



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:44 PM GMT

PDB ID : 1Q95
Title : Aspartate Transcarbamylase (ATCase) of Escherichia coli: A New Crystalline R State Bound to PALA, or to Product Analogues Phosphate and Citrate
Authors : Huang, J.; Lipscomb, W.N.
Deposited on : 2003-08-22
Resolution : 2.46 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

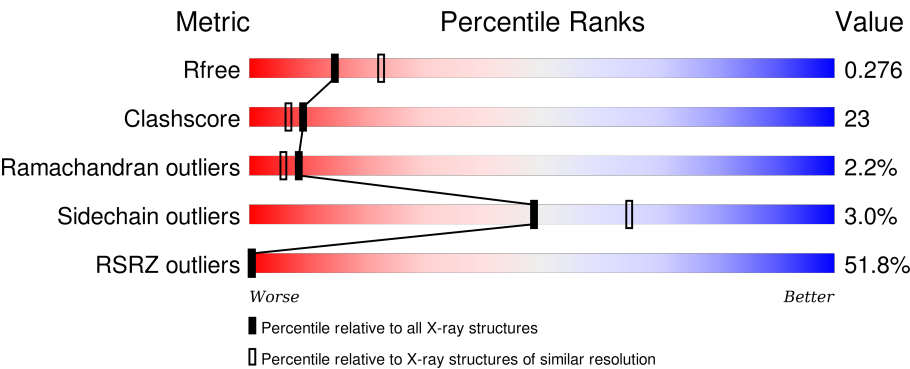
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	310	<div><div>44%</div><div>70%</div><div>27%</div><div>..</div></div>
1	B	310	<div><div>38%</div><div>71%</div><div>26%</div><div>.</div></div>
1	C	310	<div><div>46%</div><div>70%</div><div>27%</div><div>.</div></div>
1	D	310	<div><div>55%</div><div>66%</div><div>31%</div><div>.</div></div>
1	E	310	<div><div>61%</div><div>67%</div><div>30%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	F	310	<div><div><div>44%</div><div>69%</div><div>29%</div></div><div></div><div></div></div>
2	G	153	<div><div><div>49%</div><div>52%</div><div>45%</div></div><div></div><div></div></div>
2	H	153	<div><div><div>45%</div><div>54%</div><div>43%</div></div><div></div><div></div></div>
2	I	153	<div><div><div>82%</div><div>48%</div><div>48%</div></div><div></div><div></div></div>
2	J	153	<div><div><div>34%</div><div>55%</div><div>41%</div><div>5%</div></div><div></div><div></div></div>
2	K	153	<div><div><div>59%</div><div>52%</div><div>45%</div></div><div></div><div></div></div>
2	L	153	<div><div><div>89%</div><div>27%</div><div>63%</div><div>10%</div></div><div></div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22620 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 catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	B	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	D	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	E	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	F	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

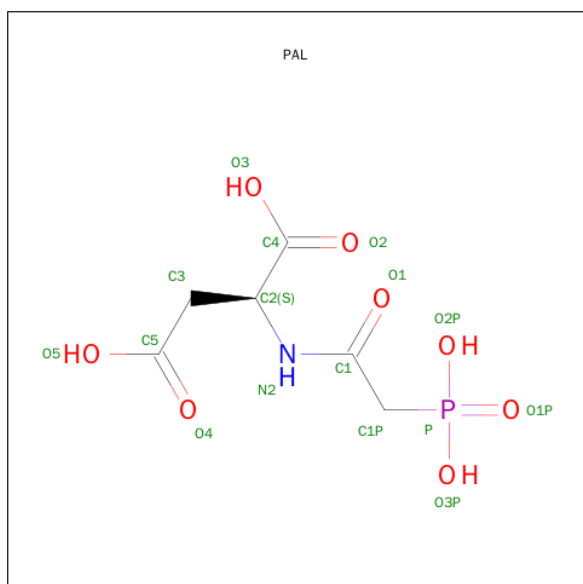
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	H	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	I	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	J	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	K	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	L	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-(PHOSPHONACETYL)-L-ASPARTIC ACID (three-letter code: PAL) (formula: $C_6H_{10}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	B	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	C	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	D	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	E	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

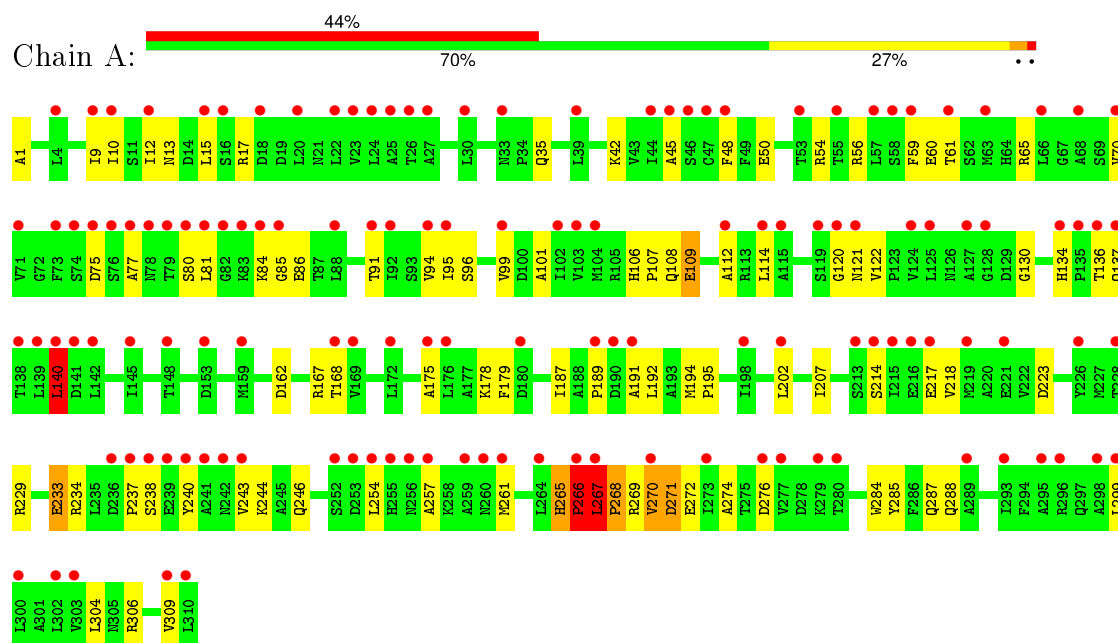
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total	O	0	0
			122	122		
5	B	120	Total	O	0	0
			120	120		
5	C	99	Total	O	0	0
			99	99		
5	D	70	Total	O	0	0
			70	70		
5	E	72	Total	O	0	0
			72	72		
5	F	128	Total	O	0	0
			128	128		
5	G	49	Total	O	0	0
			49	49		
5	H	45	Total	O	0	0
			45	45		
5	I	25	Total	O	0	0
			25	25		
5	J	41	Total	O	0	0
			41	41		
5	K	26	Total	O	0	0
			26	26		
5	L	25	Total	O	0	0
			25	25		

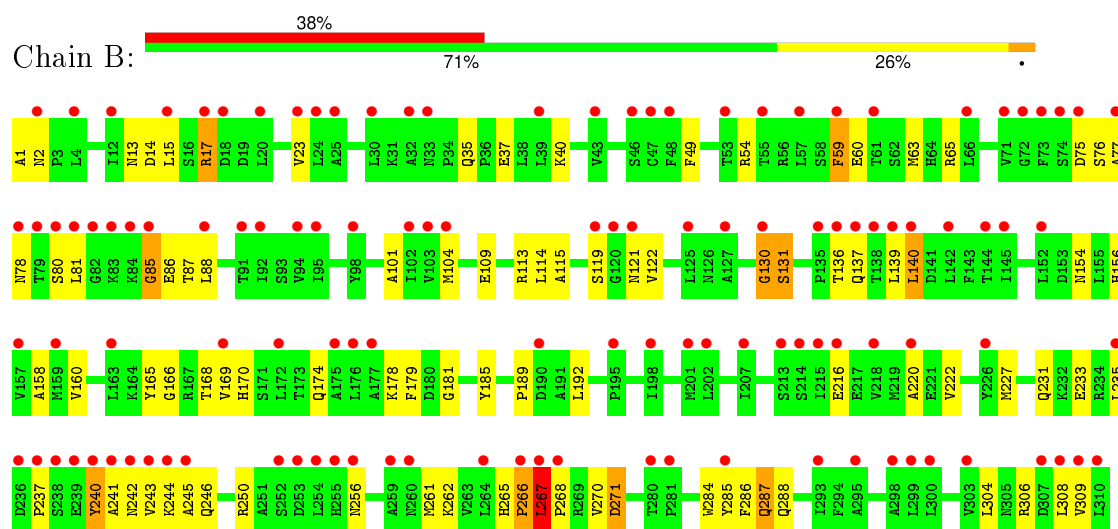
3 Residue-property plots

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

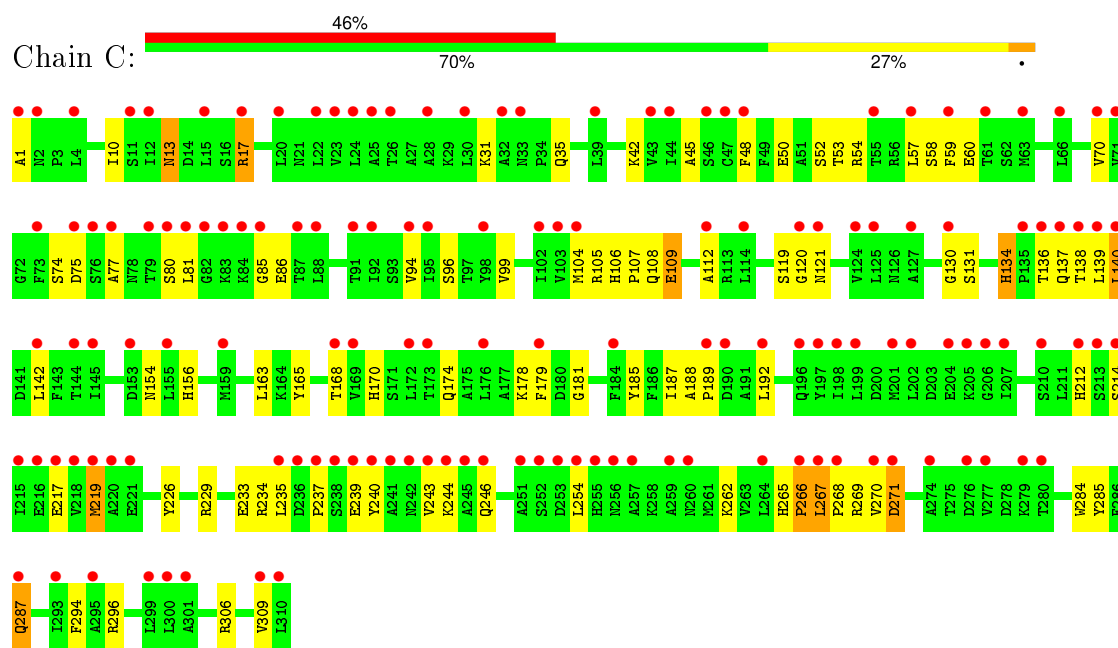
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



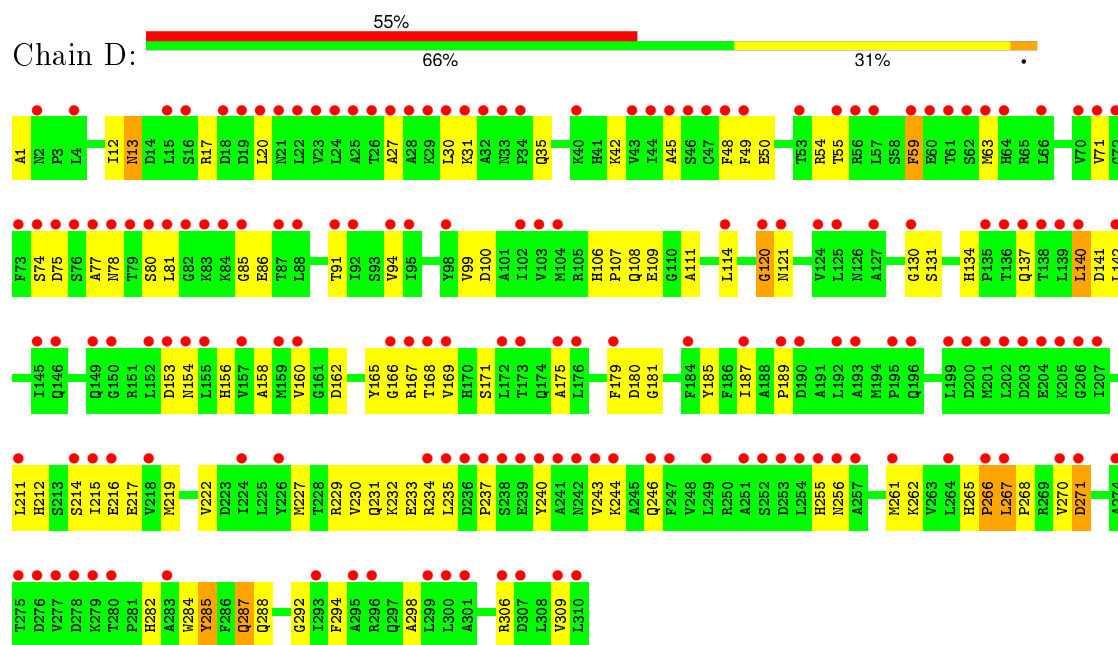
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



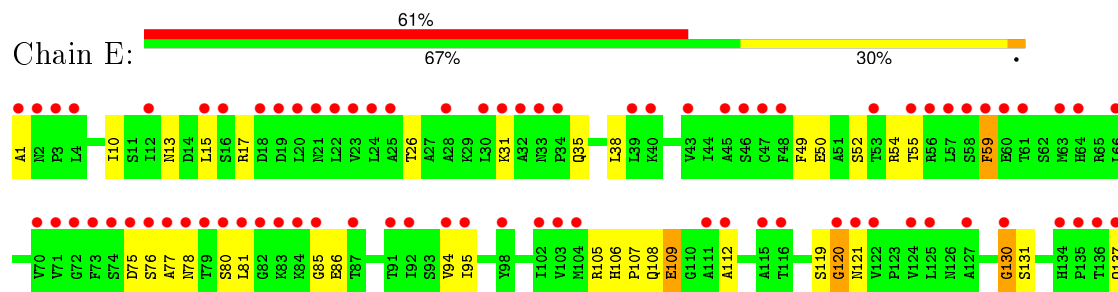
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

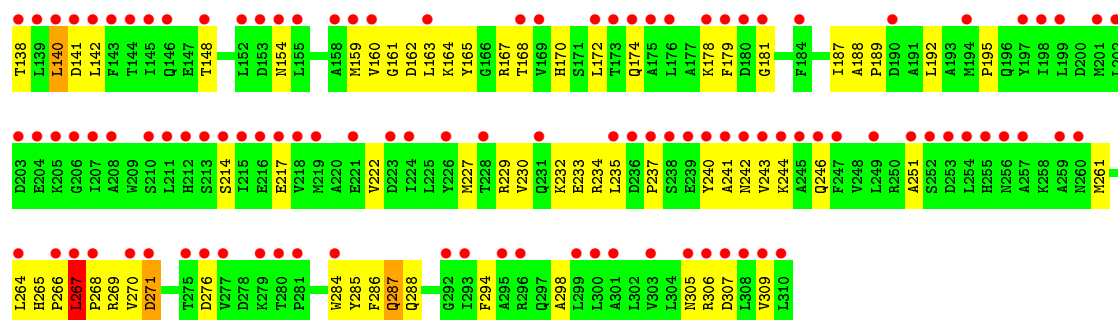


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

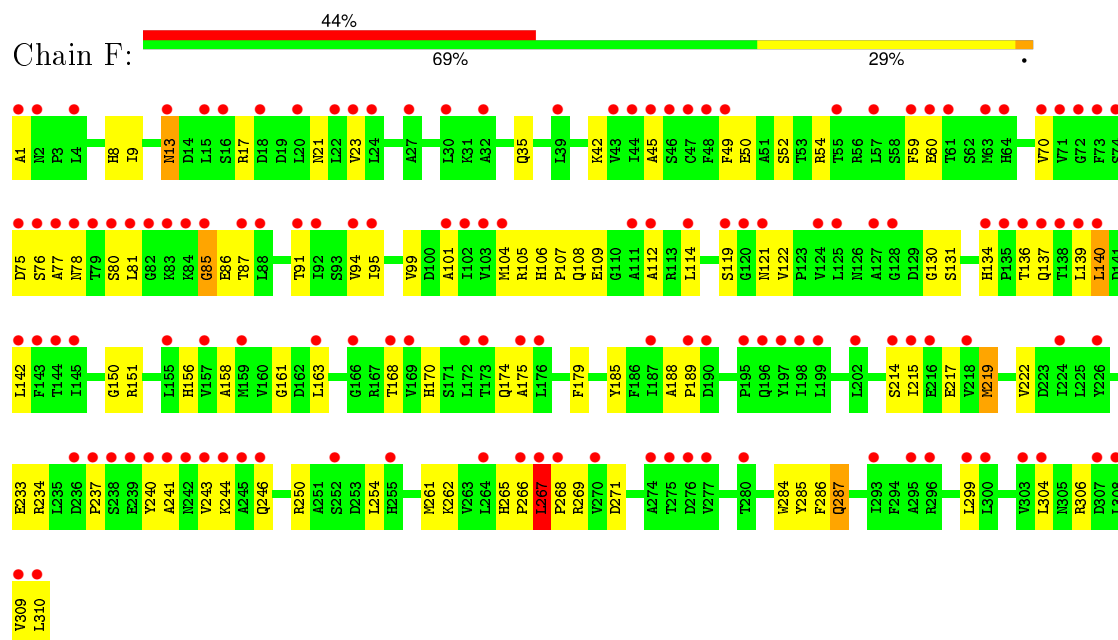


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

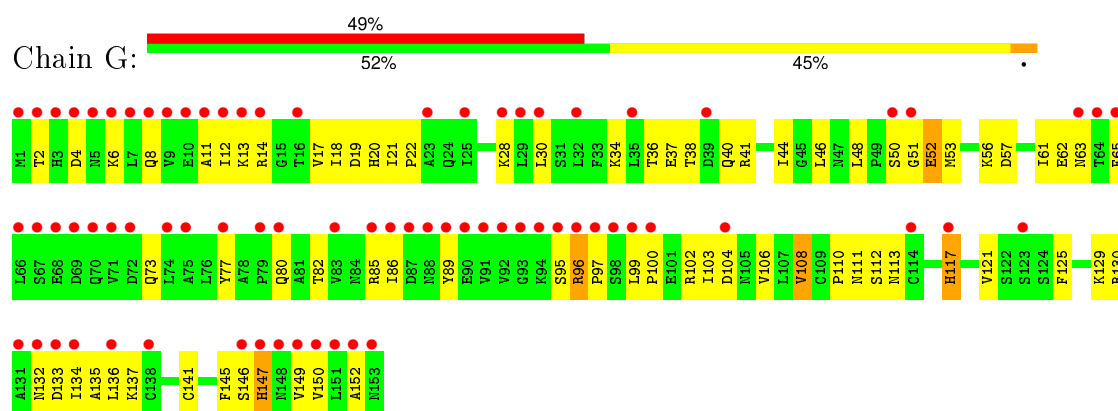




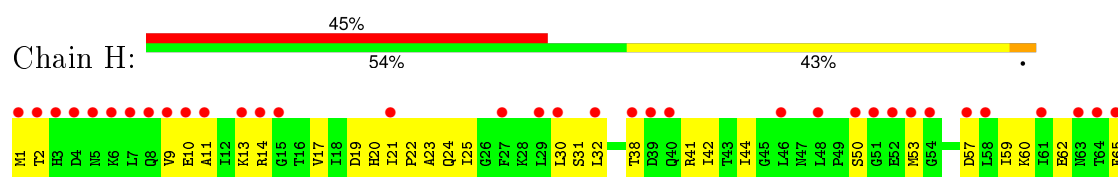
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

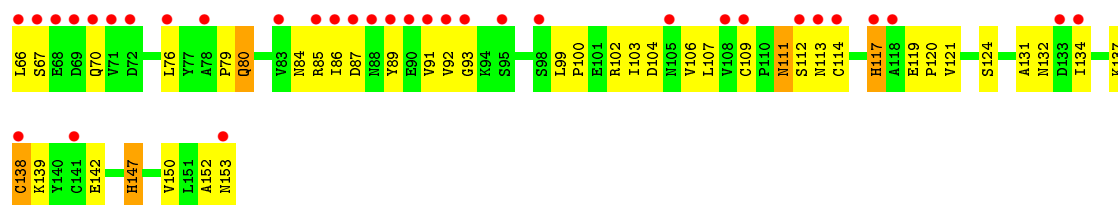


• Molecule 2: Aspartate carbamoyltransferase regulatory chain



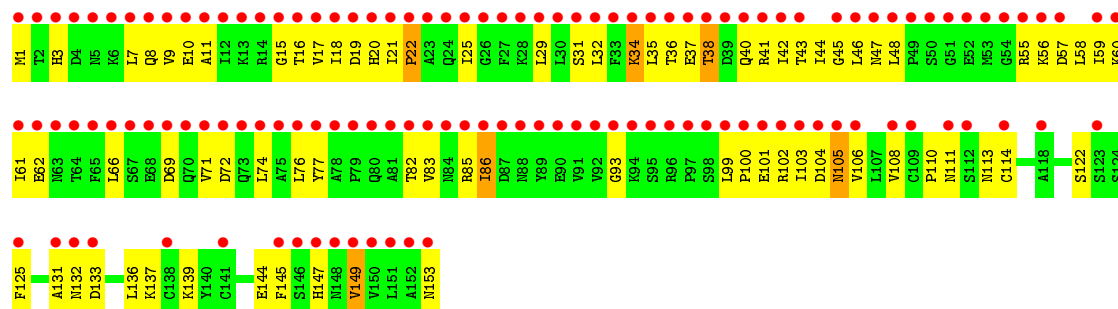
• Molecule 2: Aspartate carbamoyltransferase regulatory chain





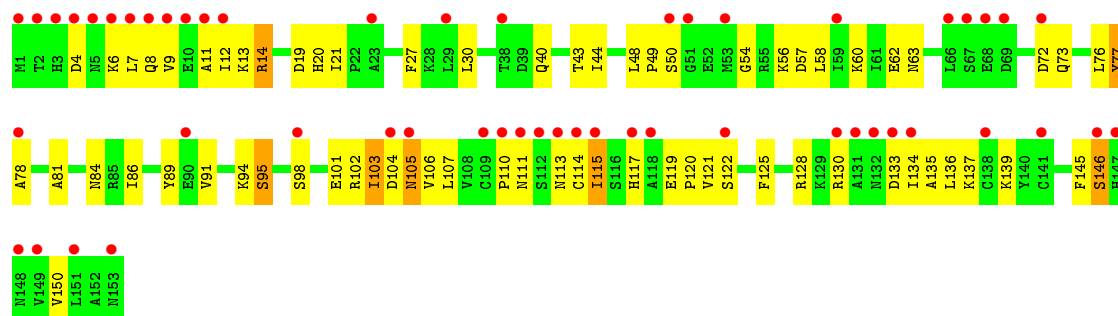
• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain I: 82% 48% 48%



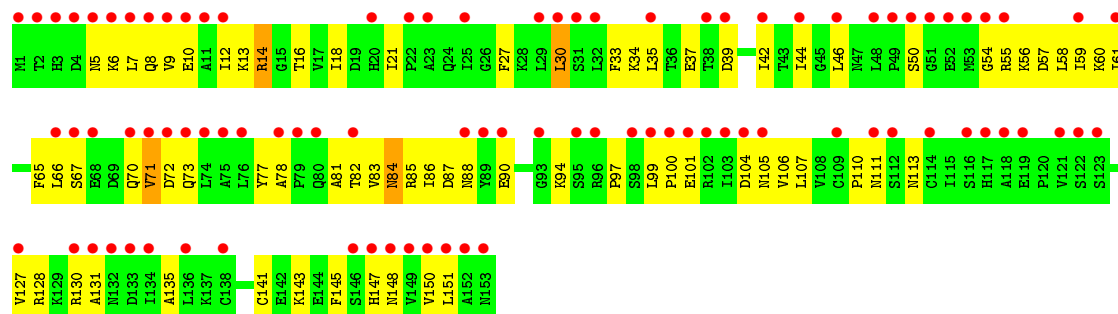
• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain J: 34% 55% 41% 5%

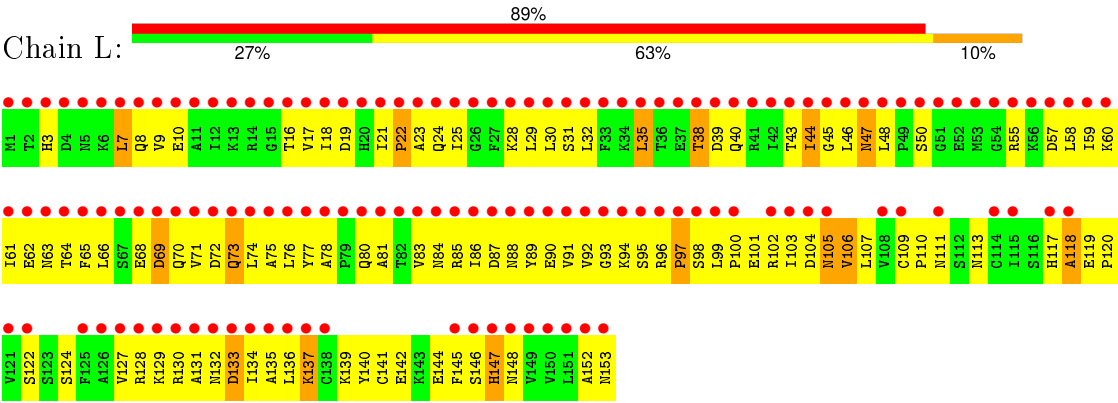


• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain K: 59% 52% 45%



• Molecule 2: Aspartate carbamoyltransferase regulatory chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.51Å 153.49Å 185.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.46 41.89 – 2.46	Depositor EDS
% Data completeness (in resolution range)	84.7 (8.00-2.46) 83.5 (41.89-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.270 0.236 , 0.276	Depositor DCC
R_{free} test set	5387 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 74.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 116771 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22620	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.44	0/2461	0.76	8/3339 (0.2%)
1	B	0.40	0/2461	0.70	3/3339 (0.1%)
1	C	0.38	0/2461	0.68	3/3339 (0.1%)
1	D	0.37	0/2461	0.65	2/3339 (0.1%)
1	E	0.35	0/2461	0.66	4/3339 (0.1%)
1	F	0.38	0/2461	0.69	3/3339 (0.1%)
2	G	0.36	0/1219	0.65	0/1647
2	H	0.36	0/1219	0.62	0/1647
2	I	0.31	0/1219	0.57	0/1647
2	J	0.36	0/1219	0.63	1/1647 (0.1%)
2	K	0.35	0/1219	0.66	1/1647 (0.1%)
2	L	0.31	0/1219	0.64	0/1647
All	All	0.37	0/22080	0.67	25/29916 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	LEU	N-CA-C	9.15	135.71	111.00
1	F	267	LEU	N-CA-C	8.21	133.16	111.00
1	B	267	LEU	N-CA-C	8.15	133.00	111.00
1	D	267	LEU	N-CA-C	8.12	132.93	111.00
1	A	267	LEU	C-N-CA	-7.68	89.75	122.00
1	E	267	LEU	N-CA-C	7.62	131.58	111.00
1	D	266	PRO	N-CA-C	-7.35	92.99	112.10
1	C	266	PRO	N-CA-C	-7.30	93.12	112.10
1	A	267	LEU	C-N-CD	7.14	143.40	128.40
1	A	267	LEU	N-CA-C	6.57	128.74	111.00
1	B	266	PRO	N-CA-C	-6.42	95.42	112.10
1	A	266	PRO	N-CA-C	-6.29	95.75	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	LEU	CA-CB-CG	-6.20	101.05	115.30
1	A	267	LEU	CA-CB-CG	-6.13	101.19	115.30
2	J	105	ASN	N-CA-C	5.71	126.42	111.00
1	F	266	PRO	N-CA-C	-5.68	97.33	112.10
1	A	140	LEU	CA-CB-CG	5.64	128.28	115.30
1	F	140	LEU	CA-CB-CG	5.49	127.92	115.30
1	E	267	LEU	C-N-CD	5.38	139.70	128.40
1	A	268	PRO	N-CA-C	-5.34	98.22	112.10
1	B	267	LEU	CA-CB-CG	-5.33	103.03	115.30
1	E	266	PRO	N-CA-C	-5.17	98.64	112.10
1	A	140	LEU	CB-CG-CD1	-5.11	102.32	111.00
2	K	71	VAL	N-CA-C	-5.10	97.22	111.00
1	E	267	LEU	CA-CB-CG	-5.02	103.75	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2422	86	0
1	B	2415	0	2422	99	0
1	C	2415	0	2422	70	0
1	D	2415	0	2422	114	0
1	E	2415	0	2422	97	0
1	F	2415	0	2422	101	0
2	G	1201	0	1219	64	0
2	H	1201	0	1219	79	0
2	I	1201	0	1219	91	0
2	J	1201	0	1219	72	0
2	K	1201	0	1219	75	0
2	L	1201	0	1219	136	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	16	0	6	1	0
4	B	16	0	6	2	0
4	C	16	0	6	0	0
4	D	16	0	6	1	0
4	E	16	0	6	1	0
4	F	16	0	6	0	0
5	A	122	0	0	4	0
5	B	120	0	0	15	0
5	C	99	0	0	9	0
5	D	70	0	0	4	0
5	E	72	0	0	8	0
5	F	128	0	0	15	0
5	G	49	0	0	1	0
5	H	45	0	0	2	0
5	I	25	0	0	2	0
5	J	41	0	0	3	0
5	K	26	0	0	2	0
5	L	25	0	0	6	0
All	All	22620	0	21882	1005	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 23.

All (1005) 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:B:241:ALA:HB2	1:F:241:ALA:HB2	1.25	1.18
2:L:10:GLU:HB3	2:L:16:THR:HG21	1.22	1.18
2:J:84:ASN:HD21	2:J:94:LYS:HD3	1.18	1.09
1:B:114:LEU:HD21	2:H:119:GLU:HG2	1.36	1.07
2:K:30:LEU:HD21	2:K:44:ILE:HD13	1.31	1.06
1:B:81:LEU:HA	1:B:86:GLU:HB3	1.35	1.06
1:A:81:LEU:HA	1:A:86:GLU:HB3	1.38	1.05
2:L:72:ASP:HB3	2:L:100:PRO:HG3	1.38	1.04
1:B:60:GLU:HA	1:B:63:MET:HE3	1.40	1.03
2:L:50:SER:HB2	2:L:55:ARG:HG2	1.39	1.02
1:B:60:GLU:HA	1:B:63:MET:CE	1.91	0.99
2:H:102:ARG:HH11	2:H:139:LYS:HE3	1.28	0.98
2:H:30:LEU:HD21	2:H:44:ILE:HD13	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:VAL:HG11	1:E:54:ARG:HG2	1.46	0.95
2:I:10:GLU:HG2	2:I:11:ALA:H	1.30	0.95
1:F:81:LEU:HA	1:F:86:GLU:HB3	1.48	0.94
2:I:21:ILE:HB	2:I:57:ASP:HB2	1.50	0.94
1:D:81:LEU:HA	1:D:86:GLU:HB3	1.51	0.93
2:L:32:LEU:HD22	2:L:152:ALA:HB3	1.48	0.92
2:L:101:GLU:HA	2:L:127:VAL:HG22	1.53	0.91
2:L:105:ASN:OD1	2:L:122:SER:HB3	1.71	0.91
1:C:267:LEU:HD21	1:C:285:TYR:HB2	1.51	0.91
1:B:54:ARG:HD3	1:B:267:LEU:HB2	1.51	0.90
2:I:15:GLY:HA3	2:I:62:GLU:HA	1.52	0.90
2:K:128:ARG:HH11	2:K:128:ARG:HB3	1.37	0.89
2:L:87:ASP:HB2	2:L:92:VAL:HG21	1.54	0.89
2:J:7:LEU:HD22	2:J:48:LEU:HB3	1.55	0.89
2:L:44:ILE:HG22	2:L:45:GLY:H	1.37	0.88
2:H:67:SER:H	2:H:70:GLN:HE21	1.20	0.88
1:C:81:LEU:HA	1:C:86:GLU:HB3	1.55	0.87
1:E:243:VAL:HG13	1:E:244:LYS:HD2	1.57	0.87
2:I:46:LEU:HD21	2:I:58:LEU:H	1.39	0.87
2:K:67:SER:HB3	2:K:85:ARG:NH2	1.88	0.87
1:E:81:LEU:HA	1:E:86:GLU:HB3	1.55	0.87
2:I:76:LEU:HD22	2:I:103:ILE:HD13	1.57	0.86
1:B:109:GLU:HG3	1:B:130:GLY:O	1.75	0.85
2:L:71:VAL:HG22	2:L:97:PRO:HG2	1.58	0.85
1:D:94:VAL:HG11	1:E:54:ARG:CG	2.06	0.84
1:C:54:ARG:HD3	1:C:267:LEU:HB2	1.60	0.84
2:L:21:ILE:HB	2:L:57:ASP:HB2	1.60	0.83
1:B:85:GLY:HA2	5:B:1119:HOH:O	1.79	0.83
1:E:237:PRO:HA	1:E:240:TYR:CE2	2.13	0.82
1:D:267:LEU:HD21	1:D:285:TYR:HB2	1.59	0.82
1:E:159:MET:HE2	1:E:172:LEU:HD23	1.59	0.82
1:E:284:TRP:CD2	1:E:287:GLN:HG3	2.15	0.82
1:C:42:LYS:HE3	5:C:1015:HOH:O	1.80	0.82
1:F:243:VAL:HG13	1:F:244:LYS:HD2	1.61	0.82
2:J:14:ARG:HA	2:J:86:ILE:O	1.79	0.82
1:B:241:ALA:CB	1:F:241:ALA:HB2	2.09	0.81
2:G:12:ILE:HG22	2:G:13:LYS:H	1.46	0.81
1:A:265:HIS:ND1	1:A:266:PRO:O	2.13	0.81
2:L:81:ALA:N	2:L:96:ARG:HH12	1.79	0.81
2:I:48:LEU:HD11	2:I:58:LEU:HG	1.63	0.80
1:F:310:LEU:HG	5:F:1046:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:VAL:HG22	2:H:60:LYS:HG2	1.65	0.79
1:D:237:PRO:HA	1:D:240:TYR:CE2	2.17	0.79
2:J:12:ILE:HD11	2:J:62:GLU:HA	1.63	0.79
1:B:284:TRP:CE2	1:B:287:GLN:HG3	2.19	0.78
2:H:13:LYS:HD3	2:H:89:TYR:CE1	2.18	0.78
2:J:12:ILE:HD11	2:J:62:GLU:CA	2.12	0.78
1:D:108:GLN:HG3	2:J:113:ASN:ND2	2.00	0.77
2:K:130:ARG:NE	2:K:135:ALA:HB2	1.99	0.77
1:D:284:TRP:CE2	1:D:287:GLN:HG3	2.20	0.77
2:L:72:ASP:CB	2:L:100:PRO:HG3	2.15	0.77
1:A:35:GLN:NE2	1:A:309:VAL:HG13	1.99	0.76
2:I:108:VAL:HG21	2:I:153:ASN:HD22	1.50	0.76
1:E:35:GLN:NE2	1:E:309:VAL:HG13	2.00	0.76
1:C:119:SER:C	5:C:1042:HOH:O	2.23	0.76
2:L:61:ILE:HB	2:L:63:ASN:HD21	1.48	0.76
2:H:102:ARG:NH1	2:H:139:LYS:HE3	2.02	0.75
2:I:20:HIS:HA	2:I:56:LYS:HG3	1.66	0.75
1:A:121:ASN:HB3	5:A:1070:HOH:O	1.86	0.75
1:A:54:ARG:HD3	1:A:267:LEU:HB2	1.68	0.75
2:J:84:ASN:ND2	2:J:94:LYS:HD3	1.97	0.75
2:H:99:LEU:HD12	2:H:100:PRO:HD2	1.69	0.75
1:C:189:PRO:HB3	1:C:246:GLN:NE2	2.01	0.75
1:C:284:TRP:CE2	1:C:287:GLN:HG3	2.22	0.75
2:I:19:ASP:HB2	2:I:82:THR:HG23	1.70	0.74
2:L:31:SER:O	2:L:32:LEU:HD23	1.87	0.74
1:A:243:VAL:HG13	1:A:244:LYS:HD2	1.69	0.74
2:I:99:LEU:HD12	2:I:100:PRO:HD2	1.68	0.74
1:B:243:VAL:HG13	1:B:244:LYS:HD2	1.67	0.74
2:I:111:ASN:HD22	2:I:114:CYS:HB2	1.52	0.74
1:A:257:ALA:HB1	1:A:261:MET:CE	2.17	0.74
5:B:1055:HOH:O	2:H:137:LYS:HE2	1.88	0.74
2:L:10:GLU:CB	2:L:16:THR:HG21	2.13	0.73
2:I:10:GLU:HA	2:I:44:ILE:HD12	1.70	0.73
1:A:265:HIS:C	1:A:266:PRO:O	2.23	0.73
2:K:34:LYS:HE2	2:K:37:GLU:OE1	1.88	0.73
1:D:31:LYS:HE2	1:D:294:PHE:CE2	2.24	0.73
1:B:267:LEU:HD12	1:C:94:VAL:CG1	2.19	0.73
1:F:35:GLN:NE2	1:F:309:VAL:HG13	2.04	0.73
1:D:54:ARG:HD3	1:D:267:LEU:HB2	1.70	0.73
2:I:61:ILE:HG22	2:I:62:GLU:H	1.53	0.72
1:D:42:LYS:HE3	5:D:1018:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:105:ASN:OD1	2:J:122:SER:HB3	1.88	0.72
1:F:287:GLN:HE21	1:F:287:GLN:H	1.37	0.72
2:L:25:ILE:HG23	2:L:28:LYS:HB2	1.70	0.72
1:B:75:ASP:HB3	5:B:1069:HOH:O	1.89	0.72
1:D:114:LEU:HG	2:J:115:ILE:HG21	1.72	0.72
2:J:7:LEU:HD23	2:J:49:PRO:HD2	1.71	0.71
2:J:58:LEU:HD21	2:J:60:LYS:HE3	1.71	0.71
1:F:170:HIS:O	1:F:174:GLN:HG3	1.89	0.71
2:I:35:LEU:HD22	2:I:40:GLN:HG3	1.72	0.71
1:C:121:ASN:HA	5:C:1033:HOH:O	1.88	0.71
2:L:69:ASP:HA	5:L:2023:HOH:O	1.90	0.71
2:L:8:GLN:HG3	5:L:2024:HOH:O	1.89	0.71
2:J:84:ASN:HD21	2:J:94:LYS:CD	2.01	0.71
2:J:13:LYS:HB2	2:J:89:TYR:CZ	2.25	0.71
1:B:119:SER:C	5:B:1051:HOH:O	2.27	0.71
1:B:265:HIS:CD2	1:B:266:PRO:O	2.44	0.71
1:D:35:GLN:NE2	1:D:309:VAL:HG13	2.06	0.71
2:K:70:GLN:HG3	2:K:73:GLN:HE21	1.55	0.71
2:J:9:VAL:HG13	2:J:43:THR:HG21	1.71	0.70
2:H:109:CYS:HB2	2:H:138:CYS:SG	2.30	0.70
2:G:28:LYS:HD3	2:G:77:TYR:OH	1.92	0.70
1:B:54:ARG:HD3	1:B:267:LEU:CB	2.20	0.70
2:H:111:ASN:ND2	2:H:113:ASN:H	1.89	0.70
2:I:46:LEU:CD2	2:I:58:LEU:H	2.05	0.70
2:L:43:THR:HB	2:L:60:LYS:O	1.92	0.70
1:B:54:ARG:CD	1:B:267:LEU:HB2	2.19	0.70
1:D:243:VAL:HG13	1:D:244:LYS:HD2	1.73	0.70
1:F:287:GLN:NE2	1:F:287:GLN:H	1.90	0.70
2:G:41:ARG:HD3	5:J:2024:HOH:O	1.90	0.70
2:K:99:LEU:HD22	2:K:127:VAL:HG11	1.74	0.70
1:F:78:ASN:HB2	5:F:1047:HOH:O	1.92	0.70
1:C:237:PRO:HA	1:C:240:TYR:CE2	2.26	0.70
1:C:214:SER:OG	1:C:217:GLU:HG3	1.92	0.69
1:A:130:GLY:O	1:A:167:ARG:HD3	1.91	0.69
1:C:284:TRP:CD2	1:C:287:GLN:HG3	2.27	0.69
2:I:56:LYS:HE2	2:I:58:LEU:HD21	1.73	0.69
1:C:189:PRO:HB3	1:C:246:GLN:HE22	1.55	0.69
2:L:50:SER:HA	2:L:55:ARG:HA	1.73	0.69
1:B:60:GLU:HA	1:B:63:MET:HE2	1.75	0.69
2:J:30:LEU:HD11	2:J:44:ILE:HD13	1.74	0.69
1:C:108:GLN:HG3	5:I:2007:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:GLU:HG2	2:I:11:ALA:N	2.07	0.68
1:B:114:LEU:CD2	2:H:119:GLU:HG2	2.19	0.68
1:F:76:SER:HB2	5:F:1029:HOH:O	1.92	0.68
2:L:73:GLN:NE2	2:L:106:VAL:HG21	2.08	0.68
2:L:19:ASP:O	2:L:21:ILE:HG13	1.93	0.68
2:K:50:SER:HB2	2:K:56:LYS:HG2	1.75	0.68
1:F:243:VAL:HG13	1:F:244:LYS:CD	2.24	0.68
1:A:214:SER:OG	1:A:217:GLU:HG3	1.94	0.68
1:F:23:VAL:HG11	1:F:139:LEU:HD13	1.76	0.67
1:E:159:MET:CE	1:E:172:LEU:HD23	2.22	0.67
2:L:61:ILE:HB	2:L:63:ASN:ND2	2.08	0.67
1:B:220:ALA:HB2	1:B:256:ASN:ND2	2.09	0.67
1:A:189:PRO:HB3	1:A:246:GLN:NE2	2.10	0.67
1:E:243:VAL:HG13	1:E:244:LYS:CD	2.23	0.67
2:H:41:ARG:HD3	2:H:62:GLU:OE2	1.95	0.67
1:F:49:PHE:HE2	1:F:81:LEU:HD13	1.59	0.67
1:D:111:ALA:HB2	2:J:115:ILE:HD11	1.77	0.67
1:F:189:PRO:HB3	1:F:246:GLN:NE2	2.10	0.67
2:L:128:ARG:HB3	2:L:128:ARG:NH1	2.10	0.67
1:F:284:TRP:CE2	1:F:287:GLN:HG3	2.31	0.66
1:B:192:LEU:HD11	1:B:242:ASN:HB3	1.77	0.66
2:I:85:ARG:HG2	5:I:2020:HOH:O	1.95	0.66
2:K:84:ASN:N	2:K:84:ASN:HD22	1.93	0.66
2:L:44:ILE:HG22	2:L:45:GLY:N	2.09	0.66
1:E:140:LEU:HD21	1:E:288:GLN:HG2	1.76	0.66
1:F:119:SER:C	5:F:1054:HOH:O	2.33	0.66
2:L:75:ALA:HB1	2:L:99:LEU:HD23	1.77	0.66
1:C:287:GLN:H	1:C:287:GLN:NE2	1.94	0.66
1:B:241:ALA:HB2	1:F:241:ALA:CB	2.15	0.66
2:J:9:VAL:HG13	2:J:43:THR:CG2	2.25	0.66
1:B:23:VAL:HG11	1:B:139:LEU:HD13	1.77	0.66
2:L:85:ARG:HH21	2:L:93:GLY:HA3	1.60	0.66
1:D:81:LEU:HD12	1:D:91:THR:OG1	1.96	0.66
2:K:70:GLN:CG	2:K:73:GLN:HE21	2.08	0.66
2:L:72:ASP:OD1	2:L:97:PRO:HB3	1.95	0.65
2:G:36:THR:HG21	2:J:27:PHE:CD2	2.31	0.65
1:E:15:LEU:O	1:E:178:LYS:HE3	1.96	0.65
1:B:114:LEU:CD1	2:H:121:VAL:HG11	2.25	0.65
1:D:49:PHE:HE2	1:D:81:LEU:HD13	1.61	0.65
2:I:10:GLU:CG	2:I:11:ALA:H	2.06	0.65
2:I:9:VAL:HG13	2:I:47:ASN:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:GLN:HE22	1:F:309:VAL:HG13	1.60	0.65
2:L:17:VAL:HG21	5:L:2007:HOH:O	1.96	0.65
2:H:79:PRO:HD2	2:H:80:GLN:NE2	2.12	0.65
1:A:81:LEU:HD11	5:A:1017:HOH:O	1.96	0.65
2:L:32:LEU:HD22	2:L:152:ALA:CB	2.26	0.65
1:B:75:ASP:OD2	1:B:77:ALA:HB3	1.96	0.65
2:K:33:PHE:HB2	2:K:35:LEU:HG	1.77	0.64
1:B:166:GLY:O	1:B:169:VAL:HG22	1.96	0.64
2:L:72:ASP:HB3	2:L:100:PRO:CG	2.23	0.64
2:H:30:LEU:HD13	2:H:59:ILE:HD13	1.78	0.64
2:H:30:LEU:HD21	2:H:44:ILE:CD1	2.25	0.64
1:F:237:PRO:HA	1:F:240:TYR:CE2	2.32	0.64
1:D:108:GLN:HB3	2:J:115:ILE:HD12	1.79	0.64
2:H:152:ALA:O	2:H:153:ASN:HB2	1.96	0.64
1:D:45:ALA:HB2	1:D:99:VAL:HG11	1.79	0.64
1:D:284:TRP:CD2	1:D:287:GLN:HG3	2.32	0.64
1:B:216:GLU:HG3	5:B:1046:HOH:O	1.97	0.64
2:I:131:ALA:O	2:I:132:ASN:HB2	1.97	0.64
1:E:154:ASN:HA	1:E:181:GLY:O	1.98	0.64
1:B:109:GLU:CG	1:B:130:GLY:O	2.44	0.64
2:K:16:THR:OG1	2:K:65:PHE:HA	1.96	0.64
1:C:265:HIS:CD2	1:C:266:PRO:O	2.50	0.64
2:L:104:ASP:OD1	2:L:124:SER:HB2	1.97	0.64
1:C:240:TYR:O	1:C:243:VAL:HG12	1.97	0.64
1:F:189:PRO:HB3	1:F:246:GLN:HE22	1.62	0.64
1:E:94:VAL:CG1	1:F:267:LEU:HD12	2.27	0.64
1:C:229:ARG:HD3	1:C:268:PRO:O	1.98	0.64
2:J:133:ASP:OD1	2:J:146:SER:HB2	1.98	0.64
2:K:70:GLN:OE1	2:K:72:ASP:HB2	1.98	0.63
2:K:67:SER:HB3	2:K:85:ARG:HH22	1.63	0.63
2:I:58:LEU:O	2:I:60:LYS:HG3	1.98	0.63
1:A:35:GLN:HE22	1:A:309:VAL:HG13	1.62	0.63
1:B:237:PRO:HA	1:B:240:TYR:CE2	2.33	0.63
1:A:1:ALA:HA	1:A:306:ARG:HG2	1.80	0.63
1:E:284:TRP:CE2	1:E:287:GLN:HG3	2.33	0.63
2:K:83:VAL:C	2:K:84:ASN:HD22	2.02	0.63
2:I:56:LYS:HE2	2:I:58:LEU:CD2	2.28	0.62
1:D:229:ARG:HD3	1:D:268:PRO:O	1.99	0.62
2:K:110:PRO:HB2	2:K:145:PHE:CE2	2.33	0.62
1:A:237:PRO:HA	1:A:240:TYR:CE2	2.34	0.62
1:F:81:LEU:HD22	5:F:1029:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:76:LEU:HD23	2:J:134:ILE:HD12	1.81	0.62
1:F:284:TRP:CD2	1:F:287:GLN:HG3	2.34	0.62
2:G:30:LEU:HD11	2:G:44:ILE:HD13	1.82	0.62
1:F:42:LYS:HE3	5:F:1086:HOH:O	1.99	0.62
1:E:137:GLN:HG2	1:E:168:THR:HG22	1.81	0.62
1:D:261:MET:HG2	1:D:262:LYS:N	2.14	0.62
1:E:49:PHE:HE2	1:E:81:LEU:HD13	1.63	0.62
2:L:71:VAL:HG23	2:L:83:VAL:HG21	1.82	0.62
1:F:85:GLY:HA2	5:F:1062:HOH:O	2.00	0.62
2:I:61:ILE:HG22	2:I:62:GLU:N	2.14	0.62
1:F:158:ALA:HB2	1:F:222:VAL:HG11	1.81	0.62
1:D:140:LEU:HD23	1:D:141:ASP:N	2.14	0.62
1:F:137:GLN:HG2	1:F:168:THR:HG22	1.81	0.61
2:I:56:LYS:HG2	2:I:57:ASP:N	2.15	0.61
2:H:76:LEU:HD23	2:H:99:LEU:HD11	1.82	0.61
1:A:114:LEU:HD22	2:G:121:VAL:HG11	1.81	0.61
2:H:10:GLU:HG2	2:H:11:ALA:N	2.14	0.61
1:F:267:LEU:HD11	1:F:286:PHE:CD1	2.34	0.61
2:H:14:ARG:HA	2:H:86:ILE:O	2.01	0.61
2:J:130:ARG:HD2	2:J:135:ALA:HB2	1.80	0.61
1:F:75:ASP:OD2	1:F:77:ALA:HB3	2.00	0.61
1:E:189:PRO:HB3	1:E:246:GLN:NE2	2.16	0.61
1:F:17:ARG:HD2	1:F:179:PHE:CE1	2.35	0.61
2:H:107:LEU:HB3	2:H:150:VAL:HG12	1.82	0.61
2:I:111:ASN:ND2	2:I:114:CYS:HB2	2.16	0.61
2:K:50:SER:HB3	2:K:54:GLY:H	1.64	0.61
2:I:101:GLU:HG3	2:I:102:ARG:N	2.16	0.61
1:A:257:ALA:HB1	1:A:261:MET:HE2	1.82	0.61
2:L:128:ARG:NH2	5:L:2008:HOH:O	2.34	0.61
1:E:267:LEU:O	1:E:269:ARG:N	2.34	0.61
2:I:76:LEU:HD22	2:I:103:ILE:CD1	2.30	0.61
1:D:75:ASP:OD2	1:D:77:ALA:HB3	2.01	0.61
2:H:1:MET:CE	2:H:91:VAL:HG12	2.31	0.61
2:I:48:LEU:HD21	2:I:58:LEU:HD11	1.82	0.60
2:G:129:LYS:HD3	5:G:2030:HOH:O	2.00	0.60
2:I:15:GLY:O	2:I:86:ILE:HA	2.01	0.60
2:I:104:ASP:O	2:I:106:VAL:HG23	2.01	0.60
2:L:99:LEU:CD1	2:L:129:LYS:HB2	2.31	0.60
1:A:17:ARG:HD2	1:A:179:PHE:CD1	2.36	0.60
1:D:287:GLN:NE2	5:D:1010:HOH:O	2.34	0.60
1:E:167:ARG:HG2	5:E:1026:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:130:ARG:CZ	2:L:135:ALA:HB2	2.32	0.60
1:F:309:VAL:HG23	5:F:1026:HOH:O	2.02	0.60
1:F:267:LEU:O	1:F:269:ARG:N	2.34	0.60
2:I:137:LYS:HB2	2:I:144:GLU:HG3	1.84	0.60
2:I:56:LYS:HG2	2:I:57:ASP:H	1.67	0.59
2:L:65:PHE:H	2:L:65:PHE:HD1	1.49	0.59
1:C:75:ASP:OD2	1:C:77:ALA:HB3	2.01	0.59
1:D:189:PRO:HB3	1:D:246:GLN:NE2	2.17	0.59
2:H:91:VAL:HG13	2:H:91:VAL:O	2.03	0.59
1:A:202:LEU:HD22	1:A:207:ILE:HG21	1.83	0.59
2:G:130:ARG:CZ	2:G:135:ALA:HB2	2.32	0.59
1:B:243:VAL:HG13	1:B:244:LYS:CD	2.32	0.59
2:G:19:ASP:OD2	2:G:20:HIS:N	2.35	0.59
2:I:19:ASP:OD1	2:I:58:LEU:HD22	2.02	0.59
2:H:92:VAL:HG23	2:H:93:GLY:N	2.18	0.59
1:D:106:HIS:ND1	1:D:107:PRO:HD2	2.17	0.59
2:H:80:GLN:NE2	2:H:80:GLN:H	2.00	0.59
1:C:1:ALA:HA	1:C:306:ARG:HG2	1.84	0.59
2:G:110:PRO:HD2	2:G:145:PHE:CE2	2.37	0.59
1:D:243:VAL:HG13	1:D:244:LYS:CD	2.33	0.58
2:I:102:ARG:NH2	2:I:139:LYS:HD3	2.18	0.58
2:L:58:LEU:O	2:L:59:ILE:HG13	2.03	0.58
2:K:128:ARG:NH1	2:K:128:ARG:HB3	2.15	0.58
2:J:12:ILE:HD11	2:J:62:GLU:CB	2.32	0.58
2:J:115:ILE:HG23	2:J:119:GLU:HG3	1.85	0.58
1:A:254:LEU:HD22	1:A:261:MET:CE	2.33	0.58
2:J:111:ASN:HD22	2:J:114:CYS:HB2	1.67	0.58
1:B:220:ALA:HB2	1:B:256:ASN:HD22	1.67	0.58
1:D:140:LEU:C	1:D:140:LEU:HD23	2.24	0.58
5:B:1053:HOH:O	2:H:139:LYS:CB	2.51	0.58
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.84	0.58
2:I:31:SER:O	2:I:34:LYS:HG3	2.03	0.58
2:H:111:ASN:HD22	2:H:112:SER:N	2.02	0.58
1:D:261:MET:CE	1:D:282:HIS:HB3	2.33	0.58
2:K:67:SER:HB3	2:K:85:ARG:HH21	1.64	0.58
1:D:108:GLN:CB	2:J:115:ILE:HD12	2.33	0.58
1:E:170:HIS:O	1:E:174:GLN:HG3	2.03	0.58
1:A:194:MET:SD	1:A:195:PRO:HD2	2.43	0.58
1:F:104:MET:HE1	1:F:112:ALA:HA	1.85	0.58
2:K:55:ARG:HG2	2:K:55:ARG:HH11	1.68	0.58
2:J:110:PRO:HD2	2:J:145:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:30:LEU:HD21	2:K:44:ILE:CD1	2.21	0.57
1:F:121:ASN:HB3	5:F:1115:HOH:O	2.04	0.57
1:E:148:THR:HB	5:E:1050:HOH:O	2.03	0.57
1:D:114:LEU:CD2	2:J:121:VAL:HG11	2.33	0.57
2:H:67:SER:H	2:H:70:GLN:NE2	1.98	0.57
2:L:65:PHE:HD2	2:L:85:ARG:HD2	1.70	0.57
2:H:84:ASN:HB3	2:H:91:VAL:HG23	1.85	0.57
1:C:154:ASN:HA	1:C:181:GLY:O	2.04	0.57
1:F:49:PHE:CE2	1:F:81:LEU:HD13	2.40	0.57
1:E:80:SER:HB2	1:F:54:ARG:NH2	2.19	0.57
1:E:50:GLU:CD	1:E:234:ARG:HH22	2.07	0.57
1:D:214:SER:OG	1:D:217:GLU:HG3	2.04	0.57
1:B:35:GLN:NE2	1:B:309:VAL:HG13	2.19	0.57
2:H:119:GLU:HG3	2:H:120:PRO:HD2	1.87	0.57
1:E:240:TYR:O	1:E:243:VAL:HG12	2.05	0.57
2:G:13:LYS:HG3	2:G:89:TYR:CE1	2.39	0.57
1:A:134:HIS:CE1	1:A:137:GLN:HB2	2.39	0.57
2:I:43:THR:O	2:L:47:ASN:HB2	2.04	0.57
1:A:271:ASP:CG	1:A:271:ASP:O	2.40	0.57
1:D:229:ARG:HE	1:D:268:PRO:HB2	1.68	0.57
1:B:14:ASP:OD2	1:B:113:ARG:NH2	2.35	0.57
2:I:22:PRO:HB2	2:I:25:ILE:HG13	1.87	0.57
2:L:87:ASP:CB	2:L:92:VAL:HG21	2.31	0.57
1:C:239:GLU:HA	5:C:1036:HOH:O	2.03	0.57
1:D:17:ARG:HD2	1:D:179:PHE:CD1	2.39	0.57
1:F:240:TYR:O	1:F:243:VAL:HG12	2.05	0.57
1:A:106:HIS:HE1	1:A:108:GLN:OE1	1.88	0.57
2:I:149:VAL:HG12	2:I:149:VAL:O	2.05	0.57
1:B:114:LEU:HD11	2:H:121:VAL:HG11	1.86	0.56
2:K:128:ARG:HH11	2:K:128:ARG:CB	2.14	0.56
1:A:257:ALA:CB	1:A:261:MET:CE	2.82	0.56
2:L:46:LEU:HD22	2:L:57:ASP:HB3	1.86	0.56
2:K:100:PRO:O	2:K:127:VAL:HB	2.06	0.56
2:I:41:ARG:C	2:I:42:ILE:HD12	2.25	0.56
1:B:137:GLN:HG2	1:B:168:THR:HG22	1.87	0.56
1:D:20:LEU:HD13	1:D:142:LEU:HD11	1.88	0.56
1:E:267:LEU:HD11	1:E:286:PHE:CD1	2.41	0.56
2:K:128:ARG:HH12	2:K:135:ALA:HB3	1.70	0.56
2:I:59:ILE:HD12	2:I:59:ILE:H	1.70	0.56
1:B:122:VAL:HB	5:B:1051:HOH:O	2.05	0.56
1:D:158:ALA:HB2	1:D:222:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:8:GLN:O	2:L:10:GLU:HG3	2.05	0.56
1:F:50:GLU:CD	1:F:234:ARG:HH22	2.09	0.56
1:E:140:LEU:HD23	1:E:140:LEU:C	2.26	0.55
2:G:40:GLN:HE22	2:G:63:ASN:HB2	1.70	0.55
2:K:71:VAL:HG12	2:K:97:PRO:HB3	1.88	0.55
2:K:130:ARG:CZ	2:K:135:ALA:HB2	2.36	0.55
2:K:104:ASP:O	2:K:105:ASN:HB2	2.05	0.55
2:G:112:SER:HA	2:G:117:HIS:HE2	1.72	0.55
2:K:18:ILE:HD11	2:K:66:LEU:HD11	1.88	0.55
1:B:17:ARG:HD2	1:B:179:PHE:CE1	2.41	0.55
1:E:192:LEU:HD11	1:E:242:ASN:HB3	1.89	0.55
1:A:80:SER:HB2	1:C:54:ARG:NH2	2.21	0.55
1:D:137:GLN:HG2	1:D:168:THR:HG22	1.88	0.55
1:B:81:LEU:HG	1:B:86:GLU:O	2.06	0.55
2:L:73:GLN:HE22	2:L:106:VAL:HG21	1.71	0.55
2:I:21:ILE:HG22	2:I:25:ILE:HB	1.88	0.55
2:L:22:PRO:HD2	2:L:80:GLN:O	2.07	0.55
1:C:81:LEU:HG	1:C:86:GLU:O	2.07	0.55
1:E:49:PHE:CE2	1:E:81:LEU:HD13	2.42	0.55
1:D:265:HIS:CD2	1:D:266:PRO:O	2.60	0.55
2:H:65:PHE:CE1	2:H:85:ARG:HG3	2.42	0.55
2:L:7:LEU:O	2:L:8:GLN:HB2	2.06	0.55
1:D:94:VAL:CG1	1:E:54:ARG:HG2	2.31	0.55
1:D:81:LEU:HG	1:D:86:GLU:O	2.06	0.55
1:D:106:HIS:CG	1:D:107:PRO:HD2	2.42	0.55
2:G:112:SER:HA	2:G:117:HIS:NE2	2.20	0.55
1:F:87:THR:HB	2:L:119:GLU:OE1	2.07	0.55
1:A:114:LEU:HD13	1:A:114:LEU:C	2.27	0.55
1:C:270:VAL:O	1:C:271:ASP:CG	2.46	0.55
1:B:170:HIS:O	1:B:174:GLN:HG3	2.07	0.54
2:G:65:PHE:CD2	2:G:85:ARG:HD3	2.41	0.54
2:H:9:VAL:HG11	2:H:60:LYS:NZ	2.23	0.54
2:G:40:GLN:NE2	2:G:63:ASN:HB2	2.21	0.54
1:D:154:ASN:HA	1:D:181:GLY:O	2.08	0.54
1:C:243:VAL:HG13	1:C:244:LYS:HD2	1.87	0.54
1:B:101:ALA:HB2	1:B:304:LEU:HD21	1.89	0.54
2:L:111:ASN:HB2	2:L:145:PHE:HZ	1.73	0.54
2:I:44:ILE:HA	2:L:46:LEU:O	2.08	0.54
2:I:35:LEU:HD13	2:I:40:GLN:HG3	1.89	0.54
1:A:270:VAL:O	1:A:271:ASP:OD1	2.25	0.54
1:D:109:GLU:OE1	1:D:130:GLY:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:PHE:CE2	1:D:81:LEU:HD13	2.42	0.54
2:H:109:CYS:SG	2:H:111:ASN:HB3	2.47	0.54
1:B:240:TYR:HE1	5:B:1071:HOH:O	1.90	0.54
1:B:140:LEU:HD21	1:B:288:GLN:HG2	1.88	0.54
2:G:134:ILE:N	2:G:134:ILE:HD12	2.23	0.54
1:B:88:LEU:N	2:H:119:GLU:OE1	2.39	0.54
1:D:54:ARG:CD	1:D:267:LEU:HB2	2.37	0.54
1:B:114:LEU:HD12	2:H:121:VAL:HG11	1.90	0.54
1:D:267:LEU:HD12	1:F:94:VAL:CG1	2.37	0.54
1:D:234:ARG:HG2	1:D:234:ARG:HH11	1.72	0.54
2:G:19:ASP:OD2	2:G:56:LYS:HE3	2.06	0.54
1:A:108:GLN:HG3	2:G:113:ASN:OD1	2.07	0.54
2:L:75:ALA:HB1	2:L:99:LEU:CD2	2.38	0.54
1:F:8:HIS:O	1:F:9:ILE:HD13	2.07	0.54
1:F:101:ALA:HB2	1:F:304:LEU:HD21	1.90	0.54
1:A:257:ALA:CB	1:A:261:MET:HE1	2.38	0.53
2:G:61:ILE:N	2:G:61:ILE:HD12	2.22	0.53
2:J:30:LEU:CD1	2:J:44:ILE:HD13	2.37	0.53
2:H:131:ALA:HA	5:H:2013:HOH:O	2.08	0.53
1:B:267:LEU:HD11	1:B:286:PHE:CD1	2.43	0.53
2:H:67:SER:OG	2:H:70:GLN:HG3	2.08	0.53
2:J:78:ALA:HB1	2:J:81:ALA:HB2	1.90	0.53
1:E:75:ASP:OD2	1:E:77:ALA:HB3	2.08	0.53
2:K:107:LEU:HD21	2:K:151:LEU:HD23	1.89	0.53
2:G:14:ARG:HA	2:G:86:ILE:HG22	1.90	0.53
1:A:243:VAL:HG13	1:A:244:LYS:CD	2.38	0.53
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.43	0.53
1:C:287:GLN:H	1:C:287:GLN:HE21	1.54	0.53
1:D:131:SER:HB3	1:D:234:ARG:HD3	1.89	0.53
2:L:84:ASN:OD1	2:L:94:LYS:HG2	2.09	0.53
2:H:22:PRO:O	2:H:25:ILE:HB	2.08	0.53
1:D:94:VAL:HG22	1:E:267:LEU:HD12	1.89	0.53
1:E:35:GLN:HE22	1:E:309:VAL:HG13	1.71	0.53
1:F:261:MET:HG2	1:F:262:LYS:N	2.24	0.53
1:C:35:GLN:NE2	1:C:309:VAL:HG13	2.24	0.53
1:D:270:VAL:O	1:D:271:ASP:CG	2.47	0.53
2:I:105:ASN:HB2	2:I:122:SER:HB3	1.90	0.53
2:J:111:ASN:ND2	2:J:114:CYS:HB2	2.23	0.53
1:A:15:LEU:O	1:A:178:LYS:HE3	2.08	0.53
2:L:29:LEU:HD21	2:L:77:TYR:HB3	1.90	0.53
2:I:35:LEU:HD22	2:I:40:GLN:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PRO:HB2	4:B:1002:PAL:H31	1.90	0.53
1:A:237:PRO:HA	1:A:240:TYR:CZ	2.44	0.53
1:F:121:ASN:HA	5:F:1100:HOH:O	2.09	0.53
1:C:262:LYS:NZ	5:C:1070:HOH:O	2.42	0.53
1:B:60:GLU:HG2	1:B:63:MET:HE1	1.91	0.52
1:B:267:LEU:HD11	1:B:286:PHE:CE1	2.44	0.52
2:H:132:ASN:N	5:H:2013:HOH:O	2.30	0.52
2:H:31:SER:HB3	2:K:27:PHE:HZ	1.72	0.52
2:H:86:ILE:HG22	2:H:87:ASP:N	2.24	0.52
1:B:160:VAL:HB	1:B:227:MET:SD	2.49	0.52
2:I:66:LEU:HA	2:I:71:VAL:HB	1.91	0.52
1:E:163:LEU:HG	1:E:188:ALA:HB2	1.91	0.52
2:K:7:LEU:HD12	2:K:10:GLU:OE2	2.10	0.52
2:K:9:VAL:HG12	2:K:60:LYS:NZ	2.24	0.52
1:C:52:SER:HB2	1:C:105:ARG:NH1	2.23	0.52
1:F:94:VAL:HG23	1:F:95:ILE:N	2.24	0.52
2:K:82:THR:HG22	2:K:84:ASN:HD21	1.74	0.52
2:I:132:ASN:O	2:I:133:ASP:HB3	2.10	0.52
2:K:77:TYR:OH	2:K:151:LEU:HD22	2.09	0.52
1:E:270:VAL:O	1:E:271:ASP:CG	2.47	0.52
1:B:59:PHE:CZ	1:B:136:THR:HG21	2.45	0.52
2:K:94:LYS:HB2	2:K:94:LYS:NZ	2.25	0.52
2:K:21:ILE:HB	2:K:57:ASP:HB2	1.92	0.52
1:A:254:LEU:HD22	1:A:261:MET:HE1	1.90	0.52
2:G:40:GLN:OE1	2:G:63:ASN:HB2	2.10	0.52
1:D:215:ILE:HD11	1:D:227:MET:HE1	1.91	0.52
1:B:60:GLU:HG2	1:B:63:MET:CE	2.40	0.52
2:G:12:ILE:HG22	2:G:13:LYS:N	2.21	0.52
2:H:104:ASP:O	2:H:106:VAL:HG23	2.09	0.52
2:L:30:LEU:HD11	2:L:46:LEU:HD11	1.90	0.52
2:L:72:ASP:HA	2:L:97:PRO:HB3	1.92	0.52
1:E:80:SER:HB2	1:F:54:ARG:HH22	1.75	0.52
1:D:59:PHE:O	1:D:63:MET:HG3	2.09	0.52
1:A:12:ILE:HG21	1:A:175:ALA:HB2	1.91	0.52
1:B:15:LEU:O	1:B:178:LYS:HE3	2.10	0.52
1:D:156:HIS:HD2	1:D:185:TYR:OH	1.91	0.52
1:E:264:LEU:O	1:E:265:HIS:HB2	2.09	0.52
1:D:54:ARG:NH2	1:F:80:SER:HB2	2.25	0.52
1:A:121:ASN:HA	5:A:1030:HOH:O	2.09	0.52
1:C:265:HIS:HD2	1:C:267:LEU:HA	1.75	0.52
1:D:111:ALA:N	2:J:115:ILE:HD13	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:LEU:HD21	2:J:60:LYS:HG3	1.92	0.52
1:E:222:VAL:O	1:E:261:MET:HG3	2.10	0.52
1:E:38:LEU:HD11	1:E:305:ASN:ND2	2.25	0.51
1:A:114:LEU:CD2	2:G:121:VAL:HG11	2.40	0.51
1:F:17:ARG:HD2	1:F:179:PHE:CD1	2.44	0.51
2:G:111:ASN:O	2:G:117:HIS:NE2	2.39	0.51
2:I:20:HIS:N	2:I:56:LYS:HE3	2.25	0.51
1:D:166:GLY:O	1:D:169:VAL:HG22	2.09	0.51
2:L:105:ASN:OD1	2:L:122:SER:CB	2.51	0.51
1:A:265:HIS:O	1:A:266:PRO:O	2.28	0.51
1:D:266:PRO:HB2	4:D:1004:PAL:H31	1.93	0.51
2:J:106:VAL:O	2:J:107:LEU:HD23	2.11	0.51
2:H:67:SER:N	2:H:70:GLN:HE21	2.00	0.51
1:E:94:VAL:HG23	1:E:95:ILE:N	2.25	0.51
2:L:95:SER:O	2:L:97:PRO:HD3	2.11	0.51
1:C:120:GLY:N	5:C:1042:HOH:O	2.39	0.51
1:E:229:ARG:HD3	1:E:268:PRO:O	2.11	0.51
2:K:78:ALA:HB1	2:K:81:ALA:HB2	1.92	0.51
2:L:76:LEU:HG	2:L:134:ILE:HD12	1.93	0.51
1:E:109:GLU:OE1	1:E:130:GLY:O	2.29	0.51
1:E:10:ILE:HD12	1:E:112:ALA:HB1	1.93	0.51
1:F:106:HIS:ND1	1:F:107:PRO:HD2	2.25	0.51
2:L:66:LEU:HD13	2:L:70:GLN:O	2.11	0.51
2:K:130:ARG:HE	2:K:135:ALA:HB2	1.73	0.51
1:A:265:HIS:CG	1:A:266:PRO:O	2.63	0.51
1:F:136:THR:HG22	1:F:299:LEU:CD2	2.41	0.51
1:C:156:HIS:HD2	1:C:185:TYR:OH	1.93	0.51
2:L:100:PRO:O	2:L:127:VAL:HG21	2.10	0.50
1:E:284:TRP:CG	1:E:287:GLN:HG3	2.46	0.50
1:F:237:PRO:HA	1:F:240:TYR:CZ	2.45	0.50
1:B:78:ASN:ND2	5:B:1069:HOH:O	2.40	0.50
2:L:18:ILE:HB	2:L:84:ASN:HB2	1.92	0.50
2:H:86:ILE:HD13	2:H:91:VAL:HA	1.91	0.50
2:I:101:GLU:HG3	2:I:102:ARG:HG3	1.94	0.50
1:F:108:GLN:HG3	2:L:113:ASN:ND2	2.25	0.50
1:B:121:ASN:HA	5:B:1077:HOH:O	2.12	0.50
1:C:31:LYS:HG3	1:C:294:PHE:CE1	2.46	0.50
2:L:128:ARG:CB	2:L:128:ARG:NH1	2.74	0.50
1:B:154:ASN:HA	1:B:181:GLY:O	2.10	0.50
1:A:140:LEU:HD21	1:A:288:GLN:HG2	1.93	0.50
1:D:94:VAL:HG11	1:E:54:ARG:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:ALA:HA	1:D:306:ARG:HG2	1.93	0.50
1:B:49:PHE:HE2	1:B:81:LEU:HD13	1.76	0.50
1:D:111:ALA:HA	2:J:115:ILE:HG12	1.92	0.50
2:I:125:PHE:HA	2:I:137:LYS:O	2.12	0.50
2:I:59:ILE:HD12	2:I:59:ILE:N	2.25	0.50
1:F:131:SER:HB3	1:F:234:ARG:CD	2.41	0.50
1:E:106:HIS:CG	1:E:107:PRO:HD2	2.46	0.50
1:A:81:LEU:HA	1:A:86:GLU:CB	2.26	0.50
1:A:81:LEU:HD12	1:A:91:THR:OG1	2.12	0.50
2:L:44:ILE:CG2	2:L:45:GLY:H	2.09	0.50
1:C:50:GLU:CD	1:C:234:ARG:HH22	2.14	0.50
2:K:148:ASN:HA	5:K:2014:HOH:O	2.12	0.50
1:B:189:PRO:HB3	1:B:246:GLN:HE22	1.76	0.50
2:H:107:LEU:HB3	2:H:150:VAL:CG1	2.41	0.50
1:D:165:TYR:CE2	1:D:235:LEU:HD23	2.47	0.50
1:E:165:TYR:CE2	1:E:235:LEU:HD23	2.47	0.50
2:L:101:GLU:CA	2:L:127:VAL:HG22	2.34	0.50
1:D:80:SER:HB2	1:E:54:ARG:NH2	2.26	0.50
1:E:237:PRO:HA	1:E:240:TYR:CZ	2.45	0.50
2:J:72:ASP:HB3	2:J:98:SER:O	2.11	0.50
2:G:4:ASP:C	2:G:6:LYS:H	2.15	0.50
1:B:114:LEU:HD11	2:H:121:VAL:CG1	2.42	0.50
1:A:189:PRO:HB3	1:A:246:GLN:HE22	1.74	0.50
2:L:85:ARG:O	2:L:86:ILE:HD13	2.12	0.50
1:D:229:ARG:NE	1:D:268:PRO:HB2	2.27	0.50
1:D:230:VAL:O	1:D:232:LYS:N	2.45	0.50
2:G:2:THR:HG22	2:G:11:ALA:H	1.76	0.50
2:L:132:ASN:O	2:L:133:ASP:HB3	2.11	0.50
2:L:46:LEU:HD23	2:L:58:LEU:H	1.77	0.49
1:D:131:SER:HA	1:D:167:ARG:HB3	1.94	0.49
2:G:46:LEU:HA	2:G:57:ASP:OD1	2.12	0.49
1:D:240:TYR:O	1:D:243:VAL:HG12	2.11	0.49
2:H:14:ARG:HA	2:H:87:ASP:HA	1.94	0.49
2:I:125:PHE:CE2	2:I:145:PHE:HZ	2.29	0.49
1:C:137:GLN:HG2	1:C:168:THR:HG22	1.94	0.49
1:B:165:TYR:O	1:B:231:GLN:HG3	2.12	0.49
1:D:94:VAL:CG2	1:E:267:LEU:HD12	2.42	0.49
2:K:90:GLU:OE1	2:K:90:GLU:HA	2.11	0.49
2:I:46:LEU:HD21	2:I:58:LEU:N	2.19	0.49
1:E:161:GLY:O	1:E:188:ALA:HB2	2.12	0.49
2:G:21:ILE:HB	2:G:57:ASP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:8:GLN:HE22	2:L:48:LEU:HD13	1.78	0.49
1:C:267:LEU:HG	5:C:1011:HOH:O	2.12	0.49
1:D:114:LEU:HG	2:J:115:ILE:CG2	2.42	0.49
2:L:136:LEU:N	2:L:145:PHE:O	2.44	0.49
2:I:36:THR:HG22	2:I:37:GLU:HG3	1.93	0.49
1:F:81:LEU:HG	1:F:86:GLU:O	2.13	0.49
1:C:189:PRO:HG2	1:C:192:LEU:HB2	1.94	0.49
1:B:189:PRO:HG2	1:B:192:LEU:HB2	1.95	0.49
2:L:130:ARG:NE	2:L:135:ALA:HB2	2.28	0.49
2:L:75:ALA:CB	2:L:99:LEU:HD23	2.43	0.49
2:H:103:ILE:O	2:H:103:ILE:HG23	2.13	0.49
1:A:94:VAL:CG1	1:C:267:LEU:HD12	2.42	0.49
1:C:267:LEU:O	1:C:269:ARG:N	2.46	0.49
2:L:78:ALA:HB1	2:L:81:ALA:HB2	1.95	0.49
1:B:284:TRP:CD2	1:B:287:GLN:HG3	2.47	0.49
2:J:8:GLN:HB2	5:J:2024:HOH:O	2.12	0.49
1:C:243:VAL:HG13	1:C:244:LYS:CD	2.43	0.49
1:D:189:PRO:HB3	1:D:246:GLN:HE22	1.76	0.49
1:C:187:ILE:HG12	1:C:212:HIS:HB2	1.94	0.49
2:L:99:LEU:HD12	2:L:129:LYS:HB2	1.94	0.49
2:H:21:ILE:HB	2:H:57:ASP:HB2	1.95	0.49
1:C:109:GLU:OE2	2:I:113:ASN:HB3	2.12	0.49
1:E:227:MET:HB2	1:E:265:HIS:HD2	1.77	0.48
2:G:13:LYS:O	2:G:86:ILE:HG22	2.12	0.48
1:B:244:LYS:HB3	5:B:1100:HOH:O	2.12	0.48
2:G:34:LYS:HB3	2:G:37:GLU:OE2	2.13	0.48
2:L:152:ALA:O	2:L:153:ASN:HB2	2.11	0.48
2:I:32:LEU:HD11	2:I:77:TYR:CE2	2.48	0.48
1:D:27:ALA:HA	1:D:298:ALA:HB2	1.96	0.48
2:H:102:ARG:HG2	2:H:139:LYS:CE	2.43	0.48
5:B:1053:HOH:O	2:H:139:LYS:HB2	2.13	0.48
2:L:65:PHE:CD1	2:L:65:PHE:N	2.80	0.48
1:D:261:MET:CE	1:D:282:HIS:CG	2.96	0.48
1:D:211:LEU:O	1:D:212:HIS:CG	2.67	0.48
2:J:77:TYR:N	2:J:77:TYR:CD1	2.81	0.48
2:H:32:LEU:O	2:H:32:LEU:HD23	2.13	0.48
2:I:20:HIS:H	2:I:56:LYS:CE	2.25	0.48
1:D:261:MET:HE1	1:D:282:HIS:CG	2.49	0.48
1:E:1:ALA:HA	1:E:306:ARG:HG2	1.95	0.48
1:B:261:MET:HG2	1:B:262:LYS:N	2.27	0.48
1:F:81:LEU:HD12	1:F:91:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:87:ASP:OD2	2:L:92:VAL:HG11	2.14	0.48
2:G:12:ILE:HG21	2:G:62:GLU:OE1	2.12	0.48
1:B:240:TYR:O	1:B:243:VAL:HG12	2.14	0.48
2:L:128:ARG:CB	2:L:128:ARG:HH11	2.26	0.48
1:A:114:LEU:HD13	1:A:114:LEU:O	2.13	0.48
2:H:92:VAL:HG23	2:H:93:GLY:H	1.78	0.48
2:L:109:CYS:SG	2:L:111:ASN:HB3	2.54	0.48
2:I:44:ILE:HG12	2:L:48:LEU:CD2	2.43	0.48
1:A:267:LEU:O	1:A:269:ARG:N	2.46	0.48
2:K:107:LEU:HD13	2:K:150:VAL:HG11	1.96	0.48
1:E:251:ALA:CB	1:E:276:ASP:OD2	2.62	0.48
1:A:81:LEU:HG	1:A:86:GLU:O	2.13	0.48
2:H:111:ASN:C	2:H:111:ASN:HD22	2.16	0.48
2:K:55:ARG:NH1	2:K:55:ARG:HG2	2.29	0.48
2:L:39:ASP:OD1	2:L:40:GLN:N	2.46	0.48
1:A:229:ARG:NH1	1:A:233:GLU:OE1	2.40	0.48
1:A:191:ALA:O	1:A:192:LEU:HD23	2.13	0.48
2:H:1:MET:O	2:H:2:THR:HG23	2.14	0.48
1:F:106:HIS:CG	1:F:107:PRO:HD2	2.49	0.48
1:A:54:ARG:HH21	1:B:80:SER:HB2	1.78	0.48
2:I:25:ILE:O	2:I:29:LEU:HB2	2.14	0.48
2:J:125:PHE:HA	2:J:137:LYS:O	2.13	0.48
1:F:214:SER:OG	1:F:217:GLU:HG3	2.14	0.48
2:I:10:GLU:CG	2:I:11:ALA:N	2.72	0.48
1:B:267:LEU:HD12	1:C:94:VAL:HG11	1.92	0.48
2:H:111:ASN:HB3	2:H:114:CYS:HB2	1.95	0.48
1:E:31:LYS:HE2	1:E:294:PHE:CE2	2.49	0.48
1:F:122:VAL:HB	5:F:1054:HOH:O	2.14	0.47
1:D:141:ASP:OD1	1:D:288:GLN:NE2	2.47	0.47
2:J:103:ILE:HD11	2:J:106:VAL:CG2	2.44	0.47
2:L:38:THR:O	2:L:39:ASP:HB2	2.14	0.47
1:F:45:ALA:HB2	1:F:99:VAL:HG11	1.96	0.47
1:C:219:MET:HE3	1:C:254:LEU:HD23	1.96	0.47
2:H:79:PRO:HD2	2:H:80:GLN:HE22	1.79	0.47
1:B:270:VAL:HG12	1:B:270:VAL:O	2.14	0.47
5:F:1097:HOH:O	2:L:120:PRO:HG2	2.13	0.47
1:C:17:ARG:HD2	1:C:179:PHE:CE1	2.49	0.47
2:L:102:ARG:O	2:L:103:ILE:HD13	2.14	0.47
1:F:250:ARG:HH11	1:F:250:ARG:HG2	1.79	0.47
1:D:160:VAL:HB	1:D:227:MET:SD	2.54	0.47
2:J:50:SER:HB2	2:J:56:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1034:HOH:O	2:K:143:LYS:HE2	2.13	0.47
1:B:287:GLN:NE2	1:B:287:GLN:H	2.11	0.47
1:D:131:SER:HB3	1:D:234:ARG:CD	2.44	0.47
1:E:109:GLU:HG3	2:K:111:ASN:HD21	1.80	0.47
1:C:60:GLU:HG2	1:C:70:VAL:HG11	1.96	0.47
2:H:134:ILE:H	2:H:147:HIS:CD2	2.31	0.47
5:B:1053:HOH:O	2:H:139:LYS:HB3	2.12	0.47
2:G:17:VAL:HG23	2:G:86:ILE:CD1	2.44	0.47
1:B:237:PRO:HA	1:B:240:TYR:CZ	2.49	0.47
1:F:52:SER:HB2	1:F:105:ARG:NH1	2.29	0.47
2:J:19:ASP:OD2	2:J:20:HIS:N	2.41	0.47
2:K:131:ALA:HA	5:K:2019:HOH:O	2.14	0.47
2:J:40:GLN:OE1	2:J:63:ASN:HB2	2.15	0.47
2:H:124:SER:OG	2:H:139:LYS:HG3	2.15	0.47
2:I:16:THR:HG22	2:I:17:VAL:N	2.29	0.47
2:L:76:LEU:HD12	2:L:147:HIS:CG	2.49	0.47
2:H:14:ARG:CA	2:H:87:ASP:HA	2.44	0.47
2:G:146:SER:O	2:G:149:VAL:HG22	2.15	0.47
1:D:160:VAL:HG22	1:D:187:ILE:HB	1.96	0.47
1:B:165:TYR:CE2	1:B:235:LEU:HD23	2.48	0.47
1:B:156:HIS:HD2	1:B:185:TYR:OH	1.97	0.47
2:H:19:ASP:OD1	2:H:20:HIS:N	2.44	0.47
2:K:14:ARG:HA	2:K:86:ILE:O	2.14	0.47
1:E:265:HIS:O	1:E:267:LEU:N	2.48	0.47
1:D:267:LEU:HD12	1:F:94:VAL:HG11	1.97	0.47
2:G:18:ILE:HA	2:G:82:THR:O	2.14	0.47
1:F:60:GLU:HG2	1:F:70:VAL:HG11	1.97	0.47
2:J:11:ALA:HB1	5:J:2038:HOH:O	2.15	0.47
2:I:20:HIS:H	2:I:56:LYS:HE3	1.79	0.47
2:L:98:SER:O	2:L:99:LEU:HD23	2.14	0.47
1:D:45:ALA:HA	1:D:71:VAL:O	2.14	0.47
2:K:18:ILE:HD11	2:K:66:LEU:CD1	2.45	0.47
1:C:163:LEU:HG	1:C:188:ALA:HB2	1.96	0.47
2:K:77:TYR:CZ	2:K:151:LEU:HD22	2.50	0.47
1:F:1:ALA:HA	1:F:306:ARG:HG2	1.97	0.47
1:B:250:ARG:HH11	1:B:250:ARG:HG2	1.80	0.47
2:L:3:HIS:O	2:L:9:VAL:HG22	2.15	0.47
1:B:87:THR:HB	2:H:119:GLU:OE1	2.15	0.46
1:E:159:MET:HE2	1:E:172:LEU:CD2	2.40	0.46
1:D:12:ILE:HG13	1:D:171:SER:HB3	1.96	0.46
1:F:86:GLU:N	5:F:1062:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:84:ASN:N	2:K:84:ASN:ND2	2.60	0.46
1:E:78:ASN:OD1	1:F:75:ASP:HB2	2.15	0.46
1:C:131:SER:HB3	1:C:234:ARG:CD	2.45	0.46
2:L:25:ILE:HD12	2:L:25:ILE:N	2.29	0.46
1:D:137:GLN:NE2	1:D:140:LEU:HD22	2.30	0.46
1:B:270:VAL:O	1:B:271:ASP:CG	2.53	0.46
2:I:45:GLY:H	2:L:46:LEU:H	1.64	0.46
1:A:54:ARG:CD	1:A:267:LEU:HB2	2.43	0.46
2:I:18:ILE:HA	2:I:83:VAL:HG12	1.96	0.46
1:C:226:TYR:CZ	1:C:266:PRO:HD3	2.51	0.46
1:D:20:LEU:HD13	1:D:142:LEU:CD1	2.45	0.46
1:B:165:TYR:CD2	1:B:235:LEU:HD23	2.51	0.46
1:B:109:GLU:CD	2:H:113:ASN:HD22	2.19	0.46
1:A:17:ARG:HD2	1:A:179:PHE:CE1	2.51	0.46
1:A:238:SER:HA	1:E:241:ALA:HA	1.98	0.46
1:E:108:GLN:HG3	2:K:113:ASN:ND2	2.29	0.46
2:G:52:GLU:O	2:G:53:MET:HG2	2.16	0.46
1:D:12:ILE:HG21	1:D:175:ALA:HB2	1.98	0.46
2:G:8:GLN:HB3	2:G:48:LEU:HD22	1.97	0.46
1:A:162:ASP:OD1	1:A:162:ASP:C	2.54	0.46
2:I:48:LEU:CD1	2:I:58:LEU:HG	2.39	0.46
2:G:50:SER:HB2	2:G:56:LYS:HG2	1.98	0.46
2:G:102:ARG:HG2	2:G:104:ASP:OD2	2.15	0.46
2:K:12:ILE:HG12	2:K:13:LYS:N	2.31	0.46
1:B:130:GLY:O	1:B:131:SER:HB3	2.16	0.46
2:G:85:ARG:C	2:G:86:ILE:HD12	2.36	0.46
2:I:38:THR:O	2:I:40:GLN:NE2	2.49	0.46
1:D:17:ARG:HD2	1:D:179:PHE:CE1	2.51	0.46
2:J:21:ILE:HB	2:J:57:ASP:HB2	1.97	0.46
2:L:43:THR:HG22	2:L:60:LYS:HB2	1.98	0.45
1:E:94:VAL:HG11	1:F:267:LEU:HD12	1.96	0.45
1:F:109:GLU:HG3	2:L:111:ASN:HD21	1.82	0.45
2:K:7:LEU:HB2	2:K:10:GLU:OE1	2.17	0.45
2:L:90:GLU:HG2	2:L:91:VAL:H	1.81	0.45
1:E:81:LEU:HG	1:E:86:GLU:O	2.17	0.45
2:H:9:VAL:HG11	2:H:60:LYS:HZ3	1.79	0.45
1:F:108:GLN:HE21	2:L:113:ASN:HD21	1.63	0.45
2:L:109:CYS:HA	2:L:110:PRO:HD3	1.85	0.45
2:L:40:GLN:HA	5:L:2015:HOH:O	2.16	0.45
1:B:1:ALA:HA	1:B:306:ARG:HG2	1.97	0.45
2:H:30:LEU:HD13	2:H:59:ILE:CD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:17:VAL:HG23	2:G:86:ILE:HD13	1.98	0.45
2:G:44:ILE:HB	2:J:44:ILE:HB	1.98	0.45
2:K:107:LEU:HD22	2:K:150:VAL:HG12	1.97	0.45
2:H:119:GLU:HG3	2:H:120:PRO:CD	2.46	0.45
1:B:17:ARG:O	1:B:17:ARG:HG3	2.15	0.45
1:C:106:HIS:CG	1:C:107:PRO:HD2	2.51	0.45
2:J:4:ASP:OD2	2:J:7:LEU:HB2	2.17	0.45
1:E:52:SER:HB2	1:E:105:ARG:NH1	2.32	0.45
2:K:94:LYS:CB	2:K:94:LYS:NZ	2.79	0.45
1:C:10:ILE:HD12	1:C:112:ALA:HB1	1.99	0.45
2:L:107:LEU:HA	2:L:152:ALA:HA	1.98	0.45
2:J:7:LEU:CD2	2:J:48:LEU:HB3	2.37	0.45
2:L:24:GLN:C	2:L:25:ILE:HD12	2.37	0.45
1:E:50:GLU:HB3	1:E:105:ARG:HG2	1.99	0.45
1:F:50:GLU:HB3	1:F:105:ARG:HG2	1.97	0.45
1:C:136:THR:HA	1:C:139:LEU:HD12	1.99	0.45
1:B:37:GLU:OE2	1:B:40:LYS:HD2	2.17	0.45
1:E:160:VAL:HG22	1:E:187:ILE:HB	1.99	0.45
2:L:74:LEU:HG	5:L:2016:HOH:O	2.16	0.45
1:E:94:VAL:CG1	1:F:267:LEU:CD1	2.95	0.45
1:F:265:HIS:HD2	1:F:267:LEU:HA	1.81	0.45
2:I:102:ARG:HH21	2:I:139:LYS:HD3	1.81	0.45
1:C:271:ASP:OD1	1:C:271:ASP:C	2.56	0.45
1:E:307:ASP:HA	5:E:1045:HOH:O	2.17	0.45
2:K:30:LEU:HD13	2:K:59:ILE:HD13	1.99	0.45
2:I:17:VAL:HG13	2:I:60:LYS:HG2	1.99	0.45
2:K:16:THR:HG1	2:K:65:PHE:HA	1.80	0.45
2:J:128:ARG:O	2:J:134:ILE:HG23	2.17	0.45
1:C:48:PHE:HB2	1:C:74:SER:HA	1.99	0.45
2:G:99:LEU:HD12	2:G:100:PRO:HD2	1.98	0.45
2:L:63:ASN:O	2:L:64:THR:C	2.55	0.45
1:B:189:PRO:HB3	1:B:246:GLN:NE2	2.32	0.45
2:J:50:SER:O	2:J:54:GLY:N	2.49	0.45
1:E:121:ASN:HB3	5:E:1016:HOH:O	2.17	0.45
1:E:162:ASP:OD1	1:E:162:ASP:C	2.55	0.45
2:L:59:ILE:HG22	2:L:60:LYS:N	2.32	0.44
2:G:86:ILE:N	2:G:86:ILE:HD12	2.31	0.44
5:E:1007:HOH:O	1:F:269:ARG:HG2	2.16	0.44
1:D:266:PRO:HG2	5:D:1034:HOH:O	2.17	0.44
2:L:136:LEU:O	2:L:145:PHE:N	2.31	0.44
1:C:234:ARG:HG2	1:C:234:ARG:HH11	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:90:GLU:HG2	2:L:91:VAL:N	2.31	0.44
1:C:178:LYS:NZ	5:C:1084:HOH:O	2.50	0.44
1:E:17:ARG:HD2	1:E:179:PHE:CE1	2.52	0.44
1:D:267:LEU:HD23	1:D:267:LEU:HA	1.72	0.44
1:E:271:ASP:OD1	1:E:271:ASP:C	2.55	0.44
2:J:72:ASP:OD1	2:J:98:SER:HB3	2.16	0.44
1:E:26:THR:HB	1:E:298:ALA:HB1	1.99	0.44
2:J:139:LYS:O	2:J:139:LYS:HG2	2.16	0.44
2:L:22:PRO:HA	2:L:55:ARG:O	2.17	0.44
2:G:65:PHE:HD2	2:G:85:ARG:HD3	1.80	0.44
1:F:265:HIS:O	1:F:267:LEU:N	2.51	0.44
2:L:111:ASN:ND2	2:L:141:CYS:SG	2.87	0.44
1:B:245:ALA:HB3	1:B:271:ASP:OD1	2.17	0.44
2:J:6:LYS:O	2:J:6:LYS:HG3	2.18	0.44
1:C:58:SER:OG	1:C:296:ARG:NH1	2.49	0.44
1:B:2:ASN:HB2	1:B:308:LEU:HD21	1.99	0.44
1:F:267:LEU:O	1:F:268:PRO:C	2.53	0.44
1:E:251:ALA:HB3	1:E:276:ASP:OD2	2.18	0.44
2:I:59:ILE:CD1	2:I:59:ILE:H	2.29	0.44
1:D:55:THR:O	1:D:59:PHE:HB2	2.17	0.44
2:I:7:LEU:HD13	2:L:9:VAL:HB	2.00	0.44
1:A:75:ASP:OD2	1:A:77:ALA:HB3	2.18	0.44
1:F:215:ILE:HG22	1:F:219:MET:HE2	2.00	0.44
1:F:163:LEU:HG	1:F:188:ALA:HB2	1.98	0.44
1:B:104:MET:HE1	1:B:115:ALA:CB	2.48	0.44
1:D:216:GLU:HG3	5:D:1062:HOH:O	2.16	0.44
2:I:22:PRO:HB2	2:I:25:ILE:CG1	2.46	0.44
1:B:54:ARG:NH2	1:C:80:SER:HB2	2.32	0.44
1:D:78:ASN:OD1	1:E:75:ASP:HB2	2.18	0.44
1:F:106:HIS:ND1	1:F:107:PRO:CD	2.81	0.44
1:D:162:ASP:C	1:D:162:ASP:OD1	2.56	0.44
1:B:158:ALA:HB2	1:B:222:VAL:HG11	2.00	0.44
1:F:137:GLN:HG2	1:F:168:THR:CG2	2.46	0.44
1:E:189:PRO:HB3	1:E:246:GLN:HE22	1.82	0.44
2:L:137:LYS:HE3	2:L:142:GLU:O	2.17	0.44
1:F:8:HIS:C	1:F:9:ILE:HD13	2.38	0.44
1:C:267:LEU:HA	1:C:267:LEU:HD23	1.62	0.44
2:H:137:LYS:NZ	2:H:142:GLU:HB3	2.33	0.44
2:L:99:LEU:HD22	2:L:134:ILE:CD1	2.48	0.44
1:E:55:THR:O	1:E:59:PHE:HB2	2.18	0.44
1:A:187:ILE:HD11	1:A:218:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:HG2	1:A:70:VAL:HG11	2.00	0.44
2:I:108:VAL:HG21	2:I:153:ASN:HB2	2.00	0.44
1:F:267:LEU:HD11	1:F:286:PHE:CE1	2.53	0.44
2:K:58:LEU:HD21	2:K:60:LYS:HE3	2.00	0.44
1:F:142:LEU:HD11	1:F:175:ALA:HB1	2.00	0.44
1:B:65:ARG:HD3	5:B:1039:HOH:O	2.17	0.44
2:I:85:ARG:O	2:I:86:ILE:HB	2.18	0.43
1:A:114:LEU:CD1	1:A:114:LEU:C	2.87	0.43
2:K:73:GLN:OE1	2:K:106:VAL:HG21	2.18	0.43
2:K:82:THR:HG22	2:K:84:ASN:ND2	2.34	0.43
1:E:80:SER:CB	1:F:54:ARG:NH2	2.81	0.43
1:A:109:GLU:OE2	2:G:113:ASN:ND2	2.51	0.43
1:C:131:SER:HB3	1:C:234:ARG:HD3	2.00	0.43
1:D:48:PHE:HB2	1:D:74:SER:HA	2.00	0.43
1:A:9:ILE:HG13	1:A:299:LEU:HD11	2.01	0.43
1:B:265:HIS:C	1:B:266:PRO:O	2.48	0.43
2:I:136:LEU:O	2:I:144:GLU:HA	2.17	0.43
1:F:131:SER:HB3	1:F:234:ARG:HD2	1.99	0.43
2:K:9:VAL:C	2:K:10:GLU:HG3	2.38	0.43
2:G:102:ARG:HG2	2:G:103:ILE:N	2.33	0.43
2:I:1:MET:HB2	2:I:3:HIS:CE1	2.52	0.43
1:C:53:THR:O	1:C:57:LEU:HB2	2.18	0.43
2:L:46:LEU:CD2	2:L:57:ASP:HB3	2.47	0.43
1:A:94:VAL:HG23	1:A:95:ILE:N	2.34	0.43
2:I:15:GLY:CA	2:I:62:GLU:HA	2.36	0.43
2:K:99:LEU:HA	2:K:100:PRO:HD3	1.81	0.43
1:E:192:LEU:HD11	1:E:242:ASN:CB	2.48	0.43
1:D:160:VAL:HA	1:D:187:ILE:O	2.19	0.43
1:E:119:SER:O	1:E:120:GLY:C	2.56	0.43
2:L:88:ASN:OD1	2:L:89:TYR:HD1	2.01	0.43
1:E:86:GLU:N	5:E:1021:HOH:O	2.51	0.43
1:D:271:ASP:OD1	1:D:271:ASP:C	2.57	0.43
1:E:38:LEU:CD1	1:E:305:ASN:ND2	2.82	0.43
1:D:255:HIS:ND1	1:D:256:ASN:N	2.67	0.43
2:G:95:SER:O	2:G:96:ARG:C	2.57	0.43
2:G:36:THR:O	2:G:38:THR:N	2.50	0.43
2:L:104:ASP:HA	2:L:124:SER:HA	2.00	0.43
1:A:50:GLU:CD	1:A:234:ARG:HH22	2.22	0.43
2:I:18:ILE:O	2:I:58:LEU:HA	2.17	0.43
2:H:111:ASN:O	2:H:117:HIS:CE1	2.71	0.43
2:L:81:ALA:H	2:L:96:ARG:HH12	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LEU:HD21	2:J:121:VAL:HG11	2.00	0.43
2:L:128:ARG:HB3	2:L:128:ARG:CZ	2.48	0.43
1:E:141:ASP:OD1	1:E:288:GLN:NE2	2.51	0.43
2:K:9:VAL:HG11	2:K:58:LEU:HD23	2.01	0.43
1:A:10:ILE:HD12	1:A:112:ALA:HB1	1.99	0.43
2:K:5:ASN:O	2:K:6:LYS:HB2	2.18	0.43
1:D:13:ASN:HA	1:D:13:ASN:HD22	1.57	0.43
1:A:229:ARG:HD3	1:A:268:PRO:O	2.19	0.43
2:L:68:GLU:O	2:L:71:VAL:HG12	2.19	0.43
1:D:111:ALA:HB2	2:J:115:ILE:CD1	2.47	0.43
2:K:73:GLN:CD	2:K:106:VAL:HG21	2.38	0.43
2:H:65:PHE:CD1	2:H:85:ARG:HG3	2.54	0.43
1:A:284:TRP:O	1:A:288:GLN:HB2	2.18	0.43
1:A:140:LEU:CD2	1:A:288:GLN:HG2	2.49	0.43
1:E:230:VAL:O	1:E:232:LYS:N	2.52	0.43
1:D:30:LEU:CD2	1:D:309:VAL:HG11	2.49	0.43
1:F:52:SER:HB2	1:F:105:ARG:HH11	1.84	0.43
2:G:125:PHE:HA	2:G:137:LYS:O	2.18	0.43
2:L:107:LEU:HD23	2:L:152:ALA:HA	2.01	0.42
2:L:107:LEU:HD23	2:L:152:ALA:HB2	2.00	0.42
2:L:105:ASN:O	2:L:106:VAL:C	2.56	0.42
1:F:310:LEU:N	5:F:1046:HOH:O	2.52	0.42
2:J:110:PRO:HD2	2:J:145:PHE:CD2	2.53	0.42
2:L:72:ASP:C	2:L:74:LEU:H	2.22	0.42
2:I:29:LEU:HD11	2:I:74:LEU:CD2	2.49	0.42
2:I:9:VAL:CG1	2:I:47:ASN:HD22	2.31	0.42
2:J:103:ILE:HD11	2:J:106:VAL:HG22	2.00	0.42
1:A:45:ALA:HB2	1:A:99:VAL:HG11	2.00	0.42
2:J:136:LEU:HD12	2:J:150:VAL:HG21	2.01	0.42
1:C:96:SER:HB2	5:C:1042:HOH:O	2.19	0.42
2:L:99:LEU:CD2	2:L:134:ILE:HD11	2.49	0.42
1:D:165:TYR:CD2	1:D:235:LEU:HD23	2.54	0.42
1:F:250:ARG:HG2	1:F:250:ARG:NH1	2.34	0.42
1:A:223:ASP:O	1:A:261:MET:HA	2.19	0.42
1:D:120:GLY:O	1:D:121:ASN:CG	2.57	0.42
1:C:170:HIS:O	1:C:174:GLN:HG3	2.19	0.42
2:I:44:ILE:HG12	2:L:48:LEU:HD23	2.01	0.42
2:J:84:ASN:OD1	2:J:94:LYS:HE2	2.20	0.42
1:A:54:ARG:HH22	1:B:86:GLU:CD	2.22	0.42
2:I:56:LYS:CE	2:I:58:LEU:HD21	2.44	0.42
1:A:266:PRO:HB2	4:A:1001:PAL:H31	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:137:LYS:HE3	2:L:137:LYS:HB2	1.80	0.42
2:K:94:LYS:HB2	2:K:94:LYS:HZ2	1.84	0.42
1:E:229:ARG:NE	4:E:1005:PAL:O4	2.52	0.42
1:F:219:MET:HE3	1:F:254:LEU:HD23	2.01	0.42
1:E:267:LEU:HA	1:E:267:LEU:HD23	1.55	0.42
2:I:110:PRO:HD2	2:I:145:PHE:CE1	2.55	0.42
1:E:214:SER:OG	1:E:217:GLU:HG3	2.20	0.42
1:F:81:LEU:HD23	5:F:1084:HOH:O	2.19	0.42
1:D:31:LYS:HG3	1:D:294:PHE:CE1	2.55	0.42
1:D:134:HIS:HB2	1:D:167:ARG:HG3	2.01	0.42
2:G:129:LYS:HB2	2:G:129:LYS:NZ	2.35	0.42
2:I:56:LYS:CG	2:I:57:ASP:H	2.32	0.42
2:K:70:GLN:HB3	2:K:73:GLN:H	1.85	0.42
1:C:134:HIS:CD2	1:C:168:THR:HG22	2.54	0.42
1:A:136:THR:HG22	1:A:299:LEU:CD2	2.49	0.42
2:G:73:GLN:HB2	2:G:106:VAL:HG21	2.02	0.42
2:H:50:SER:OG	2:H:53:MET:HB2	2.19	0.42
1:E:164:LYS:HA	1:E:195:PRO:HD3	2.01	0.42
2:J:119:GLU:HA	2:J:120:PRO:HD3	1.86	0.42
2:K:70:GLN:HB3	2:K:73:GLN:HG3	2.01	0.42
1:E:94:VAL:HG12	1:F:267:LEU:HD12	2.01	0.42
2:J:111:ASN:O	2:J:117:HIS:NE2	2.44	0.42
1:A:101:ALA:HB2	1:A:304:LEU:HD21	2.01	0.42
1:A:54:ARG:NH2	1:B:80:SER:HB2	2.35	0.42
2:L:64:THR:O	2:L:64:THR:HG23	2.20	0.42
1:D:134:HIS:CE1	1:D:137:GLN:HB2	2.55	0.42
2:H:23:ALA:O	2:H:24:GLN:HB2	2.20	0.42
1:A:267:LEU:HD23	1:A:267:LEU:HA	1.63	0.41
1:A:54:ARG:NH1	1:B:86:GLU:OE2	2.49	0.41
2:L:100:PRO:O	2:L:127:VAL:CG2	2.67	0.41
2:L:44:ILE:CG2	2:L:45:GLY:N	2.76	0.41
1:A:265:HIS:O	1:A:266:PRO:C	2.58	0.41
1:D:75:ASP:HB2	1:F:78:ASN:OD1	2.20	0.41
2:L:137:LYS:HB3	2:L:144:GLU:HG3	2.02	0.41
1:A:270:VAL:O	1:A:272:GLU:OE1	2.38	0.41
1:E:138:THR:O	1:E:142:LEU:HG	2.20	0.41
1:A:61:THR:O	1:A:65:ARG:HG2	2.20	0.41
1:D:153:ASP:HB2	1:D:180:ASP:O	2.20	0.41
2:K:34:LYS:HE2	2:K:37:GLU:CD	2.41	0.41
1:E:161:GLY:O	1:E:188:ALA:CB	2.68	0.41
1:D:27:ALA:CA	1:D:298:ALA:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:86:ILE:HG22	2:K:87:ASP:N	2.34	0.41
1:E:162:ASP:HB2	1:E:230:VAL:HA	2.02	0.41
1:A:42:LYS:HE3	5:A:1054:HOH:O	2.20	0.41
2:G:22:PRO:HG3	2:G:80:GLN:OE1	2.19	0.41
2:L:21:ILE:C	2:L:23:ALA:H	2.23	0.41
2:J:94:LYS:O	2:J:95:SER:HB3	2.20	0.41
1:A:80:SER:O	1:A:84:LYS:HB2	2.21	0.41
1:B:104:MET:HE1	1:B:115:ALA:HB2	2.02	0.41
1:A:96:SER:O	1:A:122:VAL:HG21	2.20	0.41
1:F:114:LEU:HD13	1:F:114:LEU:C	2.40	0.41
2:G:132:ASN:O	2:G:133:ASP:HB2	2.21	0.41
2:L:72:ASP:HA	2:L:97:PRO:CB	2.50	0.41
2:L:135:ALA:HB1	2:L:144:GLU:HG2	2.03	0.41
1:D:162:ASP:HB2	1:D:230:VAL:HA	2.03	0.41
1:F:13:ASN:HD22	1:F:13:ASN:HA	1.62	0.41
1:F:156:HIS:HD2	1:F:185:TYR:OH	2.03	0.41
2:I:10:GLU:CA	2:I:44:ILE:HD12	2.47	0.41
2:I:21:ILE:HD12	2:I:57:ASP:HB2	2.02	0.41
2:I:21:ILE:CB	2:I:57:ASP:HB2	2.35	0.41
1:D:120:GLY:O	1:D:121:ASN:OD1	2.39	0.41
1:C:45:ALA:HB2	1:C:99:VAL:HG11	2.02	0.41
2:L:146:SER:O	2:L:148:ASN:N	2.53	0.41
1:C:165:TYR:CE2	1:C:235:LEU:HD23	2.55	0.41
2:J:102:ARG:HH11	2:J:102:ARG:HG2	1.85	0.41
1:F:81:LEU:HD23	1:F:81:LEU:O	2.21	0.41
1:B:192:LEU:HD11	1:B:242:ASN:CB	2.48	0.41
2:L:117:HIS:O	2:L:118:ALA:HB2	2.20	0.41
1:A:48:PHE:CE2	1:A:56:ARG:HB2	2.56	0.41
2:L:61:ILE:HG22	2:L:62:GLU:N	2.35	0.41
2:G:40:GLN:CD	2:G:63:ASN:HB2	2.40	0.41
2:L:139:LYS:HE2	2:L:140:TYR:CZ	2.55	0.41
1:C:138:THR:O	1:C:142:LEU:HG	2.20	0.41
1:E:227:MET:HE3	5:E:1032:HOH:O	2.20	0.41
2:J:86:ILE:HD13	2:J:91:VAL:HA	2.03	0.41
1:B:121:ASN:HB2	5:B:1066:HOH:O	2.21	0.41
1:C:140:LEU:C	1:C:140:LEU:HD23	2.41	0.41
1:F:150:GLY:O	1:F:151:ARG:HB3	2.20	0.41
2:I:56:LYS:CG	2:I:57:ASP:N	2.82	0.41
2:J:4:ASP:OD1	2:J:7:LEU:HD12	2.21	0.41
1:B:268:PRO:HD3	4:B:1002:PAL:H1P1	2.02	0.41
1:F:54:ARG:HD3	1:F:267:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:84:ASN:HB3	2:H:91:VAL:CG2	2.51	0.41
1:E:52:SER:HB2	1:E:105:ARG:HH11	1.86	0.41
1:B:17:ARG:NH1	1:B:17:ARG:HG2	2.35	0.41
1:E:109:GLU:HG3	2:K:141:CYS:HB2	2.03	0.41
2:G:2:THR:HG22	2:G:11:ALA:N	2.36	0.41
2:I:55:ARG:NH1	2:L:40:GLN:NE2	2.69	0.41
1:F:161:GLY:O	1:F:163:LEU:HG	2.21	0.41
1:A:274:ALA:CB	1:A:276:ASP:OD1	2.69	0.41
1:F:21:ASN:HA	1:F:21:ASN:HD22	1.74	0.41
2:L:35:LEU:HD23	2:L:35:LEU:HA	1.90	0.41
2:H:66:LEU:HA	2:H:70:GLN:NE2	2.36	0.41
2:L:76:LEU:CD1	2:L:134:ILE:HB	2.51	0.41
1:D:50:GLU:CD	1:D:234:ARG:HH22	2.24	0.41
2:K:7:LEU:HB2	2:K:10:GLU:CD	2.41	0.41
1:A:284:TRP:HA	1:A:287:GLN:OE1	2.21	0.41
2:J:58:LEU:CD2	2:J:60:LYS:HG3	2.51	0.40
2:K:145:PHE:CD1	2:K:145:PHE:N	2.88	0.40
1:E:246:GLN:HB2	1:E:246:GLN:HE21	1.68	0.40
2:G:135:ALA:O	2:G:136:LEU:HD23	2.21	0.40
2:G:110:PRO:HG3	2:G:150:VAL:HA	2.01	0.40
2:G:149:VAL:CG2	2:G:150:VAL:N	2.84	0.40
2:H:42:ILE:HB	2:K:46:LEU:HB2	2.03	0.40
2:H:109:CYS:CB	2:H:138:CYS:SG	3.01	0.40
1:D:42:LYS:HA	1:D:100:ASP:OD2	2.22	0.40
1:D:140:LEU:HD12	1:D:292:GLY:CA	2.51	0.40
2:H:92:VAL:CG2	2:H:93:GLY:N	2.84	0.40
2:G:112:SER:CA	2:G:117:HIS:HE2	2.33	0.40
1:F:109:GLU:OE2	2:L:113:ASN:OD1	2.39	0.40
2:G:108:VAL:HG12	2:G:152:ALA:O	2.21	0.40
2:I:20:HIS:ND1	2:I:56:LYS:HE3	2.35	0.40
1:D:108:GLN:HG3	2:J:113:ASN:HD21	1.83	0.40
2:L:25:ILE:HG21	2:L:77:TYR:O	2.21	0.40
1:B:227:MET:O	1:B:266:PRO:HD2	2.22	0.40
2:G:149:VAL:HG23	2:G:150:VAL:N	2.36	0.40
2:G:134:ILE:HD13	2:G:147:HIS:CE1	2.56	0.40
2:L:18:ILE:HB	2:L:84:ASN:HD22	1.85	0.40
2:G:102:ARG:HD3	2:G:104:ASP:OD2	2.22	0.40
2:K:42:ILE:HG12	2:K:61:ILE:HG23	2.04	0.40
2:I:10:GLU:HA	2:I:44:ILE:CD1	2.44	0.40
2:J:58:LEU:HD21	2:J:60:LYS:CE	2.47	0.40
2:J:130:ARG:CD	2:J:135:ALA:HB2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:147:HIS:O	2:K:151:LEU:HG	2.21	0.40
1:B:250:ARG:NH1	1:B:250:ARG:HG2	2.36	0.40
1:D:114:LEU:HD22	2:J:121:VAL:HG11	2.02	0.40
1:D:35:GLN:HE22	1:D:309:VAL:HG13	1.81	0.40
1:B:35:GLN:HE22	1:B:309:VAL:HG13	1.84	0.40
2:J:73:GLN:HE22	2:J:103:ILE:HD12	1.86	0.40
1:E:165:TYR:CD2	1:E:235:LEU:HD23	2.56	0.40
1:C:13:ASN:HA	1:C:13:ASN:HD22	1.61	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	308/310 (99%)	278 (90%)	25 (8%)	5 (2%)	12	11
1	B	308/310 (99%)	288 (94%)	15 (5%)	5 (2%)	12	11
1	C	308/310 (99%)	284 (92%)	21 (7%)	3 (1%)	19	21
1	D	308/310 (99%)	276 (90%)	28 (9%)	4 (1%)	15	15
1	E	308/310 (99%)	281 (91%)	22 (7%)	5 (2%)	12	11
1	F	308/310 (99%)	281 (91%)	23 (8%)	4 (1%)	15	15
2	G	151/153 (99%)	127 (84%)	19 (13%)	5 (3%)	5	2
2	H	151/153 (99%)	132 (87%)	18 (12%)	1 (1%)	26	32
2	I	151/153 (99%)	110 (73%)	31 (20%)	10 (7%)	1	0
2	J	151/153 (99%)	129 (85%)	19 (13%)	3 (2%)	9	7
2	K	151/153 (99%)	127 (84%)	22 (15%)	2 (1%)	15	15
2	L	151/153 (99%)	88 (58%)	49 (32%)	14 (9%)	1	0
All	All	2754/2778 (99%)	2401 (87%)	292 (11%)	61 (2%)	8	6

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	117	HIS
2	I	22	PRO
2	I	34	LYS
2	I	69	ASP
2	L	7	LEU
2	L	69	ASP
2	L	118	ALA
1	A	85	GLY
1	A	120	GLY
1	B	85	GLY
1	B	130	GLY
1	C	85	GLY
1	C	219	MET
1	D	120	GLY
1	E	85	GLY
1	E	120	GLY
1	E	130	GLY
1	F	219	MET
2	G	51	GLY
2	G	52	GLU
2	I	38	THR
2	I	149	VAL
2	J	14	ARG
2	K	14	ARG
2	L	35	LEU
2	L	106	VAL
2	L	147	HIS
1	B	240	TYR
1	D	231	GLN
1	F	85	GLY
1	F	130	GLY
1	F	267	LEU
2	I	8	GLN
2	K	8	GLN
2	L	44	ILE
2	L	105	ASN
1	B	76	SER
1	D	85	GLY
1	E	267	LEU
2	L	47	ASN
2	L	73	GLN
1	B	267	LEU

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Mol	Chain	Res	Type
1	E	76	SER
2	G	117	HIS
2	I	72	ASP
2	I	105	ASN
2	J	95	SER
2	L	22	PRO
2	L	38	THR
2	L	97	PRO
1	A	270	VAL
1	D	219	MET
2	I	86	ILE
2	L	131	ALA
2	G	96	ARG
1	A	266	PRO
1	C	130	GLY
1	A	267	LEU
2	I	93	GLY
2	G	97	PRO
2	J	115	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/261 (100%)	253 (97%)	8 (3%)	47	64
1	B	261/261 (100%)	252 (97%)	9 (3%)	44	61
1	C	261/261 (100%)	251 (96%)	10 (4%)	40	55
1	D	261/261 (100%)	254 (97%)	7 (3%)	52	69
1	E	261/261 (100%)	252 (97%)	9 (3%)	44	61
1	F	261/261 (100%)	253 (97%)	8 (3%)	47	64
2	G	137/137 (100%)	134 (98%)	3 (2%)	60	75
2	H	137/137 (100%)	132 (96%)	5 (4%)	42	58
2	I	137/137 (100%)	136 (99%)	1 (1%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	137/137 (100%)	132 (96%)	5 (4%)	42	58
2	K	137/137 (100%)	132 (96%)	5 (4%)	42	58
2	L	137/137 (100%)	135 (98%)	2 (2%)	72	84
All	All	2388/2388 (100%)	2316 (97%)	72 (3%)	48	65

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	59	PHE
1	A	109	GLU
1	A	140	LEU
1	A	233	GLU
1	A	265	HIS
1	A	271	ASP
1	A	285	TYR
1	B	13	ASN
1	B	17	ARG
1	B	59	PHE
1	B	131	SER
1	B	140	LEU
1	B	233	GLU
1	B	271	ASP
1	B	285	TYR
1	B	287	GLN
1	C	13	ASN
1	C	17	ARG
1	C	59	PHE
1	C	104	MET
1	C	109	GLU
1	C	134	HIS
1	C	140	LEU
1	C	233	GLU
1	C	271	ASP
1	C	287	GLN
1	D	13	ASN
1	D	59	PHE
1	D	140	LEU
1	D	233	GLU
1	D	271	ASP
1	D	285	TYR

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Mol	Chain	Res	Type
1	D	287	GLN
1	E	13	ASN
1	E	59	PHE
1	E	109	GLU
1	E	131	SER
1	E	140	LEU
1	E	233	GLU
1	E	271	ASP
1	E	285	TYR
1	E	287	GLN
1	F	13	ASN
1	F	59	PHE
1	F	134	HIS
1	F	140	LEU
1	F	233	GLU
1	F	271	ASP
1	F	285	TYR
1	F	287	GLN
2	G	108	VAL
2	G	141	CYS
2	G	147	HIS
2	H	38	THR
2	H	80	GLN
2	H	111	ASN
2	H	138	CYS
2	H	147	HIS
2	I	147	HIS
2	J	77	TYR
2	J	101	GLU
2	J	103	ILE
2	J	104	ASP
2	J	146	SER
2	K	30	LEU
2	K	39	ASP
2	K	84	ASN
2	K	88	ASN
2	K	101	GLU
2	L	133	ASP
2	L	137	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	21	ASN
1	A	35	GLN
1	A	156	HIS
1	A	246	GLN
1	A	291	ASN
1	B	13	ASN
1	B	21	ASN
1	B	35	GLN
1	B	156	HIS
1	B	242	ASN
1	B	246	GLN
1	B	287	GLN
1	B	291	ASN
1	C	13	ASN
1	C	21	ASN
1	C	35	GLN
1	C	137	GLN
1	C	156	HIS
1	C	246	GLN
1	C	287	GLN
1	C	291	ASN
1	C	297	GLN
1	D	21	ASN
1	D	35	GLN
1	D	137	GLN
1	D	156	HIS
1	D	246	GLN
1	D	287	GLN
1	D	291	ASN
1	D	297	GLN
1	D	305	ASN
1	E	13	ASN
1	E	21	ASN
1	E	35	GLN
1	E	156	HIS
1	E	246	GLN
1	E	291	ASN
1	E	297	GLN
1	E	305	ASN
1	F	13	ASN
1	F	21	ASN
1	F	35	GLN

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Mol	Chain	Res	Type
1	F	137	GLN
1	F	156	HIS
1	F	242	ASN
1	F	246	GLN
1	F	287	GLN
1	F	291	ASN
1	F	297	GLN
2	G	47	ASN
2	G	63	ASN
2	G	84	ASN
2	G	147	HIS
2	G	148	ASN
2	H	70	GLN
2	H	84	ASN
2	H	88	ASN
2	H	111	ASN
2	H	113	ASN
2	H	117	HIS
2	H	147	HIS
2	H	148	ASN
2	I	3	HIS
2	I	47	ASN
2	I	63	ASN
2	I	111	ASN
2	I	132	ASN
2	I	147	HIS
2	I	148	ASN
2	I	153	ASN
2	J	84	ASN
2	J	113	ASN
2	J	147	HIS
2	K	20	HIS
2	K	47	ASN
2	K	63	ASN
2	K	73	GLN
2	K	84	ASN
2	K	88	ASN
2	K	113	ASN
2	K	147	HIS
2	L	40	GLN
2	L	63	ASN
2	L	73	GLN

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Mol	Chain	Res	Type
2	L	113	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	PAL	A	1001	-	9,15,15	2.67	5 (55%)	12,21,21	1.04	0
4	PAL	B	1002	-	9,15,15	2.53	4 (44%)	12,21,21	1.21	1 (8%)
4	PAL	C	1003	-	9,15,15	2.33	5 (55%)	12,21,21	1.14	0
4	PAL	D	1004	-	9,15,15	2.42	4 (44%)	12,21,21	1.07	0
4	PAL	E	1005	-	9,15,15	2.00	3 (33%)	12,21,21	1.31	2 (16%)
4	PAL	F	1006	-	9,15,15	2.48	5 (55%)	12,21,21	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PAL	A	1001	-	-	0/11/17/17	0/0/0/0
4	PAL	B	1002	-	-	0/11/17/17	0/0/0/0
4	PAL	C	1003	-	-	0/11/17/17	0/0/0/0
4	PAL	D	1004	-	-	0/11/17/17	0/0/0/0
4	PAL	E	1005	-	-	0/11/17/17	0/0/0/0
4	PAL	F	1006	-	-	0/11/17/17	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	PAL	C2-N2	-3.30	1.41	1.46
4	C	1003	PAL	C2-N2	-3.17	1.42	1.46
4	D	1004	PAL	C2-N2	-3.09	1.42	1.46
4	F	1006	PAL	C2-N2	-2.92	1.42	1.46
4	B	1002	PAL	C2-N2	-2.84	1.42	1.46
4	F	1006	PAL	P-O1P	-2.78	1.44	1.50
4	E	1005	PAL	P-O1P	-2.70	1.44	1.50
4	B	1002	PAL	P-O1P	-2.59	1.44	1.50
4	A	1001	PAL	C1-N2	-2.53	1.28	1.34
4	F	1006	PAL	C1-N2	-2.48	1.29	1.34
4	C	1003	PAL	P-O2P	-2.42	1.49	1.54
4	F	1006	PAL	P-O2P	-2.31	1.49	1.54
4	A	1001	PAL	P-O1P	-2.20	1.45	1.50
4	D	1004	PAL	P-O1P	-2.18	1.45	1.50
4	C	1003	PAL	P-O1P	-2.02	1.45	1.50
4	C	1003	PAL	P-C1P	2.47	1.83	1.79
4	B	1002	PAL	P-C1P	2.68	1.83	1.79
4	E	1005	PAL	C3-C2	2.74	1.57	1.53
4	E	1005	PAL	P-C1P	3.08	1.84	1.79
4	D	1004	PAL	P-C1P	3.28	1.84	1.79
4	A	1001	PAL	P-C1P	3.32	1.84	1.79
4	C	1003	PAL	C3-C2	3.85	1.58	1.53
4	D	1004	PAL	C3-C2	4.38	1.59	1.53
4	F	1006	PAL	C3-C2	4.54	1.59	1.53
4	A	1001	PAL	C3-C2	4.90	1.60	1.53
4	B	1002	PAL	C3-C2	5.00	1.60	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1005	PAL	P-C1P-C1	-2.68	107.86	114.41
4	B	1002	PAL	P-C1P-C1	-2.63	108.00	114.41
4	E	1005	PAL	C3-C2-C4	-2.19	106.86	111.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	PAL	1	0
4	B	1002	PAL	2	0
4	D	1004	PAL	1	0
4	E	1005	PAL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	310/310 (100%)	1.96	135 (43%) 0 0	26, 41, 87, 123	0
1	B	310/310 (100%)	1.95	119 (38%) 0 0	23, 45, 101, 117	0
1	C	310/310 (100%)	2.13	143 (46%) 0 0	26, 50, 92, 116	0
1	D	310/310 (100%)	2.39	169 (54%) 0 0	32, 56, 99, 131	0
1	E	310/310 (100%)	2.63	188 (60%) 0 0	32, 58, 104, 126	0
1	F	310/310 (100%)	2.04	136 (43%) 0 0	31, 45, 94, 129	0
2	G	153/153 (100%)	2.59	75 (49%) 0 0	40, 60, 140, 153	0
2	H	153/153 (100%)	2.20	69 (45%) 0 0	36, 58, 134, 147	0
2	I	153/153 (100%)	5.21	126 (82%) 0 0	45, 125, 154, 163	0
2	J	153/153 (100%)	2.00	52 (33%) 0 0	38, 58, 133, 156	0
2	K	153/153 (100%)	3.01	91 (59%) 0 0	48, 74, 148, 169	0
2	L	153/153 (100%)	5.73	136 (88%) 0 0	49, 134, 157, 171	0
All	All	2778/2778 (100%)	2.60	1439 (51%) 0 0	23, 55, 139, 171	0

All (1439) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	54	GLY	18.8
2	L	8	GLN	15.9
2	J	2	THR	14.9
2	I	54	GLY	14.5
2	I	11	ALA	13.5
1	F	309	VAL	13.1
2	I	89	TYR	12.7
2	I	151	LEU	12.5
2	I	86	ILE	12.3
1	D	79	THR	12.2
2	L	15	GLY	12.1

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Mol	Chain	Res	Type	RSRZ
1	B	236	ASP	12.0
1	E	81	LEU	11.8
2	L	69	ASP	11.4
1	A	85	GLY	11.4
2	I	38	THR	11.2
2	L	53	MET	11.2
2	L	38	THR	11.2
2	K	1	MET	11.1
2	L	50	SER	11.0
2	G	2	THR	11.0
2	G	9	VAL	10.8
2	K	7	LEU	10.8
2	L	89	TYR	10.8
1	E	243	VAL	10.7
2	I	51	GLY	10.6
2	H	7	LEU	10.5
2	I	15	GLY	10.5
2	I	36	THR	10.5
2	I	63	ASN	10.5
2	L	3	HIS	10.4
2	L	132	ASN	10.4
1	D	236	ASP	10.3
1	A	81	LEU	10.3
1	F	81	LEU	10.2
2	I	14	ARG	10.2
2	J	7	LEU	10.0
1	B	237	PRO	10.0
2	K	9	VAL	9.9
2	K	132	ASN	9.9
2	K	3	HIS	9.8
2	L	1	MET	9.8
2	L	49	PRO	9.7
2	L	2	THR	9.6
2	L	7	LEU	9.6
2	I	98	SER	9.5
2	I	57	ASP	9.4
2	L	65	PHE	9.4
2	L	35	LEU	9.3
2	I	64	THR	9.3
2	L	12	ILE	9.3
2	L	61	ILE	9.3
2	I	3	HIS	9.2

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Mol	Chain	Res	Type	RSRZ
2	H	4	ASP	9.2
2	K	5	ASN	9.2
1	E	237	PRO	9.1
2	I	66	LEU	9.1
2	K	50	SER	9.1
1	A	79	THR	9.1
2	L	22	PRO	9.1
2	I	84	ASN	9.1
2	I	65	PHE	9.1
2	I	67	SER	9.0
2	I	88	ASN	9.0
2	L	76	LEU	9.0
2	I	69	ASP	9.0
2	L	36	THR	8.9
2	L	71	VAL	8.9
2	L	96	ARG	8.8
1	C	81	LEU	8.8
2	L	66	LEU	8.8
2	I	39	ASP	8.8
2	K	6	LYS	8.7
2	H	10	GLU	8.7
2	L	34	LYS	8.7
1	E	236	ASP	8.7
2	L	86	ILE	8.6
1	D	80	SER	8.6
2	L	6	LYS	8.6
2	L	105	ASN	8.6
2	L	91	VAL	8.5
2	L	77	TYR	8.5
2	I	43	THR	8.5
2	I	80	GLN	8.5
2	L	51	GLY	8.4
2	I	7	LEU	8.4
2	L	67	SER	8.4
1	B	81	LEU	8.3
2	H	3	HIS	8.3
2	I	12	ILE	8.3
2	L	4	ASP	8.3
2	H	5	ASN	8.2
2	L	42	ILE	8.2
2	I	40	GLN	8.2
2	L	90	GLU	8.2

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Mol	Chain	Res	Type	RSRZ
2	L	88	ASN	8.2
2	K	2	THR	8.1
2	L	92	VAL	8.1
2	I	68	GLU	8.0
2	L	133	ASP	8.0
2	I	70	GLN	8.0
2	L	52	GLU	7.9
2	L	80	GLN	7.9
2	L	11	ALA	7.9
2	L	25	ILE	7.9
2	G	93	GLY	7.9
2	I	92	VAL	7.8
2	L	39	ASP	7.8
2	L	98	SER	7.8
2	I	73	GLN	7.8
1	D	310	LEU	7.8
2	G	7	LEU	7.8
2	I	71	VAL	7.7
2	L	14	ARG	7.7
1	B	79	THR	7.6
2	H	2	THR	7.6
1	C	255	HIS	7.6
2	I	5	ASN	7.6
2	I	1	MET	7.6
1	B	243	VAL	7.6
2	L	131	ALA	7.6
1	E	85	GLY	7.5
2	I	91	VAL	7.5
1	F	243	VAL	7.5
2	J	9	VAL	7.5
2	I	152	ALA	7.5
2	J	4	ASP	7.5
2	K	10	GLU	7.4
2	K	68	GLU	7.4
2	L	5	ASN	7.4
1	C	236	ASP	7.4
2	I	23	ALA	7.4
2	G	87	ASP	7.4
2	L	33	PHE	7.4
2	K	152	ALA	7.3
1	D	81	LEU	7.3
1	B	310	LEU	7.3

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Mol	Chain	Res	Type	RSRZ
2	G	88	ASN	7.3
2	L	100	PRO	7.3
2	L	27	PHE	7.2
2	I	85	ARG	7.2
1	C	237	PRO	7.2
1	F	237	PRO	7.2
2	I	32	LEU	7.2
2	I	30	LEU	7.1
2	L	10	GLU	7.1
1	A	236	ASP	7.1
2	L	9	VAL	7.1
2	G	153	ASN	7.1
1	C	77	ALA	7.0
2	L	75	ALA	7.0
2	L	72	ASP	7.0
2	L	79	PRO	7.0
2	L	82	THR	7.0
2	L	153	ASN	7.0
2	K	54	GLY	6.9
2	I	31	SER	6.9
2	J	1	MET	6.9
2	I	2	THR	6.9
2	L	70	GLN	6.8
2	I	47	ASN	6.8
1	E	33	ASN	6.8
1	E	310	LEU	6.8
2	L	84	ASN	6.8
2	I	90	GLU	6.8
2	L	18	ILE	6.8
2	G	6	LYS	6.8
2	G	10	GLU	6.8
2	K	70	GLN	6.7
2	L	87	ASP	6.7
1	C	80	SER	6.7
1	E	255	HIS	6.7
1	E	82	GLY	6.7
2	K	153	ASN	6.7
2	J	153	ASN	6.6
2	I	17	VAL	6.6
2	L	78	ALA	6.6
2	I	95	SER	6.6
2	I	35	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
2	I	49	PRO	6.5
2	G	92	VAL	6.5
2	H	11	ALA	6.5
2	L	60	LYS	6.5
2	I	6	LYS	6.5
2	I	4	ASP	6.5
2	G	8	GLN	6.5
2	I	72	ASP	6.4
2	G	96	ARG	6.4
1	E	280	THR	6.4
1	E	309	VAL	6.4
1	F	241	ALA	6.3
2	L	148	ASN	6.3
2	L	83	VAL	6.3
2	H	1	MET	6.3
2	L	64	THR	6.3
1	C	310	LEU	6.3
2	I	79	PRO	6.3
1	E	190	ASP	6.3
2	G	133	ASP	6.3
2	I	52	GLU	6.3
2	L	63	ASN	6.3
1	E	79	THR	6.2
1	F	240	TYR	6.2
2	L	57	ASP	6.2
2	G	3	HIS	6.2
2	L	47	ASN	6.1
2	I	42	ILE	6.1
2	I	133	ASP	6.1
1	E	307	ASP	6.1
2	I	37	GLU	6.1
1	F	242	ASN	6.1
2	I	93	GLY	6.1
2	I	41	ARG	6.1
2	L	40	GLN	6.0
2	I	53	MET	6.0
2	I	149	VAL	6.0
2	L	37	GLU	6.0
2	J	132	ASN	6.0
2	L	17	VAL	5.9
2	L	68	GLU	5.9
1	E	120	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	280	THR	5.9
1	D	30	LEU	5.9
1	E	267	LEU	5.9
1	D	32	ALA	5.8
1	E	1	ALA	5.8
2	I	19	ASP	5.8
2	H	88	ASN	5.8
1	C	79	THR	5.8
1	D	255	HIS	5.8
1	A	78	ASN	5.8
1	F	79	THR	5.8
2	L	95	SER	5.7
2	K	67	SER	5.7
2	L	55	ARG	5.7
2	I	48	LEU	5.7
2	K	148	ASN	5.7
2	L	19	ASP	5.7
2	I	81	ALA	5.6
2	I	33	PHE	5.6
1	F	85	GLY	5.6
1	A	190	ASP	5.6
1	A	84	LYS	5.6
1	A	237	PRO	5.6
2	G	67	SER	5.6
2	I	9	VAL	5.6
2	I	153	ASN	5.6
1	C	189	PRO	5.6
2	G	95	SER	5.6
2	G	152	ALA	5.6
2	I	25	ILE	5.6
2	H	6	LYS	5.5
2	J	3	HIS	5.5
2	I	59	ILE	5.5
2	I	96	ARG	5.5
2	G	151	LEU	5.5
2	L	46	LEU	5.5
1	C	252	SER	5.5
2	K	4	ASP	5.5
2	K	52	GLU	5.5
2	L	43	THR	5.5
2	I	34	LYS	5.4
1	E	140	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	57	LEU	5.4
2	L	97	PRO	5.4
2	I	18	ILE	5.4
2	H	87	ASP	5.4
1	D	240	TYR	5.4
1	E	202	LEU	5.4
1	E	241	ALA	5.3
2	L	13	LYS	5.3
2	G	1	MET	5.3
1	D	94	VAL	5.3
2	G	132	ASN	5.3
1	D	84	LYS	5.3
2	I	13	LYS	5.3
2	G	97	PRO	5.3
1	E	121	ASN	5.3
1	C	82	GLY	5.3
2	J	8	GLN	5.3
2	J	10	GLU	5.3
2	I	61	ILE	5.2
1	E	252	SER	5.2
2	L	93	GLY	5.2
2	K	53	MET	5.2
1	E	214	SER	5.2
1	D	237	PRO	5.2
1	E	20	LEU	5.2
2	L	23	ALA	5.2
1	E	276	ASP	5.2
1	D	252	SER	5.2
2	J	98	SER	5.2
2	I	26	GLY	5.2
2	L	104	ASP	5.2
2	I	83	VAL	5.2
1	E	242	ASN	5.2
1	A	310	LEU	5.1
2	L	21	ILE	5.1
2	I	150	VAL	5.1
2	K	100	PRO	5.1
1	D	176	LEU	5.1
1	E	139	LEU	5.1
1	D	195	PRO	5.1
1	D	77	ALA	5.1
2	G	131	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
2	K	8	GLN	5.1
2	I	146	SER	5.1
1	D	76	SER	5.1
1	D	267	LEU	5.1
1	B	240	TYR	5.1
1	B	267	LEU	5.1
2	H	153	ASN	5.1
1	F	80	SER	5.1
2	L	147	HIS	5.1
1	D	202	LEU	5.0
2	I	10	GLU	5.0
1	A	255	HIS	5.0
1	B	255	HIS	5.0
1	B	252	SER	5.0
2	L	20	HIS	5.0
1	A	80	SER	5.0
2	I	74	LEU	5.0
1	D	82	GLY	5.0
1	E	238	SER	5.0
1	B	215	ILE	5.0
1	E	30	LEU	5.0
2	K	51	GLY	5.0
1	B	190	ASP	5.0
2	J	133	ASP	5.0
1	F	308	LEU	4.9
1	E	216	GLU	4.9
2	I	147	HIS	4.9
1	F	236	ASP	4.9
1	D	243	VAL	4.9
2	I	75	ALA	4.9
2	K	11	ALA	4.9
1	E	144	THR	4.9
2	L	62	GLU	4.9
2	K	98	SER	4.9
2	I	82	THR	4.9
2	L	134	ILE	4.9
2	I	97	PRO	4.9
2	I	50	SER	4.9
1	B	84	LYS	4.8
1	C	202	LEU	4.8
1	C	20	LEU	4.8
1	D	216	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	190	ASP	4.8
2	H	67	SER	4.8
1	D	95	ILE	4.8
2	I	46	LEU	4.8
2	K	151	LEU	4.8
2	H	9	VAL	4.8
2	L	16	THR	4.8
1	D	276	ASP	4.8
1	B	33	ASN	4.8
1	E	154	ASN	4.8
2	L	146	SER	4.8
1	E	169	VAL	4.8
2	L	94	LYS	4.8
2	L	138	CYS	4.7
2	L	151	LEU	4.7
2	G	11	ALA	4.7
2	K	101	GLU	4.7
1	C	280	THR	4.7
2	J	6	LYS	4.7
2	K	79	PRO	4.7
1	C	241	ALA	4.7
2	K	55	ARG	4.7
2	L	130	ARG	4.7
2	K	66	LEU	4.7
1	B	242	ASN	4.7
1	E	145	ILE	4.7
1	F	267	LEU	4.7
2	L	74	LEU	4.7
1	D	33	ASN	4.7
1	A	57	LEU	4.7
2	L	30	LEU	4.7
2	G	99	LEU	4.6
1	E	136	THR	4.6
1	C	15	LEU	4.6
2	I	62	GLU	4.6
1	B	85	GLY	4.6
1	D	20	LEU	4.6
2	G	98	SER	4.6
2	H	98	SER	4.6
1	D	172	LEU	4.6
1	E	95	ILE	4.6
1	E	80	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	83	LYS	4.5
2	L	81	ALA	4.5
1	C	216	GLU	4.5
1	D	309	VAL	4.5
1	D	279	LYS	4.5
2	I	24	GLN	4.5
1	C	214	SER	4.5
1	D	190	ASP	4.5
2	J	149	VAL	4.5
1	D	57	LEU	4.5
1	F	57	LEU	4.5
1	A	267	LEU	4.5
2	I	76	LEU	4.5
1	D	244	LYS	4.5
1	B	245	ALA	4.5
2	K	111	ASN	4.5
1	B	20	LEU	4.5
2	L	48	LEU	4.5
2	H	65	PHE	4.5
1	E	266	PRO	4.4
2	G	117	HIS	4.4
2	K	147	HIS	4.4
2	K	133	ASP	4.4
2	G	5	ASN	4.4
1	E	244	LYS	4.4
2	K	75	ALA	4.4
1	D	277	VAL	4.4
1	B	241	ALA	4.4
1	E	32	ALA	4.4
1	E	206	GLY	4.4
1	C	57	LEU	4.4
2	I	29	LEU	4.4
1	B	75	ASP	4.4
1	D	206	GLY	4.4
1	B	142	LEU	4.3
1	F	202	LEU	4.3
1	B	202	LEU	4.3
1	E	264	LEU	4.3
1	E	12	ILE	4.3
1	E	198	ILE	4.3
1	F	102	ILE	4.3
1	F	48	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
2	J	5	ASN	4.3
1	C	243	VAL	4.3
1	E	279	LYS	4.3
1	D	145	ILE	4.3
1	D	242	ASN	4.3
1	A	48	PHE	4.2
1	D	48	PHE	4.2
1	E	201	MET	4.2
1	E	172	LEU	4.2
1	D	85	GLY	4.2
1	C	276	ASP	4.2
2	L	85	ARG	4.2
1	B	80	SER	4.2
1	B	256	ASN	4.2
1	E	240	TYR	4.2
2	H	138	CYS	4.2
1	A	219	MET	4.2
2	K	118	ALA	4.2
2	K	146	SER	4.2
2	K	96	ARG	4.2
1	E	268	PRO	4.2
2	K	80	GLN	4.2
1	B	83	LYS	4.2
2	J	67	SER	4.2
1	E	55	THR	4.2
1	C	242	ASN	4.2
1	E	142	LEU	4.2
1	E	176	LEU	4.2
1	E	137	GLN	4.2
2	G	39	ASP	4.2
1	A	216	GLU	4.2
1	C	85	GLY	4.2
1	E	293	ILE	4.1
2	J	130	ARG	4.1
2	L	121	VAL	4.1
2	I	148	ASN	4.1
1	E	74	SER	4.1
1	F	39	LEU	4.1
2	J	118	ALA	4.1
1	D	200	ASP	4.1
2	L	32	LEU	4.1
1	C	251	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	90	GLU	4.1
2	G	94	LYS	4.1
1	F	293	ILE	4.1
1	A	120	GLY	4.1
1	B	238	SER	4.1
1	D	140	LEU	4.1
1	D	299	LEU	4.1
2	H	118	ALA	4.1
1	C	169	VAL	4.1
1	F	73	PHE	4.1
1	F	142	LEU	4.1
1	D	47	CYS	4.1
2	K	121	VAL	4.1
2	I	27	PHE	4.1
2	K	122	SER	4.1
2	L	99	LEU	4.1
2	G	148	ASN	4.1
1	D	307	ASP	4.1
1	D	74	SER	4.0
2	G	74	LEU	4.0
2	I	105	ASN	4.0
2	I	132	ASN	4.0
2	H	89	TYR	4.0
1	F	94	VAL	4.0
1	B	15	LEU	4.0
2	L	24	GLN	4.0
1	E	260	ASN	4.0
2	L	59	ILE	4.0
1	C	142	LEU	4.0
2	H	50	SER	4.0
1	E	218	VAL	4.0
2	H	15	GLY	4.0
2	J	50	SER	4.0
1	E	217	GLU	4.0
1	D	83	LYS	4.0
1	F	71	VAL	4.0
2	I	20	HIS	4.0
2	K	39	ASP	3.9
1	B	78	ASN	3.9
2	G	13	LYS	3.9
1	D	72	GLY	3.9
1	C	257	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	J	11	ALA	3.9
1	A	76	SER	3.9
1	F	76	SER	3.9
2	I	21	ILE	3.9
1	B	121	ASN	3.9
2	I	22	PRO	3.9
1	C	217	GLU	3.9
2	H	8	GLN	3.9
2	H	39	ASP	3.9
2	I	131	ALA	3.9
1	A	243	VAL	3.9
1	A	92	ILE	3.9
1	D	238	SER	3.9
2	G	4	ASP	3.9
1	C	240	TYR	3.9
1	C	198	ILE	3.9
1	E	138	THR	3.9
1	A	300	LEU	3.9
2	I	87	ASP	3.8
1	E	83	LYS	3.8
1	B	77	ALA	3.8
1	F	310	LEU	3.8
1	D	73	PHE	3.8
1	D	103	VAL	3.8
2	J	146	SER	3.8
1	A	241	ALA	3.8
1	C	266	PRO	3.8
2	G	90	GLU	3.8
1	F	74	SER	3.8
1	E	153	ASP	3.8
1	E	103	VAL	3.8
2	J	12	ILE	3.8
1	C	1	ALA	3.8
1	E	259	ALA	3.8
2	J	111	ASN	3.8
2	K	49	PRO	3.8
1	B	172	LEU	3.8
2	G	51	GLY	3.8
1	F	59	PHE	3.8
2	H	92	VAL	3.8
1	A	280	THR	3.8
1	C	190	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	18	ASP	3.8
1	A	252	SER	3.8
1	B	216	GLU	3.8
2	K	30	LEU	3.8
1	A	215	ILE	3.7
2	J	114	CYS	3.7
1	E	257	ALA	3.7
2	I	16	THR	3.7
1	E	75	ASP	3.7
1	B	94	VAL	3.7
1	F	103	VAL	3.7
1	D	253	ASP	3.7
1	D	136	THR	3.7
2	G	149	VAL	3.7
2	H	95	SER	3.7
1	B	244	LYS	3.7
1	C	173	THR	3.7
1	F	280	THR	3.7
1	F	215	ILE	3.7
2	L	135	ALA	3.7
1	C	172	LEU	3.7
2	J	151	LEU	3.7
1	C	94	VAL	3.7
1	F	244	LYS	3.7
1	E	254	LEU	3.7
1	D	28	ALA	3.6
1	D	256	ASN	3.6
1	F	46	SER	3.6
2	G	91	VAL	3.6
1	B	307	ASP	3.6
2	I	109	CYS	3.6
1	A	139	LEU	3.6
1	D	142	LEU	3.6
1	E	15	LEU	3.6
1	E	300	LEU	3.6
1	A	242	ASN	3.6
1	B	175	ALA	3.6
1	A	124	VAL	3.6
1	E	71	VAL	3.6
1	A	140	LEU	3.6
1	A	266	PRO	3.6
1	A	59	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
2	L	122	SER	3.6
2	L	58	LEU	3.6
2	K	104	ASP	3.6
1	C	144	THR	3.6
1	E	76	SER	3.6
1	D	29	LYS	3.6
1	F	307	ASP	3.6
2	L	41	ARG	3.6
1	A	138	THR	3.6
1	A	127	ALA	3.6
1	D	104	MET	3.6
2	L	28	LYS	3.6
1	A	95	ILE	3.6
1	C	196	GLN	3.6
2	K	25	ILE	3.6
1	C	33	ASN	3.6
1	D	15	LEU	3.6
1	F	114	LEU	3.6
1	E	303	VAL	3.5
1	D	24	LEU	3.5
1	D	241	ALA	3.5
1	A	121	ASN	3.5
1	C	71	VAL	3.5
1	D	71	VAL	3.5
1	C	139	LEU	3.5
1	E	4	LEU	3.5
1	F	4	LEU	3.5
1	E	115	ALA	3.5
2	H	72	ASP	3.5
1	B	235	LEU	3.5
1	D	46	SER	3.5
1	E	253	ASP	3.5
2	H	63	ASN	3.5
1	D	271	ASP	3.5
1	E	77	ALA	3.5
2	L	129	LYS	3.5
1	C	95	ILE	3.5
2	J	115	ILE	3.5
1	D	264	LEU	3.5
1	A	82	GLY	3.5
1	D	146	GLN	3.5
1	D	239	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	275	THR	3.5
1	A	254	LEU	3.5
1	C	121	ASN	3.4
1	F	172	LEU	3.5
2	I	101	GLU	3.4
1	E	53	THR	3.4
1	E	226	TYR	3.4
1	F	95	ILE	3.4
1	A	103	VAL	3.4
1	D	23	VAL	3.4
1	D	121	ASN	3.4
1	D	34	PRO	3.4
2	I	100	PRO	3.4
1	C	238	SER	3.4
1	B	293	ILE	3.4
1	D	102	ILE	3.4
1	F	92	ILE	3.4
1	F	270	VAL	3.4
1	C	213	SER	3.4
1	C	215	ILE	3.4
2	K	134	ILE	3.4
1	C	32	ALA	3.4
2	K	102	ARG	3.4
1	D	59	PHE	3.4
2	L	31	SER	3.4
1	C	254	LEU	3.4
1	B	91	THR	3.4
1	C	253	ASP	3.4
1	E	48	PHE	3.4
1	E	84	LYS	3.4
1	F	136	THR	3.4
1	A	256	ASN	3.4
1	C	256	ASN	3.4
2	J	105	ASN	3.4
2	K	88	ASN	3.4
1	E	212	HIS	3.4
2	H	86	ILE	3.4
2	L	102	ARG	3.4
2	L	128	ARG	3.4
1	A	276	ASP	3.4
1	B	140	LEU	3.3
1	B	169	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	127	ALA	3.3
2	G	147	HIS	3.3
1	F	276	ASP	3.3
1	A	102	ILE	3.3
1	B	95	ILE	3.3
2	G	89	TYR	3.3
1	B	71	VAL	3.3
2	G	150	VAL	3.3
2	K	149	VAL	3.3
1	E	127	ALA	3.3
1	C	83	LYS	3.3
1	C	73	PHE	3.3
1	D	300	LEU	3.3
1	E	130	GLY	3.3
2	G	138	CYS	3.3
1	C	48	PHE	3.3
1	A	202	LEU	3.3
1	E	256	ASN	3.3
1	F	199	LEU	3.3
2	G	86	ILE	3.3
1	E	94	VAL	3.3
1	D	246	GLN	3.3
1	F	252	SER	3.3
1	E	18	ASP	3.3
2	G	104	ASP	3.3
1	F	72	GLY	3.3
2	K	72	ASP	3.3
1	F	77	ALA	3.3
2	J	113	ASN	3.3
1	B	176	LEU	3.3
2	I	99	LEU	3.3
1	F	82	GLY	3.3
1	A	214	SER	3.3
1	D	270	VAL	3.3
1	F	238	SER	3.3
1	C	244	LYS	3.3
2	I	55	ARG	3.3
1	B	102	ILE	3.2
1	D	75	ASP	3.2
1	E	205	LYS	3.2
2	J	104	ASP	3.2
2	L	127	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	104	MET	3.2
2	L	125	PHE	3.2
1	B	82	GLY	3.2
1	F	139	LEU	3.2
2	K	90	GLU	3.2
1	C	12	ILE	3.2
2	K	20	HIS	3.2
1	F	169	VAL	3.2
1	E	219	MET	3.2
2	H	66	LEU	3.2
1	D	53	THR	3.2
2	K	127	VAL	3.2
1	E	21	ASN	3.2
2	G	68	GLU	3.2
1	C	130	GLY	3.2
1	E	72	GLY	3.2
1	E	73	PHE	3.2
1	C	125	LEU	3.2
1	C	235	LEU	3.2
1	F	84	LYS	3.2
1	C	91	THR	3.2
1	A	260	ASN	3.2
1	F	75	ASP	3.2
2	I	104	ASP	3.2
1	F	104	MET	3.2
1	A	74	SER	3.2
1	C	279	LYS	3.2
1	B	57	LEU	3.2
2	L	111	ASN	3.2
1	A	259	ALA	3.2
1	B	226	TYR	3.2
2	K	89	TYR	3.2
1	F	216	GLU	3.2
1	C	46	SER	3.2
1	D	61	THR	3.2
1	F	32	ALA	3.2
2	K	117	HIS	3.2
1	B	300	LEU	3.1
2	H	29	LEU	3.1
1	F	266	PRO	3.1
1	F	47	CYS	3.1
1	E	87	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	261	MET	3.1
1	B	299	LEU	3.1
1	D	189	PRO	3.1
1	F	125	LEU	3.1
2	L	136	LEU	3.1
1	B	198	ILE	3.1
2	L	73	GLN	3.1
1	D	274	ALA	3.1
2	L	56	LYS	3.1
1	A	46	SER	3.1
1	E	59	PHE	3.1
1	B	125	LEU	3.1
1	B	139	LEU	3.1
1	D	22	LEU	3.1
1	C	145	ILE	3.1
2	K	12	ILE	3.1
1	A	20	LEU	3.1
1	D	139	LEU	3.1
2	J	23	ALA	3.1
1	A	18	ASP	3.1
2	K	95	SER	3.1
1	A	47	CYS	3.1
2	H	141	CYS	3.1
1	A	125	LEU	3.1
1	A	293	ILE	3.1
1	E	215	ILE	3.1
2	G	12	ILE	3.1
2	I	111	ASN	3.1
1	A	23	VAL	3.1
2	H	70	GLN	3.1
1	C	59	PHE	3.1
1	C	102	ILE	3.1
1	E	180	ASP	3.1
2	L	149	VAL	3.1
1	E	299	LEU	3.0
1	F	264	LEU	3.0
2	J	148	ASN	3.0
1	E	25	ALA	3.0
2	L	103	ILE	3.0
1	B	43	VAL	3.0
1	C	270	VAL	3.0
2	I	45	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	266	PRO	3.0
1	E	63	MET	3.0
1	A	66	LEU	3.0
1	C	30	LEU	3.0
1	E	24	LEU	3.0
1	E	134	HIS	3.0
1	E	155	LEU	3.0
1	E	306	ARG	3.0
2	H	91	VAL	3.0
1	D	4	LEU	3.0
1	E	2	ASN	3.0
1	F	138	THR	3.0
1	C	103	VAL	3.0
1	F	218	VAL	3.0
2	I	138	CYS	3.0
1	F	196	GLN	3.0
1	C	17	ARG	3.0
1	A	172	LEU	3.0
1	B	264	LEU	3.0
1	F	78	ASN	3.0
2	K	136	LEU	3.0
1	B	220	ALA	3.0
1	D	92	ILE	3.0
1	D	193	ALA	3.0
2	L	45	GLY	3.0
2	H	69	ASP	3.0
1	E	23	VAL	3.0
2	K	150	VAL	3.0
1	C	104	MET	3.0
2	I	28	LYS	3.0
2	K	109	CYS	3.0
1	E	143	PHE	3.0
1	F	300	LEU	3.0
1	B	61	THR	3.0
2	I	77	TYR	3.0
1	F	127	ALA	3.0
1	C	84	LYS	3.0
1	A	71	VAL	3.0
1	A	303	VAL	3.0
1	E	78	ASN	3.0
1	C	299	LEU	3.0
2	G	29	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	55	THR	3.0
2	I	112	SER	3.0
1	A	83	LYS	3.0
1	C	176	LEU	2.9
1	E	159	MET	2.9
1	F	15	LEU	2.9
1	F	30	LEU	2.9
1	F	16	SER	2.9
2	K	123	SER	2.9
2	G	72	ASP	2.9
2	L	118	ALA	2.9
1	D	55	THR	2.9
1	D	153	ASP	2.9
1	C	221	GLU	2.9
1	A	295	ALA	2.9
1	A	44	ILE	2.9
2	K	114	CYS	2.9
1	B	157	VAL	2.9
1	B	24	LEU	2.9
1	C	219	MET	2.9
1	C	300	LEU	2.9
1	D	254	LEU	2.9
1	F	140	LEU	2.9
1	B	280	THR	2.9
1	F	87	THR	2.9
2	J	117	HIS	2.9
1	C	92	ILE	2.9
1	A	153	ASP	2.9
1	C	309	VAL	2.9
2	H	93	GLY	2.9
1	A	15	LEU	2.9
1	A	30	LEU	2.9
1	D	125	LEU	2.9
1	E	22	LEU	2.9
2	H	112	SER	2.9
2	J	112	SER	2.9
1	A	279	LYS	2.9
1	E	245	ALA	2.9
2	G	70	GLN	2.9
2	I	118	ALA	2.9
1	A	12	ILE	2.9
1	C	268	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	268	PRO	2.9
1	A	63	MET	2.9
1	C	267	LEU	2.9
1	D	235	LEU	2.9
1	E	47	CYS	2.9
1	F	23	VAL	2.9
2	H	30	LEU	2.9
2	K	74	LEU	2.9
1	C	239	GLU	2.9
1	D	91	THR	2.9
2	G	69	ASP	2.9
1	C	120	GLY	2.9
1	A	299	LEU	2.9
1	F	296	ARG	2.9
2	K	46	LEU	2.9
1	B	295	ALA	2.9
2	I	78	ALA	2.9
2	H	13	LYS	2.9
1	E	46	SER	2.8
1	D	63	MET	2.8
1	F	63	MET	2.8
1	F	155	LEU	2.8
1	A	136	THR	2.8
1	D	179	PHE	2.8
1	E	247	PHE	2.8
2	K	82	THR	2.8
1	E	181	GLY	2.8
2	K	42	ILE	2.8
1	C	23	VAL	2.8
1	E	56	ARG	2.8
1	F	274	ALA	2.8
1	D	215	ILE	2.8
2	J	147	HIS	2.8
1	E	235	LEU	2.8
1	E	308	LEU	2.8
2	L	29	LEU	2.8
1	B	17	ARG	2.8
1	C	61	THR	2.8
2	J	51	GLY	2.8
1	A	25	ALA	2.8
2	K	131	ALA	2.8
2	K	138	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	88	LEU	2.8
2	I	60	LYS	2.8
1	E	28	ALA	2.8
1	E	16	SER	2.8
1	D	155	LEU	2.8
1	E	39	LEU	2.8
2	I	8	GLN	2.8
1	D	138	THR	2.8
1	D	168	THR	2.8
1	F	144	THR	2.8
1	C	220	ALA	2.8
1	C	210	SER	2.8
1	C	246	GLN	2.8
1	C	206	GLY	2.8
1	F	159	MET	2.8
1	B	144	THR	2.8
1	C	55	THR	2.8
1	E	148	THR	2.8
1	C	76	SER	2.8
1	E	296	ARG	2.8
1	F	120	GLY	2.7
1	A	26	THR	2.7
1	A	169	VAL	2.7
2	G	146	SER	2.7
1	D	150	GLY	2.7
1	A	22	LEU	2.7
1	F	88	LEU	2.7
1	E	104	MET	2.7
1	A	189	PRO	2.7
1	D	43	VAL	2.7
1	D	278	ASP	2.7
1	E	19	ASP	2.7
1	E	277	VAL	2.7
2	L	145	PHE	2.7
1	D	16	SER	2.7
1	B	145	ILE	2.7
1	F	145	ILE	2.7
1	A	4	LEU	2.7
1	D	203	ASP	2.7
2	K	119	GLU	2.7
1	D	157	VAL	2.7
1	C	155	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	138	THR	2.7
1	E	135	PRO	2.7
1	D	218	VAL	2.7
1	A	226	TYR	2.7
1	A	240	TYR	2.7
1	B	130	GLY	2.7
2	J	90	GLU	2.7
1	C	168	THR	2.7
1	E	275	THR	2.7
1	C	124	VAL	2.7
1	C	271	ASP	2.7
1	D	293	ILE	2.7
1	C	114	LEU	2.7
1	E	301	ALA	2.7
1	D	98	TYR	2.7
1	A	217	GLU	2.6
1	D	66	LEU	2.6
1	D	88	LEU	2.6
1	F	64	HIS	2.6
1	F	189	PRO	2.6
1	C	201	MET	2.6
1	F	275	THR	2.6
2	G	64	THR	2.6
2	J	53	MET	2.6
1	B	59	PHE	2.6
1	D	166	GLY	2.6
1	D	251	ALA	2.6
1	D	301	ALA	2.6
2	G	63	ASN	2.6
1	B	98	TYR	2.6
1	E	60	GLU	2.6
1	B	88	LEU	2.6
1	C	22	LEU	2.6
1	E	91	THR	2.6
1	E	168	THR	2.6
1	D	130	GLY	2.6
1	D	27	ALA	2.6
1	E	203	ASP	2.6
2	L	150	VAL	2.6
1	E	197	TYR	2.6
1	E	125	LEU	2.6
1	E	207	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	137	GLN	2.6
1	D	201	MET	2.6
1	E	292	GLY	2.6
2	H	113	ASN	2.6
1	A	112	ALA	2.6
2	K	71	VAL	2.6
1	A	239	GLU	2.6
1	B	4	LEU	2.6
1	B	119	SER	2.6
1	E	34	PRO	2.6
2	K	48	LEU	2.6
2	K	59	ILE	2.6
2	H	14	ARG	2.6
2	J	72	ASP	2.6
1	D	159	MET	2.6
1	C	184	PHE	2.6
1	A	309	VAL	2.6
2	H	83	VAL	2.6
1	A	264	LEU	2.6
1	B	281	PRO	2.6
1	C	140	LEU	2.6
1	C	192	LEU	2.6
1	C	293	ILE	2.6
1	D	78	ASN	2.6
2	H	109	CYS	2.6
1	A	115	ALA	2.6
1	D	283	ALA	2.6
1	F	49	PHE	2.6
2	G	80	GLN	2.6
1	F	214	SER	2.6
2	I	94	LYS	2.6
1	D	266	PRO	2.6
1	F	2	ASN	2.6
1	C	87	THR	2.6
1	E	61	THR	2.6
1	B	104	MET	2.6
1	C	137	GLN	2.6
1	E	246	GLN	2.6
1	F	143	PHE	2.6
2	I	114	CYS	2.6
1	D	56	ARG	2.5
1	F	157	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	14	ARG	2.5
1	F	135	PRO	2.5
1	D	187	ILE	2.5
1	F	44	ILE	2.5
1	A	53	THR	2.5
1	F	61	THR	2.5
1	C	295	ALA	2.5
2	J	131	ALA	2.5
1	D	18	ASP	2.5
2	I	106	VAL	2.5
1	C	47	CYS	2.5
1	E	239	GLU	2.5
1	F	13	ASN	2.5
2	H	68	GLU	2.5
2	H	105	ASN	2.5
2	J	68	GLU	2.5
1	A	88	LEU	2.5
1	C	26	THR	2.5
1	C	207	ILE	2.5
1	D	26	THR	2.5
1	D	31	LYS	2.5
1	E	173	THR	2.5
2	G	25	ILE	2.5
1	B	159	MET	2.5
1	C	63	MET	2.5
1	A	180	ASP	2.5
1	E	158	ALA	2.5
1	F	111	ALA	2.5
1	A	39	LEU	2.5
1	D	211	LEU	2.5
1	A	145	ILE	2.5
1	C	136	THR	2.5
2	G	134	ILE	2.5
2	L	44	ILE	2.5
1	D	204	GLU	2.5
1	E	223	ASP	2.5
2	L	117	HIS	2.5
1	A	77	ALA	2.5
1	F	295	ALA	2.5
2	L	152	ALA	2.5
1	A	128	GLY	2.5
1	E	305	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	196	GLN	2.5
1	B	12	ILE	2.5
1	B	253	ASP	2.5
1	D	87	THR	2.5
2	G	16	THR	2.5
2	H	114	CYS	2.5
2	H	134	ILE	2.5
1	D	120	GLY	2.5
1	D	184	PHE	2.5
1	E	179	PHE	2.5
1	E	281	PRO	2.5
1	F	239	GLU	2.5
1	B	308	LEU	2.5
1	D	152	LEU	2.5
1	D	64	HIS	2.5
1	C	260	ASN	2.5
1	E	213	SER	2.5
1	A	270	VAL	2.5
1	E	70	VAL	2.5
1	A	253	ASP	2.5
1	A	134	HIS	2.5
1	A	176	LEU	2.5
1	F	55	THR	2.5
1	A	273	ILE	2.5
1	F	224	ILE	2.5
2	K	130	ARG	2.5
1	D	226	TYR	2.5
1	C	259	ALA	2.5
1	D	25	ALA	2.5
2	G	23	ALA	2.5
2	I	141	CYS	2.4
2	J	138	CYS	2.4
1	A	277	VAL	2.4
1	C	70	VAL	2.4
1	A	114	LEU	2.4
1	B	30	LEU	2.4
1	F	20	LEU	2.4
1	F	163	LEU	2.4
2	G	66	LEU	2.4
1	A	296	ARG	2.4
2	H	54	GLY	2.4
1	A	58	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	127	ALA	2.4
1	D	45	ALA	2.4
1	E	111	ALA	2.4
1	E	210	SER	2.4
1	F	45	ALA	2.4
1	F	245	ALA	2.4
2	J	78	ALA	2.4
1	F	43	VAL	2.4
1	F	304	LEU	2.4
1	A	168	THR	2.4
1	F	166	GLY	2.4
2	H	51	GLY	2.4
1	F	198	ILE	2.4
1	A	45	ALA	2.4
1	B	32	ALA	2.4
1	F	226	TYR	2.4
2	H	57	ASP	2.4
1	E	184	PHE	2.4
1	F	137	GLN	2.4
1	A	94	VAL	2.4
1	C	205	LYS	2.4
2	G	28	LYS	2.4
2	L	108	VAL	2.4
1	B	66	LEU	2.4
1	E	199	LEU	2.4
2	K	105	ASN	2.4
1	F	168	THR	2.4
1	A	16	SER	2.4
1	A	221	GLU	2.4
1	E	221	GLU	2.4
1	D	295	ALA	2.4
1	D	247	PHE	2.4
2	I	56	LYS	2.4
1	C	218	VAL	2.4
1	B	152	LEU	2.4
2	K	29	LEU	2.4
1	B	136	THR	2.4
1	F	60	GLU	2.4
2	H	52	GLU	2.4
1	A	75	ASP	2.4
1	D	207	ILE	2.4
1	D	214	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	61	ILE	2.4
1	C	112	ALA	2.4
1	E	174	GLN	2.4
2	G	65	PHE	2.4
1	D	2	ASN	2.4
1	B	303	VAL	2.4
1	D	169	VAL	2.4
1	D	192	LEU	2.4
1	D	234	ARG	2.4
2	G	85	ARG	2.4
1	D	62	SER	2.4
1	C	28	ALA	2.4
1	E	112	ALA	2.4
2	G	114	CYS	2.4
1	B	48	PHE	2.4
1	D	154	ASN	2.4
1	F	121	ASN	2.4
2	L	26	GLY	2.4
1	A	24	LEU	2.4
1	A	142	LEU	2.4
1	B	218	VAL	2.4
1	C	43	VAL	2.4
1	E	178	LYS	2.4
1	D	199	LEU	2.4
1	E	211	LEU	2.4
1	F	70	VAL	2.4
2	G	136	LEU	2.4
2	H	48	LEU	2.4
2	J	69	ASP	2.4
2	K	112	SER	2.4
1	D	224	ILE	2.4
1	E	251	ALA	2.4
1	D	135	PRO	2.3
1	B	47	CYS	2.3
1	F	128	GLY	2.3
1	A	70	VAL	2.3
1	E	152	LEU	2.3
1	F	277	VAL	2.3
1	E	58	SER	2.3
2	K	78	ALA	2.3
2	G	100	PRO	2.3
2	I	102	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	137	GLN	2.3
2	H	133	ASP	2.3
1	B	239	GLU	2.3
2	J	122	SER	2.3
1	B	260	ASN	2.3
1	D	44	ILE	2.3
1	B	268	PRO	2.3
1	F	101	ALA	2.3
2	H	78	ALA	2.3
2	K	22	PRO	2.3
1	C	179	PHE	2.3
2	I	145	PHE	2.3
2	G	35	LEU	2.3
2	L	137	LYS	2.3
1	B	74	SER	2.3
1	B	23	VAL	2.3
1	E	124	VAL	2.3
1	F	124	VAL	2.3
2	G	83	VAL	2.3
2	H	38	THR	2.3
2	H	71	VAL	2.3
1	A	289	ALA	2.3
1	B	127	ALA	2.3
2	G	75	ALA	2.3
2	K	44	ILE	2.3
1	D	306	ARG	2.3
1	F	299	LEU	2.3
2	G	50	SER	2.3
2	K	99	LEU	2.3
1	F	303	VAL	2.3
1	B	120	GLY	2.3
1	D	19	ASP	2.3
1	E	271	ASP	2.3
2	J	110	PRO	2.3
2	K	103	ILE	2.3
2	I	123	SER	2.3
1	C	39	LEU	2.3
1	C	66	LEU	2.3
2	J	66	LEU	2.3
1	B	137	GLN	2.3
1	D	149	GLN	2.3
1	C	277	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	38	THR	2.3
1	C	75	ASP	2.3
1	E	31	LYS	2.3
1	B	92	ILE	2.3
1	E	102	ILE	2.3
1	E	194	MET	2.3
1	F	1	ALA	2.3
1	A	213	SER	2.3
1	C	153	ASP	2.3
1	E	141	ASP	2.3
1	E	284	TRP	2.3
2	G	79	PRO	2.3
1	E	92	ILE	2.2
1	E	295	ALA	2.2
2	L	115	ILE	2.2
1	A	238	SER	2.2
1	B	39	LEU	2.2
2	K	32	LEU	2.2
1	C	197	TYR	2.2
1	B	195	PRO	2.2
1	C	25	ALA	2.2
1	C	44	ILE	2.2
2	H	40	GLN	2.2
1	B	213	SER	2.2
2	K	93	GLY	2.2
1	F	176	LEU	2.2
2	K	76	LEU	2.2
1	E	228	THR	2.2
1	F	173	THR	2.2
1	C	98	TYR	2.2
1	D	40	LYS	2.2
1	B	177	ALA	2.2
1	F	27	ALA	2.2
1	A	33	ASN	2.2
1	C	4	LEU	2.2
1	C	199	LEU	2.2
1	C	264	LEU	2.2
1	B	138	THR	2.2
1	F	91	THR	2.2
1	A	257	ALA	2.2
1	C	274	ALA	2.2
1	A	119	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	59	ILE	2.2
2	K	61	ILE	2.2
1	E	66	LEU	2.2
2	G	30	LEU	2.2
2	H	46	LEU	2.2
1	C	204	GLU	2.2
1	E	3	PRO	2.2
1	D	70	VAL	2.2
2	G	77	TYR	2.2
1	A	298	ALA	2.2
1	D	167	ARG	2.2
2	K	23	ALA	2.2
1	D	49	PHE	2.2
1	F	22	LEU	2.2
2	H	64	THR	2.2
1	E	270	VAL	2.2
1	B	285	TYR	2.2
1	E	45	ALA	2.2
2	K	31	SER	2.2
1	A	9	ILE	2.2
2	L	109	CYS	2.2
1	C	287	GLN	2.2
1	D	114	LEU	2.2
1	B	309	VAL	2.1
1	B	25	ALA	2.1
1	D	175	ALA	2.1
1	A	10	ILE	2.1
2	J	109	CYS	2.1
2	J	141	CYS	2.1
2	H	58	LEU	2.1
1	B	103	VAL	2.1
1	B	214	SER	2.1
1	B	259	ALA	2.1
1	E	122	VAL	2.1
1	C	159	MET	2.1
2	H	21	ILE	2.1
1	C	24	LEU	2.1
1	B	135	PRO	2.1
1	E	231	GLN	2.1
1	F	255	HIS	2.1
1	B	72	GLY	2.1
2	I	125	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	91	THR	2.1
1	D	296	ARG	2.1
2	L	114	CYS	2.1
1	A	27	ALA	2.1
1	C	301	ALA	2.1
1	E	175	ALA	2.1
1	A	198	ILE	2.1
1	D	21	ASN	2.1
1	F	246	GLN	2.1
1	B	163	LEU	2.1
2	H	76	LEU	2.1
2	J	29	LEU	2.1
1	A	135	PRO	2.1
1	B	53	THR	2.1
1	D	173	THR	2.1
2	H	117	HIS	2.1
1	B	46	SER	2.1
1	C	11	SER	2.1
2	K	116	SER	2.1
1	A	191	ALA	2.1
1	D	124	VAL	2.1
1	D	205	LYS	2.1
1	E	43	VAL	2.1
1	E	208	ALA	2.1
2	L	126	ALA	2.1
1	C	135	PRO	2.1
1	E	163	LEU	2.1
2	G	32	LEU	2.1
1	B	18	ASP	2.1
1	A	68	ALA	2.1
1	C	245	ALA	2.1
1	D	257	ALA	2.1
1	F	112	ALA	2.1
1	A	99	VAL	2.1
2	G	71	VAL	2.1
2	J	134	ILE	2.1
1	E	64	HIS	2.1
1	E	98	TYR	2.1
1	F	134	HIS	2.1
1	F	197	TYR	2.1
1	B	254	LEU	2.1
1	F	24	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	195	PRO	2.1
1	A	61	THR	2.1
2	K	73	GLN	2.0
1	A	175	ALA	2.0
2	H	85	ARG	2.0
1	E	224	ILE	2.0
1	A	302	LEU	2.0
2	H	27	PHE	2.0
2	H	32	LEU	2.0
1	B	2	ASN	2.0
1	C	2	ASN	2.0
1	E	204	GLU	2.0
1	F	175	ALA	2.0
1	D	261	MET	2.0
1	E	160	VAL	2.0
2	H	53	MET	2.0
2	H	108	VAL	2.0
1	C	212	HIS	2.0
1	F	187	ILE	2.0
2	I	103	ILE	2.0
1	A	141	ASP	2.0
1	A	73	PHE	2.0
1	A	228	THR	2.0
1	B	73	PHE	2.0
1	E	146	GLN	2.0
1	F	119	SER	2.0
2	G	123	SER	2.0
1	E	40	LYS	2.0
1	B	298	ALA	2.0
1	A	159	MET	2.0
1	B	201	MET	2.0
1	D	160	VAL	2.0
2	I	108	VAL	2.0
1	B	207	ILE	2.0
1	D	60	GLU	2.0
1	D	249	LEU	2.0
1	E	249	LEU	2.0
2	K	35	LEU	2.0
1	A	148	THR	2.0
1	B	55	THR	2.0
1	E	116	THR	2.0
2	K	38	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	PAL	E	1005	16/16	0.92	0.31	-0.40	43,59,68,71	0
4	PAL	B	1002	16/16	0.95	0.25	-0.56	35,45,53,57	0
4	PAL	C	1003	16/16	0.96	0.24	-0.65	36,50,60,60	0
4	PAL	A	1001	16/16	0.94	0.26	-0.71	36,44,48,49	0
4	PAL	D	1004	16/16	0.95	0.24	-1.04	39,49,59,61	0
4	PAL	F	1006	16/16	0.97	0.21	-1.06	35,45,57,59	0
3	ZN	K	2005	1/1	0.99	0.08	-2.64	53,53,53,53	0
3	ZN	L	2006	1/1	0.89	0.08	-2.80	53,53,53,53	0
3	ZN	J	2004	1/1	0.99	0.07	-2.84	52,52,52,52	0
3	ZN	H	2001	1/1	0.98	0.08	-3.56	50,50,50,50	0
3	ZN	I	2003	1/1	0.99	0.06	-3.90	51,51,51,51	0
3	ZN	G	2002	1/1	0.97	0.12	-3.95	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.