Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:22 PM GMT

PDB ID	:	4Y7K
Title	:	Structure of an archaeal mechanosensitive channel in closed state
Authors	:	Li, J.; Liu, Z.
Deposited on	:	2015-02-15
Resolution	:	3.50 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

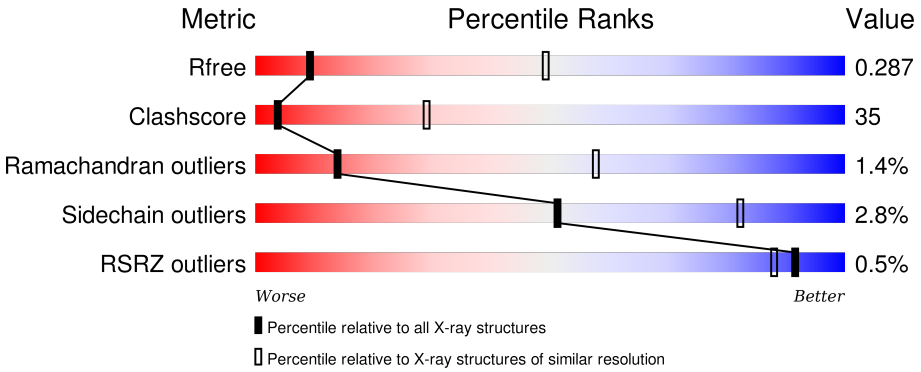
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	275	% 48% 40% • 9%
1	B	275	44% 42% • 12%
1	C	275	% 48% 38% • 12%
1	D	275	44% 41% • 12%
1	E	275	% 43% 42% • 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9218 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 Large conductance mechanosensitive channel protein,Riboflavin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1902	1252	296	344	10			
1	B	241	Total	C	N	O	S	0	0	0
			1825	1204	285	325	11			
1	C	242	Total	C	N	O	S	0	0	1
			1838	1214	284	329	11			
1	D	242	Total	C	N	O	S	0	0	0
			1812	1196	284	322	10			
1	E	242	Total	C	N	O	S	0	0	0
			1841	1216	284	330	11			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8TNK0
A	-18	GLY	-	expression tag	UNP Q8TNK0
A	-17	SER	-	expression tag	UNP Q8TNK0
A	-16	SER	-	expression tag	UNP Q8TNK0
A	-15	HIS	-	expression tag	UNP Q8TNK0
A	-14	HIS	-	expression tag	UNP Q8TNK0
A	-13	HIS	-	expression tag	UNP Q8TNK0
A	-12	HIS	-	expression tag	UNP Q8TNK0
A	-11	HIS	-	expression tag	UNP Q8TNK0
A	-10	HIS	-	expression tag	UNP Q8TNK0
A	-9	SER	-	expression tag	UNP Q8TNK0
A	-8	SER	-	expression tag	UNP Q8TNK0
A	-7	GLY	-	expression tag	UNP Q8TNK0
A	-6	LEU	-	expression tag	UNP Q8TNK0
A	-5	VAL	-	expression tag	UNP Q8TNK0
A	-4	PRO	-	expression tag	UNP Q8TNK0
A	-3	ARG	-	expression tag	UNP Q8TNK0
A	-2	GLY	-	expression tag	UNP Q8TNK0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q8TNK0
A	0	HIS	-	expression tag	UNP Q8TNK0
A	?	-	LYS	deletion	UNP Q8TNK0
B	-19	MET	-	expression tag	UNP Q8TNK0
B	-18	GLY	-	expression tag	UNP Q8TNK0
B	-17	SER	-	expression tag	UNP Q8TNK0
B	-16	SER	-	expression tag	UNP Q8TNK0
B	-15	HIS	-	expression tag	UNP Q8TNK0
B	-14	HIS	-	expression tag	UNP Q8TNK0
B	-13	HIS	-	expression tag	UNP Q8TNK0
B	-12	HIS	-	expression tag	UNP Q8TNK0
B	-11	HIS	-	expression tag	UNP Q8TNK0
B	-10	HIS	-	expression tag	UNP Q8TNK0
B	-9	SER	-	expression tag	UNP Q8TNK0
B	-8	SER	-	expression tag	UNP Q8TNK0
B	-7	GLY	-	expression tag	UNP Q8TNK0
B	-6	LEU	-	expression tag	UNP Q8TNK0
B	-5	VAL	-	expression tag	UNP Q8TNK0
B	-4	PRO	-	expression tag	UNP Q8TNK0
B	-3	ARG	-	expression tag	UNP Q8TNK0
B	-2	GLY	-	expression tag	UNP Q8TNK0
B	-1	SER	-	expression tag	UNP Q8TNK0
B	0	HIS	-	expression tag	UNP Q8TNK0
B	?	-	LYS	deletion	UNP Q8TNK0
C	-19	MET	-	expression tag	UNP Q8TNK0
C	-18	GLY	-	expression tag	UNP Q8TNK0
C	-17	SER	-	expression tag	UNP Q8TNK0
C	-16	SER	-	expression tag	UNP Q8TNK0
C	-15	HIS	-	expression tag	UNP Q8TNK0
C	-14	HIS	-	expression tag	UNP Q8TNK0
C	-13	HIS	-	expression tag	UNP Q8TNK0
C	-12	HIS	-	expression tag	UNP Q8TNK0
C	-11	HIS	-	expression tag	UNP Q8TNK0
C	-10	HIS	-	expression tag	UNP Q8TNK0
C	-9	SER	-	expression tag	UNP Q8TNK0
C	-8	SER	-	expression tag	UNP Q8TNK0
C	-7	GLY	-	expression tag	UNP Q8TNK0
C	-6	LEU	-	expression tag	UNP Q8TNK0
C	-5	VAL	-	expression tag	UNP Q8TNK0
C	-4	PRO	-	expression tag	UNP Q8TNK0
C	-3	ARG	-	expression tag	UNP Q8TNK0
C	-2	GLY	-	expression tag	UNP Q8TNK0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q8TNK0
C	0	HIS	-	expression tag	UNP Q8TNK0
C	?	-	LYS	deletion	UNP Q8TNK0
D	-19	MET	-	expression tag	UNP Q8TNK0
D	-18	GLY	-	expression tag	UNP Q8TNK0
D	-17	SER	-	expression tag	UNP Q8TNK0
D	-16	SER	-	expression tag	UNP Q8TNK0
D	-15	HIS	-	expression tag	UNP Q8TNK0
D	-14	HIS	-	expression tag	UNP Q8TNK0
D	-13	HIS	-	expression tag	UNP Q8TNK0
D	-12	HIS	-	expression tag	UNP Q8TNK0
D	-11	HIS	-	expression tag	UNP Q8TNK0
D	-10	HIS	-	expression tag	UNP Q8TNK0
D	-9	SER	-	expression tag	UNP Q8TNK0
D	-8	SER	-	expression tag	UNP Q8TNK0
D	-7	GLY	-	expression tag	UNP Q8TNK0
D	-6	LEU	-	expression tag	UNP Q8TNK0
D	-5	VAL	-	expression tag	UNP Q8TNK0
D	-4	PRO	-	expression tag	UNP Q8TNK0
D	-3	ARG	-	expression tag	UNP Q8TNK0
D	-2	GLY	-	expression tag	UNP Q8TNK0
D	-1	SER	-	expression tag	UNP Q8TNK0
D	0	HIS	-	expression tag	UNP Q8TNK0
D	?	-	LYS	deletion	UNP Q8TNK0
E	-19	MET	-	expression tag	UNP Q8TNK0
E	-18	GLY	-	expression tag	UNP Q8TNK0
E	-17	SER	-	expression tag	UNP Q8TNK0
E	-16	SER	-	expression tag	UNP Q8TNK0
E	-15	HIS	-	expression tag	UNP Q8TNK0
E	-14	HIS	-	expression tag	UNP Q8TNK0
E	-13	HIS	-	expression tag	UNP Q8TNK0
E	-12	HIS	-	expression tag	UNP Q8TNK0
E	-11	HIS	-	expression tag	UNP Q8TNK0
E	-10	HIS	-	expression tag	UNP Q8TNK0
E	-9	SER	-	expression tag	UNP Q8TNK0
E	-8	SER	-	expression tag	UNP Q8TNK0
E	-7	GLY	-	expression tag	UNP Q8TNK0
E	-6	LEU	-	expression tag	UNP Q8TNK0
E	-5	VAL	-	expression tag	UNP Q8TNK0
E	-4	PRO	-	expression tag	UNP Q8TNK0
E	-3	ARG	-	expression tag	UNP Q8TNK0
E	-2	GLY	-	expression tag	UNP Q8TNK0

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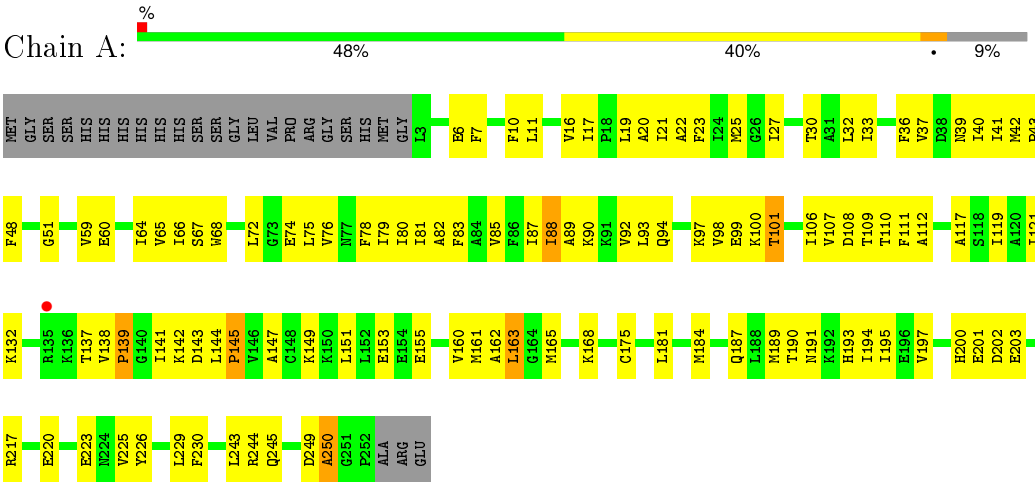
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP Q8TNK0
E	0	HIS	-	expression tag	UNP Q8TNK0
E	?	-	LYS	deletion	UNP Q8TNK0

3 Residue-property plots (i)

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

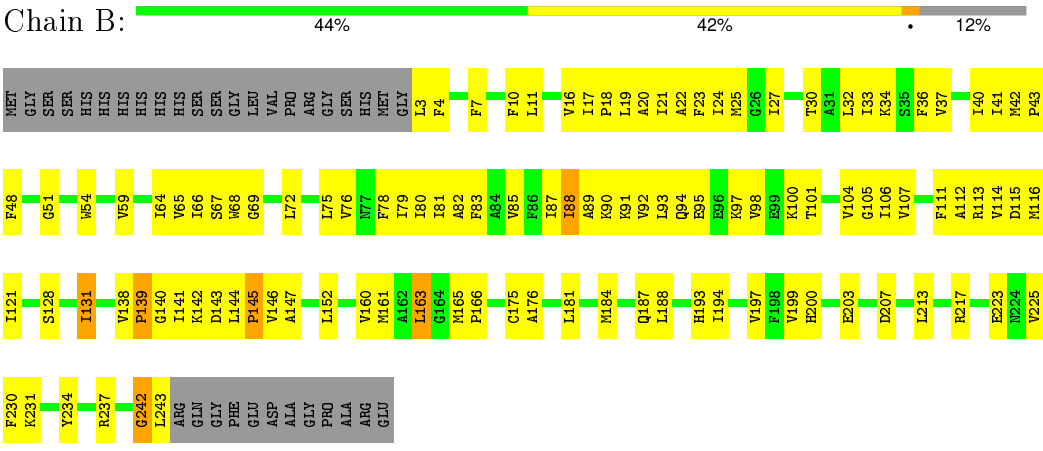
• Molecule 1: Large conductance mechanosensitive channel protein,Riboflavin synthase

Chain A:



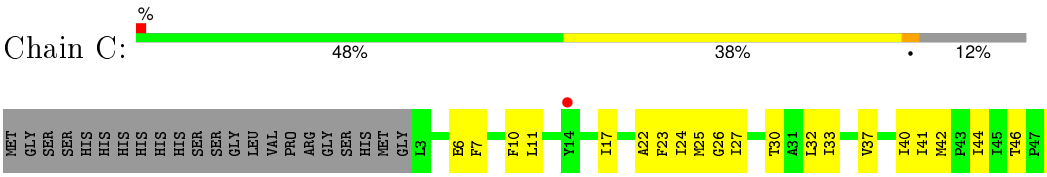
• Molecule 1: Large conductance mechanosensitive channel protein,Riboflavin synthase

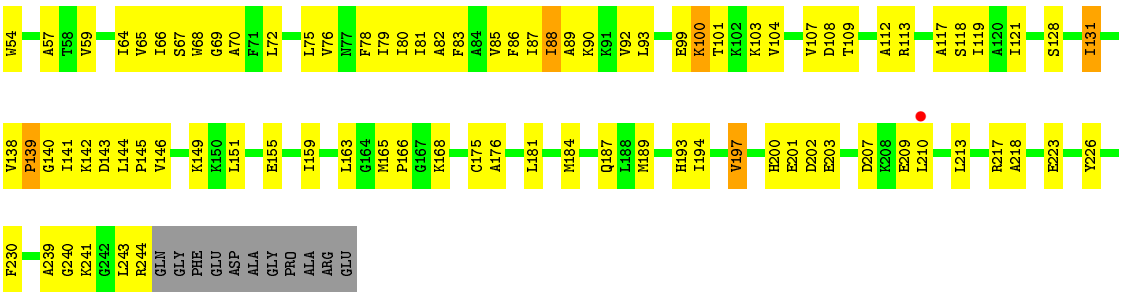
Chain B:



• Molecule 1: Large conductance mechanosensitive channel protein,Riboflavin synthase

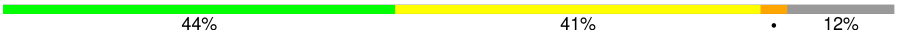
Chain C:

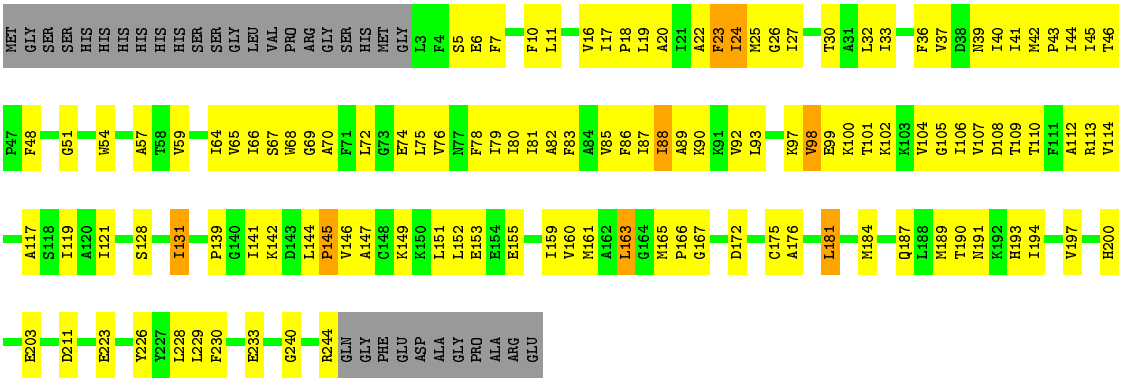




• Molecule 1: Large conductance mechanosensitive channel protein,Riboflavin synthase

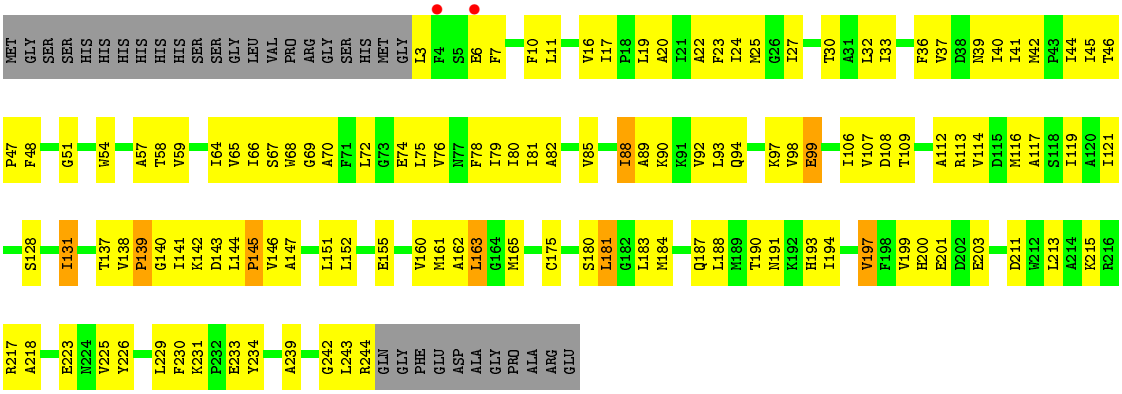
Chain D:





• Molecule 1: Large conductance mechanosensitive channel protein,Riboflavin synthase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.29Å 140.37Å 182.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.00 – 3.50 41.64 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.00-3.50) 99.3 (41.64-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.259 , 0.287 0.259 , 0.287	Depositor DCC
R_{free} test set	1455 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	151.8	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 117.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 28752 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9218	wwPDB-VP
Average B, all atoms (Å^2)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.58	0/1941	0.76	0/2628
1	B	0.65	0/1860	0.76	0/2517
1	C	0.58	0/1874	0.77	1/2538 (0.0%)
1	D	0.54	0/1848	0.73	0/2506
1	E	0.55	0/1878	0.74	0/2544
All	All	0.58	0/9401	0.75	1/12733 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	101	THR	N-CA-CB	-10.77	89.84	110.30

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	1902	0	1924	160	0
1	B	1825	0	1842	146	0
1	C	1838	0	1866	127	0
1	D	1812	0	1826	146	0
1	E	1841	0	1866	159	0
All	All	9218	0	9324	651	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 35.

All (651) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:GLU:HG2	1:C:100:LYS:H	1.00	1.09
1:C:119:ILE:H	1:C:119:ILE:HD12	1.19	1.06
1:C:99:GLU:HG2	1:C:100:LYS:N	1.70	1.06
1:E:187:GLN:HE21	1:E:194:ILE:H	1.09	1.00
1:D:163:LEU:HD13	1:D:197:VAL:HG11	1.39	0.99
1:B:163:LEU:HD13	1:B:197:VAL:HG11	1.45	0.98
1:C:187:GLN:HE21	1:C:194:ILE:H	1.05	0.98
1:C:66:ILE:HD11	1:D:44:ILE:HD11	1.46	0.96
1:A:66:ILE:HD11	1:B:44:ILE:HD11	1.47	0.96
1:C:64:ILE:HG21	1:D:44:ILE:HD13	1.45	0.95
1:D:119:ILE:H	1:D:119:ILE:HD12	1.31	0.95
1:D:187:GLN:HE21	1:D:194:ILE:H	1.13	0.95
1:D:163:LEU:HD13	1:D:197:VAL:CG1	1.97	0.94
1:E:187:GLN:NE2	1:E:194:ILE:H	1.65	0.94
1:A:51:GLY:HA2	1:E:65:VAL:HG21	1.50	0.94
1:C:187:GLN:NE2	1:C:194:ILE:H	1.66	0.92
1:E:163:LEU:HD13	1:E:197:VAL:HG11	1.51	0.92
1:A:163:LEU:HD13	1:A:197:VAL:HG11	1.51	0.91
1:A:187:GLN:HE21	1:A:194:ILE:H	1.08	0.91
1:A:187:GLN:NE2	1:A:194:ILE:H	1.67	0.91
1:C:99:GLU:CG	1:C:100:LYS:H	1.82	0.91
1:E:119:ILE:HD12	1:E:119:ILE:H	1.35	0.91
1:B:30:THR:O	1:B:33:ILE:HG22	1.72	0.90
1:A:119:ILE:H	1:A:119:ILE:HD12	1.36	0.89
1:B:243:LEU:CD2	1:B:243:LEU:CB	2.51	0.89
1:D:187:GLN:NE2	1:D:194:ILE:H	1.70	0.89
1:E:163:LEU:HD13	1:E:197:VAL:CG1	2.03	0.87
1:D:65:VAL:HG21	1:E:51:GLY:HA2	1.56	0.87
1:A:27:ILE:HG21	1:E:30:THR:HG21	1.56	0.87
1:B:65:VAL:HG21	1:C:51:GLY:HA2	1.55	0.86
1:B:163:LEU:HD13	1:B:197:VAL:CG1	2.04	0.86
1:B:187:GLN:NE2	1:B:194:ILE:H	1.74	0.86
1:B:100:LYS:C	1:B:101:THR:CA	2.44	0.86
1:A:163:LEU:HD13	1:A:197:VAL:CG1	2.07	0.85
1:D:33:ILE:HD11	1:D:80:ILE:HG22	1.61	0.83
1:A:30:THR:O	1:A:33:ILE:HG22	1.78	0.82
1:D:66:ILE:HD11	1:E:44:ILE:HD11	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLN:HE21	1:B:194:ILE:H	1.24	0.81
1:E:107:VAL:HG12	1:E:144:LEU:HD13	1.63	0.81
1:B:119:ILE:H	1:B:119:ILE:HD12	1.45	0.80
1:C:142:LYS:HE2	1:C:175:CYS:SG	2.21	0.80
1:B:142:LYS:HE2	1:B:175:CYS:SG	2.22	0.79
1:C:163:LEU:HD13	1:C:197:VAL:HG11	1.65	0.79
1:E:187:GLN:HE21	1:E:194:ILE:N	1.80	0.78
1:A:187:GLN:HE21	1:A:194:ILE:N	1.81	0.78
1:C:64:ILE:HD12	1:D:44:ILE:HA	1.66	0.77
1:D:30:THR:O	1:D:33:ILE:HG22	1.84	0.77
1:A:85:VAL:HA	1:A:88:ILE:HG22	1.67	0.77
1:A:142:LYS:HE2	1:A:175:CYS:SG	2.24	0.77
1:E:33:ILE:HG21	1:E:81:ILE:HD13	1.66	0.77
1:C:163:LEU:HD13	1:C:197:VAL:CG1	2.15	0.76
1:C:85:VAL:HA	1:C:88:ILE:HG22	1.68	0.76
1:A:33:ILE:HD11	1:A:80:ILE:HG22	1.68	0.76
1:C:33:ILE:HD11	1:C:80:ILE:HG22	1.66	0.76
1:B:85:VAL:HA	1:B:88:ILE:HG22	1.66	0.76
1:C:119:ILE:H	1:C:119:ILE:CD1	1.94	0.76
1:C:187:GLN:HE21	1:C:194:ILE:N	1.82	0.76
1:D:128:SER:O	1:D:131:ILE:HD12	1.85	0.76
1:C:30:THR:O	1:C:33:ILE:HG22	1.86	0.75
1:B:66:ILE:HD11	1:C:44:ILE:HD11	1.67	0.75
1:E:33:ILE:HD11	1:E:80:ILE:HG22	1.67	0.75
1:A:23:PHE:CE2	1:E:23:PHE:HA	2.21	0.75
1:A:75:LEU:O	1:A:79:ILE:HG12	1.87	0.75
1:A:65:VAL:HG21	1:B:51:GLY:HA2	1.68	0.75
1:E:30:THR:O	1:E:33:ILE:HG22	1.87	0.74
1:D:85:VAL:HA	1:D:88:ILE:HG22	1.69	0.74
1:D:142:LYS:HE2	1:D:175:CYS:SG	2.27	0.74
1:C:119:ILE:N	1:C:119:ILE:HD12	2.00	0.73
1:C:168:LYS:HG3	1:C:201:GLU:HB2	1.69	0.73
1:C:112:ALA:HB1	1:C:165:MET:HG3	1.70	0.73
1:E:99:GLU:H	1:E:99:GLU:CD	1.91	0.73
1:A:92:VAL:HG11	1:C:10:PHE:CE2	2.24	0.73
1:A:92:VAL:HG11	1:C:10:PHE:HE2	1.53	0.73
1:D:33:ILE:HG21	1:D:81:ILE:HD13	1.71	0.73
1:B:33:ILE:HD11	1:B:80:ILE:HG22	1.68	0.73
1:C:99:GLU:CG	1:C:100:LYS:N	2.43	0.72
1:B:128:SER:O	1:B:131:ILE:HD12	1.89	0.72
1:A:243:LEU:O	1:A:244:ARG:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:ALA:O	1:E:121:ILE:HG13	1.89	0.71
1:B:113:ARG:NH2	1:B:207:ASP:OD1	2.23	0.71
1:C:107:VAL:HG12	1:C:144:LEU:HD13	1.73	0.71
1:E:142:LYS:HE2	1:E:175:CYS:SG	2.30	0.71
1:E:75:LEU:O	1:E:79:ILE:HG12	1.91	0.70
1:E:85:VAL:HA	1:E:88:ILE:HG22	1.73	0.70
1:D:223:GLU:O	1:D:226:TYR:HB3	1.91	0.70
1:A:128:SER:O	1:A:131:ILE:HD12	1.90	0.70
1:E:78:PHE:O	1:E:81:ILE:HG22	1.92	0.70
1:A:64:ILE:HD11	1:B:47:PRO:HB3	1.73	0.70
1:E:199:VAL:HG22	1:E:217:ARG:HH21	1.56	0.69
1:E:128:SER:O	1:E:131:ILE:HD12	1.93	0.69
1:D:75:LEU:O	1:D:79:ILE:HG12	1.92	0.69
1:C:75:LEU:O	1:C:79:ILE:HG12	1.93	0.69
1:A:141:ILE:HA	1:A:144:LEU:HD23	1.75	0.68
1:B:199:VAL:HG22	1:B:217:ARG:HH21	1.58	0.68
1:C:78:PHE:O	1:C:81:ILE:HG22	1.94	0.68
1:C:200:HIS:HB2	1:C:203:GLU:HG3	1.75	0.68
1:A:119:ILE:CD1	1:A:119:ILE:H	2.06	0.68
1:E:138:VAL:HB	1:E:139:PRO:HD2	1.74	0.68
1:C:92:VAL:HG11	1:E:10:PHE:CE2	2.29	0.67
1:D:119:ILE:H	1:D:119:ILE:CD1	2.06	0.67
1:C:32:LEU:O	1:C:32:LEU:HD13	1.95	0.67
1:D:187:GLN:HE21	1:D:194:ILE:N	1.88	0.67
1:B:78:PHE:O	1:B:81:ILE:HG22	1.95	0.67
1:A:78:PHE:O	1:A:81:ILE:HG22	1.95	0.67
1:C:65:VAL:HG21	1:D:51:GLY:HA2	1.77	0.67
1:B:242:GLY:O	1:B:243:LEU:CB	2.43	0.67
1:C:88:ILE:HD13	1:C:88:ILE:O	1.95	0.66
1:E:42:MET:CE	1:E:72:LEU:HD12	2.26	0.66
1:C:30:THR:HG21	1:D:27:ILE:HG21	1.76	0.66
1:C:128:SER:O	1:C:131:ILE:HD12	1.95	0.66
1:B:187:GLN:HE21	1:B:194:ILE:N	1.93	0.66
1:A:93:LEU:HD11	1:A:97:LYS:NZ	2.11	0.66
1:E:223:GLU:O	1:E:226:TYR:HB3	1.96	0.65
1:C:33:ILE:HG21	1:C:81:ILE:HD13	1.76	0.65
1:A:200:HIS:HB2	1:A:203:GLU:HG3	1.78	0.65
1:D:163:LEU:CD1	1:D:197:VAL:HG11	2.22	0.65
1:B:200:HIS:HB2	1:B:203:GLU:HG3	1.78	0.65
1:E:112:ALA:HB1	1:E:165:MET:HG3	1.77	0.65
1:A:100:LYS:HD2	1:A:132:LYS:NZ	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ALA:HA	1:A:25:MET:CE	2.28	0.64
1:D:112:ALA:HB1	1:D:165:MET:HG3	1.79	0.64
1:D:64:ILE:HD11	1:E:47:PRO:HB3	1.80	0.64
1:A:107:VAL:HG12	1:A:144:LEU:HD13	1.79	0.64
1:C:92:VAL:HG11	1:E:10:PHE:HE2	1.62	0.64
1:A:10:PHE:CE2	1:D:92:VAL:HG11	2.33	0.64
1:D:119:ILE:HD12	1:D:119:ILE:N	2.10	0.63
1:C:138:VAL:HB	1:C:139:PRO:HD2	1.80	0.63
1:B:32:LEU:HD13	1:B:32:LEU:O	1.99	0.63
1:A:22:ALA:HA	1:A:25:MET:HE3	1.81	0.62
1:B:181:LEU:HD12	1:B:181:LEU:O	1.99	0.62
1:B:119:ILE:H	1:B:119:ILE:CD1	2.12	0.62
1:B:106:ILE:HD13	1:B:161:MET:HB2	1.81	0.62
1:B:22:ALA:HA	1:B:25:MET:CE	2.28	0.62
1:B:141:ILE:HA	1:B:144:LEU:HD23	1.81	0.62
1:D:42:MET:CE	1:D:72:LEU:HD12	2.30	0.62
1:D:200:HIS:HB2	1:D:203:GLU:HG3	1.82	0.62
1:D:107:VAL:HG12	1:D:144:LEU:HD13	1.82	0.62
1:A:100:LYS:CD	1:A:132:LYS:HZ2	2.13	0.62
1:E:200:HIS:HB2	1:E:203:GLU:HG3	1.81	0.62
1:E:72:LEU:O	1:E:76:VAL:HG12	2.00	0.61
1:E:141:ILE:HA	1:E:144:LEU:HD23	1.82	0.61
1:B:40:ILE:O	1:B:44:ILE:HG12	2.00	0.61
1:B:119:ILE:HD12	1:B:119:ILE:N	2.14	0.61
1:E:88:ILE:HD13	1:E:88:ILE:O	2.00	0.61
1:A:88:ILE:HD13	1:A:88:ILE:O	2.01	0.61
1:E:151:LEU:HA	1:E:155:GLU:HB2	1.82	0.61
1:B:107:VAL:HG12	1:B:144:LEU:HD13	1.81	0.61
1:E:72:LEU:HD13	1:E:72:LEU:O	2.00	0.61
1:C:149:LYS:HE3	1:C:189:MET:CE	2.31	0.61
1:B:30:THR:HG21	1:C:27:ILE:HG21	1.82	0.61
1:A:42:MET:CE	1:A:72:LEU:HD12	2.31	0.61
1:A:37:VAL:HA	1:A:41:ILE:HB	1.82	0.61
1:A:90:LYS:HG3	1:C:6:GLU:HG2	1.83	0.61
1:E:94:GLN:O	1:E:98:VAL:HG13	2.01	0.60
1:B:42:MET:CE	1:B:72:LEU:HD12	2.31	0.60
1:E:32:LEU:O	1:E:32:LEU:HD13	2.00	0.60
1:A:117:ALA:O	1:A:121:ILE:HG13	2.01	0.60
1:D:244:ARG:HH11	1:E:113:ARG:N	2.00	0.60
1:B:3:LEU:HG	1:B:4:PHE:H	1.66	0.60
1:B:75:LEU:O	1:B:79:ILE:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:GLY:O	1:E:244:ARG:HG3	2.02	0.60
1:D:26:GLY:HA2	1:E:24:ILE:HD11	1.83	0.60
1:A:203:GLU:CD	1:A:217:ARG:HH22	2.03	0.60
1:D:106:ILE:HD13	1:D:161:MET:HB2	1.82	0.60
1:C:40:ILE:O	1:C:44:ILE:HG12	2.01	0.60
1:A:11:LEU:HB3	1:A:17:ILE:HG13	1.83	0.60
1:D:141:ILE:HA	1:D:144:LEU:HD23	1.84	0.60
1:C:141:ILE:HA	1:C:144:LEU:HD23	1.83	0.60
1:A:106:ILE:HD13	1:A:161:MET:HB2	1.84	0.60
1:A:151:LEU:HA	1:A:155:GLU:HB2	1.82	0.60
1:E:59:VAL:HG23	1:E:68:TRP:CD1	2.37	0.59
1:C:23:PHE:HA	1:D:23:PHE:CE2	2.36	0.59
1:E:94:GLN:O	1:E:98:VAL:HG22	2.03	0.59
1:B:10:PHE:CE2	1:E:92:VAL:HG11	2.37	0.59
1:B:223:GLU:O	1:B:226:TYR:HB3	2.02	0.59
1:D:163:LEU:HA	1:D:197:VAL:HG13	1.84	0.59
1:A:10:PHE:HE2	1:D:92:VAL:HG11	1.67	0.59
1:C:90:LYS:O	1:C:93:LEU:HB3	2.02	0.59
1:D:163:LEU:HD13	1:D:197:VAL:HG13	1.85	0.59
1:D:37:VAL:HA	1:D:41:ILE:HB	1.84	0.59
1:B:112:ALA:HB1	1:B:165:MET:HG3	1.82	0.59
1:A:250:ALA:CB	1:B:113:ARG:HD3	2.33	0.59
1:C:107:VAL:CG1	1:C:144:LEU:HD13	2.32	0.59
1:B:93:LEU:HD11	1:B:97:LYS:HE2	1.85	0.59
1:B:37:VAL:HA	1:B:41:ILE:HB	1.85	0.58
1:A:249:ASP:O	1:A:250:ALA:HB2	2.03	0.58
1:D:141:ILE:O	1:D:144:LEU:HD23	2.03	0.58
1:B:163:LEU:HA	1:B:197:VAL:HG13	1.86	0.58
1:C:197:VAL:HG22	1:C:197:VAL:O	2.02	0.58
1:B:113:ARG:HB2	1:B:165:MET:CE	2.34	0.58
1:D:22:ALA:HA	1:D:25:MET:HE3	1.85	0.58
1:C:70:ALA:HB3	1:D:39:ASN:ND2	2.18	0.58
1:A:119:ILE:N	1:A:119:ILE:HD12	2.13	0.58
1:E:82:ALA:O	1:E:85:VAL:HG22	2.04	0.58
1:C:32:LEU:C	1:C:32:LEU:HD13	2.24	0.58
1:A:90:LYS:O	1:A:93:LEU:HB3	2.03	0.58
1:A:72:LEU:O	1:A:76:VAL:HG12	2.03	0.58
1:C:72:LEU:O	1:C:76:VAL:HG12	2.04	0.57
1:A:141:ILE:HA	1:A:144:LEU:CD2	2.34	0.57
1:D:78:PHE:O	1:D:81:ILE:HG22	2.02	0.57
1:E:163:LEU:HD13	1:E:197:VAL:HG13	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:VAL:HG23	1:D:68:TRP:CD1	2.39	0.57
1:A:100:LYS:HD2	1:A:132:LYS:HZ2	1.69	0.57
1:E:11:LEU:HB3	1:E:17:ILE:HG13	1.86	0.57
1:E:119:ILE:H	1:E:119:ILE:CD1	2.11	0.57
1:D:97:LYS:HE3	1:D:100:LYS:HD3	1.86	0.57
1:A:40:ILE:O	1:A:44:ILE:HG12	2.04	0.57
1:C:223:GLU:O	1:C:226:TYR:HB3	2.04	0.57
1:B:187:GLN:HE21	1:B:193:HIS:HA	1.70	0.57
1:D:88:ILE:HD13	1:D:88:ILE:O	2.05	0.57
1:E:107:VAL:CG1	1:E:144:LEU:HD13	2.33	0.57
1:A:33:ILE:HG21	1:A:81:ILE:HD13	1.87	0.56
1:A:85:VAL:HA	1:A:88:ILE:CG2	2.33	0.56
1:A:101:THR:OG1	1:A:132:LYS:HE3	2.05	0.56
1:B:139:PRO:HG2	1:B:140:GLY:H	1.69	0.56
1:A:144:LEU:O	1:A:147:ALA:HB3	2.04	0.56
1:B:85:VAL:HA	1:B:88:ILE:CG2	2.35	0.56
1:E:59:VAL:HG23	1:E:68:TRP:NE1	2.20	0.56
1:A:32:LEU:O	1:A:32:LEU:HD13	2.05	0.56
1:D:72:LEU:O	1:D:76:VAL:HG12	2.05	0.56
1:D:240:GLY:O	1:E:113:ARG:O	2.24	0.56
1:B:138:VAL:HB	1:B:139:PRO:HD2	1.87	0.56
1:C:240:GLY:O	1:D:113:ARG:O	2.24	0.56
1:D:20:ALA:O	1:D:23:PHE:HB2	2.06	0.56
1:B:10:PHE:HE2	1:E:92:VAL:HG11	1.70	0.56
1:E:184:MET:HE3	1:E:184:MET:HA	1.86	0.56
1:E:42:MET:HE1	1:E:72:LEU:HD12	1.86	0.56
1:B:90:LYS:O	1:B:93:LEU:HB3	2.06	0.56
1:E:37:VAL:HA	1:E:41:ILE:HB	1.87	0.56
1:B:22:ALA:HA	1:B:25:MET:HE3	1.87	0.56
1:B:115:ASP:OD2	1:B:118:SER:OG	2.22	0.56
1:C:139:PRO:HG2	1:C:140:GLY:H	1.71	0.55
1:D:42:MET:HE1	1:D:72:LEU:HD12	1.88	0.55
1:A:89:ALA:O	1:A:92:VAL:HG12	2.07	0.55
1:D:181:LEU:O	1:D:184:MET:HB3	2.07	0.55
1:B:65:VAL:CG2	1:C:51:GLY:HA2	2.31	0.55
1:A:78:PHE:HA	1:A:81:ILE:HG22	1.87	0.55
1:D:22:ALA:HA	1:D:25:MET:CE	2.36	0.55
1:C:37:VAL:HA	1:C:41:ILE:HB	1.89	0.55
1:B:141:ILE:HA	1:B:144:LEU:CD2	2.36	0.55
1:C:42:MET:CE	1:C:72:LEU:HD12	2.36	0.55
1:E:184:MET:CE	1:E:184:MET:HA	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HD11	1:B:44:ILE:CD1	2.27	0.55
1:D:65:VAL:CG2	1:E:51:GLY:HA2	2.32	0.55
1:C:184:MET:HE3	1:C:184:MET:HA	1.88	0.54
1:E:138:VAL:HG21	1:E:143:ASP:HB2	1.88	0.54
1:E:22:ALA:HA	1:E:25:MET:HE3	1.90	0.54
1:B:85:VAL:CA	1:B:88:ILE:HG22	2.36	0.54
1:C:149:LYS:HE3	1:C:189:MET:SD	2.48	0.54
1:D:22:ALA:CB	1:E:19:LEU:HD22	2.38	0.54
1:B:64:ILE:HG21	1:C:44:ILE:HD13	1.90	0.54
1:C:54:TRP:O	1:C:69:GLY:HA3	2.07	0.54
1:A:85:VAL:CA	1:A:88:ILE:HG22	2.37	0.54
1:D:109:THR:OG1	1:D:112:ALA:HB2	2.08	0.54
1:A:144:LEU:HB2	1:A:145:PRO:HD3	1.88	0.54
1:A:245:GLN:HA	1:A:245:GLN:NE2	2.22	0.54
1:D:117:ALA:O	1:D:121:ILE:HG13	2.07	0.54
1:C:87:ILE:HD11	1:E:3:LEU:HD13	1.90	0.54
1:D:30:THR:HG21	1:E:27:ILE:HG21	1.90	0.53
1:D:40:ILE:O	1:D:44:ILE:HG12	2.07	0.53
1:C:138:VAL:HG21	1:C:143:ASP:HB2	1.89	0.53
1:E:181:LEU:HD12	1:E:181:LEU:O	2.09	0.53
1:A:82:ALA:O	1:A:85:VAL:HG22	2.09	0.53
1:A:46:THR:HA	1:A:48:PHE:CE2	2.43	0.53
1:A:223:GLU:O	1:A:226:TYR:HB3	2.08	0.53
1:C:85:VAL:HA	1:C:88:ILE:CG2	2.36	0.53
1:E:20:ALA:O	1:E:23:PHE:HB2	2.09	0.53
1:D:59:VAL:HG23	1:D:68:TRP:NE1	2.23	0.53
1:A:39:ASN:ND2	1:E:70:ALA:HB3	2.23	0.53
1:E:106:ILE:HD13	1:E:161:MET:HB2	1.91	0.53
1:A:187:GLN:HB3	1:B:146:VAL:HG22	1.90	0.53
1:B:163:LEU:HD22	1:B:163:LEU:N	2.24	0.53
1:C:78:PHE:HA	1:C:81:ILE:HG22	1.90	0.53
1:E:144:LEU:O	1:E:147:ALA:HB3	2.07	0.53
1:E:225:VAL:O	1:E:229:LEU:HB2	2.09	0.53
1:D:54:TRP:O	1:D:69:GLY:HA3	2.09	0.53
1:B:72:LEU:O	1:B:76:VAL:HG12	2.09	0.52
1:D:228:LEU:HD21	1:E:139:PRO:CD	2.38	0.52
1:A:93:LEU:HD11	1:A:97:LYS:HZ2	1.75	0.52
1:D:149:LYS:HG2	1:D:153:GLU:OE2	2.09	0.52
1:B:11:LEU:HB3	1:B:17:ILE:HG13	1.91	0.52
1:C:187:GLN:HB3	1:D:146:VAL:HG22	1.91	0.52
1:C:141:ILE:HA	1:C:144:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD13	1:B:32:LEU:C	2.30	0.52
1:D:90:LYS:O	1:D:93:LEU:HB3	2.10	0.52
1:C:243:LEU:HD12	1:D:110:THR:HB	1.91	0.52
1:A:163:LEU:HD13	1:A:197:VAL:HG13	1.90	0.52
1:B:36:PHE:CE2	1:B:41:ILE:HD11	2.44	0.52
1:A:30:THR:HG21	1:B:27:ILE:HG21	1.92	0.52
1:C:166:PRO:HB3	1:C:176:ALA:HB2	1.92	0.52
1:E:93:LEU:O	1:E:97:LYS:HB3	2.10	0.52
1:D:82:ALA:O	1:D:85:VAL:HG22	2.09	0.52
1:D:141:ILE:HA	1:D:144:LEU:CD2	2.39	0.52
1:C:163:LEU:HD13	1:C:197:VAL:HG13	1.91	0.52
1:C:85:VAL:CA	1:C:88:ILE:HG22	2.38	0.52
1:D:11:LEU:HB3	1:D:17:ILE:HG13	1.91	0.52
1:A:100:LYS:CG	1:A:132:LYS:HZ2	2.23	0.52
1:A:59:VAL:HG23	1:A:68:TRP:NE1	2.25	0.52
1:C:59:VAL:HG23	1:C:68:TRP:NE1	2.25	0.51
1:E:163:LEU:CD1	1:E:197:VAL:HG11	2.34	0.51
1:E:78:PHE:HA	1:E:81:ILE:HG22	1.91	0.51
1:C:107:VAL:HG12	1:C:144:LEU:CD1	2.40	0.51
1:C:239:ALA:O	1:C:241:LYS:HG2	2.10	0.51
1:C:64:ILE:CG2	1:D:44:ILE:HD13	2.28	0.51
1:A:72:LEU:HD13	1:A:72:LEU:O	2.11	0.51
1:C:33:ILE:O	1:C:37:VAL:HG23	2.11	0.51
1:C:168:LYS:HG2	1:C:202:ASP:HB3	1.93	0.51
1:B:152:LEU:HD21	1:B:160:VAL:HG23	1.93	0.51
1:A:109:THR:OG1	1:A:112:ALA:HB2	2.11	0.51
1:C:11:LEU:HB3	1:C:17:ILE:HG13	1.93	0.51
1:E:119:ILE:N	1:E:119:ILE:HD12	2.16	0.51
1:B:88:ILE:HD13	1:B:88:ILE:O	2.11	0.51
1:E:90:LYS:O	1:E:93:LEU:HB3	2.10	0.51
1:E:46:THR:HG22	1:E:48:PHE:CZ	2.45	0.51
1:A:36:PHE:CE2	1:A:41:ILE:HD11	2.46	0.51
1:A:42:MET:HE1	1:A:72:LEU:HD12	1.92	0.51
1:A:112:ALA:HB1	1:A:165:MET:HG3	1.92	0.51
1:A:244:ARG:NH2	1:B:111:PHE:O	2.43	0.51
1:B:144:LEU:O	1:B:147:ALA:HB3	2.10	0.51
1:A:111:PHE:HA	1:E:243:LEU:O	2.10	0.51
1:E:22:ALA:HA	1:E:25:MET:CE	2.41	0.51
1:A:46:THR:HG22	1:A:48:PHE:CZ	2.44	0.51
1:B:89:ALA:O	1:B:92:VAL:HG12	2.10	0.51
1:B:59:VAL:HG23	1:B:68:TRP:NE1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ILE:HG21	1:E:44:ILE:HD13	1.93	0.50
1:E:89:ALA:O	1:E:92:VAL:HG12	2.11	0.50
1:D:190:THR:O	1:D:191:ASN:HB2	2.11	0.50
1:D:85:VAL:HA	1:D:88:ILE:CG2	2.39	0.50
1:D:151:LEU:HA	1:D:155:GLU:HB2	1.92	0.50
1:C:226:TYR:CD1	1:C:230:PHE:HD2	2.29	0.50
1:D:102:LYS:HB3	1:D:229:LEU:HD11	1.94	0.50
1:D:64:ILE:CD1	1:E:47:PRO:HB3	2.41	0.50
1:A:141:ILE:O	1:A:144:LEU:HD23	2.10	0.50
1:A:250:ALA:HB3	1:B:113:ARG:HD3	1.93	0.50
1:B:33:ILE:O	1:B:37:VAL:HG23	2.12	0.50
1:E:33:ILE:HD11	1:E:80:ILE:CG2	2.41	0.50
1:E:141:ILE:HA	1:E:144:LEU:CD2	2.42	0.50
1:A:243:LEU:O	1:A:244:ARG:CG	2.60	0.50
1:A:64:ILE:CD1	1:B:47:PRO:HB3	2.40	0.50
1:E:226:TYR:CD1	1:E:230:PHE:HD2	2.30	0.50
1:D:98:VAL:HG12	1:D:98:VAL:O	2.12	0.50
1:B:114:VAL:HG12	1:B:115:ASP:N	2.26	0.50
1:D:233:GLU:CD	1:D:233:GLU:H	2.15	0.50
1:B:117:ALA:O	1:B:121:ILE:HG13	2.12	0.50
1:E:187:GLN:HE21	1:E:193:HIS:HA	1.76	0.50
1:A:33:ILE:O	1:A:37:VAL:HG23	2.12	0.50
1:A:203:GLU:OE2	1:A:217:ARG:NH2	2.45	0.50
1:E:32:LEU:C	1:E:32:LEU:HD13	2.32	0.50
1:C:64:ILE:HG21	1:D:44:ILE:CD1	2.31	0.50
1:E:163:LEU:HA	1:E:197:VAL:HG13	1.94	0.50
1:E:40:ILE:O	1:E:44:ILE:HG12	2.11	0.50
1:D:144:LEU:O	1:D:147:ALA:HB3	2.12	0.50
1:B:93:LEU:CD1	1:B:97:LYS:HE2	2.41	0.50
1:D:184:MET:HA	1:D:184:MET:HE3	1.93	0.50
1:D:72:LEU:O	1:D:72:LEU:HD13	2.12	0.49
1:D:32:LEU:HD13	1:D:32:LEU:O	2.11	0.49
1:B:163:LEU:CD1	1:B:197:VAL:HG11	2.31	0.49
1:B:141:ILE:O	1:B:144:LEU:HD23	2.11	0.49
1:E:180:SER:O	1:E:183:LEU:HB2	2.12	0.49
1:A:138:VAL:HG21	1:A:143:ASP:HB2	1.93	0.49
1:B:106:ILE:CD1	1:B:161:MET:HB2	2.43	0.49
1:A:37:VAL:O	1:A:41:ILE:HB	2.13	0.49
1:B:91:LYS:O	1:B:95:GLU:HG3	2.13	0.49
1:D:89:ALA:O	1:D:92:VAL:HG12	2.13	0.49
1:B:3:LEU:HG	1:B:4:PHE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:MET:HE3	1:B:72:LEU:HD12	1.95	0.49
1:A:187:GLN:HB3	1:B:146:VAL:CG2	2.43	0.49
1:A:32:LEU:C	1:A:32:LEU:HD13	2.33	0.49
1:A:220:GLU:HB3	1:A:245:GLN:HE22	1.77	0.49
1:E:213:LEU:C	1:E:213:LEU:HD23	2.33	0.49
1:D:78:PHE:HA	1:D:81:ILE:HG22	1.94	0.49
1:D:187:GLN:HB3	1:E:146:VAL:HG22	1.95	0.49
1:A:163:LEU:HA	1:A:197:VAL:HG13	1.94	0.49
1:E:72:LEU:C	1:E:72:LEU:HD13	2.33	0.49
1:A:249:ASP:O	1:A:250:ALA:CB	2.60	0.49
1:A:184:MET:CE	1:A:184:MET:HA	2.43	0.49
1:B:78:PHE:HA	1:B:81:ILE:HG22	1.94	0.48
1:A:94:GLN:O	1:A:98:VAL:HG23	2.13	0.48
1:A:138:VAL:HB	1:A:139:PRO:HD2	1.95	0.48
1:A:106:ILE:CD1	1:A:161:MET:HB2	2.43	0.48
1:A:149:LYS:HD2	1:E:188:LEU:HD22	1.95	0.48
1:D:76:VAL:O	1:D:80:ILE:HG12	2.13	0.48
1:A:111:PHE:O	1:E:244:ARG:NH2	2.47	0.48
1:A:213:LEU:HD23	1:A:213:LEU:C	2.34	0.48
1:A:144:LEU:HD12	1:A:162:ALA:HB1	1.93	0.48
1:D:97:LYS:O	1:D:99:GLU:N	2.47	0.48
1:C:118:SER:HB2	1:C:119:ILE:HD12	1.94	0.48
1:D:197:VAL:O	1:D:197:VAL:HG22	2.13	0.48
1:B:85:VAL:O	1:B:88:ILE:HG22	2.13	0.48
1:D:85:VAL:CA	1:D:88:ILE:HG22	2.42	0.48
1:D:107:VAL:CG1	1:D:144:LEU:HD13	2.44	0.48
1:E:46:THR:HA	1:E:48:PHE:CE2	2.48	0.48
1:B:226:TYR:CD1	1:B:230:PHE:HD2	2.30	0.48
1:D:152:LEU:HD21	1:D:160:VAL:HG23	1.95	0.48
1:A:59:VAL:HG23	1:A:68:TRP:CD1	2.49	0.48
1:B:23:PHE:HA	1:C:23:PHE:CE2	2.49	0.48
1:E:113:ARG:HD2	1:E:201:GLU:OE1	2.14	0.48
1:C:22:ALA:HA	1:C:25:MET:CE	2.44	0.48
1:C:108:ASP:OD1	1:C:108:ASP:N	2.47	0.48
1:D:33:ILE:O	1:D:37:VAL:HG23	2.14	0.47
1:B:163:LEU:HD13	1:B:197:VAL:HG13	1.92	0.47
1:E:33:ILE:O	1:E:37:VAL:HG23	2.13	0.47
1:B:11:LEU:HD13	1:B:17:ILE:CG1	2.44	0.47
1:B:184:MET:HA	1:B:184:MET:HE3	1.96	0.47
1:E:190:THR:O	1:E:191:ASN:HB2	2.14	0.47
1:D:187:GLN:HE21	1:D:193:HIS:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ALA:O	1:B:85:VAL:HG22	2.15	0.47
1:C:90:LYS:HG3	1:E:6:GLU:HG2	1.96	0.47
1:A:181:LEU:HD12	1:A:181:LEU:O	2.15	0.47
1:B:42:MET:HB2	1:B:43:PRO:HD3	1.97	0.47
1:C:59:VAL:HG23	1:C:68:TRP:CD1	2.49	0.47
1:B:144:LEU:HB2	1:B:145:PRO:HD3	1.97	0.47
1:B:76:VAL:O	1:B:80:ILE:HG12	2.15	0.47
1:A:27:ILE:CG2	1:E:30:THR:HG21	2.38	0.47
1:A:138:VAL:CG2	1:A:143:ASP:HB2	2.45	0.47
1:C:82:ALA:O	1:C:85:VAL:HG22	2.15	0.47
1:E:225:VAL:O	1:E:229:LEU:CB	2.63	0.47
1:A:74:GLU:OE2	1:A:74:GLU:HA	2.15	0.47
1:B:59:VAL:HG23	1:B:68:TRP:HE1	1.80	0.47
1:B:231:LYS:O	1:B:234:TYR:HB3	2.14	0.47
1:E:108:ASP:O	1:E:137:THR:HG23	2.14	0.47
1:D:228:LEU:HD21	1:E:139:PRO:HD3	1.97	0.47
1:A:20:ALA:O	1:A:23:PHE:HB2	2.14	0.47
1:A:226:TYR:CD1	1:A:230:PHE:HD2	2.33	0.47
1:E:106:ILE:CD1	1:E:161:MET:HB2	2.44	0.47
1:E:37:VAL:O	1:E:41:ILE:HB	2.15	0.47
1:D:228:LEU:HD21	1:E:139:PRO:HD2	1.97	0.47
1:E:82:ALA:O	1:E:85:VAL:CG2	2.62	0.47
1:C:104:VAL:HG22	1:C:159:ILE:CG2	2.44	0.47
1:E:231:LYS:O	1:E:234:TYR:HB3	2.15	0.47
1:A:108:ASP:O	1:A:137:THR:HG23	2.15	0.46
1:B:113:ARG:HB2	1:B:165:MET:HE2	1.96	0.46
1:B:37:VAL:O	1:B:41:ILE:HB	2.14	0.46
1:C:26:GLY:HA2	1:D:24:ILE:HD11	1.97	0.46
1:B:113:ARG:HB2	1:B:165:MET:HE1	1.97	0.46
1:D:54:TRP:HA	1:D:57:ALA:HB2	1.97	0.46
1:A:59:VAL:HG23	1:A:68:TRP:HE1	1.81	0.46
1:D:7:PHE:O	1:D:10:PHE:HB3	2.15	0.46
1:D:144:LEU:HB2	1:D:145:PRO:HD3	1.98	0.46
1:D:244:ARG:HH11	1:E:113:ARG:H	1.61	0.46
1:B:59:VAL:HG23	1:B:68:TRP:CD1	2.51	0.46
1:C:22:ALA:HA	1:C:25:MET:HE3	1.97	0.46
1:A:163:LEU:HD22	1:A:163:LEU:N	2.30	0.46
1:B:72:LEU:HD13	1:B:72:LEU:O	2.16	0.46
1:A:44:ILE:HD11	1:E:66:ILE:HD11	1.96	0.46
1:A:190:THR:O	1:A:191:ASN:HB2	2.15	0.46
1:D:36:PHE:CE2	1:D:41:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:O	1:A:99:GLU:HB2	2.15	0.46
1:A:163:LEU:CD1	1:A:197:VAL:HG11	2.36	0.46
1:A:243:LEU:C	1:A:244:ARG:HG2	2.36	0.46
1:E:85:VAL:HA	1:E:88:ILE:CG2	2.43	0.46
1:D:226:TYR:CD1	1:D:230:PHE:HD2	2.33	0.46
1:B:3:LEU:CG	1:B:4:PHE:H	2.27	0.46
1:D:23:PHE:O	1:D:24:ILE:C	2.53	0.46
1:E:152:LEU:HD21	1:E:160:VAL:HG23	1.97	0.46
1:C:117:ALA:O	1:C:121:ILE:HG13	2.15	0.46
1:E:138:VAL:CG2	1:E:143:ASP:HB2	2.45	0.46
1:E:25:MET:HB2	1:E:25:MET:HE3	1.77	0.45
1:D:11:LEU:HD13	1:D:17:ILE:CG1	2.45	0.45
1:E:116:MET:HB3	1:E:218:ALA:HB2	1.97	0.45
1:A:85:VAL:O	1:A:88:ILE:HG22	2.16	0.45
1:A:23:PHE:HA	1:B:23:PHE:CE2	2.51	0.45
1:E:109:THR:OG1	1:E:112:ALA:HB2	2.17	0.45
1:A:11:LEU:HD13	1:A:17:ILE:CG1	2.46	0.45
1:B:46:THR:HA	1:B:48:PHE:CE2	2.52	0.45
1:D:104:VAL:HG22	1:D:159:ILE:CG2	2.46	0.45
1:A:187:GLN:HE21	1:A:193:HIS:HA	1.81	0.45
1:A:19:LEU:HD22	1:E:22:ALA:CB	2.46	0.45
1:B:94:GLN:O	1:B:98:VAL:HB	2.16	0.45
1:C:86:PHE:HD1	1:E:7:PHE:HB2	1.82	0.45
1:B:33:ILE:HG21	1:B:81:ILE:HD13	1.96	0.45
1:D:32:LEU:HD13	1:D:32:LEU:C	2.36	0.45
1:B:46:THR:HG22	1:B:48:PHE:CZ	2.52	0.45
1:A:51:GLY:HA2	1:E:65:VAL:CG2	2.33	0.45
1:E:141:ILE:O	1:E:144:LEU:HD23	2.17	0.45
1:C:59:VAL:HG23	1:C:68:TRP:HE1	1.82	0.45
1:C:109:THR:OG1	1:C:112:ALA:HB2	2.16	0.45
1:C:138:VAL:CG2	1:C:143:ASP:HB2	2.47	0.45
1:D:167:GLY:HA3	1:D:172:ASP:OD2	2.16	0.45
1:B:76:VAL:HG22	1:B:76:VAL:O	2.16	0.45
1:A:33:ILE:HD11	1:A:80:ILE:CG2	2.44	0.45
1:E:85:VAL:O	1:E:88:ILE:HG22	2.17	0.45
1:B:188:LEU:HD22	1:C:149:LYS:HD2	1.99	0.45
1:E:144:LEU:HB2	1:E:145:PRO:HD3	1.99	0.45
1:B:25:MET:HE3	1:B:25:MET:HB2	1.76	0.45
1:E:94:GLN:O	1:E:98:VAL:CG1	2.65	0.45
1:D:97:LYS:HG3	1:D:98:VAL:N	2.32	0.44
1:C:46:THR:HG22	1:C:48:PHE:CZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:THR:HA	1:D:48:PHE:CE2	2.51	0.44
1:D:41:ILE:O	1:D:45:ILE:HG13	2.18	0.44
1:E:113:ARG:HB2	1:E:165:MET:CE	2.47	0.44
1:A:6:GLU:HG2	1:D:90:LYS:HG3	1.98	0.44
1:B:54:TRP:O	1:B:69:GLY:HA3	2.17	0.44
1:D:33:ILE:HD11	1:D:80:ILE:CG2	2.39	0.44
1:E:197:VAL:O	1:E:197:VAL:HG22	2.18	0.44
1:E:144:LEU:HD12	1:E:162:ALA:HB1	1.99	0.44
1:B:128:SER:O	1:B:131:ILE:HG23	2.17	0.44
1:C:187:GLN:HE21	1:C:193:HIS:HA	1.83	0.44
1:B:107:VAL:CG1	1:B:144:LEU:HD13	2.47	0.44
1:A:76:VAL:O	1:A:80:ILE:HG12	2.18	0.44
1:E:54:TRP:HA	1:E:57:ALA:HB2	1.98	0.44
1:B:104:VAL:HG12	1:B:105:GLY:N	2.33	0.44
1:A:141:ILE:C	1:A:143:ASP:N	2.70	0.44
1:D:141:ILE:CG2	1:D:142:LYS:N	2.81	0.44
1:C:70:ALA:CB	1:D:39:ASN:ND2	2.80	0.44
1:C:46:THR:HA	1:C:48:PHE:CE2	2.53	0.44
1:D:83:PHE:O	1:D:87:ILE:HG12	2.16	0.44
1:C:65:VAL:O	1:D:43:PRO:HB3	2.17	0.44
1:E:243:LEU:N	1:E:243:LEU:HD12	2.33	0.44
1:B:138:VAL:HG21	1:B:143:ASP:HB2	1.99	0.44
1:B:152:LEU:CD2	1:B:160:VAL:HG23	2.48	0.44
1:C:25:MET:HB2	1:C:25:MET:HE3	1.81	0.44
1:C:109:THR:HA	1:C:138:VAL:O	2.17	0.44
1:E:94:GLN:O	1:E:98:VAL:CG2	2.66	0.44
1:E:233:GLU:H	1:E:233:GLU:CD	2.21	0.44
1:E:163:LEU:N	1:E:163:LEU:HD22	2.33	0.44
1:C:76:VAL:O	1:C:80:ILE:HG12	2.17	0.44
1:D:26:GLY:HA2	1:E:24:ILE:CD1	2.48	0.44
1:E:59:VAL:HG23	1:E:68:TRP:HE1	1.82	0.44
1:C:151:LEU:HA	1:C:155:GLU:HB2	2.00	0.43
1:A:107:VAL:CG1	1:A:144:LEU:HD13	2.45	0.43
1:B:131:ILE:HD13	1:B:131:ILE:H	1.83	0.43
1:C:54:TRP:HA	1:C:57:ALA:HB2	1.99	0.43
1:B:98:VAL:HG13	1:B:98:VAL:O	2.17	0.43
1:C:244:ARG:HB3	1:C:244:ARG:NH2	2.33	0.43
1:B:141:ILE:CG2	1:B:142:LYS:N	2.81	0.43
1:E:76:VAL:O	1:E:80:ILE:HG12	2.17	0.43
1:E:139:PRO:HG2	1:E:140:GLY:H	1.83	0.43
1:A:88:ILE:HD12	1:B:21:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:C	1:A:143:ASP:H	2.21	0.43
1:C:113:ARG:HB2	1:C:165:MET:CE	2.49	0.43
1:A:7:PHE:HB2	1:D:86:PHE:HD1	1.83	0.43
1:A:161:MET:SD	1:A:225:VAL:HG21	2.58	0.43
1:B:83:PHE:O	1:B:87:ILE:HG12	2.18	0.43
1:D:16:VAL:O	1:D:19:LEU:HB3	2.19	0.43
1:B:227:TYR:O	1:B:228:LEU:C	2.56	0.43
1:D:72:LEU:C	1:D:72:LEU:HD13	2.39	0.43
1:A:100:LYS:HG2	1:A:132:LYS:HZ2	1.84	0.43
1:A:72:LEU:HD13	1:A:72:LEU:C	2.39	0.43
1:E:16:VAL:O	1:E:19:LEU:HB3	2.18	0.43
1:E:11:LEU:HD13	1:E:17:ILE:CG1	2.49	0.43
1:C:83:PHE:O	1:C:87:ILE:HG12	2.19	0.43
1:A:149:LYS:HG2	1:A:153:GLU:OE2	2.19	0.43
1:C:213:LEU:C	1:C:213:LEU:HD23	2.38	0.43
1:B:42:MET:HE1	1:B:72:LEU:HD12	1.99	0.43
1:C:42:MET:HE1	1:C:72:LEU:HD12	2.01	0.43
1:C:141:ILE:O	1:C:144:LEU:HD23	2.19	0.43
1:D:108:ASP:OD1	1:D:108:ASP:N	2.50	0.43
1:E:152:LEU:CD2	1:E:160:VAL:HG23	2.49	0.43
1:D:42:MET:SD	1:D:76:VAL:HG11	2.58	0.43
1:C:163:LEU:HA	1:C:197:VAL:HG13	2.01	0.43
1:A:11:LEU:HD23	1:A:16:VAL:HB	2.00	0.43
1:B:139:PRO:HG2	1:B:143:ASP:OD2	2.19	0.43
1:A:83:PHE:O	1:A:87:ILE:HG12	2.18	0.43
1:C:209:GLU:O	1:C:210:LEU:C	2.57	0.43
1:A:160:VAL:O	1:A:195:ILE:N	2.50	0.43
1:A:23:PHE:CZ	1:E:23:PHE:HA	2.55	0.42
1:D:149:LYS:HE3	1:D:189:MET:CE	2.49	0.42
1:B:11:LEU:HD13	1:B:17:ILE:HG12	2.00	0.42
1:A:141:ILE:CA	1:A:144:LEU:HD23	2.44	0.42
1:C:89:ALA:O	1:C:92:VAL:HG12	2.19	0.42
1:D:46:THR:HG22	1:D:48:PHE:CZ	2.54	0.42
1:A:141:ILE:CG2	1:A:142:LYS:N	2.83	0.42
1:B:166:PRO:HB3	1:B:176:ALA:HB2	2.01	0.42
1:E:74:GLU:HA	1:E:74:GLU:OE2	2.20	0.42
1:D:163:LEU:N	1:D:163:LEU:HD22	2.33	0.42
1:E:42:MET:HE3	1:E:72:LEU:HD12	1.98	0.42
1:A:82:ALA:O	1:A:85:VAL:CG2	2.67	0.42
1:C:37:VAL:O	1:C:41:ILE:HB	2.19	0.42
1:B:225:VAL:O	1:B:229:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:GLN:O	1:E:191:ASN:N	2.47	0.42
1:A:42:MET:HB2	1:A:43:PRO:HD3	2.01	0.42
1:A:109:THR:HA	1:A:138:VAL:O	2.18	0.42
1:A:65:VAL:CG2	1:B:51:GLY:HA2	2.46	0.42
1:B:145:PRO:O	1:B:146:VAL:C	2.57	0.42
1:B:187:GLN:HB3	1:C:146:VAL:HG22	2.02	0.42
1:A:42:MET:HE3	1:A:72:LEU:HD12	2.02	0.42
1:A:181:LEU:O	1:A:184:MET:HB3	2.20	0.42
1:C:103:LYS:HE3	1:C:155:GLU:O	2.20	0.42
1:D:11:LEU:HD23	1:D:16:VAL:HB	2.02	0.42
1:E:119:ILE:HD11	1:E:215:LYS:HG2	2.02	0.42
1:B:20:ALA:O	1:B:23:PHE:HB2	2.20	0.42
1:A:225:VAL:O	1:A:229:LEU:HB2	2.20	0.42
1:D:104:VAL:HG12	1:D:105:GLY:N	2.35	0.42
1:D:142:LYS:CE	1:D:175:CYS:SG	3.05	0.41
1:D:17:ILE:N	1:D:18:PRO:HD2	2.35	0.41
1:C:88:ILE:HD13	1:C:88:ILE:C	2.40	0.41
1:D:131:ILE:H	1:D:131:ILE:CD1	2.33	0.41
1:D:141:ILE:CA	1:D:144:LEU:HD23	2.49	0.41
1:E:114:VAL:HG21	1:E:211:ASP:HA	2.01	0.41
1:D:166:PRO:HB3	1:D:176:ALA:HB2	2.01	0.41
1:E:88:ILE:C	1:E:88:ILE:HD13	2.41	0.41
1:C:181:LEU:HD12	1:C:181:LEU:O	2.21	0.41
1:D:36:PHE:CD1	1:D:40:ILE:HD12	2.56	0.41
1:D:42:MET:HB2	1:D:43:PRO:HD3	2.02	0.41
1:B:163:LEU:CD2	1:B:163:LEU:N	2.83	0.41
1:E:141:ILE:C	1:E:143:ASP:H	2.24	0.41
1:C:23:PHE:O	1:C:24:ILE:C	2.59	0.41
1:A:108:ASP:OD2	1:E:239:ALA:HB1	2.21	0.41
1:E:36:PHE:CE2	1:E:41:ILE:HD11	2.54	0.41
1:C:113:ARG:NH1	1:C:207:ASP:OD1	2.52	0.41
1:A:90:LYS:HG2	1:A:94:GLN:OE1	2.20	0.41
1:A:108:ASP:N	1:A:108:ASP:OD1	2.54	0.41
1:E:99:GLU:N	1:E:99:GLU:CD	2.64	0.41
1:B:131:ILE:HD13	1:B:131:ILE:N	2.35	0.41
1:B:16:VAL:O	1:B:19:LEU:HB3	2.21	0.41
1:C:217:ARG:O	1:C:218:ALA:C	2.60	0.41
1:B:33:ILE:HD11	1:B:80:ILE:CG2	2.44	0.41
1:B:72:LEU:C	1:B:72:LEU:HD13	2.40	0.41
1:A:60:GLU:HG2	1:A:65:VAL:HG22	2.02	0.41
1:D:82:ALA:O	1:D:85:VAL:CG2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ILE:CD1	1:B:131:ILE:H	2.34	0.41
1:A:200:HIS:HB3	1:A:202:ASP:OD2	2.21	0.41
1:D:106:ILE:CD1	1:D:161:MET:HB2	2.51	0.41
1:A:184:MET:HE3	1:A:184:MET:HA	2.03	0.41
1:B:234:TYR:O	1:B:237:ARG:HB3	2.21	0.41
1:B:213:LEU:HD23	1:B:213:LEU:C	2.40	0.41
1:D:74:GLU:OE2	1:D:74:GLU:HA	2.21	0.41
1:A:168:LYS:CG	1:A:201:GLU:HB2	2.51	0.41
1:D:114:VAL:HG21	1:D:211:ASP:HA	2.03	0.41
1:E:42:MET:SD	1:E:45:ILE:HD12	2.61	0.41
1:D:11:LEU:HD13	1:D:17:ILE:HG12	2.03	0.41
1:D:70:ALA:HB3	1:E:39:ASN:ND2	2.36	0.41
1:B:33:ILE:HG23	1:B:34:LYS:N	2.36	0.40
1:E:141:ILE:C	1:E:143:ASP:N	2.74	0.40
1:A:88:ILE:HD13	1:A:88:ILE:C	2.41	0.40
1:C:82:ALA:O	1:C:85:VAL:CG2	2.68	0.40
1:B:82:ALA:O	1:B:85:VAL:CG2	2.69	0.40
1:E:85:VAL:CA	1:E:88:ILE:HG22	2.45	0.40
1:C:33:ILE:HD11	1:C:80:ILE:CG2	2.44	0.40
1:D:244:ARG:NH1	1:E:113:ARG:H	2.19	0.40
1:A:11:LEU:HD13	1:A:17:ILE:HG12	2.02	0.40
1:C:239:ALA:HB1	1:D:108:ASP:OD2	2.21	0.40
1:B:116:MET:O	1:B:117:ALA:C	2.59	0.40
1:A:149:LYS:HE3	1:A:189:MET:CE	2.51	0.40
1:E:54:TRP:O	1:E:69:GLY:HA3	2.21	0.40
1:A:47:PRO:HB3	1:E:64:ILE:HD11	2.03	0.40
1:D:85:VAL:O	1:D:88:ILE:HG22	2.21	0.40
1:E:82:ALA:HA	1:E:85:VAL:HG22	2.04	0.40
1:A:21:ILE:HD11	1:E:88:ILE:HD12	2.03	0.40
1:A:7:PHE:O	1:A:10:PHE:HB3	2.21	0.40
1:B:7:PHE:O	1:B:10:PHE:HB3	2.21	0.40
1:B:17:ILE:N	1:B:18:PRO:HD2	2.36	0.40
1:C:7:PHE:CE2	1:C:11:LEU:HD11	2.56	0.40
1:D:5:SER:O	1:D:6:GLU:C	2.58	0.40
1:B:197:VAL:HG22	1:B:197:VAL:O	2.21	0.40
1:E:41:ILE:HG22	1:E:45:ILE:CD1	2.51	0.40
1:C:163:LEU:HD22	1:C:163:LEU:N	2.37	0.40
1:B:23:PHE:O	1:B:24:ILE:C	2.59	0.40
1:D:144:LEU:N	1:D:144:LEU:HD22	2.37	0.40
1:A:110:THR:HB	1:E:243:LEU:HD22	2.04	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	248/275 (90%)	228 (92%)	16 (6%)	4 (2%)	12	55
1	B	237/275 (86%)	219 (92%)	15 (6%)	3 (1%)	15	60
1	C	238/275 (86%)	223 (94%)	13 (6%)	2 (1%)	24	70
1	D	240/275 (87%)	219 (91%)	15 (6%)	6 (2%)	7	46
1	E	240/275 (87%)	221 (92%)	17 (7%)	2 (1%)	24	70
All	All	1203/1375 (88%)	1110 (92%)	76 (6%)	17 (1%)	14	58

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	THR
1	A	250	ALA
1	D	98	VAL
1	D	101	THR
1	B	145	PRO
1	A	139	PRO
1	A	145	PRO
1	B	139	PRO
1	D	23	PHE
1	E	139	PRO
1	E	145	PRO
1	C	145	PRO
1	D	145	PRO
1	B	242	GLY
1	C	139	PRO
1	D	139	PRO
1	D	24	ILE

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	194/229 (85%)	190 (98%)	4 (2%)	61 86
1	B	183/229 (80%)	179 (98%)	4 (2%)	60 85
1	C	187/229 (82%)	182 (97%)	5 (3%)	52 83
1	D	180/229 (79%)	175 (97%)	5 (3%)	51 82
1	E	186/229 (81%)	178 (96%)	8 (4%)	35 74
All	All	930/1145 (81%)	904 (97%)	26 (3%)	51 82

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	SER
1	A	88	ILE
1	A	131	ILE
1	A	163	LEU
1	B	67	SER
1	B	88	ILE
1	B	131	ILE
1	B	163	LEU
1	C	67	SER
1	C	88	ILE
1	C	100	LYS
1	C	131	ILE
1	C	197	VAL
1	D	67	SER
1	D	88	ILE
1	D	131	ILE
1	D	163	LEU
1	D	181	LEU
1	E	58	THR
1	E	67	SER
1	E	88	ILE
1	E	99	GLU
1	E	131	ILE

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Mol	Chain	Res	Type
1	E	163	LEU
1	E	181	LEU
1	E	197	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	130	ASN
1	A	187	GLN
1	A	191	ASN
1	A	224	ASN
1	A	245	GLN
1	B	39	ASN
1	B	187	GLN
1	B	191	ASN
1	B	224	ASN
1	C	130	ASN
1	C	187	GLN
1	C	191	ASN
1	C	224	ASN
1	D	39	ASN
1	D	187	GLN
1	D	191	ASN
1	D	193	HIS
1	D	224	ASN
1	E	39	ASN
1	E	187	GLN
1	E	191	ASN
1	E	224	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	250/275 (90%)	-0.23	2 (0%) 87 80	114, 173, 226, 245	0
1	B	241/275 (87%)	-0.28	0 100 100	107, 174, 223, 242	0
1	C	242/275 (88%)	-0.17	2 (0%) 87 80	109, 178, 226, 246	0
1	D	242/275 (88%)	-0.33	0 100 100	121, 181, 227, 245	0
1	E	242/275 (88%)	-0.27	2 (0%) 87 80	131, 180, 226, 246	1 (0%)
All	All	1217/1375 (88%)	-0.26	6 (0%) 91 88	107, 178, 227, 246	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	LYS	3.9
1	E	4	PHE	2.5
1	E	6	GLU	2.3
1	C	210	LEU	2.2
1	A	135	ARG	2.1
1	C	14	TYR	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.