



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:36 pm GMT

PDB ID : 3I5H
Title : The crystal structure of rigor like squid myosin S1 in the absence of nucleotide
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Cohen, C.
Deposited on : 2009-07-05
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

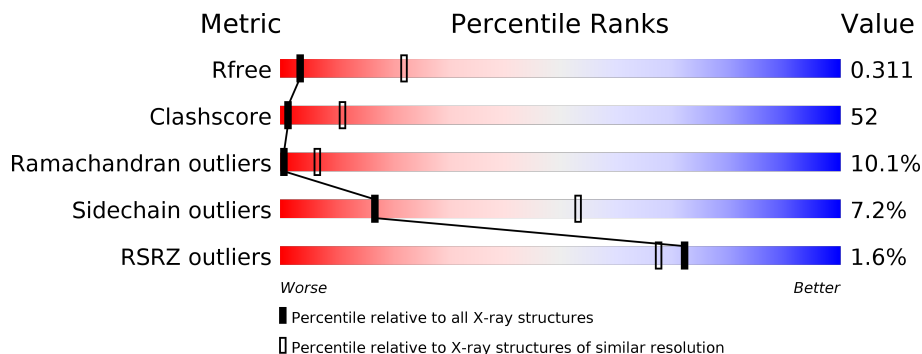
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	839	
2	B	153	
3	C	159	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8899 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 Myosin heavy chain isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	808	Total	C	N	O	S	0	0	0
			6493	4150	1111	1193	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	LYS	GLU	CONFLICT	UNP O44934
A	744	ALA	VAL	CONFLICT	UNP O44934

- Molecule 2 is a protein called Myosin regulatory light chain LC-2, mantle muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1166	733	191	233	9			

- Molecule 3 is a protein called Myosin catalytic light chain LC-1, mantle muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	156	Total	C	N	O	S	0	0	0
			1239	773	203	253	10			

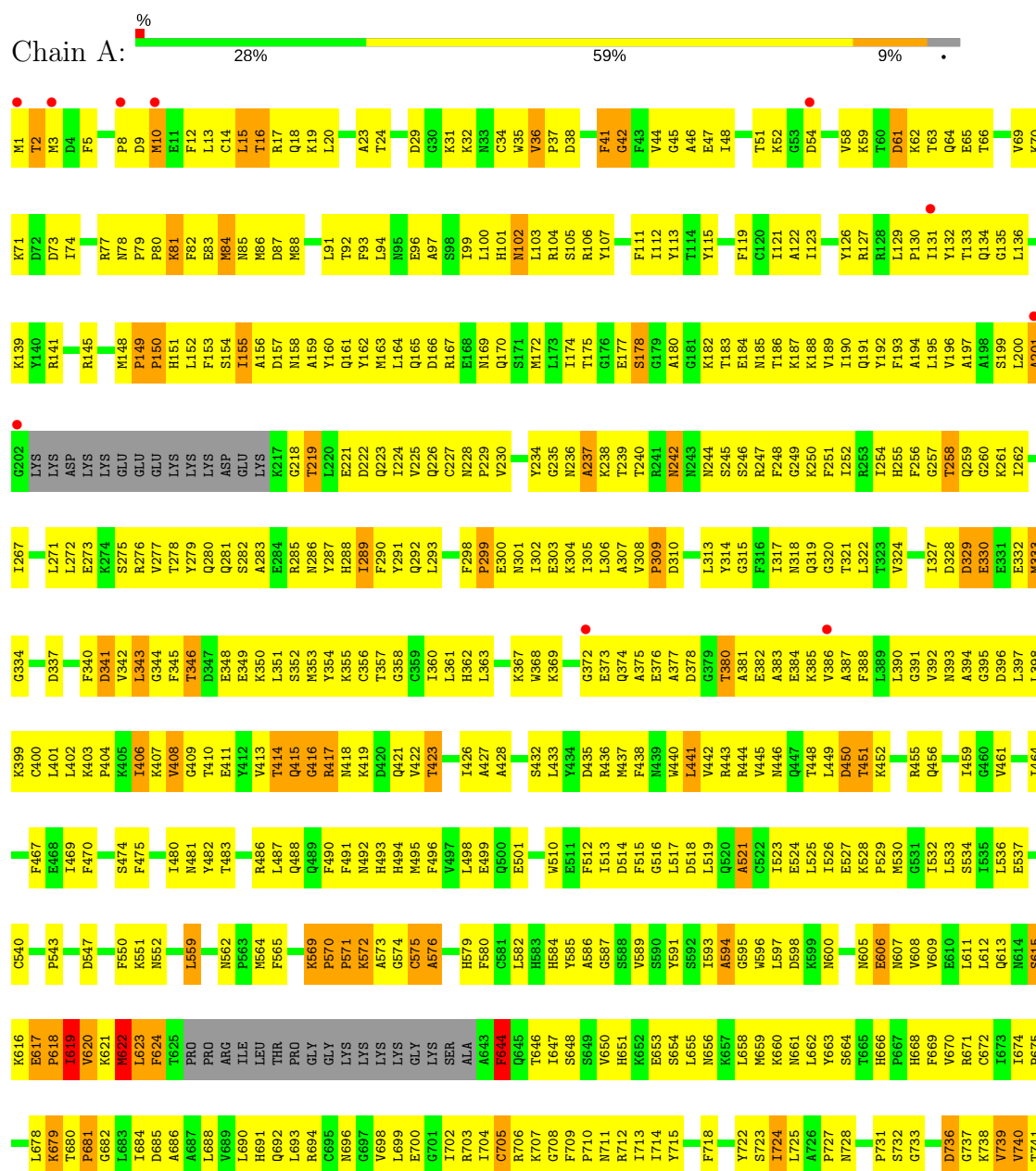
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

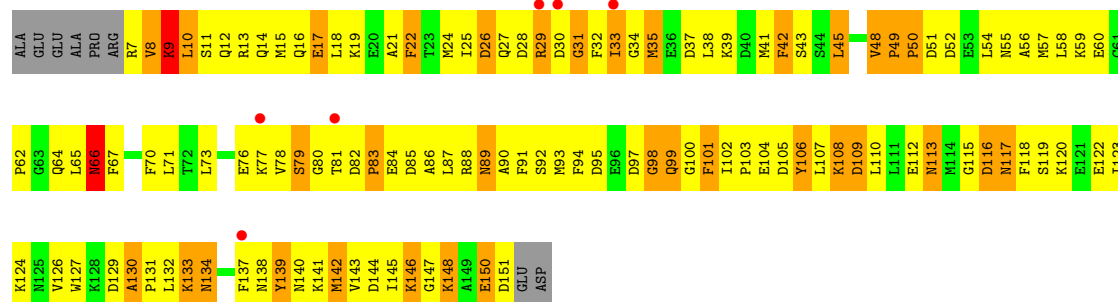
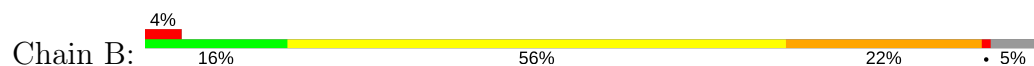
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Myosin heavy chain isoform A

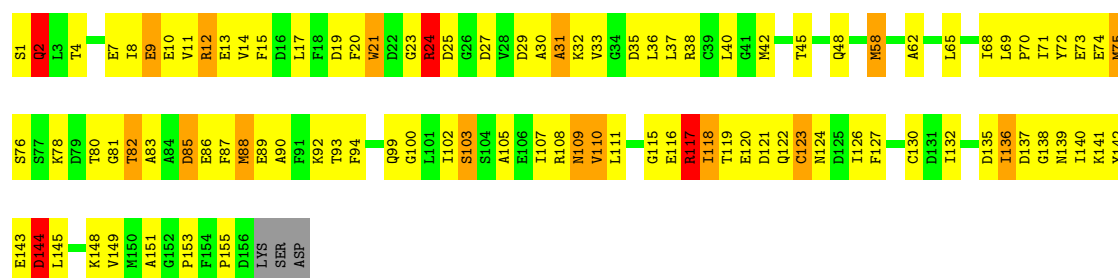




- Molecule 2: Myosin regulatory light chain LC-2, mantle muscle



- Molecule 3: Myosin catalytic light chain LC-1, mantle muscle



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	194.38Å 100.26Å 80.60Å 90.00° 105.31° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 49.25 – 3.41	Depositor EDS
% Data completeness (in resolution range)	94.9 (50.00-3.40) 95.4 (49.25-3.41)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 3.40Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.336 0.241 , 0.311	Depositor DCC
R_{free} test set	1933 reflections (9.84%)	DCC
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8899	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0/6631	0.75	0/8938
2	B	0.44	0/1186	0.82	2/1588 (0.1%)
3	C	0.56	0/1258	0.85	2/1687 (0.1%)
All	All	0.50	0/9075	0.78	4/12213 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	138	GLY	N-CA-C	-7.60	94.09	113.10
2	B	100	GLY	N-CA-C	-7.46	94.46	113.10
2	B	101	PHE	N-CA-C	5.24	125.13	111.00
3	C	58	MET	N-CA-C	5.16	124.93	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6493	0	6496	683	0
2	B	1166	0	1125	149	0
3	C	1239	0	1190	119	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8899	0	8811	918	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 52.

All (918) 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:A:259:GLN:H	1:A:261:LYS:HE2	1.03	1.13
1:A:191:GLN:HG2	1:A:221:GLU:HG2	1.28	1.11
1:A:346:THR:HB	1:A:349:GLU:HG3	1.26	1.10
1:A:302:ILE:HG21	1:A:309:PRO:HD3	1.25	1.08
1:A:155:ILE:HD11	1:A:668:HIS:HB3	1.32	1.08
1:A:617:GLU:O	1:A:620:VAL:HG23	1.54	1.07
1:A:407:LYS:HG2	1:A:411:GLU:HG2	1.37	1.06
3:C:90:ALA:O	3:C:93:THR:HG22	1.58	1.03
1:A:406:ILE:HG22	1:A:407:LYS:H	1.27	0.99
1:A:227:CYS:HB3	1:A:343:LEU:HD11	1.42	0.99
1:A:230:VAL:HG11	1:A:441:LEU:HD11	1.45	0.98
1:A:78:ASN:OD1	1:A:93:PHE:HB2	1.63	0.97
1:A:817:VAL:HA	2:B:146:LYS:HZ1	1.29	0.97
1:A:48:ILE:HA	1:A:58:VAL:HG22	1.46	0.96
1:A:620:VAL:O	1:A:624:PHE:HB2	1.65	0.96
1:A:88:MET:HE1	1:A:99:ILE:HA	1.49	0.95
1:A:259:GLN:N	1:A:261:LYS:HE2	1.84	0.92
2:B:65:LEU:HD11	2:B:70:PHE:HA	1.49	0.92
1:A:190:ILE:HG12	1:A:254:ILE:HD11	1.48	0.91
1:A:234:TYR:CZ	1:A:289:ILE:HD12	2.06	0.90
2:B:56:ALA:HA	2:B:59:LYS:HD2	1.55	0.89
2:B:26:ASP:OD2	2:B:31:GLY:HA2	1.73	0.88
1:A:194:ALA:HA	1:A:262:ILE:HD11	1.56	0.88
1:A:694:ARG:HG2	1:A:699:LEU:HD12	1.53	0.88
1:A:292:GLN:HB3	1:A:333:MET:HG2	1.55	0.87
1:A:406:ILE:HG22	1:A:407:LYS:N	1.87	0.87
1:A:133:THR:HG22	1:A:135:GLY:H	1.39	0.87
1:A:819:LYS:HE3	2:B:76:GLU:O	1.75	0.86
1:A:786:MET:SD	3:C:82:THR:OG1	2.33	0.86
1:A:572:LYS:HB2	1:A:575:CYS:HB2	1.57	0.84
1:A:442:VAL:O	1:A:445:VAL:HG22	1.78	0.83
1:A:513:ILE:HG12	1:A:517:LEU:HD12	1.59	0.83
1:A:259:GLN:HB2	1:A:261:LYS:HD3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:LEU:CD2	3:C:68:ILE:HD13	2.08	0.83
1:A:413:VAL:HG12	1:A:415:GLN:HB2	1.60	0.83
1:A:112:ILE:HG13	1:A:113:TYR:N	1.92	0.83
1:A:817:VAL:HA	2:B:146:LYS:NZ	1.92	0.83
3:C:88:MET:HE2	3:C:143:GLU:HG3	1.60	0.83
1:A:12:PHE:O	1:A:13:LEU:HD23	1.78	0.83
1:A:1:MET:SD	1:A:20:LEU:HD22	2.18	0.83
1:A:194:ALA:HA	1:A:262:ILE:CD1	2.09	0.82
1:A:47:GLU:O	1:A:58:VAL:HG13	1.78	0.82
1:A:184:GLU:O	1:A:187:LYS:HB3	1.81	0.81
2:B:101:PHE:HD1	2:B:138:ASN:HA	1.44	0.81
1:A:92:THR:HA	1:A:711:ASN:HD21	1.46	0.81
1:A:819:LYS:HE2	2:B:79:SER:HB2	1.62	0.80
2:B:147:GLY:O	2:B:148:LYS:HB2	1.78	0.80
1:A:152:LEU:O	1:A:155:ILE:HG23	1.81	0.80
1:A:136:LEU:O	1:A:139:LYS:HB2	1.82	0.80
3:C:7:GLU:O	3:C:11:VAL:HG23	1.82	0.80
1:A:155:ILE:CD1	1:A:668:HIS:HB3	2.14	0.78
1:A:800:TYR:CE1	3:C:17:LEU:HD22	2.19	0.78
1:A:46:ALA:HA	1:A:61:ASP:OD1	1.83	0.78
2:B:85:ASP:HA	2:B:88:ARG:HG3	1.63	0.78
2:B:7:ARG:O	2:B:78:VAL:HG11	1.84	0.78
3:C:130:CYS:O	3:C:148:LYS:HD3	1.84	0.78
2:B:60:GLU:HB3	2:B:73:LEU:HD11	1.66	0.78
1:A:188:LYS:HA	1:A:191:GLN:HG3	1.67	0.77
2:B:109:ASP:HA	2:B:113:ASN:OD1	1.83	0.77
1:A:360:ILE:HA	1:A:363:LEU:HD12	1.64	0.77
1:A:86:MET:HE1	1:A:149:PRO:HA	1.67	0.77
1:A:302:ILE:HD13	1:A:309:PRO:HB3	1.66	0.77
1:A:413:VAL:C	1:A:415:GLN:H	1.88	0.77
1:A:236:ASN:HB3	1:A:244:ASN:ND2	1.99	0.77
1:A:346:THR:CB	1:A:349:GLU:HG3	2.13	0.77
1:A:321:THR:HG22	1:A:322:LEU:H	1.48	0.77
3:C:132:ILE:CD1	3:C:145:LEU:HA	2.15	0.77
1:A:280:GLN:HB2	1:A:319:GLN:HB2	1.64	0.76
1:A:321:THR:HG22	1:A:322:LEU:N	2.00	0.76
2:B:65:LEU:HD11	2:B:70:PHE:CA	2.16	0.76
1:A:525:LEU:O	1:A:532:ILE:HG13	1.85	0.76
1:A:308:VAL:O	1:A:310:ASP:N	2.19	0.75
3:C:119:THR:HG22	3:C:121:ASP:H	1.49	0.75
1:A:713:ILE:HG22	1:A:714:ILE:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LYS:HB3	1:A:415:GLN:HG3	1.69	0.75
1:A:415:GLN:O	1:A:417:ARG:N	2.20	0.75
1:A:800:TYR:HE1	3:C:17:LEU:HD22	1.52	0.75
1:A:170:GLN:O	1:A:459:ILE:HA	1.86	0.74
1:A:380:THR:O	1:A:384:GLU:HG2	1.86	0.74
1:A:708:GLY:O	1:A:765:LYS:HE2	1.88	0.74
1:A:612:LEU:HB3	1:A:623:LEU:HD13	1.70	0.74
3:C:30:ALA:O	3:C:33:VAL:HG23	1.86	0.74
3:C:4:THR:OG1	3:C:7:GLU:HG3	1.86	0.74
1:A:407:LYS:O	1:A:408:VAL:HG23	1.87	0.74
2:B:145:ILE:O	2:B:148:LYS:HG3	1.87	0.74
1:A:164:LEU:HD21	1:A:260:GLY:HA2	1.68	0.74
1:A:346:THR:HG22	1:A:348:GLU:H	1.51	0.74
3:C:4:THR:O	3:C:8:ILE:HG13	1.88	0.74
1:A:368:TRP:HE1	1:A:426:ILE:CD1	2.01	0.73
1:A:36:VAL:HG22	1:A:37:PRO:HD2	1.69	0.73
1:A:259:GLN:H	1:A:261:LYS:CE	1.92	0.73
1:A:280:GLN:HB2	1:A:319:GLN:CB	2.18	0.73
2:B:13:ARG:O	2:B:17:GLU:HB2	1.88	0.73
1:A:115:TYR:CE1	1:A:150:PRO:HA	2.24	0.73
1:A:230:VAL:CG1	1:A:441:LEU:HD11	2.19	0.72
1:A:345:PHE:CE1	1:A:444:ARG:HG3	2.24	0.72
3:C:88:MET:CE	3:C:143:GLU:HG3	2.19	0.72
1:A:133:THR:H	1:A:136:LEU:HD12	1.55	0.71
2:B:25:ILE:HA	2:B:41:MET:HE2	1.71	0.71
1:A:337:ASP:O	1:A:341:ASP:OD1	2.07	0.71
1:A:170:GLN:HB2	1:A:459:ILE:HG12	1.73	0.71
3:C:102:ILE:HG13	3:C:142:TYR:HD2	1.55	0.71
1:A:368:TRP:CE3	1:A:377:ALA:HA	2.26	0.71
2:B:38:LEU:HB3	2:B:54:LEU:HD11	1.73	0.71
1:A:1:MET:N	1:A:86:MET:SD	2.63	0.70
1:A:793:GLY:O	1:A:797:ARG:HB2	1.92	0.70
1:A:808:ILE:O	1:A:812:LEU:HG	1.90	0.70
1:A:693:LEU:HD22	1:A:698:VAL:HG11	1.73	0.70
1:A:85:ASN:HD22	1:A:86:MET:H	1.38	0.70
2:B:7:ARG:C	2:B:9:LYS:H	1.92	0.70
1:A:346:THR:HB	1:A:349:GLU:CG	2.12	0.70
1:A:572:LYS:HB2	1:A:575:CYS:CB	2.22	0.70
2:B:101:PHE:CD1	2:B:138:ASN:HA	2.25	0.69
2:B:7:ARG:O	2:B:9:LYS:N	2.24	0.69
3:C:130:CYS:HB3	3:C:148:LYS:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:THR:HA	3:C:86:GLU:OE1	1.91	0.69
1:A:784:ILE:O	1:A:788:GLN:HG3	1.91	0.69
2:B:9:LYS:HA	2:B:9:LYS:HE3	1.72	0.69
3:C:123:CYS:O	3:C:126:ILE:HG22	1.91	0.69
2:B:13:ARG:HD2	2:B:13:ARG:N	2.07	0.69
1:A:397:LEU:HA	1:A:400:CYS:SG	2.32	0.69
1:A:400:CYS:SG	1:A:611:LEU:HD22	2.33	0.69
1:A:368:TRP:HE1	1:A:426:ILE:HD12	1.57	0.69
1:A:813:ILE:HG12	2:B:91:PHE:CE1	2.28	0.69
1:A:688:LEU:O	1:A:692:GLN:HG3	1.93	0.69
1:A:86:MET:HE3	1:A:150:PRO:HD3	1.75	0.68
1:A:15:LEU:HD12	1:A:19:LYS:HD3	1.74	0.68
1:A:496:PHE:CD1	1:A:514:ASP:HA	2.28	0.68
1:A:536:LEU:HA	1:A:550:PHE:CE1	2.27	0.68
2:B:99:GLN:C	2:B:101:PHE:H	1.89	0.68
1:A:112:ILE:HD11	1:A:113:TYR:CE1	2.27	0.68
3:C:135:ASP:O	3:C:136:ILE:C	2.31	0.68
1:A:91:LEU:HB2	1:A:94:LEU:HD23	1.74	0.68
1:A:800:TYR:O	1:A:804:GLN:HG3	1.93	0.68
3:C:93:THR:HG23	3:C:94:PHE:CD1	2.29	0.68
1:A:713:ILE:O	1:A:761:LYS:HA	1.94	0.67
1:A:413:VAL:O	1:A:415:GLN:N	2.27	0.67
2:B:8:VAL:O	2:B:10:LEU:N	2.27	0.67
1:A:86:MET:CE	1:A:149:PRO:HA	2.24	0.67
1:A:783:ILE:HG21	3:C:90:ALA:HB2	1.75	0.67
1:A:236:ASN:HB3	1:A:244:ASN:HD21	1.57	0.67
1:A:71:LYS:O	1:A:74:ILE:HG12	1.94	0.67
3:C:119:THR:HB	3:C:122:GLN:HG3	1.77	0.67
3:C:100:GLY:HA2	3:C:142:TYR:CZ	2.29	0.67
1:A:107:TYR:CD2	1:A:684:ILE:HD11	2.30	0.66
1:A:180:ALA:HB1	1:A:672:CYS:HB3	1.77	0.66
1:A:550:PHE:HE2	1:A:593:ILE:HD12	1.59	0.66
1:A:14:CYS:O	1:A:15:LEU:CB	2.43	0.66
1:A:658:LEU:O	1:A:661:ASN:HB2	1.94	0.66
1:A:600:ASN:ND2	1:A:646:THR:HB	2.10	0.66
1:A:156:ALA:O	1:A:159:ALA:HB3	1.95	0.66
1:A:85:ASN:ND2	1:A:86:MET:H	1.94	0.66
1:A:525:LEU:HD23	1:A:582:LEU:HD22	1.78	0.65
1:A:96:GLU:OE2	1:A:694:ARG:NH2	2.29	0.65
2:B:8:VAL:C	2:B:10:LEU:H	1.98	0.65
1:A:132:TYR:HD2	1:A:153:PHE:CZ	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:CG1	1:A:441:LEU:HD21	2.27	0.65
1:A:836:LYS:C	1:A:838:LEU:H	2.00	0.65
3:C:36:LEU:HD22	3:C:68:ILE:HD13	1.77	0.65
1:A:126:TYR:O	1:A:681:PRO:HG3	1.96	0.65
1:A:157:ASP:O	1:A:160:TYR:HB3	1.97	0.65
1:A:813:ILE:O	1:A:815:ARG:N	2.30	0.65
1:A:820:TRP:CE3	1:A:821:LEU:HD23	2.31	0.65
3:C:12:ARG:O	3:C:15:PHE:N	2.30	0.64
1:A:9:ASP:HB3	1:A:136:LEU:HD21	1.79	0.64
3:C:132:ILE:HD13	3:C:145:LEU:HA	1.78	0.64
1:A:432:SER:O	1:A:436:ARG:HG3	1.97	0.64
1:A:786:MET:HE1	3:C:80:THR:O	1.98	0.64
1:A:175:THR:O	1:A:672:CYS:HB2	1.97	0.64
1:A:239:THR:HG21	1:A:247:ARG:NH1	2.12	0.64
3:C:37:LEU:HA	3:C:40:LEU:HD12	1.79	0.64
1:A:130:PRO:O	1:A:132:TYR:N	2.31	0.64
2:B:9:LYS:HA	2:B:9:LYS:CE	2.26	0.64
2:B:65:LEU:HD21	2:B:70:PHE:HD1	1.62	0.64
1:A:256:PHE:HA	1:A:261:LYS:O	1.97	0.63
1:A:433:LEU:O	1:A:437:MET:HG3	1.98	0.63
1:A:236:ASN:CB	1:A:244:ASN:HD21	2.11	0.63
1:A:445:VAL:O	1:A:448:THR:HB	1.98	0.63
1:A:239:THR:HG23	1:A:245:SER:HB3	1.80	0.63
1:A:384:GLU:HA	1:A:387:ALA:HB3	1.81	0.63
3:C:145:LEU:O	3:C:149:VAL:HG23	1.99	0.63
1:A:88:MET:HE1	1:A:99:ILE:CA	2.24	0.63
2:B:28:ASP:O	2:B:30:ASP:N	2.32	0.63
1:A:91:LEU:HB2	1:A:94:LEU:CD2	2.28	0.63
1:A:78:ASN:HD21	1:A:91:LEU:HB3	1.62	0.63
1:A:828:TRP:CZ2	2:B:57:MET:HB3	2.33	0.63
2:B:42:PHE:HA	2:B:45:LEU:HB2	1.81	0.63
1:A:678:LEU:O	1:A:680:THR:N	2.32	0.62
1:A:84:MET:HE3	1:A:105:SER:HB2	1.81	0.62
2:B:104:GLU:HG3	2:B:127:TRP:CH2	2.32	0.62
2:B:26:ASP:CG	2:B:31:GLY:HA2	2.18	0.62
1:A:449:LEU:O	1:A:451:THR:N	2.32	0.62
1:A:236:ASN:HD22	1:A:244:ASN:ND2	1.98	0.62
1:A:58:VAL:CG1	1:A:59:LYS:N	2.63	0.62
3:C:119:THR:HG22	3:C:121:ASP:N	2.15	0.62
1:A:496:PHE:CE1	1:A:514:ASP:HA	2.33	0.62
3:C:78:LYS:HA	3:C:78:LYS:HE3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:THR:CG2	1:A:322:LEU:H	2.11	0.62
1:A:1:MET:HE1	1:A:15:LEU:C	2.20	0.62
1:A:222:ASP:O	1:A:226:GLN:HB2	2.00	0.62
2:B:8:VAL:C	2:B:10:LEU:N	2.51	0.62
3:C:36:LEU:HD21	3:C:68:ILE:HD13	1.81	0.62
1:A:492:ASN:ND2	1:A:704:ILE:HD11	2.14	0.62
2:B:25:ILE:HG22	2:B:37:ASP:HB3	1.81	0.62
2:B:28:ASP:HB2	2:B:37:ASP:OD2	2.00	0.62
1:A:85:ASN:ND2	1:A:86:MET:N	2.47	0.62
2:B:94:PHE:O	2:B:102:ILE:HG12	2.00	0.62
1:A:174:ILE:HG23	1:A:670:VAL:HG12	1.82	0.61
1:A:1:MET:HE3	1:A:14:CYS:HB3	1.82	0.61
3:C:29:ASP:OD2	3:C:58:MET:O	2.18	0.61
1:A:343:LEU:HD12	1:A:445:VAL:HG12	1.82	0.61
3:C:132:ILE:HD11	3:C:145:LEU:HA	1.81	0.61
1:A:343:LEU:CD1	1:A:445:VAL:HG12	2.31	0.61
1:A:571:PRO:HB2	1:A:575:CYS:HB3	1.83	0.61
1:A:86:MET:CE	1:A:150:PRO:HD3	2.31	0.61
1:A:186:THR:HG23	1:A:461:VAL:HG11	1.83	0.61
2:B:60:GLU:HB3	2:B:73:LEU:CD1	2.30	0.61
2:B:98:GLY:O	2:B:99:GLN:O	2.19	0.61
3:C:80:THR:HG23	3:C:80:THR:O	2.00	0.61
1:A:536:LEU:HD13	1:A:550:PHE:CZ	2.36	0.61
1:A:197:ALA:HB2	1:A:262:ILE:HG13	1.82	0.60
1:A:415:GLN:O	1:A:415:GLN:HG2	2.01	0.60
1:A:713:ILE:HD12	1:A:713:ILE:N	2.16	0.60
1:A:82:PHE:O	1:A:85:ASN:HB2	2.00	0.60
3:C:2:GLN:OE1	3:C:2:GLN:HA	2.01	0.60
1:A:450:ASP:O	1:A:450:ASP:OD1	2.19	0.60
1:A:836:LYS:C	1:A:838:LEU:N	2.54	0.60
1:A:367:LYS:HB2	1:A:378:ASP:HB3	1.84	0.60
1:A:608:VAL:HG12	1:A:612:LEU:CD1	2.32	0.60
1:A:712:ARG:C	1:A:713:ILE:HD12	2.21	0.60
1:A:191:GLN:O	1:A:194:ALA:HB3	2.01	0.60
1:A:618:PRO:O	1:A:621:LYS:N	2.34	0.60
2:B:112:GLU:HG2	2:B:113:ASN:ND2	2.16	0.60
1:A:58:VAL:HG12	1:A:59:LYS:N	2.17	0.60
2:B:118:PHE:HA	2:B:122:GLU:OE1	2.01	0.60
2:B:7:ARG:C	2:B:9:LYS:N	2.53	0.60
1:A:10:MET:HB3	1:A:14:CYS:SG	2.42	0.60
1:A:751:ASP:OD1	1:A:753:ASN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASN:O	1:A:237:ALA:HB2	2.02	0.59
1:A:257:GLY:HA3	1:A:261:LYS:HE3	1.84	0.59
2:B:32:PHE:O	2:B:34:GLY:N	2.36	0.59
3:C:107:ILE:O	3:C:110:VAL:HB	2.02	0.59
3:C:11:VAL:HG11	3:C:69:LEU:HD23	1.82	0.59
1:A:406:ILE:HD12	1:A:414:THR:HG21	1.84	0.59
1:A:830:ARG:O	1:A:833:ASN:HB2	2.03	0.59
1:A:609:VAL:O	1:A:613:GLN:HG3	2.03	0.59
3:C:30:ALA:O	3:C:32:LYS:N	2.35	0.59
1:A:1:MET:HE3	1:A:14:CYS:C	2.23	0.59
1:A:178:SER:HB3	1:A:242:ASN:HD21	1.67	0.59
1:A:310:ASP:OD1	1:A:313:LEU:HG	2.02	0.59
1:A:491:PHE:HD1	1:A:669:PHE:CE2	2.21	0.59
1:A:141:ARG:O	1:A:157:ASP:OD2	2.21	0.59
1:A:715:TYR:CE1	1:A:738:LYS:HG3	2.38	0.59
3:C:111:LEU:O	3:C:118:ILE:HB	2.01	0.59
1:A:620:VAL:HG12	1:A:624:PHE:CE1	2.37	0.58
1:A:646:THR:O	1:A:650:VAL:HG23	2.02	0.58
1:A:167:ARG:HH22	1:A:258:THR:HG23	1.67	0.58
2:B:9:LYS:HB3	2:B:78:VAL:CG1	2.34	0.58
1:A:690:LEU:HA	1:A:693:LEU:HD12	1.84	0.58
2:B:66:ASN:OD1	2:B:66:ASN:N	2.32	0.58
1:A:345:PHE:HB3	1:A:349:GLU:OE1	2.04	0.58
1:A:157:ASP:O	1:A:160:TYR:N	2.36	0.58
1:A:41:PHE:N	1:A:41:PHE:CD1	2.71	0.58
1:A:785:SER:HA	1:A:788:GLN:OE1	2.04	0.58
1:A:230:VAL:HG12	1:A:441:LEU:HD21	1.84	0.58
1:A:164:LEU:HD21	1:A:260:GLY:CA	2.33	0.58
1:A:237:ALA:HB2	1:A:287:TYR:HA	1.84	0.58
1:A:817:VAL:O	1:A:820:TRP:HB3	2.03	0.58
3:C:141:LYS:HB2	3:C:144:ASP:HB2	1.84	0.58
1:A:302:ILE:CG2	1:A:309:PRO:HD3	2.18	0.57
1:A:404:PRO:HB2	1:A:607:ASN:ND2	2.20	0.57
1:A:413:VAL:C	1:A:415:GLN:N	2.58	0.57
2:B:132:LEU:O	2:B:133:LYS:HB2	2.04	0.57
2:B:9:LYS:HB3	2:B:78:VAL:HG12	1.86	0.57
1:A:112:ILE:HG13	1:A:113:TYR:H	1.70	0.57
1:A:321:THR:CG2	1:A:322:LEU:N	2.67	0.57
1:A:723:SER:O	1:A:725:LEU:N	2.38	0.57
1:A:88:MET:HE2	1:A:102:ASN:HB3	1.87	0.57
1:A:54:ASP:HA	1:A:71:LYS:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LEU:CB	2:B:54:LEU:HD11	2.33	0.57
3:C:126:ILE:HG23	3:C:127:PHE:N	2.18	0.57
1:A:227:CYS:CB	1:A:343:LEU:HD11	2.27	0.57
1:A:174:ILE:HG23	1:A:670:VAL:CG1	2.35	0.57
2:B:143:VAL:O	2:B:146:LYS:HB2	2.04	0.57
3:C:14:VAL:HG12	3:C:36:LEU:HD12	1.85	0.57
3:C:37:LEU:HD21	3:C:72:TYR:HA	1.87	0.57
3:C:70:PRO:O	3:C:74:GLU:HG2	2.04	0.57
1:A:136:LEU:HD23	1:A:139:LYS:HD2	1.88	0.56
1:A:113:TYR:CD1	1:A:151:HIS:HA	2.40	0.56
1:A:148:MET:CE	1:A:149:PRO:HD2	2.35	0.56
1:A:300:GLU:HG3	1:A:301:ASN:H	1.70	0.56
1:A:315:GLY:HA2	1:A:318:ASN:OD1	2.06	0.56
1:A:440:TRP:HD1	1:A:443:ARG:NH1	2.03	0.56
2:B:141:LYS:O	2:B:144:ASP:HB2	2.05	0.56
1:A:80:PRO:O	1:A:82:PHE:N	2.38	0.56
2:B:26:ASP:HA	2:B:37:ASP:OD2	2.04	0.56
1:A:600:ASN:HD21	1:A:648:SER:H	1.53	0.56
2:B:28:ASP:HB2	2:B:37:ASP:CG	2.25	0.56
2:B:9:LYS:HE3	2:B:9:LYS:CA	2.36	0.56
1:A:15:LEU:HD23	1:A:20:LEU:HD13	1.88	0.56
1:A:310:ASP:CG	1:A:313:LEU:HG	2.26	0.56
1:A:475:PHE:HD1	1:A:596:TRP:CE3	2.23	0.56
1:A:88:MET:HE1	1:A:99:ILE:HG23	1.88	0.56
1:A:817:VAL:HA	2:B:146:LYS:CE	2.36	0.56
1:A:376:GLU:HA	1:A:402:LEU:HD13	1.87	0.55
1:A:685:ASP:HB3	1:A:688:LEU:HB3	1.88	0.55
1:A:786:MET:CE	3:C:82:THR:OG1	2.54	0.55
1:A:569:LYS:HD2	1:A:569:LYS:O	2.06	0.55
2:B:32:PHE:CZ	2:B:64:GLN:NE2	2.74	0.55
3:C:85:ASP:OD2	3:C:85:ASP:N	2.30	0.55
1:A:669:PHE:CD1	1:A:669:PHE:N	2.75	0.55
1:A:487:LEU:O	1:A:490:PHE:HB3	2.06	0.55
1:A:608:VAL:HG12	1:A:612:LEU:HD12	1.88	0.55
1:A:722:TYR:O	1:A:723:SER:C	2.44	0.55
2:B:106:TYR:O	2:B:110:LEU:HB2	2.07	0.55
2:B:12:GLN:HB3	2:B:13:ARG:HH11	1.71	0.55
2:B:56:ALA:HA	2:B:59:LYS:CD	2.34	0.55
1:A:200:LEU:O	1:A:201:ALA:HB2	2.06	0.55
1:A:358:GLY:O	1:A:361:LEU:N	2.38	0.55
1:A:718:PHE:CD2	1:A:741:THR:HG23	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:HD22	1:A:86:MET:N	2.01	0.55
2:B:115:GLY:O	2:B:117:ASN:N	2.40	0.55
3:C:37:LEU:O	3:C:40:LEU:HB2	2.06	0.55
1:A:189:VAL:HG12	1:A:193:PHE:CE2	2.42	0.55
1:A:238:LYS:HD2	1:A:324:VAL:HG13	1.89	0.55
1:A:474:SER:OG	1:A:475:PHE:N	2.40	0.55
1:A:488:GLN:HG2	1:A:585:TYR:CD2	2.42	0.55
2:B:123:ILE:CG2	2:B:127:TRP:HE1	2.18	0.55
1:A:693:LEU:HB3	1:A:699:LEU:HG	1.89	0.55
2:B:108:LYS:O	2:B:110:LEU:N	2.40	0.55
1:A:796:MET:HE2	3:C:35:ASP:OD1	2.06	0.55
2:B:91:PHE:CD2	2:B:139:TYR:HB2	2.41	0.55
1:A:529:PRO:O	1:A:530:MET:HB2	2.06	0.54
1:A:302:ILE:CD1	1:A:309:PRO:HB3	2.36	0.54
1:A:38:ASP:OD2	1:A:44:VAL:HG21	2.06	0.54
1:A:536:LEU:HA	1:A:550:PHE:HE1	1.72	0.54
1:A:192:TYR:CE1	1:A:196:VAL:HG11	2.42	0.54
1:A:1:MET:HE3	1:A:15:LEU:N	2.22	0.54
1:A:368:TRP:CZ2	1:A:426:ILE:HD11	2.42	0.54
2:B:108:LYS:HE3	2:B:112:GLU:OE1	2.08	0.54
2:B:25:ILE:HA	2:B:41:MET:CE	2.37	0.54
3:C:82:THR:HG21	3:C:87:PHE:CZ	2.43	0.54
1:A:248:PHE:HB3	1:A:272:LEU:HD12	1.90	0.54
1:A:736:ASP:OD1	1:A:738:LYS:N	2.40	0.54
2:B:104:GLU:HG3	2:B:127:TRP:HH2	1.73	0.54
1:A:134:GLN:HG2	1:A:195:LEU:HD13	1.88	0.54
1:A:14:CYS:O	1:A:15:LEU:HB2	2.08	0.54
1:A:440:TRP:HD1	1:A:443:ARG:CZ	2.20	0.54
1:A:823:LEU:HB3	1:A:829:TRP:CG	2.42	0.54
1:A:374:GLN:OE1	1:A:415:GLN:HG2	2.08	0.54
1:A:450:ASP:OD1	1:A:452:LYS:HG2	2.07	0.54
1:A:562:ASN:OD1	1:A:564:MET:N	2.40	0.54
2:B:67:PHE:CE2	2:B:71:LEU:HD11	2.43	0.54
3:C:30:ALA:C	3:C:32:LYS:H	2.11	0.54
1:A:88:MET:CE	1:A:102:ASN:HB3	2.38	0.54
1:A:329:ASP:O	1:A:330:GLU:C	2.46	0.54
1:A:694:ARG:HG2	1:A:699:LEU:CD1	2.34	0.54
1:A:796:MET:O	1:A:799:ALA:N	2.40	0.54
2:B:112:GLU:HB2	2:B:123:ILE:HD11	1.90	0.54
1:A:152:LEU:HD21	1:A:189:VAL:CG2	2.37	0.53
1:A:332:GLU:C	1:A:334:GLY:N	2.58	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:LEU:O	1:A:814:GLN:HB2	2.09	0.53
1:A:255:HIS:CD2	1:A:455:ARG:HD3	2.43	0.53
1:A:281:GLN:O	1:A:283:ALA:N	2.40	0.53
1:A:38:ASP:N	1:A:42:GLY:O	2.29	0.53
1:A:524:GLU:O	1:A:528:LYS:HG2	2.09	0.53
1:A:512:PHE:CE2	1:A:707:LYS:HD3	2.43	0.53
1:A:392:VAL:HG12	1:A:393:ASN:N	2.23	0.53
1:A:481:ASN:O	1:A:482:TYR:C	2.47	0.53
2:B:123:ILE:HG23	2:B:127:TRP:HE1	1.73	0.53
1:A:826:TRP:O	1:A:827:GLU:C	2.47	0.53
1:A:298:PHE:HB3	1:A:301:ASN:HD22	1.73	0.53
1:A:368:TRP:HE1	1:A:426:ILE:HD11	1.73	0.53
1:A:550:PHE:CE2	1:A:593:ILE:HD12	2.42	0.53
1:A:298:PHE:HB3	1:A:301:ASN:ND2	2.23	0.53
1:A:348:GLU:O	1:A:351:LEU:HB3	2.09	0.53
1:A:351:LEU:HD11	1:A:355:LYS:HE3	1.90	0.53
1:A:368:TRP:HH2	1:A:398:LEU:CD2	2.22	0.53
1:A:88:MET:SD	1:A:99:ILE:HG23	2.49	0.53
1:A:757:LEU:HD23	1:A:762:VAL:HG23	1.89	0.53
1:A:813:ILE:O	1:A:816:ASN:N	2.41	0.53
2:B:55:ASN:C	2:B:57:MET:H	2.11	0.53
1:A:302:ILE:HG21	1:A:309:PRO:CD	2.19	0.53
1:A:525:LEU:HD22	1:A:564:MET:HB2	1.90	0.53
1:A:739:VAL:O	1:A:742:ASP:HB3	2.09	0.53
2:B:142:MET:HE3	2:B:146:LYS:HD3	1.90	0.53
1:A:226:GLN:CG	1:A:342:VAL:HG11	2.39	0.53
1:A:724:ILE:O	1:A:727:PRO:HD3	2.08	0.53
1:A:715:TYR:CZ	1:A:738:LYS:HG3	2.44	0.53
1:A:819:LYS:O	1:A:823:LEU:HG	2.10	0.53
1:A:354:TYR:O	1:A:357:THR:HB	2.10	0.52
1:A:368:TRP:CZ3	1:A:377:ALA:HA	2.44	0.52
1:A:826:TRP:CH2	2:B:60:GLU:OE1	2.62	0.52
1:A:226:GLN:HG2	1:A:342:VAL:HG11	1.90	0.52
1:A:324:VAL:O	1:A:327:ILE:HG22	2.10	0.52
1:A:609:VAL:HG12	1:A:613:GLN:HE21	1.74	0.52
2:B:25:ILE:CG2	2:B:37:ASP:HB3	2.40	0.52
2:B:28:ASP:CB	2:B:32:PHE:O	2.58	0.52
1:A:34:CYS:O	1:A:46:ALA:N	2.36	0.52
1:A:660:LYS:HD2	1:A:660:LYS:O	2.08	0.52
1:A:675:PRO:HB2	1:A:684:ILE:HD13	1.91	0.52
1:A:170:GLN:NE2	1:A:666:HIS:HB3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:90:ALA:O	3:C:93:THR:CG2	2.47	0.52
1:A:404:PRO:HG2	1:A:414:THR:OG1	2.09	0.52
1:A:814:GLN:O	1:A:818:ARG:HG3	2.09	0.52
2:B:9:LYS:O	2:B:11:SER:N	2.42	0.52
3:C:117:ARG:HH11	3:C:117:ARG:HG3	1.75	0.52
2:B:13:ARG:CD	2:B:13:ARG:N	2.72	0.52
2:B:14:GLN:O	2:B:18:LEU:HG	2.09	0.52
1:A:794:TYR:CZ	3:C:153:PRO:HA	2.44	0.52
1:A:483:THR:HA	1:A:655:LEU:HD21	1.92	0.52
1:A:97:ALA:O	1:A:100:LEU:HB3	2.10	0.52
3:C:119:THR:HG22	3:C:120:GLU:N	2.24	0.52
1:A:113:TYR:HB3	1:A:150:PRO:HB2	1.92	0.52
1:A:341:ASP:C	1:A:344:GLY:H	2.12	0.52
1:A:407:LYS:HE2	1:A:411:GLU:OE2	2.10	0.52
1:A:79:PRO:HG2	1:A:82:PHE:CE1	2.45	0.52
2:B:119:SER:CB	2:B:122:GLU:HG3	2.40	0.52
1:A:174:ILE:O	1:A:182:LYS:HE3	2.10	0.52
1:A:218:GLY:O	1:A:223:GLN:NE2	2.38	0.52
1:A:381:ALA:O	1:A:385:LYS:HG3	2.10	0.52
1:A:712:ARG:HG2	1:A:763:PHE:CD2	2.45	0.52
1:A:786:MET:CE	3:C:80:THR:O	2.57	0.52
3:C:99:GLN:OE1	3:C:99:GLN:HA	2.09	0.52
1:A:235:GLY:O	1:A:247:ARG:N	2.38	0.51
1:A:328:ASP:O	1:A:329:ASP:C	2.48	0.51
1:A:38:ASP:CB	1:A:44:VAL:HG23	2.39	0.51
1:A:12:PHE:C	1:A:13:LEU:HD23	2.29	0.51
1:A:238:LYS:HD2	1:A:324:VAL:HG22	1.91	0.51
1:A:351:LEU:HD21	1:A:355:LYS:NZ	2.24	0.51
1:A:396:ASP:O	1:A:399:LYS:HB2	2.11	0.51
1:A:196:VAL:HA	1:A:199:SER:HB2	1.92	0.51
1:A:247:ARG:NH2	1:A:480:ILE:HD11	2.26	0.51
1:A:407:LYS:HE2	1:A:411:GLU:CD	2.31	0.51
1:A:700:GLU:CD	1:A:703:ARG:NH1	2.64	0.51
1:A:739:VAL:HG13	1:A:743:LYS:HE2	1.91	0.51
2:B:108:LYS:C	2:B:110:LEU:H	2.13	0.51
2:B:67:PHE:O	2:B:70:PHE:HB3	2.09	0.51
1:A:533:LEU:O	1:A:537:GLU:HG3	2.10	0.51
1:A:725:LEU:HD13	1:A:748:LEU:HD11	1.92	0.51
3:C:30:ALA:C	3:C:32:LYS:N	2.64	0.51
1:A:305:ILE:O	1:A:306:LEU:HB2	2.11	0.51
1:A:192:TYR:O	1:A:196:VAL:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLY:HA3	1:A:464:ILE:HD12	1.92	0.51
1:A:496:PHE:HA	1:A:515:PHE:CE2	2.45	0.51
1:A:36:VAL:CG2	1:A:37:PRO:HD2	2.39	0.51
1:A:85:ASN:HB3	1:A:102:ASN:OD1	2.11	0.51
2:B:119:SER:OG	2:B:122:GLU:HG3	2.10	0.51
2:B:25:ILE:O	2:B:26:ASP:O	2.28	0.51
1:A:482:TYR:OH	1:A:527:GLU:HG2	2.11	0.51
1:A:658:LEU:HD12	1:A:658:LEU:O	2.10	0.51
2:B:57:MET:O	2:B:60:GLU:HG3	2.10	0.51
1:A:787:PHE:HA	3:C:87:PHE:CE2	2.46	0.51
1:A:723:SER:O	1:A:724:ILE:C	2.47	0.51
3:C:12:ARG:NH1	3:C:65:LEU:CD2	2.74	0.51
2:B:26:ASP:O	2:B:27:GLN:HB3	2.11	0.50
2:B:41:MET:C	2:B:43:SER:H	2.15	0.50
1:A:418:ASN:OD1	1:A:421:GLN:HG3	2.11	0.50
1:A:618:PRO:HG2	1:A:619:ILE:H	1.75	0.50
1:A:69:VAL:HG12	1:A:70:LYS:N	2.25	0.50
1:A:806:GLN:HB3	2:B:94:PHE:CZ	2.46	0.50
2:B:150:GLU:HG3	2:B:151:ASP:H	1.74	0.50
2:B:34:GLY:O	2:B:37:ASP:N	2.44	0.50
1:A:826:TRP:CZ2	2:B:60:GLU:OE1	2.64	0.50
1:A:397:LEU:O	1:A:401:LEU:N	2.44	0.50
1:A:422:VAL:HG23	1:A:423:THR:N	2.27	0.50
1:A:174:ILE:HA	1:A:670:VAL:O	2.12	0.50
1:A:107:TYR:HA	1:A:111:PHE:O	2.12	0.50
2:B:24:MET:HG2	2:B:41:MET:HE1	1.93	0.50
3:C:15:PHE:CD2	3:C:65:LEU:HB2	2.46	0.50
1:A:415:GLN:C	1:A:417:ARG:N	2.64	0.50
1:A:565:PHE:CE1	1:A:580:PHE:CD1	3.00	0.50
1:A:5:PHE:HD1	1:A:17:ARG:HB2	1.77	0.50
2:B:138:ASN:CG	2:B:141:LYS:HD2	2.31	0.50
1:A:267:ILE:N	1:A:446:ASN:OD1	2.37	0.50
3:C:127:PHE:CE2	3:C:140:ILE:HD13	2.46	0.50
3:C:36:LEU:HD21	3:C:68:ILE:HG21	1.92	0.50
1:A:279:TYR:HA	1:A:319:GLN:OE1	2.12	0.50
1:A:831:LEU:C	1:A:833:ASN:H	2.15	0.50
1:A:828:TRP:O	1:A:829:TRP:C	2.50	0.49
1:A:621:LYS:CE	1:A:622:MET:HG3	2.42	0.49
1:A:740:VAL:O	1:A:741:THR:C	2.50	0.49
1:A:83:GLU:C	1:A:85:ASN:N	2.65	0.49
3:C:68:ILE:O	3:C:71:ILE:HB	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:CG1	1:A:113:TYR:N	2.71	0.49
1:A:257:GLY:HA3	1:A:261:LYS:HG3	1.94	0.49
1:A:787:PHE:O	1:A:791:ILE:HG13	2.13	0.49
1:A:78:ASN:ND2	1:A:91:LEU:HB3	2.26	0.49
2:B:28:ASP:HB2	2:B:37:ASP:OD1	2.12	0.49
1:A:762:VAL:O	1:A:762:VAL:HG13	2.13	0.49
2:B:139:TYR:CD1	2:B:140:ASN:N	2.80	0.49
1:A:193:PHE:HB3	1:A:256:PHE:HZ	1.76	0.49
1:A:784:ILE:HD13	3:C:110:VAL:HG13	1.93	0.49
2:B:108:LYS:C	2:B:110:LEU:N	2.65	0.49
1:A:149:PRO:HB2	1:A:150:PRO:CD	2.43	0.49
3:C:11:VAL:HG21	3:C:69:LEU:CD2	2.42	0.49
1:A:1:MET:CE	1:A:14:CYS:HB3	2.42	0.49
1:A:392:VAL:HG12	1:A:393:ASN:H	1.78	0.49
1:A:739:VAL:CG1	1:A:743:LYS:HE2	2.42	0.49
1:A:161:GLN:O	1:A:165:GLN:HB2	2.12	0.49
1:A:239:THR:O	1:A:240:THR:C	2.50	0.49
1:A:51:THR:CG2	1:A:52:LYS:N	2.75	0.49
1:A:605:ASN:O	1:A:608:VAL:HG23	2.13	0.49
2:B:122:GLU:O	2:B:126:VAL:HG23	2.12	0.49
1:A:498:LEU:O	1:A:501:GLU:N	2.44	0.49
1:A:584:HIS:O	1:A:586:ALA:N	2.46	0.49
1:A:367:LYS:HD2	1:A:367:LYS:H	1.77	0.48
1:A:406:ILE:O	1:A:411:GLU:HG2	2.13	0.48
1:A:650:VAL:O	1:A:653:GLU:N	2.46	0.48
2:B:89:ASN:HA	2:B:92:SER:OG	2.13	0.48
1:A:354:TYR:O	1:A:357:THR:N	2.45	0.48
1:A:368:TRP:HE3	1:A:377:ALA:HA	1.77	0.48
1:A:575:CYS:O	1:A:576:ALA:O	2.31	0.48
2:B:80:GLY:O	2:B:82:ASP:N	2.46	0.48
3:C:35:ASP:OD1	3:C:38:ARG:NH1	2.46	0.48
1:A:315:GLY:O	1:A:319:GLN:HG3	2.13	0.48
1:A:781:SER:O	1:A:782:LYS:C	2.51	0.48
1:A:149:PRO:O	1:A:150:PRO:O	2.31	0.48
1:A:273:GLU:OE1	1:A:276:ARG:NE	2.42	0.48
1:A:820:TRP:CZ2	2:B:145:ILE:HG21	2.48	0.48
3:C:9:GLU:O	3:C:12:ARG:HB3	2.13	0.48
1:A:104:ARG:O	1:A:107:TYR:N	2.47	0.48
1:A:250:LYS:HE3	1:A:252:ILE:HD11	1.95	0.48
1:A:407:LYS:HG2	1:A:411:GLU:CG	2.24	0.48
1:A:490:PHE:HE1	1:A:663:TYR:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ASN:C	2:B:57:MET:N	2.66	0.48
3:C:102:ILE:HG13	3:C:142:TYR:CD2	2.42	0.48
1:A:289:ILE:HG12	1:A:289:ILE:O	2.12	0.48
1:A:415:GLN:C	1:A:417:ARG:H	2.17	0.48
1:A:529:PRO:O	1:A:530:MET:CB	2.60	0.48
1:A:812:LEU:O	1:A:816:ASN:ND2	2.46	0.48
1:A:659:MET:C	1:A:661:ASN:N	2.66	0.48
3:C:103:SER:OG	3:C:105:ALA:HB3	2.14	0.48
1:A:257:GLY:CA	1:A:261:LYS:HG3	2.43	0.48
1:A:298:PHE:N	1:A:299:PRO:HD3	2.29	0.48
1:A:337:ASP:OD1	1:A:350:LYS:NZ	2.47	0.48
1:A:399:LYS:HD3	1:A:403:LYS:NZ	2.29	0.48
2:B:85:ASP:O	2:B:88:ARG:N	2.47	0.48
3:C:88:MET:O	3:C:89:GLU:C	2.51	0.48
1:A:498:LEU:O	1:A:499:GLU:C	2.50	0.47
1:A:234:TYR:O	1:A:287:TYR:CD1	2.68	0.47
1:A:417:ARG:HA	1:A:421:GLN:OE1	2.14	0.47
1:A:491:PHE:O	1:A:494:HIS:N	2.47	0.47
1:A:329:ASP:O	1:A:332:GLU:N	2.46	0.47
1:A:35:TRP:HA	1:A:35:TRP:CE3	2.48	0.47
1:A:584:HIS:O	1:A:587:GLY:N	2.39	0.47
1:A:620:VAL:HG12	1:A:624:PHE:CD1	2.49	0.47
2:B:25:ILE:HG21	2:B:33:ILE:HG23	1.95	0.47
3:C:116:GLU:O	3:C:117:ARG:O	2.33	0.47
3:C:126:ILE:CG2	3:C:127:PHE:N	2.76	0.47
1:A:194:ALA:HA	1:A:262:ILE:HD12	1.91	0.47
1:A:236:ASN:OD1	1:A:246:SER:HA	2.15	0.47
1:A:301:ASN:HA	1:A:304:LYS:HG3	1.96	0.47
1:A:368:TRP:NE1	1:A:426:ILE:HD11	2.29	0.47
1:A:786:MET:O	1:A:787:PHE:C	2.52	0.47
1:A:341:ASP:O	1:A:344:GLY:HA2	2.14	0.47
1:A:414:THR:O	1:A:416:GLY:N	2.47	0.47
1:A:83:GLU:O	1:A:85:ASN:N	2.48	0.47
1:A:698:VAL:O	1:A:702:ILE:HD12	2.15	0.47
1:A:488:GLN:HB3	1:A:519:LEU:CD1	2.44	0.47
1:A:88:MET:HE3	1:A:99:ILE:O	2.15	0.47
2:B:85:ASP:O	2:B:86:ALA:C	2.53	0.47
1:A:524:GLU:C	1:A:526:ILE:H	2.19	0.47
2:B:119:SER:O	2:B:123:ILE:HG13	2.14	0.47
1:A:342:VAL:C	1:A:344:GLY:N	2.67	0.47
2:B:102:ILE:HA	2:B:103:PRO:HD3	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ARG:HE	2:B:143:VAL:HG11	1.80	0.47
3:C:45:THR:OG1	3:C:48:GLN:HB2	2.15	0.47
1:A:2:THR:OG1	1:A:148:MET:HA	2.15	0.46
1:A:152:LEU:HD21	1:A:189:VAL:HG23	1.97	0.46
1:A:152:LEU:O	1:A:155:ILE:CG2	2.58	0.46
1:A:537:GLU:O	1:A:540:CYS:HB2	2.15	0.46
1:A:562:ASN:OD1	1:A:564:MET:HB2	2.15	0.46
1:A:525:LEU:HD21	1:A:565:PHE:HB2	1.98	0.46
2:B:116:ASP:O	2:B:117:ASN:O	2.34	0.46
3:C:9:GLU:HA	3:C:9:GLU:OE1	2.15	0.46
1:A:278:THR:O	1:A:319:GLN:NE2	2.43	0.46
1:A:172:MET:HB2	1:A:461:VAL:HG22	1.96	0.46
1:A:32:LYS:O	1:A:47:GLU:HA	2.15	0.46
1:A:644:PHE:CD1	1:A:644:PHE:N	2.84	0.46
1:A:584:HIS:C	1:A:586:ALA:N	2.69	0.46
1:A:238:LYS:HD2	1:A:324:VAL:CG1	2.45	0.46
1:A:449:LEU:C	1:A:451:THR:H	2.17	0.46
1:A:483:THR:O	1:A:486:ARG:N	2.47	0.46
1:A:618:PRO:O	1:A:619:ILE:C	2.53	0.46
2:B:87:LEU:O	2:B:90:ALA:HB3	2.16	0.46
2:B:91:PHE:O	2:B:92:SER:C	2.53	0.46
1:A:238:LYS:HD2	1:A:324:VAL:CG2	2.46	0.46
1:A:346:THR:C	1:A:348:GLU:H	2.17	0.46
1:A:438:PHE:O	1:A:442:VAL:HG23	2.15	0.46
1:A:494:HIS:O	1:A:495:MET:C	2.53	0.46
1:A:674:ILE:O	1:A:692:GLN:NE2	2.42	0.46
1:A:74:ILE:HG13	1:A:74:ILE:O	2.15	0.46
1:A:79:PRO:HG2	1:A:82:PHE:CD1	2.49	0.46
1:A:835:VAL:HG12	1:A:835:VAL:O	2.15	0.46
2:B:123:ILE:HG22	2:B:127:TRP:CD1	2.51	0.46
2:B:28:ASP:O	2:B:29:ARG:C	2.53	0.46
1:A:300:GLU:HG3	1:A:301:ASN:N	2.31	0.46
2:B:41:MET:O	2:B:43:SER:N	2.49	0.46
1:A:290:PHE:HB3	1:A:317:ILE:HD11	1.97	0.46
1:A:306:LEU:O	1:A:362:HIS:CE1	2.69	0.46
1:A:406:ILE:CG2	1:A:407:LYS:H	2.06	0.46
1:A:704:ILE:O	1:A:707:LYS:HG2	2.16	0.46
1:A:828:TRP:O	1:A:831:LEU:N	2.49	0.46
1:A:836:LYS:O	1:A:838:LEU:N	2.49	0.46
3:C:15:PHE:CE2	3:C:65:LEU:HB2	2.50	0.46
3:C:37:LEU:HD13	3:C:75:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:MET:O	1:A:789:ALA:N	2.49	0.46
2:B:134:ASN:HA	2:B:134:ASN:HD22	1.54	0.46
3:C:132:ILE:HD13	3:C:145:LEU:CA	2.44	0.46
3:C:15:PHE:CD1	3:C:68:ILE:HD12	2.51	0.46
1:A:306:LEU:HD13	1:A:385:LYS:HG2	1.98	0.46
1:A:469:ILE:HG12	1:A:589:VAL:HG22	1.98	0.46
3:C:10:GLU:O	3:C:11:VAL:C	2.53	0.46
3:C:130:CYS:HB3	3:C:148:LYS:CB	2.45	0.46
1:A:15:LEU:O	1:A:15:LEU:HG	2.16	0.46
1:A:298:PHE:CB	1:A:301:ASN:HD22	2.29	0.46
1:A:332:GLU:C	1:A:334:GLY:H	2.19	0.46
2:B:120:LYS:HA	2:B:123:ILE:HD12	1.98	0.46
1:A:183:THR:O	1:A:184:GLU:C	2.54	0.45
1:A:406:ILE:O	1:A:411:GLU:HA	2.17	0.45
1:A:44:VAL:HG12	1:A:45:GLY:N	2.31	0.45
1:A:597:LEU:HD23	1:A:597:LEU:HA	1.63	0.45
1:A:606:GLU:O	1:A:609:VAL:N	2.45	0.45
1:A:807:ARG:HG3	3:C:20:PHE:CD2	2.51	0.45
3:C:69:LEU:HB2	3:C:70:PRO:CD	2.46	0.45
1:A:87:ASP:HA	1:A:115:TYR:O	2.16	0.45
1:A:228:ASN:N	1:A:229:PRO:CD	2.79	0.45
1:A:536:LEU:CD1	1:A:550:PHE:CZ	2.99	0.45
3:C:119:THR:CG2	3:C:120:GLU:N	2.79	0.45
1:A:15:LEU:O	1:A:16:THR:C	2.55	0.45
2:B:26:ASP:CG	2:B:27:GLN:H	2.18	0.45
2:B:55:ASN:O	2:B:57:MET:N	2.49	0.45
1:A:290:PHE:HB3	1:A:317:ILE:CD1	2.46	0.45
1:A:291:TYR:CZ	1:A:317:ILE:HG23	2.52	0.45
1:A:372:GLY:O	1:A:373:GLU:HG3	2.17	0.45
1:A:693:LEU:HA	1:A:696:ASN:HB2	1.99	0.45
1:A:693:LEU:HB3	1:A:699:LEU:CG	2.47	0.45
2:B:12:GLN:OE1	2:B:13:ARG:NH1	2.50	0.45
1:A:121:ILE:HG22	1:A:122:ALA:N	2.31	0.45
1:A:273:GLU:OE1	1:A:276:ARG:NH2	2.47	0.45
1:A:234:TYR:CE1	1:A:289:ILE:HD12	2.49	0.45
2:B:137:PHE:HZ	2:B:142:MET:HG3	1.80	0.45
1:A:800:TYR:CD1	3:C:17:LEU:HD22	2.51	0.45
1:A:514:ASP:OD1	1:A:516:GLY:N	2.49	0.45
1:A:490:PHE:HD1	1:A:663:TYR:CZ	2.35	0.45
1:A:783:ILE:HG22	1:A:783:ILE:O	2.15	0.45
1:A:88:MET:CE	1:A:99:ILE:HG23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:PRO:HA	2:B:50:PRO:HD3	1.59	0.45
1:A:806:GLN:C	3:C:21:TRP:HZ2	2.19	0.45
1:A:279:TYR:CD1	1:A:319:GLN:OE1	2.70	0.45
1:A:493:HIS:O	1:A:496:PHE:HB3	2.17	0.45
1:A:36:VAL:CG2	1:A:69:VAL:HG21	2.47	0.45
2:B:26:ASP:C	2:B:28:ASP:H	2.20	0.45
1:A:141:ARG:NH1	1:A:199:SER:HB3	2.32	0.45
1:A:406:ILE:CG2	1:A:407:LYS:N	2.61	0.45
1:A:119:PHE:CZ	1:A:491:PHE:CZ	3.04	0.45
1:A:579:HIS:O	1:A:580:PHE:HB3	2.17	0.45
1:A:736:ASP:OD1	1:A:736:ASP:C	2.55	0.45
2:B:92:SER:O	2:B:94:PHE:N	2.50	0.45
1:A:375:ALA:HB2	1:A:419:LYS:N	2.32	0.45
1:A:440:TRP:O	1:A:441:LEU:C	2.55	0.45
1:A:584:HIS:O	1:A:585:TYR:C	2.54	0.45
1:A:106:ARG:NH2	1:A:150:PRO:HG2	2.32	0.45
2:B:16:GLN:C	2:B:18:LEU:N	2.67	0.45
1:A:148:MET:HE3	1:A:149:PRO:HD2	1.99	0.44
1:A:382:GLU:O	1:A:385:LYS:HB2	2.17	0.44
1:A:406:ILE:O	1:A:411:GLU:CB	2.65	0.44
1:A:510:TRP:CZ2	1:A:512:PHE:HB2	2.52	0.44
1:A:63:THR:O	1:A:65:GLU:N	2.50	0.44
1:A:693:LEU:HB2	1:A:699:LEU:HD11	1.97	0.44
1:A:14:CYS:O	1:A:15:LEU:HB3	2.16	0.44
1:A:613:GLN:HB3	1:A:624:PHE:CE2	2.53	0.44
1:A:690:LEU:HD23	1:A:693:LEU:HD12	2.00	0.44
1:A:308:VAL:HG23	1:A:308:VAL:O	2.18	0.44
1:A:693:LEU:CD2	1:A:698:VAL:HG11	2.45	0.44
1:A:706:ARG:NH1	1:A:706:ARG:HG2	2.33	0.44
2:B:95:ASP:OD1	2:B:97:ASP:O	2.35	0.44
3:C:118:ILE:HG23	3:C:122:GLN:HB2	2.00	0.44
1:A:574:GLY:O	1:A:576:ALA:N	2.49	0.44
2:B:35:MET:O	2:B:39:LYS:HG2	2.18	0.44
3:C:23:GLY:O	3:C:24:ARG:C	2.56	0.44
1:A:148:MET:HB3	1:A:148:MET:HE2	1.75	0.44
1:A:341:ASP:O	1:A:344:GLY:CA	2.65	0.44
1:A:234:TYR:OH	1:A:353:MET:HG3	2.17	0.44
1:A:380:THR:HG22	1:A:380:THR:O	2.17	0.44
1:A:523:ILE:O	1:A:526:ILE:HB	2.17	0.44
1:A:482:TYR:CD1	1:A:526:ILE:HG21	2.53	0.44
1:A:119:PHE:CE1	1:A:698:VAL:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:PHE:CD2	1:A:765:LYS:HG2	2.52	0.44
1:A:709:PHE:HB3	1:A:763:PHE:HB3	2.00	0.44
1:A:731:PRO:C	1:A:733:GLY:H	2.21	0.44
1:A:813:ILE:O	1:A:814:GLN:C	2.56	0.44
3:C:2:GLN:HA	3:C:73:GLU:OE1	2.18	0.44
3:C:74:GLU:O	3:C:76:SER:N	2.50	0.44
3:C:81:GLY:O	3:C:82:THR:CB	2.65	0.44
1:A:354:TYR:O	1:A:355:LYS:C	2.54	0.44
1:A:367:LYS:HD2	1:A:367:LYS:N	2.32	0.44
3:C:100:GLY:HA2	3:C:142:TYR:CE2	2.53	0.44
1:A:780:LEU:HD11	3:C:93:THR:HG21	1.99	0.44
1:A:219:THR:HB	1:A:221:GLU:OE1	2.18	0.44
1:A:346:THR:C	1:A:348:GLU:N	2.71	0.44
1:A:386:VAL:O	1:A:390:LEU:HG	2.18	0.44
1:A:514:ASP:C	1:A:514:ASP:OD1	2.56	0.44
1:A:785:SER:O	1:A:788:GLN:HB2	2.18	0.44
2:B:132:LEU:O	2:B:133:LYS:CB	2.65	0.44
1:A:306:LEU:O	1:A:362:HIS:HE1	1.99	0.44
1:A:415:GLN:O	1:A:416:GLY:C	2.56	0.44
1:A:565:PHE:HE1	1:A:580:PHE:CD1	2.35	0.44
1:A:620:VAL:O	1:A:624:PHE:CB	2.52	0.44
1:A:80:PRO:C	1:A:82:PHE:N	2.70	0.44
2:B:123:ILE:O	2:B:126:VAL:HB	2.18	0.44
3:C:65:LEU:O	3:C:65:LEU:HD12	2.18	0.44
1:A:227:CYS:HB3	1:A:343:LEU:CD1	2.31	0.44
1:A:655:LEU:O	1:A:656:ASN:C	2.53	0.44
1:A:768:VAL:O	1:A:771:MET:N	2.48	0.44
1:A:84:MET:CE	1:A:105:SER:HB2	2.46	0.43
1:A:157:ASP:O	1:A:160:TYR:CB	2.66	0.43
1:A:228:ASN:ND2	1:A:250:LYS:NZ	2.66	0.43
1:A:285:ARG:HG2	1:A:291:TYR:CE1	2.52	0.43
1:A:292:GLN:C	1:A:333:MET:HG2	2.38	0.43
1:A:618:PRO:HB2	1:A:622:MET:SD	2.58	0.43
3:C:1:SER:O	3:C:2:GLN:NE2	2.51	0.43
1:A:327:ILE:O	1:A:327:ILE:CG2	2.66	0.43
1:A:407:LYS:HA	1:A:410:THR:O	2.18	0.43
1:A:678:LEU:O	1:A:679:LYS:C	2.56	0.43
1:A:711:ASN:C	1:A:712:ARG:HG3	2.37	0.43
1:A:836:LYS:NZ	2:B:21:ALA:HB2	2.33	0.43
2:B:67:PHE:CZ	2:B:71:LEU:HD11	2.52	0.43
1:A:261:LYS:HG2	1:A:261:LYS:H	1.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LEU:O	1:A:352:SER:C	2.56	0.43
1:A:513:ILE:O	1:A:514:ASP:C	2.55	0.43
2:B:7:ARG:O	2:B:78:VAL:CG1	2.62	0.43
1:A:115:TYR:CD2	1:A:145:ARG:CZ	3.00	0.43
1:A:277:VAL:HA	1:A:286:ASN:HD21	1.83	0.43
1:A:357:THR:O	1:A:360:ILE:HB	2.18	0.43
1:A:442:VAL:O	1:A:443:ARG:C	2.57	0.43
1:A:690:LEU:O	1:A:691:HIS:C	2.54	0.43
1:A:804:GLN:O	1:A:805:ASP:C	2.56	0.43
1:A:808:ILE:H	1:A:808:ILE:HD12	1.83	0.43
1:A:80:PRO:C	1:A:82:PHE:H	2.21	0.43
3:C:82:THR:HG23	3:C:86:GLU:HB2	2.01	0.43
1:A:16:THR:OG1	1:A:19:LYS:HB2	2.18	0.43
1:A:38:ASP:HB2	1:A:44:VAL:HG23	1.99	0.43
1:A:58:VAL:CG1	1:A:59:LYS:H	2.31	0.43
1:A:352:SER:HB3	1:A:618:PRO:HG3	2.01	0.43
1:A:650:VAL:O	1:A:651:HIS:C	2.57	0.43
1:A:731:PRO:O	1:A:733:GLY:N	2.52	0.43
1:A:808:ILE:N	1:A:808:ILE:HD12	2.33	0.43
1:A:810:LEU:HD12	1:A:810:LEU:HA	1.85	0.43
2:B:16:GLN:O	2:B:19:LYS:N	2.49	0.43
3:C:8:ILE:HG23	3:C:69:LEU:HD11	2.00	0.43
1:A:388:PHE:O	1:A:391:GLY:N	2.51	0.43
1:A:368:TRP:HZ2	1:A:426:ILE:HD11	1.82	0.43
1:A:51:THR:HG22	1:A:52:LYS:N	2.34	0.43
1:A:547:ASP:CG	1:A:594:ALA:O	2.57	0.43
2:B:22:PHE:CE2	2:B:66:ASN:O	2.72	0.43
1:A:236:ASN:O	1:A:287:TYR:HD1	2.02	0.43
1:A:248:PHE:HA	1:A:271:LEU:O	2.19	0.43
1:A:702:ILE:HA	1:A:705:CYS:HB2	2.01	0.43
1:A:811:THR:O	1:A:812:LEU:C	2.55	0.43
3:C:93:THR:CG2	3:C:94:PHE:CD1	3.00	0.43
1:A:194:ALA:CA	1:A:262:ILE:HD11	2.39	0.43
1:A:600:ASN:HD22	1:A:647:ILE:HB	1.83	0.43
2:B:28:ASP:OD1	2:B:32:PHE:HB2	2.18	0.43
2:B:94:PHE:CD2	2:B:110:LEU:HD21	2.54	0.43
1:A:352:SER:O	1:A:356:CYS:SG	2.68	0.43
1:A:481:ASN:ND2	1:A:591:TYR:OH	2.51	0.43
1:A:644:PHE:HD1	1:A:644:PHE:N	2.16	0.43
1:A:659:MET:O	1:A:662:LEU:N	2.52	0.43
1:A:715:TYR:HB3	1:A:737:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:CE2	1:A:77:ARG:HG3	2.54	0.43
2:B:131:PRO:HD2	2:B:137:PHE:HE1	1.84	0.43
1:A:192:TYR:C	1:A:194:ALA:N	2.71	0.42
1:A:787:PHE:CA	3:C:87:PHE:CE2	3.02	0.42
1:A:375:ALA:HB2	1:A:418:ASN:C	2.39	0.42
1:A:491:PHE:O	1:A:492:ASN:C	2.57	0.42
3:C:144:ASP:O	3:C:145:LEU:C	2.57	0.42
1:A:224:ILE:C	1:A:226:GLN:N	2.72	0.42
1:A:259:GLN:HB2	1:A:261:LYS:CD	2.41	0.42
1:A:550:PHE:HE2	1:A:593:ILE:CD1	2.30	0.42
1:A:593:ILE:O	1:A:596:TRP:CD1	2.72	0.42
1:A:819:LYS:HD2	1:A:819:LYS:HA	1.75	0.42
2:B:33:ILE:HB	2:B:65:LEU:HD23	2.00	0.42
1:A:327:ILE:HG23	1:A:327:ILE:O	2.18	0.42
1:A:551:LYS:O	1:A:552:ASN:C	2.57	0.42
3:C:27:ASP:HB3	3:C:62:ALA:HB1	2.01	0.42
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.90	0.42
1:A:29:ASP:C	1:A:31:LYS:H	2.22	0.42
1:A:302:ILE:HG22	1:A:307:ALA:O	2.19	0.42
1:A:54:ASP:HA	1:A:71:LYS:CD	2.49	0.42
1:A:571:PRO:HB2	1:A:572:LYS:H	1.56	0.42
1:A:579:HIS:ND1	1:A:593:ILE:HB	2.34	0.42
2:B:104:GLU:O	2:B:105:ASP:C	2.57	0.42
2:B:10:LEU:HG	2:B:15:MET:HG3	2.01	0.42
1:A:836:LYS:HD2	2:B:17:GLU:OE2	2.18	0.42
1:A:35:TRP:HA	1:A:35:TRP:HE3	1.84	0.42
1:A:609:VAL:O	1:A:612:LEU:N	2.52	0.42
1:A:620:VAL:C	1:A:624:PHE:HB2	2.34	0.42
1:A:175:THR:HG21	1:A:671:ARG:NH1	2.35	0.42
1:A:722:TYR:HB3	1:A:725:LEU:HD12	2.01	0.42
2:B:105:ASP:O	2:B:108:LYS:HB3	2.19	0.42
3:C:148:LYS:O	3:C:151:ALA:HB3	2.19	0.42
3:C:15:PHE:CE1	3:C:68:ILE:HD12	2.54	0.42
1:A:787:PHE:N	3:C:87:PHE:HE2	2.18	0.42
1:A:301:ASN:C	1:A:303:GLU:N	2.73	0.42
1:A:29:ASP:O	1:A:31:LYS:N	2.53	0.42
1:A:343:LEU:N	1:A:343:LEU:HD23	2.34	0.42
1:A:79:PRO:O	1:A:82:PHE:HD1	2.02	0.42
3:C:12:ARG:O	3:C:13:GLU:C	2.56	0.42
1:A:104:ARG:O	1:A:105:SER:C	2.56	0.42
1:A:133:THR:HG22	1:A:135:GLY:N	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ALA:HA	1:A:288:HIS:CE1	2.55	0.42
1:A:533:LEU:O	1:A:536:LEU:HB3	2.19	0.42
1:A:731:PRO:C	1:A:733:GLY:N	2.73	0.42
1:A:745:LEU:O	1:A:746:SER:C	2.58	0.42
1:A:779:ARG:HA	1:A:779:ARG:HD2	1.72	0.42
3:C:108:ARG:O	3:C:109:ASN:C	2.58	0.42
1:A:160:TYR:OH	1:A:260:GLY:HA3	2.19	0.42
1:A:162:TYR:HD2	1:A:166:ASP:OD2	2.03	0.42
1:A:172:MET:O	1:A:461:VAL:HA	2.19	0.42
1:A:1:MET:HE1	1:A:15:LEU:O	2.20	0.42
1:A:257:GLY:CA	1:A:261:LYS:HE3	2.49	0.42
1:A:29:ASP:C	1:A:31:LYS:N	2.74	0.42
1:A:363:LEU:HG	1:A:386:VAL:HG11	2.02	0.42
1:A:396:ASP:O	1:A:400:CYS:SG	2.78	0.42
1:A:435:ASP:O	1:A:436:ARG:C	2.57	0.42
1:A:96:GLU:O	1:A:97:ALA:C	2.59	0.42
2:B:26:ASP:OD1	2:B:27:GLN:N	2.52	0.42
3:C:83:ALA:HB1	3:C:85:ASP:OD2	2.20	0.42
1:A:151:HIS:O	1:A:154:SER:OG	2.36	0.42
1:A:293:LEU:HD21	1:A:354:TYR:CD1	2.55	0.42
1:A:728:ASN:C	1:A:728:ASN:OD1	2.58	0.42
2:B:89:ASN:O	2:B:92:SER:HB2	2.20	0.42
3:C:100:GLY:HA2	3:C:142:TYR:OH	2.20	0.42
3:C:71:ILE:O	3:C:72:TYR:C	2.58	0.42
1:A:593:ILE:O	1:A:594:ALA:C	2.58	0.41
1:A:595:GLY:O	1:A:598:ASP:N	2.51	0.41
1:A:659:MET:O	1:A:660:LYS:C	2.58	0.41
1:A:71:LYS:C	1:A:73:ASP:H	2.23	0.41
1:A:799:ALA:O	1:A:800:TYR:C	2.57	0.41
2:B:133:LYS:O	2:B:134:ASN:C	2.58	0.41
3:C:120:GLU:O	3:C:124:ASN:ND2	2.54	0.41
1:A:185:ASN:O	1:A:186:THR:C	2.57	0.41
1:A:783:ILE:CG2	1:A:783:ILE:O	2.69	0.41
1:A:795:LEU:HA	1:A:795:LEU:HD23	1.76	0.41
3:C:130:CYS:O	3:C:148:LYS:CD	2.62	0.41
1:A:5:PHE:CD1	1:A:17:ARG:HB2	2.55	0.41
1:A:291:TYR:CE2	1:A:317:ILE:HG23	2.55	0.41
1:A:469:ILE:O	1:A:470:PHE:HD2	2.04	0.41
2:B:129:ASP:O	2:B:130:ALA:O	2.38	0.41
1:A:148:MET:HE2	1:A:149:PRO:HD2	2.00	0.41
1:A:427:ALA:O	1:A:428:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:THR:HB	3:C:122:GLN:CG	2.48	0.41
1:A:136:LEU:O	1:A:139:LYS:N	2.53	0.41
1:A:225:VAL:O	1:A:225:VAL:HG12	2.19	0.41
1:A:280:GLN:CB	1:A:320:GLY:N	2.83	0.41
1:A:258:THR:OG1	1:A:456:GLN:OE1	2.27	0.41
1:A:608:VAL:O	1:A:612:LEU:HB2	2.20	0.41
1:A:832:PHE:HB2	1:A:836:LYS:NZ	2.35	0.41
2:B:34:GLY:O	2:B:35:MET:C	2.58	0.41
1:A:313:LEU:C	1:A:314:TYR:CD1	2.94	0.41
1:A:358:GLY:O	1:A:361:LEU:HB2	2.20	0.41
1:A:826:TRP:CD1	1:A:828:TRP:HB2	2.55	0.41
1:A:400:CYS:SG	1:A:611:LEU:CD2	3.06	0.41
1:A:764:PHE:CD1	1:A:769:LEU:HD21	2.56	0.41
3:C:23:GLY:O	3:C:25:ASP:N	2.54	0.41
3:C:80:THR:CG2	3:C:80:THR:O	2.68	0.41
1:A:158:ASN:O	1:A:159:ALA:C	2.59	0.41
1:A:375:ALA:O	1:A:402:LEU:HD22	2.21	0.41
1:A:572:LYS:HB3	1:A:573:ALA:H	1.68	0.41
1:A:807:ARG:HG3	3:C:20:PHE:CE2	2.56	0.41
2:B:77:LYS:HE3	2:B:77:LYS:HB2	1.74	0.41
3:C:38:ARG:HA	3:C:42:MET:O	2.19	0.41
1:A:177:GLU:O	1:A:178:SER:C	2.59	0.41
1:A:248:PHE:CE2	1:A:250:LYS:HB3	2.55	0.41
1:A:391:GLY:O	1:A:615:SER:CB	2.69	0.41
1:A:723:SER:C	1:A:725:LEU:N	2.74	0.41
1:A:826:TRP:O	1:A:829:TRP:N	2.54	0.41
2:B:48:VAL:HA	2:B:49:PRO:HD3	1.77	0.41
2:B:83:PRO:HG2	2:B:86:ALA:HB2	2.02	0.41
3:C:31:ALA:HB3	3:C:58:MET:SD	2.61	0.41
1:A:24:THR:HG23	1:A:81:LYS:HA	2.02	0.41
1:A:35:TRP:CD1	1:A:77:ARG:HA	2.56	0.41
1:A:383:ALA:O	1:A:386:VAL:HG22	2.21	0.41
1:A:20:LEU:O	1:A:23:ALA:N	2.54	0.41
1:A:740:VAL:O	1:A:744:ALA:N	2.49	0.41
1:A:152:LEU:HG	1:A:152:LEU:O	2.20	0.40
1:A:58:VAL:O	1:A:66:THR:HA	2.20	0.40
1:A:700:GLU:HG3	1:A:700:GLU:O	2.21	0.40
1:A:708:GLY:O	1:A:710:PRO:HD3	2.20	0.40
1:A:808:ILE:H	1:A:808:ILE:CD1	2.34	0.40
1:A:816:ASN:HB2	2:B:87:LEU:HD21	2.02	0.40
2:B:26:ASP:C	2:B:28:ASP:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD22	1:A:123:ILE:HD11	2.03	0.40
1:A:192:TYR:C	1:A:192:TYR:CD1	2.95	0.40
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.87	0.40
1:A:369:LYS:O	1:A:375:ALA:HA	2.21	0.40
1:A:521:ALA:HB1	1:A:564:MET:HG3	2.02	0.40
1:A:490:PHE:CD1	1:A:663:TYR:CE1	3.08	0.40
1:A:739:VAL:O	1:A:740:VAL:C	2.56	0.40
1:A:348:GLU:OE2	1:A:351:LEU:HD23	2.21	0.40
1:A:422:VAL:O	1:A:423:THR:C	2.58	0.40
1:A:440:TRP:CD1	1:A:621:LYS:NZ	2.80	0.40
1:A:605:ASN:O	1:A:606:GLU:C	2.60	0.40
1:A:248:PHE:HB3	1:A:272:LEU:CD1	2.52	0.40
1:A:286:ASN:OD1	1:A:287:TYR:N	2.54	0.40
1:A:317:ILE:HD11	1:A:361:LEU:HD21	2.04	0.40
1:A:467:PHE:CE2	1:A:469:ILE:HG13	2.56	0.40
1:A:713:ILE:O	1:A:761:LYS:CA	2.67	0.40
1:A:129:LEU:HB3	1:A:130:PRO:HD2	2.04	0.40
1:A:236:ASN:O	1:A:237:ALA:CB	2.68	0.40
1:A:299:PRO:O	1:A:302:ILE:HB	2.21	0.40
1:A:394:ALA:O	1:A:395:GLY:C	2.59	0.40
1:A:397:LEU:O	1:A:401:LEU:HG	2.22	0.40
1:A:799:ALA:O	1:A:802:LYS:N	2.54	0.40
2:B:116:ASP:OD2	3:C:24:ARG:NH2	2.55	0.40
3:C:78:LYS:HA	3:C:78:LYS:CE	2.50	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	802/839 (96%)	572 (71%)	163 (20%)	67 (8%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	143/153 (94%)	85 (59%)	28 (20%)	30 (21%)	0	1
3	C	154/159 (97%)	111 (72%)	29 (19%)	14 (9%)	1	8
All	All	1099/1151 (96%)	768 (70%)	220 (20%)	111 (10%)	1	6

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	15	LEU
1	A	16	THR
1	A	64	GLN
1	A	131	ILE
1	A	150	PRO
1	A	201	ALA
1	A	282	SER
1	A	408	VAL
1	A	414	THR
1	A	415	GLN
1	A	416	GLY
1	A	450	ASP
1	A	559	LEU
1	A	576	ALA
1	A	594	ALA
1	A	606	GLU
1	A	616	LYS
1	A	679	LYS
1	A	814	GLN
2	B	26	ASP
2	B	29	ARG
2	B	48	VAL
2	B	49	PRO
2	B	50	PRO
2	B	81	THR
2	B	84	GLU
2	B	99	GLN
2	B	117	ASN
2	B	130	ALA
2	B	133	LYS
2	B	148	LYS
3	C	2	GLN
3	C	117	ARG

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Mol	Chain	Res	Type
3	C	136	ILE
3	C	139	ASN
3	C	155	PRO
1	A	62	LYS
1	A	81	LYS
1	A	178	SER
1	A	258	THR
1	A	309	PRO
1	A	330	GLU
1	A	417	ARG
1	A	571	PRO
1	A	575	CYS
1	A	686	ALA
1	A	813	ILE
1	A	827	GLU
2	B	8	VAL
2	B	9	LYS
2	B	42	PHE
2	B	66	ASN
2	B	79	SER
2	B	93	MET
2	B	116	ASP
3	C	24	ARG
3	C	31	ALA
3	C	82	THR
3	C	115	GLY
1	A	237	ALA
1	A	329	ASP
1	A	346	THR
1	A	380	THR
1	A	570	PRO
1	A	572	LYS
1	A	619	ILE
1	A	622	MET
1	A	644	PHE
1	A	742	ASP
1	A	749	GLN
2	B	35	MET
2	B	108	LYS
2	B	109	ASP
3	C	12	ARG
3	C	75	MET

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Mol	Chain	Res	Type
1	A	42	GLY
1	A	101	HIS
1	A	127	ARG
1	A	149	PRO
1	A	163	MET
1	A	169	ASN
1	A	521	ALA
1	A	739	VAL
2	B	33	ILE
2	B	83	PRO
2	B	98	GLY
2	B	150	GLU
1	A	3	MET
1	A	84	MET
1	A	275	SER
1	A	543	PRO
1	A	681	PRO
1	A	724	ILE
1	A	732	SER
2	B	10	LEU
2	B	146	LYS
3	C	21	TRP
3	C	144	ASP
1	A	406	ILE
1	A	441	LEU
1	A	617	GLU
1	A	409	GLY
2	B	62	PRO
3	C	110	VAL
1	A	740	VAL
1	A	618	PRO
1	A	768	VAL
1	A	783	ILE
1	A	682	GLY
2	B	31	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	704/731 (96%)	664 (94%)	40 (6%)	24	61
2	B	128/134 (96%)	112 (88%)	16 (12%)	5	25
3	C	134/137 (98%)	120 (90%)	14 (10%)	8	34
All	All	966/1002 (96%)	896 (93%)	70 (7%)	17	53

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	8	PRO
1	A	18	GLN
1	A	36	VAL
1	A	41	PHE
1	A	61	ASP
1	A	102	ASN
1	A	155	ILE
1	A	219	THR
1	A	242	ASN
1	A	251	PHE
1	A	289	ILE
1	A	299	PRO
1	A	333	MET
1	A	340	PHE
1	A	341	ASP
1	A	343	LEU
1	A	423	THR
1	A	451	THR
1	A	518	ASP
1	A	534	SER
1	A	559	LEU
1	A	569	LYS
1	A	570	PRO
1	A	615	SER
1	A	619	ILE
1	A	620	VAL
1	A	622	MET
1	A	623	LEU
1	A	624	PHE
1	A	644	PHE
1	A	654	SER

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Mol	Chain	Res	Type
1	A	664	SER
1	A	705	CYS
1	A	736	ASP
1	A	765	LYS
1	A	779	ARG
1	A	781	SER
1	A	827	GLU
1	A	836	LYS
2	B	9	LYS
2	B	17	GLU
2	B	22	PHE
2	B	45	LEU
2	B	51	ASP
2	B	52	ASP
2	B	58	LEU
2	B	66	ASN
2	B	89	ASN
2	B	106	TYR
2	B	107	LEU
2	B	113	ASN
2	B	124	LYS
2	B	134	ASN
2	B	139	TYR
2	B	142	MET
3	C	2	GLN
3	C	9	GLU
3	C	19	ASP
3	C	24	ARG
3	C	85	ASP
3	C	88	MET
3	C	92	LYS
3	C	103	SER
3	C	109	ASN
3	C	117	ARG
3	C	118	ILE
3	C	123	CYS
3	C	137	ASP
3	C	144	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	90	ASN
1	A	228	ASN
1	A	242	ASN
1	A	244	ASN
1	A	301	ASN
1	A	362	HIS
1	A	415	GLN
1	A	439	ASN
1	A	484	ASN
1	A	494	HIS
1	A	600	ASN
1	A	607	ASN
1	A	613	GLN
1	A	651	HIS
1	A	666	HIS
1	A	711	ASN
1	A	825	ASN
1	A	833	ASN
2	B	55	ASN
2	B	89	ASN
2	B	125	ASN
2	B	134	ASN
3	C	48	GLN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	808/839 (96%)	-0.23	12 (1%) 74 69	17, 52, 120, 162	0
2	B	145/153 (94%)	0.29	6 (4%) 38 34	26, 92, 147, 166	0
3	C	156/159 (98%)	-0.36	0 100 100	17, 40, 86, 117	0
All	All	1109/1151 (96%)	-0.18	18 (1%) 72 67	17, 55, 123, 166	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	30	ASP	5.4
2	B	137	PHE	5.1
2	B	77	LYS	4.3
1	A	202	GLY	3.8
2	B	29	ARG	3.3
2	B	33	ILE	3.2
1	A	1	MET	3.2
1	A	8	PRO	3.1
1	A	839	LEU	3.0
1	A	832	PHE	2.8
2	B	81	THR	2.5
1	A	201	ALA	2.4
1	A	54	ASP	2.3
1	A	131	ILE	2.2
1	A	372	GLY	2.2
1	A	3	MET	2.2
1	A	386	VAL	2.1
1	A	10	MET	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	C	160	1/1	0.85	0.14	-0.26	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.