Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 07:25 PM JST

PDB ID	:	4Y7J
Title	:	Structure of an archaeal mechanosensitive channel in expanded state
Authors	:	Li, J.; Liu, Z.
Deposited on	:	2015-02-15
Resolution	:	4.10 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 (i) 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 (i)) were used in the production of this report:

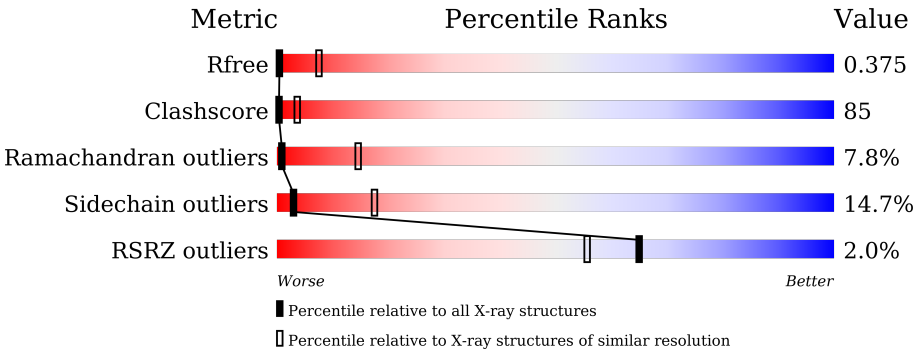
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	277	2% 24% 49% 13% • 13%
1	B	277	% 18% 51% 12% • 17%
1	C	277	% 18% 52% 13% • 16%
1	D	277	19% 52% 12% • 15%
1	E	277	4% 23% 46% 12% • 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BNG	B	301	-	-	X	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8893 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	241	Total	C	N	O	S	0	0	0
			1829	1207	281	329	12			
1	B	230	Total	C	N	O	S	0	0	0
			1757	1151	275	320	11			
1	C	234	Total	C	N	O	S	0	0	0
			1778	1171	282	313	12			
1	D	235	Total	C	N	O	S	0	0	1
			1789	1181	274	322	12			
1	E	231	Total	C	N	O	S	0	0	1
			1719	1133	270	305	11			

There are 100 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
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
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
C	-1	SER	-	expression tag	UNP Q8TNK0
C	0	HIS	-	expression tag	UNP Q8TNK0

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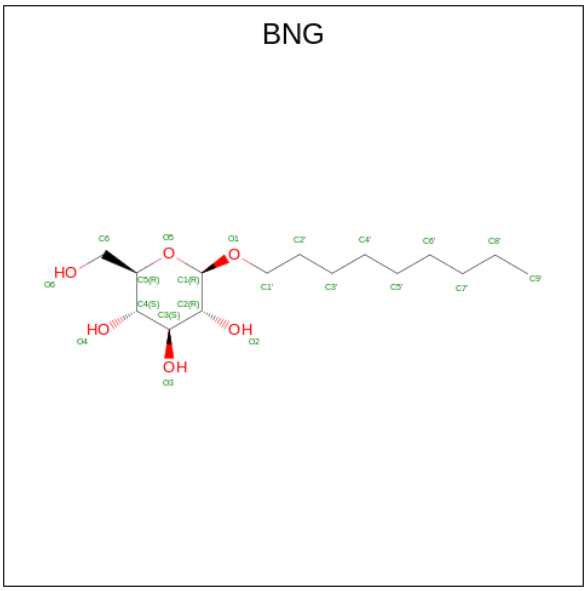
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP Q8TNK0
D	-18	GLY	-	expression tag	UNP Q8TNK0
D	-17	SER	-	expression tag	UNP Q8TNK0
D	-16	SER	-	expression tag	UNP Q8TNK0
D	-15	HIS	-	expression tag	UNP Q8TNK0
D	-14	HIS	-	expression tag	UNP Q8TNK0
D	-13	HIS	-	expression tag	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
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
E	-1	SER	-	expression tag	UNP Q8TNK0
E	0	HIS	-	expression tag	UNP Q8TNK0

- Molecule 2 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



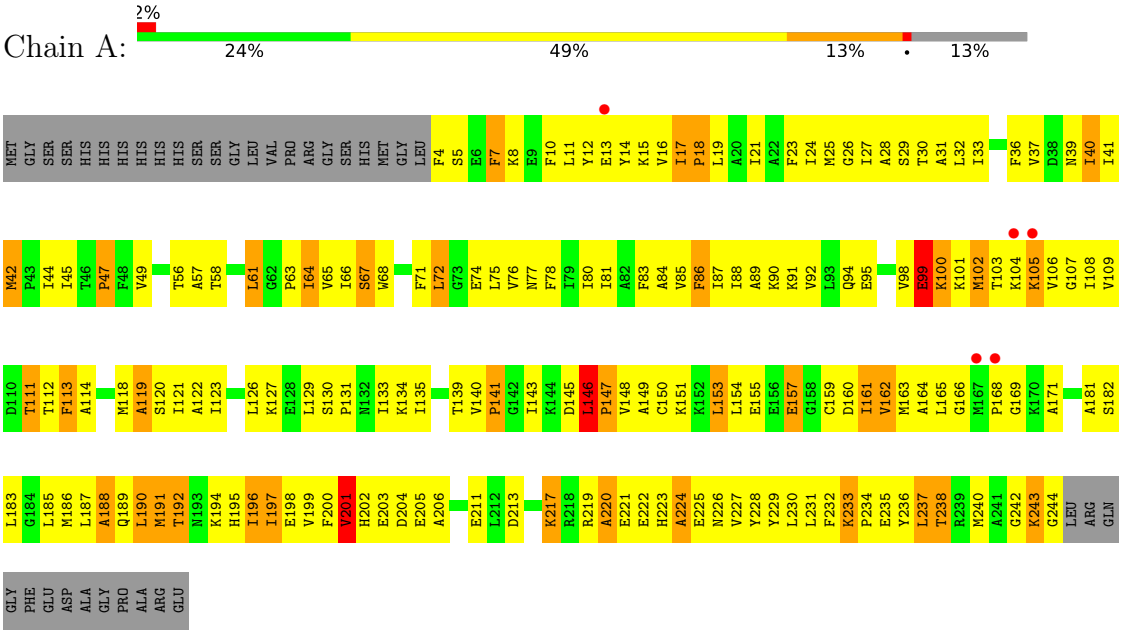
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 21 15 6	0	0

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.

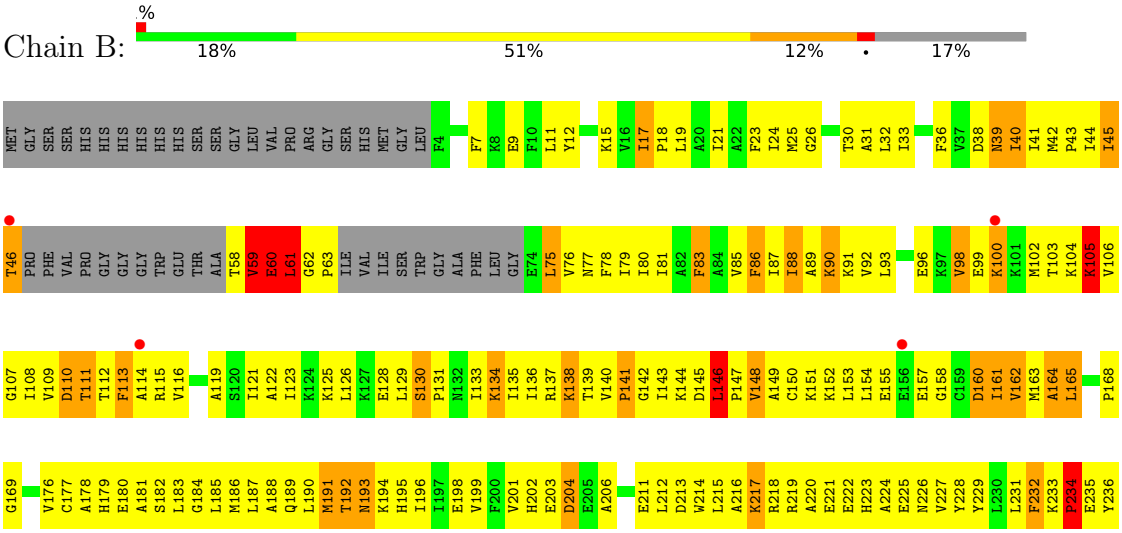
• Molecule 1: Large conductance mechanosensitive channel protein,Riboflavin synthase

Chain A:



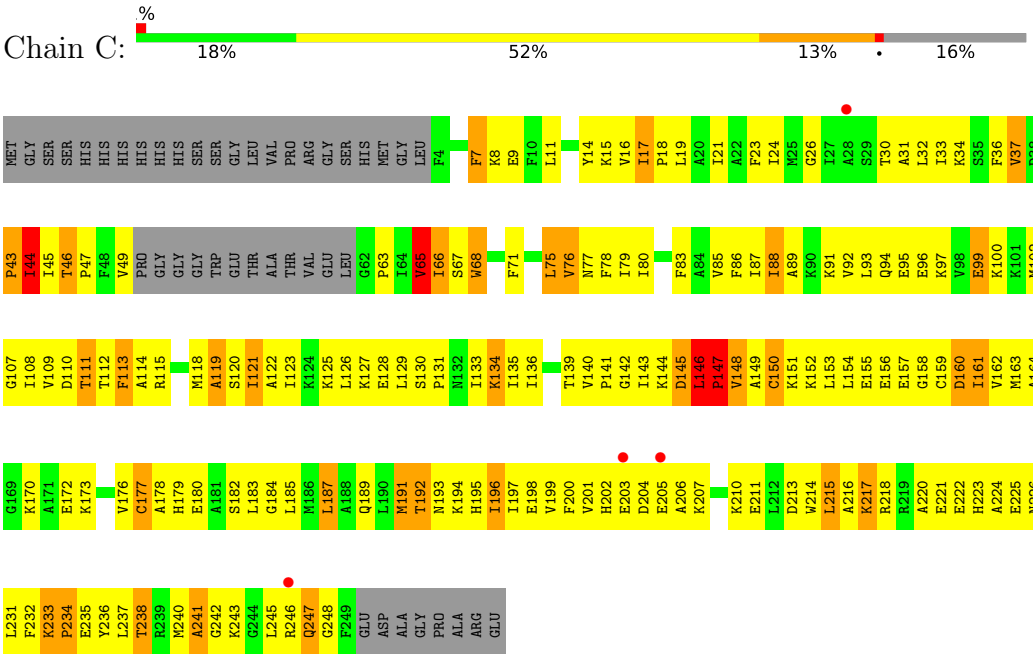
• Molecule 1: Large conductance mechanosensitive channel protein,Riboflavin synthase

Chain B:



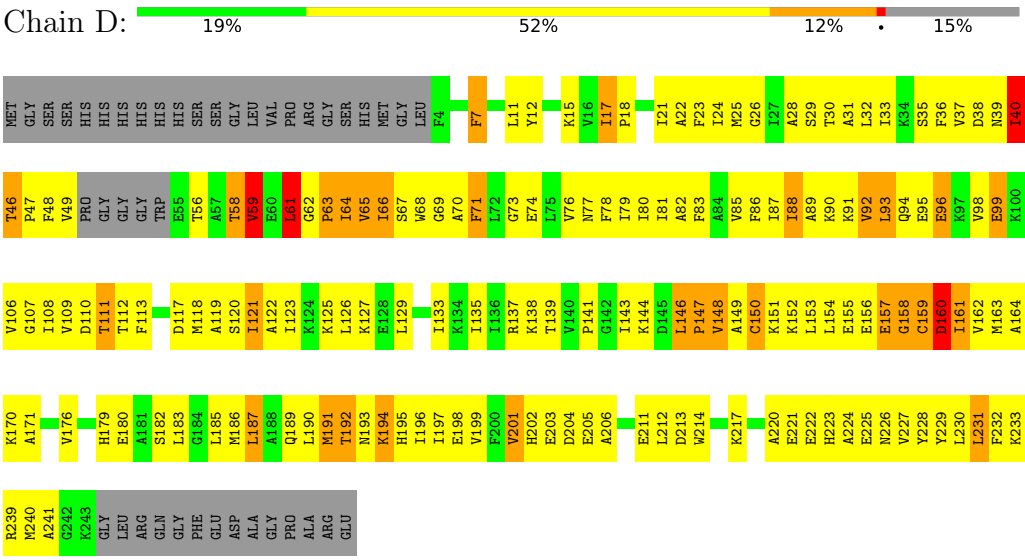
• Molecule 1: Large conductance mechanosensitive channel protein,Riboflavin synthase

Chain C:



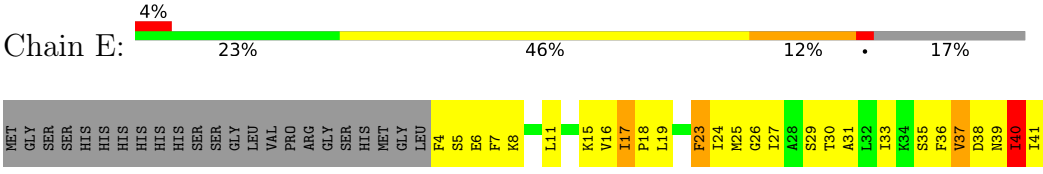
• Molecule 1: Large conductance mechanosensitive channel protein,Riboflavin synthase

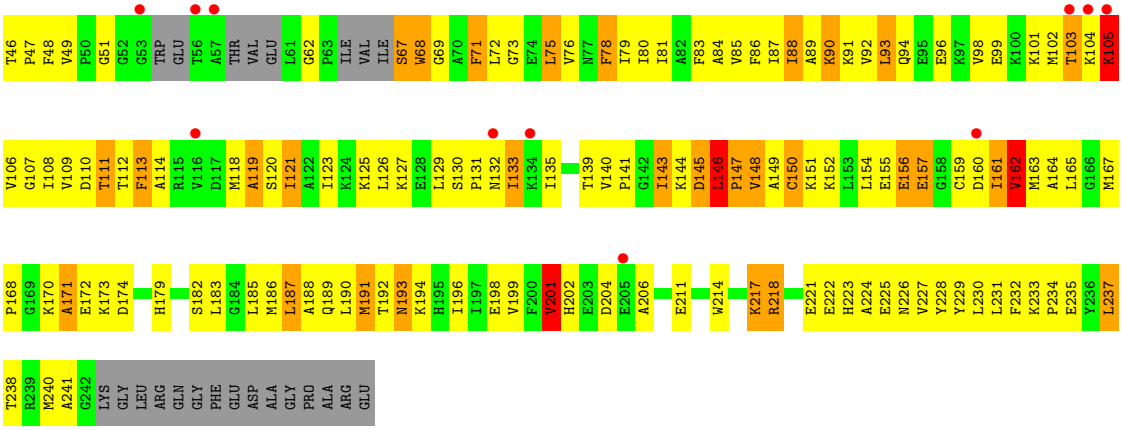
Chain D:



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

Chain E:




T46 P47 F48 V49 P50 G51 G52 G53 TRP GLU T56 A57 THR VAL GLU L61 G62 P63 ILE VAL ILE S67 W68 G69 A70 F71 L72 G73 E74 L75 V76 N77 F78 I79 I80 I81 A82 F83 A84 V85 F86 I87 I88 A89 K90 K91 V92 L93 Q94 E95 E96 K97 V98 E99 K100 K101 M102 T103 K104 K105
V106 G107 I108 V109 D110 T111 T112 F113 A114 R115 V116 D117 M118 A119 S120 I121 A122 I123 K124 K125 L126 K127 E128 L129 S130 P131 N132 I133 K134 I135 T139 V140 P141 G142 I143 K144 D145 L146 P147 V148 A149 C150 K151 K152 L153 L154 E155 E156 E157 G158 C159 D160 I161 V162 M163 A164 L165 G166 M167
P168 G169 K170 A171 E172 K173 D174 H179 S182 L183 G184 L185 M186 L187 A188 Q189 L190 M191 T192 N193 K194 H195 I196 I197 E198 V199 F200 V201 H202 E203 D204 E205 A206 E211 W214 K217 R218 E221 E222 H223 A224 E225 N226 V227 Y228 Y229 L230 L231 F232 K233 P234 E235 Y236 L237
T238 R239 M240 A241 G242 LYS GLY LEU ARG GLN GLY PHE GLU ASP ALA GLY PRO ALA ARG GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	147.36Å 149.25Å 99.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.10 41.14 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-4.10) 99.6 (41.14-4.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.321 , 0.376 0.320 , 0.375	Depositor DCC
R_{free} test set	899 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	168.8	Xtriage
Anisotropy	0.783	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 199.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.086 for k,h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8893	wwPDB-VP
Average B, all atoms (Å^2)	274.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BNG

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	0.68	0/1866	0.95	4/2527 (0.2%)
1	B	0.70	0/1786	1.08	12/2408 (0.5%)
1	C	0.62	0/1809	0.98	3/2440 (0.1%)
1	D	0.69	3/1821 (0.2%)	0.99	8/2463 (0.3%)
1	E	0.60	0/1750	0.92	6/2366 (0.3%)
All	All	0.66	3/9032 (0.0%)	0.99	33/12204 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	PHE	CG-CD2	6.67	1.48	1.38
1	D	71	PHE	CG-CD1	6.60	1.48	1.38
1	D	71	PHE	CB-CG	6.23	1.61	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	164	ALA	N-CA-C	-11.78	79.19	111.00
1	C	68	TRP	N-CA-C	9.45	136.53	111.00
1	D	106	VAL	CB-CA-C	-9.01	94.28	111.40
1	B	59	VAL	N-CA-C	8.80	134.76	111.00
1	B	40	ILE	N-CA-C	7.96	132.50	111.00
1	E	103	THR	N-CA-C	7.86	132.22	111.00
1	E	40	ILE	CG1-CB-CG2	7.74	128.44	111.40
1	D	99	GLU	N-CA-C	7.64	131.62	111.00
1	B	165	LEU	N-CA-C	-7.59	90.51	111.00
1	D	40	ILE	N-CA-C	-7.22	91.49	111.00
1	B	98	VAL	CB-CA-C	-6.90	98.29	111.40
1	D	61	LEU	CA-CB-CG	6.73	130.78	115.30
1	A	201	VAL	N-CA-C	-6.54	93.34	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	MET	N-CA-C	-6.42	93.66	111.00
1	B	59	VAL	CA-C-N	-6.32	103.29	117.20
1	D	63	PRO	N-CA-C	-5.98	96.55	112.10
1	E	62	GLY	N-CA-C	-5.98	98.16	113.10
1	C	170	LYS	N-CA-C	5.96	127.10	111.00
1	D	58	THR	N-CA-C	-5.85	95.20	111.00
1	C	65	VAL	C-N-CA	5.70	135.95	121.70
1	B	59	VAL	CB-CA-C	-5.68	100.61	111.40
1	D	56	THR	N-CA-C	-5.47	96.23	111.00
1	B	142	GLY	N-CA-C	-5.43	99.52	113.10
1	B	40	ILE	CB-CA-C	-5.30	100.99	111.60
1	E	62	GLY	C-N-CD	5.27	139.46	128.40
1	A	153	LEU	CA-CB-CG	5.18	127.22	115.30
1	E	40	ILE	CB-CA-C	-5.18	101.24	111.60
1	B	141	PRO	N-CA-C	5.16	125.51	112.10
1	B	105	LYS	N-CA-C	5.14	124.89	111.00
1	E	105	LYS	N-CA-C	5.14	124.88	111.00
1	B	59	VAL	C-N-CA	5.09	134.43	121.70
1	A	190	LEU	CA-CB-CG	-5.02	103.75	115.30
1	D	22	ALA	C-N-CA	-5.00	109.19	121.70

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	1829	0	1849	338	0
1	B	1757	0	1787	301	0
1	C	1778	0	1801	323	0
1	D	1789	0	1819	348	2
1	E	1719	0	1728	322	0
2	B	21	0	30	12	0
All	All	8893	0	9014	1527	2

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 85.

All (1527) 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:D:71:PHE:CD1	1:E:40:ILE:CD1	1.77	1.63
1:D:71:PHE:CE1	1:E:40:ILE:CD1	1.75	1.57
1:D:71:PHE:CG	1:E:40:ILE:HD13	1.37	1.54
1:D:71:PHE:CE1	1:E:40:ILE:HD11	1.02	1.54
1:D:71:PHE:CD1	1:E:40:ILE:HD11	1.32	1.47
1:B:164:ALA:O	1:B:199:VAL:CG2	1.68	1.38
1:D:71:PHE:CD2	1:E:40:ILE:HD13	1.61	1.35
1:D:71:PHE:CZ	1:E:40:ILE:CD1	2.16	1.28
1:A:168:PRO:HD2	1:A:201:VAL:O	1.31	1.24
1:B:215:LEU:HD11	1:B:219:ARG:HH21	1.03	1.17
1:B:164:ALA:O	1:B:199:VAL:HG21	1.40	1.16
1:B:193:ASN:O	1:B:194:LYS:HD2	1.46	1.12
1:B:36:PHE:O	1:B:40:ILE:HB	1.51	1.11
1:C:37:VAL:HG22	1:C:88:ILE:HG13	1.13	1.11
1:A:67:SER:O	1:A:71:PHE:CD2	2.06	1.09
1:B:243:LYS:HA	1:B:254:PRO:HB3	1.32	1.09
1:E:123:ILE:HD12	1:E:135:ILE:HD13	1.27	1.09
1:A:123:ILE:HD12	1:A:135:ILE:HD13	1.20	1.08
1:B:164:ALA:O	1:B:199:VAL:HG23	1.40	1.08
1:D:63:PRO:O	1:D:66:ILE:HG13	1.50	1.08
1:A:240:MET:HE2	1:A:240:MET:HA	1.32	1.08
1:D:62:GLY:CA	1:D:65:VAL:HG12	1.84	1.08
1:D:62:GLY:HA2	1:D:65:VAL:HG12	1.13	1.07
1:D:71:PHE:CZ	1:E:40:ILE:HD12	1.88	1.07
1:E:105:LYS:O	1:E:159:CYS:HA	1.53	1.07
1:E:121:ILE:HG21	1:E:217:LYS:HB2	1.35	1.07
1:A:129:LEU:HD23	1:A:228:TYR:CB	1.84	1.07
1:C:189:GLN:HB3	1:D:148:VAL:HG22	1.37	1.07
1:C:65:VAL:HG22	1:C:66:ILE:H	0.94	1.07
1:C:66:ILE:HG12	1:C:68:TRP:CD1	1.91	1.06
1:E:68:TRP:O	1:E:72:LEU:HG	1.55	1.06
1:A:112:THR:HB	1:A:141:PRO:HA	1.36	1.05
1:E:182:SER:HA	1:E:185:LEU:HD12	1.38	1.05
1:E:72:LEU:HA	1:E:75:LEU:HD23	1.38	1.04
1:D:222:GLU:O	1:D:225:GLU:HB3	1.58	1.04
1:C:65:VAL:CG2	1:C:66:ILE:H	1.67	1.03
1:D:71:PHE:CG	1:E:40:ILE:CD1	2.20	1.03
1:D:68:TRP:HE1	1:E:44:ILE:HD13	1.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:O	1:A:45:ILE:HG12	1.58	1.02
1:B:126:LEU:HG	1:B:133:ILE:HD12	1.41	1.02
1:C:87:ILE:HG22	1:C:91:LYS:HE2	1.38	1.02
1:E:161:ILE:HG21	1:E:231:LEU:HD11	1.41	1.02
1:D:71:PHE:CD1	1:E:40:ILE:HD13	1.61	1.02
1:A:151:LYS:HG2	1:A:155:GLU:OE2	1.60	1.00
1:E:222:GLU:O	1:E:225:GLU:HB3	1.59	0.99
1:A:36:PHE:O	1:A:40:ILE:HG12	1.62	0.98
1:B:122:ALA:HB1	1:B:224:ALA:HB2	1.45	0.98
1:D:21:ILE:O	1:D:24:ILE:HG22	1.61	0.98
1:B:165:LEU:HD23	1:B:199:VAL:HG11	1.43	0.98
1:C:183:LEU:O	1:C:187:LEU:HD12	1.62	0.98
1:D:160:ASP:O	1:D:161:ILE:HG22	1.63	0.97
1:E:154:LEU:HD11	1:E:196:ILE:HD11	1.44	0.97
1:C:134:LYS:H	1:C:134:LYS:HD2	1.27	0.97
1:D:123:ILE:HD12	1:D:135:ILE:HD13	1.45	0.97
2:B:301:BNG:H5'2	1:D:23:PHE:CZ	1.99	0.97
1:D:25:MET:O	1:D:29:SER:OG	1.82	0.97
1:A:153:LEU:O	1:A:157:GLU:HG3	1.65	0.97
1:C:65:VAL:HG22	1:C:66:ILE:N	1.79	0.96
1:D:149:ALA:O	1:D:153:LEU:HD12	1.66	0.96
1:A:182:SER:HA	1:A:185:LEU:HD12	1.47	0.95
1:D:153:LEU:HB3	1:D:159:CYS:SG	2.06	0.95
1:D:71:PHE:CE2	1:E:40:ILE:CD1	2.50	0.95
1:C:17:ILE:HD12	1:C:17:ILE:H	1.32	0.95
1:D:79:ILE:HG23	1:D:83:PHE:CD2	2.02	0.94
1:A:89:ALA:O	1:A:92:VAL:HG12	1.66	0.94
1:A:161:ILE:HG12	1:A:162:VAL:H	1.31	0.94
1:B:185:LEU:O	1:B:188:ALA:HB3	1.66	0.94
1:B:222:GLU:O	1:B:225:GLU:HB3	1.68	0.94
1:C:115:ARG:HG3	1:C:167:MET:SD	2.07	0.94
1:C:150:CYS:HB2	1:C:196:ILE:HD11	1.50	0.93
1:E:218:ARG:HA	1:E:218:ARG:HH21	1.32	0.93
1:E:218:ARG:HA	1:E:218:ARG:NH2	1.84	0.93
1:A:85:VAL:O	1:A:88:ILE:HG12	1.68	0.93
1:A:16:VAL:HG11	1:E:25:MET:SD	2.09	0.93
1:B:229:TYR:HB3	1:B:237:LEU:HD11	1.52	0.92
1:B:227:VAL:O	1:B:231:LEU:HD13	1.69	0.92
1:C:126:LEU:HG	1:C:133:ILE:HD12	1.50	0.92
1:D:186:MET:O	1:D:190:LEU:HD12	1.69	0.92
1:E:151:LYS:HE3	1:E:191:MET:HG2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:HG13	1:A:41:ILE:N	1.83	0.91
1:B:151:LYS:HG2	1:B:155:GLU:OE2	1.70	0.91
1:B:146:LEU:HD23	1:B:146:LEU:H	1.34	0.91
1:B:119:ALA:O	1:B:123:ILE:HG12	1.69	0.90
1:E:161:ILE:HD13	1:E:227:VAL:HG13	1.53	0.90
1:A:222:GLU:O	1:A:225:GLU:HB3	1.72	0.90
1:A:78:PHE:O	1:A:81:ILE:HG13	1.70	0.90
1:B:237:LEU:HD12	1:B:237:LEU:H	1.34	0.90
1:C:149:ALA:O	1:C:153:LEU:HD12	1.71	0.90
1:A:168:PRO:CD	1:A:201:VAL:O	2.19	0.90
1:D:73:GLY:O	1:D:76:VAL:HG12	1.71	0.90
1:E:193:ASN:O	1:E:194:LYS:HD2	1.72	0.90
1:A:126:LEU:HG	1:A:133:ILE:HD12	1.53	0.90
1:D:71:PHE:CE2	1:E:40:ILE:HD13	2.07	0.89
1:A:94:GLN:O	1:A:98:VAL:HG22	1.70	0.89
1:A:61:LEU:HD12	1:A:61:LEU:H	1.38	0.89
1:D:119:ALA:O	1:D:123:ILE:HG12	1.73	0.89
1:D:71:PHE:CD2	1:E:40:ILE:CD1	2.50	0.88
1:E:161:ILE:HD11	1:E:227:VAL:HG22	1.55	0.88
1:B:85:VAL:O	1:B:88:ILE:HG22	1.73	0.88
1:C:66:ILE:HG13	1:C:67:SER:H	1.36	0.88
1:D:23:PHE:O	1:D:26:GLY:N	2.06	0.88
1:E:226:ASN:HA	1:E:229:TYR:CD2	2.09	0.87
1:C:63:PRO:HG2	1:C:65:VAL:HB	1.57	0.87
1:C:65:VAL:O	1:C:66:ILE:HG23	1.74	0.87
1:C:111:THR:CG2	1:C:166:GLY:HA2	2.05	0.87
1:B:215:LEU:HD11	1:B:219:ARG:NH2	1.89	0.86
1:D:63:PRO:O	1:D:66:ILE:CG1	2.22	0.86
1:E:78:PHE:O	1:E:81:ILE:HG22	1.73	0.86
1:A:165:LEU:HD23	1:A:199:VAL:HG21	1.53	0.86
1:C:161:ILE:O	1:C:162:VAL:HG23	1.76	0.86
1:E:85:VAL:O	1:E:88:ILE:HG22	1.74	0.86
1:B:125:LYS:HE3	1:B:129:LEU:HD11	1.57	0.86
1:C:149:ALA:O	1:C:153:LEU:CD1	2.24	0.86
1:D:122:ALA:HB1	1:D:224:ALA:HB2	1.56	0.86
1:A:87:ILE:HG22	1:A:91:LYS:HE3	1.58	0.86
1:A:154:LEU:HD11	1:A:196:ILE:HD11	1.55	0.85
1:B:246:ARG:HG3	1:B:252:ALA:HB3	1.57	0.85
1:D:71:PHE:HA	1:E:39:ASN:HD22	1.41	0.85
1:D:46:THR:H	1:D:47:PRO:CD	1.88	0.85
1:E:89:ALA:O	1:E:92:VAL:HG12	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ILE:HG13	1:E:163:MET:HB2	1.59	0.85
1:E:186:MET:HA	1:E:189:GLN:OE1	1.76	0.85
1:A:37:VAL:HG21	1:A:85:VAL:HG22	1.59	0.85
1:B:189:GLN:HE21	1:B:196:ILE:H	1.25	0.85
1:D:66:ILE:HD12	1:D:67:SER:N	1.92	0.84
1:E:185:LEU:HD13	1:E:198:GLU:HG2	1.57	0.84
1:D:17:ILE:HD12	1:D:17:ILE:H	1.41	0.84
1:D:85:VAL:O	1:D:88:ILE:HG22	1.77	0.84
1:A:99:GLU:O	1:A:100:LYS:HB2	1.77	0.84
1:A:129:LEU:HD23	1:A:228:TYR:HB3	1.60	0.84
1:C:154:LEU:HD11	1:C:196:ILE:HG13	1.59	0.84
1:E:17:ILE:HD12	1:E:17:ILE:H	1.42	0.84
1:D:36:PHE:O	1:D:40:ILE:HB	1.78	0.84
1:A:185:LEU:O	1:A:188:ALA:HB3	1.77	0.83
1:E:107:GLY:O	1:E:162:VAL:HA	1.77	0.83
1:D:43:PRO:O	1:D:47:PRO:HD3	1.79	0.83
1:D:187:LEU:HD23	1:D:191:MET:CE	2.08	0.83
1:D:143:ILE:HG23	1:D:144:LYS:HG3	1.60	0.83
1:E:98:VAL:HA	1:E:101:LYS:HD2	1.60	0.83
1:D:63:PRO:HA	1:D:66:ILE:HG23	1.60	0.83
1:E:69:GLY:HA2	1:E:72:LEU:HD12	1.57	0.83
1:B:103:THR:C	1:B:104:LYS:HD2	1.98	0.83
1:A:112:THR:CB	1:A:141:PRO:HA	2.09	0.82
1:B:75:LEU:HD12	1:B:76:VAL:N	1.95	0.82
1:C:76:VAL:O	1:C:80:ILE:HG13	1.79	0.82
1:D:146:LEU:O	1:D:149:ALA:HB3	1.79	0.82
1:D:25:MET:O	1:D:29:SER:CB	2.28	0.82
1:E:164:ALA:O	1:E:199:VAL:HB	1.79	0.82
1:B:112:THR:HB	1:B:141:PRO:HA	1.62	0.81
1:B:219:ARG:HG2	1:B:223:HIS:NE2	1.94	0.81
1:C:146:LEU:O	1:C:149:ALA:HB3	1.80	0.81
1:D:25:MET:SD	1:E:16:VAL:HG11	2.20	0.81
1:B:125:LYS:O	1:B:129:LEU:HD13	1.80	0.81
1:B:126:LEU:HD23	1:B:135:ILE:HD11	1.60	0.81
1:D:62:GLY:HA2	1:D:65:VAL:CG1	2.05	0.81
1:A:101:LYS:O	1:A:103:THR:HG23	1.80	0.81
1:C:46:THR:O	1:C:49:VAL:HG12	1.78	0.81
1:C:161:ILE:HG12	1:C:162:VAL:N	1.95	0.81
1:E:48:PHE:CD2	1:E:49:VAL:HG23	2.16	0.81
1:E:73:GLY:O	1:E:76:VAL:HG12	1.81	0.81
1:E:98:VAL:HA	1:E:101:LYS:HZ3	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:C	1:A:147:PRO:HD2	2.00	0.81
1:A:197:ILE:H	1:A:197:ILE:HD13	1.45	0.81
1:A:227:VAL:O	1:A:231:LEU:HD13	1.81	0.81
1:A:160:ASP:O	1:A:194:LYS:HG3	1.81	0.81
1:D:25:MET:O	1:D:29:SER:N	2.14	0.81
1:D:108:ILE:HG13	1:D:163:MET:HB2	1.62	0.80
1:A:123:ILE:HD12	1:A:135:ILE:CD1	2.09	0.80
1:E:150:CYS:O	1:E:154:LEU:HG	1.81	0.80
1:D:186:MET:O	1:D:189:GLN:HB2	1.80	0.80
1:A:98:VAL:HG23	1:A:98:VAL:O	1.81	0.80
1:C:105:LYS:HE3	1:C:158:GLY:HA3	1.64	0.80
1:C:110:ASP:O	1:C:139:THR:HG23	1.82	0.80
1:A:197:ILE:HD13	1:A:197:ILE:N	1.97	0.80
1:C:213:ASP:O	1:C:216:ALA:HB3	1.80	0.80
1:B:153:LEU:O	1:B:157:GLU:HG2	1.82	0.80
1:B:161:ILE:HG12	1:B:162:VAL:H	1.45	0.79
1:E:182:SER:O	1:E:185:LEU:HB2	1.82	0.79
1:B:139:THR:HG22	1:B:140:VAL:H	1.44	0.79
1:C:223:HIS:CE1	1:C:247:GLN:HB3	2.17	0.79
1:C:85:VAL:O	1:C:88:ILE:HG22	1.83	0.79
1:C:189:GLN:HB3	1:D:148:VAL:CG2	2.12	0.79
1:D:164:ALA:HB3	1:D:199:VAL:H	1.48	0.79
1:A:148:VAL:HG22	1:E:189:GLN:HB3	1.65	0.79
1:B:232:PHE:O	1:B:234:PRO:HD3	1.83	0.79
1:C:159:CYS:O	1:C:161:ILE:N	2.15	0.79
1:A:185:LEU:O	1:A:189:GLN:HG3	1.83	0.79
1:A:15:LYS:HB3	1:A:18:PRO:HG2	1.65	0.79
1:A:118:MET:HE1	1:A:166:GLY:N	1.98	0.79
1:C:245:LEU:CB	1:C:245:LEU:CD2	2.61	0.79
1:C:233:LYS:HE2	1:C:236:TYR:HB2	1.65	0.78
1:D:46:THR:H	1:D:47:PRO:HD2	1.48	0.78
1:A:77:ASN:O	1:A:80:ILE:HG22	1.83	0.78
1:D:187:LEU:HB3	1:D:191:MET:HE1	1.65	0.78
1:E:217:LYS:NZ	1:E:217:LYS:HB3	1.97	0.78
1:A:146:LEU:HG	1:A:147:PRO:HD3	1.66	0.78
1:A:153:LEU:HA	1:A:157:GLU:CD	2.04	0.78
1:D:123:ILE:CD1	1:D:135:ILE:HD13	2.13	0.78
1:B:17:ILE:H	1:B:17:ILE:HD12	1.48	0.78
1:B:61:LEU:CD1	1:B:63:PRO:HB3	2.14	0.78
1:C:37:VAL:CG2	1:C:88:ILE:HG13	2.06	0.78
1:C:111:THR:HG21	1:C:166:GLY:HA2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASP:O	1:B:216:ALA:HB3	1.84	0.78
1:C:66:ILE:HG12	1:C:68:TRP:HD1	1.49	0.78
1:D:102:MET:CE	1:D:231:LEU:HD23	2.13	0.78
1:E:35:SER:HA	1:E:38:ASP:HB3	1.66	0.78
1:E:111:THR:HG21	1:E:114:ALA:HB2	1.65	0.78
1:B:111:THR:CG2	1:B:114:ALA:HB2	2.14	0.78
1:B:165:LEU:HA	1:B:199:VAL:HB	1.66	0.78
1:D:63:PRO:O	1:D:66:ILE:N	2.16	0.78
1:D:179:HIS:NE2	1:D:183:LEU:HD11	1.99	0.78
1:D:229:TYR:HB3	1:D:237:LEU:HD11	1.65	0.78
1:D:79:ILE:HG23	1:D:83:PHE:HD2	1.48	0.77
1:C:121:ILE:HG21	1:C:217:LYS:O	1.84	0.77
1:C:164:ALA:HB3	1:C:199:VAL:H	1.48	0.77
1:B:162:VAL:HG13	1:B:163:MET:O	1.83	0.77
1:E:44:ILE:O	1:E:47:PRO:HD2	1.83	0.77
1:A:40:ILE:O	1:A:44:ILE:HG22	1.84	0.77
1:C:238:THR:O	1:C:241:ALA:HB2	1.85	0.76
1:D:94:GLN:O	1:D:98:VAL:HG23	1.85	0.76
1:C:118:MET:HB2	1:C:165:LEU:HD13	1.67	0.76
1:C:164:ALA:HB3	1:C:198:GLU:HA	1.66	0.76
1:B:106:VAL:HG12	1:B:108:ILE:CD1	2.16	0.76
1:D:182:SER:HA	1:D:185:LEU:HD12	1.67	0.76
1:E:81:ILE:O	1:E:85:VAL:HG23	1.84	0.76
1:E:36:PHE:O	1:E:40:ILE:HG13	1.84	0.76
1:E:87:ILE:O	1:E:90:LYS:HG3	1.85	0.76
2:B:301:BNG:C6'	1:D:23:PHE:HZ	1.99	0.76
1:D:113:PHE:HB2	1:D:141:PRO:O	1.86	0.76
1:C:110:ASP:C	1:C:139:THR:HG23	2.06	0.76
1:D:187:LEU:HD23	1:D:191:MET:HE2	1.67	0.76
1:A:200:PHE:O	1:A:201:VAL:HG13	1.86	0.76
1:E:37:VAL:CG1	1:E:81:ILE:HG13	2.16	0.76
1:A:146:LEU:H	1:A:146:LEU:HD23	1.50	0.75
1:C:232:PHE:O	1:C:234:PRO:HD3	1.85	0.75
1:E:98:VAL:CA	1:E:101:LYS:HZ3	1.99	0.75
1:C:121:ILE:HD11	1:C:217:LYS:HZ2	1.51	0.75
1:D:77:ASN:O	1:D:81:ILE:HG12	1.87	0.75
1:E:151:LYS:HG2	1:E:155:GLU:OE2	1.87	0.75
1:D:21:ILE:O	1:D:24:ILE:CG2	2.34	0.75
1:E:42:MET:O	1:E:46:THR:HG23	1.84	0.75
1:E:98:VAL:HG13	1:E:101:LYS:HD2	1.69	0.75
1:C:235:GLU:O	1:C:238:THR:HB	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LYS:HA	1:C:128:GLU:OE1	1.85	0.75
1:D:46:THR:N	1:D:47:PRO:HD2	2.02	0.75
1:A:139:THR:HG22	1:A:140:VAL:H	1.52	0.75
1:C:243:LYS:HD2	1:C:243:LYS:N	2.02	0.75
1:B:145:ASP:C	1:B:147:PRO:HD2	2.08	0.74
1:D:71:PHE:CD1	1:E:40:ILE:CG1	2.69	0.74
1:D:150:CYS:HB2	1:D:196:ILE:HD13	1.69	0.74
1:E:123:ILE:HG23	1:E:135:ILE:CD1	2.17	0.74
1:A:150:CYS:HA	1:A:153:LEU:HD13	1.69	0.74
1:B:7:PHE:HE1	1:E:86:PHE:HB3	1.51	0.74
1:C:102:MET:C	1:C:103:THR:CA	2.56	0.74
1:D:96:GLU:N	1:D:96:GLU:OE2	2.21	0.74
1:E:186:MET:O	1:E:189:GLN:HB2	1.88	0.74
1:B:110:ASP:O	1:B:139:THR:HG23	1.87	0.73
1:B:111:THR:HG21	1:B:114:ALA:HB2	1.69	0.73
1:B:161:ILE:HG13	1:B:195:HIS:O	1.89	0.73
1:C:44:ILE:C	1:C:47:PRO:HD2	2.08	0.73
1:E:110:ASP:O	1:E:139:THR:HG23	1.87	0.73
1:A:90:LYS:HE2	1:C:7:PHE:HD1	1.52	0.73
1:E:235:GLU:O	1:E:238:THR:HB	1.89	0.73
1:A:7:PHE:HE2	1:D:90:LYS:HB2	1.54	0.73
1:A:61:LEU:H	1:A:61:LEU:CD1	2.01	0.73
1:B:108:ILE:HG13	1:B:163:MET:HB2	1.71	0.73
1:D:89:ALA:O	1:D:92:VAL:HG12	1.88	0.73
1:B:178:ALA:O	1:B:182:SER:OG	2.04	0.73
1:C:161:ILE:HG12	1:C:162:VAL:H	1.54	0.73
1:E:111:THR:CG2	1:E:114:ALA:HB2	2.18	0.73
1:A:129:LEU:HD23	1:A:228:TYR:HB2	1.69	0.73
1:B:140:VAL:HG21	1:B:145:ASP:HB3	1.71	0.73
2:B:301:BNG:H3'1	2:B:301:BNG:H7'2	1.71	0.73
1:A:5:SER:HA	1:A:8:LYS:HE2	1.69	0.72
1:D:161:ILE:HG13	1:D:195:HIS:O	1.89	0.72
1:A:182:SER:O	1:A:185:LEU:HB2	1.89	0.72
1:D:64:ILE:O	1:D:67:SER:HB3	1.89	0.72
1:C:237:LEU:HD12	1:C:237:LEU:H	1.54	0.72
1:B:161:ILE:HG12	1:B:162:VAL:N	2.03	0.72
1:D:65:VAL:HG22	1:D:68:TRP:HB2	1.71	0.72
1:A:150:CYS:O	1:A:154:LEU:HG	1.89	0.72
1:A:154:LEU:CD1	1:A:196:ILE:HD11	2.18	0.72
1:B:7:PHE:CE1	1:E:86:PHE:HB3	2.24	0.72
1:B:36:PHE:HA	1:B:40:ILE:HG13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLU:OE1	1:B:247:GLN:HG3	1.89	0.72
1:A:143:ILE:O	1:A:146:LEU:HD21	1.89	0.72
1:C:217:LYS:O	1:C:220:ALA:HB3	1.89	0.72
1:A:126:LEU:HG	1:A:133:ILE:CD1	2.20	0.72
1:D:40:ILE:HG22	1:D:41:ILE:H	1.54	0.72
1:B:193:ASN:C	1:B:194:LYS:HD2	2.09	0.72
1:C:157:GLU:HG3	1:C:159:CYS:SG	2.28	0.72
1:A:111:THR:HG21	1:A:114:ALA:HB2	1.70	0.71
1:A:226:ASN:HA	1:A:229:TYR:CD2	2.25	0.71
1:B:42:MET:HB3	1:B:43:PRO:HD3	1.72	0.71
1:C:193:ASN:HB3	1:D:152:LYS:HG2	1.70	0.71
1:D:35:SER:HA	1:D:38:ASP:HB3	1.72	0.71
1:A:229:TYR:HA	1:A:233:LYS:HB3	1.72	0.71
1:C:66:ILE:HG12	1:C:68:TRP:NE1	2.04	0.71
1:D:161:ILE:O	1:D:162:VAL:HG23	1.90	0.71
1:A:139:THR:HG22	1:A:140:VAL:N	2.06	0.71
1:B:36:PHE:C	1:B:40:ILE:HB	2.11	0.71
1:B:182:SER:HA	1:B:185:LEU:HD12	1.71	0.71
1:B:187:LEU:HB3	1:B:191:MET:CE	2.20	0.71
1:D:46:THR:N	1:D:47:PRO:CD	2.53	0.71
1:E:68:TRP:HE3	1:E:68:TRP:N	1.89	0.71
1:B:76:VAL:O	1:B:80:ILE:HG13	1.90	0.71
1:C:111:THR:CG2	1:C:114:ALA:HB2	2.20	0.71
1:D:123:ILE:HD12	1:D:135:ILE:HG21	1.73	0.71
1:B:240:MET:O	1:B:243:LYS:HB2	1.91	0.71
1:D:78:PHE:O	1:D:82:ALA:N	2.16	0.71
1:D:183:LEU:O	1:D:187:LEU:HD12	1.91	0.71
1:E:227:VAL:O	1:E:231:LEU:HD13	1.91	0.71
1:C:77:ASN:HA	1:C:80:ILE:HD12	1.73	0.71
1:D:164:ALA:O	1:D:199:VAL:HB	1.91	0.70
1:E:108:ILE:HG23	1:E:165:LEU:HD12	1.72	0.70
1:C:227:VAL:HG12	1:C:231:LEU:HD13	1.73	0.70
1:D:61:LEU:HB3	1:D:65:VAL:HB	1.73	0.70
1:C:143:ILE:O	1:C:146:LEU:HG	1.91	0.70
1:A:186:MET:O	1:A:190:LEU:N	2.20	0.70
1:D:193:ASN:HA	1:E:148:VAL:HG12	1.74	0.70
1:A:15:LYS:C	1:A:18:PRO:HD2	2.12	0.70
1:B:150:CYS:O	1:B:154:LEU:HG	1.91	0.70
1:D:68:TRP:NE1	1:E:44:ILE:HD13	2.01	0.70
1:D:186:MET:HA	1:D:189:GLN:OE1	1.91	0.70
1:E:133:ILE:O	1:E:133:ILE:HG13	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:HB	1:B:141:PRO:HD2	1.72	0.70
1:D:25:MET:HG2	1:E:16:VAL:CG1	2.21	0.70
1:C:107:GLY:O	1:C:162:VAL:HG22	1.92	0.70
1:D:62:GLY:CA	1:D:65:VAL:CG1	2.66	0.70
1:A:109:VAL:HG21	1:A:153:LEU:HD11	1.73	0.70
1:A:129:LEU:HD23	1:A:228:TYR:CG	2.27	0.70
1:A:237:LEU:O	1:A:240:MET:N	2.25	0.70
1:B:139:THR:HG22	1:B:140:VAL:N	2.07	0.70
1:C:88:ILE:HD13	1:C:88:ILE:O	1.92	0.70
1:C:229:TYR:HB3	1:C:237:LEU:HD11	1.74	0.70
1:D:102:MET:HE2	1:D:231:LEU:HD23	1.74	0.70
1:D:153:LEU:HA	1:D:157:GLU:OE2	1.92	0.69
1:B:223:HIS:O	1:B:227:VAL:HG23	1.92	0.69
1:C:125:LYS:O	1:C:128:GLU:HB3	1.92	0.69
1:C:217:LYS:NZ	1:C:217:LYS:HB3	2.07	0.69
1:D:126:LEU:HG	1:D:133:ILE:CD1	2.23	0.69
1:E:125:LYS:HG2	1:E:221:GLU:HG3	1.74	0.69
1:E:154:LEU:HD11	1:E:196:ILE:CD1	2.21	0.69
2:B:301:BNG:C5'	1:D:23:PHE:HZ	2.05	0.69
1:E:112:THR:HB	1:E:141:PRO:HA	1.73	0.69
2:B:301:BNG:C5'	1:D:23:PHE:CZ	2.75	0.69
1:C:148:VAL:O	1:C:152:LYS:HG3	1.93	0.69
1:A:68:TRP:HE3	1:A:72:LEU:HD21	1.57	0.69
1:E:49:VAL:HG12	1:E:49:VAL:O	1.91	0.69
1:A:229:TYR:HB3	1:A:233:LYS:O	1.92	0.69
1:A:240:MET:HE2	1:A:240:MET:CA	2.18	0.69
1:E:183:LEU:O	1:E:187:LEU:HD12	1.92	0.69
1:A:127:LYS:CA	1:A:133:ILE:HD11	2.22	0.69
1:B:183:LEU:O	1:B:186:MET:HB3	1.92	0.69
1:A:61:LEU:HD12	1:A:61:LEU:N	2.08	0.69
1:C:41:ILE:HG23	1:C:91:LYS:HE3	1.75	0.69
1:A:165:LEU:HA	1:A:199:VAL:HB	1.73	0.68
1:B:146:LEU:HG	1:B:147:PRO:HD3	1.75	0.68
1:C:222:GLU:OE1	1:C:248:GLY:N	2.27	0.68
1:B:89:ALA:O	1:B:92:VAL:HG12	1.93	0.68
1:C:111:THR:HG22	1:C:166:GLY:HA2	1.73	0.68
1:D:71:PHE:HA	1:E:39:ASN:ND2	2.08	0.68
1:C:121:ILE:HG13	1:C:217:LYS:HB3	1.75	0.68
1:A:45:ILE:HG22	1:A:45:ILE:O	1.93	0.68
1:A:240:MET:HA	1:A:240:MET:CE	2.18	0.68
1:B:61:LEU:HD12	1:B:63:PRO:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LYS:HG2	1:C:155:GLU:OE2	1.94	0.68
1:D:67:SER:OG	1:E:43:PRO:HB2	1.92	0.68
1:A:121:ILE:HG21	1:A:217:LYS:HB2	1.75	0.68
1:B:189:GLN:HE21	1:B:196:ILE:N	1.91	0.68
1:B:189:GLN:CG	1:B:196:ILE:HB	2.23	0.68
1:C:83:PHE:O	1:C:87:ILE:HG12	1.93	0.68
1:D:44:ILE:HG23	1:D:45:ILE:HG12	1.75	0.68
1:A:127:LYS:N	1:A:133:ILE:HD11	2.09	0.68
1:B:75:LEU:HD23	1:C:40:ILE:HG13	1.76	0.68
1:C:145:ASP:C	1:C:147:PRO:HD2	2.15	0.68
1:C:140:VAL:HB	1:C:141:PRO:HD2	1.75	0.67
1:C:187:LEU:HB3	1:C:191:MET:HE1	1.76	0.67
1:A:4:PHE:O	1:A:8:LYS:HG3	1.94	0.67
1:C:49:VAL:HG13	1:C:49:VAL:O	1.94	0.67
1:D:61:LEU:HD12	1:D:65:VAL:HG23	1.76	0.67
1:E:161:ILE:O	1:E:162:VAL:HG23	1.93	0.67
1:A:67:SER:O	1:A:71:PHE:CE2	2.47	0.67
1:D:235:GLU:O	1:D:238:THR:HB	1.95	0.67
1:A:68:TRP:CE3	1:A:72:LEU:HD21	2.28	0.67
1:A:151:LYS:O	1:A:155:GLU:HG3	1.94	0.67
1:C:185:LEU:HD13	1:C:198:GLU:HG2	1.75	0.67
1:A:161:ILE:CG1	1:A:162:VAL:H	2.08	0.67
1:D:12:TYR:O	1:D:15:LYS:HG3	1.95	0.67
1:E:98:VAL:HG22	1:E:101:LYS:NZ	2.09	0.67
1:E:111:THR:OG1	1:E:113:PHE:N	2.27	0.67
1:A:108:ILE:HG13	1:A:163:MET:HB2	1.75	0.67
1:B:112:THR:HG1	1:B:139:THR:HG22	1.60	0.67
1:E:151:LYS:HE2	1:E:191:MET:HB3	1.75	0.67
1:C:122:ALA:HB1	1:C:224:ALA:HB2	1.76	0.67
1:C:139:THR:HG22	1:C:140:VAL:H	1.60	0.67
1:D:79:ILE:HG12	1:D:83:PHE:HE2	1.60	0.67
1:D:146:LEU:HG	1:D:147:PRO:HD3	1.76	0.67
1:A:127:LYS:HA	1:A:133:ILE:HD11	1.77	0.66
1:C:46:THR:O	1:C:49:VAL:CG1	2.42	0.66
1:E:37:VAL:HG11	1:E:81:ILE:HG13	1.77	0.66
1:A:189:GLN:O	1:A:192:THR:O	2.12	0.66
1:D:121:ILE:HG21	1:D:217:LYS:O	1.93	0.66
1:A:161:ILE:HG12	1:A:162:VAL:N	2.09	0.66
1:D:58:THR:O	1:D:59:VAL:HG13	1.95	0.66
1:A:109:VAL:CG2	1:A:153:LEU:HD11	2.25	0.66
1:C:153:LEU:HA	1:C:157:GLU:OE2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:SER:HA	1:C:185:LEU:HD12	1.76	0.66
1:D:63:PRO:C	1:D:66:ILE:HG13	2.16	0.66
1:D:26:GLY:O	1:D:30:THR:HG22	1.95	0.66
1:A:146:LEU:O	1:A:149:ALA:HB3	1.95	0.66
1:C:153:LEU:O	1:C:157:GLU:HG2	1.95	0.66
1:D:61:LEU:HD12	1:D:65:VAL:CG2	2.25	0.66
1:D:187:LEU:HD23	1:D:191:MET:HE1	1.78	0.66
1:A:234:PRO:HG2	1:A:235:GLU:OE2	1.94	0.66
1:B:143:ILE:O	1:B:146:LEU:HD21	1.95	0.66
1:E:240:MET:O	1:E:241:ALA:C	2.34	0.66
1:A:65:VAL:O	1:A:66:ILE:HG13	1.96	0.66
1:A:141:PRO:HD3	1:E:230:LEU:HD21	1.77	0.66
1:C:189:GLN:O	1:C:192:THR:O	2.13	0.66
1:B:179:HIS:NE2	1:B:183:LEU:HD11	2.11	0.66
1:B:187:LEU:HB3	1:B:191:MET:HE1	1.78	0.66
1:E:121:ILE:CG2	1:E:217:LYS:HB2	2.22	0.66
1:B:189:GLN:O	1:B:192:THR:O	2.13	0.65
1:C:126:LEU:HG	1:C:133:ILE:CD1	2.25	0.65
1:A:149:ALA:O	1:A:153:LEU:HD12	1.95	0.65
1:A:42:MET:CE	1:A:81:ILE:HG22	2.26	0.65
1:A:99:GLU:HA	1:A:99:GLU:OE1	1.95	0.65
1:D:127:LYS:HA	1:D:133:ILE:HD11	1.76	0.65
1:E:118:MET:O	1:E:121:ILE:HG12	1.95	0.65
1:B:126:LEU:HG	1:B:133:ILE:CD1	2.23	0.65
1:B:61:LEU:HD13	1:B:63:PRO:HB3	1.78	0.65
1:E:67:SER:OG	1:E:68:TRP:HZ3	1.79	0.65
1:E:143:ILE:HD11	1:E:167:MET:O	1.96	0.65
1:E:48:PHE:HD2	1:E:49:VAL:HG23	1.60	0.65
1:C:36:PHE:O	1:C:40:ILE:HB	1.96	0.65
1:C:229:TYR:HA	1:C:233:LYS:HB3	1.79	0.65
1:D:65:VAL:CG2	1:D:68:TRP:HB2	2.26	0.65
1:D:187:LEU:CB	1:D:191:MET:HE1	2.26	0.65
1:E:79:ILE:O	1:E:83:PHE:N	2.24	0.65
1:E:107:GLY:HA3	1:E:162:VAL:HG22	1.79	0.65
1:D:23:PHE:O	1:D:24:ILE:C	2.29	0.65
1:B:182:SER:HA	1:B:185:LEU:CD1	2.27	0.65
1:A:190:LEU:HD23	1:B:151:LYS:HD2	1.77	0.65
1:B:228:TYR:O	1:B:232:PHE:HD1	1.80	0.65
1:B:123:ILE:HD12	1:B:135:ILE:HG21	1.79	0.64
1:B:243:LYS:HG3	1:B:254:PRO:HG3	1.78	0.64
1:E:72:LEU:O	1:E:75:LEU:HG	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ILE:O	1:B:90:LYS:HG3	1.98	0.64
1:B:99:GLU:O	1:B:100:LYS:HG2	1.96	0.64
1:C:102:MET:O	1:C:232:PHE:CE1	2.50	0.64
1:E:149:ALA:O	1:E:152:LYS:N	2.31	0.64
1:D:107:GLY:O	1:D:162:VAL:HG22	1.97	0.64
1:A:25:MET:HG3	1:E:86:PHE:CZ	2.32	0.64
1:A:30:THR:HG23	1:A:31:ALA:N	2.13	0.64
1:B:161:ILE:CG1	1:B:162:VAL:H	2.10	0.64
1:C:168:PRO:HG2	1:C:202:HIS:N	2.12	0.64
1:A:104:LYS:HB2	1:A:134:LYS:CG	2.28	0.64
1:A:107:GLY:C	1:A:108:ILE:HD12	2.18	0.64
1:C:121:ILE:HD11	1:C:217:LYS:NZ	2.12	0.64
1:A:101:LYS:HB3	1:A:101:LYS:NZ	2.13	0.64
2:B:301:BNG:H3'1	2:B:301:BNG:C7'	2.27	0.64
1:E:41:ILE:O	1:E:45:ILE:HB	1.98	0.64
1:A:236:TYR:O	1:A:240:MET:HG2	1.98	0.64
1:D:147:PRO:O	1:D:148:VAL:C	2.36	0.64
1:B:113:PHE:HD1	1:B:113:PHE:O	1.81	0.63
1:A:232:PHE:O	1:A:234:PRO:HD3	1.96	0.63
1:E:33:ILE:O	1:E:36:PHE:HB3	1.99	0.63
1:D:102:MET:HE1	1:D:231:LEU:HD23	1.78	0.63
1:D:189:GLN:O	1:D:192:THR:O	2.16	0.63
1:A:146:LEU:CG	1:A:147:PRO:HD3	2.28	0.63
1:C:150:CYS:CB	1:C:196:ILE:HD11	2.25	0.63
1:C:63:PRO:C	1:C:65:VAL:N	2.52	0.63
1:D:62:GLY:N	1:D:65:VAL:CG1	2.61	0.63
1:D:93:LEU:HD22	1:D:93:LEU:O	1.98	0.63
1:D:104:LYS:HA	1:D:104:LYS:HE3	1.79	0.63
1:B:153:LEU:O	1:B:157:GLU:CG	2.46	0.63
1:B:59:VAL:C	1:B:60:GLU:HG3	2.18	0.63
1:B:184:GLY:HA2	1:B:187:LEU:HD13	1.81	0.63
1:C:164:ALA:CB	1:C:198:GLU:HA	2.29	0.63
1:D:227:VAL:HG12	1:D:231:LEU:HD12	1.81	0.63
1:E:15:LYS:HB3	1:E:18:PRO:HG2	1.79	0.63
1:A:15:LYS:O	1:A:18:PRO:HD2	1.99	0.63
1:B:88:ILE:HD13	1:B:88:ILE:O	1.99	0.63
1:E:98:VAL:CG2	1:E:101:LYS:HZ3	2.12	0.63
1:B:183:LEU:O	1:B:187:LEU:HD12	1.99	0.62
1:E:69:GLY:HA2	1:E:72:LEU:CD1	2.28	0.62
1:A:87:ILE:HG22	1:A:91:LYS:CE	2.27	0.62
1:A:165:LEU:HD23	1:A:199:VAL:HG11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HG13	1:B:217:LYS:CB	2.29	0.62
1:C:46:THR:H	1:C:47:PRO:HD2	1.65	0.62
1:A:17:ILE:HD12	1:A:17:ILE:H	1.63	0.62
1:A:123:ILE:HG23	1:A:135:ILE:HD13	1.82	0.62
1:A:183:LEU:O	1:A:187:LEU:HD12	1.99	0.62
1:B:121:ILE:HG13	1:B:217:LYS:HB2	1.81	0.62
1:D:150:CYS:HA	1:D:153:LEU:HD13	1.82	0.62
1:E:98:VAL:HG22	1:E:101:LYS:HZ3	1.63	0.62
1:A:41:ILE:O	1:A:44:ILE:HG23	2.00	0.62
1:A:189:GLN:HB3	1:B:148:VAL:HG13	1.81	0.62
1:D:195:HIS:HE1	1:E:149:ALA:HB2	1.65	0.62
1:E:225:GLU:HG2	1:E:229:TYR:CE2	2.34	0.62
1:C:107:GLY:HA2	1:C:136:ILE:H	1.64	0.62
1:A:90:LYS:HE2	1:C:7:PHE:CD1	2.35	0.61
1:C:7:PHE:CZ	1:C:11:LEU:HD11	2.34	0.61
1:D:63:PRO:C	1:D:66:ILE:H	2.02	0.61
1:D:234:PRO:HG2	1:D:235:GLU:H	1.65	0.61
1:D:237:LEU:HD12	1:D:237:LEU:H	1.65	0.61
1:C:134:LYS:HD2	1:C:134:LYS:N	2.08	0.61
1:B:126:LEU:HD23	1:B:135:ILE:CD1	2.29	0.61
1:D:231:LEU:HD22	1:D:232:PHE:CZ	2.35	0.61
1:C:7:PHE:CE1	1:C:11:LEU:HG	2.36	0.61
1:C:113:PHE:HB2	1:C:142:GLY:HA2	1.82	0.61
1:B:115:ARG:O	1:B:116:VAL:HG23	2.00	0.61
1:C:113:PHE:HB2	1:C:141:PRO:O	2.00	0.61
1:E:76:VAL:O	1:E:80:ILE:HG13	2.01	0.61
1:D:233:LYS:HE2	1:D:236:TYR:HB2	1.83	0.61
1:B:148:VAL:O	1:B:152:LYS:HG3	2.01	0.61
1:B:199:VAL:O	1:B:201:VAL:HG13	2.01	0.61
1:D:37:VAL:CG2	1:D:88:ILE:HG13	2.30	0.61
1:A:7:PHE:CE2	1:D:90:LYS:HB2	2.35	0.61
1:A:30:THR:HG23	1:A:31:ALA:H	1.65	0.61
1:C:125:LYS:O	1:C:129:LEU:HD13	1.99	0.61
1:C:154:LEU:HD21	1:C:162:VAL:HB	1.83	0.61
1:C:162:VAL:CG1	1:C:163:MET:N	2.62	0.61
1:E:107:GLY:O	1:E:108:ILE:HD12	2.01	0.61
1:A:100:LYS:HE2	1:B:12:TYR:CG	2.36	0.61
1:B:137:ARG:O	1:B:138:LYS:HB2	2.00	0.61
1:B:190:LEU:O	1:C:151:LYS:HE3	2.01	0.61
1:C:66:ILE:CG1	1:C:68:TRP:HD1	2.13	0.61
1:C:213:ASP:O	1:C:217:LYS:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:THR:OG1	1:C:114:ALA:HB2	2.01	0.60
1:C:201:VAL:HG23	1:C:201:VAL:O	2.00	0.60
1:B:144:LYS:O	1:B:147:PRO:HD2	2.01	0.60
1:C:66:ILE:CG1	1:C:68:TRP:CD1	2.76	0.60
1:D:154:LEU:HD11	1:D:196:ILE:HG13	1.82	0.60
1:D:23:PHE:C	1:D:26:GLY:H	2.05	0.60
1:D:88:ILE:HD13	1:D:88:ILE:O	2.00	0.60
1:A:197:ILE:N	1:A:197:ILE:CD1	2.65	0.60
1:B:23:PHE:CE2	2:B:301:BNG:H3	2.36	0.60
1:D:77:ASN:HA	1:D:80:ILE:HD12	1.83	0.60
1:D:108:ILE:HD11	1:D:163:MET:HG3	1.83	0.60
1:A:226:ASN:HA	1:A:229:TYR:HD2	1.66	0.60
1:D:229:TYR:CB	1:D:237:LEU:HD11	2.32	0.60
1:A:111:THR:HG21	1:A:114:ALA:CB	2.32	0.60
1:C:102:MET:O	1:C:232:PHE:HE1	1.84	0.60
1:D:103:THR:C	1:D:104:LYS:HD2	2.22	0.60
1:D:111:THR:HG21	1:D:166:GLY:HA2	1.84	0.60
1:C:93:LEU:O	1:C:96:GLU:HB3	2.02	0.60
1:D:194:LYS:H	1:E:148:VAL:HG11	1.67	0.60
1:B:78:PHE:CE1	1:C:32:LEU:HA	2.37	0.60
1:C:178:ALA:HA	1:C:200:PHE:HE2	1.66	0.60
1:B:193:ASN:O	1:B:194:LYS:CD	2.35	0.60
1:C:109:VAL:O	1:C:165:LEU:HB2	2.01	0.60
1:D:61:LEU:HB3	1:D:65:VAL:CB	2.31	0.60
1:D:81:ILE:O	1:D:85:VAL:HG23	2.01	0.60
1:B:182:SER:CA	1:B:185:LEU:HD12	2.32	0.59
1:D:79:ILE:HG12	1:D:83:PHE:CE2	2.37	0.59
1:D:110:ASP:O	1:D:139:THR:HG23	2.01	0.59
1:D:159:CYS:O	1:D:161:ILE:N	2.34	0.59
1:A:148:VAL:CG2	1:E:189:GLN:HB3	2.31	0.59
1:D:223:HIS:C	1:D:225:GLU:N	2.51	0.59
1:E:98:VAL:HA	1:E:101:LYS:NZ	2.14	0.59
1:B:177:CYS:O	1:B:180:GLU:HB2	2.02	0.59
1:D:121:ILE:HG21	1:D:217:LYS:HB2	1.84	0.59
1:A:39:ASN:HB3	1:E:71:PHE:CD2	2.38	0.59
1:B:153:LEU:HA	1:B:157:GLU:OE2	2.03	0.59
1:A:100:LYS:O	1:A:102:MET:O	2.20	0.59
1:B:226:ASN:HA	1:B:229:TYR:HD2	1.68	0.59
1:D:111:THR:HG22	1:D:165:LEU:O	2.02	0.59
1:D:127:LYS:CA	1:D:133:ILE:HD11	2.32	0.59
1:E:68:TRP:N	1:E:68:TRP:CE3	2.69	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:HG13	1:A:41:ILE:H	1.67	0.59
1:C:161:ILE:HG13	1:C:195:HIS:O	2.02	0.59
1:D:65:VAL:HA	1:D:68:TRP:HD1	1.68	0.59
1:D:125:LYS:HG2	1:D:221:GLU:HG3	1.85	0.59
1:E:98:VAL:HA	1:E:101:LYS:CD	2.30	0.59
1:A:104:LYS:O	1:A:105:LYS:HB2	2.02	0.59
1:A:109:VAL:HG21	1:A:153:LEU:CD1	2.33	0.59
1:B:146:LEU:HD23	1:B:146:LEU:N	2.14	0.59
1:C:46:THR:N	1:C:47:PRO:HD2	2.18	0.59
1:E:186:MET:O	1:E:190:LEU:HD12	2.02	0.59
1:A:36:PHE:O	1:A:40:ILE:CG1	2.45	0.59
1:B:176:VAL:O	1:B:180:GLU:HG3	2.03	0.59
1:D:11:LEU:O	1:D:15:LYS:HA	2.03	0.59
1:D:64:ILE:HG12	1:E:44:ILE:HD12	1.85	0.59
1:D:183:LEU:O	1:D:187:LEU:CD1	2.51	0.58
1:D:151:LYS:O	1:D:155:GLU:N	2.33	0.58
1:A:148:VAL:O	1:A:151:LYS:HB3	2.02	0.58
1:A:163:MET:HE3	1:A:223:HIS:HB2	1.85	0.58
1:B:111:THR:OG1	1:B:112:THR:N	2.34	0.58
1:B:184:GLY:O	1:B:185:LEU:C	2.42	0.58
1:C:214:TRP:HE1	1:C:218:ARG:HD2	1.68	0.58
1:E:75:LEU:O	1:E:79:ILE:HG13	2.03	0.58
1:A:41:ILE:HG13	1:A:88:ILE:HG21	1.84	0.58
1:B:23:PHE:CZ	2:B:301:BNG:H3	2.39	0.58
1:B:153:LEU:HA	1:B:157:GLU:CD	2.23	0.58
1:C:107:GLY:C	1:C:108:ILE:HD12	2.22	0.58
1:D:223:HIS:O	1:D:227:VAL:HG23	2.04	0.58
1:A:98:VAL:O	1:A:99:GLU:HB2	2.03	0.58
1:B:121:ILE:CG1	1:B:217:LYS:HZ2	2.15	0.58
1:C:223:HIS:CE1	1:C:247:GLN:CB	2.86	0.58
1:D:25:MET:HG2	1:D:29:SER:HB3	1.83	0.58
1:D:25:MET:HG2	1:E:16:VAL:HG13	1.85	0.58
1:E:185:LEU:O	1:E:189:GLN:HG3	2.04	0.58
1:D:166:GLY:O	1:D:201:VAL:HG22	2.03	0.58
1:A:98:VAL:O	1:A:98:VAL:CG2	2.52	0.58
1:A:165:LEU:CA	1:A:199:VAL:HB	2.33	0.58
1:A:186:MET:CE	1:B:180:GLU:HB3	2.34	0.58
1:B:165:LEU:CD2	1:B:199:VAL:HG11	2.28	0.58
1:E:168:PRO:HD2	1:E:201:VAL:C	2.24	0.58
1:B:134:LYS:H	1:B:134:LYS:HD2	1.69	0.58
1:E:88:ILE:HD13	1:E:88:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:O	1:C:79:ILE:HG13	2.03	0.58
1:D:65:VAL:O	1:D:68:TRP:N	2.37	0.58
1:A:17:ILE:HB	1:A:18:PRO:HD3	1.86	0.57
1:A:107:GLY:O	1:A:162:VAL:HG22	2.04	0.57
1:A:111:THR:OG1	1:A:114:ALA:N	2.34	0.57
1:B:111:THR:O	1:B:139:THR:HG21	2.03	0.57
1:B:122:ALA:CB	1:B:224:ALA:HB2	2.27	0.57
1:C:41:ILE:O	1:C:45:ILE:HB	2.04	0.57
1:D:37:VAL:O	1:D:40:ILE:O	2.21	0.57
1:D:105:LYS:CE	1:D:158:GLY:HA3	2.34	0.57
1:A:213:ASP:O	1:A:217:LYS:HG2	2.04	0.57
1:A:164:ALA:O	1:A:165:LEU:C	2.43	0.57
1:A:242:GLY:O	1:A:243:LYS:CB	2.52	0.57
1:C:86:PHE:CD1	1:E:7:PHE:HZ	2.22	0.57
1:D:111:THR:HG21	1:D:166:GLY:CA	2.35	0.57
1:E:46:THR:C	1:E:48:PHE:H	2.08	0.57
1:B:189:GLN:HG2	1:B:196:ILE:HB	1.84	0.57
1:B:233:LYS:HE2	1:B:236:TYR:HB2	1.86	0.57
1:C:17:ILE:HD12	1:C:17:ILE:N	2.13	0.57
1:C:161:ILE:HD11	1:C:197:ILE:CG1	2.34	0.57
1:D:227:VAL:HG12	1:D:231:LEU:CD1	2.35	0.57
1:A:164:ALA:HB3	1:A:199:VAL:H	1.69	0.57
1:A:224:ALA:O	1:A:227:VAL:HB	2.05	0.57
1:C:110:ASP:O	1:C:139:THR:CG2	2.51	0.57
1:A:32:LEU:HD13	1:A:32:LEU:C	2.24	0.57
1:A:119:ALA:HA	1:A:165:LEU:CD1	2.35	0.57
1:C:163:MET:CE	1:C:199:VAL:HG21	2.35	0.57
1:D:105:LYS:HE2	1:D:158:GLY:HA3	1.87	0.57
1:A:146:LEU:H	1:A:146:LEU:CD2	2.13	0.57
1:A:202:HIS:N	1:A:205:GLU:OE2	2.35	0.57
1:C:42:MET:H	1:C:43:PRO:HD2	1.69	0.57
1:D:71:PHE:CE2	1:E:40:ILE:HD12	2.27	0.57
1:E:223:HIS:O	1:E:224:ALA:C	2.42	0.57
1:A:42:MET:HE3	1:A:81:ILE:HG22	1.86	0.57
1:A:206:ALA:HA	1:A:211:GLU:OE2	2.05	0.57
1:D:206:ALA:HA	1:D:211:GLU:OE2	2.05	0.57
1:A:105:LYS:HA	1:A:134:LYS:O	2.05	0.57
1:B:121:ILE:HD11	1:B:217:LYS:HZ2	1.70	0.57
1:C:123:ILE:HD12	1:C:135:ILE:HG21	1.86	0.57
1:D:63:PRO:CD	1:D:64:ILE:H	2.17	0.57
1:D:164:ALA:HB3	1:D:198:GLU:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PHE:HE1	1:A:11:LEU:HD21	1.70	0.57
1:A:143:ILE:HA	1:A:146:LEU:HD21	1.85	0.57
1:B:145:ASP:O	1:B:148:VAL:HG22	2.05	0.57
1:B:182:SER:N	1:B:185:LEU:HD12	2.20	0.57
1:C:113:PHE:HD1	1:C:113:PHE:O	1.88	0.57
1:C:213:ASP:OD1	1:C:217:LYS:HD2	2.05	0.57
1:B:187:LEU:O	1:B:190:LEU:N	2.37	0.56
1:C:42:MET:O	1:C:47:PRO:HD3	2.05	0.56
1:C:126:LEU:C	1:C:133:ILE:HD11	2.25	0.56
1:D:148:VAL:O	1:D:152:LYS:HG3	2.04	0.56
1:A:100:LYS:O	1:A:100:LYS:HG2	2.05	0.56
1:C:139:THR:HG22	1:C:140:VAL:N	2.21	0.56
1:C:154:LEU:HD11	1:C:196:ILE:CG1	2.32	0.56
1:C:164:ALA:HB3	1:C:199:VAL:N	2.17	0.56
1:E:182:SER:HA	1:E:185:LEU:CD1	2.26	0.56
1:C:107:GLY:HA2	1:C:136:ILE:O	2.04	0.56
1:B:161:ILE:CG1	1:B:162:VAL:N	2.67	0.56
1:D:126:LEU:HG	1:D:133:ILE:HD13	1.85	0.56
1:D:162:VAL:CG1	1:D:163:MET:N	2.67	0.56
1:E:83:PHE:O	1:E:87:ILE:HG12	2.05	0.56
1:E:125:LYS:O	1:E:125:LYS:HG3	2.05	0.56
1:C:129:LEU:HD23	1:C:228:TYR:CD2	2.39	0.56
1:D:78:PHE:HE2	1:E:35:SER:CB	2.19	0.56
1:D:154:LEU:HD11	1:D:196:ILE:CG1	2.36	0.56
1:D:194:LYS:H	1:E:148:VAL:CG1	2.19	0.56
1:B:98:VAL:O	1:B:98:VAL:HG12	2.05	0.56
1:B:105:LYS:HE3	1:B:158:GLY:HA3	1.86	0.56
1:B:151:LYS:O	1:B:155:GLU:HG3	2.05	0.56
1:B:161:ILE:HG21	1:B:231:LEU:HD11	1.87	0.56
1:C:123:ILE:CD1	1:C:135:ILE:HG21	2.36	0.56
1:A:240:MET:HE2	1:A:244:GLY:C	2.26	0.56
1:C:87:ILE:CG2	1:C:91:LYS:HE2	2.24	0.56
1:C:163:MET:HE2	1:C:199:VAL:HG21	1.88	0.56
1:C:234:PRO:HG2	1:C:235:GLU:H	1.71	0.56
1:E:217:LYS:HB3	1:E:217:LYS:HZ2	1.70	0.56
1:C:210:LYS:O	1:C:213:ASP:HB3	2.06	0.55
1:C:218:ARG:O	1:C:222:GLU:HG3	2.06	0.55
1:D:143:ILE:O	1:D:146:LEU:HD21	2.06	0.55
1:D:202:HIS:N	1:D:205:GLU:OE2	2.39	0.55
1:E:110:ASP:O	1:E:139:THR:CG2	2.53	0.55
1:B:125:LYS:CB	1:B:221:GLU:HG3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:THR:H	1:C:47:PRO:CD	2.19	0.55
1:C:230:LEU:HD11	1:D:141:PRO:HD3	1.88	0.55
1:B:86:PHE:O	1:D:7:PHE:HZ	1.89	0.55
1:B:125:LYS:CE	1:B:129:LEU:HD11	2.34	0.55
1:E:123:ILE:HG23	1:E:135:ILE:HD13	1.87	0.55
1:B:106:VAL:HG12	1:B:108:ILE:HD11	1.89	0.55
1:B:176:VAL:HG12	1:B:180:GLU:OE2	2.07	0.55
1:B:185:LEU:O	1:B:188:ALA:CB	2.50	0.55
1:D:78:PHE:CE2	1:E:35:SER:CB	2.90	0.55
1:D:127:LYS:N	1:D:133:ILE:HD11	2.22	0.55
1:C:150:CYS:O	1:C:154:LEU:HG	2.07	0.55
1:D:78:PHE:CE2	1:E:35:SER:HB3	2.42	0.55
1:D:143:ILE:HA	1:D:146:LEU:HD21	1.88	0.55
1:D:161:ILE:HG12	1:D:162:VAL:N	2.22	0.55
1:E:27:ILE:HA	1:E:30:THR:HG22	1.88	0.55
1:E:98:VAL:O	1:E:101:LYS:HB2	2.06	0.55
1:B:222:GLU:OE1	1:B:247:GLN:HA	2.07	0.55
1:C:66:ILE:HG13	1:C:67:SER:N	2.13	0.55
1:D:125:LYS:O	1:D:129:LEU:HD13	2.06	0.55
1:A:112:THR:HB	1:A:141:PRO:CA	2.24	0.55
1:A:28:ALA:O	1:A:32:LEU:HB2	2.07	0.55
1:C:179:HIS:CD2	1:C:183:LEU:HD11	2.42	0.55
1:C:233:LYS:O	1:C:237:LEU:HD11	2.07	0.55
1:D:30:THR:OG1	1:E:24:ILE:HB	2.07	0.55
1:B:168:PRO:O	1:B:203:GLU:OE2	2.25	0.54
1:D:167:MET:SD	1:D:203:GLU:HG2	2.47	0.54
1:E:145:ASP:O	1:E:147:PRO:N	2.40	0.54
1:E:155:GLU:C	1:E:156:GLU:HG3	2.27	0.54
1:E:206:ALA:HA	1:E:211:GLU:OE2	2.07	0.54
1:E:223:HIS:O	1:E:226:ASN:N	2.40	0.54
1:A:229:TYR:HB2	1:A:237:LEU:HD11	1.88	0.54
1:D:37:VAL:HA	1:D:41:ILE:HB	1.89	0.54
1:E:156:GLU:O	1:E:157:GLU:CB	2.56	0.54
1:A:123:ILE:HG23	1:A:135:ILE:CD1	2.37	0.54
1:D:49:VAL:HG13	1:D:49:VAL:O	2.07	0.54
1:A:40:ILE:O	1:A:44:ILE:CG2	2.55	0.54
1:A:145:ASP:C	1:A:147:PRO:CD	2.75	0.54
1:B:21:ILE:O	1:B:24:ILE:HG22	2.07	0.54
1:B:129:LEU:HD12	1:B:129:LEU:N	2.23	0.54
1:B:217:LYS:O	1:B:220:ALA:N	2.40	0.54
1:B:232:PHE:CD1	1:B:232:PHE:N	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:ILE:HG22	1:E:144:LYS:HG3	1.89	0.54
1:C:121:ILE:HG21	1:C:220:ALA:HB3	1.89	0.54
1:D:164:ALA:H	1:D:199:VAL:HG23	1.72	0.54
1:D:227:VAL:O	1:D:231:LEU:HD12	2.08	0.54
1:E:179:HIS:O	1:E:183:LEU:HG	2.08	0.54
1:A:201:VAL:HG12	1:A:219:ARG:NH2	2.23	0.54
1:A:146:LEU:HG	1:A:147:PRO:CD	2.34	0.54
1:A:164:ALA:HB3	1:A:198:GLU:HA	1.89	0.54
1:B:15:LYS:O	1:B:18:PRO:HD2	2.07	0.54
1:E:234:PRO:O	1:E:237:LEU:HD12	2.07	0.54
1:B:33:ILE:O	1:B:36:PHE:HB3	2.07	0.54
1:C:78:PHE:CE2	1:D:32:LEU:HA	2.43	0.54
1:C:37:VAL:HG22	1:C:88:ILE:CG1	2.09	0.53
1:D:162:VAL:O	1:D:197:ILE:N	2.31	0.53
1:E:151:LYS:HZ2	1:E:155:GLU:CD	2.11	0.53
1:A:235:GLU:O	1:A:238:THR:HB	2.08	0.53
1:B:234:PRO:HG2	1:B:235:GLU:N	2.24	0.53
1:E:139:THR:HG22	1:E:140:VAL:N	2.23	0.53
1:A:118:MET:O	1:A:120:SER:N	2.42	0.53
1:B:224:ALA:O	1:B:227:VAL:HB	2.08	0.53
1:D:40:ILE:HG22	1:D:41:ILE:N	2.21	0.53
1:D:101:LYS:NZ	1:D:101:LYS:HB3	2.23	0.53
1:D:164:ALA:N	1:D:197:ILE:O	2.37	0.53
1:E:121:ILE:HG13	1:E:217:LYS:HB3	1.88	0.53
1:A:101:LYS:O	1:A:102:MET:C	2.44	0.53
1:A:165:LEU:HD23	1:A:199:VAL:CG2	2.31	0.53
1:B:87:ILE:HG22	1:B:91:LYS:HE2	1.89	0.53
1:C:87:ILE:O	1:C:91:LYS:HG3	2.08	0.53
1:C:179:HIS:CD2	1:C:183:LEU:HD21	2.43	0.53
1:D:103:THR:H	1:D:104:LYS:HD2	1.73	0.53
1:D:223:HIS:C	1:D:225:GLU:H	2.12	0.53
1:E:168:PRO:HD2	1:E:201:VAL:O	2.08	0.53
1:A:223:HIS:O	1:A:226:ASN:N	2.42	0.53
1:D:15:LYS:HB3	1:D:18:PRO:HG2	1.90	0.53
1:A:228:TYR:CE1	1:A:232:PHE:CE1	2.97	0.53
1:C:30:THR:HG23	1:C:31:ALA:N	2.24	0.53
1:C:149:ALA:O	1:C:153:LEU:HD13	2.05	0.53
1:C:187:LEU:CB	1:C:191:MET:HE1	2.39	0.53
1:C:233:LYS:CE	1:C:236:TYR:HB2	2.37	0.53
1:E:140:VAL:HB	1:E:141:PRO:HD2	1.90	0.53
1:B:169:GLY:HA2	1:B:203:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLY:O	1:A:30:THR:HG22	2.09	0.53
1:B:161:ILE:HD13	1:B:227:VAL:HG13	1.90	0.53
1:D:17:ILE:HG22	1:D:21:ILE:HD11	1.90	0.53
1:A:42:MET:HE1	1:A:81:ILE:CG2	2.39	0.53
1:A:165:LEU:CD2	1:A:199:VAL:HG11	2.39	0.53
1:C:78:PHE:CD2	1:D:35:SER:HB3	2.44	0.53
1:C:121:ILE:HG13	1:C:217:LYS:CB	2.39	0.53
1:A:40:ILE:CG1	1:A:41:ILE:N	2.67	0.52
1:B:121:ILE:CD1	1:B:217:LYS:HZ2	2.23	0.52
1:B:235:GLU:O	1:B:238:THR:HB	2.09	0.52
1:E:146:LEU:O	1:E:149:ALA:HB3	2.09	0.52
1:E:229:TYR:N	1:E:229:TYR:CD1	2.74	0.52
1:A:29:SER:O	1:A:32:LEU:HB3	2.10	0.52
1:A:98:VAL:O	1:A:99:GLU:CB	2.57	0.52
1:B:39:ASN:O	1:B:43:PRO:HD2	2.09	0.52
1:B:62:GLY:N	1:B:63:PRO:HA	2.24	0.52
1:A:118:MET:O	1:A:121:ILE:N	2.43	0.52
1:D:160:ASP:O	1:D:161:ILE:CG2	2.48	0.52
1:A:33:ILE:O	1:A:36:PHE:HB3	2.10	0.52
1:A:163:MET:CE	1:A:165:LEU:HD21	2.40	0.52
1:C:179:HIS:O	1:C:183:LEU:HG	2.08	0.52
1:E:170:LYS:O	1:E:174:ASP:HB2	2.10	0.52
1:C:122:ALA:CB	1:C:224:ALA:HB2	2.39	0.52
1:C:243:LYS:HD2	1:C:243:LYS:H	1.74	0.52
1:A:143:ILE:C	1:A:146:LEU:HD21	2.29	0.52
1:D:157:GLU:HG3	1:D:159:CYS:SG	2.50	0.52
1:D:161:ILE:CG1	1:D:162:VAL:N	2.73	0.52
1:E:108:ILE:CG2	1:E:165:LEU:HD12	2.39	0.52
1:A:47:PRO:HG2	1:A:49:VAL:O	2.10	0.52
1:A:153:LEU:HA	1:A:157:GLU:OE2	2.08	0.52
1:B:17:ILE:CD1	1:B:18:PRO:HD3	2.40	0.52
1:B:61:LEU:HD12	1:B:63:PRO:CB	2.39	0.52
1:D:222:GLU:C	1:D:225:GLU:HB3	2.29	0.52
1:A:129:LEU:CD2	1:A:228:TYR:HB3	2.37	0.52
1:A:161:ILE:HD13	1:A:231:LEU:HD11	1.92	0.52
1:A:161:ILE:HG21	1:A:231:LEU:HD11	1.90	0.52
1:C:19:LEU:HD13	1:C:23:PHE:HB2	1.92	0.52
1:C:226:ASN:O	1:C:230:LEU:HD12	2.10	0.52
1:D:108:ILE:HG23	1:D:165:LEU:HG	1.90	0.52
1:D:111:THR:CG2	1:D:166:GLY:HA2	2.39	0.52
1:D:123:ILE:HG23	1:D:135:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:HIS:O	1:D:183:LEU:HG	2.09	0.52
1:E:123:ILE:HD12	1:E:135:ILE:HG21	1.92	0.52
1:A:42:MET:O	1:A:44:ILE:N	2.43	0.52
1:A:186:MET:HE1	1:B:180:GLU:HB3	1.92	0.52
1:D:133:ILE:O	1:D:133:ILE:HG13	2.10	0.52
1:D:153:LEU:O	1:D:157:GLU:HG2	2.10	0.52
1:E:37:VAL:HG12	1:E:81:ILE:HG13	1.89	0.52
1:B:119:ALA:O	1:B:123:ILE:CG1	2.51	0.51
1:C:196:ILE:HG22	1:C:196:ILE:O	2.10	0.51
1:D:179:HIS:CD2	1:D:183:LEU:HD21	2.45	0.51
1:E:107:GLY:CA	1:E:162:VAL:HG22	2.39	0.51
1:E:121:ILE:HG13	1:E:217:LYS:CB	2.40	0.51
1:A:39:ASN:HD21	1:E:68:TRP:HA	1.75	0.51
1:C:242:GLY:HA3	1:D:117:ASP:HB2	1.91	0.51
1:D:107:GLY:O	1:D:108:ILE:HD12	2.11	0.51
1:A:223:HIS:O	1:A:224:ALA:C	2.49	0.51
1:A:225:GLU:HG2	1:A:229:TYR:OH	2.10	0.51
1:B:77:ASN:HA	1:B:80:ILE:HD12	1.92	0.51
1:C:119:ALA:O	1:C:123:ILE:HG12	2.09	0.51
1:C:162:VAL:HG12	1:C:163:MET:N	2.24	0.51
1:D:109:VAL:O	1:D:165:LEU:HB2	2.10	0.51
1:D:161:ILE:HD11	1:D:197:ILE:CG1	2.41	0.51
1:E:68:TRP:C	1:E:72:LEU:HG	2.27	0.51
1:B:42:MET:CB	1:B:43:PRO:HD3	2.40	0.51
1:A:139:THR:CG2	1:A:140:VAL:H	2.21	0.51
1:B:206:ALA:HA	1:B:211:GLU:OE2	2.10	0.51
1:C:217:LYS:HZ2	1:C:217:LYS:HB3	1.73	0.51
1:E:111:THR:HA	1:E:140:VAL:O	2.11	0.51
1:A:7:PHE:HE1	1:A:11:LEU:CD2	2.23	0.51
1:D:156:GLU:O	1:D:157:GLU:HB3	2.10	0.51
1:D:164:ALA:O	1:D:199:VAL:CB	2.58	0.51
1:E:26:GLY:O	1:E:30:THR:N	2.43	0.51
1:E:161:ILE:CD1	1:E:227:VAL:HG13	2.35	0.51
1:E:235:GLU:HA	1:E:238:THR:HB	1.92	0.51
1:B:129:LEU:O	1:B:130:SER:HB2	2.11	0.51
1:C:44:ILE:HA	1:C:47:PRO:CG	2.41	0.51
1:E:67:SER:C	1:E:68:TRP:HE3	2.14	0.51
1:A:84:ALA:O	1:A:88:ILE:HG23	2.11	0.51
1:B:111:THR:OG1	1:B:114:ALA:HB2	2.11	0.51
1:D:123:ILE:CD1	1:D:135:ILE:HG21	2.41	0.51
1:C:122:ALA:HB1	1:C:224:ALA:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:LYS:C	1:E:18:PRO:HD2	2.31	0.51
1:B:143:ILE:C	1:B:146:LEU:HD21	2.31	0.51
1:C:245:LEU:O	1:C:247:GLN:OE1	2.28	0.51
1:E:49:VAL:C	1:E:51:GLY:N	2.64	0.51
1:E:67:SER:OG	1:E:68:TRP:CZ3	2.58	0.51
1:E:217:LYS:HB3	1:E:217:LYS:HZ3	1.73	0.51
1:C:134:LYS:H	1:C:134:LYS:CD	2.11	0.50
1:B:30:THR:HG23	1:B:31:ALA:N	2.27	0.50
1:B:107:GLY:HA2	1:B:136:ILE:H	1.74	0.50
1:C:227:VAL:O	1:C:231:LEU:HD13	2.12	0.50
1:D:162:VAL:HG12	1:D:163:MET:N	2.25	0.50
1:E:4:PHE:C	1:E:6:GLU:H	2.15	0.50
1:E:7:PHE:CE2	1:E:11:LEU:HD11	2.46	0.50
1:E:110:ASP:C	1:E:139:THR:HG23	2.30	0.50
1:A:240:MET:O	1:A:244:GLY:N	2.39	0.50
1:C:125:LYS:HD3	1:C:221:GLU:OE1	2.10	0.50
1:D:162:VAL:CG1	1:D:163:MET:H	2.24	0.50
1:E:106:VAL:HG11	1:E:126:LEU:CD2	2.41	0.50
1:A:19:LEU:HD13	1:A:19:LEU:O	2.12	0.50
1:B:163:MET:CE	1:B:165:LEU:HD21	2.41	0.50
1:D:70:ALA:O	1:D:74:GLU:HG2	2.12	0.50
1:D:235:GLU:HA	1:D:238:THR:OG1	2.12	0.50
1:E:123:ILE:HG23	1:E:135:ILE:HD12	1.91	0.50
1:E:168:PRO:HB2	1:E:202:HIS:HA	1.93	0.50
1:A:129:LEU:CD2	1:A:228:TYR:CB	2.76	0.50
1:B:78:PHE:C	1:B:78:PHE:CD1	2.84	0.50
1:B:214:TRP:O	1:B:215:LEU:C	2.50	0.50
1:B:217:LYS:O	1:B:218:ARG:C	2.49	0.50
1:C:30:THR:HG23	1:C:31:ALA:H	1.77	0.50
1:D:46:THR:H	1:D:47:PRO:HD3	1.74	0.50
1:A:95:GLU:OE1	1:A:95:GLU:HA	2.12	0.50
1:A:106:VAL:HG12	1:A:108:ILE:CD1	2.42	0.50
1:A:119:ALA:HA	1:A:165:LEU:HD13	1.93	0.50
1:A:182:SER:CA	1:A:185:LEU:HD12	2.29	0.50
1:B:121:ILE:HG13	1:B:217:LYS:HZ2	1.76	0.50
1:C:86:PHE:CE1	1:D:25:MET:SD	3.04	0.50
1:C:143:ILE:HG21	1:C:177:CYS:SG	2.51	0.50
1:E:188:ALA:O	1:E:191:MET:HB2	2.12	0.50
1:A:154:LEU:HD11	1:A:196:ILE:CD1	2.34	0.50
1:A:226:ASN:O	1:A:227:VAL:C	2.50	0.50
1:A:236:TYR:CZ	1:A:240:MET:SD	3.05	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ILE:O	1:C:24:ILE:HG22	2.12	0.50
1:C:95:GLU:O	1:C:97:LYS:HG3	2.12	0.50
1:D:74:GLU:HG3	1:E:39:ASN:ND2	2.27	0.50
1:E:127:LYS:HA	1:E:133:ILE:HD11	1.93	0.50
1:A:72:LEU:O	1:A:76:VAL:HG12	2.12	0.50
1:A:229:TYR:HB3	1:A:233:LYS:HB3	1.93	0.50
1:A:237:LEU:HA	1:A:240:MET:HB2	1.93	0.50
1:B:40:ILE:HG22	1:B:41:ILE:N	2.26	0.50
1:B:212:LEU:C	1:B:212:LEU:HD23	2.31	0.50
1:C:37:VAL:HG13	1:C:88:ILE:HB	1.94	0.50
1:C:108:ILE:N	1:C:136:ILE:O	2.45	0.50
1:C:233:LYS:HG2	1:C:236:TYR:HB3	1.92	0.50
1:C:164:ALA:N	1:C:197:ILE:O	2.41	0.50
1:E:5:SER:HA	1:E:8:LYS:HE2	1.93	0.50
1:E:99:GLU:CD	1:E:99:GLU:O	2.50	0.50
1:A:107:GLY:O	1:A:162:VAL:HA	2.11	0.49
1:A:164:ALA:H	1:A:199:VAL:HG23	1.76	0.49
1:B:33:ILE:HD11	1:B:88:ILE:HD12	1.93	0.49
1:D:28:ALA:O	1:D:32:LEU:HB2	2.11	0.49
1:D:121:ILE:HG13	1:D:217:LYS:CB	2.42	0.49
1:D:126:LEU:HD13	1:D:224:ALA:O	2.11	0.49
1:D:189:GLN:HB3	1:E:148:VAL:HG22	1.94	0.49
1:E:98:VAL:CA	1:E:101:LYS:HD2	2.37	0.49
1:E:143:ILE:HG22	1:E:144:LYS:N	2.27	0.49
1:C:233:LYS:HG2	1:C:236:TYR:CB	2.42	0.49
1:E:151:LYS:O	1:E:155:GLU:HG3	2.11	0.49
1:E:151:LYS:CE	1:E:191:MET:HB3	2.40	0.49
1:C:33:ILE:HG12	1:C:88:ILE:HD12	1.95	0.49
1:A:7:PHE:HD1	1:A:7:PHE:O	1.94	0.49
1:C:153:LEU:O	1:C:157:GLU:CG	2.60	0.49
1:B:125:LYS:HD3	1:B:221:GLU:OE1	2.12	0.49
1:B:168:PRO:HD2	1:B:202:HIS:HA	1.93	0.49
1:C:46:THR:N	1:C:47:PRO:CD	2.76	0.49
1:D:164:ALA:HB3	1:D:199:VAL:N	2.23	0.49
1:A:71:PHE:CD2	1:B:40:ILE:HA	2.47	0.49
1:A:165:LEU:CD2	1:A:199:VAL:HG21	2.35	0.49
1:A:219:ARG:O	1:A:222:GLU:N	2.45	0.49
1:A:233:LYS:CG	1:A:236:TYR:HB2	2.42	0.49
1:B:217:LYS:O	1:B:220:ALA:HB3	2.12	0.49
2:B:301:BNG:H6'2	1:D:23:PHE:HZ	1.76	0.49
1:D:227:VAL:O	1:D:231:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:GLU:O	1:E:99:GLU:N	2.42	0.49
1:A:118:MET:O	1:A:121:ILE:HG12	2.13	0.49
1:D:45:ILE:O	1:D:45:ILE:HG22	2.13	0.49
1:A:41:ILE:O	1:A:44:ILE:CG2	2.61	0.49
1:A:112:THR:OG1	1:A:140:VAL:O	2.27	0.49
1:B:79:ILE:HG22	1:B:83:PHE:HD2	1.78	0.49
1:B:246:ARG:HB2	1:B:252:ALA:H	1.77	0.49
1:D:48:PHE:O	1:D:49:VAL:HG12	2.13	0.49
1:E:79:ILE:O	1:E:83:PHE:CB	2.61	0.49
1:E:127:LYS:N	1:E:133:ILE:HD11	2.28	0.49
1:C:39:ASN:O	1:C:40:ILE:HD13	2.13	0.49
1:C:105:LYS:CE	1:C:158:GLY:HA3	2.40	0.49
1:D:170:LYS:O	1:D:171:ALA:HB3	2.13	0.49
1:E:119:ALA:HA	1:E:165:LEU:HD13	1.94	0.49
1:E:143:ILE:O	1:E:146:LEU:CD2	2.61	0.49
1:A:7:PHE:CE1	1:A:11:LEU:HD21	2.48	0.49
1:B:108:ILE:CD1	1:B:108:ILE:N	2.76	0.49
1:D:121:ILE:CG2	1:D:217:LYS:O	2.60	0.49
1:E:107:GLY:C	1:E:108:ILE:HD12	2.33	0.49
1:A:39:ASN:ND2	1:E:68:TRP:HA	2.28	0.48
1:A:225:GLU:HG2	1:A:229:TYR:CZ	2.48	0.48
1:C:63:PRO:C	1:C:65:VAL:H	2.05	0.48
1:C:89:ALA:O	1:C:92:VAL:HG12	2.12	0.48
1:C:115:ARG:NE	1:C:203:GLU:OE1	2.46	0.48
1:D:39:ASN:O	1:D:40:ILE:HD13	2.13	0.48
1:E:156:GLU:O	1:E:157:GLU:HB2	2.12	0.48
1:E:222:GLU:C	1:E:225:GLU:HB3	2.31	0.48
1:E:224:ALA:O	1:E:227:VAL:N	2.46	0.48
1:A:195:HIS:HE1	1:B:149:ALA:HB2	1.77	0.48
1:B:15:LYS:HB3	1:B:18:PRO:HG2	1.95	0.48
1:B:17:ILE:HD12	1:B:18:PRO:HD3	1.94	0.48
1:C:30:THR:O	1:C:33:ILE:HG22	2.13	0.48
1:D:78:PHE:CE2	1:E:35:SER:HB2	2.48	0.48
1:E:143:ILE:O	1:E:146:LEU:HG	2.14	0.48
1:A:104:LYS:O	1:A:105:LYS:CB	2.61	0.48
1:B:25:MET:HG2	1:C:16:VAL:HG11	1.94	0.48
1:B:75:LEU:HD12	1:B:75:LEU:C	2.33	0.48
1:C:65:VAL:HG13	1:C:66:ILE:N	2.29	0.48
1:D:161:ILE:O	1:D:162:VAL:CG2	2.61	0.48
1:D:176:VAL:HG12	1:D:180:GLU:OE2	2.13	0.48
1:A:7:PHE:O	1:A:10:PHE:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ASN:HA	1:C:229:TYR:CD2	2.48	0.48
1:D:25:MET:CG	1:E:16:VAL:CG1	2.91	0.48
1:A:146:LEU:N	1:A:147:PRO:CD	2.76	0.48
1:A:219:ARG:O	1:A:220:ALA:C	2.51	0.48
1:A:64:ILE:O	1:A:64:ILE:HG23	2.13	0.48
1:A:106:VAL:HG12	1:A:108:ILE:HD12	1.95	0.48
1:D:168:PRO:HD2	1:D:201:VAL:O	2.12	0.48
1:E:69:GLY:O	1:E:72:LEU:N	2.46	0.48
1:E:145:ASP:C	1:E:147:PRO:HD2	2.34	0.48
1:A:162:VAL:HG13	1:A:163:MET:N	2.29	0.48
1:B:36:PHE:O	1:B:40:ILE:CB	2.43	0.48
1:C:115:ARG:CG	1:C:167:MET:SD	2.92	0.48
1:D:203:GLU:C	1:D:205:GLU:H	2.17	0.48
1:E:36:PHE:C	1:E:40:ILE:HG13	2.32	0.48
1:A:67:SER:O	1:A:71:PHE:CG	2.61	0.48
1:A:240:MET:CE	1:A:244:GLY:C	2.82	0.48
1:C:193:ASN:O	1:C:194:LYS:HD2	2.14	0.48
1:E:94:GLN:O	1:E:98:VAL:HG23	2.14	0.48
1:E:111:THR:HG1	1:E:114:ALA:H	1.61	0.48
1:E:224:ALA:O	1:E:225:GLU:C	2.52	0.48
1:A:25:MET:HG3	1:E:86:PHE:CE1	2.48	0.48
1:A:237:LEU:HA	1:A:240:MET:CG	2.43	0.48
1:B:125:LYS:HE3	1:B:129:LEU:CD1	2.36	0.48
1:B:181:ALA:C	1:B:185:LEU:HD12	2.34	0.48
2:B:301:BNG:C7'	2:B:301:BNG:C3'	2.92	0.48
1:D:78:PHE:HE2	1:E:35:SER:HB3	1.78	0.48
1:A:39:ASN:ND2	1:E:71:PHE:CB	2.77	0.48
1:A:226:ASN:HD22	1:A:237:LEU:CD2	2.27	0.48
1:A:232:PHE:O	1:A:234:PRO:CD	2.60	0.48
1:C:32:LEU:HD13	1:C:33:ILE:N	2.29	0.48
1:D:25:MET:CG	1:D:29:SER:HB3	2.44	0.48
1:D:143:ILE:CA	1:D:146:LEU:HD21	2.44	0.48
1:D:149:ALA:O	1:D:153:LEU:CD1	2.52	0.48
1:A:11:LEU:HD11	1:D:86:PHE:HE1	1.77	0.47
1:A:227:VAL:O	1:A:231:LEU:CD1	2.56	0.47
1:B:108:ILE:O	1:B:137:ARG:HA	2.14	0.47
1:C:147:PRO:HA	1:C:150:CYS:SG	2.54	0.47
1:A:122:ALA:HB2	1:A:220:ALA:HB1	1.95	0.47
1:A:229:TYR:HA	1:A:233:LYS:CB	2.43	0.47
1:B:236:TYR:O	1:B:240:MET:HG2	2.13	0.47
1:C:119:ALA:HA	1:C:165:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:VAL:HG13	1:C:163:MET:H	1.79	0.47
1:C:214:TRP:O	1:C:215:LEU:C	2.53	0.47
1:D:234:PRO:O	1:D:237:LEU:HD12	2.13	0.47
1:E:224:ALA:O	1:E:227:VAL:HB	2.14	0.47
1:B:189:GLN:HB3	1:C:148:VAL:HG22	1.95	0.47
1:D:123:ILE:HG23	1:D:135:ILE:CD1	2.44	0.47
1:A:42:MET:C	1:A:44:ILE:N	2.66	0.47
1:A:81:ILE:O	1:A:85:VAL:HG23	2.14	0.47
1:A:146:LEU:N	1:A:147:PRO:HD2	2.29	0.47
1:A:151:LYS:HE3	1:E:190:LEU:O	2.14	0.47
1:B:26:GLY:O	1:B:30:THR:HG22	2.14	0.47
1:B:143:ILE:HA	1:B:146:LEU:HD21	1.95	0.47
1:C:179:HIS:NE2	1:C:183:LEU:HD11	2.30	0.47
1:D:25:MET:CG	1:E:16:VAL:HG11	2.44	0.47
1:A:226:ASN:HD22	1:A:237:LEU:HD21	1.79	0.47
1:B:154:LEU:HD21	1:B:162:VAL:HB	1.95	0.47
1:C:173:LYS:O	1:C:176:VAL:HG23	2.14	0.47
1:D:185:LEU:HD13	1:D:198:GLU:HG2	1.95	0.47
1:E:168:PRO:HD3	1:E:201:VAL:H	1.79	0.47
1:B:32:LEU:HD13	1:B:33:ILE:N	2.30	0.47
1:B:139:THR:CG2	1:B:140:VAL:H	2.20	0.47
1:C:15:LYS:HB3	1:C:18:PRO:HG2	1.96	0.47
1:C:234:PRO:CG	1:C:235:GLU:H	2.27	0.47
1:E:46:THR:C	1:E:48:PHE:N	2.67	0.47
1:E:140:VAL:CB	1:E:141:PRO:HD2	2.42	0.47
1:A:86:PHE:CE2	1:C:7:PHE:CE1	3.03	0.47
1:A:100:LYS:C	1:A:102:MET:N	2.65	0.47
1:A:111:THR:O	1:A:139:THR:CG2	2.62	0.47
1:A:149:ALA:C	1:A:153:LEU:HD12	2.34	0.47
1:A:153:LEU:O	1:A:157:GLU:CG	2.50	0.47
1:A:160:ASP:O	1:A:194:LYS:CG	2.59	0.47
1:B:104:LYS:HB3	1:B:105:LYS:H	1.53	0.47
1:B:134:LYS:H	1:B:134:LYS:CD	2.27	0.47
1:B:139:THR:CG2	1:B:140:VAL:N	2.77	0.47
1:B:143:ILE:O	1:B:146:LEU:CD2	2.62	0.47
1:C:107:GLY:O	1:C:108:ILE:HD12	2.14	0.47
1:D:94:GLN:O	1:D:98:VAL:CG2	2.59	0.47
1:E:107:GLY:HA3	1:E:162:VAL:CG2	2.45	0.47
1:E:112:THR:CB	1:E:141:PRO:HA	2.43	0.47
1:E:130:SER:O	1:E:133:ILE:HG12	2.14	0.47
1:E:228:TYR:CE1	1:E:232:PHE:CD2	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:PRO:HG2	1:E:235:GLU:CD	2.35	0.47
1:A:42:MET:C	1:A:44:ILE:H	2.17	0.47
1:A:181:ALA:O	1:A:182:SER:C	2.52	0.47
1:B:19:LEU:CD1	2:B:301:BNG:H61	2.45	0.47
1:C:153:LEU:HD12	1:C:153:LEU:H	1.80	0.47
1:C:162:VAL:CG1	1:C:163:MET:H	2.28	0.47
1:E:103:THR:O	1:E:104:LYS:HB2	2.14	0.47
1:A:14:TYR:HD2	1:A:16:VAL:CG2	2.28	0.47
1:A:189:GLN:HB3	1:B:148:VAL:CG1	2.45	0.47
1:A:229:TYR:CB	1:A:233:LYS:HB3	2.45	0.47
1:B:226:ASN:HA	1:B:229:TYR:CD2	2.48	0.47
1:C:202:HIS:N	1:C:205:GLU:OE2	2.48	0.47
1:B:125:LYS:O	1:B:129:LEU:CD1	2.58	0.47
1:C:146:LEU:O	1:C:150:CYS:SG	2.72	0.47
1:E:15:LYS:HD3	1:E:18:PRO:HG2	1.96	0.47
1:E:23:PHE:CD1	1:E:23:PHE:C	2.88	0.47
1:E:123:ILE:CD1	1:E:135:ILE:HG21	2.45	0.47
1:A:21:ILE:O	1:A:24:ILE:HG22	2.14	0.46
1:B:121:ILE:HG13	1:B:217:LYS:HB3	1.97	0.46
1:C:217:LYS:HB3	1:C:217:LYS:HZ3	1.80	0.46
1:C:243:LYS:N	1:C:243:LYS:CD	2.73	0.46
1:E:92:VAL:O	1:E:96:GLU:HG2	2.14	0.46
1:E:149:ALA:O	1:E:151:LYS:N	2.48	0.46
1:A:19:LEU:O	1:A:23:PHE:HB2	2.14	0.46
1:A:87:ILE:CG2	1:A:91:LYS:HE3	2.39	0.46
1:B:78:PHE:O	1:B:81:ILE:HG22	2.16	0.46
1:B:125:LYS:HB2	1:B:221:GLU:OE1	2.14	0.46
1:C:63:PRO:HB2	1:C:65:VAL:CA	2.44	0.46
1:C:120:SER:O	1:C:121:ILE:C	2.53	0.46
1:D:65:VAL:C	1:D:67:SER:N	2.67	0.46
1:D:150:CYS:HB2	1:D:196:ILE:CD1	2.42	0.46
1:E:44:ILE:O	1:E:44:ILE:HG13	2.15	0.46
1:A:71:PHE:O	1:A:75:LEU:CB	2.63	0.46
1:D:123:ILE:HD12	1:D:135:ILE:CD1	2.33	0.46
1:D:143:ILE:C	1:D:146:LEU:HD21	2.35	0.46
1:E:26:GLY:HA2	1:E:29:SER:OG	2.16	0.46
1:E:111:THR:OG1	1:E:112:THR:N	2.45	0.46
1:E:126:LEU:O	1:E:133:ILE:HD13	2.15	0.46
1:E:147:PRO:C	1:E:149:ALA:N	2.69	0.46
1:A:226:ASN:O	1:A:230:LEU:N	2.43	0.46
1:A:227:VAL:C	1:A:231:LEU:HD13	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:HB	1:B:141:PRO:CD	2.44	0.46
1:C:104:LYS:N	1:C:104:LYS:CD	2.77	0.46
1:D:151:LYS:HG2	1:D:155:GLU:OE2	2.15	0.46
1:A:56:THR:O	1:A:58:THR:N	2.49	0.46
1:B:110:ASP:OD1	1:B:138:LYS:O	2.34	0.46
1:C:168:PRO:HB2	1:C:202:HIS:HA	1.97	0.46
1:D:63:PRO:CA	1:D:66:ILE:HG23	2.40	0.46
1:D:150:CYS:HA	1:D:153:LEU:CD1	2.45	0.46
1:E:121:ILE:CD1	1:E:217:LYS:HZ2	2.28	0.46
1:A:183:LEU:O	1:A:187:LEU:CD1	2.64	0.46
1:A:225:GLU:HG2	1:A:229:TYR:CE2	2.50	0.46
1:B:19:LEU:HD11	2:B:301:BNG:H61	1.97	0.46
1:B:75:LEU:HD23	1:C:40:ILE:CG1	2.43	0.46
1:B:90:LYS:HB3	1:D:7:PHE:CZ	2.50	0.46
1:B:121:ILE:HG21	1:B:217:LYS:HB2	1.98	0.46
1:C:121:ILE:CD1	1:C:217:LYS:HZ2	2.25	0.46
1:D:158:GLY:O	1:D:159:CYS:C	2.53	0.46
1:E:40:ILE:HG22	1:E:41:ILE:N	2.30	0.46
1:E:98:VAL:CG1	1:E:101:LYS:HD2	2.41	0.46
1:E:151:LYS:NZ	1:E:155:GLU:CD	2.68	0.46
1:C:34:LYS:O	1:C:37:VAL:HG23	2.15	0.46
1:C:65:VAL:C	1:C:68:TRP:CD1	2.89	0.46
1:D:33:ILE:HD11	1:D:88:ILE:HD12	1.98	0.46
1:D:152:LYS:HB3	1:D:156:GLU:OE2	2.16	0.46
1:E:96:GLU:O	1:E:99:GLU:HB3	2.15	0.46
1:C:17:ILE:HB	1:C:18:PRO:HD3	1.98	0.46
1:C:168:PRO:HG2	1:C:201:VAL:C	2.36	0.46
1:D:64:ILE:CG1	1:E:44:ILE:HD12	2.44	0.46
1:E:26:GLY:O	1:E:30:THR:HG22	2.15	0.46
1:E:44:ILE:O	1:E:47:PRO:CD	2.60	0.46
1:E:160:ASP:OD2	1:E:194:LYS:HE3	2.15	0.46
1:A:118:MET:O	1:A:119:ALA:C	2.55	0.46
1:B:187:LEU:O	1:B:191:MET:N	2.40	0.46
1:C:16:VAL:HG12	1:C:16:VAL:O	2.15	0.46
1:C:161:ILE:HD13	1:C:227:VAL:HG13	1.97	0.46
1:C:233:LYS:O	1:C:237:LEU:CD1	2.64	0.46
1:D:193:ASN:ND2	1:E:155:GLU:OE2	2.47	0.46
1:A:127:LYS:HA	1:A:133:ILE:CD1	2.46	0.46
1:A:148:VAL:O	1:A:151:LYS:CB	2.64	0.46
1:B:108:ILE:N	1:B:108:ILE:HD12	2.30	0.46
1:B:111:THR:OG1	1:B:114:ALA:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:N	1:B:147:PRO:HD2	2.30	0.46
1:D:189:GLN:HB3	1:E:148:VAL:CG2	2.45	0.46
1:D:201:VAL:O	1:D:201:VAL:HG23	2.16	0.46
1:B:163:MET:HE2	1:B:165:LEU:HD21	1.98	0.45
1:B:234:PRO:CG	1:B:235:GLU:N	2.79	0.45
1:C:44:ILE:HA	1:C:47:PRO:HG3	1.98	0.45
1:C:152:LYS:O	1:C:156:GLU:N	2.39	0.45
1:E:127:LYS:CA	1:E:133:ILE:HD11	2.46	0.45
1:A:36:PHE:CZ	1:A:40:ILE:HD11	2.50	0.45
1:C:111:THR:HG23	1:C:114:ALA:HB2	1.95	0.45
1:D:122:ALA:HB2	1:D:220:ALA:O	2.16	0.45
1:E:93:LEU:HD22	1:E:93:LEU:HA	1.82	0.45
1:A:14:TYR:HD2	1:A:16:VAL:HG23	1.81	0.45
1:A:143:ILE:O	1:A:146:LEU:CD2	2.60	0.45
1:A:196:ILE:O	1:A:196:ILE:HG22	2.16	0.45
1:A:237:LEU:O	1:A:238:THR:C	2.53	0.45
1:B:112:THR:CB	1:B:140:VAL:O	2.63	0.45
1:B:239:ARG:O	1:B:240:MET:C	2.54	0.45
1:C:214:TRP:O	1:C:216:ALA:N	2.49	0.45
1:C:214:TRP:NE1	1:C:218:ARG:HD2	2.31	0.45
1:E:19:LEU:HD13	1:E:19:LEU:O	2.16	0.45
1:E:30:THR:HG23	1:E:31:ALA:N	2.31	0.45
1:E:44:ILE:C	1:E:46:THR:H	2.18	0.45
1:E:121:ILE:HD13	1:E:121:ILE:H	1.81	0.45
1:E:229:TYR:HB3	1:E:237:LEU:HD11	1.99	0.45
1:B:7:PHE:HE2	1:B:11:LEU:HD11	1.82	0.45
1:C:41:ILE:CG2	1:C:91:LYS:HE3	2.44	0.45
1:C:71:PHE:CZ	1:D:43:PRO:HG2	2.52	0.45
1:D:25:MET:HG2	1:E:16:VAL:HG11	1.97	0.45
1:D:179:HIS:HD2	1:D:183:LEU:HD21	1.80	0.45
1:A:42:MET:CE	1:A:81:ILE:CG2	2.90	0.45
1:A:130:SER:HA	1:A:131:PRO:HD3	1.70	0.45
1:B:58:THR:HG22	1:B:59:VAL:N	2.32	0.45
1:B:146:LEU:O	1:B:149:ALA:N	2.50	0.45
1:C:167:MET:HA	1:C:168:PRO:HD3	1.65	0.45
1:C:183:LEU:N	1:C:183:LEU:HD23	2.32	0.45
1:C:206:ALA:HA	1:C:211:GLU:OE2	2.15	0.45
1:D:129:LEU:HD23	1:D:228:TYR:CD2	2.51	0.45
1:E:183:LEU:N	1:E:183:LEU:HD23	2.31	0.45
1:E:228:TYR:O	1:E:231:LEU:HB2	2.16	0.45
1:A:109:VAL:CG2	1:A:153:LEU:CD1	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLU:O	1:A:225:GLU:CB	2.56	0.45
1:B:128:GLU:C	1:B:130:SER:N	2.70	0.45
1:E:126:LEU:HD13	1:E:224:ALA:HB1	1.99	0.45
1:A:39:ASN:CB	1:E:71:PHE:CD2	3.00	0.45
1:B:7:PHE:CE2	1:B:11:LEU:HG	2.52	0.45
1:D:61:LEU:CB	1:D:65:VAL:HG21	2.47	0.45
1:D:61:LEU:HB2	1:D:65:VAL:HG21	1.98	0.45
1:D:118:MET:SD	1:D:220:ALA:HB2	2.56	0.45
1:E:146:LEU:HD12	1:E:185:LEU:HD21	1.97	0.45
1:A:118:MET:HE2	1:A:166:GLY:O	2.16	0.45
1:A:229:TYR:CA	1:A:233:LYS:HB3	2.45	0.45
1:C:42:MET:N	1:C:43:PRO:HD2	2.29	0.45
1:A:30:THR:CG2	1:A:31:ALA:N	2.79	0.45
1:A:37:VAL:HG11	1:A:85:VAL:HG22	1.99	0.45
1:A:143:ILE:CA	1:A:146:LEU:HD21	2.47	0.45
1:B:106:VAL:CG1	1:B:108:ILE:HD11	2.47	0.45
1:B:229:TYR:HD1	1:B:233:LYS:HB3	1.81	0.45
1:C:161:ILE:O	1:C:162:VAL:CG2	2.58	0.45
1:C:207:LYS:H	1:C:211:GLU:CD	2.20	0.45
1:D:58:THR:C	1:D:59:VAL:HG22	2.36	0.45
1:E:145:ASP:O	1:E:146:LEU:C	2.56	0.45
1:E:146:LEU:CD1	1:E:185:LEU:HD21	2.47	0.45
1:B:189:GLN:NE2	1:C:145:ASP:OD1	2.50	0.45
1:B:244:GLY:N	1:B:254:PRO:HD3	2.32	0.45
1:C:214:TRP:C	1:C:216:ALA:N	2.69	0.45
1:B:162:VAL:HG13	1:B:163:MET:N	2.31	0.44
1:B:165:LEU:HD23	1:B:199:VAL:CG1	2.32	0.44
1:C:154:LEU:CD1	1:C:196:ILE:HG13	2.39	0.44
1:D:37:VAL:HG22	1:D:88:ILE:HG13	2.00	0.44
1:D:169:GLY:HA2	1:D:203:GLU:OE2	2.17	0.44
1:E:106:VAL:HG12	1:E:107:GLY:H	1.82	0.44
1:A:36:PHE:HD2	1:A:88:ILE:HD12	1.82	0.44
1:B:111:THR:HG1	1:B:114:ALA:H	1.61	0.44
1:C:102:MET:O	1:C:232:PHE:CD1	2.70	0.44
1:C:125:LYS:C	1:C:128:GLU:HB3	2.37	0.44
1:D:102:MET:HG2	1:D:231:LEU:O	2.17	0.44
1:D:152:LYS:O	1:D:156:GLU:N	2.50	0.44
1:E:46:THR:O	1:E:48:PHE:N	2.50	0.44
1:E:146:LEU:CG	1:E:147:PRO:HD3	2.47	0.44
1:E:156:GLU:O	1:E:157:GLU:CG	2.65	0.44
1:B:90:LYS:HA	1:B:93:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:C	1:D:65:VAL:HG11	2.38	0.44
1:D:158:GLY:O	1:D:160:ASP:N	2.50	0.44
1:D:167:MET:HA	1:D:168:PRO:HD3	1.59	0.44
1:D:226:ASN:HD22	1:D:229:TYR:HD2	1.64	0.44
1:E:111:THR:OG1	1:E:114:ALA:N	2.46	0.44
1:E:165:LEU:HD23	1:E:199:VAL:HG11	1.99	0.44
1:B:122:ALA:HB1	1:B:224:ALA:CB	2.33	0.44
1:D:21:ILE:C	1:D:24:ILE:HG22	2.33	0.44
1:D:30:THR:HG23	1:D:31:ALA:N	2.33	0.44
1:D:65:VAL:HA	1:D:68:TRP:CD1	2.49	0.44
1:D:157:GLU:O	1:D:159:CYS:N	2.50	0.44
1:B:106:VAL:CG1	1:B:108:ILE:CD1	2.93	0.44
1:B:110:ASP:OD1	1:B:110:ASP:N	2.49	0.44
1:B:112:THR:OG1	1:B:139:THR:HG22	2.15	0.44
1:B:145:ASP:O	1:B:148:VAL:CG2	2.65	0.44
1:B:212:LEU:O	1:B:213:ASP:C	2.56	0.44
1:D:110:ASP:N	1:D:110:ASP:OD1	2.50	0.44
1:E:111:THR:HG1	1:E:114:ALA:N	2.16	0.44
1:A:74:GLU:OE2	1:A:74:GLU:HA	2.18	0.44
1:A:111:THR:OG1	1:A:112:THR:N	2.51	0.44
1:A:196:ILE:O	1:A:197:ILE:C	2.54	0.44
1:B:112:THR:OG1	1:B:140:VAL:O	2.26	0.44
1:C:145:ASP:O	1:C:146:LEU:C	2.56	0.44
1:E:125:LYS:CG	1:E:221:GLU:HG3	2.47	0.44
1:A:66:ILE:HG22	1:A:67:SER:H	1.83	0.44
1:C:145:ASP:O	1:C:147:PRO:N	2.51	0.44
1:C:231:LEU:HD23	1:C:232:PHE:CZ	2.52	0.44
1:E:118:MET:HE1	1:E:199:VAL:HG12	2.00	0.44
1:B:75:LEU:O	1:B:79:ILE:HG13	2.17	0.44
1:B:146:LEU:C	1:B:150:CYS:SG	2.96	0.44
1:C:240:MET:O	1:C:241:ALA:O	2.36	0.44
1:E:167:MET:HA	1:E:168:PRO:HD3	1.89	0.44
1:B:59:VAL:O	1:B:60:GLU:HG3	2.17	0.44
1:C:7:PHE:CD1	1:C:7:PHE:C	2.91	0.44
1:C:7:PHE:C	1:C:9:GLU:H	2.21	0.44
1:C:130:SER:HA	1:C:131:PRO:HD3	1.83	0.44
1:C:182:SER:O	1:C:185:LEU:N	2.51	0.44
1:D:164:ALA:N	1:D:199:VAL:HG23	2.32	0.44
1:D:179:HIS:CD2	1:D:183:LEU:HD11	2.51	0.44
1:E:111:THR:HG23	1:E:114:ALA:HB2	1.96	0.44
1:E:126:LEU:C	1:E:133:ILE:HD11	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ALA:O	1:E:150:CYS:C	2.56	0.44
1:E:183:LEU:C	1:E:187:LEU:HD12	2.37	0.44
1:A:19:LEU:HD13	1:A:23:PHE:HB2	2.00	0.43
1:A:67:SER:HB3	1:A:71:PHE:HE2	1.83	0.43
1:A:106:VAL:HG11	1:A:126:LEU:HD21	2.00	0.43
1:A:165:LEU:H	1:A:165:LEU:HG	1.57	0.43
1:B:111:THR:O	1:B:139:THR:CG2	2.65	0.43
1:D:30:THR:HA	1:D:33:ILE:HG22	2.00	0.43
1:E:113:PHE:HB2	1:E:141:PRO:O	2.18	0.43
1:A:66:ILE:HG22	1:A:67:SER:N	2.33	0.43
1:A:186:MET:HB3	1:A:190:LEU:HD12	1.99	0.43
1:B:113:PHE:O	1:B:113:PHE:CD1	2.66	0.43
1:C:66:ILE:HG12	1:C:68:TRP:HE1	1.80	0.43
1:A:37:VAL:HG11	1:A:85:VAL:CG2	2.48	0.43
1:A:83:PHE:O	1:A:87:ILE:HG12	2.18	0.43
1:A:113:PHE:CD2	1:A:143:ILE:HG22	2.54	0.43
1:B:228:TYR:O	1:B:232:PHE:CD1	2.65	0.43
1:C:123:ILE:HD12	1:C:135:ILE:HD13	2.00	0.43
1:C:161:ILE:HD11	1:C:197:ILE:HG13	1.99	0.43
1:D:66:ILE:HD12	1:D:66:ILE:C	2.37	0.43
1:E:119:ALA:HA	1:E:165:LEU:CD1	2.48	0.43
1:B:199:VAL:O	1:B:199:VAL:HG12	2.17	0.43
1:C:65:VAL:C	1:C:66:ILE:HG23	2.37	0.43
1:C:118:MET:O	1:C:119:ALA:C	2.56	0.43
1:A:119:ALA:O	1:A:123:ILE:HG12	2.18	0.43
1:A:234:PRO:HD2	1:A:235:GLU:OE1	2.18	0.43
1:B:126:LEU:O	1:B:133:ILE:HD11	2.19	0.43
1:C:125:LYS:HE3	1:C:129:LEU:HD11	2.01	0.43
1:C:152:LYS:HB3	1:C:156:GLU:OE2	2.18	0.43
1:E:148:VAL:O	1:E:152:LYS:HG3	2.17	0.43
1:E:164:ALA:HB3	1:E:198:GLU:HA	2.00	0.43
1:E:171:ALA:C	1:E:173:LYS:H	2.22	0.43
1:A:187:LEU:O	1:A:191:MET:N	2.51	0.43
1:B:165:LEU:HD23	1:B:199:VAL:HG21	2.01	0.43
1:C:112:THR:HG22	1:C:112:THR:O	2.19	0.43
1:D:74:GLU:OE1	1:D:74:GLU:HA	2.19	0.43
1:D:83:PHE:O	1:D:87:ILE:HG12	2.18	0.43
1:D:165:LEU:CD2	1:D:199:VAL:HG21	2.48	0.43
1:D:212:LEU:C	1:D:212:LEU:HD23	2.39	0.43
1:E:23:PHE:CD1	1:E:24:ILE:N	2.87	0.43
1:E:113:PHE:O	1:E:113:PHE:HD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:LYS:HB2	1:E:221:GLU:OE1	2.18	0.43
1:B:182:SER:O	1:B:185:LEU:HB2	2.18	0.43
1:D:15:LYS:C	1:D:18:PRO:HD2	2.39	0.43
1:E:80:ILE:O	1:E:84:ALA:N	2.38	0.43
1:A:229:TYR:O	1:A:232:PHE:N	2.52	0.43
1:B:187:LEU:HA	1:B:190:LEU:HB2	2.00	0.43
1:B:193:ASN:HB3	1:C:152:LYS:HG2	2.01	0.43
1:C:113:PHE:CB	1:C:142:GLY:HA2	2.48	0.43
1:D:167:MET:CE	1:D:212:LEU:HD21	2.49	0.43
1:E:234:PRO:HG2	1:E:235:GLU:H	1.83	0.43
1:B:189:GLN:HB3	1:C:148:VAL:CG2	2.48	0.43
1:C:176:VAL:HG12	1:C:180:GLU:HG3	2.00	0.43
1:D:15:LYS:O	1:D:18:PRO:HD2	2.19	0.43
1:D:237:LEU:HA	1:D:240:MET:HB2	2.00	0.43
1:E:131:PRO:O	1:E:133:ILE:N	2.52	0.43
1:C:127:LYS:HA	1:C:133:ILE:HD11	2.00	0.43
1:D:120:SER:O	1:D:122:ALA:N	2.52	0.43
1:D:121:ILE:HG13	1:D:217:LYS:HB2	1.99	0.43
1:D:195:HIS:HA	1:E:148:VAL:HG21	2.01	0.43
1:A:118:MET:HE1	1:A:165:LEU:C	2.40	0.42
1:A:236:TYR:CE1	1:A:240:MET:SD	3.12	0.42
1:C:65:VAL:O	1:C:68:TRP:CD1	2.72	0.42
1:C:245:LEU:CD2	1:C:245:LEU:N	2.82	0.42
1:D:25:MET:O	1:D:29:SER:CA	2.67	0.42
1:D:39:ASN:O	1:D:40:ILE:HG12	2.19	0.42
1:D:125:LYS:CB	1:D:221:GLU:HG3	2.49	0.42
1:E:107:GLY:C	1:E:162:VAL:HG22	2.39	0.42
1:E:186:MET:O	1:E:190:LEU:CD1	2.66	0.42
1:A:149:ALA:O	1:A:150:CYS:C	2.56	0.42
1:B:60:GLU:HB2	1:B:61:LEU:H	1.05	0.42
1:B:146:LEU:O	1:B:150:CYS:SG	2.75	0.42
1:B:149:ALA:O	1:B:153:LEU:HD12	2.19	0.42
1:D:63:PRO:C	1:D:65:VAL:N	2.72	0.42
1:D:187:LEU:CD2	1:D:191:MET:HE1	2.48	0.42
1:E:78:PHE:HA	1:E:81:ILE:HG22	2.01	0.42
1:E:96:GLU:O	1:E:99:GLU:CB	2.68	0.42
1:E:125:LYS:NZ	1:E:129:LEU:HD11	2.34	0.42
1:A:163:MET:HE1	1:A:165:LEU:HD21	2.02	0.42
1:B:25:MET:SD	1:C:16:VAL:HG21	2.59	0.42
1:B:45:ILE:O	1:B:46:THR:C	2.58	0.42
1:B:229:TYR:CD1	1:B:233:LYS:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLY:HA2	1:B:252:ALA:O	2.18	0.42
1:C:111:THR:HG21	1:C:114:ALA:HB2	1.98	0.42
1:C:127:LYS:N	1:C:133:ILE:HD11	2.35	0.42
1:D:239:ARG:C	1:D:241:ALA:H	2.22	0.42
1:A:121:ILE:HG21	1:A:217:LYS:CB	2.47	0.42
1:D:21:ILE:HA	1:D:24:ILE:HG22	2.01	0.42
1:D:79:ILE:HG23	1:D:83:PHE:CE2	2.51	0.42
1:D:96:GLU:OE2	1:D:96:GLU:CA	2.67	0.42
1:A:71:PHE:O	1:A:75:LEU:N	2.41	0.42
1:B:198:GLU:OE1	1:C:144:LYS:HB3	2.18	0.42
1:C:26:GLY:O	1:C:30:THR:HG22	2.19	0.42
1:C:63:PRO:CG	1:C:65:VAL:HB	2.36	0.42
1:E:90:LYS:HZ3	1:E:91:LYS:CG	2.33	0.42
1:E:121:ILE:HD13	1:E:121:ILE:N	2.33	0.42
1:E:125:LYS:O	1:E:125:LYS:CG	2.67	0.42
1:A:189:GLN:HE21	1:A:196:ILE:N	2.17	0.42
1:A:229:TYR:HA	1:A:233:LYS:H	1.85	0.42
1:B:129:LEU:CD1	1:B:129:LEU:H	2.32	0.42
1:B:130:SER:HA	1:B:131:PRO:HD3	1.67	0.42
1:C:122:ALA:HB2	1:C:220:ALA:O	2.20	0.42
1:C:128:GLU:OE2	1:C:129:LEU:CD1	2.67	0.42
1:C:182:SER:O	1:C:183:LEU:C	2.58	0.42
1:D:151:LYS:O	1:D:152:LYS:C	2.58	0.42
1:D:164:ALA:CB	1:D:198:GLU:HA	2.48	0.42
1:E:147:PRO:O	1:E:149:ALA:N	2.53	0.42
1:E:187:LEU:O	1:E:188:ALA:C	2.57	0.42
1:A:108:ILE:O	1:A:108:ILE:HG22	2.19	0.42
1:A:186:MET:HE3	1:B:180:GLU:HB3	2.00	0.42
1:B:158:GLY:O	1:B:160:ASP:N	2.53	0.42
1:C:168:PRO:HG2	1:C:202:HIS:HA	2.01	0.42
1:D:42:MET:O	1:D:43:PRO:C	2.58	0.42
1:D:119:ALA:CB	1:D:137:ARG:NH2	2.83	0.42
1:E:222:GLU:O	1:E:226:ASN:OD1	2.37	0.42
1:A:19:LEU:HD13	1:A:19:LEU:C	2.40	0.42
1:A:165:LEU:HA	1:A:199:VAL:CB	2.48	0.42
1:B:190:LEU:HD23	1:C:151:LYS:HD2	2.01	0.42
1:E:90:LYS:O	1:E:94:GLN:HG3	2.19	0.42
1:E:118:MET:HB2	1:E:165:LEU:HD22	2.00	0.42
1:A:189:GLN:HE21	1:A:196:ILE:H	1.68	0.42
1:B:125:LYS:O	1:B:125:LYS:HG3	2.19	0.42
1:B:250:GLU:O	1:B:251:ASP:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:MET:O	1:C:44:ILE:N	2.47	0.42
1:D:63:PRO:CD	1:D:64:ILE:N	2.78	0.42
1:A:219:ARG:O	1:A:221:GLU:N	2.53	0.42
1:B:7:PHE:C	1:B:9:GLU:N	2.73	0.42
1:B:98:VAL:O	1:B:98:VAL:CG1	2.66	0.42
1:C:33:ILE:CG1	1:C:88:ILE:HD12	2.50	0.42
1:C:100:LYS:HA	1:C:100:LYS:HD3	1.71	0.42
1:D:122:ALA:CB	1:D:224:ALA:HB2	2.38	0.42
1:D:125:LYS:CG	1:D:221:GLU:HG3	2.48	0.42
1:D:189:GLN:O	1:D:192:THR:C	2.58	0.42
1:E:164:ALA:O	1:E:199:VAL:CB	2.60	0.42
1:A:88:ILE:CG1	1:A:89:ALA:N	2.82	0.41
1:A:229:TYR:O	1:A:233:LYS:N	2.53	0.41
1:B:144:LYS:O	1:B:147:PRO:HG2	2.20	0.41
1:D:65:VAL:O	1:D:69:GLY:N	2.41	0.41
1:D:121:ILE:HG21	1:D:217:LYS:C	2.40	0.41
1:E:120:SER:O	1:E:121:ILE:C	2.58	0.41
1:A:240:MET:CA	1:A:240:MET:CE	2.91	0.41
1:B:15:LYS:C	1:B:18:PRO:HD2	2.40	0.41
1:C:7:PHE:O	1:C:9:GLU:N	2.53	0.41
1:C:230:LEU:HD11	1:D:141:PRO:CD	2.49	0.41
1:D:25:MET:SD	1:E:16:VAL:CG1	3.00	0.41
1:D:221:GLU:O	1:D:223:HIS:N	2.53	0.41
1:A:30:THR:CG2	1:A:31:ALA:H	2.30	0.41
1:B:112:THR:OG1	1:B:139:THR:CG2	2.68	0.41
1:C:184:GLY:O	1:C:185:LEU:C	2.58	0.41
1:D:68:TRP:NE1	1:E:44:ILE:HG21	2.35	0.41
1:A:233:LYS:O	1:A:237:LEU:HD12	2.21	0.41
1:C:17:ILE:O	1:C:21:ILE:HG13	2.20	0.41
1:C:99:GLU:HG3	1:C:100:LYS:HG2	2.03	0.41
1:C:128:GLU:HG2	1:C:129:LEU:HD12	2.02	0.41
1:C:161:ILE:CG1	1:C:162:VAL:N	2.75	0.41
1:D:110:ASP:OD1	1:D:138:LYS:O	2.38	0.41
1:E:39:ASN:O	1:E:43:PRO:HG3	2.21	0.41
1:A:129:LEU:CD2	1:A:228:TYR:HB2	2.46	0.41
1:B:18:PRO:HB3	1:C:14:TYR:HE2	1.85	0.41
1:B:107:GLY:HA2	1:B:136:ILE:O	2.21	0.41
1:B:112:THR:HB	1:B:140:VAL:O	2.20	0.41
1:B:246:ARG:O	1:B:247:GLN:C	2.58	0.41
1:C:63:PRO:HB2	1:C:65:VAL:HA	2.03	0.41
1:C:126:LEU:C	1:C:128:GLU:N	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ASP:C	1:C:147:PRO:CD	2.87	0.41
1:D:11:LEU:O	1:D:15:LYS:CA	2.69	0.41
1:D:39:ASN:O	1:D:40:ILE:CD1	2.69	0.41
1:D:111:THR:CG2	1:D:166:GLY:CA	2.97	0.41
1:A:15:LYS:HA	1:A:17:ILE:HD12	2.03	0.41
1:A:72:LEU:O	1:A:76:VAL:N	2.44	0.41
1:A:140:VAL:HB	1:A:141:PRO:HD2	2.01	0.41
1:B:108:ILE:CG2	1:B:109:VAL:N	2.83	0.41
1:B:146:LEU:CG	1:B:147:PRO:HD3	2.48	0.41
1:C:85:VAL:HG11	1:D:28:ALA:CB	2.51	0.41
1:D:71:PHE:CD1	1:E:40:ILE:HG12	2.52	0.41
1:E:25:MET:O	1:E:29:SER:N	2.46	0.41
1:E:39:ASN:C	1:E:43:PRO:HG3	2.39	0.41
1:B:158:GLY:O	1:B:160:ASP:OD1	2.39	0.41
1:B:202:HIS:HB3	1:B:204:ASP:OD1	2.20	0.41
1:C:7:PHE:C	1:C:9:GLU:N	2.74	0.41
1:C:65:VAL:HG22	1:C:66:ILE:O	2.21	0.41
1:D:162:VAL:HG13	1:D:163:MET:H	1.85	0.41
1:E:109:VAL:O	1:E:165:LEU:HB2	2.19	0.41
1:E:150:CYS:HB3	1:E:196:ILE:CD1	2.51	0.41
1:E:225:GLU:HG2	1:E:229:TYR:CZ	2.56	0.41
1:A:106:VAL:CG1	1:A:108:ILE:HD11	2.50	0.41
1:B:149:ALA:O	1:B:152:LYS:N	2.54	0.41
1:B:244:GLY:HA2	1:B:253:GLY:C	2.41	0.41
1:C:19:LEU:HD13	1:C:19:LEU:O	2.20	0.41
1:C:71:PHE:HZ	1:D:43:PRO:HG2	1.84	0.41
1:C:93:LEU:HD13	1:C:93:LEU:C	2.41	0.41
1:E:108:ILE:HG23	1:E:165:LEU:CD1	2.47	0.41
1:E:233:LYS:O	1:E:233:LYS:HG2	2.21	0.41
1:A:7:PHE:CD1	1:A:11:LEU:HG	2.56	0.41
1:A:143:ILE:O	1:A:146:LEU:HD11	2.20	0.41
1:A:164:ALA:N	1:A:199:VAL:HG23	2.36	0.41
1:A:228:TYR:CE1	1:A:232:PHE:CD1	3.08	0.41
1:B:115:ARG:O	1:B:116:VAL:CG2	2.66	0.41
1:B:144:LYS:H	1:B:144:LYS:HG3	1.67	0.41
1:B:179:HIS:CD2	1:B:183:LEU:HD11	2.55	0.41
1:C:17:ILE:N	1:C:18:PRO:CD	2.84	0.41
1:C:32:LEU:HD13	1:C:32:LEU:C	2.41	0.41
1:C:86:PHE:HB3	1:E:7:PHE:CZ	2.56	0.41
1:C:94:GLN:OE1	1:C:94:GLN:HA	2.20	0.41
1:C:111:THR:OG1	1:C:112:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ASP:O	1:D:217:LYS:HG2	2.21	0.41
1:D:230:LEU:HD11	1:E:141:PRO:CD	2.50	0.41
1:E:146:LEU:CB	1:E:147:PRO:HD3	2.51	0.41
1:E:151:LYS:CG	1:E:155:GLU:OE2	2.64	0.41
1:A:17:ILE:N	1:A:18:PRO:CD	2.84	0.41
1:A:45:ILE:O	1:A:45:ILE:CG2	2.64	0.41
1:B:61:LEU:CD1	1:B:63:PRO:CB	2.91	0.41
1:B:165:LEU:HA	1:B:199:VAL:CB	2.42	0.41
1:B:229:TYR:CE1	1:B:233:LYS:HD3	2.56	0.41
1:B:237:LEU:HA	1:B:240:MET:CG	2.51	0.41
1:C:15:LYS:O	1:C:18:PRO:HD2	2.21	0.41
1:C:78:PHE:HE2	1:D:32:LEU:HA	1.86	0.41
1:C:168:PRO:HG2	1:C:202:HIS:CA	2.50	0.41
1:E:46:THR:OG1	1:E:47:PRO:HD3	2.21	0.41
1:E:214:TRP:O	1:E:218:ARG:HB2	2.20	0.41
1:A:66:ILE:O	1:A:67:SER:OG	2.29	0.40
1:A:75:LEU:HD11	1:B:32:LEU:HD22	2.03	0.40
1:A:86:PHE:CE2	1:C:7:PHE:HE1	2.38	0.40
1:A:225:GLU:CG	1:A:229:TYR:OH	2.69	0.40
1:B:223:HIS:O	1:B:224:ALA:C	2.60	0.40
1:C:63:PRO:HB2	1:C:65:VAL:H	1.86	0.40
1:C:213:ASP:OD1	1:C:213:ASP:C	2.59	0.40
1:C:223:HIS:C	1:C:225:GLU:N	2.73	0.40
1:D:95:GLU:HB2	1:D:96:GLU:OE2	2.21	0.40
1:D:161:ILE:HD11	1:D:197:ILE:HG12	2.03	0.40
1:D:202:HIS:O	1:D:205:GLU:HG3	2.21	0.40
1:D:223:HIS:O	1:D:225:GLU:N	2.54	0.40
1:E:69:GLY:HA2	1:E:72:LEU:CG	2.51	0.40
1:E:75:LEU:HG	1:E:76:VAL:N	2.36	0.40
1:A:27:ILE:HA	1:A:30:THR:HG22	2.04	0.40
1:A:169:GLY:HA2	1:A:203:GLU:OE2	2.21	0.40
1:A:242:GLY:O	1:A:243:LYS:HB2	2.20	0.40
1:B:187:LEU:HB3	1:B:191:MET:HE3	1.98	0.40
1:B:228:TYR:CD1	1:B:232:PHE:CE1	3.09	0.40
1:C:40:ILE:HG22	1:C:41:ILE:HD13	2.03	0.40
1:C:235:GLU:O	1:C:238:THR:CB	2.63	0.40
1:D:146:LEU:O	1:D:149:ALA:CB	2.62	0.40
1:D:221:GLU:O	1:D:222:GLU:C	2.59	0.40
1:E:106:VAL:HG12	1:E:107:GLY:N	2.37	0.40
1:A:12:TYR:O	1:A:13:GLU:HB3	2.21	0.40
1:A:105:LYS:N	1:A:134:LYS:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:CG1	1:A:163:MET:N	2.84	0.40
1:B:125:LYS:HB3	1:B:221:GLU:HG3	2.04	0.40
1:C:121:ILE:CG2	1:C:220:ALA:HB3	2.52	0.40
1:D:61:LEU:HD12	1:D:65:VAL:HG21	2.03	0.40
1:D:105:LYS:HE3	1:D:158:GLY:HA3	2.02	0.40
1:E:7:PHE:CZ	1:E:11:LEU:HD21	2.56	0.40
1:A:108:ILE:CG2	1:A:165:LEU:HD12	2.52	0.40
1:B:103:THR:O	1:B:104:LYS:HD2	2.21	0.40
1:B:129:LEU:N	1:B:129:LEU:CD1	2.84	0.40
1:B:145:ASP:O	1:B:147:PRO:HD2	2.21	0.40
1:C:93:LEU:O	1:C:96:GLU:CB	2.69	0.40
1:C:125:LYS:HB2	1:C:221:GLU:HG3	2.03	0.40
1:E:121:ILE:CD1	1:E:121:ILE:H	2.35	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:GLY:N	1:D:62:GLY:O[2_645]	2.13	0.07
1:D:62:GLY:O	1:D:62:GLY:O[2_645]	2.15	0.05

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	239/277 (86%)	168 (70%)	49 (20%)	22 (9%)	1	12
1	B	224/277 (81%)	143 (64%)	66 (30%)	15 (7%)	1	17
1	C	228/277 (82%)	161 (71%)	45 (20%)	22 (10%)	0	10
1	D	229/277 (83%)	167 (73%)	46 (20%)	16 (7%)	1	16
1	E	223/277 (80%)	163 (73%)	46 (21%)	14 (6%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1143/1385 (82%)	802 (70%)	252 (22%)	89 (8%)	1 14

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	SER
1	A	99	GLU
1	A	100	LYS
1	A	105	LYS
1	A	119	ALA
1	A	243	LYS
1	B	61	LEU
1	B	161	ILE
1	C	44	ILE
1	C	65	VAL
1	C	66	ILE
1	C	160	ASP
1	C	161	ILE
1	C	241	ALA
1	D	59	VAL
1	D	157	GLU
1	D	161	ILE
1	D	194	LYS
1	E	119	ALA
1	E	157	GLU
1	E	161	ILE
1	E	193	ASN
1	A	159	CYS
1	A	233	LYS
1	B	44	ILE
1	B	102	MET
1	B	138	LYS
1	B	245	LEU
1	C	8	LYS
1	C	145	ASP
1	C	247	GLN
1	D	40	ILE
1	D	46	THR
1	D	121	ILE
1	D	160	ASP
1	A	57	ALA
1	A	171	ALA

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Mol	Chain	Res	Type
1	A	220	ALA
1	B	60	GLU
1	B	100	LYS
1	B	193	ASN
1	B	251	ASP
1	C	119	ALA
1	C	168	PRO
1	C	172	GLU
1	D	159	CYS
1	E	146	LEU
1	E	171	ALA
1	A	64	ILE
1	C	121	ILE
1	D	99	GLU
1	D	147	PRO
1	D	158	GLY
1	E	132	ASN
1	E	150	CYS
1	E	172	GLU
1	A	162	VAL
1	A	188	ALA
1	B	130	SER
1	B	146	LEU
1	B	247	GLN
1	C	46	THR
1	C	146	LEU
1	C	215	LEU
1	C	234	PRO
1	C	238	THR
1	E	147	PRO
1	A	47	PRO
1	A	141	PRO
1	A	146	LEU
1	A	224	ALA
1	E	42	MET
1	E	201	VAL
1	A	196	ILE
1	C	233	LYS
1	D	201	VAL
1	A	161	ILE
1	D	41	ILE
1	E	133	ILE

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Mol	Chain	Res	Type
1	B	234	PRO
1	C	43	PRO
1	D	148	VAL
1	E	162	VAL
1	A	147	PRO
1	B	45	ILE
1	C	147	PRO
1	C	42	MET
1	D	42	MET
1	A	63	PRO

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	185/231 (80%)	164 (89%)	21 (11%)	5 25
1	B	181/231 (78%)	152 (84%)	29 (16%)	2 15
1	C	178/231 (77%)	152 (85%)	26 (15%)	3 18
1	D	184/231 (80%)	159 (86%)	25 (14%)	3 20
1	E	171/231 (74%)	140 (82%)	31 (18%)	1 11
All	All	899/1155 (78%)	767 (85%)	132 (15%)	3 17

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	17	ILE
1	A	18	PRO
1	A	40	ILE
1	A	42	MET
1	A	61	LEU
1	A	72	LEU
1	A	86	PHE
1	A	99	GLU

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Mol	Chain	Res	Type
1	A	111	THR
1	A	113	PHE
1	A	146	LEU
1	A	157	GLU
1	A	191	MET
1	A	192	THR
1	A	197	ILE
1	A	201	VAL
1	A	204	ASP
1	A	217	LYS
1	A	237	LEU
1	A	238	THR
1	B	17	ILE
1	B	38	ASP
1	B	39	ASN
1	B	46	THR
1	B	59	VAL
1	B	60	GLU
1	B	61	LEU
1	B	75	LEU
1	B	83	PHE
1	B	86	PHE
1	B	88	ILE
1	B	90	LYS
1	B	96	GLU
1	B	105	LYS
1	B	110	ASP
1	B	111	THR
1	B	113	PHE
1	B	134	LYS
1	B	146	LEU
1	B	148	VAL
1	B	160	ASP
1	B	162	VAL
1	B	191	MET
1	B	192	THR
1	B	204	ASP
1	B	217	LYS
1	B	232	PHE
1	B	234	PRO
1	B	249	PHE
1	C	7	PHE

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Mol	Chain	Res	Type
1	C	17	ILE
1	C	37	VAL
1	C	44	ILE
1	C	75	LEU
1	C	76	VAL
1	C	88	ILE
1	C	99	GLU
1	C	105	LYS
1	C	111	THR
1	C	113	PHE
1	C	134	LYS
1	C	146	LEU
1	C	147	PRO
1	C	148	VAL
1	C	150	CYS
1	C	160	ASP
1	C	165	LEU
1	C	177	CYS
1	C	187	LEU
1	C	191	MET
1	C	192	THR
1	C	196	ILE
1	C	204	ASP
1	C	217	LYS
1	C	246	ARG
1	D	7	PHE
1	D	17	ILE
1	D	59	VAL
1	D	61	LEU
1	D	64	ILE
1	D	65	VAL
1	D	66	ILE
1	D	88	ILE
1	D	91	LYS
1	D	92	VAL
1	D	93	LEU
1	D	96	GLU
1	D	105	LYS
1	D	111	THR
1	D	112	THR
1	D	146	LEU
1	D	150	CYS

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Mol	Chain	Res	Type
1	D	160	ASP
1	D	187	LEU
1	D	191	MET
1	D	192	THR
1	D	204	ASP
1	D	214	TRP
1	D	231	LEU
1	D	237	LEU
1	E	17	ILE
1	E	23	PHE
1	E	37	VAL
1	E	40	ILE
1	E	67	SER
1	E	68	TRP
1	E	71	PHE
1	E	75	LEU
1	E	78	PHE
1	E	88	ILE
1	E	90	LYS
1	E	93	LEU
1	E	102	MET
1	E	105	LYS
1	E	111	THR
1	E	113	PHE
1	E	121	ILE
1	E	143	ILE
1	E	145	ASP
1	E	146	LEU
1	E	148	VAL
1	E	156	GLU
1	E	162	VAL
1	E	187	LEU
1	E	191	MET
1	E	192	THR
1	E	201	VAL
1	E	204	ASP
1	E	217	LYS
1	E	218	ARG
1	E	237	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	189	GLN
1	A	226	ASN
1	B	189	GLN
1	C	179	HIS
1	C	223	HIS
1	D	179	HIS
1	D	195	HIS
1	D	226	ASN
1	E	39	ASN
1	E	179	HIS
1	E	195	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BNG	B	301	-	21,21,21	0.44	0	26,26,26	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BNG	B	301	-	-	7/12/32/32	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	BNG	C4-C5-C6-O6
2	B	301	BNG	O5-C5-C6-O6
2	B	301	BNG	C3'-C4'-C5'-C6'
2	B	301	BNG	O1-C1'-C2'-C3'
2	B	301	BNG	C1'-C2'-C3'-C4'
2	B	301	BNG	C2'-C3'-C4'-C5'
2	B	301	BNG	C6'-C7'-C8'-C9'

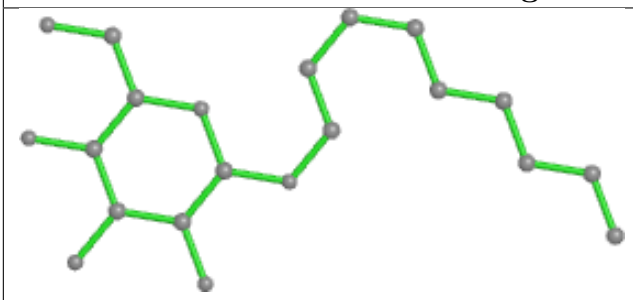
There are no ring outliers.

1 monomer is involved in 12 short contacts:

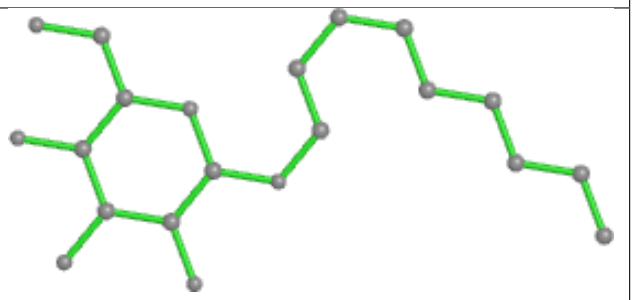
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	BNG	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

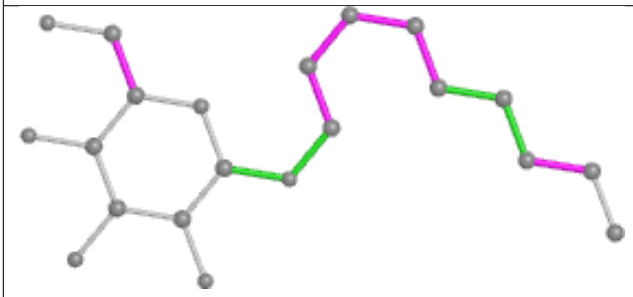
Ligand BNG B 301



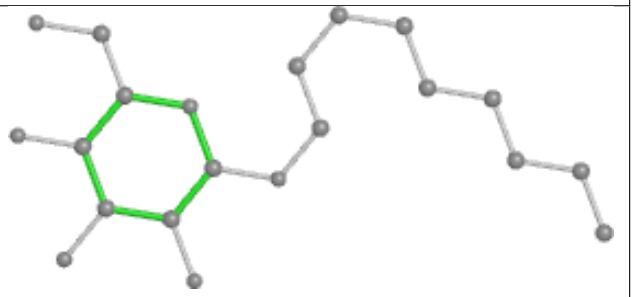
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	241/277 (87%)	-0.35	5 (2%) 63 54	87, 254, 449, 499	0
1	B	230/277 (83%)	-0.31	4 (1%) 70 60	90, 231, 472, 500	0
1	C	234/277 (84%)	-0.24	4 (1%) 70 60	107, 227, 437, 500	0
1	D	235/277 (84%)	-0.27	0 100 100	97, 243, 483, 500	0
1	E	231/277 (83%)	-0.09	11 (4%) 30 26	89, 292, 475, 500	0
All	All	1171/1385 (84%)	-0.25	24 (2%) 65 56	87, 247, 463, 500	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	57	ALA	6.0
1	E	56	THR	5.9
1	E	104	LYS	5.4
1	E	105	LYS	4.7
1	C	205	GLU	4.3
1	A	168	PRO	4.3
1	E	103	THR	3.7
1	E	134	LYS	3.7
1	C	246	ARG	3.4
1	E	53	GLY	3.1
1	B	46	THR	2.8
1	A	104	LYS	2.6
1	A	13	GLU	2.5
1	B	114	ALA	2.5
1	E	116	VAL	2.4
1	B	156	GLU	2.4
1	A	167	MET	2.4
1	C	28	ALA	2.3
1	C	203	GLU	2.2
1	E	205	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	132	ASN	2.1
1	B	100	LYS	2.1
1	E	160	ASP	2.0
1	A	105	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

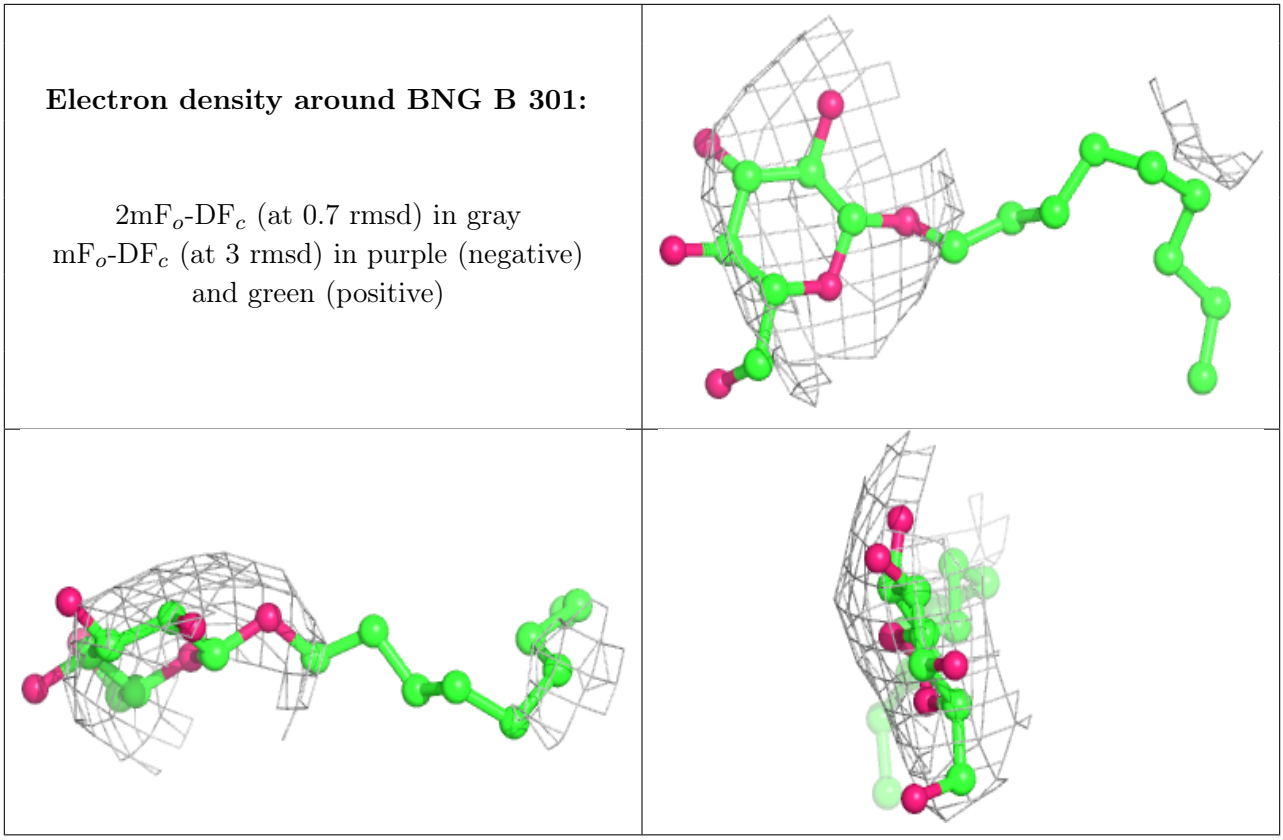
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BNG	B	301	21/21	0.47	0.61	302,345,374,378	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BNG B 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.