



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 10:35 PM EST

PDB ID : 3TVI
Title : Crystal structure of Clostridium acetobutylicum aspartate kinase (CaAK): An important allosteric enzyme for industrial amino acids production
Authors : Manjasetty, B.A.; Chance, M.R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2011-09-20
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.16
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

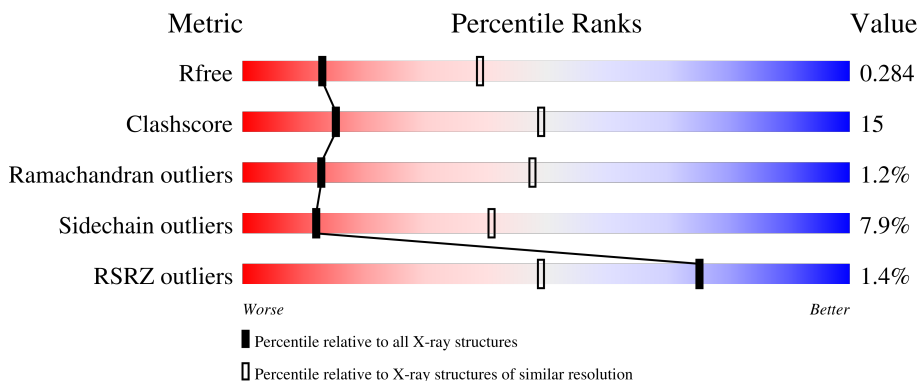
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	446	
1	B	446	
1	C	446	
1	D	446	
1	E	446	

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Mol	Chain	Length	Quality of chain	
1	F	446	70%	24%
1	G	446	66%	28%
1	H	446	67%	26%
1	I	446	68%	26%
1	J	446	70%	23%
1	K	446	66%	27%
1	L	446	69%	26%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ASP	A	451	-	-	-	X
2	ASP	G	457	-	-	-	X
2	ASP	H	458	-	-	-	X
2	ASP	L	462	-	-	-	X
3	LYS	A	501	-	-	-	X
3	LYS	C	503	-	-	-	X
3	LYS	D	504	-	-	-	X
3	LYS	G	507	-	-	X	X
3	LYS	H	508	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39043 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 Aspartokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	429	Total 3228	C 2045	N 530	O 638	S 7	Se 8	0	0	0
1	B	438	Total 3304	C 2104	N 538	O 647	S 7	Se 8	0	0	0
1	C	433	Total 3271	C 2078	N 536	O 643	S 7	Se 7	0	0	0
1	D	437	Total 3296	C 2093	N 539	O 649	S 7	Se 8	0	0	0
1	E	439	Total 3293	C 2091	N 539	O 648	S 7	Se 8	0	0	0
1	F	434	Total 3267	C 2073	N 533	O 647	S 7	Se 7	0	0	0
1	G	436	Total 3288	C 2089	N 537	O 648	S 7	Se 7	0	1	0
1	H	435	Total 3217	C 2041	N 524	O 638	S 6	Se 8	0	0	0
1	I	428	Total 3191	C 2024	N 521	O 633	S 6	Se 7	0	0	0
1	J	433	Total 3204	C 2032	N 525	O 633	S 6	Se 8	0	0	0
1	K	429	Total 3170	C 2005	N 518	O 633	S 6	Se 8	0	0	0
1	L	428	Total 3192	C 2021	N 522	O 636	S 6	Se 7	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q97MC0
A	1	LEU	-	expression tag	UNP Q97MC0
A	438	GLU	-	expression tag	UNP Q97MC0
A	439	GLY	-	expression tag	UNP Q97MC0
A	440	HIS	-	expression tag	UNP Q97MC0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	441	HIS	-	expression tag	UNP Q97MC0
A	442	HIS	-	expression tag	UNP Q97MC0
A	443	HIS	-	expression tag	UNP Q97MC0
A	444	HIS	-	expression tag	UNP Q97MC0
A	445	HIS	-	expression tag	UNP Q97MC0
B	0	SER	-	expression tag	UNP Q97MC0
B	1	LEU	-	expression tag	UNP Q97MC0
B	438	GLU	-	expression tag	UNP Q97MC0
B	439	GLY	-	expression tag	UNP Q97MC0
B	440	HIS	-	expression tag	UNP Q97MC0
B	441	HIS	-	expression tag	UNP Q97MC0
B	442	HIS	-	expression tag	UNP Q97MC0
B	443	HIS	-	expression tag	UNP Q97MC0
B	444	HIS	-	expression tag	UNP Q97MC0
B	445	HIS	-	expression tag	UNP Q97MC0
C	0	SER	-	expression tag	UNP Q97MC0
C	1	LEU	-	expression tag	UNP Q97MC0
C	438	GLU	-	expression tag	UNP Q97MC0
C	439	GLY	-	expression tag	UNP Q97MC0
C	440	HIS	-	expression tag	UNP Q97MC0
C	441	HIS	-	expression tag	UNP Q97MC0
C	442	HIS	-	expression tag	UNP Q97MC0
C	443	HIS	-	expression tag	UNP Q97MC0
C	444	HIS	-	expression tag	UNP Q97MC0
C	445	HIS	-	expression tag	UNP Q97MC0
D	0	SER	-	expression tag	UNP Q97MC0
D	1	LEU	-	expression tag	UNP Q97MC0
D	438	GLU	-	expression tag	UNP Q97MC0
D	439	GLY	-	expression tag	UNP Q97MC0
D	440	HIS	-	expression tag	UNP Q97MC0
D	441	HIS	-	expression tag	UNP Q97MC0
D	442	HIS	-	expression tag	UNP Q97MC0
D	443	HIS	-	expression tag	UNP Q97MC0
D	444	HIS	-	expression tag	UNP Q97MC0
D	445	HIS	-	expression tag	UNP Q97MC0
E	0	SER	-	expression tag	UNP Q97MC0
E	1	LEU	-	expression tag	UNP Q97MC0
E	438	GLU	-	expression tag	UNP Q97MC0
E	439	GLY	-	expression tag	UNP Q97MC0
E	440	HIS	-	expression tag	UNP Q97MC0
E	441	HIS	-	expression tag	UNP Q97MC0
E	442	HIS	-	expression tag	UNP Q97MC0

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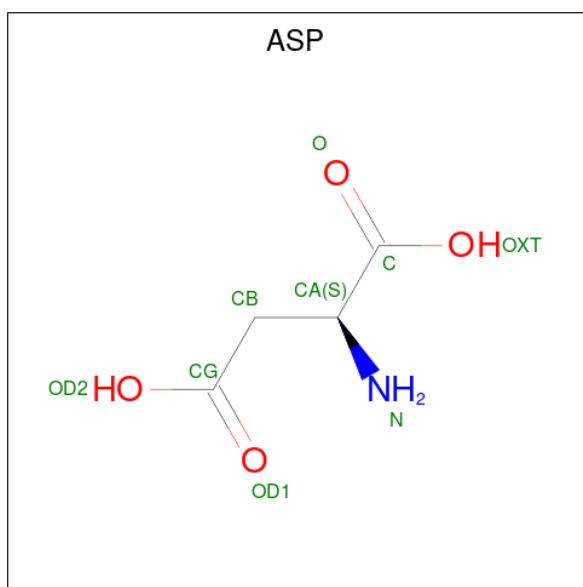
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E	444	HIS	-	expression tag	UNP Q97MC0
E	445	HIS	-	expression tag	UNP Q97MC0
F	0	SER	-	expression tag	UNP Q97MC0
F	1	LEU	-	expression tag	UNP Q97MC0
F	438	GLU	-	expression tag	UNP Q97MC0
F	439	GLY	-	expression tag	UNP Q97MC0
F	440	HIS	-	expression tag	UNP Q97MC0
F	441	HIS	-	expression tag	UNP Q97MC0
F	442	HIS	-	expression tag	UNP Q97MC0
F	443	HIS	-	expression tag	UNP Q97MC0
F	444	HIS	-	expression tag	UNP Q97MC0
F	445	HIS	-	expression tag	UNP Q97MC0
G	0	SER	-	expression tag	UNP Q97MC0
G	1	LEU	-	expression tag	UNP Q97MC0
G	438	GLU	-	expression tag	UNP Q97MC0
G	439	GLY	-	expression tag	UNP Q97MC0
G	440	HIS	-	expression tag	UNP Q97MC0
G	441	HIS	-	expression tag	UNP Q97MC0
G	442	HIS	-	expression tag	UNP Q97MC0
G	443	HIS	-	expression tag	UNP Q97MC0
G	444	HIS	-	expression tag	UNP Q97MC0
G	445	HIS	-	expression tag	UNP Q97MC0
H	0	SER	-	expression tag	UNP Q97MC0
H	1	LEU	-	expression tag	UNP Q97MC0
H	438	GLU	-	expression tag	UNP Q97MC0
H	439	GLY	-	expression tag	UNP Q97MC0
H	440	HIS	-	expression tag	UNP Q97MC0
H	441	HIS	-	expression tag	UNP Q97MC0
H	442	HIS	-	expression tag	UNP Q97MC0
H	443	HIS	-	expression tag	UNP Q97MC0
H	444	HIS	-	expression tag	UNP Q97MC0
H	445	HIS	-	expression tag	UNP Q97MC0
I	0	SER	-	expression tag	UNP Q97MC0
I	1	LEU	-	expression tag	UNP Q97MC0
I	438	GLU	-	expression tag	UNP Q97MC0
I	439	GLY	-	expression tag	UNP Q97MC0
I	440	HIS	-	expression tag	UNP Q97MC0
I	441	HIS	-	expression tag	UNP Q97MC0
I	442	HIS	-	expression tag	UNP Q97MC0
I	443	HIS	-	expression tag	UNP Q97MC0
I	444	HIS	-	expression tag	UNP Q97MC0

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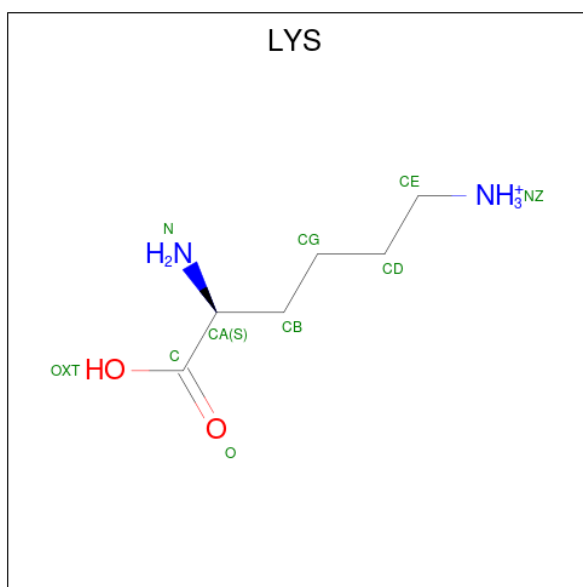
Chain	Residue	Modelled	Actual	Comment	Reference
I	445	HIS	-	expression tag	UNP Q97MC0
J	0	SER	-	expression tag	UNP Q97MC0
J	1	LEU	-	expression tag	UNP Q97MC0
J	438	GLU	-	expression tag	UNP Q97MC0
J	439	GLY	-	expression tag	UNP Q97MC0
J	440	HIS	-	expression tag	UNP Q97MC0
J	441	HIS	-	expression tag	UNP Q97MC0
J	442	HIS	-	expression tag	UNP Q97MC0
J	443	HIS	-	expression tag	UNP Q97MC0
J	444	HIS	-	expression tag	UNP Q97MC0
J	445	HIS	-	expression tag	UNP Q97MC0
K	0	SER	-	expression tag	UNP Q97MC0
K	1	LEU	-	expression tag	UNP Q97MC0
K	438	GLU	-	expression tag	UNP Q97MC0
K	439	GLY	-	expression tag	UNP Q97MC0
K	440	HIS	-	expression tag	UNP Q97MC0
K	441	HIS	-	expression tag	UNP Q97MC0
K	442	HIS	-	expression tag	UNP Q97MC0
K	443	HIS	-	expression tag	UNP Q97MC0
K	444	HIS	-	expression tag	UNP Q97MC0
K	445	HIS	-	expression tag	UNP Q97MC0
L	0	SER	-	expression tag	UNP Q97MC0
L	1	LEU	-	expression tag	UNP Q97MC0
L	438	GLU	-	expression tag	UNP Q97MC0
L	439	GLY	-	expression tag	UNP Q97MC0
L	440	HIS	-	expression tag	UNP Q97MC0
L	441	HIS	-	expression tag	UNP Q97MC0
L	442	HIS	-	expression tag	UNP Q97MC0
L	443	HIS	-	expression tag	UNP Q97MC0
L	444	HIS	-	expression tag	UNP Q97MC0
L	445	HIS	-	expression tag	UNP Q97MC0

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: C₄H₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	9	4	1	4	0	0
2	D	1	9	4	1	4	0	0
2	E	1	9	4	1	4	0	0
2	G	1	9	4	1	4	0	0
2	H	1	9	4	1	4	0	0
2	I	1	8	4	1	3	0	0
2	L	1	9	4	1	4	0	0

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: C₆H₁₅N₂O₂).

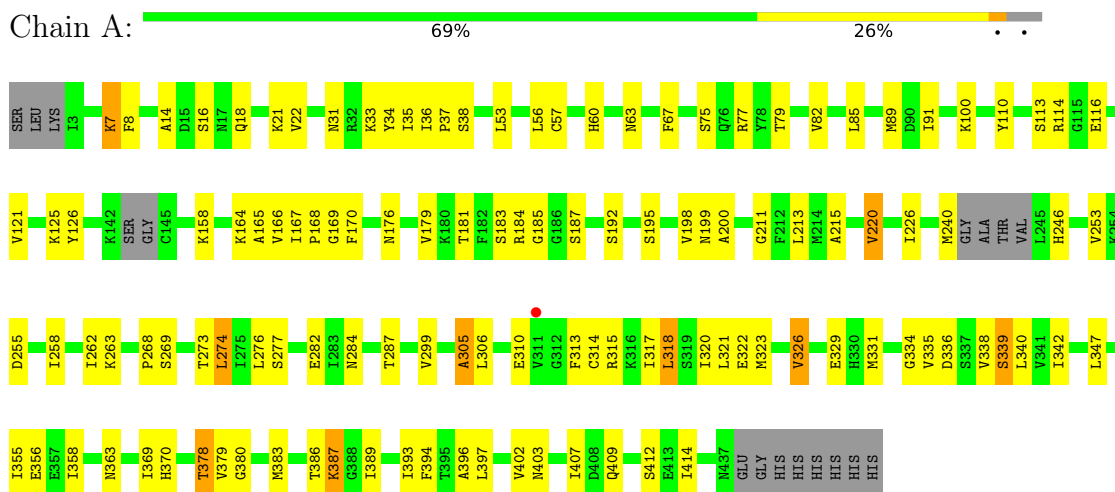


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 10	6	2	2	0	0
3	B	1	Total 10	6	2	2	0	0
3	C	1	Total 10	6	2	2	0	0
3	D	1	Total 10	6	2	2	0	0
3	G	1	Total 10	6	2	2	0	0
3	H	1	Total 10	6	2	2	0	0

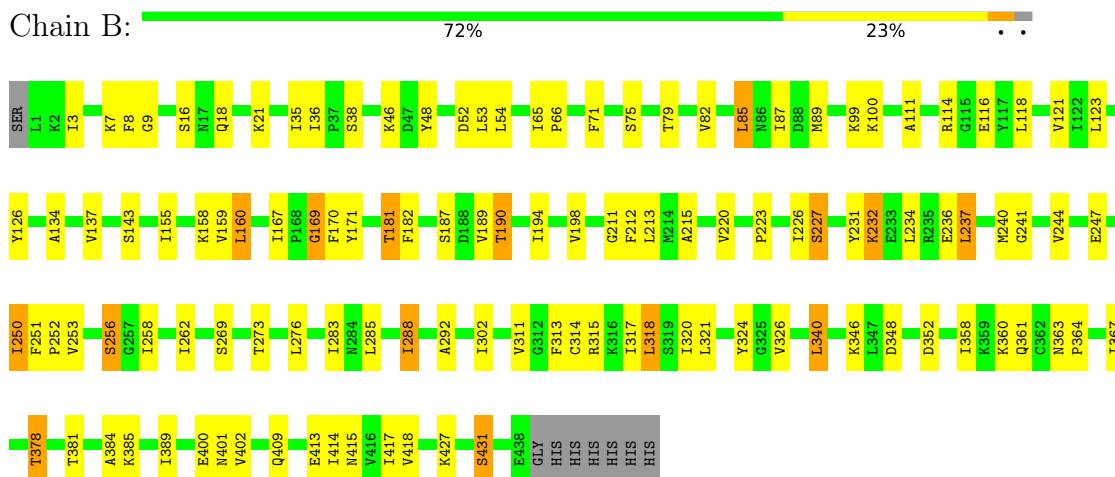
3 Residue-property plots

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

- Molecule 1: Aspartokinase

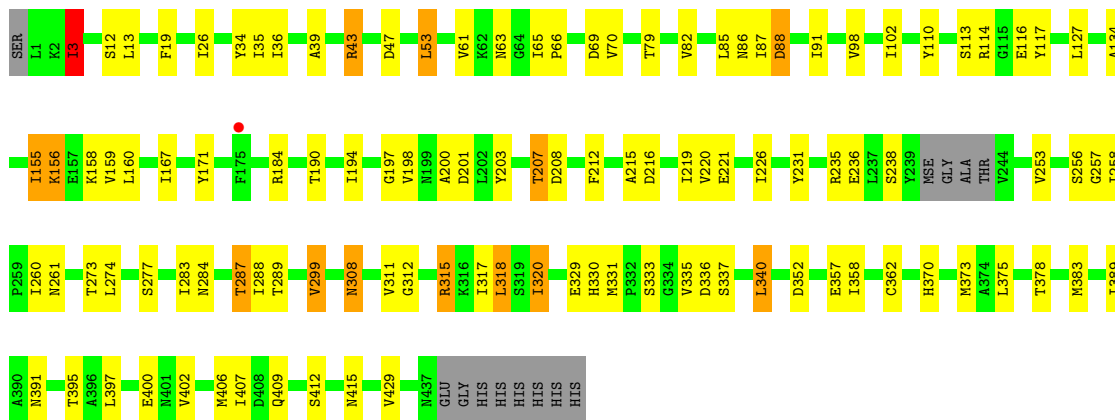


- Molecule 1: Aspartokinase



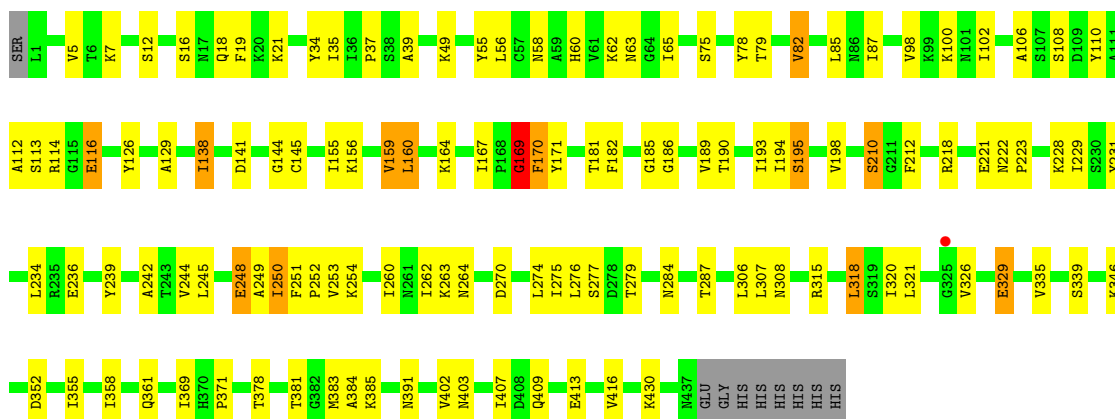
- Molecule 1: Aspartokinase





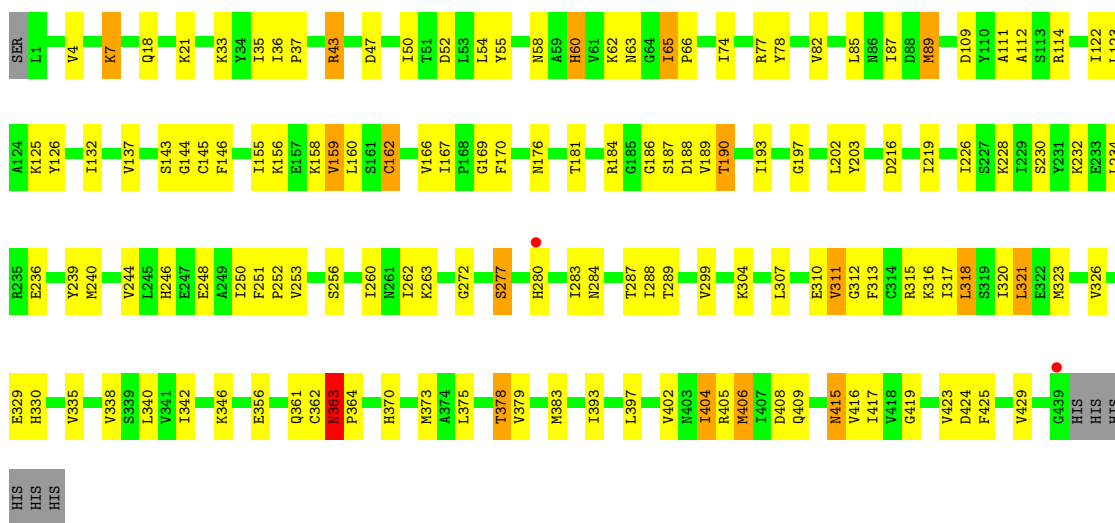
- Molecule 1: Aspartokinase

Chain D: 70% 25%



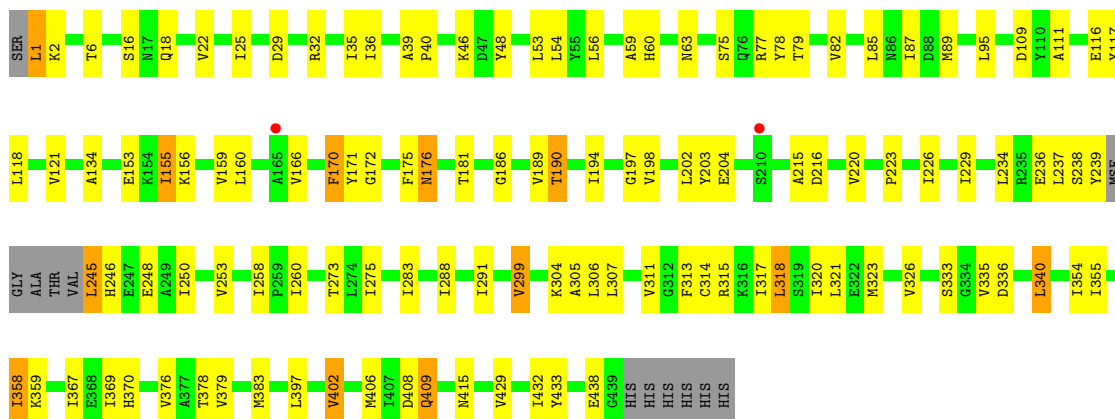
- Molecule 1: Aspartokinase

Chain E: 67% 28%



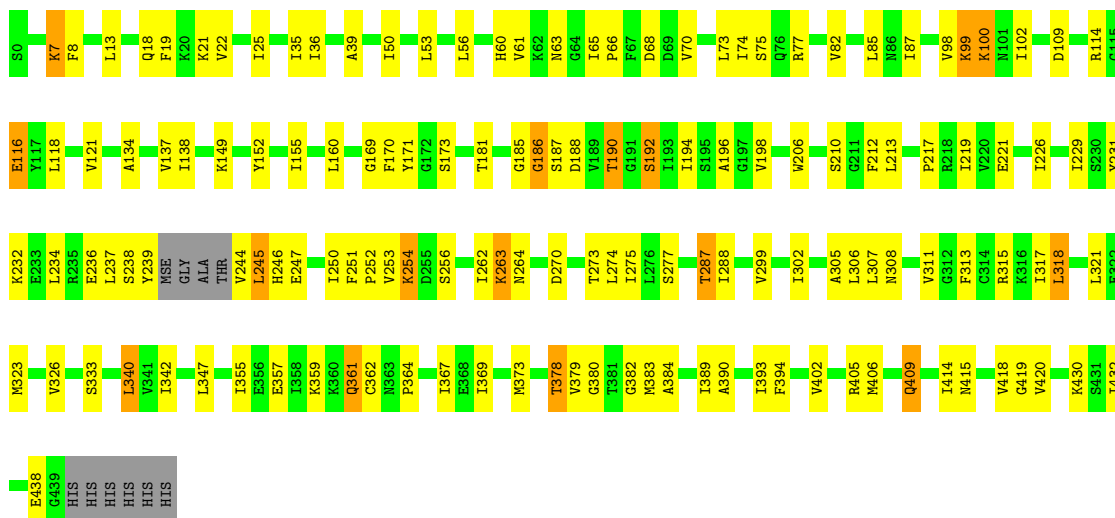
- Molecule 1: Aspartokinase

Chain F:  70% 24%



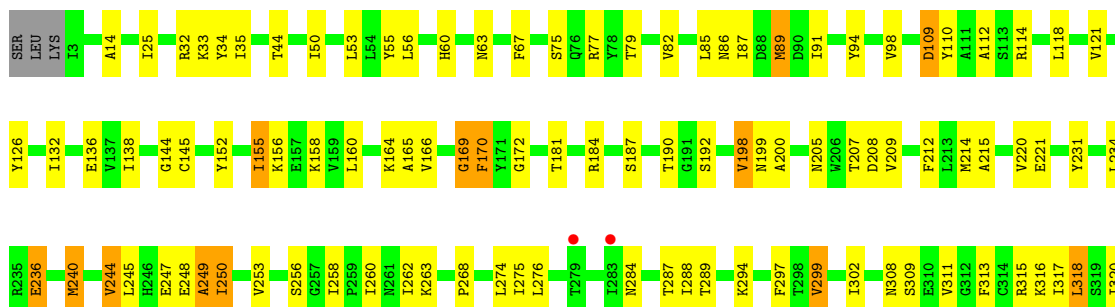
• Molecule 1: Aspartokinase

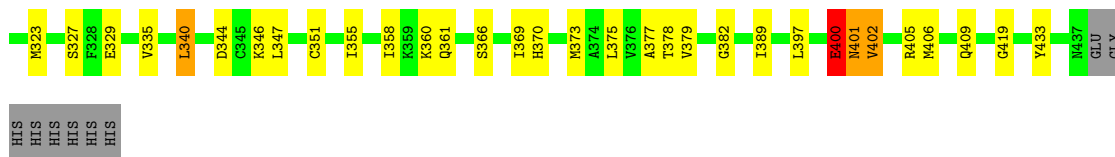
Chain G:  66% 28%



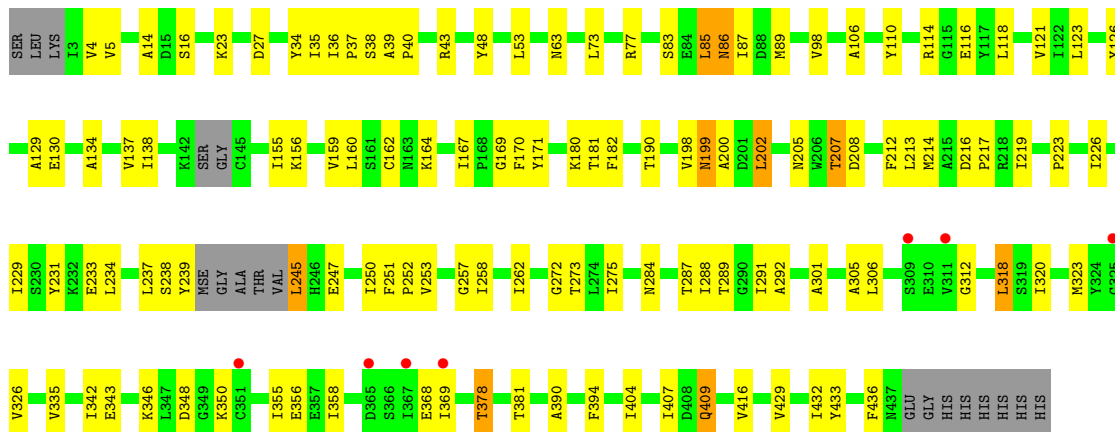
• Molecule 1: Aspartokinase

Chain H:  67% 26%

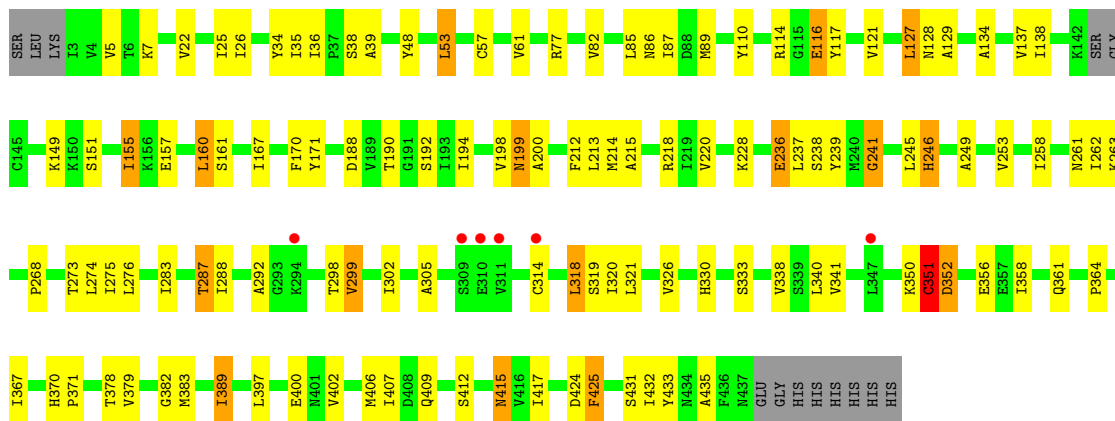




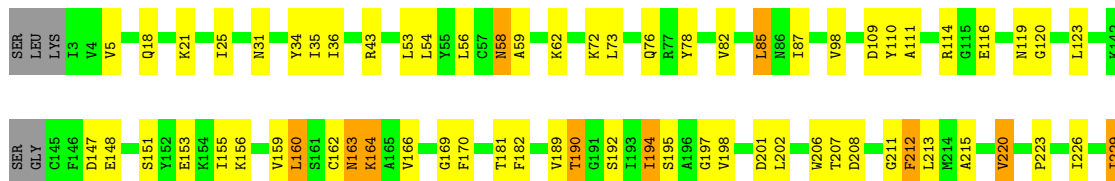
• Molecule 1: Aspartokinase

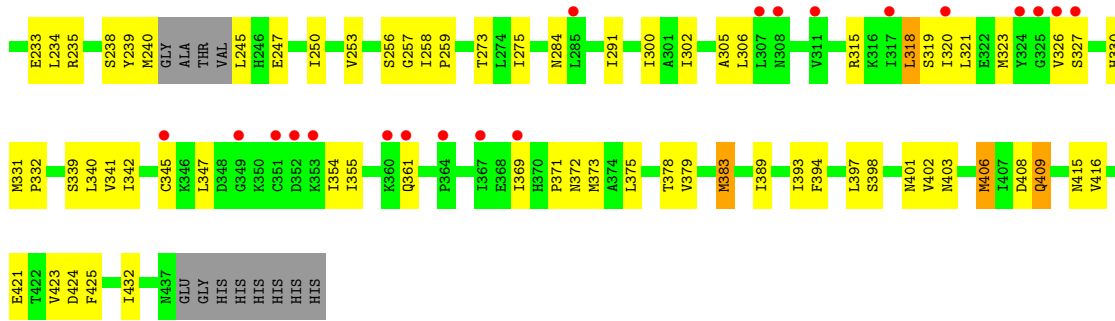


• Molecule 1: Aspartokinase

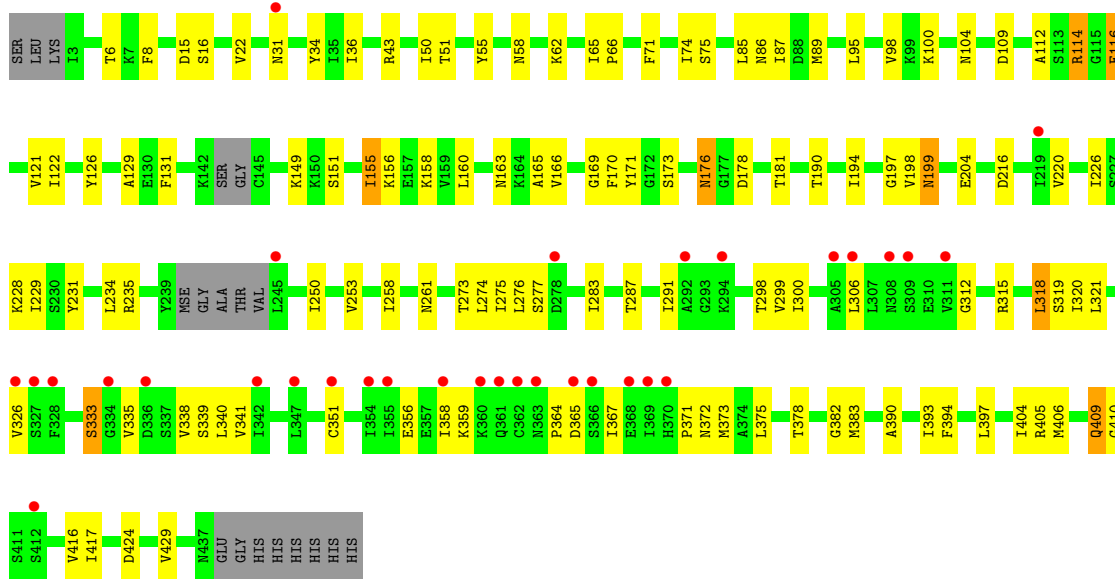


• Molecule 1: Aspartokinase





● Molecule 1: Aspartokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.04Å 274.22Å 114.04Å 90.00° 113.69° 90.00°	Depositor
Resolution (Å)	44.16 – 3.00 44.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.1 (44.16-3.00) 92.2 (44.16-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.206 , 0.273 0.209 , 0.284	Depositor DCC
R_{free} test set	924 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.018 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	39043	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/3270	0.58	0/4409
1	B	0.38	0/3349	0.57	0/4516
1	C	0.37	0/3317	0.55	0/4479
1	D	0.43	0/3341	0.58	0/4509
1	E	0.38	0/3339	0.56	0/4510
1	F	0.35	0/3311	0.51	0/4471
1	G	0.40	0/3338	0.58	0/4504
1	H	0.37	0/3260	0.57	1/4407 (0.0%)
1	I	0.34	0/3234	0.50	0/4371
1	J	0.35	0/3245	0.53	0/4383
1	K	0.36	0/3210	0.51	0/4336
1	L	0.35	0/3234	0.51	0/4369
All	All	0.37	0/39448	0.55	1/53264 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	H	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	400	GLU	N-CA-C	5.09	124.74	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	169	GLY	Peptide
1	D	169	GLY	Peptide
1	H	169	GLY	Peptide
1	H	400	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3228	0	3156	81	0
1	B	3304	0	3281	88	0
1	C	3271	0	3214	107	0
1	D	3296	0	3257	95	0
1	E	3293	0	3224	112	0
1	F	3267	0	3209	93	0
1	G	3288	0	3244	118	0
1	H	3217	0	3103	103	0
1	I	3191	0	3092	105	0
1	J	3204	0	3116	103	0
1	K	3170	0	3042	109	0
1	L	3192	0	3093	110	0
2	A	9	0	3	2	0
2	D	9	0	3	0	0
2	E	9	0	3	1	0
2	G	9	0	3	1	0
2	H	9	0	3	1	0
2	I	8	0	3	0	0
2	L	9	0	3	0	0
3	A	10	0	12	0	0
3	B	10	0	12	0	0
3	C	10	0	12	3	0
3	D	10	0	12	0	0
3	G	10	0	12	7	0
3	H	10	0	12	1	0
All	All	39043	0	38124	1150	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 15.

All (1150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:169:GLY:O	1:K:190:THR:HG21	1.41	1.19
1:D:189:VAL:HA	1:D:249:ALA:CB	1.76	1.14
1:D:189:VAL:HA	1:D:249:ALA:HB3	1.30	1.08
1:G:288:ILE:HD13	1:G:383:MSE:HE2	1.35	1.08
1:L:160:LEU:HD13	1:L:198:VAL:HG13	1.37	1.06
1:C:226:ILE:O	1:C:273:THR:HG22	1.57	1.04
1:C:215:ALA:HB3	1:C:220:VAL:HG11	1.37	1.01
1:J:137:VAL:HG13	1:J:155:ILE:HG22	1.42	0.98
1:I:155:ILE:HG23	1:I:159:VAL:HG21	1.45	0.97
1:D:383:MSE:HE1	1:D:416:VAL:HG23	1.45	0.95
1:A:355:ILE:HD11	1:A:369:ILE:HD11	1.44	0.95
1:I:318:LEU:HD11	1:J:318:LEU:HD11	1.43	0.95
1:D:169:GLY:O	1:D:190:THR:HG21	1.69	0.93
1:G:308[B]:ASN:CG	3:G:507:LYS:HG3	1.90	0.93
1:F:155:ILE:HG23	1:F:198:VAL:HG23	1.51	0.92
1:H:320:ILE:HD13	1:H:358:ILE:HG22	1.51	0.92
1:C:383:MSE:HB2	1:C:389:ILE:HG21	1.52	0.92
1:F:253:VAL:HG13	1:F:258:ILE:HB	1.53	0.90
1:G:288:ILE:CD1	1:G:383:MSE:HE2	2.01	0.90
1:G:364:PRO:HG2	1:G:367:ILE:HD11	1.53	0.90
1:G:308[B]:ASN:OD1	3:G:507:LYS:HG3	1.72	0.89
1:C:397:LEU:HD22	1:C:402:VAL:HG21	1.54	0.88
1:E:189:VAL:O	1:E:193:ILE:HD12	1.75	0.86
1:C:85:LEU:HD23	1:C:87:ILE:HD11	1.57	0.85
1:I:155:ILE:HG23	1:I:159:VAL:CG2	2.06	0.85
1:G:212:PHE:H	1:G:273:THR:CG2	1.90	0.84
1:J:215:ALA:HB3	1:J:220:VAL:HG11	1.60	0.83
1:K:341:VAL:HG11	1:K:375:LEU:HD11	1.60	0.83
1:H:373:MSE:HE3	1:H:405:ARG:HB2	1.59	0.83
1:H:355:ILE:HD13	1:H:369:ILE:HD11	1.59	0.83
1:F:288:ILE:HD12	1:F:383:MSE:HE2	1.59	0.83
1:G:373:MSE:HE1	1:G:406:MSE:HB2	1.58	0.83
1:E:50:ILE:HD11	1:E:77:ARG:HG3	1.60	0.83
1:I:226:ILE:O	1:I:273:THR:HG22	1.79	0.82
1:D:383:MSE:CE	1:D:416:VAL:HG23	2.08	0.82
1:D:320:ILE:HD13	1:D:358:ILE:HG22	1.61	0.82
1:L:155:ILE:HG23	1:L:198:VAL:HG23	1.60	0.81
1:K:320:ILE:HG23	1:K:323:MSE:HE2	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASN:O	1:A:287:THR:HG22	1.81	0.81
1:E:335:VAL:HG13	1:F:239:TYR:CD1	2.15	0.81
1:A:274:LEU:HD22	1:A:276:LEU:HD11	1.62	0.80
1:L:253:VAL:HG11	1:L:258:ILE:O	1.81	0.80
1:K:211:GLY:HA3	1:K:273:THR:HG23	1.63	0.80
1:J:155:ILE:CD1	1:J:198:VAL:HG13	2.11	0.80
1:J:127:LEU:O	1:J:129:ALA:N	2.15	0.80
1:D:189:VAL:HG23	1:D:249:ALA:HB2	1.63	0.80
1:L:98:VAL:HG13	1:L:114:ARG:HG2	1.62	0.79
1:B:16:SER:HB2	1:B:85:LEU:HD13	1.62	0.79
1:D:189:VAL:HA	1:D:249:ALA:HB2	1.61	0.79
1:J:157:GLU:O	1:J:161:SER:OG	2.01	0.78
1:C:308:ASN:HD21	3:C:503:LYS:HE2	1.47	0.78
1:F:186:GLY:O	1:F:189:VAL:HG12	1.83	0.78
1:K:226:ILE:O	1:K:273:THR:HG22	1.83	0.78
1:K:155:ILE:HG23	1:K:159:VAL:CG1	2.14	0.78
1:A:14:ALA:O	1:A:77:ARG:NH2	2.16	0.78
1:F:82:VAL:HG21	1:F:89:MSE:HE2	1.65	0.78
1:G:50:ILE:HD11	1:G:77:ARG:HG2	1.66	0.78
1:J:253:VAL:HG13	1:J:258:ILE:HB	1.65	0.78
1:K:238:SER:OG	1:L:335:VAL:CG1	2.32	0.78
1:L:320:ILE:HD13	1:L:358:ILE:HG22	1.64	0.78
1:C:87:ILE:HG22	1:C:88:ASP:H	1.48	0.78
1:B:288:ILE:HD11	1:B:378:THR:OG1	1.84	0.77
1:D:189:VAL:CB	1:D:249:ALA:HB2	2.15	0.77
1:G:379:VAL:C	1:G:383:MSE:HE3	2.05	0.77
1:A:318:LEU:HD11	1:B:318:LEU:HD11	1.65	0.77
1:G:134:ALA:HB3	1:G:171:TYR:CE1	2.20	0.77
1:C:320:ILE:HD11	1:C:358:ILE:HG23	1.67	0.77
1:I:245:LEU:HD23	1:I:245:LEU:N	2.00	0.77
1:K:406:MSE:HE2	1:K:408:ASP:HB2	1.66	0.76
1:J:261:ASN:HD22	1:J:274:LEU:HD13	1.50	0.76
1:L:87:ILE:HG21	1:L:89:MSE:HE3	1.67	0.75
1:L:155:ILE:HD11	1:L:194:ILE:HD13	1.69	0.75
1:E:406:MSE:HE2	1:E:408:ASP:HB2	1.67	0.75
1:F:155:ILE:HD12	1:F:198:VAL:HG23	1.67	0.75
1:J:397:LEU:O	1:J:402:VAL:HG12	1.87	0.74
1:G:373:MSE:HE3	1:G:405:ARG:CB	2.18	0.74
1:F:63:ASN:HD22	1:G:53:LEU:HD12	1.52	0.74
1:E:397:LEU:HD22	1:E:402:VAL:HG11	1.70	0.74
1:D:189:VAL:CA	1:D:249:ALA:CB	2.64	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLY:O	1:A:187:SER:HA	1.88	0.73
1:H:313:PHE:CE2	1:H:317:ILE:HD11	2.23	0.73
1:I:253:VAL:HG13	1:I:258:ILE:HB	1.70	0.73
1:H:373:MSE:HE2	1:H:419:GLY:HA3	1.70	0.73
1:B:215:ALA:HB3	1:B:220:VAL:HG11	1.69	0.73
1:G:238:SER:HB3	1:G:244:VAL:HG11	1.71	0.73
1:G:355:ILE:CD1	1:G:369:ILE:HD11	2.19	0.73
1:E:423:VAL:HG13	1:E:424:ASP:OD1	1.89	0.73
1:G:288:ILE:CD1	1:G:383:MSE:CE	2.67	0.73
1:G:373:MSE:HE3	1:G:405:ARG:HB3	1.70	0.73
1:J:237:LEU:HD12	1:J:241:GLY:HA3	1.70	0.73
1:G:212:PHE:H	1:G:273:THR:HG23	1.52	0.72
1:F:170:PHE:O	1:F:170:PHE:CG	2.43	0.72
1:D:155:ILE:HG23	1:D:159:VAL:CG1	2.19	0.72
1:C:155:ILE:HD11	1:C:194:ILE:HD13	1.72	0.72
1:K:355:ILE:HD11	1:K:369:ILE:HD11	1.72	0.71
1:F:245:LEU:HD22	1:F:246:HIS:H	1.54	0.71
1:B:75:SER:O	1:B:79:THR:HG23	1.90	0.71
1:B:116:GLU:HG3	1:B:170:PHE:HB3	1.73	0.70
1:D:355:ILE:HD11	1:D:369:ILE:HD11	1.72	0.70
1:I:239:TYR:HB2	1:I:292:ALA:HB1	1.73	0.70
1:H:82:VAL:HG21	1:H:89:MSE:CE	2.20	0.70
1:K:238:SER:OG	1:L:335:VAL:HG11	1.91	0.70
1:H:85:LEU:HD23	1:H:126:TYR:CZ	2.26	0.70
1:H:284:ASN:HB2	1:H:287:THR:HG21	1.74	0.70
1:E:373:MSE:HE3	1:E:405:ARG:CB	2.22	0.70
1:E:373:MSE:HE1	1:E:406:MSE:CB	2.21	0.69
1:G:39:ALA:HB3	2:G:457:ASP:OD2	1.91	0.69
1:F:291:ILE:HG21	1:F:429:VAL:HG13	1.74	0.69
1:E:323:MSE:HE1	1:E:361:GLN:HE22	1.57	0.69
1:G:355:ILE:HD11	1:G:369:ILE:HD11	1.74	0.69
1:D:189:VAL:CA	1:D:249:ALA:HB2	2.21	0.69
1:G:118:LEU:O	1:G:121:VAL:HG22	1.93	0.69
1:C:39:ALA:HB2	1:C:116:GLU:OE1	1.91	0.69
1:F:299:VAL:HG12	1:F:370:HIS:HB2	1.74	0.69
1:E:323:MSE:HE2	1:G:315:ARG:NH2	2.07	0.69
1:F:155:ILE:HD13	1:F:159:VAL:HG21	1.73	0.69
1:C:3:ILE:HD11	1:C:200:ALA:HA	1.74	0.69
1:D:189:VAL:CG2	1:D:249:ALA:HB2	2.21	0.69
1:H:82:VAL:HG21	1:H:89:MSE:HE2	1.74	0.69
1:E:52:ASP:HB3	1:H:63:ASN:HD21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:274:LEU:HD23	1:H:276:LEU:HD11	1.74	0.68
1:L:318:LEU:HD12	1:L:319:SER:N	2.07	0.68
1:C:220:VAL:HG13	1:C:220:VAL:O	1.93	0.68
1:K:318:LEU:CD2	1:L:318:LEU:HD21	2.23	0.68
1:E:299:VAL:HG13	1:E:370:HIS:HB2	1.76	0.68
1:H:215:ALA:HB3	1:H:220:VAL:HG11	1.75	0.68
1:E:35:ILE:C	1:E:36:ILE:HD12	2.14	0.68
1:G:409:GLN:HE21	1:G:409:GLN:C	1.96	0.68
1:I:155:ILE:CG2	1:I:159:VAL:HG21	2.23	0.67
1:A:274:LEU:CD2	1:A:276:LEU:HD11	2.25	0.67
1:K:109:ASP:OD2	1:K:181:THR:HG22	1.94	0.67
1:D:234:LEU:HD22	1:D:275:ILE:HD13	1.77	0.67
1:C:320:ILE:CD1	1:C:358:ILE:HG23	2.25	0.67
1:K:194:ILE:HG22	1:K:195:SER:N	2.10	0.66
1:H:187:SER:OG	2:H:458:ASP:OD2	2.08	0.66
1:L:34:TYR:CD1	1:L:165:ALA:HB3	2.31	0.66
1:D:155:ILE:HG23	1:D:159:VAL:HG13	1.78	0.66
1:F:56:LEU:O	1:F:59:ALA:HB3	1.95	0.66
1:H:323:MSE:HE1	1:H:361:GLN:NE2	2.11	0.66
1:B:415:ASN:HD21	1:B:417:ILE:HD11	1.61	0.66
1:E:36:ILE:N	1:E:36:ILE:HD12	2.10	0.66
1:E:373:MSE:HE3	1:E:405:ARG:HB2	1.76	0.66
1:L:375:LEU:HD22	1:L:417:ILE:HG22	1.78	0.65
1:H:160:LEU:HD13	1:H:198:VAL:HG13	1.77	0.65
1:D:320:ILE:HG21	1:D:358:ILE:CG2	2.26	0.65
1:L:341:VAL:HG11	1:L:406:MSE:HE1	1.77	0.65
1:C:284:ASN:O	1:C:287:THR:HG22	1.97	0.65
1:F:355:ILE:CD1	1:F:369:ILE:HD11	2.27	0.65
1:A:320:ILE:HD13	1:A:358:ILE:HG22	1.79	0.65
1:J:39:ALA:N	1:J:116:GLU:OE2	2.29	0.65
1:D:18:GLN:HE22	1:D:21:LYS:NZ	1.95	0.65
1:E:373:MSE:HE1	1:E:406:MSE:HB3	1.79	0.65
1:L:378:THR:HG21	1:L:393:ILE:HD13	1.79	0.65
1:I:14:ALA:O	1:I:77:ARG:NH2	2.30	0.64
1:C:318:LEU:HD11	1:D:318:LEU:HD11	1.80	0.64
1:K:213:LEU:H	1:K:213:LEU:HD12	1.63	0.64
1:H:253:VAL:HG13	1:H:258:ILE:HB	1.79	0.64
1:E:60:HIS:ND1	1:H:56:LEU:HD21	2.12	0.64
1:F:1:LEU:H1	1:F:1:LEU:HD13	1.63	0.64
1:K:238:SER:OG	1:L:335:VAL:HG13	1.96	0.64
1:K:326:VAL:HG11	1:K:347:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:HIS:HB3	1:E:248:GLU:HG2	1.80	0.64
1:E:60:HIS:CE1	1:H:56:LEU:HD21	2.33	0.64
1:J:155:ILE:C	1:J:155:ILE:HD12	2.18	0.64
1:B:169:GLY:O	1:B:190:THR:HG21	1.98	0.64
1:E:85:LEU:HD11	1:E:126:TYR:CZ	2.33	0.64
1:F:321:LEU:HD23	1:F:326:VAL:HG21	1.80	0.64
1:E:323:MSE:HG2	1:G:311:VAL:HG11	1.79	0.64
1:K:169:GLY:C	1:K:190:THR:HG21	2.17	0.64
1:H:308:ASN:HA	3:H:508:LYS:HA	1.80	0.64
1:D:320:ILE:HG21	1:D:358:ILE:HG22	1.80	0.63
1:G:137:VAL:HG12	1:G:138:ILE:HG13	1.80	0.63
1:I:409:GLN:CB	1:I:416:VAL:HG22	2.29	0.63
1:L:198:VAL:HG12	1:L:198:VAL:O	1.98	0.63
1:C:215:ALA:CB	1:C:220:VAL:HG11	2.22	0.63
1:A:378:THR:O	1:A:383:MSE:HE1	1.99	0.63
1:C:216:ASP:O	1:C:220:VAL:HG12	1.99	0.63
1:H:355:ILE:CD1	1:H:369:ILE:HD11	2.28	0.63
1:J:320:ILE:CD1	1:J:358:ILE:HG22	2.29	0.63
1:A:89:MSE:HE1	1:A:121:VAL:HG23	1.81	0.62
1:D:253:VAL:HG21	1:D:260:ILE:HD11	1.81	0.62
1:J:137:VAL:CG1	1:J:155:ILE:HG22	2.25	0.62
1:C:79:THR:HG22	1:C:91:ILE:HG21	1.80	0.62
1:E:253:VAL:HG21	1:E:260:ILE:HD11	1.81	0.62
1:G:379:VAL:CA	1:G:383:MSE:HE3	2.29	0.62
1:H:82:VAL:CG2	1:H:89:MSE:HE2	2.28	0.62
2:E:455:ASP:N	2:E:455:ASP:OD1	2.31	0.62
1:A:215:ALA:HB3	1:A:220:VAL:HG11	1.81	0.62
1:B:53:LEU:HD21	1:C:65:ILE:HD11	1.81	0.62
1:J:151:SER:O	1:J:155:ILE:HG23	2.00	0.62
1:H:313:PHE:HE2	1:H:317:ILE:HD11	1.63	0.62
1:K:318:LEU:HD21	1:L:318:LEU:HD21	1.82	0.62
1:B:237:LEU:HD12	1:B:292:ALA:CB	2.29	0.62
1:G:380:GLY:N	1:G:383:MSE:HE3	2.14	0.61
1:H:317:ILE:CG2	1:H:340:LEU:HD21	2.30	0.61
1:C:299:VAL:HG13	1:C:370:HIS:HB2	1.82	0.61
1:H:109:ASP:OD2	1:H:181:THR:HG22	2.01	0.61
1:J:320:ILE:HD13	1:J:358:ILE:HG22	1.80	0.61
1:D:98:VAL:HG22	1:D:114:ARG:HD2	1.82	0.61
1:F:220:VAL:HG21	1:F:433:TYR:CD1	2.35	0.61
1:K:169:GLY:O	1:K:190:THR:CG2	2.34	0.61
1:J:215:ALA:CB	1:J:220:VAL:HG11	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:330:HIS:NE2	1:J:417:ILE:HD13	2.15	0.61
1:D:212:PHE:CD1	1:D:244:VAL:HG12	2.36	0.61
1:E:330:HIS:CG	1:E:406:MSE:HE1	2.35	0.61
1:G:373:MSE:HE2	1:G:419:GLY:HA3	1.83	0.61
1:L:85:LEU:HD23	1:L:126:TYR:CE1	2.36	0.61
1:F:155:ILE:HD11	1:F:194:ILE:CD1	2.31	0.61
1:I:291:ILE:HG21	1:I:429:VAL:HG13	1.83	0.61
1:I:320:ILE:HD12	1:I:358:ILE:HG22	1.83	0.61
1:F:321:LEU:HD23	1:F:326:VAL:CG2	2.30	0.60
1:B:35:ILE:C	1:B:36:ILE:HD12	2.21	0.60
1:C:261:ASN:HD22	1:C:274:LEU:HD13	1.66	0.60
1:J:155:ILE:HD11	1:J:198:VAL:HG13	1.84	0.60
1:I:159:VAL:HG23	1:I:160:LEU:H	1.67	0.60
1:L:359:LYS:HE3	1:L:367:ILE:HD12	1.83	0.60
1:J:194:ILE:O	1:J:198:VAL:HG22	2.02	0.60
1:E:313:PHE:HE2	1:E:317:ILE:HD11	1.67	0.60
1:J:283:ILE:HG23	1:J:283:ILE:O	2.01	0.60
1:A:110:TYR:HD2	1:A:179:VAL:HG21	1.67	0.60
1:A:63:ASN:HD22	1:D:56:LEU:HD22	1.66	0.60
1:C:231:TYR:CE2	1:C:277:SER:HA	2.36	0.60
1:D:114:ARG:HA	1:D:114:ARG:HH11	1.67	0.60
1:H:138:ILE:HD11	1:H:190:THR:HG23	1.84	0.60
1:K:35:ILE:N	1:K:35:ILE:HD12	2.16	0.60
1:E:313:PHE:CE2	1:E:317:ILE:HD11	2.36	0.60
1:H:323:MSE:HE1	1:H:361:GLN:HE22	1.67	0.60
1:D:321:LEU:HG	1:D:326:VAL:HG23	1.84	0.59
1:G:155:ILE:CD1	1:G:194:ILE:HD13	2.32	0.59
1:E:65:ILE:HD13	1:E:66:PRO:O	2.02	0.59
1:K:5:VAL:HG22	1:K:34:TYR:HB2	1.83	0.59
1:D:245:LEU:HD23	1:D:250:ILE:HD11	1.83	0.59
1:G:226:ILE:O	1:G:273:THR:HG22	2.03	0.59
1:I:53:LEU:HG	1:L:65:ILE:HD11	1.84	0.59
1:D:320:ILE:CD1	1:D:358:ILE:HG22	2.32	0.59
1:I:155:ILE:HG22	1:I:156:LYS:N	2.16	0.59
1:F:299:VAL:HA	1:F:340:LEU:O	2.03	0.59
1:I:284:ASN:O	1:I:287:THR:HG22	2.02	0.59
1:L:116:GLU:HG3	1:L:170:PHE:CB	2.32	0.59
1:L:287:THR:HG22	1:L:382:GLY:HA3	1.84	0.59
1:C:335:VAL:HG11	1:D:236:GLU:HA	1.84	0.59
1:C:36:ILE:HG12	1:C:190:THR:HG22	1.85	0.59
1:H:89:MSE:HE1	1:H:91:ILE:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:CYS:HA	1:A:317:ILE:HD12	1.84	0.59
1:C:261:ASN:ND2	1:C:274:LEU:HD13	2.17	0.59
1:J:26:ILE:HD12	1:J:35:ILE:HD11	1.84	0.59
1:L:65:ILE:HG22	1:L:66:PRO:O	2.03	0.59
1:A:342:ILE:HG21	1:A:347:LEU:HD13	1.84	0.59
1:H:274:LEU:CD2	1:H:276:LEU:HD11	2.32	0.59
1:B:52:ASP:HB3	1:C:63:ASN:HD21	1.68	0.58
1:D:212:PHE:CE1	1:D:244:VAL:HG12	2.37	0.58
1:I:318:LEU:HD21	1:J:318:LEU:CD2	2.33	0.58
1:L:98:VAL:CG1	1:L:114:ARG:HG2	2.31	0.58
1:E:54:LEU:HD23	1:E:74:ILE:HD13	1.85	0.58
1:I:291:ILE:HD11	1:I:432:ILE:HG22	1.84	0.58
1:J:341:VAL:HG21	1:J:406:MSE:SE	2.53	0.58
1:A:263:LYS:NZ	1:A:268:PRO:O	2.37	0.58
1:C:207:THR:OG1	1:C:208:ASP:N	2.36	0.58
1:C:373:MSE:HE3	1:C:375:LEU:HD21	1.86	0.58
1:E:251:PHE:CG	1:E:252:PRO:HD3	2.38	0.58
1:F:237:LEU:HD11	1:F:379:VAL:HB	1.84	0.58
1:L:6:THR:HG22	1:L:204:GLU:HB2	1.84	0.58
1:D:212:PHE:CZ	1:D:262:ILE:HD13	2.38	0.58
1:K:421:GLU:HG3	1:K:423:VAL:HG12	1.86	0.58
1:C:236:GLU:HG2	1:C:415:ASN:HB2	1.86	0.58
1:C:391:ASN:OD1	1:D:391:ASN:OD1	2.22	0.58
1:F:36:ILE:HG21	1:F:190:THR:HG22	1.86	0.58
1:H:35:ILE:HB	1:H:166:VAL:HG22	1.86	0.58
1:H:373:MSE:CE	1:H:405:ARG:HB2	2.32	0.58
1:K:110:TYR:CZ	1:K:114:ARG:HD2	2.39	0.58
1:K:163:ASN:O	1:K:164:LYS:C	2.43	0.58
1:K:202:LEU:HD12	1:K:259:PRO:O	2.03	0.58
1:I:355:ILE:HD11	1:I:369:ILE:HD11	1.86	0.57
1:B:232:LYS:HG3	1:B:414:ILE:HD11	1.86	0.57
1:G:239:TYR:CD2	1:H:335:VAL:HG22	2.38	0.57
1:G:287:THR:HG22	1:G:382:GLY:HA3	1.84	0.57
1:A:274:LEU:CD2	1:A:276:LEU:CD1	2.82	0.57
1:B:169:GLY:C	1:B:190:THR:HG21	2.25	0.57
1:D:5:VAL:HG21	1:D:195:SER:HA	1.86	0.57
1:I:301:ALA:HB3	1:I:368:GLU:HB2	1.86	0.57
1:A:213:LEU:O	1:A:240:MSE:CE	2.53	0.57
1:C:253:VAL:HG13	1:C:258:ILE:HB	1.86	0.57
1:E:137:VAL:HG13	1:E:155:ILE:HG13	1.85	0.57
1:G:357:GLU:OE2	1:G:361:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ILE:HD11	1:C:429:VAL:CG1	2.35	0.57
1:C:395:THR:HA	1:D:391:ASN:HD21	1.68	0.57
1:K:321:LEU:HG	1:K:326:VAL:HG23	1.86	0.57
1:A:18:GLN:O	1:A:22:VAL:HG23	2.05	0.57
1:H:256:SER:HB3	1:H:258:ILE:HD12	1.87	0.57
1:I:134:ALA:HB3	1:I:171:TYR:CE2	2.40	0.57
1:I:390:ALA:HB1	1:I:394:PHE:CE2	2.40	0.57
1:I:4:VAL:HG13	1:I:202:LEU:HD23	1.87	0.57
1:C:315:ARG:HB2	1:D:318:LEU:HD13	1.87	0.57
1:G:302:ILE:HD12	1:G:317:ILE:HD13	1.86	0.57
1:J:214:MSE:HE2	1:J:433:TYR:CE2	2.39	0.57
1:A:331:MSE:HE2	1:A:340:LEU:HD11	1.86	0.57
1:G:212:PHE:H	1:G:273:THR:HG21	1.70	0.57
1:K:332:PRO:HG3	1:K:406:MSE:HE3	1.87	0.57
1:E:307:LEU:HD22	1:E:313:PHE:CD2	2.40	0.56
1:F:85:LEU:HD23	1:F:87:ILE:HD11	1.87	0.56
1:H:110:TYR:CZ	1:H:114:ARG:HD2	2.38	0.56
1:A:393:ILE:O	1:A:396:ALA:HB3	2.05	0.56
1:B:240:MSE:N	1:B:241:GLY:HA2	2.20	0.56
1:F:155:ILE:HG22	1:F:156:LYS:N	2.21	0.56
1:E:54:LEU:HD13	1:E:111:ALA:O	2.04	0.56
1:K:160:LEU:HG	1:K:198:VAL:HG13	1.87	0.56
1:D:18:GLN:HE22	1:D:21:LYS:HZ3	1.53	0.56
1:F:220:VAL:HG13	1:F:223:PRO:HG3	1.87	0.56
1:A:187:SER:OG	2:A:451:ASP:OD2	2.22	0.56
1:B:36:ILE:HD12	1:B:36:ILE:N	2.20	0.56
1:L:226:ILE:O	1:L:273:THR:HG22	2.05	0.56
1:H:132:ILE:HD13	1:H:158:LYS:O	2.06	0.56
1:L:359:LYS:CE	1:L:367:ILE:HD12	2.36	0.56
1:D:75:SER:O	1:D:79:THR:HG23	2.05	0.56
1:I:137:VAL:HG12	1:I:138:ILE:HG13	1.87	0.56
1:I:5:VAL:HG22	1:I:34:TYR:HB2	1.88	0.56
1:L:409:GLN:HE21	1:L:410:GLY:N	2.04	0.56
1:C:318:LEU:HD23	1:C:331:MSE:HE1	1.88	0.56
1:I:137:VAL:HG13	1:I:155:ILE:HG13	1.86	0.56
1:D:284:ASN:O	1:D:287:THR:HG22	2.06	0.56
1:E:202:LEU:HD12	1:E:203:TYR:N	2.21	0.56
1:H:287:THR:HG22	1:H:382:GLY:HA3	1.87	0.56
1:E:239:TYR:CG	1:F:335:VAL:HG13	2.41	0.55
1:G:305:ALA:C	1:G:306:LEU:HD22	2.26	0.55
1:E:54:LEU:CD2	1:E:74:ILE:HD13	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ILE:O	1:C:273:THR:CG2	2.44	0.55
1:C:219:ILE:HD11	1:C:429:VAL:HG11	1.87	0.55
1:G:383:MSE:HB2	1:G:389:ILE:HG21	1.88	0.55
1:G:7:LYS:HZ1	1:G:188:ASP:CG	2.09	0.55
1:A:18:GLN:HE22	1:A:21:LYS:HE3	1.71	0.55
1:F:234:LEU:HD22	1:F:275:ILE:HD13	1.88	0.55
1:E:239:TYR:CD2	1:F:335:VAL:HG13	2.42	0.55
1:G:373:MSE:HE3	1:G:405:ARG:HB2	1.87	0.55
1:L:231:TYR:CE2	1:L:277:SER:HA	2.41	0.55
1:L:87:ILE:HG21	1:L:89:MSE:CE	2.36	0.55
1:D:78:TYR:O	1:D:82:VAL:HG12	2.07	0.55
1:E:4:VAL:HG22	1:E:202:LEU:HB3	1.87	0.55
1:G:213:LEU:HD13	1:G:217:PRO:HG3	1.89	0.55
1:B:65:ILE:CG2	1:B:66:PRO:HD2	2.36	0.55
1:K:155:ILE:HG23	1:K:159:VAL:HG13	1.88	0.55
1:L:116:GLU:HG3	1:L:170:PHE:HB3	1.88	0.55
1:A:38:SER:HB3	2:A:451:ASP:OD2	2.07	0.55
1:C:335:VAL:HG12	1:D:239:TYR:CD2	2.42	0.55
1:D:263:LYS:NZ	1:D:270:ASP:O	2.39	0.55
1:F:109:ASP:CG	1:F:181:THR:HG22	2.26	0.55
1:H:302:ILE:HD11	1:H:358:ILE:HD12	1.87	0.55
1:C:397:LEU:HD22	1:C:402:VAL:CG2	2.33	0.55
1:G:160:LEU:HD13	1:G:198:VAL:HG13	1.89	0.55
1:I:37:PRO:HB3	1:I:123:LEU:HD12	1.89	0.55
1:J:137:VAL:HG13	1:J:155:ILE:CG2	2.28	0.55
1:L:34:TYR:HD1	1:L:165:ALA:HB3	1.70	0.55
1:B:326:VAL:HG12	1:B:346:LYS:O	2.07	0.55
1:B:9:GLY:HA2	1:B:38:SER:OG	2.07	0.55
1:H:198:VAL:O	1:H:200:ALA:N	2.40	0.55
1:H:247:GLU:HA	1:H:249:ALA:N	2.22	0.55
1:C:43:ARG:H	1:C:43:ARG:CD	2.19	0.54
1:E:326:VAL:HG12	1:E:346:LYS:O	2.06	0.54
1:I:288:ILE:HG22	1:I:289:THR:N	2.23	0.54
1:K:402:VAL:HG23	1:K:424:ASP:HB3	1.89	0.54
1:K:54:LEU:HD13	1:K:111:ALA:O	2.07	0.54
1:L:390:ALA:HB1	1:L:394:PHE:CE2	2.42	0.54
1:B:65:ILE:HD11	1:C:53:LEU:HD11	1.89	0.54
1:E:315:ARG:HA	1:E:318:LEU:HD12	1.89	0.54
1:A:226:ILE:O	1:A:273:THR:HG22	2.06	0.54
1:A:397:LEU:HB3	1:A:402:VAL:HG13	1.88	0.54
1:B:3:ILE:HD12	1:B:3:ILE:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:PHE:O	1:D:170:PHE:CG	2.61	0.54
1:I:39:ALA:N	1:I:116:GLU:OE2	2.39	0.54
1:L:8:PHE:CZ	1:L:22:VAL:HG13	2.43	0.54
1:C:256:SER:O	1:C:258:ILE:N	2.41	0.54
1:L:253:VAL:O	1:L:253:VAL:HG12	2.07	0.54
1:F:314:CYS:O	1:F:318:LEU:HD12	2.08	0.54
1:A:18:GLN:NE2	1:A:21:LYS:HE3	2.22	0.54
1:B:384:ALA:HB2	1:B:413:GLU:O	2.07	0.54
1:H:320:ILE:HA	1:H:323:MSE:HE3	1.90	0.54
1:I:155:ILE:O	1:I:159:VAL:HG22	2.08	0.54
1:B:253:VAL:HG13	1:B:258:ILE:HB	1.90	0.54
1:F:155:ILE:HD11	1:F:194:ILE:HD13	1.88	0.54
1:K:318:LEU:HD21	1:L:318:LEU:CG	2.38	0.54
1:K:393:ILE:HG22	1:K:397:LEU:HD12	1.89	0.54
1:L:364:PRO:HG3	1:L:367:ILE:HD11	1.89	0.54
1:D:231:TYR:CE1	1:D:250:ILE:HG23	2.43	0.54
1:E:202:LEU:HD12	1:E:203:TYR:H	1.73	0.54
1:H:247:GLU:HA	1:H:248:GLU:C	2.28	0.54
1:J:321:LEU:CD2	1:J:326:VAL:HG23	2.38	0.54
1:C:155:ILE:O	1:C:159:VAL:HG12	2.08	0.53
1:H:86:ASN:HD22	1:H:86:ASN:N	2.04	0.53
1:L:169:GLY:O	1:L:190:THR:OG1	2.14	0.53
1:A:274:LEU:HD22	1:A:276:LEU:CD1	2.36	0.53
1:H:87:ILE:HG22	1:H:89:MSE:HG2	1.90	0.53
1:L:75:SER:CB	1:L:95:LEU:HD13	2.38	0.53
1:B:237:LEU:HD12	1:B:292:ALA:HB3	1.90	0.53
1:E:288:ILE:HG22	1:E:289:THR:N	2.23	0.53
1:F:379:VAL:C	1:F:383:MSE:HE3	2.29	0.53
1:G:378:THR:C	1:G:383:MSE:HE1	2.28	0.53
1:I:106:ALA:HB1	1:I:110:TYR:CD1	2.43	0.53
1:I:404:ILE:HG21	1:I:407:ILE:HD11	1.89	0.53
1:K:25:ILE:HG21	1:K:206:TRP:CZ2	2.44	0.53
1:C:155:ILE:HG22	1:C:156:LYS:N	2.24	0.53
1:A:63:ASN:ND2	1:D:56:LEU:HD22	2.23	0.53
1:E:226:ILE:HG22	1:E:228:LYS:O	2.09	0.53
1:K:114:ARG:HA	1:K:114:ARG:NE	2.24	0.53
1:A:379:VAL:HA	1:A:383:MSE:CE	2.38	0.53
1:B:212:PHE:H	1:B:273:THR:CG2	2.21	0.53
1:C:235:ARG:NH1	1:C:236:GLU:OE2	2.41	0.53
1:C:315:ARG:HA	1:C:318:LEU:HD11	1.91	0.53
1:K:421:GLU:CG	1:K:423:VAL:HG12	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:321:LEU:HD12	1:L:340:LEU:HD23	1.89	0.53
1:H:212:PHE:CZ	1:H:244:VAL:HA	2.43	0.53
1:J:351:CYS:SG	1:J:352:ASP:N	2.81	0.53
1:J:87:ILE:HG21	1:J:89:MSE:CE	2.39	0.53
1:L:34:TYR:CE2	1:L:198:VAL:HG11	2.43	0.53
1:B:212:PHE:H	1:B:273:THR:HG21	1.73	0.53
1:C:212:PHE:H	1:C:273:THR:HG23	1.73	0.53
1:B:65:ILE:HD11	1:C:53:LEU:CD1	2.38	0.53
1:F:35:ILE:HD12	1:F:35:ILE:N	2.24	0.53
1:A:125:LYS:O	1:A:126:TYR:C	2.47	0.53
1:C:110:TYR:CZ	1:C:114:ARG:HD2	2.44	0.53
1:F:155:ILE:HD13	1:F:159:VAL:CG2	2.39	0.53
1:H:247:GLU:HB3	1:H:250:ILE:HD13	1.91	0.53
1:H:34:TYR:CD1	1:H:165:ALA:HB3	2.44	0.53
1:J:134:ALA:HB3	1:J:171:TYR:CE1	2.43	0.53
1:C:320:ILE:CD1	1:C:358:ILE:CG2	2.86	0.53
1:J:22:VAL:HA	1:J:25:ILE:HD12	1.91	0.53
1:J:237:LEU:HD13	1:J:292:ALA:HB2	1.91	0.53
1:K:300:ILE:HG22	1:K:302:ILE:HG13	1.91	0.53
1:C:238:SER:HB2	1:D:335:VAL:HG11	1.91	0.53
1:D:306:LEU:O	1:D:308:ASN:N	2.42	0.53
1:H:34:TYR:HD1	1:H:165:ALA:HB3	1.73	0.53
1:F:317:ILE:HA	1:F:320:ILE:HD12	1.90	0.52
1:F:354:ILE:O	1:F:358:ILE:HG22	2.08	0.52
1:G:155:ILE:CD1	1:G:194:ILE:CD1	2.87	0.52
1:H:170:PHE:O	1:H:170:PHE:CG	2.60	0.52
1:H:320:ILE:CD1	1:H:358:ILE:HG22	2.33	0.52
1:H:87:ILE:HD11	1:H:126:TYR:HB2	1.91	0.52
1:J:333:SER:HB3	1:J:338:VAL:HG23	1.90	0.52
1:J:364:PRO:HG3	1:J:367:ILE:HD11	1.90	0.52
1:G:53:LEU:HB3	1:G:74:ILE:HD11	1.91	0.52
1:I:155:ILE:CG2	1:I:159:VAL:CG2	2.84	0.52
1:I:159:VAL:HG12	1:I:167:ILE:HD11	1.90	0.52
1:I:170:PHE:CZ	1:I:181:THR:HG21	2.44	0.52
1:I:318:LEU:HD21	1:J:318:LEU:HG	1.92	0.52
1:C:79:THR:HA	1:C:82:VAL:HG12	1.91	0.52
1:D:58:ASN:HD21	1:D:62:LYS:HE3	1.74	0.52
1:L:383:MSE:HE1	1:L:416:VAL:HG23	1.90	0.52
1:A:318:LEU:HD11	1:B:318:LEU:CD1	2.38	0.52
1:G:288:ILE:HD13	1:G:383:MSE:CE	2.21	0.52
1:B:215:ALA:HB3	1:B:220:VAL:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:MSE:HE2	1:E:419:GLY:HA3	1.91	0.52
1:K:332:PRO:CG	1:K:406:MSE:HE3	2.39	0.52
1:K:383:MSE:CE	1:K:416:VAL:HG23	2.39	0.52
1:K:318:LEU:HD21	1:L:318:LEU:CD2	2.39	0.52
1:L:320:ILE:HG21	1:L:358:ILE:CG2	2.39	0.52
1:L:375:LEU:HD21	1:L:406:MSE:HE3	1.91	0.52
1:F:82:VAL:HG21	1:F:89:MSE:CE	2.38	0.52
1:G:302:ILE:CD1	1:G:317:ILE:HD13	2.39	0.52
1:I:159:VAL:HG23	1:I:160:LEU:N	2.24	0.52
1:I:390:ALA:HB1	1:I:394:PHE:HE2	1.74	0.52
1:J:213:LEU:HD12	1:J:213:LEU:N	2.25	0.52
1:B:82:VAL:HG23	1:B:87:ILE:HB	1.90	0.52
1:E:143:SER:O	1:E:145:CYS:N	2.42	0.52
1:J:117:TYR:O	1:J:121:VAL:HG13	2.09	0.52
1:J:241:GLY:CA	1:J:292:ALA:HB1	2.40	0.52
1:J:321:LEU:HD23	1:J:326:VAL:HG23	1.92	0.52
1:D:320:ILE:HD13	1:D:358:ILE:HA	1.92	0.52
1:D:352:ASP:HA	1:D:355:ILE:HD12	1.91	0.52
1:F:226:ILE:CG2	1:F:229:ILE:HB	2.40	0.52
1:G:232:LYS:HG2	1:G:414:ILE:HD11	1.91	0.52
1:I:85:LEU:O	1:I:86:ASN:C	2.48	0.52
1:J:35:ILE:N	1:J:35:ILE:HD12	2.25	0.52
1:L:129:ALA:HB3	1:L:166:VAL:HG23	1.92	0.52
1:B:326:VAL:HG23	1:B:326:VAL:O	2.10	0.52
1:B:53:LEU:HD11	1:C:65:ILE:HD11	1.91	0.52
1:C:320:ILE:HD12	1:C:357:GLU:HB3	1.92	0.52
1:K:318:LEU:HD12	1:K:319:SER:N	2.24	0.52
1:L:155:ILE:HG21	1:L:197:GLY:HA3	1.92	0.52
1:B:187:SER:O	1:B:190:THR:HG23	2.10	0.51
1:B:211:GLY:HA2	1:B:262:ILE:HG22	1.92	0.51
1:I:318:LEU:HD21	1:J:318:LEU:HD21	1.90	0.51
1:I:326:VAL:HG12	1:I:346:LYS:O	2.11	0.51
1:K:114:ARG:N	1:K:114:ARG:HE	2.07	0.51
1:G:238:SER:CB	1:G:244:VAL:HG11	2.39	0.51
1:G:245:LEU:HD12	1:G:246:HIS:N	2.25	0.51
1:F:355:ILE:HD11	1:F:369:ILE:HD11	1.92	0.51
1:G:155:ILE:HD12	1:G:194:ILE:HD13	1.93	0.51
1:H:236:GLU:HB3	1:H:379:VAL:HG21	1.91	0.51
1:H:50:ILE:HD11	1:H:77:ARG:HD3	1.91	0.51
1:I:409:GLN:HG2	1:J:407:ILE:HD12	1.92	0.51
1:K:326:VAL:HG11	1:K:347:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:216:ASP:O	1:L:220:VAL:HG12	2.10	0.51
1:B:313:PHE:CE2	1:B:317:ILE:HD11	2.45	0.51
1:C:320:ILE:HD13	1:C:358:ILE:CG2	2.40	0.51
1:J:262:ILE:CD1	1:J:275:ILE:HD11	2.40	0.51
1:J:34:TYR:C	1:J:35:ILE:HD12	2.31	0.51
1:A:57:CYS:HG	1:A:67:PHE:HD1	1.58	0.51
1:C:79:THR:HG22	1:C:91:ILE:CG2	2.41	0.51
1:I:198:VAL:O	1:I:199:ASN:C	2.48	0.51
1:I:250:ILE:O	1:I:250:ILE:HG22	2.11	0.51
1:K:58:ASN:HD21	1:K:62:LYS:HE3	1.76	0.51
1:L:364:PRO:CG	1:L:367:ILE:HD11	2.40	0.51
1:C:43:ARG:H	1:C:43:ARG:HD3	1.75	0.51
1:H:85:LEU:HD23	1:H:126:TYR:CE1	2.45	0.51
1:A:35:ILE:HB	1:A:166:VAL:HG22	1.93	0.51
1:A:315:ARG:HA	1:B:318:LEU:HD13	1.93	0.51
1:I:137:VAL:HG22	1:I:155:ILE:HA	1.93	0.51
1:K:18:GLN:HE22	1:K:21:LYS:HZ2	1.59	0.51
1:E:65:ILE:HG12	1:E:66:PRO:HD2	1.93	0.51
1:G:19:PHE:HB3	1:G:85:LEU:HD21	1.93	0.51
1:J:87:ILE:HG21	1:J:89:MSE:HE3	1.93	0.51
1:E:323:MSE:HE2	1:G:315:ARG:HH22	1.74	0.51
1:G:318:LEU:HD11	1:H:318:LEU:HD11	1.93	0.51
1:K:305:ALA:C	1:K:306:LEU:HD12	2.32	0.51
1:J:188:ASP:HB3	1:J:249:ALA:HB1	1.92	0.50
1:K:394:PHE:O	1:K:398:SER:N	2.44	0.50
1:B:160:LEU:O	1:B:160:LEU:HD12	2.12	0.50
1:B:237:LEU:HD12	1:B:292:ALA:HB2	1.92	0.50
1:B:314:CYS:HA	1:B:317:ILE:HD12	1.93	0.50
1:D:16:SER:HB2	1:D:85:LEU:HD12	1.93	0.50
1:I:138:ILE:HD13	1:I:190:THR:HG22	1.93	0.50
1:I:305:ALA:HB1	1:I:306:LEU:HD12	1.93	0.50
1:E:373:MSE:HE1	1:E:406:MSE:HB2	1.94	0.50
1:I:305:ALA:CB	1:I:306:LEU:HD12	2.42	0.50
1:E:250:ILE:CG2	1:E:250:ILE:O	2.60	0.50
1:G:169:GLY:C	1:G:190:THR:HG21	2.32	0.50
1:H:152:TYR:HA	1:H:155:ILE:HD12	1.93	0.50
1:K:36:ILE:N	1:K:36:ILE:HD12	2.26	0.50
1:L:283:ILE:O	1:L:283:ILE:HG23	2.11	0.50
1:C:383:MSE:CB	1:C:389:ILE:HG21	2.34	0.50
1:C:3:ILE:HD12	1:C:3:ILE:O	2.11	0.50
1:G:379:VAL:CA	1:G:383:MSE:CE	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:213:LEU:HD23	1:K:223:PRO:O	2.11	0.50
1:G:18:GLN:HE22	1:G:21:LYS:HZ2	1.60	0.50
1:J:48:TYR:CD1	1:J:53:LEU:HD22	2.47	0.50
1:L:100:LYS:O	1:L:104:ASN:ND2	2.44	0.50
1:E:321:LEU:HD11	1:E:342:ILE:HD11	1.92	0.50
1:H:118:LEU:O	1:H:121:VAL:HG22	2.12	0.50
1:H:98:VAL:HG22	1:H:114:ARG:HD3	1.93	0.50
1:I:320:ILE:CD1	1:I:358:ILE:HG22	2.41	0.50
1:I:16:SER:HB3	1:I:85:LEU:HD13	1.94	0.50
1:L:320:ILE:CD1	1:L:358:ILE:HG22	2.38	0.50
1:A:226:ILE:O	1:A:273:THR:CG2	2.59	0.50
1:G:263:LYS:NZ	1:G:270:ASP:O	2.34	0.50
1:B:226:ILE:O	1:B:273:THR:HG22	2.11	0.50
1:G:313:PHE:N	3:G:507:LYS:O	2.45	0.50
1:J:212:PHE:N	1:J:273:THR:OG1	2.39	0.50
1:J:402:VAL:HG23	1:J:424:ASP:HB3	1.92	0.50
1:K:147:ASP:OD2	1:K:148:GLU:N	2.44	0.50
1:B:240:MSE:N	1:B:241:GLY:CA	2.75	0.49
1:C:61:VAL:HG21	1:C:102:ILE:O	2.12	0.49
1:A:56:LEU:HD22	1:D:63:ASN:ND2	2.26	0.49
1:E:18:GLN:HE22	1:E:21:LYS:NZ	2.10	0.49
1:F:159:VAL:HB	1:F:198:VAL:HG21	1.93	0.49
1:I:23:LYS:O	1:I:27:ASP:OD1	2.30	0.49
1:K:318:LEU:HD23	1:L:318:LEU:HD21	1.93	0.49
1:K:235:ARG:O	1:K:238:SER:HB3	2.12	0.49
1:L:34:TYR:HE2	1:L:198:VAL:HG11	1.77	0.49
1:E:132:ILE:HD11	1:E:162:CYS:SG	2.52	0.49
1:E:373:MSE:HE2	1:E:419:GLY:C	2.32	0.49
1:H:60:HIS:CG	1:H:67:PHE:HB3	2.47	0.49
1:A:318:LEU:HD13	1:B:315:ARG:HA	1.95	0.49
1:E:155:ILE:HG23	1:E:159:VAL:CG1	2.42	0.49
1:J:288:ILE:HD13	1:J:383:MSE:SE	2.62	0.49
1:B:317:ILE:O	1:B:321:LEU:HD13	2.13	0.49
1:I:253:VAL:CG1	1:I:258:ILE:O	2.60	0.49
1:J:110:TYR:CZ	1:J:114:ARG:HD2	2.47	0.49
1:L:320:ILE:HG21	1:L:358:ILE:HG22	1.95	0.49
1:E:373:MSE:HE3	1:E:405:ARG:HB3	1.92	0.49
1:E:7:LYS:NZ	1:E:188:ASP:OD1	2.46	0.49
1:F:78:TYR:CE1	1:F:118:LEU:HD12	2.48	0.49
1:H:400:GLU:H	1:H:401:ASN:HA	1.77	0.49
1:L:160:LEU:HB2	1:L:198:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:75:SER:HB3	1:L:95:LEU:HD13	1.93	0.49
1:A:379:VAL:HA	1:A:383:MSE:HE2	1.93	0.49
1:H:207:THR:HG23	1:H:209:VAL:H	1.77	0.49
1:I:169:GLY:O	1:I:190:THR:CG2	2.60	0.49
1:I:213:LEU:HD12	1:I:217:PRO:HD3	1.94	0.49
1:I:213:LEU:HD13	1:I:223:PRO:HG2	1.94	0.49
1:L:397:LEU:HD12	1:L:404:ILE:HD11	1.95	0.49
1:G:198:VAL:CG1	1:G:198:VAL:O	2.60	0.49
1:G:379:VAL:C	1:G:383:MSE:CE	2.77	0.49
1:A:167:ILE:N	1:A:167:ILE:HD12	2.28	0.49
1:C:65:ILE:HG22	1:C:66:PRO:O	2.12	0.49
1:F:155:ILE:HD12	1:F:198:VAL:CG2	2.40	0.49
1:F:198:VAL:O	1:F:198:VAL:HG12	2.13	0.49
1:I:409:GLN:HB3	1:I:416:VAL:HG22	1.94	0.49
1:K:369:ILE:HG22	1:K:371:PRO:HD3	1.95	0.49
1:B:320:ILE:HD11	1:B:361:GLN:HE21	1.78	0.48
1:F:291:ILE:CG2	1:F:429:VAL:HG13	2.42	0.48
1:H:14:ALA:O	1:H:77:ARG:NH2	2.43	0.48
1:H:373:MSE:HE2	1:H:419:GLY:CA	2.42	0.48
1:L:155:ILE:HG22	1:L:156:LYS:N	2.28	0.48
1:A:7:LYS:HD2	1:A:8:PHE:N	2.28	0.48
1:B:194:ILE:O	1:B:198:VAL:HG12	2.13	0.48
1:F:75:SER:HB2	1:F:95:LEU:HD13	1.94	0.48
1:G:35:ILE:HD12	1:G:35:ILE:N	2.28	0.48
1:J:198:VAL:O	1:J:199:ASN:C	2.50	0.48
1:I:262:ILE:O	1:I:272:GLY:HA3	2.14	0.48
1:A:79:THR:HG22	1:A:91:ILE:CG2	2.44	0.48
1:A:387:LYS:HD2	1:B:401:ASN:HD22	1.79	0.48
1:D:182:PHE:CE2	1:D:190:THR:HG22	2.48	0.48
1:E:54:LEU:HD23	1:E:74:ILE:CD1	2.43	0.48
1:G:308[B]:ASN:OD1	3:G:507:LYS:CG	2.54	0.48
1:H:155:ILE:CG2	1:H:198:VAL:HG23	2.43	0.48
1:J:287:THR:HG22	1:J:382:GLY:HA3	1.95	0.48
1:L:169:GLY:HA2	1:L:190:THR:HG21	1.95	0.48
1:A:320:ILE:CD1	1:A:358:ILE:HG22	2.41	0.48
1:H:262:ILE:HD11	1:H:275:ILE:HD11	1.96	0.48
1:I:130:GLU:CB	1:I:162:CYS:SG	3.02	0.48
1:K:85:LEU:HD22	1:K:87:ILE:HD11	1.96	0.48
1:A:253:VAL:CG1	1:A:258:ILE:O	2.61	0.48
1:D:320:ILE:HG21	1:D:358:ILE:HG23	1.96	0.48
1:D:19:PHE:HB3	1:D:85:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:205:ASN:ND2	1:H:245:LEU:HD22	2.28	0.48
1:A:305:ALA:HB1	1:A:306:LEU:HD12	1.94	0.48
1:C:335:VAL:HG23	1:C:336:ASP:N	2.28	0.48
1:C:87:ILE:HG22	1:C:88:ASP:N	2.24	0.48
1:E:383:MSE:CE	1:E:416:VAL:HG23	2.44	0.48
1:I:170:PHE:CZ	1:I:181:THR:CG2	2.97	0.48
1:L:228:LYS:HE2	1:L:276:LEU:HD21	1.94	0.48
1:A:363:ASN:ND2	1:A:363:ASN:O	2.47	0.48
1:H:169:GLY:HA2	1:H:190:THR:HG21	1.95	0.48
1:I:216:ASP:HB3	1:I:219:ILE:HD13	1.95	0.48
1:I:288:ILE:HD11	1:I:436:PHE:CZ	2.48	0.48
1:J:402:VAL:HG23	1:J:424:ASP:CB	2.44	0.48
1:B:364:PRO:HG3	1:B:367:ILE:HD11	1.96	0.48
1:B:364:PRO:CG	1:B:367:ILE:HD11	2.43	0.48
1:G:390:ALA:HB1	1:G:394:PHE:CE2	2.49	0.48
1:H:55:TYR:CZ	1:H:112:ALA:HB2	2.49	0.48
1:H:288:ILE:CG2	1:H:289:THR:N	2.76	0.48
1:I:198:VAL:O	1:I:198:VAL:HG12	2.14	0.48
1:I:198:VAL:O	1:I:200:ALA:N	2.46	0.48
1:K:238:SER:O	1:K:239:TYR:C	2.53	0.48
1:A:274:LEU:HD23	1:A:276:LEU:CD1	2.44	0.48
1:E:169:GLY:C	1:E:190:THR:HG21	2.34	0.48
1:G:18:GLN:HE22	1:G:21:LYS:NZ	2.11	0.48
1:K:347:LEU:HD11	1:K:354:ILE:CD1	2.44	0.48
1:A:192:SER:HB3	1:A:253:VAL:HG23	1.96	0.47
1:A:383:MSE:HE3	1:A:414:ILE:C	2.34	0.47
1:B:302:ILE:HD13	1:B:358:ILE:HD11	1.96	0.47
1:D:186:GLY:O	1:D:189:VAL:HG12	2.13	0.47
1:H:299:VAL:HG13	1:H:370:HIS:HB2	1.96	0.47
1:I:36:ILE:N	1:I:36:ILE:HD12	2.28	0.47
1:I:318:LEU:HD21	1:J:318:LEU:CG	2.44	0.47
1:K:114:ARG:CA	1:K:114:ARG:NE	2.77	0.47
1:I:53:LEU:CG	1:L:65:ILE:HD11	2.44	0.47
1:L:85:LEU:HD23	1:L:126:TYR:CD1	2.49	0.47
1:A:334:GLY:O	1:A:336:ASP:N	2.47	0.47
1:C:318:LEU:HD13	1:D:315:ARG:CB	2.44	0.47
1:E:304:LYS:CB	1:E:363:ASN:HD21	2.27	0.47
1:F:216:ASP:O	1:F:220:VAL:HG12	2.14	0.47
1:L:89:MSE:HE1	1:L:122:ILE:HA	1.96	0.47
1:B:213:LEU:HD13	1:B:223:PRO:HG2	1.96	0.47
1:C:155:ILE:HG21	1:C:197:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:359:LYS:HE2	1:F:367:ILE:HD12	1.96	0.47
1:G:379:VAL:HA	1:G:383:MSE:HE3	1.95	0.47
1:G:231:TYR:CE2	1:G:277:SER:HA	2.49	0.47
1:J:137:VAL:HG12	1:J:138:ILE:HG12	1.95	0.47
1:J:318:LEU:C	1:J:318:LEU:HD12	2.34	0.47
1:B:381:THR:HA	1:B:414:ILE:HG22	1.97	0.47
1:E:320:ILE:HA	1:E:323:MSE:HE3	1.95	0.47
1:F:35:ILE:HB	1:F:166:VAL:HG22	1.95	0.47
1:G:333:SER:HB2	3:G:507:LYS:NZ	2.30	0.47
1:H:250:ILE:HG12	1:H:250:ILE:O	2.15	0.47
1:I:335:VAL:CG2	1:J:239:TYR:CB	2.92	0.47
1:K:409:GLN:HE21	1:K:416:VAL:HG22	1.79	0.47
1:F:323:MSE:HE2	1:H:316:LYS:NZ	2.30	0.47
1:G:152:TYR:CE1	1:G:196:ALA:HB3	2.49	0.47
1:I:229:ILE:HD11	1:I:237:LEU:HD12	1.96	0.47
1:K:82:VAL:HG23	1:K:87:ILE:HB	1.97	0.47
1:E:253:VAL:O	1:E:256:SER:O	2.33	0.47
1:I:234:LEU:HD23	1:I:234:LEU:C	2.35	0.47
1:J:397:LEU:HD22	1:J:402:VAL:HG11	1.96	0.47
1:J:397:LEU:O	1:J:402:VAL:CG1	2.62	0.47
1:J:431:SER:O	1:J:435:ALA:HB2	2.15	0.47
1:L:58:ASN:HD21	1:L:62:LYS:CE	2.28	0.47
1:C:113:SER:OG	1:C:114:ARG:NH1	2.48	0.47
1:C:35:ILE:N	1:C:35:ILE:HD12	2.29	0.47
1:E:36:ILE:CD1	1:E:36:ILE:N	2.77	0.47
1:F:250:ILE:HD12	1:F:250:ILE:C	2.35	0.47
1:G:359:LYS:CE	1:G:367:ILE:HD12	2.45	0.47
1:L:341:VAL:HG21	1:L:406:MSE:SE	2.65	0.47
1:D:251:PHE:CG	1:D:252:PRO:HD3	2.49	0.47
1:E:155:ILE:O	1:E:159:VAL:HG13	2.14	0.47
1:E:78:TYR:O	1:E:82:VAL:HG12	2.15	0.47
1:H:231:TYR:OH	1:H:253:VAL:HG12	2.15	0.47
1:I:137:VAL:HG13	1:I:155:ILE:CG1	2.45	0.47
1:A:33:LYS:O	1:A:164:LYS:HA	2.15	0.47
1:E:262:ILE:O	1:E:272:GLY:HA3	2.15	0.47
1:H:240:MSE:SE	1:H:377:ALA:HB2	2.64	0.47
1:H:358:ILE:C	1:H:360:LYS:H	2.19	0.47
1:J:424:ASP:O	1:J:425:PHE:C	2.53	0.47
1:K:35:ILE:C	1:K:36:ILE:HD12	2.35	0.47
1:A:110:TYR:CZ	1:A:114:ARG:HD2	2.50	0.47
1:A:213:LEU:O	1:A:240:MSE:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLY:HA2	1:B:38:SER:HG	1.79	0.47
1:C:212:PHE:CD2	1:C:273:THR:HG21	2.49	0.47
1:F:134:ALA:HB3	1:F:171:TYR:CE1	2.50	0.47
1:I:212:PHE:H	1:I:273:THR:HG23	1.79	0.47
1:J:155:ILE:HD13	1:J:198:VAL:HG13	1.92	0.47
1:J:241:GLY:HA2	1:J:292:ALA:HB1	1.97	0.47
1:J:412:SER:HB3	1:J:415:ASN:HD22	1.79	0.47
1:A:34:TYR:CD1	1:A:165:ALA:HB3	2.50	0.46
1:D:229:ILE:HG22	1:D:274:LEU:O	2.14	0.46
1:E:239:TYR:CE2	1:E:240:MSE:HE2	2.50	0.46
1:I:238:SER:HA	1:I:245:LEU:CD1	2.45	0.46
1:J:82:VAL:O	1:J:85:LEU:O	2.32	0.46
1:A:313:PHE:CE1	1:A:317:ILE:HD11	2.50	0.46
1:E:284:ASN:O	1:E:287:THR:HG22	2.14	0.46
1:E:362:CYS:O	1:E:364:PRO:HD3	2.14	0.46
1:G:362:CYS:O	1:G:364:PRO:HD3	2.14	0.46
1:H:82:VAL:O	1:H:85:LEU:O	2.33	0.46
1:K:215:ALA:HB3	1:K:220:VAL:HG11	1.97	0.46
1:L:114:ARG:CA	1:L:114:ARG:NE	2.78	0.46
1:C:3:ILE:CG1	1:C:3:ILE:O	2.64	0.46
1:G:359:LYS:HE3	1:G:367:ILE:HD12	1.97	0.46
1:A:339:SER:O	1:A:340:LEU:HD12	2.14	0.46
1:B:234:LEU:HD11	1:B:244:VAL:HB	1.96	0.46
1:B:65:ILE:HG22	1:B:66:PRO:CD	2.46	0.46
3:C:503:LYS:NZ	1:D:329:GLU:O	2.43	0.46
1:H:33:LYS:O	1:H:164:LYS:HA	2.16	0.46
1:K:182:PHE:CE1	1:K:190:THR:HG22	2.50	0.46
1:B:181:THR:HG23	1:B:182:PHE:O	2.16	0.46
1:D:221:GLU:C	1:D:223:PRO:HD3	2.35	0.46
1:G:192:SER:HB2	1:G:253:VAL:HG23	1.97	0.46
1:I:207:THR:OG1	1:I:208:ASP:N	2.46	0.46
1:J:236:GLU:HB3	1:J:379:VAL:HG21	1.97	0.46
1:K:378:THR:HG21	1:K:393:ILE:HD13	1.96	0.46
1:L:198:VAL:O	1:L:199:ASN:C	2.54	0.46
1:B:220:VAL:HG13	1:B:223:PRO:HB3	1.97	0.46
1:C:311:VAL:HG13	1:C:312:GLY:HA2	1.96	0.46
1:C:330:HIS:ND1	1:C:406:MSE:HE1	2.31	0.46
1:D:167:ILE:N	1:D:167:ILE:HD12	2.30	0.46
1:F:155:ILE:CG2	1:F:156:LYS:N	2.79	0.46
1:F:60:HIS:CE1	1:G:60:HIS:HE1	2.33	0.46
1:G:61:VAL:HG21	1:G:102:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:256:SER:CB	1:H:258:ILE:HD12	2.45	0.46
1:I:287:THR:HG23	1:I:288:ILE:O	2.16	0.46
1:J:245:LEU:HB3	1:J:246:HIS:CA	2.46	0.46
1:J:298:THR:HG23	1:J:371:PRO:HA	1.98	0.46
1:J:321:LEU:HD12	1:J:340:LEU:HD23	1.97	0.46
1:A:116:GLU:HG3	1:A:170:PHE:HB3	1.97	0.46
1:C:320:ILE:HD13	1:C:358:ILE:HG22	1.98	0.46
1:E:335:VAL:HG22	1:F:239:TYR:CD2	2.51	0.46
1:E:60:HIS:O	1:E:65:ILE:HG22	2.15	0.46
1:G:379:VAL:N	1:G:383:MSE:HE1	2.30	0.46
1:H:198:VAL:O	1:H:198:VAL:HG12	2.15	0.46
1:I:39:ALA:HB1	1:I:40:PRO:HD2	1.98	0.46
1:J:212:PHE:CE2	1:J:262:ILE:HD13	2.50	0.46
1:J:379:VAL:HG22	1:J:415:ASN:HB2	1.98	0.46
1:I:53:LEU:CD1	1:L:65:ILE:HD11	2.46	0.46
1:L:71:PHE:HA	1:L:74:ILE:HD12	1.98	0.46
1:C:235:ARG:O	1:C:238:SER:OG	2.32	0.46
1:E:55:TYR:CE1	1:E:112:ALA:HB2	2.51	0.46
1:G:317:ILE:CG2	1:G:340:LEU:HD21	2.45	0.46
1:B:247:GLU:HA	1:B:250:ILE:HD11	1.98	0.46
1:B:251:PHE:N	1:B:252:PRO:CD	2.78	0.46
1:D:251:PHE:CD2	1:D:252:PRO:HD3	2.50	0.46
1:D:320:ILE:HD13	1:D:358:ILE:CG2	2.41	0.46
1:D:326:VAL:HG12	1:D:346:LYS:O	2.16	0.46
1:D:384:ALA:HA	1:D:385:LYS:HA	1.74	0.46
1:I:288:ILE:HD11	1:I:436:PHE:CE1	2.51	0.46
1:L:234:LEU:HD22	1:L:275:ILE:HD13	1.98	0.46
1:L:373:MSE:HE3	1:L:405:ARG:HB3	1.98	0.46
1:B:134:ALA:HB3	1:B:171:TYR:CE1	2.50	0.46
1:B:253:VAL:O	1:B:256:SER:O	2.33	0.46
1:D:284:ASN:O	1:D:287:THR:CG2	2.64	0.46
1:E:240:MSE:HE3	1:E:417:ILE:HD13	1.96	0.46
1:F:283:ILE:HD12	1:F:283:ILE:N	2.31	0.46
1:B:35:ILE:HD12	1:B:35:ILE:N	2.30	0.45
1:C:318:LEU:HD23	1:C:331:MSE:CE	2.45	0.45
1:F:313:PHE:CE2	1:F:317:ILE:HD11	2.52	0.45
1:J:167:ILE:HD12	1:J:194:ILE:HG12	1.98	0.45
1:J:383:MSE:HB2	1:J:389:ILE:HG21	1.97	0.45
1:B:7:LYS:HG3	1:B:8:PHE:N	2.31	0.45
1:C:288:ILE:CG2	1:C:289:THR:N	2.79	0.45
1:G:393:ILE:HG23	1:G:432:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LEU:HD22	1:C:19:PHE:CZ	2.52	0.45
1:I:87:ILE:CG2	1:I:89:MSE:HG2	2.46	0.45
1:J:214:MSE:HE2	1:J:433:TYR:CD2	2.51	0.45
1:C:283:ILE:HD13	1:J:228:LYS:HD3	1.97	0.45
1:L:298:THR:HG23	1:L:371:PRO:HA	1.97	0.45
1:B:231:TYR:OH	1:B:253:VAL:HG12	2.17	0.45
1:E:283:ILE:O	1:E:283:ILE:HG23	2.17	0.45
1:I:129:ALA:HB1	1:I:164:LYS:C	2.36	0.45
1:L:321:LEU:CD1	1:L:340:LEU:HD23	2.46	0.45
1:C:335:VAL:HG23	1:C:336:ASP:H	1.80	0.45
1:A:310:GLU:HB2	1:A:313:PHE:HB2	1.98	0.45
1:F:155:ILE:HG21	1:F:198:VAL:N	2.32	0.45
1:F:321:LEU:O	1:F:326:VAL:HG22	2.17	0.45
1:H:170:PHE:O	1:H:170:PHE:CD2	2.70	0.45
1:L:318:LEU:HD12	1:L:318:LEU:C	2.36	0.45
1:A:75:SER:O	1:A:79:THR:HG23	2.16	0.45
1:B:198:VAL:HG22	1:B:198:VAL:O	2.15	0.45
1:F:315:ARG:HA	1:F:318:LEU:HD12	1.97	0.45
1:K:256:SER:O	1:K:258:ILE:N	2.50	0.45
1:K:85:LEU:CD2	1:K:87:ILE:HD11	2.46	0.45
1:L:50:ILE:O	1:L:51:THR:C	2.54	0.45
1:A:284:ASN:HB2	1:A:287:THR:HG21	1.98	0.45
1:A:380:GLY:N	1:A:383:MSE:HE2	2.32	0.45
1:B:137:VAL:HG22	1:B:155:ILE:HG13	1.99	0.45
1:C:3:ILE:HD11	1:C:200:ALA:CA	2.43	0.45
1:G:19:PHE:CB	1:G:85:LEU:HD21	2.47	0.45
1:H:262:ILE:HD11	1:H:275:ILE:CD1	2.47	0.45
1:I:306:LEU:HD12	1:I:306:LEU:N	2.32	0.45
1:J:85:LEU:HD23	1:J:87:ILE:HD11	1.98	0.45
1:K:339:SER:C	1:K:340:LEU:HD12	2.36	0.45
1:C:34:TYR:CE2	1:C:198:VAL:HG11	2.52	0.45
1:C:373:MSE:HE3	1:C:375:LEU:CD2	2.47	0.45
1:G:321:LEU:O	1:G:326:VAL:HG22	2.16	0.45
1:G:35:ILE:C	1:G:36:ILE:HD12	2.37	0.45
1:J:262:ILE:HD12	1:J:275:ILE:HD11	2.00	0.45
1:A:36:ILE:N	1:A:36:ILE:HD12	2.32	0.44
1:G:210:SER:HA	1:G:264:ASN:HB2	1.98	0.44
1:G:251:PHE:HB3	1:G:252:PRO:HD3	1.98	0.44
1:G:82:VAL:HG23	1:G:87:ILE:HB	1.98	0.44
1:I:155:ILE:HG23	1:I:159:VAL:HG22	1.96	0.44
1:J:236:GLU:CB	1:J:379:VAL:HG21	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:ILE:N	1:L:36:ILE:HD12	2.32	0.44
1:C:397:LEU:HB3	1:C:402:VAL:HG22	1.97	0.44
1:F:307:LEU:C	1:F:307:LEU:HD23	2.37	0.44
1:G:198:VAL:HG12	1:G:198:VAL:O	2.17	0.44
1:K:234:LEU:CD1	1:K:275:ILE:HG21	2.46	0.44
1:K:406:MSE:HE2	1:K:408:ASP:CB	2.41	0.44
1:D:110:TYR:O	1:D:114:ARG:HG2	2.18	0.44
1:D:160:LEU:HG	1:D:198:VAL:HG23	2.00	0.44
1:F:304:LYS:O	1:F:336:ASP:HB3	2.18	0.44
1:H:87:ILE:CG2	1:H:89:MSE:HG2	2.46	0.44
1:I:181:THR:HG22	1:I:182:PHE:O	2.18	0.44
1:J:302:ILE:HD12	1:J:338:VAL:HG13	1.99	0.44
1:L:15:ASP:O	1:L:16:SER:C	2.56	0.44
1:A:16:SER:HB2	1:A:85:LEU:CD1	2.47	0.44
1:A:318:LEU:HD13	1:B:315:ARG:CB	2.48	0.44
1:D:141:ASP:C	1:D:141:ASP:OD1	2.56	0.44
1:H:75:SER:O	1:H:79:THR:HG23	2.17	0.44
1:C:98:VAL:HG22	1:C:114:ARG:HD3	1.99	0.44
1:D:315:ARG:O	1:D:318:LEU:HD12	2.17	0.44
1:E:137:VAL:HG13	1:E:155:ILE:CG1	2.48	0.44
1:F:1:LEU:N	1:F:1:LEU:HD22	2.33	0.44
1:H:192:SER:HB3	1:H:253:VAL:HG23	1.99	0.44
1:H:25:ILE:HG23	1:H:32:ARG:NH1	2.32	0.44
1:K:159:VAL:O	1:K:162:CYS:HB2	2.18	0.44
1:F:176:ASN:HD22	1:F:176:ASN:C	2.19	0.44
1:G:306:LEU:O	1:G:307:LEU:C	2.55	0.44
1:I:134:ALA:HB3	1:I:171:TYR:CZ	2.53	0.44
1:I:48:TYR:CE2	1:I:73:LEU:HD22	2.53	0.44
1:J:57:CYS:O	1:J:61:VAL:HG23	2.17	0.44
1:K:110:TYR:CE1	1:K:114:ARG:HD2	2.52	0.44
1:K:72:LYS:O	1:K:76:GLN:HB2	2.17	0.44
1:A:387:LYS:CD	1:B:401:ASN:HD22	2.31	0.44
1:B:170:PHE:CG	1:B:170:PHE:O	2.71	0.44
1:D:210:SER:HA	1:D:264:ASN:HB2	1.99	0.44
1:E:216:ASP:HB3	1:E:219:ILE:HD12	2.00	0.44
1:E:373:MSE:HE2	1:E:419:GLY:CA	2.48	0.44
1:G:25:ILE:HD13	1:G:206:TRP:CZ3	2.53	0.44
1:I:38:SER:HA	1:I:116:GLU:OE2	2.17	0.44
1:J:299:VAL:HG12	1:J:370:HIS:HB2	2.00	0.44
1:L:176:ASN:HD22	1:L:176:ASN:H	1.64	0.44
1:B:100:LYS:HD2	1:B:100:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ALA:HB2	1:D:413:GLU:O	2.17	0.44
1:F:54:LEU:HD13	1:F:111:ALA:O	2.18	0.44
1:G:359:LYS:O	1:G:362:CYS:O	2.35	0.44
1:I:251:PHE:N	1:I:252:PRO:CD	2.80	0.44
1:K:34:TYR:C	1:K:35:ILE:HD12	2.38	0.44
1:L:291:ILE:HG21	1:L:429:VAL:HG13	1.98	0.44
1:D:55:TYR:CE1	1:D:112:ALA:HB2	2.52	0.44
1:F:376:VAL:HG11	1:F:432:ILE:HD13	1.99	0.44
1:H:138:ILE:HG22	1:H:172:GLY:HA3	2.00	0.44
1:H:302:ILE:CD1	1:H:358:ILE:HD12	2.47	0.44
1:L:261:ASN:HD22	1:L:274:LEU:HD12	1.83	0.44
1:L:299:VAL:HG22	1:L:300:ILE:N	2.33	0.44
1:L:321:LEU:O	1:L:321:LEU:HD23	2.18	0.44
1:D:222:ASN:O	1:D:223:PRO:C	2.54	0.43
1:E:383:MSE:HE1	1:E:416:VAL:HG23	2.00	0.43
1:E:50:ILE:HD11	1:E:77:ARG:CG	2.39	0.43
1:I:214:MSE:HE2	1:I:433:TYR:CD2	2.53	0.43
1:K:123:LEU:HA	1:K:123:LEU:HD23	1.89	0.43
1:C:3:ILE:CD1	1:C:200:ALA:HA	2.47	0.43
1:C:3:ILE:HG13	1:C:3:ILE:O	2.18	0.43
1:C:407:ILE:HG21	1:D:407:ILE:HG21	1.99	0.43
1:D:113:SER:HB2	1:D:171:TYR:CD2	2.52	0.43
1:D:34:TYR:CE2	1:D:198:VAL:HG21	2.52	0.43
1:H:144:GLY:HA2	1:H:145:CYS:HA	1.76	0.43
1:B:71:PHE:CE2	1:B:99:LYS:HB2	2.53	0.43
1:C:155:ILE:CG2	1:C:156:LYS:N	2.80	0.43
1:E:85:LEU:HD11	1:E:126:TYR:OH	2.18	0.43
1:E:404:ILE:HD13	1:E:404:ILE:N	2.33	0.43
1:E:82:VAL:HG23	1:E:87:ILE:HB	2.00	0.43
1:F:53:LEU:HD12	1:G:63:ASN:HD22	1.83	0.43
1:G:39:ALA:HB2	1:G:116:GLU:OE2	2.18	0.43
1:J:241:GLY:HA3	1:J:292:ALA:HB1	2.00	0.43
1:K:189:VAL:HG13	1:K:190:THR:N	2.33	0.43
1:L:114:ARG:HA	1:L:114:ARG:NE	2.33	0.43
1:K:318:LEU:HD13	1:L:315:ARG:CB	2.48	0.43
1:C:220:VAL:O	1:C:220:VAL:CG1	2.64	0.43
1:C:333:SER:HB2	3:C:503:LYS:HD3	2.00	0.43
1:E:166:VAL:C	1:E:167:ILE:HG13	2.39	0.43
1:F:194:ILE:O	1:F:198:VAL:N	2.52	0.43
1:H:294:LYS:HB3	1:H:297:PHE:HE2	1.83	0.43
1:H:344:ASP:O	1:H:347:LEU:HD23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:231:TYR:CE1	1:I:275:ILE:HG22	2.54	0.43
1:I:378:THR:HG21	1:I:432:ILE:HD13	2.00	0.43
1:J:116:GLU:HG3	1:J:170:PHE:HB3	2.01	0.43
1:K:378:THR:HG21	1:K:393:ILE:CD1	2.49	0.43
1:K:56:LEU:O	1:K:59:ALA:HB3	2.18	0.43
1:L:151:SER:O	1:L:155:ILE:HB	2.19	0.43
1:E:317:ILE:CG2	1:E:340:LEU:HD21	2.48	0.43
1:F:260:ILE:HB	1:F:275:ILE:HB	2.01	0.43
1:H:397:LEU:HD22	1:H:402:VAL:HG11	2.00	0.43
1:I:35:ILE:HD12	1:I:35:ILE:N	2.33	0.43
1:K:253:VAL:CG1	1:K:258:ILE:O	2.67	0.43
1:L:229:ILE:HG22	1:L:274:LEU:O	2.19	0.43
1:L:372:ASN:O	1:L:405:ARG:NH1	2.51	0.43
1:B:384:ALA:CB	1:B:413:GLU:O	2.66	0.43
1:B:427:LYS:O	1:B:431:SER:OG	2.35	0.43
1:B:52:ASP:HB3	1:C:63:ASN:ND2	2.31	0.43
1:D:102:ILE:HA	1:D:106:ALA:HB3	1.99	0.43
1:E:404:ILE:HD13	1:E:404:ILE:H	1.83	0.43
1:E:63:ASN:HD22	1:H:53:LEU:HD12	1.82	0.43
1:F:406:MSE:HE3	1:F:408:ASP:HB2	2.00	0.43
1:H:274:LEU:HD23	1:H:276:LEU:CD1	2.45	0.43
1:J:160:LEU:HB2	1:J:198:VAL:HG12	2.01	0.43
1:K:212:PHE:HD1	1:K:213:LEU:N	2.15	0.43
1:K:234:LEU:C	1:K:234:LEU:HD23	2.39	0.43
1:L:55:TYR:CE1	1:L:112:ALA:HB2	2.53	0.43
1:K:318:LEU:HD21	1:L:318:LEU:HG	2.00	0.43
1:E:155:ILE:HG23	1:E:159:VAL:HG13	2.01	0.43
1:F:39:ALA:HB1	1:F:40:PRO:CD	2.48	0.43
1:F:48:TYR:HB3	1:G:65:ILE:HD11	2.00	0.43
1:J:110:TYR:O	1:J:114:ARG:HG2	2.19	0.43
1:C:114:ARG:HA	1:C:114:ARG:NE	2.34	0.43
1:C:317:ILE:CG2	1:C:340:LEU:HD21	2.48	0.43
1:D:253:VAL:CG2	1:D:260:ILE:HD11	2.47	0.43
1:G:13:LEU:HD22	1:G:19:PHE:CZ	2.54	0.43
1:J:263:LYS:NZ	1:J:268:PRO:O	2.52	0.43
1:K:291:ILE:CD1	1:K:432:ILE:HG22	2.49	0.43
1:K:383:MSE:HE3	1:K:416:VAL:HG23	2.01	0.43
1:E:240:MSE:CE	1:E:417:ILE:HD13	2.49	0.43
1:E:85:LEU:HD21	1:E:126:TYR:CD2	2.54	0.43
1:G:185:GLY:O	1:G:186:GLY:C	2.58	0.43
1:H:55:TYR:CE1	1:H:112:ALA:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:318:LEU:C	1:J:318:LEU:CD1	2.87	0.43
1:K:98:VAL:HG13	1:K:114:ARG:HG3	2.01	0.43
1:A:262:ILE:HD12	1:A:262:ILE:N	2.34	0.43
1:A:397:LEU:HB3	1:A:402:VAL:CG1	2.49	0.43
1:A:60:HIS:CE1	1:D:60:HIS:CE1	3.07	0.43
1:E:37:PRO:HB3	1:E:123:LEU:HD12	2.01	0.43
1:E:18:GLN:HE22	1:E:21:LYS:HZ2	1.66	0.43
1:J:116:GLU:HG3	1:J:170:PHE:CB	2.49	0.43
1:K:198:VAL:HG12	1:K:198:VAL:O	2.19	0.43
1:K:327:SER:O	1:K:342:ILE:HG23	2.18	0.43
1:K:233:GLU:HB2	1:K:379:VAL:CG1	2.49	0.43
1:L:155:ILE:HG21	1:L:197:GLY:C	2.39	0.43
1:B:159:VAL:HG11	1:B:167:ILE:HD11	2.01	0.42
1:D:242:ALA:O	1:D:244:VAL:HG22	2.19	0.42
1:F:155:ILE:HG21	1:F:197:GLY:C	2.39	0.42
1:F:226:ILE:HG22	1:F:229:ILE:HB	2.01	0.42
1:F:409:GLN:HE21	1:F:409:GLN:C	2.22	0.42
1:G:65:ILE:HG22	1:G:66:PRO:O	2.19	0.42
1:K:155:ILE:HG22	1:K:156:LYS:N	2.33	0.42
1:E:316:LYS:NZ	1:G:323:MSE:HE2	2.33	0.42
1:F:397:LEU:HD22	1:F:402:VAL:HG11	2.01	0.42
1:H:253:VAL:HG11	1:H:260:ILE:HD11	2.00	0.42
1:I:87:ILE:HD11	1:I:126:TYR:HB2	2.02	0.42
1:J:350:LYS:O	1:J:351:CYS:C	2.56	0.42
1:J:397:LEU:O	1:J:400:GLU:O	2.37	0.42
1:J:86:ASN:HD22	1:J:86:ASN:N	2.17	0.42
1:K:192:SER:HB3	1:K:253:VAL:HG23	2.01	0.42
1:K:300:ILE:HG22	1:K:302:ILE:CG1	2.49	0.42
1:B:137:VAL:HG22	1:B:155:ILE:CG1	2.49	0.42
1:C:318:LEU:CD2	1:C:331:MSE:HE1	2.48	0.42
1:E:277:SER:HB3	1:E:280:HIS:CD2	2.54	0.42
1:E:310:GLU:O	1:E:311:VAL:C	2.58	0.42
1:G:187:SER:HA	1:G:190:THR:HG23	2.00	0.42
1:H:110:TYR:CE1	1:H:114:ARG:HD2	2.54	0.42
1:I:87:ILE:HG22	1:I:89:MSE:HG2	2.02	0.42
1:J:36:ILE:HG21	1:J:190:THR:HG22	2.01	0.42
1:J:432:ILE:O	1:J:435:ALA:HB3	2.19	0.42
1:A:321:LEU:O	1:A:326:VAL:HG23	2.18	0.42
1:C:26:ILE:HG21	1:C:127:LEU:HD13	2.02	0.42
1:E:375:LEU:HD23	1:E:419:GLY:CA	2.49	0.42
1:E:379:VAL:HG22	1:E:415:ASN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:LYS:NZ	1:G:188:ASP:CG	2.72	0.42
1:G:226:ILE:O	1:G:273:THR:CG2	2.66	0.42
1:J:155:ILE:O	1:J:155:ILE:HD12	2.19	0.42
1:L:226:ILE:C	1:L:273:THR:HG22	2.40	0.42
1:K:318:LEU:CD2	1:L:315:ARG:HA	2.50	0.42
1:L:383:MSE:CE	1:L:416:VAL:HG23	2.50	0.42
1:D:189:VAL:HG23	1:D:249:ALA:CB	2.42	0.42
1:D:87:ILE:HD11	1:D:126:TYR:HB2	2.01	0.42
1:E:321:LEU:HD23	1:E:326:VAL:O	2.19	0.42
1:E:58:ASN:HD21	1:E:62:LYS:HE3	1.83	0.42
1:H:87:ILE:HG22	1:H:89:MSE:CG	2.50	0.42
1:I:342:ILE:HG22	1:I:343:GLU:O	2.19	0.42
1:J:276:LEU:HD12	1:J:276:LEU:N	2.34	0.42
1:J:276:LEU:CD1	1:J:276:LEU:N	2.83	0.42
1:L:116:GLU:HG3	1:L:170:PHE:HB2	2.00	0.42
1:D:212:PHE:CZ	1:D:262:ILE:CD1	3.01	0.42
1:H:207:THR:OG1	1:H:208:ASP:N	2.50	0.42
1:I:291:ILE:CD1	1:I:432:ILE:HG22	2.49	0.42
1:A:110:TYR:O	1:A:113:SER:OG	2.28	0.42
1:A:37:PRO:HD2	1:A:168:PRO:HA	2.02	0.42
1:B:283:ILE:O	1:B:285:LEU:HD12	2.20	0.42
1:B:48:TYR:CD1	1:B:53:LEU:HD22	2.55	0.42
1:D:85:LEU:HD23	1:D:126:TYR:CD1	2.54	0.42
1:E:89:MSE:CE	1:E:125:LYS:CB	2.98	0.42
1:E:362:CYS:C	1:E:364:PRO:HD3	2.40	0.42
1:F:226:ILE:C	1:F:273:THR:HG22	2.39	0.42
1:K:163:ASN:N	1:K:163:ASN:HD22	2.17	0.42
1:K:35:ILE:N	1:K:35:ILE:CD1	2.83	0.42
1:C:283:ILE:HG21	1:J:274:LEU:HD22	2.02	0.42
1:D:129:ALA:HB2	1:D:164:LYS:HD3	2.01	0.42
1:F:202:LEU:HD12	1:F:203:TYR:H	1.85	0.42
1:F:25:ILE:O	1:F:32:ARG:NH1	2.49	0.42
1:G:213:LEU:CD1	1:G:217:PRO:HG3	2.50	0.42
1:G:8:PHE:CD1	1:G:22:VAL:HG22	2.55	0.42
1:K:151:SER:O	1:K:155:ILE:HD13	2.19	0.42
1:C:36:ILE:N	1:C:36:ILE:HD12	2.35	0.42
1:D:39:ALA:HB2	1:D:116:GLU:OE2	2.19	0.42
1:B:89:MSE:HA	1:G:100:LYS:HG2	2.02	0.42
1:G:229:ILE:O	1:G:229:ILE:HG23	2.20	0.42
1:I:118:LEU:O	1:I:121:VAL:HG22	2.20	0.42
1:I:245:LEU:N	1:I:245:LEU:CD2	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:PRO:HB3	1:I:123:LEU:CD1	2.50	0.42
1:J:288:ILE:CD1	1:J:383:MSE:SE	3.18	0.42
1:K:318:LEU:HD22	1:L:315:ARG:HA	2.01	0.42
1:E:239:TYR:HD2	1:F:335:VAL:HG22	1.83	0.42
1:F:79:THR:HA	1:F:82:VAL:HG12	2.02	0.42
1:G:262:ILE:HD11	1:G:275:ILE:HD11	2.01	0.42
1:K:213:LEU:HD22	1:K:223:PRO:HD2	2.02	0.42
1:K:331:MSE:HE1	1:L:318:LEU:HD23	2.01	0.42
1:K:383:MSE:HB3	1:K:389:ILE:HG21	2.02	0.42
1:B:324:TYR:HB2	1:B:326:VAL:HG22	2.01	0.41
1:C:3:ILE:HD13	1:C:198:VAL:HG12	2.02	0.41
1:E:288:ILE:CG2	1:E:289:THR:N	2.82	0.41
1:A:195:SER:O	1:A:198:VAL:O	2.38	0.41
1:A:394:PHE:CZ	1:A:407:ILE:HD13	2.56	0.41
1:E:7:LYS:HZ1	1:E:188:ASP:CG	2.22	0.41
1:F:117:TYR:O	1:F:121:VAL:HG13	2.19	0.41
1:G:274:LEU:HA	1:G:274:LEU:HD12	1.87	0.41
1:J:253:VAL:CG1	1:J:258:ILE:HB	2.45	0.41
1:K:318:LEU:C	1:K:318:LEU:HD12	2.40	0.41
1:L:378:THR:O	1:L:378:THR:HG23	2.20	0.41
1:A:383:MSE:HB2	1:A:389:ILE:HG21	2.02	0.41
1:F:215:ALA:HB3	1:F:220:VAL:HG11	2.01	0.41
1:F:60:HIS:CE1	1:G:56:LEU:HD21	2.56	0.41
1:L:121:VAL:HG12	1:L:131:PHE:CE1	2.55	0.41
1:L:333:SER:HA	1:L:338:VAL:HA	2.02	0.41
1:B:87:ILE:HD13	1:B:126:TYR:HB2	2.02	0.41
1:E:43:ARG:NH1	1:E:47:ASP:OD1	2.54	0.41
1:F:6:THR:HG22	1:F:204:GLU:HB2	2.01	0.41
1:F:359:LYS:HG3	1:F:367:ILE:HD11	2.02	0.41
1:G:379:VAL:HG12	1:G:380:GLY:N	2.36	0.41
1:G:219:ILE:HG22	1:G:430:LYS:HG3	2.02	0.41
1:H:297:PHE:CE1	1:H:375:LEU:HD12	2.55	0.41
1:I:98:VAL:HG13	1:I:114:ARG:HG3	2.02	0.41
1:L:178:ASP:OD1	1:L:178:ASP:N	2.53	0.41
1:C:43:ARG:CD	1:C:47:ASP:OD2	2.68	0.41
1:E:89:MSE:HE1	1:E:122:ILE:HA	2.03	0.41
1:E:375:LEU:HA	1:E:375:LEU:HD23	1.95	0.41
1:E:425:PHE:O	1:E:429:VAL:HG23	2.20	0.41
1:G:253:VAL:O	1:G:254:LYS:C	2.58	0.41
1:K:247:GLU:HB2	1:L:306:LEU:HD11	2.02	0.41
1:A:211:GLY:HA3	1:A:273:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:VAL:CG1	1:B:167:ILE:HD11	2.50	0.41
1:C:134:ALA:HB3	1:C:171:TYR:CE1	2.56	0.41
1:D:320:ILE:CG2	1:D:358:ILE:HG22	2.50	0.41
1:D:35:ILE:HD12	1:D:35:ILE:N	2.36	0.41
1:H:433:TYR:C	1:H:433:TYR:CD1	2.94	0.41
1:I:214:MSE:HE2	1:I:433:TYR:CE2	2.56	0.41
1:K:207:THR:OG1	1:K:208:ASP:N	2.54	0.41
1:C:167:ILE:HD12	1:C:167:ILE:N	2.35	0.41
1:C:69:ASP:OD1	1:C:70:VAL:HG23	2.21	0.41
1:H:263:LYS:NZ	1:H:268:PRO:O	2.51	0.41
1:J:198:VAL:O	1:J:200:ALA:N	2.53	0.41
1:K:120:GLY:O	1:K:166:VAL:HG11	2.21	0.41
1:A:299:VAL:CG1	1:A:370:HIS:HB2	2.51	0.41
1:B:118:LEU:O	1:B:121:VAL:HG22	2.20	0.41
1:F:155:ILE:HG22	1:F:156:LYS:HD2	2.03	0.41
1:F:160:LEU:HB2	1:F:198:VAL:HG22	2.02	0.41
1:I:326:VAL:HG13	1:I:350:LYS:HD2	2.03	0.41
1:I:409:GLN:CG	1:I:416:VAL:HG22	2.51	0.41
1:K:78:TYR:HE2	1:K:119:ASN:OD1	2.03	0.41
1:L:321:LEU:C	1:L:321:LEU:HD23	2.40	0.41
1:A:322:GLU:HA	1:B:311:VAL:HG12	2.02	0.41
1:B:381:THR:O	1:B:384:ALA:HB3	2.20	0.41
1:C:3:ILE:HD13	1:C:198:VAL:CG1	2.49	0.41
1:C:65:ILE:HG23	1:C:66:PRO:HD2	2.02	0.41
1:E:251:PHE:CD2	1:E:252:PRO:HD3	2.55	0.41
1:G:262:ILE:CD1	1:G:275:ILE:HD11	2.51	0.41
1:G:321:LEU:HG	1:G:326:VAL:HG23	2.03	0.41
1:B:54:LEU:HD13	1:B:111:ALA:O	2.21	0.41
1:B:18:GLN:HE22	1:B:21:LYS:NZ	2.18	0.41
1:D:185:GLY:HA3	1:D:189:VAL:CG1	2.51	0.41
1:E:156:LYS:NZ	1:E:197:GLY:O	2.51	0.41
1:G:212:PHE:HB2	1:G:273:THR:HG21	2.02	0.41
1:G:68:ASP:OD1	1:G:99:LYS:NZ	2.42	0.41
1:K:315:ARG:HA	1:L:318:LEU:HD11	2.03	0.41
1:K:233:GLU:HB2	1:K:379:VAL:HG11	2.03	0.41
1:B:226:ILE:O	1:B:227:SER:C	2.59	0.41
1:C:260:ILE:O	1:C:274:LEU:HD12	2.21	0.41
1:D:248:GLU:HA	1:D:249:ALA:HA	1.70	0.41
1:D:228:LYS:HD3	1:D:276:LEU:HD11	2.03	0.41
1:F:155:ILE:HG23	1:F:198:VAL:CG2	2.34	0.41
1:F:18:GLN:O	1:F:22:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:VAL:O	1:G:73:LEU:HB2	2.21	0.41
1:H:214:MSE:HE1	1:H:288:ILE:HG21	2.03	0.41
1:H:373:MSE:HE1	1:H:406:MSE:HB2	2.02	0.41
1:J:5:VAL:HG21	1:J:194:ILE:HG22	2.03	0.41
1:K:155:ILE:HG23	1:K:159:VAL:HG11	1.96	0.41
1:L:321:LEU:CD2	1:L:326:VAL:HG23	2.51	0.41
1:I:53:LEU:HD11	1:L:65:ILE:HD11	2.03	0.41
1:B:321:LEU:HD21	1:B:340:LEU:HD23	2.02	0.40
1:C:156:LYS:HG3	1:C:160:LEU:HD23	2.04	0.40
1:D:60:HIS:CD2	1:D:65:ILE:HD11	2.56	0.40
1:E:375:LEU:HD23	1:E:419:GLY:HA2	2.03	0.40
1:F:317:ILE:O	1:F:320:ILE:HB	2.21	0.40
1:G:134:ALA:HB3	1:G:171:TYR:CZ	2.55	0.40
1:K:194:ILE:O	1:K:197:GLY:N	2.53	0.40
1:K:229:ILE:O	1:K:275:ILE:HA	2.20	0.40
1:L:339:SER:C	1:L:340:LEU:HD12	2.41	0.40
1:A:383:MSE:CB	1:A:389:ILE:HG21	2.52	0.40
1:D:138:ILE:HD13	1:D:193:ILE:HG21	2.03	0.40
1:E:321:LEU:HG	1:E:326:VAL:HG23	2.03	0.40
1:E:85:LEU:HD23	1:E:87:ILE:HD11	2.03	0.40
1:G:98:VAL:HG13	1:G:114:ARG:HG3	2.03	0.40
1:G:342:ILE:HG21	1:G:347:LEU:HD13	2.03	0.40
1:H:358:ILE:HD13	1:H:358:ILE:HG21	1.86	0.40
1:L:176:ASN:HD22	1:L:176:ASN:N	2.19	0.40
1:E:137:VAL:CG1	1:E:155:ILE:CG1	2.99	0.40
1:E:378:THR:HG21	1:E:393:ILE:HD13	2.03	0.40
1:G:355:ILE:HD13	1:G:369:ILE:HD11	1.99	0.40
1:I:87:ILE:HD11	1:I:126:TYR:HD1	1.85	0.40
1:I:288:ILE:HG22	1:I:289:THR:H	1.86	0.40
1:I:233:GLU:CG	1:I:381:THR:HG23	2.52	0.40
1:K:330:HIS:CB	1:K:406:MSE:HE1	2.51	0.40
1:C:331:MSE:HG3	1:C:340:LEU:HD12	2.03	0.40
1:F:226:ILE:HG21	1:F:229:ILE:HB	2.03	0.40
1:G:373:MSE:HE1	1:G:406:MSE:CB	2.40	0.40
1:G:418:VAL:HG12	1:G:420:VAL:HG13	2.02	0.40
1:H:94:TYR:O	1:H:98:VAL:HG23	2.21	0.40
1:L:114:ARG:N	1:L:114:ARG:HE	2.19	0.40
1:A:198:VAL:O	1:A:200:ALA:N	2.54	0.40
1:A:321:LEU:HG	1:A:326:VAL:HG23	2.03	0.40
1:C:283:ILE:CG2	1:C:284:ASN:N	2.84	0.40
1:D:156:LYS:HA	1:D:160:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:SER:CB	1:F:95:LEU:HD13	2.51	0.40
1:G:231:TYR:CD2	1:G:277:SER:HA	2.57	0.40
1:J:318:LEU:HD12	1:J:319:SER:N	2.37	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	423/446 (95%)	385 (91%)	34 (8%)	4 (1%)	17	55
1	B	436/446 (98%)	406 (93%)	28 (6%)	2 (0%)	29	68
1	C	429/446 (96%)	381 (89%)	45 (10%)	3 (1%)	22	60
1	D	435/446 (98%)	397 (91%)	33 (8%)	5 (1%)	14	50
1	E	437/446 (98%)	401 (92%)	28 (6%)	8 (2%)	8	37
1	F	430/446 (96%)	387 (90%)	38 (9%)	5 (1%)	13	48
1	G	433/446 (97%)	400 (92%)	28 (6%)	5 (1%)	13	48
1	H	433/446 (97%)	386 (89%)	40 (9%)	7 (2%)	9	40
1	I	422/446 (95%)	377 (89%)	39 (9%)	6 (1%)	11	43
1	J	429/446 (96%)	386 (90%)	36 (8%)	7 (2%)	9	40
1	K	423/446 (95%)	381 (90%)	37 (9%)	5 (1%)	13	48
1	L	422/446 (95%)	383 (91%)	36 (8%)	3 (1%)	22	60
All	All	5152/5352 (96%)	4670 (91%)	422 (8%)	60 (1%)	13	48

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	307	LEU

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Mol	Chain	Res	Type
1	E	144	GLY
1	G	170	PHE
1	H	199	ASN
1	I	199	ASN
1	J	128	ASN
1	J	199	ASN
1	J	351	CYS
1	K	425	PHE
1	L	351	CYS
1	A	199	ASN
1	A	335	VAL
1	C	257	GLY
1	D	169	GLY
1	E	170	PHE
1	F	29	ASP
1	F	172	GLY
1	F	305	ALA
1	G	186	GLY
1	G	254	LYS
1	H	184	ARG
1	H	244	VAL
1	I	86	ASN
1	I	257	GLY
1	I	348	ASP
1	J	305	ALA
1	K	170	PHE
1	K	257	GLY
1	A	185	GLY
1	A	305	ALA
1	E	176	ASN
1	G	438	GLU
1	H	155	ILE
1	H	249	ALA
1	J	425	PHE
1	K	164	LYS
1	B	348	ASP
1	E	311	VAL
1	F	438	GLU
1	B	227	SER
1	C	86	ASN
1	F	16	SER
1	H	198	VAL

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Mol	Chain	Res	Type
1	I	247	GLU
1	J	246	HIS
1	L	199	ASN
1	G	384	ALA
1	H	170	PHE
1	D	144	GLY
1	I	312	GLY
1	J	241	GLY
1	L	312	GLY
1	E	186	GLY
1	C	3	ILE
1	E	363	ASN
1	K	194	ILE
1	D	37	PRO
1	E	244	VAL
1	D	371	PRO
1	E	312	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/377 (92%)	318 (91%)	30 (9%)	10	37
1	B	359/377 (95%)	328 (91%)	31 (9%)	10	37
1	C	354/377 (94%)	325 (92%)	29 (8%)	11	39
1	D	358/377 (95%)	326 (91%)	32 (9%)	9	35
1	E	354/377 (94%)	320 (90%)	34 (10%)	8	32
1	F	353/377 (94%)	327 (93%)	26 (7%)	13	44
1	G	357/377 (95%)	328 (92%)	29 (8%)	11	40
1	H	338/377 (90%)	312 (92%)	26 (8%)	13	42
1	I	340/377 (90%)	326 (96%)	14 (4%)	30	67
1	J	339/377 (90%)	314 (93%)	25 (7%)	13	44
1	K	334/377 (89%)	304 (91%)	30 (9%)	9	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	341/377 (90%)	319 (94%)	22 (6%)	17 50
All	All	4175/4524 (92%)	3847 (92%)	328 (8%)	12 41

All (328) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	31	ASN
1	A	53	LEU
1	A	82	VAL
1	A	100	LYS
1	A	158	LYS
1	A	176	ASN
1	A	181	THR
1	A	183	SER
1	A	184	ARG
1	A	220	VAL
1	A	246	HIS
1	A	255	ASP
1	A	269	SER
1	A	274	LEU
1	A	277	SER
1	A	282	GLU
1	A	318	LEU
1	A	323	MSE
1	A	326	VAL
1	A	329	GLU
1	A	338	VAL
1	A	339	SER
1	A	356	GLU
1	A	378	THR
1	A	386	THR
1	A	387	LYS
1	A	403	ASN
1	A	409	GLN
1	A	412	SER
1	B	46	LYS
1	B	85	LEU
1	B	114	ARG
1	B	123	LEU
1	B	143	SER
1	B	158	LYS

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Mol	Chain	Res	Type
1	B	160	LEU
1	B	181	THR
1	B	189	VAL
1	B	190	THR
1	B	232	LYS
1	B	236	GLU
1	B	237	LEU
1	B	250	ILE
1	B	256	SER
1	B	269	SER
1	B	276	LEU
1	B	288	ILE
1	B	318	LEU
1	B	340	LEU
1	B	352	ASP
1	B	360	LYS
1	B	363	ASN
1	B	378	THR
1	B	385	LYS
1	B	389	ILE
1	B	400	GLU
1	B	402	VAL
1	B	409	GLN
1	B	418	VAL
1	B	431	SER
1	C	3	ILE
1	C	12	SER
1	C	43	ARG
1	C	53	LEU
1	C	88	ASP
1	C	117	TYR
1	C	155	ILE
1	C	156	LYS
1	C	158	LYS
1	C	184	ARG
1	C	201	ASP
1	C	203	TYR
1	C	207	THR
1	C	221	GLU
1	C	287	THR
1	C	299	VAL
1	C	308	ASN

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Mol	Chain	Res	Type
1	C	315	ARG
1	C	318	LEU
1	C	320	ILE
1	C	329	GLU
1	C	337	SER
1	C	340	LEU
1	C	352	ASP
1	C	362	CYS
1	C	378	THR
1	C	400	GLU
1	C	409	GLN
1	C	412	SER
1	D	7	LYS
1	D	12	SER
1	D	49	LYS
1	D	82	VAL
1	D	100	LYS
1	D	108	SER
1	D	116	GLU
1	D	138	ILE
1	D	145	CYS
1	D	159	VAL
1	D	160	LEU
1	D	170	PHE
1	D	181	THR
1	D	194	ILE
1	D	195	SER
1	D	210	SER
1	D	218	ARG
1	D	248	GLU
1	D	250	ILE
1	D	254	LYS
1	D	277	SER
1	D	279	THR
1	D	318	LEU
1	D	329	GLU
1	D	339	SER
1	D	361	GLN
1	D	378	THR
1	D	381	THR
1	D	402	VAL
1	D	403	ASN

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Mol	Chain	Res	Type
1	D	409	GLN
1	D	430	LYS
1	E	7	LYS
1	E	33	LYS
1	E	43	ARG
1	E	60	HIS
1	E	65	ILE
1	E	89	MSE
1	E	109	ASP
1	E	114	ARG
1	E	146	PHE
1	E	158	LYS
1	E	159	VAL
1	E	160	LEU
1	E	162	CYS
1	E	181	THR
1	E	184	ARG
1	E	187	SER
1	E	190	THR
1	E	230	SER
1	E	232	LYS
1	E	234	LEU
1	E	236	GLU
1	E	263	LYS
1	E	277	SER
1	E	318	LEU
1	E	321	LEU
1	E	329	GLU
1	E	338	VAL
1	E	356	GLU
1	E	363	ASN
1	E	378	THR
1	E	404	ILE
1	E	406	MSE
1	E	409	GLN
1	E	415	ASN
1	F	1	LEU
1	F	2	LYS
1	F	46	LYS
1	F	77	ARG
1	F	116	GLU
1	F	153	GLU

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Mol	Chain	Res	Type
1	F	155	ILE
1	F	170	PHE
1	F	175	PHE
1	F	176	ASN
1	F	190	THR
1	F	236	GLU
1	F	238	SER
1	F	245	LEU
1	F	248	GLU
1	F	299	VAL
1	F	306	LEU
1	F	311	VAL
1	F	318	LEU
1	F	333	SER
1	F	340	LEU
1	F	358	ILE
1	F	378	THR
1	F	402	VAL
1	F	409	GLN
1	F	415	ASN
1	G	7	LYS
1	G	75	SER
1	G	99	LYS
1	G	100	LYS
1	G	109	ASP
1	G	116	GLU
1	G	149	LYS
1	G	173	SER
1	G	181	THR
1	G	190	THR
1	G	192	SER
1	G	221	GLU
1	G	234	LEU
1	G	236	GLU
1	G	237	LEU
1	G	245	LEU
1	G	247	GLU
1	G	250	ILE
1	G	256	SER
1	G	263	LYS
1	G	287	THR
1	G	299	VAL

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Mol	Chain	Res	Type
1	G	318	LEU
1	G	340	LEU
1	G	361	GLN
1	G	378	THR
1	G	402	VAL
1	G	409	GLN
1	G	415	ASN
1	H	44	THR
1	H	89	MSE
1	H	109	ASP
1	H	136	GLU
1	H	156	LYS
1	H	221	GLU
1	H	234	LEU
1	H	236	GLU
1	H	240	MSE
1	H	250	ILE
1	H	299	VAL
1	H	309	SER
1	H	311	VAL
1	H	315	ARG
1	H	318	LEU
1	H	327	SER
1	H	329	GLU
1	H	340	LEU
1	H	346	LYS
1	H	351	CYS
1	H	366	SER
1	H	378	THR
1	H	389	ILE
1	H	401	ASN
1	H	402	VAL
1	H	409	GLN
1	I	43	ARG
1	I	63	ASN
1	I	83	SER
1	I	85	LEU
1	I	180	LYS
1	I	202	LEU
1	I	205	ASN
1	I	207	THR
1	I	245	LEU

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Mol	Chain	Res	Type
1	I	318	LEU
1	I	323	MSE
1	I	356	GLU
1	I	378	THR
1	I	409	GLN
1	J	7	LYS
1	J	38	SER
1	J	53	LEU
1	J	77	ARG
1	J	116	GLU
1	J	127	LEU
1	J	149	LYS
1	J	155	ILE
1	J	160	LEU
1	J	192	SER
1	J	218	ARG
1	J	236	GLU
1	J	238	SER
1	J	287	THR
1	J	299	VAL
1	J	314	CYS
1	J	318	LEU
1	J	351	CYS
1	J	352	ASP
1	J	356	GLU
1	J	361	GLN
1	J	378	THR
1	J	389	ILE
1	J	409	GLN
1	J	415	ASN
1	K	31	ASN
1	K	43	ARG
1	K	53	LEU
1	K	58	ASN
1	K	73	LEU
1	K	85	LEU
1	K	116	GLU
1	K	153	GLU
1	K	160	LEU
1	K	163	ASN
1	K	190	THR
1	K	201	ASP

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Mol	Chain	Res	Type
1	K	212	PHE
1	K	220	VAL
1	K	229	ILE
1	K	240	MSE
1	K	245	LEU
1	K	250	ILE
1	K	284	ASN
1	K	318	LEU
1	K	345	CYS
1	K	361	GLN
1	K	372	ASN
1	K	373	MSE
1	K	383	MSE
1	K	401	ASN
1	K	403	ASN
1	K	406	MSE
1	K	409	GLN
1	K	415	ASN
1	L	31	ASN
1	L	43	ARG
1	L	86	ASN
1	L	109	ASP
1	L	114	ARG
1	L	116	GLU
1	L	149	LYS
1	L	155	ILE
1	L	158	LYS
1	L	163	ASN
1	L	171	TYR
1	L	173	SER
1	L	176	ASN
1	L	181	THR
1	L	235	ARG
1	L	250	ILE
1	L	318	LEU
1	L	333	SER
1	L	356	GLU
1	L	365	ASP
1	L	409	GLN
1	L	424	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	58	ASN
1	A	63	ASN
1	A	76	GLN
1	A	176	ASN
1	A	266	ASN
1	A	363	ASN
1	A	372	ASN
1	A	391	ASN
1	A	437	ASN
1	B	18	GLN
1	B	58	ASN
1	B	63	ASN
1	B	246	HIS
1	B	266	ASN
1	B	401	ASN
1	B	409	GLN
1	B	415	ASN
1	B	437	ASN
1	C	18	GLN
1	C	63	ASN
1	C	261	ASN
1	C	266	ASN
1	C	308	ASN
1	C	361	GLN
1	C	401	ASN
1	C	409	GLN
1	C	437	ASN
1	D	17	ASN
1	D	18	GLN
1	D	58	ASN
1	D	60	HIS
1	D	86	ASN
1	D	222	ASN
1	D	246	HIS
1	D	266	ASN
1	D	361	GLN
1	D	372	ASN
1	D	391	ASN
1	D	403	ASN
1	D	437	ASN
1	E	18	GLN
1	E	31	ASN

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Mol	Chain	Res	Type
1	E	58	ASN
1	E	60	HIS
1	E	163	ASN
1	E	199	ASN
1	E	266	ASN
1	E	280	HIS
1	E	361	GLN
1	E	363	ASN
1	E	409	GLN
1	F	17	ASN
1	F	18	GLN
1	F	58	ASN
1	F	63	ASN
1	F	176	ASN
1	F	199	ASN
1	F	222	ASN
1	F	261	ASN
1	F	266	ASN
1	F	409	GLN
1	F	437	ASN
1	G	18	GLN
1	G	58	ASN
1	G	60	HIS
1	G	63	ASN
1	G	266	ASN
1	G	361	GLN
1	G	409	GLN
1	H	18	GLN
1	H	60	HIS
1	H	63	ASN
1	H	86	ASN
1	H	101	ASN
1	H	205	ASN
1	H	266	ASN
1	H	361	GLN
1	H	401	ASN
1	H	409	GLN
1	I	18	GLN
1	I	31	ASN
1	I	205	ASN
1	I	266	ASN
1	I	409	GLN

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Mol	Chain	Res	Type
1	J	18	GLN
1	J	58	ASN
1	J	63	ASN
1	J	86	ASN
1	J	101	ASN
1	J	163	ASN
1	J	261	ASN
1	J	266	ASN
1	J	401	ASN
1	J	409	GLN
1	J	415	ASN
1	K	18	GLN
1	K	58	ASN
1	K	63	ASN
1	K	163	ASN
1	K	222	ASN
1	K	266	ASN
1	K	284	ASN
1	K	372	ASN
1	K	401	ASN
1	K	409	GLN
1	K	437	ASN
1	L	18	GLN
1	L	58	ASN
1	L	163	ASN
1	L	176	ASN
1	L	261	ASN
1	L	266	ASN
1	L	409	GLN
1	L	437	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ASP	A	451	-	2,8,8	0.31	0	1,10,10	0.80	0
2	ASP	E	455	-	2,8,8	0.41	0	1,10,10	1.41	0
3	LYS	H	508	-	5,9,9	0.63	0	4,10,10	0.36	0
2	ASP	H	458	-	2,8,8	0.36	0	1,10,10	1.02	0
3	LYS	B	502	-	5,9,9	0.28	0	4,10,10	0.25	0
2	ASP	I	459	-	4,7,8	2.23	1 (25%)	3,8,10	1.64	1 (33%)
2	ASP	G	457	-	2,8,8	0.30	0	1,10,10	1.53	0
3	LYS	C	503	-	5,9,9	0.25	0	4,10,10	0.41	0
3	LYS	A	501	-	5,9,9	0.47	0	4,10,10	0.43	0
2	ASP	D	454	-	2,8,8	0.26	0	1,10,10	0.54	0
2	ASP	L	462	-	2,8,8	0.25	0	1,10,10	0.36	0
3	LYS	D	504	-	5,9,9	0.51	0	4,10,10	0.45	0
3	LYS	G	507	-	5,9,9	0.57	0	4,10,10	0.33	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
2	ASP	A	451	-	-	0/2/8/8	-
2	ASP	E	455	-	-	1/2/8/8	-
3	LYS	H	508	-	-	0/5/9/9	-
2	ASP	H	458	-	-	1/2/8/8	-
3	LYS	B	502	-	-	0/5/9/9	-
2	ASP	I	459	-	-	2/4/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ASP	G	457	-	-	0/2/8/8	-
3	LYS	C	503	-	-	0/5/9/9	-
3	LYS	A	501	-	-	0/5/9/9	-
2	ASP	D	454	-	-	1/2/8/8	-
2	ASP	L	462	-	-	0/2/8/8	-
3	LYS	D	504	-	-	0/5/9/9	-
3	LYS	G	507	-	-	2/5/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	459	ASP	OXT-C	-4.43	1.23	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	459	ASP	OXT-C-CA	2.47	121.27	111.52

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	455	ASP	N-CA-CB-CG
2	H	458	ASP	N-CA-CB-CG
2	I	459	ASP	N-CA-CB-CG
2	I	459	ASP	C-CA-CB-CG
3	G	507	LYS	C-CA-CB-CG
2	D	454	ASP	N-CA-CB-CG
3	G	507	LYS	N-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	451	ASP	2	0
2	E	455	ASP	1	0
3	H	508	LYS	1	0
2	H	458	ASP	1	0
2	G	457	ASP	1	0
3	C	503	LYS	3	0
3	G	507	LYS	7	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	421/446 (94%)	-0.45	1 (0%) 95 87	42, 62, 111, 135	0
1	B	430/446 (96%)	-0.37	0 100 100	43, 66, 108, 135	1 (0%)
1	C	426/446 (95%)	-0.38	1 (0%) 95 87	53, 82, 112, 133	0
1	D	429/446 (96%)	-0.41	1 (0%) 95 87	36, 58, 123, 175	1 (0%)
1	E	431/446 (96%)	-0.38	2 (0%) 91 75	48, 74, 111, 142	1 (0%)
1	F	427/446 (95%)	-0.26	2 (0%) 91 75	58, 101, 135, 154	0
1	G	429/446 (96%)	-0.51	0 100 100	39, 61, 87, 101	0
1	H	427/446 (95%)	-0.38	2 (0%) 91 75	51, 80, 110, 140	0
1	I	421/446 (94%)	-0.10	7 (1%) 70 41	67, 105, 166, 195	1 (0%)
1	J	425/446 (95%)	-0.26	6 (1%) 75 49	58, 93, 154, 194	0
1	K	421/446 (94%)	-0.09	20 (4%) 30 11	54, 97, 191, 220	1 (0%)
1	L	421/446 (94%)	0.21	32 (7%) 13 4	61, 120, 203, 273	1 (0%)
All	All	5108/5352 (95%)	-0.28	74 (1%) 75 49	36, 82, 149, 273	6 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	362	CYS	9.0
1	L	347	LEU	8.3
1	L	366	SER	7.0
1	L	363	ASN	6.6
1	L	308	ASN	5.4
1	L	351	CYS	5.3
1	K	353	LYS	5.1
1	L	311	VAL	5.0
1	K	317	ILE	4.8
1	L	365	ASP	4.8
1	L	336	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	L	358	ILE	4.7
1	L	326	VAL	4.6
1	I	311	VAL	4.6
1	L	355	ILE	4.5
1	L	309	SER	4.5
1	K	364	PRO	4.4
1	L	370	HIS	4.2
1	K	324	TYR	4.0
1	I	369	ILE	4.0
1	J	311	VAL	3.8
1	K	285	LEU	3.8
1	L	306	LEU	3.6
1	L	368	GLU	3.5
1	D	325	GLY	3.4
1	K	325	GLY	3.4
1	L	361	GLN	3.4
1	J	347	LEU	3.3
1	I	367	ILE	3.3
1	K	352	ASP	3.2
1	L	305	ALA	3.2
1	K	345	CYS	3.1
1	I	351	CYS	3.1
1	L	360	LYS	3.1
1	K	369	ILE	3.0
1	E	439	GLY	3.0
1	K	326	VAL	2.9
1	K	349	GLY	2.8
1	E	280	HIS	2.7
1	J	310	GLU	2.7
1	L	219	ILE	2.7
1	L	292	ALA	2.7
1	J	309	SER	2.6
1	K	307	LEU	2.6
1	I	325	GLY	2.6
1	J	294	LYS	2.6
1	L	334	GLY	2.6
1	L	369	ILE	2.5
1	H	279	THR	2.5
1	L	342	ILE	2.5
1	L	245	LEU	2.5
1	K	367	ILE	2.5
1	L	412	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	320	ILE	2.5
1	K	327	SER	2.5
1	H	283	ILE	2.5
1	L	31	ASN	2.4
1	K	351	CYS	2.4
1	L	327	SER	2.4
1	L	354	ILE	2.4
1	C	175	PHE	2.4
1	I	365	ASP	2.3
1	I	309	SER	2.3
1	J	314	CYS	2.3
1	L	278	ASP	2.2
1	F	165	ALA	2.2
1	L	328	PHE	2.1
1	K	308	ASN	2.1
1	K	311	VAL	2.1
1	K	361	GLN	2.1
1	A	311	VAL	2.0
1	K	360	LYS	2.0
1	F	210	SER	2.0
1	L	294	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LYS	G	507	10/10	0.29	0.78	56,64,67,68	10
3	LYS	H	508	10/10	0.57	0.56	70,72,76,81	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	LYS	C	503	10/10	0.58	0.60	71,73,73,73	10
2	ASP	A	451	9/9	0.60	0.50	55,59,60,61	9
2	ASP	G	457	9/9	0.68	0.44	53,55,58,58	9
3	LYS	A	501	10/10	0.69	0.46	59,62,65,66	10
2	ASP	H	458	9/9	0.75	0.41	64,66,71,74	9
2	ASP	L	462	9/9	0.75	0.42	74,78,86,87	9
3	LYS	B	502	10/10	0.75	0.38	56,58,59,60	10
2	ASP	I	459	8/9	0.76	0.39	63,64,69,73	8
3	LYS	D	504	10/10	0.76	0.40	59,61,62,62	10
2	ASP	D	454	9/9	0.76	0.35	61,69,78,81	9
2	ASP	E	455	9/9	0.80	0.36	62,63,64,66	9

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.