Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 05:26 PM EDT

PDB ID	:	3M85
Title	:	Archaeoglobus fulgidus exosome y70a with RNA bound to the active site
Authors	:	Hartung, S.; Hopfner, K.-P.
Deposited on	:	2010-03-17
Resolution	:	3.00 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 (1)) were used in the production of this report:

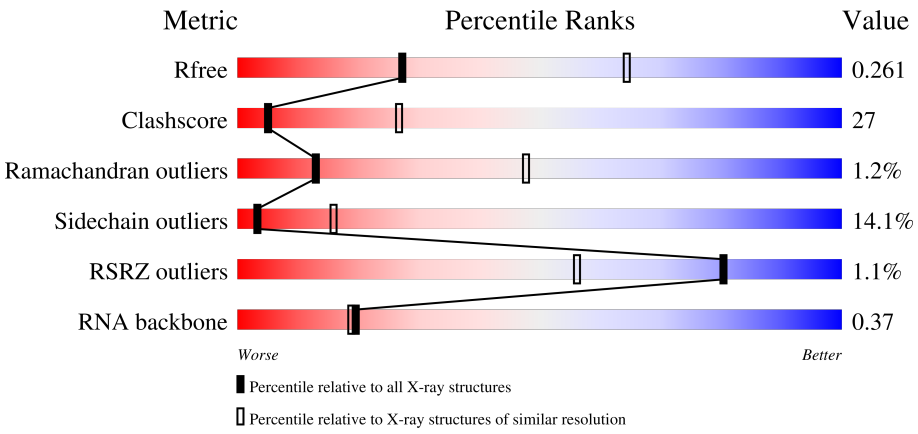
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	179	.% 55% 40% 6%
1	B	179	2% 44% 44% 12%
1	C	179	2% 56% 39% 5%
2	D	258	45% 40% 8% 6%

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Mol	Chain	Length	Quality of chain
2	E	258	% 51% 37% 6% 5%
2	F	258	54% 33% 8% 5%
3	G	259	46% 45% 8%
3	H	259	2% 49% 41% 9%
3	I	259	2% 62% 33% 5%
4	X	6	17% 50% 33%
4	Y	6	17% 17% 33% 17% 33%
4	Z	6	33% 17% 17% 33%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16110 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 Putative uncharacterized protein AF_0206.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	179	1371	855	242	266	8	18	0	0
1	B	179	1371	855	242	266	8	61	0	0
1	C	179	1371	855	242	266	8	16	0	0

- Molecule 2 is a protein called Probable exosome complex exonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	243	1902	1198	334	357	13	33	0	0
2	E	245	1920	1209	337	361	13	48	0	0
2	F	246	1926	1213	337	363	13	14	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	65	GLU	ARG	engineered mutation	UNP O29757
E	65	GLU	ARG	engineered mutation	UNP O29757
F	65	GLU	ARG	engineered mutation	UNP O29757

- Molecule 3 is a protein called Probable exosome complex exonuclease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	258	1997	1259	331	401	6	77	0	0
3	H	258	1997	1259	331	401	6	46	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	259	2006	1265	332	403	6	62	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	70	ALA	TYR	engineered mutation	UNP O29756
H	70	ALA	TYR	engineered mutation	UNP O29756
I	70	ALA	TYR	engineered mutation	UNP O29756

- Molecule 4 is a RNA chain called 5'-R(*CP*UP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	X	4	80	36	12	28	4	1	0	0
4	Y	4	80	36	12	28	4	1	0	0
4	Z	4	80	36	12	28	4	1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0
5	B	1	1	1	0	0
5	C	1	1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	D	1	1	1	0	0
6	F	5	5	5	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: Putative uncharacterized protein AF_0206

Chain A: %
55% 40% 6%

M1 V4 M5 P6 S12 A13 E14 E15 Y16 V22 Y23 E24 G27 F30 A31 A34 G35 K36 L37 I38 I39 K40 V43 E47 S48 I49 S50 P53 V56 K57 G58 D59 V60 V61 V65 V66 D67 I68 R69 N70 S71 I72 I75 E76 V77 K81

R85 R90 I94 L95 H96 V97 S98 N99 V100 D101 E102 G103 Y104 V105 K106 E107 I108 S109 V112 G113 Y114 L115 D116 I117 L118 K119 I123 G124 R128 T131 K132 E135 V138 L139 R140 A141 L142 C143 S144 N145 M150 P160 E161 C162 G163 R164 V165 E166 K167 R168

T172 D173 Y174 W179

• Molecule 1: Putative uncharacterized protein AF_0206

Chain B: 2%
44% 44% 12%

M1 M5 P6 G7 I10 G11 Y16 V17 K18 V22 Y23 E24 E25 E28 L29 F30 L37 I38 I39 V46 I52 P53 E54 I55 V56 K57 G58 D59 V60 V61 R64 V65 V66 D67 I72 A73 L74 I75 E76 V77 S78 S79 K80 E83 N84 R85 G86 P87

I92 G93 I94 L95 H96 V97 S98 N99 V100 D101 E102 G103 Y104 V105 K106 E107 I108 S109 E110 A111 V112 G113 Y114 L115 D116 I117 L118 K119 A120 R121 V122 I123 G124 D125 N126 L127 R128 L129 S130 T131 K132 E133 G137 V138 L139 R140 A141 L142 C143 S144 N145 C146 K147 T148 E149 M150 V151 R152 E153

G154 D155 I156 L157 K158 C159 P160 E161 R164 V165 E166 K167 R168 K169 I170 S171 T172 D173 Y174 G175 K176 W179

• Molecule 1: Putative uncharacterized protein AF_0206

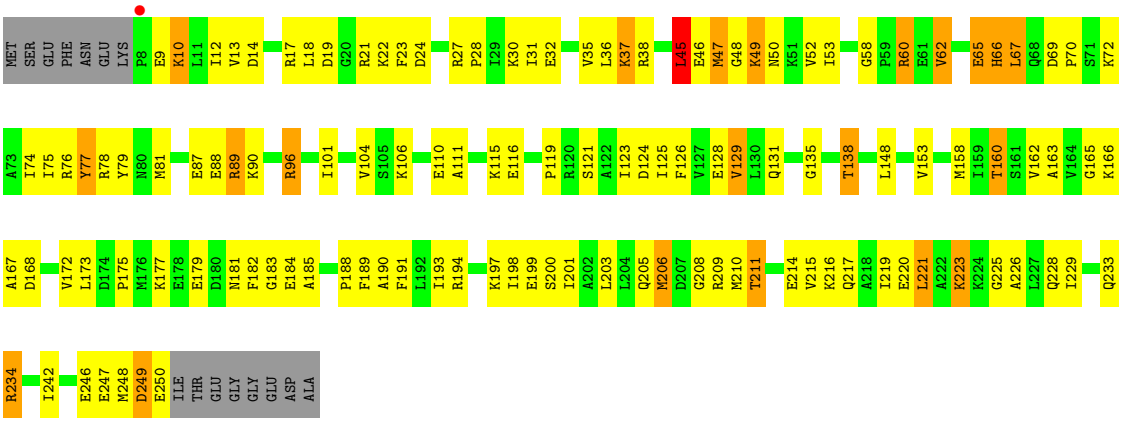
Chain C: 2%
56% 39% 5%

M1 M5 R9 E25 E28 L29 L37 D41 R42 V43 P53 E54 I55 D59 V60 V61 L62 V65 L68 R69 N70 S71 I72 A73 L74 I75 E76 V77 S78 S79 E83 P87 S88 N89 R90 G91 I92 G93 I94 L95 H96 V97 S98 N99 V100 D101 E102 G103

Y104 V105 K106 E107 I108 A111 V112 G113 Y114 L115 D116 I117 L118 K119 V122 I123 G124 D125 N126 L127 R128 L129 S130 T131 K132 E133 E134 E135 M136 G137 V138 L139 R140 A141 L142 C143 S144 N145 C146 K147 T148 R152 E153 I156 L157 K158 C159 P160 E161 C162 K167 R168 K169 I170 S171

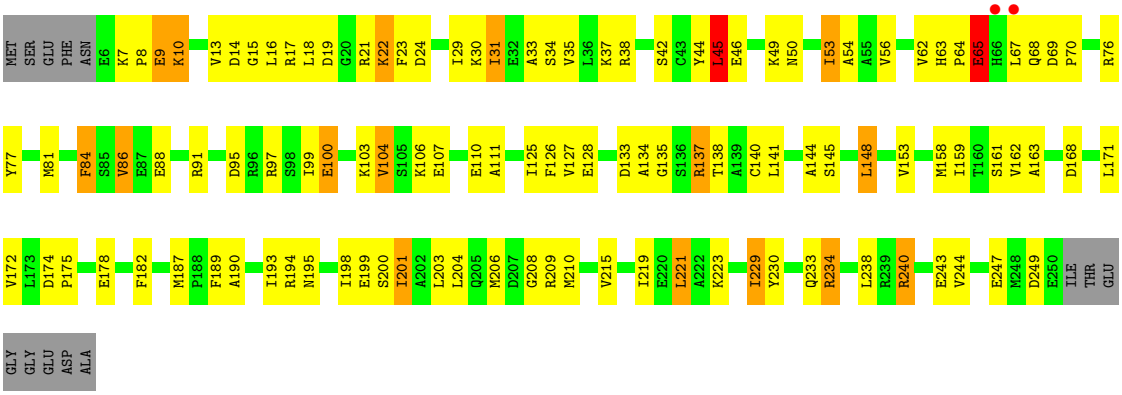
• Molecule 2: Probable exosome complex exonuclease 1

Chain D:



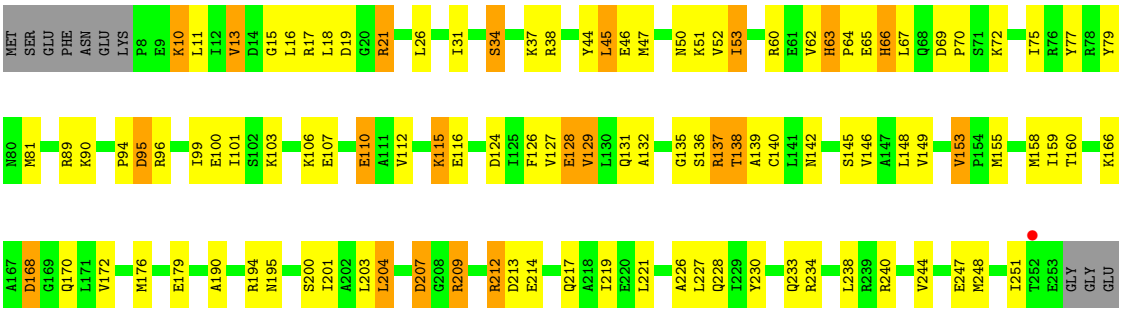
• Molecule 2: Probable exosome complex exonuclease 1

Chain E:



• Molecule 2: Probable exosome complex exonuclease 1

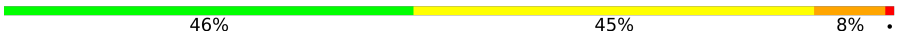
Chain F:

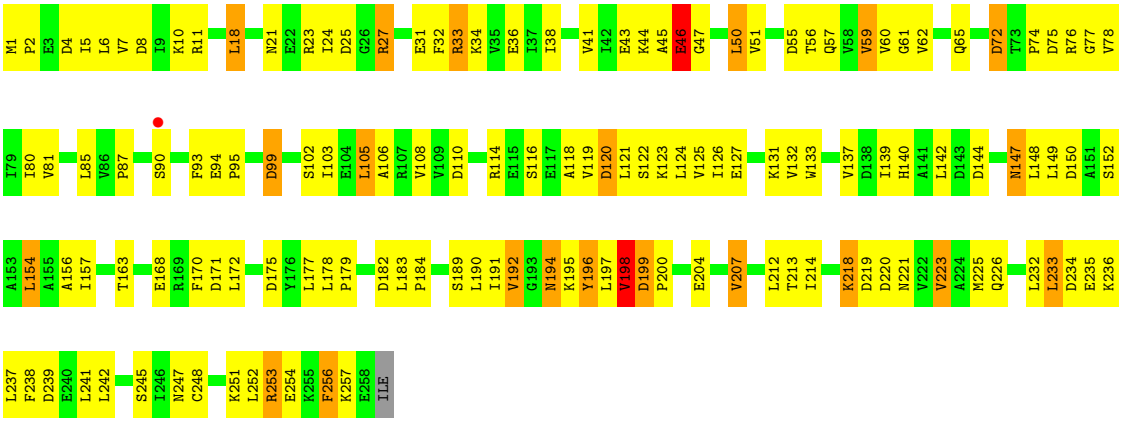


ASP
ALA

• Molecule 3: Probable exosome complex exonuclease 2

Chain G:



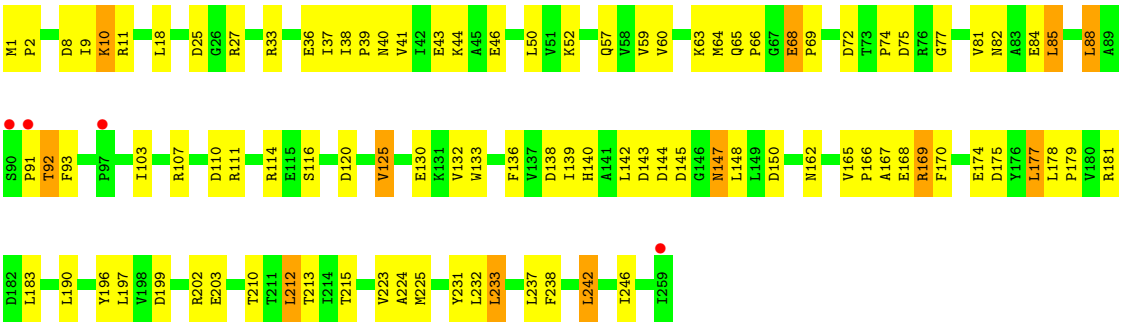


• Molecule 3: Probable exosome complex exonuclease 2

Chain H:

• Molecule 3: Probable exosome complex exonuclease 2

Chain I:

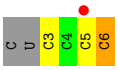


• Molecule 4: 5'-R(*CP*UP*CP*CP*CP*C)-3'

Chain X:

• Molecule 4: 5'-R(*CP*UP*CP*CP*CP*C)-3'

Chain Y:



• Molecule 4: 5'-R(*CP*UP*CP*CP*CP*C)-3'

Chain Z:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	138.02Å 138.02Å 262.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.00 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-3.00) 99.9 (19.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_129)	Depositor
R, R_{free}	0.191 , 0.278 0.178 , 0.261	Depositor DCC
R_{free} test set	5167 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å^2)	64.5	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16110	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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 (i)

5.1 Standard geometry (i)

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

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	0.41	0/1385	0.61	0/1855
1	B	0.39	0/1385	0.55	0/1855
1	C	0.40	0/1385	0.53	0/1855
2	D	0.47	0/1929	0.64	1/2588 (0.0%)
2	E	0.45	0/1947	0.63	1/2612 (0.0%)
2	F	0.51	0/1953	0.67	0/2621
3	G	0.38	0/2025	0.62	1/2748 (0.0%)
3	H	0.48	0/2025	0.64	0/2748
3	I	0.48	0/2034	0.65	0/2759
4	X	1.02	0/87	1.77	3/132 (2.3%)
4	Y	0.79	0/87	1.35	1/132 (0.8%)
4	Z	0.92	0/87	1.55	2/132 (1.5%)
All	All	0.46	0/16329	0.65	9/22037 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	6	C	C4'-C3'-C2'	-7.15	95.45	102.60
4	Z	6	C	C4'-C3'-C2'	-6.83	95.77	102.60
2	D	45	LEU	CA-CB-CG	6.65	130.59	115.30
4	Z	6	C	O4'-C1'-N1	6.22	113.18	108.20
4	Y	6	C	C4'-C3'-C2'	-6.00	96.60	102.60
3	G	199	ASP	N-CA-C	5.98	127.14	111.00
2	E	45	LEU	CA-CB-CG	5.51	127.96	115.30
4	X	4	C	O4'-C1'-N1	5.26	112.41	108.20
4	X	4	C	C4'-C3'-C2'	-5.22	97.38	102.60

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	1371	0	1408	67	0
1	B	1371	0	1410	91	0
1	C	1371	0	1409	70	0
2	D	1902	0	1948	117	0
2	E	1920	0	1966	113	0
2	F	1926	0	1972	101	0
3	G	1997	0	2021	150	0
3	H	1997	0	2021	140	0
3	I	2006	0	2032	83	0
4	X	80	0	45	1	0
4	Y	80	0	45	2	0
4	Z	80	0	45	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	5	0	0	0	0
All	All	16110	0	16322	856	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (856) 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)
3:G:23:ARG:HH22	3:G:198:VAL:HG13	1.13	1.14
1:B:128:ARG:HG2	1:B:128:ARG:HH21	1.19	1.04
3:G:23:ARG:HH12	3:G:198:VAL:HG21	1.22	1.04
3:H:75:ASP:O	3:H:76:ARG:HG2	1.58	1.03
2:F:18:LEU:H	2:F:18:LEU:HD12	1.17	1.01
3:G:23:ARG:NH2	3:G:198:VAL:HG13	1.77	1.00
2:F:81:MET:HB2	2:F:90:LYS:HE2	1.44	1.00
1:B:156:ILE:HD11	1:B:167:LYS:HA	1.41	0.97
1:C:65:VAL:HG21	1:C:112:VAL:HG11	1.44	0.96
3:G:23:ARG:HH12	3:G:198:VAL:CG2	1.79	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:GLN:NE2	3:H:44:LYS:H	1.65	0.94
2:F:131:GLN:HE21	3:H:44:LYS:H	1.08	0.93
1:B:143:CYS:HB3	1:B:146:CYS:SG	2.08	0.93
1:A:40:LYS:O	1:A:43:VAL:HG12	1.69	0.92
3:G:198:VAL:HB	3:G:199:ASP:CA	2.00	0.92
3:G:1:MET:N	3:G:4:ASP:HB3	1.85	0.92
3:G:124:LEU:HB3	3:G:133:TRP:HB2	1.50	0.91
2:D:198:ILE:HD12	2:D:223:LYS:HB3	1.50	0.91
2:F:18:LEU:HD12	2:F:18:LEU:N	1.84	0.90
3:G:198:VAL:HB	3:G:199:ASP:C	1.92	0.89
2:D:160:THR:HG23	2:D:233:GLN:HE22	1.37	0.89
1:B:145:ASN:H	1:B:145:ASN:HD22	0.93	0.89
1:C:97:VAL:HG22	1:C:108:ILE:HG23	1.55	0.88
2:D:160:THR:HG23	2:D:233:GLN:NE2	1.87	0.88
3:G:234:ASP:HB3	3:G:237:LEU:HD13	1.54	0.88
2:E:161:SER:HB2	2:E:189:PHE:O	1.74	0.87
1:B:145:ASN:H	1:B:145:ASN:ND2	1.72	0.87
3:H:257:LYS:N	3:H:257:LYS:HD2	1.91	0.86
1:C:119:LYS:HB2	1:C:139:LEU:HD11	1.57	0.86
1:B:128:ARG:HH21	1:B:128:ARG:CG	1.88	0.86
1:C:65:VAL:HG21	1:C:112:VAL:CG1	2.05	0.85
1:A:97:VAL:HG13	1:A:108:ILE:HB	1.59	0.85
1:B:145:ASN:HD22	1:B:145:ASN:N	1.74	0.84
3:G:23:ARG:HH22	3:G:198:VAL:CG1	1.90	0.84
3:G:214:ILE:HG12	3:G:225:MET:HE3	1.59	0.84
3:I:91:PRO:HD2	3:I:202:ARG:HH12	1.41	0.84
3:H:250:ARG:HH21	3:H:250:ARG:HG3	1.44	0.83
3:G:1:MET:H3	3:G:4:ASP:HB3	1.43	0.83
3:G:144:ASP:HA	3:G:148:LEU:HD21	1.60	0.83
2:F:38:ARG:HH11	3:H:202:ARG:HD2	1.44	0.82
3:G:27:ARG:NH1	3:G:198:VAL:HG11	1.93	0.82
2:D:208:GLY:O	3:G:223:VAL:HA	1.79	0.82
2:E:10:LYS:HA	2:E:10:LYS:NZ	1.94	0.82
3:G:218:LYS:HG2	3:G:219:ASP:N	1.94	0.82
3:H:72:ASP:O	3:H:74:PRO:HD3	1.80	0.81
1:A:99:ASN:HA	1:A:132:LYS:HE3	1.61	0.81
2:E:56:VAL:HG21	2:E:148:LEU:HD13	1.62	0.80
1:C:65:VAL:HG22	1:C:75:ILE:HG12	1.64	0.80
3:G:139:ILE:HD13	3:G:152:SER:HB3	1.62	0.79
2:D:206:MET:CG	3:G:225:MET:HG3	2.12	0.79
1:B:57:LYS:HE2	1:B:124:GLY:HA2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:18:LEU:H	2:F:18:LEU:CD1	1.94	0.79
2:F:112:VAL:HG21	2:F:159:ILE:HD11	1.64	0.79
1:B:173:ASP:HA	1:B:176:LYS:HD3	1.64	0.78
1:C:153:GLU:HG3	1:C:158:LYS:HE2	1.66	0.78
1:C:65:VAL:HG23	1:C:118:LEU:HD13	1.64	0.77
3:G:196:TYR:HD1	3:G:241:LEU:HD13	1.47	0.77
1:A:119:LYS:HB2	1:A:139:LEU:HD11	1.66	0.77
2:E:15:GLY:O	2:E:16:LEU:HD23	1.84	0.77
2:F:66:HIS:H	2:F:66:HIS:CD2	1.98	0.77
3:G:80:ILE:HD12	4:Y:3:C:H1'	1.65	0.77
2:E:63:HIS:CD2	2:E:64:PRO:HA	2.20	0.77
3:G:196:TYR:H	3:G:196:TYR:HD2	1.30	0.76
2:D:128:GLU:HG2	3:I:140:HIS:CE1	2.21	0.76
1:B:16:TYR:CE2	1:B:39:ILE:HD13	2.21	0.76
3:G:23:ARG:NH1	3:G:198:VAL:CG2	2.48	0.76
3:I:59:VAL:CG2	3:I:142:LEU:HD11	2.17	0.75
3:I:177:LEU:H	3:I:177:LEU:HD22	1.50	0.75
1:C:108:ILE:HD13	1:C:108:ILE:H	1.51	0.75
2:E:128:GLU:HG2	3:G:140:HIS:CE1	2.21	0.75
3:H:191:ILE:HD11	3:H:212:LEU:HB2	1.68	0.75
3:G:168:GLU:HB2	3:G:175:ASP:OD1	1.87	0.75
2:D:67:LEU:H	2:D:67:LEU:HD22	1.52	0.74
2:E:209:ARG:HH12	3:H:117:GLU:HG3	1.51	0.74
3:I:110:ASP:OD2	3:I:114:ARG:NH2	2.20	0.74
3:G:157:ILE:HG23	3:G:256:PHE:CZ	2.21	0.74
2:E:111:ALA:HB1	3:H:232:LEU:HG	1.70	0.74
3:G:27:ARG:CZ	3:G:198:VAL:HG11	2.18	0.74
3:G:25:ASP:OD1	3:G:27:ARG:HB2	1.87	0.73
2:D:206:MET:HG2	3:G:225:MET:HG3	1.70	0.73
3:H:90:SER:HA	3:H:202:ARG:HH12	1.53	0.73
1:A:164:ARG:HG3	1:A:165:VAL:H	1.53	0.73
3:G:23:ARG:NH1	3:G:198:VAL:HG21	1.99	0.73
3:H:1:MET:N	3:H:2:PRO:HD3	2.04	0.72
1:B:22:VAL:HG23	1:B:46:VAL:HG23	1.72	0.72
3:G:196:TYR:CD1	3:G:241:LEU:HD13	2.24	0.72
2:F:19:ASP:OD2	2:F:21:ARG:HD3	1.90	0.72
3:G:41:VAL:HG21	3:G:50:LEU:HB3	1.70	0.72
3:H:196:TYR:CD2	3:H:241:LEU:HD13	2.25	0.72
2:E:206:MET:CE	3:H:222:VAL:HG12	2.20	0.71
2:F:145:SER:OG	2:F:159:ILE:HB	1.91	0.71
1:A:65:VAL:HG21	1:A:112:VAL:HG12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:27:ARG:NH1	3:H:199:ASP:O	2.16	0.71
3:I:168:GLU:O	3:I:169:ARG:HB3	1.91	0.71
2:E:209:ARG:NH1	3:H:117:GLU:HG3	2.05	0.71
3:G:72:ASP:O	3:G:74:PRO:HD3	1.89	0.71
2:D:17:ARG:CZ	2:D:172:VAL:HB	2.21	0.71
3:G:62:VAL:HG22	3:G:137:VAL:HG22	1.72	0.70
1:B:128:ARG:HG2	1:B:128:ARG:NH2	1.97	0.70
1:A:30:PHE:CE2	2:D:194:ARG:HD3	2.26	0.70
1:B:126:ASN:HB2	1:B:128:ARG:NH2	2.07	0.70
2:E:219:ILE:HD11	3:H:238:PHE:CE2	2.27	0.70
3:H:46:GLU:HG2	3:H:166:PRO:HG3	1.73	0.69
1:A:69:ARG:HB2	1:A:72:ILE:HG22	1.73	0.69
1:C:173:ASP:HA	1:C:176:LYS:HE2	1.74	0.69
2:F:129:VAL:HG21	2:F:132:ALA:HB2	1.75	0.69
2:D:19:ASP:OD1	2:D:21:ARG:HG3	1.91	0.69
3:G:120:ASP:OD1	3:G:123:LYS:HG3	1.92	0.69
1:C:90:ARG:NH1	3:H:2:PRO:HB2	2.07	0.69
2:F:17:ARG:HD2	2:F:179:GLU:OE1	1.91	0.69
3:I:38:ILE:HD13	3:I:38:ILE:N	2.06	0.69
1:C:75:ILE:HD13	1:C:118:LEU:HD22	1.73	0.69
3:H:124:LEU:HB2	3:H:133:TRP:HB2	1.74	0.69
3:I:43:GLU:CD	3:I:43:GLU:H	1.96	0.69
1:C:117:ILE:HD13	1:C:140:ARG:HD2	1.74	0.69
3:H:191:ILE:CD1	3:H:212:LEU:HB2	2.23	0.69
3:G:56:THR:HG23	3:G:148:LEU:HD23	1.75	0.68
3:I:59:VAL:HG23	3:I:142:LEU:HD11	1.73	0.68
2:D:198:ILE:HD12	2:D:223:LYS:CB	2.22	0.68
3:G:36:GLU:HG2	3:G:38:ILE:HD11	1.75	0.68
1:B:143:CYS:CB	1:B:146:CYS:SG	2.81	0.68
1:A:5:MET:HG3	2:D:234:ARG:HG3	1.76	0.68
1:B:16:TYR:CE2	1:B:39:ILE:HG21	2.29	0.68
1:B:55:ILE:HG22	1:B:122:VAL:HG21	1.76	0.68
2:F:213:ASP:O	2:F:217:GLN:HG3	1.94	0.68
3:H:125:VAL:HA	3:H:132:VAL:CG2	2.23	0.68
3:H:1:MET:H3	3:H:2:PRO:HD3	1.57	0.67
3:H:89:ALA:HB1	3:H:144:ASP:H	1.59	0.67
2:E:50:ASN:ND2	2:E:133:ASP:HB3	2.09	0.67
1:B:151:VAL:HG12	1:B:158:LYS:O	1.94	0.67
3:I:25:ASP:OD2	3:I:27:ARG:HD3	1.95	0.67
3:G:43:GLU:HG2	3:G:44:LYS:H	1.59	0.67
1:C:76:GLU:O	1:C:76:GLU:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:VAL:HG22	2:D:67:LEU:HD23	1.77	0.67
2:F:10:LYS:HD2	2:F:168:ASP:OD1	1.95	0.67
3:G:196:TYR:O	3:G:197:LEU:HD12	1.95	0.66
3:H:87:PRO:HA	3:H:93:PHE:HB2	1.76	0.66
2:E:7:LYS:HB3	2:E:182:PHE:CE2	2.30	0.66
3:I:125:VAL:HA	3:I:132:VAL:HG23	1.78	0.66
2:E:203:LEU:C	2:E:203:LEU:HD23	2.16	0.66
3:G:157:ILE:HG23	3:G:256:PHE:HZ	1.59	0.66
2:F:34:SER:HB2	2:F:240:ARG:HD3	1.78	0.66
3:G:59:VAL:HG22	3:G:142:LEU:HD11	1.77	0.65
2:E:10:LYS:HA	2:E:10:LYS:HZ3	1.61	0.65
3:G:60:VAL:HG11	3:G:156:ALA:HA	1.77	0.65
2:F:38:ARG:NH1	3:H:202:ARG:HD2	2.11	0.65
2:E:190:ALA:HB3	2:E:203:LEU:HB3	1.77	0.65
2:F:89:ARG:HD2	3:H:136:PHE:CG	2.32	0.65
1:B:57:LYS:HE2	1:B:124:GLY:CA	2.27	0.65
2:D:67:LEU:HD22	2:D:67:LEU:N	2.10	0.65
2:D:163:ALA:O	2:D:175:PRO:HD3	1.97	0.65
1:A:65:VAL:HG21	1:A:112:VAL:CG1	2.27	0.64
2:D:17:ARG:HH12	2:D:173:LEU:H	1.45	0.64
2:E:135:GLY:HA2	2:E:137:ARG:NH1	2.12	0.64
1:C:93:GLY:HA2	1:C:127:LEU:HB2	1.80	0.64
1:B:159:CYS:SG	1:B:161:GLU:N	2.70	0.64
2:D:173:LEU:HD13	2:D:221:LEU:HD13	1.79	0.64
3:H:89:ALA:HB1	3:H:144:ASP:N	2.11	0.64
1:B:173:ASP:HA	1:B:176:LYS:CD	2.28	0.64
3:H:125:VAL:HA	3:H:132:VAL:HG23	1.79	0.64
3:G:212:LEU:HD23	3:G:213:THR:H	1.63	0.64
1:B:109:SER:O	1:B:110:GLU:HB3	1.97	0.64
1:B:10:ILE:O	1:B:11:GLY:O	2.16	0.64
2:D:78:ARG:HB3	2:D:126:PHE:HD2	1.63	0.63
3:G:18:LEU:HD22	3:G:195:LYS:HD2	1.78	0.63
1:B:65:VAL:HG11	1:B:116:ASP:OD2	1.97	0.63
3:H:42:ILE:HG22	3:H:42:ILE:O	1.99	0.63
1:C:53:PRO:HB3	1:C:83:GLU:OE2	1.98	0.63
3:H:168:GLU:HG3	3:H:175:ASP:CG	2.18	0.63
2:D:111:ALA:HB1	3:G:232:LEU:HG	1.80	0.63
2:D:131:GLN:HE22	3:I:43:GLU:HB2	1.64	0.63
1:B:96:HIS:HD2	1:B:98:SER:H	1.47	0.63
3:I:46:GLU:HG2	3:I:166:PRO:HG3	1.80	0.63
1:A:167:LYS:HD3	1:A:168:ARG:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:10:LYS:HE3	3:I:203:GLU:OE2	1.99	0.63
1:C:73:ALA:HB3	1:C:95:LEU:HB3	1.79	0.62
1:C:75:ILE:HD12	1:C:129:LEU:HD12	1.81	0.62
2:F:66:HIS:CD2	2:F:66:HIS:N	2.68	0.62
2:F:137:ARG:HH11	2:F:137:ARG:HG2	1.65	0.62
1:A:119:LYS:HE2	1:A:179:TRP:OXT	1.99	0.62
1:C:145:ASN:O	1:C:146:CYS:HB3	2.00	0.62
1:B:24:GLU:HG2	1:B:25:GLU:N	2.15	0.62
1:B:143:CYS:O	1:B:147:LYS:HD2	2.00	0.62
2:F:15:GLY:O	2:F:16:LEU:HD23	1.99	0.62
2:F:66:HIS:H	2:F:66:HIS:HD2	1.45	0.62
3:G:11:ARG:HG3	3:G:207:VAL:HA	1.82	0.62
1:C:133:GLU:HB2	1:C:136:MET:HG2	1.81	0.61
3:I:37:ILE:C	3:I:38:ILE:HD13	2.20	0.61
2:D:210:MET:HE1	2:D:215:VAL:HG22	1.82	0.61
3:G:218:LYS:HG2	3:G:219:ASP:H	1.65	0.61
1:A:116:ASP:OD1	1:A:168:ARG:NH1	2.34	0.61
1:B:142:LEU:HD23	1:B:149:GLU:HA	1.82	0.61
1:C:146:CYS:SG	1:C:148:THR:HG23	2.40	0.61
3:H:242:LEU:O	3:H:246:ILE:HG13	2.00	0.61
3:I:147:ASN:ND2	3:I:150:ASP:H	1.99	0.61
2:E:219:ILE:HD11	3:H:238:PHE:HE2	1.64	0.61
1:C:99:ASN:HA	1:C:132:LYS:HE3	1.82	0.61
2:F:230:TYR:HA	2:F:233:GLN:HE21	1.66	0.61
3:H:127:GLU:OE2	3:H:131:LYS:HD3	2.00	0.61
2:F:149:VAL:HG22	2:F:155:MET:HE3	1.82	0.61
3:G:85:LEU:O	3:G:93:PHE:HB3	2.00	0.61
3:H:89:ALA:HB2	3:H:142:LEU:O	2.01	0.61
3:G:46:GLU:H	3:G:46:GLU:CD	2.03	0.60
3:G:196:TYR:HD2	3:G:196:TYR:N	1.96	0.60
1:C:111:ALA:O	1:C:168:ARG:HB3	2.00	0.60
2:D:188:PRO:HD2	2:D:205:GLN:O	2.00	0.60
2:D:135:GLY:O	2:D:138:THR:HG22	2.01	0.60
2:E:193:ILE:HD12	2:E:230:TYR:HB2	1.81	0.60
2:D:22:LYS:HG2	2:D:23:PHE:H	1.66	0.60
2:E:44:TYR:CE2	2:E:46:GLU:HG3	2.37	0.60
3:G:147:ASN:ND2	3:G:150:ASP:H	1.99	0.60
2:F:131:GLN:HE21	3:H:44:LYS:N	1.90	0.60
3:G:196:TYR:C	3:G:197:LEU:HD12	2.22	0.60
2:F:128:GLU:HG2	3:H:140:HIS:NE2	2.17	0.60
3:G:214:ILE:HG12	3:G:225:MET:CE	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:ALA:HB3	2:D:203:LEU:HB3	1.82	0.60
2:E:10:LYS:O	2:E:10:LYS:HD3	2.01	0.60
1:B:110:GLU:O	1:B:168:ARG:HD3	2.02	0.60
2:F:101:ILE:HD13	2:F:137:ARG:HG3	1.84	0.60
2:F:149:VAL:HG22	2:F:155:MET:CE	2.32	0.60
1:C:167:LYS:O	1:C:167:LYS:HG3	2.02	0.59
1:A:117:ILE:HG21	3:I:9:ILE:HD11	1.84	0.59
1:B:16:TYR:HE2	1:B:39:ILE:HG21	1.67	0.59
3:G:254:GLU:C	3:G:256:PHE:H	2.04	0.59
3:H:161:MET:HG2	3:H:180:VAL:HG11	1.84	0.59
3:I:68:GLU:CD	3:I:68:GLU:H	2.05	0.59
1:A:164:ARG:CG	1:A:165:VAL:N	2.65	0.59
3:H:25:ASP:OD2	3:H:27:ARG:HD3	2.02	0.59
2:E:10:LYS:HA	2:E:10:LYS:HZ2	1.66	0.59
1:A:150:MET:HE2	1:A:166:GLU:HB2	1.85	0.59
3:G:219:ASP:O	3:G:220:ASP:HB2	2.03	0.59
3:H:110:ASP:OD2	3:H:114:ARG:NH2	2.35	0.59
1:C:93:GLY:CA	1:C:127:LEU:HB2	2.33	0.59
1:A:144:SER:HB2	1:A:166:GLU:OE1	2.02	0.59
2:D:87:GLU:O	3:I:63:LYS:HE2	2.03	0.59
2:F:103:LYS:O	2:F:107:GLU:HG3	2.02	0.59
2:F:127:VAL:HG11	2:F:140:CYS:HB3	1.83	0.58
3:G:170:PHE:O	3:G:172:LEU:HD12	2.03	0.58
1:C:61:VAL:HG11	1:C:77:VAL:CG1	2.33	0.58
3:G:27:ARG:NH1	3:G:199:ASP:O	2.36	0.58
1:B:100:VAL:O	1:B:169:LYS:CD	2.52	0.58
2:F:96:ARG:NH1	3:I:82:ASN:OD1	2.37	0.58
3:G:242:LEU:HD23	3:G:242:LEU:O	2.04	0.58
3:H:127:GLU:HB2	3:H:131:LYS:H	1.68	0.58
2:D:247:GLU:O	2:D:250:GLU:HG2	2.03	0.58
3:G:198:VAL:HB	3:G:199:ASP:O	2.03	0.58
3:H:196:TYR:CG	3:H:241:LEU:HD13	2.39	0.58
1:C:159:CYS:SG	1:C:162:CYS:HB3	2.44	0.58
2:E:206:MET:HB3	3:H:225:MET:HG3	1.85	0.58
3:H:256:PHE:C	3:H:258:GLU:H	2.07	0.58
2:E:95:ASP:O	2:E:99:ILE:HG13	2.04	0.58
2:F:116:GLU:H	2:F:116:GLU:CD	2.06	0.58
3:G:1:MET:H1	3:G:5:ILE:HD12	1.68	0.57
3:G:25:ASP:OD1	3:G:27:ARG:HD3	2.04	0.57
1:B:53:PRO:HG2	1:B:85:ARG:O	2.04	0.57
1:C:75:ILE:CD1	1:C:118:LEU:HD22	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:22:LYS:HD3	2:E:24:ASP:OD1	2.04	0.57
2:F:38:ARG:HG3	3:H:202:ARG:NH1	2.19	0.57
1:C:9:ARG:HG2	1:C:9:ARG:NH2	2.19	0.57
2:E:100:GLU:O	2:E:104:VAL:HG22	2.04	0.57
2:F:31:ILE:HG12	2:F:45:LEU:HD22	1.86	0.57
2:F:126:PHE:CE2	3:H:87:PRO:HG2	2.39	0.57
4:Y:5:C:H2'	4:Y:6:C:O4'	2.03	0.57
1:B:76:GLU:O	1:B:76:GLU:HG3	2.03	0.57
2:F:219:ILE:HD11	3:I:238:PHE:CE2	2.38	0.57
3:I:177:LEU:HD22	3:I:177:LEU:N	2.18	0.57
3:I:196:TYR:C	3:I:197:LEU:HD12	2.24	0.57
1:A:101:ASP:OD1	1:A:102:GLU:N	2.37	0.57
2:E:243:GLU:O	2:E:247:GLU:HG2	2.05	0.57
2:F:69:ASP:HB3	2:F:72:LYS:O	2.05	0.57
2:D:76:ARG:HG3	2:D:124:ASP:OD2	2.04	0.57
2:D:165:GLY:HA3	2:D:175:PRO:HG3	1.86	0.57
3:H:250:ARG:HG3	3:H:250:ARG:NH2	2.19	0.57
1:A:13:ALA:N	1:A:27:GLY:O	2.37	0.57
2:D:18:LEU:HD12	2:D:18:LEU:H	1.69	0.57
2:E:45:LEU:C	2:E:45:LEU:HD12	2.25	0.57
2:E:63:HIS:HD2	2:E:64:PRO:O	1.87	0.57
1:C:117:ILE:HG21	3:H:9:ILE:HD11	1.87	0.57
1:C:119:LYS:HB2	1:C:139:LEU:CD1	2.33	0.57
2:D:209:ARG:HD3	3:G:221:ASN:HD22	1.69	0.57
2:E:128:GLU:HG2	3:G:140:HIS:HE1	1.67	0.57
2:E:203:LEU:HD23	2:E:204:LEU:N	2.19	0.56
2:F:138:THR:HG22	2:F:139:ALA:N	2.20	0.56
1:A:53:PRO:HG2	1:A:85:ARG:O	2.05	0.56
2:D:242:ILE:O	2:D:246:GLU:HG3	2.06	0.56
2:E:64:PRO:HG2	2:E:67:LEU:HB2	1.87	0.56
2:E:206:MET:HE2	3:H:222:VAL:HG12	1.87	0.56
2:F:44:TYR:OH	2:F:51:LYS:HD3	2.06	0.56
2:F:95:ASP:N	2:F:95:ASP:OD2	2.38	0.56
3:H:190:LEU:HD13	3:H:192:VAL:HG23	1.86	0.56
2:F:207:ASP:OD1	3:I:111:ARG:HG2	2.06	0.56
3:H:33:ARG:HD3	3:H:199:ASP:OD1	2.05	0.56
1:C:71:SER:O	1:C:97:VAL:HG23	2.05	0.56
1:A:119:LYS:NZ	1:A:135:GLU:HG2	2.21	0.56
2:F:17:ARG:HD3	2:F:172:VAL:HG11	1.86	0.56
2:D:31:ILE:HG12	2:D:45:LEU:HD22	1.87	0.56
3:H:214:ILE:HD13	3:H:242:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:242:LEU:O	3:I:246:ILE:HG13	2.06	0.56
1:A:97:VAL:HA	1:A:100:VAL:HG23	1.87	0.56
2:E:95:ASP:OD2	2:E:97:ARG:HB3	2.06	0.56
3:G:59:VAL:CG2	3:G:142:LEU:HD11	2.35	0.56
3:I:27:ARG:NH1	3:I:199:ASP:O	2.39	0.56
3:H:87:PRO:HA	3:H:93:PHE:CB	2.36	0.56
3:H:185:VAL:O	3:H:215:THR:HG23	2.06	0.56
1:B:96:HIS:CD2	1:B:98:SER:H	2.24	0.56
1:B:60:VAL:CG2	1:B:121:ARG:HH11	2.19	0.55
2:E:34:SER:HB3	2:E:240:ARG:HD3	1.88	0.55
1:C:119:LYS:HE2	1:C:135:GLU:HG2	1.89	0.55
2:D:203:LEU:C	2:D:203:LEU:HD23	2.27	0.55
1:A:75:ILE:HD13	1:A:95:LEU:HB2	1.87	0.55
2:D:200:SER:CB	3:G:232:LEU:HB3	2.36	0.55
2:F:89:ARG:HD2	3:H:136:PHE:CD1	2.42	0.55
2:F:128:GLU:HG2	3:H:140:HIS:CE1	2.40	0.55
3:G:99:ASP:O	3:G:103:ILE:HG12	2.07	0.55
2:F:248:MET:O	2:F:251:ILE:HG22	2.07	0.55
3:G:23:ARG:NH1	3:G:198:VAL:HG22	2.22	0.55
3:G:33:ARG:HD2	3:G:199:ASP:OD1	2.06	0.55
2:E:208:GLY:O	3:H:223:VAL:HA	2.07	0.55
1:B:161:GLU:OE2	1:B:161:GLU:HA	2.06	0.55
2:E:210:MET:HE2	2:E:215:VAL:HG22	1.88	0.55
1:B:169:LYS:NZ	1:B:169:LYS:HB3	2.22	0.55
2:D:17:ARG:NH1	2:D:173:LEU:H	2.04	0.55
2:D:206:MET:HG3	3:G:225:MET:HG3	1.88	0.55
1:C:87:PRO:HD2	1:C:90:ARG:HD2	1.89	0.55
3:H:190:LEU:HB2	3:H:200:PRO:HG3	1.88	0.55
1:B:100:VAL:O	1:B:169:LYS:HD2	2.07	0.54
1:B:114:TYR:O	1:B:115:LEU:HB2	2.07	0.54
2:E:103:LYS:HE2	2:E:107:GLU:OE2	2.06	0.54
1:A:141:ALA:CB	1:A:168:ARG:HH12	2.20	0.54
1:C:112:VAL:HG12	1:C:113:GLY:N	2.22	0.54
3:H:251:LYS:HD2	3:H:251:LYS:N	2.23	0.54
1:C:61:VAL:HG12	1:C:62:LEU:N	2.22	0.54
3:H:116:SER:OG	3:H:184:PRO:HG3	2.07	0.54
1:A:5:MET:HG3	2:D:234:ARG:CG	2.38	0.54
1:B:156:ILE:HG13	1:B:157:LEU:H	1.72	0.54
2:D:210:MET:CE	2:D:215:VAL:HG22	2.38	0.54
1:B:56:VAL:HG13	1:B:57:LYS:N	2.21	0.54
1:C:9:ARG:HD3	2:F:195:ASN:HD21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:153:VAL:HG23	2:E:153:VAL:O	2.08	0.54
1:C:138:VAL:O	1:C:171:SER:HB3	2.08	0.54
2:F:45:LEU:HB3	2:F:52:VAL:HG22	1.89	0.54
2:F:94:PRO:HB2	2:F:99:ILE:HD11	1.89	0.54
2:F:131:GLN:NE2	3:H:44:LYS:N	2.47	0.54
3:G:38:ILE:N	3:G:38:ILE:HD12	2.23	0.54
3:G:46:GLU:O	3:G:163:THR:HA	2.08	0.54
3:H:77:GLY:HA2	3:H:132:VAL:HG11	1.90	0.54
1:C:90:ARG:HH12	3:H:2:PRO:HB2	1.73	0.53
1:C:152:ARG:HA	1:C:157:LEU:HD23	1.90	0.53
2:D:220:GLU:OE2	2:D:220:GLU:HA	2.08	0.53
3:I:166:PRO:O	3:I:170:PHE:HD1	1.91	0.53
1:C:143:CYS:SG	1:C:145:ASN:O	2.66	0.53
2:E:8:PRO:C	2:E:10:LYS:H	2.12	0.53
2:F:47:MET:SD	2:F:138:THR:CG2	2.97	0.53
2:F:145:SER:HG	2:F:159:ILE:HB	1.72	0.53
3:G:76:ARG:HB3	3:G:121:LEU:HB3	1.90	0.53
1:A:97:VAL:HG12	1:A:105:VAL:HG13	1.89	0.53
1:B:10:ILE:HG22	1:B:11:GLY:N	2.23	0.53
2:D:35:VAL:HG23	2:D:36:LEU:HG	1.90	0.53
3:I:43:GLU:CD	3:I:43:GLU:N	2.60	0.53
1:A:141:ALA:HB1	1:A:168:ARG:HH12	1.74	0.53
2:F:45:LEU:HB3	2:F:52:VAL:CG2	2.39	0.53
2:D:216:LYS:HE2	3:G:239:ASP:CG	2.28	0.53
3:I:215:THR:HB	3:I:224:ALA:HB3	1.89	0.53
1:A:100:VAL:O	1:A:131:THR:HB	2.08	0.53
2:E:8:PRO:O	2:E:9:GLU:HG2	2.08	0.53
3:G:46:GLU:N	3:G:46:GLU:OE1	2.40	0.53
3:H:76:ARG:HA	3:H:122:SER:HA	1.90	0.53
3:H:188:THR:OG1	3:H:213:THR:HG23	2.09	0.53
2:E:158:MET:CE	2:E:233:GLN:NE2	2.72	0.53
3:H:66:PRO:HD3	3:H:133:TRP:CZ3	2.44	0.53
1:A:164:ARG:CG	1:A:165:VAL:H	2.21	0.53
1:C:62:LEU:HD12	1:C:118:LEU:O	2.08	0.53
2:E:135:GLY:HA2	2:E:137:ARG:HH12	1.72	0.53
1:A:117:ILE:HD12	1:A:140:ARG:HH21	1.74	0.52
1:B:120:ALA:HB1	1:B:129:LEU:HB3	1.91	0.52
1:B:123:ILE:O	1:B:128:ARG:HB2	2.09	0.52
3:H:85:LEU:O	3:H:93:PHE:CD1	2.61	0.52
1:C:123:ILE:HG13	1:C:130:SER:HB2	1.90	0.52
2:F:19:ASP:OD1	2:F:21:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:69:PRO:CD	3:I:130:GLU:HA	2.39	0.52
2:E:19:ASP:OD1	2:E:21:ARG:HG3	2.09	0.52
3:G:237:LEU:O	3:G:238:PHE:C	2.45	0.52
3:H:53:LEU:O	3:H:56:THR:HB	2.09	0.52
3:I:39:PRO:O	3:I:40:ASN:HB2	2.09	0.52
2:E:206:MET:HE1	3:H:222:VAL:HG12	1.89	0.52
3:G:254:GLU:C	3:G:256:PHE:N	2.63	0.52
3:H:120:ASP:OD2	3:H:122:SER:OG	2.24	0.52
1:B:145:ASN:ND2	1:B:146:CYS:SG	2.83	0.52
2:D:13:VAL:O	2:D:14:ASP:HB2	2.09	0.52
3:H:42:ILE:HG22	3:H:45:ALA:CB	2.39	0.52
1:C:5:MET:HG3	2:F:234:ARG:HG3	1.91	0.52
2:E:106:LYS:HE2	2:E:110:GLU:OE1	2.10	0.52
2:E:201:ILE:CD1	2:E:204:LEU:HB2	2.40	0.52
3:H:81:VAL:HB	3:H:110:ASP:HB2	1.92	0.52
1:A:143:CYS:SG	1:A:145:ASN:HB3	2.50	0.52
1:C:61:VAL:HG13	1:C:79:SER:O	2.10	0.52
3:H:90:SER:CA	3:H:202:ARG:HH12	2.21	0.52
1:C:9:ARG:HG2	1:C:9:ARG:HH21	1.74	0.52
2:F:110:GLU:CG	2:F:115:LYS:HE2	2.40	0.52
2:F:204:LEU:HD11	3:I:225:MET:HE1	1.92	0.52
2:E:37:LYS:HD2	3:G:55:ASP:OD1	2.09	0.52
2:F:81:MET:HA	2:F:129:VAL:HG13	1.92	0.52
1:A:164:ARG:HG3	1:A:165:VAL:N	2.21	0.52
1:B:169:LYS:HB3	1:B:169:LYS:HZ2	1.75	0.52
1:C:95:LEU:HD23	1:C:129:LEU:HB2	1.92	0.52
2:E:64:PRO:O	2:E:65:GLU:HB3	2.08	0.52
2:F:244:VAL:O	2:F:247:GLU:HG2	2.10	0.52
2:D:160:THR:CG2	2:D:233:GLN:NE2	2.69	0.51
1:A:81:LYS:HB2	1:A:179:TRP:CZ3	2.45	0.51
2:E:31:ILE:HG12	2:E:45:LEU:HD22	1.93	0.51
2:E:128:GLU:CG	3:G:140:HIS:CE1	2.92	0.51
3:G:212:LEU:HD23	3:G:213:THR:N	2.24	0.51
3:G:1:MET:H2	3:G:4:ASP:HB3	1.73	0.51
3:G:196:TYR:HB3	3:G:241:LEU:HD22	1.91	0.51
3:I:60:VAL:HG22	3:I:139:ILE:HA	1.92	0.51
2:D:21:ARG:CZ	2:D:27:ARG:HG3	2.41	0.51
2:D:191:PHE:CG	2:D:198:ILE:HD13	2.45	0.51
3:G:45:ALA:O	3:G:47:GLY:N	2.44	0.51
3:G:105:LEU:HD11	3:G:149:LEU:HA	1.93	0.51
1:C:177:GLY:O	3:H:9:ILE:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:VAL:CG1	1:C:113:GLY:N	2.74	0.51
3:G:1:MET:N	3:G:5:ILE:HD12	2.25	0.51
3:I:132:VAL:HG22	3:I:133:TRP:N	2.25	0.51
1:A:75:ILE:HD12	1:A:75:ILE:N	2.25	0.50
2:E:21:ARG:NH1	2:E:174:ASP:O	2.44	0.50
3:H:9:ILE:O	3:H:12:ASP:HB2	2.10	0.50
3:H:220:ASP:OD2	3:H:250:ARG:NH2	2.43	0.50
1:B:5:MET:HG3	2:E:234:ARG:HG3	1.92	0.50
2:E:103:LYS:O	2:E:107:GLU:HG3	2.10	0.50
2:E:210:MET:CE	2:E:215:VAL:HA	2.42	0.50
1:B:126:ASN:O	1:B:127:LEU:HB2	2.11	0.50
3:G:77:GLY:HA2	3:G:132:VAL:CG2	2.41	0.50
3:I:69:PRO:HD2	3:I:130:GLU:HA	1.94	0.50
1:A:162:CYS:SG	1:A:164:ARG:HB3	2.52	0.50
1:B:5:MET:HG3	2:E:234:ARG:CG	2.41	0.50
2:E:163:ALA:O	2:E:175:PRO:HD3	2.12	0.50
2:F:209:ARG:HH22	3:I:116:SER:C	2.14	0.50
3:G:31:GLU:O	3:G:198:VAL:HG12	2.12	0.50
3:G:192:VAL:HG22	3:G:192:VAL:O	2.12	0.50
3:H:219:ASP:O	3:H:220:ASP:HB2	2.10	0.50
1:B:77:VAL:HG21	1:B:127:LEU:HD13	1.93	0.49
2:D:89:ARG:O	2:D:89:ARG:HG2	2.12	0.49
2:D:209:ARG:HD3	3:G:221:ASN:ND2	2.27	0.49
3:H:250:ARG:HH21	3:H:250:ARG:CG	2.15	0.49
2:E:206:MET:CB	3:H:225:MET:HG3	2.42	0.49
3:G:198:VAL:HB	3:G:199:ASP:CB	2.42	0.49
2:D:17:ARG:NH1	2:D:172:VAL:HB	2.26	0.49
2:D:30:LYS:HE3	2:D:46:GLU:OE2	2.12	0.49
2:E:13:VAL:O	2:E:14:ASP:C	2.50	0.49
2:E:84:PHE:CD1	3:G:61:GLY:HA3	2.47	0.49
1:A:6:PRO:HA	1:A:31:ALA:O	2.12	0.49
2:D:198:ILE:HD11	2:D:226:ALA:HB3	1.94	0.49
2:E:144:ALA:O	2:E:148:LEU:HD22	2.13	0.49
3:H:250:ARG:NH2	3:H:250:ARG:CG	2.74	0.49
3:H:257:LYS:HD2	3:H:257:LYS:H	1.75	0.49
1:A:22:VAL:HG13	1:A:30:PHE:O	2.12	0.49
2:D:46:GLU:HA	2:D:50:ASN:O	2.12	0.49
2:E:50:ASN:HD22	2:E:50:ASN:H	1.60	0.49
2:F:129:VAL:CG2	2:F:132:ALA:HB2	2.42	0.49
3:H:75:ASP:C	3:H:76:ARG:HG2	2.31	0.49
2:F:212:ARG:HG2	3:I:242:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:168:GLU:HG3	3:H:175:ASP:OD2	2.12	0.49
1:A:123:ILE:HD12	1:A:124:GLY:N	2.27	0.49
1:B:67:ASP:HB3	1:B:74:LEU:HB2	1.95	0.49
1:C:76:GLU:O	1:C:76:GLU:CG	2.60	0.49
3:I:33:ARG:NH2	3:I:199:ASP:OD2	2.45	0.49
1:A:119:LYS:HB2	1:A:139:LEU:CD1	2.41	0.49
3:H:214:ILE:HG12	3:H:225:MET:CE	2.43	0.49
1:B:156:ILE:HD11	1:B:167:LYS:CA	2.28	0.49
2:D:193:ILE:CD1	2:D:198:ILE:HG12	2.43	0.49
3:H:38:ILE:HD12	3:H:38:ILE:N	2.27	0.49
2:D:10:LYS:HD3	2:D:168:ASP:OD1	2.11	0.49
2:E:64:PRO:O	2:E:65:GLU:CB	2.61	0.49
3:G:23:ARG:NH2	3:G:198:VAL:HG22	2.28	0.49
3:G:32:PHE:CE1	3:G:199:ASP:HB2	2.48	0.49
2:E:133:ASP:OD2	2:E:134:ALA:N	2.46	0.48
2:F:176:MET:HG2	2:F:179:GLU:OE2	2.13	0.48
1:B:121:ARG:HD2	1:B:133:GLU:OE1	2.13	0.48
2:D:184:GLU:O	2:D:185:ALA:HB2	2.13	0.48
2:F:11:LEU:HA	2:F:18:LEU:HD11	1.94	0.48
2:F:137:ARG:H	2:F:137:ARG:HD3	1.77	0.48
3:G:77:GLY:O	3:G:121:LEU:HD23	2.13	0.48
3:I:103:ILE:O	3:I:107:ARG:HG3	2.13	0.48
1:A:104:TYR:HD2	1:A:105:VAL:H	1.61	0.48
2:D:17:ARG:HH12	2:D:173:LEU:N	2.09	0.48
2:D:81:MET:HE2	2:D:90:LYS:HD3	1.96	0.48
3:G:110:ASP:OD2	3:G:114:ARG:NH2	2.45	0.48
2:D:166:LYS:HB3	2:D:185:ALA:HB3	1.95	0.48
2:E:141:LEU:HD11	2:E:203:LEU:CD1	2.44	0.48
1:B:61:VAL:HB	1:B:77:VAL:HG13	1.95	0.48
2:F:60:ARG:NH1	3:H:91:PRO:HB3	2.29	0.48
2:D:163:ALA:O	2:D:175:PRO:CD	2.61	0.48
2:E:8:PRO:O	2:E:10:LYS:N	2.45	0.48
3:G:225:MET:HE1	3:G:238:PHE:CZ	2.49	0.48
3:I:36:GLU:HB2	3:I:52:LYS:HB2	1.95	0.48
1:A:71:SER:O	1:A:97:VAL:HG22	2.14	0.48
1:C:123:ILE:CG1	1:C:130:SER:HB2	2.43	0.48
3:G:23:ARG:NH2	3:G:198:VAL:CG1	2.61	0.48
2:F:64:PRO:CB	2:F:66:HIS:CD2	2.97	0.48
1:A:4:VAL:O	1:A:34:ALA:HA	2.14	0.48
1:B:18:LYS:HG2	1:B:22:VAL:O	2.14	0.48
2:F:47:MET:SD	2:F:138:THR:HG22	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:SER:HB3	2:F:158:MET:CE	2.44	0.48
3:I:74:PRO:O	3:I:75:ASP:HB3	2.13	0.48
1:C:152:ARG:HD2	1:C:170:ILE:HG21	1.96	0.47
2:D:69:ASP:OD1	2:D:70:PRO:CD	2.62	0.47
2:E:10:LYS:HD3	2:E:10:LYS:C	2.34	0.47
2:F:75:ILE:HG22	2:F:106:LYS:HG3	1.95	0.47
3:H:157:ILE:HG23	3:H:256:PHE:HE1	1.77	0.47
1:A:150:MET:CE	1:A:166:GLU:HB2	2.44	0.47
1:B:10:ILE:HG22	1:B:11:GLY:H	1.78	0.47
2:D:189:PHE:CE2	2:D:219:ILE:HG12	2.49	0.47
2:D:217:GLN:O	2:D:220:GLU:N	2.44	0.47
3:G:51:VAL:O	3:G:57:GLN:HA	2.14	0.47
3:H:154:LEU:O	3:H:157:ILE:HG22	2.15	0.47
1:A:119:LYS:HD2	1:A:139:LEU:HD21	1.96	0.47
2:E:86:VAL:HG11	4:Z:6:C:C2	2.49	0.47
2:F:50:ASN:OD1	2:F:136:SER:HB3	2.14	0.47
2:F:60:ARG:NH2	2:F:124:ASP:OD1	2.47	0.47
2:D:65:GLU:OE2	2:D:66:HIS:N	2.45	0.47
2:D:69:ASP:OD1	2:D:70:PRO:HD2	2.14	0.47
3:G:196:TYR:N	3:G:196:TYR:CD2	2.69	0.47
3:I:77:GLY:HA2	3:I:132:VAL:CG2	2.45	0.47
3:I:174:GLU:HG2	3:I:175:ASP:N	2.29	0.47
3:G:75:ASP:O	3:G:76:ARG:HG2	2.15	0.47
3:G:77:GLY:HA2	3:G:132:VAL:HG21	1.97	0.47
1:B:102:GLU:HB2	1:B:132:LYS:HB3	1.94	0.47
2:D:81:MET:HA	2:D:129:VAL:HG22	1.97	0.47
2:D:249:ASP:O	2:D:250:GLU:C	2.52	0.47
2:F:53:ILE:HG23	3:H:88:LEU:HD21	1.95	0.47
3:H:51:VAL:HG23	3:H:155:ALA:HB2	1.96	0.47
1:B:164:ARG:HG2	1:B:165:VAL:N	2.30	0.47
1:C:9:ARG:HH21	1:C:9:ARG:CG	2.27	0.47
2:D:167:ALA:O	2:D:168:ASP:C	2.53	0.47
2:D:205:GLN:HE21	3:G:226:GLN:HE22	1.62	0.47
2:E:42:SER:HA	2:E:54:ALA:O	2.15	0.47
3:G:24:ILE:HD11	3:G:204:GLU:HG3	1.96	0.47
3:H:1:MET:N	3:H:2:PRO:CD	2.76	0.47
3:I:41:VAL:HG21	3:I:50:LEU:HB2	1.95	0.47
3:I:196:TYR:O	3:I:196:TYR:CD1	2.68	0.47
1:B:64:ARG:CZ	3:G:5:ILE:HG13	2.45	0.47
2:D:210:MET:CE	2:D:215:VAL:HA	2.44	0.47
2:F:110:GLU:HG2	2:F:115:LYS:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ILE:CG2	1:B:122:VAL:HG21	2.44	0.47
2:E:219:ILE:O	2:E:223:LYS:HG3	2.15	0.47
3:H:38:ILE:HA	3:H:39:PRO:HD3	1.73	0.47
3:I:1:MET:HB2	3:I:2:PRO:HD3	1.97	0.47
3:I:147:ASN:HD21	3:I:150:ASP:H	1.63	0.47
1:A:56:VAL:HG22	1:A:59:ASP:OD1	2.15	0.47
3:G:23:ARG:CZ	3:G:198:VAL:HG22	2.44	0.47
2:E:138:THR:HG22	2:E:161:SER:OG	2.15	0.46
2:F:145:SER:HB3	2:F:158:MET:HE1	1.97	0.46
2:E:53:ILE:HG23	2:E:128:GLU:HB3	1.97	0.46
3:G:118:ALA:HA	3:G:182:ASP:H	1.80	0.46
1:C:55:ILE:O	1:C:89:ASN:ND2	2.48	0.46
3:H:35:VAL:HA	3:H:52:LYS:O	2.15	0.46
3:H:157:ILE:HG23	3:H:256:PHE:CE1	2.50	0.46
2:D:52:VAL:CG1	2:D:53:ILE:N	2.78	0.46
3:G:65:GLN:HA	3:G:133:TRP:HZ3	1.81	0.46
1:A:138:VAL:O	1:A:174:TYR:HD1	1.99	0.46
2:D:211:THR:HG23	2:D:214:GLU:HB2	1.98	0.46
3:H:72:ASP:OD1	3:H:72:ASP:C	2.54	0.46
2:D:181:ASN:O	2:D:182:PHE:CD2	2.68	0.46
2:E:8:PRO:O	2:E:9:GLU:CG	2.62	0.46
2:E:23:PHE:CE2	2:E:24:ASP:HB3	2.50	0.46
2:F:126:PHE:CD2	3:H:87:PRO:HB2	2.51	0.46
1:A:114:TYR:O	1:A:115:LEU:HB2	2.16	0.46
1:B:100:VAL:HG23	1:B:169:LYS:HD2	1.98	0.46
1:B:131:THR:HG21	1:B:137:GLY:HA2	1.97	0.46
1:C:28:GLU:O	1:C:29:LEU:HD23	2.16	0.46
2:F:190:ALA:HB3	2:F:203:LEU:HB3	1.97	0.46
3:G:1:MET:O	3:G:1:MET:HG3	2.15	0.46
1:B:59:ASP:OD2	1:B:80:LYS:HE3	2.16	0.46
2:F:95:ASP:O	2:F:99:ILE:HG12	2.16	0.46
3:H:25:ASP:OD2	3:H:27:ARG:CD	2.64	0.46
3:I:92:THR:O	3:I:92:THR:HG23	2.15	0.46
1:C:68:LEU:HD22	1:C:108:ILE:CG1	2.46	0.46
2:D:89:ARG:HD3	3:I:136:PHE:CG	2.51	0.46
2:D:200:SER:HB3	3:G:232:LEU:HB3	1.96	0.46
2:E:49:LYS:HA	2:E:49:LYS:HD3	1.62	0.46
2:D:58:GLY:HA2	2:D:60:ARG:HG2	1.97	0.46
2:D:79:TYR:CD2	2:D:79:TYR:O	2.69	0.46
2:E:194:ARG:O	2:E:195:ASN:HB3	2.15	0.46
3:G:18:LEU:HD23	3:G:18:LEU:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:198:VAL:CB	3:G:199:ASP:C	2.75	0.46
3:H:79:ILE:HG12	3:H:135:VAL:HB	1.98	0.46
3:H:221:ASN:N	3:H:221:ASN:HD22	2.14	0.46
1:A:48:SER:C	1:A:50:SER:H	2.18	0.45
3:G:251:LYS:HB2	3:G:251:LYS:HE3	1.77	0.45
3:I:225:MET:CE	3:I:238:PHE:CE1	2.99	0.45
1:B:57:LYS:HA	1:B:122:VAL:HG12	1.99	0.45
1:B:120:ALA:CB	1:B:129:LEU:HB3	2.46	0.45
2:D:148:LEU:HD22	2:D:153:VAL:HG21	1.98	0.45
2:E:19:ASP:CG	2:E:21:ARG:HG3	2.37	0.45
2:E:56:VAL:HG22	2:E:125:ILE:HG12	1.98	0.45
3:H:85:LEU:HD22	3:H:102:SER:HA	1.98	0.45
1:A:12:SER:O	1:A:15:GLU:HB3	2.17	0.45
1:B:110:GLU:HG2	1:B:167:LYS:O	2.16	0.45
3:I:225:MET:HE2	3:I:225:MET:HB3	1.62	0.45
3:H:58:VAL:HG11	3:H:151:ALA:HB1	1.98	0.45
3:I:57:GLN:HG2	3:I:143:ASP:HB3	1.99	0.45
3:I:196:TYR:C	3:I:196:TYR:CD1	2.89	0.45
1:B:152:ARG:HH11	1:B:170:ILE:HD12	1.81	0.45
2:D:179:GLU:O	2:D:183:GLY:HA3	2.16	0.45
2:F:64:PRO:HB3	2:F:66:HIS:CD2	2.52	0.45
3:H:3:GLU:OE1	3:H:4:ASP:OD1	2.35	0.45
3:G:183:LEU:HD13	3:G:253:ARG:HG2	1.98	0.45
2:D:173:LEU:HD12	2:D:173:LEU:HA	1.81	0.45
2:E:141:LEU:CD1	2:E:203:LEU:HD13	2.47	0.45
3:H:125:VAL:HA	3:H:132:VAL:HG22	1.96	0.45
3:I:144:ASP:HB2	3:I:148:LEU:HD11	1.98	0.45
2:D:77:TYR:HA	2:D:125:ILE:O	2.17	0.45
2:D:47:MET:HE3	2:D:47:MET:HB3	1.66	0.45
2:E:107:GLU:HA	2:E:110:GLU:HG3	1.99	0.45
2:F:63:HIS:HA	2:F:64:PRO:C	2.37	0.45
3:H:89:ALA:HB2	3:H:142:LEU:C	2.37	0.45
3:H:124:LEU:O	3:H:132:VAL:HG22	2.17	0.45
2:D:77:TYR:C	2:D:77:TYR:CD2	2.90	0.45
2:D:77:TYR:HB3	2:D:106:LYS:HB2	1.99	0.45
2:E:201:ILE:HG23	3:H:233:LEU:O	2.17	0.44
3:G:126:ILE:HB	3:G:131:LYS:C	2.37	0.44
1:A:35:GLY:HA3	1:A:47:GLU:O	2.18	0.44
3:G:116:SER:CB	3:G:184:PRO:HG3	2.47	0.44
3:H:251:LYS:HD2	3:H:251:LYS:H	1.82	0.44
2:D:10:LYS:HE2	2:D:12:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:ARG:HD3	3:G:103:ILE:HD12	1.99	0.44
3:G:1:MET:N	3:G:2:PRO:HA	2.32	0.44
3:H:17:LYS:HD2	3:H:17:LYS:HA	1.67	0.44
3:I:65:GLN:HA	3:I:133:TRP:HZ3	1.82	0.44
3:I:210:THR:HB	3:I:231:TYR:CD2	2.52	0.44
1:A:72:ILE:O	1:A:72:ILE:CG2	2.65	0.44
2:F:135:GLY:O	2:F:138:THR:HB	2.17	0.44
3:I:63:LYS:HB3	3:I:63:LYS:HE3	1.89	0.44
1:A:97:VAL:HA	1:A:100:VAL:CG2	2.47	0.44
2:D:225:GLY:O	2:D:229:ILE:HG13	2.17	0.44
2:F:45:LEU:HD13	2:F:46:GLU:N	2.32	0.44
3:G:122:SER:O	3:G:125:VAL:HG23	2.18	0.44
1:B:86:GLY:HA2	1:B:87:PRO:HD3	1.87	0.44
1:B:150:MET:HE1	1:B:159:CYS:HB2	1.99	0.44
2:D:37:LYS:HD3	2:D:37:LYS:HA	1.62	0.44
2:D:211:THR:HG23	2:D:214:GLU:CG	2.48	0.44
1:A:13:ALA:HB2	1:A:27:GLY:O	2.18	0.44
1:B:56:VAL:CG1	1:B:57:LYS:N	2.81	0.44
2:D:75:ILE:HD12	2:D:123:ILE:HB	2.00	0.44
3:H:2:PRO:HD2	3:H:3:GLU:H	1.83	0.44
3:I:81:VAL:HB	3:I:110:ASP:HB2	2.00	0.44
1:A:108:ILE:CG1	1:A:108:ILE:O	2.66	0.44
2:D:72:LYS:O	2:D:119:PRO:HA	2.18	0.44
2:E:67:LEU:HD23	2:E:67:LEU:HA	1.82	0.44
2:F:110:GLU:HG3	2:F:115:LYS:HE2	2.00	0.44
3:H:169:ARG:HD2	3:H:170:PHE:CE2	2.53	0.44
3:I:232:LEU:HD23	3:I:232:LEU:HA	1.82	0.44
2:E:33:ALA:HB3	2:E:240:ARG:HG2	1.99	0.43
3:G:32:PHE:CD1	3:G:199:ASP:HB2	2.53	0.43
3:I:41:VAL:HG21	3:I:50:LEU:CB	2.48	0.43
3:I:165:VAL:HA	3:I:166:PRO:HD3	1.88	0.43
1:B:157:LEU:HD21	1:B:168:ARG:HB2	2.01	0.43
2:D:131:GLN:NE2	3:I:44:LYS:H	2.16	0.43
2:D:219:ILE:HG21	3:G:235:GLU:OE2	2.17	0.43
2:E:221:LEU:HD23	2:E:221:LEU:HA	1.72	0.43
2:F:127:VAL:HG11	2:F:140:CYS:CB	2.48	0.43
3:H:14:VAL:HG21	3:H:204:GLU:HA	2.00	0.43
1:B:52:ILE:HA	1:B:53:PRO:HD3	1.89	0.43
2:D:110:GLU:O	2:D:115:LYS:HE2	2.17	0.43
2:F:51:LYS:HG3	2:F:131:GLN:HB3	2.01	0.43
2:F:81:MET:HB2	2:F:90:LYS:CE	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:VAL:HG22	2:D:67:LEU:CD2	2.45	0.43
2:F:13:VAL:O	2:F:13:VAL:HG22	2.18	0.43
2:E:81:MET:CE	2:E:86:VAL:HG13	2.49	0.43
3:G:2:PRO:HA	3:G:5:ILE:CD1	2.48	0.43
3:G:46:GLU:HG2	3:G:62:VAL:O	2.19	0.43
3:G:108:VAL:HG11	3:G:149:LEU:HD11	2.00	0.43
3:H:46:GLU:CG	3:H:166:PRO:HG3	2.46	0.43
3:H:201:SER:HB2	3:H:204:GLU:H	1.83	0.43
1:C:159:CYS:HA	1:C:160:PRO:HD3	1.76	0.43
2:E:141:LEU:HD11	2:E:203:LEU:HD13	2.00	0.43
3:G:1:MET:H1	3:G:5:ILE:CD1	2.30	0.43
3:H:21:ASN:CG	3:H:21:ASN:O	2.57	0.43
1:B:121:ARG:HG3	1:B:122:VAL:N	2.33	0.43
1:C:59:ASP:O	1:C:122:VAL:HG23	2.18	0.43
2:F:209:ARG:NH2	3:I:116:SER:HA	2.34	0.43
3:G:170:PHE:O	3:G:171:ASP:HB2	2.19	0.43
3:H:214:ILE:HG12	3:H:225:MET:HE2	2.00	0.43
3:I:64:MET:HG3	3:I:166:PRO:HD3	2.00	0.43
1:A:99:ASN:O	1:A:132:LYS:HG3	2.19	0.43
1:B:138:VAL:HG21	1:B:168:ARG:HD2	1.99	0.43
2:E:29:ILE:CD1	2:E:229:ILE:HD13	2.48	0.43
3:G:178:LEU:HD23	3:G:179:PRO:N	2.33	0.43
3:H:165:VAL:HA	3:H:166:PRO:HD3	1.78	0.43
2:D:219:ILE:O	2:D:223:LYS:HG2	2.18	0.43
3:G:144:ASP:CA	3:G:148:LEU:HD21	2.40	0.43
3:H:242:LEU:HD23	3:H:242:LEU:HA	1.78	0.43
2:E:30:LYS:C	2:E:31:ILE:HG13	2.39	0.43
3:I:237:LEU:O	3:I:237:LEU:HD23	2.18	0.43
1:A:38:ILE:HD11	1:A:47:GLU:OE2	2.19	0.42
1:A:68:LEU:HD11	1:A:112:VAL:O	2.18	0.42
1:B:121:ARG:O	1:B:129:LEU:HA	2.19	0.42
1:C:68:LEU:HD22	1:C:108:ILE:HG13	2.00	0.42
1:C:77:VAL:HG23	1:C:93:GLY:H	1.84	0.42
2:E:127:VAL:HG11	2:E:140:CYS:HB3	2.01	0.42
3:G:77:GLY:HA2	3:G:132:VAL:HB	2.01	0.42
3:H:64:MET:HE2	3:H:135:VAL:HG22	2.01	0.42
3:H:190:LEU:HB2	3:H:200:PRO:CG	2.48	0.42
1:B:65:VAL:HG12	1:B:116:ASP:O	2.19	0.42
2:D:60:ARG:H	2:D:60:ARG:HG3	1.72	0.42
2:E:203:LEU:C	2:E:203:LEU:CD2	2.84	0.42
3:H:3:GLU:H	3:H:3:GLU:CD	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:MET:HB2	1:B:174:TYR:OH	2.19	0.42
1:C:142:LEU:HD22	1:C:147:LYS:O	2.19	0.42
2:E:53:ILE:CG2	2:E:128:GLU:HB3	2.49	0.42
3:G:236:LYS:O	3:G:239:ASP:HB2	2.19	0.42
3:H:107:ARG:HH11	4:Z:5:C:P	2.43	0.42
3:I:57:GLN:HG2	3:I:143:ASP:CB	2.49	0.42
3:I:77:GLY:HA2	3:I:132:VAL:HG22	2.00	0.42
1:A:99:ASN:HA	1:A:132:LYS:CE	2.41	0.42
1:A:101:ASP:HA	1:A:132:LYS:HA	2.01	0.42
1:B:103:GLY:O	1:B:104:TYR:HB2	2.20	0.42
3:G:234:ASP:OD1	3:G:234:ASP:C	2.58	0.42
3:H:190:LEU:HD13	3:H:192:VAL:CG2	2.49	0.42
1:B:128:ARG:CG	1:B:128:ARG:NH2	2.58	0.42
1:C:108:ILE:H	1:C:108:ILE:CD1	2.27	0.42
2:F:26:LEU:HD12	2:F:228:GLN:HE21	1.85	0.42
2:F:69:ASP:CG	2:F:72:LYS:HG2	2.39	0.42
2:F:142:ASN:O	2:F:146:VAL:HG23	2.19	0.42
3:G:242:LEU:HD23	3:G:242:LEU:C	2.40	0.42
3:H:124:LEU:H	3:H:124:LEU:HG	1.48	0.42
1:A:56:VAL:HG23	1:A:57:LYS:O	2.19	0.42
1:B:22:VAL:HG23	1:B:46:VAL:CG2	2.47	0.42
2:D:24:ASP:HB3	2:D:221:LEU:HD21	2.01	0.42
2:D:69:ASP:HA	2:D:70:PRO:HD3	1.83	0.42
2:D:194:ARG:NH2	2:D:199:GLU:OE2	2.53	0.42
3:G:81:VAL:O	3:G:106:ALA:HB1	2.19	0.42
3:G:178:LEU:HA	3:G:179:PRO:HD3	1.83	0.42
1:C:179:TRP:CE3	1:C:179:TRP:OXT	2.73	0.42
2:D:77:TYR:HE2	2:D:79:TYR:HB2	1.83	0.42
2:D:129:VAL:O	2:D:129:VAL:CG2	2.68	0.42
2:E:17:ARG:NH2	2:E:21:ARG:NH1	2.68	0.42
2:E:22:LYS:H	2:E:22:LYS:HG3	1.63	0.42
3:H:2:PRO:HD2	3:H:3:GLU:CD	2.40	0.42
1:C:41:ASP:C	1:C:43:VAL:H	2.23	0.42
2:D:17:ARG:NH1	2:D:23:PHE:O	2.52	0.42
3:G:191:ILE:HD12	3:G:191:ILE:N	2.35	0.42
3:H:89:ALA:HB2	3:H:143:ASP:HA	2.01	0.42
3:I:120:ASP:HA	3:I:181:ARG:NH2	2.34	0.42
3:I:178:LEU:HG	3:I:179:PRO:HD2	2.02	0.42
1:B:7:GLY:O	1:B:30:PHE:HD2	2.03	0.42
1:B:55:ILE:H	1:B:55:ILE:HG12	1.47	0.42
2:D:101:ILE:O	2:D:104:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:77:TYR:HA	2:E:125:ILE:O	2.20	0.42
2:F:37:LYS:HE2	3:H:145:ASP:OD1	2.19	0.42
3:H:127:GLU:O	3:H:128:GLU:C	2.57	0.42
3:I:225:MET:CE	3:I:238:PHE:HE1	2.33	0.42
1:B:101:ASP:O	1:B:102:GLU:HB3	2.20	0.42
1:B:157:LEU:O	1:B:165:VAL:HG13	2.20	0.42
2:D:165:GLY:HA3	2:D:175:PRO:CG	2.48	0.42
3:G:198:VAL:HB	3:G:199:ASP:HB3	2.02	0.42
2:D:197:LYS:HD3	2:D:197:LYS:HA	1.91	0.41
2:E:24:ASP:OD1	2:E:24:ASP:N	2.53	0.41
2:E:53:ILE:HG13	2:E:54:ALA:N	2.33	0.41
2:F:96:ARG:HD3	3:I:103:ILE:HD13	2.02	0.41
3:H:178:LEU:HA	3:H:179:PRO:HD3	1.88	0.41
3:I:225:MET:HE3	3:I:238:PHE:CE1	2.54	0.41
1:B:131:THR:HG22	1:B:131:THR:O	2.19	0.41
1:B:150:MET:CE	1:B:159:CYS:HB2	2.50	0.41
1:C:53:PRO:HG2	1:C:87:PRO:HA	2.01	0.41
2:D:148:LEU:HA	2:D:148:LEU:HD23	1.66	0.41
2:E:198:ILE:H	2:E:198:ILE:HG12	1.52	0.41
2:F:148:LEU:HD23	2:F:153:VAL:HG11	2.01	0.41
3:G:126:ILE:H	3:G:132:VAL:HA	1.85	0.41
3:I:212:LEU:HD22	3:I:213:THR:N	2.35	0.41
1:A:77:VAL:O	1:A:90:ARG:HB2	2.20	0.41
1:A:115:LEU:HD21	2:F:70:PRO:HB2	2.02	0.41
1:A:15:GLU:HG2	1:A:16:TYR:CD1	2.55	0.41
1:B:143:CYS:HB2	1:B:150:MET:HE1	2.01	0.41
3:G:198:VAL:CB	3:G:199:ASP:CA	2.87	0.41
3:H:41:VAL:HG23	3:H:42:ILE:HD13	2.02	0.41
3:H:89:ALA:O	3:H:93:PHE:CD1	2.73	0.41
3:H:100:GLU:H	3:H:100:GLU:HG3	1.68	0.41
3:H:170:PHE:O	3:H:172:LEU:HD13	2.20	0.41
3:I:39:PRO:HB3	3:I:162:ASN:ND2	2.35	0.41
2:D:47:MET:O	2:D:48:GLY:C	2.57	0.41
3:H:29:PHE:O	3:H:198:VAL:HG23	2.21	0.41
3:I:85:LEU:O	3:I:93:PHE:CG	2.72	0.41
1:C:152:ARG:HH21	1:C:170:ILE:CG2	2.33	0.41
2:D:49:LYS:HE3	2:D:49:LYS:HA	2.01	0.41
2:E:126:PHE:CE2	3:G:87:PRO:HG2	2.55	0.41
2:E:158:MET:HE2	2:E:233:GLN:NE2	2.35	0.41
2:F:64:PRO:CB	2:F:66:HIS:HD2	2.33	0.41
3:G:127:GLU:HG2	3:G:131:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PRO:O	1:A:161:GLU:C	2.58	0.41
1:B:157:LEU:HD12	1:B:166:GLU:O	2.21	0.41
2:D:248:MET:O	2:D:250:GLU:CG	2.69	0.41
2:E:35:VAL:N	2:E:42:SER:OG	2.54	0.41
3:G:8:ASP:O	3:G:11:ARG:HB3	2.20	0.41
3:G:190:LEU:C	3:G:190:LEU:HD13	2.41	0.41
1:C:97:VAL:HG22	1:C:108:ILE:CG2	2.39	0.41
2:E:201:ILE:HD13	2:E:204:LEU:HB2	2.02	0.41
3:G:194:ASN:HA	3:G:237:LEU:HD21	2.03	0.41
3:G:199:ASP:HA	3:G:200:PRO:HD2	1.97	0.41
3:I:59:VAL:HG23	3:I:142:LEU:CD1	2.47	0.41
1:B:28:GLU:C	1:B:29:LEU:HD23	2.40	0.41
1:C:115:LEU:HD11	2:E:70:PRO:HB2	2.02	0.41
2:D:67:LEU:N	2:D:67:LEU:CD2	2.80	0.41
2:D:158:MET:CE	2:D:233:GLN:NE2	2.84	0.41
2:F:166:LYS:HE3	2:F:214:GLU:OE1	2.20	0.41
3:G:38:ILE:HD13	3:G:50:LEU:HD23	2.03	0.41
3:H:216:THR:HG21	3:H:246:ILE:HG23	2.03	0.41
2:E:134:ALA:O	2:E:135:GLY:C	2.58	0.41
3:G:27:ARG:NE	3:G:33:ARG:HG3	2.36	0.41
3:H:6:LEU:HD23	3:H:6:LEU:HA	1.88	0.41
3:H:88:LEU:HD12	3:H:88:LEU:HA	1.78	0.41
1:A:104:TYR:HD2	1:A:105:VAL:N	2.18	0.40
1:A:167:LYS:HD3	1:A:168:ARG:H	1.83	0.40
1:B:96:HIS:O	1:B:100:VAL:HG12	2.20	0.40
2:D:27:ARG:HB3	2:D:28:PRO:CD	2.51	0.40
2:D:166:LYS:HD2	2:D:214:GLU:OE2	2.21	0.40
2:E:38:ARG:HA	2:E:38:ARG:HD3	1.87	0.40
2:E:201:ILE:HD11	2:E:204:LEU:HB2	2.02	0.40
2:F:201:ILE:HB	3:I:233:LEU:HB3	2.03	0.40
3:G:118:ALA:O	3:G:119:VAL:HG23	2.21	0.40
3:G:197:LEU:C	3:G:198:VAL:CG2	2.89	0.40
3:H:78:VAL:HG12	3:H:79:ILE:N	2.36	0.40
1:A:143:CYS:C	1:A:145:ASN:H	2.24	0.40
1:B:22:VAL:O	1:B:22:VAL:HG12	2.22	0.40
2:E:10:LYS:O	2:E:168:ASP:OD1	2.39	0.40
2:E:23:PHE:CD2	2:E:23:PHE:C	2.94	0.40
2:E:187:MET:HG2	2:E:189:PHE:CE1	2.56	0.40
2:F:19:ASP:OD1	2:F:21:ARG:CG	2.69	0.40
2:F:160:THR:HG21	2:F:226:ALA:O	2.21	0.40
3:G:212:LEU:CD1	3:G:233:LEU:HD11	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:169:ARG:O	3:I:169:ARG:HG2	2.20	0.40
1:B:159:CYS:HA	1:B:160:PRO:HD3	1.90	0.40
2:D:74:ILE:C	2:D:75:ILE:HD13	2.41	0.40
2:D:217:GLN:O	2:D:220:GLU:HB2	2.21	0.40
2:E:17:ARG:CZ	2:E:172:VAL:HB	2.52	0.40
2:E:50:ASN:HD21	2:E:133:ASP:HB3	1.85	0.40
3:G:25:ASP:CG	3:G:27:ARG:HB2	2.41	0.40
3:G:25:ASP:C	3:G:27:ARG:H	2.24	0.40
3:G:154:LEU:HD12	3:G:154:LEU:HA	1.89	0.40
3:G:248:CYS:O	3:G:252:LEU:HG	2.22	0.40
3:H:147:ASN:HD22	3:H:147:ASN:HA	1.68	0.40
3:I:8:ASP:O	3:I:11:ARG:HB3	2.21	0.40
3:I:68:GLU:HA	3:I:69:PRO:HD3	1.95	0.40
1:C:76:GLU:HA	1:C:92:ILE:HD13	2.03	0.40
1:C:102:GLU:HG2	1:C:132:LYS:HD3	2.03	0.40
1:C:125:ASP:C	1:C:127:LEU:N	2.73	0.40
2:E:229:ILE:O	2:E:230:TYR:C	2.60	0.40
2:F:79:TYR:CD2	2:F:79:TYR:C	2.95	0.40
3:I:33:ARG:NH1	3:I:145:ASP:O	2.55	0.40
3:I:65:GLN:HA	3:I:66:PRO:HD3	1.83	0.40
3:I:107:ARG:HH12	4:X:5:C:P	2.43	0.40
2:D:166:LYS:HE2	2:D:184:GLU:OE1	2.22	0.40
2:E:69:ASP:OD1	2:E:69:ASP:C	2.59	0.40
2:E:69:ASP:HA	2:E:70:PRO:HD3	1.99	0.40
2:F:53:ILE:CG2	3:H:88:LEU:HD21	2.51	0.40
3:H:252:LEU:HD23	3:H:252:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	177/179 (99%)	158 (89%)	16 (9%)	3 (2%)	9	39
1	B	177/179 (99%)	148 (84%)	23 (13%)	6 (3%)	3	20
1	C	177/179 (99%)	158 (89%)	17 (10%)	2 (1%)	14	50
2	D	241/258 (93%)	212 (88%)	28 (12%)	1 (0%)	34	72
2	E	243/258 (94%)	224 (92%)	16 (7%)	3 (1%)	13	48
2	F	244/258 (95%)	236 (97%)	7 (3%)	1 (0%)	34	72
3	G	256/259 (99%)	215 (84%)	37 (14%)	4 (2%)	9	40
3	H	256/259 (99%)	229 (90%)	25 (10%)	2 (1%)	19	57
3	I	257/259 (99%)	236 (92%)	19 (7%)	2 (1%)	19	57
All	All	2028/2088 (97%)	1816 (90%)	188 (9%)	24 (1%)	13	48

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	11	GLY
1	B	108	ILE
3	G	72	ASP
3	I	88	LEU
1	A	160	PRO
1	A	164	ARG
1	B	126	ASN
1	B	155	ASP
2	E	65	GLU
3	G	46	GLU
3	G	95	PRO
3	I	167	ALA
1	C	42	ARG
3	G	198	VAL
3	H	90	SER
2	D	177	LYS
2	E	9	GLU
2	F	65	GLU
3	H	87	PRO
1	A	103	GLY
1	B	123	ILE
1	B	156	ILE
1	C	100	VAL
2	E	31	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	149/149 (100%)	132 (89%)	17 (11%)	5 24
1	B	149/149 (100%)	117 (78%)	32 (22%)	1 5
1	C	149/149 (100%)	135 (91%)	14 (9%)	8 32
2	D	202/214 (94%)	171 (85%)	31 (15%)	2 13
2	E	204/214 (95%)	172 (84%)	32 (16%)	2 13
2	F	205/214 (96%)	174 (85%)	31 (15%)	3 14
3	G	225/226 (100%)	190 (84%)	35 (16%)	2 13
3	H	225/226 (100%)	192 (85%)	33 (15%)	3 15
3	I	226/226 (100%)	207 (92%)	19 (8%)	11 38
All	All	1734/1767 (98%)	1490 (86%)	244 (14%)	3 16

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	37	LEU
1	A	61	VAL
1	A	66	VAL
1	A	72	ILE
1	A	94	ILE
1	A	95	LEU
1	A	97	VAL
1	A	104	TYR
1	A	107	GLU
1	A	108	ILE
1	A	109	SER
1	A	115	LEU
1	A	128	ARG
1	A	144	SER
1	A	162	CYS
1	A	172	THR
1	B	22	VAL

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Mol	Chain	Res	Type
1	B	24	GLU
1	B	28	GLU
1	B	37	LEU
1	B	55	ILE
1	B	56	VAL
1	B	72	ILE
1	B	78	SER
1	B	83	GLU
1	B	84	ASN
1	B	85	ARG
1	B	92	ILE
1	B	94	ILE
1	B	97	VAL
1	B	106	LYS
1	B	108	ILE
1	B	112	VAL
1	B	118	LEU
1	B	127	LEU
1	B	128	ARG
1	B	130	SER
1	B	132	LYS
1	B	139	LEU
1	B	140	ARG
1	B	143	CYS
1	B	145	ASN
1	B	146	CYS
1	B	152	ARG
1	B	157	LEU
1	B	158	LYS
1	B	167	LYS
1	B	171	SER
1	C	1	MET
1	C	9	ARG
1	C	25	GLU
1	C	37	LEU
1	C	72	ILE
1	C	95	LEU
1	C	108	ILE
1	C	140	ARG
1	C	145	ASN
1	C	146	CYS
1	C	153	GLU

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Mol	Chain	Res	Type
1	C	156	ILE
1	C	162	CYS
1	C	168	ARG
2	D	9	GLU
2	D	10	LYS
2	D	32	GLU
2	D	37	LYS
2	D	38	ARG
2	D	45	LEU
2	D	47	MET
2	D	49	LYS
2	D	60	ARG
2	D	62	VAL
2	D	65	GLU
2	D	66	HIS
2	D	67	LEU
2	D	77	TYR
2	D	88	GLU
2	D	89	ARG
2	D	96	ARG
2	D	116	GLU
2	D	121	SER
2	D	129	VAL
2	D	138	THR
2	D	160	THR
2	D	162	VAL
2	D	201	ILE
2	D	206	MET
2	D	211	THR
2	D	221	LEU
2	D	223	LYS
2	D	228	GLN
2	D	234	ARG
2	D	249	ASP
2	E	10	LYS
2	E	18	LEU
2	E	22	LYS
2	E	45	LEU
2	E	53	ILE
2	E	62	VAL
2	E	65	GLU
2	E	68	GLN

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Mol	Chain	Res	Type
2	E	76	ARG
2	E	84	PHE
2	E	86	VAL
2	E	88	GLU
2	E	91	ARG
2	E	100	GLU
2	E	104	VAL
2	E	137	ARG
2	E	145	SER
2	E	148	LEU
2	E	159	ILE
2	E	162	VAL
2	E	171	LEU
2	E	178	GLU
2	E	199	GLU
2	E	200	SER
2	E	201	ILE
2	E	221	LEU
2	E	229	ILE
2	E	234	ARG
2	E	238	LEU
2	E	240	ARG
2	E	244	VAL
2	E	249	ASP
2	F	10	LYS
2	F	13	VAL
2	F	21	ARG
2	F	34	SER
2	F	45	LEU
2	F	53	ILE
2	F	62	VAL
2	F	63	HIS
2	F	66	HIS
2	F	67	LEU
2	F	77	TYR
2	F	95	ASP
2	F	100	GLU
2	F	110	GLU
2	F	115	LYS
2	F	128	GLU
2	F	129	VAL
2	F	137	ARG

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Mol	Chain	Res	Type
2	F	138	THR
2	F	153	VAL
2	F	168	ASP
2	F	170	GLN
2	F	194	ARG
2	F	200	SER
2	F	204	LEU
2	F	207	ASP
2	F	209	ARG
2	F	212	ARG
2	F	221	LEU
2	F	227	LEU
2	F	238	LEU
3	G	6	LEU
3	G	7	VAL
3	G	10	LYS
3	G	18	LEU
3	G	21	ASN
3	G	27	ARG
3	G	33	ARG
3	G	34	LYS
3	G	46	GLU
3	G	50	LEU
3	G	59	VAL
3	G	78	VAL
3	G	90	SER
3	G	94	GLU
3	G	99	ASP
3	G	102	SER
3	G	105	LEU
3	G	120	ASP
3	G	147	ASN
3	G	154	LEU
3	G	177	LEU
3	G	189	SER
3	G	192	VAL
3	G	194	ASN
3	G	196	TYR
3	G	198	VAL
3	G	207	VAL
3	G	218	LYS
3	G	223	VAL

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Mol	Chain	Res	Type
3	G	233	LEU
3	G	245	SER
3	G	247	ASN
3	G	253	ARG
3	G	256	PHE
3	G	257	LYS
3	H	3	GLU
3	H	4	ASP
3	H	16	SER
3	H	17	LYS
3	H	18	LEU
3	H	71	PRO
3	H	76	ARG
3	H	80	ILE
3	H	82	ASN
3	H	85	LEU
3	H	88	LEU
3	H	100	GLU
3	H	104	GLU
3	H	124	LEU
3	H	126	ILE
3	H	132	VAL
3	H	147	ASN
3	H	154	LEU
3	H	168	GLU
3	H	172	LEU
3	H	182	ASP
3	H	183	LEU
3	H	190	LEU
3	H	212	LEU
3	H	223	VAL
3	H	225	MET
3	H	228	SER
3	H	233	LEU
3	H	237	LEU
3	H	242	LEU
3	H	251	LYS
3	H	257	LYS
3	H	258	GLU
3	I	10	LYS
3	I	18	LEU
3	I	68	GLU

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Mol	Chain	Res	Type
3	I	72	ASP
3	I	84	GLU
3	I	85	LEU
3	I	88	LEU
3	I	92	THR
3	I	125	VAL
3	I	138	ASP
3	I	147	ASN
3	I	169	ARG
3	I	177	LEU
3	I	183	LEU
3	I	190	LEU
3	I	212	LEU
3	I	223	VAL
3	I	233	LEU
3	I	242	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	B	96	HIS
1	B	145	ASN
1	C	84	ASN
2	D	68	GLN
2	D	131	GLN
2	D	217	GLN
2	D	233	GLN
2	E	50	ASN
2	E	63	HIS
2	E	66	HIS
2	E	80	ASN
2	E	131	GLN
2	E	205	GLN
2	E	233	GLN
2	F	66	HIS
2	F	68	GLN
2	F	131	GLN
2	F	170	GLN
2	F	181	ASN
2	F	195	ASN
2	F	233	GLN

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Mol	Chain	Res	Type
3	G	82	ASN
3	G	147	ASN
3	G	221	ASN
3	H	147	ASN
3	I	147	ASN
3	I	162	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	X	3/6 (50%)	0	0
4	Y	3/6 (50%)	0	0
4	Z	3/6 (50%)	0	0
All	All	9/18 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	179/179 (100%)	-0.42	1 (0%)	89	72	43, 63, 95, 115	6 (3%)
1	B	179/179 (100%)	-0.16	4 (2%)	62	33	42, 84, 121, 136	15 (8%)
1	C	179/179 (100%)	-0.37	3 (1%)	70	41	33, 70, 101, 133	8 (4%)
2	D	242/258 (93%)	-0.62	1 (0%)	92	79	34, 55, 88, 119	7 (2%)
2	E	243/258 (94%)	-0.66	2 (0%)	86	65	32, 49, 83, 108	9 (3%)
2	F	246/258 (95%)	-0.77	1 (0%)	92	79	26, 38, 75, 104	4 (1%)
3	G	253/259 (97%)	-0.48	1 (0%)	92	79	44, 67, 110, 125	12 (4%)
3	H	258/259 (99%)	-0.67	5 (1%)	66	37	26, 43, 86, 95	10 (3%)
3	I	256/259 (98%)	-0.69	4 (1%)	72	44	26, 41, 90, 121	11 (4%)
4	X	4/6 (66%)	0.61	0	100	100	75, 81, 83, 84	0
4	Y	4/6 (66%)	1.37	1 (25%)	0	0	93, 105, 109, 109	0
4	Z	4/6 (66%)	0.91	0	100	100	90, 90, 96, 98	0
All	All	2047/2106 (97%)	-0.55	23 (1%)	80	56	26, 54, 100, 136	82 (4%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	GLU	3.6
1	B	104	TYR	3.2
3	H	92	THR	3.2
3	H	90	SER	3.1
3	I	97	PRO	3.1
3	H	89	ALA	2.8
2	E	66	HIS	2.7
3	I	259	ILE	2.6
2	D	8	PRO	2.6
3	I	90	SER	2.5
1	A	104	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	104	TYR	2.4
1	B	154	GLY	2.3
3	I	91	PRO	2.2
1	C	70	ASN	2.2
3	G	90	SER	2.2
4	Y	5	C	2.2
3	H	96	GLY	2.1
1	C	106	LYS	2.1
2	F	252	THR	2.1
3	H	91	PRO	2.1
1	B	67	ASP	2.1
2	E	67	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	B	180	1/1	0.96	0.07	118,118,118,118	0
5	ZN	C	180	1/1	0.97	0.04	81,81,81,81	0
5	ZN	A	180	1/1	0.98	0.06	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.