Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 12:57 PM EDT

PDB ID	:	5DDJ
Title	:	Crystal structure of recombinant foot-and-mouth-disease virus O1M-S2093Y empty capsid
Authors	:	Kotecha, A.; Seago, J.; Scott, K.; Burman, A.; Loureiro, S.; Ren, J.; Porta, C.; Ginn, H.M.; Jackson, T.; Perez-Martin, E.; Siebert, C.A.; Paul, G.; Huiskonen, J.T.; Jones, I.M.; Esnouf, R.M.; Fry, E.E.; Maree, F.F.; Charleston, B.; Stuart, D.I.
Deposited on	:	2015-08-25
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

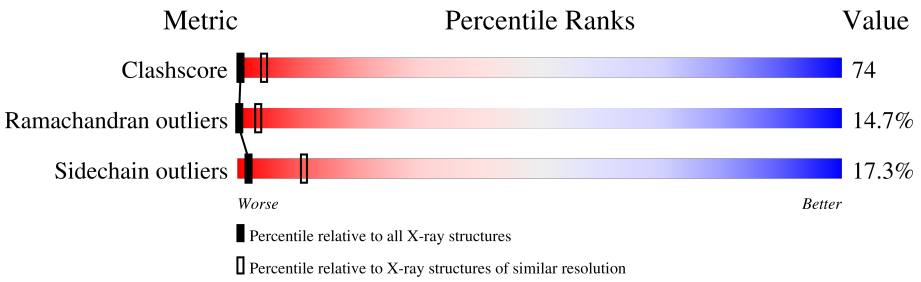
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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%

Mol	Chain	Length	Quality of chain
1	1	211	16% 48% 21% • 13%
2	2	218	21% 52% 22% • •
3	3	220	29% 52% 18% •
4	4	85	16% 32% 6% 46%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5131 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 Foot and mouth disease virus, VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	184	1437	910	258	266	3	0	0	0

- Molecule 2 is a protein called Foot and mouth disease virus, VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	210	1656	1057	282	310	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	93	TYR	SER	engineered mutation	UNP Q6PMW3

- Molecule 3 is a protein called Foot and mouth disease virus, VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	220	1685	1079	274	323	9	0	0	0

- Molecule 4 is a protein called Genome polyprotein.

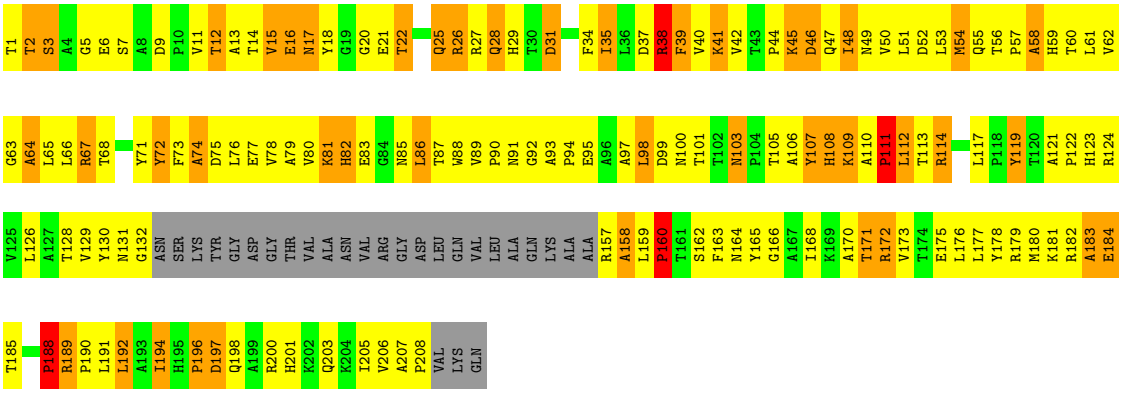
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	46	353	222	57	72	2	0	0	0

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. 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. 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.

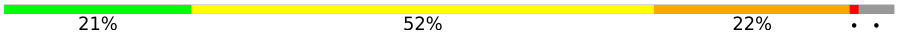
- Molecule 1: Foot and mouth disease virus, VP1

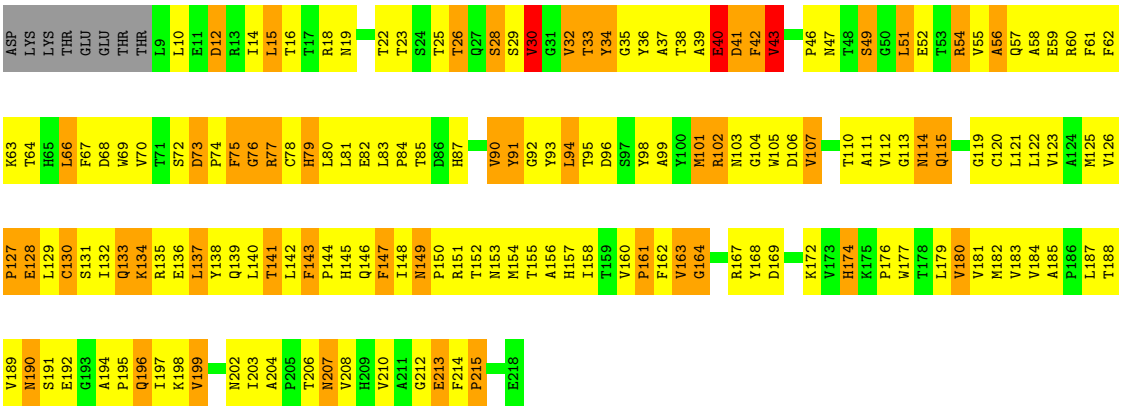
Chain 1:



- Molecule 2: Foot and mouth disease virus, VP2

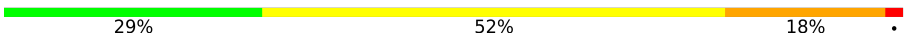
Chain 2:

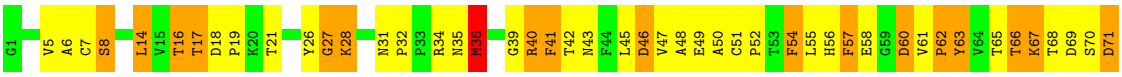




- Molecule 3: Foot and mouth disease virus, VP3

Chain 3:





R72 V73 L74 A75 Q76 L79 H85 M86 S87 N88 T89 F90 L91 A92 G93 L94 A95 Q96 Y97 Y98 T99 Q100 Y101 S102 G103 T104 I105 N106 L107 H108 F109 M110 F111 T112 G113 P114 A117 R120 Y121 M122 I123 A124 Y125 A126 P127 P128 G129 M130 E131 P132 P133 K134 T135 P136 E137 A138

A139 A140 H141 C142 I143 E146 W147 D148 T149 G150 L151 N152 S153 K154 F155 T156 F157 S158 I159 P160 Y161 L162 S163 D166 Y167 A168 Y169 D173 T174 A175 E176 T177 T178 N179 V180 Q181 V184 C185 L186 F187 Q188 I189 T190 H191 G192 K193 A194 D195 G196 D197 A198 L199 V200 V201 L202 A203

S204 A205 G206 K207 D208 F209 E210 L211 R212 L213 P214 V215 D216 A217 R218 T219 Q220

- Molecule 4: Genome polyprotein

Chain 4: 16% 32% 6% 46%

GLY ALA GLY GLN SER SER PRO ALA THR GLY SER GLN ASN GLN S15 G16 I21 I22 N23 N24 Y25 Y26 M27 Q28 Q29 Y30 Q31 N32 L38 G39 ASP ASN ALA THR SER GLY GLY SER ASN GLU GLY SER THR ASP THR THR SER THR HIS THR THR ASN THR GLN ASN N65 D66 W67

F68 S69 K70 L71 S74 A75 F76 S77 G78 L79 F80 G81 A82 L83 L84 A85

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	344.08Å 344.08Å 344.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 3.50 45.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	77.8 (49.66-3.50) 77.8 (45.98-3.50)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.48Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.361 , (Not available) 0.361 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 87.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.499 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.70	EDS
Total number of atoms	5131	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% 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)

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	1	0.49	0/1471	0.82	1/2012 (0.0%)
2	2	0.52	0/1701	0.83	1/2323 (0.0%)
3	3	0.56	0/1735	0.83	2/2370 (0.1%)
4	4	0.59	0/359	0.73	0/481
All	All	0.53	0/5266	0.82	4/7186 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	28	SER	N-CA-C	-5.67	95.70	111.00
3	3	213	LEU	CA-CB-CG	5.58	128.14	115.30
1	1	81	LYS	N-CA-C	-5.21	96.94	111.00
3	3	79	LEU	CA-CB-CG	5.06	126.95	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	107	TYR	Sidechain

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	1	1437	0	1443	268	0
2	2	1656	0	1610	295	0
3	3	1685	0	1610	217	0
4	4	353	0	324	35	0
All	All	5131	0	4987	746	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 74.

All (746) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:32:VAL:HG22	2:2:33:THR:H	1.02	1.11
2:2:91:TYR:HA	2:2:94:LEU:HD22	1.12	1.10
2:2:78:CYS:HB2	2:2:180:VAL:HG23	1.26	1.07
1:1:94:PRO:HG2	1:1:97:ALA:HB2	1.37	1.04
1:1:34:PHE:HA	4:4:16:GLY:HA2	1.35	1.04
1:1:122:PRO:HB3	3:3:167:TYR:HB2	1.39	1.04
4:4:65:ASN:HB2	4:4:69:SER:HB2	1.39	1.03
1:1:44:PRO:HB3	1:1:176:LEU:HB2	1.40	0.99
1:1:12:THR:HG22	1:1:13:ALA:H	1.27	0.98
1:1:131:ASN:HB2	2:2:129:LEU:H	1.31	0.96
2:2:133:GLN:HB2	2:2:136:GLU:HG3	1.47	0.96
3:3:40:ARG:HG2	3:3:41:PHE:H	1.29	0.95
2:2:148:ILE:HD11	2:2:156:ALA:HB2	1.46	0.95
3:3:133:PRO:HG2	3:3:187:PHE:HZ	1.33	0.93
4:4:84:LEU:HG	4:4:85:ALA:H	1.34	0.93
2:2:91:TYR:CA	2:2:94:LEU:HD22	1.99	0.92
2:2:32:VAL:HG22	2:2:33:THR:N	1.86	0.91
2:2:32:VAL:CG2	2:2:33:THR:H	1.84	0.90
3:3:103:GLY:HA3	3:3:209:PHE:HA	1.53	0.90
2:2:10:LEU:HG	2:2:12:ASP:H	1.37	0.89
1:1:67:ARG:HH11	1:1:67:ARG:HG2	1.36	0.89
3:3:65:THR:HB	3:3:196:GLY:HA2	1.55	0.88
3:3:180:VAL:HG23	3:3:181:GLN:HE22	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:79:LEU:HD23	3:3:184:VAL:HB	1.58	0.85
1:1:65:LEU:O	1:1:68:THR:HG22	1.74	0.85
3:3:104:THR:HG23	3:3:208:ASP:HB3	1.57	0.85
1:1:83:GLU:HB2	1:1:172:ARG:HB3	1.58	0.85
2:2:214:PHE:HB3	2:2:215:PRO:HD2	1.59	0.85
2:2:73:ASP:OD2	2:2:183:VAL:HG21	1.77	0.84
2:2:22:THR:HG23	2:2:60:ARG:HD2	1.59	0.84
1:1:15:VAL:HB	1:1:22:THR:HG23	1.58	0.84
2:2:90:VAL:O	2:2:94:LEU:HD13	1.78	0.84
1:1:38:ARG:HH11	1:1:38:ARG:HG2	1.43	0.83
1:1:130:TYR:H	1:1:159:LEU:HD11	1.44	0.83
3:3:121:TYR:CD1	3:3:199:LEU:HD22	2.14	0.82
2:2:91:TYR:HA	2:2:94:LEU:CD2	2.05	0.82
1:1:35:ILE:HD12	1:1:38:ARG:CZ	2.10	0.82
3:3:180:VAL:HG23	3:3:181:GLN:NE2	1.95	0.81
2:2:189:VAL:HG23	2:2:190:ASN:H	1.45	0.81
2:2:32:VAL:O	2:2:33:THR:HG23	1.81	0.81
2:2:18:ARG:HA	2:2:23:THR:HG22	1.63	0.81
2:2:14:ILE:HG22	2:2:15:LEU:N	1.95	0.80
2:2:78:CYS:HB2	2:2:180:VAL:CG2	2.07	0.80
1:1:119:TYR:OH	1:1:121:ALA:HB3	1.80	0.80
1:1:192:LEU:HB2	2:2:135:ARG:NH1	1.96	0.79
2:2:103:ASN:HD22	2:2:104:GLY:H	1.31	0.79
2:2:134:LYS:CD	2:2:134:LYS:H	1.93	0.79
1:1:35:ILE:HG13	1:1:61:LEU:HD21	1.64	0.79
2:2:84:PRO:HB3	2:2:91:TYR:OH	1.82	0.79
1:1:53:LEU:O	1:1:56:THR:HG22	1.84	0.78
1:1:25:GLN:H	1:1:25:GLN:NE2	1.82	0.78
1:1:76:LEU:HB3	1:1:117:LEU:HB2	1.64	0.78
1:1:122:PRO:HB3	3:3:167:TYR:CB	2.14	0.77
2:2:14:ILE:HG22	2:2:15:LEU:H	1.49	0.77
2:2:43:VAL:HG11	2:2:102:ARG:CZ	2.14	0.77
3:3:96:GLN:HG3	3:3:97:TYR:H	1.49	0.77
3:3:124:ALA:HB3	3:3:187:PHE:HE1	1.47	0.77
3:3:120:ARG:HG3	3:3:120:ARG:HH11	1.49	0.77
3:3:133:PRO:HG2	3:3:187:PHE:CZ	2.19	0.77
1:1:130:TYR:CE2	1:1:132:GLY:HA3	2.19	0.77
3:3:102:SER:HA	3:3:161:TYR:CE1	2.20	0.77
1:1:83:GLU:HG3	1:1:172:ARG:HE	1.49	0.77
1:1:85:ASN:ND2	1:1:107:TYR:HA	2.00	0.76
2:2:54:ARG:CZ	2:2:56:ALA:HB2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:98:TYR:HE1	3:3:214:PRO:HG3	1.49	0.75
2:2:90:VAL:HG23	2:2:91:TYR:H	1.52	0.75
3:3:160:PRO:HB2	3:3:162:LEU:CD2	2.17	0.75
1:1:80:VAL:HG13	1:1:173:VAL:HG23	1.66	0.75
1:1:119:TYR:CZ	1:1:121:ALA:HB3	2.22	0.74
2:2:103:ASN:HB3	2:2:208:VAL:HB	1.68	0.74
3:3:57:PHE:HB2	3:3:61:VAL:O	1.88	0.74
2:2:129:LEU:HG	2:2:130:CYS:H	1.53	0.74
2:2:148:ILE:HA	2:2:153:ASN:HD21	1.53	0.74
1:1:93:ALA:HB1	3:3:215:VAL:HG21	1.68	0.73
2:2:187:LEU:HD23	2:2:188:THR:N	2.03	0.73
2:2:134:LYS:H	2:2:134:LYS:HZ2	1.36	0.73
2:2:87:HIS:CD2	2:2:91:TYR:HB3	2.23	0.73
2:2:133:GLN:HA	2:2:134:LYS:NZ	2.03	0.73
2:2:78:CYS:HB3	2:2:182:MET:CA	2.19	0.73
2:2:137:LEU:HD22	2:2:182:MET:SD	2.29	0.73
1:1:73:PHE:HE1	1:1:182:ARG:HH12	1.37	0.73
2:2:61:PHE:HA	2:2:203:ILE:O	1.88	0.73
3:3:110:MET:O	3:3:199:LEU:HA	1.88	0.73
1:1:45:LYS:N	1:1:49:ASN:HD21	1.86	0.72
3:3:67:LYS:HZ1	3:3:74:LEU:HA	1.53	0.72
2:2:91:TYR:O	2:2:95:THR:HG23	1.89	0.72
3:3:176:GLU:HG2	3:3:179:ASN:HA	1.71	0.72
1:1:12:THR:H	4:4:75:ALA:HB1	1.54	0.72
3:3:40:ARG:HG2	3:3:41:PHE:N	2.04	0.72
2:2:134:LYS:H	2:2:134:LYS:HD2	1.54	0.72
1:1:51:LEU:HD11	1:1:168:ILE:HG23	1.72	0.71
3:3:94:LEU:HD12	3:3:95:ALA:N	2.05	0.71
1:1:192:LEU:HD12	2:2:135:ARG:HH11	1.53	0.71
1:1:188:PRO:HD2	2:2:36:TYR:CZ	2.25	0.71
2:2:18:ARG:C	2:2:19:ASN:HD22	1.93	0.71
3:3:96:GLN:HG3	3:3:97:TYR:N	2.06	0.71
1:1:79:ALA:HA	1:1:113:THR:O	1.90	0.71
3:3:67:LYS:NZ	3:3:74:LEU:HA	2.05	0.71
3:3:114:PRO:HG2	3:3:117:ALA:HB2	1.73	0.70
2:2:28:SER:HB3	2:2:153:ASN:HA	1.73	0.70
1:1:63:GLY:O	1:1:66:LEU:HB3	1.92	0.70
2:2:104:GLY:O	2:2:206:THR:HG22	1.91	0.70
1:1:101:THR:HA	1:1:105:THR:OG1	1.90	0.70
2:2:141:THR:HA	2:2:145:HIS:CE1	2.27	0.70
1:1:122:PRO:CB	3:3:167:TYR:HB2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:123:VAL:O	2:2:145:HIS:HB2	1.92	0.69
3:3:186:LEU:HD12	3:3:187:PHE:N	2.08	0.69
1:1:107:TYR:CG	3:3:14:LEU:HD23	2.28	0.69
2:2:102:ARG:HG2	2:2:102:ARG:HH11	1.58	0.69
3:3:27:GLY:O	3:3:28:LYS:HB2	1.93	0.69
3:3:75:ALA:O	3:3:76:GLN:HB2	1.90	0.69
2:2:114:ASN:HB2	2:2:115:GLN:OE1	1.93	0.69
2:2:40:GLU:CD	2:2:102:ARG:HH22	1.94	0.69
2:2:59:GLU:HG3	2:2:206:THR:HA	1.75	0.68
2:2:102:ARG:HG2	2:2:167:ARG:O	1.91	0.68
1:1:94:PRO:O	1:1:97:ALA:N	2.27	0.68
1:1:67:ARG:HG2	1:1:67:ARG:NH1	2.08	0.68
1:1:171:THR:O	1:1:172:ARG:HB2	1.94	0.68
2:2:54:ARG:NE	2:2:56:ALA:HB2	2.09	0.68
3:3:40:ARG:CG	3:3:41:PHE:H	2.04	0.68
2:2:67:PHE:HB3	2:2:79:HIS:CG	2.28	0.68
2:2:73:ASP:OD1	2:2:77:ARG:HG3	1.94	0.68
1:1:44:PRO:CB	1:1:176:LEU:HB2	2.18	0.68
1:1:93:ALA:HB2	3:3:99:THR:CG2	2.24	0.68
2:2:83:LEU:N	2:2:177:TRP:O	2.22	0.68
2:2:141:THR:HA	2:2:145:HIS:NE2	2.09	0.68
1:1:42:VAL:HG11	1:1:55:GLN:HG3	1.76	0.68
2:2:146:GLN:CG	2:2:158:ILE:HG23	2.24	0.68
2:2:51:LEU:HD11	3:3:143:ILE:HD13	1.75	0.67
1:1:192:LEU:N	1:1:192:LEU:HD23	2.09	0.67
1:1:207:ALA:HB1	1:1:208:PRO:HD2	1.75	0.67
1:1:188:PRO:HD2	2:2:36:TYR:OH	1.94	0.67
1:1:182:ARG:HH21	4:4:32:ASN:HB3	1.58	0.67
2:2:47:ASN:HB2	3:3:163:SER:O	1.94	0.67
1:1:179:ARG:HD3	1:1:181:LYS:HE2	1.75	0.67
3:3:105:ILE:HG13	3:3:159:ILE:HD11	1.76	0.67
2:2:82:GLU:O	2:2:83:LEU:HD13	1.95	0.67
1:1:41:LYS:HD2	1:1:41:LYS:O	1.95	0.66
1:1:15:VAL:HG11	1:1:21:GLU:O	1.95	0.66
1:1:35:ILE:HA	1:1:38:ARG:NH1	2.10	0.66
1:1:129:VAL:HA	1:1:159:LEU:HD21	1.77	0.66
2:2:172:LYS:HE3	3:3:129:GLY:O	1.94	0.66
2:2:189:VAL:HG23	2:2:190:ASN:N	2.11	0.66
4:4:65:ASN:HB2	4:4:69:SER:CB	2.22	0.66
1:1:15:VAL:O	1:1:17:ASN:N	2.29	0.66
1:1:160:PRO:HB2	1:1:163:PHE:CD1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:146:GLN:HG3	2:2:158:ILE:HG23	1.76	0.66
3:3:66:THR:OG1	3:3:195:ASP:HA	1.96	0.66
1:1:92:GLY:HA2	3:3:169:TYR:CE2	2.31	0.66
2:2:87:HIS:HB3	2:2:92:GLY:HA3	1.78	0.66
1:1:76:LEU:HB3	1:1:117:LEU:CB	2.25	0.66
2:2:122:LEU:O	2:2:181:VAL:HA	1.95	0.66
3:3:87:SER:O	3:3:88:ASN:HB3	1.96	0.66
2:2:42:PHE:O	2:2:167:ARG:HD3	1.96	0.65
2:2:103:ASN:HD22	2:2:104:GLY:N	1.92	0.65
2:2:134:LYS:HD2	2:2:134:LYS:N	2.11	0.65
3:3:55:LEU:HD12	3:3:201:VAL:O	1.95	0.65
2:2:214:PHE:CE1	3:3:127:PRO:HG2	2.31	0.65
3:3:108:HIS:CG	3:3:156:THR:HG22	2.31	0.65
3:3:86:MET:O	3:3:92:ALA:HB3	1.96	0.65
2:2:163:VAL:HG23	2:2:164:GLY:H	1.61	0.65
2:2:213:GLU:O	3:3:127:PRO:HD3	1.96	0.65
3:3:127:PRO:HB2	3:3:128:PRO:HD2	1.78	0.65
2:2:14:ILE:CG2	2:2:15:LEU:H	2.10	0.64
2:2:115:GLN:CD	2:2:115:GLN:H	1.99	0.64
2:2:78:CYS:HB3	2:2:182:MET:HB3	1.78	0.64
2:2:197:ILE:O	2:2:197:ILE:HG22	1.97	0.64
1:1:72:TYR:HA	1:1:185:THR:HA	1.79	0.64
3:3:139:ALA:C	3:3:141:HIS:H	2.01	0.64
1:1:11:VAL:HG12	1:1:11:VAL:O	1.98	0.64
1:1:44:PRO:C	1:1:49:ASN:HD21	2.00	0.64
1:1:129:VAL:CA	1:1:159:LEU:HD21	2.27	0.64
2:2:133:GLN:HB2	2:2:136:GLU:CG	2.23	0.64
2:2:162:PHE:HZ	2:2:169:ASP:HB2	1.62	0.64
1:1:88:TRP:CZ2	1:1:166:GLY:HA3	2.32	0.64
2:2:47:ASN:O	3:3:162:LEU:HA	1.98	0.64
1:1:157:ARG:O	1:1:158:ALA:HB2	1.98	0.64
1:1:71:TYR:OH	2:2:128:GLU:HG2	1.97	0.64
2:2:126:VAL:HG22	2:2:143:PHE:HB2	1.80	0.63
1:1:130:TYR:N	1:1:159:LEU:HD11	2.12	0.63
2:2:129:LEU:CG	2:2:130:CYS:H	2.10	0.63
3:3:74:LEU:HD13	3:3:188:GLN:HB2	1.81	0.63
2:2:22:THR:CG2	2:2:60:ARG:HD2	2.28	0.63
1:1:47:GLN:HA	1:1:173:VAL:HG12	1.81	0.63
2:2:63:LYS:HE3	2:2:202:ASN:ND2	2.14	0.63
3:3:86:MET:HA	3:3:89:THR:CG2	2.29	0.63
4:4:21:ILE:HD12	4:4:22:ILE:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:148:ILE:HD11	2:2:156:ALA:CB	2.24	0.63
2:2:18:ARG:CA	2:2:23:THR:HG22	2.28	0.63
3:3:35:ASN:O	3:3:36:MET:C	2.37	0.63
2:2:14:ILE:CG2	2:2:15:LEU:N	2.62	0.63
3:3:45:LEU:HD11	3:3:211:LEU:HB2	1.80	0.62
4:4:67:TRP:CZ2	4:4:71:LEU:HD22	2.33	0.62
1:1:46:ASP:O	1:1:47:GLN:HG3	1.99	0.62
1:1:107:TYR:HB2	3:3:14:LEU:HB3	1.82	0.62
1:1:77:GLU:HB3	1:1:179:ARG:HB3	1.81	0.62
3:3:120:ARG:HG3	3:3:120:ARG:NH1	2.11	0.62
1:1:40:VAL:O	1:1:177:LEU:HA	1.99	0.62
3:3:192:GLY:C	3:3:194:ALA:N	2.52	0.62
1:1:1:THR:HG23	4:4:78:GLY:O	2.00	0.62
2:2:40:GLU:CD	2:2:102:ARG:NH2	2.53	0.62
1:1:86:LEU:HD11	1:1:168:ILE:HB	1.82	0.62
1:1:130:TYR:H	1:1:159:LEU:CD1	2.13	0.62
1:1:35:ILE:HA	1:1:38:ARG:CZ	2.30	0.61
1:1:93:ALA:HB2	3:3:99:THR:HG21	1.82	0.61
1:1:73:PHE:HE1	1:1:182:ARG:NH1	1.98	0.61
1:1:94:PRO:CG	1:1:97:ALA:HB2	2.22	0.61
2:2:70:VAL:HG23	2:2:73:ASP:HB2	1.81	0.61
3:3:106:ASN:O	3:3:107:LEU:HD13	1.99	0.61
2:2:140:LEU:O	2:2:142:LEU:N	2.29	0.61
3:3:126:ALA:HB2	3:3:142:CYS:SG	2.40	0.61
3:3:113:GLY:HA3	3:3:197:ASP:OD2	2.01	0.61
1:1:3:SER:HA	4:4:80:PHE:CE1	2.36	0.61
1:1:122:PRO:HG3	3:3:100:GLN:CD	2.20	0.61
1:1:38:ARG:HG2	1:1:38:ARG:NH1	2.15	0.61
2:2:58:ALA:HB2	2:2:90:VAL:HB	1.82	0.61
1:1:123:HIS:HE2	1:1:162:SER:HB2	1.65	0.61
2:2:43:VAL:CG1	2:2:102:ARG:NH1	2.64	0.60
2:2:128:GLU:OE1	2:2:176:PRO:HB3	2.01	0.60
1:1:76:LEU:O	1:1:117:LEU:N	2.33	0.60
1:1:93:ALA:CB	3:3:215:VAL:HG21	2.31	0.60
2:2:102:ARG:HH11	2:2:102:ARG:CG	2.14	0.60
1:1:12:THR:HG22	1:1:13:ALA:N	2.10	0.60
1:1:54:MET:HE1	1:1:128:THR:HG22	1.84	0.60
1:1:72:TYR:HB2	1:1:185:THR:HG22	1.84	0.60
2:2:64:THR:HG21	2:2:81:LEU:HD21	1.83	0.60
2:2:129:LEU:HG	2:2:130:CYS:N	2.16	0.60
1:1:55:GLN:HG3	1:1:56:THR:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:134:LYS:HZ2	2:2:134:LYS:N	1.98	0.60
1:1:3:SER:OG	1:1:11:VAL:HG11	2.01	0.60
2:2:22:THR:OG1	2:2:60:ARG:HB2	2.02	0.60
2:2:133:GLN:HA	2:2:134:LYS:HZ3	1.65	0.60
2:2:43:VAL:HG11	2:2:102:ARG:NH1	2.17	0.60
2:2:190:ASN:CG	2:2:191:SER:H	2.06	0.60
3:3:94:LEU:C	3:3:96:GLN:H	2.06	0.60
2:2:37:ALA:HB3	2:2:161:PRO:CB	2.32	0.59
2:2:75:PHE:CG	2:2:75:PHE:O	2.54	0.59
3:3:66:THR:HG22	3:3:188:GLN:CD	2.23	0.59
3:3:112:THR:OG1	3:3:198:ALA:HB3	2.02	0.59
3:3:202:LEU:HD12	3:3:202:LEU:N	2.17	0.59
1:1:94:PRO:O	1:1:95:GLU:C	2.40	0.59
1:1:42:VAL:HG13	1:1:56:THR:HA	1.83	0.59
1:1:80:VAL:HG12	1:1:82:HIS:HB3	1.83	0.59
2:2:78:CYS:HB3	2:2:182:MET:HA	1.84	0.59
2:2:102:ARG:CZ	2:2:102:ARG:HB2	2.32	0.59
2:2:160:VAL:HG21	2:2:177:TRP:CZ3	2.37	0.59
3:3:120:ARG:NH1	3:3:146:GLU:HG2	2.17	0.59
1:1:79:ALA:HB1	1:1:112:LEU:CD1	2.33	0.59
2:2:83:LEU:O	2:2:177:TRP:HB2	2.02	0.59
2:2:126:VAL:HG22	2:2:143:PHE:CB	2.33	0.59
1:1:188:PRO:HG3	2:2:142:LEU:O	2.03	0.59
3:3:160:PRO:HB2	3:3:162:LEU:HD23	1.83	0.59
2:2:146:GLN:HG3	2:2:157:HIS:O	2.03	0.59
2:2:163:VAL:O	2:2:164:GLY:O	2.20	0.59
1:1:74:ALA:O	1:1:119:TYR:HB2	2.02	0.59
2:2:84:PRO:HB3	2:2:91:TYR:HH	1.68	0.59
3:3:55:LEU:HD21	3:3:86:MET:SD	2.43	0.59
2:2:103:ASN:CB	2:2:208:VAL:HB	2.32	0.58
2:2:67:PHE:HB3	2:2:79:HIS:ND1	2.19	0.58
2:2:115:GLN:OE1	2:2:115:GLN:N	2.35	0.58
1:1:48:ILE:HD12	1:1:48:ILE:H	1.68	0.58
2:2:25:THR:HG22	2:2:26:THR:N	2.19	0.58
4:4:67:TRP:O	4:4:70:LYS:HB2	2.02	0.58
2:2:203:ILE:HG22	2:2:204:ALA:N	2.18	0.58
4:4:81:GLY:O	4:4:82:ALA:HB2	2.02	0.58
3:3:17:THR:O	3:3:18:ASP:C	2.40	0.58
2:2:34:TYR:N	2:2:34:TYR:CD1	2.69	0.58
2:2:55:VAL:HG22	2:2:55:VAL:O	2.03	0.58
3:3:73:VAL:HG22	3:3:187:PHE:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:6:ALA:O	3:3:8:SER:N	2.34	0.58
1:1:83:GLU:HG3	1:1:172:ARG:NE	2.17	0.58
4:4:65:ASN:N	4:4:65:ASN:HD22	2.02	0.58
3:3:55:LEU:HB3	3:3:85:HIS:HB3	1.86	0.57
2:2:78:CYS:HB3	2:2:182:MET:CB	2.33	0.57
2:2:87:HIS:HB3	2:2:92:GLY:CA	2.34	0.57
3:3:52:PRO:HB3	3:3:204:SER:HB3	1.85	0.57
2:2:32:VAL:HG13	2:2:33:THR:N	2.18	0.57
4:4:21:ILE:CD1	4:4:22:ILE:HG23	2.34	0.57
2:2:122:LEU:HB2	2:2:184:VAL:HG23	1.87	0.57
3:3:69:ASP:OD2	3:3:71:ASP:HB2	2.04	0.57
1:1:182:ARG:HH11	1:1:182:ARG:HG2	1.70	0.57
1:1:198:GLN:C	1:1:200:ARG:H	2.08	0.57
2:2:14:ILE:O	2:2:15:LEU:HB2	2.05	0.57
2:2:51:LEU:CD1	3:3:143:ILE:HD13	2.35	0.57
2:2:103:ASN:ND2	2:2:104:GLY:H	2.02	0.57
3:3:104:THR:HG23	3:3:208:ASP:CB	2.32	0.57
3:3:108:HIS:O	3:3:201:VAL:HA	2.05	0.56
1:1:160:PRO:HB2	1:1:163:PHE:CE1	2.40	0.56
2:2:34:TYR:N	2:2:34:TYR:HD1	2.03	0.56
3:3:79:LEU:HD23	3:3:184:VAL:CB	2.33	0.56
3:3:134:LYS:NZ	3:3:134:LYS:HB3	2.20	0.56
2:2:54:ARG:HH12	2:2:208:VAL:CG1	2.19	0.56
3:3:79:LEU:HD21	3:3:159:ILE:HD12	1.87	0.56
4:4:65:ASN:O	4:4:66:ASP:C	2.43	0.56
1:1:67:ARG:HH11	1:1:67:ARG:CG	2.12	0.56
2:2:213:GLU:CD	3:3:143:ILE:HG12	2.25	0.56
2:2:29:SER:O	2:2:30:VAL:HG12	2.05	0.56
1:1:35:ILE:HG13	1:1:35:ILE:O	2.06	0.56
1:1:130:TYR:CZ	1:1:132:GLY:HA3	2.41	0.56
2:2:194:ALA:HB1	2:2:195:PRO:HD2	1.88	0.56
3:3:49:GLU:HG3	3:3:205:ALA:O	2.05	0.56
2:2:81:LEU:HD23	2:2:179:LEU:HD23	1.88	0.56
3:3:32:PRO:HD2	3:3:34:ARG:HH12	1.69	0.56
3:3:103:GLY:O	3:3:161:TYR:HB2	2.06	0.56
4:4:84:LEU:HG	4:4:85:ALA:N	2.13	0.56
3:3:114:PRO:HG2	3:3:117:ALA:CB	2.35	0.56
1:1:35:ILE:HD12	1:1:38:ARG:NE	2.22	0.55
1:1:44:PRO:C	1:1:49:ASN:ND2	2.59	0.55
2:2:54:ARG:HH12	2:2:208:VAL:HG12	1.71	0.55
2:2:98:TYR:CE2	2:2:210:VAL:HG21	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:163:VAL:HG22	2:2:177:TRP:CZ2	2.40	0.55
3:3:75:ALA:CB	3:3:186:LEU:HD23	2.37	0.55
3:3:31:ASN:HB3	3:3:32:PRO:CD	2.36	0.55
3:3:75:ALA:HB2	3:3:186:LEU:HD23	1.88	0.55
3:3:86:MET:O	3:3:88:ASN:N	2.40	0.55
1:1:2:THR:O	1:1:3:SER:HB3	2.07	0.55
1:1:72:TYR:CD1	1:1:73:PHE:N	2.75	0.55
2:2:143:PHE:N	2:2:143:PHE:CD2	2.74	0.55
3:3:40:ARG:O	3:3:41:PHE:HB3	2.07	0.55
1:1:73:PHE:O	1:1:74:ALA:HB2	2.07	0.55
3:3:66:THR:HG22	3:3:188:GLN:NE2	2.22	0.55
2:2:49:SER:C	2:2:51:LEU:H	2.11	0.55
3:3:70:SER:O	3:3:72:ARG:HG3	2.06	0.55
1:1:71:TYR:O	1:1:72:TYR:HB3	2.06	0.55
1:1:188:PRO:HG3	4:4:68:PHE:HZ	1.72	0.55
1:1:29:HIS:HA	1:1:34:PHE:CE2	2.42	0.54
2:2:140:LEU:C	2:2:142:LEU:H	2.10	0.54
3:3:86:MET:HA	3:3:89:THR:HG23	1.88	0.54
3:3:94:LEU:C	3:3:96:GLN:N	2.59	0.54
3:3:131:GLU:HG3	3:3:132:PRO:HD2	1.88	0.54
2:2:36:TYR:CE2	2:2:144:PRO:HD3	2.42	0.54
2:2:68:ASP:OD1	2:2:198:LYS:HG2	2.07	0.54
3:3:46:ASP:O	3:3:50:ALA:CB	2.55	0.54
3:3:99:THR:HG23	3:3:215:VAL:HB	1.89	0.54
1:1:11:VAL:HG13	4:4:76:PHE:CE1	2.42	0.54
1:1:119:TYR:HD1	1:1:165:TYR:OH	1.91	0.54
1:1:44:PRO:HA	1:1:176:LEU:HD22	1.90	0.54
2:2:102:ARG:NH1	2:2:102:ARG:HB2	2.23	0.54
2:2:167:ARG:HB2	2:2:167:ARG:CZ	2.38	0.54
3:3:147:TRP:CD1	3:3:148:ASP:N	2.75	0.54
1:1:130:TYR:H	1:1:159:LEU:HD21	1.72	0.54
2:2:111:ALA:HB2	2:2:199:VAL:HG13	1.89	0.54
2:2:133:GLN:HA	2:2:134:LYS:HZ2	1.72	0.54
3:3:139:ALA:O	3:3:141:HIS:N	2.40	0.54
1:1:67:ARG:NH1	1:1:67:ARG:CG	2.69	0.53
3:3:6:ALA:C	3:3:8:SER:H	2.11	0.53
1:1:37:ASP:OD1	1:1:37:ASP:O	2.26	0.53
1:1:72:TYR:CD1	1:1:72:TYR:C	2.82	0.53
1:1:129:VAL:HG13	1:1:129:VAL:O	2.08	0.53
3:3:137:GLU:CD	3:3:137:GLU:H	2.11	0.53
3:3:49:GLU:HA	3:3:205:ALA:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:70:VAL:O	2:2:73:ASP:HB3	2.08	0.53
2:2:127:PRO:O	2:2:128:GLU:C	2.47	0.53
3:3:192:GLY:C	3:3:194:ALA:H	2.10	0.53
1:1:196:PRO:HG3	1:1:201:HIS:HB2	1.90	0.53
2:2:98:TYR:CE2	2:2:210:VAL:HG11	2.44	0.53
2:2:115:GLN:HA	2:2:150:PRO:O	2.09	0.53
2:2:155:THR:HG22	2:2:156:ALA:N	2.23	0.53
3:3:121:TYR:CE1	3:3:199:LEU:HD22	2.43	0.53
1:1:124:ARG:HH12	2:2:41:ASP:HB2	1.74	0.53
2:2:135:ARG:HA	2:2:138:TYR:HE2	1.74	0.53
3:3:101:TYR:HB3	3:3:211:LEU:CD1	2.39	0.53
1:1:97:ALA:HA	3:3:217:ALA:CB	2.39	0.53
1:1:103:ASN:O	1:1:105:THR:N	2.42	0.53
2:2:72:SER:O	2:2:73:ASP:C	2.46	0.53
2:2:98:TYR:CZ	2:2:210:VAL:HG21	2.43	0.53
2:2:112:VAL:O	2:2:197:ILE:HG12	2.09	0.53
1:1:97:ALA:HA	3:3:217:ALA:HB2	1.91	0.52
2:2:102:ARG:O	2:2:208:VAL:HG23	2.10	0.52
2:2:25:THR:HG22	2:2:26:THR:H	1.74	0.52
2:2:78:CYS:O	2:2:79:HIS:C	2.48	0.52
3:3:75:ALA:O	3:3:76:GLN:CB	2.56	0.52
1:1:37:ASP:HB3	4:4:16:GLY:HA3	1.90	0.52
3:3:155:PHE:CZ	3:3:157:PHE:HB2	2.44	0.52
1:1:40:VAL:O	1:1:40:VAL:HG13	2.09	0.52
1:1:190:PRO:HA	2:2:139:GLN:OE1	2.08	0.52
3:3:101:TYR:HB3	3:3:211:LEU:HD12	1.91	0.52
1:1:3:SER:CB	1:1:11:VAL:HG11	2.40	0.52
1:1:72:TYR:HD1	1:1:73:PHE:N	2.08	0.52
2:2:87:HIS:NE2	2:2:91:TYR:HB3	2.24	0.52
3:3:134:LYS:HD2	3:3:134:LYS:N	2.24	0.52
1:1:192:LEU:HD23	1:1:192:LEU:H	1.75	0.52
2:2:47:ASN:O	3:3:161:TYR:O	2.28	0.52
3:3:167:TYR:O	3:3:168:ALA:CB	2.58	0.52
1:1:25:GLN:H	1:1:25:GLN:CD	2.12	0.52
1:1:31:ASP:HB3	1:1:34:PHE:HB3	1.92	0.51
1:1:35:ILE:O	1:1:35:ILE:HG23	2.10	0.51
2:2:54:ARG:HD2	2:2:56:ALA:H	1.75	0.51
2:2:113:GLY:HA3	2:2:197:ILE:HD11	1.92	0.51
3:3:73:VAL:HG21	3:3:134:LYS:HA	1.92	0.51
1:1:82:HIS:HB2	1:1:172:ARG:O	2.09	0.51
1:1:86:LEU:HD21	1:1:168:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:103:ASN:ND2	2:2:104:GLY:N	2.57	0.51
3:3:139:ALA:C	3:3:141:HIS:N	2.63	0.51
1:1:42:VAL:HG11	1:1:55:GLN:HE21	1.74	0.51
1:1:188:PRO:O	1:1:189:ARG:HG2	2.11	0.51
2:2:40:GLU:OE2	2:2:102:ARG:NH2	2.43	0.51
3:3:67:LYS:HZ3	3:3:74:LEU:HD12	1.76	0.51
1:1:119:TYR:HE1	1:1:126:LEU:HD12	1.76	0.51
2:2:167:ARG:CB	2:2:167:ARG:NH1	2.73	0.51
1:1:42:VAL:CG1	1:1:55:GLN:HE21	2.24	0.51
2:2:55:VAL:O	2:2:57:GLN:N	2.44	0.51
2:2:106:ASP:C	2:2:107:VAL:HG23	2.31	0.51
2:2:196:GLN:HE22	2:2:198:LYS:HG2	1.76	0.51
1:1:119:TYR:HD1	1:1:165:TYR:CZ	2.29	0.51
3:3:109:PHE:CG	3:3:147:TRP:CH2	2.99	0.51
2:2:102:ARG:HG3	2:2:168:TYR:HA	1.93	0.51
3:3:109:PHE:O	3:3:154:LYS:HA	2.11	0.51
1:1:26:ARG:HD3	1:1:26:ARG:N	2.26	0.50
1:1:27:ARG:O	1:1:29:HIS:N	2.44	0.50
1:1:71:TYR:O	1:1:185:THR:HB	2.11	0.50
2:2:18:ARG:C	2:2:19:ASN:ND2	2.63	0.50
2:2:60:ARG:O	2:2:204:ALA:HA	2.12	0.50
3:3:120:ARG:HD2	3:3:189:ILE:HG21	1.93	0.50
3:3:178:THR:O	3:3:179:ASN:O	2.27	0.50
1:1:119:TYR:HE1	1:1:126:LEU:CD1	2.23	0.50
2:2:99:ALA:HB2	2:2:214:PHE:CZ	2.47	0.50
2:2:35:GLY:O	2:2:37:ALA:N	2.42	0.50
2:2:69:TRP:CD2	2:2:187:LEU:HD12	2.46	0.50
1:1:64:ALA:O	1:1:67:ARG:N	2.44	0.50
2:2:140:LEU:N	2:2:140:LEU:HD22	2.26	0.50
2:2:142:LEU:HB2	2:2:143:PHE:CE2	2.47	0.50
4:4:79:LEU:HD21	4:4:83:LEU:HB2	1.94	0.50
3:3:67:LYS:NZ	3:3:74:LEU:HD12	2.26	0.50
1:1:47:GLN:HG2	1:1:172:ARG:N	2.26	0.50
1:1:79:ALA:HB3	1:1:177:LEU:HD13	1.92	0.50
2:2:146:GLN:HG2	2:2:158:ILE:HG23	1.94	0.50
1:1:6:GLU:OE1	2:2:152:THR:HG21	2.12	0.50
1:1:192:LEU:HB2	2:2:135:ARG:HH12	1.72	0.50
4:4:28:GLN:C	4:4:30:TYR:H	2.15	0.50
1:1:25:GLN:NE2	1:1:25:GLN:N	2.57	0.49
3:3:73:VAL:HG13	3:3:75:ALA:O	2.11	0.49
3:3:161:TYR:C	3:3:162:LEU:HD22	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:102:ARG:HD2	2:2:168:TYR:CZ	2.47	0.49
2:2:135:ARG:O	2:2:138:TYR:HD2	1.94	0.49
1:1:130:TYR:N	1:1:159:LEU:HD21	2.26	0.49
1:1:171:THR:O	1:1:172:ARG:CB	2.60	0.49
3:3:56:HIS:ND1	3:3:57:PHE:N	2.58	0.49
3:3:123:ILE:O	3:3:123:ILE:HG13	2.11	0.49
1:1:109:LYS:HE3	1:1:109:LYS:C	2.33	0.49
3:3:160:PRO:HB2	3:3:162:LEU:HD21	1.93	0.49
1:1:51:LEU:HD22	1:1:165:TYR:O	2.12	0.49
1:1:194:ILE:O	1:1:196:PRO:HD3	2.12	0.49
3:3:131:GLU:CG	3:3:132:PRO:HD2	2.42	0.49
2:2:148:ILE:HD13	2:2:153:ASN:HD21	1.77	0.49
2:2:148:ILE:HD13	2:2:153:ASN:ND2	2.27	0.49
3:3:97:TYR:HA	3:3:215:VAL:O	2.13	0.49
3:3:137:GLU:CD	3:3:137:GLU:N	2.66	0.49
1:1:52:ASP:C	1:1:53:LEU:HD22	2.33	0.49
1:1:54:MET:HA	1:1:67:ARG:NH2	2.28	0.49
2:2:196:GLN:HE22	2:2:198:LYS:CG	2.26	0.49
3:3:154:LYS:NZ	3:3:154:LYS:HB3	2.28	0.49
1:1:42:VAL:N	1:1:176:LEU:O	2.46	0.49
1:1:80:VAL:HG11	1:1:86:LEU:HD23	1.93	0.49
1:1:85:ASN:ND2	1:1:107:TYR:CG	2.80	0.49
2:2:81:LEU:O	2:2:83:LEU:HD22	2.12	0.49
3:3:48:ALA:HB1	3:3:91:LEU:HG	1.94	0.49
3:3:73:VAL:CG1	3:3:75:ALA:O	2.60	0.49
1:1:9:ASP:O	1:1:11:VAL:HG23	2.13	0.48
3:3:108:HIS:N	3:3:108:HIS:CD2	2.81	0.48
1:1:15:VAL:HG12	1:1:16:GLU:N	2.27	0.48
2:2:43:VAL:HG11	2:2:102:ARG:NE	2.29	0.48
4:4:81:GLY:O	4:4:82:ALA:CB	2.60	0.48
3:3:133:PRO:C	3:3:134:LYS:HZ3	2.16	0.48
2:2:78:CYS:O	2:2:80:LEU:HD12	2.12	0.48
2:2:94:LEU:HD13	2:2:94:LEU:H	1.78	0.48
2:2:212:GLY:O	2:2:213:GLU:HB3	2.12	0.48
1:1:28:GLN:O	1:1:31:ASP:HB2	2.13	0.48
1:1:206:VAL:HG23	1:1:206:VAL:O	2.14	0.48
2:2:125:MET:O	2:2:177:TRP:HZ3	1.95	0.48
2:2:133:GLN:NE2	2:2:136:GLU:OE1	2.46	0.48
3:3:109:PHE:CG	3:3:147:TRP:HH2	2.31	0.48
1:1:54:MET:SD	1:1:128:THR:HG22	2.53	0.48
1:1:68:THR:HA	1:1:189:ARG:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:95:GLU:O	1:1:98:LEU:HG	2.14	0.48
2:2:129:LEU:CG	2:2:130:CYS:N	2.75	0.48
2:2:214:PHE:HB3	2:2:215:PRO:CD	2.39	0.48
2:2:28:SER:HB3	2:2:154:MET:N	2.28	0.48
2:2:213:GLU:OE2	3:3:143:ILE:HG12	2.13	0.48
1:1:74:ALA:O	1:1:165:TYR:OH	2.11	0.48
1:1:157:ARG:O	1:1:158:ALA:CB	2.61	0.48
2:2:66:LEU:HB2	2:2:199:VAL:O	2.13	0.48
1:1:3:SER:HA	4:4:80:PHE:CD1	2.48	0.47
1:1:109:LYS:HG3	1:1:110:ALA:N	2.29	0.47
2:2:18:ARG:CB	2:2:23:THR:HG22	2.44	0.47
2:2:54:ARG:NH1	2:2:208:VAL:H	2.12	0.47
3:3:86:MET:HA	3:3:89:THR:HG21	1.94	0.47
3:3:120:ARG:HG2	3:3:189:ILE:CG1	2.44	0.47
3:3:192:GLY:O	3:3:194:ALA:N	2.47	0.47
2:2:63:LYS:HD2	2:2:63:LYS:N	2.29	0.47
2:2:160:VAL:HG22	2:2:161:PRO:HD2	1.96	0.47
3:3:124:ALA:HB3	3:3:187:PHE:CE1	2.38	0.47
1:1:75:ASP:OD1	1:1:119:TYR:N	2.46	0.47
1:1:194:ILE:HG21	1:1:201:HIS:CD2	2.50	0.47
3:3:92:ALA:C	3:3:94:LEU:H	2.16	0.47
1:1:15:VAL:O	1:1:16:GLU:C	2.52	0.47
1:1:35:ILE:HD11	1:1:61:LEU:HD11	1.96	0.47
4:4:79:LEU:CD2	4:4:83:LEU:HB2	2.45	0.47
2:2:106:ASP:HB3	2:2:204:ALA:HB3	1.96	0.47
1:1:130:TYR:CD2	1:1:160:PRO:HG2	2.49	0.47
1:1:196:PRO:O	1:1:197:ASP:CG	2.53	0.47
2:2:102:ARG:O	2:2:208:VAL:HA	2.15	0.47
2:2:102:ARG:HB3	2:2:162:PHE:CZ	2.50	0.47
3:3:98:TYR:CE1	3:3:214:PRO:HG3	2.39	0.47
1:1:188:PRO:C	1:1:189:ARG:HG2	2.36	0.47
2:2:41:ASP:O	2:2:42:PHE:C	2.53	0.47
1:1:56:THR:HG22	1:1:67:ARG:HH21	1.79	0.47
3:3:26:TYR:O	3:3:27:GLY:O	2.32	0.47
1:1:53:LEU:HB3	1:1:66:LEU:HD21	1.97	0.47
1:1:54:MET:HE1	1:1:128:THR:CG2	2.44	0.47
1:1:192:LEU:HD13	2:2:135:ARG:HG2	1.96	0.47
2:2:63:LYS:HE3	2:2:202:ASN:HD21	1.78	0.47
2:2:102:ARG:NH1	2:2:102:ARG:CG	2.72	0.47
3:3:72:ARG:HD3	3:3:188:GLN:O	2.15	0.47
2:2:167:ARG:HH11	2:2:167:ARG:HB3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:51:LEU:HD12	1:1:51:LEU:N	2.30	0.46
1:1:62:VAL:O	1:1:66:LEU:HB2	2.15	0.46
2:2:46:PRO:HG2	2:2:47:ASN:H	1.80	0.46
3:3:109:PHE:CB	3:3:147:TRP:CH2	2.99	0.46
2:2:143:PHE:O	2:2:144:PRO:C	2.54	0.46
2:2:163:VAL:HG23	2:2:164:GLY:N	2.30	0.46
2:2:167:ARG:HB2	2:2:167:ARG:NH1	2.30	0.46
3:3:74:LEU:CD1	3:3:188:GLN:HB2	2.45	0.46
1:1:188:PRO:CG	2:2:142:LEU:O	2.62	0.46
2:2:133:GLN:N	2:2:133:GLN:OE1	2.49	0.46
2:2:134:LYS:H	2:2:134:LYS:NZ	2.09	0.46
3:3:91:LEU:HD12	3:3:91:LEU:N	2.31	0.46
3:3:191:HIS:HB2	3:3:194:ALA:HB3	1.98	0.46
1:1:82:HIS:HD2	1:1:170:ALA:CB	2.29	0.46
1:1:130:TYR:H	1:1:159:LEU:CG	2.27	0.46
2:2:54:ARG:NH1	2:2:208:VAL:CG1	2.79	0.46
2:2:59:GLU:O	2:2:60:ARG:HB3	2.15	0.46
2:2:189:VAL:O	2:2:190:ASN:HB3	2.16	0.46
1:1:54:MET:HA	1:1:67:ARG:HH22	1.80	0.46
2:2:43:VAL:HB	2:2:168:TYR:OH	2.15	0.46
2:2:52:GLU:HA	2:2:210:VAL:O	2.14	0.46
2:2:54:ARG:NH1	2:2:208:VAL:HG13	2.31	0.46
2:2:121:LEU:HD21	2:2:199:VAL:HG21	1.97	0.46
1:1:48:ILE:H	1:1:48:ILE:CD1	2.21	0.46
1:1:93:ALA:CA	3:3:99:THR:HG22	2.46	0.46
1:1:194:ILE:HG21	1:1:201:HIS:NE2	2.31	0.46
2:2:114:ASN:O	2:2:150:PRO:HB3	2.16	0.46
1:1:81:LYS:H	1:1:175:GLU:HB2	1.81	0.46
2:2:181:VAL:HG23	2:2:181:VAL:O	2.16	0.46
3:3:94:LEU:O	3:3:96:GLN:N	2.49	0.46
4:4:21:ILE:HD12	4:4:22:ILE:N	2.31	0.46
4:4:67:TRP:CZ2	4:4:71:LEU:CD2	2.98	0.46
1:1:88:TRP:CE2	1:1:166:GLY:HA3	2.50	0.46
1:1:110:ALA:HA	1:1:111:PRO:HA	1.78	0.46
3:3:94:LEU:HD12	3:3:94:LEU:C	2.35	0.46
2:2:134:LYS:O	2:2:137:LEU:HB2	2.16	0.45
2:2:206:THR:O	2:2:207:ASN:C	2.54	0.45
3:3:120:ARG:NH1	3:3:146:GLU:CG	2.79	0.45
1:1:42:VAL:CB	1:1:55:GLN:HE21	2.28	0.45
1:1:58:ALA:HB2	1:1:67:ARG:CZ	2.45	0.45
1:1:198:GLN:C	1:1:200:ARG:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:137:LEU:O	2:2:140:LEU:CD2	2.64	0.45
2:2:140:LEU:C	2:2:142:LEU:N	2.70	0.45
4:4:23:ASN:O	4:4:24:ASN:C	2.54	0.45
1:1:42:VAL:HB	1:1:55:GLN:HE21	1.81	0.45
1:1:192:LEU:N	1:1:192:LEU:CD2	2.79	0.45
2:2:67:PHE:CD2	2:2:77:ARG:HD2	2.51	0.45
2:2:135:ARG:HA	2:2:138:TYR:CE2	2.52	0.45
3:3:120:ARG:CD	3:3:189:ILE:HG21	2.46	0.45
4:4:38:LEU:C	4:4:38:LEU:HD23	2.35	0.45
1:1:91:ASN:ND2	3:3:169:TYR:OH	2.48	0.45
2:2:83:LEU:O	2:2:177:TRP:O	2.35	0.45
1:1:89:VAL:CG1	1:1:93:ALA:HB3	2.47	0.45
1:1:182:ARG:HA	4:4:15:SER:HB3	1.98	0.45
3:3:136:PRO:HA	3:3:139:ALA:HB3	1.97	0.45
2:2:139:GLN:C	2:2:141:THR:N	2.67	0.45
2:2:139:GLN:HB3	2:2:142:LEU:HD11	1.97	0.45
3:3:74:LEU:HD13	3:3:188:GLN:CB	2.46	0.45
2:2:36:TYR:N	2:2:36:TYR:CD2	2.85	0.45
2:2:203:ILE:CG2	2:2:204:ALA:N	2.79	0.45
2:2:54:ARG:HD2	2:2:55:VAL:N	2.31	0.45
2:2:98:TYR:CD2	2:2:210:VAL:HG11	2.51	0.45
4:4:22:ILE:C	4:4:24:ASN:H	2.19	0.45
1:1:42:VAL:CG1	1:1:56:THR:HA	2.47	0.45
1:1:109:LYS:HE2	1:1:110:ALA:HB3	1.99	0.45
2:2:28:SER:HB3	2:2:154:MET:H	1.82	0.45
2:2:84:PRO:HA	2:2:105:TRP:CZ2	2.52	0.45
2:2:133:GLN:N	2:2:133:GLN:CD	2.70	0.45
3:3:62:PRO:HG2	3:3:63:TYR:H	1.82	0.45
3:3:76:GLN:OE1	3:3:132:PRO:HG2	2.16	0.45
1:1:107:TYR:CB	3:3:14:LEU:HD23	2.47	0.44
1:1:123:HIS:HE2	1:1:162:SER:CB	2.29	0.44
1:1:63:GLY:O	1:1:67:ARG:HD2	2.17	0.44
2:2:76:GLY:O	2:2:77:ARG:C	2.55	0.44
2:2:138:TYR:O	2:2:139:GLN:HG2	2.17	0.44
3:3:46:ASP:O	3:3:50:ALA:HB3	2.16	0.44
4:4:65:ASN:O	4:4:66:ASP:O	2.35	0.44
1:1:58:ALA:HB1	1:1:67:ARG:HD3	2.00	0.44
1:1:64:ALA:O	1:1:65:LEU:C	2.54	0.44
3:3:212:ARG:HG3	3:3:213:LEU:HD22	1.98	0.44
1:1:57:PRO:C	1:1:59:HIS:H	2.20	0.44
1:1:188:PRO:HD3	4:4:68:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:119:GLY:HA2	2:2:185:ALA:CB	2.48	0.44
1:1:189:ARG:O	2:2:142:LEU:HD13	2.17	0.44
2:2:54:ARG:HD3	2:2:208:VAL:O	2.18	0.44
3:3:124:ALA:CB	3:3:187:PHE:HE1	2.25	0.44
3:3:147:TRP:CD1	3:3:147:TRP:C	2.90	0.44
1:1:78:VAL:HG13	1:1:117:LEU:HD12	2.00	0.44
1:1:53:LEU:HB3	1:1:66:LEU:CD2	2.48	0.44
1:1:58:ALA:HA	1:1:67:ARG:NE	2.33	0.44
1:1:123:HIS:NE2	1:1:162:SER:HB2	2.32	0.44
1:1:77:GLU:OE2	1:1:114:ARG:NH1	2.51	0.44
2:2:75:PHE:O	2:2:75:PHE:CD1	2.71	0.44
2:2:94:LEU:CD1	2:2:94:LEU:N	2.81	0.44
1:1:183:ALA:O	1:1:184:GLU:HB3	2.18	0.44
3:3:67:LYS:HE2	3:3:74:LEU:HD12	1.99	0.44
3:3:167:TYR:O	3:3:168:ALA:HB3	2.17	0.44
2:2:54:ARG:NH2	2:2:59:GLU:OE2	2.51	0.43
1:1:79:ALA:HB3	1:1:177:LEU:CD1	2.49	0.43
1:1:119:TYR:O	1:1:119:TYR:CD2	2.71	0.43
2:2:189:VAL:CG2	2:2:190:ASN:N	2.81	0.43
3:3:101:TYR:CB	3:3:211:LEU:CD1	2.96	0.43
2:2:91:TYR:CD2	2:2:91:TYR:C	2.91	0.43
3:3:104:THR:CG2	3:3:208:ASP:HB3	2.37	0.43
1:1:131:ASN:HB2	2:2:129:LEU:N	2.14	0.43
2:2:39:ALA:O	2:2:40:GLU:HB2	2.17	0.43
2:2:163:VAL:C	2:2:164:GLY:O	2.55	0.43
3:3:79:LEU:HD23	3:3:184:VAL:CG1	2.49	0.43
3:3:120:ARG:HD3	3:3:189:ILE:HG13	2.00	0.43
1:1:37:ASP:CB	4:4:16:GLY:HA3	2.48	0.43
2:2:132:ILE:HG12	2:2:133:GLN:N	2.33	0.43
2:2:213:GLU:O	3:3:127:PRO:CD	2.65	0.43
3:3:65:THR:HA	3:3:197:ASP:O	2.18	0.43
3:3:199:LEU:O	3:3:199:LEU:HG	2.19	0.43
1:1:82:HIS:HB2	1:1:173:VAL:HA	2.00	0.43
2:2:137:LEU:HD23	2:2:137:LEU:HA	1.81	0.43
3:3:66:THR:HG22	3:3:188:GLN:OE1	2.18	0.43
1:1:18:TYR:CD2	1:1:18:TYR:N	2.82	0.43
1:1:48:ILE:HD12	1:1:48:ILE:N	2.33	0.43
1:1:57:PRO:O	1:1:59:HIS:N	2.49	0.43
1:1:82:HIS:O	1:1:108:HIS:CE1	2.71	0.43
2:2:127:PRO:HG3	2:2:177:TRP:CH2	2.53	0.43
3:3:31:ASN:HB3	3:3:34:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:67:LYS:HG2	3:3:71:ASP:O	2.17	0.43
1:1:40:VAL:HG21	1:1:56:THR:OG1	2.19	0.43
1:1:87:THR:OG1	1:1:105:THR:HG23	2.19	0.43
1:1:100:ASN:O	1:1:103:ASN:HB2	2.18	0.43
1:1:192:LEU:CD1	2:2:135:ARG:HG2	2.48	0.43
2:2:14:ILE:O	2:2:15:LEU:CB	2.66	0.43
3:3:135:THR:O	3:3:137:GLU:N	2.52	0.43
3:3:180:VAL:HG23	3:3:181:GLN:CD	2.37	0.43
1:1:89:VAL:HG21	1:1:98:LEU:HA	2.01	0.43
1:1:122:PRO:HG3	3:3:100:GLN:NE2	2.33	0.43
3:3:105:ILE:O	3:3:159:ILE:HG12	2.18	0.43
1:1:122:PRO:HG3	3:3:100:GLN:OE1	2.18	0.43
1:1:191:LEU:N	2:2:139:GLN:OE1	2.45	0.43
2:2:36:TYR:N	2:2:36:TYR:HD2	2.16	0.43
2:2:75:PHE:CD1	2:2:75:PHE:C	2.91	0.43
3:3:154:LYS:HG2	3:3:155:PHE:H	1.84	0.43
2:2:40:GLU:OE1	2:2:102:ARG:NH1	2.45	0.42
1:1:5:GLY:C	1:1:7:SER:H	2.23	0.42
2:2:47:ASN:HA	3:3:161:TYR:CD2	2.54	0.42
2:2:58:ALA:CB	2:2:90:VAL:HB	2.46	0.42
2:2:90:VAL:C	2:2:94:LEU:HD13	2.37	0.42
3:3:161:TYR:OH	3:3:167:TYR:O	2.37	0.42
1:1:45:LYS:CA	1:1:49:ASN:HD21	2.31	0.42
1:1:65:LEU:N	1:1:65:LEU:HD12	2.33	0.42
1:1:79:ALA:HB1	1:1:112:LEU:HD13	2.01	0.42
2:2:126:VAL:HA	2:2:127:PRO:HD3	1.64	0.42
1:1:42:VAL:O	1:1:176:LEU:HB3	2.19	0.42
1:1:95:GLU:O	1:1:98:LEU:CD1	2.67	0.42
1:1:119:TYR:CE1	1:1:126:LEU:CD1	3.02	0.42
1:1:176:LEU:HG	1:1:178:TYR:CE1	2.55	0.42
2:2:28:SER:HB2	2:2:154:MET:HB2	2.01	0.42
2:2:47:ASN:HB3	3:3:166:ASP:HA	2.01	0.42
2:2:148:ILE:CD1	2:2:153:ASN:ND2	2.83	0.42
2:2:122:LEU:HB2	2:2:184:VAL:CG2	2.48	0.42
3:3:76:GLN:OE1	3:3:132:PRO:CG	2.68	0.42
3:3:101:TYR:CB	3:3:211:LEU:HD12	2.49	0.42
2:2:90:VAL:HG23	2:2:91:TYR:N	2.28	0.42
1:1:79:ALA:HB3	1:1:177:LEU:HB2	2.02	0.42
3:3:18:ASP:HA	3:3:19:PRO:HD3	1.78	0.42
3:3:68:THR:O	3:3:68:THR:HG22	2.19	0.42
3:3:27:GLY:O	3:3:28:LYS:CB	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:36:MET:CE	3:3:36:MET:HA	2.50	0.42
3:3:91:LEU:HD21	3:3:205:ALA:N	2.35	0.42
1:1:6:GLU:HG2	2:2:149:ASN:HB3	2.01	0.42
1:1:11:VAL:HG22	4:4:76:PHE:CZ	2.55	0.42
1:1:14:THR:O	1:1:15:VAL:C	2.57	0.42
1:1:191:LEU:HA	1:1:191:LEU:HD23	1.80	0.42
3:3:74:LEU:HD11	3:3:188:GLN:OE1	2.20	0.42
3:3:135:THR:C	3:3:137:GLU:N	2.72	0.42
1:1:55:GLN:CG	1:1:56:THR:N	2.82	0.42
1:1:107:TYR:CD1	3:3:14:LEU:HD23	2.55	0.42
2:2:62:PHE:CZ	2:2:203:ILE:HB	2.54	0.42
2:2:67:PHE:N	2:2:79:HIS:CD2	2.88	0.42
1:1:45:LYS:O	1:1:46:ASP:HB2	2.19	0.41
2:2:34:TYR:HD1	2:2:34:TYR:H	1.68	0.41
2:2:102:ARG:HB3	2:2:162:PHE:CE1	2.55	0.41
2:2:212:GLY:O	2:2:213:GLU:CB	2.68	0.41
3:3:54:PHE:HA	3:3:202:LEU:HA	2.02	0.41
3:3:73:VAL:CG2	3:3:134:LYS:HA	2.50	0.41
3:3:191:HIS:HE1	3:3:195:ASP:HB3	1.85	0.41
1:1:93:ALA:HA	3:3:99:THR:HG22	2.01	0.41
1:1:124:ARG:HH22	2:2:41:ASP:CG	2.23	0.41
2:2:58:ALA:CB	2:2:94:LEU:HD21	2.50	0.41
3:3:169:TYR:CD1	3:3:169:TYR:N	2.84	0.41
1:1:16:GLU:O	1:1:17:ASN:C	2.59	0.41
1:1:83:GLU:OE2	1:1:172:ARG:NH2	2.53	0.41
1:1:119:TYR:CE1	1:1:126:LEU:HD12	2.55	0.41
1:1:38:ARG:O	1:1:39:PHE:O	2.38	0.41
1:1:119:TYR:HA	1:1:165:TYR:CE2	2.56	0.41
2:2:160:VAL:CG2	2:2:177:TRP:CZ3	3.03	0.41
3:3:106:ASN:HD21	3:3:206:GLY:HA2	1.84	0.41
3:3:200:VAL:O	3:3:200:VAL:HG13	2.21	0.41
4:4:67:TRP:O	4:4:70:LYS:N	2.53	0.41
1:1:76:LEU:HD12	1:1:77:GLU:H	1.85	0.41
2:2:19:ASN:ND2	2:2:19:ASN:N	2.69	0.41
3:3:55:LEU:C	3:3:56:HIS:O	2.58	0.41
3:3:109:PHE:HD1	3:3:199:LEU:HG	1.85	0.41
3:3:88:ASN:OD1	3:3:89:THR:N	2.53	0.41
1:1:53:LEU:C	1:1:55:GLN:H	2.22	0.41
1:1:54:MET:CE	1:1:128:THR:HG22	2.48	0.41
1:1:85:ASN:ND2	1:1:106:ALA:O	2.54	0.41
2:2:120:CYS:N	2:2:185:ALA:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:191:SER:OG	2:2:192:GLU:N	2.54	0.41
2:2:206:THR:O	2:2:208:VAL:N	2.54	0.41
1:1:51:LEU:HD23	1:1:76:LEU:HD23	2.03	0.41
1:1:93:ALA:HB1	3:3:215:VAL:CG2	2.44	0.41
1:1:132:GLY:HA2	2:2:174:HIS:CD2	2.56	0.41
2:2:55:VAL:O	2:2:55:VAL:HG13	2.20	0.41
3:3:42:THR:HG22	3:3:42:THR:O	2.21	0.41
3:3:50:ALA:C	3:3:51:CYS:SG	2.99	0.41
1:1:196:PRO:C	1:1:197:ASP:OD1	2.59	0.40
3:3:86:MET:O	3:3:89:THR:N	2.52	0.40
3:3:108:HIS:CG	3:3:156:THR:CG2	3.01	0.40
1:1:190:PRO:HG2	2:2:136:GLU:HB3	2.03	0.40
1:1:192:LEU:HB2	2:2:135:ARG:HH11	1.82	0.40
2:2:120:CYS:HB3	2:2:147:PHE:CE2	2.55	0.40
2:2:196:GLN:HG2	2:2:197:ILE:N	2.36	0.40
3:3:90:PHE:CE2	3:3:94:LEU:HD23	2.56	0.40
2:2:90:VAL:O	2:2:93:TYR:N	2.55	0.40
3:3:32:PRO:HD2	3:3:34:ARG:HH22	1.87	0.40
3:3:67:LYS:CE	3:3:74:LEU:HD12	2.51	0.40
1:1:79:ALA:CB	1:1:177:LEU:HD13	2.51	0.40
1:1:51:LEU:N	1:1:51:LEU:CD1	2.85	0.40
2:2:77:ARG:O	2:2:182:MET:HA	2.22	0.40
2:2:101:MET:O	2:2:169:ASP:O	2.40	0.40
3:3:46:ASP:O	3:3:50:ALA:HB2	2.22	0.40
3:3:136:PRO:HG3	3:3:187:PHE:CB	2.52	0.40
3:3:173:ASP:C	3:3:175:ALA:H	2.25	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	1	180/211 (85%)	108 (60%)	42 (23%)	30 (17%)	0 2
2	2	208/218 (95%)	124 (60%)	56 (27%)	28 (14%)	0 4
3	3	218/220 (99%)	139 (64%)	50 (23%)	29 (13%)	0 4
4	4	42/85 (49%)	24 (57%)	10 (24%)	8 (19%)	0 2
All	All	648/734 (88%)	395 (61%)	158 (24%)	95 (15%)	0 3

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	15	VAL
1	1	16	GLU
1	1	38	ARG
1	1	39	PHE
1	1	45	LYS
1	1	158	ALA
1	1	160	PRO
1	1	172	ARG
1	1	184	GLU
1	1	194	ILE
2	2	32	VAL
2	2	74	PRO
2	2	90	VAL
2	2	207	ASN
2	2	215	PRO
3	3	7	CYS
3	3	14	LEU
3	3	17	THR
3	3	27	GLY
3	3	60	ASP
3	3	63	TYR
3	3	76	GLN
3	3	168	ALA
3	3	179	ASN
3	3	189	ILE
4	4	27	MET
4	4	74	SER
4	4	82	ALA
1	1	3	SER
1	1	17	ASN
1	1	20	GLY
1	1	28	GLN
1	1	108	HIS

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Mol	Chain	Res	Type
1	1	171	THR
1	1	205	ILE
2	2	30	VAL
2	2	42	PHE
2	2	91	TYR
2	2	141	THR
2	2	164	GLY
2	2	174	HIS
3	3	8	SER
3	3	16	THR
3	3	28	LYS
3	3	36	MET
3	3	39	GLY
3	3	40	ARG
3	3	41	PHE
3	3	43	ASN
3	3	73	VAL
3	3	87	SER
3	3	88	ASN
3	3	134	LYS
3	3	140	ALA
3	3	218	ARG
4	4	66	ASP
4	4	81	GLY
1	1	46	ASP
1	1	90	PRO
1	1	99	ASP
1	1	183	ALA
1	1	196	PRO
2	2	15	LEU
2	2	114	ASN
2	2	128	GLU
2	2	190	ASN
2	2	213	GLU
3	3	89	THR
4	4	25	TYR
1	1	74	ALA
1	1	111	PRO
1	1	197	ASP
2	2	12	ASP
2	2	38	THR
2	2	40	GLU

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Mol	Chain	Res	Type
2	2	49	SER
2	2	56	ALA
2	2	137	LEU
3	3	127	PRO
3	3	133	PRO
3	3	149	THR
4	4	29	GLN
1	1	12	THR
1	1	58	ALA
1	1	64	ALA
2	2	43	VAL
2	2	73	ASP
2	2	107	VAL
3	3	62	PRO
1	1	188	PRO
2	2	127	PRO
2	2	130	CYS
4	4	31	GLN
1	1	35	ILE
2	2	76	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	153/173 (88%)	124 (81%)	29 (19%)	1 8
2	2	182/190 (96%)	149 (82%)	33 (18%)	1 9
3	3	176/176 (100%)	145 (82%)	31 (18%)	2 10
4	4	37/67 (55%)	35 (95%)	2 (5%)	22 55
All	All	548/606 (90%)	453 (83%)	95 (17%)	2 11

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	THR

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Mol	Chain	Res	Type
1	1	22	THR
1	1	25	GLN
1	1	26	ARG
1	1	31	ASP
1	1	38	ARG
1	1	41	LYS
1	1	48	ILE
1	1	50	VAL
1	1	54	MET
1	1	60	THR
1	1	67	ARG
1	1	72	TYR
1	1	82	HIS
1	1	86	LEU
1	1	98	LEU
1	1	103	ASN
1	1	109	LYS
1	1	111	PRO
1	1	112	LEU
1	1	114	ARG
1	1	119	TYR
1	1	160	PRO
1	1	164	ASN
1	1	180	MET
1	1	188	PRO
1	1	189	ARG
1	1	192	LEU
1	1	203	GLN
2	2	16	THR
2	2	26	THR
2	2	30	VAL
2	2	33	THR
2	2	34	TYR
2	2	40	GLU
2	2	41	ASP
2	2	43	VAL
2	2	51	LEU
2	2	54	ARG
2	2	66	LEU
2	2	75	PHE
2	2	77	ARG
2	2	79	HIS

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Mol	Chain	Res	Type
2	2	85	THR
2	2	94	LEU
2	2	96	ASP
2	2	101	MET
2	2	102	ARG
2	2	110	THR
2	2	115	GLN
2	2	131	SER
2	2	133	GLN
2	2	134	LYS
2	2	143	PHE
2	2	147	PHE
2	2	149	ASN
2	2	151	ARG
2	2	161	PRO
2	2	163	VAL
2	2	180	VAL
2	2	196	GLN
2	2	199	VAL
3	3	5	VAL
3	3	16	THR
3	3	21	THR
3	3	36	MET
3	3	46	ASP
3	3	47	VAL
3	3	54	PHE
3	3	57	PHE
3	3	58	GLU
3	3	60	ASP
3	3	66	THR
3	3	67	LYS
3	3	71	ASP
3	3	85	HIS
3	3	105	ILE
3	3	107	LEU
3	3	110	MET
3	3	122	MET
3	3	123	ILE
3	3	127	PRO
3	3	134	LYS
3	3	143	ILE
3	3	147	TRP

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Mol	Chain	Res	Type
3	3	151	LEU
3	3	153	SER
3	3	154	LYS
3	3	155	PHE
3	3	166	ASP
3	3	179	ASN
3	3	186	LEU
3	3	218	ARG
4	4	65	ASN
4	4	79	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	23	GLN
1	1	25	GLN
1	1	49	ASN
1	1	55	GLN
1	1	82	HIS
1	1	91	ASN
1	1	108	HIS
2	2	19	ASN
2	2	103	ASN
2	2	149	ASN
2	2	196	GLN
3	3	31	ASN
3	3	100	GLN
3	3	141	HIS
3	3	191	HIS
3	3	220	GLN
4	4	23	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.