLU:O	1:E:240:LYS:HB3	1.98	0.62
1:F:230:GLU:CD	1:F:230:GLU:H	2.01	0.62
1:I:187:LYS:HD2	1:I:188:GLU:CD	2.20	0.62
1:M:76:LYS:HA	1:M:76:LYS:HE2	1.81	0.62
1:N:43:LEU:HD11	1:N:101:VAL:HG23	1.82	0.62
1:A:52:THR:HB	1:B:80:VAL:HG13	1.80	0.62
1:K:31:THR:O	1:K:32:LYS:HB2	1.99	0.62
1:K:230:GLU:CD	1:K:230:GLU:H	2.02	0.62
1:A:99:ILE:HA	1:A:119:VAL:CG1	2.30	0.62
1:A:228:GLN:HB3	1:A:230:GLU:OE1	1.99	0.62
1:F:80:VAL:O	1:F:81:ALA:HB2	1.98	0.62
1:F:100:ILE:HB	1:F:121:ILE:HD13	1.81	0.62
1:I:249:ARG:NH1	1:I:276:LEU:HD21	2.14	0.62
1:L:31:THR:CG2	1:L:33:ARG:HB2	2.30	0.62
1:N:270:ASP:HB3	1:N:272:ASP:OD1	2.00	0.62
1:D:190:ARG:HB2	1:D:190:ARG:CZ	2.30	0.62
1:E:81:ALA:O	1:E:83:GLY:N	2.32	0.62
1:L:131:HIS:CD2	1:L:133:THR:HG23	2.35	0.62
1:M:270:ASP:HB3	1:M:272:ASP:OD1	2.00	0.61
1:N:48:TYR:CD1	1:N:75:LEU:HD13	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:SER:C	1:C:79:SER:H	2.03	0.61
1:I:209:LYS:HE2	3:I:422:HOH:O	2.00	0.61
1:A:87:ILE:HD12	1:E:235:PRO:HD2	1.82	0.61
1:A:290:PRO:HA	1:A:293:MET:HE2	1.82	0.61
1:M:187:LYS:H	1:M:187:LYS:HZ3	1.47	0.61
1:C:103:ARG:HG2	1:C:103:ARG:NH1	2.08	0.61
1:I:72:MET:HB2	1:K:56:LEU:HD11	1.82	0.61
1:J:90:ILE:O	1:J:94:SER:HB2	1.99	0.61
1:B:236:ASN:OD1	1:F:271:TYR:HB3	2.01	0.61
1:C:6:SER:HA	1:C:130:GLN:HG2	1.81	0.61
1:J:180:GLU:OE2	1:J:205:LYS:HD2	2.00	0.61
1:K:217:ASP:C	1:K:219:ILE:H	2.02	0.61
1:M:287:TYR:O	1:M:291:VAL:HG13	2.01	0.61
1:C:75:LEU:O	1:C:81:ALA:HB2	2.00	0.61
1:I:90:ILE:O	1:I:94:SER:HB2	1.99	0.61
1:I:230:GLU:H	1:I:230:GLU:CD	2.03	0.61
1:I:268:GLU:H	1:I:268:GLU:CD	2.04	0.61
1:L:180:GLU:HG3	1:L:205:LYS:HD2	1.83	0.61
1:N:73:THR:CG2	1:N:74:ASP:H	2.14	0.61
1:B:271:TYR:HB3	1:F:236:ASN:OD1	2.01	0.61
1:A:52:THR:CB	1:B:80:VAL:HG13	2.31	0.61
1:B:100:ILE:HB	1:B:121:ILE:HD13	1.83	0.61
1:I:287:TYR:O	1:I:291:VAL:HG13	2.01	0.61
1:B:29:LEU:HD11	1:B:293:MET:CE	2.31	0.60
1:J:235:PRO:HD2	1:L:87:ILE:CD1	2.04	0.60
1:K:119:VAL:HG13	1:K:120:PRO:HD2	1.83	0.60
1:L:119:VAL:HG13	1:L:120:PRO:HD2	1.83	0.60
1:A:53:ARG:NH2	1:A:264:PRO:HB3	2.15	0.60
1:D:94:SER:OG	1:D:118:GLN:HG2	2.01	0.60
1:L:270:ASP:HB3	1:L:272:ASP:OD1	2.01	0.60
1:D:100:ILE:HB	1:D:121:ILE:HD13	1.81	0.60
1:F:270:ASP:HB3	1:F:272:ASP:OD1	2.01	0.60
1:B:2:LYS:HD2	1:B:303:ASN:ND2	2.16	0.60
1:B:304:GLU:OE2	1:B:304:GLU:HA	2.02	0.60
1:F:268:GLU:CD	1:F:268:GLU:H	2.04	0.60
1:B:76:LYS:HA	1:B:76:LYS:NZ	2.15	0.60
1:B:131:HIS:CD2	1:B:133:THR:HG23	2.36	0.60
1:J:128:SER:O	1:J:130:GLN:N	2.35	0.60
1:I:190:ARG:HG3	1:I:190:ARG:HH11	1.65	0.60
1:I:270:ASP:HB3	1:I:272:ASP:OD1	2.01	0.60
1:J:43:LEU:HD11	1:J:101:VAL:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:SER:OG	1:L:118:GLN:HG2	2.02	0.60
1:A:4:LEU:HD11	1:A:10:ILE:HD11	1.84	0.60
1:A:73:THR:CG2	1:A:74:ASP:N	2.65	0.60
1:C:27:GLU:O	1:C:31:THR:HG23	2.02	0.60
1:C:249:ARG:HG3	1:C:249:ARG:NH1	2.12	0.60
1:B:144:ARG:HG3	1:B:144:ARG:NH1	2.14	0.60
1:D:119:VAL:HG13	1:D:120:PRO:HD2	1.84	0.60
1:I:31:THR:HG21	3:I:411:HOH:O	2.01	0.60
1:J:237:GLU:O	1:J:240:LYS:HB3	2.01	0.60
1:M:125:GLY:HA2	1:M:130:GLN:O	2.00	0.60
1:N:268:GLU:H	1:N:268:GLU:CD	2.05	0.60
1:C:203:ASN:HB3	3:C:423:HOH:O	2.00	0.60
1:N:157:VAL:O	1:N:225:THR:HG22	2.01	0.60
1:B:128:SER:HB3	1:B:164:ARG:CG	2.22	0.60
1:E:73:THR:HG22	1:E:74:ASP:N	2.16	0.60
1:J:157:VAL:O	1:J:225:THR:HG22	2.02	0.60
1:B:125:GLY:HA2	1:B:130:GLN:O	2.00	0.59
1:D:188:GLU:CD	1:D:188:GLU:H	2.05	0.59
1:J:289:ILE:HG22	1:J:293:MET:HE1	1.83	0.59
1:D:29:LEU:HD11	1:D:293:MET:CE	2.31	0.59
1:D:214:ASP:OD2	3:D:401:HOH:O	2.17	0.59
1:I:144:ARG:HH11	1:I:144:ARG:HG3	1.67	0.59
1:M:90:ILE:O	1:M:94:SER:HB2	2.02	0.59
1:A:268:GLU:CD	1:A:268:GLU:H	2.05	0.59
1:D:212:LEU:O	1:D:215:LEU:HB3	2.01	0.59
1:E:270:ASP:HB3	1:E:272:ASP:OD1	2.01	0.59
1:I:180:GLU:OE2	1:I:205:LYS:HD2	2.02	0.59
1:I:249:ARG:HB2	1:I:272:ASP:OD2	2.03	0.59
1:C:297:LYS:O	1:C:301:GLU:HG3	2.03	0.59
1:F:123:ASN:ND2	1:F:125:GLY:N	2.50	0.59
1:K:158:GLY:HA2	1:K:227:ILE:HD11	1.85	0.59
1:L:49:GLU:OE2	1:L:127:GLY:HA2	2.02	0.59
1:N:128:SER:CB	1:N:164:ARG:HG3	2.33	0.59
1:B:73:THR:HG22	1:B:74:ASP:H	1.68	0.59
1:F:4:LEU:HD11	1:F:10:ILE:HD11	1.85	0.59
1:J:270:ASP:HB3	1:J:272:ASP:OD1	2.02	0.59
1:J:287:TYR:O	1:J:291:VAL:HG13	2.02	0.59
1:N:119:VAL:HG13	1:N:120:PRO:HD2	1.85	0.59
1:I:129:ASN:HA	1:I:164:ARG:HD2	1.84	0.59
1:L:31:THR:C	1:L:33:ARG:H	2.04	0.59
1:N:215:LEU:HD22	1:N:219:ILE:CD1	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:SER:HB3	1:A:164:ARG:HG3	1.85	0.59
1:D:229:LYS:H	1:D:229:LYS:HD2	1.67	0.59
1:I:72:MET:HG3	1:K:52:THR:HG21	1.83	0.59
1:I:290:PRO:HA	1:I:293:MET:HE2	1.84	0.59
1:N:29:LEU:HD11	1:N:293:MET:CE	2.32	0.59
1:D:268:GLU:H	1:D:268:GLU:CD	2.06	0.59
1:A:270:ASP:HB3	1:A:272:ASP:OD1	2.03	0.58
1:B:270:ASP:HB3	1:B:272:ASP:OD1	2.03	0.58
1:E:4:LEU:HD11	1:E:10:ILE:HD11	1.84	0.58
1:L:268:GLU:CD	1:L:268:GLU:H	2.06	0.58
1:A:29:LEU:HD11	1:A:293:MET:CE	2.33	0.58
1:D:250:GLU:HG2	1:D:251:TYR:N	2.18	0.58
1:F:287:TYR:O	1:F:291:VAL:HG13	2.02	0.58
1:I:2:LYS:HA	1:I:303:ASN:HD21	1.67	0.58
1:I:104:HIS:HB3	1:I:109:ALA:HB1	1.85	0.58
1:C:228:GLN:HB3	1:C:230:GLU:OE1	2.03	0.58
1:D:104:HIS:HB3	1:D:109:ALA:HB1	1.83	0.58
1:E:268:GLU:CD	1:E:268:GLU:H	2.07	0.58
1:F:289:ILE:HG22	1:F:293:MET:HE1	1.83	0.58
1:A:158:GLY:HA2	1:A:227:ILE:HD11	1.84	0.58
1:C:289:ILE:HG22	1:C:293:MET:HE1	1.86	0.58
1:K:209:LYS:HG2	1:K:214:ASP:HB2	1.84	0.58
1:B:233:PRO:HG3	1:D:106:SER:HB3	1.85	0.58
1:C:153:LYS:HD2	1:C:218:ASP:O	2.03	0.58
1:L:4:LEU:HD11	1:L:10:ILE:HD11	1.85	0.58
1:M:158:GLY:HA2	1:M:227:ILE:HD11	1.85	0.58
1:E:74:ASP:O	1:E:80:VAL:HB	2.03	0.58
1:L:104:HIS:HB3	1:L:109:ALA:HB1	1.86	0.58
1:I:29:LEU:HD11	1:I:293:MET:HE1	1.84	0.58
1:I:94:SER:OG	1:I:118:GLN:HG2	2.03	0.58
1:K:104:HIS:HB3	1:K:109:ALA:HB1	1.86	0.58
1:K:268:GLU:CD	1:K:268:GLU:H	2.07	0.58
1:L:27:GLU:HA	1:L:30:ASN:ND2	2.19	0.58
1:N:94:SER:OG	1:N:118:GLN:HG2	2.04	0.58
1:B:8:LYS:HG2	1:B:171:TYR:CZ	2.38	0.58
1:B:290:PRO:HA	1:B:293:MET:CE	2.34	0.58
1:J:29:LEU:HD11	1:J:293:MET:HE1	1.85	0.58
1:J:187:LYS:HE2	1:J:187:LYS:N	2.16	0.58
1:K:287:TYR:O	1:K:291:VAL:HG13	2.03	0.58
1:K:289:ILE:HG22	1:K:293:MET:HE1	1.84	0.58
1:L:211:SER:HB3	1:L:214:ASP:OD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:TYR:O	1:A:291:VAL:HG13	2.03	0.58
1:N:180:GLU:HB2	1:N:205:LYS:HE3	1.85	0.58
1:B:268:GLU:CD	1:B:268:GLU:H	2.04	0.58
1:C:119:VAL:HG13	1:C:120:PRO:HD2	1.85	0.58
1:N:125:GLY:O	1:N:127:GLY:N	2.30	0.58
1:E:29:LEU:HD11	1:E:293:MET:CE	2.32	0.57
1:J:49:GLU:CD	1:J:105:PRO:HG3	2.24	0.57
1:K:180:GLU:OE2	1:K:205:LYS:HD2	2.04	0.57
1:K:249:ARG:O	1:K:253:GLU:HG3	2.04	0.57
1:D:290:PRO:HA	1:D:293:MET:HE2	1.85	0.57
1:J:29:LEU:HD11	1:J:293:MET:CE	2.34	0.57
1:K:270:ASP:HB3	1:K:272:ASP:OD1	2.03	0.57
1:L:128:SER:CB	1:L:164:ARG:HG3	2.27	0.57
1:B:75:LEU:HD23	1:B:80:VAL:HG12	1.85	0.57
1:I:249:ARG:HH12	1:I:276:LEU:HD21	1.68	0.57
1:K:43:LEU:HD11	1:K:101:VAL:HG23	1.86	0.57
1:M:2:LYS:HA	1:M:303:ASN:HD21	1.68	0.57
1:M:4:LEU:HD11	1:M:10:ILE:HD11	1.85	0.57
1:M:73:THR:CG2	1:M:74:ASP:H	2.16	0.57
1:C:196:ILE:HG23	1:C:206:PHE:CZ	2.39	0.57
1:D:287:TYR:O	1:D:291:VAL:HG13	2.04	0.57
1:F:76:LYS:HE2	1:F:76:LYS:CA	2.30	0.57
1:L:109:ALA:HB3	1:L:126:ASP:OD2	2.04	0.57
1:L:297:LYS:O	1:L:301:GLU:HG3	2.03	0.57
1:N:155:ALA:HB2	1:N:219:ILE:HD13	1.86	0.57
1:C:7:MET:H	1:C:130:GLN:NE2	2.02	0.57
1:C:209:LYS:HG2	1:C:214:ASP:HB3	1.86	0.57
1:E:209:LYS:HG2	1:E:214:ASP:HB2	1.87	0.57
1:K:237:GLU:O	1:K:240:LYS:HB3	2.05	0.57
1:N:289:ILE:HG22	1:N:293:MET:HE1	1.87	0.57
1:C:43:LEU:HD11	1:C:101:VAL:HG23	1.86	0.57
1:I:75:LEU:HA	1:I:80:VAL:HB	1.87	0.57
1:I:119:VAL:HG13	1:I:120:PRO:HD2	1.86	0.57
1:N:73:THR:CG2	1:N:74:ASP:N	2.68	0.57
1:D:2:LYS:HA	1:D:303:ASN:HD21	1.70	0.57
1:I:250:GLU:OE1	1:I:250:GLU:N	2.35	0.57
1:J:297:LYS:O	1:J:301:GLU:HG3	2.03	0.57
1:K:213:ASP:C	1:K:215:LEU:H	2.08	0.57
1:M:268:GLU:CD	1:M:268:GLU:H	2.06	0.57
1:F:248:LYS:O	1:F:252:VAL:HG23	2.05	0.57
1:I:196:ILE:HG23	1:I:206:PHE:CZ	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLU:O	1:J:277:PRO:CG	2.53	0.57
1:D:56:LEU:HD11	1:E:72:MET:HB2	1.87	0.57
1:D:187:LYS:HD3	1:D:210:GLU:OE1	2.05	0.57
1:D:190:ARG:HH11	1:D:190:ARG:HG3	1.70	0.57
1:E:180:GLU:OE2	1:E:205:LYS:HD3	2.04	0.57
1:F:157:VAL:O	1:F:225:THR:HG22	2.03	0.57
1:I:297:LYS:O	1:I:301:GLU:HG3	2.05	0.57
1:J:158:GLY:HA2	1:J:227:ILE:HD11	1.87	0.57
1:K:100:ILE:HB	1:K:121:ILE:HD13	1.86	0.57
1:K:297:LYS:O	1:K:301:GLU:HG3	2.04	0.57
1:M:157:VAL:O	1:M:225:THR:HG22	2.05	0.57
1:N:128:SER:OG	1:N:164:ARG:HG3	2.05	0.57
1:N:297:LYS:O	1:N:301:GLU:HG3	2.05	0.57
1:B:209:LYS:HE2	3:J:413:HOH:O	2.04	0.56
1:C:94:SER:OG	1:C:118:GLN:HG2	2.04	0.56
1:J:104:HIS:HB3	1:J:109:ALA:HB1	1.87	0.56
1:K:31:THR:HG22	1:K:33:ARG:CB	2.35	0.56
1:M:75:LEU:O	1:M:81:ALA:HB2	2.05	0.56
1:A:104:HIS:HB3	1:A:109:ALA:HB1	1.87	0.56
1:B:157:VAL:O	1:B:225:THR:HG22	2.05	0.56
1:D:75:LEU:HD23	1:D:80:VAL:CG1	2.35	0.56
1:F:49:GLU:CD	1:F:127:GLY:HA2	2.24	0.56
1:K:94:SER:OG	1:K:118:GLN:HG2	2.05	0.56
1:L:100:ILE:HB	1:L:121:ILE:HD13	1.87	0.56
1:A:128:SER:CB	1:A:164:ARG:HG3	2.36	0.56
1:A:289:ILE:HG22	1:A:293:MET:HE1	1.86	0.56
1:B:53:ARG:HG3	1:B:53:ARG:HH11	1.71	0.56
1:C:100:ILE:HB	1:C:121:ILE:HD13	1.87	0.56
1:C:268:GLU:CD	1:C:268:GLU:H	2.08	0.56
1:D:157:VAL:O	1:D:225:THR:HG22	2.06	0.56
1:F:215:LEU:HD22	1:F:219:ILE:HD11	1.85	0.56
1:L:43:LEU:HD11	1:L:101:VAL:HG23	1.87	0.56
1:N:287:TYR:O	1:N:291:VAL:HG13	2.04	0.56
1:A:196:ILE:HG23	1:A:206:PHE:CZ	2.41	0.56
1:E:43:LEU:HD11	1:E:101:VAL:HG23	1.86	0.56
1:F:155:ALA:HB2	1:F:219:ILE:HD13	1.88	0.56
1:J:125:GLY:C	1:J:127:GLY:N	2.57	0.56
1:K:125:GLY:HA2	1:K:130:GLN:O	2.05	0.56
1:M:77:SER:O	1:M:79:SER:N	2.39	0.56
1:N:4:LEU:HD11	1:N:10:ILE:HD11	1.87	0.56
1:A:94:SER:OG	1:A:118:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:SER:CB	1:E:103:ARG:HH12	2.13	0.56
1:E:56:LEU:HD11	1:F:72:MET:HB2	1.86	0.56
1:K:180:GLU:HG3	1:K:205:LYS:CG	2.33	0.56
1:L:193:LYS:O	1:L:197:GLU:HG2	2.05	0.56
1:B:297:LYS:O	1:B:301:GLU:HG3	2.05	0.56
1:M:104:HIS:HB3	1:M:109:ALA:HB1	1.87	0.56
1:B:104:HIS:HB3	1:B:109:ALA:HB1	1.88	0.56
1:C:248:LYS:O	1:C:252:VAL:HG23	2.05	0.56
1:I:128:SER:O	1:I:130:GLN:N	2.34	0.56
1:K:4:LEU:HD11	1:K:10:ILE:HD11	1.87	0.56
1:L:217:ASP:O	1:L:256:LYS:HE2	2.05	0.56
1:L:289:ILE:HG22	1:L:293:MET:HE1	1.88	0.56
1:M:290:PRO:HA	1:M:293:MET:HE2	1.86	0.56
1:A:125:GLY:HA2	1:A:130:GLN:O	2.06	0.56
1:F:305:GLY:O	1:F:306:GLU:HB2	2.06	0.56
1:K:6:SER:HA	1:K:130:GLN:HG2	1.88	0.56
1:M:248:LYS:O	1:M:252:VAL:HG23	2.06	0.56
1:N:230:GLU:H	1:N:230:GLU:CD	2.08	0.56
1:D:297:LYS:O	1:D:301:GLU:HG3	2.06	0.56
1:I:125:GLY:C	1:I:127:GLY:H	2.09	0.56
1:L:2:LYS:HA	1:L:303:ASN:HD21	1.70	0.56
1:N:108:GLY:HA2	3:N:425:HOH:O	2.06	0.56
1:C:2:LYS:HA	1:C:303:ASN:HD21	1.71	0.56
1:C:53:ARG:NH1	1:C:53:ARG:HG3	2.21	0.56
1:D:4:LEU:HD11	1:D:10:ILE:HD11	1.88	0.56
1:D:48:TYR:HB3	1:D:76:LYS:CG	2.31	0.56
1:D:217:ASP:HB2	1:D:255:LYS:HD3	1.88	0.56
1:L:190:ARG:HG3	1:L:190:ARG:HH11	1.71	0.56
1:M:297:LYS:O	1:M:301:GLU:HG3	2.06	0.56
1:E:104:HIS:HB3	1:E:109:ALA:HB1	1.87	0.55
1:L:213:ASP:C	1:L:215:LEU:H	2.09	0.55
1:N:180:GLU:HG3	1:N:205:LYS:CG	2.35	0.55
1:A:27:GLU:HG2	1:A:28:LEU:N	2.21	0.55
1:C:4:LEU:HD11	1:C:10:ILE:HD11	1.88	0.55
1:C:129:ASN:HD22	1:C:130:GLN:H	1.55	0.55
1:D:10:ILE:HG23	1:D:14:GLU:HB3	1.88	0.55
1:D:213:ASP:O	1:D:215:LEU:N	2.33	0.55
1:D:213:ASP:C	1:D:215:LEU:H	2.10	0.55
1:E:290:PRO:HA	1:E:293:MET:CE	2.36	0.55
1:I:187:LYS:HD2	1:I:188:GLU:OE1	2.05	0.55
1:I:215:LEU:HB3	1:I:219:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:31:THR:HG22	1:K:33:ARG:H	1.72	0.55
1:L:128:SER:O	1:L:129:ASN:HB3	2.06	0.55
1:C:215:LEU:HD13	1:C:219:ILE:CD1	2.37	0.55
1:D:3:HIS:HB2	3:D:451:HOH:O	2.07	0.55
1:D:144:ARG:HG2	1:D:144:ARG:HH11	1.72	0.55
1:D:248:LYS:O	1:D:252:VAL:HG23	2.07	0.55
1:F:94:SER:OG	1:F:118:GLN:HG2	2.06	0.55
1:I:157:VAL:O	1:I:225:THR:HG22	2.06	0.55
1:K:196:ILE:HG23	1:K:206:PHE:CZ	2.42	0.55
1:L:31:THR:HG22	1:L:33:ARG:N	2.17	0.55
1:B:4:LEU:HD11	1:B:10:ILE:HD11	1.88	0.55
1:B:51:SER:CB	1:B:103:ARG:HH12	2.17	0.55
1:J:100:ILE:HB	1:J:121:ILE:HD13	1.88	0.55
1:N:4:LEU:CD1	1:N:10:ILE:HD11	2.36	0.55
1:D:125:GLY:HA2	1:D:130:GLN:O	2.07	0.55
1:I:237:GLU:O	1:I:240:LYS:HB3	2.06	0.55
1:L:196:ILE:HG23	1:L:206:PHE:CZ	2.42	0.55
1:L:248:LYS:O	1:L:252:VAL:HG23	2.06	0.55
1:N:100:ILE:HB	1:N:121:ILE:HD13	1.89	0.55
1:A:249:ARG:HB2	1:A:272:ASP:OD2	2.06	0.55
1:E:289:ILE:HG22	1:E:293:MET:HE1	1.87	0.55
1:F:216:ASP:OD1	1:F:218:ASP:HB2	2.07	0.55
1:I:216:ASP:O	1:I:219:ILE:HG12	2.07	0.55
1:N:51:SER:CB	1:N:103:ARG:HH12	2.18	0.55
1:B:90:ILE:O	1:B:94:SER:HB2	2.07	0.55
1:C:104:HIS:HB3	1:C:109:ALA:HB1	1.87	0.55
1:D:305:GLY:O	1:D:306:GLU:CB	2.55	0.55
1:F:43:LEU:HD11	1:F:101:VAL:HG23	1.88	0.55
1:I:48:TYR:HB3	1:I:76:LYS:HG2	1.89	0.55
1:J:187:LYS:HA	1:J:190:ARG:NH2	2.21	0.55
1:L:53:ARG:HD2	3:L:406:HOH:O	2.06	0.55
1:B:119:VAL:HG13	1:B:120:PRO:HD2	1.88	0.54
1:E:4:LEU:CD1	1:E:10:ILE:HD11	2.36	0.54
1:E:100:ILE:HB	1:E:121:ILE:HD13	1.88	0.54
1:E:306:GLU:OE1	1:E:306:GLU:N	2.41	0.54
1:F:28:LEU:HA	1:F:31:THR:OG1	2.07	0.54
1:L:31:THR:HG22	1:L:33:ARG:HB2	1.88	0.54
1:M:77:SER:C	1:M:79:SER:H	2.11	0.54
1:F:104:HIS:HB3	1:F:109:ALA:HB1	1.89	0.54
1:F:119:VAL:HG13	1:F:120:PRO:HD2	1.87	0.54
1:F:128:SER:O	1:F:130:GLN:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:268:GLU:CD	1:J:268:GLU:H	2.10	0.54
1:I:158:GLY:HA2	1:I:227:ILE:HD11	1.90	0.54
1:M:193:LYS:HG3	3:M:423:HOH:O	2.08	0.54
1:N:128:SER:O	1:N:130:GLN:N	2.40	0.54
1:N:158:GLY:HA2	1:N:227:ILE:HD11	1.89	0.54
1:E:209:LYS:CG	1:E:214:ASP:HB2	2.38	0.54
1:I:129:ASN:H	1:I:164:ARG:HG3	1.72	0.54
1:M:128:SER:O	1:M:129:ASN:HB3	2.07	0.54
1:A:75:LEU:HD23	1:A:80:VAL:O	2.07	0.54
1:C:209:LYS:CG	1:C:214:ASP:HB3	2.37	0.54
1:D:4:LEU:CD1	1:D:10:ILE:HD11	2.38	0.54
1:F:287:TYR:O	1:F:290:PRO:HD2	2.08	0.54
1:I:4:LEU:CD1	1:I:10:ILE:HD11	2.37	0.54
1:C:72:MET:HG2	1:C:75:LEU:HD11	1.88	0.54
1:D:43:LEU:HD11	1:D:101:VAL:HG23	1.90	0.54
1:F:99:ILE:HG13	1:F:120:PRO:HB2	1.89	0.54
1:L:125:GLY:O	1:L:127:GLY:N	2.37	0.54
1:D:33:ARG:HH11	1:D:33:ARG:CB	2.04	0.54
1:D:51:SER:CB	1:D:103:ARG:HH12	2.15	0.54
1:J:45:THR:HG23	1:J:47:PHE:CE1	2.43	0.54
1:M:129:ASN:HA	1:M:164:ARG:HD2	1.90	0.54
1:D:290:PRO:HA	1:D:293:MET:CE	2.37	0.54
1:F:129:ASN:O	1:F:130:GLN:HB2	2.07	0.54
1:K:4:LEU:CD1	1:K:10:ILE:HD11	2.38	0.54
1:L:4:LEU:CD1	1:L:10:ILE:HD11	2.38	0.54
1:L:290:PRO:HA	1:L:293:MET:CE	2.37	0.54
1:B:53:ARG:NH1	1:B:53:ARG:HG3	2.22	0.54
1:D:196:ILE:HG23	1:D:206:PHE:CZ	2.44	0.54
1:K:46:VAL:HG13	1:K:75:LEU:HD11	1.89	0.54
1:N:72:MET:SD	1:N:75:LEU:HD21	2.48	0.54
1:F:126:ASP:C	1:F:128:SER:H	2.10	0.53
1:I:229:LYS:HG2	1:I:238:TYR:CE2	2.43	0.53
1:J:48:TYR:CZ	1:J:75:LEU:HD22	2.42	0.53
1:K:128:SER:O	1:K:129:ASN:CG	2.46	0.53
1:B:191:LEU:HD12	1:B:192:PRO:HD2	1.89	0.53
1:I:43:LEU:HD11	1:I:101:VAL:HG23	1.89	0.53
1:I:100:ILE:HB	1:I:121:ILE:HD13	1.88	0.53
1:I:216:ASP:HB3	1:I:218:ASP:OD1	2.08	0.53
1:L:157:VAL:O	1:L:225:THR:HG22	2.08	0.53
1:M:4:LEU:CD1	1:M:10:ILE:HD11	2.38	0.53
1:M:78:SER:HA	1:M:81:ALA:HB3	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ASP:C	1:D:215:LEU:N	2.58	0.53
1:F:73:THR:HG22	1:F:74:ASP:N	2.24	0.53
1:F:289:ILE:HG22	1:F:293:MET:CE	2.38	0.53
1:I:74:ASP:HB2	3:I:418:HOH:O	2.08	0.53
1:I:191:LEU:HD12	1:I:192:PRO:HD2	1.90	0.53
1:L:7:MET:HB2	1:L:130:GLN:NE2	2.22	0.53
1:N:75:LEU:HA	1:N:80:VAL:CG1	2.37	0.53
1:I:23:ARG:HA	1:I:140:TYR:OH	2.08	0.53
1:J:4:LEU:HD11	1:J:10:ILE:HD11	1.89	0.53
1:D:289:ILE:HG22	1:D:293:MET:CE	2.39	0.53
1:E:196:ILE:HG23	1:E:206:PHE:CZ	2.43	0.53
1:J:196:ILE:HG23	1:J:206:PHE:CZ	2.43	0.53
1:N:104:HIS:HB3	1:N:109:ALA:HB1	1.89	0.53
1:E:297:LYS:O	1:E:301:GLU:HG3	2.09	0.53
1:J:75:LEU:C	1:J:77:SER:H	2.11	0.53
1:L:75:LEU:O	1:L:81:ALA:HB2	2.09	0.53
1:M:51:SER:CB	1:M:103:ARG:HH12	2.14	0.53
1:N:249:ARG:NH1	1:N:276:LEU:HD21	2.24	0.53
1:A:72:MET:HB2	1:C:56:LEU:HD11	1.91	0.53
1:C:53:ARG:HG3	1:C:53:ARG:HH11	1.73	0.53
1:L:28:LEU:O	1:L:31:THR:HB	2.09	0.53
1:L:45:THR:HG23	1:L:47:PHE:CE1	2.44	0.53
1:M:73:THR:CG2	1:M:74:ASP:N	2.71	0.53
1:N:209:LYS:HG2	1:N:214:ASP:HB2	1.89	0.53
1:N:290:PRO:HA	1:N:293:MET:CE	2.38	0.53
1:A:289:ILE:HG22	1:A:293:MET:CE	2.38	0.53
1:I:229:LYS:HG2	1:I:238:TYR:CZ	2.44	0.53
1:J:248:LYS:O	1:J:252:VAL:HG23	2.08	0.53
1:A:119:VAL:HG13	1:A:120:PRO:CD	2.39	0.53
1:A:100:ILE:HB	1:A:121:ILE:HD13	1.91	0.53
1:B:271:TYR:CZ	1:F:235:PRO:HB3	2.44	0.53
1:C:4:LEU:CD1	1:C:10:ILE:HD11	2.39	0.53
1:C:7:MET:HB2	1:C:130:GLN:NE2	2.24	0.53
1:F:4:LEU:CD1	1:F:10:ILE:HD11	2.38	0.53
1:I:72:MET:HG2	1:I:75:LEU:HD11	1.91	0.53
1:L:75:LEU:HA	1:L:80:VAL:HB	1.91	0.53
1:M:100:ILE:HB	1:M:121:ILE:HD13	1.90	0.53
1:N:196:ILE:HG23	1:N:206:PHE:CZ	2.43	0.53
1:D:45:THR:HG23	1:D:47:PHE:CE1	2.44	0.52
1:E:157:VAL:O	1:E:225:THR:HG22	2.08	0.52
1:E:158:GLY:HA2	1:E:227:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:THR:HG23	1:F:47:PHE:CE1	2.44	0.52
1:J:75:LEU:HG	1:J:80:VAL:HG12	1.90	0.52
1:K:216:ASP:O	1:K:219:ILE:HD12	2.09	0.52
1:L:73:THR:CG2	1:L:74:ASP:N	2.63	0.52
1:L:158:GLY:HA2	1:L:227:ILE:HD11	1.90	0.52
1:M:45:THR:HG23	1:M:47:PHE:CE1	2.44	0.52
1:M:51:SER:CB	1:M:103:ARG:NH1	2.72	0.52
1:A:43:LEU:HD11	1:A:101:VAL:HG23	1.90	0.52
1:B:235:PRO:HB2	1:F:271:TYR:CD2	2.44	0.52
1:C:27:GLU:HA	1:C:30:ASN:HD22	1.74	0.52
1:D:8:LYS:HG2	1:D:171:TYR:CZ	2.45	0.52
1:E:45:THR:HG23	1:E:47:PHE:CE1	2.44	0.52
1:K:157:VAL:O	1:K:225:THR:HG22	2.09	0.52
1:K:215:LEU:HB3	1:K:219:ILE:CD1	2.39	0.52
1:N:303:ASN:O	1:N:304:GLU:HB3	2.09	0.52
1:A:144:ARG:HG2	1:A:287:TYR:OH	2.09	0.52
1:B:148:ARG:NH2	3:B:415:HOH:O	2.42	0.52
1:D:126:ASP:CB	1:D:129:ASN:HD21	2.19	0.52
1:I:190:ARG:HB2	1:I:190:ARG:CZ	2.39	0.52
1:C:125:GLY:HA2	1:C:130:GLN:O	2.09	0.52
1:J:289:ILE:HG22	1:J:293:MET:CE	2.39	0.52
1:A:52:THR:HG21	1:B:72:MET:HG3	1.91	0.52
1:C:126:ASP:HB2	1:C:129:ASN:ND2	2.24	0.52
1:F:291:VAL:O	1:F:295:ILE:HG13	2.10	0.52
1:I:290:PRO:HA	1:I:293:MET:CE	2.39	0.52
1:A:290:PRO:HA	1:A:293:MET:CE	2.40	0.52
1:B:43:LEU:HD11	1:B:101:VAL:HG23	1.92	0.52
1:F:158:GLY:O	1:F:160:LEU:HG	2.09	0.52
1:J:28:LEU:O	1:J:31:THR:CB	2.57	0.52
1:F:80:VAL:O	1:F:81:ALA:CB	2.58	0.52
1:F:297:LYS:O	1:F:301:GLU:HG3	2.10	0.52
1:I:45:THR:HG23	1:I:47:PHE:CE1	2.45	0.52
1:N:45:THR:HG23	1:N:47:PHE:CE1	2.44	0.52
1:A:14:GLU:HB2	3:A:417:HOH:O	2.09	0.52
1:C:73:THR:HG22	1:C:74:ASP:N	2.25	0.52
1:D:48:TYR:CZ	1:D:75:LEU:HD13	2.45	0.52
1:I:53:ARG:HD2	3:I:401:HOH:O	2.10	0.52
1:C:287:TYR:O	1:C:290:PRO:HD2	2.10	0.52
1:D:128:SER:O	1:D:130:GLN:N	2.39	0.52
1:K:263:LEU:HB3	1:K:264:PRO:HA	1.92	0.52
1:M:240:LYS:HD3	1:M:240:LYS:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:23:ARG:HA	1:N:140:TYR:OH	2.10	0.52
1:B:158:GLY:HA2	1:B:227:ILE:HD11	1.92	0.52
1:B:196:ILE:HG23	1:B:206:PHE:CZ	2.45	0.52
1:E:76:LYS:HA	1:E:76:LYS:CE	2.34	0.52
1:J:140:TYR:CE2	1:J:144:ARG:HG3	2.45	0.52
1:L:228:GLN:HB3	1:L:230:GLU:OE1	2.10	0.52
1:N:216:ASP:HB2	1:N:218:ASP:OD1	2.10	0.52
1:B:33:ARG:O	1:B:34:PRO:C	2.46	0.51
1:E:51:SER:CB	1:E:103:ARG:NH1	2.73	0.51
1:F:48:TYR:CD2	1:F:75:LEU:HB2	2.44	0.51
1:F:51:SER:CB	1:F:103:ARG:NH1	2.72	0.51
1:J:128:SER:C	1:J:130:GLN:H	2.13	0.51
1:L:75:LEU:HD23	1:L:80:VAL:O	2.09	0.51
1:A:4:LEU:CD1	1:A:10:ILE:HD11	2.39	0.51
1:A:31:THR:O	1:A:32:LYS:HB2	2.10	0.51
1:M:215:LEU:HD22	1:M:219:ILE:CD1	2.39	0.51
1:M:289:ILE:HG22	1:M:293:MET:CE	2.40	0.51
1:N:248:LYS:O	1:N:252:VAL:HG23	2.11	0.51
1:B:76:LYS:HA	1:B:76:LYS:HZ3	1.75	0.51
1:B:289:ILE:HG22	1:B:293:MET:CE	2.41	0.51
1:A:233:PRO:HG3	1:E:106:SER:HB3	1.91	0.51
1:C:158:GLY:O	1:C:160:LEU:HG	2.10	0.51
1:D:48:TYR:HA	1:D:75:LEU:HB2	1.92	0.51
1:E:158:GLY:O	1:E:160:LEU:HG	2.10	0.51
1:J:73:THR:HG22	1:J:74:ASP:H	1.75	0.51
1:K:51:SER:CB	1:K:103:ARG:HH12	2.17	0.51
1:K:112:LEU:HD22	1:N:233:PRO:HB2	1.92	0.51
1:N:289:ILE:HG22	1:N:293:MET:CE	2.41	0.51
1:A:297:LYS:O	1:A:301:GLU:HG3	2.10	0.51
1:B:27:GLU:O	1:B:31:THR:HG23	2.10	0.51
1:K:51:SER:CB	1:K:103:ARG:NH1	2.74	0.51
1:L:56:LEU:HD11	1:M:72:MET:HB2	1.91	0.51
1:D:191:LEU:HD12	1:D:192:PRO:HD2	1.92	0.51
1:F:290:PRO:HA	1:F:293:MET:CE	2.41	0.51
1:M:289:ILE:HG22	1:M:293:MET:HE1	1.91	0.51
1:A:7:MET:H	1:A:130:GLN:NE2	2.08	0.51
1:B:234:ASP:CA	1:D:112:LEU:HD21	2.40	0.51
1:C:123:ASN:ND2	1:C:125:GLY:H	2.09	0.51
1:C:157:VAL:O	1:C:225:THR:HG22	2.10	0.51
1:C:249:ARG:NH1	1:C:276:LEU:HD21	2.20	0.51
1:E:53:ARG:NH2	1:F:82:LYS:HB2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:128:SER:O	1:L:129:ASN:CB	2.59	0.51
1:L:187:LYS:HA	1:L:190:ARG:NH2	2.26	0.51
1:M:209:LYS:CG	1:M:214:ASP:CB	2.89	0.51
1:N:30:ASN:O	1:N:32:LYS:HG3	2.11	0.51
1:A:14:GLU:O	1:A:18:ILE:HG13	2.11	0.51
1:C:278:GLN:CD	1:C:278:GLN:H	2.14	0.51
1:D:92:VAL:HG13	1:F:285:SER:OG	2.10	0.51
1:D:289:ILE:HG22	1:D:293:MET:HE1	1.93	0.51
1:M:291:VAL:O	1:M:295:ILE:HG13	2.11	0.51
1:A:49:GLU:HG3	1:A:49:GLU:O	2.11	0.51
1:D:51:SER:CB	1:D:103:ARG:NH1	2.72	0.51
1:L:180:GLU:HA	1:L:205:LYS:HG3	1.92	0.51
1:N:229:LYS:HG2	1:N:238:TYR:CZ	2.46	0.51
1:J:191:LEU:HD12	1:J:192:PRO:HD2	1.92	0.50
1:J:217:ASP:O	1:J:256:LYS:HE2	2.11	0.50
1:N:219:ILE:O	1:N:257:PHE:HB3	2.10	0.50
1:B:48:TYR:CZ	1:B:75:LEU:HD13	2.47	0.50
1:C:125:GLY:C	1:C:127:GLY:N	2.64	0.50
1:J:290:PRO:HA	1:J:293:MET:CE	2.41	0.50
1:M:290:PRO:HA	1:M:293:MET:CE	2.41	0.50
1:A:148:ARG:NH1	3:A:432:HOH:O	2.44	0.50
1:J:158:GLY:O	1:J:160:LEU:HG	2.11	0.50
1:K:215:LEU:HB3	1:K:219:ILE:HD11	1.93	0.50
1:K:229:LYS:HG2	1:K:238:TYR:CZ	2.46	0.50
1:L:287:TYR:O	1:L:290:PRO:HD2	2.11	0.50
1:A:278:GLN:CD	1:A:278:GLN:H	2.15	0.50
1:B:158:GLY:O	1:B:160:LEU:HG	2.11	0.50
1:E:75:LEU:HD23	1:E:80:VAL:O	2.12	0.50
1:I:51:SER:CB	1:I:103:ARG:HH12	2.21	0.50
1:K:272:ASP:HB3	3:K:427:HOH:O	2.12	0.50
1:N:73:THR:O	1:N:80:VAL:HG11	2.11	0.50
1:B:265:ARG:HD2	1:B:265:ARG:C	2.32	0.50
1:B:287:TYR:O	1:B:290:PRO:HD2	2.12	0.50
1:B:289:ILE:HG22	1:B:293:MET:HE1	1.93	0.50
1:D:23:ARG:NE	1:D:144:ARG:NH1	2.60	0.50
1:E:53:ARG:HH22	1:F:82:LYS:CB	2.24	0.50
1:F:31:THR:HG23	1:F:33:ARG:NH2	2.26	0.50
1:F:75:LEU:HB3	1:F:81:ALA:HB2	1.92	0.50
1:F:191:LEU:HD12	1:F:192:PRO:HD2	1.94	0.50
1:J:180:GLU:HG3	1:J:205:LYS:HD2	1.92	0.50
1:L:49:GLU:OE2	1:L:127:GLY:CA	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:HG23	1:B:47:PHE:CE1	2.46	0.50
1:C:180:GLU:HG3	1:C:205:LYS:HG3	1.93	0.50
1:E:216:ASP:HB2	1:E:218:ASP:OD1	2.11	0.50
1:M:196:ILE:HG23	1:M:206:PHE:CZ	2.47	0.50
1:C:290:PRO:HA	1:C:293:MET:CE	2.40	0.50
1:E:75:LEU:C	1:E:77:SER:H	2.14	0.50
1:I:74:ASP:C	1:I:76:LYS:H	2.14	0.50
1:M:23:ARG:HA	1:M:140:TYR:OH	2.12	0.50
1:I:125:GLY:HA2	1:I:130:GLN:O	2.11	0.50
1:J:4:LEU:CD1	1:J:10:ILE:HD11	2.41	0.50
1:B:234:ASP:HA	1:D:112:LEU:HD21	1.93	0.50
1:D:140:TYR:CE2	1:D:144:ARG:HD3	2.47	0.50
1:E:228:GLN:HB3	1:E:230:GLU:HG2	1.94	0.50
1:I:209:LYS:HG2	1:I:214:ASP:CB	2.40	0.50
1:B:278:GLN:CD	1:B:278:GLN:H	2.15	0.49
1:D:144:ARG:HG2	1:D:144:ARG:NH1	2.27	0.49
3:D:420:HOH:O	1:F:32:LYS:HD2	2.12	0.49
1:K:191:LEU:HD12	1:K:192:PRO:HD2	1.94	0.49
1:K:290:PRO:HA	1:K:293:MET:CE	2.40	0.49
1:L:158:GLY:O	1:L:160:LEU:HG	2.12	0.49
1:N:77:SER:O	1:N:81:ALA:HB3	2.11	0.49
1:A:27:GLU:CG	1:A:28:LEU:N	2.74	0.49
1:B:161:LYS:HA	1:B:192:PRO:HD3	1.95	0.49
1:F:196:ILE:HG23	1:F:206:PHE:CZ	2.47	0.49
1:J:87:ILE:HD12	1:L:235:PRO:CD	2.35	0.49
1:A:106:SER:HB3	1:E:233:PRO:HG3	1.94	0.49
1:C:76:LYS:HA	1:C:76:LYS:CE	2.24	0.49
1:E:73:THR:HG22	1:E:74:ASP:H	1.76	0.49
1:I:53:ARG:NH1	3:I:401:HOH:O	2.40	0.49
1:I:289:ILE:HG22	1:I:293:MET:CE	2.42	0.49
1:I:289:ILE:HG22	1:I:293:MET:HE1	1.94	0.49
1:L:75:LEU:CD2	1:L:80:VAL:O	2.61	0.49
1:A:74:ASP:O	1:A:80:VAL:HB	2.12	0.49
1:D:48:TYR:O	1:D:76:LYS:HB2	2.12	0.49
1:I:126:ASP:HB2	1:I:129:ASN:ND2	2.21	0.49
1:A:51:SER:CB	1:A:103:ARG:NH1	2.75	0.49
1:A:230:GLU:N	1:A:230:GLU:OE2	2.46	0.49
1:A:299:LEU:O	1:A:303:ASN:ND2	2.46	0.49
1:I:209:LYS:CG	1:I:214:ASP:CB	2.91	0.49
1:K:217:ASP:O	1:K:219:ILE:N	2.46	0.49
1:M:191:LEU:HD12	1:M:192:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:209:LYS:HG2	1:N:214:ASP:CB	2.42	0.49
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.77	0.49
1:I:287:TYR:O	1:I:290:PRO:HD2	2.11	0.49
1:L:49:GLU:OE1	1:L:105:PRO:HG3	2.13	0.49
1:L:180:GLU:N	1:L:205:LYS:HE3	2.28	0.49
1:N:180:GLU:HG3	1:N:205:LYS:CD	2.43	0.49
1:D:278:GLN:H	1:D:278:GLN:CD	2.15	0.49
1:I:76:LYS:HA	1:I:76:LYS:CE	2.38	0.49
1:C:77:SER:C	1:C:79:SER:N	2.66	0.49
1:D:217:ASP:O	1:D:218:ASP:HB3	2.12	0.49
1:F:53:ARG:HG3	1:F:53:ARG:HH11	1.77	0.49
1:I:248:LYS:O	1:I:252:VAL:HG23	2.13	0.49
1:L:51:SER:CB	1:L:103:ARG:HH12	2.21	0.49
1:L:187:LYS:CD	1:L:190:ARG:HH21	2.24	0.49
1:A:10:ILE:HG23	1:A:14:GLU:HB3	1.94	0.49
1:A:27:GLU:HG2	1:A:28:LEU:H	1.78	0.49
1:B:75:LEU:HD23	1:B:80:VAL:CG1	2.43	0.49
1:B:87:ILE:HG22	1:B:91:ARG:HH21	1.76	0.49
1:D:137:LEU:HD12	1:D:137:LEU:C	2.33	0.49
1:D:187:LYS:CD	1:D:190:ARG:NH2	2.70	0.49
1:J:119:VAL:HG13	1:J:120:PRO:CD	2.42	0.49
1:J:188:GLU:H	1:J:188:GLU:CD	2.15	0.49
1:L:191:LEU:HD12	1:L:192:PRO:HD2	1.95	0.49
1:B:230:GLU:OE2	1:B:230:GLU:N	2.46	0.49
1:B:235:PRO:HB3	1:F:271:TYR:CZ	2.47	0.49
1:E:125:GLY:C	1:E:127:GLY:N	2.64	0.49
1:E:131:HIS:HE1	3:E:455:HOH:O	1.94	0.49
1:J:56:LEU:HD11	1:K:72:MET:HB2	1.95	0.49
1:N:217:ASP:OD2	1:N:255:LYS:HA	2.13	0.49
1:D:46:VAL:HG13	1:D:75:LEU:HD11	1.94	0.48
1:D:217:ASP:HB2	1:D:255:LYS:HD2	1.95	0.48
1:K:73:THR:CG2	1:K:74:ASP:H	2.26	0.48
1:L:263:LEU:HB3	1:L:264:PRO:HA	1.95	0.48
1:E:263:LEU:HB3	1:E:264:PRO:HA	1.95	0.48
1:J:215:LEU:HB3	1:J:219:ILE:HD11	1.95	0.48
1:J:287:TYR:O	1:J:290:PRO:HD2	2.13	0.48
1:L:80:VAL:HG12	1:L:80:VAL:O	2.14	0.48
1:M:49:GLU:CD	1:M:127:GLY:HA2	2.33	0.48
1:B:4:LEU:CD1	1:B:10:ILE:HD11	2.43	0.48
1:B:129:ASN:O	1:B:130:GLN:NE2	2.46	0.48
1:C:158:GLY:HA2	1:C:227:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ASN:ND2	1:D:125:GLY:H	2.11	0.48
1:K:75:LEU:HA	1:K:80:VAL:HB	1.95	0.48
1:K:248:LYS:O	1:K:252:VAL:HG23	2.13	0.48
1:N:47:PHE:C	1:N:75:LEU:HD12	2.34	0.48
1:N:180:GLU:CB	1:N:205:LYS:HE3	2.43	0.48
1:A:158:GLY:O	1:A:160:LEU:HG	2.14	0.48
1:B:106:SER:CB	1:D:233:PRO:HG3	2.37	0.48
1:B:155:ALA:CB	1:B:219:ILE:HD13	2.42	0.48
1:D:219:ILE:O	1:D:257:PHE:HB3	2.13	0.48
1:D:263:LEU:HB3	1:D:264:PRO:HA	1.95	0.48
1:E:248:LYS:O	1:E:252:VAL:HG23	2.14	0.48
1:I:272:ASP:HA	3:I:414:HOH:O	2.12	0.48
1:A:190:ARG:HG3	1:A:190:ARG:NH1	2.27	0.48
1:B:73:THR:CG2	1:B:74:ASP:N	2.75	0.48
1:C:112:LEU:CD2	1:F:233:PRO:HB2	2.44	0.48
1:C:180:GLU:OE2	1:C:205:LYS:HD2	2.13	0.48
1:D:31:THR:O	1:D:33:ARG:N	2.47	0.48
1:E:99:ILE:HG13	1:E:120:PRO:HB2	1.94	0.48
1:I:77:SER:C	1:I:79:SER:H	2.16	0.48
1:I:137:LEU:HD12	1:I:137:LEU:C	2.34	0.48
1:I:180:GLU:HG3	1:I:205:LYS:HG3	1.95	0.48
1:K:153:LYS:HD2	1:K:218:ASP:O	2.13	0.48
1:M:27:GLU:HA	1:M:30:ASN:ND2	2.29	0.48
1:N:47:PHE:O	1:N:75:LEU:HD12	2.13	0.48
1:N:158:GLY:O	1:N:160:LEU:HG	2.14	0.48
1:B:14:GLU:O	1:B:18:ILE:HG13	2.14	0.48
1:B:51:SER:CB	1:B:103:ARG:NH1	2.74	0.48
1:E:23:ARG:NH2	1:E:27:GLU:OE1	2.46	0.48
1:E:119:VAL:HG13	1:E:120:PRO:CD	2.43	0.48
1:I:14:GLU:O	1:I:18:ILE:HG13	2.13	0.48
1:L:23:ARG:HA	1:L:140:TYR:OH	2.14	0.48
1:L:72:MET:HG2	1:L:75:LEU:HD21	1.95	0.48
1:L:289:ILE:HG22	1:L:293:MET:CE	2.42	0.48
1:A:52:THR:HG22	1:B:72:MET:HE3	1.96	0.48
1:D:287:TYR:O	1:D:290:PRO:HD2	2.13	0.48
1:J:233:PRO:HB2	1:L:112:LEU:HD22	1.95	0.48
1:K:45:THR:HG23	1:K:47:PHE:CE1	2.49	0.48
1:K:75:LEU:HD23	1:K:80:VAL:HG12	1.95	0.48
1:M:27:GLU:HA	1:M:30:ASN:HD22	1.79	0.48
1:C:217:ASP:OD2	1:C:255:LYS:HA	2.14	0.48
1:C:289:ILE:HG22	1:C:293:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ILE:HA	1:F:119:VAL:HG13	1.94	0.48
1:K:186:PRO:HG3	1:K:245:TYR:CE1	2.48	0.48
1:D:45:THR:O	1:D:45:THR:HG22	2.13	0.48
1:E:213:ASP:C	1:E:215:LEU:H	2.16	0.48
1:K:73:THR:CG2	1:K:74:ASP:N	2.76	0.48
1:L:278:GLN:H	1:L:278:GLN:CD	2.17	0.48
1:N:217:ASP:OD2	1:N:255:LYS:HD3	2.14	0.48
1:C:7:MET:HB2	1:C:130:GLN:HE22	1.79	0.47
1:C:137:LEU:C	1:C:137:LEU:HD12	2.34	0.47
1:F:249:ARG:NH1	1:F:276:LEU:HD21	2.29	0.47
1:J:73:THR:CG2	1:J:74:ASP:N	2.76	0.47
1:J:216:ASP:O	1:J:218:ASP:OD1	2.32	0.47
1:K:287:TYR:O	1:K:290:PRO:HD2	2.13	0.47
1:L:137:LEU:HD12	1:L:137:LEU:C	2.34	0.47
1:A:140:TYR:CE2	1:A:144:ARG:HD3	2.49	0.47
1:A:175:LEU:HB3	3:A:419:HOH:O	2.13	0.47
1:B:123:ASN:HD22	1:B:124:ALA:N	2.12	0.47
1:C:51:SER:CB	1:C:103:ARG:NH1	2.76	0.47
1:L:235:PRO:O	1:L:239:GLU:HG2	2.14	0.47
1:N:48:TYR:HA	1:N:75:LEU:HB2	1.95	0.47
1:A:186:PRO:HG3	1:A:245:TYR:CE1	2.49	0.47
1:I:158:GLY:O	1:I:160:LEU:HG	2.14	0.47
1:I:291:VAL:O	1:I:295:ILE:HG13	2.14	0.47
1:K:187:LYS:HG3	1:K:210:GLU:OE1	2.13	0.47
1:N:191:LEU:HD12	1:N:192:PRO:HD2	1.96	0.47
1:A:53:ARG:HB3	3:A:401:HOH:O	2.13	0.47
1:A:144:ARG:HG3	1:A:144:ARG:NH1	2.30	0.47
1:B:291:VAL:O	1:B:295:ILE:HG13	2.14	0.47
1:I:73:THR:HG22	3:I:418:HOH:O	2.15	0.47
1:K:10:ILE:HG23	1:K:14:GLU:HB3	1.95	0.47
1:K:217:ASP:OD2	1:K:255:LYS:HA	2.14	0.47
1:B:99:ILE:HG13	1:B:120:PRO:HB2	1.97	0.47
1:B:143:MET:CE	1:B:148:ARG:HA	2.43	0.47
1:E:249:ARG:O	1:E:253:GLU:HG3	2.15	0.47
1:F:128:SER:C	1:F:130:GLN:H	2.18	0.47
1:I:29:LEU:HD11	1:I:293:MET:CE	2.45	0.47
1:K:137:LEU:C	1:K:137:LEU:HD12	2.35	0.47
1:L:129:ASN:O	1:L:130:GLN:HB2	2.15	0.47
1:M:230:GLU:N	1:M:230:GLU:OE2	2.48	0.47
1:B:155:ALA:HB2	1:B:219:ILE:CD1	2.42	0.47
1:E:14:GLU:O	1:E:18:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ILE:HG23	1:F:14:GLU:HB3	1.97	0.47
1:J:51:SER:CB	1:J:103:ARG:HH12	2.19	0.47
1:J:229:LYS:HG3	3:J:406:HOH:O	2.14	0.47
1:K:180:GLU:HB2	1:K:205:LYS:HE3	1.95	0.47
1:M:99:ILE:HG13	1:M:120:PRO:HB2	1.96	0.47
1:M:123:ASN:ND2	1:M:125:GLY:N	2.63	0.47
1:A:265:ARG:HD2	1:A:265:ARG:C	2.35	0.47
1:A:298:LYS:HE3	3:A:446:HOH:O	2.13	0.47
1:C:112:LEU:HD22	1:F:233:PRO:HB2	1.96	0.47
1:D:73:THR:CG2	1:D:74:ASP:N	2.67	0.47
1:D:99:ILE:HA	1:D:119:VAL:HG13	1.96	0.47
1:E:137:LEU:HD12	1:E:137:LEU:C	2.35	0.47
1:F:287:TYR:C	1:F:290:PRO:HD2	2.35	0.47
1:I:72:MET:HE3	1:K:56:LEU:HD12	1.97	0.47
1:I:73:THR:CG2	1:I:74:ASP:N	2.77	0.47
1:J:209:LYS:CG	1:J:214:ASP:CB	2.92	0.47
1:L:287:TYR:C	1:L:290:PRO:HD2	2.35	0.47
1:A:248:LYS:O	1:A:252:VAL:HG23	2.15	0.47
1:F:215:LEU:HD22	1:F:219:ILE:CD1	2.45	0.47
1:I:48:TYR:HD2	1:I:76:LYS:HE3	1.79	0.47
1:I:228:GLN:HB3	1:I:230:GLU:HG2	1.97	0.47
1:L:99:ILE:HA	1:L:119:VAL:HG13	1.95	0.47
1:M:76:LYS:HA	1:M:76:LYS:NZ	2.29	0.47
1:B:87:ILE:HG22	1:B:91:ARG:NH2	2.30	0.47
1:B:99:ILE:HA	1:B:119:VAL:HG13	1.95	0.47
1:C:6:SER:HA	1:C:130:GLN:CG	2.45	0.47
1:C:51:SER:CB	1:C:103:ARG:HH12	2.19	0.47
1:E:150:ASP:OD1	1:E:177:GLU:N	2.43	0.47
1:F:75:LEU:C	1:F:77:SER:H	2.18	0.47
1:L:10:ILE:HG23	1:L:14:GLU:HB3	1.97	0.47
1:A:191:LEU:HD12	1:A:192:PRO:HD2	1.97	0.47
1:B:87:ILE:CG2	1:B:91:ARG:NH2	2.78	0.47
1:C:123:ASN:ND2	1:C:125:GLY:N	2.63	0.47
1:D:129:ASN:O	1:D:130:GLN:NE2	2.48	0.47
1:E:191:LEU:HD12	1:E:192:PRO:HD2	1.96	0.47
1:I:82:LYS:HB2	1:K:53:ARG:NH2	2.30	0.47
1:L:6:SER:CB	1:L:130:GLN:HG2	2.45	0.47
1:B:8:LYS:HG2	1:B:171:TYR:CE2	2.50	0.46
1:B:148:ARG:HB2	3:B:409:HOH:O	2.15	0.46
1:D:46:VAL:HG13	1:D:75:LEU:CD1	2.45	0.46
1:D:140:TYR:CZ	1:D:144:ARG:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:GLU:N	1:E:230:GLU:OE2	2.47	0.46
1:I:228:GLN:HB3	1:I:230:GLU:OE1	2.15	0.46
1:J:291:VAL:O	1:J:295:ILE:HG13	2.15	0.46
1:K:87:ILE:CD1	1:N:235:PRO:HD2	2.17	0.46
1:M:249:ARG:HD2	1:M:249:ARG:C	2.35	0.46
1:N:128:SER:HB3	1:N:164:ARG:HG3	1.97	0.46
1:N:278:GLN:CD	1:N:278:GLN:H	2.16	0.46
1:B:6:SER:HA	1:B:130:GLN:HG2	1.98	0.46
1:B:109:ALA:HB3	1:B:126:ASP:OD1	2.15	0.46
1:B:123:ASN:O	1:B:132:PRO:HD2	2.15	0.46
1:D:190:ARG:HH11	1:D:190:ARG:CG	2.28	0.46
1:F:23:ARG:HA	1:F:140:TYR:OH	2.14	0.46
1:I:73:THR:HG22	1:I:74:ASP:H	1.78	0.46
1:J:209:LYS:HG2	1:J:214:ASP:HB2	1.98	0.46
1:N:9:ASP:HA	3:N:416:HOH:O	2.15	0.46
1:B:304:GLU:HA	3:B:417:HOH:O	2.16	0.46
1:C:287:TYR:C	1:C:290:PRO:HD2	2.36	0.46
1:E:148:ARG:HH11	1:E:148:ARG:HG2	1.79	0.46
1:E:161:LYS:HA	1:E:192:PRO:HD3	1.98	0.46
1:I:31:THR:HG22	1:I:33:ARG:HB2	1.97	0.46
1:J:2:LYS:HB3	1:J:303:ASN:OD1	2.14	0.46
1:J:190:ARG:HG2	1:J:208:GLU:OE1	2.15	0.46
1:L:31:THR:C	1:L:33:ARG:N	2.68	0.46
1:L:144:ARG:HG3	1:L:144:ARG:HH11	1.80	0.46
1:L:148:ARG:HG2	1:L:148:ARG:HH11	1.80	0.46
1:L:265:ARG:HD2	1:L:265:ARG:C	2.36	0.46
1:N:287:TYR:O	1:N:290:PRO:HD2	2.15	0.46
1:A:104:HIS:O	1:A:126:ASP:HA	2.16	0.46
1:A:140:TYR:O	1:A:144:ARG:HB2	2.16	0.46
1:A:148:ARG:HG2	1:A:148:ARG:HH11	1.79	0.46
1:I:10:ILE:HG22	1:I:15:ILE:HG13	1.98	0.46
1:I:190:ARG:HH11	1:I:190:ARG:CG	2.28	0.46
1:K:153:LYS:HD3	1:K:218:ASP:OD2	2.14	0.46
1:K:158:GLY:O	1:K:160:LEU:HG	2.15	0.46
1:L:219:ILE:O	1:L:257:PHE:HB3	2.14	0.46
1:N:249:ARG:O	1:N:251:TYR:N	2.49	0.46
1:A:45:THR:HG23	1:A:47:PHE:CE1	2.51	0.46
1:A:209:LYS:HG2	1:A:214:ASP:HB3	1.98	0.46
1:C:99:ILE:HA	1:C:119:VAL:HG13	1.97	0.46
1:E:73:THR:CG2	1:E:74:ASP:N	2.79	0.46
1:F:51:SER:CB	1:F:103:ARG:HH12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:51:SER:CB	1:I:103:ARG:NH1	2.76	0.46
1:J:51:SER:CB	1:J:103:ARG:NH1	2.76	0.46
1:J:73:THR:CG2	1:J:74:ASP:H	2.29	0.46
1:K:31:THR:C	1:K:33:ARG:H	2.17	0.46
1:K:119:VAL:HG13	1:K:120:PRO:CD	2.46	0.46
1:L:31:THR:O	1:L:33:ARG:N	2.48	0.46
1:L:87:ILE:HG22	1:L:91:ARG:HH21	1.80	0.46
1:N:265:ARG:HD2	1:N:265:ARG:C	2.35	0.46
1:A:298:LYS:HG3	3:A:448:HOH:O	2.15	0.46
1:I:77:SER:O	1:I:79:SER:N	2.46	0.46
1:I:180:GLU:HG3	1:I:205:LYS:CG	2.46	0.46
1:J:212:LEU:O	1:J:215:LEU:CD1	2.61	0.46
1:K:161:LYS:HA	1:K:192:PRO:HD3	1.97	0.46
1:K:263:LEU:HD22	3:K:405:HOH:O	2.15	0.46
1:L:53:ARG:NH1	1:L:53:ARG:CG	2.76	0.46
1:L:180:GLU:HG3	1:L:205:LYS:CD	2.46	0.46
1:N:249:ARG:O	1:N:252:VAL:N	2.48	0.46
1:B:248:LYS:O	1:B:252:VAL:HG23	2.16	0.46
1:D:123:ASN:ND2	1:D:125:GLY:N	2.63	0.46
1:D:287:TYR:C	1:D:290:PRO:HD2	2.36	0.46
1:I:99:ILE:HG13	1:I:120:PRO:HB2	1.98	0.46
1:I:128:SER:CB	1:I:164:ARG:HG3	2.34	0.46
1:I:265:ARG:HD2	1:I:265:ARG:C	2.36	0.46
1:K:278:GLN:H	1:K:278:GLN:CD	2.18	0.46
1:M:75:LEU:HD12	1:M:75:LEU:N	2.31	0.46
1:M:188:GLU:CD	1:M:188:GLU:H	2.19	0.46
1:B:148:ARG:HG2	1:B:148:ARG:HH11	1.81	0.46
1:B:271:TYR:CD2	1:F:235:PRO:HB2	2.50	0.46
1:K:184:VAL:HG21	1:K:215:LEU:HD11	1.97	0.46
1:N:51:SER:CB	1:N:103:ARG:NH1	2.75	0.46
1:A:81:ALA:O	1:C:53:ARG:NH2	2.48	0.46
1:A:255:LYS:HE3	3:A:434:HOH:O	2.15	0.46
1:I:29:LEU:HD21	1:I:293:MET:HE1	1.97	0.46
1:I:263:LEU:HB3	1:I:264:PRO:HA	1.98	0.46
1:J:49:GLU:HG2	1:J:105:PRO:HG3	1.95	0.46
1:J:150:ASP:OD1	1:J:177:GLU:N	2.48	0.46
1:J:230:GLU:N	1:J:230:GLU:OE2	2.49	0.46
1:C:265:ARG:C	1:C:265:ARG:HD2	2.36	0.46
1:D:6:SER:HA	1:D:130:GLN:HG2	1.97	0.46
1:D:218:ASP:OD2	1:D:218:ASP:C	2.55	0.46
1:E:98:ASP:O	1:E:119:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:LEU:C	1:J:137:LEU:HD12	2.36	0.46
1:J:209:LYS:HG2	1:J:214:ASP:CB	2.45	0.46
1:K:289:ILE:HG22	1:K:293:MET:CE	2.46	0.46
1:N:263:LEU:HB3	1:N:264:PRO:HA	1.97	0.46
1:B:52:THR:HG21	1:C:72:MET:HG3	1.98	0.45
1:L:51:SER:CB	1:L:103:ARG:NH1	2.78	0.45
1:L:190:ARG:HD3	1:L:208:GLU:OE1	2.16	0.45
1:B:233:PRO:HB2	1:D:112:LEU:CD2	2.46	0.45
1:C:191:LEU:HD12	1:C:192:PRO:HD2	1.98	0.45
1:C:230:GLU:N	1:C:230:GLU:OE2	2.49	0.45
1:E:52:THR:HG21	1:F:72:MET:HG3	1.97	0.45
1:J:265:ARG:C	1:J:265:ARG:HD2	2.37	0.45
1:K:217:ASP:C	1:K:219:ILE:N	2.69	0.45
1:B:73:THR:CG2	1:B:74:ASP:H	2.27	0.45
1:B:106:SER:HB3	1:D:233:PRO:CG	2.42	0.45
1:B:287:TYR:C	1:B:290:PRO:HD2	2.37	0.45
1:D:52:THR:OG1	1:E:80:VAL:HG13	2.16	0.45
1:F:74:ASP:O	1:F:80:VAL:HB	2.15	0.45
1:F:126:ASP:HB2	1:F:129:ASN:HD21	1.81	0.45
1:I:287:TYR:C	1:I:290:PRO:HD2	2.35	0.45
1:J:31:THR:HG23	1:J:33:ARG:CZ	2.45	0.45
1:L:81:ALA:O	1:L:82:LYS:HB2	2.15	0.45
1:M:119:VAL:HG13	1:M:120:PRO:CD	2.45	0.45
1:M:137:LEU:C	1:M:137:LEU:HD12	2.36	0.45
1:M:148:ARG:HH11	1:M:148:ARG:HG2	1.79	0.45
1:M:237:GLU:O	1:M:240:LYS:HB3	2.16	0.45
1:D:8:LYS:HG2	1:D:171:TYR:CE2	2.52	0.45
1:J:98:ASP:O	1:J:119:VAL:HG13	2.16	0.45
1:K:10:ILE:HG22	1:K:15:ILE:HG13	1.98	0.45
1:K:33:ARG:HA	1:K:34:PRO:HD3	1.66	0.45
1:L:125:GLY:C	1:L:127:GLY:N	2.70	0.45
1:M:123:ASN:HD22	1:M:124:ALA:N	2.14	0.45
1:N:14:GLU:O	1:N:18:ILE:HG13	2.17	0.45
1:B:200:LYS:CE	1:J:253:GLU:OE1	2.64	0.45
1:D:119:VAL:HG13	1:D:120:PRO:CD	2.45	0.45
1:D:158:GLY:O	1:D:160:LEU:HG	2.16	0.45
1:K:99:ILE:HG13	1:K:120:PRO:HB2	1.97	0.45
1:A:137:LEU:C	1:A:137:LEU:HD12	2.37	0.45
3:A:437:HOH:O	1:C:53:ARG:HD3	2.16	0.45
1:D:148:ARG:HG2	1:D:148:ARG:HH11	1.81	0.45
1:F:76:LYS:HA	1:F:76:LYS:CE	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:287:TYR:C	1:J:290:PRO:HD2	2.37	0.45
1:N:186:PRO:HG3	1:N:245:TYR:CE1	2.52	0.45
1:C:187:LYS:HD3	1:C:210:GLU:OE1	2.17	0.45
1:D:161:LYS:HA	1:D:192:PRO:HD3	1.99	0.45
1:E:128:SER:HB3	1:E:164:ARG:HG3	1.99	0.45
1:E:289:ILE:HG22	1:E:293:MET:CE	2.46	0.45
1:F:158:GLY:HA2	1:F:227:ILE:HD11	1.97	0.45
1:I:217:ASP:OD2	1:I:255:LYS:HA	2.17	0.45
1:K:123:ASN:ND2	1:K:125:GLY:N	2.65	0.45
1:M:99:ILE:HA	1:M:119:VAL:HG13	1.98	0.45
1:M:158:GLY:O	1:M:160:LEU:HG	2.17	0.45
1:A:6:SER:CB	1:A:130:GLN:HG2	2.46	0.45
1:C:174:SER:HB2	1:C:204:ILE:CD1	2.47	0.45
1:D:140:TYR:OH	1:D:144:ARG:HD2	2.17	0.45
1:J:14:GLU:O	1:J:18:ILE:HG13	2.16	0.45
1:J:278:GLN:H	1:J:278:GLN:CD	2.20	0.45
1:K:123:ASN:ND2	1:K:125:GLY:H	2.15	0.45
1:L:23:ARG:HG3	1:L:23:ARG:HH11	1.81	0.45
1:N:49:GLU:OE2	1:N:127:GLY:HA2	2.16	0.45
1:N:98:ASP:O	1:N:119:VAL:HG13	2.16	0.45
1:N:150:ASP:OD1	1:N:177:GLU:N	2.48	0.45
1:B:216:ASP:HB2	1:B:218:ASP:OD1	2.17	0.45
1:B:235:PRO:CB	1:F:271:TYR:CE2	3.00	0.45
1:B:235:PRO:HG3	1:D:85:SER:HB2	1.99	0.45
1:C:186:PRO:HG3	1:C:245:TYR:CE1	2.52	0.45
1:E:219:ILE:HB	3:E:416:HOH:O	2.17	0.45
1:I:53:ARG:HH21	1:J:82:LYS:HB2	1.81	0.45
1:I:125:GLY:C	1:I:127:GLY:N	2.69	0.45
1:K:98:ASP:O	1:K:119:VAL:HG13	2.17	0.45
1:L:99:ILE:HG13	1:L:120:PRO:HB2	1.99	0.45
1:E:299:LEU:O	1:E:303:ASN:ND2	2.38	0.45
1:J:99:ILE:HG13	1:J:120:PRO:HB2	1.99	0.45
1:N:193:LYS:O	1:N:197:GLU:HG2	2.17	0.45
1:A:103:ARG:NH1	1:A:103:ARG:CG	2.76	0.44
1:C:68:GLU:HG2	3:C:439:HOH:O	2.16	0.44
1:D:215:LEU:HD13	1:D:215:LEU:O	2.17	0.44
1:F:14:GLU:O	1:F:18:ILE:HG13	2.16	0.44
1:F:104:HIS:HA	1:F:105:PRO:HD3	1.85	0.44
1:M:83:GLY:HA2	3:M:412:HOH:O	2.16	0.44
1:M:123:ASN:ND2	1:M:125:GLY:H	2.15	0.44
1:N:228:GLN:HB3	1:N:230:GLU:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LYS:O	1:C:27:GLU:HG2	2.17	0.44
1:C:77:SER:O	1:C:79:SER:N	2.50	0.44
1:E:27:GLU:OE2	1:E:27:GLU:HA	2.17	0.44
1:E:246:LYS:HE2	1:E:270:ASP:CG	2.38	0.44
1:I:230:GLU:CD	1:I:230:GLU:N	2.69	0.44
1:C:291:VAL:O	1:C:295:ILE:HG13	2.16	0.44
1:D:217:ASP:OD1	1:D:256:LYS:N	2.40	0.44
1:E:186:PRO:HG3	1:E:245:TYR:CE1	2.51	0.44
1:M:287:TYR:O	1:M:290:PRO:HD2	2.17	0.44
1:N:210:GLU:O	1:N:210:GLU:HG3	2.17	0.44
1:A:287:TYR:O	1:A:290:PRO:HD2	2.17	0.44
1:D:14:GLU:O	1:D:18:ILE:HG13	2.17	0.44
1:F:174:SER:HB2	1:F:204:ILE:CD1	2.47	0.44
1:F:231:ARG:HH11	1:F:231:ARG:HG2	1.82	0.44
1:J:263:LEU:HB3	1:J:264:PRO:HA	2.00	0.44
1:K:128:SER:CB	1:K:164:ARG:HG3	2.39	0.44
1:K:299:LEU:O	1:K:303:ASN:ND2	2.48	0.44
1:L:215:LEU:HB3	1:L:219:ILE:CD1	2.47	0.44
1:A:51:SER:CB	1:A:103:ARG:HH12	2.18	0.44
1:J:87:ILE:HG22	1:J:91:ARG:HH21	1.83	0.44
1:L:282:PHE:O	1:L:285:SER:HB3	2.18	0.44
1:M:87:ILE:HG22	1:M:91:ARG:HH21	1.81	0.44
1:A:48:TYR:CE1	1:A:75:LEU:HD13	2.52	0.44
1:C:45:THR:HG23	1:C:47:PHE:CE1	2.53	0.44
1:D:30:ASN:C	1:D:32:LYS:H	2.21	0.44
1:E:48:TYR:CD2	1:E:75:LEU:HB2	2.53	0.44
1:I:99:ILE:HA	1:I:119:VAL:HG13	1.98	0.44
1:I:180:GLU:HB2	1:I:205:LYS:HE3	1.99	0.44
1:K:126:ASP:CB	1:K:129:ASN:HD21	2.04	0.44
1:K:287:TYR:C	1:K:290:PRO:HD2	2.37	0.44
1:N:230:GLU:CD	1:N:230:GLU:N	2.70	0.44
1:D:215:LEU:O	1:D:216:ASP:O	2.34	0.44
1:F:87:ILE:HG22	1:F:91:ARG:HH21	1.83	0.44
1:J:282:PHE:O	1:J:285:SER:HB3	2.17	0.44
1:K:19:LEU:HD22	1:K:140:TYR:HA	1.98	0.44
1:L:72:MET:SD	1:L:75:LEU:HD21	2.58	0.44
1:L:249:ARG:HB2	1:L:272:ASP:OD2	2.18	0.44
1:N:228:GLN:NE2	1:N:231:ARG:HH12	2.15	0.44
1:B:123:ASN:ND2	1:B:125:GLY:N	2.66	0.44
1:F:31:THR:CG2	1:F:33:ARG:CZ	2.96	0.44
1:I:72:MET:CG	1:I:75:LEU:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:161:LYS:HA	1:J:192:PRO:HD3	2.00	0.44
1:M:209:LYS:HG3	1:M:214:ASP:CB	2.46	0.44
1:M:287:TYR:C	1:M:290:PRO:HD2	2.37	0.44
1:N:246:LYS:HE2	1:N:270:ASP:CG	2.38	0.44
1:A:45:THR:O	1:A:45:THR:HG22	2.17	0.44
1:A:73:THR:O	1:A:80:VAL:HG11	2.18	0.44
1:D:73:THR:O	1:D:74:ASP:HB3	2.18	0.44
1:K:265:ARG:HD2	1:K:265:ARG:C	2.37	0.44
1:L:180:GLU:OE2	1:L:205:LYS:HD2	2.18	0.44
1:N:205:LYS:HB2	3:N:418:HOH:O	2.17	0.44
1:A:80:VAL:O	1:A:80:VAL:HG12	2.18	0.43
1:A:157:VAL:O	1:A:225:THR:HG22	2.18	0.43
1:D:153:LYS:HB2	1:D:219:ILE:HA	2.00	0.43
1:E:249:ARG:NH2	1:E:272:ASP:O	2.51	0.43
1:J:72:MET:HG2	1:J:75:LEU:HD11	2.00	0.43
1:N:48:TYR:CD2	1:N:75:LEU:HB2	2.52	0.43
1:B:129:ASN:HB2	3:B:446:HOH:O	2.17	0.43
1:E:287:TYR:O	1:E:290:PRO:HD2	2.18	0.43
1:F:47:PHE:HA	1:F:103:ARG:HB3	1.99	0.43
1:F:217:ASP:OD1	1:F:217:ASP:O	2.37	0.43
1:I:87:ILE:HD12	1:M:235:PRO:CD	2.42	0.43
1:M:153:LYS:O	1:M:219:ILE:HG23	2.19	0.43
1:N:228:GLN:HE21	1:N:231:ARG:NH1	2.14	0.43
1:N:287:TYR:C	1:N:290:PRO:HD2	2.38	0.43
1:A:72:MET:HG3	1:C:52:THR:HG21	1.99	0.43
1:A:87:ILE:HG22	1:A:91:ARG:HH21	1.83	0.43
1:A:205:LYS:HE2	1:A:207:TYR:OH	2.18	0.43
1:B:46:VAL:O	1:B:102:LEU:HD12	2.17	0.43
1:C:262:PRO:O	1:C:263:LEU:HB2	2.19	0.43
1:E:190:ARG:HG3	1:E:190:ARG:HH11	1.83	0.43
1:I:19:LEU:HD22	1:I:140:TYR:HA	2.00	0.43
1:K:48:TYR:HA	1:K:75:LEU:HB2	2.01	0.43
1:K:70:ILE:O	1:K:70:ILE:HG13	2.18	0.43
1:K:209:LYS:HG3	1:K:214:ASP:CB	2.45	0.43
1:N:303:ASN:O	1:N:304:GLU:CB	2.65	0.43
1:C:75:LEU:HA	1:C:80:VAL:HB	2.01	0.43
1:C:282:PHE:O	1:C:285:SER:HB3	2.19	0.43
1:E:53:ARG:HD3	3:E:430:HOH:O	2.18	0.43
1:E:144:ARG:HG2	1:E:287:TYR:OH	2.19	0.43
1:F:128:SER:OG	1:F:164:ARG:HG3	2.18	0.43
1:J:75:LEU:HA	1:J:80:VAL:CG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:87:ILE:CG2	1:L:91:ARG:NH2	2.82	0.43
1:M:278:GLN:H	1:M:278:GLN:CD	2.19	0.43
1:A:287:TYR:C	1:A:290:PRO:HD2	2.39	0.43
1:B:103:ARG:HD2	1:B:124:ALA:O	2.18	0.43
1:B:153:LYS:HG2	1:B:180:GLU:HB3	2.01	0.43
1:D:265:ARG:HD2	1:D:265:ARG:C	2.39	0.43
1:I:278:GLN:CD	1:I:278:GLN:H	2.15	0.43
1:J:129:ASN:O	1:J:130:GLN:HB2	2.18	0.43
1:K:209:LYS:NZ	1:K:214:ASP:O	2.48	0.43
1:B:271:TYR:CE2	1:F:235:PRO:CB	3.01	0.43
1:C:14:GLU:O	1:C:18:ILE:HG13	2.19	0.43
1:J:53:ARG:HG3	1:J:53:ARG:HH11	1.83	0.43
1:K:150:ASP:OD1	1:K:177:GLU:N	2.47	0.43
1:L:180:GLU:CG	1:L:205:LYS:HD2	2.48	0.43
1:A:126:ASP:OD1	1:A:129:ASN:OD1	2.36	0.43
1:I:23:ARG:NH2	1:I:144:ARG:HH21	2.17	0.43
1:L:119:VAL:HG13	1:L:120:PRO:CD	2.48	0.43
1:A:123:ASN:ND2	1:A:125:GLY:N	2.66	0.43
1:A:140:TYR:CZ	1:A:144:ARG:HD3	2.53	0.43
1:B:23:ARG:HB3	3:B:425:HOH:O	2.18	0.43
1:C:73:THR:CG2	1:C:74:ASP:N	2.82	0.43
1:F:70:ILE:HG13	1:F:70:ILE:O	2.18	0.43
1:F:150:ASP:OD1	1:F:177:GLU:N	2.47	0.43
1:F:265:ARG:HD2	1:F:265:ARG:C	2.38	0.43
1:I:282:PHE:O	1:I:285:SER:HB3	2.18	0.43
1:J:180:GLU:HG3	1:J:205:LYS:CD	2.49	0.43
1:J:234:ASP:HA	1:L:112:LEU:HD21	2.01	0.43
1:K:75:LEU:O	1:K:77:SER:N	2.52	0.43
1:K:148:ARG:HG2	1:K:148:ARG:HH11	1.83	0.43
1:L:174:SER:HB2	1:L:204:ILE:CD1	2.48	0.43
1:N:53:ARG:HD2	3:N:401:HOH:O	2.17	0.43
1:N:119:VAL:HG13	1:N:120:PRO:CD	2.49	0.43
1:B:174:SER:HB2	1:B:204:ILE:CD1	2.49	0.43
1:I:31:THR:C	1:I:33:ARG:N	2.72	0.43
1:I:73:THR:CG2	1:I:74:ASP:H	2.31	0.43
1:J:72:MET:SD	1:J:75:LEU:HD21	2.59	0.43
1:K:14:GLU:O	1:K:18:ILE:HG13	2.18	0.43
1:K:153:LYS:HG2	1:K:180:GLU:HB3	2.00	0.43
1:M:104:HIS:HA	1:M:105:PRO:HD3	1.87	0.43
1:M:265:ARG:C	1:M:265:ARG:HD2	2.38	0.43
1:N:137:LEU:HD12	1:N:137:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:148:ARG:HG2	1:N:148:ARG:HH11	1.84	0.43
1:A:128:SER:HB3	1:A:129:ASN:H	1.61	0.43
1:F:6:SER:HA	1:F:130:GLN:HG3	2.01	0.43
1:F:299:LEU:O	1:F:303:ASN:ND2	2.50	0.43
1:J:219:ILE:HD12	1:J:219:ILE:H	1.84	0.43
1:C:45:THR:HG22	1:C:45:THR:O	2.18	0.42
1:K:190:ARG:HG3	1:K:208:GLU:OE1	2.20	0.42
1:K:217:ASP:O	1:K:217:ASP:OD1	2.36	0.42
1:M:14:GLU:O	1:M:18:ILE:HG13	2.18	0.42
1:B:47:PHE:HA	1:B:103:ARG:HB3	2.02	0.42
1:C:249:ARG:HH21	1:C:272:ASP:HB2	1.81	0.42
1:F:301:GLU:CA	1:F:304:GLU:HG3	2.42	0.42
1:I:45:THR:O	1:I:45:THR:HG22	2.19	0.42
1:I:148:ARG:HG2	1:I:148:ARG:HH11	1.83	0.42
1:I:150:ASP:OD1	1:I:177:GLU:N	2.47	0.42
1:I:257:PHE:CD1	1:I:257:PHE:C	2.93	0.42
1:K:53:ARG:NH1	1:K:53:ARG:HG3	2.33	0.42
1:N:99:ILE:HA	1:N:119:VAL:HG13	1.98	0.42
1:E:48:TYR:CZ	1:E:75:LEU:HD13	2.54	0.42
1:F:282:PHE:O	1:F:285:SER:HB3	2.19	0.42
1:I:72:MET:HE3	1:K:52:THR:HG22	2.01	0.42
1:J:209:LYS:CG	1:J:214:ASP:HB2	2.49	0.42
1:J:216:ASP:O	1:J:218:ASP:N	2.45	0.42
1:M:98:ASP:O	1:M:119:VAL:HG13	2.20	0.42
1:N:10:ILE:HG22	1:N:15:ILE:HG13	2.02	0.42
1:C:47:PHE:HA	1:C:103:ARG:HB3	2.02	0.42
1:D:98:ASP:O	1:D:119:VAL:HG13	2.19	0.42
1:D:158:GLY:HA2	1:D:227:ILE:HD11	2.01	0.42
1:E:287:TYR:C	1:E:290:PRO:HD2	2.39	0.42
1:J:230:GLU:CD	1:J:230:GLU:N	2.68	0.42
1:M:49:GLU:O	1:M:49:GLU:HG3	2.20	0.42
1:N:291:VAL:O	1:N:295:ILE:HG13	2.19	0.42
1:A:246:LYS:HE2	1:A:270:ASP:CG	2.39	0.42
1:C:47:PHE:O	1:C:74:ASP:N	2.51	0.42
1:C:161:LYS:HA	1:C:192:PRO:HD3	2.01	0.42
1:D:33:ARG:HG3	1:D:35:LEU:HD23	2.02	0.42
1:E:278:GLN:H	1:E:278:GLN:CD	2.19	0.42
1:I:125:GLY:O	1:I:127:GLY:N	2.42	0.42
1:I:187:LYS:O	1:I:190:ARG:NH2	2.53	0.42
1:M:87:ILE:HD13	1:M:116:TYR:CZ	2.55	0.42
1:A:87:ILE:CG2	1:A:91:ARG:NH2	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ARG:NH2	1:C:144:ARG:NH2	2.67	0.42
1:C:98:ASP:O	1:C:119:VAL:HG13	2.19	0.42
1:C:129:ASN:ND2	1:C:130:GLN:N	2.66	0.42
1:F:10:ILE:HG22	1:F:15:ILE:HG13	2.01	0.42
1:F:143:MET:CE	1:F:148:ARG:HA	2.50	0.42
1:J:143:MET:CE	1:J:148:ARG:HA	2.49	0.42
1:K:48:TYR:CE2	1:K:75:LEU:HB3	2.54	0.42
1:N:229:LYS:HG2	1:N:238:TYR:CE2	2.55	0.42
1:B:143:MET:HE1	1:B:148:ARG:HA	2.02	0.42
1:D:72:MET:HG3	1:F:52:THR:HG21	2.02	0.42
1:D:231:ARG:HG2	1:D:231:ARG:HH11	1.84	0.42
1:D:257:PHE:CD1	1:D:257:PHE:C	2.92	0.42
1:I:144:ARG:HG3	1:I:144:ARG:NH1	2.34	0.42
1:I:144:ARG:NH2	3:I:402:HOH:O	2.48	0.42
1:I:207:TYR:CD1	1:I:207:TYR:N	2.87	0.42
1:I:249:ARG:NH1	1:I:249:ARG:HG3	2.34	0.42
1:J:53:ARG:HG3	1:J:53:ARG:NH1	2.35	0.42
1:J:75:LEU:N	1:J:75:LEU:HD12	2.34	0.42
1:J:187:LYS:H	1:J:187:LYS:HD3	1.81	0.42
1:K:87:ILE:HD13	1:K:116:TYR:CZ	2.55	0.42
1:K:104:HIS:O	1:K:126:ASP:HA	2.20	0.42
1:N:19:LEU:HD22	1:N:140:TYR:HA	2.00	0.42
1:N:99:ILE:HG13	1:N:120:PRO:HB2	2.01	0.42
1:N:128:SER:C	1:N:130:GLN:H	2.22	0.42
1:N:228:GLN:HE21	1:N:228:GLN:HB2	1.61	0.42
1:B:22:ALA:HA	1:B:294:ALA:HB2	2.02	0.42
1:C:6:SER:CA	1:C:130:GLN:HG2	2.49	0.42
1:C:148:ARG:HH11	1:C:148:ARG:HG2	1.85	0.42
1:D:125:GLY:C	1:D:127:GLY:H	2.23	0.42
1:E:73:THR:CG2	1:E:74:ASP:H	2.33	0.42
1:I:161:LYS:HA	1:I:192:PRO:HD3	2.02	0.42
1:I:252:VAL:CG1	1:I:278:GLN:CG	2.98	0.42
1:K:99:ILE:HA	1:K:119:VAL:HG13	2.00	0.42
1:K:291:VAL:O	1:K:295:ILE:HG13	2.19	0.42
1:L:104:HIS:HA	1:L:105:PRO:HD3	1.88	0.42
1:M:77:SER:C	1:M:79:SER:N	2.73	0.42
1:A:82:LYS:HB2	1:C:53:ARG:HH22	1.84	0.42
1:B:219:ILE:O	1:B:257:PHE:HB3	2.20	0.42
1:D:53:ARG:HG3	1:D:53:ARG:HH11	1.84	0.42
1:E:10:ILE:HG22	1:E:15:ILE:HG13	2.02	0.42
1:E:75:LEU:CD2	1:E:80:VAL:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:SER:HB2	1:E:204:ILE:CD1	2.50	0.42
1:F:207:TYR:CD1	1:F:207:TYR:N	2.87	0.42
1:F:263:LEU:HB3	1:F:264:PRO:HA	2.01	0.42
1:I:180:GLU:HG3	1:I:205:LYS:CD	2.50	0.42
1:K:75:LEU:O	1:K:81:ALA:HB2	2.20	0.42
1:N:123:ASN:HD22	1:N:124:ALA:N	2.17	0.42
1:C:231:ARG:HG2	1:C:231:ARG:HH11	1.85	0.42
1:E:249:ARG:HB3	1:E:272:ASP:OD2	2.20	0.42
1:F:28:LEU:O	1:F:31:THR:HB	2.20	0.42
1:F:230:GLU:CD	1:F:230:GLU:N	2.72	0.42
1:K:23:ARG:HA	1:K:140:TYR:OH	2.20	0.42
1:K:49:GLU:HG3	1:K:49:GLU:O	2.20	0.42
1:K:129:ASN:O	1:K:130:GLN:HB2	2.20	0.42
1:L:27:GLU:HA	1:L:30:ASN:HD22	1.82	0.42
1:L:87:ILE:HG22	1:L:91:ARG:NH2	2.34	0.42
1:M:263:LEU:HB3	1:M:264:PRO:HA	2.02	0.42
1:D:129:ASN:OD1	1:D:130:GLN:N	2.53	0.41
1:D:150:ASP:OD1	1:D:177:GLU:N	2.50	0.41
1:E:87:ILE:HD13	1:E:116:TYR:CZ	2.55	0.41
1:I:174:SER:HB2	1:I:204:ILE:CD1	2.49	0.41
1:J:47:PHE:HA	1:J:103:ARG:HB3	2.02	0.41
1:L:257:PHE:CD1	1:L:257:PHE:C	2.93	0.41
1:M:252:VAL:CG1	1:M:278:GLN:CG	2.98	0.41
1:A:98:ASP:O	1:A:119:VAL:HG13	2.20	0.41
1:A:161:LYS:HA	1:A:192:PRO:HD3	2.02	0.41
1:C:33:ARG:HA	1:C:34:PRO:HD3	1.85	0.41
1:C:123:ASN:HD22	1:C:124:ALA:N	2.18	0.41
1:E:87:ILE:HG22	1:E:91:ARG:HH21	1.84	0.41
1:F:87:ILE:HD13	1:F:116:TYR:CZ	2.56	0.41
1:L:230:GLU:CD	1:L:230:GLU:N	2.71	0.41
1:N:128:SER:HB3	1:N:129:ASN:H	1.53	0.41
1:B:263:LEU:HB3	1:B:264:PRO:HA	2.02	0.41
1:C:27:GLU:HA	1:C:30:ASN:ND2	2.35	0.41
1:D:291:VAL:O	1:D:295:ILE:HG13	2.20	0.41
1:J:156:PHE:CD2	1:J:166:VAL:HG13	2.55	0.41
1:J:174:SER:HB2	1:J:204:ILE:CD1	2.50	0.41
1:J:187:LYS:HB3	1:J:190:ARG:NH2	2.35	0.41
1:N:78:SER:O	1:N:82:LYS:CG	2.68	0.41
1:N:80:VAL:O	1:N:81:ALA:HB2	2.20	0.41
1:A:207:TYR:CD1	1:A:207:TYR:N	2.88	0.41
1:A:291:VAL:O	1:A:295:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:THR:HG22	1:C:72:MET:HE3	2.01	0.41
1:B:252:VAL:CG1	1:B:278:GLN:CG	2.98	0.41
1:C:10:ILE:HG22	1:C:15:ILE:HG13	2.02	0.41
1:F:137:LEU:HB3	1:F:291:VAL:HG21	2.02	0.41
1:F:148:ARG:HH11	1:F:148:ARG:HG2	1.84	0.41
1:I:210:GLU:O	1:I:210:GLU:HG2	2.20	0.41
1:J:45:THR:O	1:J:45:THR:HG22	2.19	0.41
1:J:60:THR:HB	1:J:289:ILE:HD12	2.01	0.41
1:K:125:GLY:O	1:K:127:GLY:N	2.53	0.41
1:M:10:ILE:HG22	1:M:15:ILE:HG13	2.03	0.41
1:A:209:LYS:CG	1:A:214:ASP:HB3	2.51	0.41
1:B:249:ARG:HB2	1:B:272:ASP:OD2	2.20	0.41
1:C:80:VAL:O	1:C:80:VAL:HG12	2.20	0.41
1:D:31:THR:CB	1:D:33:ARG:HG2	2.47	0.41
1:F:126:ASP:HB2	1:F:129:ASN:OD1	2.21	0.41
1:I:119:VAL:HG13	1:I:120:PRO:CD	2.50	0.41
1:J:99:ILE:HA	1:J:119:VAL:HG13	1.98	0.41
1:K:182:TYR:CD2	1:K:215:LEU:CD2	3.03	0.41
1:L:207:TYR:N	1:L:207:TYR:CD1	2.88	0.41
1:M:52:THR:HG21	1:N:72:MET:HG3	2.01	0.41
1:N:161:LYS:HA	1:N:192:PRO:HD3	2.03	0.41
1:B:144:ARG:NH1	1:B:144:ARG:CG	2.78	0.41
1:B:215:LEU:HD13	1:B:219:ILE:HD12	2.01	0.41
1:D:103:ARG:HD2	1:D:124:ALA:O	2.21	0.41
1:F:22:ALA:HA	1:F:294:ALA:HB2	2.02	0.41
1:I:23:ARG:NE	1:I:144:ARG:HE	2.18	0.41
1:I:256:LYS:HE2	1:I:256:LYS:HB3	1.89	0.41
1:J:112:LEU:O	1:J:115:GLU:HB2	2.21	0.41
1:J:187:LYS:HB3	1:J:190:ARG:HH22	1.86	0.41
1:K:6:SER:HA	1:K:130:GLN:CG	2.50	0.41
1:K:123:ASN:HD22	1:K:124:ALA:N	2.19	0.41
1:L:53:ARG:NH2	1:M:82:LYS:HB2	2.35	0.41
1:A:263:LEU:HB3	1:A:264:PRO:HA	2.03	0.41
1:C:217:ASP:OD1	1:C:217:ASP:O	2.37	0.41
1:D:71:THR:HG22	1:D:72:MET:N	2.36	0.41
1:D:155:ALA:HB2	1:D:219:ILE:HG21	2.03	0.41
1:E:77:SER:O	1:E:79:SER:N	2.54	0.41
1:F:252:VAL:CG1	1:F:278:GLN:CG	2.98	0.41
1:K:240:LYS:O	1:K:240:LYS:HG2	2.20	0.41
1:K:249:ARG:C	1:K:251:TYR:H	2.24	0.41
1:L:252:VAL:CG1	1:L:278:GLN:CG	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:10:ILE:HG23	1:N:14:GLU:HB2	2.03	0.41
1:N:104:HIS:HA	1:N:105:PRO:HD3	1.85	0.41
1:A:304:GLU:HG3	1:A:306:GLU:CG	2.44	0.41
1:F:246:LYS:HE2	1:F:270:ASP:CG	2.40	0.41
1:I:4:LEU:HD12	1:I:4:LEU:HA	1.93	0.41
1:I:254:GLY:O	1:I:255:LYS:C	2.59	0.41
1:J:2:LYS:HA	1:J:303:ASN:ND2	2.31	0.41
1:J:128:SER:CB	1:J:164:ARG:HG3	2.33	0.41
1:J:252:VAL:CG1	1:J:278:GLN:CG	2.99	0.41
1:K:47:PHE:HA	1:K:103:ARG:HB3	2.02	0.41
1:L:224:VAL:CG1	1:L:268:GLU:HB3	2.51	0.41
1:M:73:THR:C	1:M:75:LEU:HD12	2.41	0.41
1:M:174:SER:HB2	1:M:204:ILE:CD1	2.50	0.41
1:N:46:VAL:HG13	1:N:75:LEU:HD11	2.03	0.41
1:N:53:ARG:CG	3:N:401:HOH:O	2.69	0.41
1:A:6:SER:HA	1:A:130:GLN:CG	2.51	0.41
1:A:87:ILE:HG22	1:A:91:ARG:NH2	2.36	0.41
1:A:150:ASP:OD1	1:A:177:GLU:N	2.50	0.41
1:B:137:LEU:HD12	1:B:137:LEU:C	2.41	0.41
1:C:104:HIS:HA	1:C:105:PRO:HD3	1.85	0.41
1:D:103:ARG:NH1	1:D:103:ARG:CG	2.79	0.41
1:D:228:GLN:HE21	1:D:228:GLN:HB2	1.56	0.41
1:E:215:LEU:HD13	1:E:219:ILE:CD1	2.51	0.41
1:F:156:PHE:CD2	1:F:166:VAL:HG13	2.56	0.41
1:F:230:GLU:N	1:F:230:GLU:OE2	2.54	0.41
1:I:87:ILE:HG22	1:I:91:ARG:HH21	1.86	0.41
1:J:76:LYS:HD3	1:J:76:LYS:HA	1.86	0.41
1:J:207:TYR:CD1	1:J:207:TYR:N	2.89	0.41
1:K:174:SER:HB2	1:K:204:ILE:CD1	2.50	0.41
1:L:291:VAL:O	1:L:295:ILE:HG13	2.21	0.41
1:M:187:LYS:H	1:M:187:LYS:HE2	1.84	0.41
1:M:187:LYS:HZ3	1:M:187:LYS:N	2.17	0.41
1:M:231:ARG:HG2	1:M:231:ARG:HH11	1.86	0.41
1:N:47:PHE:HA	1:N:103:ARG:HB3	2.03	0.41
1:N:70:ILE:O	1:N:70:ILE:HG13	2.21	0.41
1:N:125:GLY:C	1:N:127:GLY:N	2.72	0.41
1:N:174:SER:HB2	1:N:204:ILE:CD1	2.50	0.41
1:N:181:MET:O	1:N:206:PHE:HA	2.20	0.41
1:C:246:LYS:HE2	1:C:270:ASP:CG	2.41	0.41
1:D:282:PHE:O	1:D:285:SER:HB3	2.21	0.41
1:E:282:PHE:O	1:E:285:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:LEU:N	1:F:75:LEU:CD1	2.82	0.41
1:F:126:ASP:C	1:F:128:SER:N	2.74	0.41
1:F:301:GLU:HA	1:F:304:GLU:CG	2.41	0.41
1:I:31:THR:O	1:I:33:ARG:N	2.54	0.41
1:J:6:SER:CB	1:J:130:GLN:HG2	2.51	0.41
1:L:288:GLY:O	1:L:292:ARG:HG3	2.21	0.41
1:M:186:PRO:HA	1:M:187:LYS:HZ1	1.84	0.41
1:C:153:LYS:HG2	1:C:180:GLU:HB3	2.02	0.40
1:C:257:PHE:CD1	1:C:257:PHE:C	2.95	0.40
1:D:70:ILE:O	1:D:70:ILE:HG13	2.21	0.40
1:E:291:VAL:O	1:E:295:ILE:HG13	2.22	0.40
1:I:103:ARG:NH1	1:I:103:ARG:CG	2.77	0.40
1:I:230:GLU:N	1:I:230:GLU:OE2	2.54	0.40
1:J:226:ARG:HD3	1:J:264:PRO:O	2.21	0.40
1:K:219:ILE:O	1:K:257:PHE:HB3	2.22	0.40
1:L:2:LYS:HG3	1:L:3:HIS:CD2	2.56	0.40
1:L:72:MET:HG3	1:N:52:THR:HG21	2.01	0.40
1:M:7:MET:HG2	1:M:132:PRO:HA	2.03	0.40
1:M:87:ILE:CG2	1:M:91:ARG:NH2	2.84	0.40
1:M:108:GLY:O	1:M:109:ALA:C	2.60	0.40
1:B:125:GLY:C	1:B:127:GLY:H	2.25	0.40
1:B:207:TYR:CD1	1:B:207:TYR:N	2.89	0.40
1:D:31:THR:C	1:D:33:ARG:N	2.74	0.40
1:D:285:SER:OG	1:E:92:VAL:HG13	2.21	0.40
1:E:190:ARG:HG2	1:E:208:GLU:OE1	2.21	0.40
1:F:6:SER:CB	1:F:130:GLN:HG2	2.51	0.40
1:F:45:THR:O	1:F:45:THR:HG22	2.21	0.40
1:F:278:GLN:H	1:F:278:GLN:CD	2.16	0.40
1:I:180:GLU:HG3	1:I:205:LYS:HD2	2.03	0.40
1:I:249:ARG:HG3	1:I:249:ARG:HH11	1.86	0.40
1:K:87:ILE:HG22	1:K:91:ARG:HH21	1.86	0.40
1:K:137:LEU:HB3	1:K:291:VAL:HG21	2.03	0.40
1:L:10:ILE:HG22	1:L:15:ILE:HG13	2.04	0.40
1:M:80:VAL:HG12	1:M:80:VAL:O	2.21	0.40
1:M:87:ILE:HG22	1:M:91:ARG:NH2	2.36	0.40
1:M:161:LYS:HA	1:M:192:PRO:HD3	2.03	0.40
1:N:75:LEU:O	1:N:81:ALA:HB2	2.21	0.40
1:A:249:ARG:CZ	1:A:276:LEU:HD21	2.52	0.40
1:A:257:PHE:CD1	1:A:257:PHE:C	2.95	0.40
1:B:45:THR:O	1:B:45:THR:HG22	2.21	0.40
1:B:265:ARG:NH2	1:B:271:TYR:CD2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:THR:O	1:F:56:LEU:HD21	2.21	0.40
1:F:257:PHE:C	1:F:257:PHE:CD1	2.94	0.40
1:I:48:TYR:O	1:I:76:LYS:CG	2.68	0.40
1:M:207:TYR:CD1	1:M:207:TYR:N	2.89	0.40
1:A:306:GLU:CA	1:C:32:LYS:HG3	2.38	0.40
1:B:144:ARG:HG2	1:B:287:TYR:CZ	2.56	0.40
1:B:217:ASP:O	1:B:217:ASP:OD1	2.39	0.40
1:C:207:TYR:CD1	1:C:207:TYR:N	2.90	0.40
1:E:265:ARG:C	1:E:265:ARG:HD2	2.42	0.40
1:K:44:ALA:HB3	1:K:100:ILE:HG12	2.04	0.40
1:L:228:GLN:NE2	1:L:231:ARG:HH12	2.20	0.40
1:L:230:GLU:N	1:L:230:GLU:OE2	2.53	0.40
1:A:123:ASN:HD22	1:A:124:ALA:N	2.20	0.40
1:B:83:GLY:HA3	3:B:457:HOH:O	2.20	0.40
1:D:49:GLU:CD	1:D:127:GLY:HA2	2.40	0.40
1:D:190:ARG:CG	1:D:190:ARG:NH1	2.84	0.40
1:E:240:LYS:HE3	3:E:426:HOH:O	2.22	0.40
1:F:25:MET:CE	1:F:28:LEU:HD12	2.52	0.40
1:F:206:PHE:CD1	1:F:206:PHE:C	2.94	0.40
1:L:6:SER:HA	1:L:130:GLN:CG	2.52	0.40
1:M:133:THR:H	1:M:133:THR:HG22	1.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	304/306 (99%)	274 (90%)	26 (9%)	4 (1%)	12 45
1	B	302/306 (99%)	272 (90%)	28 (9%)	2 (1%)	22 60
1	C	304/306 (99%)	267 (88%)	29 (10%)	8 (3%)	5 27
1	D	304/306 (99%)	272 (90%)	26 (9%)	6 (2%)	7 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	304/306 (99%)	270 (89%)	28 (9%)	6 (2%)	7 34
1	F	304/306 (99%)	273 (90%)	22 (7%)	9 (3%)	4 24
1	I	302/306 (99%)	273 (90%)	23 (8%)	6 (2%)	7 34
1	J	302/306 (99%)	272 (90%)	26 (9%)	4 (1%)	12 45
1	K	303/306 (99%)	265 (88%)	31 (10%)	7 (2%)	6 30
1	L	303/306 (99%)	265 (88%)	31 (10%)	7 (2%)	6 30
1	M	303/306 (99%)	278 (92%)	22 (7%)	3 (1%)	15 53
1	N	302/306 (99%)	267 (88%)	27 (9%)	8 (3%)	5 27
All	All	3637/3672 (99%)	3248 (89%)	319 (9%)	70 (2%)	8 36

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ALA
1	B	109	ALA
1	C	109	ALA
1	D	32	LYS
1	D	109	ALA
1	D	129	ASN
1	D	216	ASP
1	E	82	LYS
1	E	109	ALA
1	F	81	ALA
1	F	109	ALA
1	F	128	SER
1	F	129	ASN
1	I	109	ALA
1	J	109	ALA
1	J	129	ASN
1	J	217	ASP
1	K	109	ALA
1	L	109	ALA
1	L	129	ASN
1	M	78	SER
1	M	109	ALA
1	N	109	ALA
1	N	129	ASN
1	C	32	LYS
1	C	250	GLU

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Mol	Chain	Res	Type
1	D	218	ASP
1	E	78	SER
1	F	74	ASP
1	F	80	VAL
1	F	130	GLN
1	I	78	SER
1	I	129	ASN
1	I	255	LYS
1	K	218	ASP
1	M	128	SER
1	N	81	ALA
1	N	125	GLY
1	N	130	GLN
1	N	250	GLU
1	A	129	ASN
1	C	78	SER
1	C	217	ASP
1	E	74	ASP
1	E	129	ASN
1	I	128	SER
1	K	250	GLU
1	L	130	GLN
1	C	130	GLN
1	K	76	LYS
1	K	240	LYS
1	L	125	GLY
1	L	214	ASP
1	N	77	SER
1	N	126	ASP
1	C	129	ASN
1	E	214	ASP
1	F	78	SER
1	F	217	ASP
1	J	130	GLN
1	K	214	ASP
1	K	302	ASP
1	L	32	LYS
1	L	78	SER
1	A	304	GLU
1	D	128	SER
1	I	32	LYS
1	A	34	PRO

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Mol	Chain	Res	Type
1	C	33	ARG
1	B	80	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/275 (100%)	264 (96%)	11 (4%)	31	68
1	B	274/275 (100%)	263 (96%)	11 (4%)	31	68
1	C	275/275 (100%)	262 (95%)	13 (5%)	26	63
1	D	275/275 (100%)	262 (95%)	13 (5%)	26	63
1	E	275/275 (100%)	261 (95%)	14 (5%)	24	60
1	F	275/275 (100%)	262 (95%)	13 (5%)	26	63
1	I	274/275 (100%)	261 (95%)	13 (5%)	26	63
1	J	274/275 (100%)	260 (95%)	14 (5%)	24	60
1	K	274/275 (100%)	260 (95%)	14 (5%)	24	60
1	L	274/275 (100%)	265 (97%)	9 (3%)	38	73
1	M	274/275 (100%)	263 (96%)	11 (4%)	31	68
1	N	274/275 (100%)	263 (96%)	11 (4%)	31	68
All	All	3293/3300 (100%)	3146 (96%)	147 (4%)	27	64

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	133	THR
1	A	137	LEU
1	A	209	LYS
1	A	229	LYS
1	A	230	GLU
1	A	250	GLU
1	A	257	PHE

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Mol	Chain	Res	Type
1	A	265	ARG
1	A	278	GLN
1	A	281	TYR
1	B	76	LYS
1	B	123	ASN
1	B	130	GLN
1	B	133	THR
1	B	137	LEU
1	B	197	GLU
1	B	209	LYS
1	B	230	GLU
1	B	257	PHE
1	B	265	ARG
1	B	278	GLN
1	C	76	LYS
1	C	123	ASN
1	C	129	ASN
1	C	133	THR
1	C	137	LEU
1	C	209	LYS
1	C	228	GLN
1	C	230	GLU
1	C	237	GLU
1	C	257	PHE
1	C	265	ARG
1	C	275	ASP
1	C	278	GLN
1	D	33	ARG
1	D	123	ASN
1	D	130	GLN
1	D	133	THR
1	D	137	LEU
1	D	144	ARG
1	D	209	LYS
1	D	214	ASP
1	D	215	LEU
1	D	230	GLU
1	D	257	PHE
1	D	265	ARG
1	D	278	GLN
1	E	31	THR
1	E	49	GLU

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Mol	Chain	Res	Type
1	E	76	LYS
1	E	123	ASN
1	E	133	THR
1	E	137	LEU
1	E	209	LYS
1	E	214	ASP
1	E	230	GLU
1	E	257	PHE
1	E	265	ARG
1	E	275	ASP
1	E	278	GLN
1	E	306	GLU
1	F	53	ARG
1	F	76	LYS
1	F	123	ASN
1	F	133	THR
1	F	137	LEU
1	F	144	ARG
1	F	209	LYS
1	F	210	GLU
1	F	230	GLU
1	F	237	GLU
1	F	257	PHE
1	F	265	ARG
1	F	278	GLN
1	I	75	LEU
1	I	123	ASN
1	I	133	THR
1	I	137	LEU
1	I	187	LYS
1	I	209	LYS
1	I	219	ILE
1	I	228	GLN
1	I	230	GLU
1	I	237	GLU
1	I	257	PHE
1	I	265	ARG
1	I	278	GLN
1	J	123	ASN
1	J	133	THR
1	J	137	LEU
1	J	187	LYS

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Mol	Chain	Res	Type
1	J	209	LYS
1	J	215	LEU
1	J	217	ASP
1	J	228	GLN
1	J	230	GLU
1	J	237	GLU
1	J	257	PHE
1	J	265	ARG
1	J	278	GLN
1	J	281	TYR
1	K	123	ASN
1	K	133	THR
1	K	137	LEU
1	K	187	LYS
1	K	209	LYS
1	K	216	ASP
1	K	230	GLU
1	K	237	GLU
1	K	239	GLU
1	K	257	PHE
1	K	265	ARG
1	K	275	ASP
1	K	278	GLN
1	K	281	TYR
1	L	123	ASN
1	L	133	THR
1	L	137	LEU
1	L	209	LYS
1	L	230	GLU
1	L	257	PHE
1	L	265	ARG
1	L	278	GLN
1	L	281	TYR
1	M	76	LYS
1	M	123	ASN
1	M	133	THR
1	M	137	LEU
1	M	209	LYS
1	M	228	GLN
1	M	230	GLU
1	M	237	GLU
1	M	257	PHE

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Mol	Chain	Res	Type
1	M	265	ARG
1	M	278	GLN
1	N	30	ASN
1	N	53	ARG
1	N	123	ASN
1	N	133	THR
1	N	137	LEU
1	N	209	LYS
1	N	210	GLU
1	N	230	GLU
1	N	257	PHE
1	N	265	ARG
1	N	278	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	129	ASN
1	A	130	GLN
1	A	228	GLN
1	B	123	ASN
1	B	130	GLN
1	B	228	GLN
1	C	30	ASN
1	C	123	ASN
1	C	129	ASN
1	C	131	HIS
1	C	228	GLN
1	D	104	HIS
1	D	123	ASN
1	D	130	GLN
1	D	178	ASN
1	D	228	GLN
1	D	303	ASN
1	E	30	ASN
1	E	123	ASN
1	E	228	GLN
1	F	123	ASN
1	F	131	HIS
1	F	228	GLN
1	I	30	ASN

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Mol	Chain	Res	Type
1	I	123	ASN
1	I	129	ASN
1	I	130	GLN
1	I	228	GLN
1	I	303	ASN
1	J	30	ASN
1	J	104	HIS
1	J	123	ASN
1	J	178	ASN
1	J	228	GLN
1	K	104	HIS
1	K	123	ASN
1	K	129	ASN
1	K	130	GLN
1	K	228	GLN
1	L	30	ASN
1	L	123	ASN
1	L	130	GLN
1	L	228	GLN
1	L	303	ASN
1	M	30	ASN
1	M	123	ASN
1	M	228	GLN
1	M	303	ASN
1	N	30	ASN
1	N	123	ASN
1	N	130	GLN
1	N	228	GLN
1	N	303	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
2	SO4	L	307	-	4,4,4	0.34	0	6,6,6	0.17	0
2	SO4	A	307	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	D	307	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	I	307	-	4,4,4	0.35	0	6,6,6	0.17	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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	306/306 (100%)	-0.27	6 (1%) 65 36	16, 45, 106, 200	0
1	B	304/306 (99%)	-0.41	4 (1%) 77 51	11, 42, 101, 172	0
1	C	306/306 (100%)	-0.25	8 (2%) 56 27	15, 59, 114, 160	0
1	D	306/306 (100%)	-0.26	8 (2%) 56 27	17, 44, 96, 164	0
1	E	306/306 (100%)	-0.23	4 (1%) 77 51	11, 50, 97, 164	0
1	F	306/306 (100%)	-0.31	5 (1%) 72 44	22, 50, 116, 180	0
1	I	304/306 (99%)	0.41	24 (7%) 12 4	41, 100, 160, 191	0
1	J	304/306 (99%)	-0.11	10 (3%) 46 20	28, 66, 124, 170	0
1	K	305/306 (99%)	0.01	9 (2%) 50 22	34, 77, 137, 197	0
1	L	305/306 (99%)	0.46	18 (5%) 22 7	39, 97, 154, 186	0
1	M	305/306 (99%)	0.01	17 (5%) 24 8	27, 73, 133, 194	0
1	N	304/306 (99%)	-0.00	6 (1%) 65 36	29, 76, 136, 183	0
All	All	3661/3672 (99%)	-0.08	119 (3%) 46 20	11, 64, 137, 200	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	78	SER	7.4
1	B	78	SER	7.2
1	M	79	SER	6.9
1	K	79	SER	6.6
1	K	78	SER	6.4
1	J	79	SER	6.2
1	L	149	ILE	5.6
1	F	306	GLU	5.1
1	N	79	SER	5.1
1	L	79	SER	5.0
1	A	305	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	78	SER	4.8
1	A	127	GLY	4.7
1	K	305	GLY	4.6
1	F	78	SER	4.6
1	N	80	VAL	4.5
1	I	161	LYS	4.5
1	M	81	ALA	4.3
1	E	78	SER	4.1
1	M	74	ASP	4.1
1	I	80	VAL	4.0
1	K	80	VAL	4.0
1	J	127	GLY	3.9
1	C	79	SER	3.9
1	L	212	LEU	3.9
1	K	81	ALA	3.9
1	N	77	SER	3.8
1	J	80	VAL	3.7
1	E	127	GLY	3.6
1	L	199	LEU	3.6
1	I	214	ASP	3.5
1	B	77	SER	3.4
1	M	77	SER	3.4
1	J	77	SER	3.3
1	E	80	VAL	3.3
1	I	176	PHE	3.2
1	I	81	ALA	3.2
1	I	149	ILE	3.1
1	A	126	ASP	3.1
1	M	163	GLY	3.1
1	B	80	VAL	3.1
1	M	80	VAL	3.1
1	D	78	SER	3.0
1	L	80	VAL	3.0
1	M	78	SER	3.0
1	L	78	SER	2.8
1	K	77	SER	2.8
1	L	176	PHE	2.8
1	I	126	ASP	2.8
1	L	150	ASP	2.8
1	N	74	ASP	2.8
1	J	81	ALA	2.8
1	M	82	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	187	LYS	2.7
1	A	78	SER	2.7
1	I	207	TYR	2.7
1	I	127	GLY	2.7
1	C	127	GLY	2.7
1	L	155	ALA	2.6
1	I	202	LYS	2.6
1	D	305	GLY	2.6
1	K	127	GLY	2.6
1	I	203	ASN	2.6
1	K	163	GLY	2.6
1	M	197	GLU	2.6
1	I	186	PRO	2.6
1	M	126	ASP	2.6
1	I	79	SER	2.5
1	M	49	GLU	2.5
1	L	1	MET	2.5
1	J	126	ASP	2.5
1	L	232	PHE	2.5
1	D	80	VAL	2.5
1	D	306	GLU	2.5
1	A	77	SER	2.5
1	I	208	GLU	2.5
1	I	157	VAL	2.4
1	L	31	THR	2.4
1	C	81	ALA	2.4
1	B	79	SER	2.4
1	L	148	ARG	2.4
1	I	215	LEU	2.4
1	L	227	ILE	2.4
1	N	78	SER	2.4
1	D	79	SER	2.3
1	C	129	ASN	2.3
1	L	152	ILE	2.3
1	M	232	PHE	2.3
1	F	304	GLU	2.3
1	F	77	SER	2.3
1	I	216	ASP	2.2
1	J	106	SER	2.2
1	N	128	SER	2.2
1	M	303	ASN	2.2
1	D	77	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	226	ARG	2.2
1	M	198	ASP	2.2
1	I	197	GLU	2.2
1	C	80	VAL	2.2
1	M	304	GLU	2.2
1	C	128	SER	2.2
1	E	79	SER	2.2
1	I	220	ASP	2.2
1	K	75	LEU	2.2
1	D	81	ALA	2.2
1	I	16	LEU	2.2
1	L	177	GLU	2.1
1	A	79	SER	2.1
1	D	217	ASP	2.1
1	J	128	SER	2.1
1	I	232	PHE	2.1
1	J	82	LYS	2.1
1	L	222	LEU	2.1
1	F	79	SER	2.1
1	L	242	LYS	2.1
1	M	127	GLY	2.1
1	I	78	SER	2.0
1	M	106	SER	2.0
1	I	251	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	I	307	5/5	0.96	0.24	63,63,63,63	0
2	SO4	L	307	5/5	0.97	0.26	63,63,63,63	0
2	SO4	A	307	5/5	0.99	0.17	46,46,46,46	0
2	SO4	D	307	5/5	0.99	0.20	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.