



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:38 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

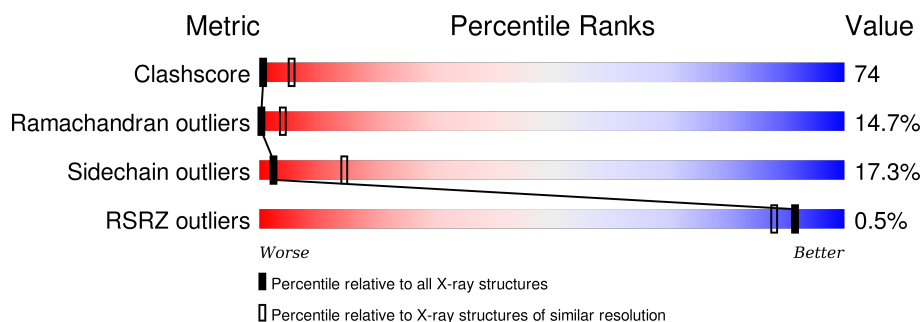
1 Overall quality at a glance

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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

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

2 Entry composition

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
1	1	184	Total	C	N	O	S	0	0	0
			1437	910	258	266	3			

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

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

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
3	3	220	Total	C	N	O	S	0	0	0
			1685	1079	274	323	9			

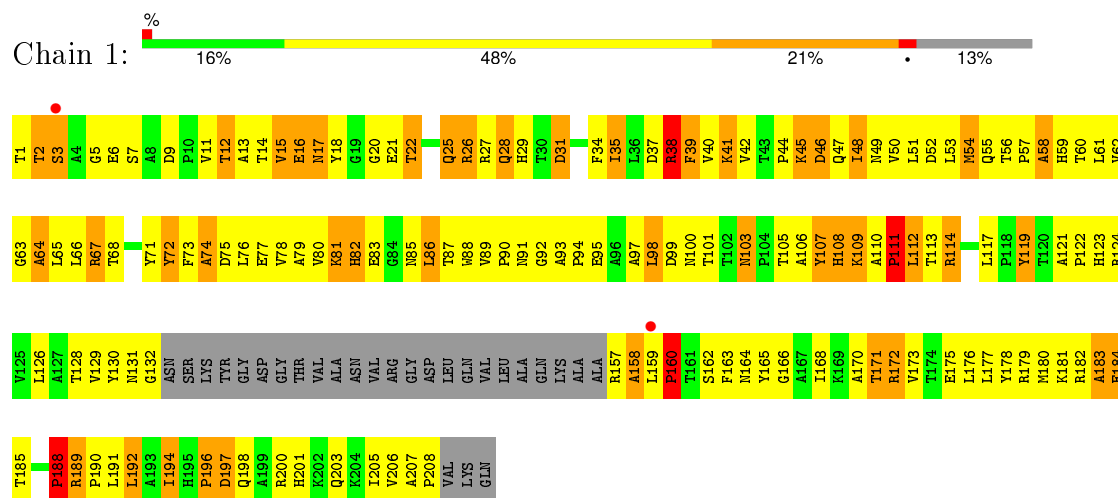
- Molecule 4 is a protein called Genome polypeptide.

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

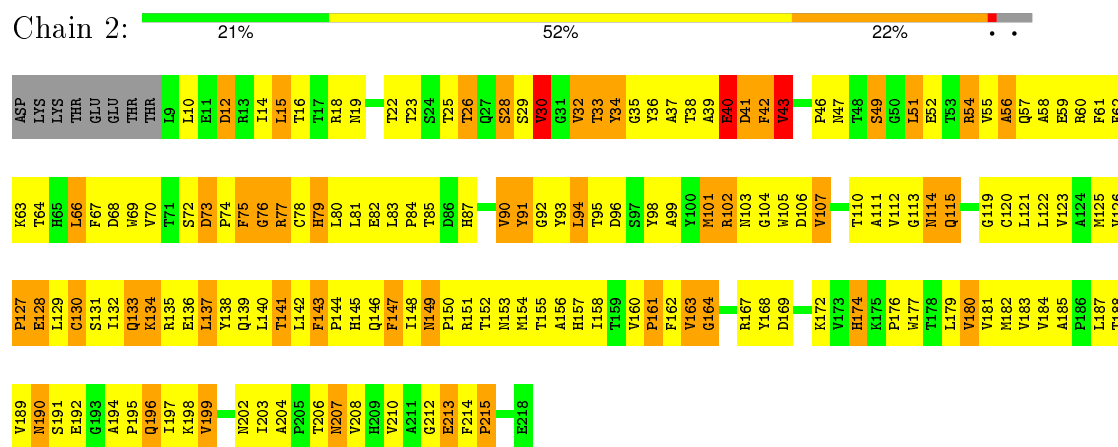
3 Residue-property plots

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

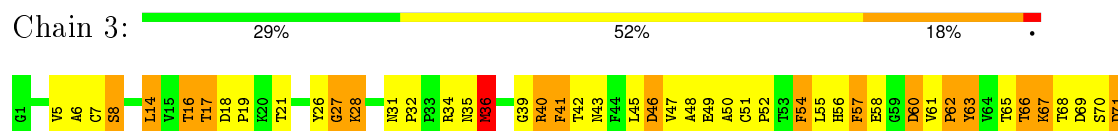
• Molecule 1: Foot and mouth disease virus, VP1

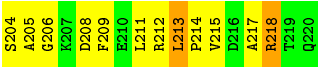
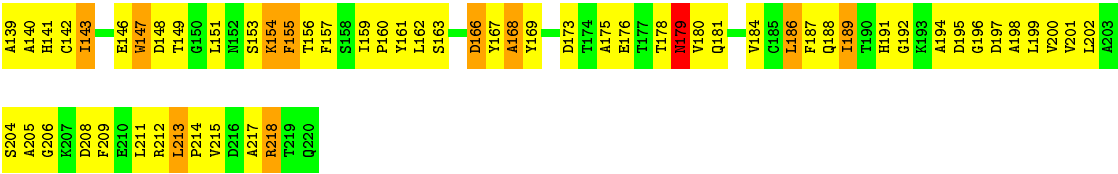
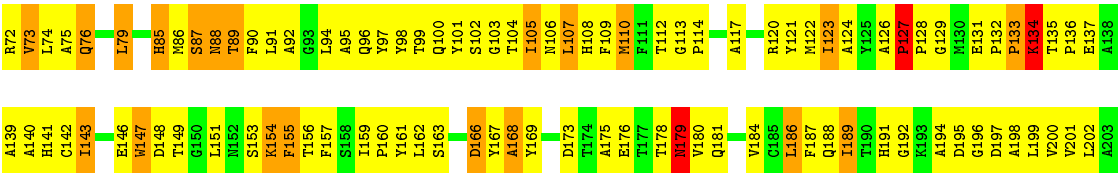


• Molecule 2: Foot and mouth disease virus, VP2

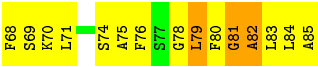


• Molecule 3: Foot and mouth disease virus, VP3





● Molecule 4: Genome polypeptide



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.361 , (Not available) 0.361 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 , 87.3	EDS
Estimated twinning fraction	0.499 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	1 of 65915 reflections (0.002%)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	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($^{\circ}$)	Ideal($^{\circ}$)
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 ⓘ

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
2:2:90:VAL:O	2:2:94:LEU:HD13	1.78	0.84
1:1:15:VAL:HB	1:1:22:THR:HG23	1.58	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:H	2:2:134:LYS:CD	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
3:3:133:PRO:HG2	3:3:187:PHE:CZ	2.19	0.77
3:3:120:ARG:HG3	3:3:120:ARG:HH11	1.49	0.77
3:3:102:SER:HA	3:3:161:TYR:CE1	2.20	0.77
1:1:130:TYR:CE2	1:1:132:GLY:HA3	2.19	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
3:3:75:ALA:O	3:3:76:GLN:HB2	1.90	0.69
2:2:102:ARG:HH11	2:2:102:ARG:HG2	1.58	0.69
1:1:107:TYR:CG	3:3:14:LEU:HD23	2.28	0.69
3:3:27:GLY:O	3:3:28:LYS:HB2	1.93	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
1:1:171:THR:O	1:1:172:ARG:HB2	1.94	0.68
1:1:67:ARG:HG2	1:1:67:ARG:NH1	2.08	0.68
3:3:40:ARG:CG	3:3:41:PHE:H	2.04	0.68
2:2:54:ARG:NE	2:2:56:ALA:HB2	2.09	0.68
2:2:73:ASP:OD1	2:2:77:ARG:HG3	1.94	0.68
2:2:67:PHE:HB3	2:2:79:HIS:CG	2.28	0.68
1:1:44:PRO:CB	1:1:176:LEU:HB2	2.18	0.68
2:2:141:THR:HA	2:2:145:HIS:NE2	2.09	0.68
2:2:83:LEU:N	2:2:177:TRP:O	2.22	0.68
1:1:93:ALA:HB2	3:3:99:THR:CG2	2.24	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
4:4:65:ASN:HB2	4:4:69:SER:CB	2.22	0.66
2:2:189:VAL:HG23	2:2:190:ASN:N	2.11	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)
3:3:66:THR:OG1	3:3:195:ASP:HA	1.96	0.66
2:2:146:GLN:HG3	2:2:158:ILE:HG23	1.76	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
2:2:103:ASN:HD22	2:2:104:GLY:N	1.92	0.65
2:2:42:PHE:O	2:2:167:ARG:HD3	1.96	0.65
2:2:134:LYS:N	2:2:134:LYS:HD2	2.11	0.65
3:3:55:LEU:HD12	3:3:201:VAL:O	1.95	0.65
3:3:108:HIS:CG	3:3:156:THR:HG22	2.31	0.65
2:2:214:PHE:CE1	3:3:127:PRO:HG2	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
1:1:44:PRO:C	1:1:49:ASN:HD21	2.00	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
1:1:129:VAL:CA	1:1:159:LEU:HD21	2.27	0.64
1:1:11:VAL:O	1:1:11:VAL:HG12	1.98	0.64
2:2:47:ASN:O	3:3:162:LEU:HA	1.98	0.64
1:1:88:TRP:CZ2	1:1:166:GLY:HA3	2.32	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
2:2:129:LEU:CG	2:2:130:CYS:H	2.10	0.63
1:1:130:TYR:N	1:1:159:LEU:HD11	2.12	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
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
2:2:63:LYS:HE3	2:2:202:ASN:ND2	2.14	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
2:2:40:GLU:CD	2:2:102:ARG:NH2	2.53	0.62
1:1:1:THR:HG23	4:4:78:GLY:O	2.00	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
1:1:122:PRO:HG3	3:3:100:GLN:CD	2.20	0.61
1:1:3:SER:HA	4:4:80:PHE:CE1	2.36	0.61
2:2:58:ALA:HB2	2:2:90:VAL:HB	1.82	0.61
1:1:38:ARG:HG2	1:1:38:ARG:NH1	2.15	0.61
1:1:123:HIS:HE2	1:1:162:SER:HB2	1.65	0.61
2:2:128:GLU:OE1	2:2:176:PRO:HB3	2.01	0.60
2:2:43:VAL:CG1	2:2:102:ARG:NH1	2.64	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
1:1:54: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
1:1:12:THR:HG22	1:1:13:ALA:N	2.10	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:N	2:2:134:LYS:HZ2	1.98	0.60
2:2:133:GLN:HA	2:2:134:LYS:HZ3	1.65	0.60
2:2:22:THR:OG1	2:2:60:ARG:HB2	2.02	0.60
1:1:3:SER:OG	1:1:11:VAL:HG11	2.01	0.60
3:3:94:LEU:C	3:3:96:GLN:H	2.06	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
2:2:37:ALA:HB3	2:2:161:PRO:CB	2.32	0.59
3:3:66:THR:HG22	3:3:188:GLN:CD	2.23	0.59
3:3:202:LEU:HD12	3:3:202:LEU:N	2.17	0.59
3:3:112:THR:OG1	3:3:198:ALA:HB3	2.02	0.59
2:2:75:PHE:O	2:2:75:PHE:CG	2.54	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
2:2:160:VAL:HG21	2:2:177:TRP:CZ3	2.37	0.59
2:2:102:ARG:CZ	2:2:102:ARG:HB2	2.32	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
2:2:126:VAL:HG22	2:2:143:PHE:CB	2.33	0.59
2:2:83:LEU:O	2:2:177:TRP:HB2	2.02	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
2:2:163:VAL:O	2:2:164:GLY:O	2.20	0.59
2:2:146:GLN:HG3	2:2:157:HIS:O	2.03	0.59
2:2:84:PRO:HB3	2:2:91:TYR:HH	1.68	0.59
1:1:74:ALA:O	1:1:119:TYR:HB2	2.02	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
2:2:25:THR:HG22	2:2:26:THR:N	2.19	0.58
1:1:48:ILE:H	1:1:48:ILE:HD12	1.68	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
3:3:73:VAL:HG22	3:3:187:PHE:CD2	2.39	0.58
2:2:55:VAL:HG22	2:2:55:VAL:O	2.03	0.58
2:2:34:TYR:CD1	2:2:34:TYR:N	2.69	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
2:2:87:HIS:HB3	2:2:92:GLY:CA	2.34	0.57
2:2:78:CYS:HB3	2:2:182:MET:CB	2.33	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
3:3:104:THR:HG23	3:3:208:ASP:CB	2.32	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
2:2:14:ILE:O	2:2:15:LEU:HB2	2.05	0.57
3:3:108:HIS:O	3:3:201:VAL:HA	2.05	0.56
3:3:134:LYS:NZ	3:3:134:LYS:HB3	2.20	0.56
3:3:79:LEU:HD23	3:3:184:VAL:CB	2.33	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
4:4:65:ASN:O	4:4:66:ASP:C	2.43	0.56
3:3:79:LEU:HD21	3:3:159:ILE:HD12	1.87	0.56
2:2:54:ARG:HH12	2:2:208:VAL:CG1	2.19	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
3:3:103: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
3:3:32:PRO:HD2	3:3:34:ARG:HH12	1.69	0.56
3:3:114:PRO:HG2	3:3:117:ALA:CB	2.35	0.56
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
1:1:35:ILE:HD12	1:1:38:ARG:NE	2.22	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
3:3:75:ALA:HB2	3:3:186:LEU:HD23	1.88	0.55
3:3:31:ASN:HB3	3:3:32:PRO:CD	2.36	0.55
3:3:86:MET:O	3:3:88:ASN:N	2.40	0.55
1:1:72:TYR:CD1	1:1:73:PHE:N	2.75	0.55
2:2:143:PHE:CD2	2:2:143:PHE:N	2.74	0.55
3:3:40:ARG:O	3:3:41:PHE:HB3	2.07	0.55
1:1:2:THR:O	1:1:3:SER: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
3:3:99:THR:HG23	3:3:215:VAL:HB	1.89	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
1:1:119:TYR:HD1	1:1:165:TYR:OH	1.91	0.54
1:1:11:VAL:HG13	4:4:76:PHE:CE1	2.42	0.54
1:1:44:PRO:HA	1:1:176:LEU:HD22	1.90	0.54
2:2:102:ARG:HB2	2:2:102:ARG:NH1	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
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
1:1:130: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
1:1:67:ARG:CG	1:1:67:ARG:NH1	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:O	1:1:129:VAL:HG13	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)
2:2:127:PRO:O	2:2:128:GLU:C	2.47	0.53
2:2:70:VAL:O	2:2:73:ASP:HB3	2.08	0.53
3:3:192:GLY:C	3:3:194:ALA:H	2.10	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
2:2:115:GLN:HA	2:2:150:PRO:O	2.09	0.53
2:2:98:TYR:CE2	2:2:210:VAL:HG11	2.44	0.53
1:1:196:PRO:HG3	1:1:201:HIS:HB2	1.90	0.53
2:2:135:ARG:HA	2:2:138:TYR:HE2	1.74	0.53
1:1:124:ARG:HH12	2:2:41:ASP:HB2	1.74	0.53
3:3:101:TYR:HB3	3:3:211:LEU:CD1	2.39	0.53
2:2:72:SER:O	2:2:73:ASP:C	2.46	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
2:2:98: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:HG13	1:1:40:VAL:O	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
2:2:87:HIS:NE2	2:2:91:TYR:HB3	2.24	0.52
1:1:72:TYR:HD1	1:1:73:PHE:N	2.08	0.52
3:3:134:LYS:N	3:3:134:LYS:HD2	2.24	0.52
1:1:3:SER:CB	1:1:11:VAL:HG11	2.40	0.52
1:1:192:LEU:H	1:1:192:LEU:HD23	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
3:3:73:VAL:HG21	3:3:134:LYS:HA	1.92	0.51
2:2:54:ARG:HD2	2:2:56:ALA:H	1.75	0.51
1:1:35:ILE:HG23	1:1:35:ILE:O	2.10	0.51
2:2:113:GLY:HA3	2:2:197:ILE:HD11	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)
3:3:139:ALA:C	3:3:141:HIS:N	2.63	0.51
2:2:103:ASN:ND2	2:2:104:GLY:N	2.57	0.51
1:1:188:PRO:O	1:1:189:ARG:HG2	2.11	0.51
1:1:42:VAL:HG11	1:1:55:GLN:HE21	1.74	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
2:2:106:ASP:C	2:2:107:VAL:HG23	2.31	0.51
2:2:55:VAL:O	2:2:57:GLN:N	2.44	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
1:1:71:TYR:O	1:1:185:THR:HB	2.11	0.50
1:1:27:ARG:O	1:1:29:HIS:N	2.44	0.50
2:2:60:ARG:O	2:2:204:ALA:HA	2.12	0.50
2:2:18:ARG:C	2:2:19:ASN:ND2	2.63	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
1:1:26:ARG:HD3	1:1:26:ARG:N	2.26	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
3:3:161:TYR:C	3:3:162:LEU:HD22	2.33	0.49
3:3:73:VAL:HG13	3:3:75:ALA:O	2.11	0.49
1:1:25:GLN:N	1:1:25:GLN:NE2	2.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:135:ARG:O	2:2:138:TYR:HD2	1.94	0.49
2:2:102:ARG:HD2	2:2:168:TYR:CZ	2.47	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
1:1:130:TYR:N	1:1:159:LEU:HD21	2.26	0.49
3:3:123:ILE:HG13	3:3:123:ILE:O	2.11	0.49
3:3:160:PRO:HB2	3:3:162:LEU:HD21	1.93	0.49
1:1:109:LYS:HE3	1:1:109:LYS:C	2.33	0.49
1:1:51:LEU:HD22	1:1:165:TYR:O	2.12	0.49
3:3:131:GLU:CG	3:3:132:PRO:HD2	2.42	0.49
1:1:194:ILE:O	1:1:196:PRO:HD3	2.12	0.49
2:2:148:ILE:HD13	2:2:153:ASN:HD21	1.77	0.49
3:3:97:TYR:HA	3:3:215:VAL:O	2.13	0.49
2:2:148:ILE:HD13	2:2:153:ASN:ND2	2.27	0.49
3:3:137:GLU:N	3:3:137:GLU:CD	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
3:3:154:LYS:HB3	3:3:154:LYS:NZ	2.28	0.49
2:2:196:GLN:HE22	2:2:198:LYS:CG	2.26	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
2:2:81:LEU:O	2:2:83:LEU:HD22	2.12	0.49
3:3:73:VAL:CG1	3:3:75:ALA:O	2.60	0.49
1:1:85:ASN:ND2	1:1:107:TYR:CG	2.80	0.49
3:3:48:ALA:HB1	3:3:91:LEU:HG	1.94	0.49
3:3:108:HIS:N	3:3:108:HIS:CD2	2.81	0.48
1:1:9:ASP:O	1:1:11:VAL:HG23	2.13	0.48
2:2:43:VAL:HG11	2:2:102:ARG:NE	2.29	0.48
1:1:15:VAL:HG12	1:1:16:GLU:N	2.27	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
2:2:94:LEU:HD13	2:2:94:LEU:H	1.78	0.48
2:2:78:CYS:O	2:2:80:LEU:HD12	2.12	0.48
2:2:212:GLY:O	2:2:213:GLU:HB3	2.12	0.48
2:2:133:GLN:NE2	2:2:136:GLU:OE1	2.46	0.48
2:2:125:MET:O	2:2:177:TRP:HZ3	1.95	0.48
1:1:28:GLN:O	1:1:31:ASP:HB2	2.13	0.48
3:3:109:PHE:CG	3:3:147:TRP:HH2	2.31	0.48
1:1:206:VAL:HG23	1:1:206:VAL:O	2.14	0.48
1:1:68:THR:HA	1:1:189:ARG:HB2	1.96	0.48
1:1:54:MET:SD	1:1:128:THR:HG22	2.53	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
3:3:86:MET:HA	3:3:89:THR:HG21	1.94	0.47
2:2:54:ARG:NH1	2:2:208:VAL:H	2.12	0.47
2:2:18:ARG:CB	2:2:23:THR:HG22	2.44	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
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
2:2:160: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
2:2:63:LYS:N	2:2:63:LYS:HD2	2.29	0.47
1:1:75:ASP:OD1	1:1:119:TYR:N	2.46	0.47
3:3:92:ALA:C	3:3:94:LEU:H	2.16	0.47
1:1:194:ILE:HG21	1:1:201:HIS:CD2	2.50	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
2:2:102:ARG:HB3	2:2:162:PHE:CZ	2.50	0.47
2:2:102:ARG:O	2:2:208:VAL:HA	2.15	0.47
1:1:130:TYR:CD2	1:1:160:PRO:HG2	2.49	0.47
3:3:98:TYR:CE1	3:3:214:PRO:HG3	2.39	0.47
1:1:196:PRO:O	1:1:197:ASP:CG	2.53	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
1:1:192:LEU:HD13	2:2:135:ARG:HG2	1.96	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
2:2:102:ARG:CG	2:2:102:ARG:NH1	2.72	0.47
3:3:72:ARG:HD3	3:3:188:GLN:O	2.15	0.47
2:2:63:LYS:HE3	2:2:202:ASN:HD21	1.78	0.47
2:2:167:ARG:HB3	2:2:167:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:51:LEU:N	1:1:51:LEU:HD12	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
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
1:1:188:PRO:CG	2:2:142:LEU:O	2.62	0.46
3:3:191:HIS:HB2	3:3:194:ALA:HB3	1.98	0.46
3:3:91:LEU:HD12	3:3:91:LEU:N	2.31	0.46
1:1:82:HIS:HD2	1:1:170:ALA:CB	2.29	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
1:1:130:TYR:H	1:1:159:LEU:CG	2.27	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
2:2:54:ARG:NH1	2:2:208:VAL:HG13	2.31	0.46
2:2:52:GLU:HA	2:2:210:VAL:O	2.14	0.46
2:2:121:LEU:HD21	2:2:199:VAL:HG21	1.97	0.46
1:1:93:ALA:CA	3:3:99:THR:HG22	2.46	0.46
2:2:114:ASN:O	2:2:150:PRO:HB3	2.16	0.46
1:1:48:ILE:H	1:1:48:ILE:CD1	2.21	0.46
1:1:194:ILE:HG21	1:1:201:HIS:NE2	2.31	0.46
3:3:94:LEU:O	3:3:96:GLN:N	2.49	0.46
2:2:181:VAL:HG23	2:2:181:VAL:O	2.16	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
1:1:81:LYS:H	1:1:175:GLU:HB2	1.81	0.46
3:3:94:LEU:HD12	3:3:94:LEU:C	2.35	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
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
2:2:137:LEU:O	2:2:140:LEU:CD2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:198:GLN:C	1:1:200:ARG:N	2.70	0.45
1:1:192:LEU:N	1:1:192:LEU:CD2	2.79	0.45
1:1:42:VAL:HB	1:1:55:GLN:HE21	1.81	0.45
2:2:135:ARG:HA	2:2:138:TYR:CE2	2.52	0.45
2:2:67:PHE:CD2	2:2:77:ARG:HD2	2.51	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
2:2:83:LEU:O	2:2:177:TRP:O	2.35	0.45
1:1:91:ASN:ND2	3:3:169:TYR:OH	2.48	0.45
1:1:182:ARG:HA	4:4:15:SER:HB3	1.98	0.45
1:1:89:VAL:CG1	1:1:93:ALA:HB3	2.47	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:CD2	2:2:36:TYR:N	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
4:4:22:ILE:C	4:4:24:ASN:H	2.19	0.45
2:2:98:TYR:CD2	2:2:210:VAL:HG11	2.51	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
2:2:84: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
2:2:28:SER:HB3	2:2:154:MET:H	1.82	0.45
3:3:76:GLN:OE1	3:3:132:PRO:HG2	2.16	0.45
3:3:62:PRO:HG2	3:3:63:TYR:H	1.82	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
2:2:138:TYR:O	2:2:139:GLN:HG2	2.17	0.44
2:2:76:GLY:O	2:2:77:ARG:C	2.55	0.44
4:4:65:ASN:O	4:4:66:ASP:O	2.35	0.44
3:3:46:ASP:O	3:3:50:ALA:HB3	2.16	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
1:1:188:PRO:HD3	4:4:68:PHE:CE2	2.53	0.44
1:1:57:PRO:C	1:1:59:HIS:H	2.20	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
3:3:124:ALA:CB	3:3:187:PHE:HE1	2.25	0.44
2:2:54:ARG:HD3	2:2:208:VAL:O	2.18	0.44
3:3:147:TRP:C	3:3:147:TRP:CD1	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
2:2:94:LEU:CD1	2:2:94:LEU:N	2.81	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
3:3:167:TYR:O	3:3:168:ALA:HB3	2.17	0.44
3:3:67:LYS:HE2	3:3:74:LEU:HD12	1.99	0.44
1:1:183:ALA:O	1:1:184:GLU:HB3	2.18	0.44
2:2:54:ARG:NH2	2:2:59:GLU:OE2	2.51	0.43
1:1:119:TYR:CD2	1:1:119:TYR:O	2.71	0.43
1:1:79:ALA:HB3	1:1:177:LEU:CD1	2.49	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:C	2:2:91:TYR:CD2	2.91	0.43
3:3:104:THR:CG2	3:3:208:ASP:HB3	2.37	0.43
2:2:163:VAL:C	2:2:164:GLY:O	2.55	0.43
1:1:131:ASN:HB2	2:2:129:LEU:N	2.14	0.43
3:3:79:LEU:HD23	3:3:184:VAL:CG1	2.49	0.43
2:2:39:ALA:O	2:2:40:GLU:HB2	2.17	0.43
3:3:120:ARG:HD3	3:3:189:ILE:HG13	2.00	0.43
2:2:132:ILE:HG12	2:2:133:GLN:N	2.33	0.43
1:1:37:ASP:CB	4:4:16:GLY:HA3	2.48	0.43
3:3:65:THR:HA	3:3:197:ASP:O	2.18	0.43
2:2:213:GLU:O	3:3:127:PRO:CD	2.65	0.43
3:3:199:LEU:HG	3:3:199:LEU:O	2.19	0.43
1:1:82:HIS:HB2	1:1:173:VAL:HA	2.00	0.43
2:2:137:LEU:HA	2:2:137:LEU:HD23	1.81	0.43
3:3:66:THR:HG22	3:3:188:GLN:OE1	2.18	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
3:3:67:LYS:HG2	3:3:71:ASP:O	2.17	0.43
1:1:48:ILE:HD12	1:1:48:ILE:N	2.33	0.43
3:3:31:ASN:HB3	3:3:34:ARG:NH2	2.33	0.43
1:1:57:PRO:O	1:1:59:HIS:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:18:TYR:CD2	1:1:18:TYR:N	2.82	0.43
1:1:40:VAL:HG21	1:1:56:THR:OG1	2.19	0.43
1:1:192:LEU:CD1	2:2:135:ARG:HG2	2.48	0.43
3:3:180:VAL:HG23	3:3:181:GLN:CD	2.37	0.43
2:2:14:ILE:O	2:2:15:LEU:CB	2.66	0.43
1:1:100:ASN:O	1:1:103:ASN:HB2	2.18	0.43
1:1:87:THR:OG1	1:1:105:THR:HG23	2.19	0.43
3:3:135:THR:O	3:3:137:GLU:N	2.52	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
1:1:191: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
1:1:122:PRO:HG3	3:3:100:GLN:OE1	2.18	0.43
3:3:154:LYS:HG2	3:3:155:PHE:H	1.84	0.43
2:2:75:PHE:C	2:2:75:PHE:CD1	2.91	0.43
2:2:40:GLU:OE1	2:2:102:ARG:NH1	2.45	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
2:2:47:ASN:HA	3:3:161:TYR:CD2	2.54	0.42
3:3:161:TYR:OH	3:3:167:TYR:O	2.37	0.42
1:1:5:GLY:C	1:1:7:SER:H	2.23	0.42
1:1:45:LYS:CA	1:1:49:ASN:HD21	2.31	0.42
1:1:65:LEU:HD12	1:1:65:LEU:N	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
1:1:119: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
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
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
2:2:28:SER:HB2	2:2:154:MET:HB2	2.01	0.42
3:3:76:GLN:OE1	3:3:132:PRO:CG	2.68	0.42
2:2:122:LEU:HB2	2:2:184:VAL:CG2	2.48	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:HA	3:3:36:MET:CE	2.50	0.42
3:3:91:LEU:HD21	3:3:205:ALA:N	2.35	0.42
1:1:191:LEU:HD23	1:1:191:LEU:HA	1.80	0.42
1:1:14:THR:O	1:1:15:VAL:C	2.57	0.42
3:3:74:LEU:HD11	3:3:188:GLN:OE1	2.20	0.42
1:1:11:VAL:HG22	4:4:76:PHE:CZ	2.55	0.42
3:3:135:THR:C	3:3:137:GLU:N	2.72	0.42
1:1:6:GLU:HG2	2:2:149:ASN:HB3	2.01	0.42
1:1:55:GLN:CG	1:1:56:THR:N	2.82	0.42
2:2:67:PHE:N	2:2:79:HIS:CD2	2.88	0.42
2:2:62:PHE:CZ	2:2:203:ILE:HB	2.54	0.42
1:1:107:TYR:CD1	3:3:14:LEU:HD23	2.55	0.42
1:1:45:LYS:O	1:1:46:ASP:HB2	2.19	0.41
3:3:73:VAL:CG2	3:3:134:LYS:HA	2.50	0.41
2:2:212:GLY:O	2:2:213:GLU:CB	2.68	0.41
2:2:102:ARG:HB3	2:2:162:PHE:CE1	2.55	0.41
3:3:191:HIS:HE1	3:3:195:ASP:HB3	1.85	0.41
3:3:54:PHE:HA	3:3:202:LEU:HA	2.02	0.41
2:2:34:TYR:H	2:2:34:TYR:HD1	1.68	0.41
2:2:58:ALA:CB	2:2:94:LEU:HD21	2.50	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
3:3:169:TYR:N	3:3:169:TYR:CD1	2.84	0.41
1:1:119:TYR:CE1	1:1:126:LEU:HD12	2.55	0.41
1:1:83:GLU:OE2	1:1:172:ARG:NH2	2.53	0.41
1:1:16:GLU:O	1:1:17:ASN:C	2.59	0.41
1:1:119:TYR:HA	1:1:165:TYR:CE2	2.56	0.41
1:1:38:ARG:O	1:1:39:PHE:O	2.38	0.41
2:2:160:VAL:CG2	2:2:177:TRP:CZ3	3.03	0.41
4:4:67:TRP:O	4:4:70:LYS:N	2.53	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
1:1:76:LEU:HD12	1:1:77:GLU:H	1.85	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
2:2:19:ASN:ND2	2:2:19:ASN:N	2.69	0.41
3:3:88:ASN:OD1	3:3:89:THR:N	2.53	0.41
1:1:54:MET:CE	1:1:128:THR:HG22	2.48	0.41
1:1:53:LEU:C	1:1:55:GLN:H	2.22	0.41
2:2:206:THR:O	2:2:208:VAL:N	2.54	0.41
2:2:191:SER:OG	2:2:192:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:2:55:VAL:O	2:2:55:VAL:HG13	2.20	0.41
1:1:132:GLY:HA2	2:2:174:HIS:CD2	2.56	0.41
3:3:50:ALA:C	3:3:51:CYS:SG	2.99	0.41
3:3:42:THR:HG22	3:3:42:THR:O	2.21	0.41
3:3:108:HIS:CG	3:3:156:THR:CG2	3.01	0.40
3:3:86:MET:O	3:3:89:THR:N	2.52	0.40
1:1:196:PRO:C	1:1:197:ASP:OD1	2.59	0.40
1:1:192:LEU:HB2	2:2:135:ARG:HH11	1.82	0.40
1:1:190:PRO:HG2	2:2:136:GLU:HB3	2.03	0.40
3:3:90:PHE:CE2	3:3:94:LEU:HD23	2.56	0.40
2:2:196:GLN:HG2	2:2:197:ILE:N	2.36	0.40
2:2:120:CYS:HB3	2:2:147:PHE:CE2	2.55	0.40
2:2:90:VAL:O	2:2:93:TYR:N	2.55	0.40
3:3:67:LYS:CE	3:3:74:LEU:HD12	2.51	0.40
3:3:32:PRO:HD2	3:3:34:ARG:HH22	1.87	0.40
1:1:79:ALA:CB	1:1:177:LEU:HD13	2.51	0.40
1:1:51:LEU:CD1	1:1:51:LEU:N	2.85	0.40
2:2:77:ARG:O	2:2:182:MET:HA	2.22	0.40
3:3:136:PRO:HG3	3:3:187:PHE:CB	2.52	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
3:3:173: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	3
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	5
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	4

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 ⓘ

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%)	2	10
2	2	182/190 (96%)	149 (82%)	33 (18%)	2	12
3	3	176/176 (100%)	145 (82%)	31 (18%)	2	13
4	4	37/67 (55%)	35 (95%)	2 (5%)	27	67
All	All	548/606 (90%)	453 (83%)	95 (17%)	2	14

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

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	1	184/211 (87%)	-0.17	2 (1%) 82 73	11, 41, 73, 98	0
2	2	210/218 (96%)	-0.24	0 100 100	12, 43, 76, 130	0
3	3	220/220 (100%)	-0.12	0 100 100	12, 44, 86, 116	0
4	4	46/85 (54%)	0.02	1 (2%) 65 55	21, 62, 95, 111	0
All	All	660/734 (89%)	-0.16	3 (0%) 91 88	11, 44, 84, 130	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	4	15	SER	2.9
1	1	159	LEU	2.9
1	1	3	SER	2.2

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.