



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 02:46 AM EDT

PDB ID : 3AB2
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 : 4.02b-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

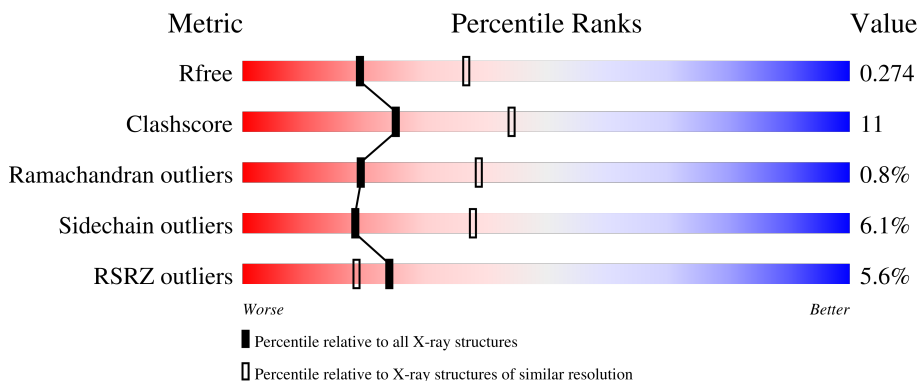
1 Overall quality at a glance

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.



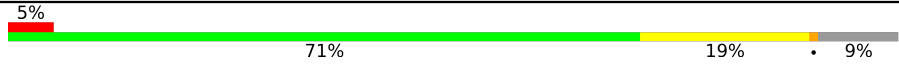

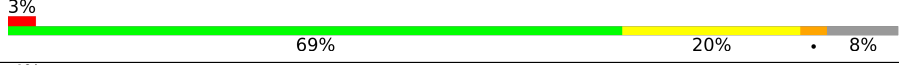


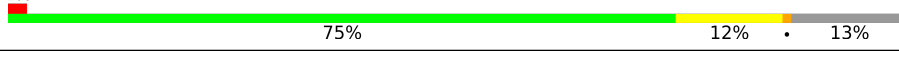
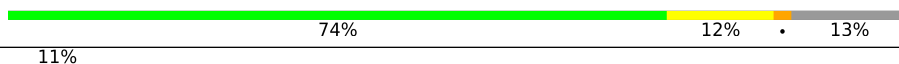

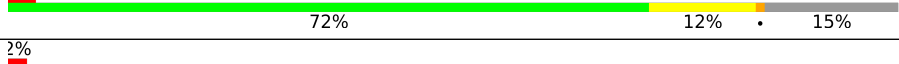

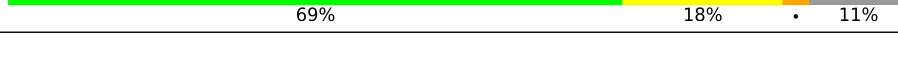
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	 6% 69% 20% • 8%
1	C	421	 4% 73% 15% • 10%
1	E	421	 4% 70% 19% • 9%
1	G	421	 6% 76% 14% • 9%
1	I	421	 4% 70% 18% • 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 [i](#)

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
			Total	C	N	O	S			
1	A	386	Total 2841	C 1761	N 492	O 574	S 14	0	0	0
1	C	380	Total 2793	C 1737	N 478	O 564	S 14	0	0	0
1	E	383	Total 2814	C 1749	N 484	O 567	S 14	0	0	0
1	G	383	Total 2803	C 1742	N 483	O 564	S 14	0	0	0
1	I	377	Total 2748	C 1711	N 469	O 554	S 14	0	0	0
1	K	382	Total 2793	C 1733	N 480	O 566	S 14	0	0	0
1	M	380	Total 2796	C 1738	N 482	O 562	S 14	0	0	0
1	O	386	Total 2851	C 1767	N 493	O 577	S 14	0	0	0

- Molecule 2 is a protein called Aspartokinase.

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

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

There are 56 discrepancies between the modelled and reference sequences:

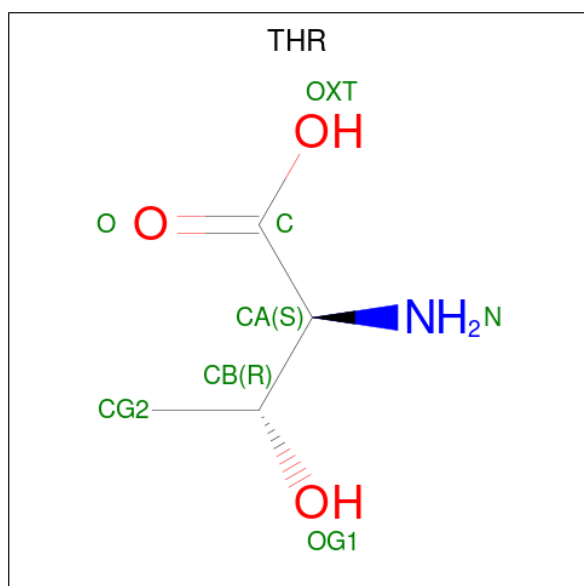
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P26512
B	173	HIS	-	expression tag	UNP P26512
B	174	HIS	-	expression tag	UNP P26512
B	175	HIS	-	expression tag	UNP P26512
B	176	HIS	-	expression tag	UNP P26512
B	177	HIS	-	expression tag	UNP P26512
B	178	HIS	-	expression 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 (three-letter code: THR) (formula: C₄H₉NO₃).



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	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		
3	O	1	Total	C	N	O	0	0
			8	4	1	3		
3	P	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is water.

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

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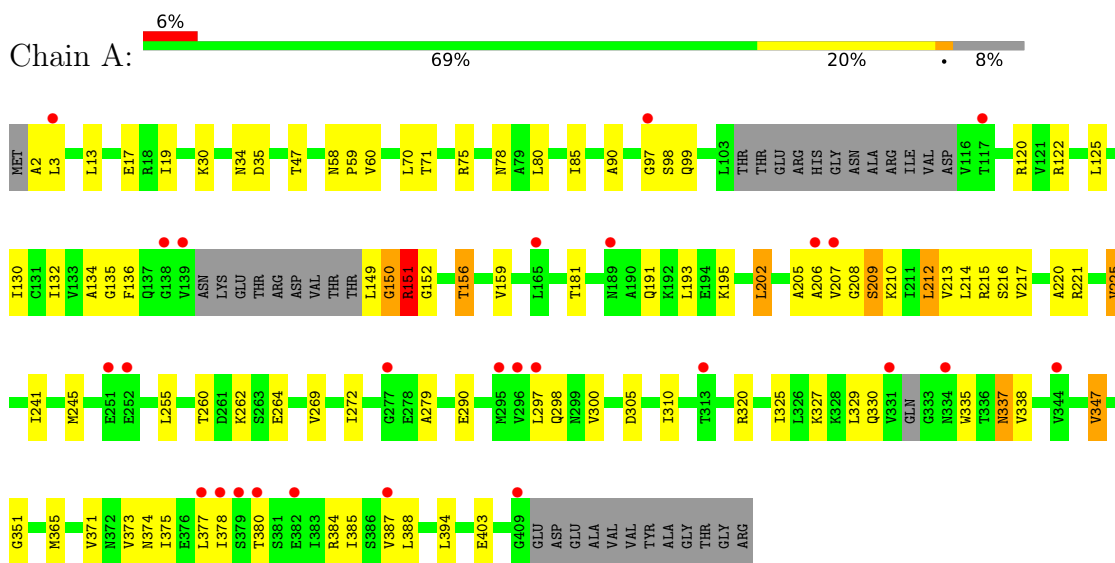
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	8	Total O 8 8	0	0
4	G	18	Total O 18 18	0	0
4	H	9	Total O 9 9	0	0
4	I	16	Total O 16 16	0	0
4	J	6	Total O 6 6	0	0
4	K	25	Total O 25 25	0	0
4	L	5	Total O 5 5	0	0
4	M	21	Total O 21 21	0	0
4	N	4	Total O 4 4	0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

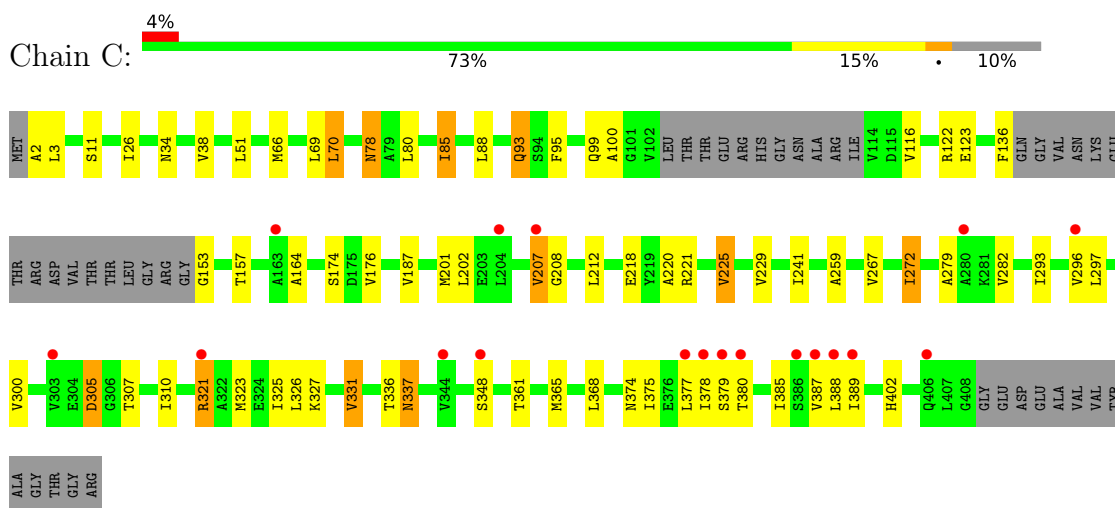
3 Residue-property plots [i](#)

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

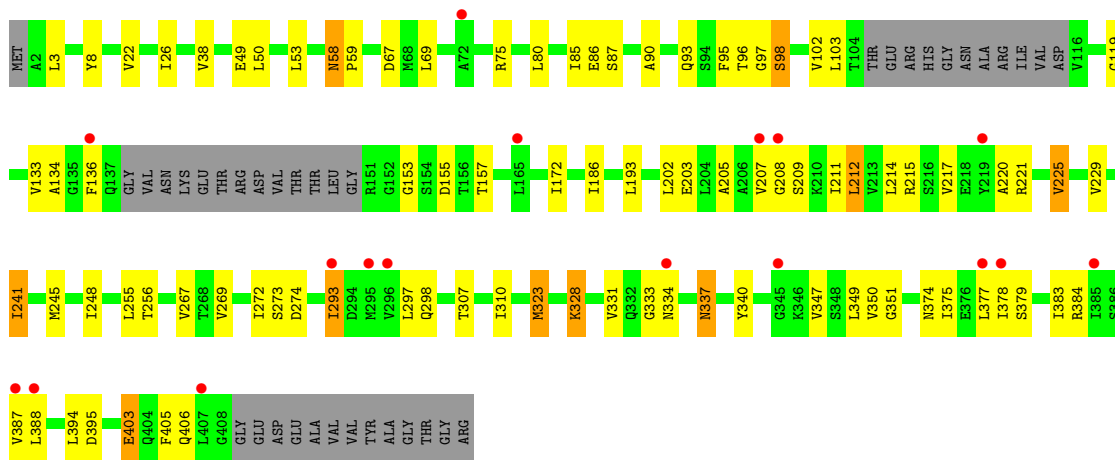


- Molecule 1: Aspartokinase

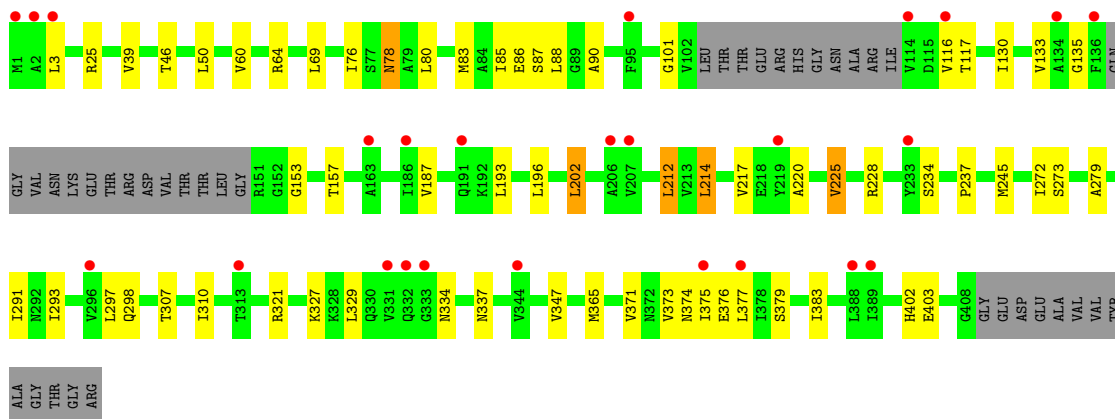
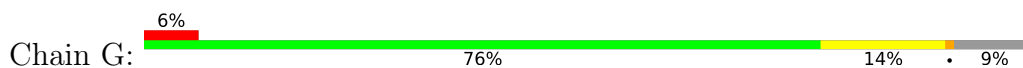


- Molecule 1: Aspartokinase

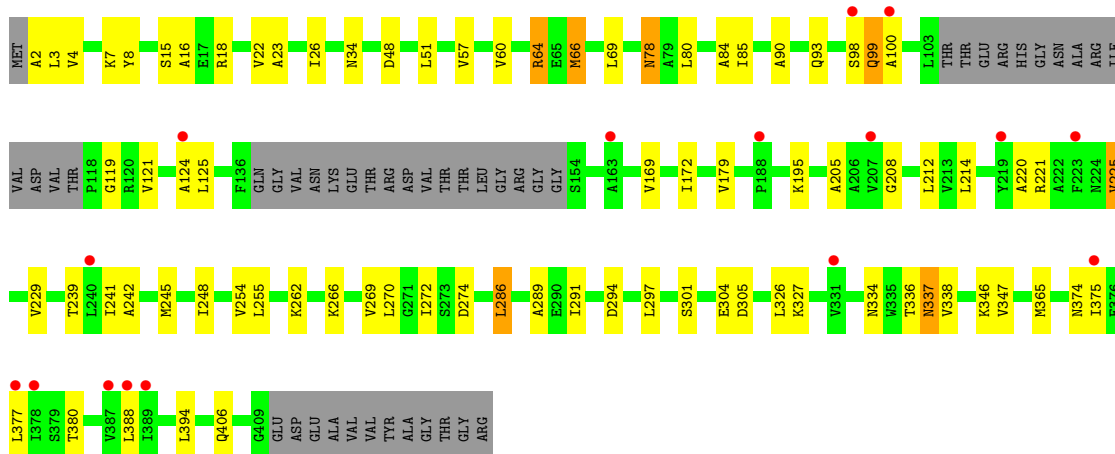




• Molecule 1: Aspartokinase

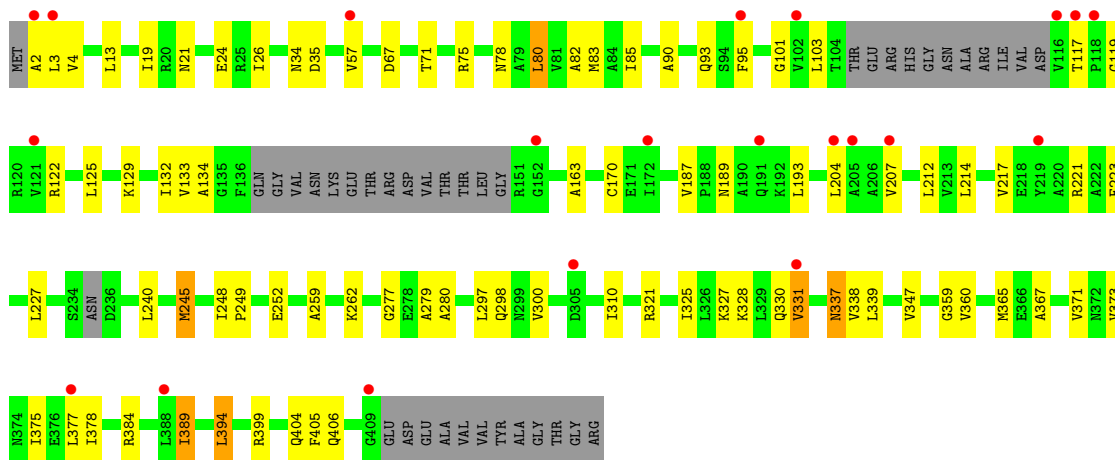


• Molecule 1: Aspartokinase



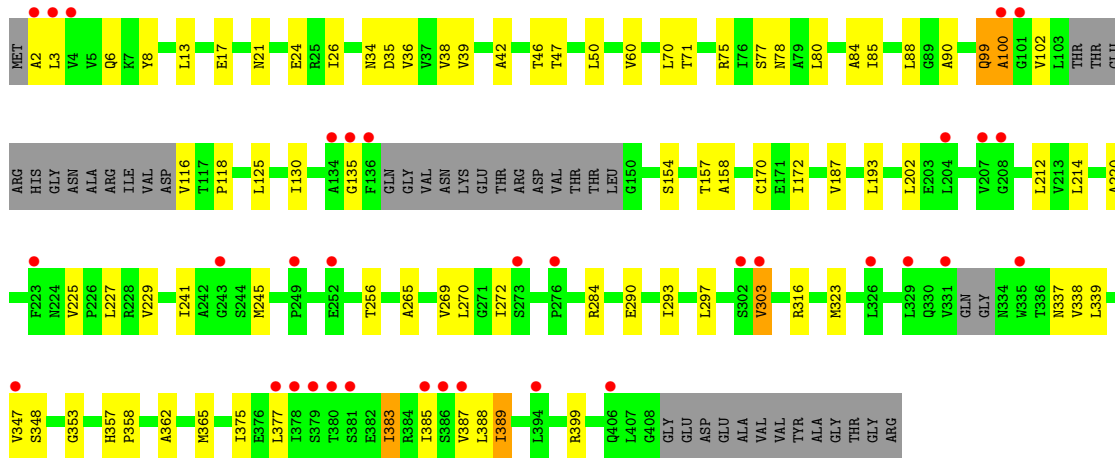
• Molecule 1: Aspartokinase

Chain K: 5% 71% 19% 9%



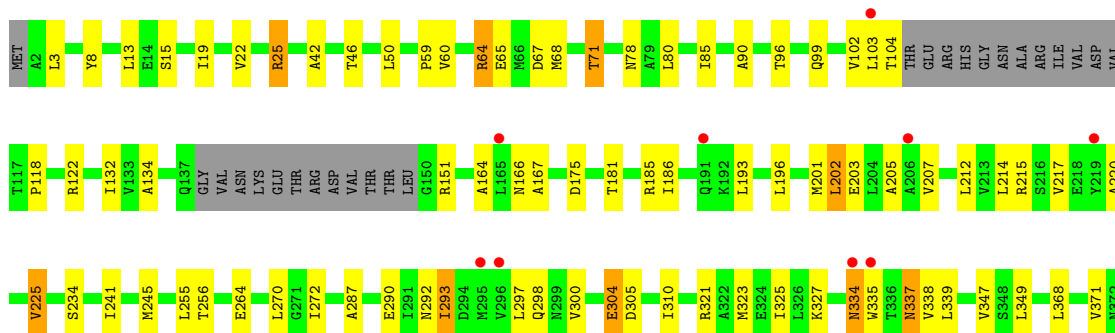
• Molecule 1: Aspartokinase

Chain M: 8% 71% 19% 10%



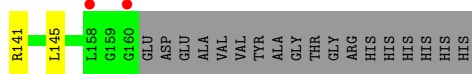
• Molecule 1: Aspartokinase

Chain O: 3% 69% 20% 8%

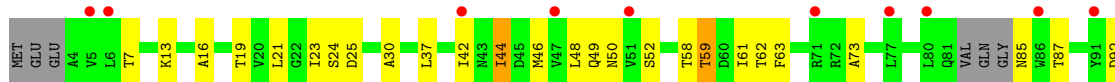




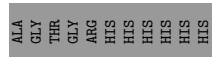
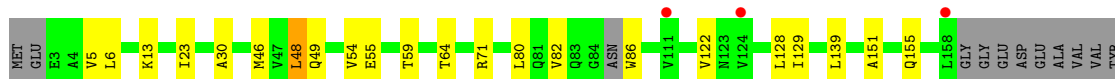
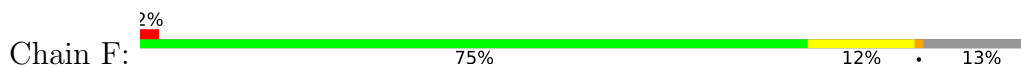
• Molecule 2: Aspartokinase



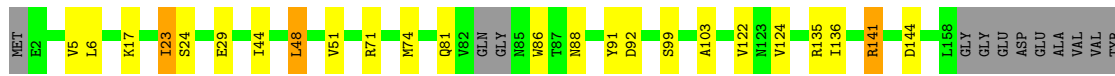
• Molecule 2: Aspartokinase



• Molecule 2: Aspartokinase

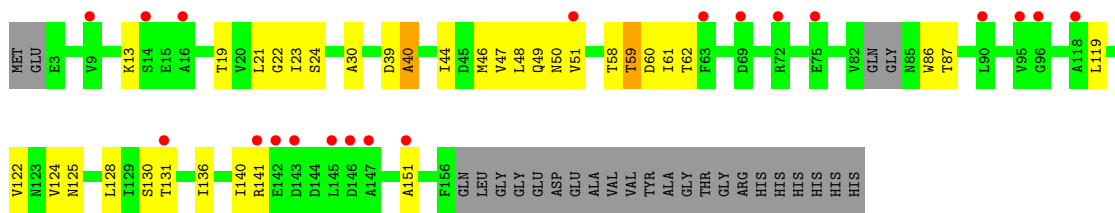


• Molecule 2: Aspartokinase

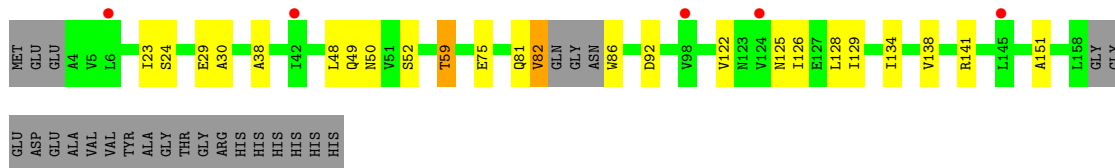


• Molecule 2: Aspartokinase

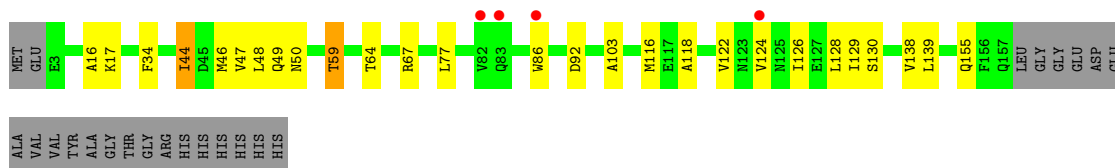




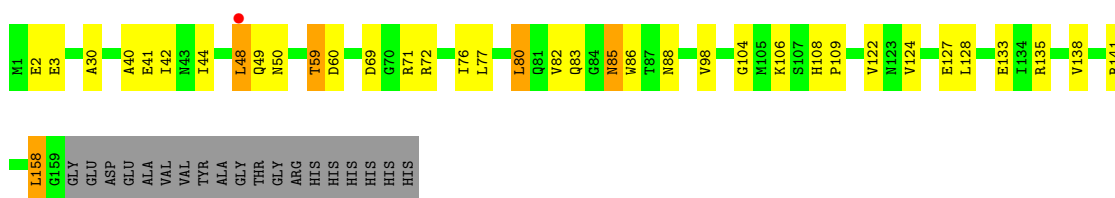
• Molecule 2: Aspartokinase



• 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) 97.1 (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)	Xtrriage
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	Xtrriage
Anisotropy	0.195	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.32	0/2867	0.53	0/3883
1	C	0.31	0/2820	0.50	0/3825
1	E	0.31	0/2841	0.50	0/3853
1	G	0.32	0/2830	0.52	0/3839
1	I	0.31	0/2774	0.50	0/3765
1	K	0.31	0/2818	0.49	0/3823
1	M	0.30	0/2822	0.49	0/3824
1	O	0.33	0/2878	0.52	0/3899
2	B	0.32	0/1194	0.52	0/1618
2	D	0.29	0/1125	0.49	0/1528
2	F	0.31	0/1176	0.51	0/1590
2	H	0.32	0/1171	0.53	0/1586
2	J	0.28	0/1090	0.46	0/1481
2	L	0.30	0/1141	0.47	0/1547
2	N	0.28	0/1146	0.45	0/1557
2	P	0.33	0/1207	0.56	0/1633
All	All	0.31	0/31900	0.50	0/43251

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2841	0	2834	72	0
1	C	2793	0	2791	60	0
1	E	2814	0	2809	62	0
1	G	2803	0	2793	48	0
1	I	2748	0	2735	66	0
1	K	2793	0	2773	67	0
1	M	2796	0	2799	66	0
1	O	2851	0	2852	82	0
2	B	1183	0	1169	27	0
2	D	1116	0	1094	39	0
2	F	1166	0	1169	18	0
2	H	1161	0	1155	22	0
2	J	1082	0	1027	33	0
2	L	1131	0	1114	22	0
2	N	1135	0	1117	22	0
2	P	1196	0	1194	29	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	678	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 (678) 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
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:N:46:MET:HE1	2:N:139:LEU:HD21	1.35	1.04
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: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
2:F:46:MET:HE1	2:F:139:LEU:HD21	1.52	0.89
1:E:267:VAL:HG13	1:E:323:MET:HE1	1.56	0.87
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
1:G:116:VAL:O	1:G:117:THR:HG22	1.75	0.87
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:267:VAL:HG22	1:C:323:MET:HE1	1.61	0.81
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
2:N:46:MET:HE3	2:N:139:LEU:HD11	1.66	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
2:F:46:MET:HE3	2:F:139:LEU:HD11	1.66	0.76
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
2:F:48:LEU:HD12	2:F:128:LEU:HD21	1.69	0.74
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:M:78:ASN:HB3	1:O:68:MET:HE1	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:267:VAL:CG1	1:E: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:I:85:ILE:CG2	1:I:90:ALA:HB3	2.20	0.71
2:F:46:MET:CE	2:F:139:LEU:HD21	2.20	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:L:50:ASN:O	2:L:59:THR:HG21	1.91	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:G:80:LEU:HD23	1:G:83:MET:HE1	1.74	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
1:E:96:THR:HG23	1:E:136:PHE:CZ	2.28	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
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
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:HE1	1.75	0.67
2:D:46:MET:HE1	2:D:139:LEU:HD21	1.76	0.66
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
2:H:44:ILE:HD12	2:H:44:ILE:C	2.15	0.66
1:I:85:ILE:HG22	1:I:90:ALA:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:46:MET:CE	2:D:139:LEU:HD21	2.26	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: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
1:I:380:THR:HG21	2:J:46:MET:HA	1.81	0.63
1:K:80:LEU:HA	1:K:83:MET:HE2	1.80	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:78:ASN:C	1:I:78:ASN:HD22	2.04	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: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
1:I:57:VAL:CG2	1:K:83:MET:HE3	2.32	0.60
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
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
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
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:G:376:GLU:C	1:G:377:LEU:HD12	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:M:78:ASN:CB	1:O:68:MET:HE1	2.34	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: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
1:E:269:VAL:CG1	1:E:272:ILE:HD11	2.35	0.56
1:C:51:LEU:HD23	1:C:66:MET:HE1	1.87	0.56
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: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
2:B:127:GLU:C	2:B:128:LEU:HD12	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:ASN:C	1:G:78:ASN:HD22	2.11	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:P:2:GLU:C	2:P:108:HIS:NE2	2.61	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:C:267:VAL:HG22	1:C:323:MET:CE	2.36	0.54
1:K:204:LEU:HD23	1:K:259:ALA:HB2	1.90	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
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:E:80:LEU:HD13	1:G:69:LEU:HD13	1.91	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
1:C:78:ASN:C	1:C:78:ASN:HD22	2.12	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
1:I:294:ASP:OD2	1:I:346:LYS:NZ	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:323:MET:HA	1:E:323:MET:HE2	1.91	0.52
2:H:23:ILE:HD12	2:H:23:ILE:C	2.30	0.52
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:C:66:MET:HE3	1:C:70:LEU:HD13	1.92	0.52
2:F:5:VAL:C	2:F:6:LEU:HD12	2.30	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
2:L:126:ILE:HG21	2:L:129:ILE:HG12	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:205:ALA:HB1	1:I:214:LEU:HD11	1.92	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: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
1:A:2:ALA:HB3	1:A:34:ASN:HD22	1.77	0.50
1:C:201:MET:CE	1:C:212:LEU:HD13	2.42	0.50
1:M:78:ASN:CG	1:O:68:MET:HE1	2.32	0.50
1:A:150:GLY:CA	1:A:151:ARG:CB	2.90	0.50
1:E:58:ASN:HD22	1:E:58:ASN:C	2.14	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:140:ILE:HD11	2:D:145:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:3:LEU:HD22	1:O:167:ALA:CB	2.42	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
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
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: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:I:57:VAL:HG21	1:K:83:MET:HE3	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: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
2:N:46:MET:CE	2:N:139:LEU:HD11	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:A:377:LEU:HD23	1:A:377:LEU:C	2.36	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:270:LEU:C	1:I:336:THR:HG22	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:201:MET:HE2	1:C:212:LEU:HD13	1.96	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: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
1:M:75:ARG:CZ	1:O:68:MET:HE2	2.45	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
2:F:46:MET:HE2	2:F:64:THR:HG21	1.98	0.46
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
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: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: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
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
2:N:46:MET:HE3	2:N:64:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:MET:HE3	2:B:134:ILE:HA	1.98	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
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
2:N:46:MET:CE	2:N:64:THR:HG21	2.47	0.44
2:P:127:GLU:C	2:P:128:LEU:HD12	2.37	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:B:85:ASN:HD22	2:B:86:TRP:N	2.15	0.44
1:E:245:MET:SD	1:E:383:ILE:HG21	2.58	0.44
2:J:21:LEU:HD23	2:J:60:ASP:CG	2.38	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
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:E:172:ILE:HD12	1:E:172:ILE:N	2.33	0.43
2:H:44:ILE:C	2:H:44:ILE:CD1	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:149:LEU:O	1:A:150:GLY:C	2.56	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:215:ARG:NH2	4:A:517:HOH:O	2.51	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:270:LEU:HD11	1:O:339:LEU:HD11	2.01	0.42
2:D:46:MET:HE3	2:D:139:LEU:HD21	2.00	0.42
1:G:220:ALA:HA	1:G:225:VAL:CG1	2.48	0.42
2:P:2:GLU:O	2:P:108:HIS:NE2	2.52	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: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:A:152:GLY:HA3	1:A:156:THR:CG2	2.49	0.42
1:C:293:ILE:HD12	1:C:293:ILE:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:26:ILE:HB	1:M:85:ILE:HD11	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
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
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:O:196:LEU:CD1	1:O:256:THR:CG2	2.97	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
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: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:I:78:ASN:C	1:I:78:ASN:ND2	2.74	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
2:F:46:MET:CE	2:F:64:THR:HG21	2.50	0.41
1:I:377:LEU:C	1:I:377:LEU:HD23	2.41	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: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: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
1:M:6:GLN:OE1	1:M:26:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:21:LEU:C	2:D:87:THR:HG22	2.41	0.40
2:F:6:LEU:HD12	2:F:6:LEU:N	2.36	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
2:N:17:LYS:HG2	2:N:92:ASP:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/421 (90%)	356 (94%)	16 (4%)	6 (2%)	9	19
1	C	374/421 (89%)	357 (96%)	15 (4%)	2 (0%)	29	52
1	E	377/421 (90%)	355 (94%)	16 (4%)	6 (2%)	9	19
1	G	377/421 (90%)	356 (94%)	20 (5%)	1 (0%)	41	64
1	I	371/421 (88%)	353 (95%)	14 (4%)	4 (1%)	14	30
1	K	374/421 (89%)	361 (96%)	10 (3%)	3 (1%)	19	39
1	M	372/421 (88%)	353 (95%)	15 (4%)	4 (1%)	14	30
1	O	380/421 (90%)	369 (97%)	9 (2%)	2 (0%)	29	52
2	B	158/178 (89%)	151 (96%)	6 (4%)	1 (1%)	25	47
2	D	148/178 (83%)	141 (95%)	7 (5%)	0	100	100
2	F	151/178 (85%)	143 (95%)	7 (5%)	1 (1%)	22	43
2	H	151/178 (85%)	149 (99%)	2 (1%)	0	100	100
2	J	148/178 (83%)	136 (92%)	11 (7%)	1 (1%)	22	43
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%)	8	15
All	All	4217/4792 (88%)	4019 (95%)	164 (4%)	34 (1%)	19	39

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/336 (89%)	277 (92%)	23 (8%)	13	25
1	C	296/336 (88%)	276 (93%)	20 (7%)	16	32
1	E	297/336 (88%)	278 (94%)	19 (6%)	17	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	294/336 (88%)	278 (95%)	16 (5%)	22	44
1	I	288/336 (86%)	274 (95%)	14 (5%)	25	48
1	K	293/336 (87%)	278 (95%)	15 (5%)	24	46
1	M	296/336 (88%)	283 (96%)	13 (4%)	28	53
1	O	303/336 (90%)	280 (92%)	23 (8%)	13	26
2	B	126/146 (86%)	113 (90%)	13 (10%)	7	13
2	D	117/146 (80%)	109 (93%)	8 (7%)	16	32
2	F	126/146 (86%)	119 (94%)	7 (6%)	21	42
2	H	125/146 (86%)	118 (94%)	7 (6%)	21	42
2	J	108/146 (74%)	104 (96%)	4 (4%)	34	60
2	L	121/146 (83%)	117 (97%)	4 (3%)	38	64
2	N	119/146 (82%)	115 (97%)	4 (3%)	37	63
2	P	129/146 (88%)	117 (91%)	12 (9%)	9	17
All	All	3338/3856 (87%)	3136 (94%)	202 (6%)	18	38

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	17	GLU
1	A	80	LEU
1	A	99	GLN
1	A	120	ARG
1	A	122	ARG
1	A	136	PHE
1	A	151	ARG
1	A	156	THR
1	A	191	GLN
1	A	195	LYS
1	A	202	LEU
1	A	212	LEU
1	A	221	ARG
1	A	225	VAL
1	A	245	MET
1	A	264	GLU
1	A	290	GLU
1	A	305	ASP

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Mol	Chain	Res	Type
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
1	C	3	LEU
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	202	LEU
1	C	207	VAL
1	C	221	ARG
1	C	225	VAL
1	C	272	ILE
1	C	321	ARG
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	120	ARG

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Mol	Chain	Res	Type
2	D	140	ILE
2	D	141	ARG
2	D	143	ASP
1	E	3	LEU
1	E	58	ASN
1	E	67	ASP
1	E	75	ARG
1	E	86	GLU
1	E	87	SER
1	E	93	GLN
1	E	155	ASP
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	293	ILE
1	E	323	MET
1	E	328	LYS
1	E	337	ASN
1	E	403	GLU
2	F	13	LYS
2	F	48	LEU
2	F	55	GLU
2	F	71	ARG
2	F	80	LEU
2	F	86	TRP
2	F	155	GLN
1	G	3	LEU
1	G	64	ARG
1	G	78	ASN
1	G	86	GLU
1	G	87	SER
1	G	88	LEU
1	G	202	LEU
1	G	212	LEU
1	G	214	LEU
1	G	225	VAL
1	G	293	ILE
1	G	329	LEU
1	G	334	ASN

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Mol	Chain	Res	Type
1	G	337	ASN
1	G	347	VAL
1	G	403	GLU
2	H	6	LEU
2	H	23	ILE
2	H	48	LEU
2	H	71	ARG
2	H	81	GLN
2	H	88	ASN
2	H	141	ARG
1	I	7	LYS
1	I	18	ARG
1	I	64	ARG
1	I	66	MET
1	I	78	ASN
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	337	ASN
2	J	13	LYS
2	J	44	ILE
2	J	59	THR
2	J	86	TRP
1	K	21	ASN
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	337	ASN
1	K	339	LEU
1	K	389	ILE
1	K	394	LEU

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Mol	Chain	Res	Type
1	K	406	GLN
2	L	59	THR
2	L	75	GLU
2	L	82	VAL
2	L	125	ASN
1	M	17	GLU
1	M	21	ASN
1	M	24	GLU
1	M	50	LEU
1	M	80	LEU
1	M	99	GLN
1	M	202	LEU
1	M	270	LEU
1	M	284	ARG
1	M	337	ASN
1	M	339	LEU
1	M	383	ILE
1	M	389	ILE
2	N	44	ILE
2	N	59	THR
2	N	77	LEU
2	N	86	TRP
1	O	25	ARG
1	O	64	ARG
1	O	65	GLU
1	O	71	THR
1	O	80	LEU
1	O	122	ARG
1	O	166	ASN
1	O	175	ASP
1	O	202	LEU
1	O	212	LEU
1	O	225	VAL
1	O	245	MET
1	O	255	LEU
1	O	264	GLU
1	O	290	GLU
1	O	293	ILE
1	O	323	MET
1	O	334	ASN
1	O	335	TRP
1	O	337	ASN

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Mol	Chain	Res	Type
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	71	ARG
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 (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	93	GLN
1	A	235	ASN
1	A	292	ASN
1	A	298	GLN
1	A	334	ASN
1	A	337	ASN
1	A	343	GLN
1	A	374	ASN
2	B	43	ASN
2	B	81	GLN
2	B	85	ASN
2	B	88	ASN
1	C	21	ASN
1	C	34	ASN
1	C	78	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	43	ASN

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Mol	Chain	Res	Type
1	E	58	ASN
1	E	93	GLN
1	E	189	ASN
1	E	191	GLN
1	E	224	ASN
1	E	292	ASN
1	E	298	GLN
1	E	337	ASN
1	E	374	ASN
1	E	406	GLN
2	F	43	ASN
2	F	88	ASN
1	G	34	ASN
1	G	78	ASN
1	G	166	ASN
1	G	189	ASN
1	G	224	ASN
1	G	298	GLN
1	G	334	ASN
1	G	337	ASN
1	G	343	GLN
1	G	374	ASN
2	H	88	ASN
1	I	34	ASN
1	I	78	ASN
1	I	93	GLN
1	I	99	GLN
1	I	292	ASN
1	I	332	GLN
1	I	334	ASN
1	I	337	ASN
1	I	343	GLN
1	I	372	ASN
2	J	43	ASN
1	K	21	ASN
1	K	34	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

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Mol	Chain	Res	Type
1	K	406	GLN
2	L	123	ASN
1	M	34	ASN
1	M	191	GLN
1	M	292	ASN
1	M	337	ASN
1	M	343	GLN
1	M	374	ASN
2	N	43	ASN
1	O	21	ASN
1	O	34	ASN
1	O	99	GLN
1	O	166	ASN
1	O	235	ASN
1	O	292	ASN
1	O	298	GLN
1	O	334	ASN
1	O	337	ASN
1	O	374	ASN
1	O	404	GLN
2	P	43	ASN
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 monosaccharides 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	F	501	-	6,7,7	1.04	1 (16%)	7,9,9	1.42	1 (14%)
3	THR	J	501	-	6,7,7	0.91	1 (16%)	7,9,9	1.27	1 (14%)
3	THR	O	501	-	6,7,7	0.95	1 (16%)	7,9,9	1.28	2 (28%)
3	THR	C	501	-	6,7,7	0.99	1 (16%)	7,9,9	1.34	1 (14%)
3	THR	K	501	-	6,7,7	0.97	1 (16%)	7,9,9	1.23	1 (14%)
3	THR	D	501	-	6,7,7	0.96	1 (16%)	7,9,9	1.23	1 (14%)
3	THR	A	501	-	6,7,7	0.96	1 (16%)	7,9,9	1.31	1 (14%)
3	THR	N	501	-	6,7,7	0.96	1 (16%)	7,9,9	1.27	1 (14%)
3	THR	P	501	-	6,7,7	0.98	1 (16%)	7,9,9	1.37	2 (28%)
3	THR	G	501	-	6,7,7	1.02	1 (16%)	7,9,9	1.33	1 (14%)
3	THR	M	501	-	6,7,7	0.94	1 (16%)	7,9,9	1.41	1 (14%)
3	THR	L	501	-	6,7,7	0.95	1 (16%)	7,9,9	1.15	1 (14%)
3	THR	B	501	-	6,7,7	0.98	1 (16%)	7,9,9	1.41	2 (28%)
3	THR	H	501	-	6,7,7	0.91	1 (16%)	7,9,9	1.26	1 (14%)
3	THR	E	501	-	6,7,7	0.89	1 (16%)	7,9,9	1.44	2 (28%)

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. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	THR	F	501	-	-	4/8/8/8	-
3	THR	J	501	-	-	1/8/8/8	-
3	THR	O	501	-	-	0/8/8/8	-
3	THR	C	501	-	-	1/8/8/8	-
3	THR	K	501	-	-	0/8/8/8	-
3	THR	D	501	-	-	4/8/8/8	-
3	THR	A	501	-	-	3/8/8/8	-
3	THR	N	501	-	-	0/8/8/8	-
3	THR	P	501	-	-	4/8/8/8	-
3	THR	G	501	-	-	6/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	THR	M	501	-	-	0/8/8/8	-
3	THR	L	501	-	-	4/8/8/8	-
3	THR	B	501	-	-	0/8/8/8	-
3	THR	H	501	-	-	0/8/8/8	-
3	THR	E	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	-2.31	1.23	1.30
3	C	501	THR	OXT-C	-2.24	1.23	1.30
3	G	501	THR	OXT-C	-2.23	1.23	1.30
3	K	501	THR	OXT-C	-2.18	1.23	1.30
3	P	501	THR	OXT-C	-2.17	1.23	1.30
3	L	501	THR	OXT-C	-2.16	1.23	1.30
3	N	501	THR	OXT-C	-2.15	1.23	1.30
3	D	501	THR	OXT-C	-2.15	1.23	1.30
3	B	501	THR	OXT-C	-2.14	1.23	1.30
3	O	501	THR	OXT-C	-2.11	1.23	1.30
3	M	501	THR	OXT-C	-2.09	1.23	1.30
3	J	501	THR	OXT-C	-2.09	1.23	1.30
3	H	501	THR	OXT-C	-2.09	1.23	1.30
3	A	501	THR	OXT-C	-2.07	1.23	1.30
3	E	501	THR	OXT-C	-2.03	1.23	1.30

All (19) 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	124.09
3	M	501	THR	OXT-C-O	-3.04	117.19	124.09
3	C	501	THR	OXT-C-O	-2.92	117.47	124.09
3	B	501	THR	OXT-C-O	-2.91	117.49	124.09
3	G	501	THR	OXT-C-O	-2.90	117.50	124.09
3	E	501	THR	OXT-C-O	-2.87	117.57	124.09
3	P	501	THR	OXT-C-O	-2.85	117.62	124.09
3	A	501	THR	OXT-C-O	-2.84	117.64	124.09
3	J	501	THR	OXT-C-O	-2.67	118.02	124.09
3	D	501	THR	OXT-C-O	-2.67	118.03	124.09
3	N	501	THR	OXT-C-O	-2.64	118.09	124.09
3	K	501	THR	OXT-C-O	-2.60	118.20	124.09
3	O	501	THR	OXT-C-O	-2.59	118.22	124.09
3	H	501	THR	OXT-C-O	-2.53	118.33	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	501	THR	OXT-C-O	-2.43	118.57	124.09
3	E	501	THR	OXT-C-CA	2.28	122.20	114.22
3	B	501	THR	OXT-C-CA	2.16	121.78	114.22
3	P	501	THR	OXT-C-CA	2.14	121.70	114.22
3	O	501	THR	OXT-C-CA	2.03	121.32	114.22

There are no chirality outliers.

All (27) 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	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	G	501	THR	O-C-CA-N
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	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	F	501	THR	6	0
3	J	501	THR	6	0
3	C	501	THR	4	0
3	K	501	THR	6	0
3	D	501	THR	7	0
3	A	501	THR	7	0
3	P	501	THR	5	0
3	G	501	THR	5	0
3	L	501	THR	4	0
3	B	501	THR	1	0
3	H	501	THR	3	0
3	E	501	THR	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/421 (91%)	0.36	26 (6%) 17 13	43, 56, 73, 82	1 (0%)
1	C	380/421 (90%)	0.29	18 (4%) 31 25	43, 61, 86, 96	0
1	E	383/421 (90%)	0.35	17 (4%) 34 27	42, 58, 76, 94	0
1	G	383/421 (90%)	0.35	25 (6%) 18 14	38, 56, 73, 83	0
1	I	377/421 (89%)	0.32	16 (4%) 36 29	50, 69, 90, 98	0
1	K	382/421 (90%)	0.35	21 (5%) 25 19	42, 62, 79, 93	0
1	M	380/421 (90%)	0.45	34 (8%) 9 6	48, 65, 79, 88	0
1	O	386/421 (91%)	0.17	11 (2%) 53 46	37, 50, 69, 82	0
2	B	160/178 (89%)	0.29	7 (4%) 34 27	46, 61, 79, 89	0
2	D	152/178 (85%)	0.98	31 (20%) 1 0	60, 79, 103, 111	0
2	F	155/178 (87%)	0.16	3 (1%) 66 62	43, 59, 79, 87	0
2	H	155/178 (87%)	0.02	0 100 100	34, 50, 73, 83	0
2	J	152/178 (85%)	0.80	20 (13%) 3 2	60, 85, 103, 108	0
2	L	152/178 (85%)	0.27	5 (3%) 46 39	48, 68, 90, 96	0
2	N	155/178 (87%)	0.33	4 (2%) 56 50	59, 75, 93, 104	0
2	P	159/178 (89%)	-0.00	1 (0%) 89 88	36, 47, 66, 72	0
All	All	4297/4792 (89%)	0.34	239 (5%) 24 19	34, 61, 87, 111	1 (0%)

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	116	VAL	7.1
2	N	82	VAL	6.4
1	A	409	GLY	6.1
1	M	303	VAL	5.9
1	G	114	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
2	J	147	ALA	5.0
2	D	80	LEU	5.0
1	M	100	ALA	4.9
2	J	16	ALA	4.8
2	D	124	VAL	4.8
2	D	91	TYR	4.6
2	D	156	PHE	4.6
1	G	1	MET	4.5
1	M	331	VAL	4.5
1	O	411	ASP	4.4
2	D	148	ALA	4.4
2	N	83	GLN	4.3
1	G	331	VAL	4.3
2	J	118	ALA	4.3
2	D	71	ARG	4.3
1	K	95	PHE	4.2
1	M	2	ALA	4.2
1	G	332	GLN	4.2
2	D	147	ALA	4.0
2	D	77	LEU	3.9
2	F	158	LEU	3.9
1	I	377	LEU	3.9
2	D	42	ILE	3.8
2	J	146	ASP	3.8
2	F	124	VAL	3.8
1	C	380	THR	3.7
1	G	2	ALA	3.7
2	J	9	VAL	3.6
2	D	143	ASP	3.6
2	L	42	ILE	3.6
1	M	406	GLN	3.5
1	M	207	VAL	3.5
1	C	387	VAL	3.4
1	C	378	ILE	3.4
1	G	3	LEU	3.3
1	O	219	TYR	3.3
1	M	335	TRP	3.3
1	K	152	GLY	3.3
1	A	206	ALA	3.3
1	A	378	ILE	3.3
1	I	331	VAL	3.2
1	G	219	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	251	GLU	3.1
1	M	136	PHE	3.1
1	A	117	THR	3.1
1	C	388	LEU	3.1
2	L	145	LEU	3.1
2	B	42	ILE	3.1
1	K	331	VAL	3.1
1	M	347	VAL	3.1
2	D	122	VAL	3.1
1	A	334	ASN	3.0
1	G	377	LEU	3.0
2	D	158	LEU	3.0
2	J	69	ASP	3.0
1	A	277	GLY	3.0
1	E	219	TYR	3.0
2	D	152	LEU	3.0
1	A	296	VAL	3.0
1	G	388	LEU	3.0
1	K	219	TYR	2.9
1	M	135	GLY	2.9
2	J	145	LEU	2.9
2	D	86	TRP	2.9
1	M	380	THR	2.9
1	A	97	GLY	2.8
2	D	150	ARG	2.8
1	A	139	VAL	2.8
1	K	117	THR	2.8
1	M	3	LEU	2.8
1	M	302	SER	2.8
1	A	207	VAL	2.8
1	M	252	GLU	2.8
1	A	377	LEU	2.8
1	M	208	GLY	2.8
1	E	296	VAL	2.8
1	I	219	TYR	2.8
1	M	394	LEU	2.8
2	D	6	LEU	2.8
2	N	86	TRP	2.7
2	J	63	PHE	2.7
2	P	48	LEU	2.7
1	M	385	ILE	2.7
2	D	145	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	72	ALA	2.7
2	D	98	VAL	2.7
1	I	375	ILE	2.7
1	K	409	GLY	2.7
1	E	387	VAL	2.7
1	C	348	SER	2.7
2	D	125	ASN	2.7
2	N	124	VAL	2.7
1	K	118	PRO	2.7
2	D	121	ASP	2.7
2	J	51	VAL	2.6
2	D	100	LEU	2.6
1	G	163	ALA	2.6
2	J	151	ALA	2.6
1	M	273	SER	2.6
1	G	344	VAL	2.6
1	A	3	LEU	2.6
1	G	136	PHE	2.6
1	A	382	GLU	2.6
1	I	98	SER	2.6
1	O	409	GLY	2.6
2	D	118	ALA	2.6
1	E	293	ILE	2.6
1	G	296	VAL	2.6
1	I	388	LEU	2.6
2	B	158	LEU	2.6
1	E	345	GLY	2.6
1	E	388	LEU	2.5
1	I	378	ILE	2.5
1	E	136	PHE	2.5
1	A	295	MET	2.5
2	B	73	ALA	2.5
1	C	377	LEU	2.5
1	I	207	VAL	2.5
1	C	379	SER	2.5
1	E	295	MET	2.5
1	E	334	ASN	2.5
2	D	157	GLN	2.5
2	D	151	ALA	2.5
1	K	204	LEU	2.5
1	M	387	VAL	2.5
2	D	144	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	134	ALA	2.5
2	J	131	THR	2.5
2	L	124	VAL	2.4
1	E	165	LEU	2.4
1	G	233	TYR	2.4
2	J	75	GLU	2.4
1	C	207	VAL	2.4
2	B	82	VAL	2.4
1	A	165	LEU	2.4
1	O	296	VAL	2.4
2	B	160	GLY	2.4
1	M	329	LEU	2.4
1	M	377	LEU	2.4
2	J	72	ARG	2.4
2	L	98	VAL	2.4
1	G	206	ALA	2.4
1	M	381	SER	2.4
1	I	188	PRO	2.4
1	M	249	PRO	2.3
1	C	321	ARG	2.3
1	M	204	LEU	2.3
1	A	387	VAL	2.3
2	D	146	ASP	2.3
1	I	163	ALA	2.3
1	E	208	GLY	2.3
1	G	186	ILE	2.3
1	G	389	ILE	2.3
1	M	378	ILE	2.3
1	K	205	ALA	2.3
1	I	387	VAL	2.3
1	M	4	VAL	2.3
2	B	91	TYR	2.3
1	E	377	LEU	2.3
1	M	276	PRO	2.3
1	K	102	VAL	2.3
1	O	334	ASN	2.3
1	M	243	GLY	2.3
1	I	124	ALA	2.3
1	I	223	PHE	2.3
1	C	303	VAL	2.2
2	D	5	VAL	2.2
1	K	305	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	280	ALA	2.2
1	K	388	LEU	2.2
1	G	95	PHE	2.2
1	G	313	THR	2.2
1	I	240	LEU	2.2
1	O	335	TRP	2.2
2	L	6	LEU	2.2
1	C	386	SER	2.2
1	M	386	SER	2.2
1	E	385	ILE	2.2
1	G	134	ALA	2.2
1	I	389	ILE	2.2
1	A	313	THR	2.2
1	K	377	LEU	2.2
1	O	165	LEU	2.2
1	C	344	VAL	2.2
1	A	252	GLU	2.2
1	A	138	GLY	2.2
2	J	143	ASP	2.2
1	K	57	VAL	2.2
1	A	379	SER	2.2
1	K	191	GLN	2.2
1	K	2	ALA	2.2
2	D	149	ALA	2.2
2	J	14	SER	2.2
1	E	207	VAL	2.1
1	A	380	THR	2.1
1	O	191	GLN	2.1
1	A	189	ASN	2.1
2	B	8	GLY	2.1
1	G	116	VAL	2.1
1	I	100	ALA	2.1
1	K	207	VAL	2.1
1	E	378	ILE	2.1
1	G	375	ILE	2.1
1	M	223	PHE	2.1
1	M	326	LEU	2.1
1	M	379	SER	2.1
1	A	331	VAL	2.1
1	A	344	VAL	2.1
1	O	206	ALA	2.1
2	D	47	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	51	VAL	2.1
1	K	3	LEU	2.1
1	C	406	GLN	2.1
1	G	207	VAL	2.1
2	D	140	ILE	2.1
2	J	141	ARG	2.1
1	K	121	VAL	2.0
1	K	172	ILE	2.0
1	O	103	LEU	2.0
1	C	163	ALA	2.0
1	C	296	VAL	2.0
2	J	142	GLU	2.0
1	A	297	LEU	2.0
1	C	204	LEU	2.0
1	C	389	ILE	2.0
1	E	407	LEU	2.0
1	M	101	GLY	2.0
2	J	90	LEU	2.0
1	O	295	MET	2.0
1	G	191	GLN	2.0
2	F	111	VAL	2.0
2	J	95	VAL	2.0
1	G	333	GLY	2.0
2	J	96	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	THR	M	501	8/8	0.89	0.18	39,39,39,39	0
3	THR	E	501	8/8	0.94	0.12	40,40,41,41	0
3	THR	J	501	8/8	0.94	0.21	51,51,51,51	0
3	THR	L	501	8/8	0.94	0.16	51,52,52,52	0
3	THR	D	501	8/8	0.94	0.12	35,35,35,35	0
3	THR	C	501	8/8	0.95	0.12	71,71,71,71	0
3	THR	K	501	8/8	0.95	0.17	50,50,50,50	0
3	THR	N	501	8/8	0.95	0.14	38,38,38,38	0
3	THR	P	501	8/8	0.95	0.12	35,36,36,36	0
3	THR	F	501	8/8	0.96	0.15	28,28,28,28	0
3	THR	H	501	8/8	0.96	0.14	37,37,37,38	0
3	THR	B	501	8/8	0.97	0.12	38,39,39,39	0
3	THR	G	501	8/8	0.97	0.10	29,30,30,30	0
3	THR	A	501	8/8	0.97	0.09	40,40,40,40	0
3	THR	O	501	8/8	0.99	0.08	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.