



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:27 PM UTC

PDB ID : 3I5G / pdb_00003i5g
Title : Crystal structure of rigor-like squid myosin S1
Authors : Yang, Y.; Gourinath, S.; Kovacs, M.; Nyitray, L.; Reutzel, R.; Himmel, D.M.; O'Neill-Hennessey, E.; Reshetnikova, L.; Szent-Gyorgyi, A.G.; Brown, J.H.; Cohen, C.
Deposited on : 2009-07-05
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

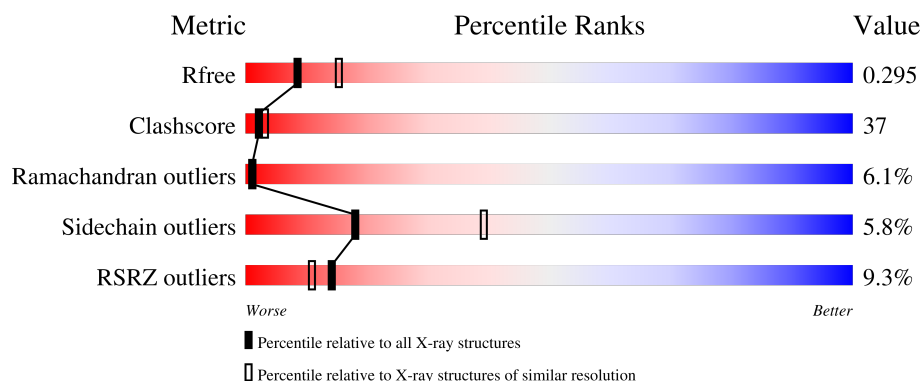
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 6 unique types of molecules in this entry. The entry contains 8985 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

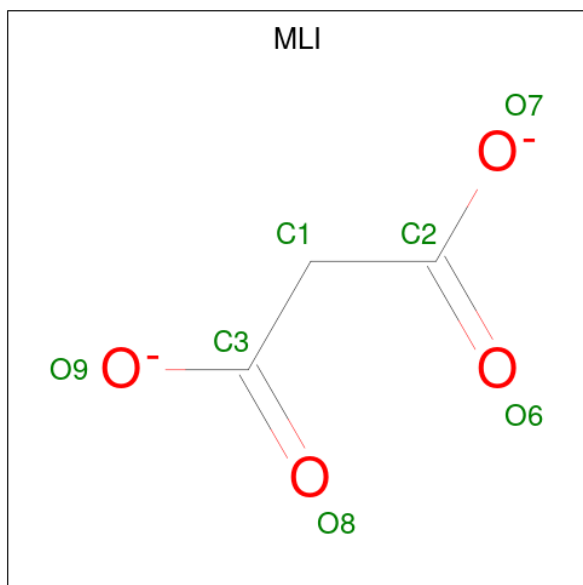
- Molecule 2 is a protein called Myosin regulatory light chain LC-2, mantle muscle.

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 MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

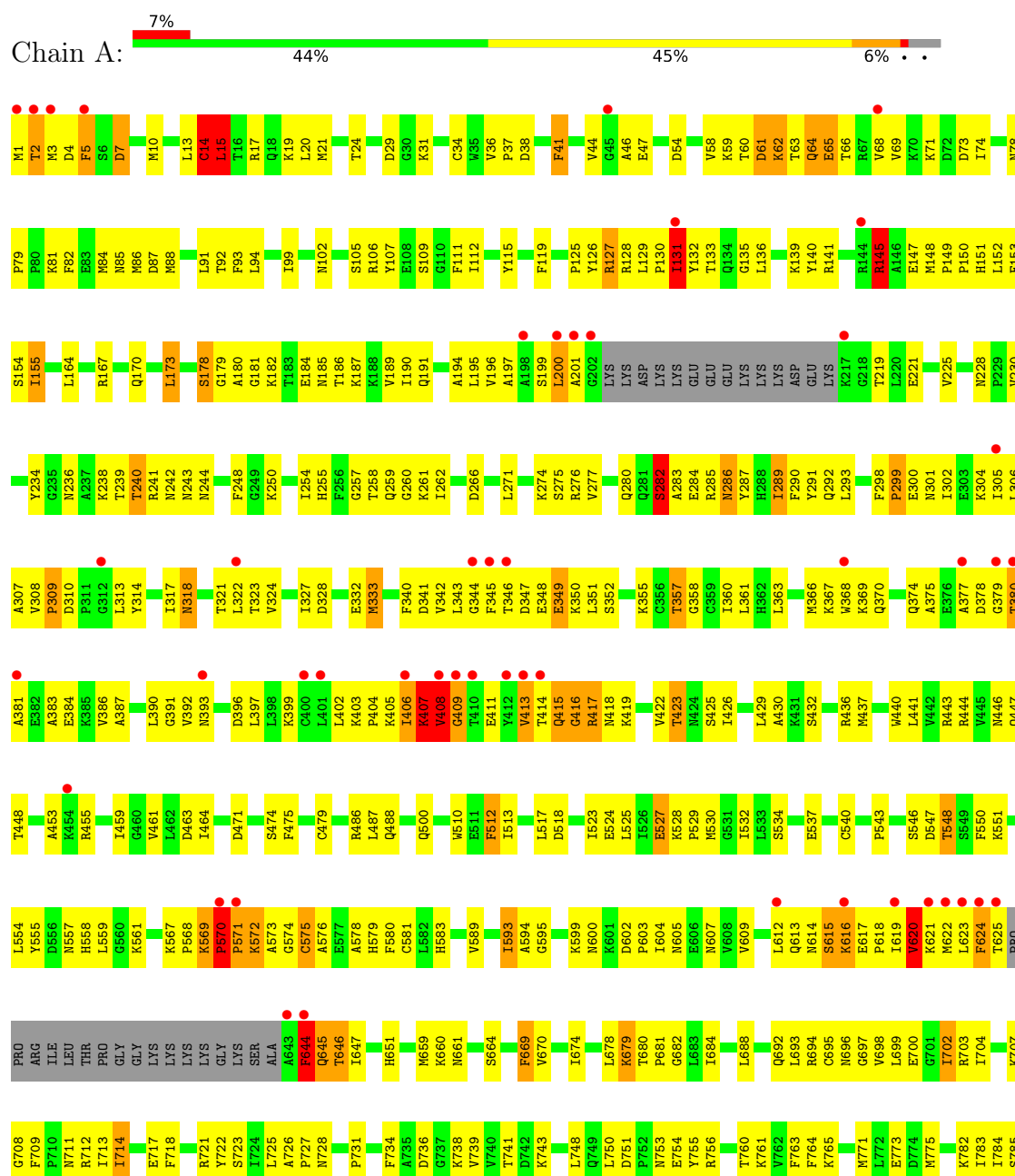
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	51	Total	O	0	0
			51	51		
6	C	28	Total	O	0	0
			28	28		

3 Residue-property plots

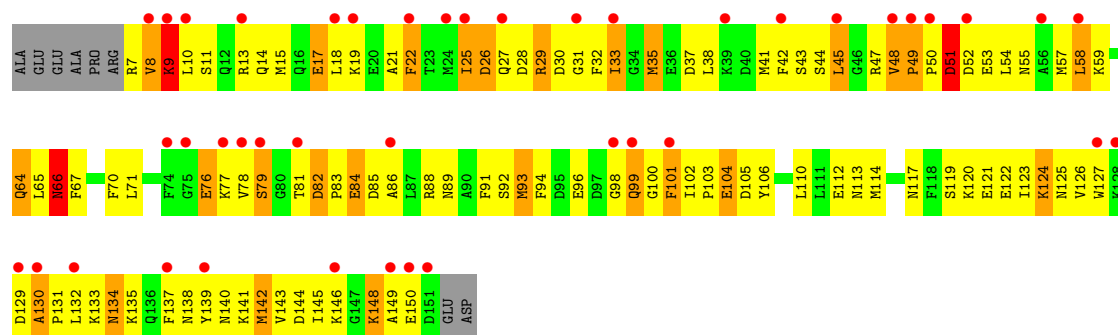
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Myosin heavy chain isoform A

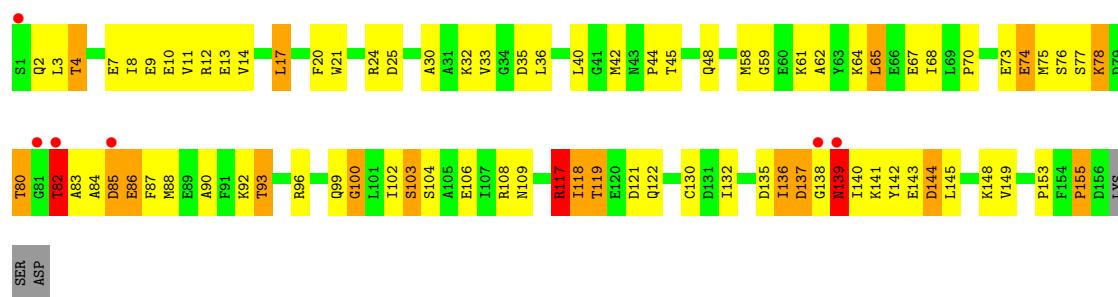




- Molecule 2: Myosin regulatory light chain LC-2, mantle muscle



- 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	194.14Å 101.75Å 80.65Å 90.00° 105.74° 90.00°	Depositor
Resolution (Å)	46.73 – 2.60 46.73 – 2.61	Depositor EDS
% Data completeness (in resolution range)	92.3 (46.73-2.60) 93.4 (46.73-2.61)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.252 , 0.297 0.251 , 0.295	Depositor DCC
R_{free} test set	4327 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8985	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: MLI, 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	0.52	1/6631 (0.0%)	1.05	46/8938 (0.5%)
2	B	0.41	0/1186	1.28	9/1588 (0.6%)
3	C	0.57	1/1258 (0.1%)	1.15	10/1687 (0.6%)
All	All	0.52	2/9075 (0.0%)	1.10	65/12213 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	80	THR	CA-CB	5.80	1.60	1.52
1	A	796	MET	SD-CE	-5.14	1.66	1.79

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100	GLY	N-CA-C	-18.92	93.34	113.58
2	B	48	VAL	N-CA-C	10.79	119.05	109.02
2	B	102	ILE	N-CA-C	10.51	120.42	108.96
2	B	149	ALA	N-CA-C	-8.96	100.76	112.41
3	C	84	ALA	N-CA-C	-8.73	101.72	111.07
2	B	76	GLU	N-CA-C	-8.26	104.34	114.75
1	A	409	GLY	N-CA-C	-7.99	103.20	115.66
3	C	144	ASP	N-CA-C	-7.58	102.96	111.07
1	A	557	ASN	N-CA-C	7.51	120.35	111.71
3	C	138	GLY	N-CA-C	-7.42	95.58	113.18
1	A	349	GLU	N-CA-C	-7.37	103.18	111.14
1	A	343	LEU	N-CA-C	-7.34	104.20	113.01
3	C	74	GLU	N-CA-C	-7.25	103.07	110.97
1	A	15	LEU	N-CA-C	-7.15	95.57	110.80
1	A	697	GLY	N-CA-C	-7.00	105.40	115.27
1	A	527	GLU	N-CA-C	7.00	122.10	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	LYS	CA-C-N	6.82	127.40	120.38
1	A	569	LYS	C-N-CA	6.82	127.40	120.38
1	A	595	GLY	N-CA-C	6.81	123.19	115.08
1	A	14	CYS	N-CA-C	6.76	123.68	110.56
2	B	101	PHE	N-CA-C	6.74	125.16	110.80
2	B	82	ASP	N-CA-C	-6.60	101.75	109.93
1	A	131	ILE	N-CA-C	6.48	122.82	109.34
1	A	837	PRO	N-CA-C	-6.38	105.54	113.84
3	C	139	ASN	N-CA-C	6.20	124.01	110.80
1	A	180	ALA	N-CA-C	-6.12	105.97	113.50
3	C	93	THR	N-CA-C	-6.05	104.75	111.71
1	A	615	SER	CB-CA-C	-6.02	109.64	116.63
2	B	44	SER	N-CA-C	-5.94	106.09	113.15
1	A	572	LYS	N-CA-C	5.87	118.42	109.62
1	A	304	LYS	N-CA-C	-5.85	105.03	111.82
1	A	471	ASP	N-CA-C	-5.79	105.47	112.54
1	A	669	PHE	N-CA-C	5.78	118.30	108.02
1	A	271	LEU	N-CA-C	5.69	119.24	111.39
1	A	554	LEU	N-CA-C	-5.69	104.46	111.40
3	C	82	THR	N-CA-C	5.64	122.81	110.80
1	A	646	THR	N-CA-C	5.63	117.75	109.24
1	A	109	SER	N-CA-C	-5.61	104.68	112.30
1	A	645	GLN	N-CA-C	5.59	122.70	110.80
1	A	2	THR	N-CA-C	5.52	117.66	108.99
1	A	333	MET	N-CA-C	-5.51	105.38	111.71
1	A	357	THR	N-CA-C	-5.45	105.24	111.07
1	A	318	ASN	N-CA-C	5.44	119.77	113.18
1	A	21	MET	N-CA-C	-5.43	104.60	111.11
1	A	614	ASN	N-CA-C	5.39	117.88	109.52
1	A	695	CYS	CA-C-N	5.32	127.41	120.28
1	A	695	CYS	C-N-CA	5.32	127.41	120.28
1	A	7	ASP	CA-C-N	5.32	126.49	119.84
1	A	7	ASP	C-N-CA	5.32	126.49	119.84
3	C	100	GLY	N-CA-C	-5.29	107.74	115.63
1	A	408	VAL	N-CA-C	-5.25	98.42	109.34
2	B	100	GLY	CA-C-O	5.20	124.25	119.83
1	A	407	LYS	N-CA-C	5.19	121.85	110.80
1	A	512	PHE	N-CA-C	5.15	117.07	108.99
1	A	34	CYS	N-CA-C	5.13	115.11	107.88
1	A	615	SER	N-CA-C	5.08	116.66	108.08
1	A	145	ARG	N-CA-C	5.07	121.61	110.80
1	A	447	GLN	N-CA-C	-5.06	105.84	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	PRO	CA-C-N	5.04	125.32	119.47
1	A	79	PRO	C-N-CA	5.04	125.32	119.47
1	A	558	HIS	N-CA-C	5.04	121.53	110.80
1	A	600	ASN	N-CA-C	5.04	118.58	112.23
3	C	45	THR	N-CA-C	-5.02	103.78	110.55
3	C	64	LYS	N-CA-C	-5.02	103.32	110.59
1	A	488	GLN	N-CA-C	-5.00	105.91	111.36

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	466	0
2	B	1166	0	1125	139	0
3	C	1239	0	1190	79	0
4	A	7	0	2	0	0
5	C	1	0	0	0	0
6	A	51	0	0	3	0
6	C	28	0	0	2	0
All	All	8985	0	8813	654	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 37.

All (654) 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:167:ARG:HH22	1:A:258:THR:HG23	1.13	1.10
1:A:191:GLN:HG2	1:A:221:GLU:HG2	1.28	1.08
1:A:259:GLN:HB2	1:A:261:LYS:HD3	1.39	1.04
2:B:9:LYS:HA	2:B:9:LYS:HE3	1.40	1.04
1:A:750:LEU:HD13	1:A:771:MET:HE1	1.48	0.96
1:A:133:THR:HG22	1:A:135:GLY:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LYS:HB3	1:A:415:GLN:HG3	1.50	0.91
1:A:786:MET:HE1	3:C:80:THR:O	1.71	0.90
1:A:678:LEU:O	1:A:680:THR:HG23	1.71	0.89
1:A:404:PRO:HB2	1:A:607:ASN:ND2	1.87	0.88
1:A:408:VAL:HG12	1:A:409:GLY:H	1.39	0.88
1:A:479:CYS:HB3	1:A:651:HIS:CE1	2.08	0.87
1:A:796:MET:HE3	3:C:35:ASP:CG	2.00	0.87
1:A:84:MET:HE1	1:A:105:SER:HB2	1.57	0.86
1:A:78:ASN:OD1	1:A:93:PHE:HB2	1.74	0.86
1:A:836:LYS:NZ	2:B:21:ALA:HB2	1.90	0.86
1:A:191:GLN:CG	1:A:221:GLU:HG2	2.04	0.86
1:A:550:PHE:HE2	1:A:593:ILE:HD12	1.41	0.85
3:C:82:THR:HG21	3:C:87:PHE:CE2	2.12	0.85
1:A:234:TYR:CZ	1:A:289:ILE:HD12	2.10	0.85
1:A:13:LEU:HD21	1:A:131:ILE:HG23	1.59	0.85
3:C:130:CYS:O	3:C:148:LYS:HD3	1.76	0.85
1:A:86:MET:CE	1:A:149:PRO:HA	2.08	0.84
1:A:817:VAL:HA	2:B:146:LYS:NZ	1.92	0.84
2:B:25:ILE:HG22	2:B:37:ASP:HB3	1.59	0.84
1:A:524:GLU:O	1:A:528:LYS:HG2	1.78	0.83
2:B:84:GLU:HG3	2:B:85:ASP:H	1.42	0.83
1:A:612:LEU:HB3	1:A:623:LEU:HD13	1.57	0.83
2:B:142:MET:HE1	2:B:146:LYS:HD3	1.58	0.83
1:A:230:VAL:HG11	1:A:441:LEU:HD11	1.61	0.83
3:C:70:PRO:O	3:C:74:GLU:HG2	1.78	0.83
2:B:101:PHE:HD1	2:B:138:ASN:HA	1.44	0.82
1:A:54:ASP:HA	1:A:71:LYS:HD3	1.61	0.82
1:A:437:MET:HG3	1:A:622:MET:HE1	1.60	0.81
1:A:167:ARG:HH22	1:A:258:THR:CG2	1.94	0.80
1:A:239:THR:O	1:A:241:ARG:N	2.14	0.80
1:A:817:VAL:HA	2:B:146:LYS:HZ1	1.46	0.80
1:A:324:VAL:O	1:A:327:ILE:HG22	1.80	0.80
1:A:834:LYS:HD2	2:B:45:LEU:HD11	1.62	0.80
2:B:131:PRO:HB3	2:B:141:LYS:HD3	1.63	0.79
1:A:805:ASP:HB3	2:B:93:MET:HE1	1.63	0.79
1:A:86:MET:HE3	1:A:149:PRO:HA	1.64	0.78
1:A:300:GLU:HG3	1:A:301:ASN:H	1.49	0.78
3:C:90:ALA:O	3:C:93:THR:HG22	1.84	0.78
2:B:28:ASP:OD1	2:B:29:ARG:HG2	1.83	0.78
1:A:617:GLU:O	1:A:620:VAL:HG23	1.84	0.78
1:A:293:LEU:HA	1:A:333:MET:HE3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LYS:O	1:A:408:VAL:HG23	1.84	0.77
2:B:7:ARG:C	2:B:9:LYS:H	1.90	0.77
1:A:86:MET:HE3	1:A:150:PRO:HD3	1.66	0.76
1:A:167:ARG:NH2	1:A:258:THR:HG23	1.97	0.76
1:A:248:PHE:HE1	1:A:250:LYS:HB3	1.50	0.76
1:A:408:VAL:HG12	1:A:409:GLY:N	1.98	0.76
2:B:7:ARG:O	2:B:78:VAL:HG11	1.86	0.75
2:B:142:MET:CE	2:B:146:LYS:HD3	2.16	0.75
1:A:240:THR:H	1:A:284:GLU:HG2	1.51	0.75
1:A:786:MET:SD	3:C:82:THR:OG1	2.45	0.75
1:A:1:MET:SD	1:A:20:LEU:HD22	2.27	0.75
1:A:406:ILE:HG22	1:A:407:LYS:N	2.01	0.74
1:A:620:VAL:HG12	1:A:624:PHE:CE1	2.23	0.74
2:B:28:ASP:HB2	2:B:37:ASP:OD2	1.87	0.74
3:C:132:ILE:HD13	3:C:145:LEU:HA	1.68	0.74
2:B:145:ILE:HA	2:B:148:LYS:HD3	1.68	0.74
1:A:819:LYS:HE2	2:B:79:SER:HB2	1.70	0.73
2:B:119:SER:O	2:B:123:ILE:HG13	1.89	0.73
1:A:88:MET:HE3	1:A:102:ASN:HB3	1.70	0.72
1:A:300:GLU:HG3	1:A:301:ASN:N	2.03	0.72
1:A:513:ILE:HG12	1:A:517:LEU:HD12	1.72	0.72
1:A:191:GLN:HG2	1:A:221:GLU:CG	2.13	0.72
3:C:88:MET:HE3	3:C:142:TYR:HE1	1.53	0.72
1:A:190:ILE:HG12	1:A:254:ILE:HD11	1.71	0.71
1:A:298:PHE:HB3	1:A:301:ASN:HD22	1.56	0.71
1:A:292:GLN:HB3	1:A:333:MET:HE2	1.73	0.71
2:B:42:PHE:HA	2:B:45:LEU:HB2	1.73	0.71
1:A:86:MET:CE	1:A:150:PRO:HD3	2.20	0.70
3:C:132:ILE:CD1	3:C:145:LEU:HA	2.21	0.70
1:A:571:PRO:HB2	1:A:575:CYS:HB3	1.72	0.70
2:B:101:PHE:HB2	2:B:137:PHE:O	1.91	0.70
2:B:28:ASP:HB2	2:B:37:ASP:CG	2.17	0.70
2:B:38:LEU:HB3	2:B:54:LEU:HD11	1.74	0.70
2:B:26:ASP:C	2:B:28:ASP:H	1.98	0.70
2:B:131:PRO:HB2	2:B:138:ASN:HB3	1.74	0.70
1:A:236:ASN:HD22	1:A:244:ASN:ND2	1.90	0.70
1:A:310:ASP:HB3	1:A:313:LEU:HD12	1.74	0.69
2:B:7:ARG:C	2:B:9:LYS:N	2.47	0.69
3:C:3:LEU:HD21	3:C:73:GLU:HB3	1.74	0.69
1:A:259:GLN:H	1:A:261:LYS:HE2	1.56	0.69
2:B:26:ASP:CG	2:B:27:GLN:H	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LYS:CB	1:A:415:GLN:HG3	2.23	0.69
1:A:713:ILE:HD12	1:A:713:ILE:N	2.08	0.69
1:A:88:MET:CE	1:A:99:ILE:HA	2.22	0.68
1:A:302:ILE:HG21	1:A:309:PRO:HD3	1.75	0.68
1:A:834:LYS:O	1:A:837:PRO:HD2	1.94	0.68
1:A:195:LEU:O	1:A:199:SER:HB2	1.94	0.68
1:A:802:LYS:O	1:A:806:GLN:HG3	1.93	0.68
1:A:58:VAL:HG12	1:A:59:LYS:N	2.08	0.67
3:C:88:MET:HE1	3:C:143:GLU:HB2	1.75	0.67
1:A:3:MET:HE2	1:A:3:MET:H	1.60	0.67
1:A:360:ILE:HA	1:A:363:LEU:HD12	1.77	0.67
1:A:36:VAL:CG2	1:A:69:VAL:HG21	2.24	0.67
1:A:58:VAL:CG1	1:A:59:LYS:N	2.58	0.67
2:B:8:VAL:C	2:B:10:LEU:H	2.01	0.67
3:C:14:VAL:HG12	3:C:36:LEU:HD12	1.77	0.67
1:A:82:PHE:O	1:A:85:ASN:HB2	1.94	0.66
1:A:221:GLU:O	1:A:225:VAL:HG23	1.95	0.66
1:A:290:PHE:HB3	1:A:317:ILE:CD1	2.25	0.66
1:A:572:LYS:O	1:A:574:GLY:N	2.28	0.66
1:A:708:GLY:O	1:A:765:LYS:HE3	1.96	0.66
1:A:727:PRO:HG2	3:C:86:GLU:HG3	1.78	0.66
1:A:748:LEU:HD22	1:A:775:MET:HE1	1.77	0.66
1:A:133:THR:HG22	1:A:135:GLY:N	2.08	0.65
1:A:618:PRO:O	1:A:622:MET:HG3	1.96	0.65
1:A:731:PRO:HG2	1:A:734:PHE:CD1	2.32	0.65
2:B:120:LYS:HA	2:B:123:ILE:HD12	1.78	0.65
3:C:104:SER:HB3	3:C:140:ILE:HG13	1.77	0.65
2:B:8:VAL:O	2:B:10:LEU:N	2.29	0.65
3:C:153:PRO:O	3:C:155:PRO:HD3	1.97	0.65
1:A:693:LEU:HA	1:A:696:ASN:HD22	1.62	0.64
1:A:694:ARG:HG2	1:A:699:LEU:HD12	1.79	0.64
2:B:148:LYS:HE3	2:B:150:GLU:HA	1.79	0.64
1:A:182:LYS:HE3	1:A:463:ASP:OD2	1.97	0.64
1:A:248:PHE:CE1	1:A:250:LYS:HB3	2.33	0.64
1:A:836:LYS:HG2	1:A:839:LEU:HD11	1.80	0.64
1:A:1:MET:HE1	1:A:5:PHE:HB3	1.79	0.64
1:A:487:LEU:CD2	1:A:659:MET:HE1	2.28	0.64
1:A:413:VAL:C	1:A:415:GLN:H	2.06	0.63
1:A:236:ASN:HB3	1:A:244:ASN:ND2	2.13	0.63
2:B:8:VAL:C	2:B:10:LEU:N	2.56	0.63
1:A:61:ASP:O	1:A:63:THR:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLN:O	1:A:417:ARG:N	2.32	0.63
1:A:391:GLY:O	1:A:615:SER:HB3	1.99	0.63
3:C:4:THR:O	3:C:8:ILE:HG13	1.99	0.62
1:A:139:LYS:O	1:A:148:MET:HE2	1.99	0.62
2:B:94:PHE:CD2	2:B:110:LEU:HD21	2.34	0.62
1:A:404:PRO:HB2	1:A:607:ASN:HD22	1.64	0.62
1:A:374:GLN:OE1	1:A:415:GLN:HG2	2.00	0.62
2:B:26:ASP:CG	2:B:27:GLN:N	2.58	0.62
1:A:406:ILE:O	1:A:411:GLU:HG2	2.00	0.61
1:A:259:GLN:HB2	1:A:261:LYS:CD	2.25	0.61
1:A:178:SER:OG	1:A:179:GLY:N	2.33	0.61
1:A:569:LYS:HD2	1:A:569:LYS:O	2.00	0.61
1:A:74:ILE:HG13	1:A:74:ILE:O	1.99	0.61
1:A:187:LYS:O	1:A:191:GLN:HG3	2.00	0.61
1:A:194:ALA:HA	1:A:262:ILE:HD12	1.82	0.61
1:A:530:MET:HA	1:A:530:MET:HE2	1.80	0.61
3:C:135:ASP:O	3:C:136:ILE:C	2.43	0.61
1:A:391:GLY:HA3	1:A:616:LYS:HG2	1.82	0.61
1:A:619:ILE:HG23	1:A:623:LEU:HD12	1.83	0.61
1:A:709:PHE:HB3	1:A:763:PHE:HB3	1.82	0.61
1:A:10:MET:HB3	1:A:14:CYS:HB2	1.82	0.61
1:A:784:ILE:O	1:A:788:GLN:HG3	2.00	0.61
2:B:13:ARG:HD2	2:B:13:ARG:N	2.15	0.61
3:C:88:MET:HE3	3:C:142:TYR:CE1	2.36	0.61
1:A:390:LEU:HA	1:A:619:ILE:CD1	2.30	0.61
1:A:754:GLU:HA	1:A:754:GLU:OE1	2.01	0.61
2:B:122:GLU:HA	2:B:125:ASN:HD22	1.65	0.61
1:A:186:THR:HG23	1:A:461:VAL:HG11	1.82	0.61
1:A:317:ILE:CD1	1:A:361:LEU:HD21	2.30	0.61
1:A:280:GLN:HG2	1:A:285:ARG:HA	1.82	0.60
1:A:620:VAL:O	1:A:624:PHE:HB2	1.99	0.60
1:A:1:MET:HE3	1:A:15:LEU:O	2.02	0.60
1:A:321:THR:HG22	1:A:322:LEU:N	2.15	0.60
1:A:537:GLU:O	1:A:540:CYS:HB2	2.02	0.60
1:A:317:ILE:HD12	1:A:361:LEU:HD21	1.83	0.60
1:A:832:PHE:CE1	1:A:836:LYS:HE2	2.36	0.60
1:A:432:SER:O	1:A:436:ARG:HG3	2.01	0.60
1:A:1:MET:CE	1:A:5:PHE:HB3	2.32	0.60
1:A:2:THR:OG1	1:A:148:MET:HA	2.02	0.60
1:A:230:VAL:CG1	1:A:441:LEU:HD11	2.31	0.60
1:A:579:HIS:ND1	1:A:593:ILE:HB	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:ASP:OD1	3:C:136:ILE:N	2.34	0.59
1:A:54:ASP:HA	1:A:71:LYS:CD	2.32	0.59
1:A:379:GLY:C	1:A:381:ALA:H	2.10	0.59
2:B:137:PHE:HZ	2:B:142:MET:HG3	1.67	0.59
1:A:345:PHE:CE1	1:A:444:ARG:HB3	2.38	0.59
2:B:42:PHE:HA	2:B:45:LEU:CB	2.33	0.59
1:A:290:PHE:HB3	1:A:317:ILE:HD11	1.84	0.59
1:A:131:ILE:HG22	1:A:151:HIS:CE1	2.38	0.59
1:A:47:GLU:O	1:A:58:VAL:HG13	2.03	0.58
2:B:101:PHE:CD1	2:B:138:ASN:HA	2.31	0.58
2:B:123:ILE:HG22	2:B:127:TRP:CD1	2.38	0.58
1:A:258:THR:N	1:A:261:LYS:HE2	2.18	0.58
1:A:293:LEU:HD23	1:A:333:MET:CE	2.33	0.58
1:A:298:PHE:CB	1:A:301:ASN:HD22	2.15	0.58
1:A:406:ILE:HG22	1:A:407:LYS:H	1.66	0.58
3:C:14:VAL:CG1	3:C:36:LEU:HD12	2.34	0.58
1:A:836:LYS:HZ3	2:B:21:ALA:HB2	1.68	0.58
1:A:257:GLY:C	1:A:261:LYS:HE2	2.29	0.58
1:A:711:ASN:HB2	1:A:764:PHE:HB2	1.86	0.57
2:B:7:ARG:O	2:B:9:LYS:N	2.37	0.57
1:A:555:TYR:OH	1:A:567:LYS:HE3	2.04	0.57
1:A:836:LYS:HG2	1:A:839:LEU:CG	2.34	0.57
2:B:132:LEU:HD21	2:B:137:PHE:HD1	1.68	0.57
3:C:78:LYS:HA	3:C:78:LYS:HE3	1.87	0.57
1:A:436:ARG:CZ	1:A:623:LEU:HD23	2.35	0.57
3:C:99:GLN:OE1	3:C:99:GLN:HA	2.02	0.57
1:A:1:MET:N	1:A:86:MET:SD	2.74	0.57
1:A:119:PHE:CE1	1:A:698:VAL:HA	2.40	0.57
1:A:624:PHE:O	1:A:625:THR:C	2.47	0.57
1:A:755:TYR:O	1:A:756:ARG:HG2	2.05	0.57
1:A:2:THR:OG1	1:A:149:PRO:HD3	2.04	0.57
1:A:107:TYR:HA	1:A:111:PHE:O	2.05	0.57
1:A:834:LYS:C	1:A:837:PRO:HD2	2.30	0.57
1:A:305:ILE:HG23	1:A:358:GLY:HA3	1.85	0.56
3:C:82:THR:HG21	3:C:87:PHE:CZ	2.40	0.56
1:A:1:MET:CE	1:A:15:LEU:O	2.53	0.56
1:A:293:LEU:HD23	1:A:333:MET:HE3	1.87	0.56
1:A:609:VAL:HG12	1:A:613:GLN:HE21	1.71	0.56
3:C:135:ASP:O	3:C:137:ASP:N	2.38	0.56
3:C:141:LYS:HB2	3:C:144:ASP:HB2	1.87	0.56
1:A:832:PHE:HE1	1:A:836:LYS:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PRO:O	1:A:132:TYR:N	2.38	0.56
1:A:743:LYS:HD2	6:A:1062:HOH:O	2.05	0.56
3:C:80:THR:O	3:C:80:THR:HG23	2.06	0.56
1:A:36:VAL:HG21	1:A:69:VAL:HG21	1.88	0.56
2:B:25:ILE:HG12	2:B:41:MET:HE3	1.88	0.56
1:A:404:PRO:CB	1:A:607:ASN:HD22	2.19	0.56
1:A:500:GLN:HG3	1:A:510:TRP:NE1	2.21	0.56
2:B:10:LEU:HB2	2:B:78:VAL:HG21	1.88	0.56
1:A:298:PHE:HB3	1:A:301:ASN:ND2	2.19	0.56
1:A:390:LEU:HA	1:A:619:ILE:HD11	1.88	0.56
1:A:828:TRP:CZ2	2:B:57:MET:HB3	2.40	0.56
3:C:104:SER:HB3	3:C:140:ILE:CG1	2.35	0.56
1:A:259:GLN:H	1:A:261:LYS:CE	2.19	0.56
1:A:755:TYR:HA	1:A:763:PHE:O	2.06	0.56
2:B:26:ASP:C	2:B:28:ASP:N	2.64	0.55
1:A:3:MET:HE2	1:A:3:MET:N	2.20	0.55
1:A:126:TYR:O	1:A:681:PRO:HG3	2.06	0.55
1:A:347:ASP:HA	1:A:350:LYS:HB3	1.87	0.55
1:A:688:LEU:O	1:A:692:GLN:HG3	2.06	0.55
1:A:786:MET:HB3	3:C:82:THR:OG1	2.05	0.55
2:B:99:GLN:C	2:B:101:PHE:H	2.11	0.55
1:A:568:PRO:HG3	1:A:578:ALA:CB	2.36	0.55
1:A:613:GLN:HB3	1:A:624:PHE:CE2	2.41	0.55
1:A:413:VAL:CG1	1:A:413:VAL:O	2.54	0.55
1:A:739:VAL:HG13	1:A:743:LYS:HE2	1.87	0.55
1:A:151:HIS:CD2	1:A:153:PHE:H	2.24	0.55
1:A:344:GLY:O	1:A:345:PHE:CD2	2.59	0.55
1:A:529:PRO:O	1:A:530:MET:HB2	2.06	0.55
1:A:190:ILE:HG12	1:A:254:ILE:CD1	2.36	0.55
2:B:28:ASP:O	2:B:29:ARG:C	2.49	0.55
2:B:66:ASN:OD1	2:B:66:ASN:N	2.33	0.55
2:B:96:GLU:H	2:B:96:GLU:CD	2.15	0.55
1:A:88:MET:HE1	1:A:99:ILE:HG23	1.87	0.55
1:A:308:VAL:O	1:A:310:ASP:N	2.38	0.55
1:A:422:VAL:HG23	1:A:423:THR:N	2.22	0.55
3:C:117:ARG:HG3	3:C:117:ARG:HH11	1.71	0.55
1:A:550:PHE:CE2	1:A:593:ILE:HD12	2.32	0.55
2:B:142:MET:HE1	2:B:146:LYS:CD	2.36	0.55
1:A:4:ASP:HB3	1:A:7:ASP:HB2	1.89	0.54
2:B:13:ARG:O	2:B:17:GLU:HB2	2.08	0.54
1:A:525:LEU:O	1:A:532:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LYS:HE2	1:A:555:TYR:CE1	2.41	0.54
2:B:101:PHE:CZ	2:B:140:ASN:HB2	2.43	0.54
1:A:259:GLN:CB	1:A:261:LYS:HD3	2.26	0.54
1:A:819:LYS:HE3	2:B:76:GLU:O	2.08	0.54
2:B:38:LEU:CB	2:B:54:LEU:HD11	2.38	0.54
1:A:240:THR:H	1:A:284:GLU:CG	2.19	0.54
1:A:342:VAL:C	1:A:344:GLY:H	2.16	0.54
1:A:487:LEU:HD23	1:A:659:MET:HE1	1.88	0.54
1:A:704:ILE:O	1:A:707:LYS:HG2	2.08	0.54
1:A:830:ARG:O	1:A:833:ASN:HB2	2.06	0.54
2:B:26:ASP:HA	2:B:37:ASP:OD2	2.07	0.54
1:A:88:MET:HE2	1:A:99:ILE:HA	1.89	0.54
1:A:126:TYR:CE1	1:A:679:LYS:HA	2.43	0.54
1:A:513:ILE:HD11	1:A:517:LEU:HD13	1.89	0.54
3:C:153:PRO:C	3:C:155:PRO:HD3	2.33	0.54
1:A:368:TRP:HZ2	1:A:426:ILE:HD11	1.72	0.53
2:B:114:MET:HE2	3:C:21:TRP:HE3	1.71	0.53
1:A:58:VAL:CG1	1:A:59:LYS:H	2.20	0.53
1:A:693:LEU:HB3	1:A:699:LEU:HG	1.90	0.53
2:B:141:LYS:O	2:B:145:ILE:HG13	2.08	0.53
1:A:324:VAL:HB	1:A:327:ILE:HG21	1.90	0.53
1:A:793:GLY:HA3	1:A:797:ARG:HH21	1.73	0.53
1:A:817:VAL:O	1:A:821:LEU:HG	2.08	0.53
1:A:107:TYR:CD2	1:A:684:ILE:HD11	2.43	0.53
2:B:9:LYS:HA	2:B:9:LYS:CE	2.21	0.53
3:C:119:THR:HG22	3:C:121:ASP:N	2.24	0.53
1:A:46:ALA:CB	1:A:60:THR:HA	2.38	0.53
1:A:141:ARG:NH2	1:A:200:LEU:HD23	2.24	0.53
1:A:145:ARG:HG3	1:A:154:SER:OG	2.09	0.53
1:A:678:LEU:O	1:A:679:LYS:C	2.52	0.53
1:A:805:ASP:HB3	2:B:93:MET:CE	2.36	0.53
1:A:817:VAL:HA	2:B:146:LYS:HZ3	1.71	0.53
1:A:1:MET:HE2	1:A:5:PHE:CG	2.44	0.53
1:A:379:GLY:O	1:A:381:ALA:N	2.42	0.53
3:C:103:SER:HA	3:C:139:ASN:CG	2.34	0.53
1:A:133:THR:C	1:A:135:GLY:H	2.15	0.52
1:A:831:LEU:HD11	2:B:57:MET:HE1	1.90	0.52
2:B:28:ASP:HB2	2:B:37:ASP:OD1	2.09	0.52
3:C:74:GLU:O	3:C:77:SER:HB2	2.08	0.52
3:C:83:ALA:HB1	3:C:85:ASP:OD2	2.09	0.52
1:A:5:PHE:N	1:A:5:PHE:CD2	2.70	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:O	1:A:155:ILE:HG23	2.09	0.52
1:A:404:PRO:HG2	1:A:414:THR:OG1	2.08	0.52
1:A:725:LEU:HD13	1:A:748:LEU:HD11	1.91	0.52
1:A:415:GLN:O	1:A:416:GLY:C	2.52	0.52
1:A:836:LYS:HG2	1:A:839:LEU:CD1	2.38	0.52
1:A:78:ASN:ND2	1:A:92:THR:H	2.08	0.52
1:A:796:MET:HE3	3:C:35:ASP:OD1	2.10	0.52
3:C:80:THR:HA	6:C:1003:HOH:O	2.08	0.52
2:B:25:ILE:CG2	2:B:37:ASP:HB3	2.37	0.52
2:B:89:ASN:O	2:B:92:SER:HB2	2.10	0.52
1:A:2:THR:HG21	1:A:148:MET:CA	2.40	0.52
1:A:14:CYS:O	1:A:15:LEU:CB	2.58	0.52
1:A:54:ASP:OD1	1:A:71:LYS:HD3	2.10	0.52
1:A:307:ALA:HB1	1:A:314:TYR:OH	2.09	0.52
1:A:721:ARG:NH2	1:A:773:GLU:OE2	2.39	0.52
1:A:782:LYS:O	1:A:786:MET:HG3	2.10	0.52
1:A:380:THR:O	1:A:384:GLU:HG2	2.10	0.52
1:A:785:SER:HA	1:A:788:GLN:OE1	2.09	0.52
2:B:28:ASP:O	2:B:30:ASP:N	2.43	0.52
2:B:144:ASP:O	2:B:148:LYS:HA	2.10	0.51
3:C:118:ILE:HG23	3:C:122:GLN:HB2	1.93	0.51
1:A:266:ASP:HB2	1:A:446:ASN:OD1	2.10	0.51
1:A:617:GLU:C	1:A:620:VAL:HG23	2.34	0.51
1:A:568:PRO:HG3	1:A:578:ALA:HB3	1.91	0.51
2:B:65:LEU:HD11	2:B:70:PHE:HA	1.93	0.51
3:C:100:GLY:HA2	3:C:142:TYR:CE2	2.45	0.51
3:C:30:ALA:O	3:C:33:VAL:HG23	2.11	0.51
1:A:24:THR:HG22	1:A:24:THR:O	2.10	0.51
1:A:342:VAL:C	1:A:344:GLY:N	2.66	0.51
1:A:836:LYS:HZ2	2:B:21:ALA:HB2	1.72	0.51
1:A:786:MET:O	1:A:789:ALA:HB3	2.11	0.51
1:A:41:PHE:CD1	1:A:41:PHE:N	2.78	0.51
1:A:5:PHE:HD1	1:A:17:ARG:HB2	1.75	0.51
1:A:173:LEU:N	1:A:173:LEU:HD23	2.26	0.51
3:C:14:VAL:HG12	3:C:36:LEU:CD1	2.40	0.51
1:A:46:ALA:HB1	1:A:59:LYS:O	2.11	0.50
1:A:804:GLN:HG2	3:C:17:LEU:HD13	1.92	0.50
1:A:406:ILE:CG1	1:A:414:THR:HG21	2.42	0.50
1:A:437:MET:CG	1:A:622:MET:HE1	2.36	0.50
1:A:92:THR:HA	1:A:711:ASN:HD21	1.76	0.50
1:A:126:TYR:O	1:A:127:ARG:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:O	1:A:189:VAL:HG23	2.10	0.50
1:A:479:CYS:HB3	1:A:651:HIS:HE1	1.73	0.50
2:B:99:GLN:HA	2:B:101:PHE:CE2	2.46	0.50
3:C:12:ARG:NH1	3:C:65:LEU:CD2	2.75	0.50
1:A:408:VAL:CG1	1:A:409:GLY:H	2.10	0.50
1:A:812:LEU:HD22	2:B:82:ASP:CG	2.37	0.50
1:A:404:PRO:CB	1:A:607:ASN:ND2	2.67	0.50
1:A:290:PHE:HB3	1:A:317:ILE:HD13	1.94	0.50
1:A:390:LEU:O	1:A:619:ILE:HD12	2.11	0.50
1:A:440:TRP:CD1	1:A:621:LYS:HD2	2.47	0.50
1:A:199:SER:O	1:A:200:LEU:C	2.55	0.49
1:A:324:VAL:HB	1:A:327:ILE:CG2	2.42	0.49
1:A:479:CYS:HB3	1:A:651:HIS:ND1	2.27	0.49
1:A:836:LYS:C	1:A:838:LEU:N	2.65	0.49
1:A:291:TYR:CE2	1:A:317:ILE:HG23	2.47	0.49
1:A:599:LYS:O	1:A:647:ILE:HD12	2.13	0.49
1:A:181:GLY:HA2	6:A:1056:HOH:O	2.11	0.49
1:A:239:THR:O	1:A:240:THR:C	2.55	0.49
1:A:239:THR:HA	1:A:284:GLU:HG2	1.95	0.49
1:A:341:ASP:O	1:A:344:GLY:HA2	2.12	0.49
1:A:529:PRO:O	1:A:530:MET:CB	2.60	0.49
3:C:36:LEU:CD2	3:C:68:ILE:HD13	2.41	0.49
1:A:88:MET:HE1	1:A:99:ILE:HA	1.94	0.49
1:A:289:ILE:HG23	1:A:290:PHE:N	2.26	0.49
2:B:25:ILE:O	2:B:26:ASP:O	2.31	0.49
1:A:155:ILE:HD13	1:A:670:VAL:CG2	2.42	0.49
1:A:276:ARG:HG2	1:A:286:ASN:HA	1.95	0.49
1:A:523:ILE:O	1:A:527:GLU:HG2	2.13	0.49
2:B:9:LYS:HB3	2:B:78:VAL:CG1	2.42	0.49
1:A:112:ILE:HG21	1:A:125:PRO:HB3	1.95	0.49
2:B:114:MET:HE2	3:C:21:TRP:CE3	2.48	0.49
1:A:191:GLN:O	1:A:194:ALA:HB3	2.13	0.49
1:A:500:GLN:HG3	1:A:510:TRP:CD1	2.48	0.49
1:A:572:LYS:H	1:A:575:CYS:HB3	1.77	0.49
2:B:148:LYS:HG3	2:B:150:GLU:H	1.78	0.48
1:A:274:LYS:O	1:A:277:VAL:HG23	2.12	0.48
1:A:414:THR:O	1:A:416:GLY:N	2.46	0.48
1:A:826:TRP:O	1:A:827:GLU:C	2.56	0.48
3:C:36:LEU:HD21	3:C:68:ILE:HD13	1.94	0.48
3:C:85:ASP:OD2	3:C:85:ASP:N	2.35	0.48
1:A:136:LEU:O	1:A:139:LYS:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:LYS:HD3	2:B:47:ARG:NH2	2.28	0.48
2:B:85:ASP:O	2:B:86:ALA:C	2.56	0.48
1:A:61:ASP:C	1:A:63:THR:H	2.22	0.48
1:A:88:MET:HE1	1:A:99:ILE:O	2.13	0.48
2:B:88:ARG:HG2	2:B:143:VAL:HG21	1.94	0.48
3:C:30:ALA:C	3:C:32:LYS:H	2.19	0.48
3:C:100:GLY:HA2	3:C:142:TYR:CZ	2.48	0.48
1:A:255:HIS:CG	1:A:455:ARG:HD3	2.48	0.48
1:A:59:LYS:HE2	1:A:64:GLN:OE1	2.14	0.48
2:B:10:LEU:HA	2:B:14:GLN:OE1	2.14	0.48
2:B:148:LYS:HE3	2:B:150:GLU:CA	2.42	0.48
1:A:88:MET:HE1	1:A:99:ILE:CG2	2.43	0.48
1:A:133:THR:C	1:A:135:GLY:N	2.72	0.48
1:A:832:PHE:HE1	1:A:836:LYS:CE	2.27	0.48
2:B:99:GLN:HA	2:B:101:PHE:CD2	2.49	0.48
3:C:73:GLU:HA	3:C:76:SER:OG	2.13	0.48
1:A:321:THR:CG2	1:A:322:LEU:N	2.77	0.47
1:A:406:ILE:HD12	1:A:414:THR:HG21	1.96	0.47
1:A:85:ASN:HD22	1:A:86:MET:H	1.61	0.47
1:A:129:LEU:HD13	1:A:131:ILE:HD11	1.96	0.47
1:A:518:ASP:OD2	1:A:703:ARG:NH2	2.47	0.47
1:A:604:ILE:H	1:A:644:PHE:HA	1.79	0.47
1:A:621:LYS:HB3	1:A:621:LYS:HE2	1.44	0.47
1:A:645:GLN:OE1	1:A:645:GLN:HA	2.14	0.47
1:A:375:ALA:O	1:A:402:LEU:HD22	2.14	0.47
1:A:390:LEU:HD22	1:A:619:ILE:CD1	2.45	0.47
2:B:132:LEU:HD23	2:B:137:PHE:HA	1.97	0.47
1:A:236:ASN:HD22	1:A:244:ASN:HD21	1.61	0.47
1:A:317:ILE:HD12	1:A:361:LEU:CD2	2.44	0.47
1:A:513:ILE:CG1	1:A:517:LEU:HD12	2.43	0.47
2:B:85:ASP:O	2:B:88:ARG:N	2.47	0.47
2:B:101:PHE:HD1	2:B:138:ASN:CA	2.22	0.47
1:A:88:MET:CE	1:A:99:ILE:HG23	2.44	0.47
1:A:282:SER:HB3	1:A:283:ALA:H	1.55	0.47
1:A:242:ASN:HD22	1:A:243:ASN:N	2.13	0.47
1:A:258:THR:HG22	1:A:258:THR:O	2.15	0.47
1:A:298:PHE:N	1:A:299:PRO:HD3	2.30	0.47
1:A:559:LEU:C	1:A:561:LYS:H	2.23	0.47
1:A:786:MET:CB	3:C:82:THR:OG1	2.63	0.47
2:B:9:LYS:O	2:B:11:SER:N	2.46	0.47
3:C:11:VAL:HA	3:C:40:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:HA	2:B:67:PHE:CE1	2.50	0.47
2:B:25:ILE:HG23	2:B:37:ASP:O	2.14	0.47
2:B:144:ASP:O	2:B:148:LYS:N	2.48	0.47
3:C:132:ILE:HA	6:C:1004:HOH:O	2.14	0.47
1:A:141:ARG:HH22	1:A:200:LEU:HD23	1.80	0.47
1:A:289:ILE:HD13	1:A:357:THR:HG21	1.96	0.47
1:A:486:ARG:HG2	1:A:523:ILE:HD13	1.97	0.47
1:A:644:PHE:CD1	1:A:644:PHE:N	2.82	0.47
2:B:66:ASN:HB2	2:B:67:PHE:H	1.49	0.47
3:C:44:PRO:HA	3:C:48:GLN:OE1	2.15	0.47
1:A:184:GLU:O	1:A:187:LYS:HB3	2.15	0.46
1:A:711:ASN:C	1:A:712:ARG:HG3	2.40	0.46
2:B:129:ASP:CG	2:B:130:ALA:N	2.73	0.46
1:A:2:THR:HB	1:A:147:GLU:O	2.14	0.46
1:A:64:GLN:O	1:A:65:GLU:HB2	2.14	0.46
1:A:141:ARG:HD3	1:A:196:VAL:HG12	1.97	0.46
1:A:669:PHE:N	1:A:669:PHE:CD1	2.84	0.46
1:A:58:VAL:O	1:A:66:THR:HA	2.16	0.46
1:A:239:THR:O	1:A:242:ASN:N	2.44	0.46
1:A:546:SER:C	1:A:548:THR:N	2.71	0.46
1:A:572:LYS:HB3	1:A:575:CYS:HB2	1.97	0.46
1:A:661:ASN:N	1:A:661:ASN:HD22	2.14	0.46
1:A:760:THR:OG1	1:A:761:LYS:HG3	2.14	0.46
1:A:513:ILE:HD11	1:A:517:LEU:CD1	2.45	0.46
2:B:142:MET:HE1	2:B:146:LYS:NZ	2.30	0.46
1:A:151:HIS:HD2	1:A:153:PHE:H	1.60	0.46
1:A:391:GLY:O	1:A:615:SER:CB	2.64	0.46
2:B:35:MET:CE	2:B:54:LEU:HD23	2.46	0.46
1:A:63:THR:O	1:A:64:GLN:O	2.33	0.46
1:A:321:THR:HG22	1:A:323:THR:H	1.81	0.46
3:C:135:ASP:OD1	3:C:136:ILE:HG13	2.16	0.46
1:A:46:ALA:HA	1:A:61:ASP:OD1	2.15	0.46
1:A:179:GLY:C	1:A:674:ILE:HG12	2.41	0.46
2:B:9:LYS:HE3	2:B:9:LYS:CA	2.28	0.46
3:C:88:MET:O	3:C:92:LYS:HG3	2.16	0.46
1:A:547:ASP:OD2	1:A:594:ALA:HA	2.15	0.46
3:C:96:ARG:NH2	3:C:106:GLU:OE2	2.49	0.46
3:C:132:ILE:HD13	3:C:145:LEU:CA	2.44	0.46
1:A:88:MET:HE1	1:A:99:ILE:CA	2.45	0.46
1:A:141:ARG:NH1	1:A:199:SER:OG	2.48	0.46
1:A:1:MET:HE2	1:A:5:PHE:CD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLY:O	1:A:361:LEU:HB2	2.16	0.45
1:A:714:ILE:HG13	1:A:717:GLU:OE1	2.16	0.45
2:B:122:GLU:O	2:B:126:VAL:HG23	2.15	0.45
1:A:196:VAL:HA	1:A:199:SER:HB2	1.97	0.45
1:A:238:LYS:HD2	1:A:324:VAL:HG22	1.99	0.45
1:A:197:ALA:HB2	1:A:262:ILE:HG13	1.98	0.45
1:A:620:VAL:O	1:A:621:LYS:C	2.59	0.45
1:A:831:LEU:HD21	2:B:42:PHE:CZ	2.51	0.45
1:A:2:THR:HG1	1:A:148:MET:HA	1.80	0.45
1:A:131:ILE:O	1:A:151:HIS:HE1	2.00	0.45
1:A:436:ARG:HH11	1:A:623:LEU:HA	1.81	0.45
1:A:748:LEU:HD23	1:A:748:LEU:HA	1.83	0.45
2:B:119:SER:C	2:B:121:GLU:N	2.75	0.45
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.81	0.45
1:A:386:VAL:HG23	1:A:387:ALA:N	2.32	0.45
1:A:819:LYS:HD2	1:A:819:LYS:HA	1.86	0.45
2:B:26:ASP:CG	2:B:31:GLY:HA2	2.41	0.45
3:C:42:MET:HE1	3:C:75:MET:HG3	1.98	0.45
3:C:139:ASN:HB3	3:C:140:ILE:H	1.37	0.45
1:A:2:THR:HG21	1:A:148:MET:HA	1.98	0.45
1:A:63:THR:O	1:A:64:GLN:HB2	2.17	0.45
1:A:807:ARG:HG3	3:C:20:PHE:CD2	2.52	0.45
1:A:293:LEU:N	1:A:333:MET:HE2	2.32	0.45
1:A:351:LEU:HD21	1:A:355:LYS:HE3	1.97	0.45
1:A:593:ILE:HD13	1:A:593:ILE:HA	1.61	0.45
1:A:783:ILE:HA	1:A:786:MET:HG3	1.98	0.45
2:B:106:TYR:CE2	2:B:110:LEU:HD13	2.52	0.45
3:C:9:GLU:OE1	3:C:9:GLU:HA	2.17	0.45
1:A:24:THR:O	1:A:24:THR:CG2	2.64	0.45
1:A:546:SER:C	1:A:548:THR:H	2.25	0.45
1:A:581:CYS:HB2	1:A:589:VAL:O	2.17	0.45
2:B:84:GLU:HG3	2:B:85:ASP:N	2.22	0.45
2:B:98:GLY:O	2:B:99:GLN:O	2.35	0.45
1:A:194:ALA:HA	1:A:262:ILE:CD1	2.45	0.44
1:A:406:ILE:HG13	1:A:414:THR:HG21	1.98	0.44
1:A:579:HIS:ND1	1:A:593:ILE:N	2.56	0.44
3:C:82:THR:CG2	3:C:87:PHE:CZ	3.00	0.44
1:A:369:LYS:HD2	1:A:370:GLN:H	1.82	0.44
2:B:25:ILE:HG21	2:B:33:ILE:HG23	2.00	0.44
1:A:36:VAL:HG12	1:A:44:VAL:O	2.18	0.44
1:A:37:PRO:HD3	6:A:1035:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ARG:NH1	1:A:623:LEU:HA	2.31	0.44
1:A:128:ARG:HG2	1:A:128:ARG:NH1	2.32	0.44
1:A:230:VAL:HG12	1:A:441:LEU:HD21	1.98	0.44
1:A:286:ASN:OD1	1:A:287:TYR:N	2.41	0.44
1:A:348:GLU:O	1:A:351:LEU:HB3	2.17	0.44
1:A:86:MET:HE3	1:A:149:PRO:CA	2.42	0.44
1:A:87:ASP:HA	1:A:115:TYR:O	2.18	0.44
1:A:379:GLY:C	1:A:381:ALA:N	2.74	0.44
1:A:413:VAL:O	1:A:413:VAL:HG13	2.17	0.44
1:A:836:LYS:HE3	2:B:17:GLU:CD	2.42	0.44
2:B:48:VAL:HA	2:B:49:PRO:HD3	1.63	0.44
2:B:55:ASN:O	2:B:58:LEU:HB2	2.17	0.44
2:B:96:GLU:CD	2:B:96:GLU:N	2.75	0.44
3:C:117:ARG:HG3	3:C:117:ARG:NH1	2.33	0.44
1:A:2:THR:OG1	1:A:149:PRO:CD	2.65	0.44
1:A:64:GLN:OE1	1:A:64:GLN:HA	2.18	0.44
1:A:91:LEU:HB2	1:A:94:LEU:CD2	2.48	0.44
1:A:736:ASP:OD1	1:A:738:LYS:N	2.51	0.44
1:A:700:GLU:CD	1:A:703:ARG:NH1	2.76	0.44
1:A:292:GLN:C	1:A:333:MET:HE2	2.43	0.44
1:A:413:VAL:C	1:A:415:GLN:N	2.74	0.44
2:B:104:GLU:O	2:B:105:ASP:C	2.61	0.44
1:A:85:ASN:ND2	1:A:86:MET:N	2.66	0.44
1:A:437:MET:HA	1:A:622:MET:HE3	1.99	0.44
3:C:67:GLU:O	3:C:70:PRO:HG2	2.17	0.44
2:B:32:PHE:CE2	2:B:64:GLN:NE2	2.86	0.43
3:C:119:THR:HG22	3:C:121:ASP:H	1.82	0.43
1:A:238:LYS:HD2	1:A:324:VAL:HG13	2.01	0.43
2:B:132:LEU:CD2	2:B:137:PHE:HD1	2.31	0.43
3:C:118:ILE:CG2	3:C:119:THR:N	2.80	0.43
1:A:832:PHE:CE1	1:A:836:LYS:CE	3.00	0.43
2:B:38:LEU:O	2:B:41:MET:HB3	2.18	0.43
2:B:137:PHE:CZ	2:B:142:MET:HG3	2.50	0.43
1:A:440:TRP:CD1	1:A:621:LYS:HZ2	2.36	0.43
1:A:617:GLU:HA	1:A:620:VAL:CG2	2.49	0.43
1:A:71:LYS:O	1:A:74:ILE:HG12	2.19	0.43
1:A:474:SER:OG	1:A:475:PHE:N	2.50	0.43
2:B:134:ASN:HD22	2:B:134:ASN:HA	1.59	0.43
1:A:396:ASP:O	1:A:399:LYS:HB2	2.19	0.43
1:A:512:PHE:CE2	1:A:707:LYS:HD3	2.54	0.43
1:A:645:GLN:HB3	1:A:646:THR:H	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:ASP:C	1:A:753:ASN:H	2.27	0.43
1:A:830:ARG:O	1:A:834:LYS:HG3	2.18	0.43
2:B:10:LEU:HG	2:B:15:MET:CG	2.49	0.43
2:B:51:ASP:O	2:B:52:ASP:C	2.61	0.43
2:B:124:LYS:C	2:B:126:VAL:N	2.75	0.43
1:A:61:ASP:C	1:A:63:THR:N	2.75	0.43
1:A:86:MET:HE2	1:A:150:PRO:HD3	1.99	0.43
1:A:404:PRO:C	1:A:405:LYS:HG3	2.44	0.43
1:A:809:GLY:O	1:A:813:ILE:HG13	2.18	0.43
1:A:836:LYS:C	1:A:838:LEU:H	2.26	0.43
3:C:65:LEU:HD12	3:C:65:LEU:O	2.18	0.43
1:A:129:LEU:CD1	1:A:131:ILE:HD11	2.49	0.43
1:A:352:SER:HB3	1:A:618:PRO:HG3	2.00	0.43
1:A:660:LYS:HD2	1:A:660:LYS:O	2.19	0.43
2:B:50:PRO:HB2	2:B:53:GLU:HG3	2.01	0.43
1:A:190:ILE:CG1	1:A:254:ILE:HD11	2.44	0.42
1:A:230:VAL:CG1	1:A:441:LEU:HD21	2.49	0.42
1:A:425:SER:OG	1:A:605:ASN:ND2	2.52	0.42
1:A:440:TRP:HD1	1:A:443:ARG:NH1	2.17	0.42
1:A:530:MET:HE2	1:A:530:MET:CA	2.48	0.42
1:A:836:LYS:HG2	1:A:839:LEU:HG	2.00	0.42
1:A:383:ALA:HA	1:A:386:VAL:HG22	2.01	0.42
1:A:550:PHE:HE2	1:A:593:ILE:CD1	2.22	0.42
1:A:793:GLY:HA3	1:A:797:ARG:NH2	2.34	0.42
2:B:43:SER:C	2:B:45:LEU:H	2.26	0.42
3:C:102:ILE:HG13	3:C:142:TYR:HD2	1.83	0.42
1:A:293:LEU:HD23	1:A:333:MET:HE1	2.00	0.42
1:A:731:PRO:HG2	1:A:734:PHE:HD1	1.82	0.42
2:B:112:GLU:HG3	2:B:123:ILE:HD11	2.02	0.42
1:A:1:MET:CE	1:A:5:PHE:CG	3.03	0.42
1:A:407:LYS:HA	1:A:411:GLU:HA	2.00	0.42
2:B:35:MET:HE2	2:B:35:MET:HB3	1.91	0.42
2:B:50:PRO:HB2	2:B:53:GLU:CD	2.45	0.42
1:A:91:LEU:HB2	1:A:94:LEU:HD23	2.00	0.42
1:A:170:GLN:HB2	1:A:459:ILE:HG12	2.01	0.42
2:B:103:PRO:O	2:B:104:GLU:C	2.61	0.42
3:C:4:THR:HG23	3:C:7:GLU:HG3	2.00	0.42
1:A:782:LYS:HZ3	3:C:80:THR:HG21	1.84	0.42
2:B:28:ASP:CB	2:B:32:PHE:O	2.67	0.42
2:B:41:MET:C	2:B:43:SER:H	2.28	0.42
2:B:124:LYS:O	2:B:125:ASN:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:O	1:A:308:VAL:HG23	2.19	0.42
1:A:603:PRO:CB	1:A:644:PHE:HB3	2.50	0.42
1:A:61:ASP:HB2	1:A:62:LYS:H	1.67	0.42
1:A:345:PHE:HE1	1:A:444:ARG:HB3	1.83	0.42
1:A:375:ALA:HB2	1:A:418:ASN:C	2.45	0.42
1:A:579:HIS:O	1:A:580:PHE:HB3	2.18	0.42
1:A:829:TRP:HZ3	2:B:77:LYS:HD3	1.84	0.42
1:A:24:THR:HG23	1:A:81:LYS:HA	2.01	0.42
1:A:352:SER:CB	1:A:618:PRO:HG3	2.49	0.42
1:A:793:GLY:CA	1:A:797:ARG:HH21	2.32	0.42
1:A:836:LYS:O	1:A:839:LEU:HG	2.20	0.42
2:B:15:MET:HE2	2:B:71:LEU:HD13	2.01	0.42
2:B:22:PHE:CE2	2:B:66:ASN:O	2.72	0.42
2:B:58:LEU:HD23	2:B:58:LEU:HA	1.90	0.42
2:B:88:ARG:CG	2:B:143:VAL:HG11	2.50	0.42
3:C:102:ILE:HG13	3:C:142:TYR:CD2	2.55	0.42
3:C:130:CYS:HB2	3:C:132:ILE:HD12	2.01	0.42
1:A:698:VAL:O	1:A:702:ILE:HD12	2.20	0.42
2:B:134:ASN:O	2:B:135:LYS:C	2.63	0.42
2:B:145:ILE:O	2:B:148:LYS:HB2	2.19	0.42
3:C:119:THR:CG2	3:C:121:ASP:H	2.33	0.42
1:A:140:TYR:O	1:A:141:ARG:C	2.62	0.41
1:A:236:ASN:HB3	1:A:244:ASN:HD21	1.82	0.41
1:A:314:TYR:C	1:A:318:ASN:ND2	2.78	0.41
2:B:119:SER:C	2:B:121:GLU:H	2.27	0.41
1:A:58:VAL:HG13	1:A:59:LYS:H	1.85	0.41
1:A:568:PRO:CG	1:A:578:ALA:HB3	2.50	0.41
3:C:61:LYS:HG2	3:C:62:ALA:N	2.35	0.41
1:A:368:TRP:O	1:A:419:LYS:HE3	2.21	0.41
1:A:415:GLN:C	1:A:417:ARG:N	2.77	0.41
1:A:602:ASP:N	1:A:603:PRO:CD	2.84	0.41
1:A:700:GLU:OE2	1:A:703:ARG:NH1	2.50	0.41
1:A:718:PHE:CD2	1:A:741:THR:HG23	2.55	0.41
2:B:78:VAL:O	2:B:79:SER:C	2.63	0.41
1:A:512:PHE:HZ	1:A:707:LYS:O	2.03	0.41
2:B:150:GLU:HA	2:B:150:GLU:OE1	2.21	0.41
1:A:71:LYS:C	1:A:73:ASP:H	2.27	0.41
1:A:709:PHE:CD2	1:A:765:LYS:HG2	2.56	0.41
1:A:85:ASN:O	1:A:106:ARG:HD2	2.21	0.41
1:A:414:THR:C	1:A:416:GLY:H	2.27	0.41
1:A:429:LEU:O	1:A:430:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:PRO:HG2	2:B:53:GLU:OE1	2.21	0.41
1:A:396:ASP:O	1:A:397:LEU:C	2.63	0.41
2:B:133:LYS:O	2:B:134:ASN:C	2.64	0.41
3:C:10:GLU:O	3:C:11:VAL:C	2.63	0.41
1:A:15:LEU:HD12	1:A:19:LYS:HD3	2.03	0.41
1:A:366:MET:HE2	1:A:368:TRP:CZ2	2.55	0.41
1:A:754:GLU:OE1	1:A:754:GLU:CA	2.67	0.41
1:A:38:ASP:OD2	1:A:44:VAL:HG21	2.20	0.41
1:A:46:ALA:HB2	1:A:60:THR:HA	2.02	0.41
1:A:615:SER:O	1:A:616:LYS:C	2.63	0.41
1:A:722:TYR:O	1:A:723:SER:C	2.64	0.41
2:B:14:GLN:O	2:B:18:LEU:HG	2.21	0.41
1:A:29:ASP:C	1:A:31:LYS:N	2.79	0.41
1:A:328:ASP:O	1:A:332:GLU:HG2	2.21	0.41
1:A:569:LYS:HA	1:A:570:PRO:HD3	1.97	0.41
1:A:726:ALA:N	1:A:727:PRO:HD3	2.36	0.41
1:A:68:VAL:O	1:A:68:VAL:HG12	2.21	0.40
1:A:164:LEU:HD21	1:A:260:GLY:HA2	2.02	0.40
1:A:392:VAL:HG12	1:A:393:ASN:N	2.36	0.40
1:A:487:LEU:HD21	1:A:659:MET:HE1	2.01	0.40
1:A:728:ASN:OD1	1:A:728:ASN:C	2.63	0.40
1:A:756:ARG:HG2	1:A:756:ARG:NH1	2.35	0.40
1:A:820:TRP:CE3	1:A:821:LEU:HD23	2.57	0.40
2:B:91:PHE:CD2	2:B:139:TYR:HB2	2.57	0.40
3:C:25:ASP:C	3:C:25:ASP:OD1	2.64	0.40
3:C:104:SER:O	3:C:108:ARG:HG3	2.21	0.40
1:A:234:TYR:CE1	1:A:289:ILE:HD12	2.53	0.40
1:A:85:ASN:HD22	1:A:86:MET:N	2.19	0.40
1:A:349:GLU:C	1:A:351:LEU:N	2.80	0.40
1:A:406:ILE:CD1	1:A:414:THR:HG21	2.52	0.40
1:A:801:LYS:O	1:A:801:LYS:HG2	2.21	0.40
1:A:15:LEU:CD1	1:A:19:LYS:HD3	2.51	0.40
2:B:58:LEU:O	2:B:59:LYS:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	686 (86%)	79 (10%)	37 (5%)	2	2
2	B	143/153 (94%)	97 (68%)	26 (18%)	20 (14%)	0	0
3	C	154/159 (97%)	134 (87%)	10 (6%)	10 (6%)	1	1
All	All	1099/1151 (96%)	917 (83%)	115 (10%)	67 (6%)	1	1

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	131	ILE
1	A	178	SER
1	A	200	LEU
1	A	240	THR
1	A	408	VAL
1	A	453	ALA
1	A	573	ALA
1	A	576	ALA
1	A	679	LYS
2	B	26	ASP
2	B	29	ARG
2	B	81	THR
2	B	99	GLN
3	C	136	ILE
3	C	139	ASN
3	C	155	PRO
1	A	15	LEU
1	A	64	GLN
1	A	286	ASN
1	A	377	ALA
1	A	378	ASP
1	A	380	THR
1	A	415	GLN

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Mol	Chain	Res	Type
1	A	416	GLY
1	A	571	PRO
1	A	644	PHE
2	B	9	LYS
2	B	49	PRO
2	B	51	ASP
2	B	66	ASN
2	B	79	SER
2	B	117	ASN
3	C	58	MET
3	C	59	GLY
3	C	82	THR
1	A	65	GLU
1	A	127	ARG
1	A	306	LEU
1	A	309	PRO
1	A	575	CYS
2	B	84	GLU
2	B	93	MET
2	B	104	GLU
2	B	130	ALA
3	C	24	ARG
3	C	117	ARG
1	A	145	ARG
1	A	275	SER
1	A	282	SER
1	A	406	ILE
1	A	682	GLY
1	A	827	GLU
3	C	2	GLN
1	A	201	ALA
1	A	228	ASN
1	A	417	ARG
2	B	64	GLN
3	C	137	ASP
1	A	616	LYS
2	B	83	PRO
2	B	148	LYS
1	A	570	PRO
1	A	620	VAL
2	B	8	VAL
2	B	25	ILE

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Mol	Chain	Res	Type
2	B	33	ILE

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%)	673 (96%)	31 (4%)	25	50
2	B	128/134 (96%)	116 (91%)	12 (9%)	8	18
3	C	134/137 (98%)	121 (90%)	13 (10%)	8	17
All	All	966/1002 (96%)	910 (94%)	56 (6%)	18	39

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	14	CYS
1	A	41	PHE
1	A	61	ASP
1	A	155	ILE
1	A	173	LEU
1	A	219	THR
1	A	282	SER
1	A	289	ILE
1	A	299	PRO
1	A	340	PHE
1	A	346	THR
1	A	367	LYS
1	A	407	LYS
1	A	413	VAL
1	A	423	THR
1	A	448	THR
1	A	464	ILE
1	A	534	SER
1	A	543	PRO
1	A	548	THR

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Mol	Chain	Res	Type
1	A	570	PRO
1	A	583	HIS
1	A	593	ILE
1	A	620	VAL
1	A	624	PHE
1	A	644	PHE
1	A	664	SER
1	A	702	ILE
1	A	714	ILE
1	A	827	GLU
2	B	9	LYS
2	B	17	GLU
2	B	22	PHE
2	B	35	MET
2	B	45	LEU
2	B	51	ASP
2	B	58	LEU
2	B	66	ASN
2	B	113	ASN
2	B	124	LYS
2	B	134	ASN
2	B	142	MET
3	C	4	THR
3	C	13	GLU
3	C	17	LEU
3	C	65	LEU
3	C	78	LYS
3	C	85	ASP
3	C	86	GLU
3	C	103	SER
3	C	109	ASN
3	C	117	ARG
3	C	118	ILE
3	C	119	THR
3	C	149	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	85	ASN
1	A	151	HIS

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Mol	Chain	Res	Type
1	A	165	GLN
1	A	169	ASN
1	A	242	ASN
1	A	243	ASN
1	A	244	ASN
1	A	301	ASN
1	A	424	ASN
1	A	494	HIS
1	A	552	ASN
1	A	605	ASN
1	A	607	ASN
1	A	645	GLN
1	A	661	ASN
1	A	696	ASN
1	A	711	ASN
1	A	804	GLN
1	A	806	GLN
1	A	833	ASN
2	B	64	GLN
2	B	89	ASN
2	B	99	GLN
2	B	117	ASN
2	B	125	ASN
2	B	134	ASN
3	C	50	HIS
3	C	109	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MLI	A	1001	-	6,6,6	1.80	2 (33%)	7,7,7	1.93	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLI	A	1001	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	MLI	C1-C2	2.90	1.55	1.51
4	A	1001	MLI	O9-C3	-2.30	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	MLI	O9-C3-O8	3.53	132.40	123.33
4	A	1001	MLI	O7-C2-O6	-2.02	118.13	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	MLI	C2-C1-C3-O9
4	A	1001	MLI	C2-C1-C3-O8

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

6.1 Protein, DNA and RNA chains

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%)	0.38	55 (6%) 23 19	18, 49, 88, 115	0
2	B	145/153 (94%)	1.55	42 (28%) 1 1	54, 93, 114, 121	0
3	C	156/159 (98%)	0.26	6 (3%) 44 38	24, 44, 65, 75	0
All	All	1109/1151 (96%)	0.51	103 (9%) 14 11	18, 51, 103, 121	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	SER	5.1
2	B	77	LYS	4.8
1	A	5	PHE	4.6
3	C	82	THR	4.2
1	A	643	ALA	3.9
2	B	75	GLY	3.9
1	A	835	VAL	3.9
1	A	412	TYR	3.8
1	A	622	MET	3.7
2	B	45	LEU	3.7
1	A	570	PRO	3.7
1	A	200	LEU	3.6
1	A	829	TRP	3.6
1	A	832	PHE	3.5
2	B	137	PHE	3.5
1	A	624	PHE	3.4
1	A	2	THR	3.4
1	A	322	LEU	3.4
1	A	346	THR	3.3
3	C	85	ASP	3.3
3	C	139	ASN	3.3
2	B	81	THR	3.3
2	B	48	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	623	LEU	3.2
1	A	839	LEU	3.2
1	A	838	LEU	3.2
2	B	58	LEU	3.2
2	B	146	LYS	3.1
1	A	1	MET	3.1
1	A	345	PHE	3.1
1	A	836	LYS	3.0
3	C	138	GLY	3.0
2	B	56	ALA	3.0
2	B	52	ASP	3.0
2	B	78	VAL	2.9
1	A	831	LEU	2.9
2	B	10	LEU	2.9
1	A	198	ALA	2.9
2	B	9	LYS	2.8
2	B	129	ASP	2.8
1	A	3	MET	2.8
1	A	625	THR	2.8
2	B	98	GLY	2.7
1	A	644	PHE	2.7
2	B	8	VAL	2.7
1	A	305	ILE	2.7
2	B	25	ILE	2.7
1	A	409	GLY	2.7
2	B	33	ILE	2.7
1	A	408	VAL	2.7
1	A	406	ILE	2.7
1	A	414	THR	2.6
2	B	42	PHE	2.5
2	B	79	SER	2.5
1	A	201	ALA	2.5
2	B	22	PHE	2.5
2	B	74	PHE	2.5
2	B	86	ALA	2.5
2	B	151	ASP	2.4
2	B	50	PRO	2.4
1	A	377	ALA	2.4
2	B	18	LEU	2.4
1	A	410	THR	2.4
1	A	413	VAL	2.4
1	A	612	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	401	LEU	2.3
1	A	454	LYS	2.3
2	B	19	LYS	2.3
1	A	616	LYS	2.3
1	A	571	PRO	2.3
1	A	368	TRP	2.3
2	B	27	GLN	2.3
1	A	400	CYS	2.2
1	A	217	LYS	2.2
1	A	131	ILE	2.2
2	B	99	GLN	2.2
2	B	132	LEU	2.2
2	B	24	MET	2.2
2	B	101	PHE	2.2
2	B	149	ALA	2.2
1	A	621	LYS	2.2
1	A	828	TRP	2.2
1	A	45	GLY	2.2
2	B	31	GLY	2.2
2	B	49	PRO	2.1
1	A	344	GLY	2.1
1	A	619	ILE	2.1
2	B	130	ALA	2.1
2	B	127	TRP	2.1
1	A	380	THR	2.1
2	B	139	TYR	2.1
1	A	379	GLY	2.1
2	B	13	ARG	2.1
1	A	393	ASN	2.1
2	B	39	LYS	2.1
1	A	202	GLY	2.1
1	A	312	GLY	2.1
3	C	81	GLY	2.1
1	A	381	ALA	2.0
2	B	128	LYS	2.0
1	A	68	VAL	2.0
2	B	150	GLU	2.0
1	A	144	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	MLI	A	1001	7/7	0.75	0.17	44,48,51,53	0
5	CA	C	1001	1/1	0.95	0.07	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.