Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 12:59 AM EDT

PDB ID	:	3AB4
Title	:	Crystal structure of feedback inhibition resistant mutant of aspartate kinase from Corynebacterium glutamicum in complex with lysine and threonine
Authors	:	Yoshida, A.; Tomita, T.; Kuzuyama, T.; Nishiyama, M.
Deposited on	:	2009-11-30
Resolution	:	2.47 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

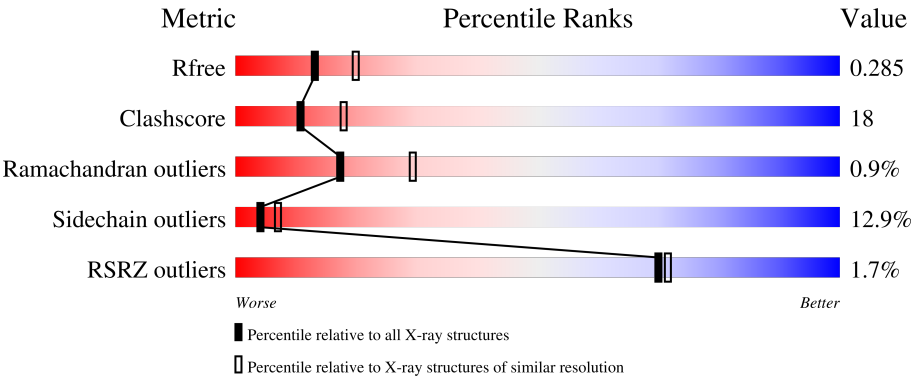
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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

Mol	Chain	Length	Quality of chain
1	A	421	62% 21% 5% 12%
1	C	421	60% 22% 5% 13%
1	E	421	59% 22% 7% 13%
1	G	421	% 61% 19% 5% 15%
1	I	421	% 57% 23% 5% 14%

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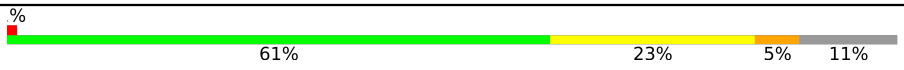
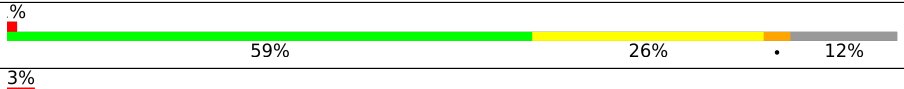
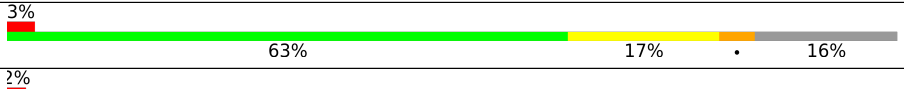
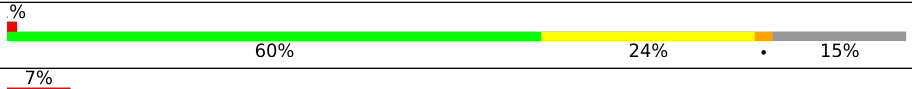
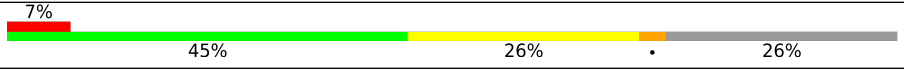
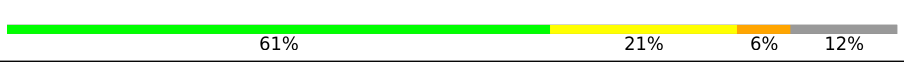
Mol	Chain	Length	Quality of chain
1	K	421	
1	M	421	
1	O	421	
2	B	178	
2	D	178	
2	F	178	
2	H	178	
2	J	178	
2	L	178	
2	N	178	
2	P	178	

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
3	THR	B	201	-	-	X	-
3	THR	C	501	-	-	X	-
3	THR	D	201	-	-	X	-
3	THR	F	201	-	-	X	-
3	THR	G	501	-	-	X	-
3	THR	H	201	-	-	X	-
3	THR	I	501	-	-	X	-
3	THR	K	501	-	-	X	-
3	THR	O	501	-	-	X	-
4	LYS	K	601	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30970 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
1	A	370	Total	C	N	O	S	0	0	0
			2711	1687	463	547	14			
1	C	367	Total	C	N	O	S	0	0	0
			2705	1686	463	542	14			
1	E	368	Total	C	N	O	S	0	0	0
			2682	1669	462	537	14			
1	G	357	Total	C	N	O	S	0	0	0
			2600	1620	443	523	14			
1	I	360	Total	C	N	O	S	0	0	0
			2634	1645	445	530	14			
1	K	373	Total	C	N	O	S	0	0	0
			2736	1704	469	549	14			
1	M	377	Total	C	N	O	S	0	0	0
			2772	1725	479	554	14			
1	O	364	Total	C	N	O	S	0	0	0
			2642	1637	457	534	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	PHE	SER	SEE REMARK 999	UNP P26512
C	301	PHE	SER	SEE REMARK 999	UNP P26512
E	301	PHE	SER	SEE REMARK 999	UNP P26512
G	301	PHE	SER	SEE REMARK 999	UNP P26512
I	301	PHE	SER	SEE REMARK 999	UNP P26512
K	301	PHE	SER	SEE REMARK 999	UNP P26512
M	301	PHE	SER	SEE REMARK 999	UNP P26512
O	301	PHE	SER	SEE REMARK 999	UNP P26512

- Molecule 2 is a protein called Aspartokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	157	Total	C	N	O	S	0	0	0
			1175	729	203	238	5			
2	D	150	Total	C	N	O	S	0	0	0
			1133	706	198	224	5			
2	F	148	Total	C	N	O	S	0	0	0
			1077	671	184	217	5			
2	H	151	Total	C	N	O	S	0	0	0
			1108	691	188	224	5			
2	J	132	Total	C	N	O	S	0	0	0
			974	608	167	195	4			
2	L	156	Total	C	N	O	S	0	0	0
			1176	735	201	235	5			
2	N	155	Total	C	N	O	S	0	0	0
			1153	716	199	233	5			
2	P	149	Total	C	N	O	S	0	0	0
			1107	687	191	225	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P26512
B	52	PHE	SER	SEE REMARK 999	UNP P26512
B	173	HIS	-	expression tag	UNP P26512
B	174	HIS	-	expression tag	UNP P26512
B	175	HIS	-	expression tag	UNP P26512
B	176	HIS	-	expression tag	UNP P26512
B	177	HIS	-	expression tag	UNP P26512
B	178	HIS	-	expression tag	UNP P26512
D	1	MET	-	initiating methionine	UNP P26512
D	52	PHE	SER	SEE REMARK 999	UNP P26512
D	173	HIS	-	expression tag	UNP P26512
D	174	HIS	-	expression tag	UNP P26512
D	175	HIS	-	expression tag	UNP P26512
D	176	HIS	-	expression tag	UNP P26512
D	177	HIS	-	expression tag	UNP P26512
D	178	HIS	-	expression tag	UNP P26512
F	1	MET	-	initiating methionine	UNP P26512
F	52	PHE	SER	SEE REMARK 999	UNP P26512
F	173	HIS	-	expression tag	UNP P26512
F	174	HIS	-	expression tag	UNP P26512
F	175	HIS	-	expression tag	UNP P26512
F	176	HIS	-	expression tag	UNP P26512
F	177	HIS	-	expression tag	UNP P26512
F	178	HIS	-	expression tag	UNP P26512

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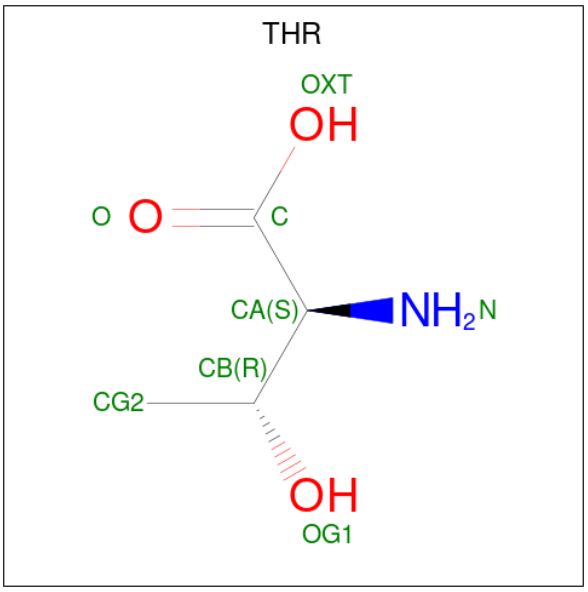
Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	initiating methionine	UNP P26512
H	52	PHE	SER	SEE REMARK 999	UNP P26512
H	173	HIS	-	expression tag	UNP P26512
H	174	HIS	-	expression tag	UNP P26512
H	175	HIS	-	expression tag	UNP P26512
H	176	HIS	-	expression tag	UNP P26512
H	177	HIS	-	expression tag	UNP P26512
H	178	HIS	-	expression tag	UNP P26512
J	1	MET	-	initiating methionine	UNP P26512
J	52	PHE	SER	SEE REMARK 999	UNP P26512
J	173	HIS	-	expression tag	UNP P26512
J	174	HIS	-	expression tag	UNP P26512
J	175	HIS	-	expression tag	UNP P26512
J	176	HIS	-	expression tag	UNP P26512
J	177	HIS	-	expression tag	UNP P26512
J	178	HIS	-	expression tag	UNP P26512
L	1	MET	-	initiating methionine	UNP P26512
L	52	PHE	SER	SEE REMARK 999	UNP P26512
L	173	HIS	-	expression tag	UNP P26512
L	174	HIS	-	expression tag	UNP P26512
L	175	HIS	-	expression tag	UNP P26512
L	176	HIS	-	expression tag	UNP P26512
L	177	HIS	-	expression tag	UNP P26512
L	178	HIS	-	expression tag	UNP P26512
N	1	MET	-	initiating methionine	UNP P26512
N	52	PHE	SER	SEE REMARK 999	UNP P26512
N	173	HIS	-	expression tag	UNP P26512
N	174	HIS	-	expression tag	UNP P26512
N	175	HIS	-	expression tag	UNP P26512
N	176	HIS	-	expression tag	UNP P26512
N	177	HIS	-	expression tag	UNP P26512
N	178	HIS	-	expression tag	UNP P26512
P	1	MET	-	initiating methionine	UNP P26512
P	52	PHE	SER	SEE REMARK 999	UNP P26512
P	173	HIS	-	expression tag	UNP P26512
P	174	HIS	-	expression tag	UNP P26512
P	175	HIS	-	expression tag	UNP P26512
P	176	HIS	-	expression tag	UNP P26512
P	177	HIS	-	expression tag	UNP P26512
P	178	HIS	-	expression tag	UNP P26512

- Molecule 3 is THREONINE (three-letter code: THR) (formula: $C_4H_9NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	C	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		
3	E	1	Total	C	N	O	0	0
			8	4	1	3		
3	F	1	Total	C	N	O	0	0
			8	4	1	3		
3	G	1	Total	C	N	O	0	0
			8	4	1	3		
3	H	1	Total	C	N	O	0	0
			8	4	1	3		
3	I	1	Total	C	N	O	0	0
			8	4	1	3		
3	J	1	Total	C	N	O	0	0
			8	4	1	3		
3	K	1	Total	C	N	O	0	0
			8	4	1	3		
3	L	1	Total	C	N	O	0	0
			8	4	1	3		
3	M	1	Total	C	N	O	0	0
			8	4	1	3		
3	N	1	Total	C	N	O	0	0
			8	4	1	3		

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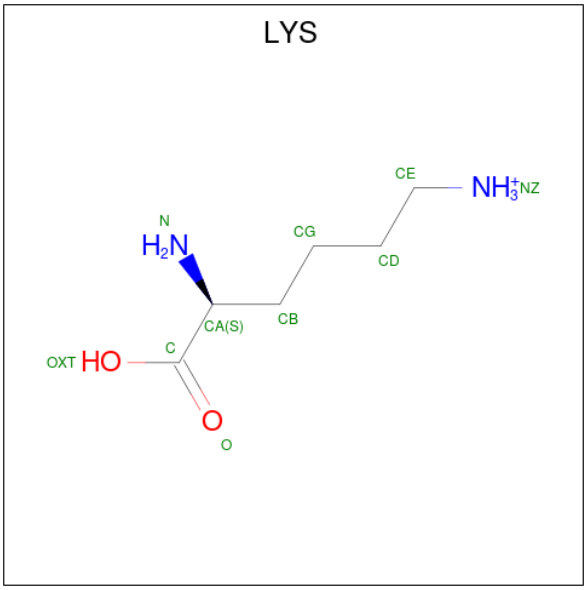
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total C N O 8 4 1 3	0	0
3	P	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 10 6 2 2	0	0
4	C	1	Total C N O 10 6 2 2	0	0
4	E	1	Total C N O 10 6 2 2	0	0
4	G	1	Total C N O 10 6 2 2	0	0
4	K	1	Total C N O 10 6 2 2	0	0
4	M	1	Total C N O 10 6 2 2	0	0
4	O	1	Total C N O 10 6 2 2	0	0

- Molecule 5 is water.

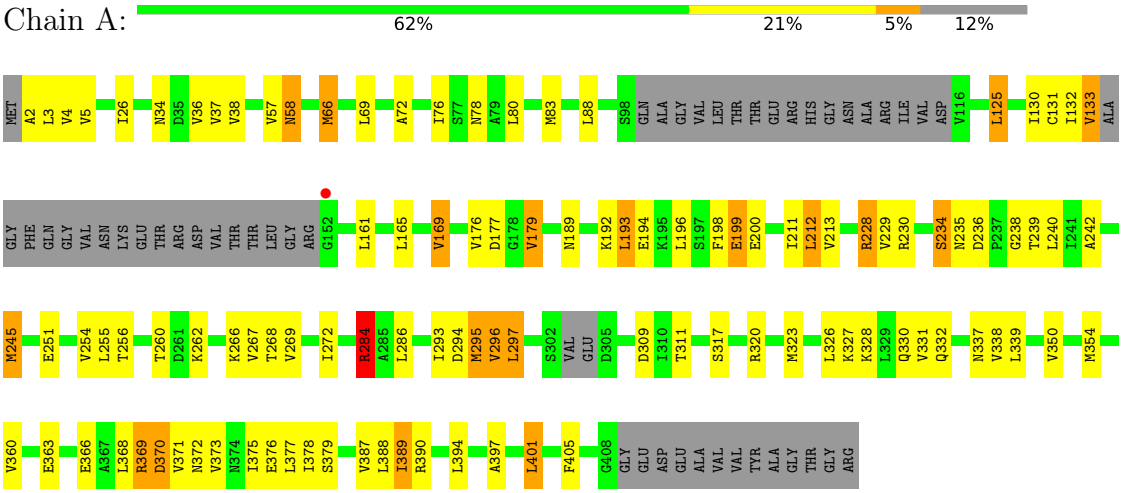
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	46	Total O 46 46	0	0
5	B	36	Total O 36 36	0	0
5	C	25	Total O 25 25	0	0
5	D	13	Total O 13 13	0	0
5	E	30	Total O 30 30	0	0
5	F	5	Total O 5 5	0	0
5	G	27	Total O 27 27	0	0
5	H	11	Total O 11 11	0	0
5	I	22	Total O 22 22	0	0
5	J	3	Total O 3 3	0	0
5	K	41	Total O 41 41	0	0
5	L	22	Total O 22 22	0	0
5	M	52	Total O 52 52	0	0
5	N	24	Total O 24 24	0	0
5	O	22	Total O 22 22	0	0
5	P	8	Total O 8 8	0	0

3 Residue-property plots (i)

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

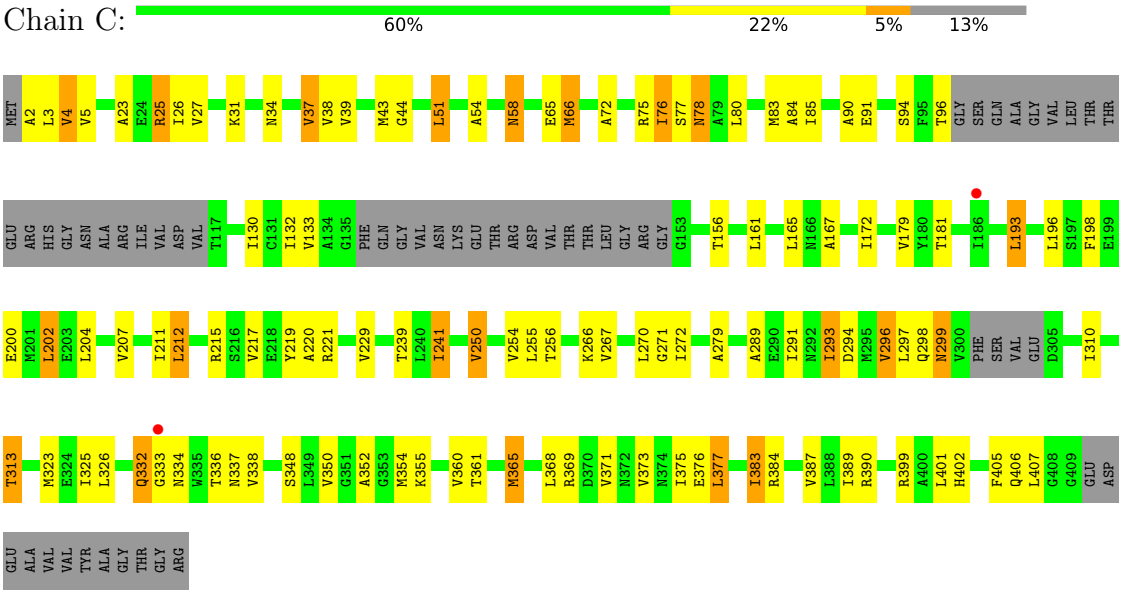
• Molecule 1: Aspartokinase

Chain A:



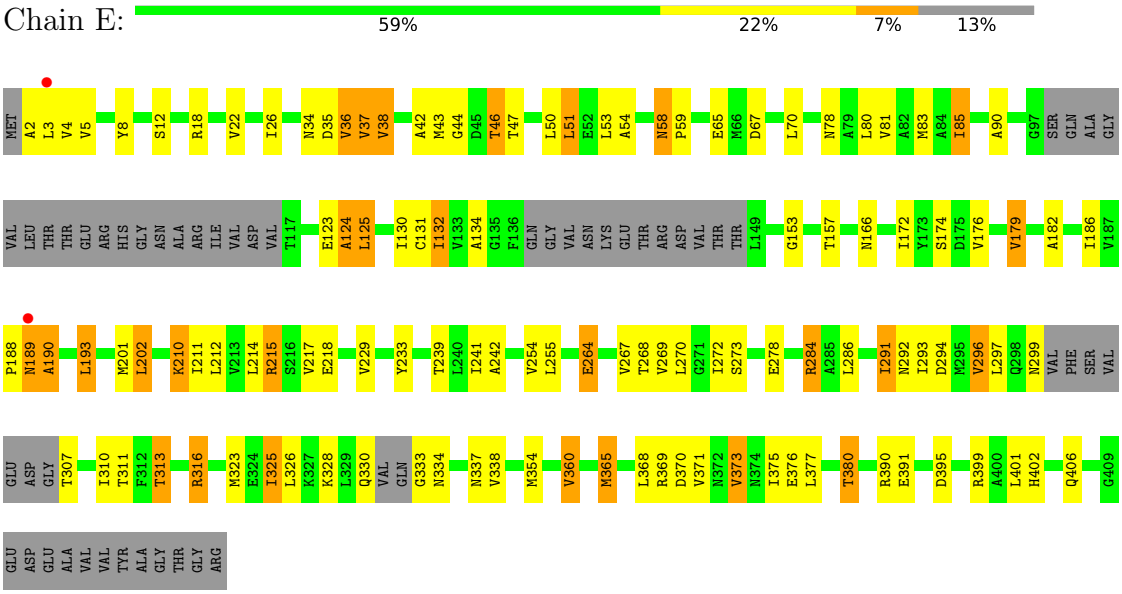
• Molecule 1: Aspartokinase

Chain C:



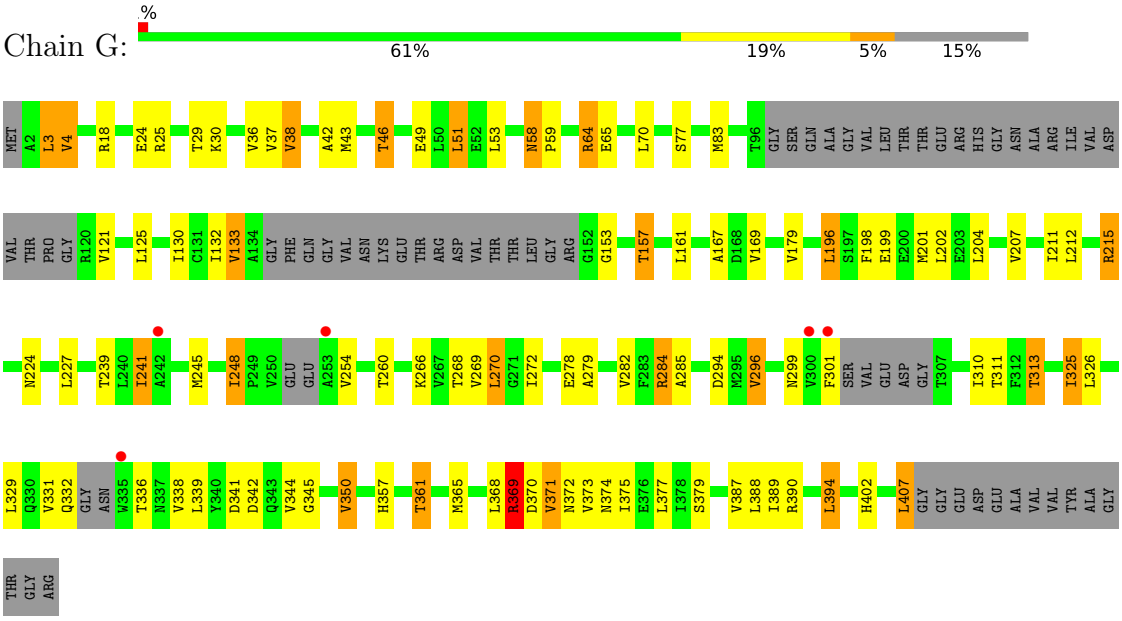
• Molecule 1: Aspartokinase

Chain E:



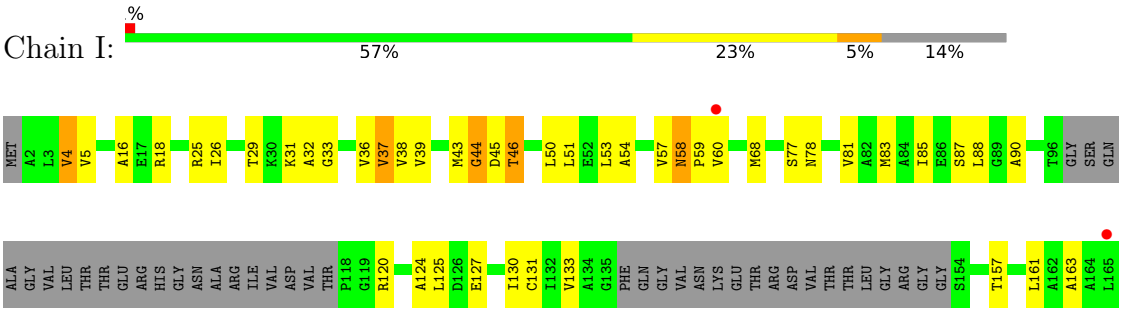
• Molecule 1: Aspartokinase

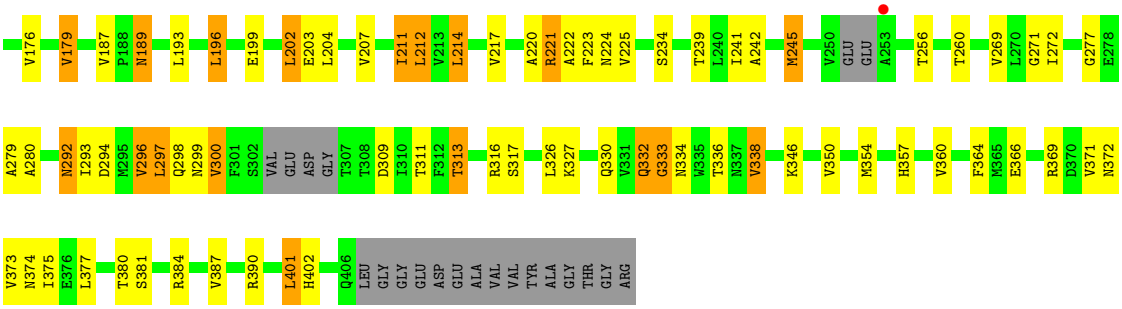
Chain G:



• Molecule 1: Aspartokinase

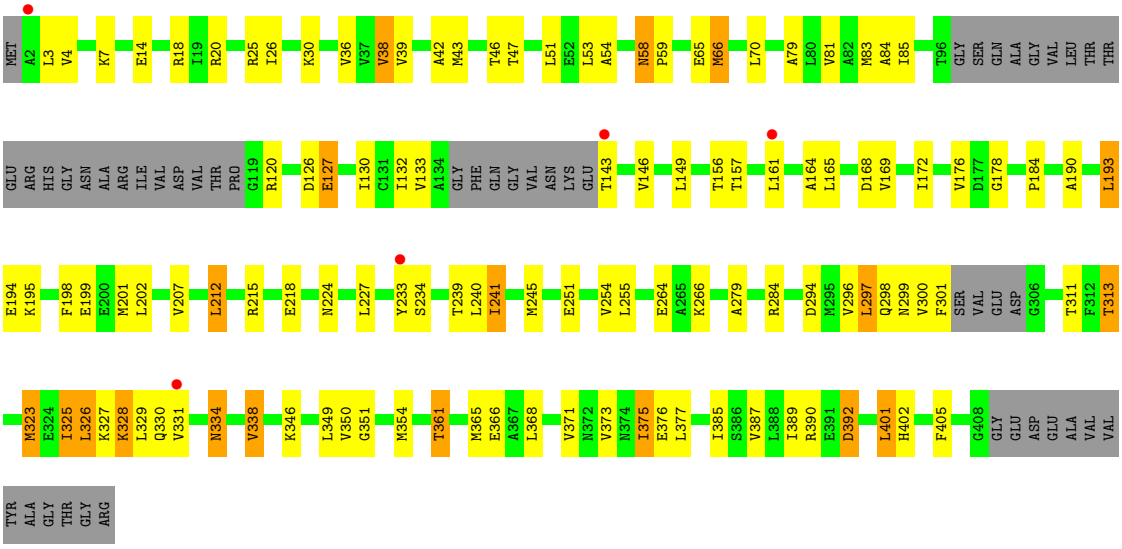
Chain I:





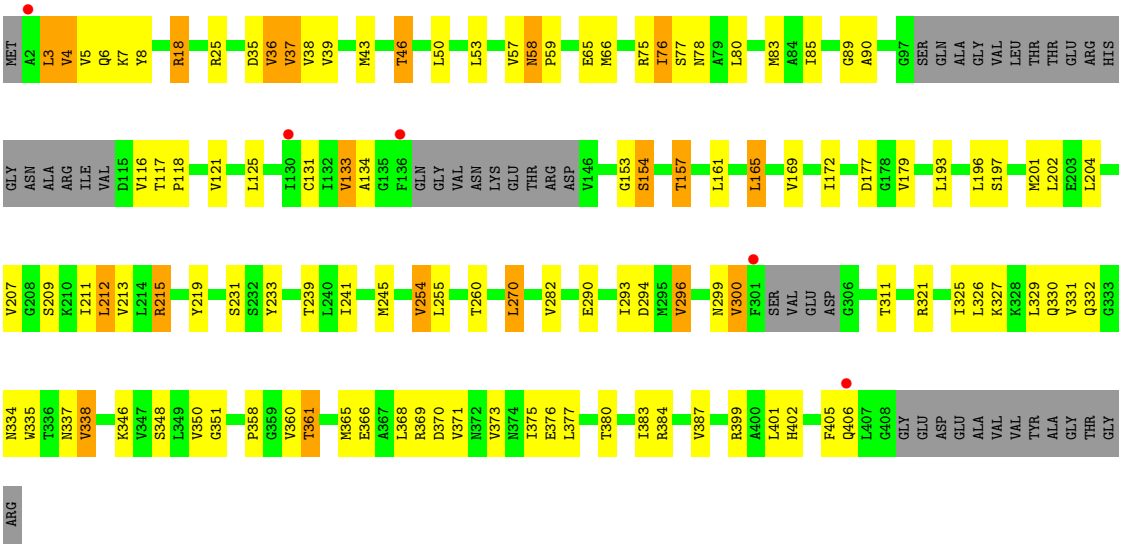
• Molecule 1: Aspartokinase

Chain K:



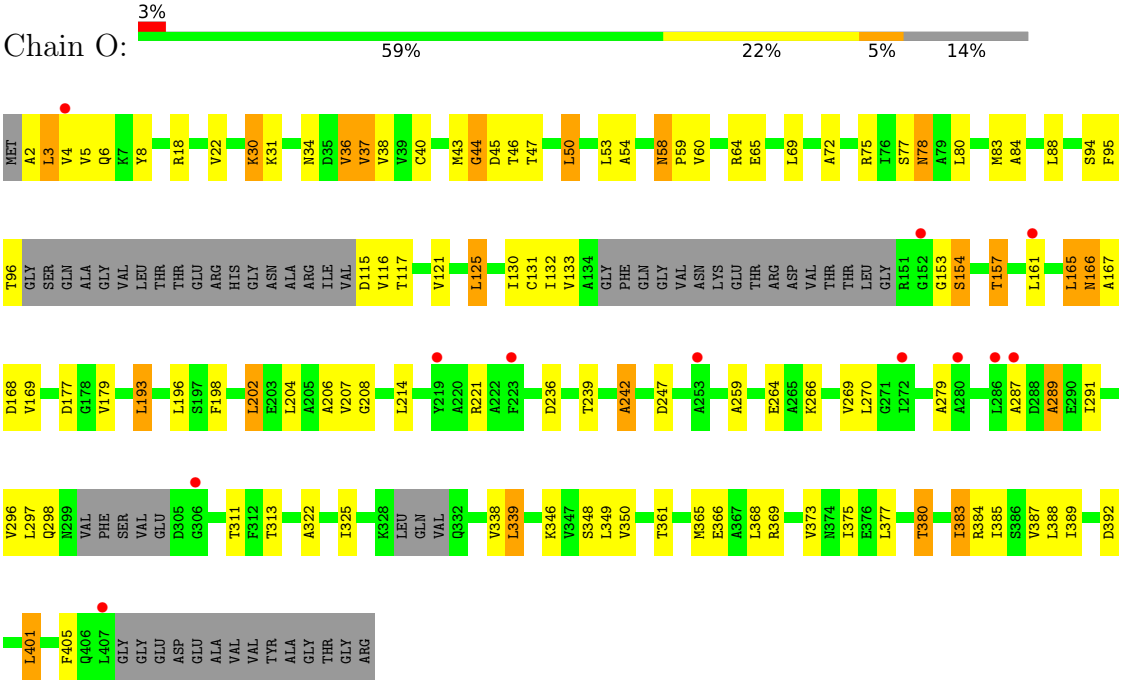
• Molecule 1: Aspartokinase

Chain M:



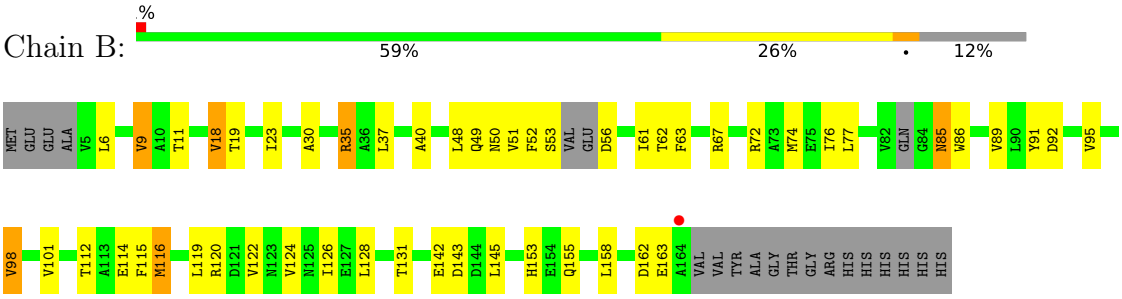
• Molecule 1: Aspartokinase

Chain O:



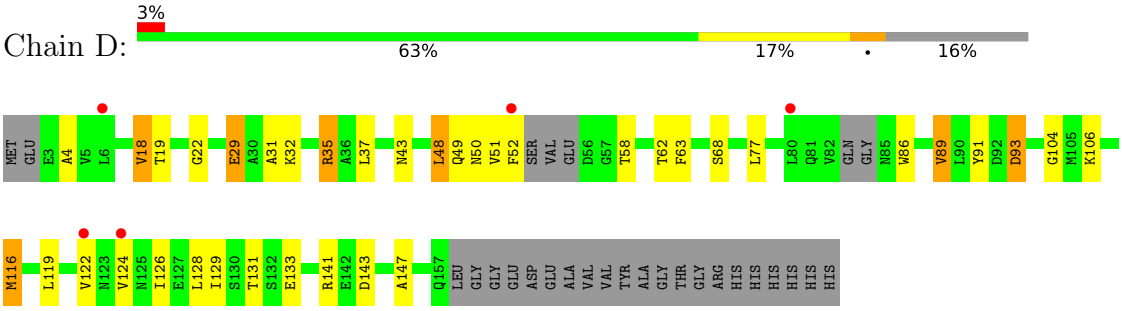
• Molecule 2: Aspartokinase

Chain B:



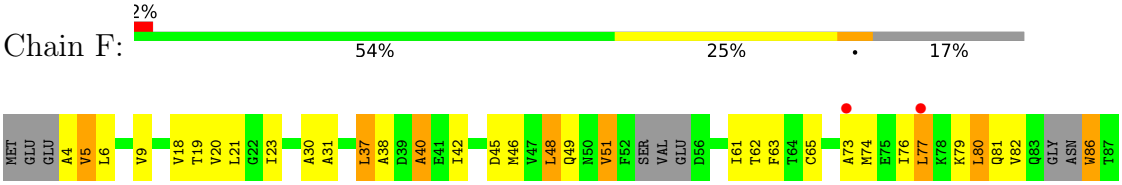
• Molecule 2: Aspartokinase

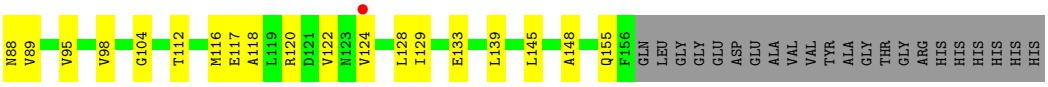
Chain D:



• Molecule 2: Aspartokinase

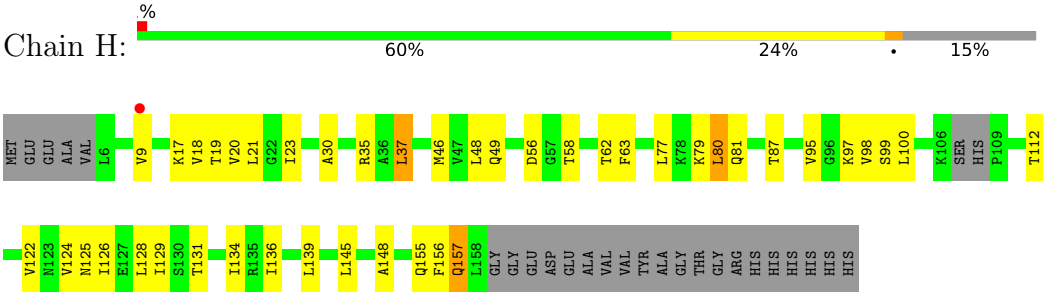
Chain F:





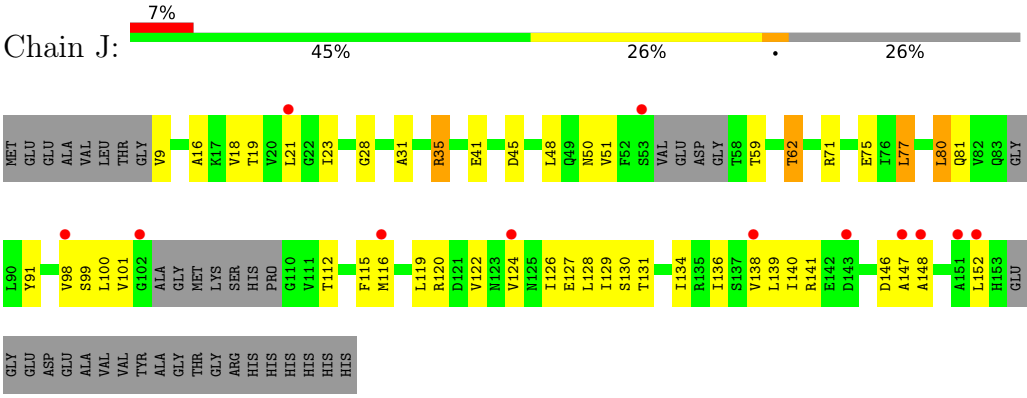
• Molecule 2: Aspartokinase

Chain H:



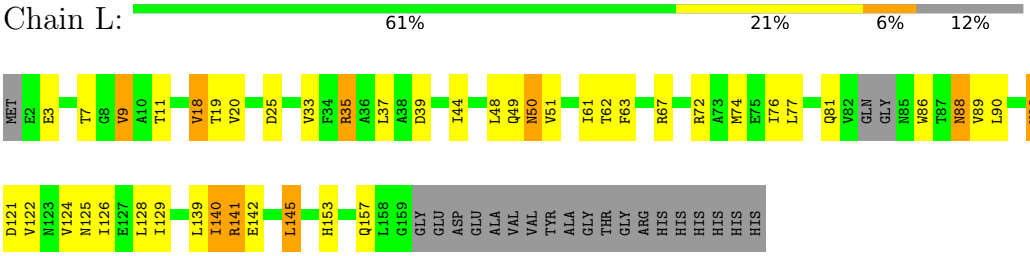
• Molecule 2: Aspartokinase

Chain J:



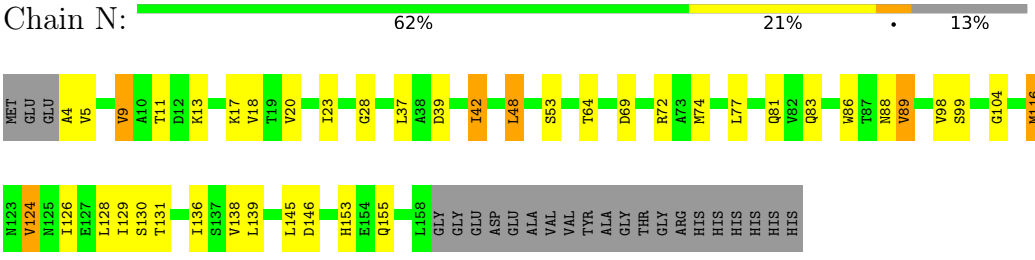
• Molecule 2: Aspartokinase

Chain L:



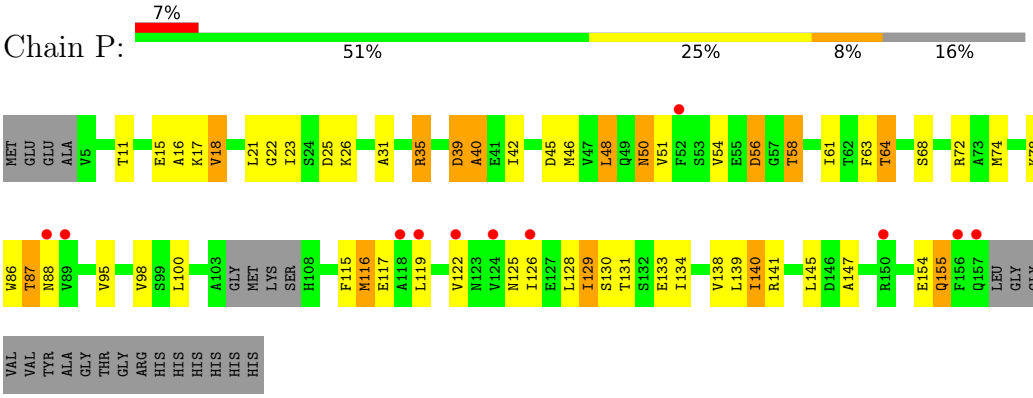
• Molecule 2: Aspartokinase

Chain N:



• Molecule 2: Aspartokinase

Chain P:


7%
51%
25%
8%
16%
MET GLU GLU ALA V5 T11 E15 A16 K17 V18 L21 G22 I23 S24 D25 K26 A31 R35 D39 A40 E41 I42 D45 M46 V47 L48 Q49 N50 V51 F52 S53 V54 E55 D56 G57 T58 I61 T62 F63 T64 S68 R72 A73 M74 K78 Q81 V82
W86 T87 N88 V89 V95 V98 S99 L100 A103 GLY MET LYS SER H108 F115 M116 E117 A118 L119 V122 N123 V124 N125 I126 E127 L128 I129 S130 T131 S132 E133 I134 V138 L139 I140 R141 L145 D146 A147 R150 E154 Q155 F156 Q157 LEU GLY GLY GLU ASP GLU ALA
VAL VAL TYR ALA GLY THR GLY ARG HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	99.03Å 112.87Å 120.01Å 76.03° 71.07° 74.50°	Depositor
Resolution (Å)	39.74 – 2.47 44.03 – 2.47	Depositor EDS
% Data completeness (in resolution range)	95.7 (39.74-2.47) 95.7 (44.03-2.47)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.223 , 0.288 0.225 , 0.285	Depositor DCC
R_{free} test set	8052 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	30970	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.49	0/2736	0.64	1/3712 (0.0%)
1	C	0.44	0/2730	0.64	0/3702
1	E	0.46	0/2706	0.63	0/3670
1	G	0.45	0/2623	0.64	1/3564 (0.0%)
1	I	0.42	0/2659	0.61	0/3610
1	K	0.48	0/2760	0.67	1/3743 (0.0%)
1	M	0.52	0/2797	0.69	0/3794
1	O	0.42	0/2665	0.59	0/3619
2	B	0.51	0/1185	0.72	0/1602
2	D	0.42	0/1142	0.62	0/1543
2	F	0.38	0/1085	0.59	0/1473
2	H	0.42	0/1118	0.59	0/1516
2	J	0.38	0/980	0.59	0/1329
2	L	0.49	0/1187	0.67	0/1606
2	N	0.48	0/1164	0.65	0/1580
2	P	0.38	0/1115	0.59	0/1512
All	All	0.45	0/30652	0.64	3/41575 (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	A	0	1
1	M	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	369	ARG	NE-CZ-NH1	5.66	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	284	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	K	392	ASP	CB-CG-OD1	5.24	123.01	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370	ASP	Peptide
1	M	380	THR	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	2711	0	2702	95	0
1	C	2705	0	2721	143	0
1	E	2682	0	2672	106	0
1	G	2600	0	2554	87	0
1	I	2634	0	2613	92	0
1	K	2736	0	2729	95	0
1	M	2772	0	2790	130	0
1	O	2642	0	2590	103	0
2	B	1175	0	1155	61	0
2	D	1133	0	1140	38	0
2	F	1077	0	1053	52	0
2	H	1108	0	1076	42	0
2	J	974	0	934	41	0
2	L	1176	0	1177	44	1
2	N	1153	0	1138	39	1
2	P	1107	0	1090	60	0
3	A	8	0	6	0	0
3	B	8	0	6	6	0
3	C	8	0	6	6	0
3	D	8	0	6	5	0
3	E	8	0	6	0	0
3	F	8	0	6	6	0
3	G	8	0	6	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	8	0	6	6	0
3	I	8	0	6	4	0
3	J	8	0	6	2	0
3	K	8	0	6	6	0
3	L	8	0	6	1	0
3	M	8	0	6	0	0
3	N	8	0	6	0	0
3	O	8	0	6	4	0
3	P	8	0	6	1	0
4	A	10	0	12	0	0
4	C	10	0	12	5	0
4	E	10	0	12	2	0
4	G	10	0	12	2	0
4	K	10	0	12	6	0
4	M	10	0	12	5	0
4	O	10	0	12	2	0
5	A	46	0	0	1	0
5	B	36	0	0	0	0
5	C	25	0	0	2	0
5	D	13	0	0	1	0
5	E	30	0	0	0	0
5	F	5	0	0	0	0
5	G	27	0	0	1	0
5	H	11	0	0	0	0
5	I	22	0	0	1	0
5	J	3	0	0	0	0
5	K	41	0	0	0	0
5	L	22	0	0	0	0
5	M	52	0	0	1	0
5	N	24	0	0	0	0
5	O	22	0	0	1	0
5	P	8	0	0	0	0
All	All	30970	0	30314	1116	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1116) 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:E:43:MET:O	1:E:46:THR:HG22	1.34	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:LEU:CD2	1:E:291:ILE:HD11	1.69	1.21
2:H:20:VAL:HG12	2:H:23:ILE:HD11	1.19	1.17
1:C:297:LEU:HD22	1:C:377:LEU:HD21	1.26	1.16
2:N:116:MET:HE2	2:N:126:ILE:HD13	1.23	1.14
1:E:286:LEU:HD22	1:E:291:ILE:HD11	1.14	1.12
1:M:179:VAL:CG1	1:M:239:THR:HG21	1.81	1.11
2:N:116:MET:CE	2:N:126:ILE:HD13	1.79	1.11
1:C:172:ILE:HD11	1:C:229:VAL:HG22	1.31	1.09
1:M:245:MET:SD	1:M:383:ILE:HD11	1.92	1.08
2:J:48:LEU:HD13	2:J:128:LEU:HD11	1.34	1.08
1:K:279:ALA:HB2	3:K:501:THR:HG23	1.35	1.07
1:E:286:LEU:HD22	1:E:291:ILE:CD1	1.85	1.06
1:O:43:MET:O	1:O:46:THR:HG23	1.57	1.05
1:C:279:ALA:HB2	3:C:501:THR:CG2	1.88	1.04
2:F:49:GLN:HE22	3:F:201:THR:HG21	0.90	1.04
1:C:297:LEU:CD2	1:C:377:LEU:HD21	1.86	1.04
1:C:267:VAL:HG13	1:C:323:MET:HE3	1.37	1.02
1:G:211:ILE:HG23	1:G:212:LEU:HD22	1.36	1.02
1:A:297:LEU:CD1	1:A:377:LEU:HD21	1.91	1.00
1:M:270:LEU:HD21	1:M:337:ASN:HB3	1.42	1.00
1:M:43:MET:O	1:M:46:THR:HG23	1.62	1.00
2:N:48:LEU:CD1	2:N:128:LEU:HD21	1.90	1.00
2:F:49:GLN:NE2	3:F:201:THR:HG21	1.76	1.00
2:B:116:MET:CE	2:B:126:ILE:HD13	1.93	0.98
1:E:299:ASN:HD21	2:F:62:THR:HG21	1.28	0.98
1:O:80:LEU:HD23	1:O:83:MET:HE1	1.48	0.96
1:A:133:VAL:HG21	1:A:161:LEU:HD11	1.47	0.95
1:A:354:MET:HB2	1:A:360:VAL:HG11	1.46	0.95
1:G:43:MET:O	1:G:46:THR:HG22	1.66	0.95
1:A:311:THR:HG23	2:B:50:ASN:HD21	1.29	0.95
1:I:43:MET:O	1:I:46:THR:HG23	1.67	0.94
1:M:58:ASN:ND2	1:M:59:PRO:O	1.98	0.94
1:C:289:ALA:CB	1:C:325:ILE:HD11	1.98	0.94
1:I:354:MET:HB2	1:I:360:VAL:HG11	1.45	0.94
1:I:279:ALA:HB2	3:I:501:THR:HG23	1.48	0.93
1:G:279:ALA:HB2	3:G:501:THR:CG2	1.99	0.93
1:C:297:LEU:HD22	1:C:377:LEU:CD2	1.98	0.93
2:H:112:THR:HG22	2:H:136:ILE:HD11	1.51	0.92
2:B:30:ALA:HB2	3:B:201:THR:HG23	1.52	0.92
1:M:245:MET:SD	1:M:383:ILE:CD1	2.59	0.91
1:O:291:ILE:HD11	1:O:322:ALA:HB2	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:VAL:CG1	1:C:323:MET:HE3	2.01	0.90
2:B:19:THR:OG1	2:B:62:THR:HG22	1.72	0.90
1:E:254:VAL:HG22	1:E:255:LEU:H	1.37	0.89
1:O:80:LEU:HD23	1:O:83:MET:CE	2.03	0.89
2:F:49:GLN:HE22	3:F:201:THR:CG2	1.83	0.88
1:O:179:VAL:HG22	1:O:239:THR:HG21	1.56	0.88
1:O:279:ALA:HB2	3:O:501:THR:HG22	1.54	0.88
1:A:297:LEU:HD13	1:A:377:LEU:HD21	1.55	0.87
1:E:380:THR:HG21	2:F:46:MET:HA	1.54	0.87
1:C:375:ILE:HG23	1:C:387:VAL:CG2	2.03	0.87
2:B:116:MET:HE2	2:B:126:ILE:HD13	1.57	0.87
2:B:116:MET:HE2	2:B:126:ILE:CD1	2.06	0.86
2:F:118:ALA:HB2	2:F:155:GLN:HG3	1.58	0.86
1:C:133:VAL:HG21	1:C:161:LEU:HD11	1.57	0.86
1:M:179:VAL:HG12	1:M:239:THR:HG21	1.55	0.86
1:M:361:THR:HG22	4:M:601:LYS:HG2	1.57	0.86
2:F:122:VAL:HG12	2:F:124:VAL:HG23	1.56	0.86
2:D:48:LEU:HD13	2:D:128:LEU:HD21	1.59	0.85
1:O:78:ASN:C	1:O:78:ASN:HD22	1.80	0.84
1:E:267:VAL:HG13	1:E:323:MET:HE1	1.60	0.84
1:K:43:MET:O	1:K:46:THR:HG23	1.77	0.84
1:M:299:ASN:O	1:M:300:VAL:HG22	1.77	0.83
1:C:179:VAL:HG22	1:C:239:THR:HG21	1.60	0.83
2:P:122:VAL:HG11	2:P:147:ALA:HB1	1.61	0.83
1:C:207:VAL:HG11	1:C:348:SER:OG	1.79	0.83
1:C:279:ALA:HB2	3:C:501:THR:HG22	1.58	0.83
2:B:116:MET:HE1	2:B:126:ILE:HD13	1.59	0.83
1:C:297:LEU:CD2	1:C:377:LEU:CD2	2.54	0.82
1:K:294:ASP:HB3	1:K:313:THR:HG22	1.61	0.82
1:A:80:LEU:HD23	1:A:83:MET:CE	2.09	0.82
2:N:48:LEU:HD13	2:N:128:LEU:HD21	1.59	0.82
1:M:153:GLY:O	1:M:157:THR:HG22	1.80	0.82
2:H:95:VAL:HG11	2:H:139:LEU:HD13	1.62	0.81
2:N:128:LEU:HD13	2:N:139:LEU:HD12	1.61	0.81
2:H:122:VAL:HG13	2:H:124:VAL:HG13	1.59	0.81
2:D:48:LEU:CD1	2:D:128:LEU:HD21	2.11	0.81
1:A:311:THR:HG23	2:B:50:ASN:ND2	1.96	0.80
1:M:204:LEU:HG	1:M:350:VAL:HG11	1.62	0.80
2:L:125:ASN:O	2:L:140:ILE:HG23	1.82	0.80
1:I:204:LEU:HG	1:I:350:VAL:HG21	1.63	0.79
1:O:80:LEU:HA	1:O:83:MET:HE2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:285:ALA:HB1	1:G:325:ILE:HD11	1.64	0.79
1:A:375:ILE:HB	3:B:201:THR:HG22	1.63	0.79
1:G:377:LEU:HD22	1:G:388:LEU:HD12	1.65	0.79
2:H:30:ALA:HB2	3:H:201:THR:CG2	2.12	0.79
1:K:227:LEU:HB2	1:K:241:ILE:HG23	1.65	0.79
1:C:133:VAL:HG21	1:C:161:LEU:CD1	2.13	0.78
1:M:211:ILE:HG22	1:M:212:LEU:HD13	1.64	0.78
2:B:18:VAL:HG22	2:B:63:PHE:CZ	2.19	0.78
1:K:58:ASN:ND2	1:K:59:PRO:O	2.16	0.78
1:E:179:VAL:HG13	1:E:239:THR:HG21	1.65	0.78
1:G:361:THR:HG22	4:G:601:LYS:OXT	1.83	0.78
1:O:380:THR:HG21	2:P:46:MET:HA	1.66	0.78
1:G:268:THR:HG22	1:G:270:LEU:HD22	1.65	0.77
2:F:42:ILE:HD11	2:F:65:CYS:CB	2.15	0.77
1:I:54:ALA:HB1	1:K:83:MET:HE1	1.67	0.77
2:B:85:ASN:N	2:B:85:ASN:HD22	1.82	0.76
1:E:218:GLU:HG2	2:F:5:VAL:HG21	1.66	0.76
1:G:301:PHE:CZ	2:H:21:LEU:HD21	2.20	0.76
1:E:369:ARG:NH1	1:E:370:ASP:OD1	2.19	0.76
2:B:116:MET:CE	2:B:126:ILE:CD1	2.62	0.76
1:E:215:ARG:H	1:E:215:ARG:HD3	1.49	0.76
1:M:215:ARG:CZ	2:N:5:VAL:HG11	2.15	0.76
2:B:85:ASN:ND2	2:B:86:TRP:CD1	2.54	0.75
1:C:207:VAL:HG12	1:C:207:VAL:O	1.87	0.75
1:K:279:ALA:CB	3:K:501:THR:HG23	2.14	0.75
1:E:54:ALA:HB1	1:G:83:MET:HE1	1.69	0.75
2:D:51:VAL:O	2:D:52:PHE:CB	2.35	0.75
1:A:36:VAL:HG23	1:A:130:ILE:HG23	1.68	0.75
1:A:267:VAL:HG13	1:A:323:MET:CE	2.16	0.74
2:N:116:MET:HE2	2:N:126:ILE:CD1	2.11	0.74
1:E:172:ILE:HG21	1:E:212:LEU:CD1	2.18	0.74
2:P:138:VAL:HG23	2:P:140:ILE:HD11	1.70	0.74
1:G:279:ALA:HB2	3:G:501:THR:HG21	1.69	0.74
1:E:267:VAL:HG13	1:E:323:MET:CE	2.17	0.74
1:E:132:ILE:HD12	1:E:132:ILE:C	2.06	0.73
1:I:371:VAL:O	1:I:373:VAL:N	2.21	0.73
1:E:254:VAL:HG22	1:E:255:LEU:N	2.04	0.73
2:L:125:ASN:O	2:L:140:ILE:CG2	2.36	0.73
1:O:375:ILE:HG23	1:O:387:VAL:HG22	1.71	0.73
1:A:294:ASP:O	1:A:295:MET:O	2.07	0.73
1:C:80:LEU:HD23	1:C:83:MET:CE	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LEU:HD23	1:C:83:MET:HE1	1.71	0.73
2:F:19:THR:OG1	2:F:62:THR:HG22	1.87	0.73
1:A:262:LYS:HG2	1:A:394:LEU:CD2	2.19	0.72
1:E:80:LEU:HD23	1:E:83:MET:CE	2.18	0.72
1:I:279:ALA:HB2	3:I:501:THR:CG2	2.17	0.72
1:C:375:ILE:HG23	1:C:387:VAL:HG21	1.71	0.72
1:M:25:ARG:NH1	5:M:641:HOH:O	2.22	0.72
1:G:179:VAL:HG13	1:G:239:THR:HG21	1.71	0.72
1:G:371:VAL:HG22	1:G:373:VAL:HG23	1.72	0.72
1:A:296:VAL:HG13	2:B:131:THR:CG2	2.20	0.71
1:I:39:VAL:HG22	1:I:133:VAL:HG13	1.71	0.71
1:C:75:ARG:HE	1:C:96:THR:HG21	1.55	0.71
1:I:202:LEU:HD13	1:I:217:VAL:HG12	1.73	0.71
1:I:202:LEU:HD13	1:I:217:VAL:CG1	2.21	0.71
3:K:501:THR:HG22	2:L:126:ILE:HB	1.72	0.71
1:E:58:ASN:HD22	1:E:58:ASN:C	1.93	0.71
1:M:204:LEU:CD2	1:M:350:VAL:HG11	2.20	0.71
1:M:375:ILE:HG23	1:M:387:VAL:CG1	2.21	0.71
1:G:43:MET:O	1:G:46:THR:CG2	2.39	0.71
2:H:112:THR:HG22	2:H:136:ILE:CD1	2.19	0.71
1:M:361:THR:CG2	4:M:601:LYS:HG2	2.20	0.71
1:K:299:ASN:HD21	2:L:62:THR:HG23	1.54	0.70
1:M:179:VAL:HG12	1:M:239:THR:CG2	2.21	0.70
1:C:371:VAL:HG12	1:C:371:VAL:O	1.89	0.70
1:K:264:GLU:HB3	1:K:313:THR:HG23	1.72	0.70
1:K:26:ILE:HG22	1:K:130:ILE:HD13	1.73	0.70
1:G:198:PHE:HA	1:G:241:ILE:HD11	1.74	0.70
2:P:125:ASN:O	2:P:140:ILE:HG23	1.91	0.70
2:B:18:VAL:CG2	2:B:63:PHE:CZ	2.75	0.70
2:B:53:SER:HG	2:B:56:ASP:N	1.87	0.70
1:C:375:ILE:HG23	1:C:387:VAL:HG23	1.73	0.70
1:A:5:VAL:HG22	1:A:37:VAL:CG1	2.22	0.70
1:K:279:ALA:HB2	3:K:501:THR:CG2	2.17	0.70
1:A:66:MET:CE	1:A:69:LEU:HD23	2.22	0.70
2:H:48:LEU:HD23	2:H:49:GLN:N	2.06	0.70
2:N:116:MET:CE	2:N:126:ILE:CD1	2.63	0.70
2:B:30:ALA:HB2	3:B:201:THR:CG2	2.19	0.70
1:M:361:THR:HG22	4:M:601:LYS:OXT	1.91	0.70
1:O:207:VAL:HG11	1:O:348:SER:OG	1.92	0.70
1:G:344:VAL:HG11	1:G:388:LEU:HD13	1.74	0.69
1:M:375:ILE:HG23	1:M:387:VAL:HG11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:HD11	1:A:256:THR:HG21	1.74	0.69
1:O:296:VAL:HG22	2:P:129:ILE:HD11	1.74	0.69
1:E:80:LEU:HA	1:E:83:MET:HE2	1.74	0.69
2:H:131:THR:HB	2:H:136:ILE:HD13	1.73	0.69
2:D:119:LEU:HB3	2:D:124:VAL:HG23	1.74	0.69
2:P:45:ASP:HB3	2:P:64:THR:HG22	1.74	0.69
1:E:2:ALA:HB3	1:E:34:ASN:ND2	2.08	0.69
1:I:57:VAL:HG11	1:K:84:ALA:HB2	1.75	0.69
1:G:329:LEU:O	1:G:332:GLN:NE2	2.26	0.69
1:G:270:LEU:N	1:G:270:LEU:HD23	2.07	0.69
1:O:361:THR:HG22	1:O:385:ILE:HD11	1.73	0.69
1:O:349:LEU:HD22	1:O:405:PHE:CE2	2.27	0.69
2:B:85:ASN:HD22	2:B:85:ASN:H	1.39	0.68
1:M:245:MET:CE	1:M:383:ILE:HD11	2.24	0.68
2:B:85:ASN:N	2:B:85:ASN:ND2	2.41	0.68
2:L:74:MET:HG2	2:L:89:VAL:HG22	1.75	0.68
1:C:51:LEU:HD12	1:C:66:MET:CE	2.24	0.68
1:G:369:ARG:HG2	1:G:369:ARG:HH11	1.60	0.67
1:K:201:MET:CB	1:K:241:ILE:HD12	2.25	0.67
1:M:383:ILE:HG22	1:M:383:ILE:O	1.93	0.67
1:E:174:SER:OG	1:E:176:VAL:HG22	1.94	0.67
1:M:204:LEU:CG	1:M:350:VAL:HG11	2.24	0.67
1:C:289:ALA:CB	1:C:325:ILE:CD1	2.72	0.67
1:G:58:ASN:C	1:G:58:ASN:HD22	1.97	0.67
1:G:179:VAL:CG1	1:G:239:THR:HG21	2.24	0.67
1:K:294:ASP:HB2	2:L:106:LYS:HD2	1.76	0.67
1:O:38:VAL:HG22	1:O:132:ILE:HD13	1.76	0.67
1:E:212:LEU:HD21	1:E:229:VAL:CG2	2.24	0.67
1:G:369:ARG:NH1	1:G:370:ASP:OD1	2.28	0.67
2:H:30:ALA:HB2	3:H:201:THR:HG23	1.77	0.67
2:J:19:THR:HG1	2:J:62:THR:HG1	1.42	0.67
1:M:321:ARG:O	1:M:325:ILE:HD13	1.94	0.67
1:A:58:ASN:C	1:A:58:ASN:HD22	1.98	0.67
2:J:122:VAL:HG23	2:J:124:VAL:HG23	1.76	0.67
1:K:361:THR:HG23	4:K:601:LYS:O	1.93	0.67
1:E:80:LEU:HD23	1:E:83:MET:HE1	1.76	0.67
1:E:189:ASN:O	1:E:190:ALA:CB	2.41	0.67
1:C:270:LEU:HD12	1:C:337:ASN:HB3	1.77	0.66
1:G:377:LEU:HD22	1:G:388:LEU:CD1	2.25	0.66
1:C:294:ASP:HB3	1:C:313:THR:CG2	2.25	0.66
1:M:83:MET:HE1	1:O:54:ALA:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:ILE:O	1:G:329:LEU:HD13	1.95	0.66
1:E:286:LEU:HD23	1:E:291:ILE:HD11	1.69	0.66
2:H:112:THR:CG2	2:H:136:ILE:HD11	2.25	0.66
1:A:268:THR:HG23	1:A:311:THR:HG22	1.78	0.66
1:A:311:THR:HG21	2:B:50:ASN:OD1	1.96	0.66
1:K:168:ASP:O	1:K:169:VAL:HG13	1.96	0.66
1:C:5:VAL:HG22	1:C:37:VAL:HG13	1.78	0.66
1:E:81:VAL:O	1:E:85:ILE:HG23	1.96	0.66
1:I:204:LEU:CD2	1:I:350:VAL:HG21	2.27	0.65
1:I:214:LEU:HD21	2:J:134:ILE:CG2	2.25	0.65
1:C:279:ALA:HB2	3:C:501:THR:HG23	1.75	0.65
1:A:211:ILE:HG22	1:A:212:LEU:HD13	1.79	0.65
1:A:2:ALA:HB1	1:A:34:ASN:OD1	1.97	0.65
1:M:80:LEU:HD23	1:M:83:MET:HE1	1.79	0.65
1:M:179:VAL:HG13	1:M:239:THR:HG21	1.75	0.65
2:P:126:ILE:CG2	2:P:129:ILE:HG22	2.27	0.65
2:H:23:ILE:HD12	2:H:23:ILE:N	2.12	0.65
1:C:39:VAL:HG22	1:C:133:VAL:CG2	2.27	0.65
1:C:207:VAL:CG1	1:C:348:SER:OG	2.44	0.65
1:E:43:MET:O	1:E:46:THR:CG2	2.28	0.65
2:B:49:GLN:OE1	3:B:201:THR:HG21	1.96	0.65
1:C:196:LEU:CD1	1:C:256:THR:HG21	2.27	0.65
1:E:123:GLU:O	1:E:124:ALA:CB	2.44	0.64
1:K:199:GLU:HA	1:K:202:LEU:HD23	1.79	0.64
1:M:351:GLY:C	1:M:383:ILE:HG23	2.17	0.64
2:D:19:THR:OG1	2:D:62:THR:HG22	1.97	0.64
1:E:354:MET:HB2	1:E:360:VAL:HG11	1.78	0.64
1:A:267:VAL:HG13	1:A:323:MET:HE1	1.79	0.64
2:F:5:VAL:O	2:F:6:LEU:HD23	1.98	0.64
1:O:58:ASN:C	1:O:58:ASN:HD22	1.99	0.64
1:A:66:MET:HE1	1:A:69:LEU:HD23	1.80	0.64
1:A:80:LEU:HA	1:A:83:MET:HE2	1.78	0.64
2:B:101:VAL:HB	2:B:163:GLU:CB	2.28	0.64
1:C:80:LEU:HA	1:C:83:MET:HE2	1.79	0.64
1:K:164:ALA:O	1:K:165:LEU:HB2	1.98	0.64
2:P:140:ILE:HG22	2:P:141:ARG:H	1.62	0.64
2:L:19:THR:HG23	2:L:62:THR:HG22	1.79	0.63
2:N:98:VAL:HG13	2:N:145:LEU:HD12	1.80	0.63
1:E:264:GLU:HG2	1:E:313:THR:HG23	1.80	0.63
2:P:140:ILE:N	2:P:140:ILE:HD12	2.13	0.63
1:C:299:ASN:HD21	2:D:62:THR:HG21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:128:LEU:HD23	2:F:129:ILE:N	2.14	0.63
1:A:80:LEU:HD23	1:A:83:MET:HE1	1.81	0.63
2:L:122:VAL:HG13	2:L:124:VAL:CG1	2.28	0.63
1:M:196:LEU:HD22	1:M:241:ILE:HG13	1.80	0.63
1:A:262:LYS:HG2	1:A:394:LEU:HD23	1.81	0.63
1:E:78:ASN:OD1	1:E:134:ALA:HB2	1.98	0.63
1:E:268:THR:HG21	2:F:51:VAL:HG11	1.80	0.63
1:A:311:THR:CG2	2:B:50:ASN:OD1	2.47	0.62
1:I:204:LEU:CG	1:I:350:VAL:HG21	2.27	0.62
1:O:78:ASN:C	1:O:78:ASN:ND2	2.51	0.62
1:C:371:VAL:O	1:C:371:VAL:CG1	2.47	0.62
1:A:262:LYS:CD	1:A:394:LEU:HD23	2.29	0.62
1:A:284:ARG:HG2	1:A:284:ARG:HH11	1.64	0.62
2:F:42:ILE:HD11	2:F:65:CYS:HB2	1.81	0.62
1:I:179:VAL:HG13	1:I:239:THR:HG21	1.82	0.62
1:O:157:THR:O	1:O:161:LEU:HD23	1.99	0.62
1:I:83:MET:HE1	1:K:54:ALA:HB1	1.80	0.62
2:N:42:ILE:HD13	2:N:69:ASP:HB3	1.82	0.62
2:B:19:THR:CB	2:B:62:THR:HG22	2.29	0.62
1:G:207:VAL:HG12	1:G:207:VAL:O	1.98	0.62
1:M:204:LEU:HD21	1:M:350:VAL:CG1	2.29	0.62
1:C:39:VAL:HG22	1:C:133:VAL:HG22	1.80	0.62
1:C:204:LEU:HD23	1:C:350:VAL:CG1	2.30	0.61
2:F:98:VAL:HG11	2:F:148:ALA:HB3	1.82	0.61
1:K:327:LYS:HE2	1:K:338:VAL:HG13	1.81	0.61
1:G:272:ILE:HD12	1:G:310:ILE:HG13	1.82	0.61
1:O:207:VAL:HG21	1:O:384:ARG:HD2	1.82	0.61
1:C:58:ASN:C	1:C:58:ASN:HD22	2.04	0.61
2:D:19:THR:HG23	2:D:62:THR:CG2	2.30	0.61
1:O:296:VAL:CG2	2:P:129:ILE:HD11	2.31	0.61
1:C:3:LEU:HD23	1:C:4:VAL:N	2.15	0.61
1:G:279:ALA:HB2	3:G:501:THR:HG23	1.80	0.61
1:A:199:GLU:HG2	1:A:245:MET:HG2	1.82	0.61
1:C:204:LEU:HD23	1:C:350:VAL:HG11	1.82	0.61
1:I:296:VAL:HG13	2:J:131:THR:CG2	2.30	0.61
1:C:289:ALA:HB3	1:C:325:ILE:CD1	2.30	0.61
2:D:122:VAL:HG13	2:D:124:VAL:HG22	1.83	0.61
2:P:122:VAL:HG12	2:P:122:VAL:O	2.00	0.61
2:B:23:ILE:HD13	2:B:61:ILE:HD12	1.81	0.61
1:C:196:LEU:HD11	1:C:256:THR:HG21	1.83	0.61
1:C:202:LEU:HD22	1:C:217:VAL:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:ALA:HB3	1:I:131:CYS:SG	2.41	0.61
1:O:5:VAL:HG22	1:O:37:VAL:HG22	1.83	0.61
1:E:189:ASN:O	1:E:190:ALA:HB2	2.01	0.61
2:F:122:VAL:CG1	2:F:122:VAL:O	2.49	0.61
2:H:56:ASP:HB2	2:H:58:THR:HG22	1.81	0.61
1:C:297:LEU:HD21	1:C:377:LEU:CD2	2.31	0.60
1:E:297:LEU:HD22	1:E:377:LEU:HD23	1.83	0.60
1:G:325:ILE:HD13	1:G:325:ILE:C	2.21	0.60
1:M:133:VAL:HG21	1:M:161:LEU:HD11	1.82	0.60
2:L:122:VAL:HG13	2:L:124:VAL:HG13	1.83	0.60
1:O:298:GLN:HB3	2:P:129:ILE:HG23	1.83	0.60
1:I:207:VAL:HG11	1:I:384:ARG:HD2	1.83	0.60
1:M:204:LEU:CD2	1:M:350:VAL:CG1	2.79	0.60
1:O:179:VAL:CG2	1:O:239:THR:HG21	2.30	0.60
1:C:156:THR:HG23	1:C:219:TYR:CE1	2.36	0.60
1:K:298:GLN:OE1	3:K:501:THR:HG21	2.00	0.60
1:E:36:VAL:CG2	1:E:130:ILE:HG23	2.32	0.60
1:C:75:ARG:NE	1:C:96:THR:HG21	2.16	0.60
1:C:172:ILE:HD13	1:C:212:LEU:HD23	1.84	0.60
2:F:30:ALA:HB2	3:F:201:THR:HG23	1.84	0.60
1:O:179:VAL:HG23	1:O:193:LEU:HD22	1.83	0.60
2:P:98:VAL:HG22	2:P:145:LEU:HD12	1.82	0.60
1:E:8:TYR:CE2	1:E:26:ILE:HD11	2.37	0.60
1:C:202:LEU:HD22	1:C:217:VAL:CG1	2.32	0.60
1:M:57:VAL:CG1	1:O:84:ALA:HB2	2.32	0.60
1:C:27:VAL:HG12	1:C:31:LYS:HD3	1.83	0.60
1:K:26:ILE:HD13	1:K:38:VAL:HG11	1.84	0.60
1:M:209:SER:HB3	1:M:211:ILE:HD12	1.84	0.60
1:E:42:ALA:HB1	1:E:46:THR:CG2	2.32	0.59
1:E:153:GLY:O	1:E:157:THR:HG22	2.02	0.59
1:G:58:ASN:ND2	1:G:59:PRO:O	2.35	0.59
1:K:172:ILE:HG12	1:K:212:LEU:HD11	1.83	0.59
1:O:264:GLU:HB3	1:O:313:THR:CG2	2.32	0.59
1:C:289:ALA:HB3	1:C:325:ILE:HD11	1.84	0.59
2:B:19:THR:HG23	2:B:62:THR:HG22	1.84	0.59
1:M:121:VAL:O	1:M:125:LEU:HB2	2.03	0.59
1:O:153:GLY:O	1:O:157:THR:HG22	2.03	0.59
1:I:25:ARG:NH2	1:I:234:SER:O	2.27	0.59
1:M:361:THR:HG22	4:M:601:LYS:CG	2.30	0.59
2:B:19:THR:CG2	2:B:62:THR:HG22	2.33	0.59
1:C:85:ILE:HG22	1:C:90:ALA:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:PHE:CD1	1:C:241:ILE:HD11	2.38	0.59
2:L:88:ASN:OD1	2:L:90:LEU:HD21	2.03	0.59
2:L:120:ARG:HG3	2:L:121:ASP:N	2.17	0.59
1:M:196:LEU:HD23	1:M:197:SER:O	2.03	0.59
1:M:361:THR:CG2	4:M:601:LYS:OXT	2.51	0.59
1:O:377:LEU:HD13	1:O:388:LEU:HD12	1.84	0.59
2:P:46:MET:HB2	2:P:64:THR:HB	1.84	0.59
2:B:11:THR:HG22	2:B:98:VAL:HG13	1.85	0.59
1:K:368:LEU:HG	1:K:373:VAL:CG2	2.33	0.59
1:O:204:LEU:HD22	1:O:259:ALA:HB2	1.84	0.59
1:C:76:ILE:HD12	1:C:80:LEU:HD12	1.85	0.59
2:F:20:VAL:HG13	2:F:86:TRP:CD1	2.36	0.59
3:O:501:THR:N	2:P:126:ILE:O	2.36	0.59
2:P:126:ILE:HG22	2:P:129:ILE:HG22	1.85	0.59
1:G:341:ASP:OD2	1:G:342:ASP:O	2.21	0.58
1:K:368:LEU:HD13	1:K:401:LEU:HD11	1.83	0.58
2:D:116:MET:HE2	2:D:126:ILE:HD13	1.85	0.58
1:E:215:ARG:H	1:E:215:ARG:CD	2.17	0.58
1:E:254:VAL:CG2	1:E:255:LEU:H	2.14	0.58
1:E:286:LEU:CD2	1:E:291:ILE:CD1	2.57	0.58
2:J:23:ILE:N	2:J:59:THR:O	2.33	0.58
1:I:346:LYS:NZ	5:I:506:HOH:O	2.31	0.58
1:I:269:VAL:HG12	1:I:272:ILE:HD11	1.84	0.58
2:N:48:LEU:HD13	2:N:128:LEU:CD2	2.33	0.58
1:M:57:VAL:HG13	1:O:84:ALA:HB2	1.86	0.58
1:A:387:VAL:HG12	1:A:389:ILE:HG23	1.85	0.58
1:G:294:ASP:HB3	1:G:313:THR:HG22	1.85	0.58
2:F:79:LYS:HA	2:F:82:VAL:HG12	1.85	0.58
2:J:147:ALA:O	2:J:148:ALA:HB3	2.04	0.58
1:A:397:ALA:O	1:A:401:LEU:HD22	2.03	0.58
1:M:116:VAL:HG12	1:M:116:VAL:O	2.03	0.57
1:M:368:LEU:O	1:M:373:VAL:HG22	2.03	0.57
1:M:369:ARG:NH1	1:M:370:ASP:OD1	2.37	0.57
1:I:125:LEU:O	1:I:127:GLU:O	2.22	0.57
2:L:81:GLN:OE1	2:L:89:VAL:HG12	2.04	0.57
1:O:311:THR:CB	2:P:50:ASN:HD21	2.16	0.57
2:P:42:ILE:HD11	2:P:72:ARG:NH1	2.19	0.57
2:J:126:ILE:HG21	2:J:129:ILE:HG12	1.85	0.57
1:M:78:ASN:HD21	1:M:134:ALA:HB2	1.69	0.57
1:M:154:SER:HA	1:M:157:THR:CG2	2.34	0.57
2:L:98:VAL:HG22	2:L:145:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:ALA:HB2	1:K:53:LEU:HD13	1.86	0.57
1:G:361:THR:HG22	4:G:601:LYS:HG2	1.86	0.57
1:K:51:LEU:CD2	1:K:70:LEU:HD21	2.34	0.57
1:A:36:VAL:CG2	1:A:130:ILE:HG23	2.33	0.57
1:E:36:VAL:HG22	1:E:130:ILE:HG23	1.86	0.57
1:G:279:ALA:CB	3:G:501:THR:CG2	2.80	0.57
1:I:193:LEU:HD21	1:I:256:THR:HG23	1.87	0.57
1:M:196:LEU:HD21	1:M:201:MET:HB2	1.87	0.57
1:O:270:LEU:HD11	1:O:339:LEU:HD21	1.87	0.57
1:A:377:LEU:HD13	1:A:388:LEU:HD12	1.86	0.57
2:D:19:THR:HG23	2:D:62:THR:HG22	1.87	0.57
1:A:389:ILE:HD11	1:A:394:LEU:HD13	1.87	0.57
1:E:202:LEU:HD22	1:E:217:VAL:HG12	1.87	0.57
1:I:364:PHE:CE1	1:I:401:LEU:HD21	2.39	0.57
1:O:121:VAL:HG12	1:O:125:LEU:HD22	1.87	0.57
1:C:289:ALA:HB2	1:C:325:ILE:HD11	1.87	0.56
1:G:227:LEU:HB2	1:G:241:ILE:HG23	1.86	0.56
1:K:47:THR:O	1:K:51:LEU:HD23	2.05	0.56
1:K:354:MET:O	4:K:601:LYS:HB2	2.05	0.56
1:C:267:VAL:CG1	1:C:323:MET:CE	2.79	0.56
1:M:311:THR:HG21	1:M:377:LEU:HD21	1.87	0.56
2:D:116:MET:CE	2:D:126:ILE:HD13	2.36	0.56
1:G:371:VAL:CG2	1:G:372:ASN:N	2.69	0.56
1:I:223:PHE:O	1:I:225:VAL:N	2.39	0.56
1:M:270:LEU:HD23	1:M:270:LEU:H	1.70	0.56
1:A:354:MET:CB	1:A:360:VAL:HG11	2.28	0.56
1:E:18:ARG:NH1	1:E:233:TYR:CZ	2.74	0.56
1:G:153:GLY:O	1:G:157:THR:HG22	2.06	0.56
1:M:85:ILE:HG23	1:M:90:ALA:HB3	1.88	0.56
2:P:22:GLY:HA3	2:P:87:THR:HG22	1.88	0.56
1:A:179:VAL:HG13	1:A:239:THR:HG21	1.87	0.56
1:A:368:LEU:O	1:A:371:VAL:O	2.23	0.56
2:J:80:LEU:HD23	2:J:86:TRP:CZ2	2.40	0.56
1:K:42:ALA:HB1	1:K:46:THR:OG1	2.05	0.56
1:M:118:PRO:HA	1:M:121:VAL:HG12	1.88	0.56
1:M:179:VAL:HG12	1:M:239:THR:CB	2.35	0.56
1:C:196:LEU:HD11	1:C:200:GLU:HB3	1.88	0.56
1:G:278:GLU:O	1:G:282:VAL:HG23	2.06	0.56
1:I:380:THR:HG23	1:I:381:SER:O	2.06	0.56
2:N:98:VAL:HG13	2:N:145:LEU:CD1	2.36	0.56
1:C:207:VAL:O	1:C:207:VAL:CG1	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:THR:OG1	2:B:62:THR:CG2	2.52	0.55
1:E:270:LEU:HD12	1:E:337:ASN:HB3	1.88	0.55
2:L:19:THR:OG1	2:L:62:THR:HG22	2.06	0.55
1:M:371:VAL:HG12	1:M:373:VAL:HG13	1.87	0.55
1:O:179:VAL:HG23	1:O:193:LEU:CD2	2.36	0.55
2:B:116:MET:CE	2:B:116:MET:HA	2.36	0.55
1:E:272:ILE:HD13	1:E:310:ILE:HG13	1.87	0.55
1:G:375:ILE:O	3:H:201:THR:N	2.39	0.55
2:P:81:GLN:HE21	2:P:88:ASN:HA	1.70	0.55
1:A:297:LEU:HD21	2:B:48:LEU:HG	1.88	0.55
1:A:309:ASP:HB2	2:B:51:VAL:HG21	1.88	0.55
1:C:172:ILE:HD13	1:C:212:LEU:CD2	2.36	0.55
2:D:4:ALA:HB2	2:D:104:GLY:O	2.06	0.55
1:E:375:ILE:O	3:F:201:THR:N	2.39	0.55
1:E:85:ILE:CD1	1:E:90:ALA:HB3	2.37	0.55
1:E:176:VAL:HG21	1:E:211:ILE:HG23	1.88	0.55
1:G:371:VAL:CG2	1:G:373:VAL:HG23	2.37	0.55
1:I:298:GLN:OE1	3:I:501:THR:HG21	2.07	0.55
1:K:218:GLU:OE1	2:L:7:THR:HG21	2.07	0.55
1:M:133:VAL:CG2	1:M:161:LEU:HD11	2.36	0.55
1:M:368:LEU:HG	1:M:373:VAL:HG21	1.88	0.55
1:C:202:LEU:CD2	1:C:217:VAL:HG12	2.37	0.55
1:G:201:MET:HG2	1:G:241:ILE:HD13	1.88	0.55
1:I:269:VAL:CG1	1:I:272:ILE:HD11	2.36	0.55
1:I:374:ASN:OD1	3:J:201:THR:N	2.39	0.55
1:K:201:MET:HB3	1:K:241:ILE:HD12	1.88	0.55
1:A:5:VAL:HG22	1:A:37:VAL:HG13	1.87	0.55
1:A:179:VAL:HG22	1:A:193:LEU:HD23	1.88	0.55
1:I:44:GLY:O	1:I:45:ASP:HB2	2.07	0.55
1:O:361:THR:HG22	4:O:601:LYS:HG2	1.89	0.55
1:M:270:LEU:CD2	1:M:337:ASN:HB3	2.29	0.55
1:M:351:GLY:O	1:M:383:ILE:HG23	2.06	0.55
2:P:115:PHE:O	2:P:119:LEU:HD23	2.06	0.55
2:D:122:VAL:HG21	2:D:147:ALA:HB1	1.88	0.55
1:M:57:VAL:HG11	1:O:80:LEU:O	2.07	0.55
1:C:241:ILE:C	1:C:241:ILE:HD12	2.28	0.54
2:P:39:ASP:O	2:P:40:ALA:HB2	2.07	0.54
1:I:327:LYS:HE2	1:I:338:VAL:HG13	1.90	0.54
2:D:49:GLN:OE1	3:D:201:THR:HG21	2.07	0.54
1:G:38:VAL:HG22	1:G:132:ILE:HD12	1.90	0.54
1:M:58:ASN:C	1:M:58:ASN:HD22	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:44:GLY:O	1:O:45:ASP:HB2	2.08	0.54
1:C:217:VAL:O	1:C:220:ALA:HB3	2.07	0.54
1:C:296:VAL:HG13	2:D:131:THR:CG2	2.37	0.54
1:E:42:ALA:HB1	1:E:46:THR:HG21	1.90	0.54
1:G:198:PHE:HA	1:G:241:ILE:CD1	2.37	0.54
1:G:341:ASP:O	1:G:344:VAL:HG23	2.07	0.54
2:H:9:VAL:HG12	2:H:100:LEU:HD13	1.88	0.54
4:K:601:LYS:N	2:L:44:ILE:H	2.06	0.54
1:O:8:TYR:CE1	1:O:22:VAL:HG13	2.43	0.54
1:E:182:ALA:HB2	1:E:402:HIS:HD1	1.73	0.54
4:K:601:LYS:N	2:L:44:ILE:N	2.55	0.54
1:A:234:SER:OG	1:A:235:ASN:N	2.40	0.54
2:B:18:VAL:HG22	2:B:63:PHE:CE2	2.43	0.54
2:H:37:LEU:HD21	2:H:63:PHE:CE2	2.43	0.54
1:K:299:ASN:OD1	2:L:62:THR:HG21	2.08	0.54
1:C:179:VAL:HG12	1:C:211:ILE:HD13	1.90	0.54
1:E:294:ASP:HB3	1:E:313:THR:CG2	2.38	0.54
1:C:38:VAL:HG13	1:C:132:ILE:HD13	1.89	0.54
1:E:218:GLU:HG2	2:F:5:VAL:CG2	2.35	0.54
1:E:269:VAL:HG12	1:E:272:ILE:HD11	1.89	0.54
1:G:36:VAL:HG13	1:G:130:ILE:HG12	1.90	0.54
2:P:17:LYS:HB3	2:P:95:VAL:HG21	1.89	0.54
1:M:368:LEU:HD23	1:M:375:ILE:CD1	2.38	0.53
1:E:123:GLU:O	1:E:124:ALA:HB3	2.07	0.53
1:K:328:LYS:O	1:K:331:VAL:HG12	2.09	0.53
1:A:339:LEU:HD22	1:M:89:GLY:CA	2.37	0.53
1:I:369:ARG:HD3	2:J:28:GLY:HA3	1.89	0.53
1:M:245:MET:SD	1:M:383:ILE:HD13	2.47	0.53
1:A:72:ALA:HB3	1:C:76:ILE:HG22	1.89	0.53
1:G:42:ALA:HB1	1:G:46:THR:HG23	1.89	0.53
1:G:224:ASN:ND2	5:G:616:HOH:O	2.40	0.53
1:O:291:ILE:CD1	1:O:322:ALA:HB2	2.33	0.53
1:C:291:ILE:HD11	1:C:325:ILE:HD12	1.91	0.53
2:H:81:GLN:NE2	2:H:87:THR:O	2.41	0.53
1:K:311:THR:CB	2:L:50:ASN:HD21	2.21	0.53
2:P:11:THR:HB	2:P:145:LEU:HD21	1.91	0.53
2:P:18:VAL:HG13	2:P:63:PHE:CE1	2.44	0.53
2:B:85:ASN:ND2	2:B:86:TRP:NE1	2.57	0.53
2:F:19:THR:CB	2:F:62:THR:HG22	2.38	0.53
2:H:17:LYS:HD2	2:H:62:THR:HG21	1.91	0.53
2:P:119:LEU:HG	2:P:126:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:LYS:CB	1:G:344:VAL:HG21	2.38	0.53
1:G:268:THR:CG2	1:G:270:LEU:HD22	2.37	0.53
1:I:26:ILE:HG22	1:I:130:ILE:HD13	1.91	0.53
2:B:116:MET:HA	2:B:116:MET:HE3	1.91	0.53
1:E:368:LEU:O	1:E:371:VAL:O	2.26	0.53
1:I:207:VAL:HG11	1:I:384:ARG:CD	2.39	0.53
1:K:368:LEU:HD23	1:K:375:ILE:HD11	1.91	0.53
2:L:50:ASN:ND2	2:L:51:VAL:H	2.06	0.53
1:A:125:LEU:HD13	1:A:131:CYS:SG	2.49	0.53
1:E:325:ILE:N	1:E:325:ILE:HD13	2.23	0.53
1:M:118:PRO:O	1:M:121:VAL:HG12	2.08	0.53
1:M:154:SER:HA	1:M:157:THR:HG23	1.90	0.53
1:M:270:LEU:HD23	1:M:337:ASN:O	2.08	0.53
1:A:26:ILE:HG22	1:A:130:ILE:HD13	1.91	0.52
1:G:402:HIS:HA	1:G:407:LEU:HD23	1.90	0.52
1:K:300:VAL:O	1:K:301:PHE:CB	2.57	0.52
1:E:42:ALA:HB3	1:E:47:THR:HG23	1.91	0.52
2:H:46:MET:HE3	2:H:97:LYS:HE3	1.92	0.52
1:K:375:ILE:CD1	1:K:375:ILE:N	2.72	0.52
1:C:266:LYS:HE3	2:D:51:VAL:HG11	1.91	0.52
1:I:279:ALA:CB	3:I:501:THR:HG23	2.30	0.52
1:K:361:THR:CG2	4:K:601:LYS:O	2.55	0.52
1:M:4:VAL:O	1:M:36:VAL:HA	2.10	0.52
1:A:57:VAL:HG13	1:C:84:ALA:HB2	1.92	0.52
1:A:198:PHE:CE2	1:A:242:ALA:O	2.62	0.52
1:E:201:MET:CE	1:E:212:LEU:HD23	2.39	0.52
1:E:299:ASN:ND2	2:F:62:THR:HG21	2.11	0.52
2:F:98:VAL:CG1	2:F:145:LEU:HD12	2.39	0.52
1:M:368:LEU:HD23	1:M:375:ILE:HD11	1.92	0.52
2:N:98:VAL:CG1	2:N:145:LEU:HD12	2.39	0.52
1:G:301:PHE:HZ	2:H:21:LEU:HD21	1.73	0.52
1:A:262:LYS:CG	1:A:394:LEU:HD23	2.40	0.52
2:D:19:THR:CB	2:D:62:THR:HG22	2.39	0.52
1:O:154:SER:HA	1:O:157:THR:HG23	1.89	0.52
1:O:383:ILE:HD13	1:O:383:ILE:H	1.74	0.52
2:F:122:VAL:HG12	2:F:122:VAL:O	2.10	0.52
3:G:501:THR:CG2	3:G:501:THR:OXT	2.58	0.52
1:K:371:VAL:O	1:K:371:VAL:CG1	2.57	0.52
1:C:332:GLN:O	1:C:334:ASN:N	2.43	0.52
1:K:58:ASN:C	1:K:58:ASN:HD22	2.13	0.52
1:O:207:VAL:HG11	1:O:348:SER:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:122:VAL:CG1	2:P:147:ALA:HB1	2.37	0.52
1:G:345:GLY:HA3	1:G:394:LEU:HD21	1.92	0.52
1:M:375:ILE:HG23	1:M:387:VAL:HG13	1.92	0.52
1:G:326:LEU:HD12	1:G:329:LEU:HD22	1.91	0.52
1:O:95:PHE:HB3	1:O:116:VAL:HG23	1.92	0.52
1:I:366:GLU:OE2	2:J:35:ARG:NH1	2.42	0.51
1:K:368:LEU:HG	1:K:373:VAL:HG21	1.92	0.51
2:N:122:VAL:HG13	2:N:124:VAL:CG1	2.39	0.51
1:O:94:SER:HA	1:O:132:ILE:HG23	1.91	0.51
1:A:192:LYS:NZ	1:A:236:ASP:OD2	2.41	0.51
1:A:296:VAL:HG13	2:B:131:THR:HG21	1.91	0.51
1:I:189:ASN:C	1:I:189:ASN:HD22	2.14	0.51
1:K:323:MET:SD	1:M:59:PRO:HG2	2.51	0.51
1:O:40:CYS:SG	1:O:132:ILE:HD11	2.50	0.51
1:C:179:VAL:O	1:C:179:VAL:HG23	2.08	0.51
1:C:294:ASP:HB3	1:C:313:THR:HG22	1.91	0.51
2:F:19:THR:HG23	2:F:62:THR:HG22	1.91	0.51
1:G:270:LEU:HD21	1:G:339:LEU:HG	1.92	0.51
2:P:21:LEU:O	2:P:87:THR:HG22	2.11	0.51
2:P:31:ALA:O	2:P:35:ARG:HB2	2.10	0.51
1:E:42:ALA:CB	1:E:46:THR:HG23	2.40	0.51
2:F:42:ILE:HD13	2:F:73:ALA:CB	2.41	0.51
1:K:255:LEU:HA	1:K:351:GLY:HA3	1.92	0.51
1:O:38:VAL:CG2	1:O:132:ILE:HD13	2.41	0.51
1:A:330:GLN:NE2	1:A:337:ASN:HA	2.25	0.51
1:C:51:LEU:HD12	1:C:66:MET:HE3	1.91	0.51
1:K:299:ASN:OD1	2:L:62:THR:CG2	2.59	0.51
2:P:140:ILE:HG22	2:P:141:ARG:N	2.24	0.51
1:K:25:ARG:NH1	1:K:234:SER:O	2.41	0.51
2:L:18:VAL:HG22	2:L:63:PHE:CE2	2.46	0.51
1:O:279:ALA:HB2	3:O:501:THR:CG2	2.36	0.51
1:A:323:MET:HE1	1:A:338:VAL:CG2	2.40	0.51
2:N:98:VAL:HG23	2:N:138:VAL:HG22	1.93	0.51
1:A:76:ILE:CD1	1:C:72:ALA:HB3	2.40	0.51
1:A:76:ILE:HD13	1:C:72:ALA:HB3	1.93	0.51
1:A:294:ASP:O	1:A:295:MET:C	2.50	0.51
1:E:215:ARG:CD	1:E:215:ARG:N	2.73	0.51
1:E:330:GLN:O	1:E:333:GLY:N	2.44	0.51
2:L:19:THR:CG2	2:L:62:THR:HG22	2.41	0.51
1:M:204:LEU:HD21	1:M:350:VAL:HG12	1.92	0.51
1:M:369:ARG:HD3	2:N:28:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:LEU:HD13	1:G:167:ALA:HA	1.91	0.51
1:I:133:VAL:HG11	1:I:161:LEU:CD2	2.41	0.51
1:O:50:LEU:HG	1:O:69:LEU:HD11	1.91	0.51
1:O:58:ASN:HD22	1:O:59:PRO:N	2.09	0.51
1:K:299:ASN:ND2	2:L:62:THR:HG23	2.23	0.50
2:B:114:GLU:OE2	2:B:155:GLN:NE2	2.36	0.50
1:E:132:ILE:HD12	1:E:132:ILE:O	2.12	0.50
1:K:198:PHE:O	1:K:202:LEU:HD22	2.11	0.50
1:K:207:VAL:HG12	1:K:207:VAL:O	2.12	0.50
1:O:279:ALA:CB	3:O:501:THR:HG22	2.33	0.50
1:E:273:SER:HA	1:E:307:THR:HG22	1.92	0.50
1:G:269:VAL:HA	1:G:338:VAL:HG12	1.93	0.50
3:G:501:THR:N	2:H:125:ASN:OD1	2.44	0.50
1:K:349:LEU:HD22	1:K:405:PHE:CE2	2.47	0.50
2:L:20:VAL:HG13	2:L:86:TRP:CE3	2.46	0.50
2:F:37:LEU:HD21	2:F:63:PHE:CZ	2.46	0.50
1:K:297:LEU:HD23	1:K:377:LEU:HG	1.93	0.50
2:L:25:ASP:O	1:O:31:LYS:NZ	2.45	0.50
1:C:279:ALA:CB	3:C:501:THR:HG22	2.36	0.50
1:K:387:VAL:HG12	1:K:389:ILE:HG23	1.92	0.50
2:P:15:GLU:CD	2:P:64:THR:HG21	2.32	0.50
1:E:186:ILE:HD12	1:E:395:ASP:OD2	2.12	0.50
1:I:60:VAL:HG23	1:I:60:VAL:O	2.12	0.50
1:M:207:VAL:HG21	1:M:384:ARG:HD2	1.94	0.50
1:A:196:LEU:HD11	1:A:200:GLU:HB3	1.93	0.50
2:B:72:ARG:NH1	2:B:76:ILE:HD11	2.27	0.50
1:C:355:LYS:HB2	1:C:383:ILE:CD1	2.42	0.50
1:C:355:LYS:HB2	1:C:383:ILE:HD12	1.94	0.50
2:F:23:ILE:HD13	2:F:61:ILE:HG13	1.94	0.50
2:B:112:THR:O	2:B:116:MET:HG2	2.11	0.50
1:C:26:ILE:HG13	1:C:85:ILE:HD11	1.94	0.50
1:G:4:VAL:HG21	1:G:29:THR:HG21	1.94	0.50
1:M:282:VAL:HG22	1:M:335:TRP:CZ3	2.47	0.50
1:C:23:ALA:HB1	1:C:85:ILE:HD13	1.93	0.49
1:C:365:MET:CE	1:C:375:ILE:HD13	2.42	0.49
1:E:125:LEU:HD13	1:E:131:CYS:SG	2.52	0.49
1:K:254:VAL:HG22	1:K:255:LEU:H	1.77	0.49
2:P:122:VAL:O	2:P:122:VAL:CG1	2.60	0.49
1:A:369:ARG:HG3	1:A:370:ASP:N	2.26	0.49
1:A:196:LEU:CD1	1:A:256:THR:HG21	2.41	0.49
2:D:128:LEU:HD23	2:D:129:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:LEU:HD23	2:H:48:LEU:C	2.32	0.49
1:I:4:VAL:HG21	1:I:29:THR:HG21	1.93	0.49
2:N:120:ARG:HG3	2:N:121:ASP:N	2.26	0.49
4:C:601:LYS:N	2:D:43:ASN:HD21	2.11	0.49
2:D:22:GLY:HA2	2:D:58:THR:HG21	1.95	0.49
2:J:80:LEU:HD23	2:J:86:TRP:HZ2	1.77	0.49
1:K:371:VAL:HG12	1:K:373:VAL:HG13	1.93	0.49
1:M:241:ILE:N	1:M:241:ILE:HD12	2.27	0.49
1:C:298:GLN:OE1	3:C:501:THR:HG21	2.12	0.49
1:E:85:ILE:HD13	1:E:90:ALA:HB3	1.95	0.49
2:H:56:ASP:CB	2:H:58:THR:HG22	2.43	0.49
1:K:207:VAL:HG13	1:K:346:LYS:CE	2.43	0.49
1:O:196:LEU:O	1:O:242:ALA:N	2.37	0.49
1:O:380:THR:CG2	2:P:46:MET:HA	2.41	0.49
1:A:3:LEU:HD21	1:A:165:LEU:HB3	1.95	0.49
1:A:284:ARG:HG2	1:A:284:ARG:NH1	2.22	0.49
1:E:58:ASN:HD22	1:E:59:PRO:N	2.10	0.49
1:M:6:GLN:NE2	1:M:8:TYR:OH	2.45	0.49
1:C:196:LEU:HD13	1:C:256:THR:HG21	1.94	0.49
1:K:402:HIS:O	1:K:405:PHE:O	2.31	0.49
1:I:297:LEU:HD12	2:J:130:SER:HA	1.95	0.49
1:O:38:VAL:HG22	1:O:132:ILE:CD1	2.41	0.49
2:B:72:ARG:O	2:B:76:ILE:HD13	2.13	0.49
1:C:156:THR:HG23	1:C:219:TYR:CD1	2.48	0.49
1:E:212:LEU:HD21	1:E:229:VAL:HG22	1.93	0.49
1:E:284:ARG:HG2	2:F:117:GLU:OE2	2.13	0.49
1:O:96:THR:HG22	1:O:115:ASP:HB2	1.95	0.49
1:C:207:VAL:HG12	5:C:605:HOH:O	2.13	0.48
1:G:285:ALA:CB	1:G:329:LEU:HD21	2.43	0.48
1:I:25:ARG:HH22	1:I:234:SER:C	2.13	0.48
2:N:69:ASP:OD2	2:N:72:ARG:NH1	2.46	0.48
1:O:311:THR:OG1	2:P:50:ASN:ND2	2.39	0.48
1:G:285:ALA:CB	1:G:325:ILE:HD11	2.39	0.48
1:I:87:SER:OG	1:I:88:LEU:HD22	2.13	0.48
2:L:9:VAL:HG13	2:L:153:HIS:CE1	2.47	0.48
2:L:19:THR:CB	2:L:62:THR:HG22	2.43	0.48
1:M:207:VAL:O	1:M:207:VAL:HG13	2.11	0.48
1:M:331:VAL:HG23	1:M:332:GLN:HG3	1.95	0.48
2:B:30:ALA:CB	3:B:201:THR:HG23	2.35	0.48
1:C:204:LEU:CD2	1:C:350:VAL:HG13	2.44	0.48
1:C:365:MET:HB3	2:D:31:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:TYR:CE2	1:E:26:ILE:CD1	2.96	0.48
1:C:215:ARG:HG2	1:C:219:TYR:CE1	2.48	0.48
1:E:85:ILE:C	1:E:85:ILE:HD12	2.34	0.48
1:E:294:ASP:OD1	1:E:313:THR:HG21	2.13	0.48
2:J:100:LEU:C	2:J:100:LEU:HD23	2.34	0.48
1:K:371:VAL:O	1:K:371:VAL:HG12	2.13	0.48
1:E:186:ILE:HD12	1:E:395:ASP:CG	2.34	0.48
1:I:214:LEU:HD21	2:J:134:ILE:HG22	1.94	0.48
1:I:369:ARG:HB2	2:J:28:GLY:HA2	1.94	0.48
1:O:3:LEU:HD11	1:O:165:LEU:HB3	1.95	0.48
2:P:56:ASP:HB2	2:P:58:THR:HB	1.94	0.48
2:F:79:LYS:O	2:F:80:LEU:HB2	2.13	0.48
1:M:296:VAL:HG13	2:N:131:THR:OG1	2.13	0.48
1:A:262:LYS:HG2	1:A:394:LEU:HD21	1.95	0.48
1:A:296:VAL:HG13	2:B:131:THR:HG23	1.94	0.48
1:E:375:ILE:HB	3:F:201:THR:HG22	1.96	0.48
2:H:128:LEU:HB3	2:H:139:LEU:HB2	1.94	0.48
1:K:361:THR:HG22	4:K:601:LYS:HG2	1.95	0.48
1:C:377:LEU:O	1:C:387:VAL:HG23	2.14	0.48
1:G:133:VAL:CG2	1:G:161:LEU:HD11	2.43	0.48
1:C:172:ILE:O	1:C:172:ILE:HG13	2.14	0.48
1:C:179:VAL:O	1:C:179:VAL:CG2	2.61	0.48
1:C:204:LEU:CD2	1:C:350:VAL:CG1	2.92	0.48
2:H:95:VAL:CG1	2:H:139:LEU:HB3	2.44	0.48
2:N:74:MET:SD	2:N:89:VAL:HG23	2.54	0.48
2:P:100:LEU:HD22	2:P:155:GLN:HE22	1.79	0.48
2:H:23:ILE:N	2:H:23:ILE:CD1	2.76	0.48
1:O:266:LYS:HE3	1:O:377:LEU:HD11	1.94	0.48
1:A:262:LYS:HD3	1:A:394:LEU:HD23	1.94	0.47
1:C:255:LEU:HD13	1:C:405:PHE:CD1	2.49	0.47
1:I:57:VAL:CG1	1:K:84:ALA:HB2	2.42	0.47
2:J:48:LEU:HD11	2:J:128:LEU:HD21	1.96	0.47
2:J:119:LEU:HD11	2:J:152:LEU:HD11	1.95	0.47
2:N:99:SER:HA	2:N:136:ILE:O	2.14	0.47
1:O:125:LEU:HD13	1:O:131:CYS:SG	2.54	0.47
1:O:269:VAL:HA	1:O:338:VAL:HG12	1.95	0.47
2:B:19:THR:HG23	2:B:62:THR:CG2	2.43	0.47
2:F:18:VAL:HG22	2:F:63:PHE:CE2	2.49	0.47
1:M:35:ASP:HB3	1:M:125:LEU:HG	1.97	0.47
2:P:23:ILE:HD12	2:P:61:ILE:HG13	1.95	0.47
1:E:214:LEU:HD13	2:F:133:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:277:GLY:O	1:I:280:ALA:HB3	2.14	0.47
2:J:19:THR:OG1	2:J:62:THR:OG1	2.22	0.47
1:M:329:LEU:HD23	1:M:335:TRP:CZ2	2.49	0.47
2:P:98:VAL:HG22	2:P:145:LEU:CD1	2.44	0.47
1:C:3:LEU:HD23	1:C:3:LEU:C	2.34	0.47
1:C:133:VAL:O	1:C:133:VAL:HG23	2.14	0.47
1:E:179:VAL:HG22	1:E:193:LEU:HD23	1.96	0.47
1:G:301:PHE:CZ	2:H:19:THR:HG21	2.49	0.47
1:M:327:LYS:HG2	1:M:338:VAL:HG13	1.95	0.47
1:E:26:ILE:HG22	1:E:130:ILE:HD13	1.97	0.47
1:O:165:LEU:O	1:O:167:ALA:N	2.48	0.47
1:A:297:LEU:HD13	1:A:377:LEU:CD2	2.38	0.47
1:C:94:SER:HA	1:C:132:ILE:HG23	1.95	0.47
2:J:139:LEU:O	2:J:140:ILE:HD12	2.14	0.47
1:K:176:VAL:HG12	1:K:178:GLY:H	1.80	0.47
3:K:501:THR:N	2:L:125:ASN:OD1	2.47	0.47
1:M:211:ILE:HG22	1:M:212:LEU:CD1	2.40	0.47
1:O:206:ALA:HB1	2:P:133:GLU:HB2	1.96	0.47
1:A:366:GLU:OE2	2:B:35:ARG:NH1	2.47	0.47
1:C:298:GLN:HE22	3:C:501:THR:HB	1.80	0.47
1:E:12:SER:HA	1:E:18:ARG:HH12	1.79	0.47
1:C:90:ALA:HB1	1:C:130:ILE:CD1	2.45	0.47
1:I:196:LEU:HD12	1:I:196:LEU:N	2.30	0.47
1:I:327:LYS:NZ	1:I:330:GLN:HE22	2.12	0.47
1:O:296:VAL:C	1:O:297:LEU:HD12	2.35	0.47
1:G:196:LEU:N	1:G:196:LEU:HD12	2.30	0.47
2:L:72:ARG:O	2:L:76:ILE:HG12	2.14	0.47
1:C:91:GLU:CD	2:P:54:VAL:HG11	2.35	0.46
1:I:77:SER:O	1:I:81:VAL:HG23	2.15	0.46
1:M:3:LEU:HD11	1:M:165:LEU:HB3	1.97	0.46
1:M:154:SER:O	1:M:157:THR:HG23	2.15	0.46
1:O:291:ILE:HG23	1:O:291:ILE:O	2.15	0.46
1:C:85:ILE:HG21	1:C:130:ILE:HD13	1.96	0.46
1:E:78:ASN:CG	1:E:132:ILE:HD13	2.35	0.46
1:E:297:LEU:HB2	1:E:311:THR:CG2	2.45	0.46
1:E:360:VAL:HG12	4:E:601:LYS:HB2	1.96	0.46
1:G:387:VAL:HG12	1:G:389:ILE:HG23	1.97	0.46
1:O:58:ASN:ND2	1:O:60:VAL:H	2.12	0.46
2:B:48:LEU:HD22	2:B:128:LEU:HD23	1.97	0.46
1:C:179:VAL:HG12	1:C:211:ILE:CD1	2.45	0.46
1:C:354:MET:O	4:C:601:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:VAL:CG2	2:B:63:PHE:CE2	2.98	0.46
2:B:53:SER:OG	2:B:56:ASP:N	2.45	0.46
1:C:298:GLN:O	2:D:128:LEU:HG	2.16	0.46
2:F:38:ALA:O	2:F:40:ALA:O	2.33	0.46
2:J:98:VAL:HG12	2:J:138:VAL:CG2	2.46	0.46
1:M:196:LEU:CD2	1:M:201:MET:HB2	2.45	0.46
1:C:207:VAL:HG11	1:C:348:SER:HG	1.79	0.46
2:D:122:VAL:O	2:D:122:VAL:HG22	2.16	0.46
1:K:143:THR:O	1:K:146:VAL:HG22	2.15	0.46
1:O:204:LEU:CD2	1:O:259:ALA:HB2	2.46	0.46
2:B:40:ALA:HB1	2:B:72:ARG:NH2	2.30	0.46
1:C:181:THR:HG23	1:C:193:LEU:HD13	1.97	0.46
2:D:48:LEU:HD13	2:D:128:LEU:CD2	2.39	0.46
1:G:369:ARG:HH11	1:G:369:ARG:CG	2.27	0.46
1:M:76:ILE:HG22	1:O:72:ALA:HB3	1.97	0.46
2:N:20:VAL:HG13	2:N:86:TRP:CE3	2.50	0.46
1:O:30:LYS:HB3	1:O:36:VAL:CG1	2.45	0.46
1:C:297:LEU:HD21	1:C:377:LEU:HD23	1.96	0.46
2:F:95:VAL:HG11	2:F:139:LEU:HD13	1.98	0.46
1:G:371:VAL:HG23	1:G:372:ASN:N	2.30	0.46
2:N:11:THR:HG22	2:N:98:VAL:HG12	1.98	0.46
1:C:27:VAL:CG2	1:C:85:ILE:HG23	2.46	0.46
1:G:64:ARG:NH1	1:G:65:GLU:OE2	2.49	0.46
1:M:80:LEU:HD23	1:M:83:MET:CE	2.43	0.46
1:O:361:THR:CG2	4:O:601:LYS:HG2	2.46	0.46
1:A:58:ASN:C	1:A:58:ASN:ND2	2.69	0.46
1:C:43:MET:SD	1:C:76:ILE:HD11	2.56	0.46
1:C:375:ILE:HB	3:D:201:THR:CG2	2.46	0.46
2:D:106:LYS:HB2	2:D:133:GLU:HG2	1.97	0.46
1:E:38:VAL:HG22	1:E:132:ILE:HG22	1.98	0.46
1:E:201:MET:HE2	1:E:212:LEU:HD23	1.97	0.46
2:F:19:THR:CG2	2:F:62:THR:HG22	2.45	0.46
1:M:3:LEU:CD1	1:M:165:LEU:HB3	2.45	0.46
1:M:329:LEU:HD23	1:M:335:TRP:CH2	2.51	0.46
2:N:128:LEU:HB3	2:N:139:LEU:HB2	1.97	0.46
1:A:363:GLU:HG3	5:A:624:HOH:O	2.16	0.46
1:I:271:GLY:HA3	1:I:336:THR:HG23	1.97	0.46
1:I:300:VAL:HG12	2:J:127:GLU:O	2.15	0.46
1:K:172:ILE:N	1:K:172:ILE:HD12	2.30	0.46
1:M:207:VAL:HG11	1:M:348:SER:CB	2.46	0.46
1:O:6:GLN:NE2	1:O:8:TYR:OH	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:296:VAL:HG12	2:P:131:THR:CG2	2.46	0.46
1:E:365:MET:HB3	2:F:31:ALA:HB2	1.98	0.45
1:K:368:LEU:HD13	1:K:401:LEU:CD1	2.45	0.45
2:L:125:ASN:HD22	2:L:141:ARG:NH1	2.14	0.45
1:O:375:ILE:CG2	1:O:387:VAL:HG22	2.44	0.45
1:A:78:ASN:ND2	1:A:132:ILE:HG22	2.31	0.45
1:A:80:LEU:HD23	1:A:83:MET:HE2	1.96	0.45
1:A:83:MET:HE1	1:C:54:ALA:HA	1.98	0.45
1:C:375:ILE:O	3:D:201:THR:N	2.50	0.45
2:D:29:GLU:OE2	2:D:32:LYS:NZ	2.50	0.45
1:G:296:VAL:HG13	2:H:131:THR:CG2	2.46	0.45
1:G:296:VAL:HG12	2:H:131:THR:OG1	2.16	0.45
1:I:39:VAL:HG22	1:I:133:VAL:CG1	2.43	0.45
1:O:287:ALA:O	1:O:289:ALA:N	2.48	0.45
1:O:296:VAL:HG13	2:P:129:ILE:HG13	1.98	0.45
1:E:292:ASN:C	1:E:293:ILE:HD12	2.37	0.45
1:K:207:VAL:HG13	1:K:346:LYS:NZ	2.31	0.45
1:M:383:ILE:O	1:M:383:ILE:CG2	2.61	0.45
1:O:289:ALA:HB3	1:O:291:ILE:HG22	1.99	0.45
2:B:122:VAL:HG13	2:B:122:VAL:O	2.15	0.45
2:D:19:THR:CG2	2:D:62:THR:HG22	2.45	0.45
2:H:156:PHE:O	2:H:157:GLN:CB	2.64	0.45
1:I:176:VAL:HG11	1:I:211:ILE:HD12	1.97	0.45
1:I:296:VAL:HG13	2:J:131:THR:HG21	1.99	0.45
1:M:85:ILE:CG2	1:M:90:ALA:HB3	2.47	0.45
1:O:18:ARG:HD3	5:O:609:HOH:O	2.17	0.45
1:G:64:ARG:CD	1:G:64:ARG:H	2.30	0.45
2:J:115:PHE:O	2:J:119:LEU:HD13	2.16	0.45
1:A:228:ARG:HG2	1:A:230:ARG:HD2	1.99	0.45
1:A:269:VAL:CG1	1:A:272:ILE:HD11	2.46	0.45
1:C:361:THR:OG1	4:C:601:LYS:HG2	2.16	0.45
1:E:212:LEU:HD21	1:E:229:VAL:HG21	1.96	0.45
2:H:119:LEU:HD12	2:H:126:ILE:HG12	1.99	0.45
1:I:179:VAL:CG1	1:I:239:THR:HG21	2.46	0.45
1:K:184:PRO:HB3	1:K:190:ALA:HB3	1.99	0.45
1:K:375:ILE:N	1:K:375:ILE:HD12	2.32	0.45
1:M:376:GLU:O	1:M:377:LEU:HD12	2.16	0.45
2:N:17:LYS:HB3	2:N:64:THR:HG22	1.99	0.45
2:D:22:GLY:HA2	2:D:58:THR:CG2	2.47	0.45
1:G:270:LEU:N	1:G:270:LEU:CD2	2.78	0.45
1:I:202:LEU:CD1	1:I:217:VAL:HG12	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:99:SER:HA	2:J:136:ILE:O	2.17	0.45
1:O:207:VAL:HG21	1:O:384:ARG:CD	2.47	0.45
2:B:74:MET:HE3	2:B:91:TYR:CD2	2.52	0.45
1:G:36:VAL:CG1	1:G:130:ILE:HG12	2.47	0.45
1:G:245:MET:O	1:G:248:ILE:HG12	2.16	0.45
1:G:266:LYS:HB2	1:G:344:VAL:HG21	1.98	0.45
1:M:133:VAL:HG11	1:M:161:LEU:HD13	1.99	0.45
1:M:209:SER:CB	1:M:211:ILE:HD12	2.46	0.45
1:A:297:LEU:HD23	2:B:48:LEU:HD23	1.99	0.45
1:A:311:THR:HG23	2:B:50:ASN:CG	2.37	0.45
1:C:156:THR:CG2	1:C:219:TYR:CE1	2.99	0.45
2:F:19:THR:OG1	2:F:62:THR:CG2	2.63	0.45
1:K:51:LEU:HD22	1:K:70:LEU:HD21	1.98	0.45
1:K:164:ALA:O	1:K:165:LEU:CB	2.64	0.45
1:A:212:LEU:HD11	1:A:229:VAL:HG22	1.99	0.44
1:C:3:LEU:HD22	1:C:167:ALA:HB2	1.99	0.44
1:G:49:GLU:O	1:G:53:LEU:HD23	2.17	0.44
1:G:266:LYS:HB3	1:G:344:VAL:HG21	1.98	0.44
1:I:59:PRO:O	1:I:60:VAL:HG22	2.17	0.44
1:I:68:MET:HG2	1:K:79:ALA:HB2	1.99	0.44
1:I:299:ASN:ND2	2:J:62:THR:HB	2.32	0.44
1:I:203:GLU:CD	2:J:134:ILE:HD11	2.38	0.44
2:L:50:ASN:HD22	2:L:51:VAL:H	1.65	0.44
1:M:215:ARG:NH1	2:N:5:VAL:HG11	2.31	0.44
2:P:81:GLN:NE2	2:P:88:ASN:HA	2.32	0.44
1:A:297:LEU:HD11	1:A:379:SER:HB3	1.99	0.44
2:D:91:TYR:CE2	2:D:93:ASP:HB3	2.51	0.44
1:G:204:LEU:HG	1:G:350:VAL:HG21	1.99	0.44
1:G:279:ALA:CB	3:G:501:THR:HG23	2.44	0.44
1:M:296:VAL:O	2:N:130:SER:HA	2.17	0.44
1:O:322:ALA:O	1:O:325:ILE:HG22	2.17	0.44
2:B:67:ARG:NH1	2:B:142:GLU:OE2	2.50	0.44
2:P:22:GLY:HA2	2:P:58:THR:CG2	2.48	0.44
1:E:296:VAL:CG2	2:F:129:ILE:HG21	2.47	0.44
2:F:76:ILE:O	2:F:77:LEU:CB	2.66	0.44
2:H:79:LYS:O	2:H:80:LEU:HB2	2.18	0.44
2:J:31:ALA:O	2:J:35:ARG:HB2	2.18	0.44
1:K:156:THR:HG21	2:L:3:GLU:OE1	2.18	0.44
2:P:82:VAL:HG12	2:P:82:VAL:O	2.17	0.44
2:B:122:VAL:HG12	2:B:124:VAL:HG13	1.99	0.44
1:G:58:ASN:C	1:G:58:ASN:ND2	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:ASN:C	1:I:58:ASN:HD22	2.21	0.44
1:O:214:LEU:HD22	2:P:134:ILE:CG2	2.48	0.44
1:C:207:VAL:HG21	1:C:384:ARG:HD2	1.99	0.44
2:H:30:ALA:HB2	3:H:201:THR:HG22	1.97	0.44
1:I:204:LEU:HD21	1:I:350:VAL:CG2	2.48	0.44
1:I:369:ARG:HB2	2:J:28:GLY:CA	2.48	0.44
1:K:126:ASP:O	1:K:127:GLU:HB2	2.16	0.44
1:K:168:ASP:O	1:K:169:VAL:CG1	2.63	0.44
2:B:92:ASP:CG	2:B:95:VAL:HG23	2.38	0.44
1:C:26:ILE:HB	1:C:85:ILE:HD12	1.99	0.44
1:C:198:PHE:HA	1:C:241:ILE:CD1	2.48	0.44
1:C:271:GLY:HA3	1:C:336:THR:HG23	1.99	0.44
2:F:79:LYS:O	2:F:80:LEU:CB	2.66	0.44
1:K:368:LEU:CD1	1:K:401:LEU:CD1	2.96	0.44
1:M:76:ILE:HG13	1:M:77:SER:N	2.33	0.44
1:M:330:GLN:HE21	1:M:338:VAL:HG12	1.83	0.44
1:O:58:ASN:HD22	1:O:60:VAL:H	1.66	0.44
1:C:179:VAL:CG2	1:C:239:THR:HG21	2.41	0.44
1:C:297:LEU:CD1	1:C:377:LEU:HD21	2.48	0.44
1:E:292:ASN:O	1:E:293:ILE:HD12	2.17	0.44
2:N:81:GLN:NE2	2:N:88:ASN:HA	2.33	0.44
1:A:389:ILE:HD11	1:A:394:LEU:CD1	2.47	0.43
1:E:80:LEU:HA	1:E:83:MET:CE	2.46	0.43
4:E:601:LYS:HE2	2:F:45:ASP:O	2.18	0.43
1:G:301:PHE:HZ	2:H:19:THR:HG21	1.83	0.43
1:I:5:VAL:HG13	1:I:37:VAL:CG2	2.48	0.43
1:K:325:ILE:HG22	1:K:326:LEU:HD13	1.98	0.43
2:N:4:ALA:HB2	2:N:104:GLY:O	2.18	0.43
2:N:128:LEU:HD23	2:N:129:ILE:N	2.33	0.43
1:O:2:ALA:HB3	1:O:34:ASN:HD22	1.83	0.43
1:O:266:LYS:CE	1:O:377:LEU:HD11	2.48	0.43
1:A:83:MET:CE	1:C:54:ALA:HA	2.49	0.43
1:A:240:LEU:HG	1:A:242:ALA:HB2	2.00	0.43
1:C:78:ASN:C	1:C:78:ASN:HD22	2.22	0.43
2:H:128:LEU:HD23	2:H:128:LEU:C	2.39	0.43
2:L:33:VAL:HG13	2:L:77:LEU:HD21	1.99	0.43
2:L:48:LEU:HD13	2:L:128:LEU:HD11	2.00	0.43
1:M:196:LEU:HD23	1:M:196:LEU:C	2.38	0.43
2:P:139:LEU:C	2:P:140:ILE:HD12	2.38	0.43
1:A:267:VAL:HG13	1:A:323:MET:HE3	1.99	0.43
1:G:299:ASN:ND2	2:H:62:THR:OG1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:GLN:OE1	3:H:201:THR:HG21	2.18	0.43
2:H:99:SER:HA	2:H:136:ILE:O	2.18	0.43
1:K:126:ASP:O	1:K:127:GLU:CB	2.65	0.43
1:K:201:MET:HB2	1:K:241:ILE:HD12	1.99	0.43
1:O:168:ASP:O	1:O:169:VAL:HG13	2.18	0.43
2:B:115:PHE:HD2	2:B:116:MET:HE3	1.84	0.43
1:C:196:LEU:HD13	1:C:256:THR:CG2	2.48	0.43
1:K:366:GLU:OE2	2:L:35:ARG:HG2	2.18	0.43
1:M:177:ASP:HA	1:M:231:SER:HB2	1.99	0.43
1:I:204:LEU:CD2	1:I:350:VAL:CG2	2.96	0.43
2:J:126:ILE:HG21	2:J:129:ILE:CG1	2.48	0.43
1:K:193:LEU:O	1:K:239:THR:HG23	2.18	0.43
1:M:37:VAL:HG12	1:M:125:LEU:HD11	1.99	0.43
1:M:215:ARG:CZ	2:N:5:VAL:CG1	2.92	0.43
2:N:9:VAL:HG13	2:N:153:HIS:CE1	2.54	0.43
2:P:74:MET:O	2:P:78:LYS:N	2.44	0.43
1:K:361:THR:O	1:K:365:MET:HG2	2.19	0.43
2:L:25:ASP:OD1	3:L:201:THR:N	2.51	0.43
1:M:212:LEU:HD13	1:M:212:LEU:N	2.33	0.43
1:O:165:LEU:O	1:O:166:ASN:C	2.56	0.43
1:C:198:PHE:HB3	1:C:221:ARG:HB3	1.99	0.43
1:E:311:THR:HG21	1:E:377:LEU:HD21	1.99	0.43
1:M:196:LEU:CD2	1:M:197:SER:O	2.67	0.43
2:P:48:LEU:HD11	2:P:130:SER:HB2	2.01	0.43
1:A:331:VAL:O	1:A:332:GLN:HB2	2.18	0.43
2:B:6:LEU:O	2:B:158:LEU:HD11	2.19	0.43
2:D:116:MET:HE3	2:D:126:ILE:CD1	2.48	0.43
1:G:245:MET:HA	1:G:248:ILE:HD13	2.00	0.43
2:H:98:VAL:HG22	2:H:145:LEU:HD12	2.01	0.43
1:I:199:GLU:HG2	1:I:245:MET:HG3	2.01	0.43
1:M:215:ARG:HG2	2:N:5:VAL:HG13	2.00	0.43
1:M:299:ASN:O	1:M:300:VAL:CG2	2.58	0.43
1:A:255:LEU:CD1	1:A:405:PHE:CD1	3.02	0.43
1:C:352:ALA:HA	1:C:383:ILE:CG1	2.48	0.43
1:G:215:ARG:HD3	1:G:215:ARG:HA	1.88	0.43
2:H:128:LEU:HD23	2:H:129:ILE:N	2.33	0.43
1:M:5:VAL:HG13	1:M:37:VAL:HG22	2.01	0.43
1:M:215:ARG:NE	2:N:5:VAL:HG11	2.34	0.43
4:C:601:LYS:N	2:D:43:ASN:ND2	2.66	0.43
1:M:133:VAL:HG11	1:M:161:LEU:CD1	2.48	0.42
1:M:172:ILE:HG21	1:M:212:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HG23	1:A:169:VAL:HG23	2.00	0.42
1:E:51:LEU:HD13	1:E:70:LEU:HD21	2.01	0.42
1:G:211:ILE:CG2	1:G:212:LEU:HD22	2.26	0.42
1:I:57:VAL:HG13	1:K:20:ARG:HG3	2.00	0.42
1:M:207:VAL:HG11	1:M:348:SER:HB2	2.02	0.42
1:O:296:VAL:HG12	2:P:131:THR:OG1	2.19	0.42
1:A:267:VAL:CG1	1:A:323:MET:CE	2.94	0.42
1:A:371:VAL:HG12	1:A:372:ASN:H	1.84	0.42
2:D:35:ARG:NH1	5:D:314:HOH:O	2.51	0.42
2:F:122:VAL:HG12	2:F:124:VAL:CG2	2.38	0.42
1:K:199:GLU:CG	1:K:245:MET:HG2	2.49	0.42
2:L:128:LEU:HD22	2:L:139:LEU:HG	2.01	0.42
1:M:369:ARG:O	1:M:371:VAL:O	2.37	0.42
1:M:402:HIS:O	1:M:405:PHE:O	2.37	0.42
1:C:254:VAL:HG22	1:C:255:LEU:H	1.84	0.42
1:I:31:LYS:O	1:I:33:GLY:N	2.53	0.42
1:I:241:ILE:O	1:I:241:ILE:HG22	2.19	0.42
1:M:125:LEU:HD13	1:M:131:CYS:SG	2.59	0.42
1:M:254:VAL:HG13	1:M:255:LEU:N	2.35	0.42
1:C:198:PHE:HA	1:C:241:ILE:HD11	2.01	0.42
1:C:376:GLU:OE1	1:C:390:ARG:HD2	2.20	0.42
2:D:19:THR:O	2:D:89:VAL:HA	2.19	0.42
1:I:85:ILE:HG23	1:I:90:ALA:HB3	2.02	0.42
1:K:376:GLU:OE2	1:K:390:ARG:HD2	2.19	0.42
1:M:213:VAL:HG23	1:M:213:VAL:O	2.19	0.42
1:M:334:ASN:HB3	1:M:335:TRP:CE3	2.54	0.42
1:M:376:GLU:C	1:M:377:LEU:HD12	2.40	0.42
1:O:8:TYR:CZ	1:O:22:VAL:HG13	2.54	0.42
1:A:377:LEU:HD23	1:A:378:ILE:N	2.35	0.42
1:C:2:ALA:HB3	1:C:34:ASN:HD22	1.85	0.42
1:C:31:LYS:HB3	2:P:25:ASP:HB3	2.01	0.42
1:C:402:HIS:CE1	1:C:407:LEU:HB3	2.55	0.42
1:E:42:ALA:CB	1:E:46:THR:CG2	2.98	0.42
1:E:254:VAL:CG2	1:E:255:LEU:N	2.74	0.42
1:G:296:VAL:HG13	2:H:131:THR:HG23	2.01	0.42
1:K:81:VAL:O	1:K:85:ILE:HG12	2.19	0.42
1:M:327:LYS:HG2	1:M:338:VAL:CG1	2.49	0.42
1:O:38:VAL:O	1:O:132:ILE:HD12	2.20	0.42
2:B:122:VAL:O	2:B:122:VAL:CG1	2.68	0.42
1:C:51:LEU:HD12	1:C:66:MET:HE1	1.97	0.42
1:C:293:ILE:O	2:D:106:LYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:ASN:HD21	2:F:62:THR:CG2	2.16	0.42
2:F:112:THR:O	2:F:116:MET:HG2	2.19	0.42
1:I:375:ILE:O	3:J:201:THR:N	2.52	0.42
2:P:15:GLU:OE1	2:P:64:THR:CG2	2.68	0.42
1:I:124:ALA:CB	1:I:131:CYS:SG	3.08	0.42
2:J:128:LEU:HB3	2:J:139:LEU:HB2	2.01	0.42
1:K:195:LYS:HA	1:K:240:LEU:O	2.19	0.42
2:L:128:LEU:HB3	2:L:139:LEU:HB2	2.02	0.42
1:M:368:LEU:HB3	1:M:373:VAL:HG23	2.02	0.42
2:N:48:LEU:CD1	2:N:128:LEU:CD2	2.80	0.42
1:O:368:LEU:HB3	1:O:373:VAL:HG13	2.01	0.42
2:B:119:LEU:HB3	2:B:124:VAL:CG2	2.50	0.42
2:D:18:VAL:HG13	2:D:63:PHE:CE1	2.55	0.42
2:F:81:GLN:OE1	2:F:89:VAL:HG23	2.20	0.42
1:I:212:LEU:HD12	1:I:212:LEU:HA	1.90	0.42
1:I:294:ASP:HB3	1:I:313:THR:CG2	2.50	0.42
1:I:296:VAL:HG13	2:J:131:THR:HG23	2.01	0.42
1:M:207:VAL:O	1:M:207:VAL:CG1	2.67	0.42
1:O:207:VAL:HG13	1:O:346:LYS:HE2	2.02	0.42
1:O:375:ILE:HG23	1:O:387:VAL:CG2	2.46	0.42
1:A:376:GLU:OE2	1:A:390:ARG:HD2	2.20	0.42
1:C:375:ILE:O	3:D:201:THR:HG22	2.20	0.42
1:G:51:LEU:HD13	1:G:70:LEU:HD21	2.02	0.42
2:L:142:GLU:O	2:L:145:LEU:HB2	2.20	0.42
1:O:179:VAL:HG22	1:O:239:THR:CG2	2.39	0.42
1:C:58:ASN:C	1:C:58:ASN:ND2	2.72	0.41
1:C:365:MET:HE2	1:C:375:ILE:HD13	2.02	0.41
1:K:18:ARG:NH2	1:K:233:TYR:CE2	2.88	0.41
2:B:119:LEU:HB3	2:B:124:VAL:HG23	2.01	0.41
1:G:374:ASN:OD1	3:H:201:THR:N	2.53	0.41
1:I:187:VAL:HG11	1:I:402:HIS:CD2	2.55	0.41
1:I:364:PHE:CZ	1:I:401:LEU:HD21	2.55	0.41
2:J:16:ALA:HB1	2:J:91:TYR:CE1	2.55	0.41
2:J:100:LEU:HD23	2:J:101:VAL:N	2.36	0.41
1:K:38:VAL:HG13	1:K:132:ILE:HG12	2.02	0.41
1:K:51:LEU:HD13	1:K:66:MET:CE	2.50	0.41
1:E:316:ARG:HH22	1:E:391:GLU:CD	2.24	0.41
2:J:80:LEU:H	2:J:80:LEU:HD22	1.84	0.41
2:L:49:GLN:HE21	2:L:61:ILE:HG12	1.85	0.41
1:M:368:LEU:HG	1:M:373:VAL:CG2	2.51	0.41
1:O:401:LEU:HD12	1:O:401:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:GLN:HE22	3:B:201:THR:HB	1.85	0.41
2:J:21:LEU:HD12	2:J:88:ASN:HB3	2.02	0.41
1:O:30:LYS:HG2	1:O:130:ILE:HD11	2.03	0.41
1:O:266:LYS:NZ	2:P:51:VAL:HG12	2.35	0.41
1:O:366:GLU:OE1	2:P:35:ARG:NH1	2.53	0.41
1:O:375:ILE:O	3:P:201:THR:N	2.54	0.41
2:B:9:VAL:HG13	2:B:153:HIS:CE1	2.55	0.41
1:C:3:LEU:HD22	1:C:167:ALA:CB	2.51	0.41
2:D:141:ARG:HA	2:D:141:ARG:NE	2.36	0.41
1:E:51:LEU:CD1	1:E:70:LEU:HD21	2.51	0.41
1:I:220:ALA:O	1:I:223:PHE:O	2.38	0.41
2:J:77:LEU:HB3	2:J:89:VAL:HG11	2.03	0.41
1:C:272:ILE:CD1	1:C:310:ILE:HD12	2.50	0.41
1:C:299:ASN:HD21	2:D:62:THR:CG2	2.32	0.41
2:F:21:LEU:HD12	2:F:88:ASN:HB3	2.03	0.41
2:F:42:ILE:HD11	2:F:65:CYS:SG	2.60	0.41
2:F:76:ILE:O	2:F:77:LEU:HG	2.20	0.41
2:F:128:LEU:HD23	2:F:128:LEU:C	2.40	0.41
2:P:15:GLU:CD	2:P:64:THR:CG2	2.89	0.41
2:P:115:PHE:HD2	2:P:116:MET:HE3	1.85	0.41
2:F:4:ALA:HB2	2:F:104:GLY:O	2.20	0.41
1:K:327:LYS:NZ	1:K:330:GLN:HE22	2.19	0.41
1:M:18:ARG:NE	1:M:233:TYR:OH	2.38	0.41
1:M:204:LEU:HD21	1:M:350:VAL:HG11	1.94	0.41
1:M:294:ASP:OD1	1:M:346:LYS:NZ	2.54	0.41
2:N:98:VAL:HG23	2:N:138:VAL:CG2	2.50	0.41
1:O:125:LEU:HD12	1:O:125:LEU:HA	1.95	0.41
1:A:72:ALA:CB	1:C:76:ILE:HG22	2.51	0.41
1:A:286:LEU:HD13	1:A:293:ILE:HD11	2.02	0.41
1:C:365:MET:HE3	1:C:375:ILE:HD13	2.03	0.41
1:I:309:ASP:HB2	2:J:51:VAL:CG2	2.50	0.41
2:J:112:THR:O	2:J:116:MET:HG2	2.21	0.41
1:O:198:PHE:O	1:O:202:LEU:HD22	2.20	0.41
1:O:202:LEU:HD13	1:O:202:LEU:HA	1.91	0.41
1:O:377:LEU:HD13	1:O:388:LEU:CD1	2.50	0.41
1:C:204:LEU:HD23	1:C:350:VAL:HG13	2.02	0.41
1:E:376:GLU:O	1:E:377:LEU:HD12	2.21	0.41
2:F:48:LEU:HD13	2:F:128:LEU:HD11	2.02	0.41
1:I:58:ASN:ND2	1:I:59:PRO:O	2.54	0.41
1:I:163:ALA:HB1	1:I:223:PHE:CG	2.56	0.41
1:I:332:GLN:O	1:I:333:GLY:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:380:THR:HG21	2:J:45:ASP:O	2.20	0.41
1:M:83:MET:HE2	1:M:83:MET:HB2	1.87	0.41
1:M:366:GLU:HG2	1:M:369:ARG:NH2	2.36	0.41
1:M:368:LEU:CD2	1:M:375:ILE:HD11	2.50	0.41
2:N:116:MET:HE3	2:N:126:ILE:CD1	2.49	0.41
2:P:16:ALA:O	2:P:64:THR:HA	2.20	0.41
1:C:27:VAL:HG23	1:C:85:ILE:HG23	2.02	0.41
1:E:5:VAL:HG22	1:E:37:VAL:HG13	2.02	0.41
1:I:54:ALA:CB	1:K:83:MET:HE1	2.45	0.41
1:K:7:LYS:HA	1:K:39:VAL:O	2.21	0.41
1:K:298:GLN:O	2:L:128:LEU:HG	2.21	0.41
1:A:177:ASP:O	1:A:238:GLY:HA2	2.21	0.40
1:E:210:LYS:HB2	1:E:210:LYS:NZ	2.36	0.40
1:E:368:LEU:HB3	1:E:373:VAL:HG22	2.02	0.40
2:F:42:ILE:CD1	2:F:73:ALA:CB	2.99	0.40
1:I:294:ASP:HB3	1:I:313:THR:HG22	2.03	0.40
1:M:7:LYS:HA	1:M:39:VAL:O	2.21	0.40
2:P:22:GLY:HA2	2:P:58:THR:HG23	2.02	0.40
1:A:327:LYS:HG2	1:A:338:VAL:CG1	2.51	0.40
1:C:375:ILE:HB	3:D:201:THR:HG23	2.03	0.40
1:G:38:VAL:CG2	1:G:132:ILE:HD12	2.50	0.40
1:G:284:ARG:HG2	2:H:117:GLU:OE2	2.21	0.40
1:G:368:LEU:HD12	1:G:375:ILE:HD11	2.02	0.40
1:K:157:THR:O	1:K:161:LEU:HD23	2.21	0.40
4:C:601:LYS:HB2	5:C:609:HOH:O	2.22	0.40
2:D:19:THR:HG23	2:D:62:THR:HG23	2.02	0.40
1:E:2:ALA:HB3	1:E:34:ASN:HD21	1.84	0.40
2:H:119:LEU:HD22	2:H:148:ALA:HB1	2.03	0.40
1:I:16:ALA:HB2	1:K:53:LEU:CD1	2.51	0.40
1:I:189:ASN:C	1:I:189:ASN:ND2	2.74	0.40
1:K:266:LYS:NZ	2:L:51:VAL:HG11	2.37	0.40
1:M:118:PRO:CA	1:M:121:VAL:HG12	2.50	0.40
1:O:2:ALA:HB3	1:O:34:ASN:ND2	2.36	0.40
1:O:5:VAL:HA	1:O:37:VAL:O	2.21	0.40
1:A:323:MET:O	1:A:327:LYS:HB2	2.21	0.40
1:A:323:MET:SD	1:A:338:VAL:HG22	2.62	0.40
1:C:25:ARG:HB3	1:C:25:ARG:HH11	1.86	0.40
1:E:229:VAL:HG23	1:E:241:ILE:CD1	2.51	0.40
1:I:221:ARG:HG3	1:I:222:ALA:N	2.36	0.40
1:I:292:ASN:OD1	1:I:292:ASN:N	2.51	0.40
2:J:100:LEU:C	2:J:100:LEU:CD2	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:126:ILE:HG21	2:L:129:ILE:HG12	2.03	0.40
2:N:42:ILE:HD11	2:N:72:ARG:HG2	2.03	0.40
2:N:122:VAL:O	2:N:122:VAL:HG22	2.21	0.40
2:P:39:ASP:O	2:P:40:ALA:CB	2.68	0.40
1:E:18:ARG:O	1:E:22:VAL:HG23	2.21	0.40
1:K:368:LEU:CD1	1:K:401:LEU:HD11	2.49	0.40
1:M:375:ILE:HD13	1:M:387:VAL:HG11	2.04	0.40
2:P:128:LEU:HD22	2:P:139:LEU:HG	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:ASP:OD2	2:N:39:ASP:OD2[1_655]	2.12	0.08

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	362/421 (86%)	346 (96%)	15 (4%)	1 (0%)	41 59
1	C	359/421 (85%)	341 (95%)	15 (4%)	3 (1%)	19 33
1	E	358/421 (85%)	335 (94%)	16 (4%)	7 (2%)	7 11
1	G	345/421 (82%)	329 (95%)	15 (4%)	1 (0%)	41 59
1	I	350/421 (83%)	327 (93%)	15 (4%)	8 (2%)	6 9
1	K	365/421 (87%)	349 (96%)	14 (4%)	2 (0%)	29 46
1	M	369/421 (88%)	355 (96%)	13 (4%)	1 (0%)	41 59
1	O	354/421 (84%)	326 (92%)	23 (6%)	5 (1%)	11 18
2	B	151/178 (85%)	141 (93%)	8 (5%)	2 (1%)	12 19
2	D	144/178 (81%)	136 (94%)	8 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	142/178 (80%)	133 (94%)	5 (4%)	4 (3%)	5 6
2	H	147/178 (83%)	140 (95%)	5 (3%)	2 (1%)	11 18
2	J	124/178 (70%)	115 (93%)	9 (7%)	0	100 100
2	L	152/178 (85%)	145 (95%)	7 (5%)	0	100 100
2	N	153/178 (86%)	149 (97%)	4 (3%)	0	100 100
2	P	145/178 (82%)	136 (94%)	7 (5%)	2 (1%)	11 18
All	All	4020/4792 (84%)	3803 (95%)	179 (4%)	38 (1%)	17 29

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	MET
1	C	333	GLY
1	E	124	ALA
1	E	190	ALA
2	F	74	MET
1	I	224	ASN
1	I	372	ASN
1	K	127	GLU
1	K	334	ASN
1	M	300	VAL
1	O	166	ASN
2	P	40	ALA
2	B	162	ASP
1	C	44	GLY
1	E	242	ALA
2	F	77	LEU
2	H	80	LEU
2	H	157	GLN
1	I	44	GLY
1	I	333	GLY
1	I	334	ASN
1	O	44	GLY
2	B	143	ASP
1	E	44	GLY
1	I	32	ALA
2	P	39	ASP
1	E	334	ASN
2	F	40	ALA
1	I	242	ALA

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Mol	Chain	Res	Type
1	O	242	ALA
1	O	289	ALA
1	C	250	VAL
1	E	189	ASN
1	E	188	PRO
2	F	80	LEU
1	G	331	VAL
1	O	208	GLY
1	I	211	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	286/336 (85%)	252 (88%)	34 (12%)	5 9
1	C	287/336 (85%)	253 (88%)	34 (12%)	5 9
1	E	280/336 (83%)	239 (85%)	41 (15%)	3 5
1	G	270/336 (80%)	227 (84%)	43 (16%)	2 4
1	I	277/336 (82%)	238 (86%)	39 (14%)	3 5
1	K	286/336 (85%)	250 (87%)	36 (13%)	4 7
1	M	294/336 (88%)	254 (86%)	40 (14%)	3 6
1	O	272/336 (81%)	236 (87%)	36 (13%)	4 6
2	B	125/146 (86%)	113 (90%)	12 (10%)	8 15
2	D	122/146 (84%)	109 (89%)	13 (11%)	6 11
2	F	112/146 (77%)	105 (94%)	7 (6%)	18 32
2	H	115/146 (79%)	109 (95%)	6 (5%)	23 41
2	J	99/146 (68%)	84 (85%)	15 (15%)	3 4
2	L	127/146 (87%)	113 (89%)	14 (11%)	6 10
2	N	123/146 (84%)	107 (87%)	16 (13%)	4 7
2	P	117/146 (80%)	99 (85%)	18 (15%)	2 4
All	All	3192/3856 (83%)	2788 (87%)	404 (13%)	4 7

All (404) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	58	ASN
1	A	66	MET
1	A	88	LEU
1	A	125	LEU
1	A	133	VAL
1	A	169	VAL
1	A	176	VAL
1	A	179	VAL
1	A	189	ASN
1	A	193	LEU
1	A	194	GLU
1	A	199	GLU
1	A	212	LEU
1	A	213	VAL
1	A	228	ARG
1	A	234	SER
1	A	245	MET
1	A	251	GLU
1	A	254	VAL
1	A	260	THR
1	A	266	LYS
1	A	284	ARG
1	A	296	VAL
1	A	297	LEU
1	A	317	SER
1	A	320	ARG
1	A	326	LEU
1	A	328	LYS
1	A	350	VAL
1	A	369	ARG
1	A	373	VAL
1	A	389	ILE
1	A	401	LEU
2	B	9	VAL
2	B	18	VAL
2	B	35	ARG
2	B	37	LEU
2	B	52	PHE
2	B	77	LEU
2	B	85	ASN
2	B	89	VAL

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Mol	Chain	Res	Type
2	B	98	VAL
2	B	116	MET
2	B	120	ARG
2	B	145	LEU
1	C	4	VAL
1	C	25	ARG
1	C	37	VAL
1	C	51	LEU
1	C	58	ASN
1	C	65	GLU
1	C	66	MET
1	C	76	ILE
1	C	77	SER
1	C	78	ASN
1	C	165	LEU
1	C	193	LEU
1	C	202	LEU
1	C	212	LEU
1	C	241	ILE
1	C	250	VAL
1	C	293	ILE
1	C	296	VAL
1	C	299	ASN
1	C	313	THR
1	C	326	LEU
1	C	332	GLN
1	C	338	VAL
1	C	360	VAL
1	C	365	MET
1	C	368	LEU
1	C	369	ARG
1	C	373	VAL
1	C	377	LEU
1	C	383	ILE
1	C	389	ILE
1	C	399	ARG
1	C	401	LEU
1	C	406	GLN
2	D	18	VAL
2	D	29	GLU
2	D	35	ARG
2	D	37	LEU

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Mol	Chain	Res	Type
2	D	48	LEU
2	D	50	ASN
2	D	68	SER
2	D	77	LEU
2	D	86	TRP
2	D	89	VAL
2	D	93	ASP
2	D	116	MET
2	D	143	ASP
1	E	3	LEU
1	E	4	VAL
1	E	35	ASP
1	E	36	VAL
1	E	37	VAL
1	E	38	VAL
1	E	46	THR
1	E	50	LEU
1	E	51	LEU
1	E	53	LEU
1	E	58	ASN
1	E	65	GLU
1	E	67	ASP
1	E	85	ILE
1	E	125	LEU
1	E	132	ILE
1	E	166	ASN
1	E	179	VAL
1	E	193	LEU
1	E	202	LEU
1	E	210	LYS
1	E	215	ARG
1	E	264	GLU
1	E	278	GLU
1	E	284	ARG
1	E	291	ILE
1	E	296	VAL
1	E	313	THR
1	E	316	ARG
1	E	325	ILE
1	E	326	LEU
1	E	328	LYS
1	E	338	VAL

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Mol	Chain	Res	Type
1	E	360	VAL
1	E	365	MET
1	E	373	VAL
1	E	380	THR
1	E	390	ARG
1	E	399	ARG
1	E	401	LEU
1	E	406	GLN
2	F	5	VAL
2	F	9	VAL
2	F	37	LEU
2	F	48	LEU
2	F	51	VAL
2	F	86	TRP
2	F	120	ARG
1	G	3	LEU
1	G	4	VAL
1	G	18	ARG
1	G	24	GLU
1	G	25	ARG
1	G	30	LYS
1	G	37	VAL
1	G	38	VAL
1	G	46	THR
1	G	51	LEU
1	G	58	ASN
1	G	64	ARG
1	G	77	SER
1	G	121	VAL
1	G	125	LEU
1	G	133	VAL
1	G	157	THR
1	G	169	VAL
1	G	196	LEU
1	G	199	GLU
1	G	202	LEU
1	G	215	ARG
1	G	241	ILE
1	G	248	ILE
1	G	254	VAL
1	G	260	THR
1	G	270	LEU

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Mol	Chain	Res	Type
1	G	284	ARG
1	G	296	VAL
1	G	311	THR
1	G	313	THR
1	G	325	ILE
1	G	336	THR
1	G	350	VAL
1	G	357	HIS
1	G	361	THR
1	G	365	MET
1	G	369	ARG
1	G	371	VAL
1	G	379	SER
1	G	390	ARG
1	G	394	LEU
1	G	407	LEU
2	H	18	VAL
2	H	35	ARG
2	H	37	LEU
2	H	77	LEU
2	H	134	ILE
2	H	155	GLN
1	I	4	VAL
1	I	18	ARG
1	I	36	VAL
1	I	37	VAL
1	I	38	VAL
1	I	46	THR
1	I	50	LEU
1	I	51	LEU
1	I	53	LEU
1	I	58	ASN
1	I	78	ASN
1	I	120	ARG
1	I	157	THR
1	I	179	VAL
1	I	189	ASN
1	I	196	LEU
1	I	202	LEU
1	I	212	LEU
1	I	214	LEU
1	I	221	ARG

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Mol	Chain	Res	Type
1	I	245	MET
1	I	260	THR
1	I	292	ASN
1	I	293	ILE
1	I	296	VAL
1	I	297	LEU
1	I	300	VAL
1	I	311	THR
1	I	313	THR
1	I	316	ARG
1	I	317	SER
1	I	326	LEU
1	I	332	GLN
1	I	338	VAL
1	I	357	HIS
1	I	377	LEU
1	I	387	VAL
1	I	390	ARG
1	I	401	LEU
2	J	9	VAL
2	J	18	VAL
2	J	35	ARG
2	J	41	GLU
2	J	50	ASN
2	J	62	THR
2	J	71	ARG
2	J	75	GLU
2	J	77	LEU
2	J	80	LEU
2	J	81	GLN
2	J	88	ASN
2	J	120	ARG
2	J	141	ARG
2	J	146	ASP
1	K	3	LEU
1	K	4	VAL
1	K	14	GLU
1	K	30	LYS
1	K	36	VAL
1	K	38	VAL
1	K	58	ASN
1	K	65	GLU

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Mol	Chain	Res	Type
1	K	66	MET
1	K	120	ARG
1	K	133	VAL
1	K	149	LEU
1	K	193	LEU
1	K	194	GLU
1	K	212	LEU
1	K	215	ARG
1	K	224	ASN
1	K	241	ILE
1	K	251	GLU
1	K	284	ARG
1	K	296	VAL
1	K	297	LEU
1	K	313	THR
1	K	323	MET
1	K	325	ILE
1	K	326	LEU
1	K	328	LYS
1	K	329	LEU
1	K	334	ASN
1	K	338	VAL
1	K	350	VAL
1	K	361	THR
1	K	375	ILE
1	K	385	ILE
1	K	392	ASP
1	K	401	LEU
2	L	9	VAL
2	L	11	THR
2	L	18	VAL
2	L	35	ARG
2	L	37	LEU
2	L	50	ASN
2	L	67	ARG
2	L	88	ASN
2	L	98	VAL
2	L	120	ARG
2	L	140	ILE
2	L	141	ARG
2	L	145	LEU
2	L	157	GLN

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Mol	Chain	Res	Type
1	M	3	LEU
1	M	4	VAL
1	M	18	ARG
1	M	36	VAL
1	M	37	VAL
1	M	38	VAL
1	M	46	THR
1	M	50	LEU
1	M	53	LEU
1	M	58	ASN
1	M	65	GLU
1	M	66	MET
1	M	75	ARG
1	M	76	ILE
1	M	117	THR
1	M	133	VAL
1	M	154	SER
1	M	157	THR
1	M	165	LEU
1	M	169	VAL
1	M	193	LEU
1	M	202	LEU
1	M	212	LEU
1	M	215	ARG
1	M	219	TYR
1	M	254	VAL
1	M	260	THR
1	M	270	LEU
1	M	290	GLU
1	M	293	ILE
1	M	296	VAL
1	M	326	LEU
1	M	338	VAL
1	M	358	PRO
1	M	360	VAL
1	M	361	THR
1	M	365	MET
1	M	399	ARG
1	M	401	LEU
1	M	406	GLN
2	N	9	VAL
2	N	13	LYS

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Mol	Chain	Res	Type
2	N	18	VAL
2	N	23	ILE
2	N	37	LEU
2	N	42	ILE
2	N	48	LEU
2	N	53	SER
2	N	77	LEU
2	N	83	GLN
2	N	89	VAL
2	N	116	MET
2	N	120	ARG
2	N	124	VAL
2	N	146	ASP
2	N	155	GLN
1	O	3	LEU
1	O	4	VAL
1	O	30	LYS
1	O	36	VAL
1	O	37	VAL
1	O	47	THR
1	O	50	LEU
1	O	53	LEU
1	O	58	ASN
1	O	64	ARG
1	O	65	GLU
1	O	75	ARG
1	O	77	SER
1	O	78	ASN
1	O	88	LEU
1	O	117	THR
1	O	125	LEU
1	O	133	VAL
1	O	154	SER
1	O	157	THR
1	O	165	LEU
1	O	177	ASP
1	O	193	LEU
1	O	202	LEU
1	O	221	ARG
1	O	236	ASP
1	O	247	ASP
1	O	339	LEU

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Mol	Chain	Res	Type
1	O	350	VAL
1	O	365	MET
1	O	369	ARG
1	O	380	THR
1	O	383	ILE
1	O	389	ILE
1	O	392	ASP
1	O	401	LEU
2	P	18	VAL
2	P	26	LYS
2	P	35	ARG
2	P	48	LEU
2	P	50	ASN
2	P	56	ASP
2	P	58	THR
2	P	64	THR
2	P	68	SER
2	P	81	GLN
2	P	86	TRP
2	P	87	THR
2	P	116	MET
2	P	117	GLU
2	P	129	ILE
2	P	140	ILE
2	P	154	GLU
2	P	155	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	58	ASN
1	A	189	ASN
1	A	402	HIS
2	B	43	ASN
2	B	88	ASN
1	C	6	GLN
1	C	21	ASN
1	C	34	ASN
1	C	58	ASN
1	C	78	ASN
1	C	166	ASN

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Mol	Chain	Res	Type
1	C	292	ASN
1	C	299	ASN
1	C	330	GLN
1	C	334	ASN
1	C	402	HIS
1	C	406	GLN
2	D	50	ASN
2	D	85	ASN
1	E	6	GLN
1	E	34	ASN
1	E	58	ASN
1	E	166	ASN
1	E	299	ASN
1	E	330	GLN
1	E	334	ASN
2	F	43	ASN
2	F	49	GLN
2	F	108	HIS
1	G	6	GLN
1	G	58	ASN
1	G	224	ASN
1	G	299	ASN
1	G	402	HIS
1	G	406	GLN
2	H	43	ASN
2	H	81	GLN
2	H	85	ASN
2	H	94	GLN
2	H	123	ASN
1	I	6	GLN
1	I	34	ASN
1	I	58	ASN
1	I	78	ASN
1	I	189	ASN
1	I	224	ASN
1	I	330	GLN
1	I	374	ASN
1	I	402	HIS
2	J	43	ASN
2	J	88	ASN
2	J	153	HIS
1	K	6	GLN

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Mol	Chain	Res	Type
1	K	34	ASN
1	K	58	ASN
1	K	330	GLN
1	K	374	ASN
1	K	402	HIS
2	L	43	ASN
2	L	49	GLN
2	L	50	ASN
2	L	88	ASN
2	L	125	ASN
1	M	6	GLN
1	M	58	ASN
1	M	93	GLN
1	M	189	ASN
1	M	224	ASN
1	M	330	GLN
1	M	402	HIS
1	M	404	GLN
2	N	43	ASN
2	N	83	GLN
1	O	6	GLN
1	O	34	ASN
1	O	58	ASN
1	O	78	ASN
1	O	224	ASN
1	O	337	ASN
2	P	50	ASN
2	P	81	GLN
2	P	85	ASN
2	P	94	GLN

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)

23 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	$\#\|Z\| > 2$
3	THR	A	501	-	6,7,7	0.92	1 (16%)	7,9,9	1.12	1 (14%)
3	THR	M	501	-	6,7,7	1.00	1 (16%)	7,9,9	1.45	2 (28%)
3	THR	J	201	-	6,7,7	1.02	1 (16%)	7,9,9	1.43	1 (14%)
4	LYS	M	601	-	8,9,9	0.95	1 (12%)	9,10,10	1.56	2 (22%)
3	THR	F	201	-	6,7,7	1.09	1 (16%)	7,9,9	1.43	2 (28%)
4	LYS	E	601	-	8,9,9	0.82	1 (12%)	9,10,10	1.14	1 (11%)
4	LYS	C	601	-	8,9,9	0.83	1 (12%)	9,10,10	1.19	1 (11%)
3	THR	D	201	-	6,7,7	0.96	1 (16%)	7,9,9	1.24	1 (14%)
3	THR	O	501	-	6,7,7	0.98	1 (16%)	7,9,9	1.32	2 (28%)
4	LYS	O	601	-	8,9,9	0.86	1 (12%)	9,10,10	1.24	2 (22%)
3	THR	I	501	-	6,7,7	0.94	1 (16%)	7,9,9	1.17	1 (14%)
3	THR	C	501	-	6,7,7	0.85	0	7,9,9	1.26	2 (28%)
3	THR	P	201	-	6,7,7	1.10	1 (16%)	7,9,9	1.47	1 (14%)
4	LYS	A	601	-	8,9,9	0.74	0	9,10,10	0.97	0
3	THR	E	501	-	6,7,7	0.97	1 (16%)	7,9,9	1.42	2 (28%)
3	THR	K	501	-	6,7,7	0.96	0	7,9,9	1.41	1 (14%)
3	THR	L	201	-	6,7,7	0.94	1 (16%)	7,9,9	1.35	1 (14%)
3	THR	N	201	-	6,7,7	0.91	0	7,9,9	1.03	1 (14%)
3	THR	H	201	-	6,7,7	0.99	0	7,9,9	1.34	1 (14%)
3	THR	G	501	-	6,7,7	0.90	0	7,9,9	1.27	2 (28%)
3	THR	B	201	-	6,7,7	1.06	0	7,9,9	1.13	1 (14%)
4	LYS	G	601	-	8,9,9	0.76	0	9,10,10	1.36	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LYS	K	601	-	8,9,9	0.99	1 (12%)	9,10,10	1.41	2 (22%)

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
3	THR	A	501	-	-	0/8/8/8	-
3	THR	M	501	-	-	0/8/8/8	-
3	THR	J	201	-	-	0/8/8/8	-
4	LYS	M	601	-	-	2/9/9/9	-
3	THR	F	201	-	-	3/8/8/8	-
4	LYS	E	601	-	-	1/9/9/9	-
4	LYS	C	601	-	-	4/9/9/9	-
3	THR	D	201	-	-	0/8/8/8	-
3	THR	O	501	-	-	0/8/8/8	-
4	LYS	O	601	-	-	4/9/9/9	-
3	THR	I	501	-	-	2/8/8/8	-
3	THR	C	501	-	-	0/8/8/8	-
3	THR	P	201	-	-	0/8/8/8	-
4	LYS	A	601	-	-	2/9/9/9	-
3	THR	E	501	-	-	3/8/8/8	-
3	THR	K	501	-	-	4/8/8/8	-
3	THR	L	201	-	-	0/8/8/8	-
3	THR	N	201	-	-	0/8/8/8	-
3	THR	H	201	-	-	4/8/8/8	-
3	THR	G	501	-	-	4/8/8/8	-
3	THR	B	201	-	-	4/8/8/8	-
4	LYS	G	601	-	-	1/9/9/9	-
4	LYS	K	601	-	-	3/9/9/9	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	201	THR	OXT-C	-2.46	1.22	1.30
3	J	201	THR	OXT-C	-2.41	1.22	1.30
3	P	201	THR	OXT-C	-2.40	1.22	1.30
4	M	601	LYS	OXT-C	-2.39	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	601	LYS	OXT-C	-2.34	1.22	1.30
3	M	501	THR	OXT-C	-2.25	1.23	1.30
3	O	501	THR	OXT-C	-2.23	1.23	1.30
3	E	501	THR	OXT-C	-2.22	1.23	1.30
4	E	601	LYS	OXT-C	-2.22	1.23	1.30
4	O	601	LYS	OXT-C	-2.17	1.23	1.30
4	C	601	LYS	OXT-C	-2.15	1.23	1.30
3	L	201	THR	OXT-C	-2.09	1.23	1.30
3	D	201	THR	OXT-C	-2.07	1.23	1.30
3	I	501	THR	OXT-C	-2.07	1.23	1.30
3	A	501	THR	OXT-C	-2.04	1.23	1.30

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	601	LYS	OXT-C-O	-3.71	115.67	124.09
3	P	201	THR	OXT-C-O	-3.37	116.44	124.09
3	J	201	THR	OXT-C-O	-3.15	116.94	124.09
3	F	201	THR	OXT-C-O	-3.07	117.12	124.09
3	K	501	THR	OXT-C-O	-3.04	117.19	124.09
3	M	501	THR	OXT-C-O	-3.02	117.24	124.09
4	K	601	LYS	OXT-C-CA	2.97	123.49	113.38
3	E	501	THR	OXT-C-O	-2.93	117.45	124.09
3	H	201	THR	OXT-C-O	-2.88	117.54	124.09
3	L	201	THR	OXT-C-O	-2.85	117.61	124.09
4	O	601	LYS	OXT-C-O	-2.81	117.70	124.09
4	C	601	LYS	OXT-C-O	-2.81	117.71	124.09
4	G	601	LYS	OXT-C-O	-2.80	117.74	124.09
4	G	601	LYS	OXT-C-CA	2.66	122.46	113.38
3	O	501	THR	OXT-C-O	-2.61	118.16	124.09
3	D	201	THR	OXT-C-O	-2.60	118.18	124.09
4	E	601	LYS	OXT-C-O	-2.58	118.23	124.09
3	I	501	THR	OXT-C-O	-2.56	118.29	124.09
3	G	501	THR	OXT-C-O	-2.49	118.44	124.09
4	M	601	LYS	OXT-C-CA	2.37	121.44	113.38
3	C	501	THR	OXT-C-O	-2.34	118.78	124.09
3	A	501	THR	OXT-C-O	-2.27	118.93	124.09
3	M	501	THR	OXT-C-CA	2.26	122.12	114.22
4	K	601	LYS	OXT-C-O	-2.25	118.98	124.09
3	B	201	THR	OXT-C-O	-2.23	119.02	124.09
3	C	501	THR	OXT-C-CA	2.19	121.88	114.22
3	O	501	THR	OXT-C-CA	2.14	121.72	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	501	THR	OXT-C-CA	2.14	121.71	114.22
3	N	201	THR	OXT-C-O	-2.08	119.36	124.09
4	O	601	LYS	OXT-C-CA	2.08	120.45	113.38
3	G	501	THR	OXT-C-CA	2.07	121.46	114.22
3	F	201	THR	OXT-C-CA	2.05	121.40	114.22

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	THR	N-CA-CB-OG1
3	B	201	THR	C-CA-CB-OG1
3	B	201	THR	C-CA-CB-CG2
3	E	501	THR	O-C-CA-CB
3	E	501	THR	OXT-C-CA-CB
3	G	501	THR	C-CA-CB-OG1
3	G	501	THR	C-CA-CB-CG2
3	H	201	THR	N-CA-CB-OG1
3	H	201	THR	N-CA-CB-CG2
3	H	201	THR	C-CA-CB-OG1
3	H	201	THR	C-CA-CB-CG2
3	I	501	THR	C-CA-CB-OG1
3	K	501	THR	N-CA-CB-OG1
3	K	501	THR	N-CA-CB-CG2
3	K	501	THR	C-CA-CB-OG1
3	K	501	THR	C-CA-CB-CG2
4	A	601	LYS	C-CA-CB-CG
4	C	601	LYS	N-CA-CB-CG
4	K	601	LYS	C-CA-CB-CG
4	O	601	LYS	N-CA-CB-CG
4	O	601	LYS	C-CA-CB-CG
4	M	601	LYS	CA-CB-CG-CD
4	A	601	LYS	CA-CB-CG-CD
4	E	601	LYS	CE-CD-CG-CB
4	G	601	LYS	CG-CD-CE-NZ
3	B	201	THR	N-CA-CB-CG2
3	G	501	THR	N-CA-CB-CG2
4	O	601	LYS	CE-CD-CG-CB
4	C	601	LYS	CG-CD-CE-NZ
3	E	501	THR	OXT-C-CA-N
3	F	201	THR	N-CA-CB-OG1
4	C	601	LYS	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
4	M	601	LYS	C-CA-CB-CG
3	F	201	THR	C-CA-CB-OG1
4	K	601	LYS	CG-CD-CE-NZ
3	F	201	THR	N-CA-CB-CG2
4	K	601	LYS	CE-CD-CG-CB
4	C	601	LYS	CE-CD-CG-CB
3	G	501	THR	N-CA-CB-OG1
4	O	601	LYS	CG-CD-CE-NZ
3	I	501	THR	C-CA-CB-CG2

There are no ring outliers.

18 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	201	THR	2	0
4	M	601	LYS	5	0
3	F	201	THR	6	0
4	E	601	LYS	2	0
4	C	601	LYS	5	0
3	D	201	THR	5	0
3	O	501	THR	4	0
4	O	601	LYS	2	0
3	I	501	THR	4	0
3	C	501	THR	6	0
3	P	201	THR	1	0
3	K	501	THR	6	0
3	L	201	THR	1	0
3	H	201	THR	6	0
3	G	501	THR	7	0
3	B	201	THR	6	0
4	G	601	LYS	2	0
4	K	601	LYS	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	370/421 (87%)	-0.07	1 (0%) 94 94	29, 45, 72, 83	0
1	C	367/421 (87%)	0.07	2 (0%) 91 91	38, 56, 69, 80	0
1	E	368/421 (87%)	-0.01	2 (0%) 91 91	35, 53, 72, 84	0
1	G	357/421 (84%)	-0.03	5 (1%) 75 77	38, 54, 74, 99	0
1	I	360/421 (85%)	0.06	3 (0%) 86 87	39, 61, 78, 101	0
1	K	373/421 (88%)	-0.04	5 (1%) 77 78	29, 50, 73, 90	0
1	M	377/421 (89%)	-0.02	5 (1%) 77 78	30, 45, 64, 74	0
1	O	364/421 (86%)	0.15	12 (3%) 46 49	37, 65, 88, 100	0
2	B	157/178 (88%)	-0.14	1 (0%) 89 90	27, 42, 66, 82	0
2	D	150/178 (84%)	0.13	5 (3%) 46 49	41, 61, 82, 92	0
2	F	148/178 (83%)	0.23	3 (2%) 65 67	46, 69, 91, 98	0
2	H	151/178 (84%)	0.03	1 (0%) 87 89	39, 65, 85, 94	0
2	J	132/178 (74%)	0.42	12 (9%) 9 8	55, 75, 91, 96	0
2	L	156/178 (87%)	-0.23	0 100 100	27, 44, 61, 69	0
2	N	155/178 (87%)	-0.10	0 100 100	31, 45, 63, 69	0
2	P	149/178 (83%)	0.38	12 (8%) 12 11	45, 71, 106, 120	0
All	All	4134/4792 (86%)	0.03	69 (1%) 70 71	27, 54, 81, 120	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	148	ALA	5.4
2	F	73	ALA	5.3
2	P	122	VAL	5.2
1	O	253	ALA	4.4
2	B	164	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	M	301	PHE	4.3
1	O	407	LEU	4.2
1	C	333	GLY	4.1
1	G	242	ALA	3.8
2	P	119	LEU	3.7
1	C	186	ILE	3.6
1	A	152	GLY	3.4
2	F	77	LEU	3.3
1	G	301	PHE	3.2
2	P	156	PHE	3.2
2	P	124	VAL	3.1
1	M	136	PHE	3.0
1	O	223	PHE	3.0
2	P	118	ALA	3.0
1	O	306	GLY	2.8
2	J	147	ALA	2.8
1	I	253	ALA	2.8
2	J	116	MET	2.8
2	P	88	ASN	2.7
2	F	124	VAL	2.7
2	J	143	ASP	2.7
1	O	272	ILE	2.7
2	P	52	PHE	2.7
2	J	152	LEU	2.7
2	D	6	LEU	2.6
2	J	21	LEU	2.6
1	O	280	ALA	2.6
2	J	98	VAL	2.6
1	O	286	LEU	2.6
1	O	287	ALA	2.5
1	K	161	LEU	2.5
2	P	157	GLN	2.5
2	P	150	ARG	2.5
1	G	300	VAL	2.5
2	D	52	PHE	2.4
2	J	151	ALA	2.4
1	M	130	ILE	2.4
1	M	406	GLN	2.4
1	E	189	ASN	2.4
2	J	124	VAL	2.4
1	G	335	TRP	2.4
1	E	3	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	165	LEU	2.4
1	O	219	TYR	2.3
1	K	2	ALA	2.3
2	J	138	VAL	2.3
1	K	233	TYR	2.3
2	P	126	ILE	2.3
1	M	2	ALA	2.3
1	O	4	VAL	2.3
2	D	80	LEU	2.2
1	G	253	ALA	2.2
2	D	124	VAL	2.2
2	P	82	VAL	2.2
1	K	143	THR	2.2
2	J	53	SER	2.2
2	P	89	VAL	2.1
1	O	161	LEU	2.1
2	H	9	VAL	2.1
2	J	102	GLY	2.1
1	I	60	VAL	2.1
1	O	152	GLY	2.1
1	K	331	VAL	2.0
2	D	122	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LYS	K	601	10/10	0.87	0.17	23,31,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	THR	H	201	8/8	0.92	0.22	36,36,37,38	0
3	THR	P	201	8/8	0.92	0.17	29,29,29,30	0
3	THR	G	501	8/8	0.92	0.26	9,9,10,11	0
3	THR	D	201	8/8	0.93	0.18	29,30,31,32	0
3	THR	I	501	8/8	0.93	0.29	43,43,43,44	0
4	LYS	O	601	10/10	0.93	0.13	31,32,32,32	0
3	THR	F	201	8/8	0.94	0.24	2,2,2,2	0
4	LYS	A	601	10/10	0.94	0.16	21,26,27,27	0
4	LYS	E	601	10/10	0.94	0.12	25,26,27,27	0
3	THR	C	501	8/8	0.94	0.20	42,42,42,42	0
4	LYS	M	601	10/10	0.94	0.16	16,17,18,18	0
3	THR	O	501	8/8	0.94	0.32	49,49,49,49	0
4	LYS	C	601	10/10	0.95	0.14	31,32,32,33	0
3	THR	E	501	8/8	0.95	0.29	41,42,42,43	0
4	LYS	G	601	10/10	0.95	0.11	25,26,26,26	0
3	THR	J	201	8/8	0.96	0.08	37,37,37,37	0
3	THR	K	501	8/8	0.96	0.16	33,34,34,34	0
3	THR	L	201	8/8	0.96	0.13	22,24,24,24	0
3	THR	B	201	8/8	0.96	0.17	28,29,29,31	0
3	THR	N	201	8/8	0.97	0.09	23,24,24,24	0
3	THR	A	501	8/8	0.97	0.13	25,26,26,27	0
3	THR	M	501	8/8	0.98	0.14	25,25,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.