Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 11:56 pm GMT

PDB ID	:	2V7H
Title	:	Crystal structure of an immunogen specific anti-mannopyranoside monoclonal antibody Fab fragment
Authors	:	Krishnan, L.; Sahni, G.; Kaur, K.J.; Salunke, D.M.
Deposited on	:	2007-07-30
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

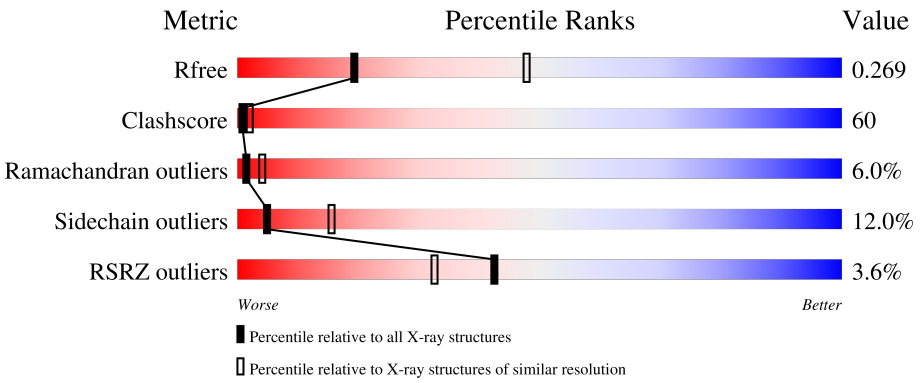
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	214	2%, 36%, 56%, 8%
1	L	214	5%, 32%, 60%, 8%
2	B	220	5%, 28%, 54%, 15%, • •
2	H	220	2%, 30%, 53%, 14%, •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6704 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 MONOCLONAL ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1644	1018	280	339	7	0	0	0
1	L	214	1648	1017	280	344	7	0	0	0

- Molecule 2 is a protein called MONOCLONAL ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	216	1645	1042	271	325	7	0	0	0
2	H	220	1661	1049	274	331	7	0	0	0

- Molecule 3 is water.

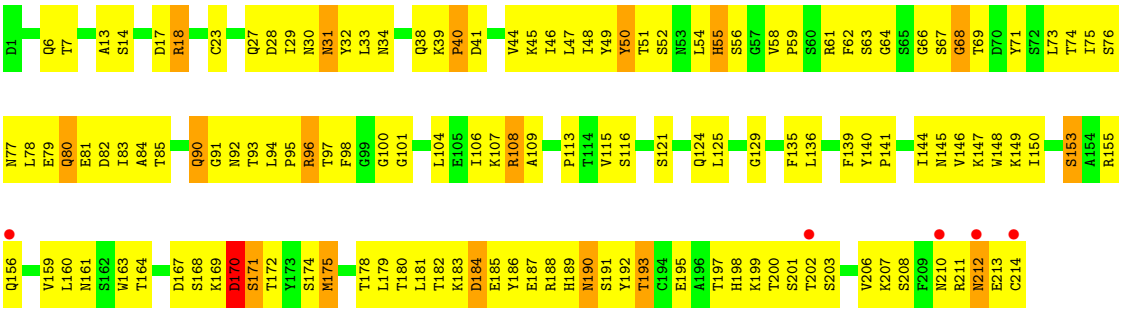
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	24	24	24	0	0
3	B	32	32	32	0	0
3	L	28	28	28	0	0
3	H	22	22	22	0	0

3 Residue-property plots (i)

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

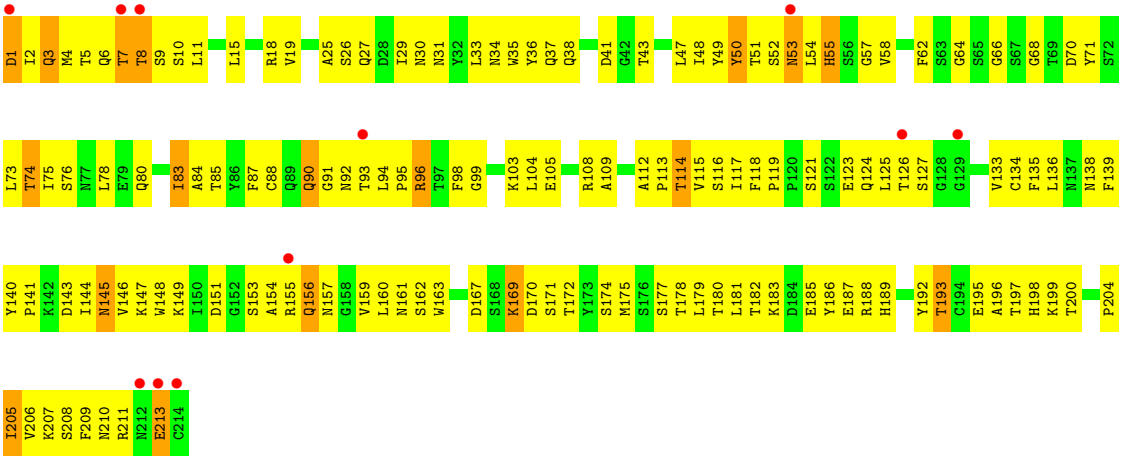
• Molecule 1: MONOCLONAL ANTIBODY

Chain A:



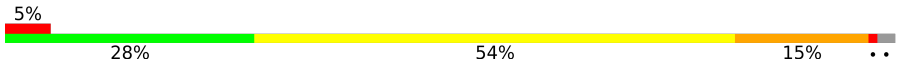
• Molecule 1: MONOCLONAL ANTIBODY

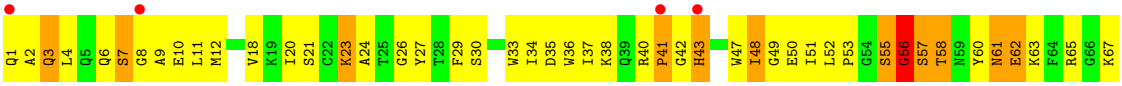
Chain L:

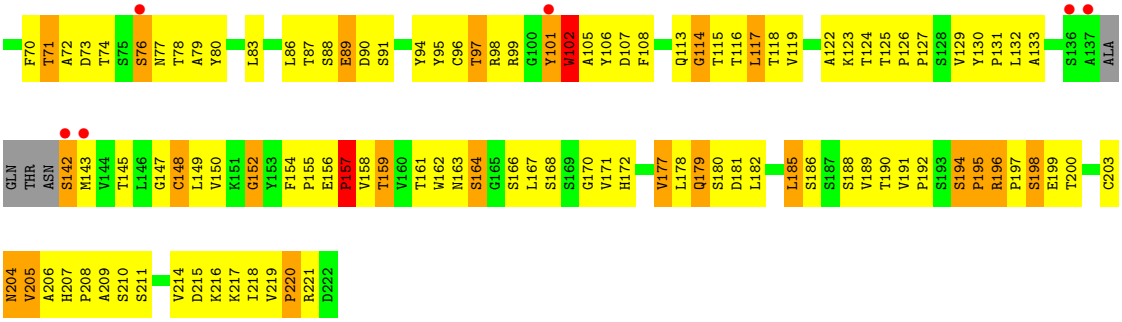


• Molecule 2: MONOCLONAL ANTIBODY

Chain B:

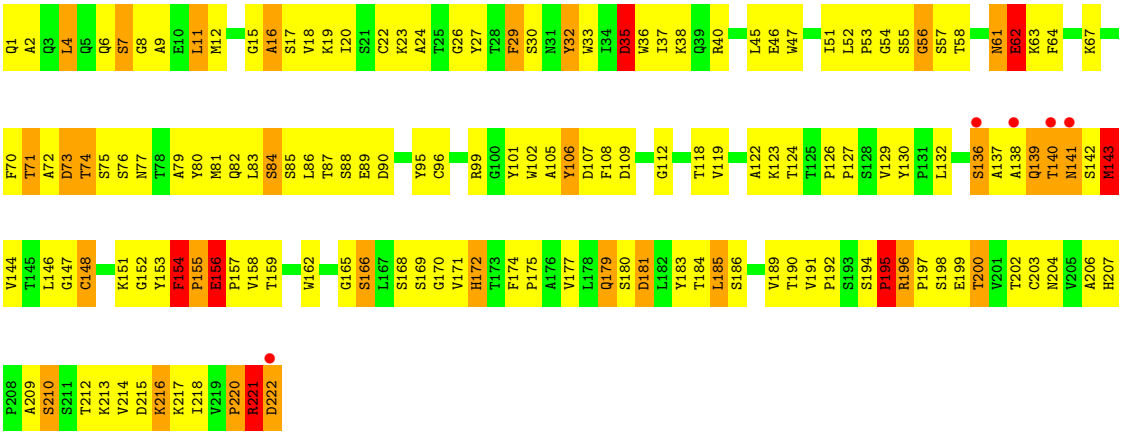






- Molecule 2: MONOCLONAL ANTIBODY

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	40.02Å 79.74Å 132.28Å 90.00° 90.75° 90.00°	Depositor
Resolution (Å)	17.46 – 2.80 17.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.2 (17.46-2.80) 94.7 (17.46-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.50 (at 2.78Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.242 , 0.268 0.242 , 0.269	Depositor DCC
R_{free} test set	1922 reflections (9.70%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6704	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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	A	0.49	0/1677	0.76	2/2276 (0.1%)
1	L	0.47	0/1681	0.83	2/2284 (0.1%)
2	B	0.51	0/1691	0.82	2/2309 (0.1%)
2	H	0.50	0/1707	0.80	4/2333 (0.2%)
All	All	0.49	0/6756	0.80	10/9202 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	9	SER	N-CA-C	7.05	130.02	111.00
2	B	56	GLY	N-CA-C	-6.88	95.91	113.10
2	H	156	GLU	N-CA-C	6.14	127.58	111.00
1	A	170	ASP	N-CA-C	-6.01	94.76	111.00
2	H	35	ASP	CB-CG-OD1	5.89	123.60	118.30
1	L	10	SER	N-CA-C	-5.77	95.42	111.00
2	H	154	PHE	C-N-CD	-5.15	109.27	120.60
2	B	143	MET	N-CA-C	5.14	124.87	111.00
2	H	143	MET	N-CA-C	-5.12	97.19	111.00
1	A	55	HIS	CB-CA-C	-5.06	100.28	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1644	0	1558	198	1
1	L	1648	0	1559	203	0
2	B	1645	0	1585	215	0
2	H	1661	0	1590	195	1
3	A	24	0	0	2	0
3	B	32	0	0	4	0
3	H	22	0	0	1	0
3	L	28	0	0	5	0
All	All	6704	0	6292	771	1

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 60.

All (771) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:ILE:HG21	1:L:52:SER:HA	1.22	1.17
2:B:12:MET:HG3	2:B:18:VAL:HG12	1.23	1.16
1:L:48:ILE:CG2	1:L:52:SER:HA	1.78	1.12
1:L:108:ARG:NH1	1:L:171:SER:H	1.46	1.12
1:L:108:ARG:NH1	1:L:170:ASP:HB2	1.67	1.08
1:L:193:THR:HB	1:L:208:SER:HB3	1.34	1.07
2:H:18:VAL:HG23	2:H:86:LEU:HD11	1.13	1.07
2:B:117:LEU:HD12	2:B:118:THR:N	1.69	1.06
2:B:12:MET:HG3	2:B:18:VAL:CG1	1.84	1.06
1:L:108:ARG:HH12	1:L:170:ASP:CB	1.70	1.05
1:L:213:GLU:HG2	2:H:136:SER:OG	1.61	1.01
1:L:7:THR:O	1:L:8:THR:HG23	1.59	1.00
2:H:155:PRO:O	2:H:157:PRO:HD2	1.62	1.00
1:L:80:GLN:O	1:L:83:ILE:HG22	1.61	1.00
1:L:198:HIS:ND1	1:L:200:THR:HB	1.77	0.99
1:L:31:ASN:HD22	1:L:51:THR:HG21	1.28	0.98
2:H:30:SER:HA	2:H:53:PRO:HB2	1.42	0.98
2:B:6:GLN:NE2	2:B:114:GLY:HA2	1.78	0.98
1:L:108:ARG:HH12	1:L:170:ASP:HB2	0.84	0.97
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.47	0.96
2:B:117:LEU:HD12	2:B:118:THR:H	1.28	0.94
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.32	0.93
1:L:108:ARG:HH11	1:L:171:SER:H	0.96	0.92
2:H:11:LEU:HD11	2:H:154:PHE:CE2	2.06	0.91
1:L:48:ILE:HG21	1:L:52:SER:CA	2.00	0.91
2:H:126:PRO:HG3	2:H:210:SER:OG	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.49	0.91
2:B:131:PRO:HB2	2:B:218:ILE:HD13	1.51	0.91
2:H:154:PHE:HD2	2:H:155:PRO:HD3	1.35	0.90
1:A:147:LYS:HB3	1:A:155:ARG:NH1	1.87	0.90
2:H:194:SER:HB2	2:H:195:PRO:HD3	1.54	0.89
2:H:214:VAL:HG11	2:H:216:LYS:CE	2.02	0.89
2:H:18:VAL:CG2	2:H:86:LEU:HD11	2.01	0.89
1:A:51:THR:HG22	1:A:51:THR:O	1.72	0.88
1:L:146:VAL:HG21	1:L:175:MET:HE2	1.56	0.88
2:B:35:ASP:HB2	2:B:97:THR:HG22	1.56	0.88
1:L:199:LYS:HD2	1:L:199:LYS:N	1.89	0.87
1:A:136:LEU:HD11	1:A:146:VAL:HG22	1.57	0.87
2:B:220:PRO:O	2:B:221:ARG:HG3	1.74	0.87
1:A:125:LEU:O	1:A:183:LYS:HE3	1.74	0.86
2:B:159:THR:HB	2:B:206:ALA:HB3	1.57	0.86
1:L:41:ASP:OD1	1:L:43:THR:HG23	1.75	0.86
2:H:38:LYS:HE2	2:H:40:ARG:HD3	1.58	0.85
2:B:196:ARG:HG2	2:B:197:PRO:HA	1.58	0.85
1:L:162:SER:OG	2:H:175:PRO:HD2	1.75	0.85
1:L:31:ASN:ND2	1:L:51:THR:HG21	1.92	0.85
1:A:48:ILE:HG21	1:A:52:SER:HA	1.59	0.85
1:A:136:LEU:HD11	1:A:146:VAL:CG2	2.06	0.85
1:L:187:GLU:HA	1:L:211:ARG:HH12	1.40	0.84
1:A:155:ARG:HG3	1:A:156:GLN:H	1.41	0.84
2:H:11:LEU:HD11	2:H:154:PHE:HE2	1.43	0.84
1:A:193:THR:HG23	1:A:208:SER:HB3	1.59	0.84
2:B:57:SER:O	2:B:58:THR:HG23	1.78	0.84
1:L:182:THR:OG1	1:L:185:GLU:HG3	1.77	0.83
1:A:108:ARG:CD	1:A:109:ALA:H	1.91	0.83
1:A:51:THR:HG23	1:A:71:TYR:CD2	2.14	0.82
1:L:115:VAL:HG22	1:L:136:LEU:HD22	1.61	0.82
1:L:139:PHE:CE2	1:L:174:SER:HA	2.15	0.82
1:A:147:LYS:HG3	1:A:195:GLU:HB3	1.62	0.82
1:L:187:GLU:HA	1:L:211:ARG:NH1	1.94	0.82
1:L:7:THR:O	1:L:8:THR:CG2	2.28	0.81
2:H:215:ASP:O	2:H:216:LYS:HD2	1.79	0.81
1:A:170:ASP:OD1	1:A:172:THR:HG22	1.80	0.81
2:H:12:MET:HE1	2:H:16:ALA:HB1	1.63	0.80
2:H:154:PHE:CD2	2:H:155:PRO:N	2.49	0.80
1:A:31:ASN:CB	1:A:51:THR:OG1	2.29	0.80
1:L:94:LEU:O	1:L:96:ARG:N	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:ARG:HH12	2:H:99:ARG:HD2	1.46	0.80
1:A:52:SER:HB3	1:A:64:GLY:HA3	1.62	0.80
1:L:162:SER:O	1:L:175:MET:HG3	1.82	0.80
1:A:51:THR:HG23	1:A:71:TYR:CE2	2.17	0.80
1:A:85:THR:HG21	2:B:43:HIS:HE1	1.46	0.79
2:H:154:PHE:CD2	2:H:155:PRO:HD3	2.18	0.79
1:A:83:ILE:HG13	1:A:83:ILE:O	1.82	0.79
1:L:149:LYS:HA	1:L:154:ALA:O	1.81	0.79
2:H:61:ASN:C	2:H:63:LYS:H	1.81	0.79
1:A:31:ASN:CA	1:A:51:THR:OG1	2.31	0.79
2:H:146:LEU:HD11	2:H:196:ARG:HG3	1.62	0.78
2:H:154:PHE:O	2:H:156:GLU:N	2.15	0.78
2:H:61:ASN:O	2:H:63:LYS:N	2.16	0.78
2:H:154:PHE:HD2	2:H:155:PRO:CD	1.96	0.78
2:H:147:GLY:O	2:H:218:ILE:HD11	1.83	0.78
2:H:214:VAL:HG11	2:H:216:LYS:HE2	1.65	0.77
2:H:154:PHE:HB3	2:H:155:PRO:CD	2.15	0.77
1:A:108:ARG:HD2	1:A:109:ALA:H	1.49	0.77
2:B:142:SER:O	2:B:192:PRO:HA	1.84	0.77
1:A:34:ASN:HD22	1:A:49:TYR:HA	1.49	0.77
1:A:80:GLN:NE2	1:A:171:SER:OG	2.18	0.76
2:H:27:TYR:CE1	2:H:29:PHE:HA	2.20	0.76
2:B:207:HIS:HD2	2:B:210:SER:OG	1.67	0.76
2:H:159:THR:HB	2:H:206:ALA:HB3	1.67	0.76
1:L:139:PHE:HE2	1:L:174:SER:HA	1.50	0.75
1:L:147:LYS:NZ	1:L:149:LYS:HE3	2.00	0.75
1:L:48:ILE:HD12	1:L:73:LEU:HD12	1.66	0.75
2:B:129:VAL:HG21	2:B:214:VAL:HG11	1.67	0.75
1:L:108:ARG:HH11	1:L:171:SER:N	1.78	0.75
1:L:4:MET:HB2	1:L:98:PHE:O	1.87	0.75
1:A:160:LEU:HD11	2:B:179:GLN:HG2	1.69	0.74
1:A:190:ASN:O	1:A:210:ASN:HA	1.87	0.74
1:A:18:ARG:HG3	1:A:76:SER:HA	1.68	0.74
1:A:6:GLN:HG3	1:A:100:GLY:H	1.52	0.74
2:H:89:GLU:N	2:H:89:GLU:OE1	2.20	0.74
2:B:71:THR:HG22	2:B:80:TYR:CD1	2.22	0.74
1:L:31:ASN:HD22	1:L:51:THR:CG2	2.01	0.74
1:L:147:LYS:HZ2	1:L:149:LYS:HE3	1.53	0.74
1:A:170:ASP:OD1	1:A:170:ASP:O	2.04	0.74
1:L:126:THR:O	1:L:126:THR:HG22	1.88	0.74
2:B:101:TYR:O	2:B:102:TRP:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ALA:HB2	2:B:218:ILE:HG23	1.70	0.73
2:H:154:PHE:CD2	2:H:155:PRO:CD	2.72	0.73
1:L:108:ARG:NH1	1:L:171:SER:N	2.30	0.73
1:A:168:SER:O	1:A:169:LYS:HD2	1.89	0.73
2:B:33:TRP:CH2	2:B:57:SER:HB2	2.23	0.73
1:L:146:VAL:HG21	1:L:175:MET:CE	2.18	0.73
2:B:2:ALA:HA	2:B:26:GLY:HA3	1.71	0.73
2:B:97:THR:HG21	2:B:108:PHE:HB3	1.71	0.72
1:A:63:SER:OG	1:A:74:THR:CG2	2.37	0.72
1:L:48:ILE:HG22	1:L:52:SER:HA	1.69	0.72
1:L:55:HIS:HB3	1:L:58:VAL:HG22	1.71	0.72
1:A:155:ARG:HG3	1:A:156:GLN:N	2.05	0.72
1:A:155:ARG:CG	1:A:156:GLN:N	2.52	0.72
2:B:4:LEU:HD22	2:B:24:ALA:HB2	1.70	0.72
2:B:194:SER:O	2:B:198:SER:HB3	1.90	0.71
2:H:67:LYS:O	2:H:83:LEU:HA	1.89	0.71
2:H:18:VAL:HG23	2:H:86:LEU:CD1	2.07	0.71
1:L:148:TRP:H	1:L:155:ARG:HG3	1.56	0.71
2:B:8:GLY:HA3	2:B:20:ILE:HA	1.72	0.71
2:H:105:ALA:O	2:H:107:ASP:N	2.21	0.70
1:A:31:ASN:HB3	1:A:51:THR:HG1	1.56	0.70
2:B:61:ASN:HD22	2:B:62:GLU:N	1.89	0.70
2:H:132:LEU:HB2	2:H:147:GLY:HA3	1.73	0.70
1:L:6:GLN:HE22	1:L:87:PHE:HA	1.55	0.70
2:H:146:LEU:CD1	2:H:196:ARG:HG3	2.21	0.70
2:B:6:GLN:HE22	2:B:114:GLY:HA2	1.55	0.70
1:L:2:ILE:HD12	1:L:93:THR:HG22	1.74	0.70
2:H:6:GLN:O	2:H:7:SER:HB2	1.92	0.70
1:L:211:ARG:HG3	1:L:211:ARG:HH11	1.57	0.70
1:A:187:GLU:HA	1:A:211:ARG:CZ	2.22	0.70
2:B:62:GLU:OE1	2:B:65:ARG:HD3	1.92	0.70
1:A:34:ASN:ND2	2:B:107:ASP:HB3	2.06	0.69
2:B:101:TYR:HD1	2:B:102:TRP:N	1.90	0.69
2:B:33:TRP:CD1	2:B:52:LEU:HD13	2.27	0.69
2:B:97:THR:HG23	2:B:98:ARG:N	2.07	0.69
2:H:154:PHE:CB	2:H:155:PRO:CD	2.70	0.69
1:L:121:SER:O	1:L:125:LEU:HB2	1.92	0.69
2:H:180:SER:O	2:H:181:ASP:HB2	1.90	0.69
1:L:50:TYR:O	1:L:51:THR:HG22	1.93	0.69
1:A:33:LEU:CD2	1:A:71:TYR:HB2	2.23	0.68
2:B:145:THR:HG22	2:B:190:THR:OG1	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:HH11	1:A:96:ARG:CG	2.03	0.68
2:B:122:ALA:HB3	2:B:154:PHE:CE2	2.29	0.67
1:L:90:GLN:NE2	1:L:92:ASN:H	1.92	0.67
1:A:146:VAL:O	1:A:155:ARG:NH1	2.26	0.67
2:H:155:PRO:O	2:H:157:PRO:CD	2.41	0.67
2:H:132:LEU:HB2	2:H:147:GLY:CA	2.24	0.67
1:A:73:LEU:HD12	1:A:74:THR:N	2.09	0.67
1:L:118:PHE:HE1	1:L:135:PHE:HD2	1.42	0.67
1:L:193:THR:CB	1:L:208:SER:HB3	2.20	0.67
2:B:33:TRP:CE2	2:B:52:LEU:HB2	2.30	0.67
2:H:9:ALA:HB3	2:H:18:VAL:HG13	1.77	0.67
2:H:12:MET:HG3	2:H:18:VAL:HG22	1.76	0.67
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.75	0.67
1:L:108:ARG:HG2	1:L:109:ALA:N	2.09	0.66
2:H:154:PHE:HB3	2:H:155:PRO:HD2	1.75	0.66
1:L:112:ALA:CB	1:L:200:THR:HG21	2.25	0.66
2:B:6:GLN:NE2	2:B:94:TYR:O	2.28	0.66
1:A:73:LEU:HD12	1:A:74:THR:H	1.59	0.66
1:A:52:SER:HB3	1:A:64:GLY:CA	2.24	0.66
1:A:31:ASN:HB3	1:A:51:THR:OG1	1.95	0.66
1:A:38:GLN:HB2	1:A:44:VAL:HG22	1.77	0.66
1:L:48:ILE:HD12	1:L:73:LEU:CD1	2.25	0.66
1:L:62:PHE:CE1	1:L:75:ILE:HG12	2.31	0.66
1:A:198:HIS:CE1	1:A:200:THR:HG23	2.30	0.65
1:L:34:ASN:O	1:L:88:CYS:HA	1.96	0.65
1:L:112:ALA:HB2	1:L:200:THR:HG21	1.77	0.65
2:H:154:PHE:O	2:H:155:PRO:C	2.34	0.65
1:A:31:ASN:O	1:A:51:THR:OG1	2.12	0.65
2:B:192:PRO:O	2:B:195:PRO:HD2	1.96	0.65
2:B:194:SER:HB2	2:B:195:PRO:HD3	1.79	0.65
1:L:199:LYS:HD2	1:L:199:LYS:H	1.60	0.65
2:H:18:VAL:HG12	2:H:19:LYS:N	2.12	0.65
1:L:167:ASP:OD2	1:L:169:LYS:HB2	1.97	0.64
1:A:108:ARG:CD	1:A:109:ALA:N	2.60	0.64
1:L:15:LEU:HA	1:L:78:LEU:HD23	1.80	0.64
2:B:61:ASN:ND2	2:B:63:LYS:HG3	2.12	0.64
1:L:115:VAL:O	1:L:207:LYS:HG3	1.97	0.64
2:H:61:ASN:C	2:H:63:LYS:N	2.51	0.64
2:H:147:GLY:O	2:H:218:ILE:CD1	2.45	0.64
1:L:155:ARG:HG2	1:L:159:VAL:HG21	1.78	0.64
1:L:47:LEU:HA	1:L:58:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:GLN:O	1:L:83:ILE:CG2	2.44	0.64
1:A:6:GLN:CD	1:A:101:GLY:H	2.01	0.64
2:H:185:LEU:HD12	2:H:186:SER:N	2.12	0.64
1:A:32:TYR:O	1:A:90:GLN:HA	1.98	0.63
1:A:160:LEU:HD13	2:B:177:VAL:HG21	1.79	0.63
1:A:193:THR:HG23	1:A:208:SER:CB	2.28	0.63
2:B:76:SER:O	2:B:77:ASN:HB2	1.97	0.63
1:L:48:ILE:CG2	1:L:52:SER:CA	2.64	0.63
1:A:29:ILE:O	1:A:29:ILE:HG22	1.98	0.63
2:B:7:SER:HA	2:B:115:THR:OG1	1.98	0.63
2:B:4:LEU:CD2	2:B:24:ALA:CB	2.77	0.63
2:H:33:TRP:NE1	2:H:52:LEU:HD13	2.12	0.63
1:L:198:HIS:CE1	1:L:200:THR:HB	2.32	0.63
2:B:61:ASN:HD22	2:B:61:ASN:C	2.02	0.63
1:A:49:TYR:CE1	1:A:55:HIS:O	2.51	0.63
1:A:136:LEU:CD1	1:A:146:VAL:CG2	2.77	0.63
1:L:41:ASP:OD1	1:L:41:ASP:C	2.36	0.63
1:A:108:ARG:HD3	1:A:109:ALA:H	1.63	0.62
2:H:155:PRO:C	2:H:157:PRO:HD2	2.18	0.62
2:H:214:VAL:CG1	2:H:216:LYS:CE	2.77	0.62
2:B:124:THR:HA	2:B:154:PHE:O	1.98	0.62
2:B:67:LYS:HE2	2:B:90:ASP:OD1	1.99	0.62
2:H:36:TRP:C	2:H:37:ILE:HD12	2.20	0.62
1:L:108:ARG:CG	1:L:109:ALA:N	2.63	0.62
2:B:4:LEU:HD22	2:B:24:ALA:CB	2.29	0.62
2:B:163:ASN:HB3	2:B:166:SER:HB2	1.82	0.61
2:H:129:VAL:HB	2:H:216:LYS:HE3	1.80	0.61
2:H:197:PRO:HB3	2:H:220:PRO:HG2	1.82	0.61
1:A:198:HIS:CG	1:A:199:LYS:H	2.18	0.61
1:L:41:ASP:OD1	1:L:43:THR:CG2	2.47	0.61
1:L:29:ILE:HD11	1:L:33:LEU:HB2	1.81	0.61
1:L:52:SER:HB3	1:L:64:GLY:HA3	1.81	0.61
1:L:94:LEU:O	1:L:96:ARG:HG2	1.99	0.61
2:B:71:THR:HG22	2:B:80:TYR:HD1	1.65	0.61
2:H:126:PRO:HG3	2:H:210:SER:CB	2.30	0.61
2:H:194:SER:HB2	2:H:195:PRO:CD	2.28	0.61
1:A:160:LEU:HD11	2:B:179:GLN:CG	2.29	0.61
1:A:32:TYR:HB2	1:A:92:ASN:HB2	1.82	0.61
1:A:124:GLN:HG2	1:A:129:GLY:O	2.00	0.61
2:B:56:GLY:O	2:B:57:SER:O	2.19	0.61
2:B:71:THR:CG2	2:B:80:TYR:CD1	2.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:LEU:HD13	1:L:180:THR:N	2.16	0.61
1:A:33:LEU:HD23	1:A:71:TYR:CB	2.31	0.60
1:A:51:THR:O	1:A:51:THR:CG2	2.43	0.60
2:B:71:THR:HG22	2:B:80:TYR:HB2	1.81	0.60
1:L:18:ARG:HA	1:L:76:SER:O	2.01	0.60
1:L:36:TYR:CE2	2:H:108:PHE:HB2	2.36	0.60
2:H:214:VAL:HG11	2:H:216:LYS:HE3	1.83	0.60
1:A:147:LYS:CA	1:A:155:ARG:HH11	2.14	0.60
1:L:155:ARG:HE	1:L:156:GLN:N	2.00	0.60
2:B:35:ASP:HB2	2:B:97:THR:CG2	2.31	0.60
2:B:156:GLU:OE1	2:B:157:PRO:HA	2.01	0.60
1:A:14:SER:O	1:A:17:ASP:HB2	2.02	0.60
1:A:58:VAL:HB	1:A:59:PRO:CD	2.31	0.60
2:B:61:ASN:HD21	2:B:63:LYS:HG3	1.66	0.60
2:B:181:ASP:O	2:B:182:LEU:HD23	2.01	0.60
1:A:115:VAL:HA	1:A:135:PHE:O	2.01	0.60
2:B:51:ILE:HG13	2:B:58:THR:HG23	1.82	0.60
2:H:207:HIS:NE2	2:H:209:ALA:HB3	2.17	0.60
1:A:210:ASN:O	1:A:213:GLU:HG2	2.02	0.60
2:B:131:PRO:HB2	2:B:218:ILE:CD1	2.27	0.60
1:A:136:LEU:CD1	1:A:146:VAL:HG22	2.31	0.59
1:A:160:LEU:HD13	2:B:177:VAL:CG2	2.31	0.59
2:B:30:SER:HA	2:B:53:PRO:HG2	1.84	0.59
1:L:55:HIS:N	1:L:55:HIS:CD2	2.69	0.59
1:L:213:GLU:CG	2:H:136:SER:OG	2.43	0.59
2:B:52:LEU:HD12	2:B:53:PRO:HD2	1.83	0.59
1:A:78:LEU:HD11	1:A:104:LEU:HD21	1.85	0.59
1:L:159:VAL:HG22	1:L:179:LEU:HD23	1.84	0.59
2:H:191:VAL:HB	2:H:192:PRO:HD2	1.82	0.59
1:A:85:THR:HG21	2:B:43:HIS:CE1	2.32	0.59
2:B:10:GLU:HG3	2:B:116:THR:O	2.03	0.59
2:H:132:LEU:HB2	2:H:147:GLY:C	2.23	0.59
1:L:118:PHE:HE1	1:L:135:PHE:CD2	2.21	0.59
1:A:96:ARG:HG3	1:A:96:ARG:NH1	2.12	0.59
2:B:214:VAL:HG22	2:B:215:ASP:N	2.18	0.59
1:A:33:LEU:HD23	1:A:71:TYR:HB2	1.84	0.59
1:A:108:ARG:HD2	1:A:109:ALA:N	2.18	0.59
2:B:6:GLN:HE22	2:B:95:TYR:HA	1.68	0.58
2:H:158:VAL:HG11	2:H:185:LEU:CD2	2.32	0.58
1:A:38:GLN:CB	1:A:44:VAL:HG22	2.33	0.58
1:A:51:THR:HG23	1:A:71:TYR:HD2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:ILE:HG13	3:L:2001:HOH:O	2.01	0.58
1:A:147:LYS:HA	1:A:155:ARG:HH11	1.68	0.58
1:A:46:ILE:HG12	1:A:47:LEU:N	2.19	0.58
1:A:98:PHE:CZ	2:B:37:ILE:HD13	2.39	0.58
2:B:132:LEU:HD23	2:B:148:CYS:N	2.19	0.58
1:A:31:ASN:C	1:A:51:THR:OG1	2.41	0.58
2:H:126:PRO:HG3	2:H:210:SER:HG	1.66	0.58
2:B:29:PHE:O	2:B:53:PRO:HG3	2.03	0.58
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.36	0.58
1:A:141:PRO:HD2	1:A:198:HIS:NE2	2.19	0.58
1:L:160:LEU:O	1:L:177:SER:HA	2.03	0.58
2:B:33:TRP:HZ3	2:B:50:GLU:O	1.87	0.58
2:B:167:LEU:HD23	2:B:189:VAL:HG21	1.86	0.58
1:L:5:THR:HG22	1:L:7:THR:H	1.69	0.58
1:A:48:ILE:CG2	1:A:52:SER:HA	2.31	0.57
1:A:83:ILE:HG22	1:A:106:ILE:HG13	1.85	0.57
2:H:151:LYS:HA	2:H:184:THR:HG23	1.86	0.57
2:B:161:THR:HG22	2:B:162:TRP:N	2.20	0.57
1:L:157:ASN:HA	3:L:2022:HOH:O	2.04	0.57
1:A:136:LEU:HD11	1:A:146:VAL:HG21	1.86	0.57
2:B:24:ALA:HB3	2:B:29:PHE:CE1	2.39	0.57
2:B:78:THR:HG23	2:B:80:TYR:CE1	2.40	0.57
1:L:62:PHE:CD1	1:L:75:ILE:HG12	2.40	0.57
2:H:71:THR:O	2:H:80:TYR:N	2.36	0.57
2:B:71:THR:CG2	2:B:80:TYR:HB2	2.34	0.57
1:A:149:LYS:HA	1:A:153:SER:O	2.03	0.57
2:H:156:GLU:HB2	2:H:183:TYR:CE1	2.39	0.57
1:A:30:ASN:O	1:A:31:ASN:HB2	2.04	0.57
1:A:48:ILE:HG23	1:A:54:LEU:O	2.04	0.57
2:B:61:ASN:O	2:B:63:LYS:N	2.37	0.57
2:B:86:LEU:HA	2:B:90:ASP:OD2	2.05	0.57
2:B:145:THR:CG2	2:B:190:THR:OG1	2.53	0.57
1:L:124:GLN:HB2	2:H:130:TYR:CD2	2.39	0.57
2:B:57:SER:O	2:B:58:THR:CG2	2.51	0.56
2:H:126:PRO:HB3	2:H:212:THR:OG1	2.05	0.56
2:H:158:VAL:HG11	2:H:185:LEU:HD23	1.85	0.56
2:H:214:VAL:HG12	2:H:215:ASP:N	2.19	0.56
1:L:6:GLN:HE21	1:L:99:GLY:HA3	1.69	0.56
1:A:48:ILE:HG21	1:A:52:SER:CA	2.33	0.56
2:B:185:LEU:HD12	2:B:185:LEU:C	2.26	0.56
1:L:125:LEU:O	1:L:183:LYS:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:LEU:O	1:L:95:PRO:C	2.40	0.56
2:B:132:LEU:HB2	2:B:147:GLY:CA	2.36	0.56
2:B:207:HIS:NE2	2:B:209:ALA:HB3	2.20	0.56
2:B:131:PRO:CB	2:B:218:ILE:HD13	2.31	0.56
1:A:63:SER:OG	1:A:74:THR:HG22	2.06	0.56
2:H:158:VAL:HG23	2:H:206:ALA:O	2.06	0.56
1:A:28:ASP:HA	1:A:68:GLY:O	2.06	0.55
2:B:211:SER:OG	2:H:74:THR:HG21	2.06	0.55
2:H:32:TYR:N	2:H:32:TYR:CD1	2.75	0.55
2:H:73:ASP:OD2	2:H:75:SER:HB2	2.06	0.55
1:A:61:ARG:HH21	1:A:82:ASP:CG	2.10	0.55
2:H:207:HIS:CD2	2:H:209:ALA:HB3	2.41	0.55
1:A:46:ILE:HG12	1:A:47:LEU:H	1.71	0.55
1:A:124:GLN:HB2	2:B:130:TYR:CZ	2.41	0.55
2:B:101:TYR:CD1	2:B:102:TRP:N	2.73	0.55
2:B:200:THR:HG23	2:B:217:LYS:CD	2.37	0.55
2:H:32:TYR:O	2:H:53:PRO:HD2	2.05	0.55
1:A:121:SER:OG	2:B:130:TYR:HB3	2.07	0.55
1:A:39:LYS:HA	1:A:84:ALA:CB	2.36	0.55
1:L:48:ILE:HA	1:L:54:LEU:O	2.07	0.55
2:H:105:ALA:O	2:H:107:ASP:OD1	2.24	0.55
1:A:107:LYS:HA	1:A:140:TYR:OH	2.06	0.55
1:A:199:LYS:HG2	1:A:199:LYS:O	2.06	0.55
2:B:35:ASP:CB	2:B:97:THR:HG22	2.34	0.55
1:A:167:ASP:HB3	1:A:170:ASP:O	2.06	0.55
2:B:35:ASP:O	2:B:96:CYS:HA	2.06	0.55
2:B:163:ASN:O	2:B:166:SER:N	2.35	0.55
1:L:155:ARG:HE	1:L:156:GLN:H	1.55	0.55
2:H:6:GLN:O	2:H:7:SER:CB	2.55	0.55
2:B:127:PRO:HB2	2:B:150:VAL:CG1	2.37	0.55
1:L:155:ARG:HH21	1:L:156:GLN:HA	1.71	0.55
2:H:84:SER:O	2:H:85:SER:C	2.45	0.55
1:A:168:SER:C	1:A:169:LYS:HD2	2.27	0.54
2:H:12:MET:HE1	2:H:16:ALA:CB	2.36	0.54
2:H:81:MET:HE3	2:H:83:LEU:HD11	1.88	0.54
2:H:139:GLN:HG2	2:H:140:THR:HG23	1.88	0.54
2:B:35:ASP:OD2	2:B:108:PHE:CD1	2.60	0.54
1:A:187:GLU:HA	1:A:211:ARG:NH1	2.22	0.54
1:L:117:ILE:O	2:H:139:GLN:OE1	2.25	0.54
1:A:193:THR:CG2	1:A:208:SER:HB3	2.36	0.54
2:B:36:TRP:O	2:B:48:ILE:HB	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:MET:CE	2:H:16:ALA:HB1	2.36	0.54
2:B:219:VAL:HG23	2:B:219:VAL:O	2.08	0.54
2:H:37:ILE:HD12	2:H:37:ILE:N	2.23	0.54
2:H:156:GLU:HB2	2:H:183:TYR:HE1	1.72	0.54
2:H:202:THR:HG23	2:H:216:LYS:O	2.06	0.54
2:B:51:ILE:HG13	2:B:58:THR:CG2	2.38	0.54
2:B:97:THR:CG2	2:B:108:PHE:HB3	2.37	0.54
2:H:37:ILE:HG21	2:H:45:LEU:HG	1.90	0.54
2:H:146:LEU:HD11	2:H:196:ARG:CG	2.36	0.54
1:A:63:SER:O	1:A:73:LEU:HD12	2.08	0.54
2:H:30:SER:HB2	2:H:54:GLY:CA	2.38	0.54
1:L:115:VAL:HG22	1:L:136:LEU:CD2	2.35	0.54
1:L:11:LEU:HA	3:L:2002:HOH:O	2.07	0.53
2:H:214:VAL:HG12	2:H:216:LYS:CD	2.39	0.53
1:A:96:ARG:CG	1:A:96:ARG:NH1	2.65	0.53
2:B:168:SER:O	2:B:171:VAL:HG12	2.08	0.53
1:L:113:PRO:HG3	1:L:144:ILE:CD1	2.38	0.53
2:B:61:ASN:C	2:B:63:LYS:H	2.11	0.53
1:L:2:ILE:HD12	1:L:93:THR:CG2	2.38	0.53
2:H:212:THR:HG22	2:H:213:LYS:N	2.24	0.53
1:A:107:LYS:HD2	1:A:140:TYR:OH	2.07	0.53
1:A:163:TRP:CD1	1:A:175:MET:HG3	2.44	0.53
1:L:31:ASN:ND2	1:L:51:THR:CG2	2.67	0.53
2:H:168:SER:O	2:H:170:GLY:N	2.38	0.53
1:A:155:ARG:CG	1:A:156:GLN:H	2.05	0.53
1:L:196:ALA:HB3	1:L:205:ILE:HG23	1.90	0.53
2:B:51:ILE:HD12	2:B:70:PHE:CB	2.39	0.53
1:A:170:ASP:OD1	1:A:172:THR:CG2	2.56	0.53
2:B:11:LEU:HD12	2:B:118:THR:O	2.09	0.53
1:L:148:TRP:HB2	1:L:155:ARG:HG3	1.91	0.53
1:L:118:PHE:CE1	1:L:135:PHE:HD2	2.25	0.52
1:L:133:VAL:HG22	1:L:178:THR:HG23	1.91	0.52
1:L:196:ALA:O	1:L:205:ILE:HG22	2.09	0.52
1:A:147:LYS:HA	1:A:155:ARG:CD	2.39	0.52
1:L:33:LEU:HD13	1:L:33:LEU:C	2.30	0.52
1:L:96:ARG:HG3	2:H:47:TRP:CE2	2.44	0.52
2:H:8:GLY:HA3	2:H:20:ILE:HA	1.91	0.52
2:B:52:LEU:N	2:B:57:SER:OG	2.36	0.52
1:L:73:LEU:HG	1:L:74:THR:N	2.24	0.52
2:H:18:VAL:HG12	2:H:19:LYS:H	1.73	0.52
2:H:55:SER:OG	2:H:56:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:OG	3:A:2007:HOH:O	2.15	0.52
2:B:73:ASP:OD2	2:B:76:SER:OG	2.26	0.52
2:B:51:ILE:HD12	2:B:70:PHE:HB3	1.92	0.52
1:A:75:ILE:HG21	1:A:78:LEU:HD12	1.90	0.52
1:L:163:TRP:O	2:H:175:PRO:HG2	2.10	0.52
1:A:52:SER:HB3	1:A:64:GLY:C	2.30	0.52
2:B:129:VAL:CG2	2:B:214:VAL:HG11	2.39	0.52
2:H:122:ALA:HB3	2:H:154:PHE:CD1	2.45	0.52
1:A:115:VAL:HG12	1:A:116:SER:N	2.24	0.52
2:B:74:THR:N	3:B:2014:HOH:O	2.37	0.52
1:L:179:LEU:HD11	1:L:181:LEU:HD21	1.91	0.52
1:A:31:ASN:C	1:A:51:THR:HG1	2.09	0.51
2:H:141:ASN:O	2:H:142:SER:HB3	2.10	0.51
1:A:93:THR:O	1:A:94:LEU:HD23	2.10	0.51
2:B:192:PRO:C	2:B:195:PRO:HD2	2.31	0.51
1:L:66:GLY:HA3	1:L:71:TYR:CD2	2.46	0.51
1:L:175:MET:HA	2:H:174:PHE:HE1	1.75	0.51
2:H:12:MET:O	2:H:119:VAL:HA	2.11	0.51
1:A:58:VAL:HB	1:A:59:PRO:HD2	1.92	0.51
1:L:96:ARG:HG3	2:H:47:TRP:CZ2	2.46	0.51
2:H:38:LYS:HE2	2:H:40:ARG:CD	2.37	0.51
1:A:180:THR:O	1:A:181:LEU:HD23	2.10	0.51
2:B:147:GLY:O	2:B:218:ILE:HD11	2.10	0.51
1:A:182:THR:O	1:A:183:LYS:C	2.49	0.51
2:H:142:SER:O	2:H:143:MET:HG3	2.10	0.51
1:L:182:THR:HG1	1:L:185:GLU:HG3	1.72	0.51
2:H:214:VAL:CG1	2:H:216:LYS:CD	2.89	0.51
2:B:101:TYR:HD1	2:B:102:TRP:H	1.52	0.51
2:H:37:ILE:HG23	2:H:46:GLU:O	2.11	0.51
1:A:108:ARG:HD3	1:A:109:ALA:N	2.25	0.50
2:B:71:THR:HG21	3:H:2002:HOH:O	2.11	0.50
1:L:52:SER:HB2	1:L:64:GLY:C	2.31	0.50
2:H:27:TYR:CZ	2:H:29:PHE:HA	2.45	0.50
1:A:49:TYR:O	1:A:50:TYR:C	2.49	0.50
1:A:198:HIS:CG	1:A:199:LYS:N	2.79	0.50
2:B:33:TRP:CE3	2:B:51:ILE:C	2.85	0.50
2:B:159:THR:O	2:B:205:VAL:HA	2.11	0.50
1:L:31:ASN:O	1:L:51:THR:N	2.44	0.50
2:H:33:TRP:CD1	2:H:52:LEU:HD13	2.46	0.50
2:H:101:TYR:O	2:H:102:TRP:CD1	2.64	0.50
1:A:147:LYS:CB	1:A:155:ARG:NH1	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:HA	2:B:23:LYS:O	2.11	0.50
2:B:200:THR:HG23	2:B:217:LYS:HD2	1.92	0.50
1:L:52:SER:HB3	1:L:64:GLY:CA	2.41	0.50
2:H:162:TRP:CH2	2:H:203:CYS:HB3	2.46	0.50
1:A:39:LYS:HA	1:A:84:ALA:HB1	1.94	0.50
1:A:74:THR:O	1:A:74:THR:HG23	2.10	0.50
1:A:6:GLN:HG3	1:A:100:GLY:N	2.23	0.50
2:B:50:GLU:O	2:B:58:THR:HA	2.12	0.50
1:L:124:GLN:HB2	2:H:130:TYR:CE2	2.46	0.50
1:L:140:TYR:HA	1:L:141:PRO:C	2.32	0.50
1:L:160:LEU:HD13	2:H:177:VAL:HG11	1.94	0.50
1:L:213:GLU:CG	1:L:213:GLU:O	2.59	0.50
1:L:138:ASN:HA	1:L:172:THR:HB	1.94	0.50
2:H:144:VAL:O	2:H:190:THR:HG23	2.12	0.50
2:H:195:PRO:O	2:H:199:GLU:N	2.38	0.50
2:B:102:TRP:O	2:B:105:ALA:HB3	2.11	0.50
2:B:161:THR:HG23	3:B:2028:HOH:O	2.12	0.50
2:B:207:HIS:CE1	2:B:209:ALA:HB3	2.46	0.50
2:H:18:VAL:O	2:H:82:GLN:HA	2.11	0.50
1:A:95:PRO:HB3	3:B:2010:HOH:O	2.11	0.49
2:B:4:LEU:CD2	2:B:24:ALA:HB1	2.41	0.49
1:L:161:ASN:HD22	1:L:177:SER:HB2	1.77	0.49
2:H:35:ASP:O	2:H:96:CYS:HA	2.12	0.49
2:B:113:GLN:O	2:B:114:GLY:O	2.30	0.49
2:B:164:SER:HA	2:B:204:ASN:HD21	1.76	0.49
1:A:33:LEU:CD2	1:A:71:TYR:CB	2.89	0.49
2:B:6:GLN:O	2:B:7:SER:HB3	2.12	0.49
2:B:34:ILE:CD1	2:B:79:ALA:HB2	2.42	0.49
2:B:97:THR:HG21	2:B:108:PHE:CB	2.39	0.49
2:B:181:ASP:C	2:B:182:LEU:HD23	2.32	0.49
2:H:36:TRP:CZ3	2:H:96:CYS:HB3	2.46	0.49
2:B:48:ILE:O	2:B:61:ASN:HB2	2.12	0.49
2:H:61:ASN:C	2:H:61:ASN:HD22	2.16	0.49
2:H:155:PRO:HB2	2:H:209:ALA:CB	2.43	0.49
2:H:214:VAL:CG1	2:H:216:LYS:HE2	2.36	0.49
1:A:61:ARG:HD2	1:A:77:ASN:O	2.13	0.49
2:B:127:PRO:HB2	2:B:150:VAL:HG13	1.95	0.49
2:H:137:ALA:C	2:H:139:GLN:H	2.13	0.49
2:H:210:SER:HG	2:H:212:THR:HG1	1.59	0.49
1:A:98:PHE:HZ	2:B:37:ILE:HD13	1.75	0.49
1:A:210:ASN:H	1:A:213:GLU:CD	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:ARG:CG	1:L:159:VAL:HG21	2.41	0.49
2:H:29:PHE:CE2	2:H:53:PRO:HB3	2.46	0.49
1:L:50:TYR:O	1:L:51:THR:CG2	2.61	0.49
1:L:123:GLU:OE1	1:L:123:GLU:N	2.36	0.49
1:A:46:ILE:CG1	1:A:47:LEU:H	2.25	0.49
2:B:155:PRO:HD2	2:B:209:ALA:HB1	1.95	0.49
1:L:2:ILE:HG22	1:L:4:MET:CE	2.43	0.49
1:L:33:LEU:H	1:L:51:THR:H	1.60	0.49
1:L:167:ASP:O	1:L:170:ASP:O	2.31	0.49
1:A:66:GLY:CA	1:A:71:TYR:HA	2.43	0.49
1:A:90:GLN:HE22	1:A:93:THR:H	1.61	0.49
1:A:39:LYS:O	1:A:40:PRO:O	2.31	0.48
1:A:145:ASN:HB3	1:A:197:THR:HB	1.95	0.48
2:B:196:ARG:CG	2:B:197:PRO:HA	2.35	0.48
1:L:186:TYR:CE2	1:L:211:ARG:HG3	2.48	0.48
1:A:96:ARG:HH12	2:B:50:GLU:CD	2.17	0.48
1:A:18:ARG:HA	1:A:76:SER:O	2.14	0.48
1:A:51:THR:O	1:A:52:SER:HB2	2.12	0.48
2:B:158:VAL:HA	2:B:206:ALA:O	2.14	0.48
2:H:154:PHE:C	2:H:156:GLU:N	2.67	0.48
1:A:190:ASN:N	1:A:190:ASN:HD22	2.12	0.48
2:B:159:THR:O	2:B:159:THR:HG22	2.14	0.48
1:L:3:GLN:HG3	1:L:26:SER:HB3	1.96	0.48
1:A:46:ILE:CG1	1:A:47:LEU:N	2.77	0.48
1:A:31:ASN:HA	1:A:51:THR:OG1	2.09	0.48
2:B:6:GLN:NE2	2:B:114:GLY:CA	2.65	0.48
1:L:48:ILE:HG22	1:L:49:TYR:N	2.27	0.48
1:L:126:THR:O	1:L:126:THR:CG2	2.58	0.48
2:H:214:VAL:CG1	2:H:215:ASP:N	2.77	0.48
2:H:1:GLN:O	2:H:26:GLY:HA3	2.13	0.48
2:H:51:ILE:O	2:H:53:PRO:HD3	2.13	0.48
1:L:195:GLU:HG2	1:L:204:PRO:HB3	1.96	0.48
1:A:124:GLN:HB2	2:B:130:TYR:CE2	2.49	0.47
1:A:201:SER:C	1:A:203:SER:H	2.16	0.47
2:B:33:TRP:HH2	2:B:58:THR:H	1.62	0.47
2:B:132:LEU:HD23	2:B:148:CYS:CA	2.44	0.47
1:L:108:ARG:HD2	1:L:171:SER:HB2	1.95	0.47
1:L:118:PHE:CE1	1:L:135:PHE:CD2	3.00	0.47
1:L:160:LEU:HD11	2:H:179:GLN:HE21	1.79	0.47
2:H:192:PRO:O	2:H:195:PRO:HD2	2.14	0.47
1:A:58:VAL:CB	1:A:59:PRO:CD	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:THR:HA	1:A:208:SER:HB3	1.97	0.47
2:B:35:ASP:OD2	2:B:108:PHE:CE1	2.67	0.47
2:B:195:PRO:O	2:B:199:GLU:N	2.47	0.47
2:H:159:THR:O	2:H:206:ALA:N	2.41	0.47
1:L:2:ILE:HG22	1:L:4:MET:HE3	1.96	0.47
1:L:19:VAL:O	1:L:74:THR:HA	2.14	0.47
2:H:61:ASN:HB3	2:H:64:PHE:HB2	1.97	0.47
2:H:37:ILE:CG2	2:H:38:LYS:N	2.78	0.47
2:H:67:LYS:HB2	2:H:67:LYS:HE2	1.68	0.47
2:H:154:PHE:CG	2:H:155:PRO:N	2.79	0.47
1:A:66:GLY:HA2	1:A:71:TYR:HA	1.95	0.47
1:A:83:ILE:O	1:A:83:ILE:CG1	2.60	0.47
1:L:179:LEU:HD13	1:L:179:LEU:C	2.35	0.47
1:A:80:GLN:O	1:A:80:GLN:HG3	2.14	0.47
2:B:2:ALA:HB2	2:B:26:GLY:O	2.15	0.47
2:B:161:THR:O	2:B:203:CYS:HA	2.14	0.47
1:L:36:TYR:HE2	2:H:108:PHE:O	1.98	0.47
1:L:105:GLU:O	1:L:105:GLU:HG3	2.15	0.47
1:L:211:ARG:NH1	1:L:211:ARG:HG3	2.25	0.47
2:H:12:MET:HE2	2:H:17:SER:O	2.14	0.47
2:H:147:GLY:O	2:H:148:CYS:HB2	2.15	0.47
2:H:197:PRO:HB3	2:H:220:PRO:CG	2.44	0.47
1:L:113:PRO:HG3	1:L:144:ILE:HD12	1.95	0.47
1:L:145:ASN:HB3	1:L:197:THR:O	2.15	0.47
1:L:96:ARG:NH1	2:H:99:ARG:HD2	2.23	0.47
2:H:212:THR:HG22	2:H:213:LYS:H	1.80	0.47
2:B:24:ALA:HB3	2:B:29:PHE:HE1	1.80	0.46
2:H:137:ALA:O	2:H:139:GLN:N	2.43	0.46
1:A:55:HIS:HB3	1:A:56:SER:H	1.60	0.46
1:A:91:GLY:HA3	2:B:106:TYR:HB2	1.96	0.46
1:A:147:LYS:HB3	1:A:155:ARG:CZ	2.43	0.46
1:L:140:TYR:HA	1:L:141:PRO:O	2.16	0.46
2:B:65:ARG:C	2:B:67:LYS:H	2.18	0.46
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.16	0.46
2:H:122:ALA:HB3	2:H:154:PHE:CE1	2.51	0.46
2:H:158:VAL:HA	2:H:206:ALA:O	2.15	0.46
1:A:80:GLN:HA	1:A:106:ILE:CD1	2.46	0.46
1:A:164:THR:HG23	1:A:174:SER:O	2.15	0.46
2:B:177:VAL:CG2	2:B:177:VAL:O	2.63	0.46
2:B:197:PRO:HG3	2:B:220:PRO:HG3	1.97	0.46
1:L:175:MET:CA	2:H:174:PHE:HE1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:192:TYR:N	1:L:192:TYR:CD1	2.83	0.46
2:H:24:ALA:HB3	2:H:29:PHE:CD1	2.50	0.46
1:A:29:ILE:HG22	1:A:32:TYR:H	1.80	0.46
3:A:2017:HOH:O	2:B:145:THR:HG21	2.15	0.46
2:B:179:GLN:OE1	2:B:179:GLN:O	2.34	0.46
1:L:148:TRP:HZ2	1:L:177:SER:O	1.99	0.46
1:L:163:TRP:NE1	1:L:175:MET:SD	2.88	0.46
2:H:9:ALA:HB3	2:H:18:VAL:CG1	2.43	0.46
2:H:46:GLU:OE1	2:H:63:LYS:NZ	2.38	0.46
1:A:148:TRP:H	1:A:155:ARG:HB3	1.81	0.46
2:B:33:TRP:CZ2	2:B:57:SER:HB2	2.51	0.46
1:L:52:SER:O	1:L:53:ASN:CB	2.63	0.46
1:A:49:TYR:HE1	1:A:55:HIS:O	1.97	0.46
1:L:52:SER:CB	1:L:64:GLY:C	2.84	0.46
1:L:143:ASP:OD2	1:L:199:LYS:HD3	2.15	0.46
1:L:210:ASN:N	1:L:210:ASN:HD22	2.13	0.46
1:A:61:ARG:CZ	1:A:79:GLU:HG3	2.46	0.46
1:A:61:ARG:HB2	1:A:76:SER:OG	2.16	0.46
2:H:6:GLN:OE1	2:H:112:GLY:HA3	2.15	0.46
2:H:36:TRP:HA	2:H:95:TYR:O	2.15	0.46
1:A:160:LEU:CD1	2:B:177:VAL:HG21	2.45	0.46
1:A:170:ASP:O	1:A:172:THR:N	2.49	0.46
2:B:57:SER:O	2:B:58:THR:CB	2.64	0.46
2:B:155:PRO:O	2:B:207:HIS:HE1	1.98	0.46
1:L:83:ILE:HG13	1:L:104:LEU:O	2.16	0.46
2:B:152:GLY:HA2	2:B:182:LEU:HB3	1.97	0.46
2:H:196:ARG:HE	2:H:196:ARG:HB3	1.33	0.46
1:A:27:GLN:O	1:A:28:ASP:C	2.53	0.45
1:L:7:THR:C	1:L:8:THR:HG23	2.30	0.45
1:L:35:TRP:HA	1:L:87:PHE:O	2.16	0.45
2:H:12:MET:CE	2:H:16:ALA:CB	2.94	0.45
2:B:48:ILE:HG22	2:B:49:GLY:N	2.32	0.45
2:B:97:THR:HG21	2:B:108:PHE:CG	2.51	0.45
1:L:85:THR:HA	1:L:103:LYS:HA	1.99	0.45
2:H:61:ASN:ND2	2:H:63:LYS:HB3	2.32	0.45
1:A:115:VAL:CG1	1:A:116:SER:N	2.79	0.45
1:L:36:TYR:CZ	2:H:108:PHE:HB2	2.51	0.45
1:L:199:LYS:N	1:L:199:LYS:CD	2.67	0.45
2:B:1:GLN:O	2:B:3:GLN:HG3	2.17	0.45
1:L:90:GLN:HE21	1:L:92:ASN:H	1.64	0.45
1:A:115:VAL:HG12	1:A:207:LYS:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:PHE:CD2	2:H:77:ASN:HA	2.52	0.45
1:A:159:VAL:HA	1:A:178:THR:O	2.16	0.45
2:B:196:ARG:HE	2:B:196:ARG:HB3	1.39	0.45
2:B:220:PRO:C	2:B:221:ARG:CG	2.85	0.45
2:H:158:VAL:CG1	2:H:185:LEU:CD2	2.94	0.45
2:B:102:TRP:CE3	2:B:105:ALA:N	2.85	0.45
1:L:147:LYS:HZ3	1:L:149:LYS:HE3	1.80	0.45
2:H:162:TRP:HA	2:H:202:THR:O	2.17	0.45
1:A:98:PHE:HZ	2:B:37:ILE:CD1	2.29	0.45
2:B:214:VAL:CG2	2:B:215:ASP:N	2.80	0.45
2:H:1:GLN:CD	2:H:2:ALA:H	2.20	0.45
1:A:31:ASN:CB	1:A:51:THR:HG1	2.16	0.45
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.52	0.45
2:H:185:LEU:HD12	2:H:185:LEU:C	2.37	0.45
2:B:195:PRO:O	2:B:199:GLU:HB2	2.16	0.45
1:A:80:GLN:HE22	1:A:171:SER:N	2.15	0.44
2:B:220:PRO:C	2:B:221:ARG:HG3	2.35	0.44
2:H:33:TRP:HB2	2:H:99:ARG:HB3	1.99	0.44
2:B:204:ASN:HB3	2:B:215:ASP:OD1	2.16	0.44
2:H:37:ILE:HG22	2:H:38:LYS:N	2.32	0.44
2:H:141:ASN:OD1	2:H:141:ASN:N	2.31	0.44
2:B:29:PHE:HB2	2:B:77:ASN:OD1	2.18	0.44
1:L:193:THR:HA	1:L:208:SER:HA	1.99	0.44
1:L:205:ILE:HG23	1:L:205:ILE:O	2.17	0.44
2:H:126:PRO:HB3	2:H:212:THR:HG1	1.81	0.44
2:H:158:VAL:CG1	2:H:185:LEU:HD21	2.47	0.44
1:A:147:LYS:HB3	1:A:155:ARG:HH11	1.78	0.44
2:B:180:SER:C	2:B:182:LEU:H	2.21	0.44
1:A:113:PRO:HB3	1:A:139:PHE:HB3	2.00	0.44
2:B:18:VAL:HG21	2:B:117:LEU:HD22	2.00	0.44
1:L:115:VAL:HA	1:L:135:PHE:O	2.17	0.44
2:B:37:ILE:HG22	2:B:38:LYS:N	2.32	0.44
2:B:170:GLY:O	2:B:189:VAL:HA	2.18	0.44
2:B:178:LEU:HD12	2:B:178:LEU:HA	1.87	0.44
1:L:33:LEU:HD13	1:L:34:ASN:N	2.32	0.44
2:H:192:PRO:HG2	2:H:195:PRO:HD2	1.99	0.44
2:B:129:VAL:HG21	2:B:214:VAL:CG1	2.41	0.44
2:H:191:VAL:HG23	2:H:192:PRO:O	2.18	0.44
1:A:79:GLU:O	1:A:81:GLU:N	2.46	0.44
1:A:147:LYS:HA	1:A:155:ARG:HD3	1.98	0.44
1:L:206:VAL:O	1:L:207:LYS:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:209:PHE:HB2	2:H:136:SER:HB2	1.99	0.44
2:B:162:TRP:CE2	2:B:203:CYS:HB3	2.53	0.44
2:H:12:MET:CE	2:H:17:SER:O	2.65	0.44
1:A:13:ALA:O	1:A:106:ILE:HA	2.18	0.43
1:A:48:ILE:HA	1:A:54:LEU:O	2.18	0.43
1:A:34:ASN:HD22	1:A:49:TYR:CA	2.24	0.43
2:B:38:LYS:HE2	2:B:40:ARG:CG	2.49	0.43
1:A:206:VAL:HG13	1:A:206:VAL:O	2.18	0.43
2:B:220:PRO:O	2:B:221:ARG:CG	2.58	0.43
1:L:108:ARG:HG2	1:L:109:ALA:O	2.19	0.43
1:L:113:PRO:CA	1:L:139:PHE:HB3	2.49	0.43
2:B:172:HIS:N	2:B:188:SER:O	2.51	0.43
2:B:205:VAL:HG13	2:B:214:VAL:CG1	2.49	0.43
1:L:145:ASN:OD1	1:L:197:THR:HB	2.18	0.43
2:B:11:LEU:HD22	2:B:155:PRO:HG3	2.01	0.43
2:B:36:TRP:HA	2:B:95:TYR:O	2.18	0.43
2:B:125:THR:HA	2:B:126:PRO:HD3	1.83	0.43
1:L:41:ASP:OD2	3:L:2006:HOH:O	2.21	0.43
2:H:15:GLY:O	2:H:85:SER:HA	2.19	0.43
1:A:29:ILE:O	1:A:29:ILE:CG2	2.66	0.43
1:A:51:THR:HG23	1:A:71:TYR:HE2	1.75	0.43
2:B:27:TYR:CZ	2:B:98:ARG:HD3	2.54	0.43
1:A:52:SER:CB	1:A:64:GLY:C	2.87	0.43
2:B:131:PRO:HD3	2:B:216:LYS:HG2	2.01	0.43
2:B:132:LEU:HD21	2:B:149:LEU:HB2	2.00	0.43
2:H:51:ILE:HB	2:H:58:THR:HG22	2.01	0.43
1:A:67:SER:O	1:A:69:THR:N	2.47	0.43
2:B:67:LYS:O	2:B:83:LEU:HD23	2.19	0.43
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.91	0.43
2:H:30:SER:HB2	2:H:54:GLY:HA2	2.00	0.43
2:H:123:LYS:O	2:H:124:THR:C	2.57	0.43
1:A:139:PHE:CE2	1:A:174:SER:HA	2.54	0.43
1:A:144:ILE:HG12	1:A:145:ASN:N	2.34	0.43
2:B:11:LEU:HD22	2:B:155:PRO:HB3	2.00	0.43
1:L:51:THR:O	1:L:51:THR:HG23	2.18	0.43
1:L:161:ASN:HB2	1:L:163:TRP:CH2	2.54	0.43
2:H:165:GLY:O	2:H:166:SER:C	2.57	0.43
2:B:34:ILE:HG22	2:B:35:ASP:N	2.34	0.42
1:L:114:THR:HG22	1:L:114:THR:O	2.20	0.42
1:A:182:THR:O	1:A:185:GLU:N	2.50	0.42
1:A:189:HIS:O	1:A:211:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:GLN:HB2	2:H:130:TYR:CG	2.54	0.42
1:L:148:TRP:O	1:L:149:LYS:HG3	2.19	0.42
1:L:155:ARG:NE	1:L:156:GLN:H	2.17	0.42
2:H:1:GLN:OE1	2:H:1:GLN:HA	2.18	0.42
1:A:52:SER:O	1:A:54:LEU:N	2.50	0.42
1:A:66:GLY:HA3	1:A:71:TYR:CD2	2.54	0.42
2:B:61:ASN:HA	3:B:2010:HOH:O	2.20	0.42
1:L:29:ILE:CD1	1:L:33:LEU:HB2	2.46	0.42
1:A:212:ASN:HD22	1:A:212:ASN:HA	1.65	0.42
2:B:194:SER:CB	2:B:195:PRO:HD3	2.46	0.42
1:L:146:VAL:CG2	1:L:175:MET:CE	2.94	0.42
2:H:61:ASN:HD22	2:H:62:GLU:N	2.17	0.42
2:H:194:SER:O	2:H:198:SER:OG	2.38	0.42
1:A:90:GLN:NE2	1:A:92:ASN:H	2.18	0.42
2:B:40:ARG:O	2:B:42:GLY:N	2.53	0.42
2:B:67:LYS:O	2:B:67:LYS:HG3	2.20	0.42
1:L:116:SER:OG	2:H:140:THR:HG21	2.19	0.42
1:L:136:LEU:CD1	1:L:146:VAL:HG22	2.50	0.42
2:H:18:VAL:CG1	2:H:19:LYS:N	2.80	0.42
2:B:6:GLN:HG2	2:B:7:SER:H	1.85	0.42
2:B:10:GLU:CG	2:B:116:THR:O	2.67	0.42
1:L:94:LEU:HD23	1:L:96:ARG:HE	1.85	0.42
2:B:60:TYR:CE1	2:B:70:PHE:CD1	3.08	0.42
1:L:41:ASP:OD1	1:L:43:THR:N	2.53	0.42
1:L:49:TYR:CZ	1:L:54:LEU:HB3	2.54	0.42
2:H:4:LEU:HG	2:H:22:CYS:SG	2.59	0.42
2:H:171:VAL:HG22	2:H:172:HIS:N	2.34	0.42
2:B:87:THR:O	2:B:119:VAL:HB	2.20	0.41
2:B:189:VAL:O	2:B:189:VAL:HG13	2.20	0.41
2:H:200:THR:O	2:H:200:THR:CG2	2.68	0.41
2:B:27:TYR:CE2	2:B:98:ARG:HD3	2.54	0.41
2:B:41:PRO:C	2:B:43:HIS:H	2.24	0.41
2:B:132:LEU:HB2	2:B:147:GLY:HA3	2.02	0.41
1:L:31:ASN:ND2	1:L:51:THR:CB	2.83	0.41
2:H:192:PRO:HG2	2:H:195:PRO:CD	2.50	0.41
1:A:147:LYS:HA	1:A:155:ARG:HD2	2.03	0.41
1:L:183:LYS:NZ	1:L:187:GLU:OE1	2.51	0.41
2:H:70:PHE:HA	2:H:80:TYR:O	2.19	0.41
1:A:51:THR:O	1:A:52:SER:CB	2.68	0.41
1:A:59:PRO:HB2	1:A:62:PHE:CD1	2.56	0.41
2:B:60:TYR:CE1	2:B:70:PHE:CE1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4:MET:HE2	1:L:25:ALA:HA	2.02	0.41
2:B:89:GLU:H	2:B:89:GLU:HG2	1.68	0.41
2:B:94:TYR:N	2:B:115:THR:O	2.51	0.41
2:B:106:TYR:N	2:B:106:TYR:CD1	2.88	0.41
2:B:132:LEU:HD22	2:B:132:LEU:N	2.35	0.41
1:L:30:ASN:HA	3:L:2010:HOH:O	2.21	0.41
1:A:44:VAL:HG12	1:A:45:LYS:N	2.36	0.41
1:L:211:ARG:NH1	1:L:211:ARG:CG	2.82	0.41
2:B:23:LYS:HB3	2:B:23:LYS:HE3	1.55	0.41
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.56	0.41
2:B:167:LEU:HD21	2:B:191:VAL:CG1	2.50	0.41
1:L:91:GLY:HA3	2:H:106:TYR:HB2	2.02	0.41
1:A:147:LYS:CB	1:A:155:ARG:HH11	2.33	0.41
2:B:99:ARG:HA	2:B:107:ASP:O	2.20	0.41
2:B:145:THR:HG23	2:B:190:THR:HG23	2.03	0.41
1:L:38:GLN:O	1:L:84:ALA:HB1	2.21	0.41
2:H:81:MET:CE	2:H:83:LEU:HD11	2.50	0.41
1:A:79:GLU:C	1:A:81:GLU:H	2.22	0.41
2:B:61:ASN:C	2:B:63:LYS:N	2.73	0.41
2:B:63:LYS:C	2:B:65:ARG:H	2.24	0.41
2:B:162:TRP:CD2	2:B:203:CYS:HB3	2.55	0.41
2:B:191:VAL:HB	2:B:192:PRO:HD2	2.02	0.41
2:B:208:PRO:O	2:B:209:ALA:C	2.59	0.41
1:L:1:ASP:HB2	1:L:2:ILE:H	1.54	0.41
1:L:113:PRO:HG3	1:L:144:ILE:HD11	2.03	0.41
1:L:149:LYS:HG2	1:L:153:SER:O	2.20	0.41
1:L:213:GLU:O	1:L:213:GLU:HG3	2.20	0.41
2:H:189:VAL:O	2:H:189:VAL:HG13	2.20	0.41
1:A:40:PRO:C	1:A:41:ASP:OD1	2.60	0.41
1:A:161:ASN:HB3	1:A:175:MET:HE3	2.03	0.41
1:L:133:VAL:HG12	1:L:134:CYS:N	2.36	0.41
2:H:221:ARG:O	2:H:222:ASP:HB2	2.21	0.41
1:A:206:VAL:HG22	1:A:207:LYS:N	2.35	0.40
2:B:185:LEU:HD12	2:B:186:SER:N	2.36	0.40
1:A:33:LEU:H	1:A:51:THR:H	1.69	0.40
2:B:4:LEU:HD23	2:B:24:ALA:HA	2.02	0.40
1:L:41:ASP:OD1	1:L:43:THR:OG1	2.35	0.40
1:L:180:THR:O	1:L:180:THR:HG23	2.21	0.40
2:H:72:ALA:HA	2:H:79:ALA:HA	2.02	0.40
2:H:88:SER:C	2:H:90:ASP:H	2.23	0.40
1:A:39:LYS:C	1:A:40:PRO:O	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:C	1:A:184:ASP:N	2.72	0.40
2:H:63:LYS:O	2:H:63:LYS:HG2	2.21	0.40
2:H:126:PRO:HG3	2:H:210:SER:HB2	2.03	0.40
1:A:186:TYR:HA	1:A:192:TYR:OH	2.21	0.40
2:B:9:ALA:HA	2:H:76:SER:OG	2.21	0.40
1:L:160:LEU:HD23	1:L:160:LEU:HA	1.89	0.40
1:L:163:TRP:CE2	1:L:175:MET:SD	3.15	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:O	2:H:57:SER:OG[2_656]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	212/214 (99%)	173 (82%)	34 (16%)	5 (2%)	6 20
1	L	212/214 (99%)	176 (83%)	27 (13%)	9 (4%)	3 9
2	B	212/220 (96%)	173 (82%)	24 (11%)	15 (7%)	1 2
2	H	218/220 (99%)	163 (75%)	33 (15%)	22 (10%)	0 1
All	All	854/868 (98%)	685 (80%)	118 (14%)	51 (6%)	1 4

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	TYR
2	B	7	SER
2	B	55	SER

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Mol	Chain	Res	Type
2	B	57	SER
2	B	58	THR
2	B	72	ALA
2	B	157	PRO
1	L	8	THR
2	H	7	SER
2	H	62	GLU
2	H	106	TYR
2	H	154	PHE
2	H	155	PRO
2	H	156	GLU
2	H	166	SER
2	H	220	PRO
1	A	7	THR
1	A	68	GLY
2	B	48	ILE
2	B	56	GLY
2	B	62	GLU
2	B	114	GLY
1	L	68	GLY
2	H	29	PHE
2	H	148	CYS
2	H	152	GLY
2	H	169	SER
1	A	40	PRO
1	A	80	GLN
2	B	164	SER
1	L	57	GLY
1	L	169	LYS
2	H	136	SER
2	H	138	ALA
2	H	139	GLN
2	H	143	MET
2	H	195	PRO
2	H	221	ARG
2	B	41	PRO
1	L	7	THR
1	L	156	GLN
2	H	16	ALA
2	H	56	GLY
2	H	73	ASP
2	B	102	TRP

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Mol	Chain	Res	Type
2	B	220	PRO
1	L	50	TYR
2	H	140	THR
1	L	27	GLN
1	L	127	SER
2	B	152	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	A	185/191 (97%)	167 (90%)	18 (10%)	8 24
1	L	188/191 (98%)	173 (92%)	15 (8%)	12 34
2	B	183/187 (98%)	154 (84%)	29 (16%)	2 8
2	H	183/187 (98%)	156 (85%)	27 (15%)	3 9
All	All	739/756 (98%)	650 (88%)	89 (12%)	5 15

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	23	CYS
1	A	31	ASN
1	A	90	GLN
1	A	96	ARG
1	A	97	THR
1	A	108	ARG
1	A	153	SER
1	A	170	ASP
1	A	171	SER
1	A	175	MET
1	A	184	ASP
1	A	190	ASN
1	A	191	SER
1	A	193	THR

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Mol	Chain	Res	Type
1	A	202	THR
1	A	212	ASN
1	A	214	CYS
2	B	3	GLN
2	B	21	SER
2	B	23	LYS
2	B	43	HIS
2	B	55	SER
2	B	61	ASN
2	B	71	THR
2	B	76	SER
2	B	88	SER
2	B	89	GLU
2	B	91	SER
2	B	97	THR
2	B	101	TYR
2	B	102	TRP
2	B	117	LEU
2	B	123	LYS
2	B	142	SER
2	B	148	CYS
2	B	157	PRO
2	B	159	THR
2	B	177	VAL
2	B	179	GLN
2	B	185	LEU
2	B	194	SER
2	B	195	PRO
2	B	196	ARG
2	B	198	SER
2	B	204	ASN
2	B	205	VAL
1	L	1	ASP
1	L	3	GLN
1	L	53	ASN
1	L	55	HIS
1	L	70	ASP
1	L	74	THR
1	L	83	ILE
1	L	90	GLN
1	L	96	ARG
1	L	114	THR

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Mol	Chain	Res	Type
1	L	145	ASN
1	L	188	ARG
1	L	193	THR
1	L	205	ILE
1	L	213	GLU
2	H	4	LEU
2	H	11	LEU
2	H	23	LYS
2	H	32	TYR
2	H	35	ASP
2	H	61	ASN
2	H	62	GLU
2	H	71	THR
2	H	74	THR
2	H	84	SER
2	H	87	THR
2	H	109	ASP
2	H	118	THR
2	H	141	ASN
2	H	172	HIS
2	H	179	GLN
2	H	181	ASP
2	H	185	LEU
2	H	195	PRO
2	H	196	ARG
2	H	200	THR
2	H	204	ASN
2	H	210	SER
2	H	216	LYS
2	H	217	LYS
2	H	221	ARG
2	H	222	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	34	ASN
1	A	80	GLN
1	A	90	GLN
1	A	190	ASN
1	A	212	ASN

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Mol	Chain	Res	Type
2	B	6	GLN
2	B	43	HIS
2	B	61	ASN
2	B	77	ASN
2	B	172	HIS
2	B	204	ASN
2	B	207	HIS
1	L	6	GLN
1	L	30	ASN
1	L	31	ASN
1	L	38	GLN
1	L	77	ASN
1	L	80	GLN
1	L	90	GLN
1	L	161	ASN
1	L	210	ASN
1	L	212	ASN
2	H	39	GLN
2	H	61	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)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	214/214 (100%)	-0.05	5 (2%)	60	51	25, 44, 60, 76	0
1	L	214/214 (100%)	0.11	11 (5%)	28	19	24, 45, 59, 75	0
2	B	216/220 (98%)	0.14	10 (4%)	32	22	28, 45, 64, 75	0
2	H	220/220 (100%)	0.11	5 (2%)	60	51	23, 47, 68, 81	0
All	All	864/868 (99%)	0.08	31 (3%)	42	32	23, 45, 63, 81	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	140	THR	7.1
2	H	136	SER	5.6
2	H	141	ASN	4.3
2	B	137	ALA	4.2
1	A	214	CYS	4.0
2	B	8	GLY	4.0
2	H	222	ASP	3.8
1	L	8	THR	3.7
1	L	7	THR	3.4
1	A	212	ASN	3.2
2	B	101	TYR	3.2
1	L	53	ASN	2.8
1	A	210	ASN	2.7
2	B	136	SER	2.6
2	B	43	HIS	2.6
2	B	1	GLN	2.5
2	B	76	SER	2.5
1	L	129	GLY	2.5
1	L	212	ASN	2.4
1	L	214	CYS	2.3
2	B	143	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	138	ALA	2.3
1	A	156	GLN	2.2
1	L	126	THR	2.2
1	L	93	THR	2.2
2	B	41	PRO	2.2
1	L	155	ARG	2.2
2	B	142	SER	2.1
1	L	213	GLU	2.1
1	L	1	ASP	2.0
1	A	202	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.