Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 11:20 AM EDT

PDB ID	:	3I5I
Title	:	The crystal structure of squid myosin S1 in the presence of SO4 2-
Authors	:	Yang, Y.; Gourinath, S.; Kovacs, M.; Nyitray, L.; Reutzel, R.; Himmel, D.M.; O'Neall-Hennessey, E.; Reshetnikova, L.; Szent-Gyorgyi, A.G.; Brown, J.H.; Cohen, C.
Deposited on	:	2009-07-05
Resolution	:	3.30 Å(reported)

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

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

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

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

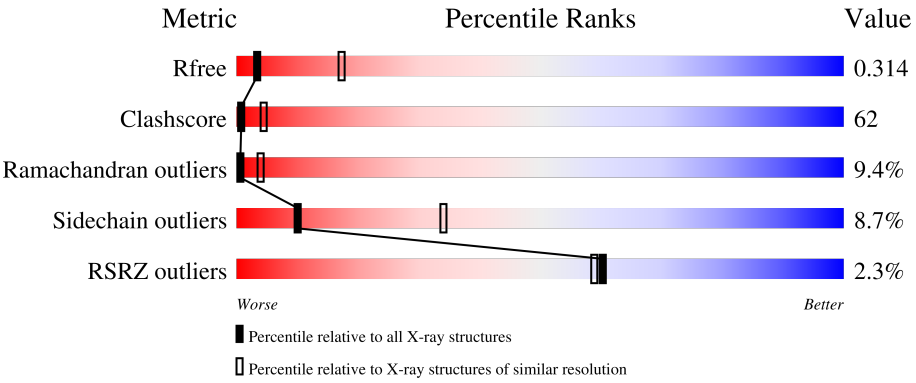
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	839	2% 32% 54% 9%
2	B	153	6% 14% 52% 25% 5%
3	C	159	% 42% 43% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	1001	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8904 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

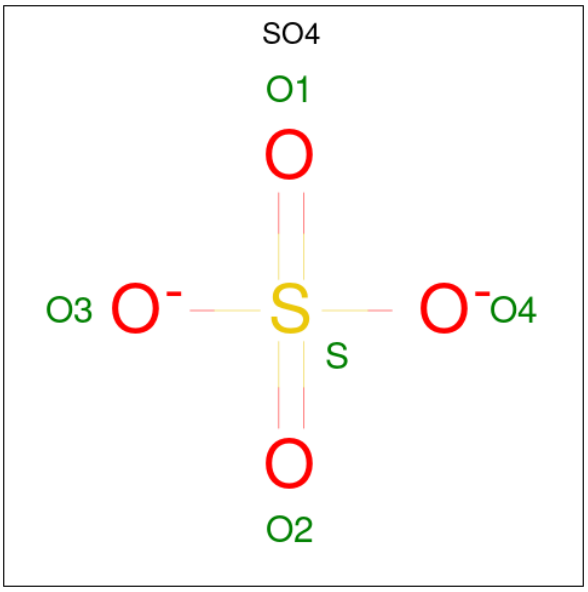
- Molecule 2 is a protein called Myosin regulatory light chain LC-2, mantle muscle.

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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

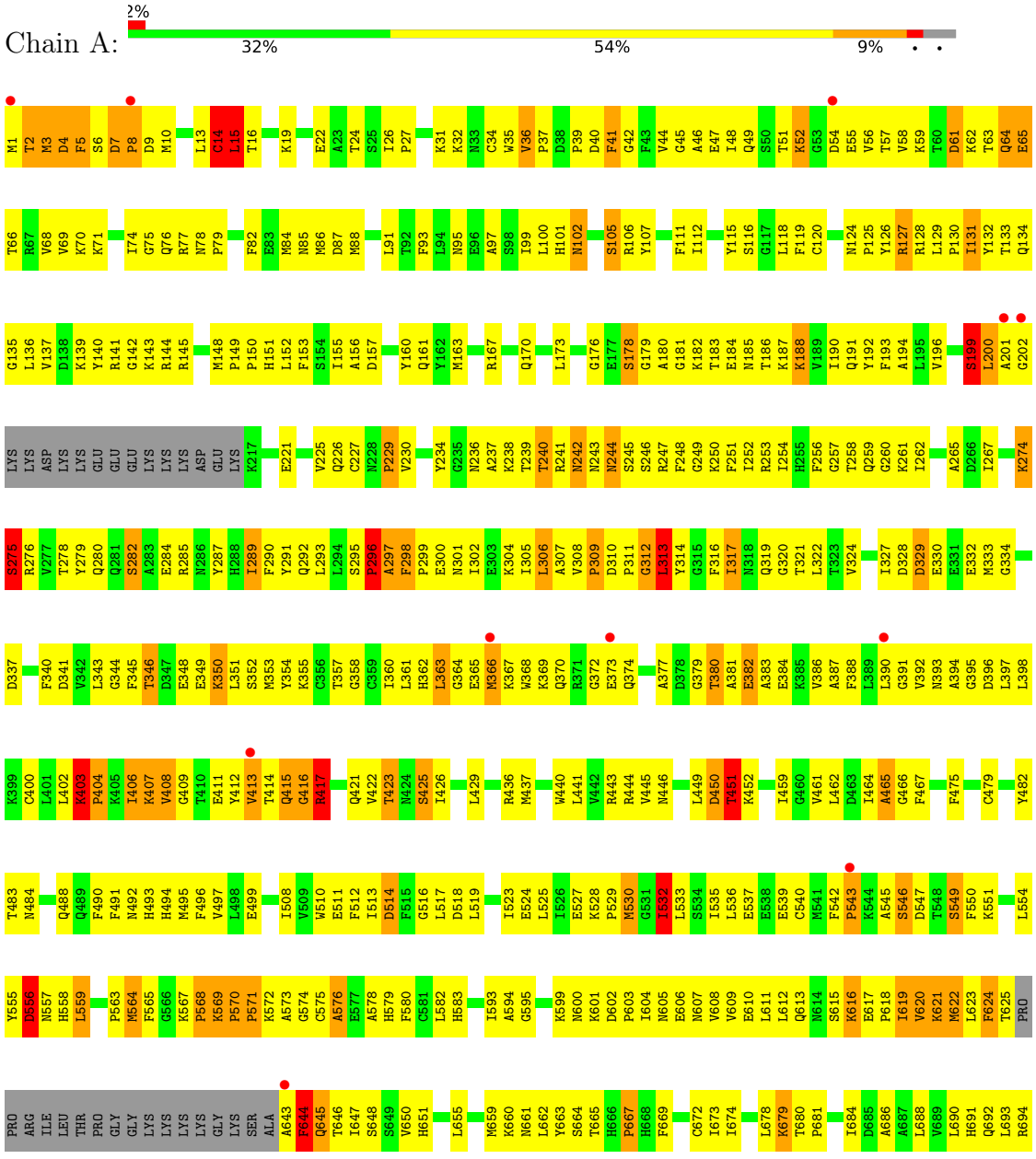
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

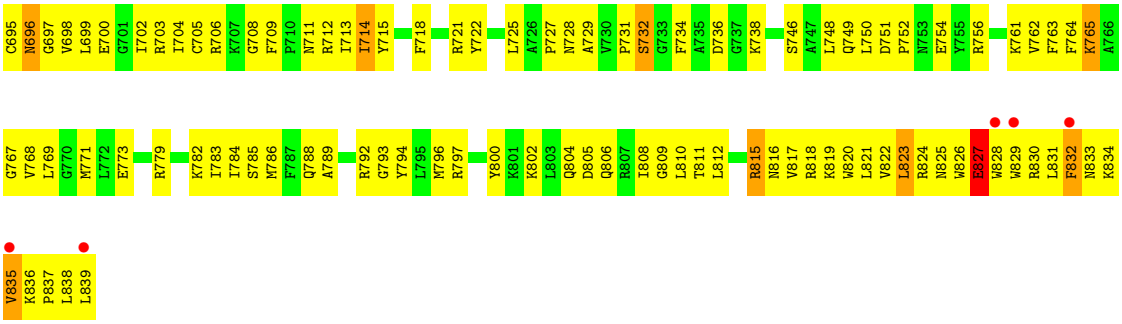
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Ca 1 1	0	0

3 Residue-property plots (i)

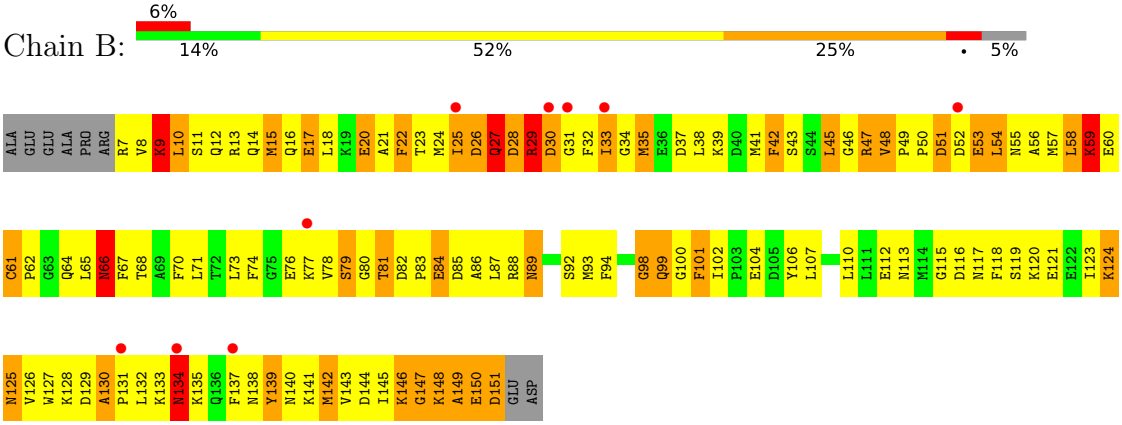
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Myosin heavy chain isoform A

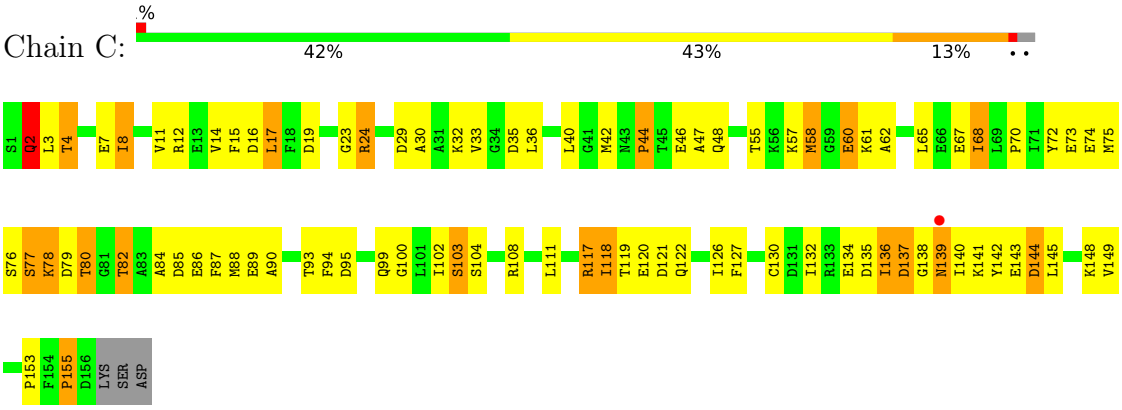




• Molecule 2: Myosin regulatory light chain LC-2, mantle muscle



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.19Å 100.15Å 80.19Å 90.00° 105.45° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.30 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-3.30) 97.2 (49.30-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.330 0.251 , 0.314	Depositor DCC
R_{free} test set	2180 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	69.7	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 68.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0/6631	0.87	12/8938 (0.1%)
2	B	0.56	0/1186	1.17	11/1588 (0.7%)
3	C	0.59	0/1258	1.01	5/1687 (0.3%)
All	All	0.53	0/9075	0.93	28/12213 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	28	ASP	N-CA-C	12.34	144.32	111.00
3	C	2	GLN	N-CA-C	10.93	140.51	111.00
2	B	27	GLN	N-CA-C	-10.82	81.79	111.00
3	C	138	GLY	N-CA-C	-10.50	86.84	113.10
2	B	100	GLY	N-CA-C	-9.60	89.09	113.10
2	B	10	LEU	N-CA-C	-8.33	88.50	111.00
1	A	403	LYS	C-N-CD	-7.51	104.08	120.60
1	A	297	ALA	N-CA-C	-6.85	92.50	111.00
2	B	151	ASP	CA-C-O	6.79	134.35	120.10
2	B	151	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	200	LEU	CA-CB-CG	-6.08	101.31	115.30
3	C	58	MET	N-CA-C	6.08	127.42	111.00
2	B	28	ASP	CA-C-N	-6.00	104.00	117.20
2	B	101	PHE	N-CA-C	5.97	127.11	111.00
1	A	451	THR	N-CA-C	-5.84	95.24	111.00
2	B	47	ARG	N-CA-C	5.79	126.64	111.00
3	C	80	THR	N-CA-C	-5.73	95.53	111.00
1	A	14	CYS	N-CA-C	5.72	126.44	111.00
1	A	3	MET	CB-CG-SD	-5.71	95.25	112.40
2	B	149	ALA	N-CA-C	-5.63	95.79	111.00
1	A	4	ASP	N-CA-C	-5.61	95.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	645	GLN	N-CA-C	5.61	126.14	111.00
1	A	199	SER	N-CA-C	5.58	126.06	111.00
2	B	28	ASP	CB-CA-C	-5.36	99.68	110.40
1	A	313	LEU	N-CA-C	5.31	125.33	111.00
3	C	17	LEU	CA-CB-CG	-5.19	103.36	115.30
1	A	15	LEU	N-CA-C	-5.12	97.17	111.00
1	A	409	GLY	N-CA-C	-5.01	100.56	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6493	0	6496	787	0
2	B	1166	0	1125	238	1
3	C	1239	0	1190	136	0
4	A	5	0	0	4	0
5	C	1	0	0	0	0
All	All	8904	0	8811	1104	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 62.

All (1104) 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:141:ARG:NH2	1:A:199:SER:HB3	1.54	1.20
1:A:191:GLN:HG2	1:A:221:GLU:HG2	1.19	1.18
2:B:26:ASP:OD1	2:B:28:ASP:HB2	1.47	1.15
1:A:293:LEU:HD23	1:A:333:MET:HE1	1.26	1.15
1:A:259:GLN:H	1:A:261:LYS:HE2	1.13	1.12
1:A:365:GLU:O	1:A:367:LYS:HD3	1.50	1.11
1:A:413:VAL:HG13	1:A:415:GLN:HB2	1.33	1.08
1:A:190:ILE:HG12	1:A:254:ILE:HD11	1.36	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ARG:O	2:B:78:VAL:HG11	1.54	1.05
1:A:572:LYS:HB3	1:A:575:CYS:HB2	1.36	1.04
2:B:84:GLU:HG3	2:B:85:ASP:H	1.22	1.03
1:A:802:LYS:HE2	1:A:806:GLN:NE2	1.75	1.01
1:A:316:PHE:HE1	1:A:364:GLY:HA2	1.21	1.00
1:A:572:LYS:H	1:A:575:CYS:HB3	1.25	1.00
1:A:404:PRO:HB3	1:A:607:ASN:HD22	1.27	1.00
1:A:620:VAL:O	1:A:624:PHE:HB2	1.62	1.00
2:B:23:THR:O	2:B:26:ASP:HB2	1.62	0.99
1:A:78:ASN:OD1	1:A:93:PHE:HB2	1.63	0.99
1:A:550:PHE:HE2	1:A:593:ILE:HD12	1.29	0.97
1:A:404:PRO:HB3	1:A:607:ASN:ND2	1.79	0.96
2:B:120:LYS:HA	2:B:123:ILE:HD12	1.45	0.96
1:A:141:ARG:HH22	1:A:199:SER:HB3	1.21	0.96
1:A:2:THR:HG21	1:A:143:LYS:NZ	1.80	0.95
2:B:25:ILE:O	2:B:37:ASP:HB3	1.67	0.95
1:A:571:PRO:HB2	1:A:575:CYS:HB3	1.46	0.94
1:A:316:PHE:CE1	1:A:364:GLY:HA2	2.02	0.94
1:A:316:PHE:CE1	1:A:364:GLY:CA	2.52	0.93
1:A:317:ILE:HD12	1:A:361:LEU:HD21	1.51	0.92
1:A:316:PHE:HE1	1:A:364:GLY:CA	1.82	0.92
1:A:403:LYS:N	1:A:404:PRO:HD2	1.80	0.91
1:A:167:ARG:HH22	1:A:258:THR:HG23	1.35	0.91
2:B:26:ASP:OD1	2:B:28:ASP:CB	2.17	0.91
3:C:4:THR:HG23	3:C:7:GLU:HG3	1.51	0.91
1:A:817:VAL:HA	2:B:146:LYS:HZ1	1.35	0.91
3:C:3:LEU:HD21	3:C:73:GLU:HB3	1.53	0.89
1:A:190:ILE:CG1	1:A:254:ILE:HD11	2.02	0.89
1:A:2:THR:HG21	1:A:143:LYS:HZ1	1.32	0.89
3:C:130:CYS:O	3:C:148:LYS:HD3	1.73	0.88
1:A:436:ARG:HH11	1:A:623:LEU:HA	1.37	0.88
1:A:569:LYS:HD2	1:A:569:LYS:O	1.73	0.88
1:A:278:THR:HG22	1:A:316:PHE:CD2	2.08	0.88
3:C:153:PRO:O	3:C:155:PRO:HD3	1.74	0.87
1:A:13:LEU:HD11	1:A:151:HIS:HD2	1.39	0.87
1:A:88:MET:HE1	1:A:99:ILE:HA	1.56	0.87
1:A:196:VAL:O	1:A:199:SER:HB2	1.74	0.86
1:A:406:ILE:HD12	1:A:414:THR:HG21	1.57	0.86
1:A:191:GLN:HG2	1:A:221:GLU:CG	2.04	0.86
1:A:413:VAL:HG13	1:A:415:GLN:CB	2.05	0.86
1:A:608:VAL:O	1:A:612:LEU:HG	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLN:N	1:A:261:LYS:HE2	1.90	0.85
1:A:297:ALA:HB3	1:A:298:PHE:CE1	2.11	0.85
1:A:836:LYS:NZ	2:B:21:ALA:HB2	1.90	0.85
2:B:9:LYS:HA	2:B:9:LYS:HE3	1.58	0.85
1:A:572:LYS:O	1:A:572:LYS:HG3	1.74	0.85
3:C:90:ALA:O	3:C:93:THR:HG22	1.77	0.84
2:B:8:VAL:C	2:B:10:LEU:H	1.79	0.84
1:A:836:LYS:HZ2	2:B:21:ALA:HB2	1.38	0.83
1:A:298:PHE:HB3	1:A:301:ASN:HD22	1.43	0.83
1:A:230:VAL:HG11	1:A:441:LEU:HD11	1.59	0.83
1:A:406:ILE:HG22	1:A:407:LYS:N	1.91	0.83
2:B:24:MET:C	2:B:26:ASP:H	1.79	0.83
1:A:406:ILE:HG22	1:A:407:LYS:H	1.42	0.82
1:A:317:ILE:HD12	1:A:361:LEU:CD2	2.09	0.82
1:A:659:MET:HE1	1:A:662:LEU:HD12	1.60	0.82
1:A:278:THR:HG22	1:A:316:PHE:CE2	2.13	0.82
1:A:400:CYS:HA	1:A:404:PRO:HD3	1.59	0.82
1:A:194:ALA:HA	1:A:262:ILE:CD1	2.09	0.82
1:A:391:GLY:O	1:A:615:SER:HB3	1.79	0.82
1:A:550:PHE:CE2	1:A:593:ILE:HD12	2.15	0.82
1:A:259:GLN:HB2	1:A:261:LYS:HD3	1.59	0.82
1:A:600:ASN:HD21	1:A:648:SER:H	1.29	0.81
2:B:8:VAL:O	2:B:10:LEU:N	2.13	0.81
2:B:142:MET:HE1	2:B:146:LYS:HD3	1.63	0.81
1:A:47:GLU:O	1:A:58:VAL:HG13	1.79	0.81
1:A:555:TYR:HE2	1:A:567:LYS:HD2	1.45	0.80
1:A:610:GLU:O	1:A:613:GLN:HB2	1.79	0.80
3:C:132:ILE:CD1	3:C:145:LEU:HA	2.11	0.80
2:B:131:PRO:HB3	2:B:141:LYS:CD	2.11	0.80
2:B:11:SER:O	2:B:15:MET:HG3	1.82	0.80
3:C:103:SER:HA	3:C:139:ASN:CG	2.02	0.80
2:B:24:MET:C	2:B:26:ASP:N	2.35	0.80
1:A:826:TRP:O	1:A:829:TRP:N	2.14	0.79
1:A:88:MET:HE1	1:A:99:ILE:HG23	1.62	0.79
1:A:86:MET:HE3	1:A:150:PRO:HD3	1.65	0.79
1:A:817:VAL:HA	2:B:146:LYS:NZ	1.97	0.79
1:A:316:PHE:CD1	1:A:364:GLY:HA3	2.18	0.78
1:A:120:CYS:HB2	1:A:155:ILE:HD11	1.64	0.78
1:A:404:PRO:HB2	1:A:414:THR:OG1	1.83	0.78
2:B:29:ARG:HG3	2:B:32:PHE:HB2	1.66	0.78
2:B:53:GLU:O	2:B:56:ALA:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ARG:NE	1:A:417:ARG:H	1.81	0.78
1:A:828:TRP:CZ2	2:B:57:MET:HB3	2.18	0.77
1:A:403:LYS:H	1:A:404:PRO:HD2	1.46	0.77
1:A:119:PHE:CE1	1:A:698:VAL:HA	2.18	0.77
1:A:280:GLN:HB2	1:A:319:GLN:HB2	1.66	0.77
1:A:599:LYS:O	1:A:647:ILE:HD12	1.85	0.77
1:A:343:LEU:CD1	1:A:445:VAL:HG12	2.14	0.77
2:B:29:ARG:HH21	2:B:34:GLY:HA2	1.49	0.77
1:A:368:TRP:CZ3	1:A:402:LEU:HD21	2.20	0.77
1:A:834:LYS:HD2	2:B:45:LEU:HD13	1.67	0.76
1:A:298:PHE:CE1	1:A:333:MET:HG3	2.20	0.76
1:A:834:LYS:HD2	2:B:45:LEU:CD1	2.15	0.76
2:B:101:PHE:HD2	2:B:139:TYR:CD2	2.04	0.76
3:C:103:SER:HA	3:C:139:ASN:CB	2.16	0.76
2:B:24:MET:O	2:B:26:ASP:N	2.19	0.76
2:B:142:MET:CE	2:B:146:LYS:HD3	2.15	0.76
1:A:390:LEU:HD22	1:A:619:ILE:HD11	1.68	0.75
1:A:806:GLN:HG2	2:B:93:MET:HE2	1.68	0.75
3:C:117:ARG:HG3	3:C:117:ARG:HH11	1.50	0.75
1:A:173:LEU:HD22	1:A:462:LEU:HD23	1.69	0.75
1:A:551:LYS:HG2	1:A:555:TYR:CE1	2.21	0.75
1:A:725:LEU:HD13	1:A:748:LEU:HD11	1.67	0.75
1:A:786:MET:HE1	3:C:80:THR:O	1.85	0.75
2:B:35:MET:HE3	2:B:54:LEU:HD23	1.68	0.75
1:A:88:MET:CE	1:A:99:ILE:HA	2.17	0.75
3:C:78:LYS:HA	3:C:78:LYS:HE3	1.69	0.75
1:A:221:GLU:O	1:A:225:VAL:HG23	1.86	0.75
1:A:731:PRO:HG2	1:A:734:PHE:HD1	1.52	0.75
2:B:34:GLY:H	2:B:37:ASP:HB2	1.52	0.75
1:A:362:HIS:C	1:A:364:GLY:H	1.89	0.74
1:A:343:LEU:HD13	1:A:445:VAL:HG12	1.66	0.74
1:A:10:MET:HB3	1:A:14:CYS:HB2	1.70	0.74
1:A:731:PRO:HG2	1:A:734:PHE:CD1	2.22	0.74
2:B:13:ARG:HD2	2:B:13:ARG:N	2.00	0.74
3:C:4:THR:HG23	3:C:7:GLU:CG	2.16	0.74
3:C:136:ILE:HG22	3:C:137:ASP:H	1.51	0.74
1:A:4:ASP:C	1:A:6:SER:H	1.89	0.74
2:B:150:GLU:HG2	2:B:151:ASP:N	2.02	0.74
1:A:296:PRO:HD2	1:A:330:GLU:HG2	1.70	0.74
1:A:366:MET:CE	1:A:386:VAL:HG21	2.18	0.74
1:A:406:ILE:CD1	1:A:414:THR:HG21	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:LYS:HE3	2:B:76:GLU:O	1.88	0.74
1:A:831:LEU:HD21	2:B:42:PHE:CE1	2.22	0.74
1:A:194:ALA:HA	1:A:262:ILE:HD12	1.69	0.74
1:A:236:ASN:HB3	1:A:244:ASN:ND2	2.03	0.73
1:A:572:LYS:N	1:A:575:CYS:HB3	2.01	0.73
1:A:133:THR:HG22	1:A:135:GLY:H	1.52	0.73
1:A:414:THR:O	1:A:416:GLY:N	2.21	0.73
1:A:406:ILE:CG1	1:A:414:THR:HG21	2.19	0.73
1:A:568:PRO:HG3	1:A:578:ALA:HB3	1.70	0.73
1:A:345:PHE:CD2	1:A:444:ARG:NH2	2.56	0.73
1:A:49:GLN:HB2	1:A:57:THR:HG22	1.68	0.73
1:A:391:GLY:O	1:A:615:SER:CB	2.37	0.72
1:A:417:ARG:HE	1:A:417:ARG:N	1.87	0.72
2:B:29:ARG:NH2	2:B:34:GLY:CA	2.52	0.72
1:A:64:GLN:OE1	1:A:64:GLN:HA	1.88	0.72
1:A:141:ARG:CZ	1:A:199:SER:HB3	2.19	0.72
1:A:754:GLU:HA	1:A:754:GLU:OE1	1.89	0.72
2:B:29:ARG:CZ	2:B:34:GLY:HA3	2.18	0.72
1:A:234:TYR:CZ	1:A:289:ILE:HD12	2.23	0.72
1:A:374:GLN:CD	1:A:415:GLN:HE21	1.92	0.72
2:B:149:ALA:O	2:B:150:GLU:HB2	1.90	0.72
1:A:694:ARG:HG2	1:A:699:LEU:HD12	1.70	0.72
1:A:786:MET:SD	3:C:82:THR:OG1	2.47	0.72
1:A:365:GLU:OE1	1:A:365:GLU:HA	1.89	0.72
1:A:436:ARG:NH1	1:A:623:LEU:HA	2.03	0.72
1:A:2:THR:HG22	1:A:2:THR:O	1.88	0.72
1:A:571:PRO:HB2	1:A:575:CYS:CB	2.19	0.71
1:A:36:VAL:CG2	1:A:69:VAL:HG21	2.19	0.71
1:A:369:LYS:HD2	1:A:370:GLN:H	1.55	0.71
2:B:67:PHE:HA	2:B:70:PHE:HB2	1.73	0.71
3:C:135:ASP:O	3:C:136:ILE:C	2.29	0.71
1:A:346:THR:HG22	1:A:348:GLU:H	1.56	0.71
1:A:136:LEU:HD23	1:A:139:LYS:HD2	1.73	0.71
2:B:14:GLN:HE22	2:B:81:THR:HG23	1.55	0.71
1:A:313:LEU:H	1:A:313:LEU:HD23	1.56	0.71
1:A:362:HIS:O	1:A:364:GLY:N	2.24	0.71
2:B:101:PHE:HB2	2:B:137:PHE:O	1.90	0.71
1:A:407:LYS:O	1:A:408:VAL:HG23	1.91	0.70
1:A:415:GLN:O	1:A:417:ARG:N	2.24	0.70
2:B:46:GLY:O	2:B:47:ARG:HG2	1.90	0.70
2:B:11:SER:O	2:B:15:MET:CG	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:GLY:O	1:A:765:LYS:HE2	1.92	0.70
1:A:831:LEU:HD21	2:B:42:PHE:CZ	2.27	0.70
2:B:131:PRO:HB3	2:B:141:LYS:CE	2.22	0.70
3:C:4:THR:CG2	3:C:7:GLU:HG3	2.21	0.69
3:C:136:ILE:HG22	3:C:137:ASP:N	2.07	0.69
1:A:464:ILE:HG23	1:A:465:ALA:N	2.07	0.69
1:A:782:LYS:O	1:A:786:MET:HG3	1.92	0.69
2:B:9:LYS:HA	2:B:9:LYS:CE	2.14	0.69
2:B:10:LEU:HB2	2:B:78:VAL:HG21	1.75	0.69
2:B:23:THR:O	2:B:26:ASP:CB	2.38	0.69
1:A:510:TRP:CE2	1:A:512:PHE:HB2	2.28	0.69
1:A:312:GLY:O	1:A:314:TYR:N	2.25	0.69
2:B:15:MET:SD	2:B:71:LEU:HD13	2.32	0.69
2:B:67:PHE:CZ	2:B:71:LEU:HD11	2.28	0.69
3:C:132:ILE:HD11	3:C:145:LEU:HA	1.73	0.69
1:A:525:LEU:O	1:A:532:ILE:HG13	1.93	0.69
1:A:620:VAL:HG12	1:A:624:PHE:CE1	2.28	0.69
1:A:84:MET:HE3	1:A:105:SER:HB2	1.74	0.68
2:B:23:THR:C	2:B:26:ASP:HB2	2.14	0.68
2:B:88:ARG:HE	2:B:143:VAL:HG11	1.57	0.68
1:A:84:MET:CE	1:A:105:SER:HB2	2.23	0.68
1:A:316:PHE:O	1:A:317:ILE:HG13	1.92	0.68
3:C:11:VAL:HA	3:C:40:LEU:HD21	1.75	0.68
1:A:345:PHE:HB3	1:A:349:GLU:OE1	1.92	0.68
1:A:537:GLU:O	1:A:540:CYS:HB2	1.93	0.68
1:A:417:ARG:H	1:A:417:ARG:HE	1.38	0.68
1:A:822:VAL:HG12	1:A:823:LEU:N	2.08	0.68
1:A:609:VAL:O	1:A:613:GLN:HG3	1.94	0.68
1:A:251:PHE:HA	1:A:461:VAL:O	1.93	0.67
2:B:7:ARG:C	2:B:9:LYS:N	2.42	0.67
1:A:194:ALA:HA	1:A:262:ILE:HD11	1.75	0.67
1:A:366:MET:HE1	1:A:386:VAL:HG21	1.75	0.67
1:A:575:CYS:O	1:A:576:ALA:O	2.13	0.67
1:A:5:PHE:O	1:A:16:THR:HG22	1.94	0.67
1:A:617:GLU:O	1:A:620:VAL:HG23	1.95	0.67
2:B:12:GLN:HB3	2:B:13:ARG:HH11	1.58	0.67
1:A:298:PHE:HB3	1:A:301:ASN:ND2	2.09	0.67
1:A:513:ILE:HG12	1:A:517:LEU:HD12	1.75	0.67
3:C:100:GLY:HA2	3:C:142:TYR:CZ	2.29	0.67
1:A:466:GLY:O	1:A:484:ASN:ND2	2.28	0.67
1:A:51:THR:HG22	1:A:52:LYS:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:GLN:C	2:B:101:PHE:H	1.81	0.67
3:C:103:SER:HA	3:C:139:ASN:HB3	1.76	0.67
2:B:124:LYS:O	2:B:126:VAL:N	2.27	0.67
2:B:149:ALA:O	2:B:150:GLU:CB	2.43	0.67
3:C:44:PRO:HA	3:C:48:GLN:OE1	1.92	0.67
3:C:100:GLY:HA2	3:C:142:TYR:CE2	2.30	0.67
1:A:619:ILE:HG22	1:A:619:ILE:O	1.95	0.66
1:A:568:PRO:HG3	1:A:578:ALA:CB	2.26	0.66
1:A:729:ALA:HA	3:C:85:ASP:OD1	1.95	0.66
1:A:155:ILE:HG22	1:A:155:ILE:O	1.95	0.66
1:A:365:GLU:O	1:A:367:LYS:CD	2.38	0.66
3:C:88:MET:HE3	3:C:142:TYR:HE1	1.60	0.66
2:B:81:THR:HG23	2:B:81:THR:O	1.96	0.66
1:A:493:HIS:O	1:A:497:VAL:HG23	1.96	0.66
1:A:620:VAL:O	1:A:624:PHE:CD1	2.49	0.66
1:A:786:MET:CE	3:C:80:THR:O	2.44	0.66
1:A:694:ARG:HG2	1:A:699:LEU:CD1	2.26	0.66
1:A:700:GLU:OE2	1:A:703:ARG:NH1	2.29	0.66
1:A:832:PHE:HE2	2:B:77:LYS:HZ3	1.41	0.66
1:A:836:LYS:HG2	1:A:839:LEU:CG	2.26	0.66
2:B:131:PRO:HB3	2:B:141:LYS:HD3	1.77	0.66
1:A:351:LEU:HD21	1:A:355:LYS:HE3	1.78	0.65
2:B:26:ASP:OD1	2:B:28:ASP:CG	2.34	0.65
2:B:29:ARG:NH2	2:B:35:MET:H	1.94	0.65
1:A:230:VAL:HG12	1:A:441:LEU:HD21	1.78	0.65
2:B:131:PRO:HB3	2:B:141:LYS:HE2	1.78	0.65
1:A:440:TRP:CD1	1:A:621:LYS:HD2	2.32	0.65
1:A:360:ILE:HA	1:A:363:LEU:HD12	1.78	0.65
2:B:131:PRO:HB2	2:B:138:ASN:HB3	1.77	0.65
1:A:278:THR:HG22	1:A:316:PHE:HD2	1.60	0.65
1:A:292:GLN:C	1:A:333:MET:HE3	2.17	0.65
2:B:35:MET:HE3	2:B:54:LEU:CD2	2.27	0.65
2:B:101:PHE:CD2	2:B:139:TYR:CD2	2.84	0.65
2:B:115:GLY:O	3:C:23:GLY:HA2	1.97	0.65
1:A:160:TYR:OH	1:A:260:GLY:O	2.14	0.65
1:A:308:VAL:O	1:A:310:ASP:N	2.30	0.65
1:A:324:VAL:O	1:A:327:ILE:HG22	1.97	0.65
1:A:362:HIS:C	1:A:364:GLY:N	2.49	0.65
1:A:572:LYS:HB3	1:A:575:CYS:CB	2.21	0.65
1:A:756:ARG:HG2	1:A:756:ARG:HH11	1.61	0.65
1:A:826:TRP:CD1	2:B:76:GLU:OE2	2.50	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ILE:CG2	2:B:127:TRP:HE1	2.10	0.65
1:A:141:ARG:NH2	1:A:199:SER:CB	2.46	0.65
3:C:3:LEU:HD21	3:C:73:GLU:CB	2.27	0.65
1:A:152:LEU:HD22	1:A:185:ASN:OD1	1.97	0.64
1:A:237:ALA:HB2	1:A:287:TYR:HA	1.78	0.64
1:A:574:GLY:O	1:A:576:ALA:N	2.30	0.64
1:A:820:TRP:O	1:A:824:ARG:HG2	1.96	0.64
2:B:8:VAL:C	2:B:10:LEU:N	2.50	0.64
1:A:85:ASN:HD22	1:A:86:MET:H	1.43	0.64
1:A:400:CYS:CA	1:A:404:PRO:HD3	2.25	0.64
1:A:316:PHE:HD1	1:A:364:GLY:HA3	1.60	0.64
3:C:29:ASP:OD2	3:C:58:MET:O	2.16	0.64
1:A:196:VAL:O	1:A:199:SER:CB	2.45	0.64
1:A:316:PHE:CD1	1:A:364:GLY:CA	2.80	0.64
1:A:290:PHE:CD1	1:A:317:ILE:HD11	2.33	0.64
1:A:830:ARG:O	1:A:834:LYS:HG3	1.98	0.64
2:B:84:GLU:HG3	2:B:85:ASP:N	2.05	0.64
1:A:15:LEU:HD22	1:A:84:MET:HG3	1.80	0.64
2:B:26:ASP:OD1	2:B:28:ASP:OD2	2.14	0.64
1:A:64:GLN:O	1:A:65:GLU:HB2	1.98	0.64
1:A:403:LYS:O	1:A:415:GLN:HA	1.98	0.64
2:B:131:PRO:HD2	2:B:137:PHE:CE1	2.33	0.64
1:A:289:ILE:HA	1:A:292:GLN:HB2	1.79	0.64
1:A:551:LYS:CG	1:A:555:TYR:HE1	2.11	0.64
2:B:150:GLU:CG	2:B:151:ASP:H	2.09	0.64
1:A:2:THR:CG2	1:A:143:LYS:NZ	2.59	0.63
1:A:285:ARG:HH21	1:A:291:TYR:CB	2.11	0.63
1:A:415:GLN:O	1:A:416:GLY:C	2.34	0.63
2:B:35:MET:CE	2:B:54:LEU:HD23	2.27	0.63
2:B:81:THR:O	2:B:81:THR:CG2	2.46	0.63
1:A:3:MET:SD	1:A:149:PRO:HG3	2.38	0.63
1:A:551:LYS:HG2	1:A:555:TYR:HE1	1.62	0.63
1:A:6:SER:O	1:A:8:PRO:N	2.31	0.63
1:A:86:MET:CE	1:A:149:PRO:HA	2.28	0.63
1:A:620:VAL:O	1:A:624:PHE:HD1	1.82	0.63
1:A:839:LEU:HD13	2:B:20:GLU:HB3	1.79	0.63
3:C:119:THR:HG22	3:C:121:ASP:N	2.14	0.63
1:A:800:TYR:CE2	1:A:804:GLN:NE2	2.67	0.63
1:A:802:LYS:HE2	1:A:806:GLN:HE21	1.61	0.63
1:A:816:ASN:HD21	2:B:82:ASP:HB2	1.63	0.63
1:A:525:LEU:HD23	1:A:582:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLN:HA	2:B:27:GLN:OE1	1.98	0.63
2:B:28:ASP:OD1	2:B:29:ARG:HG2	1.98	0.63
1:A:290:PHE:HB3	1:A:317:ILE:CD1	2.29	0.63
1:A:317:ILE:CD1	1:A:361:LEU:HD21	2.28	0.63
2:B:29:ARG:NH2	2:B:34:GLY:HA2	2.14	0.63
3:C:12:ARG:HG3	3:C:12:ARG:HH11	1.63	0.63
3:C:104:SER:HB3	3:C:140:ILE:CD1	2.29	0.63
1:A:230:VAL:CG1	1:A:441:LEU:HD11	2.28	0.62
3:C:119:THR:HG22	3:C:121:ASP:H	1.63	0.62
1:A:337:ASP:O	1:A:341:ASP:OD1	2.17	0.62
2:B:147:GLY:O	2:B:148:LYS:HG3	1.99	0.62
3:C:80:THR:O	3:C:80:THR:HG23	1.98	0.62
2:B:124:LYS:C	2:B:126:VAL:N	2.52	0.62
1:A:540:CYS:O	1:A:601:LYS:HE2	1.98	0.62
1:A:3:MET:SD	1:A:149:PRO:CG	2.88	0.62
1:A:248:PHE:HE2	1:A:250:LYS:HB3	1.64	0.62
3:C:4:THR:H	3:C:7:GLU:HG3	1.65	0.62
1:A:285:ARG:HG2	1:A:291:TYR:CE1	2.34	0.62
1:A:831:LEU:O	1:A:835:VAL:N	2.31	0.62
1:A:3:MET:CE	1:A:14:CYS:SG	2.87	0.62
1:A:78:ASN:OD1	1:A:93:PHE:CB	2.45	0.62
1:A:82:PHE:O	1:A:85:ASN:HB2	2.00	0.62
1:A:392:VAL:HG11	1:A:611:LEU:HG	1.82	0.62
2:B:26:ASP:O	2:B:27:GLN:HB2	1.98	0.62
1:A:167:ARG:NH2	1:A:258:THR:HG23	2.13	0.62
1:A:820:TRP:CE3	1:A:821:LEU:HD23	2.34	0.62
2:B:150:GLU:HG2	2:B:151:ASP:H	1.65	0.62
1:A:7:ASP:O	1:A:9:ASP:N	2.33	0.62
1:A:51:THR:HG22	1:A:52:LYS:H	1.64	0.62
1:A:344:GLY:O	1:A:345:PHE:CD2	2.53	0.62
1:A:140:TYR:CZ	1:A:148:MET:HE2	2.35	0.61
1:A:200:LEU:HD11	1:A:259:GLN:O	1.99	0.61
1:A:321:THR:HG22	1:A:322:LEU:N	2.15	0.61
1:A:693:LEU:HA	1:A:696:ASN:HD22	1.65	0.61
2:B:29:ARG:NE	2:B:34:GLY:HA3	2.15	0.61
1:A:35:TRP:HH2	1:A:101:HIS:ND1	1.98	0.61
1:A:142:GLY:HA2	1:A:161:GLN:NE2	2.15	0.61
1:A:579:HIS:ND1	1:A:593:ILE:HB	2.15	0.61
2:B:84:GLU:CG	2:B:85:ASP:H	1.97	0.61
3:C:70:PRO:O	3:C:74:GLU:HG2	1.99	0.61
1:A:3:MET:CE	1:A:10:MET:SD	2.88	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:O	1:A:229:PRO:HD2	2.00	0.61
1:A:239:THR:O	1:A:240:THR:C	2.39	0.61
2:B:112:GLU:HG3	2:B:123:ILE:HD11	1.83	0.61
2:B:7:ARG:O	2:B:9:LYS:N	2.33	0.61
2:B:133:LYS:O	2:B:135:LYS:N	2.34	0.61
1:A:191:GLN:HA	1:A:221:GLU:OE2	2.00	0.61
1:A:300:GLU:HG3	1:A:301:ASN:H	1.65	0.61
1:A:413:VAL:CG1	1:A:413:VAL:O	2.49	0.61
1:A:450:ASP:OD1	1:A:452:LYS:HG2	2.00	0.61
1:A:802:LYS:HE2	1:A:806:GLN:HE22	1.60	0.61
1:A:257:GLY:HA3	1:A:261:LYS:HE3	1.83	0.61
2:B:7:ARG:C	2:B:9:LYS:H	2.02	0.61
2:B:131:PRO:O	2:B:132:LEU:HD23	2.01	0.61
1:A:800:TYR:O	1:A:804:GLN:HG3	2.00	0.61
1:A:58:VAL:HG12	1:A:59:LYS:N	2.16	0.61
1:A:234:TYR:OH	1:A:353:MET:HG3	2.01	0.61
1:A:365:GLU:O	1:A:367:LYS:N	2.34	0.60
1:A:618:PRO:C	1:A:620:VAL:H	2.04	0.60
1:A:826:TRP:O	1:A:827:GLU:C	2.39	0.60
1:A:141:ARG:HH11	1:A:141:ARG:HG2	1.67	0.60
1:A:290:PHE:HB3	1:A:317:ILE:HD11	1.83	0.60
1:A:200:LEU:O	1:A:202:GLY:N	2.34	0.60
3:C:2:GLN:O	3:C:3:LEU:C	2.37	0.60
2:B:124:LYS:C	2:B:126:VAL:H	2.05	0.60
3:C:134:GLU:HA	3:C:139:ASN:O	2.00	0.60
1:A:3:MET:HE1	1:A:14:CYS:SG	2.42	0.60
1:A:157:ASP:OD1	1:A:161:GLN:NE2	2.34	0.60
3:C:67:GLU:O	3:C:70:PRO:HD2	2.02	0.60
1:A:239:THR:O	1:A:241:ARG:N	2.34	0.60
1:A:305:ILE:O	1:A:306:LEU:HG	2.02	0.60
1:A:400:CYS:C	1:A:404:PRO:HD3	2.22	0.60
1:A:711:ASN:C	1:A:712:ARG:HG3	2.21	0.60
1:A:4:ASP:C	1:A:6:SER:N	2.55	0.60
1:A:383:ALA:HA	1:A:386:VAL:HG22	1.84	0.60
1:A:811:THR:O	1:A:815:ARG:HB3	2.02	0.60
1:A:196:VAL:HA	1:A:199:SER:OG	2.02	0.59
1:A:828:TRP:CD1	2:B:60:GLU:OE1	2.55	0.59
1:A:839:LEU:HD13	2:B:20:GLU:CB	2.32	0.59
1:A:184:GLU:O	1:A:187:LYS:HB3	2.01	0.59
1:A:620:VAL:O	1:A:624:PHE:CB	2.43	0.59
1:A:786:MET:O	1:A:789:ALA:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ASP:OD1	1:A:450:ASP:O	2.21	0.59
1:A:85:ASN:ND2	1:A:86:MET:N	2.50	0.59
1:A:819:LYS:HE2	2:B:79:SER:HB2	1.85	0.59
2:B:101:PHE:CD1	2:B:138:ASN:HA	2.37	0.59
3:C:36:LEU:CD2	3:C:68:ILE:HD13	2.33	0.59
1:A:88:MET:HE1	1:A:99:ILE:CG2	2.33	0.59
1:A:337:ASP:OD1	1:A:350:LYS:HE3	2.02	0.59
1:A:290:PHE:CG	1:A:317:ILE:HD11	2.38	0.59
1:A:756:ARG:HG2	1:A:756:ARG:NH1	2.15	0.59
3:C:30:ALA:HA	3:C:33:VAL:HG23	1.84	0.59
1:A:617:GLU:HA	1:A:620:VAL:CG2	2.32	0.59
1:A:693:LEU:HB3	1:A:699:LEU:HG	1.84	0.59
1:A:750:LEU:HD13	1:A:771:MET:HE1	1.84	0.59
3:C:104:SER:HB3	3:C:140:ILE:HG13	1.85	0.59
1:A:830:ARG:O	1:A:833:ASN:HB2	2.03	0.58
2:B:32:PHE:CE2	2:B:64:GLN:HG2	2.37	0.58
1:A:120:CYS:HB2	1:A:155:ILE:CD1	2.32	0.58
1:A:280:GLN:HB2	1:A:320:GLY:N	2.18	0.58
1:A:617:GLU:C	1:A:620:VAL:HG23	2.23	0.58
1:A:86:MET:CE	1:A:150:PRO:HD3	2.33	0.58
1:A:611:LEU:C	1:A:613:GLN:H	2.07	0.58
1:A:820:TRP:HE1	2:B:145:ILE:HG22	1.68	0.58
1:A:826:TRP:CH2	2:B:60:GLU:CD	2.77	0.58
2:B:94:PHE:O	2:B:102:ILE:HG12	2.03	0.58
1:A:298:PHE:N	1:A:299:PRO:CD	2.67	0.58
1:A:413:VAL:O	1:A:413:VAL:HG12	2.03	0.58
1:A:547:ASP:OD2	1:A:594:ALA:HA	2.02	0.58
1:A:181:GLY:C	1:A:183:THR:N	2.51	0.58
2:B:10:LEU:HB2	2:B:78:VAL:CG2	2.33	0.58
1:A:191:GLN:CG	1:A:221:GLU:HG2	2.13	0.58
1:A:130:PRO:O	1:A:132:TYR:N	2.37	0.58
1:A:136:LEU:O	1:A:139:LYS:N	2.35	0.58
1:A:4:ASP:O	1:A:6:SER:N	2.35	0.58
1:A:278:THR:CG2	1:A:316:PHE:CE2	2.86	0.57
2:B:56:ALA:O	2:B:59:LYS:HG3	2.04	0.57
3:C:67:GLU:C	3:C:70:PRO:HD2	2.25	0.57
1:A:186:THR:HG23	1:A:461:VAL:HG11	1.84	0.57
1:A:54:ASP:HA	1:A:71:LYS:HD2	1.85	0.57
1:A:393:ASN:O	1:A:396:ASP:N	2.37	0.57
1:A:608:VAL:O	1:A:612:LEU:CG	2.49	0.57
2:B:51:ASP:O	2:B:52:ASP:C	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLU:HG3	1:A:185:ASN:N	2.19	0.57
1:A:823:LEU:O	1:A:829:TRP:CD1	2.57	0.57
2:B:94:PHE:CD2	2:B:110:LEU:HD21	2.40	0.57
3:C:57:LYS:HG3	3:C:60:GLU:HG3	1.86	0.57
1:A:391:GLY:HA3	1:A:616:LYS:HG2	1.86	0.57
2:B:41:MET:C	2:B:43:SER:H	2.07	0.57
1:A:85:ASN:HD22	1:A:86:MET:N	2.01	0.57
1:A:157:ASP:O	1:A:161:GLN:HG3	2.04	0.57
1:A:141:ARG:CZ	1:A:199:SER:CB	2.82	0.57
1:A:533:LEU:O	1:A:537:GLU:HG3	2.05	0.57
1:A:279:TYR:HA	1:A:319:GLN:OE1	2.05	0.57
1:A:348:GLU:HA	1:A:348:GLU:OE1	2.04	0.57
2:B:12:GLN:CD	2:B:13:ARG:HH12	2.08	0.57
1:A:555:TYR:HD2	1:A:559:LEU:HD11	1.71	0.56
2:B:143:VAL:O	2:B:146:LYS:HB2	2.05	0.56
3:C:15:PHE:CG	3:C:65:LEU:HD13	2.40	0.56
1:A:41:PHE:CD2	1:A:41:PHE:N	2.72	0.56
1:A:383:ALA:HA	1:A:386:VAL:CG2	2.35	0.56
2:B:22:PHE:HA	2:B:33:ILE:HD11	1.87	0.56
1:A:417:ARG:HA	1:A:421:GLN:OE1	2.06	0.56
1:A:644:PHE:N	1:A:644:PHE:HD1	2.04	0.56
1:A:836:LYS:HG2	1:A:839:LEU:HD11	1.87	0.56
3:C:132:ILE:HD12	3:C:145:LEU:HD13	1.88	0.56
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.71	0.56
1:A:836:LYS:HG2	1:A:839:LEU:HG	1.88	0.56
2:B:28:ASP:OD1	2:B:37:ASP:OD2	2.24	0.56
1:A:563:PRO:HG2	1:A:564:MET:HE2	1.86	0.56
3:C:141:LYS:HB2	3:C:144:ASP:HB2	1.86	0.56
1:A:713:ILE:HG22	1:A:714:ILE:O	2.06	0.56
3:C:102:ILE:HG22	3:C:103:SER:O	2.06	0.56
1:A:31:LYS:C	1:A:32:LYS:HG2	2.26	0.55
2:B:50:PRO:HG2	2:B:53:GLU:OE1	2.06	0.55
3:C:4:THR:O	3:C:8:ILE:HG13	2.06	0.55
1:A:35:TRP:CH2	1:A:101:HIS:ND1	2.75	0.55
1:A:302:ILE:HG21	1:A:309:PRO:HD3	1.88	0.55
1:A:305:ILE:HG23	1:A:358:GLY:HA3	1.88	0.55
1:A:87:ASP:HA	1:A:115:TYR:O	2.06	0.55
1:A:413:VAL:C	1:A:415:GLN:H	2.10	0.55
3:C:78:LYS:CE	3:C:79:ASP:H	2.19	0.55
1:A:4:ASP:OD1	1:A:6:SER:HB2	2.05	0.55
1:A:620:VAL:HG12	1:A:624:PHE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:LYS:C	1:A:838:LEU:N	2.56	0.55
1:A:836:LYS:HD3	2:B:17:GLU:O	2.06	0.55
1:A:139:LYS:O	1:A:148:MET:SD	2.64	0.55
1:A:236:ASN:HB3	1:A:244:ASN:HD21	1.69	0.55
1:A:644:PHE:N	1:A:644:PHE:CD1	2.75	0.55
2:B:7:ARG:O	2:B:8:VAL:C	2.44	0.55
2:B:132:LEU:O	2:B:133:LYS:CG	2.55	0.55
1:A:406:ILE:CG2	1:A:407:LYS:N	2.65	0.55
3:C:126:ILE:HD11	3:C:149:VAL:HG22	1.88	0.55
1:A:278:THR:CG2	1:A:316:PHE:HE2	2.20	0.55
1:A:63:THR:O	1:A:64:GLN:HB2	2.06	0.55
1:A:85:ASN:ND2	1:A:86:MET:H	2.05	0.55
1:A:191:GLN:O	1:A:194:ALA:HB3	2.06	0.55
1:A:352:SER:CB	1:A:618:PRO:HG3	2.37	0.55
1:A:820:TRP:HB3	2:B:146:LYS:HZ1	1.72	0.55
3:C:78:LYS:HG3	3:C:79:ASP:N	2.22	0.55
3:C:132:ILE:HD13	3:C:145:LEU:HA	1.88	0.55
1:A:35:TRP:CE2	1:A:77:ARG:HG3	2.42	0.55
1:A:54:ASP:HA	1:A:71:LYS:CD	2.37	0.55
2:B:74:PHE:CE2	2:B:77:LYS:NZ	2.75	0.55
3:C:4:THR:CB	3:C:7:GLU:HG3	2.37	0.55
1:A:107:TYR:OH	1:A:124:ASN:O	2.19	0.55
1:A:488:GLN:OE1	1:A:697:GLY:HA3	2.07	0.55
1:A:571:PRO:HD2	1:A:575:CYS:O	2.07	0.55
1:A:820:TRP:CZ3	1:A:821:LEU:HD23	2.41	0.55
1:A:156:ALA:HB1	1:A:193:PHE:CE1	2.42	0.54
1:A:678:LEU:O	1:A:680:THR:N	2.40	0.54
3:C:93:THR:HG23	3:C:94:PHE:CD1	2.41	0.54
1:A:579:HIS:O	1:A:580:PHE:HB3	2.07	0.54
1:A:832:PHE:HA	1:A:835:VAL:HB	1.90	0.54
1:A:836:LYS:O	1:A:837:PRO:C	2.45	0.54
2:B:85:ASP:O	2:B:88:ARG:N	2.40	0.54
3:C:117:ARG:HH11	3:C:117:ARG:CG	2.20	0.54
3:C:132:ILE:HD13	3:C:145:LEU:CA	2.37	0.54
1:A:132:TYR:CE2	1:A:188:LYS:HD3	2.43	0.54
1:A:68:VAL:HG12	1:A:68:VAL:O	2.06	0.54
1:A:248:PHE:CE2	1:A:250:LYS:HB3	2.42	0.54
1:A:818:ARG:HH21	2:B:118:PHE:HD1	1.56	0.54
2:B:14:GLN:HE22	2:B:81:THR:CG2	2.20	0.54
2:B:29:ARG:NH2	2:B:34:GLY:HA3	2.23	0.54
3:C:102:ILE:HG13	3:C:142:TYR:HD2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TYR:O	1:A:127:ARG:HB3	2.07	0.54
1:A:296:PRO:HA	1:A:299:PRO:HD3	1.89	0.54
1:A:413:VAL:CG1	1:A:415:GLN:HB2	2.22	0.54
1:A:88:MET:HE1	1:A:99:ILE:CA	2.36	0.54
1:A:155:ILE:O	1:A:155:ILE:CG2	2.56	0.54
1:A:746:SER:O	1:A:749:GLN:N	2.29	0.54
1:A:820:TRP:HB3	2:B:146:LYS:NZ	2.23	0.54
3:C:132:ILE:HD12	3:C:145:LEU:CD1	2.37	0.54
1:A:259:GLN:H	1:A:261:LYS:CE	2.03	0.54
1:A:727:PRO:HG3	3:C:86:GLU:HG2	1.90	0.54
1:A:820:TRP:NE1	2:B:145:ILE:HG22	2.23	0.54
3:C:130:CYS:O	3:C:148:LYS:CD	2.53	0.54
1:A:74:ILE:HG13	1:A:74:ILE:O	2.07	0.53
2:B:41:MET:C	2:B:43:SER:N	2.60	0.53
2:B:147:GLY:O	2:B:148:LYS:CB	2.56	0.53
1:A:332:GLU:C	1:A:334:GLY:N	2.60	0.53
2:B:32:PHE:CZ	2:B:64:GLN:NE2	2.76	0.53
2:B:120:LYS:CA	2:B:123:ILE:HD12	2.29	0.53
3:C:74:GLU:O	3:C:77:SER:HB2	2.08	0.53
1:A:352:SER:HB3	1:A:618:PRO:HG3	1.89	0.53
2:B:32:PHE:CE2	2:B:64:GLN:NE2	2.75	0.53
2:B:98:GLY:O	2:B:99:GLN:O	2.25	0.53
1:A:58:VAL:CG1	1:A:59:LYS:N	2.72	0.53
1:A:406:ILE:HG13	1:A:414:THR:HG21	1.91	0.53
3:C:4:THR:N	3:C:7:GLU:HG3	2.22	0.53
1:A:182:LYS:N	4:A:1001:SO4:O1	2.41	0.53
1:A:305:ILE:O	1:A:306:LEU:CB	2.57	0.53
1:A:313:LEU:HD23	1:A:313:LEU:N	2.18	0.53
1:A:357:THR:OG1	1:A:437:MET:HE1	2.09	0.53
1:A:400:CYS:SG	1:A:611:LEU:HD22	2.48	0.53
1:A:827:GLU:OE1	1:A:830:ARG:CZ	2.57	0.53
2:B:88:ARG:HD3	2:B:140:ASN:OD1	2.08	0.53
1:A:346:THR:C	1:A:348:GLU:N	2.61	0.53
2:B:48:VAL:HG12	2:B:48:VAL:O	2.07	0.53
1:A:3:MET:HE1	1:A:149:PRO:HG2	1.91	0.53
1:A:36:VAL:HG21	1:A:69:VAL:HG21	1.91	0.53
3:C:117:ARG:HG3	3:C:117:ARG:NH1	2.23	0.53
1:A:141:ARG:HG2	1:A:141:ARG:NH1	2.24	0.53
1:A:329:ASP:O	1:A:332:GLU:N	2.42	0.53
1:A:368:TRP:CE3	1:A:377:ALA:HA	2.44	0.53
1:A:728:ASN:OD1	1:A:728:ASN:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:PHE:CE2	2:B:66:ASN:O	2.62	0.53
2:B:66:ASN:OD1	2:B:66:ASN:N	2.35	0.53
1:A:127:ARG:NE	1:A:129:LEU:HD21	2.24	0.53
1:A:128:ARG:HG2	1:A:128:ARG:NH1	2.23	0.52
2:B:41:MET:O	2:B:43:SER:N	2.42	0.52
3:C:78:LYS:HE3	3:C:78:LYS:CA	2.36	0.52
1:A:617:GLU:HA	1:A:620:VAL:HG23	1.91	0.52
1:A:762:VAL:HG13	1:A:762:VAL:O	2.10	0.52
2:B:13:ARG:O	2:B:17:GLU:HB2	2.09	0.52
2:B:29:ARG:NH2	2:B:35:MET:N	2.57	0.52
2:B:94:PHE:CD1	2:B:94:PHE:N	2.77	0.52
1:A:467:PHE:HB3	1:A:695:CYS:HB3	1.91	0.52
2:B:58:LEU:O	2:B:60:GLU:N	2.42	0.52
1:A:236:ASN:HD22	1:A:244:ASN:ND2	2.07	0.52
1:A:298:PHE:H	1:A:299:PRO:HD3	1.73	0.52
1:A:346:THR:HG22	1:A:348:GLU:CB	2.39	0.52
1:A:826:TRP:HB3	1:A:829:TRP:HB2	1.92	0.52
1:A:831:LEU:C	1:A:833:ASN:H	2.13	0.52
2:B:32:PHE:O	2:B:34:GLY:N	2.43	0.52
1:A:383:ALA:O	1:A:386:VAL:HG23	2.09	0.52
1:A:713:ILE:CD1	1:A:769:LEU:HD21	2.39	0.52
1:A:794:TYR:CZ	3:C:153:PRO:HA	2.44	0.52
1:A:3:MET:HE1	1:A:10:MET:SD	2.49	0.52
1:A:293:LEU:N	1:A:333:MET:HE3	2.24	0.52
1:A:365:GLU:HB3	1:A:367:LYS:NZ	2.25	0.52
2:B:132:LEU:HD21	2:B:137:PHE:HD1	1.75	0.52
3:C:104:SER:O	3:C:108:ARG:HG3	2.10	0.52
1:A:51:THR:CG2	1:A:52:LYS:H	2.23	0.52
1:A:616:LYS:H	1:A:616:LYS:HD3	1.74	0.52
2:B:47:ARG:O	2:B:48:VAL:CB	2.58	0.52
2:B:67:PHE:CE1	2:B:71:LEU:HD21	2.45	0.52
2:B:85:ASP:O	2:B:86:ALA:C	2.49	0.52
2:B:145:ILE:O	2:B:148:LYS:CG	2.58	0.52
1:A:14:CYS:O	1:A:15:LEU:CB	2.58	0.52
1:A:184:GLU:HB2	1:A:188:LYS:HE3	1.92	0.52
1:A:836:LYS:HD2	2:B:17:GLU:OE2	2.09	0.52
2:B:14:GLN:NE2	2:B:81:THR:HG23	2.24	0.52
2:B:34:GLY:O	2:B:38:LEU:N	2.40	0.52
1:A:76:GLN:OE1	1:A:93:PHE:CE2	2.63	0.52
1:A:285:ARG:NH2	1:A:291:TYR:HB2	2.25	0.52
1:A:363:LEU:HD22	1:A:429:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ARG:O	1:A:706:ARG:HB2	2.10	0.52
2:B:132:LEU:CD2	2:B:137:PHE:HD1	2.22	0.52
1:A:88:MET:HA	1:A:91:LEU:HG	1.91	0.51
1:A:178:SER:O	4:A:1001:SO4:S	2.68	0.51
1:A:390:LEU:O	1:A:619:ILE:HD12	2.09	0.51
1:A:688:LEU:O	1:A:692:GLN:HG3	2.10	0.51
1:A:809:GLY:O	1:A:812:LEU:N	2.43	0.51
1:A:836:LYS:HG2	1:A:839:LEU:CD1	2.40	0.51
1:A:179:GLY:O	1:A:674:ILE:HG12	2.11	0.51
1:A:321:THR:CG2	1:A:322:LEU:N	2.73	0.51
1:A:490:PHE:HD1	1:A:663:TYR:CE2	2.29	0.51
1:A:618:PRO:O	1:A:620:VAL:N	2.43	0.51
1:A:751:ASP:HB3	1:A:754:GLU:HG2	1.92	0.51
2:B:13:ARG:N	2:B:13:ARG:CD	2.73	0.51
2:B:53:GLU:O	2:B:55:ASN:N	2.43	0.51
1:A:88:MET:CE	1:A:99:ILE:HG23	2.35	0.51
1:A:483:THR:HA	1:A:655:LEU:HD21	1.93	0.51
3:C:118:ILE:HG23	3:C:122:GLN:HB2	1.92	0.51
1:A:274:LYS:O	1:A:276:ARG:N	2.44	0.51
1:A:328:ASP:O	1:A:329:ASP:C	2.49	0.51
1:A:390:LEU:HD22	1:A:619:ILE:CD1	2.39	0.51
1:A:514:ASP:OD1	1:A:516:GLY:N	2.40	0.51
1:A:555:TYR:O	1:A:556:ASP:C	2.49	0.51
1:A:672:CYS:C	1:A:673:ILE:HG13	2.31	0.51
2:B:47:ARG:O	2:B:48:VAL:HB	2.10	0.51
1:A:293:LEU:HD13	1:A:305:ILE:CD1	2.41	0.51
2:B:89:ASN:O	2:B:92:SER:HB2	2.10	0.51
3:C:73:GLU:HA	3:C:76:SER:OG	2.10	0.51
1:A:107:TYR:CD2	1:A:684:ILE:HD11	2.46	0.51
1:A:178:SER:O	4:A:1001:SO4:O3	2.28	0.51
1:A:230:VAL:CG1	1:A:441:LEU:HD21	2.40	0.51
1:A:346:THR:HB	1:A:349:GLU:CG	2.41	0.51
1:A:417:ARG:NE	1:A:417:ARG:N	2.49	0.51
1:A:499:GLU:OE1	1:A:712:ARG:NH2	2.33	0.51
1:A:620:VAL:HG12	1:A:624:PHE:HE1	1.75	0.51
2:B:42:PHE:HA	2:B:45:LEU:HB2	1.92	0.51
1:A:180:ALA:HB1	1:A:672:CYS:HB3	1.93	0.51
2:B:147:GLY:O	2:B:148:LYS:HB2	2.09	0.51
3:C:30:ALA:CB	3:C:55:THR:HG23	2.40	0.51
1:A:351:LEU:HD11	1:A:355:LYS:HE3	1.91	0.51
2:B:34:GLY:N	2:B:37:ASP:HB2	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:ARG:HD2	2:B:13:ARG:H	1.74	0.51
2:B:145:ILE:O	2:B:148:LYS:HG3	2.11	0.51
1:A:36:VAL:HG22	1:A:69:VAL:HG21	1.94	0.50
1:A:51:THR:CG2	1:A:52:LYS:N	2.74	0.50
1:A:546:SER:N	1:A:549:SER:OG	2.43	0.50
1:A:568:PRO:CG	1:A:578:ALA:HB3	2.40	0.50
1:A:307:ALA:HB1	1:A:314:TYR:OH	2.11	0.50
1:A:645:GLN:HA	1:A:645:GLN:OE1	2.10	0.50
2:B:67:PHE:HA	2:B:70:PHE:CB	2.41	0.50
2:B:145:ILE:O	2:B:146:LYS:C	2.48	0.50
1:A:611:LEU:C	1:A:613:GLN:N	2.65	0.50
2:B:22:PHE:CD1	2:B:22:PHE:C	2.84	0.50
1:A:46:ALA:HB1	1:A:58:VAL:CG1	2.41	0.50
1:A:308:VAL:O	1:A:308:VAL:HG23	2.12	0.50
1:A:440:TRP:CD1	1:A:621:LYS:CD	2.94	0.50
1:A:292:GLN:HB3	1:A:333:MET:HE2	1.94	0.50
1:A:324:VAL:O	1:A:327:ILE:CG2	2.60	0.50
1:A:794:TYR:CD1	3:C:153:PRO:HD3	2.47	0.50
1:A:346:THR:C	1:A:348:GLU:H	2.14	0.50
1:A:363:LEU:HD23	1:A:366:MET:SD	2.52	0.50
1:A:369:LYS:CD	1:A:370:GLN:H	2.25	0.50
1:A:36:VAL:HG22	1:A:37:PRO:HD2	1.93	0.50
1:A:351:LEU:HD21	1:A:355:LYS:CE	2.42	0.49
1:A:491:PHE:O	1:A:492:ASN:C	2.50	0.49
1:A:643:ALA:O	1:A:644:PHE:O	2.30	0.49
1:A:715:TYR:CE1	1:A:738:LYS:HG3	2.47	0.49
1:A:820:TRP:CB	2:B:146:LYS:NZ	2.75	0.49
1:A:403:LYS:O	1:A:415:GLN:CA	2.60	0.49
1:A:510:TRP:CZ2	1:A:512:PHE:HB2	2.46	0.49
1:A:618:PRO:C	1:A:620:VAL:N	2.65	0.49
1:A:793:GLY:O	1:A:797:ARG:HB2	2.12	0.49
1:A:88:MET:CE	1:A:102:ASN:HB3	2.42	0.49
1:A:304:LYS:HB3	1:A:355:LYS:HE2	1.94	0.49
1:A:346:THR:HB	1:A:349:GLU:HG3	1.94	0.49
1:A:796:MET:HE2	3:C:35:ASP:OD1	2.12	0.49
1:A:832:PHE:CE2	2:B:77:LYS:HD3	2.47	0.49
1:A:396:ASP:O	1:A:400:CYS:SG	2.65	0.49
1:A:571:PRO:HB2	1:A:575:CYS:SG	2.53	0.49
1:A:800:TYR:CE1	3:C:17:LEU:HD22	2.47	0.49
2:B:12:GLN:HB3	2:B:13:ARG:NH1	2.27	0.49
1:A:249:GLY:HA3	1:A:464:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ARG:HH12	1:A:621:LYS:HD2	1.77	0.49
1:A:354:TYR:O	1:A:357:THR:HB	2.11	0.49
1:A:832:PHE:HE2	2:B:77:LYS:NZ	2.07	0.49
3:C:14:VAL:CG1	3:C:36:LEU:HD12	2.43	0.49
2:B:33:ILE:HB	2:B:65:LEU:HD23	1.95	0.49
3:C:132:ILE:CD1	3:C:145:LEU:CA	2.89	0.49
1:A:140:TYR:CE1	1:A:148:MET:HE2	2.47	0.49
1:A:153:PHE:CD2	1:A:192:TYR:CD2	3.01	0.49
1:A:569:LYS:O	1:A:570:PRO:O	2.30	0.49
1:A:602:ASP:OD1	1:A:602:ASP:O	2.31	0.49
1:A:698:VAL:HG12	1:A:699:LEU:N	2.27	0.49
2:B:131:PRO:CB	2:B:141:LYS:HD3	2.42	0.49
3:C:135:ASP:OD1	3:C:136:ILE:N	2.46	0.49
1:A:178:SER:O	4:A:1001:SO4:O2	2.30	0.48
2:B:142:MET:HE3	2:B:146:LYS:HD3	1.94	0.48
1:A:15:LEU:CD2	1:A:84:MET:HG3	2.41	0.48
1:A:173:LEU:HD22	1:A:462:LEU:CD2	2.42	0.48
1:A:236:ASN:CB	1:A:244:ASN:HD21	2.26	0.48
1:A:600:ASN:ND2	1:A:648:SER:H	2.04	0.48
3:C:74:GLU:O	3:C:77:SER:N	2.33	0.48
1:A:133:THR:HG22	1:A:134:GLN:N	2.29	0.48
1:A:479:CYS:HB3	1:A:651:HIS:CD2	2.49	0.48
1:A:518:ASP:C	1:A:519:LEU:HD23	2.34	0.48
1:A:617:GLU:HA	1:A:620:VAL:HG21	1.96	0.48
1:A:6:SER:O	1:A:8:PRO:CD	2.61	0.48
1:A:183:THR:O	1:A:184:GLU:C	2.51	0.48
1:A:311:PRO:O	1:A:312:GLY:O	2.30	0.48
1:A:115:TYR:CD1	1:A:150:PRO:HG3	2.49	0.48
1:A:193:PHE:CE2	1:A:459:ILE:HG21	2.49	0.48
1:A:298:PHE:HE1	1:A:333:MET:HG3	1.72	0.48
1:A:417:ARG:HE	1:A:417:ARG:CA	2.27	0.48
1:A:572:LYS:C	1:A:574:GLY:H	2.17	0.48
3:C:88:MET:CE	3:C:142:TYR:HE1	2.25	0.48
1:A:374:GLN:NE2	1:A:415:GLN:HG2	2.28	0.48
3:C:104:SER:HB3	3:C:140:ILE:CG1	2.44	0.48
1:A:71:LYS:O	1:A:74:ILE:HG12	2.14	0.48
1:A:136:LEU:CD2	1:A:139:LYS:HD2	2.42	0.48
1:A:352:SER:O	1:A:353:MET:C	2.51	0.48
1:A:713:ILE:O	1:A:761:LYS:HA	2.13	0.48
1:A:722:TYR:O	1:A:725:LEU:HB2	2.14	0.48
1:A:529:PRO:O	1:A:530:MET:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:PHE:N	1:A:669:PHE:CD1	2.82	0.48
3:C:12:ARG:HG3	3:C:12:ARG:NH1	2.27	0.48
1:A:406:ILE:O	1:A:407:LYS:HB3	2.13	0.48
2:B:7:ARG:O	2:B:78:VAL:CG1	2.44	0.48
2:B:35:MET:O	2:B:39:LYS:HG3	2.13	0.48
1:A:95:ASN:O	1:A:99:ILE:HG12	2.15	0.47
1:A:367:LYS:NZ	1:A:382:GLU:CD	2.67	0.47
2:B:14:GLN:O	2:B:18:LEU:HG	2.14	0.47
2:B:55:ASN:O	2:B:58:LEU:HB2	2.14	0.47
3:C:16:ASP:HA	3:C:19:ASP:OD1	2.14	0.47
1:A:16:THR:OG1	1:A:19:LYS:HG3	2.15	0.47
1:A:88:MET:HE3	1:A:99:ILE:O	2.14	0.47
1:A:193:PHE:HB3	1:A:256:PHE:HZ	1.79	0.47
1:A:227:CYS:HB3	1:A:445:VAL:HG11	1.96	0.47
1:A:345:PHE:CE2	1:A:444:ARG:NH2	2.64	0.47
1:A:388:PHE:O	1:A:391:GLY:N	2.47	0.47
1:A:406:ILE:HB	1:A:414:THR:CG2	2.44	0.47
1:A:3:MET:SD	1:A:149:PRO:HD3	2.55	0.47
1:A:115:TYR:CZ	1:A:150:PRO:HA	2.49	0.47
3:C:4:THR:HG23	3:C:7:GLU:CD	2.34	0.47
3:C:14:VAL:HG12	3:C:36:LEU:CD1	2.45	0.47
1:A:59:LYS:HE2	1:A:64:GLN:HE22	1.80	0.47
1:A:293:LEU:HA	1:A:333:MET:CE	2.44	0.47
1:A:367:LYS:HD3	1:A:367:LYS:N	2.29	0.47
1:A:536:LEU:HD13	1:A:550:PHE:CZ	2.50	0.47
1:A:550:PHE:HE2	1:A:593:ILE:CD1	2.14	0.47
2:B:52:ASP:O	2:B:55:ASN:HB3	2.14	0.47
3:C:117:ARG:CG	3:C:117:ARG:NH1	2.76	0.47
1:A:831:LEU:C	1:A:833:ASN:N	2.68	0.47
2:B:8:VAL:HG23	2:B:9:LYS:HD2	1.97	0.47
1:A:337:ASP:OD1	1:A:350:LYS:NZ	2.48	0.47
1:A:403:LYS:N	1:A:404:PRO:CD	2.67	0.47
1:A:539:GLU:OE2	1:A:549:SER:HB2	2.15	0.47
1:A:690:LEU:O	1:A:691:HIS:C	2.51	0.47
2:B:127:TRP:O	2:B:128:LYS:C	2.53	0.47
3:C:42:MET:CE	3:C:75:MET:HG3	2.44	0.47
1:A:337:ASP:OD1	1:A:350:LYS:CE	2.62	0.47
1:A:382:GLU:O	1:A:386:VAL:HG22	2.14	0.47
1:A:603:PRO:CB	1:A:644:PHE:HB3	2.45	0.47
1:A:617:GLU:CA	1:A:620:VAL:HG23	2.45	0.47
2:B:10:LEU:HG	2:B:15:MET:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:VAL:HG21	3:C:40:LEU:HD23	1.96	0.47
1:A:99:ILE:HG13	1:A:702:ILE:HD13	1.97	0.47
1:A:692:GLN:O	1:A:696:ASN:ND2	2.47	0.47
2:B:10:LEU:HA	2:B:14:GLN:OE1	2.15	0.47
2:B:32:PHE:CD2	2:B:64:GLN:HG2	2.50	0.47
2:B:60:GLU:HB3	2:B:73:LEU:HD11	1.97	0.47
3:C:135:ASP:O	3:C:136:ILE:O	2.32	0.47
1:A:84:MET:HE1	1:A:105:SER:HB2	1.97	0.47
1:A:107:TYR:HA	1:A:111:PHE:O	2.15	0.47
1:A:170:GLN:O	1:A:459:ILE:HA	2.15	0.47
1:A:346:THR:HB	1:A:349:GLU:H	1.80	0.47
1:A:379:GLY:O	1:A:380:THR:OG1	2.19	0.47
1:A:551:LYS:O	1:A:555:TYR:HD1	1.97	0.47
2:B:29:ARG:O	2:B:32:PHE:HD1	1.98	0.47
1:A:160:TYR:OH	1:A:260:GLY:HA3	2.15	0.46
1:A:346:THR:HG22	1:A:348:GLU:HB3	1.96	0.46
1:A:351:LEU:O	1:A:355:LYS:N	2.41	0.46
1:A:358:GLY:O	1:A:361:LEU:HB2	2.14	0.46
1:A:368:TRP:CE3	1:A:402:LEU:HD21	2.50	0.46
1:A:386:VAL:HG23	1:A:387:ALA:N	2.29	0.46
1:A:495:MET:HE1	1:A:704:ILE:HB	1.97	0.46
1:A:727:PRO:HB2	3:C:85:ASP:HB3	1.96	0.46
1:A:836:LYS:HA	1:A:839:LEU:CD2	2.45	0.46
2:B:25:ILE:O	2:B:37:ASP:CB	2.53	0.46
3:C:153:PRO:C	3:C:155:PRO:HD3	2.34	0.46
1:A:348:GLU:O	1:A:349:GLU:C	2.53	0.46
1:A:547:ASP:CG	1:A:595:GLY:H	2.18	0.46
1:A:783:ILE:HG21	3:C:86:GLU:O	2.16	0.46
2:B:39:LYS:HE2	2:B:54:LEU:HD22	1.97	0.46
1:A:42:GLY:HA3	1:A:686:ALA:CB	2.45	0.46
1:A:115:TYR:CE1	1:A:150:PRO:HA	2.50	0.46
1:A:160:TYR:OH	1:A:260:GLY:CA	2.63	0.46
1:A:413:VAL:C	1:A:415:GLN:N	2.68	0.46
1:A:785:SER:HA	1:A:788:GLN:OE1	2.16	0.46
1:A:2:THR:CG2	1:A:143:LYS:HZ3	2.28	0.46
1:A:44:VAL:CG1	1:A:45:GLY:N	2.79	0.46
1:A:184:GLU:CG	1:A:185:ASN:N	2.79	0.46
1:A:242:ASN:HD22	1:A:243:ASN:N	2.13	0.46
1:A:300:GLU:HG3	1:A:301:ASN:N	2.29	0.46
1:A:646:THR:O	1:A:650:VAL:HG23	2.16	0.46
1:A:713:ILE:HD11	1:A:769:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:ARG:NH1	3:C:65:LEU:CD2	2.78	0.46
1:A:79:PRO:HG2	1:A:82:PHE:CD1	2.50	0.46
1:A:513:ILE:O	1:A:514:ASP:C	2.53	0.46
1:A:528:LYS:HA	1:A:529:PRO:HD3	1.81	0.46
1:A:551:LYS:HE2	1:A:555:TYR:CE1	2.51	0.46
1:A:572:LYS:O	1:A:573:ALA:HB3	2.16	0.46
2:B:29:ARG:O	2:B:31:GLY:N	2.49	0.46
2:B:132:LEU:O	2:B:133:LYS:HG2	2.15	0.46
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.83	0.46
1:A:365:GLU:O	1:A:366:MET:C	2.54	0.46
1:A:398:LEU:O	1:A:402:LEU:HB2	2.16	0.46
1:A:422:VAL:HG23	1:A:423:THR:N	2.31	0.46
1:A:190:ILE:HG23	1:A:254:ILE:CD1	2.46	0.46
1:A:712:ARG:HG2	1:A:763:PHE:CD2	2.51	0.46
1:A:718:PHE:CE1	1:A:722:TYR:CD1	3.04	0.46
2:B:146:LYS:HD2	2:B:146:LYS:HA	1.39	0.46
1:A:97:ALA:O	1:A:100:LEU:HB3	2.16	0.46
1:A:450:ASP:OD1	1:A:452:LYS:CG	2.63	0.46
2:B:12:GLN:CD	2:B:13:ARG:NH1	2.69	0.46
2:B:130:ALA:HA	2:B:131:PRO:HD3	1.75	0.46
2:B:132:LEU:HD23	2:B:137:PHE:HA	1.97	0.46
1:A:1:MET:O	1:A:2:THR:OG1	2.26	0.46
1:A:572:LYS:O	1:A:572:LYS:CG	2.52	0.46
1:A:258:THR:O	1:A:258:THR:CG2	2.63	0.45
2:B:28:ASP:O	2:B:30:ASP:N	2.49	0.45
1:A:192:TYR:CE1	1:A:196:VAL:HG11	2.50	0.45
1:A:200:LEU:HD13	1:A:259:GLN:OE1	2.17	0.45
1:A:292:GLN:HB3	1:A:333:MET:CE	2.45	0.45
1:A:392:VAL:HG12	1:A:393:ASN:N	2.31	0.45
1:A:31:LYS:O	1:A:32:LYS:HG2	2.17	0.45
1:A:240:THR:H	1:A:284:GLU:HG2	1.81	0.45
1:A:280:GLN:CB	1:A:320:GLY:N	2.80	0.45
1:A:384:GLU:HA	1:A:387:ALA:HB3	1.98	0.45
1:A:402:LEU:C	1:A:403:LYS:HG2	2.33	0.45
1:A:425:SER:OG	1:A:605:ASN:ND2	2.50	0.45
1:A:690:LEU:O	1:A:693:LEU:N	2.50	0.45
1:A:779:ARG:HD2	1:A:779:ARG:HA	1.59	0.45
1:A:817:VAL:O	1:A:820:TRP:N	2.49	0.45
1:A:36:VAL:CG2	1:A:37:PRO:HD2	2.47	0.45
1:A:61:ASP:O	1:A:63:THR:N	2.48	0.45
1:A:261:LYS:H	1:A:261:LYS:HG2	1.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:ARG:CD	2:B:13:ARG:H	2.29	0.45
1:A:142:GLY:HA2	1:A:161:GLN:HE21	1.79	0.45
1:A:289:ILE:O	1:A:289:ILE:HG12	2.16	0.45
1:A:608:VAL:HG12	1:A:612:LEU:CD1	2.47	0.45
1:A:805:ASP:O	1:A:808:ILE:HB	2.17	0.45
3:C:30:ALA:O	3:C:33:VAL:HG23	2.16	0.45
3:C:61:LYS:HG2	3:C:62:ALA:N	2.31	0.45
1:A:496:PHE:CD1	1:A:514:ASP:HA	2.51	0.45
1:A:750:LEU:HD13	1:A:771:MET:CE	2.47	0.45
3:C:136:ILE:CG2	3:C:137:ASP:N	2.76	0.45
1:A:346:THR:CG2	1:A:348:GLU:HB3	2.47	0.45
1:A:555:TYR:HD2	1:A:559:LEU:CD1	2.29	0.45
1:A:563:PRO:HB2	1:A:564:MET:HE1	1.98	0.45
2:B:87:LEU:HB3	2:B:143:VAL:HG22	1.97	0.45
2:B:123:ILE:HG22	2:B:127:TRP:HE1	1.81	0.45
1:A:2:THR:HG21	1:A:143:LYS:CE	2.47	0.45
1:A:9:ASP:HB3	1:A:136:LEU:HD21	1.98	0.45
1:A:63:THR:C	1:A:64:GLN:O	2.53	0.45
1:A:715:TYR:CZ	1:A:738:LYS:HG3	2.52	0.45
2:B:35:MET:O	2:B:38:LEU:HB2	2.17	0.45
1:A:176:GLY:O	1:A:182:LYS:HE3	2.17	0.45
1:A:363:LEU:HA	1:A:366:MET:SD	2.56	0.45
3:C:7:GLU:O	3:C:11:VAL:HG23	2.16	0.45
3:C:119:THR:CG2	3:C:120:GLU:N	2.79	0.45
1:A:35:TRP:HA	1:A:35:TRP:CE3	2.52	0.45
1:A:386:VAL:HG23	1:A:387:ALA:H	1.82	0.45
1:A:832:PHE:CZ	2:B:77:LYS:HD3	2.52	0.45
1:A:374:GLN:CD	1:A:415:GLN:NE2	2.67	0.44
1:A:444:ARG:HD2	1:A:444:ARG:HA	1.48	0.44
1:A:524:GLU:O	1:A:528:LYS:HB2	2.18	0.44
1:A:619:ILE:O	1:A:619:ILE:CG2	2.65	0.44
1:A:709:PHE:CD2	1:A:765:LYS:HG2	2.52	0.44
1:A:48:ILE:HA	1:A:58:VAL:HG22	2.00	0.44
1:A:407:LYS:O	1:A:408:VAL:CG2	2.63	0.44
1:A:440:TRP:CD1	1:A:621:LYS:CE	3.01	0.44
1:A:817:VAL:HA	2:B:146:LYS:CE	2.47	0.44
1:A:826:TRP:HB3	1:A:829:TRP:CB	2.47	0.44
1:A:836:LYS:HZ3	2:B:21:ALA:HB2	1.80	0.44
3:C:78:LYS:HE3	3:C:79:ASP:H	1.82	0.44
1:A:131:ILE:O	1:A:131:ILE:HG22	2.17	0.44
1:A:176:GLY:O	1:A:182:LYS:CE	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:PRO:O	1:A:530:MET:CB	2.66	0.44
1:A:604:ILE:H	1:A:644:PHE:HA	1.83	0.44
1:A:678:LEU:O	1:A:679:LYS:C	2.55	0.44
1:A:615:SER:O	1:A:620:VAL:HG22	2.18	0.44
2:B:48:VAL:O	2:B:50:PRO:HD3	2.17	0.44
2:B:53:GLU:O	2:B:54:LEU:C	2.56	0.44
3:C:44:PRO:CA	3:C:48:GLN:OE1	2.65	0.44
1:A:199:SER:O	1:A:200:LEU:HD23	2.17	0.44
1:A:329:ASP:O	1:A:330:GLU:C	2.55	0.44
1:A:519:LEU:O	1:A:523:ILE:HG13	2.17	0.44
2:B:50:PRO:O	2:B:53:GLU:HB2	2.18	0.44
3:C:36:LEU:HD21	3:C:68:ILE:HD13	2.00	0.44
3:C:82:THR:HG21	3:C:87:PHE:CE2	2.53	0.44
1:A:199:SER:C	1:A:200:LEU:HD23	2.37	0.44
2:B:28:ASP:CG	2:B:29:ARG:HG2	2.38	0.44
3:C:117:ARG:H	3:C:117:ARG:HD2	1.83	0.44
1:A:6:SER:O	1:A:8:PRO:HD3	2.18	0.44
1:A:136:LEU:O	1:A:137:VAL:C	2.56	0.44
1:A:407:LYS:HB3	1:A:411:GLU:HG2	1.99	0.44
1:A:571:PRO:HD2	1:A:576:ALA:O	2.18	0.44
2:B:28:ASP:OD2	2:B:37:ASP:OD2	2.36	0.44
1:A:19:LYS:O	1:A:22:GLU:HB3	2.18	0.44
1:A:153:PHE:CD2	1:A:192:TYR:HD2	2.35	0.44
1:A:351:LEU:CD2	1:A:355:LYS:HE3	2.45	0.44
1:A:624:PHE:O	1:A:625:THR:C	2.57	0.44
1:A:65:GLU:HA	1:A:65:GLU:OE1	2.18	0.43
1:A:181:GLY:O	1:A:182:LYS:C	2.57	0.43
1:A:280:GLN:HB2	1:A:319:GLN:CB	2.42	0.43
1:A:351:LEU:CG	1:A:355:LYS:HE3	2.48	0.43
1:A:786:MET:CE	3:C:82:THR:OG1	2.66	0.43
2:B:28:ASP:OD1	2:B:37:ASP:CG	2.56	0.43
2:B:151:ASP:N	2:B:151:ASP:OD1	2.51	0.43
1:A:392:VAL:HG11	1:A:611:LEU:CG	2.48	0.43
1:A:414:THR:C	1:A:416:GLY:H	2.21	0.43
2:B:147:GLY:O	2:B:148:LYS:CG	2.66	0.43
1:A:794:TYR:OH	3:C:153:PRO:HA	2.18	0.43
1:A:274:LYS:O	1:A:275:SER:C	2.57	0.43
1:A:285:ARG:CG	1:A:291:TYR:CE1	3.00	0.43
1:A:563:PRO:HG2	1:A:564:MET:H	1.82	0.43
1:A:78:ASN:HD21	1:A:91:LEU:HB3	1.82	0.43
1:A:247:ARG:HD2	1:A:247:ARG:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:O	1:A:265:ALA:HA	2.18	0.43
1:A:290:PHE:CB	1:A:317:ILE:HD11	2.47	0.43
1:A:298:PHE:N	1:A:299:PRO:HD3	2.33	0.43
1:A:449:LEU:O	1:A:451:THR:N	2.50	0.43
1:A:482:TYR:OH	1:A:527:GLU:HG2	2.19	0.43
1:A:751:ASP:OD1	1:A:752:PRO:HD2	2.19	0.43
1:A:784:ILE:O	1:A:788:GLN:HG3	2.18	0.43
1:A:812:LEU:O	1:A:816:ASN:HB2	2.19	0.43
2:B:29:ARG:HH22	2:B:35:MET:H	1.62	0.43
2:B:124:LYS:O	2:B:125:ASN:C	2.57	0.43
2:B:133:LYS:O	2:B:134:ASN:C	2.57	0.43
1:A:49:GLN:OE1	1:A:49:GLN:HA	2.19	0.43
1:A:321:THR:CG2	1:A:322:LEU:H	2.32	0.43
1:A:382:GLU:H	1:A:382:GLU:HG3	1.39	0.43
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.43	0.43
1:A:817:VAL:O	1:A:820:TRP:HB3	2.18	0.43
1:A:832:PHE:CE2	2:B:77:LYS:NZ	2.71	0.43
2:B:77:LYS:HE3	2:B:77:LYS:HB2	1.80	0.43
3:C:42:MET:HE2	3:C:75:MET:HG3	2.01	0.43
3:C:57:LYS:HG2	3:C:60:GLU:OE2	2.18	0.43
1:A:56:VAL:CG1	1:A:57:THR:N	2.81	0.43
1:A:106:ARG:O	1:A:111:PHE:HB2	2.19	0.43
1:A:380:THR:O	1:A:380:THR:HG22	2.18	0.43
3:C:102:ILE:O	3:C:103:SER:C	2.56	0.43
1:A:2:THR:CG2	1:A:143:LYS:HZ1	2.17	0.43
1:A:32:LYS:HD3	1:A:48:ILE:O	2.18	0.43
1:A:51:THR:O	1:A:52:LYS:HB2	2.17	0.43
1:A:293:LEU:HD13	1:A:305:ILE:HD11	2.00	0.43
1:A:709:PHE:HB3	1:A:763:PHE:HB3	2.00	0.43
1:A:711:ASN:HB2	1:A:764:PHE:HB2	2.00	0.43
3:C:93:THR:CG2	3:C:94:PHE:CD1	3.02	0.43
1:A:34:CYS:HB2	1:A:75:GLY:O	2.19	0.43
1:A:120:CYS:CB	1:A:155:ILE:CD1	2.96	0.43
2:B:29:ARG:O	2:B:30:ASP:C	2.57	0.43
2:B:101:PHE:HD2	2:B:139:TYR:CE2	2.36	0.43
3:C:78:LYS:HG3	3:C:79:ASP:H	1.83	0.43
3:C:89:GLU:HA	3:C:89:GLU:OE1	2.19	0.43
1:A:69:VAL:HG12	1:A:70:LYS:N	2.34	0.43
1:A:440:TRP:HZ2	1:A:444:ARG:NH1	2.17	0.43
1:A:721:ARG:NH2	1:A:773:GLU:OE2	2.47	0.43
1:A:816:ASN:ND2	2:B:82:ASP:HB2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:PHE:C	2:B:70:PHE:H	2.21	0.43
2:B:119:SER:C	2:B:121:GLU:N	2.67	0.43
3:C:35:ASP:O	3:C:36:LEU:C	2.56	0.43
1:A:63:THR:O	1:A:64:GLN:O	2.37	0.42
1:A:250:LYS:HE3	1:A:252:ILE:HD11	2.01	0.42
1:A:302:ILE:HG22	1:A:307:ALA:O	2.19	0.42
1:A:615:SER:O	1:A:616:LYS:O	2.37	0.42
1:A:823:LEU:C	1:A:825:ASN:H	2.22	0.42
2:B:32:PHE:O	2:B:37:ASP:OD2	2.37	0.42
2:B:145:ILE:O	2:B:148:LYS:HG2	2.19	0.42
3:C:40:LEU:HD13	3:C:72:TYR:CE1	2.54	0.42
1:A:56:VAL:HG12	1:A:58:VAL:HG23	2.01	0.42
1:A:118:LEU:HD13	1:A:494:HIS:HD2	1.84	0.42
1:A:305:ILE:O	1:A:306:LEU:CG	2.66	0.42
1:A:332:GLU:C	1:A:334:GLY:H	2.20	0.42
1:A:381:ALA:O	1:A:384:GLU:HG2	2.19	0.42
1:A:800:TYR:CE1	3:C:17:LEU:CD2	3.02	0.42
2:B:101:PHE:CE1	2:B:138:ASN:OD1	2.72	0.42
1:A:181:GLY:C	1:A:183:THR:H	2.22	0.42
1:A:437:MET:HG3	1:A:622:MET:CE	2.50	0.42
1:A:466:GLY:O	1:A:484:ASN:CG	2.57	0.42
1:A:661:ASN:O	1:A:665:THR:HG23	2.20	0.42
3:C:82:THR:HG21	3:C:87:PHE:CZ	2.54	0.42
1:A:346:THR:HG22	1:A:348:GLU:N	2.30	0.42
1:A:826:TRP:O	1:A:828:TRP:N	2.52	0.42
1:A:557:ASN:HB3	1:A:558:HIS:CD2	2.54	0.42
2:B:39:LYS:CE	2:B:54:LEU:HD22	2.50	0.42
2:B:56:ALA:HA	2:B:59:LYS:CG	2.48	0.42
3:C:99:GLN:OE1	3:C:99:GLN:HA	2.20	0.42
1:A:192:TYR:CD1	1:A:192:TYR:C	2.93	0.42
1:A:258:THR:O	1:A:258:THR:HG22	2.18	0.42
1:A:348:GLU:O	1:A:351:LEU:HB3	2.20	0.42
1:A:488:GLN:O	1:A:491:PHE:HB3	2.19	0.42
1:A:567:LYS:HA	1:A:580:PHE:HA	2.02	0.42
1:A:660:LYS:HD2	1:A:660:LYS:O	2.19	0.42
1:A:736:ASP:OD1	1:A:738:LYS:N	2.52	0.42
1:A:800:TYR:CZ	1:A:804:GLN:NE2	2.84	0.42
1:A:816:ASN:ND2	2:B:87:LEU:HD21	2.34	0.42
3:C:104:SER:HB3	3:C:140:ILE:HD11	2.00	0.42
1:A:35:TRP:CZ2	1:A:77:ARG:HG3	2.54	0.42
1:A:362:HIS:O	1:A:365:GLU:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HG21	2:B:33:ILE:HG23	2.02	0.42
3:C:119:THR:HG22	3:C:120:GLU:N	2.34	0.42
1:A:234:TYR:CE1	1:A:289:ILE:HD12	2.54	0.42
1:A:728:ASN:C	3:C:85:ASP:CG	2.78	0.42
1:A:826:TRP:CZ2	2:B:60:GLU:OE1	2.73	0.42
3:C:102:ILE:HG13	3:C:142:TYR:CD2	2.52	0.42
1:A:118:LEU:CD1	1:A:494:HIS:HD2	2.33	0.42
1:A:163:MET:HE2	1:A:163:MET:HB3	1.92	0.42
1:A:236:ASN:HA	1:A:245:SER:O	2.20	0.42
1:A:367:LYS:O	1:A:368:TRP:CD2	2.73	0.42
2:B:142:MET:O	2:B:143:VAL:C	2.58	0.42
1:A:187:LYS:O	1:A:191:GLN:HG3	2.19	0.42
1:A:267:ILE:N	1:A:446:ASN:OD1	2.43	0.42
1:A:397:LEU:O	1:A:398:LEU:C	2.59	0.42
1:A:440:TRP:CZ2	1:A:444:ARG:NH1	2.88	0.42
1:A:551:LYS:O	1:A:554:LEU:HB2	2.20	0.42
1:A:593:ILE:HD13	1:A:593:ILE:HA	1.80	0.42
1:A:612:LEU:HD23	1:A:612:LEU:HA	1.87	0.42
2:B:129:ASP:O	2:B:130:ALA:O	2.38	0.42
1:A:192:TYR:CE1	1:A:196:VAL:CG1	3.02	0.41
1:A:259:GLN:HB2	1:A:261:LYS:CD	2.40	0.41
1:A:363:LEU:O	1:A:426:ILE:HG21	2.20	0.41
1:A:415:GLN:C	1:A:417:ARG:N	2.73	0.41
2:B:28:ASP:CG	2:B:37:ASP:OD2	2.58	0.41
2:B:61:CYS:O	2:B:62:PRO:C	2.59	0.41
2:B:131:PRO:HD2	2:B:137:PHE:HE1	1.79	0.41
3:C:29:ASP:O	3:C:32:LYS:N	2.53	0.41
1:A:280:GLN:HB3	1:A:320:GLY:HA3	2.02	0.41
1:A:828:TRP:NE1	2:B:60:GLU:OE1	2.53	0.41
2:B:74:PHE:CD2	2:B:77:LYS:NZ	2.84	0.41
2:B:106:TYR:O	2:B:110:LEU:HB2	2.19	0.41
2:B:150:GLU:O	2:B:151:ASP:C	2.58	0.41
1:A:58:VAL:O	1:A:66:THR:HA	2.20	0.41
1:A:450:ASP:O	1:A:450:ASP:CG	2.58	0.41
2:B:83:PRO:HD2	2:B:86:ALA:HB3	2.01	0.41
3:C:15:PHE:HE1	3:C:68:ILE:HD12	1.85	0.41
1:A:79:PRO:HG2	1:A:82:PHE:CE1	2.55	0.41
1:A:305:ILE:HG12	1:A:355:LYS:HA	2.03	0.41
1:A:542:PHE:O	1:A:545:ALA:N	2.36	0.41
1:A:693:LEU:HD22	1:A:698:VAL:HG11	2.01	0.41
1:A:792:ARG:NH2	3:C:117:ARG:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:GLU:HA	3:C:120:GLU:OE1	2.20	0.41
1:A:24:THR:HG22	1:A:24:THR:O	2.20	0.41
1:A:618:PRO:O	1:A:621:LYS:N	2.54	0.41
3:C:95:ASP:OD2	3:C:100:GLY:N	2.53	0.41
3:C:111:LEU:O	3:C:118:ILE:HB	2.19	0.41
3:C:117:ARG:CZ	3:C:117:ARG:HB3	2.50	0.41
1:A:464:ILE:HG23	1:A:465:ALA:H	1.80	0.41
1:A:820:TRP:CZ3	1:A:821:LEU:CD2	3.04	0.41
3:C:84:ALA:O	3:C:85:ASP:C	2.59	0.41
1:A:369:LYS:HG3	1:A:370:GLN:N	2.36	0.41
1:A:665:THR:O	1:A:667:PRO:HD3	2.19	0.41
1:A:836:LYS:HG2	1:A:839:LEU:HD21	2.02	0.41
1:A:193:PHE:CZ	1:A:459:ILE:HG21	2.56	0.41
1:A:258:THR:N	1:A:261:LYS:HE2	2.36	0.41
1:A:479:CYS:HB3	1:A:651:HIS:NE2	2.35	0.41
1:A:602:ASP:N	1:A:603:PRO:CD	2.84	0.41
2:B:81:THR:O	2:B:82:ASP:C	2.58	0.41
2:B:141:LYS:O	2:B:144:ASP:HB2	2.21	0.41
3:C:14:VAL:HG12	3:C:36:LEU:HD12	2.03	0.41
1:A:192:TYR:HE1	1:A:196:VAL:HG11	1.86	0.41
1:A:290:PHE:HB3	1:A:317:ILE:HD13	2.00	0.41
1:A:305:ILE:O	1:A:306:LEU:HB2	2.19	0.41
1:A:372:GLY:O	1:A:373:GLU:HG3	2.20	0.41
1:A:393:ASN:O	1:A:395:GLY:N	2.54	0.41
1:A:412:TYR:CG	1:A:413:VAL:N	2.89	0.41
1:A:525:LEU:HD21	1:A:565:PHE:HB2	2.03	0.41
1:A:615:SER:O	1:A:616:LYS:C	2.59	0.41
1:A:809:GLY:O	1:A:812:LEU:HB2	2.21	0.41
3:C:46:GLU:O	3:C:47:ALA:C	2.57	0.41
3:C:132:ILE:CD1	3:C:145:LEU:CD1	2.98	0.41
3:C:141:LYS:HD2	3:C:144:ASP:OD2	2.21	0.41
1:A:3:MET:HE2	1:A:14:CYS:SG	2.61	0.41
1:A:51:THR:O	1:A:52:LYS:CB	2.68	0.41
1:A:132:TYR:CZ	1:A:188:LYS:HD3	2.56	0.41
1:A:406:ILE:C	1:A:407:LYS:HD3	2.42	0.41
1:A:569:LYS:HA	1:A:570:PRO:HD2	1.69	0.41
1:A:718:PHE:CE1	1:A:722:TYR:HD1	2.39	0.41
1:A:810:LEU:HD12	1:A:810:LEU:HA	1.92	0.41
2:B:58:LEU:O	2:B:59:LYS:C	2.59	0.41
2:B:131:PRO:HB3	2:B:141:LYS:CG	2.50	0.41
2:B:144:ASP:O	2:B:145:ILE:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASP:CB	1:A:41:PHE:HD2	2.34	0.40
1:A:200:LEU:CD1	1:A:259:GLN:O	2.68	0.40
1:A:238:LYS:HD2	1:A:324:VAL:HG22	2.04	0.40
1:A:280:GLN:CB	1:A:319:GLN:HB2	2.45	0.40
1:A:645:GLN:HB3	1:A:646:THR:H	1.63	0.40
1:A:650:VAL:O	1:A:651:HIS:C	2.59	0.40
3:C:61:LYS:HB2	3:C:61:LYS:HE3	1.89	0.40
1:A:26:ILE:HB	1:A:27:PRO:CD	2.50	0.40
1:A:141:ARG:NH1	1:A:199:SER:OG	2.53	0.40
1:A:181:GLY:O	1:A:185:ASN:HB2	2.22	0.40
1:A:299:PRO:O	1:A:302:ILE:HB	2.21	0.40
1:A:380:THR:O	1:A:380:THR:CG2	2.70	0.40
1:A:412:TYR:CE2	1:A:413:VAL:O	2.74	0.40
1:A:528:LYS:HD2	1:A:529:PRO:HD2	2.03	0.40
1:A:767:GLY:O	1:A:768:VAL:C	2.59	0.40
3:C:12:ARG:NH1	3:C:65:LEU:HD23	2.36	0.40
1:A:369:LYS:CG	1:A:370:GLN:N	2.84	0.40
1:A:659:MET:O	1:A:660:LYS:C	2.59	0.40
1:A:815:ARG:NH2	2:B:82:ASP:OD1	2.52	0.40
2:B:116:ASP:OD2	3:C:24:ARG:NH2	2.55	0.40
2:B:123:ILE:HG23	2:B:127:TRP:HE1	1.86	0.40
3:C:132:ILE:CD1	3:C:145:LEU:HD13	2.52	0.40
3:C:143:GLU:O	3:C:144:ASP:C	2.60	0.40
1:A:479:CYS:SG	1:A:651:HIS:CD2	3.14	0.40
1:A:572:LYS:O	1:A:574:GLY:N	2.48	0.40
1:A:3:MET:HE2	1:A:3:MET:HB3	2.00	0.40
1:A:112:ILE:HG21	1:A:125:PRO:HB3	2.03	0.40
1:A:236:ASN:HD22	1:A:244:ASN:HD21	1.67	0.40
1:A:358:GLY:HA2	1:A:361:LEU:HD12	2.03	0.40
1:A:796:MET:CE	3:C:35:ASP:CG	2.90	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLN:OE1	2:B:68:THR:OG1[2_556]	2.10	0.10

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%)	625 (78%)	109 (14%)	68 (8%)	1 5
2	B	143/153 (94%)	89 (62%)	26 (18%)	28 (20%)	0 0
3	C	154/159 (97%)	130 (84%)	17 (11%)	7 (4%)	2 15
All	All	1099/1151 (96%)	844 (77%)	152 (14%)	103 (9%)	0 4

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	8	PRO
1	A	52	LYS
1	A	61	ASP
1	A	62	LYS
1	A	65	GLU
1	A	131	ILE
1	A	178	SER
1	A	201	ALA
1	A	240	THR
1	A	275	SER
1	A	306	LEU
1	A	309	PRO
1	A	313	LEU
1	A	366	MET
1	A	380	THR
1	A	394	ALA
1	A	404	PRO
1	A	408	VAL
1	A	415	GLN
1	A	417	ARG
1	A	570	PRO
1	A	571	PRO
1	A	576	ALA

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Mol	Chain	Res	Type
1	A	616	LYS
2	B	9	LYS
2	B	27	GLN
2	B	48	VAL
2	B	99	GLN
2	B	117	ASN
2	B	130	ALA
2	B	134	ASN
2	B	148	LYS
2	B	150	GLU
3	C	2	GLN
3	C	24	ARG
3	C	136	ILE
3	C	139	ASN
1	A	5	PHE
1	A	15	LEU
1	A	127	ARG
1	A	145	ARG
1	A	274	LYS
1	A	296	PRO
1	A	312	GLY
1	A	317	ILE
1	A	346	THR
1	A	363	LEU
1	A	416	GLY
1	A	450	ASP
1	A	530	MET
1	A	644	PHE
1	A	679	LYS
1	A	827	GLU
2	B	25	ILE
2	B	30	ASP
2	B	54	LEU
2	B	59	LYS
2	B	66	ASN
2	B	84	GLU
2	B	98	GLY
2	B	125	ASN
3	C	82	THR
3	C	155	PRO
1	A	14	CYS
1	A	105	SER

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Mol	Chain	Res	Type
1	A	282	SER
1	A	350	LYS
1	A	406	ILE
1	A	514	ASP
1	A	532	ILE
1	A	681	PRO
1	A	823	LEU
2	B	42	PHE
2	B	51	ASP
2	B	79	SER
2	B	104	GLU
2	B	146	LYS
3	C	60	GLU
1	A	55	GLU
1	A	64	GLN
1	A	199	SER
1	A	403	LYS
1	A	465	ALA
1	A	475	PHE
1	A	543	PRO
1	A	556	ASP
1	A	732	SER
1	A	835	VAL
2	B	33	ILE
2	B	49	PRO
2	B	53	GLU
1	A	7	ASP
1	A	606	GLU
1	A	619	ILE
1	A	696	ASN
2	B	29	ARG
1	A	329	ASP
1	A	568	PRO
2	B	80	GLY
1	A	298	PHE
1	A	229	PRO
2	B	147	GLY

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	704/731 (96%)	653 (93%)	51 (7%)	14 41
2	B	128/134 (96%)	107 (84%)	21 (16%)	2 10
3	C	134/137 (98%)	122 (91%)	12 (9%)	9 32
All	All	966/1002 (96%)	882 (91%)	84 (9%)	10 34

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	CYS
1	A	36	VAL
1	A	39	PRO
1	A	41	PHE
1	A	102	ASN
1	A	116	SER
1	A	144	ARG
1	A	188	LYS
1	A	242	ASN
1	A	244	ASN
1	A	246	SER
1	A	275	SER
1	A	282	SER
1	A	289	ILE
1	A	295	SER
1	A	296	PRO
1	A	340	PHE
1	A	382	GLU
1	A	403	LYS
1	A	407	LYS
1	A	413	VAL
1	A	417	ARG
1	A	423	THR
1	A	425	SER
1	A	451	THR
1	A	508	ILE
1	A	511	GLU
1	A	532	ILE
1	A	535	ILE
1	A	543	PRO

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Mol	Chain	Res	Type
1	A	546	SER
1	A	549	SER
1	A	556	ASP
1	A	559	LEU
1	A	564	MET
1	A	569	LYS
1	A	583	HIS
1	A	620	VAL
1	A	621	LYS
1	A	622	MET
1	A	624	PHE
1	A	644	PHE
1	A	664	SER
1	A	667	PRO
1	A	705	CYS
1	A	714	ILE
1	A	732	SER
1	A	765	LYS
1	A	815	ARG
1	A	827	GLU
1	A	832	PHE
2	B	9	LYS
2	B	15	MET
2	B	17	GLU
2	B	20	GLU
2	B	22	PHE
2	B	26	ASP
2	B	29	ARG
2	B	35	MET
2	B	45	LEU
2	B	58	LEU
2	B	59	LYS
2	B	61	CYS
2	B	66	ASN
2	B	81	THR
2	B	89	ASN
2	B	107	LEU
2	B	113	ASN
2	B	124	LYS
2	B	134	ASN
2	B	139	TYR
2	B	142	MET

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Mol	Chain	Res	Type
3	C	4	THR
3	C	8	ILE
3	C	44	PRO
3	C	68	ILE
3	C	77	SER
3	C	78	LYS
3	C	103	SER
3	C	117	ARG
3	C	118	ILE
3	C	127	PHE
3	C	137	ASP
3	C	144	ASP

Sometimes 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	161	GLN
1	A	242	ASN
1	A	244	ASN
1	A	301	ASN
1	A	362	HIS
1	A	374	GLN
1	A	415	GLN
1	A	439	ASN
1	A	484	ASN
1	A	494	HIS
1	A	600	ASN
1	A	605	ASN
1	A	607	ASN
1	A	651	HIS
1	A	661	ASN
1	A	666	HIS
1	A	696	ASN
1	A	711	ASN
1	A	806	GLN
1	A	816	ASN
1	A	833	ASN
2	B	89	ASN
2	B	134	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 monosaccharides 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	SO4	A	1001	-	4,4,4	0.20	0	6,6,6	0.09	0

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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	SO4	4	0

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, 95^{th} 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%)	-0.03	16 (1%) 65 64	13, 64, 137, 163	0
2	B	145/153 (94%)	0.51	9 (6%) 20 20	34, 100, 146, 163	0
3	C	156/159 (98%)	-0.12	1 (0%) 89 90	13, 47, 106, 152	0
All	All	1109/1151 (96%)	0.03	26 (2%) 60 59	13, 66, 140, 163	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	30	ASP	6.2
2	B	77	LYS	4.8
1	A	202	GLY	4.6
3	C	139	ASN	4.1
1	A	643	ALA	3.8
2	B	137	PHE	3.7
1	A	835	VAL	3.4
1	A	832	PHE	3.1
1	A	543	PRO	3.0
2	B	33	ILE	2.9
2	B	52	ASP	2.9
1	A	8	PRO	2.8
1	A	839	LEU	2.8
2	B	25	ILE	2.6
1	A	366	MET	2.6
1	A	201	ALA	2.6
1	A	828	TRP	2.6
2	B	131	PRO	2.6
1	A	390	LEU	2.5
1	A	829	TRP	2.3
2	B	31	GLY	2.2
1	A	1	MET	2.2
1	A	413	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	373	GLU	2.1
1	A	54	ASP	2.0
2	B	134	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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(Å^2)	Q<0.9
5	CA	C	2001	1/1	0.79	0.14	58,58,58,58	0
4	SO4	A	1001	5/5	0.93	0.41	58,58,58,58	5

6.5 Other polymers (i)

There are no such residues in this entry.