



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:30 AM UTC

PDB ID : 3AB2 / pdb_00003ab2
Title : Crystal structure of aspartate kinase from *Corynebacterium glutamicum* in complex with threonine
Authors : Yoshida, A.; Tomita, T.; Kuzuyama, T.; Nishiyama, M.
Deposited on : 2009-11-30
Resolution : 2.59 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

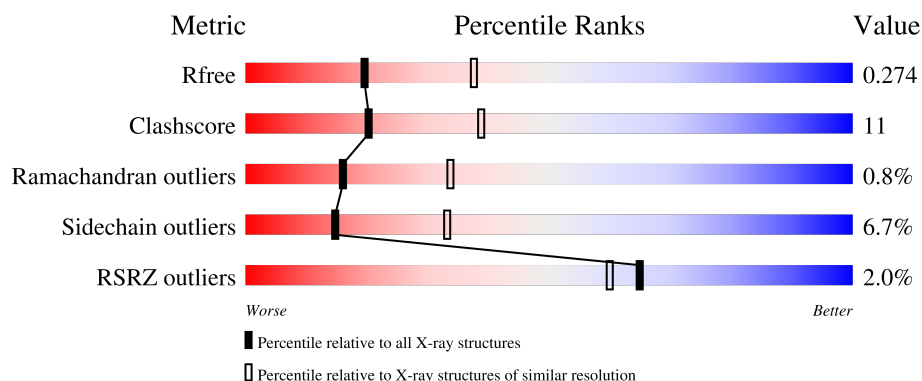
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	421	0.2% 68% 20% • 8%
1	C	421	2% 70% 18% • 10%
1	E	421	0.2% 68% 19% • 9%
1	G	421	2% 75% 14% • 9%
1	I	421	3% 69% 19% • 10%

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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	A	501	-	-	X	-
3	THR	C	501	-	-	X	-
3	THR	D	501	-	-	X	-
3	THR	F	501	-	-	X	-
3	THR	G	501	-	-	X	-
3	THR	J	501	-	-	X	-
3	THR	K	501	-	-	X	-
3	THR	L	501	-	-	X	-
3	THR	P	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31975 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	386	Total	C	N	O	S	0	0	0
			2841	1761	492	574	14			
1	C	380	Total	C	N	O	S	0	0	0
			2793	1737	478	564	14			
1	E	383	Total	C	N	O	S	0	0	0
			2814	1749	484	567	14			
1	G	383	Total	C	N	O	S	0	0	0
			2803	1742	483	564	14			
1	I	377	Total	C	N	O	S	0	0	0
			2748	1711	469	554	14			
1	K	382	Total	C	N	O	S	0	0	0
			2793	1733	480	566	14			
1	M	380	Total	C	N	O	S	0	0	0
			2796	1738	482	562	14			
1	O	386	Total	C	N	O	S	0	0	0
			2851	1767	493	577	14			

- Molecule 2 is a protein called Aspartokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1183	734	202	242	5			
2	D	152	Total	C	N	O	S	0	0	0
			1116	694	191	226	5			
2	F	155	Total	C	N	O	S	0	0	0
			1166	725	202	234	5			
2	H	155	Total	C	N	O	S	0	0	0
			1161	721	202	233	5			
2	J	152	Total	C	N	O	S	0	0	0
			1082	665	193	219	5			
2	L	152	Total	C	N	O	S	0	0	0
			1131	703	193	230	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	155	Total	C	N	O	S	0	0	0
			1135	707	196	227	5			
2	P	159	Total	C	N	O	S	0	0	0
			1196	741	207	243	5			

There are 56 discrepancies between the modelled and reference sequences:

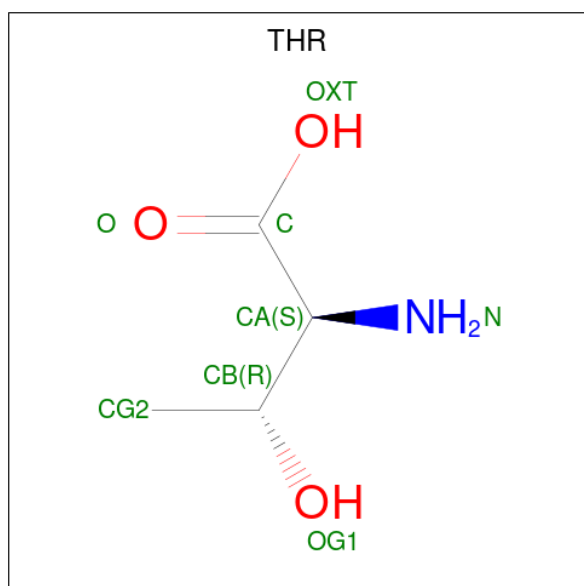
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P26512
B	173	HIS	-	expression tag	UNP P26512
B	174	HIS	-	expression tag	UNP P26512
B	175	HIS	-	expression tag	UNP P26512
B	176	HIS	-	expression tag	UNP P26512
B	177	HIS	-	expression tag	UNP P26512
B	178	HIS	-	expression tag	UNP P26512
D	1	MET	-	initiating methionine	UNP P26512
D	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	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
H	1	MET	-	initiating methionine	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	178	HIS	-	expression tag	UNP P26512
L	1	MET	-	initiating methionine	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	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	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 (CCD ID: THR) (formula: $C_4H_9NO_3$).



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

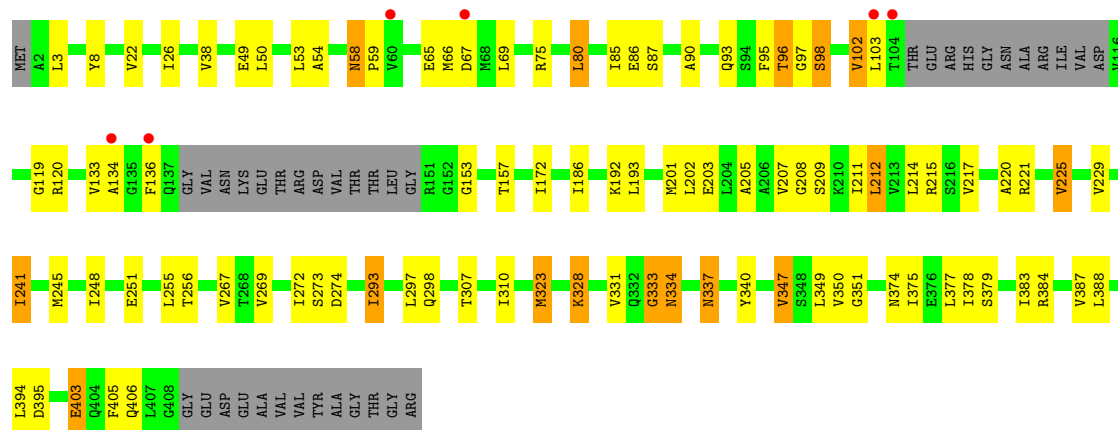
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	36	Total O 36 36	0	0
4	B	11	Total O 11 11	0	0
4	C	18	Total O 18 18	0	0
4	D	3	Total O 3 3	0	0
4	E	23	Total O 23 23	0	0

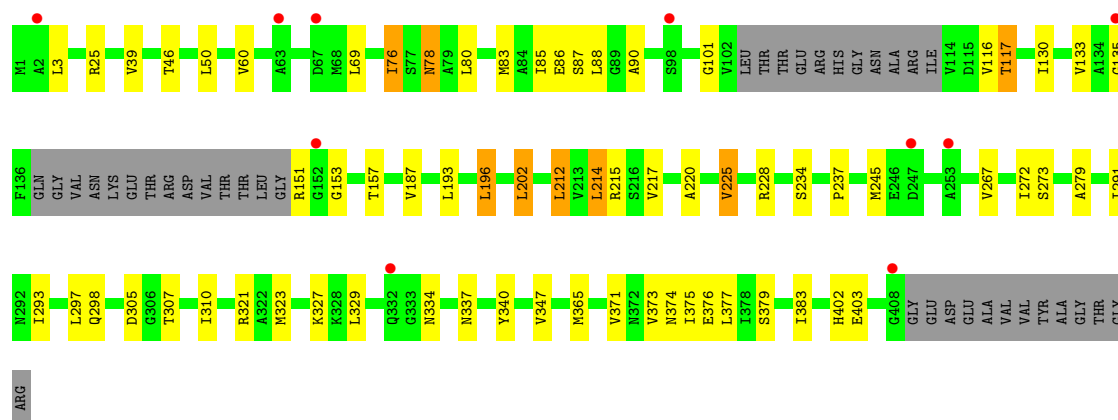
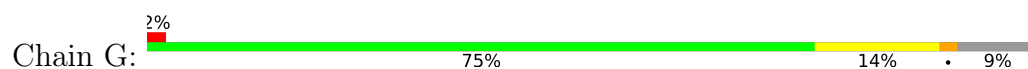
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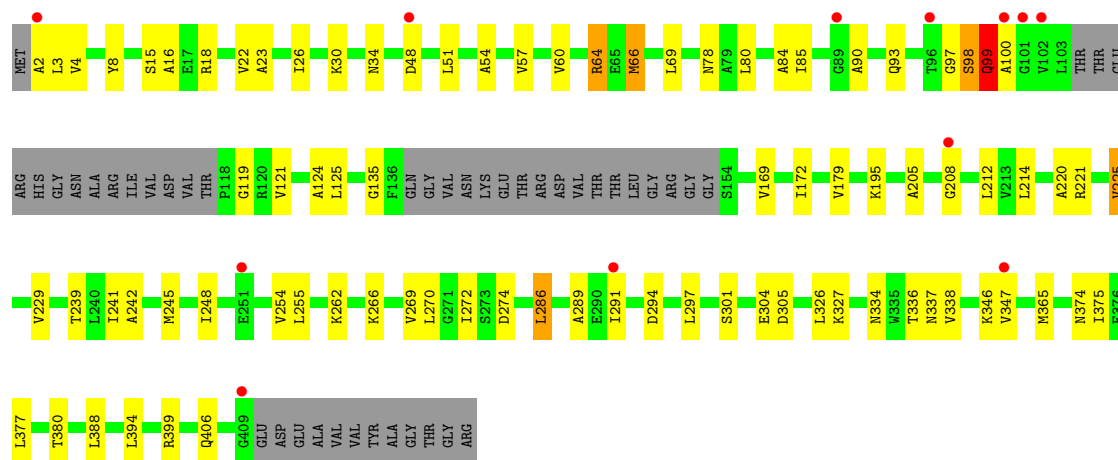
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	8	Total 8	O 8	0	0
4	G	18	Total 18	O 18	0	0
4	H	9	Total 9	O 9	0	0
4	I	16	Total 16	O 16	0	0
4	J	6	Total 6	O 6	0	0
4	K	25	Total 25	O 25	0	0
4	L	5	Total 5	O 5	0	0
4	M	21	Total 21	O 21	0	0
4	N	4	Total 4	O 4	0	0
4	O	31	Total 31	O 31	0	0
4	P	12	Total 12	O 12	0	0



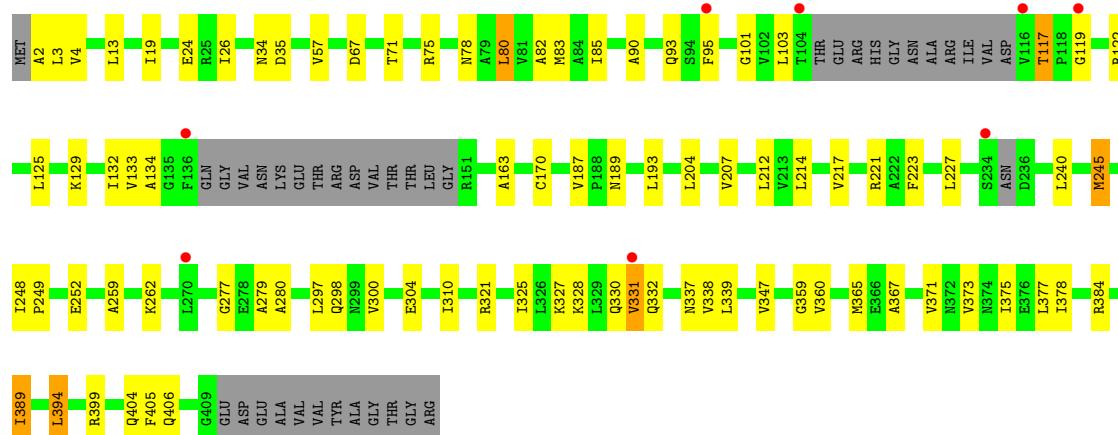
• Molecule 1: Aspartokinase



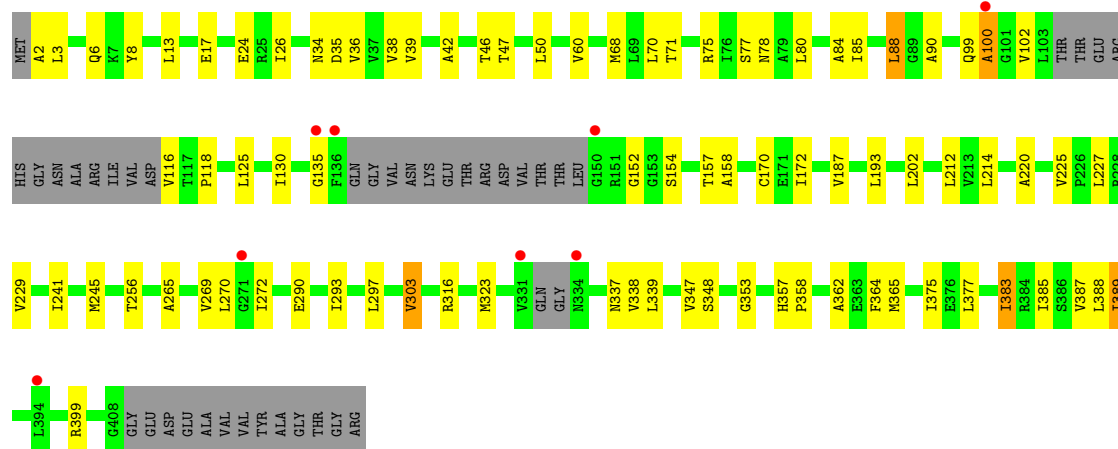
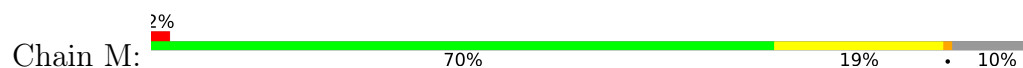
• Molecule 1: Aspartokinase



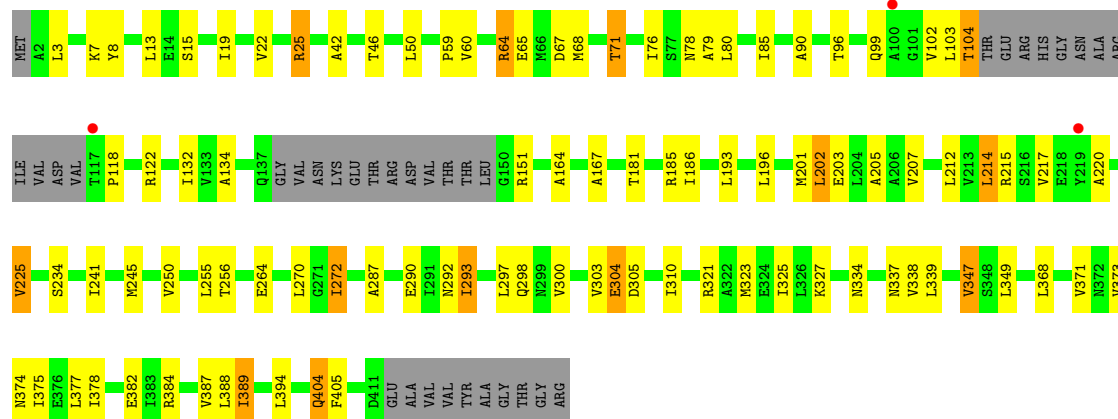
• Molecule 1: Aspartokinase



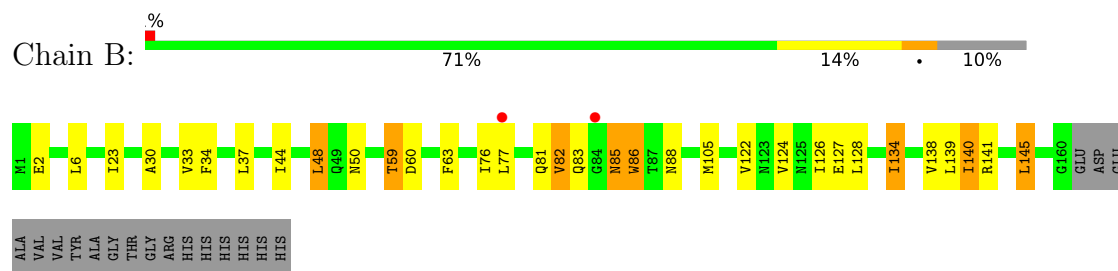
• Molecule 1: Aspartokinase



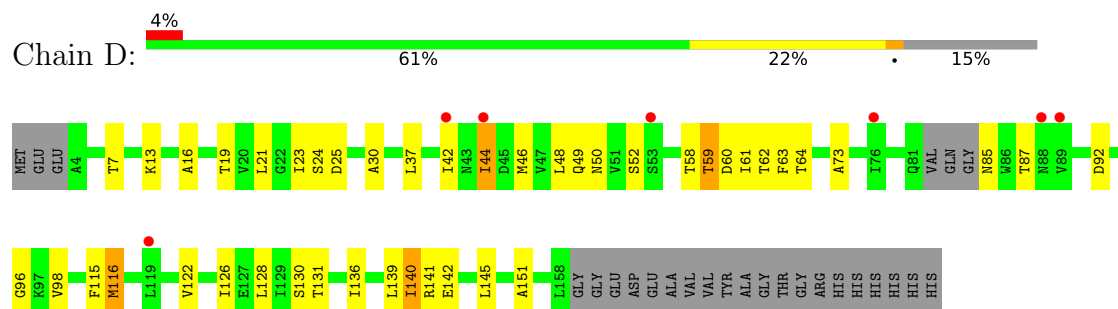
• Molecule 1: Aspartokinase



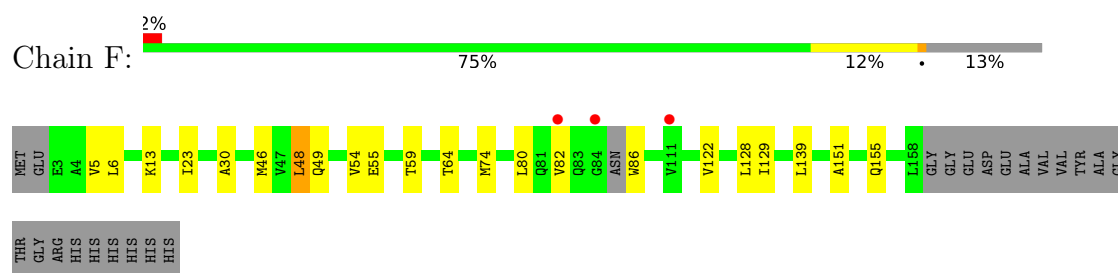
- Molecule 2: Aspartokinase



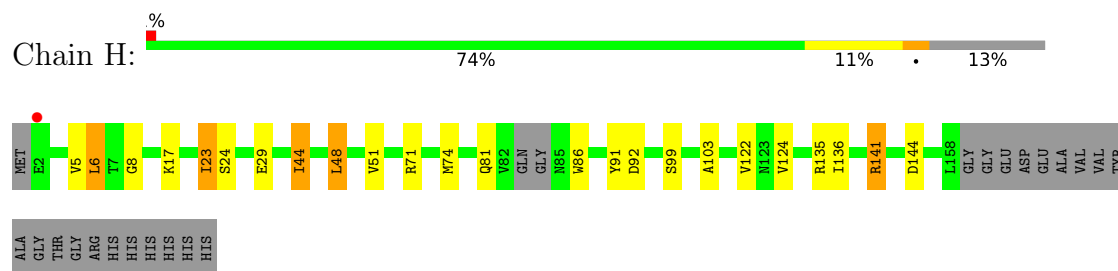
- Molecule 2: Aspartokinase



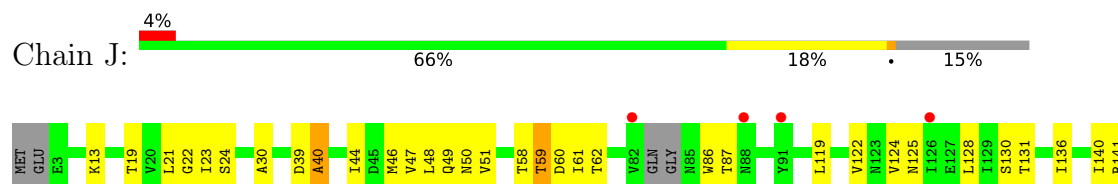
- Molecule 2: Aspartokinase

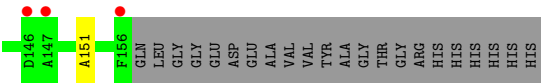


- Molecule 2: Aspartokinase

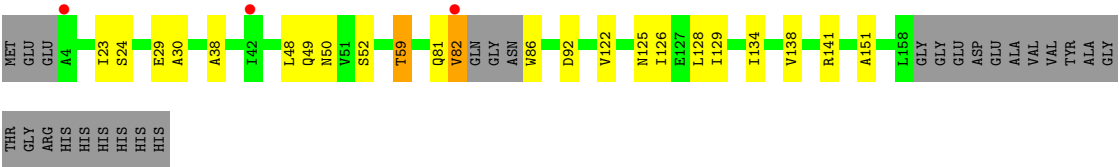


- Molecule 2: Aspartokinase





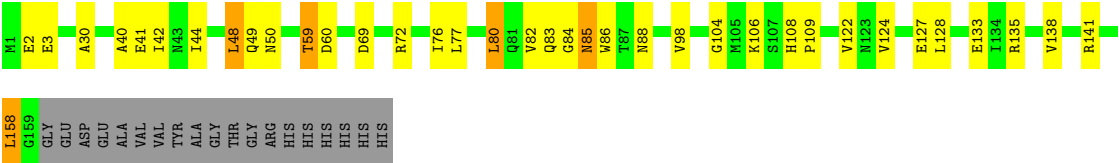
● Molecule 2: Aspartokinase



● Molecule 2: Aspartokinase



● Molecule 2: Aspartokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	101.83Å 119.09Å 124.38Å 71.85° 69.48° 72.72°	Depositor
Resolution (Å)	42.04 – 2.59 42.04 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.1 (42.04-2.59) 97.2 (42.04-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.232 , 0.280 0.227 , 0.274	Depositor DCC
R_{free} test set	7701 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31975	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/2867	0.74	0/3883
1	C	0.44	0/2820	0.72	0/3825
1	E	0.43	0/2841	0.72	0/3853
1	G	0.44	0/2830	0.74	0/3839
1	I	0.43	0/2774	0.75	1/3765 (0.0%)
1	K	0.45	1/2818 (0.0%)	0.72	0/3823
1	M	0.43	0/2822	0.73	1/3824 (0.0%)
1	O	0.46	0/2878	0.75	0/3899
2	B	0.46	0/1194	0.73	0/1618
2	D	0.44	0/1125	0.72	0/1528
2	F	0.42	0/1176	0.71	0/1590
2	H	0.43	0/1171	0.73	1/1586 (0.1%)
2	J	0.41	0/1090	0.70	0/1481
2	L	0.41	0/1141	0.67	0/1547
2	N	0.41	0/1146	0.66	0/1557
2	P	0.46	0/1207	0.74	0/1633
All	All	0.44	1/31900 (0.0%)	0.73	3/43251 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	117	THR	CA-CB	5.82	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8	GLY	N-CA-C	5.73	118.86	110.38
1	M	152	GLY	N-CA-C	-5.62	107.57	113.58
1	I	99	GLN	N-CA-C	-5.50	107.14	112.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2841	0	2834	76	0
1	C	2793	0	2791	68	0
1	E	2814	0	2809	66	0
1	G	2803	0	2793	52	0
1	I	2748	0	2735	70	0
1	K	2793	0	2773	69	0
1	M	2796	0	2799	69	0
1	O	2851	0	2852	86	0
2	B	1183	0	1169	27	0
2	D	1116	0	1094	42	0
2	F	1166	0	1169	18	0
2	H	1161	0	1155	23	0
2	J	1082	0	1027	34	0
2	L	1131	0	1114	24	0
2	N	1135	0	1117	25	0
2	P	1196	0	1194	30	0
3	A	8	0	6	7	0
3	B	8	0	6	1	0
3	C	8	0	6	4	0
3	D	8	0	6	7	0
3	E	8	0	6	1	0
3	F	8	0	6	6	0
3	G	8	0	6	5	0
3	H	8	0	6	3	0
3	J	8	0	6	6	0
3	K	8	0	6	6	0
3	L	8	0	6	4	0
3	M	8	0	6	0	0
3	N	8	0	6	0	0
3	O	8	0	6	0	0
3	P	8	0	6	5	0
4	A	36	0	0	1	0
4	B	11	0	0	0	0
4	C	18	0	0	1	0
4	D	3	0	0	0	0
4	E	23	0	0	0	0
4	F	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	18	0	0	0	0
4	H	9	0	0	0	0
4	I	16	0	0	1	0
4	J	6	0	0	0	0
4	K	25	0	0	0	0
4	L	5	0	0	0	0
4	M	21	0	0	0	0
4	N	4	0	0	0	0
4	O	31	0	0	0	0
4	P	12	0	0	0	0
All	All	31975	0	31515	717	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (717) 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)
2:L:30:ALA:HB2	3:L:501:THR:HG23	1.26	1.14
2:B:48:LEU:HD11	2:B:128:LEU:HD23	1.30	1.12
1:C:297:LEU:HD13	1:C:377:LEU:HD21	1.31	1.10
2:H:23:ILE:HD11	3:H:501:THR:HG22	1.30	1.10
2:F:46:MET:HE1	2:F:139:LEU:HD21	1.34	1.09
1:K:279:ALA:HB2	3:K:501:THR:HG22	1.32	1.08
1:G:298:GLN:HE22	3:G:501:THR:HG21	1.16	1.06
1:A:279:ALA:HB2	3:A:501:THR:CG2	1.84	1.06
2:D:46:MET:HE1	2:D:139:LEU:HD21	1.36	1.03
2:J:30:ALA:HB2	3:J:501:THR:HG23	1.03	1.02
1:O:368:LEU:HD12	1:O:375:ILE:HD11	1.41	1.02
2:D:30:ALA:HB2	3:D:501:THR:HG23	1.38	1.01
2:J:30:ALA:CB	3:J:501:THR:HG23	1.92	1.00
1:O:297:LEU:HD22	1:O:377:LEU:HD21	1.42	0.99
1:A:13:LEU:HD22	1:A:19:ILE:HD13	1.43	0.99
2:N:46:MET:HE1	2:N:139:LEU:HD21	1.42	0.98
1:C:201:MET:HE2	1:C:212:LEU:HD13	1.46	0.98
2:J:30:ALA:HB2	3:J:501:THR:CG2	1.96	0.96
1:C:279:ALA:HB2	3:C:501:THR:HG22	1.47	0.95
2:D:23:ILE:HG21	2:D:61:ILE:HD13	1.54	0.90
1:G:279:ALA:HB2	3:G:501:THR:HG23	1.56	0.87
1:O:67:ASP:O	1:O:71:THR:HG23	1.74	0.87
2:J:19:THR:HG23	2:J:62:THR:HG22	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:VAL:O	1:G:117:THR:HG22	1.75	0.87
1:C:267:VAL:HG22	1:C:323:MET:HE1	1.57	0.87
1:E:267:VAL:HG13	1:E:323:MET:HE1	1.57	0.86
1:O:297:LEU:CD2	1:O:377:LEU:HD21	2.05	0.86
1:A:85:ILE:HG23	1:A:90:ALA:HB3	1.57	0.86
2:D:50:ASN:O	2:D:59:THR:HG21	1.75	0.85
2:F:30:ALA:HB2	3:F:501:THR:HG23	1.56	0.85
1:M:220:ALA:HA	1:M:225:VAL:HG12	1.60	0.84
1:A:220:ALA:HA	1:A:225:VAL:HG13	1.60	0.83
2:J:50:ASN:O	2:J:59:THR:HG21	1.78	0.83
1:O:375:ILE:HB	3:P:501:THR:HG22	1.59	0.83
1:M:75:ARG:CZ	1:O:68:MET:HE3	2.09	0.83
1:A:205:ALA:HB1	1:A:214:LEU:HD11	1.60	0.83
2:N:50:ASN:O	2:N:59:THR:HG21	1.79	0.82
2:N:122:VAL:HG23	2:N:124:VAL:HG23	1.58	0.82
1:A:279:ALA:HB2	3:A:501:THR:HG22	1.61	0.82
1:C:374:ASN:HD21	3:D:501:THR:N	1.77	0.82
2:D:30:ALA:HB2	3:D:501:THR:CG2	2.10	0.82
1:O:78:ASN:HB2	1:O:134:ALA:HB2	1.60	0.81
1:I:245:MET:O	1:I:248:ILE:HG22	1.82	0.80
1:C:361:THR:HG21	2:D:44:ILE:HG21	1.63	0.80
2:L:52:SER:HA	2:L:59:THR:HG23	1.64	0.80
1:E:50:LEU:HD22	1:E:69:LEU:HD11	1.65	0.79
1:O:300:VAL:CG1	2:P:128:LEU:HD11	2.12	0.79
1:K:279:ALA:HB2	3:K:501:THR:CG2	2.11	0.79
1:A:377:LEU:HD13	1:A:388:LEU:HD12	1.64	0.78
1:M:293:ILE:HD12	1:M:293:ILE:O	1.83	0.78
2:D:62:THR:HG21	2:D:128:LEU:HD21	1.66	0.78
2:P:49:GLN:OE1	3:P:501:THR:HG21	1.84	0.78
1:O:300:VAL:HG13	2:P:128:LEU:HD11	1.64	0.77
1:K:297:LEU:HD13	1:K:377:LEU:HD21	1.65	0.77
1:E:85:ILE:HG22	1:E:90:ALA:HB3	1.67	0.77
2:N:48:LEU:HG	2:N:128:LEU:HD21	1.67	0.77
1:A:90:ALA:HB1	1:A:130:ILE:HD13	1.65	0.77
1:O:297:LEU:HD22	1:O:377:LEU:CD2	2.14	0.77
2:D:49:GLN:OE1	3:D:501:THR:HG21	1.85	0.77
1:G:60:VAL:HG21	1:I:327:LYS:HG3	1.66	0.76
1:I:172:ILE:HD13	1:I:212:LEU:HD22	1.68	0.75
1:K:13:LEU:HD22	1:K:19:ILE:HD13	1.68	0.75
1:M:78:ASN:CG	1:O:68:MET:HE1	2.11	0.75
2:F:48:LEU:HD12	2:F:128:LEU:HD21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:196:LEU:HD11	1:O:256:THR:HG21	1.68	0.74
1:K:85:ILE:HG23	1:K:90:ALA:HB3	1.70	0.74
2:L:30:ALA:HB2	3:L:501:THR:CG2	2.14	0.74
2:B:50:ASN:O	2:B:59:THR:HG21	1.87	0.74
1:K:279:ALA:CB	3:K:501:THR:HG22	2.16	0.74
1:K:212:LEU:HD23	1:K:217:VAL:HG22	1.69	0.74
1:O:377:LEU:HD13	1:O:388:LEU:HD12	1.69	0.73
1:C:297:LEU:HD13	1:C:377:LEU:CD2	2.13	0.73
1:G:279:ALA:HB2	3:G:501:THR:CG2	2.19	0.72
1:C:267:VAL:CG2	1:C:323:MET:HE1	2.19	0.72
2:L:23:ILE:HD11	2:L:29:GLU:HB3	1.71	0.71
1:K:321:ARG:NH2	1:K:325:ILE:HD11	2.05	0.71
3:C:501:THR:O	2:D:126:ILE:HD13	1.89	0.71
1:C:2:ALA:HB3	1:C:34:ASN:HD22	1.55	0.71
1:E:69:LEU:HD22	1:G:83:MET:HE1	1.72	0.71
1:I:85:ILE:CG2	1:I:90:ALA:HB3	2.20	0.71
1:E:267:VAL:CG1	1:E:323:MET:HE1	2.20	0.71
2:H:44:ILE:HD12	2:H:44:ILE:C	2.15	0.71
1:G:117:THR:O	1:G:117:THR:HG23	1.89	0.70
1:A:337:ASN:HD22	1:A:338:VAL:H	1.39	0.70
1:I:212:LEU:HD21	1:I:229:VAL:HG22	1.73	0.70
2:D:46:MET:HE3	2:D:64:THR:HG21	1.73	0.70
2:L:50:ASN:O	2:L:59:THR:HG21	1.91	0.70
2:F:46:MET:HE3	2:F:64:THR:HG21	1.73	0.70
1:E:134:ALA:HB3	1:E:136:PHE:HE2	1.57	0.70
1:I:220:ALA:HA	1:I:225:VAL:HG13	1.74	0.69
2:L:48:LEU:HD22	2:L:128:LEU:HD23	1.72	0.69
1:K:298:GLN:HE22	3:K:501:THR:HG21	1.56	0.69
1:M:85:ILE:CG2	1:M:90:ALA:HB3	2.22	0.69
1:I:99:GLN:HE21	1:I:99:GLN:HA	1.58	0.69
1:C:2:ALA:HB3	1:C:34:ASN:ND2	2.07	0.69
1:E:347:VAL:HG22	1:E:394:LEU:CD2	2.23	0.69
2:N:46:MET:HE3	2:N:64:THR:HG21	1.75	0.69
1:E:96:THR:HG23	1:E:136:PHE:CZ	2.28	0.69
1:I:57:VAL:HG21	1:K:83:MET:HE3	1.74	0.69
1:K:85:ILE:CG2	1:K:90:ALA:HB3	2.23	0.69
2:P:76:ILE:O	2:P:80:LEU:HD22	1.93	0.69
2:N:46:MET:HE1	2:N:139:LEU:CD2	2.22	0.68
1:E:245:MET:O	1:E:248:ILE:HG22	1.93	0.68
2:D:96:GLY:HA3	2:D:145:LEU:HD11	1.76	0.68
1:I:8:TYR:CE2	1:I:26:ILE:HD11	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:26:ILE:HD12	1:M:38:VAL:CG2	2.24	0.68
1:K:207:VAL:HG11	1:K:384:ARG:HD2	1.76	0.68
2:L:30:ALA:CB	3:L:501:THR:HG23	2.16	0.67
1:E:328:LYS:O	1:E:331:VAL:HG22	1.94	0.67
1:I:380:THR:HG21	2:J:47:VAL:H	1.59	0.67
2:B:30:ALA:O	2:B:33:VAL:HG12	1.93	0.67
1:K:80:LEU:HD12	1:K:83:MET:HE2	1.74	0.67
1:O:368:LEU:CD1	1:O:375:ILE:HD11	2.22	0.66
2:P:30:ALA:HB2	3:P:501:THR:HG23	1.76	0.66
1:A:279:ALA:HB2	3:A:501:THR:HG23	1.76	0.66
1:A:245:MET:HE2	1:A:383:ILE:HD13	1.78	0.66
1:I:85:ILE:HG22	1:I:90:ALA:HB3	1.78	0.66
1:C:174:SER:OG	1:C:176:VAL:HG12	1.96	0.66
2:P:50:ASN:O	2:P:59:THR:HG21	1.96	0.65
2:D:52:SER:HA	2:D:59:THR:HG23	1.78	0.65
1:E:377:LEU:HD13	1:E:388:LEU:HD12	1.78	0.65
1:I:78:ASN:C	1:I:78:ASN:HD22	2.04	0.65
2:B:128:LEU:HD22	2:B:139:LEU:HD12	1.78	0.65
1:C:212:LEU:HD11	1:C:229:VAL:HG21	1.77	0.65
2:H:23:ILE:HD11	3:H:501:THR:CG2	2.18	0.65
1:O:3:LEU:HD22	1:O:167:ALA:HB2	1.79	0.65
1:G:377:LEU:HD11	2:H:51:VAL:CG1	2.25	0.65
1:M:99:GLN:O	1:M:100:ALA:HB2	1.96	0.65
1:E:347:VAL:HG22	1:E:394:LEU:HD23	1.79	0.65
1:G:60:VAL:O	1:G:60:VAL:HG23	1.97	0.65
1:C:279:ALA:HB2	3:C:501:THR:CG2	2.24	0.65
2:B:23:ILE:HD12	2:B:86:TRP:CD1	2.32	0.65
1:O:13:LEU:HD22	1:O:19:ILE:HD13	1.77	0.64
1:K:337:ASN:HD22	1:K:338:VAL:H	1.44	0.64
1:G:291:ILE:HD11	1:G:321:ARG:HG3	1.78	0.64
1:K:337:ASN:HD22	1:K:338:VAL:N	1.95	0.64
1:A:207:VAL:HG11	1:A:384:ARG:HD2	1.79	0.64
2:J:48:LEU:HD11	2:J:130:SER:HB2	1.80	0.64
1:O:85:ILE:CG2	1:O:90:ALA:HB3	2.27	0.64
1:M:99:GLN:O	1:M:100:ALA:CB	2.45	0.63
1:E:85:ILE:CG2	1:E:90:ALA:HB3	2.28	0.63
1:M:78:ASN:ND2	1:O:68:MET:HE1	2.13	0.63
1:O:404:GLN:HE21	1:O:404:GLN:HA	1.63	0.63
1:K:80:LEU:HD12	1:K:83:MET:CE	2.29	0.63
2:P:80:LEU:O	2:P:85:ASN:ND2	2.31	0.63
1:C:220:ALA:HA	1:C:225:VAL:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:380:THR:HG21	2:J:46:MET:HA	1.81	0.63
1:C:116:VAL:HG11	1:C:164:ALA:HB2	1.80	0.63
2:F:122:VAL:HG11	2:F:151:ALA:HB2	1.79	0.63
1:K:67:ASP:O	1:K:71:THR:HG22	1.98	0.63
1:M:193:LEU:HD21	1:M:256:THR:HG23	1.79	0.63
1:G:298:GLN:HE22	3:G:501:THR:CG2	2.04	0.63
1:G:376:GLU:C	1:G:377:LEU:HD12	2.23	0.63
1:K:347:VAL:HG22	1:K:394:LEU:HD23	1.80	0.63
2:B:48:LEU:HD11	2:B:128:LEU:CD2	2.19	0.62
2:F:46:MET:CE	2:F:139:LEU:HD21	2.20	0.62
2:P:48:LEU:HD23	2:P:48:LEU:N	2.14	0.62
1:A:156:THR:HA	1:A:159:VAL:HG12	1.80	0.62
1:A:300:VAL:HG12	2:B:128:LEU:HD11	1.81	0.62
2:D:128:LEU:HD22	2:D:139:LEU:HD12	1.82	0.62
1:A:150:GLY:HA3	1:A:151:ARG:CB	2.29	0.62
2:B:85:ASN:HD22	2:B:86:TRP:H	1.46	0.62
1:C:207:VAL:HG21	1:C:348:SER:OG	1.99	0.62
1:G:371:VAL:HG23	1:G:373:VAL:HG23	1.82	0.61
1:M:26:ILE:HD12	1:M:38:VAL:HG22	1.82	0.61
1:M:35:ASP:HB3	1:M:125:LEU:HD22	1.82	0.61
2:N:46:MET:CE	2:N:139:LEU:HD21	2.27	0.61
1:E:212:LEU:HD13	1:E:217:VAL:HG21	1.82	0.61
1:M:297:LEU:HD13	1:M:377:LEU:HD11	1.83	0.61
1:M:42:ALA:HB1	1:M:46:THR:HB	1.83	0.61
1:I:57:VAL:CG2	1:K:83:MET:HE3	2.29	0.61
1:G:267:VAL:HG13	1:G:323:MET:HE1	1.82	0.61
1:G:298:GLN:NE2	3:G:501:THR:HG21	2.01	0.60
1:I:254:VAL:HG12	1:I:255:LEU:H	1.66	0.60
2:B:127:GLU:C	2:B:128:LEU:HD12	2.27	0.60
2:D:44:ILE:HD13	2:D:44:ILE:H	1.66	0.60
1:C:293:ILE:HD13	1:C:296:VAL:HG23	1.84	0.60
1:E:50:LEU:HD21	1:G:76:ILE:HD12	1.83	0.60
1:C:374:ASN:ND2	3:D:501:THR:N	2.50	0.60
1:A:298:GLN:HE22	3:A:501:THR:HG21	1.64	0.60
2:F:46:MET:HE1	2:F:139:LEU:CD2	2.19	0.60
1:G:80:LEU:HA	1:G:83:MET:HE3	1.84	0.59
1:I:375:ILE:HB	3:J:501:THR:HG22	1.84	0.59
1:M:85:ILE:HG22	1:M:90:ALA:HB3	1.84	0.59
2:P:48:LEU:HD11	2:P:128:LEU:HD23	1.84	0.59
1:C:272:ILE:HD12	1:C:310:ILE:HD12	1.84	0.59
1:E:153:GLY:O	1:E:157:THR:HG23	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:44:ILE:HD13	2:N:44:ILE:H	1.67	0.59
1:O:220:ALA:HA	1:O:225:VAL:HG13	1.83	0.59
1:A:2:ALA:HB3	1:A:34:ASN:ND2	2.18	0.59
1:G:78:ASN:C	1:G:78:ASN:HD22	2.11	0.59
2:J:39:ASP:O	2:J:40:ALA:HB2	2.02	0.59
1:I:48:ASP:HA	1:I:51:LEU:HD23	1.84	0.59
2:P:2:GLU:C	2:P:108:HIS:NE2	2.61	0.59
1:C:279:ALA:CB	3:C:501:THR:HG22	2.29	0.59
2:J:49:GLN:OE1	3:J:501:THR:HG21	2.03	0.59
1:O:337:ASN:HD22	1:O:338:VAL:H	1.50	0.59
1:M:269:VAL:HG11	1:M:272:ILE:HD11	1.83	0.58
1:O:374:ASN:ND2	3:P:501:THR:N	2.51	0.58
1:C:26:ILE:HB	1:C:85:ILE:HD11	1.83	0.58
2:D:42:ILE:HD13	2:D:73:ALA:HB2	1.85	0.58
1:M:71:THR:HG23	1:M:135:GLY:CA	2.33	0.58
2:D:23:ILE:HG21	2:D:61:ILE:CD1	2.31	0.58
1:E:297:LEU:HD11	1:E:379:SER:HB2	1.85	0.58
1:G:273:SER:HA	1:G:307:THR:HG22	1.85	0.58
1:E:49:GLU:O	1:E:53:LEU:HD23	2.04	0.58
1:G:220:ALA:HA	1:G:225:VAL:HG13	1.86	0.58
2:F:49:GLN:OE1	3:F:501:THR:HG21	2.04	0.57
1:C:78:ASN:C	1:C:78:ASN:HD22	2.12	0.57
1:G:377:LEU:HD11	2:H:51:VAL:HG12	1.86	0.57
2:H:122:VAL:HG23	2:H:124:VAL:HG23	1.85	0.57
1:K:371:VAL:HG23	1:K:373:VAL:HG23	1.86	0.57
2:J:119:LEU:O	2:J:124:VAL:HG12	2.04	0.57
2:N:46:MET:HE1	2:N:139:LEU:HD11	1.86	0.57
1:E:375:ILE:HB	3:F:501:THR:HG22	1.87	0.57
1:O:347:VAL:HG22	1:O:394:LEU:HD23	1.87	0.57
1:E:220:ALA:HA	1:E:225:VAL:HG13	1.86	0.57
2:D:122:VAL:HG21	2:D:151:ALA:HB2	1.85	0.57
1:A:156:THR:HG22	1:A:216:SER:HB3	1.87	0.57
1:A:60:VAL:HG11	1:O:327:LYS:HG3	1.87	0.56
2:H:23:ILE:HD12	2:H:23:ILE:C	2.30	0.56
2:P:42:ILE:HD12	2:P:69:ASP:HB3	1.86	0.56
1:A:209:SER:O	1:A:210:LYS:HB2	2.04	0.56
2:F:5:VAL:C	2:F:6:LEU:HD12	2.30	0.56
1:E:269:VAL:CG1	1:E:272:ILE:HD11	2.35	0.56
1:I:294:ASP:OD2	1:I:346:LYS:NZ	2.38	0.56
1:C:323:MET:HE3	1:C:340:TYR:CD1	2.40	0.56
1:I:66:MET:HE2	1:I:66:MET:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:286:LEU:CD2	1:I:326:LEU:HD21	2.36	0.56
1:A:297:LEU:HD13	1:A:377:LEU:HD21	1.88	0.56
1:O:13:LEU:HD22	1:O:19:ILE:CD1	2.35	0.56
1:E:350:VAL:HG22	1:E:384:ARG:HG3	1.87	0.56
1:O:85:ILE:HG22	1:O:90:ALA:HB3	1.88	0.56
1:C:201:MET:HE2	1:C:212:LEU:CD1	2.30	0.56
1:G:377:LEU:HD11	2:H:51:VAL:HG13	1.88	0.56
1:I:377:LEU:HD13	1:I:388:LEU:HD12	1.87	0.56
1:O:201:MET:HA	1:O:201:MET:HE3	1.88	0.56
1:G:85:ILE:CG2	1:G:90:ALA:HB3	2.36	0.56
1:K:297:LEU:HD13	1:K:377:LEU:CD2	2.36	0.55
1:O:196:LEU:CD1	1:O:256:THR:HG21	2.36	0.55
2:N:118:ALA:HB2	2:N:155:GLN:HG3	1.89	0.55
1:A:71:THR:HG23	1:A:135:GLY:HA3	1.87	0.55
2:P:106:LYS:HB2	2:P:133:GLU:HG2	1.88	0.55
2:H:23:ILE:HD13	2:H:29:GLU:HB3	1.88	0.55
2:P:48:LEU:CD1	2:P:128:LEU:HD23	2.37	0.55
1:G:327:LYS:HG3	1:I:60:VAL:HG11	1.88	0.55
1:E:58:ASN:HD22	1:E:58:ASN:C	2.14	0.55
1:G:153:GLY:O	1:G:157:THR:HG23	2.07	0.55
1:G:297:LEU:HD11	1:G:379:SER:HB3	1.87	0.55
2:J:48:LEU:HG	2:J:128:LEU:HD23	1.88	0.55
1:K:310:ILE:HD11	3:K:501:THR:HG21	1.88	0.55
1:M:2:ALA:HB3	1:M:34:ASN:HD22	1.71	0.55
1:O:300:VAL:HG12	2:P:128:LEU:HD11	1.87	0.55
1:O:118:PRO:HG3	1:O:164:ALA:HB1	1.89	0.54
1:I:365:MET:SD	1:I:375:ILE:HD13	2.46	0.54
1:K:327:LYS:O	1:K:331:VAL:HG23	2.07	0.54
1:O:13:LEU:HB3	1:O:19:ILE:HD11	1.90	0.54
2:D:48:LEU:CD1	2:D:128:LEU:HD23	2.38	0.54
2:F:23:ILE:HG22	2:F:59:THR:O	2.07	0.54
2:B:140:ILE:HD11	2:B:145:LEU:HD12	1.87	0.54
1:O:205:ALA:HB1	1:O:214:LEU:HD11	1.88	0.54
1:I:66:MET:CE	1:I:69:LEU:HD23	2.38	0.54
1:C:218:GLU:OE2	2:D:7:THR:HG21	2.07	0.54
1:K:367:ALA:HB2	1:K:404:GLN:HG2	1.90	0.54
1:K:204:LEU:HD23	1:K:259:ALA:HB2	1.90	0.54
2:N:46:MET:HE3	2:N:64:THR:CG2	2.38	0.54
1:C:282:VAL:HG13	1:C:326:LEU:HD21	1.90	0.53
1:C:375:ILE:HB	3:D:501:THR:HG22	1.90	0.53
2:D:48:LEU:HD21	2:D:130:SER:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:331:VAL:HG12	1:K:331:VAL:O	2.09	0.53
1:M:47:THR:HG23	1:M:70:LEU:HD22	1.89	0.53
1:O:272:ILE:HD12	1:O:310:ILE:HD12	1.91	0.53
1:A:297:LEU:HD11	1:A:378:ILE:O	2.09	0.53
1:C:51:LEU:HD23	1:C:66:MET:HE1	1.89	0.53
2:D:115:PHE:HD2	2:D:116:MET:HE3	1.73	0.53
1:E:80:LEU:HD13	1:G:69:LEU:HD13	1.91	0.53
1:C:267:VAL:HG22	1:C:323:MET:CE	2.36	0.53
1:E:297:LEU:HG	1:E:377:LEU:HD21	1.91	0.53
1:A:30:LYS:HD2	1:A:130:ILE:HD11	1.91	0.53
1:A:85:ILE:HG23	1:A:90:ALA:CB	2.34	0.53
1:C:208:GLY:HA3	1:C:259:ALA:HB1	1.90	0.53
1:E:349:LEU:HD22	1:E:405:PHE:CE1	2.44	0.53
1:K:298:GLN:HE21	1:K:310:ILE:HG12	1.73	0.53
1:K:2:ALA:HB3	1:K:34:ASN:ND2	2.23	0.53
1:K:327:LYS:HG3	1:M:60:VAL:HG11	1.90	0.53
2:F:30:ALA:HB2	3:F:501:THR:CG2	2.32	0.53
2:F:30:ALA:CB	3:F:501:THR:HG23	2.35	0.53
1:I:64:ARG:NH2	4:I:434:HOH:O	2.41	0.53
1:A:371:VAL:HG23	1:A:373:VAL:HG23	1.90	0.53
1:K:187:VAL:HG22	1:K:399:ARG:HG3	1.91	0.53
1:O:374:ASN:HD21	3:P:501:THR:N	2.07	0.53
2:J:23:ILE:HG22	2:J:59:THR:O	2.09	0.53
1:O:103:LEU:O	1:O:104:THR:HG22	2.09	0.53
2:D:24:SER:HA	2:D:58:THR:HG22	1.89	0.52
1:I:172:ILE:CD1	1:I:212:LEU:HD22	2.38	0.52
1:K:71:THR:O	1:K:75:ARG:HG2	2.09	0.52
1:O:368:LEU:HD12	1:O:375:ILE:CD1	2.26	0.52
1:M:26:ILE:HD12	1:M:38:VAL:HG21	1.90	0.52
1:O:8:TYR:CE1	1:O:22:VAL:HG13	2.44	0.52
1:E:269:VAL:HG12	1:E:272:ILE:HD11	1.92	0.52
1:M:365:MET:SD	1:M:375:ILE:HD13	2.49	0.52
1:O:297:LEU:CD2	1:O:377:LEU:CD2	2.82	0.52
1:A:132:ILE:N	1:A:132:ILE:HD12	2.25	0.52
1:A:150:GLY:CA	1:A:151:ARG:HB3	2.40	0.52
1:C:377:LEU:HD13	1:C:388:LEU:HD12	1.91	0.52
2:J:19:THR:CG2	2:J:62:THR:HG22	2.35	0.52
1:K:2:ALA:HB3	1:K:34:ASN:HD22	1.75	0.52
1:O:215:ARG:HD2	2:P:104:GLY:HA3	1.91	0.52
1:E:193:LEU:HD21	1:E:256:THR:HG23	1.91	0.52
1:K:375:ILE:HB	3:L:501:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:ILE:HG21	1:E:229:VAL:HG11	1.92	0.52
2:J:122:VAL:HG11	2:J:151:ALA:HB2	1.92	0.52
1:K:327:LYS:NZ	1:K:330:GLN:HE22	2.08	0.52
1:O:132:ILE:HD12	1:O:132:ILE:N	2.25	0.52
1:K:214:LEU:HD21	2:L:134:ILE:CG2	2.40	0.52
2:L:126:ILE:HG23	2:L:138:VAL:HB	1.92	0.52
1:M:269:VAL:CG1	1:M:272:ILE:HD11	2.40	0.52
1:K:13:LEU:CD2	1:K:19:ILE:HD13	2.39	0.51
2:L:52:SER:CA	2:L:59:THR:HG23	2.39	0.51
1:M:71:THR:HG23	1:M:135:GLY:HA2	1.91	0.51
1:E:298:GLN:HE21	1:E:310:ILE:HG12	1.75	0.51
1:I:23:ALA:HB2	1:I:84:ALA:HB1	1.93	0.51
2:L:122:VAL:HG11	2:L:151:ALA:HB2	1.91	0.51
1:M:364:PHE:CD2	1:M:365:MET:HE2	2.45	0.51
2:L:126:ILE:HG21	2:L:129:ILE:HG12	1.90	0.51
2:N:46:MET:CE	2:N:139:LEU:HD11	2.41	0.51
1:C:66:MET:HE3	1:C:70:LEU:HD13	1.92	0.51
1:I:270:LEU:C	1:I:336:THR:HG22	2.36	0.51
1:O:371:VAL:HG23	1:O:373:VAL:HG23	1.91	0.51
1:A:13:LEU:HB3	1:A:19:ILE:HD11	1.93	0.51
1:A:212:LEU:HD13	1:A:217:VAL:HG21	1.92	0.51
1:K:101:GLY:O	1:K:117:THR:HG23	2.11	0.51
1:K:214:LEU:HD21	2:L:134:ILE:HG23	1.92	0.51
1:K:245:MET:O	1:K:248:ILE:HG22	2.11	0.51
1:M:375:ILE:HG23	1:M:387:VAL:HB	1.93	0.51
1:I:205:ALA:HB1	1:I:214:LEU:HD11	1.92	0.51
1:A:377:LEU:HD23	1:A:377:LEU:C	2.36	0.51
1:M:3:LEU:HD12	1:M:35:ASP:O	2.11	0.51
2:B:140:ILE:HD11	2:B:145:LEU:CD1	2.41	0.51
1:C:11:SER:OG	4:C:508:HOH:O	2.19	0.51
1:C:212:LEU:N	1:C:212:LEU:HD12	2.26	0.51
2:B:81:GLN:O	2:B:83:GLN:N	2.43	0.50
1:E:201:MET:HA	1:E:201:MET:HE3	1.94	0.50
1:G:39:VAL:HA	1:G:133:VAL:O	2.11	0.50
1:O:287:ALA:HA	2:P:109:PRO:HB2	1.92	0.50
1:E:220:ALA:HA	1:E:225:VAL:CG1	2.41	0.50
2:F:48:LEU:HD12	2:F:128:LEU:CD2	2.41	0.50
1:I:297:LEU:CD1	2:J:48:LEU:HD12	2.42	0.50
2:P:40:ALA:HB2	2:P:76:ILE:HD13	1.94	0.50
2:P:40:ALA:O	2:P:72:ARG:NH2	2.44	0.50
1:K:347:VAL:HG23	1:K:389:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ALA:HB3	1:A:34:ASN:HD22	1.77	0.50
1:A:150:GLY:CA	1:A:151:ARG:CB	2.90	0.50
1:E:323:MET:SD	1:E:340:TYR:HB2	2.51	0.50
1:M:245:MET:SD	1:M:383:ILE:HG21	2.51	0.50
1:M:377:LEU:HD22	1:M:388:LEU:HG	1.92	0.50
2:N:116:MET:SD	2:N:126:ILE:HD13	2.52	0.50
1:O:201:MET:HG2	1:O:241:ILE:HD13	1.93	0.50
1:I:69:LEU:HD13	1:K:80:LEU:HD13	1.93	0.50
1:C:153:GLY:O	1:C:157:THR:HG23	2.11	0.50
1:E:95:PHE:HB2	1:E:133:VAL:HG22	1.94	0.50
1:E:96:THR:HG23	1:E:136:PHE:CE1	2.46	0.49
1:G:85:ILE:HG23	1:G:90:ALA:HB3	1.94	0.49
1:K:82:ALA:HB2	1:K:132:ILE:HD12	1.94	0.49
1:A:241:ILE:N	1:A:241:ILE:HD12	2.27	0.49
2:N:47:VAL:O	2:N:48:LEU:HD22	2.12	0.49
2:B:48:LEU:HD23	2:B:48:LEU:N	2.27	0.49
1:G:297:LEU:HD13	2:H:48:LEU:HD21	1.94	0.49
2:H:17:LYS:HG2	2:H:92:ASP:HB3	1.93	0.49
1:I:337:ASN:HD22	1:I:338:VAL:H	1.61	0.49
1:O:334:ASN:N	1:O:334:ASN:HD22	2.10	0.49
2:B:134:ILE:HD13	2:B:134:ILE:H	1.76	0.49
1:E:217:VAL:HG13	1:E:241:ILE:HD11	1.94	0.49
1:A:327:LYS:HG3	1:O:60:VAL:HG11	1.93	0.49
2:D:115:PHE:CD2	2:D:116:MET:HE3	2.48	0.49
2:D:140:ILE:HD11	2:D:145:LEU:HD12	1.93	0.49
1:M:84:ALA:O	1:M:88:LEU:HD22	2.12	0.49
1:O:375:ILE:HD12	1:O:387:VAL:HG21	1.94	0.49
1:A:205:ALA:HA	1:A:209:SER:HB2	1.95	0.49
1:C:26:ILE:HD13	1:C:38:VAL:HG21	1.95	0.49
1:E:323:MET:HA	1:E:323:MET:HE2	1.94	0.49
1:O:3:LEU:HD22	1:O:167:ALA:CB	2.42	0.49
2:P:127:GLU:C	2:P:128:LEU:HD12	2.37	0.49
2:J:23:ILE:HD13	2:J:61:ILE:CD1	2.42	0.49
1:A:378:ILE:HG12	1:A:387:VAL:HG12	1.93	0.49
1:E:323:MET:HA	1:E:323:MET:CE	2.42	0.49
1:K:95:PHE:O	1:K:133:VAL:HA	2.13	0.49
1:G:214:LEU:HB3	2:H:103:ALA:HB1	1.95	0.49
1:I:286:LEU:HD21	1:I:326:LEU:HD21	1.95	0.49
2:J:21:LEU:HD23	2:J:60:ASP:CG	2.38	0.49
1:G:212:LEU:HD13	1:G:217:VAL:HG21	1.95	0.48
2:H:23:ILE:HD12	2:H:24:SER:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:375:ILE:HG23	1:O:387:VAL:HB	1.95	0.48
1:A:297:LEU:CD1	1:A:377:LEU:HD21	2.42	0.48
1:C:95:PHE:HB3	1:C:100:ALA:HB2	1.94	0.48
2:B:140:ILE:HD13	2:B:140:ILE:H	1.77	0.48
1:I:93:GLN:HG2	1:I:124:ALA:HB1	1.95	0.48
1:I:297:LEU:HD11	2:J:48:LEU:HD12	1.95	0.48
2:L:23:ILE:HD13	2:L:86:TRP:NE1	2.28	0.48
1:M:68:MET:HE1	1:O:78:ASN:CG	2.38	0.48
2:H:44:ILE:C	2:H:44:ILE:CD1	2.85	0.48
1:O:207:VAL:HG11	1:O:384:ARG:HD2	1.95	0.48
1:O:272:ILE:HD12	1:O:310:ILE:CD1	2.43	0.48
1:A:374:ASN:HD21	3:B:501:THR:N	2.12	0.48
1:C:297:LEU:HD12	1:C:379:SER:HB2	1.95	0.48
1:M:71:THR:HG23	1:M:135:GLY:HA3	1.96	0.48
1:M:214:LEU:HB3	2:N:103:ALA:HB1	1.95	0.48
1:M:297:LEU:CD2	2:N:48:LEU:HD12	2.43	0.48
1:A:47:THR:HG23	1:A:70:LEU:HD22	1.95	0.48
1:C:116:VAL:CG1	1:C:164:ALA:HB2	2.43	0.48
1:I:297:LEU:HD11	2:J:48:LEU:CD1	2.43	0.48
2:L:23:ILE:HD13	2:L:86:TRP:HE1	1.78	0.48
1:M:8:TYR:CE2	1:M:26:ILE:HD11	2.49	0.48
1:A:149:LEU:O	1:A:150:GLY:C	2.56	0.48
1:E:98:SER:HA	1:E:102:VAL:HG23	1.95	0.48
1:E:374:ASN:ND2	3:F:501:THR:N	2.62	0.48
1:E:403:GLU:O	1:E:406:GLN:NE2	2.46	0.48
1:M:172:ILE:HG12	1:M:212:LEU:HD21	1.96	0.48
1:A:377:LEU:HD22	1:A:388:LEU:HG	1.95	0.47
1:C:51:LEU:HD23	1:C:66:MET:CE	2.44	0.47
2:J:19:THR:HG23	2:J:62:THR:CG2	2.35	0.47
1:O:297:LEU:HD22	1:O:377:LEU:CG	2.45	0.47
1:A:206:ALA:CB	2:B:134:ILE:HD12	2.45	0.47
1:C:327:LYS:O	1:C:331:VAL:HG23	2.15	0.47
1:C:368:LEU:CD1	1:C:375:ILE:HD11	2.45	0.47
2:H:74:MET:SD	2:H:91:TYR:HB2	2.54	0.47
1:K:3:LEU:HD23	1:K:4:VAL:N	2.29	0.47
1:K:85:ILE:HG23	1:K:90:ALA:CB	2.42	0.47
2:N:122:VAL:HG23	2:N:124:VAL:CG2	2.37	0.47
1:A:181:THR:HG22	1:A:193:LEU:HD11	1.97	0.47
1:E:186:ILE:HD12	1:E:395:ASP:OD1	2.14	0.47
1:G:25:ARG:NH2	1:G:234:SER:O	2.44	0.47
1:M:2:ALA:HB3	1:M:34:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:39:VAL:HG21	1:M:158:ALA:HA	1.96	0.47
1:O:202:LEU:HD13	1:O:217:VAL:CG1	2.45	0.47
1:A:94:SER:CB	1:C:68:MET:HE1	2.44	0.47
1:C:375:ILE:HG23	1:C:387:VAL:HB	1.96	0.47
1:G:196:LEU:HD23	1:G:196:LEU:N	2.29	0.47
1:K:298:GLN:NE2	3:K:501:THR:HG21	2.26	0.47
2:P:40:ALA:CB	2:P:76:ILE:CD1	2.93	0.47
1:A:60:VAL:O	1:A:60:VAL:HG22	2.15	0.47
1:I:4:VAL:HG23	1:I:169:VAL:HG13	1.96	0.47
1:I:241:ILE:HD12	1:I:241:ILE:N	2.29	0.47
1:K:360:VAL:HG13	1:K:405:PHE:CE1	2.50	0.47
1:C:295:MET:HE1	1:C:388:LEU:HD11	1.96	0.47
1:E:212:LEU:HD13	1:E:217:VAL:CG2	2.44	0.47
1:I:195:LYS:HE3	1:I:242:ALA:HB3	1.96	0.47
2:J:23:ILE:HG21	2:J:61:ILE:HG13	1.96	0.47
1:A:269:VAL:HG11	1:A:272:ILE:HD11	1.97	0.47
1:C:293:ILE:HD12	1:C:293:ILE:C	2.40	0.47
2:P:122:VAL:HG23	2:P:124:VAL:HG23	1.95	0.47
1:E:297:LEU:CD2	1:E:377:LEU:HD21	2.45	0.46
1:I:60:VAL:O	1:I:60:VAL:HG13	2.15	0.46
2:D:48:LEU:HD13	2:D:128:LEU:HD23	1.96	0.46
2:J:59:THR:HG22	2:J:60:ASP:H	1.80	0.46
2:B:23:ILE:HD12	2:B:86:TRP:HD1	1.79	0.46
1:G:374:ASN:HD21	3:H:501:THR:N	2.13	0.46
1:I:289:ALA:HB3	1:I:291:ILE:HD13	1.97	0.46
1:A:30:LYS:HD3	2:F:54:VAL:HG12	1.98	0.46
1:A:78:ASN:HD22	1:A:134:ALA:HB3	1.79	0.46
1:A:365:MET:SD	1:A:375:ILE:HD13	2.55	0.46
1:O:46:THR:HG22	1:O:50:LEU:HD22	1.98	0.46
1:O:96:THR:H	1:O:99:GLN:HE21	1.63	0.46
1:A:58:ASN:OD1	1:A:59:PRO:O	2.33	0.46
1:A:298:GLN:HE22	3:A:501:THR:CG2	2.29	0.46
1:M:297:LEU:HD21	2:N:48:LEU:HD12	1.97	0.46
1:O:293:ILE:HD12	2:P:109:PRO:HA	1.97	0.46
1:I:78:ASN:C	1:I:78:ASN:ND2	2.74	0.46
1:I:380:THR:HG21	2:J:46:MET:CA	2.46	0.46
1:O:389:ILE:HD13	1:O:389:ILE:H	1.81	0.46
1:G:117:THR:O	1:G:117:THR:CG2	2.58	0.46
2:J:39:ASP:O	2:J:40:ALA:CB	2.64	0.46
1:A:380:THR:HG22	1:A:385:ILE:HD13	1.97	0.46
1:E:50:LEU:HD22	1:E:69:LEU:CD1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:VAL:HG12	1:I:26:ILE:HD13	1.98	0.46
1:I:266:LYS:HE3	2:J:51:VAL:HG11	1.98	0.46
1:I:377:LEU:C	1:I:377:LEU:HD23	2.41	0.46
2:J:141:ARG:NE	2:J:141:ARG:HA	2.30	0.46
1:O:337:ASN:HD22	1:O:338:VAL:N	2.13	0.46
1:C:300:VAL:CG1	2:D:128:LEU:HD11	2.45	0.45
1:G:212:LEU:HD13	1:G:217:VAL:CG2	2.45	0.45
1:K:26:ILE:HG21	1:K:85:ILE:HD11	1.97	0.45
1:K:170:CYS:HB3	1:K:227:LEU:HD23	1.97	0.45
2:B:82:VAL:HG13	2:B:83:GLN:N	2.31	0.45
1:C:245:MET:HE1	1:C:383:ILE:HG21	1.97	0.45
1:G:365:MET:SD	1:G:375:ILE:HD13	2.56	0.45
1:I:254:VAL:HG12	1:I:255:LEU:N	2.31	0.45
1:M:303:VAL:O	1:M:303:VAL:HG22	2.15	0.45
1:A:298:GLN:HE21	1:A:310:ILE:HG12	1.82	0.45
1:A:202:LEU:CD1	1:A:217:VAL:HG12	2.45	0.45
2:B:48:LEU:CD1	2:B:128:LEU:HD23	2.21	0.45
1:E:378:ILE:HG12	1:E:387:VAL:HG12	1.99	0.45
2:F:46:MET:HE3	2:F:64:THR:CG2	2.43	0.45
2:J:22:GLY:HA3	2:J:87:THR:HG23	1.99	0.45
1:G:90:ALA:HB1	1:G:130:ILE:HD12	1.98	0.45
1:G:187:VAL:HG11	1:G:402:HIS:CG	2.52	0.45
2:H:92:ASP:OD1	2:H:141:ARG:NH1	2.49	0.45
2:D:21:LEU:C	2:D:87:THR:HG22	2.41	0.45
1:E:8:TYR:CE1	1:E:22:VAL:HG13	2.52	0.45
1:E:293:ILE:HD13	1:E:293:ILE:O	2.16	0.45
2:J:125:ASN:O	2:J:140:ILE:HG22	2.17	0.45
2:D:142:GLU:O	2:D:145:LEU:HD13	2.17	0.45
1:C:300:VAL:HG12	2:D:128:LEU:HD11	1.97	0.45
1:C:380:THR:HG22	1:C:385:ILE:HA	1.98	0.45
1:E:203:GLU:O	1:E:207:VAL:HG22	2.16	0.45
1:C:208:GLY:CA	1:C:259:ALA:HB1	2.47	0.45
1:E:273:SER:HA	1:E:307:THR:HG22	1.99	0.45
1:G:298:GLN:HE21	1:G:310:ILE:HG12	1.82	0.45
2:J:24:SER:HA	2:J:58:THR:HG22	1.99	0.45
1:M:187:VAL:HG22	1:M:399:ARG:HG3	1.98	0.44
1:O:102:VAL:HG21	1:O:151:ARG:HH21	1.81	0.44
2:D:62:THR:HG21	2:D:128:LEU:CD2	2.43	0.44
1:K:35:ASP:HB3	1:K:125:LEU:HD22	1.98	0.44
1:O:85:ILE:HG23	1:O:90:ALA:HB3	1.97	0.44
1:A:255:LEU:HA	1:A:351:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:380:THR:HG21	2:J:47:VAL:N	2.31	0.44
1:I:406:GLN:O	1:I:406:GLN:HG2	2.16	0.44
1:A:262:LYS:HB3	1:A:394:LEU:HD11	2.00	0.44
1:A:300:VAL:CG1	2:B:128:LEU:HD11	2.45	0.44
2:D:16:ALA:HB1	2:D:92:ASP:O	2.18	0.44
1:E:274:ASP:OD2	3:E:501:THR:N	2.51	0.44
1:M:172:ILE:HD11	1:M:227:LEU:HD22	1.99	0.44
1:O:25:ARG:NH2	1:O:234:SER:O	2.50	0.44
1:G:193:LEU:HD23	1:G:196:LEU:HD13	1.99	0.44
1:A:337:ASN:HD22	1:A:338:VAL:N	2.10	0.44
2:D:37:LEU:HD11	2:D:63:PHE:CZ	2.53	0.44
1:I:15:SER:OG	1:I:16:ALA:N	2.49	0.44
2:J:46:MET:HE2	2:J:48:LEU:HD21	2.00	0.44
2:B:85:ASN:HD22	2:B:86:TRP:N	2.15	0.44
2:D:60:ASP:C	2:D:61:ILE:HD12	2.43	0.44
1:E:245:MET:SD	1:E:383:ILE:HG21	2.58	0.44
1:O:272:ILE:HD12	1:O:310:ILE:HG13	2.00	0.44
1:A:202:LEU:CD1	1:A:217:VAL:CG1	2.96	0.44
1:G:297:LEU:CD1	2:H:48:LEU:CD2	2.96	0.44
1:O:59:PRO:O	1:O:60:VAL:CG1	2.66	0.44
1:O:181:THR:HG23	1:O:193:LEU:CD1	2.47	0.44
1:A:150:GLY:HA3	1:A:151:ARG:HB2	1.99	0.44
2:B:105:MET:HE3	2:B:134:ILE:HA	2.00	0.44
1:G:272:ILE:HD12	1:G:310:ILE:HG13	1.99	0.44
1:I:380:THR:CG2	2:J:47:VAL:H	2.27	0.44
1:O:272:ILE:CD1	1:O:310:ILE:HD12	2.47	0.44
1:O:349:LEU:HD22	1:O:405:PHE:CE1	2.52	0.44
1:C:93:GLN:HE21	1:C:93:GLN:HA	1.83	0.43
1:C:294:ASP:O	1:C:295:MET:C	2.61	0.43
1:E:172:ILE:HD12	1:E:172:ILE:N	2.33	0.43
1:M:26:ILE:HG22	1:M:130:ILE:HD13	1.98	0.43
1:G:245:MET:SD	1:G:383:ILE:HG21	2.57	0.43
1:O:347:VAL:HG22	1:O:394:LEU:CD2	2.46	0.43
1:E:58:ASN:HD22	1:E:59:PRO:N	2.16	0.43
1:I:100:ALA:CB	1:I:121:VAL:HG23	2.48	0.43
1:M:154:SER:O	1:M:157:THR:HG22	2.18	0.43
1:E:333:GLY:O	1:E:334:ASN:C	2.61	0.43
1:I:2:ALA:HA	1:I:34:ASN:HD22	1.84	0.43
1:I:406:GLN:O	1:I:406:GLN:CG	2.66	0.43
1:M:220:ALA:HA	1:M:225:VAL:CG1	2.39	0.43
1:M:323:MET:SD	1:M:338:VAL:HG12	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HG2	1:A:75:ARG:HH11	1.83	0.43
2:D:25:ASP:OD2	3:D:501:THR:N	2.52	0.43
1:E:209:SER:HB2	1:E:211:ILE:HD13	2.00	0.43
1:E:255:LEU:HA	1:E:351:GLY:HA3	1.99	0.43
1:G:228:ARG:HD2	1:G:237:PRO:O	2.19	0.43
1:K:227:LEU:O	1:K:240:LEU:HD12	2.18	0.43
1:M:357:HIS:HA	1:M:358:PRO:HD3	1.88	0.43
1:O:42:ALA:HB1	1:O:46:THR:HB	2.01	0.43
1:C:361:THR:HG22	2:D:44:ILE:HD12	2.00	0.43
1:I:286:LEU:HD22	1:I:326:LEU:HD21	1.99	0.43
1:K:347:VAL:HG22	1:K:394:LEU:CD2	2.48	0.43
1:A:208:GLY:O	1:A:209:SER:C	2.62	0.43
1:A:215:ARG:NH2	4:A:517:HOH:O	2.51	0.43
2:D:46:MET:CE	2:D:139:LEU:HD21	2.26	0.43
1:E:102:VAL:HG12	1:E:103:LEU:H	1.84	0.43
1:E:297:LEU:HD12	2:F:48:LEU:HD21	2.00	0.43
1:M:154:SER:HA	1:M:157:THR:HG22	1.99	0.43
2:P:3:GLU:HA	2:P:108:HIS:CE1	2.54	0.43
2:P:40:ALA:CB	2:P:76:ILE:HD13	2.49	0.43
2:P:98:VAL:HG13	2:P:138:VAL:CG2	2.48	0.43
1:A:35:ASP:HB3	1:A:125:LEU:HD22	2.01	0.43
2:H:135:ARG:O	2:H:136:ILE:HD13	2.18	0.43
1:I:255:LEU:N	1:I:255:LEU:HD12	2.33	0.43
1:I:374:ASN:HD21	3:J:501:THR:N	2.16	0.43
1:K:297:LEU:HD11	1:K:378:ILE:O	2.19	0.43
1:M:377:LEU:HG	2:N:49:GLN:O	2.19	0.43
1:C:245:MET:HE1	1:C:383:ILE:CG2	2.49	0.43
1:E:337:ASN:HD22	1:E:337:ASN:HA	1.72	0.43
1:I:274:ASP:OD2	1:I:301:SER:OG	2.37	0.43
2:L:23:ILE:HD12	2:L:24:SER:H	1.84	0.43
1:O:292:ASN:N	1:O:292:ASN:HD22	2.16	0.43
1:E:26:ILE:HD13	1:E:38:VAL:HG21	2.01	0.42
1:I:8:TYR:CE1	1:I:22:VAL:HG13	2.55	0.42
1:K:300:VAL:CG1	2:L:128:LEU:HD11	2.48	0.42
1:O:378:ILE:HG12	1:O:387:VAL:HG12	2.01	0.42
1:A:202:LEU:HD13	1:A:217:VAL:HG12	2.01	0.42
1:A:298:GLN:HE22	3:A:501:THR:CB	2.33	0.42
1:C:336:THR:HG22	1:C:337:ASN:HB2	2.01	0.42
1:G:101:GLY:O	1:G:116:VAL:HG13	2.19	0.42
1:K:78:ASN:HD22	1:K:134:ALA:HB3	1.84	0.42
1:K:365:MET:HE3	1:K:378:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:270:LEU:HD11	1:O:339:LEU:HD11	2.01	0.42
1:G:220:ALA:HA	1:G:225:VAL:CG1	2.48	0.42
2:F:48:LEU:HD11	2:F:129:ILE:O	2.19	0.42
1:O:15:SER:O	1:O:19:ILE:HG12	2.19	0.42
1:A:213:VAL:O	1:A:217:VAL:HG23	2.18	0.42
1:E:96:THR:HG23	1:E:136:PHE:HZ	1.82	0.42
1:G:323:MET:HE3	1:G:340:TYR:HB2	2.01	0.42
1:K:163:ALA:HB1	1:K:223:PHE:CD1	2.54	0.42
1:M:39:VAL:HG11	1:M:154:SER:O	2.19	0.42
1:M:85:ILE:HG23	1:M:90:ALA:HB3	1.96	0.42
1:M:229:VAL:HG23	1:M:241:ILE:HD11	2.02	0.42
2:D:19:THR:HG22	2:D:21:LEU:HD23	2.01	0.42
1:I:80:LEU:O	1:K:57:VAL:HG11	2.20	0.42
1:K:365:MET:SD	1:K:375:ILE:HD13	2.59	0.42
1:M:193:LEU:CD2	1:M:256:THR:HG23	2.49	0.42
1:O:303:VAL:O	1:O:304:GLU:C	2.63	0.42
2:P:2:GLU:O	2:P:108:HIS:NE2	2.52	0.42
1:A:152:GLY:HA3	1:A:156:THR:CG2	2.49	0.42
1:K:277:GLY:O	1:K:280:ALA:HB3	2.20	0.42
2:L:81:GLN:O	2:L:82:VAL:HG13	2.20	0.42
1:M:353:GLY:O	1:M:357:HIS:ND1	2.52	0.42
2:B:59:THR:HG22	2:B:60:ASP:H	1.85	0.42
2:H:5:VAL:CG1	2:H:103:ALA:HB3	2.48	0.42
1:I:100:ALA:HA	1:I:119:GLY:HA3	2.01	0.42
2:L:92:ASP:OD2	2:L:141:ARG:NH1	2.53	0.42
1:M:265:ALA:HB2	1:M:316:ARG:HG2	2.01	0.42
1:M:297:LEU:HD13	1:M:377:LEU:CD1	2.47	0.42
1:O:203:GLU:O	1:O:207:VAL:HG22	2.19	0.42
1:O:321:ARG:O	1:O:325:ILE:HG12	2.20	0.42
1:C:368:LEU:HD13	1:C:375:ILE:CD1	2.49	0.42
2:D:98:VAL:HG12	2:D:140:ILE:HD12	2.01	0.42
1:E:205:ALA:HB1	1:E:214:LEU:CD1	2.50	0.42
2:J:131:THR:HG22	2:J:136:ILE:HA	2.02	0.42
1:K:212:LEU:HD23	1:K:217:VAL:CG2	2.45	0.42
1:M:26:ILE:HB	1:M:85:ILE:HD11	2.01	0.42
1:M:68:MET:HE2	1:O:79:ALA:HB2	2.01	0.42
1:M:116:VAL:O	1:M:116:VAL:HG23	2.20	0.42
1:C:305:ASP:HB3	1:C:307:THR:HG22	2.01	0.42
1:I:54:ALA:HA	1:K:83:MET:HE1	2.01	0.42
2:P:158:LEU:HD13	2:P:158:LEU:HA	1.93	0.42
1:C:116:VAL:HG21	1:C:164:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ILE:N	1:C:241:ILE:HD12	2.35	0.41
2:D:13:LYS:O	2:D:13:LYS:HG2	2.20	0.41
2:H:99:SER:HA	2:H:136:ILE:O	2.20	0.41
1:M:75:ARG:NH1	1:O:68:MET:HE3	2.34	0.41
1:O:196:LEU:CD1	1:O:256:THR:CG2	2.97	0.41
2:P:84:GLY:O	2:P:85:ASN:C	2.63	0.41
1:E:269:VAL:HB	1:E:272:ILE:HD11	2.02	0.41
1:G:46:THR:O	1:G:50:LEU:HD13	2.20	0.41
1:K:93:GLN:HE21	1:K:129:LYS:HD3	1.85	0.41
2:N:46:MET:CE	2:N:64:THR:HG21	2.47	0.41
1:O:64:ARG:HD3	1:O:64:ARG:H	1.85	0.41
1:C:368:LEU:CD1	1:C:375:ILE:CD1	2.98	0.41
1:C:368:LEU:HD12	1:C:375:ILE:HD11	2.01	0.41
2:D:48:LEU:HD12	2:D:128:LEU:HD23	2.03	0.41
1:E:134:ALA:HB3	1:E:136:PHE:CE2	2.46	0.41
2:L:81:GLN:C	2:L:82:VAL:CG1	2.92	0.41
2:B:33:VAL:HG13	2:B:34:PHE:CD2	2.55	0.41
1:C:375:ILE:HG21	1:C:378:ILE:HG12	2.02	0.41
1:K:248:ILE:HD12	1:K:249:PRO:HD2	2.02	0.41
2:N:16:ALA:HB2	2:N:67:ARG:HG3	2.01	0.41
1:C:297:LEU:C	1:C:297:LEU:HD23	2.45	0.41
1:K:359:GLY:HA2	2:L:38:ALA:HB2	2.01	0.41
1:M:170:CYS:HB3	1:M:227:LEU:HD23	2.01	0.41
1:A:262:LYS:HB3	1:A:394:LEU:CD1	2.51	0.41
1:A:377:LEU:HD23	1:A:378:ILE:N	2.36	0.41
1:I:269:VAL:CG1	1:I:272:ILE:HD11	2.50	0.41
1:K:80:LEU:HA	1:K:83:MET:HE2	2.02	0.41
1:M:362:ALA:HB2	2:N:34:PHE:O	2.21	0.41
1:O:185:ARG:CG	1:O:186:ILE:HD12	2.51	0.41
1:A:260:THR:HG22	1:A:347:VAL:HG12	2.02	0.41
1:A:298:GLN:NE2	3:A:501:THR:HG21	2.33	0.41
2:D:131:THR:CG2	2:D:136:ILE:HG23	2.51	0.41
1:I:347:VAL:HG22	1:I:394:LEU:HD23	2.03	0.41
2:B:37:LEU:HD11	2:B:63:PHE:CZ	2.56	0.41
1:C:212:LEU:HD11	1:C:229:VAL:CG2	2.49	0.41
1:E:54:ALA:HB1	1:E:66:MET:HE1	2.02	0.41
2:H:5:VAL:C	2:H:6:LEU:HD13	2.46	0.41
1:I:98:SER:C	1:I:100:ALA:H	2.28	0.41
1:I:270:LEU:O	1:I:336:THR:HG22	2.21	0.41
1:K:328:LYS:NZ	1:M:290:GLU:OE2	2.54	0.41
2:L:48:LEU:N	2:L:48:LEU:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:81:GLN:C	2:L:82:VAL:HG13	2.46	0.41
1:M:6:GLN:OE1	1:M:26:ILE:HD13	2.21	0.41
1:M:347:VAL:HG23	1:M:389:ILE:HD11	2.03	0.41
2:N:48:LEU:HD21	2:N:130:SER:HB2	2.02	0.41
2:N:129:ILE:HG12	2:N:138:VAL:HG12	2.03	0.41
1:O:220:ALA:HA	1:O:225:VAL:CG1	2.49	0.41
1:O:304:GLU:HA	1:O:304:GLU:OE1	2.21	0.41
2:P:59:THR:HG22	2:P:60:ASP:H	1.85	0.41
2:P:98:VAL:HG13	2:P:138:VAL:HG23	2.03	0.41
1:A:305:ASP:OD2	1:A:305:ASP:C	2.62	0.41
1:K:365:MET:CE	1:K:378:ILE:HD13	2.50	0.41
1:K:377:LEU:HG	2:L:49:GLN:O	2.21	0.41
1:M:26:ILE:HG23	1:M:36:VAL:HG11	2.02	0.41
1:O:181:THR:CG2	1:O:193:LEU:HD11	2.50	0.41
1:A:330:GLN:HG3	1:A:335:TRP:HD1	1.87	0.40
2:B:122:VAL:HG23	2:B:124:VAL:HG23	2.02	0.40
2:D:23:ILE:CG2	2:D:61:ILE:HD13	2.39	0.40
2:H:124:VAL:HG13	2:H:144:ASP:HB3	2.03	0.40
1:I:23:ALA:CB	1:I:84:ALA:HB1	2.51	0.40
1:M:348:SER:HA	1:M:385:ILE:O	2.21	0.40
1:C:187:VAL:HG11	1:C:402:HIS:CG	2.56	0.40
1:C:321:ARG:O	1:C:325:ILE:HD13	2.21	0.40
1:C:365:MET:CE	1:C:378:ILE:HD13	2.52	0.40
1:O:272:ILE:HD12	1:O:310:ILE:CG1	2.51	0.40
1:A:325:ILE:O	1:A:329:LEU:HD23	2.21	0.40
2:F:6:LEU:HD12	2:F:6:LEU:N	2.36	0.40
1:G:323:MET:HA	1:G:323:MET:HE2	2.03	0.40
1:I:179:VAL:HB	1:I:239:THR:HG21	2.03	0.40
1:M:13:LEU:HD13	1:M:77:SER:HB3	2.03	0.40
2:B:126:ILE:HG23	2:B:138:VAL:HB	2.03	0.40
1:G:202:LEU:HD13	1:G:217:VAL:CG1	2.51	0.40
1:I:22:VAL:O	1:I:26:ILE:HD13	2.21	0.40
1:M:8:TYR:HE2	1:M:26:ILE:HD11	1.84	0.40
1:O:298:GLN:HE21	1:O:310:ILE:HG12	1.85	0.40
1:O:377:LEU:HD23	1:O:378:ILE:N	2.37	0.40
2:H:23:ILE:HG22	2:H:86:TRP:CD1	2.57	0.40
1:I:97:GLY:HA2	1:I:135:GLY:C	2.46	0.40
2:N:17:LYS:HG2	2:N:92:ASP:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/421 (90%)	356 (94%)	16 (4%)	6 (2%)	7	16
1	C	374/421 (89%)	357 (96%)	15 (4%)	2 (0%)	24	46
1	E	377/421 (90%)	355 (94%)	16 (4%)	6 (2%)	7	16
1	G	377/421 (90%)	356 (94%)	20 (5%)	1 (0%)	36	58
1	I	371/421 (88%)	353 (95%)	14 (4%)	4 (1%)	11	25
1	K	374/421 (89%)	361 (96%)	10 (3%)	3 (1%)	16	34
1	M	372/421 (88%)	353 (95%)	15 (4%)	4 (1%)	11	25
1	O	380/421 (90%)	369 (97%)	9 (2%)	2 (0%)	24	46
2	B	158/178 (89%)	151 (96%)	6 (4%)	1 (1%)	21	42
2	D	148/178 (83%)	141 (95%)	7 (5%)	0	100	100
2	F	151/178 (85%)	143 (95%)	7 (5%)	1 (1%)	18	38
2	H	151/178 (85%)	149 (99%)	2 (1%)	0	100	100
2	J	148/178 (83%)	136 (92%)	11 (7%)	1 (1%)	18	38
2	L	148/178 (83%)	143 (97%)	5 (3%)	0	100	100
2	N	153/178 (86%)	145 (95%)	8 (5%)	0	100	100
2	P	157/178 (88%)	151 (96%)	3 (2%)	3 (2%)	6	13
All	All	4217/4792 (88%)	4019 (95%)	164 (4%)	34 (1%)	16	34

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	A	151	ARG
1	A	209	SER
2	B	82	VAL
1	E	98	SER
1	E	119	GLY

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Mol	Chain	Res	Type
1	E	334	ASN
2	J	40	ALA
2	P	83	GLN
2	P	85	ASN
1	A	150	GLY
2	F	82	VAL
1	G	135	GLY
1	I	125	LEU
1	K	119	GLY
1	M	100	ALA
1	O	305	ASP
2	P	82	VAL
1	E	97	GLY
1	K	103	LEU
1	K	331	VAL
1	O	304	GLU
1	A	97	GLY
1	C	305	ASP
1	I	3	LEU
1	I	98	SER
1	M	102	VAL
1	C	331	VAL
1	E	333	GLY
1	M	118	PRO
1	M	303	VAL
1	E	208	GLY
1	I	208	GLY
1	A	208	GLY

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	300/336 (89%)	274 (91%)	26 (9%)	9	21
1	C	296/336 (88%)	273 (92%)	23 (8%)	11	26
1	E	297/336 (88%)	271 (91%)	26 (9%)	9	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	294/336 (88%)	273 (93%)	21 (7%)	13	31
1	I	288/336 (86%)	275 (96%)	13 (4%)	24	50
1	K	293/336 (87%)	278 (95%)	15 (5%)	21	45
1	M	296/336 (88%)	285 (96%)	11 (4%)	30	57
1	O	303/336 (90%)	278 (92%)	25 (8%)	10	23
2	B	126/146 (86%)	112 (89%)	14 (11%)	6	12
2	D	117/146 (80%)	111 (95%)	6 (5%)	21	45
2	F	126/146 (86%)	119 (94%)	7 (6%)	19	40
2	H	125/146 (86%)	118 (94%)	7 (6%)	19	40
2	J	108/146 (74%)	104 (96%)	4 (4%)	30	57
2	L	121/146 (83%)	118 (98%)	3 (2%)	42	69
2	N	119/146 (82%)	114 (96%)	5 (4%)	26	52
2	P	129/146 (88%)	118 (92%)	11 (8%)	10	22
All	All	3338/3856 (87%)	3121 (94%)	217 (6%)	15	35

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	17	GLU
1	A	50	LEU
1	A	80	LEU
1	A	85	ILE
1	A	86	GLU
1	A	99	GLN
1	A	122	ARG
1	A	136	PHE
1	A	151	ARG
1	A	156	THR
1	A	191	GLN
1	A	193	LEU
1	A	195	LYS
1	A	202	LEU
1	A	212	LEU
1	A	225	VAL
1	A	245	MET
1	A	264	GLU

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Mol	Chain	Res	Type
1	A	290	GLU
1	A	304	GLU
1	A	305	ASP
1	A	320	ARG
1	A	337	ASN
1	A	347	VAL
1	A	403	GLU
2	B	2	GLU
2	B	6	LEU
2	B	44	ILE
2	B	48	LEU
2	B	59	THR
2	B	76	ILE
2	B	77	LEU
2	B	85	ASN
2	B	86	TRP
2	B	88	ASN
2	B	134	ILE
2	B	140	ILE
2	B	141	ARG
2	B	145	LEU
1	C	3	LEU
1	C	30	LYS
1	C	69	LEU
1	C	70	LEU
1	C	78	ASN
1	C	80	LEU
1	C	85	ILE
1	C	88	LEU
1	C	93	GLN
1	C	99	GLN
1	C	122	ARG
1	C	123	GLU
1	C	136	PHE
1	C	199	GLU
1	C	202	LEU
1	C	207	VAL
1	C	215	ARG
1	C	221	ARG
1	C	225	VAL
1	C	248	ILE
1	C	272	ILE

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Mol	Chain	Res	Type
1	C	337	ASN
1	C	389	ILE
2	D	44	ILE
2	D	59	THR
2	D	85	ASN
2	D	116	MET
2	D	140	ILE
2	D	141	ARG
1	E	3	LEU
1	E	58	ASN
1	E	65	GLU
1	E	67	ASP
1	E	75	ARG
1	E	80	LEU
1	E	86	GLU
1	E	87	SER
1	E	93	GLN
1	E	96	THR
1	E	102	VAL
1	E	120	ARG
1	E	192	LYS
1	E	202	LEU
1	E	212	LEU
1	E	215	ARG
1	E	221	ARG
1	E	225	VAL
1	E	241	ILE
1	E	251	GLU
1	E	293	ILE
1	E	323	MET
1	E	328	LYS
1	E	337	ASN
1	E	347	VAL
1	E	403	GLU
2	F	13	LYS
2	F	48	LEU
2	F	55	GLU
2	F	74	MET
2	F	80	LEU
2	F	86	TRP
2	F	155	GLN
1	G	3	LEU

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Mol	Chain	Res	Type
1	G	76	ILE
1	G	78	ASN
1	G	86	GLU
1	G	87	SER
1	G	88	LEU
1	G	117	THR
1	G	151	ARG
1	G	196	LEU
1	G	202	LEU
1	G	212	LEU
1	G	214	LEU
1	G	215	ARG
1	G	225	VAL
1	G	293	ILE
1	G	305	ASP
1	G	329	LEU
1	G	334	ASN
1	G	337	ASN
1	G	347	VAL
1	G	403	GLU
2	H	6	LEU
2	H	23	ILE
2	H	44	ILE
2	H	48	LEU
2	H	71	ARG
2	H	81	GLN
2	H	141	ARG
1	I	18	ARG
1	I	30	LYS
1	I	64	ARG
1	I	66	MET
1	I	99	GLN
1	I	221	ARG
1	I	225	VAL
1	I	262	LYS
1	I	286	LEU
1	I	304	GLU
1	I	305	ASP
1	I	334	ASN
1	I	399	ARG
2	J	13	LYS
2	J	44	ILE

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Mol	Chain	Res	Type
2	J	59	THR
2	J	86	TRP
1	K	24	GLU
1	K	80	LEU
1	K	122	ARG
1	K	189	ASN
1	K	193	LEU
1	K	221	ARG
1	K	245	MET
1	K	252	GLU
1	K	262	LYS
1	K	304	GLU
1	K	332	GLN
1	K	339	LEU
1	K	389	ILE
1	K	394	LEU
1	K	406	GLN
2	L	59	THR
2	L	82	VAL
2	L	125	ASN
1	M	17	GLU
1	M	24	GLU
1	M	50	LEU
1	M	80	LEU
1	M	88	LEU
1	M	202	LEU
1	M	270	LEU
1	M	337	ASN
1	M	339	LEU
1	M	383	ILE
1	M	389	ILE
2	N	6	LEU
2	N	44	ILE
2	N	59	THR
2	N	77	LEU
2	N	153	HIS
1	O	7	LYS
1	O	25	ARG
1	O	64	ARG
1	O	65	GLU
1	O	71	THR
1	O	76	ILE

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Mol	Chain	Res	Type
1	O	80	LEU
1	O	104	THR
1	O	122	ARG
1	O	202	LEU
1	O	212	LEU
1	O	214	LEU
1	O	225	VAL
1	O	245	MET
1	O	250	VAL
1	O	255	LEU
1	O	264	GLU
1	O	272	ILE
1	O	290	GLU
1	O	293	ILE
1	O	323	MET
1	O	347	VAL
1	O	382	GLU
1	O	389	ILE
1	O	404	GLN
2	P	41	GLU
2	P	44	ILE
2	P	48	LEU
2	P	59	THR
2	P	77	LEU
2	P	80	LEU
2	P	86	TRP
2	P	88	ASN
2	P	135	ARG
2	P	141	ARG
2	P	158	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	78	ASN
1	A	292	ASN
1	A	298	GLN
1	A	334	ASN
1	A	337	ASN
1	A	343	GLN
1	A	404	GLN

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Mol	Chain	Res	Type
1	A	406	GLN
2	B	43	ASN
2	B	85	ASN
2	B	88	ASN
1	C	6	GLN
1	C	34	ASN
1	C	93	GLN
1	C	224	ASN
1	C	292	ASN
1	C	298	GLN
1	C	337	ASN
1	C	343	GLN
2	D	108	HIS
1	E	6	GLN
1	E	58	ASN
1	E	93	GLN
1	E	189	ASN
1	E	191	GLN
1	E	292	ASN
1	E	298	GLN
1	E	337	ASN
1	E	372	ASN
1	E	374	ASN
1	E	406	GLN
2	F	43	ASN
2	F	88	ASN
2	F	125	ASN
2	F	155	GLN
1	G	34	ASN
1	G	78	ASN
1	G	93	GLN
1	G	166	ASN
1	G	189	ASN
1	G	298	GLN
1	G	334	ASN
1	G	337	ASN
2	H	49	GLN
2	H	81	GLN
2	H	88	ASN
2	H	125	ASN
1	I	6	GLN
1	I	34	ASN

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Mol	Chain	Res	Type
1	I	78	ASN
1	I	99	GLN
1	I	292	ASN
1	I	298	GLN
1	I	334	ASN
1	I	337	ASN
1	I	343	GLN
1	I	372	ASN
1	I	374	ASN
1	I	406	GLN
2	J	43	ASN
2	J	81	GLN
2	J	85	ASN
2	J	123	ASN
1	K	21	ASN
1	K	34	ASN
1	K	78	ASN
1	K	93	GLN
1	K	189	ASN
1	K	292	ASN
1	K	298	GLN
1	K	330	GLN
1	K	332	GLN
1	K	337	ASN
1	K	343	GLN
1	K	374	ASN
2	L	108	HIS
2	L	123	ASN
1	M	34	ASN
1	M	99	GLN
1	M	191	GLN
1	M	292	ASN
1	M	337	ASN
1	M	343	GLN
1	M	404	GLN
2	N	49	GLN
1	O	21	ASN
1	O	34	ASN
1	O	99	GLN
1	O	166	ASN
1	O	189	ASN
1	O	235	ASN

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Mol	Chain	Res	Type
1	O	292	ASN
1	O	298	GLN
1	O	334	ASN
1	O	337	ASN
1	O	343	GLN
1	O	374	ASN
1	O	404	GLN
2	P	88	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	-	7,7,7	0.94	1 (14%)	8,9,9	1.28	1 (12%)
3	THR	H	501	-	7,7,7	0.89	1 (14%)	8,9,9	1.20	2 (25%)
3	THR	K	501	-	7,7,7	0.94	1 (14%)	8,9,9	1.18	1 (12%)
3	THR	B	501	-	7,7,7	0.95	1 (14%)	8,9,9	1.34	2 (25%)
3	THR	G	501	-	7,7,7	0.99	1 (14%)	8,9,9	1.28	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	THR	C	501	-	7,7,7	0.96	1 (14%)	8,9,9	1.27	1 (12%)
3	THR	D	501	-	7,7,7	0.93	1 (14%)	8,9,9	1.20	1 (12%)
3	THR	L	501	-	7,7,7	0.92	1 (14%)	8,9,9	1.09	1 (12%)
3	THR	M	501	-	7,7,7	0.93	1 (14%)	8,9,9	1.40	1 (12%)
3	THR	E	501	-	7,7,7	0.87	1 (14%)	8,9,9	1.37	2 (25%)
3	THR	J	501	-	7,7,7	0.89	1 (14%)	8,9,9	1.21	1 (12%)
3	THR	N	501	-	7,7,7	0.93	1 (14%)	8,9,9	1.21	1 (12%)
3	THR	F	501	-	7,7,7	1.01	1 (14%)	8,9,9	1.34	1 (12%)
3	THR	P	501	-	7,7,7	0.95	1 (14%)	8,9,9	1.30	2 (25%)
3	THR	O	501	-	7,7,7	0.92	1 (14%)	8,9,9	1.25	2 (25%)

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	-	-	4/8/8/8	-
3	THR	H	501	-	-	0/8/8/8	-
3	THR	K	501	-	-	0/8/8/8	-
3	THR	B	501	-	-	0/8/8/8	-
3	THR	G	501	-	-	6/8/8/8	-
3	THR	C	501	-	-	2/8/8/8	-
3	THR	D	501	-	-	4/8/8/8	-
3	THR	L	501	-	-	5/8/8/8	-
3	THR	M	501	-	-	0/8/8/8	-
3	THR	E	501	-	-	0/8/8/8	-
3	THR	J	501	-	-	1/8/8/8	-
3	THR	N	501	-	-	0/8/8/8	-
3	THR	F	501	-	-	4/8/8/8	-
3	THR	P	501	-	-	4/8/8/8	-
3	THR	O	501	-	-	0/8/8/8	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	THR	OXT-C	-2.40	1.23	1.30
3	C	501	THR	OXT-C	-2.33	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	501	THR	OXT-C	-2.32	1.23	1.30
3	K	501	THR	OXT-C	-2.27	1.23	1.30
3	P	501	THR	OXT-C	-2.26	1.23	1.30
3	L	501	THR	OXT-C	-2.25	1.23	1.30
3	N	501	THR	OXT-C	-2.24	1.23	1.30
3	D	501	THR	OXT-C	-2.24	1.23	1.30
3	B	501	THR	OXT-C	-2.23	1.23	1.30
3	O	501	THR	OXT-C	-2.20	1.23	1.30
3	M	501	THR	OXT-C	-2.18	1.23	1.30
3	J	501	THR	OXT-C	-2.18	1.23	1.30
3	H	501	THR	OXT-C	-2.18	1.23	1.30
3	A	501	THR	OXT-C	-2.15	1.23	1.30
3	E	501	THR	OXT-C	-2.12	1.23	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	501	THR	OXT-C-O	-3.13	116.98	124.08
3	M	501	THR	OXT-C-O	-3.04	117.19	124.08
3	C	501	THR	OXT-C-O	-2.92	117.47	124.08
3	B	501	THR	OXT-C-O	-2.90	117.49	124.08
3	G	501	THR	OXT-C-O	-2.90	117.50	124.08
3	E	501	THR	OXT-C-O	-2.87	117.57	124.08
3	P	501	THR	OXT-C-O	-2.85	117.62	124.08
3	A	501	THR	OXT-C-O	-2.84	117.64	124.08
3	J	501	THR	OXT-C-O	-2.67	118.02	124.08
3	D	501	THR	OXT-C-O	-2.67	118.03	124.08
3	N	501	THR	OXT-C-O	-2.64	118.09	124.08
3	K	501	THR	OXT-C-O	-2.59	118.20	124.08
3	O	501	THR	OXT-C-O	-2.58	118.22	124.08
3	H	501	THR	OXT-C-O	-2.53	118.33	124.08
3	L	501	THR	OXT-C-O	-2.43	118.57	124.08
3	E	501	THR	OXT-C-CA	2.34	122.20	114.15
3	B	501	THR	OXT-C-CA	2.21	121.78	114.15
3	P	501	THR	OXT-C-CA	2.19	121.70	114.15
3	O	501	THR	OXT-C-CA	2.08	121.32	114.15
3	H	501	THR	OXT-C-CA	2.04	121.19	114.15

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	THR	C-CA-CB-OG1
3	D	501	THR	N-CA-CB-OG1
3	D	501	THR	C-CA-CB-OG1
3	D	501	THR	C-CA-CB-CG2
3	F	501	THR	N-CA-CB-OG1
3	F	501	THR	N-CA-CB-CG2
3	F	501	THR	C-CA-CB-OG1
3	F	501	THR	C-CA-CB-CG2
3	G	501	THR	O-C-CA-N
3	G	501	THR	N-CA-CB-OG1
3	G	501	THR	C-CA-CB-OG1
3	G	501	THR	C-CA-CB-CG2
3	L	501	THR	C-CA-CB-OG1
3	P	501	THR	N-CA-CB-OG1
3	P	501	THR	N-CA-CB-CG2
3	P	501	THR	C-CA-CB-OG1
3	P	501	THR	C-CA-CB-CG2
3	C	501	THR	OXT-C-CA-N
3	J	501	THR	OXT-C-CA-N
3	L	501	THR	OXT-C-CA-N
3	D	501	THR	N-CA-CB-CG2
3	G	501	THR	N-CA-CB-CG2
3	A	501	THR	C-CA-CB-CG2
3	L	501	THR	C-CA-CB-CG2
3	G	501	THR	OXT-C-CA-N
3	C	501	THR	O-C-CA-N
3	A	501	THR	N-CA-CB-CG2
3	L	501	THR	N-CA-CB-CG2
3	A	501	THR	N-CA-CB-OG1
3	L	501	THR	N-CA-CB-OG1

There are no ring outliers.

12 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	THR	7	0
3	H	501	THR	3	0
3	K	501	THR	6	0
3	B	501	THR	1	0
3	G	501	THR	5	0
3	C	501	THR	4	0
3	D	501	THR	7	0
3	L	501	THR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	THR	1	0
3	J	501	THR	6	0
3	F	501	THR	6	0
3	P	501	THR	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/421 (91%)	0.07	5 (1%) 75 71	35, 56, 73, 82	1 (0%)
1	C	380/421 (90%)	0.15	7 (1%) 67 63	43, 61, 86, 96	0
1	E	383/421 (90%)	0.12	6 (1%) 70 66	42, 58, 76, 94	0
1	G	383/421 (90%)	0.10	10 (2%) 57 51	38, 56, 73, 83	0
1	I	377/421 (89%)	0.29	12 (3%) 50 44	50, 69, 90, 98	0
1	K	382/421 (90%)	0.13	8 (2%) 63 58	42, 62, 79, 93	0
1	M	380/421 (90%)	0.19	8 (2%) 63 58	48, 65, 79, 88	0
1	O	386/421 (91%)	-0.02	3 (0%) 82 80	37, 50, 69, 82	0
2	B	160/178 (89%)	0.11	2 (1%) 75 71	46, 61, 79, 89	0
2	D	152/178 (85%)	0.47	7 (4%) 37 32	60, 79, 103, 111	0
2	F	155/178 (87%)	0.01	3 (1%) 66 61	43, 59, 79, 87	0
2	H	155/178 (87%)	-0.14	1 (0%) 85 83	34, 50, 73, 83	0
2	J	152/178 (85%)	0.51	7 (4%) 37 32	60, 85, 103, 108	0
2	L	152/178 (85%)	0.12	3 (1%) 65 60	48, 68, 90, 96	0
2	N	155/178 (87%)	0.28	2 (1%) 75 71	59, 75, 93, 104	0
2	P	159/178 (89%)	-0.23	0 100 100	36, 47, 66, 72	0
All	All	4297/4792 (89%)	0.13	84 (1%) 65 60	34, 61, 87, 111	1 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	82	VAL	4.9
2	F	84	GLY	4.2
1	M	100	ALA	4.0
2	J	146	ASP	4.0
1	A	382	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	408	GLY	3.7
2	D	89	VAL	3.6
1	G	135	GLY	3.6
2	D	44	ILE	3.5
1	E	103	LEU	3.4
1	M	331	VAL	3.3
1	E	67	ASP	3.1
1	E	134	ALA	3.0
2	D	88	ASN	2.9
2	D	42	ILE	2.9
1	M	334	ASN	2.8
2	N	82	VAL	2.8
2	N	3	GLU	2.8
2	J	91	TYR	2.7
1	A	139	VAL	2.7
1	C	282	VAL	2.7
1	C	336	THR	2.7
2	L	4	ALA	2.7
2	D	76	ILE	2.7
1	I	89	GLY	2.6
2	H	2	GLU	2.6
2	B	84	GLY	2.6
1	A	97	GLY	2.6
1	E	136	PHE	2.5
1	G	2	ALA	2.5
1	I	291	ILE	2.5
1	G	332	GLN	2.5
1	A	334	ASN	2.5
1	I	2	ALA	2.5
1	M	135	GLY	2.5
1	K	234	SER	2.5
1	M	271	GLY	2.4
1	K	95	PHE	2.4
1	K	119	GLY	2.4
2	J	126	ILE	2.4
1	I	48	ASP	2.4
2	F	111	VAL	2.4
1	I	208	GLY	2.4
2	L	42	ILE	2.4
2	J	147	ALA	2.4
1	O	219	TYR	2.3
2	J	88	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	63	ALA	2.3
2	J	156	PHE	2.3
2	L	82	VAL	2.3
1	I	96	THR	2.3
2	D	53	SER	2.3
1	G	98	SER	2.2
1	A	102	VAL	2.2
1	C	303	VAL	2.2
1	E	60	VAL	2.2
1	M	394	LEU	2.2
1	C	294	ASP	2.2
1	G	247	ASP	2.2
1	I	251	GLU	2.2
1	K	104	THR	2.2
1	O	117	THR	2.2
1	I	101	GLY	2.2
1	K	270	LEU	2.2
1	G	253	ALA	2.2
1	M	150	GLY	2.2
1	C	136	PHE	2.2
1	C	360	VAL	2.1
1	G	152	GLY	2.1
1	C	408	GLY	2.1
1	I	409	GLY	2.1
2	D	119	LEU	2.1
1	I	347	VAL	2.1
1	M	136	PHE	2.1
1	O	100	ALA	2.1
1	G	67	ASP	2.1
1	I	102	VAL	2.0
1	K	136	PHE	2.0
2	F	82	VAL	2.0
1	I	100	ALA	2.0
2	B	77	LEU	2.0
1	E	104	THR	2.0
1	K	116	VAL	2.0
1	K	331	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	THR	M	501	8/8	0.84	0.11	39,39,39,39	0
3	THR	J	501	8/8	0.86	0.09	51,51,51,51	0
3	THR	C	501	8/8	0.87	0.10	71,71,71,71	0
3	THR	L	501	8/8	0.88	0.10	51,52,52,52	0
3	THR	D	501	8/8	0.91	0.10	35,35,35,35	0
3	THR	K	501	8/8	0.91	0.08	50,50,50,50	0
3	THR	B	501	8/8	0.92	0.07	38,39,39,39	0
3	THR	E	501	8/8	0.92	0.10	40,40,41,41	0
3	THR	N	501	8/8	0.92	0.10	38,38,38,38	0
3	THR	P	501	8/8	0.92	0.08	35,36,36,36	0
3	THR	A	501	8/8	0.93	0.06	40,40,40,40	0
3	THR	F	501	8/8	0.93	0.09	28,28,28,28	0
3	THR	G	501	8/8	0.94	0.07	29,30,30,30	0
3	THR	H	501	8/8	0.95	0.06	37,37,37,38	0
3	THR	O	501	8/8	0.98	0.05	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.