Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:33 AM GMT

PDB ID : 2R69

Title : Crystal structure of Fab 1A1D-2 complexed with E-DIII of Dengue virus at 3.8 angstrom resolution

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Deposited on : 2007-09-05
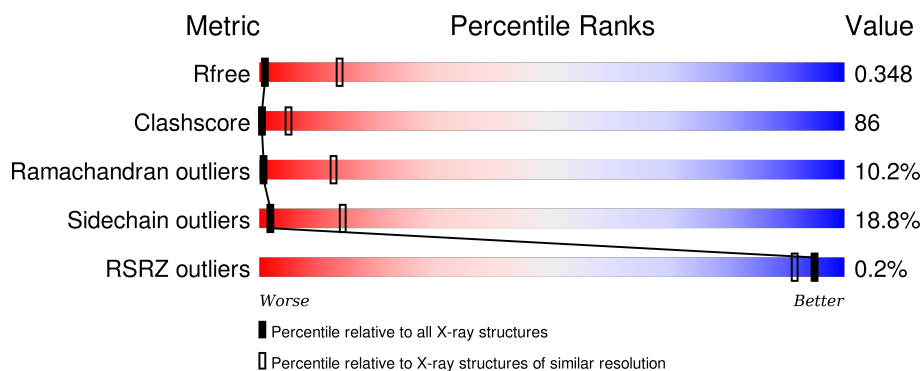
Resolution : 3.80 Å(reported)

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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
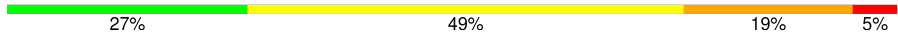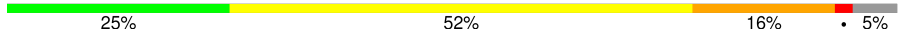*X-RAY DIFFRACTION*
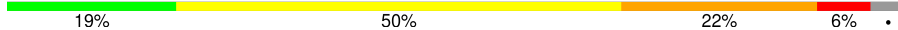
The reported resolution of this entry is 3.80 Å.

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	Percentile Ranks	Value
Rfree		0.348
Clashscore		86
Ramachandran outliers		10.2%
Sidechain outliers		18.8%
RSRZ outliers		0.2%

Worse ▬ *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 <=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	97	27% 49% 19% 5%
2	H	214	25% 52% 16% · 5%
3	L	212	19% 50% 22% 6% ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3886 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 Major envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total 768	C 495	N 126	O 143	S 4	0	0	0

- Molecule 2 is a protein called Heavy chain of 1A1D-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	203	Total 1536	C 979	N 248	O 304	S 5	0	0	0

- Molecule 3 is a protein called Light chain of 1A1D-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	204	Total 1582	C 989	N 268	O 319	S 6	0	0	0

3 Residue-property plots (i)

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: Major envelope protein E
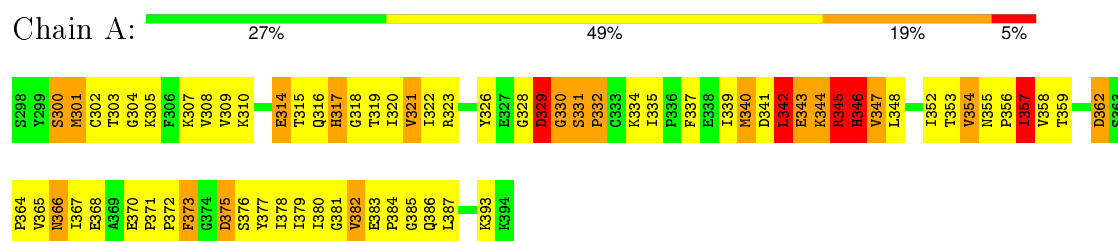
- Molecule 2: Heavy chain of 1A1D-2
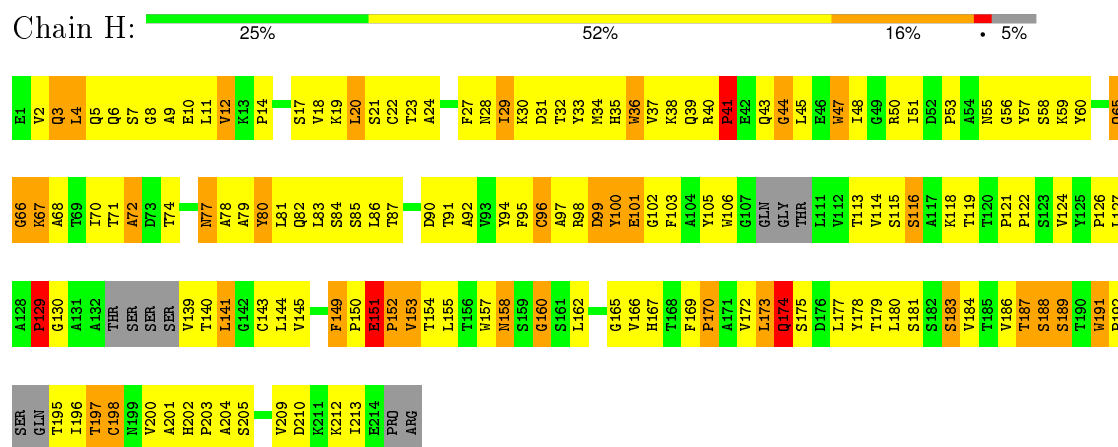
- Molecule 3: Light chain of 1A1D-2
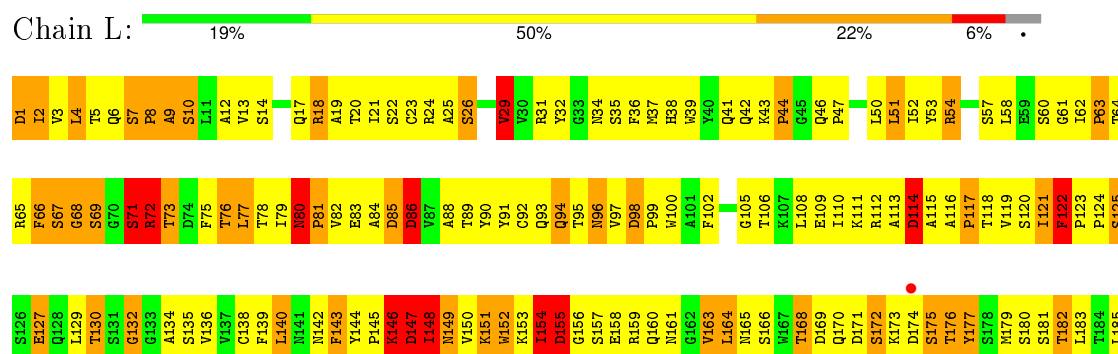
T186 K187 N194 S195 Y196 T197 C198 E199 A200 T201 SER PRO ILE VAL K207 S208 F209 ASN ARG ASN GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants $a, b, c, \alpha, \beta, \gamma$	164.77Å 66.89Å 79.41Å 90.00° 113.05° 90.00°	Depositor
Resolution (Å)	20.00 – 3.80 30.41 – 3.60	Depositor EDS
% Data completeness (in resolution range)	73.2 (20.00-3.80) 68.4 (30.41-3.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 3.56Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.313 , 0.363 0.305 , 0.348	Depositor DCC
R_{free} test set	634 reflections (10.90%)	DCC
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	0.818	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.36, < L^2 > = 0.18$	Xtriage
Outliers	0 of 6433 reflections	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	3886	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.68	0/785	1.19	10/1060 (0.9%)
2	H	0.67	2/1574 (0.1%)	1.09	9/2149 (0.4%)
3	L	0.67	0/1618	1.25	19/2199 (0.9%)
All	All	0.67	2/3977 (0.1%)	1.17	38/5408 (0.7%)

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
3	L	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	77	ASN	C-O	-5.29	1.13	1.23
2	H	47	TRP	CB-CG	5.19	1.59	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	148	ILE	N-CA-C	11.60	142.31	111.00
3	L	122	PHE	CB-CG-CD2	-10.57	113.40	120.80
3	L	147	ASP	N-CA-C	9.40	136.38	111.00
3	L	67	SER	N-CA-C	8.85	134.90	111.00
2	H	77	ASN	N-CA-C	8.28	133.36	111.00
2	H	175	SER	N-CA-C	7.92	132.40	111.00
1	A	373	PHE	N-CA-C	7.74	131.89	111.00
2	H	174	GLN	N-CA-C	-7.71	90.17	111.00
1	A	343	GLU	N-CA-C	-7.29	91.31	111.00
3	L	71	SER	N-CA-C	7.27	130.62	111.00
3	L	156	GLY	N-CA-C	-7.24	95.00	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	VAL	N-CA-C	-7.22	91.50	111.00
2	H	189	SER	N-CA-C	7.19	130.42	111.00
1	A	301	MET	N-CA-C	-7.14	91.73	111.00
1	A	345	ARG	N-CA-C	-6.96	92.22	111.00
1	A	300	SER	N-CA-C	6.38	128.23	111.00
3	L	66	PHE	N-CA-C	6.38	128.22	111.00
2	H	160	GLY	N-CA-C	-6.27	97.43	113.10
3	L	86	ASP	N-CA-C	6.27	127.92	111.00
3	L	154	ILE	N-CA-C	-6.24	94.15	111.00
3	L	175	SER	N-CA-C	6.21	127.76	111.00
2	H	129	PRO	CA-CB-CG	-6.09	92.42	104.00
3	L	146	LYS	C-N-CA	-5.88	106.99	121.70
3	L	140	LEU	N-CA-C	-5.85	95.21	111.00
1	A	347	VAL	N-CA-C	5.76	126.55	111.00
3	L	127	GLU	N-CA-C	-5.68	95.67	111.00
1	A	329	ASP	N-CA-C	5.62	126.18	111.00
3	L	121	ILE	N-CA-C	-5.62	95.83	111.00
2	H	151	GLU	N-CA-C	5.57	126.05	111.00
3	L	68	GLY	N-CA-C	5.55	126.99	113.10
2	H	72	ALA	N-CA-C	-5.48	96.21	111.00
1	A	344	LYS	N-CA-C	-5.46	96.27	111.00
2	H	80	TYR	CB-CG-CD2	-5.42	117.75	121.00
3	L	98	ASP	N-CA-C	5.40	125.57	111.00
1	A	342	LEU	N-CA-C	5.38	125.54	111.00
3	L	63	PRO	N-CA-C	-5.27	98.41	112.10
3	L	155	ASP	CA-C-N	-5.10	106.00	116.20
3	L	72	ARG	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	122	PHE	Sidechain
3	L	177	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	768	0	780	141	0
2	H	1536	0	1498	285	0
3	L	1582	0	1517	293	0
All	All	3886	0	3795	664	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 86.

All (664) 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:H:129:PRO:HG3	3:L:122:PHE:CZ	1.53	1.43
1:A:301:MET:HA	1:A:334:LYS:HB3	1.24	1.17
3:L:160:GLN:O	3:L:163:VAL:HG23	1.44	1.16
3:L:148:ILE:CG2	3:L:149:ASN:H	1.61	1.14
2:H:183:SER:HB2	3:L:139:PHE:CE1	1.84	1.11
3:L:83:GLU:HG3	3:L:84:ALA:H	1.16	1.11
3:L:77:LEU:HD12	3:L:78:THR:H	1.09	1.11
2:H:68:ALA:HB1	2:H:81:LEU:HD11	1.32	1.10
3:L:148:ILE:HG23	3:L:149:ASN:H	0.97	1.10
3:L:120:SER:HB3	3:L:139:PHE:HB2	1.27	1.09
1:A:304:GLY:HA3	1:A:326:TYR:CE1	1.87	1.09
3:L:134:ALA:HB1	3:L:185:LEU:H	1.18	1.09
2:H:196:ILE:HG22	2:H:197:THR:H	1.17	1.09
3:L:71:SER:HA	3:L:75:PHE:HE2	1.15	1.08
3:L:121:ILE:HG12	3:L:207:LYS:N	1.70	1.07
2:H:139:VAL:HB	2:H:187:THR:HA	1.37	1.06
2:H:129:PRO:HB3	3:L:122:PHE:HE2	1.21	1.06
1:A:354:VAL:HG23	1:A:355:ASN:H	1.15	1.05
3:L:121:ILE:O	3:L:122:PHE:CD1	2.10	1.04
3:L:148:ILE:HG23	3:L:149:ASN:N	1.73	1.03
1:A:352:ILE:HD11	1:A:370:GLU:HB2	1.36	1.03
2:H:81:LEU:HD12	2:H:82:GLN:H	1.15	1.03
1:A:373:PHE:HB3	1:A:393:LYS:HD3	1.42	1.02
1:A:319:THR:OG1	1:A:368:GLU:HG3	1.60	1.01
3:L:120:SER:CB	3:L:139:PHE:HB2	1.90	1.01
2:H:127:LEU:HD23	3:L:125:SER:HB2	1.37	1.01
2:H:129:PRO:CG	3:L:122:PHE:CZ	2.43	1.01
3:L:118:THR:HG22	3:L:119:VAL:H	1.25	1.01
2:H:91:THR:HG23	2:H:113:THR:HA	1.40	1.00
3:L:18:ARG:HD3	3:L:18:ARG:H	1.25	1.00
2:H:127:LEU:CD2	3:L:125:SER:H	1.74	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:PRO:HG3	3:L:122:PHE:CE2	1.97	0.99
2:H:2:VAL:HG11	2:H:98:ARG:HH22	1.27	0.99
2:H:191:TRP:HB3	2:H:192:PRO:HD3	1.42	0.98
2:H:28:ASN:ND2	2:H:30:LYS:HB2	1.78	0.98
2:H:2:VAL:CG2	2:H:98:ARG:HH12	1.76	0.97
3:L:163:VAL:O	3:L:164:LEU:HD23	1.65	0.97
1:A:341:ASP:HB2	1:A:345:ARG:HB3	1.44	0.96
1:A:304:GLY:HA3	1:A:326:TYR:HE1	1.31	0.96
2:H:129:PRO:CG	3:L:122:PHE:CE2	2.49	0.96
2:H:40:ARG:HB3	2:H:41:PRO:HD2	1.46	0.96
3:L:84:ALA:HB1	3:L:172:SER:O	1.67	0.95
1:A:331:SER:OG	1:A:332:PRO:HD3	1.67	0.94
1:A:342:LEU:HD22	1:A:377:TYR:CZ	2.01	0.94
3:L:153:LYS:HA	3:L:158:GLU:HG3	1.47	0.94
3:L:93:GLN:HG2	3:L:94:GLN:H	1.30	0.93
2:H:129:PRO:CB	3:L:122:PHE:HE2	1.81	0.93
2:H:129:PRO:CB	3:L:122:PHE:CE2	2.52	0.93
2:H:184:VAL:HG22	2:H:186:VAL:HG22	1.50	0.93
2:H:139:VAL:HB	2:H:187:THR:CA	1.98	0.93
2:H:129:PRO:HB3	3:L:122:PHE:CE2	2.04	0.92
3:L:83:GLU:O	3:L:86:ASP:HB2	1.69	0.92
3:L:108:LEU:HD12	3:L:109:GLU:H	1.35	0.92
3:L:80:ASN:HB3	3:L:81:PRO:CD	1.98	0.92
2:H:23:THR:HA	2:H:78:ALA:HB2	1.51	0.91
2:H:197:THR:HG23	2:H:210:ASP:OD1	1.70	0.91
2:H:150:PRO:HG2	2:H:202:HIS:HE2	1.34	0.89
2:H:173:LEU:HD22	2:H:178:TYR:CE1	2.07	0.89
1:A:353:THR:HG21	1:A:356:PRO:HB3	1.55	0.88
3:L:14:SER:OG	3:L:17:GLN:HG2	1.71	0.88
1:A:307:LYS:HB2	3:L:54:ARG:NH2	1.88	0.88
1:A:341:ASP:HB2	1:A:345:ARG:CB	2.03	0.88
1:A:309:VAL:HA	2:H:100:TYR:HB3	1.55	0.88
3:L:71:SER:HA	3:L:75:PHE:CE2	2.07	0.87
3:L:153:LYS:HB3	3:L:197:THR:HB	1.56	0.86
3:L:77:LEU:HD12	3:L:78:THR:N	1.91	0.86
1:A:340:MET:SD	1:A:344:LYS:HG3	2.16	0.86
3:L:120:SER:HB3	3:L:139:PHE:CB	2.06	0.86
2:H:2:VAL:HG13	2:H:2:VAL:O	1.76	0.85
3:L:80:ASN:HB3	3:L:81:PRO:HD3	1.57	0.85
1:A:342:LEU:HD23	1:A:342:LEU:N	1.92	0.85
1:A:335:ILE:O	1:A:337:PHE:N	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:CG1	2:H:98:ARG:HH22	1.88	0.84
3:L:39:TRP:HB2	3:L:52:ILE:HB	1.57	0.84
2:H:81:LEU:HD12	2:H:82:GLN:N	1.92	0.83
3:L:134:ALA:CB	3:L:185:LEU:H	1.90	0.83
3:L:50:LEU:HD12	3:L:51:LEU:H	1.44	0.83
3:L:89:THR:HA	3:L:106:THR:O	1.79	0.83
3:L:22:SER:HA	3:L:76:THR:HA	1.61	0.83
2:H:23:THR:HA	2:H:78:ALA:CB	2.09	0.83
3:L:77:LEU:CD1	3:L:78:THR:H	1.91	0.83
2:H:2:VAL:HG22	2:H:98:ARG:HH12	1.45	0.82
3:L:83:GLU:HG3	3:L:84:ALA:N	1.94	0.82
1:A:373:PHE:HB3	1:A:393:LYS:CD	2.09	0.82
1:A:305:LYS:HZ3	1:A:385:GLY:HA2	1.43	0.82
3:L:153:LYS:HA	3:L:158:GLU:CG	2.08	0.82
1:A:354:VAL:HG23	1:A:355:ASN:N	1.94	0.82
2:H:191:TRP:CB	2:H:192:PRO:HD3	2.09	0.82
3:L:97:VAL:HG12	3:L:99:PRO:HD3	1.60	0.82
2:H:139:VAL:CB	2:H:187:THR:HA	2.10	0.81
1:A:343:GLU:C	1:A:345:ARG:H	1.82	0.81
3:L:118:THR:HG22	3:L:119:VAL:N	1.95	0.81
3:L:118:THR:CG2	3:L:119:VAL:H	1.93	0.81
3:L:183:LEU:CD1	3:L:185:LEU:HD21	2.11	0.81
3:L:86:ASP:O	3:L:108:LEU:HD23	1.80	0.80
3:L:29:VAL:O	3:L:29:VAL:HG13	1.81	0.80
3:L:44:PRO:O	3:L:46:GLN:HG3	1.82	0.80
2:H:27:PHE:CE2	2:H:98:ARG:NH1	2.49	0.80
2:H:40:ARG:HG2	2:H:92:ALA:CB	2.13	0.79
3:L:120:SER:CB	3:L:139:PHE:CB	2.59	0.79
2:H:22:CYS:O	2:H:78:ALA:HB1	1.82	0.79
3:L:25:ALA:HB3	3:L:73:THR:OG1	1.84	0.79
2:H:196:ILE:HG22	2:H:197:THR:N	1.95	0.78
3:L:170:GLN:HA	3:L:176:THR:O	1.83	0.78
3:L:95:THR:HA	3:L:100:TRP:CD1	2.19	0.78
2:H:40:ARG:HH21	2:H:43:GLN:HG2	1.47	0.77
2:H:2:VAL:HG21	2:H:98:ARG:HH12	1.49	0.77
3:L:96:ASN:C	3:L:96:ASN:HD22	1.88	0.76
2:H:37:VAL:HG12	2:H:38:LYS:N	1.98	0.76
2:H:68:ALA:HB1	2:H:81:LEU:CD1	2.14	0.76
3:L:153:LYS:CA	3:L:158:GLU:HG3	2.15	0.76
2:H:50:ARG:HD3	3:L:100:TRP:HZ3	1.51	0.75
1:A:341:ASP:O	1:A:343:GLU:O	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:153:LYS:N	3:L:197:THR:O	2.20	0.75
3:L:83:GLU:CG	3:L:84:ALA:H	1.98	0.74
2:H:2:VAL:O	2:H:2:VAL:CG1	2.35	0.74
2:H:4:LEU:HD21	2:H:27:PHE:HZ	1.53	0.74
2:H:209:VAL:HG22	2:H:210:ASP:N	2.02	0.74
2:H:27:PHE:CD2	2:H:98:ARG:NH1	2.55	0.74
2:H:7:SER:OG	2:H:21:SER:OG	2.06	0.74
2:H:129:PRO:HG2	2:H:130:GLY:N	2.01	0.74
2:H:98:ARG:NH2	2:H:105:TYR:HD2	1.85	0.74
2:H:50:ARG:CD	3:L:100:TRP:HZ3	2.00	0.74
1:A:379:ILE:HA	1:A:387:LEU:O	1.87	0.73
2:H:202:HIS:CE1	2:H:205:SER:H	2.06	0.73
3:L:154:ILE:HD12	3:L:196:TYR:CE2	2.23	0.73
2:H:209:VAL:HG22	2:H:210:ASP:H	1.52	0.73
1:A:342:LEU:HD23	1:A:342:LEU:H	1.54	0.73
2:H:83:LEU:HB2	2:H:86:LEU:HD21	1.71	0.72
3:L:148:ILE:CG2	3:L:149:ASN:N	2.38	0.72
3:L:76:THR:HG23	3:L:76:THR:O	1.89	0.72
2:H:43:GLN:CD	2:H:43:GLN:H	1.93	0.72
2:H:186:VAL:HG12	2:H:188:SER:HB2	1.70	0.72
1:A:342:LEU:HD22	1:A:377:TYR:CE1	2.24	0.72
2:H:55:ASN:ND2	2:H:57:TYR:HB2	2.04	0.72
3:L:122:PHE:CD2	3:L:123:PRO:HD2	2.24	0.72
3:L:4:LEU:HA	3:L:24:ARG:O	1.89	0.72
2:H:34:MET:HG3	2:H:97:ALA:O	1.90	0.72
1:A:305:LYS:NZ	1:A:385:GLY:HA2	2.05	0.71
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.72	0.71
1:A:329:ASP:O	1:A:330:GLY:O	2.07	0.71
2:H:27:PHE:HE2	2:H:98:ARG:HH11	1.37	0.71
3:L:29:VAL:O	3:L:29:VAL:CG1	2.38	0.71
2:H:43:GLN:N	2:H:43:GLN:CD	2.43	0.71
2:H:150:PRO:HG2	2:H:202:HIS:NE2	2.04	0.71
2:H:186:VAL:C	2:H:188:SER:H	1.93	0.71
1:A:304:GLY:CA	1:A:326:TYR:HE1	2.02	0.71
3:L:21:ILE:HD12	3:L:21:ILE:N	2.05	0.71
1:A:352:ILE:HG22	1:A:352:ILE:O	1.91	0.71
1:A:343:GLU:C	1:A:345:ARG:N	2.43	0.71
1:A:375:ASP:OD2	1:A:375:ASP:N	2.24	0.71
2:H:184:VAL:HG22	2:H:186:VAL:CG2	2.20	0.70
3:L:18:ARG:N	3:L:18:ARG:HD3	2.04	0.70
3:L:31:ARG:HG2	3:L:32:TYR:HD1	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:PRO:HG3	3:L:122:PHE:HZ	1.47	0.70
2:H:4:LEU:HD13	2:H:22:CYS:SG	2.31	0.70
3:L:108:LEU:HD12	3:L:109:GLU:N	2.07	0.70
1:A:301:MET:CA	1:A:334:LYS:HB3	2.15	0.70
2:H:38:LYS:HG3	2:H:94:TYR:HE2	1.56	0.69
1:A:323:ARG:HD3	1:A:366:ASN:HD21	1.56	0.69
1:A:341:ASP:HB3	1:A:345:ARG:HD2	1.74	0.69
3:L:69:SER:HB3	3:L:76:THR:O	1.93	0.69
2:H:98:ARG:NH2	2:H:105:TYR:CD2	2.61	0.69
3:L:183:LEU:HD11	3:L:185:LEU:HD21	1.75	0.69
2:H:170:PRO:HD2	3:L:166:SER:OG	1.91	0.69
2:H:119:THR:HG22	2:H:150:PRO:HG3	1.73	0.69
3:L:68:GLY:O	3:L:69:SER:HB2	1.92	0.69
2:H:196:ILE:CG2	2:H:197:THR:H	2.00	0.69
1:A:320:ILE:HG13	1:A:320:ILE:O	1.93	0.69
2:H:139:VAL:N	2:H:187:THR:HG23	2.08	0.68
2:H:139:VAL:CG1	2:H:140:THR:N	2.56	0.68
2:H:68:ALA:CB	2:H:81:LEU:HD11	2.18	0.68
2:H:183:SER:HB2	3:L:139:PHE:HE1	1.57	0.68
3:L:121:ILE:HG22	3:L:122:PHE:N	2.09	0.67
1:A:335:ILE:HG22	1:A:337:PHE:HB2	1.76	0.67
2:H:39:GLN:HE22	3:L:42:GLN:NE2	1.91	0.67
1:A:305:LYS:HD3	1:A:385:GLY:HA3	1.76	0.67
3:L:46:GLN:HB3	3:L:47:PRO:HD2	1.77	0.67
2:H:172:VAL:C	2:H:173:LEU:HD23	2.15	0.67
3:L:62:ILE:HG23	3:L:62:ILE:O	1.94	0.67
1:A:352:ILE:CD1	1:A:370:GLU:HB2	2.18	0.67
1:A:357:ILE:HD13	1:A:357:ILE:H	1.60	0.66
2:H:55:ASN:O	2:H:57:TYR:N	2.28	0.66
1:A:307:LYS:HB2	3:L:54:ARG:HH22	1.60	0.66
3:L:110:ILE:HD11	3:L:175:SER:OG	1.96	0.66
3:L:57:SER:O	3:L:58:LEU:HD22	1.95	0.66
3:L:134:ALA:HB1	3:L:185:LEU:N	2.00	0.66
2:H:28:ASN:HD21	2:H:30:LYS:HB2	1.56	0.66
1:A:366:ASN:O	1:A:367:ILE:HD12	1.96	0.66
3:L:142:ASN:C	3:L:143:PHE:HD1	1.99	0.66
1:A:335:ILE:CG2	1:A:337:PHE:HB2	2.26	0.66
1:A:317:HIS:CD2	1:A:317:HIS:C	2.69	0.66
3:L:57:SER:C	3:L:58:LEU:HD22	2.16	0.66
3:L:21:ILE:O	3:L:77:LEU:N	2.24	0.65
2:H:55:ASN:HD21	2:H:57:TYR:HB2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HG11	2:H:98:ARG:NH2	2.07	0.65
3:L:42:GLN:O	3:L:88:ALA:HB1	1.96	0.65
3:L:93:GLN:HG2	3:L:94:GLN:N	2.06	0.65
3:L:31:ARG:HG2	3:L:32:TYR:CD1	2.32	0.65
2:H:158:ASN:HB2	2:H:162:LEU:HB2	1.78	0.65
2:H:127:LEU:HD23	3:L:125:SER:H	1.60	0.65
2:H:2:VAL:HG21	2:H:98:ARG:NH1	2.10	0.65
3:L:96:ASN:C	3:L:96:ASN:ND2	2.46	0.65
2:H:186:VAL:O	2:H:188:SER:N	2.30	0.65
2:H:40:ARG:HB3	2:H:41:PRO:CD	2.26	0.65
2:H:195:THR:HG22	2:H:212:LYS:NZ	2.11	0.65
2:H:81:LEU:CD1	2:H:82:GLN:H	2.00	0.65
2:H:150:PRO:HG3	2:H:204:ALA:CB	2.27	0.64
2:H:195:THR:HG22	2:H:212:LYS:HZ2	1.62	0.64
2:H:127:LEU:HD22	3:L:123:PRO:O	1.98	0.64
3:L:84:ALA:HB1	3:L:172:SER:C	2.17	0.64
3:L:62:ILE:CG2	3:L:62:ILE:O	2.45	0.64
3:L:43:LYS:NZ	3:L:85:ASP:OD1	2.28	0.64
3:L:80:ASN:CB	3:L:81:PRO:CD	2.75	0.64
2:H:149:PHE:O	2:H:150:PRO:C	2.35	0.64
2:H:139:VAL:HG12	2:H:140:THR:N	2.13	0.64
3:L:50:LEU:HD12	3:L:51:LEU:N	2.12	0.64
1:A:379:ILE:HG22	1:A:380:ILE:N	2.12	0.64
1:A:358:VAL:HG13	1:A:365:VAL:CG2	2.27	0.64
2:H:38:LYS:HG3	2:H:94:TYR:CE2	2.31	0.64
1:A:303:THR:O	1:A:303:THR:HG23	1.97	0.64
1:A:326:TYR:CZ	1:A:328:GLY:HA3	2.34	0.63
2:H:202:HIS:CE1	2:H:204:ALA:HB3	2.33	0.63
3:L:163:VAL:O	3:L:164:LEU:CD2	2.44	0.63
2:H:59:LYS:HD2	3:L:98:ASP:HB3	1.81	0.63
3:L:38:HIS:CE1	3:L:95:THR:OG1	2.52	0.63
3:L:51:LEU:HG	3:L:62:ILE:HD12	1.79	0.63
2:H:44:GLY:C	2:H:45:LEU:HD12	2.18	0.63
1:A:307:LYS:HD2	2:H:101:GLU:HB2	1.80	0.63
2:H:127:LEU:HD23	3:L:125:SER:CB	2.22	0.63
2:H:72:ALA:HB2	2:H:79:ALA:HA	1.81	0.62
2:H:51:ILE:HG13	2:H:58:SER:HB3	1.81	0.62
2:H:118:LYS:HD3	2:H:119:THR:H	1.63	0.62
3:L:161:ASN:O	3:L:183:LEU:CD1	2.48	0.62
1:A:340:MET:CE	1:A:344:LYS:HE3	2.29	0.62
3:L:117:PRO:HA	3:L:142:ASN:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:HIS:O	2:H:96:CYS:HA	1.99	0.62
3:L:120:SER:HB2	3:L:139:PHE:O	2.00	0.62
3:L:124:PRO:CB	3:L:135:SER:OG	2.48	0.62
1:A:376:SER:O	1:A:377:TYR:HD2	1.83	0.62
2:H:184:VAL:O	2:H:186:VAL:HG23	1.98	0.61
3:L:2:ILE:CG2	3:L:3:VAL:N	2.63	0.61
3:L:142:ASN:OD1	3:L:143:PHE:N	2.33	0.61
3:L:84:ALA:CB	3:L:172:SER:O	2.45	0.61
3:L:19:ALA:O	3:L:78:THR:HG23	2.00	0.61
2:H:139:VAL:CA	2:H:187:THR:HA	2.30	0.61
2:H:150:PRO:CG	2:H:204:ALA:HB3	2.31	0.61
2:H:2:VAL:CG2	2:H:98:ARG:NH1	2.56	0.61
2:H:186:VAL:C	2:H:188:SER:N	2.49	0.61
1:A:334:LYS:HD2	1:A:335:ILE:H	1.64	0.61
3:L:120:SER:HB2	3:L:139:PHE:HB2	1.82	0.61
2:H:99:ASP:HB2	2:H:102:GLY:O	2.01	0.61
2:H:65:GLN:HG2	2:H:66:GLY:N	2.15	0.61
3:L:120:SER:HB2	3:L:139:PHE:CB	2.29	0.61
2:H:2:VAL:O	2:H:3:GLN:OE1	2.19	0.60
3:L:163:VAL:C	3:L:164:LEU:HD23	2.21	0.60
2:H:154:THR:HB	2:H:201:ALA:HB3	1.83	0.60
2:H:98:ARG:HG3	2:H:99:ASP:OD1	2.01	0.60
1:A:344:LYS:HG2	1:A:344:LYS:O	2.01	0.60
3:L:154:ILE:HD12	3:L:196:TYR:HE2	1.65	0.60
3:L:6:GLN:HE22	3:L:91:TYR:HA	1.65	0.60
1:A:373:PHE:CB	1:A:393:LYS:HD3	2.26	0.60
2:H:172:VAL:HG12	2:H:179:THR:HB	1.83	0.60
2:H:87:THR:O	2:H:114:VAL:HG21	2.02	0.60
3:L:12:ALA:HB2	3:L:109:GLU:HB3	1.82	0.60
2:H:184:VAL:HG13	2:H:184:VAL:O	2.02	0.60
2:H:32:THR:OG1	2:H:33:TYR:N	2.35	0.59
3:L:152:TRP:CE3	3:L:152:TRP:HA	2.36	0.59
3:L:146:LYS:HG3	3:L:177:TYR:CE1	2.37	0.59
3:L:14:SER:OG	3:L:17:GLN:CG	2.49	0.59
2:H:18:VAL:O	2:H:82:GLN:HG3	2.01	0.59
3:L:136:VAL:HG12	3:L:152:TRP:CZ2	2.37	0.59
1:A:300:SER:O	1:A:334:LYS:N	2.35	0.59
1:A:379:ILE:CG2	1:A:380:ILE:N	2.65	0.59
3:L:112:ARG:HD3	3:L:175:SER:HB3	1.85	0.59
2:H:72:ALA:CB	2:H:79:ALA:HA	2.32	0.59
1:A:307:LYS:HE3	2:H:100:TYR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ILE:O	1:A:387:LEU:HB2	2.01	0.59
2:H:150:PRO:CG	2:H:204:ALA:CB	2.80	0.59
1:A:383:GLU:O	1:A:384:PRO:C	2.38	0.59
1:A:357:ILE:HD13	1:A:357:ILE:N	2.18	0.59
3:L:51:LEU:O	3:L:52:ILE:HG12	2.03	0.59
2:H:191:TRP:HB3	2:H:192:PRO:CD	2.26	0.59
3:L:62:ILE:O	3:L:63:PRO:C	2.41	0.58
1:A:305:LYS:NZ	1:A:385:GLY:CA	2.65	0.58
2:H:37:VAL:HG12	2:H:38:LYS:H	1.66	0.58
3:L:121:ILE:O	3:L:122:PHE:CG	2.55	0.58
1:A:305:LYS:CD	1:A:385:GLY:HA3	2.32	0.58
1:A:332:PRO:HA	1:A:358:VAL:O	2.03	0.58
1:A:319:THR:HG21	1:A:368:GLU:OE2	2.04	0.58
2:H:60:TYR:HE2	2:H:70:ILE:HG13	1.67	0.58
2:H:29:ILE:HG12	2:H:53:PRO:HG2	1.84	0.58
1:A:342:LEU:HD22	1:A:377:TYR:CE2	2.38	0.58
3:L:166:SER:HB3	3:L:180:SER:O	2.04	0.58
2:H:100:TYR:O	2:H:101:GLU:HB2	2.04	0.58
3:L:14:SER:HA	3:L:111:LYS:HB2	1.85	0.58
2:H:50:ARG:NE	3:L:100:TRP:CZ3	2.71	0.58
2:H:139:VAL:CG1	2:H:141:LEU:CD2	2.82	0.58
2:H:180:LEU:HD23	2:H:181:SER:N	2.18	0.58
2:H:81:LEU:CD1	2:H:82:GLN:N	2.65	0.58
3:L:121:ILE:O	3:L:122:PHE:CB	2.52	0.57
1:A:323:ARG:CD	1:A:366:ASN:HD21	2.17	0.57
1:A:309:VAL:CA	2:H:100:TYR:HB3	2.32	0.57
2:H:14:PRO:HG3	2:H:114:VAL:HG12	1.85	0.57
3:L:161:ASN:O	3:L:183:LEU:HD13	2.03	0.57
3:L:77:LEU:CD1	3:L:78:THR:N	2.60	0.57
3:L:77:LEU:CG	3:L:78:THR:N	2.68	0.57
1:A:321:VAL:HG13	1:A:368:GLU:HB2	1.87	0.57
2:H:40:ARG:NH2	2:H:43:GLN:HG2	2.18	0.57
3:L:3:VAL:HG23	3:L:26:SER:HB3	1.87	0.57
2:H:37:VAL:CG1	2:H:38:LYS:N	2.66	0.57
2:H:186:VAL:HG12	2:H:188:SER:CB	2.35	0.56
3:L:146:LYS:HG3	3:L:177:TYR:HE1	1.70	0.56
2:H:40:ARG:CB	2:H:41:PRO:HD2	2.29	0.56
1:A:342:LEU:CD2	1:A:342:LEU:N	2.64	0.56
2:H:6:GLN:HA	2:H:21:SER:O	2.04	0.56
1:A:322:ILE:HG22	1:A:323:ARG:N	2.21	0.56
1:A:366:ASN:C	1:A:367:ILE:HD12	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:163:VAL:HG12	3:L:163:VAL:O	2.04	0.56
3:L:97:VAL:HG12	3:L:99:PRO:CD	2.32	0.56
2:H:36:TRP:HA	2:H:95:PHE:O	2.05	0.56
1:A:335:ILE:C	1:A:337:PHE:N	2.58	0.56
2:H:50:ARG:NE	3:L:100:TRP:HZ3	2.04	0.56
2:H:169:PHE:CE2	3:L:168:THR:OG1	2.58	0.56
2:H:30:LYS:HA	2:H:53:PRO:HB2	1.87	0.56
2:H:173:LEU:N	2:H:173:LEU:HD23	2.21	0.56
1:A:335:ILE:C	1:A:337:PHE:H	2.06	0.56
2:H:4:LEU:HD23	2:H:24:ALA:HA	1.88	0.56
2:H:139:VAL:N	2:H:187:THR:HA	2.20	0.56
2:H:202:HIS:CE1	2:H:205:SER:N	2.73	0.56
2:H:45:LEU:HD13	3:L:91:TYR:CE2	2.41	0.56
2:H:115:SER:OG	2:H:116:SER:N	2.39	0.56
2:H:98:ARG:HH22	2:H:105:TYR:HD2	1.54	0.56
3:L:6:GLN:NE2	3:L:92:CYS:N	2.53	0.56
3:L:5:THR:N	3:L:24:ARG:O	2.39	0.56
3:L:154:ILE:CD1	3:L:196:TYR:CE2	2.89	0.55
1:A:301:MET:HA	1:A:334:LYS:CB	2.18	0.55
2:H:34:MET:HA	2:H:97:ALA:O	2.06	0.55
1:A:323:ARG:HD3	1:A:366:ASN:ND2	2.20	0.55
2:H:2:VAL:CG2	2:H:27:PHE:HD2	2.19	0.55
2:H:65:GLN:O	2:H:67:LYS:N	2.40	0.55
2:H:157:TRP:CZ3	2:H:198:CYS:SG	3.00	0.55
3:L:5:THR:OG1	3:L:24:ARG:HB2	2.07	0.55
2:H:59:LYS:CD	3:L:98:ASP:HB3	2.36	0.55
1:A:358:VAL:HG13	1:A:365:VAL:HG22	1.88	0.55
2:H:40:ARG:HG2	2:H:92:ALA:HB2	1.89	0.55
3:L:71:SER:CA	3:L:75:PHE:HE2	2.06	0.54
2:H:127:LEU:CD2	3:L:125:SER:N	2.58	0.54
2:H:139:VAL:HB	2:H:186:VAL:O	2.08	0.54
2:H:3:GLN:O	2:H:5:GLN:HG3	2.08	0.54
2:H:144:LEU:C	2:H:144:LEU:HD23	2.27	0.54
3:L:39:TRP:O	3:L:50:LEU:HD12	2.08	0.54
2:H:68:ALA:HA	2:H:82:GLN:O	2.08	0.54
1:A:353:THR:HG22	1:A:356:PRO:HD3	1.89	0.54
2:H:173:LEU:HD22	2:H:178:TYR:HE1	1.65	0.54
1:A:381:GLY:C	1:A:382:VAL:O	2.37	0.54
2:H:67:LYS:HB3	2:H:83:LEU:HD23	1.90	0.54
2:H:40:ARG:HH21	2:H:43:GLN:CG	2.19	0.54
3:L:151:LYS:O	3:L:199:GLU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:VAL:HG12	3:L:73:THR:OG1	2.08	0.54
3:L:6:GLN:NE2	3:L:92:CYS:H	2.05	0.54
2:H:169:PHE:HB3	3:L:166:SER:OG	2.07	0.54
1:A:337:PHE:CE1	1:A:367:ILE:HG21	2.42	0.54
3:L:50:LEU:O	3:L:51:LEU:HD22	2.07	0.54
2:H:209:VAL:CG2	2:H:210:ASP:N	2.70	0.54
2:H:36:TRP:HE3	2:H:95:PHE:O	1.90	0.54
1:A:379:ILE:C	1:A:380:ILE:HG13	2.28	0.53
3:L:118:THR:CG2	3:L:119:VAL:N	2.61	0.53
2:H:155:LEU:O	2:H:155:LEU:HD23	2.09	0.53
1:A:317:HIS:CD2	1:A:319:THR:HG22	2.42	0.53
3:L:31:ARG:HB3	3:L:36:PHE:CE1	2.43	0.53
2:H:209:VAL:CG2	2:H:210:ASP:H	2.18	0.53
2:H:150:PRO:HG3	2:H:204:ALA:HB3	1.91	0.53
3:L:6:GLN:NE2	3:L:105:GLY:HA2	2.24	0.53
1:A:335:ILE:CD1	1:A:367:ILE:HD11	2.39	0.53
3:L:35:SER:O	3:L:54:ARG:HA	2.09	0.53
3:L:182:THR:OG1	3:L:183:LEU:N	2.36	0.53
1:A:354:VAL:CG2	1:A:355:ASN:H	1.96	0.53
1:A:380:ILE:O	1:A:387:LEU:HD23	2.09	0.53
2:H:180:LEU:C	2:H:180:LEU:HD23	2.30	0.53
1:A:307:LYS:CB	3:L:54:ARG:HH22	2.21	0.53
1:A:376:SER:C	1:A:377:TYR:HD2	2.12	0.53
1:A:334:LYS:HG3	1:A:335:ILE:N	2.23	0.52
3:L:22:SER:CA	3:L:76:THR:HA	2.36	0.52
2:H:37:VAL:HG21	2:H:106:TRP:HZ3	1.74	0.52
3:L:154:ILE:CG2	3:L:154:ILE:O	2.56	0.52
2:H:39:GLN:NE2	3:L:42:GLN:HE22	2.07	0.52
3:L:124:PRO:HB3	3:L:135:SER:OG	2.08	0.52
2:H:126:PRO:O	3:L:125:SER:CB	2.57	0.52
3:L:95:THR:C	3:L:100:TRP:HE1	2.12	0.52
3:L:113:ALA:O	3:L:114:ASP:C	2.48	0.52
2:H:50:ARG:HD3	3:L:100:TRP:CZ3	2.38	0.52
2:H:47:TRP:CG	3:L:100:TRP:O	2.63	0.52
2:H:83:LEU:CB	2:H:86:LEU:HD21	2.39	0.52
2:H:144:LEU:HD23	2:H:145:VAL:N	2.25	0.52
3:L:187:LYS:HG2	3:L:187:LYS:O	2.10	0.52
2:H:20:LEU:CD1	2:H:21:SER:H	2.23	0.52
3:L:132:GLY:HA2	3:L:187:LYS:HB2	1.92	0.52
3:L:51:LEU:O	3:L:52:ILE:HD13	2.10	0.52
3:L:97:VAL:O	3:L:100:TRP:CD1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:102:GLY:N	3:L:38:HIS:NE2	2.57	0.51
3:L:9:ALA:O	3:L:10:SER:HB3	2.10	0.51
3:L:51:LEU:O	3:L:52:ILE:CG1	2.59	0.51
2:H:68:ALA:HB2	2:H:83:LEU:CD2	2.40	0.51
1:A:340:MET:SD	1:A:344:LYS:CG	2.96	0.51
3:L:154:ILE:HG22	3:L:154:ILE:O	2.08	0.51
2:H:39:GLN:HE22	3:L:42:GLN:CD	2.14	0.51
2:H:100:TYR:O	2:H:101:GLU:CB	2.59	0.51
2:H:27:PHE:HE2	2:H:98:ARG:NH1	1.98	0.51
3:L:124:PRO:O	3:L:125:SER:C	2.47	0.51
1:A:378:ILE:CG2	1:A:379:ILE:N	2.72	0.51
3:L:37:MET:HE1	3:L:93:GLN:O	2.11	0.51
2:H:129:PRO:CG	2:H:130:GLY:N	2.55	0.51
1:A:334:LYS:HE3	1:A:335:ILE:O	2.11	0.51
1:A:339:ILE:C	1:A:340:MET:HG2	2.30	0.51
3:L:153:LYS:CA	3:L:158:GLU:CG	2.83	0.51
3:L:151:LYS:N	3:L:199:GLU:O	2.26	0.51
2:H:172:VAL:HB	2:H:179:THR:O	2.11	0.51
2:H:150:PRO:HG3	2:H:204:ALA:HB1	1.93	0.51
1:A:321:VAL:HG12	1:A:367:ILE:O	2.11	0.51
2:H:33:TYR:O	2:H:98:ARG:HA	2.11	0.51
1:A:308:VAL:O	2:H:101:GLU:HG3	2.11	0.50
3:L:29:VAL:HG21	3:L:94:GLN:CD	2.31	0.50
1:A:345:ARG:O	1:A:346:HIS:C	2.48	0.50
3:L:154:ILE:HD13	3:L:159:ARG:CG	2.41	0.50
3:L:8:PRO:C	3:L:10:SER:H	2.14	0.50
3:L:37:MET:CE	3:L:93:GLN:O	2.59	0.50
2:H:118:LYS:HD3	2:H:119:THR:HG23	1.93	0.50
2:H:44:GLY:HA2	3:L:91:TYR:OH	2.10	0.50
2:H:4:LEU:HD21	2:H:27:PHE:CZ	2.40	0.50
3:L:142:ASN:C	3:L:143:PHE:CD1	2.82	0.50
2:H:127:LEU:HD22	3:L:125:SER:H	1.69	0.50
1:A:317:HIS:HD2	1:A:317:HIS:C	2.12	0.50
2:H:212:LYS:HG3	2:H:213:ILE:N	2.27	0.50
2:H:127:LEU:H	2:H:143:CYS:HA	1.77	0.50
3:L:2:ILE:HG23	3:L:3:VAL:N	2.25	0.50
2:H:40:ARG:HG2	2:H:92:ALA:HB3	1.92	0.50
1:A:344:LYS:O	1:A:344:LYS:CG	2.60	0.50
3:L:18:ARG:O	3:L:18:ARG:HG2	2.10	0.50
3:L:38:HIS:HB2	3:L:93:GLN:HB3	1.94	0.49
3:L:93:GLN:CG	3:L:94:GLN:H	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:76:THR:CG2	3:L:76:THR:O	2.58	0.49
2:H:6:GLN:OE1	2:H:95:PHE:HA	2.11	0.49
2:H:201:ALA:O	2:H:203:PRO:HD3	2.12	0.49
3:L:39:TRP:CD2	3:L:77:LEU:HD22	2.47	0.49
2:H:169:PHE:CD2	3:L:168:THR:OG1	2.66	0.49
2:H:212:LYS:O	2:H:213:ILE:HG12	2.12	0.49
3:L:41:GLN:HG3	3:L:90:TYR:HE1	1.77	0.49
3:L:142:ASN:C	3:L:142:ASN:OD1	2.51	0.49
1:A:316:GLN:C	1:A:318:GLY:N	2.66	0.49
2:H:139:VAL:HB	2:H:187:THR:C	2.32	0.49
2:H:11:LEU:HD11	2:H:115:SER:HB3	1.95	0.49
2:H:2:VAL:HG22	2:H:98:ARG:NH1	2.21	0.49
1:A:353:THR:O	1:A:354:VAL:C	2.50	0.49
3:L:155:ASP:HB2	3:L:195:SER:OG	2.13	0.49
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.48	0.49
3:L:2:ILE:HG23	3:L:3:VAL:H	1.78	0.49
2:H:157:TRP:CZ2	2:H:184:VAL:HG12	2.47	0.49
3:L:166:SER:HB3	3:L:180:SER:HB3	1.94	0.49
2:H:126:PRO:HA	2:H:143:CYS:HB2	1.95	0.48
3:L:112:ARG:O	3:L:144:TYR:CD2	2.66	0.48
1:A:386:GLN:H	1:A:386:GLN:CD	2.17	0.48
3:L:2:ILE:O	3:L:3:VAL:HG22	2.14	0.48
2:H:29:ILE:HG12	2:H:53:PRO:CG	2.43	0.48
3:L:154:ILE:HG22	3:L:157:SER:O	2.13	0.48
3:L:21:ILE:N	3:L:21:ILE:CD1	2.74	0.48
3:L:6:GLN:CD	3:L:92:CYS:HB3	2.34	0.48
2:H:37:VAL:CG1	2:H:38:LYS:H	2.26	0.48
1:A:334:LYS:CG	1:A:335:ILE:N	2.76	0.48
3:L:95:THR:C	3:L:100:TRP:NE1	2.67	0.48
2:H:43:GLN:N	2:H:43:GLN:NE2	2.61	0.48
2:H:100:TYR:HD1	2:H:101:GLU:N	2.12	0.48
1:A:344:LYS:O	1:A:345:ARG:C	2.51	0.48
1:A:343:GLU:O	1:A:345:ARG:N	2.42	0.48
3:L:121:ILE:CG2	3:L:122:PHE:N	2.77	0.48
3:L:37:MET:O	3:L:38:HIS:CD2	2.67	0.48
3:L:14:SER:HG	3:L:17:GLN:HG2	1.72	0.48
1:A:307:LYS:HZ1	2:H:99:ASP:HB3	1.79	0.48
3:L:51:LEU:O	3:L:52:ILE:CD1	2.61	0.48
2:H:166:VAL:HG12	2:H:167:HIS:N	2.29	0.48
1:A:335:ILE:HD11	1:A:365:VAL:HG11	1.95	0.48
2:H:197:THR:HG23	2:H:210:ASP:CG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:23:CYS:O	3:L:24:ARG:HG2	2.13	0.48
3:L:8:PRO:O	3:L:10:SER:N	2.47	0.47
1:A:341:ASP:CB	1:A:345:ARG:HD2	2.44	0.47
2:H:157:TRP:CH2	2:H:198:CYS:SG	3.06	0.47
2:H:103:PHE:CD2	2:H:103:PHE:N	2.82	0.47
2:H:139:VAL:C	2:H:140:THR:HG23	2.33	0.47
1:A:316:GLN:C	1:A:318:GLY:H	2.16	0.47
2:H:65:GLN:O	2:H:66:GLY:C	2.51	0.47
2:H:28:ASN:HD21	2:H:30:LYS:HD2	1.79	0.47
3:L:51:LEU:C	3:L:52:ILE:HG12	2.35	0.47
2:H:36:TRP:CE3	2:H:95:PHE:O	2.67	0.47
3:L:31:ARG:HB3	3:L:36:PHE:HE1	1.78	0.47
2:H:39:GLN:NE2	3:L:42:GLN:NE2	2.58	0.47
2:H:12:VAL:HG11	2:H:17:SER:O	2.15	0.47
1:A:353:THR:O	1:A:354:VAL:O	2.32	0.47
1:A:373:PHE:HB3	1:A:393:LYS:CE	2.45	0.47
3:L:71:SER:C	3:L:72:ARG:O	2.49	0.47
2:H:28:ASN:O	2:H:30:LYS:N	2.48	0.47
3:L:194:ASN:CG	3:L:195:SER:N	2.69	0.47
2:H:60:TYR:CE2	2:H:70:ILE:HG13	2.50	0.46
2:H:78:ALA:O	2:H:80:TYR:CE1	2.68	0.46
2:H:36:TRP:CE3	2:H:36:TRP:HA	2.50	0.46
2:H:80:TYR:N	2:H:80:TYR:CD1	2.82	0.46
2:H:27:PHE:HD2	2:H:98:ARG:NH1	2.12	0.46
1:A:340:MET:HE2	1:A:344:LYS:HE3	1.97	0.46
3:L:7:SER:HB3	3:L:8:PRO:CD	2.46	0.46
3:L:1:ASP:O	3:L:2:ILE:HG12	2.16	0.46
2:H:141:LEU:N	2:H:141:LEU:HD23	2.30	0.46
2:H:4:LEU:CD2	2:H:24:ALA:HB2	2.46	0.46
3:L:22:SER:HB2	3:L:75:PHE:O	2.16	0.46
3:L:153:LYS:CB	3:L:158:GLU:HG3	2.46	0.46
3:L:4:LEU:CA	3:L:24:ARG:O	2.63	0.46
3:L:122:PHE:HA	3:L:123:PRO:HD2	1.44	0.46
3:L:77:LEU:HG	3:L:78:THR:N	2.31	0.46
3:L:143:PHE:CD1	3:L:143:PHE:N	2.84	0.46
3:L:8:PRO:C	3:L:10:SER:N	2.68	0.46
3:L:116:ALA:HA	3:L:117:PRO:HD2	1.70	0.46
2:H:157:TRP:CE2	2:H:184:VAL:HG12	2.51	0.46
1:A:339:ILE:CG2	1:A:377:TYR:O	2.64	0.46
1:A:339:ILE:HG23	1:A:378:ILE:HD13	1.98	0.46
3:L:43:LYS:NZ	3:L:85:ASP:O	2.46	0.45

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:94:GLN:HG2	3:L:94:GLN:O	2.16	0.45
3:L:154:ILE:CG2	3:L:157:SER:O	2.64	0.45
3:L:53:TYR:C	3:L:54:ARG:HG3	2.35	0.45
2:H:67:LYS:HZ3	2:H:86:LEU:HA	1.82	0.45
2:H:28:ASN:O	2:H:29:ILE:C	2.54	0.45
3:L:172:SER:O	3:L:173:LYS:C	2.54	0.45
2:H:124:VAL:HG11	2:H:209:VAL:HG11	1.97	0.45
3:L:152:TRP:O	3:L:158:GLU:HB3	2.16	0.45
3:L:4:LEU:HD11	3:L:102:PHE:O	2.16	0.45
2:H:27:PHE:CE2	2:H:98:ARG:HD3	2.52	0.45
2:H:20:LEU:HD13	2:H:21:SER:H	1.80	0.45
3:L:31:ARG:O	3:L:34:ASN:O	2.34	0.45
2:H:39:GLN:CD	3:L:42:GLN:HE22	2.20	0.45
3:L:140:LEU:N	3:L:140:LEU:HD12	2.32	0.45
3:L:79:ILE:HG22	3:L:79:ILE:O	2.17	0.45
3:L:110:ILE:HD13	3:L:110:ILE:HG21	1.59	0.45
1:A:307:LYS:NZ	2:H:101:GLU:O	2.44	0.45
2:H:187:THR:O	2:H:187:THR:HG22	2.16	0.45
3:L:154:ILE:HD13	3:L:159:ARG:HG2	1.99	0.45
2:H:139:VAL:O	2:H:140:THR:CG2	2.65	0.45
3:L:7:SER:O	3:L:9:ALA:N	2.49	0.45
2:H:67:LYS:NZ	2:H:86:LEU:HA	2.31	0.44
3:L:127:GLU:HB3	3:L:130:THR:OG1	2.17	0.44
2:H:139:VAL:CG1	2:H:141:LEU:HD23	2.47	0.44
1:A:353:THR:CG2	1:A:356:PRO:HD3	2.48	0.44
3:L:115:ALA:HB3	3:L:144:TYR:N	2.33	0.44
1:A:322:ILE:O	1:A:323:ARG:HG2	2.18	0.44
1:A:334:LYS:CD	1:A:335:ILE:H	2.30	0.44
3:L:148:ILE:HG23	3:L:149:ASN:HB2	1.98	0.44
3:L:29:VAL:HG21	3:L:94:GLN:CG	2.48	0.44
3:L:150:VAL:CG2	3:L:199:GLU:O	2.65	0.44
2:H:91:THR:O	2:H:92:ALA:HB2	2.18	0.44
2:H:106:TRP:CD1	2:H:106:TRP:N	2.85	0.44
2:H:84:SER:O	2:H:85:SER:C	2.56	0.44
2:H:152:PRO:O	2:H:153:VAL:HG13	2.18	0.44
1:A:345:ARG:O	1:A:346:HIS:O	2.36	0.44
2:H:77:ASN:HB3	2:H:78:ALA:H	1.55	0.44
3:L:68:GLY:O	3:L:69:SER:CB	2.63	0.44
1:A:308:VAL:CG2	1:A:310:LYS:O	2.66	0.43
2:H:81:LEU:CG	2:H:82:GLN:N	2.81	0.43
2:H:45:LEU:HD13	3:L:91:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASP:N	1:A:362:ASP:OD1	2.38	0.43
3:L:164:LEU:O	3:L:181:SER:OG	2.22	0.43
3:L:84:ALA:C	3:L:172:SER:HB2	2.39	0.43
3:L:84:ALA:O	3:L:172:SER:HB2	2.18	0.43
1:A:352:ILE:CG2	1:A:352:ILE:O	2.62	0.43
3:L:89:THR:HG1	3:L:91:TYR:HE1	1.63	0.43
2:H:37:VAL:HG21	2:H:106:TRP:CZ3	2.52	0.43
3:L:115:ALA:H	3:L:144:TYR:HB3	1.83	0.43
2:H:174:GLN:O	2:H:177:LEU:O	2.36	0.43
1:A:337:PHE:C	1:A:337:PHE:CD2	2.91	0.43
1:A:357:ILE:HG12	1:A:358:VAL:N	2.33	0.43
3:L:51:LEU:HA	3:L:51:LEU:HD13	1.77	0.43
1:A:376:SER:C	1:A:377:TYR:CD2	2.92	0.43
2:H:72:ALA:HB2	2:H:79:ALA:CB	2.49	0.43
2:H:153:VAL:HG23	2:H:153:VAL:O	2.18	0.43
1:A:314:GLU:O	1:A:315:THR:C	2.54	0.43
3:L:120:SER:HB2	3:L:139:PHE:C	2.38	0.43
2:H:47:TRP:CB	3:L:100:TRP:O	2.66	0.43
3:L:3:VAL:O	3:L:25:ALA:HA	2.18	0.43
3:L:3:VAL:CG2	3:L:26:SER:HB3	2.47	0.43
3:L:153:LYS:NZ	3:L:199:GLU:OE1	2.50	0.43
3:L:31:ARG:CG	3:L:32:TYR:CD1	3.00	0.43
3:L:127:GLU:HA	3:L:127:GLU:OE1	2.18	0.43
3:L:95:THR:O	3:L:95:THR:HG22	2.18	0.43
2:H:68:ALA:HB2	2:H:83:LEU:HD23	1.99	0.43
1:A:355:ASN:CG	1:A:355:ASN:O	2.57	0.43
1:A:339:ILE:HG22	1:A:340:MET:N	2.34	0.43
2:H:45:LEU:N	2:H:45:LEU:HD12	2.33	0.43
3:L:51:LEU:CG	3:L:62:ILE:HD12	2.48	0.43
1:A:353:THR:CG2	1:A:356:PRO:HB3	2.36	0.43
3:L:52:ILE:HG23	3:L:57:SER:OG	2.19	0.43
3:L:183:LEU:CG	3:L:185:LEU:HD21	2.48	0.43
2:H:40:ARG:O	2:H:41:PRO:C	2.57	0.43
1:A:308:VAL:HG12	2:H:101:GLU:OE2	2.19	0.43
2:H:72:ALA:HB2	2:H:79:ALA:CA	2.49	0.43
1:A:379:ILE:C	1:A:380:ILE:CG1	2.88	0.43
3:L:29:VAL:HG21	3:L:94:GLN:HG3	2.00	0.42
3:L:12:ALA:HA	3:L:109:GLU:O	2.19	0.42
2:H:60:TYR:HE2	2:H:70:ILE:H	1.65	0.42
3:L:95:THR:HA	3:L:100:TRP:NE1	2.34	0.42
3:L:154:ILE:CD1	3:L:196:TYR:HE2	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:LYS:HA	2:H:81:LEU:O	2.19	0.42
3:L:6:GLN:HE22	3:L:92:CYS:H	1.66	0.42
2:H:169:PHE:HB3	2:H:170:PRO:HD2	2.01	0.42
2:H:195:THR:CG2	2:H:212:LYS:NZ	2.82	0.42
2:H:50:ARG:O	2:H:58:SER:HB2	2.19	0.42
3:L:13:VAL:CG1	3:L:17:GLN:HB2	2.50	0.42
3:L:89:THR:O	3:L:91:TYR:CD1	2.72	0.42
3:L:127:GLU:C	3:L:129:LEU:N	2.72	0.42
3:L:12:ALA:CB	3:L:109:GLU:HB3	2.49	0.42
2:H:2:VAL:HG21	2:H:27:PHE:HD2	1.83	0.42
2:H:70:ILE:HG22	2:H:71:THR:N	2.34	0.42
2:H:124:VAL:HG13	2:H:124:VAL:O	2.20	0.42
2:H:197:THR:CG2	2:H:198:CYS:N	2.82	0.42
1:A:341:ASP:OD1	1:A:348:LEU:HB3	2.20	0.42
1:A:331:SER:O	1:A:359:THR:O	2.37	0.42
1:A:317:HIS:NE2	1:A:319:THR:CG2	2.82	0.42
2:H:118:LYS:CD	2:H:119:THR:H	2.31	0.42
1:A:357:ILE:CD1	1:A:357:ILE:N	2.82	0.42
3:L:29:VAL:HG22	3:L:96:ASN:HB3	2.01	0.42
2:H:183:SER:CB	3:L:139:PHE:CE1	2.78	0.42
2:H:51:ILE:CD1	2:H:71:THR:HA	2.49	0.42
1:A:335:ILE:HG22	1:A:337:PHE:N	2.35	0.42
2:H:4:LEU:HA	2:H:24:ALA:HA	2.01	0.42
2:H:27:PHE:CD1	2:H:27:PHE:C	2.93	0.42
3:L:20:THR:C	3:L:21:ILE:HD12	2.38	0.42
3:L:52:ILE:HG22	3:L:53:TYR:N	2.34	0.42
2:H:139:VAL:CG1	2:H:140:THR:H	2.33	0.42
1:A:340:MET:O	1:A:377:TYR:HB2	2.20	0.42
3:L:121:ILE:CD1	3:L:207:LYS:HB2	2.50	0.41
3:L:147:ASP:HB3	3:L:148:ILE:H	1.73	0.41
2:H:67:LYS:HZ2	2:H:86:LEU:HD23	1.85	0.41
2:H:212:LYS:C	2:H:213:ILE:CG1	2.89	0.41
3:L:51:LEU:HD11	3:L:62:ILE:HB	2.02	0.41
2:H:65:GLN:C	2:H:67:LYS:N	2.73	0.41
2:H:103:PHE:HD1	2:H:106:TRP:CH2	2.38	0.41
3:L:2:ILE:C	3:L:3:VAL:CG2	2.88	0.41
1:A:341:ASP:HB2	1:A:345:ARG:HB2	1.95	0.41
2:H:139:VAL:CG1	2:H:186:VAL:O	2.68	0.41
2:H:155:LEU:HD12	2:H:200:VAL:HG22	2.02	0.41
3:L:63:PRO:O	3:L:65:ARG:N	2.52	0.41
1:A:364:PRO:HG3	2:H:31:ASP:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:PHE:O	2:H:27:PHE:CD1	2.74	0.41
3:L:145:PRO:O	3:L:147:ASP:N	2.53	0.41
1:A:383:GLU:O	1:A:385:GLY:N	2.53	0.41
3:L:108:LEU:CD1	3:L:109:GLU:H	2.19	0.41
1:A:307:LYS:HD2	2:H:101:GLU:CB	2.50	0.41
2:H:4:LEU:CD2	2:H:27:PHE:HZ	2.30	0.41
1:A:341:ASP:CB	1:A:345:ARG:CB	2.89	0.41
3:L:174:ASP:O	3:L:175:SER:HB3	2.20	0.41
3:L:134:ALA:HB2	3:L:185:LEU:C	2.41	0.41
2:H:139:VAL:HG11	2:H:186:VAL:O	2.21	0.41
3:L:4:LEU:HD12	3:L:4:LEU:H	1.85	0.41
3:L:38:HIS:HE1	3:L:95:THR:OG1	2.03	0.40
1:A:387:LEU:HA	1:A:387:LEU:HD13	1.90	0.40
3:L:154:ILE:HD13	3:L:159:ARG:HG3	2.01	0.40
2:H:28:ASN:HD21	2:H:30:LYS:CB	2.28	0.40
1:A:378:ILE:HG22	1:A:379:ILE:N	2.36	0.40
1:A:305:LYS:HZ2	1:A:385:GLY:CA	2.32	0.40
2:H:9:ALA:O	2:H:10:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/97 (98%)	64 (67%)	23 (24%)	8 (8%)	1	17
2	H	195/214 (91%)	144 (74%)	31 (16%)	20 (10%)	1	12
3	L	200/212 (94%)	133 (66%)	45 (22%)	22 (11%)	0	10
All	All	490/523 (94%)	341 (70%)	99 (20%)	50 (10%)	1	13

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	GLY
1	A	332	PRO
1	A	354	VAL
2	H	8	GLY
2	H	56	GLY
2	H	67	LYS
2	H	129	PRO
2	H	149	PHE
2	H	151	GLU
3	L	26	SER
3	L	29	VAL
3	L	67	SER
3	L	86	ASP
3	L	117	PRO
3	L	148	ILE
3	L	163	VAL
2	H	29	ILE
2	H	41	PRO
2	H	44	GLY
2	H	65	GLN
2	H	101	GLU
2	H	189	SER
3	L	61	GLY
3	L	64	THR
3	L	69	SER
1	A	331	SER
1	A	346	HIS
1	A	371	PRO
2	H	66	GLY
2	H	187	THR
3	L	44	PRO
3	L	76	THR
3	L	80	ASN
3	L	114	ASP
3	L	146	LYS
1	A	342	LEU
2	H	121	PRO
3	L	8	PRO
3	L	132	GLY
2	H	153	VAL
3	L	9	ALA
3	L	10	SER
3	L	73	THR

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Mol	Chain	Res	Type
2	H	152	PRO
2	H	165	GLY
3	L	7	SER
1	A	357	ILE
2	H	160	GLY
3	L	122	PHE
2	H	170	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	87/87 (100%)	72 (83%)	15 (17%)	2	18
2	H	171/181 (94%)	147 (86%)	24 (14%)	4	29
3	L	178/186 (96%)	135 (76%)	43 (24%)	1	7
All	All	436/454 (96%)	354 (81%)	82 (19%)	2	14

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	CYS
1	A	314	GLU
1	A	317	HIS
1	A	321	VAL
1	A	329	ASP
1	A	340	MET
1	A	342	LEU
1	A	345	ARG
1	A	346	HIS
1	A	347	VAL
1	A	357	ILE
1	A	362	ASP
1	A	366	ASN
1	A	372	PRO
1	A	375	ASP

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Mol	Chain	Res	Type
2	H	3	GLN
2	H	4	LEU
2	H	12	VAL
2	H	20	LEU
2	H	36	TRP
2	H	41	PRO
2	H	74	THR
2	H	90	ASP
2	H	96	CYS
2	H	99	ASP
2	H	100	TYR
2	H	116	SER
2	H	122	PRO
2	H	129	PRO
2	H	141	LEU
2	H	151	GLU
2	H	158	ASN
2	H	173	LEU
2	H	174	GLN
2	H	183	SER
2	H	188	SER
2	H	191	TRP
2	H	197	THR
2	H	198	CYS
3	L	1	ASP
3	L	2	ILE
3	L	4	LEU
3	L	18	ARG
3	L	29	VAL
3	L	51	LEU
3	L	54	ARG
3	L	60	SER
3	L	66	PHE
3	L	71	SER
3	L	72	ARG
3	L	77	LEU
3	L	80	ASN
3	L	81	PRO
3	L	82	VAL
3	L	85	ASP
3	L	94	GLN
3	L	96	ASN

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Mol	Chain	Res	Type
3	L	114	ASP
3	L	125	SER
3	L	130	THR
3	L	138	CYS
3	L	143	PHE
3	L	147	ASP
3	L	148	ILE
3	L	149	ASN
3	L	151	LYS
3	L	152	TRP
3	L	154	ILE
3	L	155	ASP
3	L	164	LEU
3	L	165	ASN
3	L	168	THR
3	L	169	ASP
3	L	171	ASP
3	L	172	SER
3	L	176	THR
3	L	179	MET
3	L	182	THR
3	L	194	ASN
3	L	197	THR
3	L	198	CYS
3	L	209	PHE

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

Mol	Chain	Res	Type
1	A	316	GLN
1	A	317	HIS
1	A	325	GLN
1	A	366	ASN
1	A	390	ASN
2	H	28	ASN
2	H	39	GLN
2	H	82	GLN
3	L	6	GLN
3	L	42	GLN
3	L	46	GLN
3	L	194	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 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(Å²)	Q<0.9
1	A	97/97 (100%)	-0.35	0	100	100	20, 20, 20, 20	0
2	H	203/214 (94%)	-0.40	0	100	100	20, 20, 20, 20	0
3	L	204/212 (96%)	-0.28	1 (0%)	91	85	20, 20, 20, 20	0
All	All	504/523 (96%)	-0.34	1 (0%)	95	91	20, 20, 20, 20	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	174	ASP	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.