



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:13 AM UTC

PDB ID : 3AOC / pdb_00003aoc
Title : Structures of the multidrug exporter AcrB reveal a proximal multisite drug-binding pocket
Authors : Nakashima, R.; Sakurai, K.; Yamaguchi, A.
Deposited on : 2010-09-23
Resolution : 3.34 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

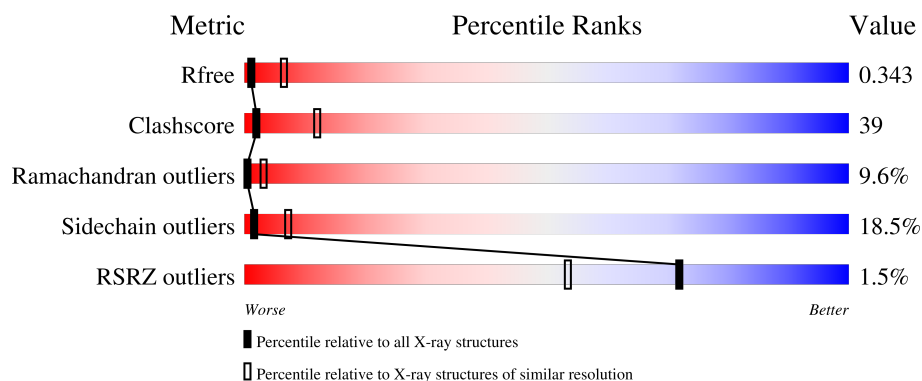
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1053	2% 34% 47% 14% . .
1	B	1053	2% 32% 47% 17% . .
1	C	1053	2% 35% 48% 13% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23378 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.

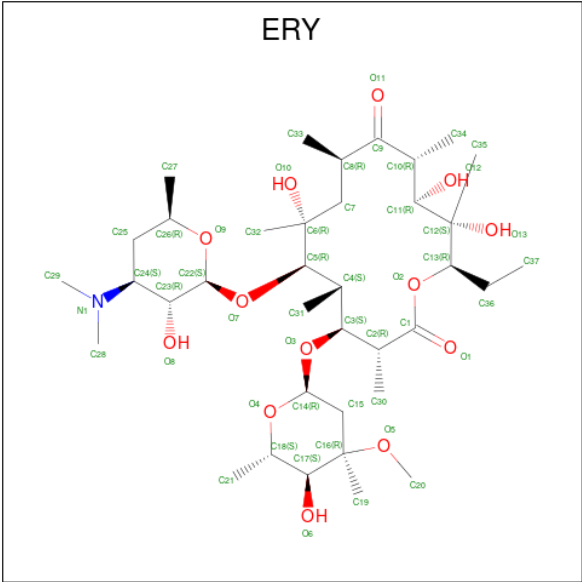
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
B	1051	HIS	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
C	1050	HIS	-	expression tag	UNP P31224
C	1051	HIS	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

- Molecule 2 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			51	37	1	13		

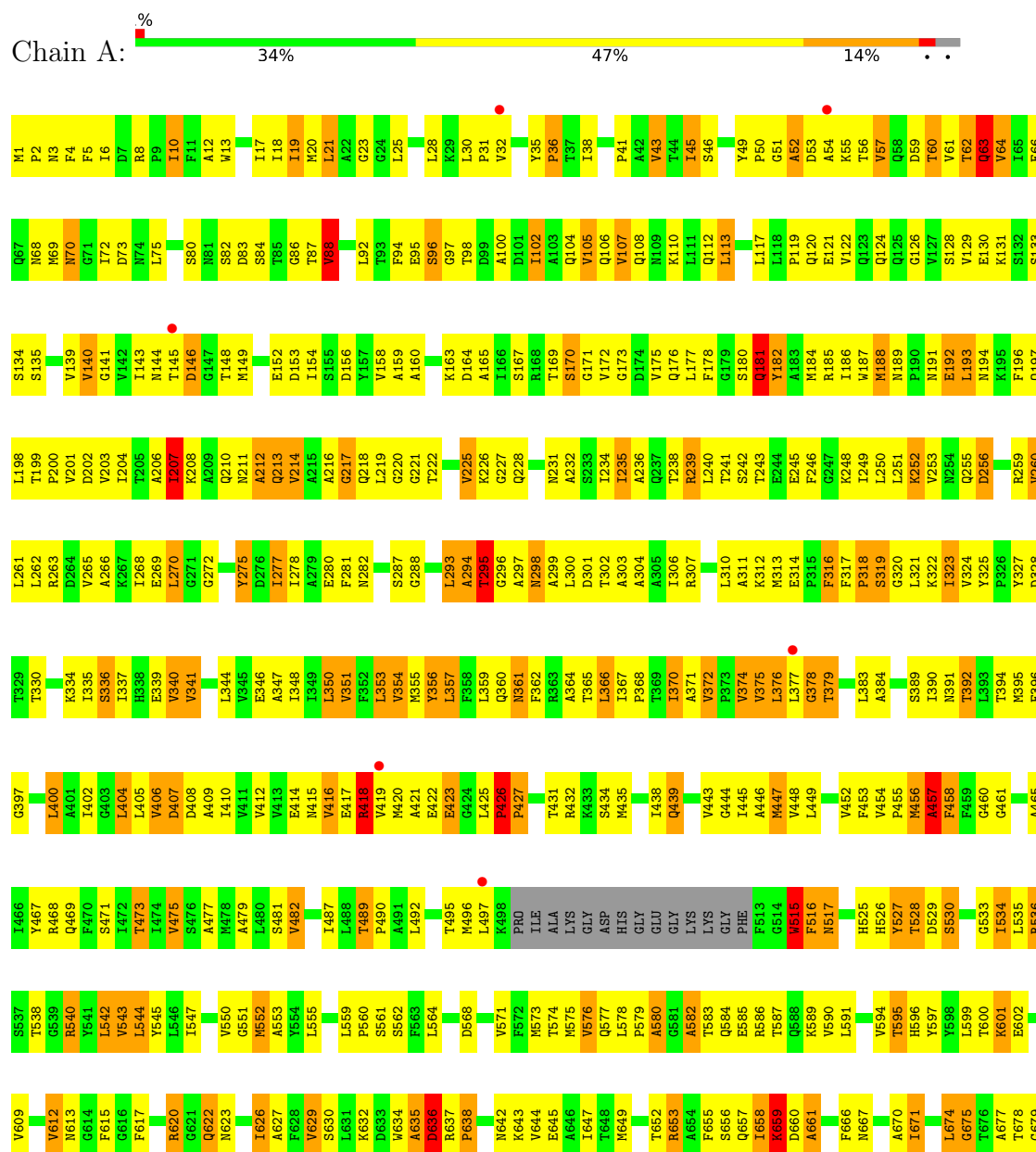
- Molecule 3 is water.

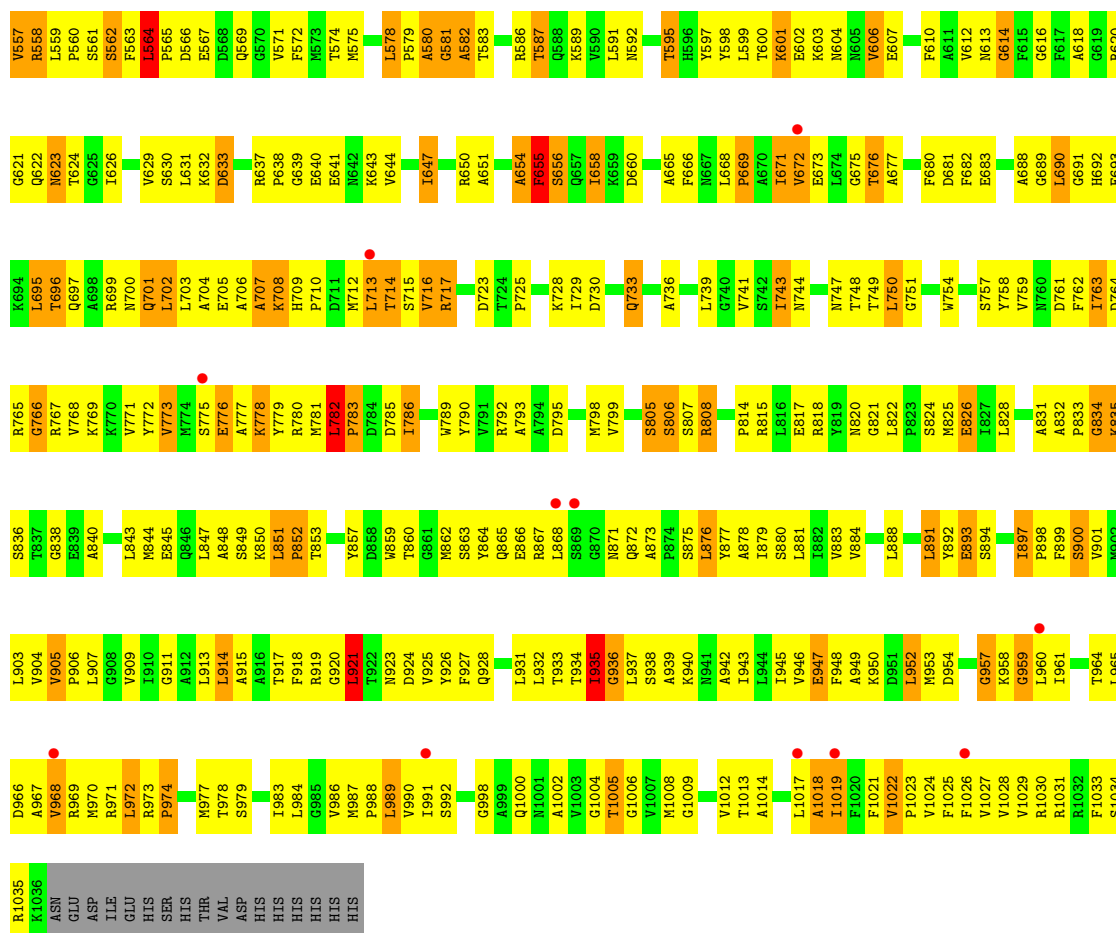
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O	0	0
			2 2		
3	B	2	Total O	0	0
			2 2		
3	C	1	Total O	0	0
			1 1		

3 Residue-property plots

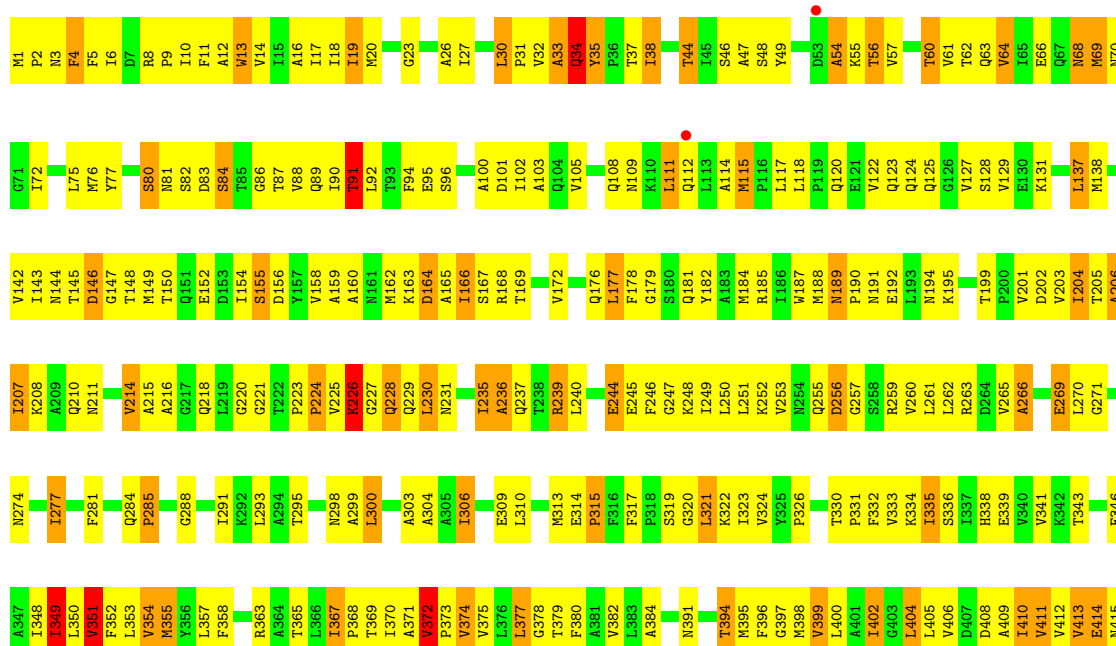
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





● Molecule 1: Acriflavine resistance protein B





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.28Å 134.21Å 162.05Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	45.73 – 3.34 45.73 – 3.34	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.73-3.34) 95.4 (45.73-3.34)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.91 (at 3.32Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.273 , 0.344 0.269 , 0.343	Depositor DCC
R_{free} test set	3329 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	97.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23378	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.79	3/7920 (0.0%)	1.09	26/10756 (0.2%)
1	B	0.78	1/7920 (0.0%)	1.10	28/10756 (0.3%)
1	C	0.81	3/7920 (0.0%)	1.12	28/10756 (0.3%)
All	All	0.79	7/23760 (0.0%)	1.10	82/32268 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	671	ILE	CA-CB	7.04	1.64	1.54
1	A	426	PRO	CA-C	5.79	1.57	1.52
1	C	1019	ILE	CA-CB	5.42	1.60	1.54
1	A	102	ILE	CA-CB	-5.26	1.49	1.54
1	A	897	ILE	CA-CB	5.19	1.56	1.54
1	B	1022	VAL	CA-CB	5.10	1.57	1.54
1	C	445	ILE	CA-CB	5.07	1.59	1.54

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	ALA	N-CA-CB	-16.75	82.18	110.49
1	B	425	LEU	CA-C-N	13.76	134.55	120.38
1	B	425	LEU	C-N-CA	13.76	134.55	120.38
1	A	717	ARG	N-CA-C	12.03	119.04	108.22
1	A	456	MET	N-CA-C	9.14	130.27	110.80
1	B	426	PRO	N-CA-C	8.73	121.35	110.70
1	A	336	SER	N-CA-C	-7.39	106.19	114.62
1	C	771	VAL	CB-CA-C	-7.20	102.17	110.73
1	B	998	GLY	N-CA-C	-7.08	106.66	115.08
1	A	52	ALA	N-CA-C	7.07	114.57	108.78
1	C	673	GLU	N-CA-C	-7.06	95.76	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	822	LEU	CA-C-N	7.06	127.48	119.93
1	B	822	LEU	C-N-CA	7.06	127.48	119.93
1	A	419	VAL	N-CA-C	-7.00	106.24	112.12
1	B	218	GLN	N-CA-C	6.98	119.55	109.14
1	B	564	LEU	CA-C-N	6.82	128.28	120.98
1	B	564	LEU	C-N-CA	6.82	128.28	120.98
1	B	516	PHE	N-CA-C	6.74	116.94	108.45
1	C	426	PRO	N-CA-C	6.50	118.63	110.70
1	B	559	LEU	CA-C-N	6.48	126.51	119.90
1	B	559	LEU	C-N-CA	6.48	126.51	119.90
1	C	685	ILE	N-CA-C	6.32	118.12	107.18
1	C	271	GLY	N-CA-C	6.28	120.99	110.56
1	A	959	GLY	N-CA-C	6.25	119.92	110.18
1	A	275	TYR	N-CA-C	6.22	120.90	112.88
1	C	309	GLU	N-CA-C	-6.18	103.86	111.40
1	C	479	ALA	N-CA-C	-6.14	106.76	114.56
1	A	851	LEU	CA-C-N	6.11	127.48	119.84
1	A	851	LEU	C-N-CA	6.11	127.48	119.84
1	A	458	PHE	N-CA-C	-6.09	104.27	113.89
1	A	622	GLN	N-CA-C	-6.09	105.98	113.41
1	A	88	VAL	CB-CA-C	-6.07	101.57	110.62
1	B	540	ARG	N-CA-C	-6.07	105.96	113.19
1	A	573	MET	N-CA-C	6.07	119.09	109.50
1	B	666	PHE	N-CA-C	6.05	118.65	109.63
1	B	701	GLN	N-CA-C	-6.01	105.80	113.01
1	A	864	TYR	N-CA-C	-6.00	105.62	113.12
1	A	87	THR	N-CA-C	5.91	119.11	109.24
1	C	339	GLU	N-CA-C	-5.88	106.65	113.88
1	A	418	ARG	N-CA-C	-5.87	103.54	112.99
1	A	296	GLY	N-CA-C	-5.81	107.16	115.64
1	C	813	SER	CA-C-N	5.65	125.75	119.87
1	C	813	SER	C-N-CA	5.65	125.75	119.87
1	A	791	VAL	N-CA-C	5.65	116.13	107.77
1	C	454	VAL	N-CA-C	5.61	120.99	108.88
1	C	959	GLY	N-CA-C	5.58	120.98	111.16
1	A	52	ALA	CA-C-O	5.58	121.18	117.94
1	C	813	SER	N-CA-C	5.57	117.51	109.04
1	A	582	ALA	N-CA-C	5.56	117.50	110.33
1	C	773	VAL	N-CA-C	-5.51	104.05	110.05
1	B	68	ASN	N-CA-C	5.48	118.44	111.69
1	C	218	GLN	N-CA-C	5.48	117.60	108.99
1	C	873	ALA	N-CA-C	5.47	120.19	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	GLN	N-CA-C	-5.45	103.31	110.33
1	C	214	VAL	N-CA-C	5.44	115.89	107.78
1	A	1011	MET	N-CA-C	-5.41	106.69	113.28
1	B	85	THR	N-CA-C	-5.35	105.58	113.61
1	C	288	GLY	N-CA-C	5.35	119.11	110.87
1	C	641	GLU	N-CA-C	-5.34	106.89	113.41
1	B	782	LEU	CA-C-N	5.30	126.47	119.84
1	B	782	LEU	C-N-CA	5.30	126.47	119.84
1	B	25	LEU	N-CA-C	-5.27	104.45	112.04
1	B	207	ILE	CB-CA-C	-5.24	105.27	111.97
1	C	679	GLY	N-CA-C	-5.22	105.63	111.63
1	A	379	THR	N-CA-C	-5.22	106.18	112.54
1	A	897	ILE	N-CA-CB	5.20	114.01	110.52
1	C	351	VAL	N-CA-C	-5.20	107.33	113.42
1	B	763	ILE	N-CA-C	5.19	114.67	106.32
1	A	811	TYR	N-CA-C	5.18	118.07	109.46
1	C	776	GLU	N-CA-C	-5.18	102.09	110.32
1	C	762	PHE	N-CA-C	-5.16	102.56	110.14
1	C	399	VAL	N-CA-C	-5.14	105.59	110.42
1	B	32	VAL	CB-CA-C	-5.12	103.03	110.81
1	C	235	ILE	N-CA-C	5.12	114.11	106.85
1	B	57	VAL	N-CA-C	-5.08	107.61	111.62
1	C	91	THR	N-CA-C	5.08	115.69	107.32
1	C	562	SER	N-CA-C	5.07	114.52	107.73
1	B	452	VAL	N-CA-C	-5.06	103.07	109.80
1	C	1029	VAL	N-CA-C	5.04	115.26	110.42
1	A	80	SER	N-CA-C	5.03	116.89	108.99
1	B	146	ASP	N-CA-C	5.03	118.53	111.74
1	B	707	ALA	N-CA-C	-5.02	105.89	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	7774	0	7931	556	0
1	B	7774	0	7931	668	0
1	C	7774	0	7931	655	0
2	C	51	0	67	11	0
3	A	2	0	0	1	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	23378	0	23860	1819	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 39.

All (1819) 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:B:456:MET:HG3	1:B:467:TYR:HB3	1.24	1.16
1:A:145:THR:HG22	1:A:320:GLY:HA3	1.15	1.13
1:A:710:PRO:HA	1:A:713:LEU:HD22	1.19	1.12
1:A:638:PRO:HD2	1:A:642:ASN:HD22	1.04	1.07
1:A:714:THR:HG23	1:A:832:ALA:HA	1.33	1.06
1:A:317:PHE:HB3	1:A:321:LEU:HB2	1.36	1.05
1:A:414:GLU:HG2	1:A:974:PRO:HG3	1.35	1.05
1:A:94:PHE:HB3	1:A:98:THR:HG21	1.39	1.02
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.41	1.02
1:A:674:LEU:HD22	1:A:675:GLY:H	1.25	1.01
1:A:945:ILE:HG13	1:A:971:ARG:HG2	1.40	1.01
1:C:577:GLN:HB3	1:C:624:THR:HG22	1.41	1.01
1:C:415:ASN:HA	1:C:418:ARG:HE	1.23	1.01
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.24	1.00
1:B:52:ALA:HB2	1:B:86:GLY:N	1.76	1.00
1:B:879:ILE:O	1:B:883:VAL:HG23	1.58	1.00
1:C:34:GLN:HE22	1:C:299:ALA:HB3	1.26	0.99
1:B:445:ILE:HG23	1:B:940:LYS:HG3	1.44	0.99
1:C:930:GLY:HA3	1:C:1007:VAL:HG22	1.43	0.98
1:A:140:VAL:HG12	1:A:141:GLY:H	1.22	0.98
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.44	0.98
1:A:447:MET:HB3	1:A:887:CYS:SG	2.04	0.98
1:C:901:VAL:HG11	1:C:943:ILE:HG13	1.43	0.97
1:A:781:MET:HE3	1:C:228:GLN:OE1	1.64	0.96
1:C:26:ALA:O	1:C:30:LEU:HB2	1.63	0.96
1:A:659:LYS:HG2	1:A:660:ASP:H	1.27	0.96
1:C:418:ARG:HH12	1:C:971:ARG:HH11	1.06	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.46	0.95
1:C:240:LEU:HD12	1:C:245:GLU:HB3	1.48	0.94
1:A:246:PHE:O	1:A:249:ILE:HG12	1.68	0.94
1:A:145:THR:CG2	1:A:320:GLY:HA3	1.97	0.94
1:C:23:GLY:HA3	1:C:377:LEU:O	1.69	0.93
1:A:756:GLY:HA2	1:A:774:MET:HB2	1.52	0.92
1:B:224:PRO:HA	1:C:781:MET:HE1	1.50	0.92
1:B:574:THR:HG23	1:B:665:ALA:HB2	1.51	0.92
1:C:713:LEU:HD11	1:C:834:GLY:HA3	1.52	0.91
1:C:959:GLY:H	1:C:962:GLU:HB2	1.36	0.90
1:C:358:PHE:HB3	1:C:977:MET:HE2	1.51	0.90
1:B:485:ALA:HA	1:B:489:THR:HB	1.54	0.90
1:A:638:PRO:HD2	1:A:642:ASN:ND2	1.87	0.89
1:B:26:ALA:O	1:B:30:LEU:HB2	1.73	0.89
1:A:710:PRO:CA	1:A:713:LEU:HD22	2.03	0.89
1:C:979:SER:O	1:C:983:ILE:HG12	1.72	0.88
1:A:795:ASP:HB2	1:A:797:GLN:HG2	1.54	0.88
1:B:743:ILE:HD12	1:B:743:ILE:H	1.37	0.88
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.55	0.87
1:B:631:LEU:HB3	1:B:637:ARG:HH12	1.39	0.87
1:B:222:THR:OG1	1:B:223:PRO:HD3	1.75	0.87
1:C:404:LEU:HD22	1:C:478:MET:HG3	1.56	0.87
1:C:409:ALA:O	1:C:413:VAL:HG12	1.72	0.87
1:C:972:LEU:H	1:C:974:PRO:HD2	1.39	0.87
1:B:986:VAL:O	1:B:990:VAL:HG23	1.75	0.86
1:C:11:PHE:O	1:C:14:VAL:HG12	1.76	0.86
1:C:513:PHE:HB2	1:C:516:PHE:HB2	1.58	0.85
1:C:692:HIS:HE1	1:C:721:LEU:HD21	1.38	0.85
1:A:612:VAL:HG23	1:A:626:ILE:HG22	1.58	0.85
1:A:525:HIS:HA	1:A:528:THR:HG22	1.59	0.85
1:C:934:THR:HG22	1:C:1011:MET:HE3	1.59	0.85
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.56	0.85
1:B:607:GLU:HG2	1:B:632:LYS:HA	1.57	0.84
1:B:583:THR:HG22	1:B:586:ARG:HD3	1.59	0.84
1:A:141:GLY:HA2	1:A:288:GLY:HA2	1.58	0.84
1:B:591:LEU:O	1:B:595:THR:HG22	1.78	0.84
1:A:731:ILE:HD12	1:A:746:ILE:HG21	1.60	0.84
1:A:140:VAL:HG12	1:A:141:GLY:N	1.88	0.83
1:C:415:ASN:HA	1:C:418:ARG:NE	1.93	0.83
1:B:24:GLY:H	1:B:27:ILE:HG23	1.44	0.83
1:C:176:GLN:NE2	1:C:620:ARG:NH1	2.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:767:ARG:HG3	1:C:767:ARG:HH11	1.43	0.83
1:C:545:TYR:OH	1:C:1021:PHE:HB3	1.78	0.83
1:B:143:ILE:HD12	1:B:144:ASN:H	1.43	0.82
1:B:736:ALA:HB1	1:B:741:VAL:CG2	2.08	0.82
1:A:13:TRP:O	1:A:17:ILE:HG12	1.77	0.82
1:B:193:LEU:HD23	1:B:265:VAL:HG11	1.59	0.82
1:A:383:LEU:HD21	1:A:473:THR:HG23	1.62	0.82
1:C:713:LEU:CD1	1:C:834:GLY:HA3	2.09	0.82
1:C:343:THR:HG21	1:C:989:LEU:HD13	1.60	0.82
1:B:157:TYR:HA	1:B:161:ASN:ND2	1.95	0.82
1:C:758:TYR:H	1:C:758:TYR:HD1	1.27	0.82
1:C:713:LEU:HD11	1:C:835:LYS:H	1.44	0.82
1:B:401:ALA:HA	1:B:404:LEU:HB2	1.61	0.82
1:B:235:ILE:HD13	1:B:235:ILE:N	1.96	0.81
1:A:750:LEU:O	1:A:754:TRP:HD1	1.64	0.81
1:A:51:GLY:O	1:C:215:ALA:HB1	1.80	0.80
1:B:715:SER:O	1:B:716:VAL:HG23	1.82	0.80
1:C:416:VAL:HG11	1:C:431:THR:HG22	1.63	0.80
1:A:140:VAL:CG1	1:A:141:GLY:H	1.94	0.80
1:A:591:LEU:CD1	1:A:613:ASN:HB3	2.11	0.80
1:B:563:PHE:HD1	1:B:866:GLU:HG3	1.46	0.80
1:A:702:LEU:HD21	1:A:844:MET:HE1	1.61	0.80
1:B:359:LEU:HD23	1:B:365:THR:HA	1.62	0.80
1:B:934:THR:C	1:B:936:GLY:H	1.90	0.79
1:C:932:LEU:HA	1:C:935:ILE:HG22	1.63	0.79
1:A:6:ILE:HD11	1:A:432:ARG:HD2	1.64	0.79
1:A:883:VAL:O	1:A:887:CYS:HB2	1.82	0.79
1:C:400:LEU:HD12	1:C:929:VAL:HG12	1.65	0.79
1:B:94:PHE:HB3	1:B:98:THR:HG21	1.64	0.79
1:B:673:GLU:O	1:B:676:THR:HG22	1.82	0.79
1:B:143:ILE:HD13	1:B:285:PRO:O	1.83	0.78
1:C:552:MET:SD	1:C:909:VAL:HG21	2.22	0.78
1:C:672:VAL:CG1	1:C:673:GLU:H	1.96	0.78
1:A:395:MET:HE2	1:A:395:MET:HA	1.65	0.78
1:C:983:ILE:HG23	1:C:1008:MET:HG2	1.65	0.78
1:A:396:PHE:CD2	1:A:1003:VAL:HG21	2.18	0.78
1:A:945:ILE:CG1	1:A:971:ARG:HG2	2.13	0.78
1:A:746:ILE:HD12	1:A:791:VAL:HG21	1.64	0.78
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.13	0.78
1:C:265:VAL:O	1:C:265:VAL:HG23	1.79	0.78
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:MET:HA	1:C:835:LYS:HG3	1.66	0.78
1:C:605:ASN:HB3	1:C:637:ARG:HD3	1.64	0.78
1:C:144:ASN:ND2	1:C:149:MET:H	1.81	0.77
1:C:680:PHE:HE1	1:C:844:MET:HE3	1.49	0.77
1:B:552:MET:SD	1:B:909:VAL:HG21	2.24	0.77
1:C:832:ALA:HB1	1:C:833:PRO:CD	2.15	0.77
1:B:149:MET:HB3	1:B:154:ILE:HG22	1.67	0.76
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.66	0.76
1:A:278:ILE:HB	1:A:613:ASN:OD1	1.86	0.76
1:B:157:TYR:HA	1:B:161:ASN:HD22	1.48	0.76
1:C:34:GLN:HE22	1:C:299:ALA:CB	1.99	0.76
1:C:894:SER:OG	1:C:897:ILE:HG12	1.86	0.76
1:A:890:ALA:HB1	1:C:11:PHE:HD1	1.50	0.76
1:B:343:THR:HG21	1:B:1000:GLN:OE1	1.84	0.76
1:B:399:VAL:O	1:B:402:ILE:HG22	1.85	0.76
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.65	0.76
1:C:588:GLN:HG2	1:C:613:ASN:HD22	1.51	0.76
1:A:404:LEU:HD21	1:A:449:LEU:HD13	1.68	0.75
1:B:213:GLN:HB2	1:B:239:ARG:HD2	1.67	0.75
1:A:43:VAL:HG11	1:A:107:VAL:HG21	1.66	0.75
1:A:396:PHE:HD2	1:A:1003:VAL:HG21	1.51	0.75
1:B:552:MET:SD	1:B:909:VAL:CG2	2.74	0.75
2:C:3402:ERY:H302	2:C:3402:ERY:H14	1.68	0.75
1:A:354:VAL:HG12	1:A:355:MET:H	1.50	0.75
1:A:344:LEU:HD13	1:A:376:LEU:HD21	1.68	0.75
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.21	0.75
1:B:934:THR:O	1:B:936:GLY:N	2.20	0.74
1:C:448:VAL:HG22	1:C:887:CYS:HB3	1.68	0.74
1:C:618:ALA:HB1	1:C:815:ARG:HH12	1.52	0.74
1:B:923:ASN:HD22	1:B:927:PHE:HD2	1.34	0.74
1:A:445:ILE:HG21	1:A:940:LYS:HG3	1.67	0.74
1:B:924:ASP:O	1:B:928:GLN:HG3	1.87	0.74
1:A:294:ALA:HB3	1:A:297:ALA:HB2	1.70	0.74
1:B:892:TYR:HB3	1:B:897:ILE:HD11	1.68	0.74
1:B:579:PRO:O	1:B:580:ALA:O	2.05	0.74
1:A:659:LYS:HG2	1:A:660:ASP:N	2.03	0.74
1:A:6:ILE:HG22	1:A:490:PRO:O	1.87	0.74
1:B:213:GLN:HG3	1:C:56:THR:HG23	1.69	0.74
1:C:176:GLN:HE22	1:C:620:ARG:NH1	1.84	0.73
1:C:375:VAL:HG11	1:C:405:LEU:HD22	1.70	0.73
1:A:707:ALA:HA	1:A:713:LEU:HD12	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD22	1:B:390:ILE:HG13	1.67	0.73
1:B:242:SER:HB2	1:B:245:GLU:OE2	1.87	0.73
1:C:754:TRP:CZ2	1:C:786:ILE:HD13	2.24	0.73
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.23	0.73
1:A:921:LEU:HG	1:A:922:THR:H	1.51	0.73
1:B:36:PRO:HD3	1:B:391:ASN:ND2	2.04	0.73
1:B:736:ALA:HB1	1:B:741:VAL:HG23	1.69	0.73
1:B:203:VAL:O	1:B:207:ILE:HG12	1.88	0.73
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.70	0.73
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.70	0.73
1:A:144:ASN:HD22	1:A:149:MET:H	1.37	0.73
1:B:68:ASN:C	1:B:70:ASN:H	1.96	0.73
1:B:213:GLN:CG	1:C:56:THR:HG23	2.18	0.73
1:B:276:ASP:O	1:B:614:GLY:HA3	1.89	0.73
1:B:441:ALA:O	1:B:445:ILE:HG12	1.88	0.73
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.69	0.72
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.71	0.72
1:A:575:MET:HE1	1:A:577:GLN:HE21	1.53	0.72
1:B:426:PRO:HB3	1:B:430:ALA:HB3	1.71	0.72
1:B:119:PRO:HB2	1:B:122:VAL:HG23	1.70	0.72
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.70	0.72
1:B:947:GLU:OE1	1:B:947:GLU:HA	1.88	0.72
1:C:92:LEU:HD12	1:C:92:LEU:H	1.53	0.72
1:A:728:LYS:HD2	1:C:235:ILE:O	1.89	0.72
1:C:681:ASP:HB3	1:C:860:THR:CG2	2.20	0.72
1:C:600:THR:O	1:C:603:LYS:HB2	1.90	0.72
1:A:597:TYR:O	1:A:601:LYS:HB3	1.89	0.72
1:A:188:MET:HA	1:A:266:ALA:HB2	1.72	0.72
1:B:560:PRO:HB2	1:B:836:SER:HB2	1.71	0.72
1:B:675:GLY:O	1:B:677:ALA:N	2.22	0.72
1:C:548:ILE:HD13	1:C:1017:LEU:HD21	1.72	0.71
1:B:188:MET:HE1	1:B:203:VAL:HG11	1.72	0.71
1:C:203:VAL:O	1:C:207:ILE:HG12	1.90	0.71
1:A:753:ALA:HB3	1:A:754:TRP:CD1	2.26	0.71
1:B:45:ILE:CD1	1:B:69:MET:HE3	2.21	0.71
1:C:3:ASN:C	1:C:5:PHE:H	1.99	0.71
1:C:617:PHE:O	2:C:3402:ERY:H332	1.90	0.71
1:C:709:HIS:HB3	1:C:712:MET:SD	2.31	0.71
1:A:170:SER:O	1:A:302:THR:HG22	1.90	0.71
1:C:137:LEU:HD23	1:C:293:LEU:HD13	1.73	0.71
1:A:4:PHE:HB3	1:A:8:ARG:NH2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:795:ASP:OD1	1:C:797:GLN:HB2	1.90	0.71
1:A:207:ILE:HB	1:A:759:VAL:HG11	1.72	0.70
1:C:143:ILE:HD11	1:C:281:PHE:HB3	1.72	0.70
1:A:10:ILE:HG21	1:B:893:GLU:O	1.90	0.70
1:A:721:LEU:HD12	1:A:814:PRO:HG2	1.73	0.70
1:C:210:GLN:O	1:C:240:LEU:HD21	1.91	0.70
1:A:782:LEU:O	1:A:785:ASP:HB2	1.91	0.70
1:C:124:GLN:CB	1:C:758:TYR:HE2	2.05	0.70
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.56	0.70
1:A:471:SER:O	1:A:475:VAL:HG12	1.90	0.70
1:B:412:VAL:HG13	1:B:435:MET:HE1	1.74	0.70
1:C:418:ARG:NH1	1:C:971:ARG:HH11	1.86	0.69
1:C:166:ILE:HG21	1:C:291:ILE:HD11	1.72	0.69
1:A:41:PRO:HB3	1:A:100:ALA:HB2	1.74	0.69
1:C:713:LEU:HD11	1:C:835:LYS:N	2.06	0.69
1:B:210:GLN:HG2	1:C:733:GLN:HE21	1.56	0.69
1:B:952:LEU:C	1:B:954:ASP:H	2.00	0.69
1:A:145:THR:HG21	1:A:322:LYS:HE2	1.73	0.69
1:A:591:LEU:HD12	1:A:613:ASN:HB3	1.74	0.69
1:A:714:THR:HG23	1:A:832:ALA:CA	2.19	0.69
1:B:932:LEU:HA	1:B:935:ILE:HG13	1.73	0.69
1:C:839:GLU:HA	1:C:842:GLU:HB3	1.74	0.69
1:A:314:GLU:HA	1:A:317:PHE:CD2	2.27	0.69
1:B:66:GLU:OE2	1:B:821:GLY:HA2	1.93	0.69
1:B:298:ASN:O	1:B:300:LEU:N	2.26	0.69
1:C:727:PHE:CE1	1:C:807:SER:HB2	2.28	0.69
1:B:460:GLY:HA2	1:B:872:GLN:HE22	1.58	0.69
1:C:265:VAL:O	1:C:266:ALA:HB2	1.91	0.69
1:A:674:LEU:CD2	1:A:675:GLY:H	2.04	0.69
1:A:707:ALA:HA	1:A:713:LEU:CD1	2.23	0.69
1:A:746:ILE:HG13	1:A:804:PHE:CE1	2.26	0.69
1:B:344:LEU:O	1:B:348:ILE:HG13	1.93	0.69
1:B:561:SER:O	1:B:838:GLY:HA3	1.93	0.69
1:B:897:ILE:HB	1:B:1026:PHE:HE1	1.58	0.69
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.23	0.68
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.75	0.68
1:C:146:ASP:HB3	1:C:148:THR:CG2	2.21	0.68
1:A:180:SER:O	1:A:181:GLN:HB3	1.91	0.68
1:B:671:ILE:HG22	1:B:676:THR:HB	1.75	0.68
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.29	0.68
1:A:2:PRO:O	1:A:6:ILE:HG23	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:ARG:CG	1:B:717:ARG:HH11	2.06	0.68
1:A:895:TRP:HZ2	1:C:13:TRP:CE3	2.10	0.68
1:B:419:VAL:O	1:B:419:VAL:HG12	1.94	0.68
1:C:705:GLU:HA	1:C:708:LYS:HE2	1.75	0.68
1:C:607:GLU:HB2	1:C:632:LYS:HG2	1.75	0.68
1:A:1021:PHE:HD1	1:A:1025:PHE:CE1	2.11	0.68
1:B:326:PRO:HG2	1:B:610:PHE:CD1	2.28	0.68
1:B:775:SER:O	1:B:780:ARG:HD3	1.93	0.68
1:B:905:VAL:HG13	1:B:906:PRO:HD3	1.76	0.68
1:C:435:MET:HA	1:C:438:ILE:HG22	1.75	0.68
1:B:121:GLU:O	1:B:125:GLN:HG2	1.94	0.68
1:A:696:THR:OG1	1:A:825:MET:HE1	1.94	0.68
1:B:18:ILE:HG22	1:B:19:ILE:HD13	1.76	0.68
1:B:880:SER:O	1:B:884:VAL:HG23	1.94	0.68
1:C:973:ARG:O	1:C:977:MET:HB2	1.94	0.68
1:A:31:PRO:HB2	1:A:389:SER:HB2	1.74	0.68
1:B:456:MET:HG3	1:B:467:TYR:CB	2.13	0.68
1:C:2:PRO:O	1:C:6:ILE:HG12	1.92	0.68
1:C:672:VAL:HG12	1:C:673:GLU:H	1.59	0.68
1:C:734:GLU:HA	1:C:737:GLN:HG2	1.76	0.68
1:C:759:VAL:HG23	1:C:771:VAL:O	1.94	0.68
1:A:23:GLY:HA3	1:A:378:GLY:HA2	1.77	0.67
1:A:299:ALA:O	1:A:303:ALA:HB2	1.94	0.67
1:A:643:LYS:O	1:A:647:ILE:HG13	1.93	0.67
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.24	0.67
1:A:207:ILE:O	1:A:211:ASN:HB3	1.94	0.67
1:B:411:VAL:HB	1:B:438:ILE:HD11	1.76	0.67
1:B:717:ARG:HH11	1:B:717:ARG:HG2	1.58	0.67
1:C:66:GLU:OE2	1:C:80:SER:HB3	1.94	0.67
1:C:767:ARG:HD3	1:C:769:LYS:HE3	1.77	0.67
1:B:408:ASP:OD1	1:B:442:LEU:HA	1.94	0.67
1:C:244:GLU:HA	1:C:263:ARG:NH2	2.05	0.67
1:C:681:ASP:CB	1:C:860:THR:HG23	2.24	0.67
1:C:185:ARG:HB2	1:C:269:GLU:O	1.94	0.67
1:C:758:TYR:CD1	1:C:758:TYR:N	2.51	0.67
1:C:979:SER:O	1:C:983:ILE:CG1	2.41	0.67
1:B:94:PHE:CB	1:B:98:THR:HG21	2.24	0.67
1:B:349:ILE:C	1:B:351:VAL:H	2.03	0.67
1:B:416:VAL:O	1:B:426:PRO:HG2	1.95	0.67
1:B:915:ALA:CB	1:B:1009:GLY:HA3	2.24	0.67
1:B:55:LYS:HE2	1:B:59:ASP:OD1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ASN:HB3	1:B:301:ASP:HB2	1.76	0.67
1:B:582:ALA:O	1:B:583:THR:HB	1.94	0.67
1:C:925:VAL:O	1:C:929:VAL:HG23	1.95	0.67
1:A:400:LEU:CD1	1:A:1003:VAL:HG13	2.24	0.67
1:A:733:GLN:OE1	1:A:743:ILE:HD11	1.95	0.67
1:B:13:TRP:HE3	1:B:488:LEU:HD21	1.60	0.67
1:C:252:LYS:HG2	1:C:260:VAL:HG12	1.76	0.67
1:C:332:PHE:CD2	1:C:569:GLN:HA	2.30	0.67
1:A:1:MET:SD	1:A:487:ILE:HD11	2.35	0.66
1:B:45:ILE:HD11	1:B:69:MET:HE3	1.77	0.66
1:C:542:LEU:HD11	1:C:1028:VAL:HG11	1.76	0.66
1:B:188:MET:HB2	1:B:775:SER:HA	1.76	0.66
1:B:348:ILE:HG12	1:B:402:ILE:HD11	1.75	0.66
1:C:56:THR:O	1:C:60:THR:HB	1.95	0.66
1:C:610:PHE:HB3	1:C:628:PHE:HB2	1.76	0.66
1:C:636:ASP:OD1	1:C:636:ASP:N	2.27	0.66
1:B:149:MET:HB3	1:B:154:ILE:CG2	2.25	0.66
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.78	0.66
1:C:679:GLY:HA2	1:C:830:GLN:HA	1.76	0.66
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.96	0.66
1:A:94:PHE:CB	1:A:98:THR:HG21	2.22	0.66
1:A:294:ALA:O	1:A:295:THR:HB	1.93	0.66
1:C:616:GLY:HA3	1:C:624:THR:HB	1.76	0.66
1:B:419:VAL:O	1:B:426:PRO:HG3	1.95	0.66
1:B:24:GLY:N	1:B:27:ILE:HG23	2.11	0.66
1:B:817:GLU:HB2	1:B:824:SER:O	1.96	0.66
1:C:986:VAL:O	1:C:986:VAL:HG12	1.96	0.66
1:B:13:TRP:CE3	1:B:488:LEU:HD21	2.30	0.65
1:B:859:TRP:HB3	1:B:863:SER:HB2	1.78	0.65
1:C:184:MET:HA	1:C:184:MET:HE3	1.78	0.65
1:C:695:LEU:HD22	1:C:825:MET:SD	2.36	0.65
1:C:911:GLY:C	1:C:1010:GLY:HA2	2.20	0.65
1:C:203:VAL:HG13	1:C:262:LEU:CD1	2.25	0.65
1:C:124:GLN:HB2	1:C:758:TYR:HE2	1.61	0.65
1:C:176:GLN:NE2	1:C:620:ARG:HH11	1.94	0.65
1:A:379:THR:HG21	1:A:477:ALA:HA	1.76	0.65
1:B:224:PRO:CA	1:C:781:MET:HE1	2.26	0.65
1:B:249:ILE:HB	1:B:262:LEU:HD12	1.78	0.65
1:C:395:MET:HA	1:C:395:MET:HE2	1.79	0.65
1:B:632:LYS:O	1:B:633:ASP:O	2.15	0.65
1:C:522:LYS:HE2	1:C:522:LYS:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:GLU:O	1:C:650:ARG:NH1	2.30	0.65
1:A:746:ILE:CD1	1:A:791:VAL:HG21	2.27	0.65
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.61	0.65
1:B:911:GLY:HA2	1:B:914:LEU:HB2	1.79	0.65
1:B:1009:GLY:O	1:B:1012:VAL:HG22	1.97	0.64
1:C:775:SER:HB3	1:C:780:ARG:HD3	1.79	0.64
1:A:141:GLY:HA2	1:A:288:GLY:CA	2.28	0.64
1:B:925:VAL:HA	1:B:928:GLN:OE1	1.97	0.64
1:A:747:ASN:HD21	1:C:237:GLN:HE21	1.45	0.64
1:B:189:ASN:O	1:B:193:LEU:HB2	1.97	0.64
1:B:213:GLN:HB2	1:B:239:ARG:HG3	1.79	0.64
1:B:157:TYR:CA	1:B:161:ASN:HD22	2.10	0.64
1:B:225:VAL:H	1:C:781:MET:HE3	1.62	0.64
1:A:591:LEU:HD11	1:A:613:ASN:HB3	1.77	0.64
1:B:563:PHE:CD1	1:B:866:GLU:HG3	2.32	0.64
1:A:171:GLY:HA3	1:A:302:THR:HG21	1.80	0.64
1:A:217:GLY:O	1:A:234:ILE:HG12	1.97	0.64
1:B:144:ASN:HD21	1:B:148:THR:H	1.44	0.64
1:B:683:GLU:OE1	1:B:826:GLU:HG3	1.98	0.64
1:B:931:LEU:O	1:B:935:ILE:HG12	1.97	0.64
1:A:714:THR:CG2	1:A:832:ALA:HA	2.19	0.64
1:B:5:PHE:HB3	1:B:12:ALA:HB2	1.80	0.64
1:C:752:ALA:O	1:C:774:MET:HA	1.98	0.64
1:A:159:ALA:HA	1:A:163:LYS:HB2	1.79	0.64
1:C:664:PHE:H	1:C:664:PHE:HD2	1.46	0.64
1:C:688:ALA:O	1:C:690:LEU:N	2.31	0.64
1:A:188:MET:HA	1:A:266:ALA:CB	2.27	0.64
1:B:356:TYR:CE2	1:B:365:THR:HG21	2.33	0.64
1:C:3:ASN:HD21	1:C:432:ARG:HG3	1.62	0.64
1:C:61:VAL:O	1:C:64:VAL:HG23	1.98	0.64
1:C:265:VAL:O	1:C:266:ALA:CB	2.46	0.64
1:A:102:ILE:HD11	1:C:101:ASP:HB3	1.80	0.63
1:A:277:ILE:HD11	1:A:615:PHE:HB3	1.80	0.63
1:B:339:GLU:O	1:B:342:LYS:HB3	1.98	0.63
1:C:394:THR:HG22	1:C:395:MET:HE3	1.79	0.63
1:C:713:LEU:HD11	1:C:834:GLY:CA	2.26	0.63
1:A:117:LEU:HD21	1:C:124:GLN:O	1.98	0.63
1:B:135:SER:HB2	1:B:676:THR:HG21	1.80	0.63
1:B:143:ILE:HD12	1:B:144:ASN:N	2.10	0.63
1:B:251:LEU:HD22	1:B:262:LEU:H	1.62	0.63
1:C:20:MET:HG3	1:C:374:VAL:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:MET:HE2	1:A:909:VAL:HB	1.80	0.63
1:A:895:TRP:HZ2	1:C:13:TRP:HE3	1.46	0.63
1:A:530:SER:O	1:A:534:ILE:HG13	1.97	0.63
1:A:886:LEU:CD1	1:C:14:VAL:HG23	2.28	0.63
1:B:762:PHE:HD2	1:B:771:VAL:HG22	1.64	0.63
1:A:731:ILE:HD12	1:A:746:ILE:CG2	2.27	0.63
1:A:154:ILE:O	1:A:158:VAL:HG23	1.99	0.63
1:C:144:ASN:HD22	1:C:149:MET:H	1.43	0.63
1:C:897:ILE:N	1:C:898:PRO:HD2	2.13	0.63
1:A:113:LEU:HG	1:C:127:VAL:HG23	1.81	0.63
1:C:463:THR:C	1:C:465:ALA:H	2.07	0.63
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.80	0.63
1:A:620:ARG:HH11	1:A:620:ARG:CG	2.11	0.63
1:A:901:VAL:O	1:A:904:VAL:HG23	1.98	0.63
1:B:99:ASP:C	1:B:99:ASP:OD2	2.40	0.63
1:C:455:PRO:O	1:C:876:LEU:HD11	1.98	0.63
1:A:713:LEU:HD23	1:A:714:THR:H	1.63	0.62
1:B:55:LYS:C	1:B:55:LYS:HD3	2.25	0.62
1:B:359:LEU:CD2	1:B:365:THR:HA	2.29	0.62
1:A:890:ALA:HB1	1:C:11:PHE:CD1	2.32	0.62
1:B:111:LEU:HD22	1:B:129:VAL:CG2	2.29	0.62
1:B:345:VAL:C	1:B:347:ALA:H	2.07	0.62
1:A:145:THR:HG23	1:A:146:ASP:H	1.65	0.62
1:B:158:VAL:HA	1:B:162:MET:CG	2.28	0.62
1:B:326:PRO:O	1:B:630:SER:HB2	2.00	0.62
1:C:246:PHE:O	1:C:249:ILE:HG12	2.00	0.62
1:C:767:ARG:HH11	1:C:767:ARG:CG	2.11	0.62
1:A:182:TYR:HB3	1:A:270:LEU:HD11	1.82	0.62
1:A:330:THR:HG22	1:A:334:LYS:HE2	1.82	0.62
1:A:144:ASN:HA	1:A:320:GLY:O	1.99	0.62
1:B:904:VAL:HG13	1:B:907:LEU:HD12	1.82	0.62
1:C:146:ASP:C	1:C:148:THR:H	2.08	0.62
1:A:717:ARG:HB2	1:A:718:PRO:HD2	1.82	0.62
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.99	0.62
1:B:346:GLU:O	1:B:988:PRO:HG3	2.00	0.62
1:B:539:GLY:C	1:B:541:TYR:H	2.07	0.62
1:C:211:ASN:HD22	1:C:240:LEU:HD23	1.65	0.62
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.82	0.62
1:A:241:THR:HG22	1:A:763:ILE:O	2.00	0.61
1:B:445:ILE:HD13	1:B:943:ILE:HG23	1.83	0.61
1:A:144:ASN:ND2	1:A:149:MET:H	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:LEU:HD21	1:A:901:VAL:HB	1.82	0.61
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.82	0.61
1:A:552:MET:CE	1:A:906:PRO:HA	2.29	0.61
1:C:372:VAL:HG21	1:C:406:VAL:HG22	1.82	0.61
1:A:713:LEU:HD23	1:A:714:THR:N	2.14	0.61
1:B:680:PHE:O	1:B:828:LEU:HD23	2.00	0.61
1:C:423:GLU:HB3	1:C:426:PRO:HD2	1.81	0.61
1:B:714:THR:HG22	1:B:831:ALA:HA	1.82	0.61
1:B:792:ARG:HG2	1:B:793:ALA:N	2.16	0.61
1:C:568:ASP:HB2	1:C:643:LYS:HG3	1.83	0.61
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.64	0.61
1:C:712:MET:SD	1:C:843:LEU:HD22	2.41	0.61
1:B:525:HIS:HA	1:B:528:THR:HG22	1.82	0.61
1:B:859:TRP:HB3	1:B:863:SER:CB	2.30	0.61
1:C:16:ALA:HB1	1:C:374:VAL:HG21	1.83	0.61
1:A:339:GLU:O	1:A:341:VAL:N	2.33	0.61
1:A:568:ASP:O	1:A:634:TRP:CH2	2.54	0.61
1:B:485:ALA:HA	1:B:489:THR:CB	2.29	0.61
1:A:216:ALA:HB2	1:B:750:LEU:HD13	1.83	0.61
1:B:57:VAL:O	1:B:61:VAL:HG12	2.01	0.61
1:C:142:VAL:HG12	1:C:154:ILE:HG23	1.83	0.61
1:C:363:ARG:HB3	1:C:496:MET:HB2	1.83	0.61
2:C:3402:ERY:H14	2:C:3402:ERY:C30	2.29	0.61
1:A:746:ILE:HG22	1:A:747:ASN:N	2.16	0.60
1:A:124:GLN:HG2	1:A:758:TYR:CE2	2.36	0.60
1:A:298:ASN:HD22	1:A:300:LEU:H	1.47	0.60
1:B:456:MET:CG	1:B:467:TYR:HB3	2.14	0.60
1:A:965:LEU:O	1:A:969:ARG:HG3	2.01	0.60
1:B:10:ILE:HG13	1:C:893:GLU:O	2.01	0.60
1:B:28:LEU:HD12	1:B:29:LYS:HG3	1.82	0.60
1:C:672:VAL:HG21	1:C:676:THR:H	1.66	0.60
1:A:750:LEU:O	1:A:754:TRP:CD1	2.51	0.60
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.37	0.60
1:C:672:VAL:HG12	1:C:673:GLU:N	2.16	0.60
1:C:958:LYS:HB3	1:C:962:GLU:CB	2.32	0.60
1:A:56:THR:O	1:A:60:THR:HB	2.01	0.60
1:B:680:PHE:HD1	1:B:859:TRP:HZ3	1.50	0.60
1:C:1016:VAL:C	1:C:1018:ALA:H	2.09	0.60
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.83	0.60
1:A:246:PHE:O	1:A:249:ILE:CG1	2.47	0.60
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:PHE:C	1:C:657:GLN:H	2.09	0.60
1:B:699:ARG:HG2	1:B:700:ASN:H	1.67	0.60
1:C:419:VAL:HG23	1:C:430:ALA:HB1	1.84	0.60
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.36	0.60
1:A:218:GLN:HB3	1:A:231:ASN:HD21	1.67	0.60
1:B:231:ASN:C	1:B:231:ASN:ND2	2.60	0.60
1:B:456:MET:HG2	1:B:457:ALA:N	2.17	0.60
1:B:575:MET:HA	1:B:626:ILE:HG22	1.83	0.60
1:C:220:GLY:HA3	1:C:231:ASN:ND2	2.17	0.60
1:C:355:MET:HB3	1:C:365:THR:HG23	1.84	0.60
1:C:713:LEU:HG	1:C:833:PRO:C	2.27	0.60
1:C:947:GLU:C	1:C:949:ALA:H	2.09	0.60
1:A:362:PHE:CZ	1:A:366:LEU:HD13	2.36	0.60
1:B:139:VAL:O	1:B:139:VAL:HG12	2.00	0.60
1:C:930:GLY:HA3	1:C:1007:VAL:CG2	2.25	0.60
1:A:921:LEU:HG	1:A:922:THR:N	2.17	0.59
1:C:322:LYS:HG2	1:C:323:ILE:O	2.02	0.59
1:C:353:LEU:C	1:C:355:MET:H	2.10	0.59
1:C:673:GLU:O	1:C:674:LEU:HB3	2.01	0.59
1:C:930:GLY:CA	1:C:1007:VAL:HG22	2.27	0.59
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.84	0.59
1:B:911:GLY:HA3	1:B:1013:THR:HG21	1.83	0.59
1:C:713:LEU:HB2	1:C:832:ALA:HB3	1.84	0.59
1:C:912:ALA:C	1:C:914:LEU:H	2.11	0.59
1:A:617:PHE:CE2	1:A:666:PHE:HZ	2.20	0.59
1:B:225:VAL:HG11	1:C:778:LYS:HB3	1.84	0.59
1:A:243:THR:O	1:A:268:ILE:HG21	2.02	0.59
1:B:973:ARG:HG2	1:B:977:MET:HE2	1.84	0.59
1:B:1022:VAL:CG2	1:B:1023:PRO:HD3	2.31	0.59
1:B:957:GLY:O	1:B:958:LYS:HG3	2.02	0.59
1:C:156:ASP:HA	1:C:181:GLN:HA	1.84	0.59
1:C:932:LEU:HA	1:C:935:ILE:CG2	2.31	0.59
1:B:68:ASN:O	1:B:70:ASN:N	2.36	0.59
1:B:703:LEU:HD12	1:B:716:VAL:HG12	1.84	0.59
1:C:608:SER:HB3	1:C:630:SER:HB2	1.84	0.59
1:C:882:ILE:O	1:C:882:ILE:HG22	2.03	0.59
1:C:961:ILE:O	1:C:965:LEU:HB2	2.02	0.59
1:A:533:GLY:O	1:A:535:LEU:HG	2.02	0.59
1:A:699:ARG:HH22	1:A:722:GLU:CD	2.10	0.59
1:B:696:THR:HG23	1:B:825:MET:HE1	1.84	0.59
1:C:354:VAL:O	1:C:354:VAL:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:899:PHE:N	1:C:899:PHE:HD1	2.00	0.59
1:C:1016:VAL:HA	1:C:1019:ILE:HG22	1.85	0.59
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.31	0.59
1:B:184:MET:H	1:B:762:PHE:HE2	1.50	0.59
1:B:364:ALA:CB	1:B:497:LEU:HG	2.32	0.59
1:C:732:ASP:O	1:C:733:GLN:C	2.45	0.59
1:A:620:ARG:HH11	1:A:620:ARG:HG2	1.68	0.59
1:B:258:SER:O	1:B:259:ARG:HG2	2.03	0.59
1:C:348:ILE:C	1:C:350:LEU:H	2.11	0.59
1:A:543:VAL:O	1:A:545:TYR:N	2.32	0.58
1:B:213:GLN:HB2	1:B:239:ARG:CD	2.31	0.58
1:B:225:VAL:H	1:C:781:MET:CE	2.16	0.58
1:B:235:ILE:N	1:B:235:ILE:CD1	2.65	0.58
1:B:695:LEU:HD12	1:B:825:MET:HE3	1.85	0.58
1:B:729:ILE:HG12	1:B:730:ASP:H	1.68	0.58
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.85	0.58
1:B:345:VAL:HA	1:B:348:ILE:HD12	1.85	0.58
1:C:1:MET:HG3	1:C:3:ASN:H	1.68	0.58
1:B:197:GLN:HA	1:B:798:MET:SD	2.43	0.58
1:B:355:MET:O	1:B:365:THR:OG1	2.21	0.58
1:B:714:THR:HG21	1:B:833:PRO:HD2	1.84	0.58
1:C:155:SER:OG	1:C:179:GLY:HA3	2.02	0.58
1:B:426:PRO:HB3	1:B:430:ALA:CB	2.32	0.58
1:C:601:LYS:C	1:C:603:LYS:H	2.11	0.58
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.85	0.58
1:A:45:ILE:HD11	1:A:69:MET:HE2	1.86	0.58
1:A:543:VAL:HG22	1:A:544:LEU:H	1.68	0.58
1:B:13:TRP:CE3	1:B:13:TRP:HA	2.37	0.58
1:B:23:GLY:N	1:B:381:ALA:HB2	2.18	0.58
1:C:149:MET:SD	1:C:321:LEU:HD23	2.44	0.58
1:C:331:PRO:O	1:C:335:ILE:HG12	2.04	0.58
1:C:527:TYR:HE2	1:C:968:VAL:O	1.86	0.58
1:A:5:PHE:CD1	1:A:12:ALA:HB2	2.38	0.58
1:A:212:ALA:O	1:A:213:GLN:HB2	2.02	0.58
1:A:240:LEU:HD23	1:A:246:PHE:HA	1.86	0.58
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.85	0.58
1:B:268:ILE:H	1:B:268:ILE:HD12	1.68	0.58
1:B:371:ALA:HA	1:B:374:VAL:HG12	1.86	0.58
1:C:144:ASN:HA	1:C:320:GLY:O	2.04	0.58
1:B:193:LEU:CD1	1:B:198:LEU:O	2.52	0.58
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:945:ILE:C	1:C:947:GLU:H	2.12	0.58
1:A:844:MET:HA	1:A:844:MET:HE3	1.86	0.57
1:A:888:LEU:HD11	1:A:943:ILE:HG12	1.86	0.57
1:A:1021:PHE:HD1	1:A:1025:PHE:HE1	1.52	0.57
1:B:728:LYS:HG2	1:B:808:ARG:HD3	1.86	0.57
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.84	0.57
1:C:986:VAL:O	1:C:990:VAL:HG23	2.03	0.57
1:A:10:ILE:HD12	1:A:10:ILE:O	2.04	0.57
1:A:75:LEU:HD13	1:A:92:LEU:HB3	1.87	0.57
1:A:348:ILE:HD11	1:A:372:VAL:CG1	2.33	0.57
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.86	0.57
1:B:370:ILE:HG22	1:B:370:ILE:O	2.02	0.57
1:C:489:THR:O	1:C:493:CYS:HB3	2.03	0.57
1:A:1035:ARG:HH11	1:A:1035:ARG:HA	1.69	0.57
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.34	0.57
1:C:554:TYR:O	1:C:556:PHE:N	2.29	0.57
1:C:643:LYS:NZ	1:C:997:SER:HB2	2.20	0.57
1:C:674:LEU:HD13	1:C:862:MET:HA	1.85	0.57
1:C:685:ILE:O	1:C:687:GLN:HG2	2.05	0.57
1:C:907:LEU:HD22	1:C:1017:LEU:HD23	1.86	0.57
1:A:820:ASN:ND2	3:A:4001:HOH:O	2.33	0.57
1:B:398:MET:HG3	1:B:473:THR:HG21	1.87	0.57
1:B:979:SER:O	1:B:983:ILE:HG12	2.03	0.57
1:B:57:VAL:CG1	1:B:58:GLN:N	2.67	0.57
1:A:659:LYS:NZ	1:A:660:ASP:O	2.38	0.57
1:A:882:ILE:O	1:A:886:LEU:HB2	2.05	0.57
1:B:349:ILE:O	1:B:351:VAL:N	2.36	0.57
1:B:673:GLU:O	1:B:676:THR:CG2	2.51	0.57
1:C:144:ASN:HD21	1:C:148:THR:N	2.02	0.57
1:A:216:ALA:CB	1:B:750:LEU:HD13	2.35	0.57
1:A:456:MET:O	1:A:458:PHE:N	2.35	0.57
1:B:425:LEU:HB2	1:B:498:LYS:O	2.04	0.57
1:C:899:PHE:N	1:C:899:PHE:CD1	2.72	0.57
1:C:641:GLU:H	1:C:641:GLU:CD	2.13	0.57
1:C:672:VAL:CG1	1:C:673:GLU:N	2.63	0.57
1:C:681:ASP:HB3	1:C:860:THR:HG23	1.87	0.57
1:C:884:VAL:C	1:C:886:LEU:H	2.13	0.57
1:B:792:ARG:HG2	1:B:793:ALA:H	1.70	0.57
1:C:88:VAL:HG12	1:C:90:ILE:HD12	1.86	0.57
1:A:871:ASN:O	1:A:874:PRO:HD2	2.04	0.56
1:B:453:PHE:HZ	1:B:933:THR:HG23	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:LEU:HD12	1:C:929:VAL:CG1	2.35	0.56
1:A:5:PHE:HD1	1:A:12:ALA:HB2	1.68	0.56
1:A:688:ALA:C	1:A:690:LEU:H	2.12	0.56
1:A:723:ASP:OD1	1:A:813:SER:N	2.38	0.56
1:B:537:SER:O	1:B:539:GLY:N	2.38	0.56
1:C:184:MET:HG2	1:C:246:PHE:CD1	2.40	0.56
1:A:199:THR:CG2	1:A:791:VAL:HA	2.35	0.56
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.40	0.56
1:A:880:SER:O	1:A:884:VAL:HG23	2.06	0.56
1:A:911:GLY:H	1:A:914:LEU:HD13	1.70	0.56
1:A:1011:MET:HE3	1:A:1014:ALA:HB3	1.87	0.56
1:B:52:ALA:HB2	1:B:85:THR:C	2.29	0.56
1:B:298:ASN:ND2	1:B:301:ASP:OD1	2.39	0.56
1:B:314:GLU:HG2	1:B:317:PHE:CE2	2.40	0.56
1:B:900:SER:HB2	1:B:1026:PHE:CZ	2.40	0.56
1:C:13:TRP:O	1:C:17:ILE:HG12	2.06	0.56
1:C:159:ALA:CB	1:C:181:GLN:HB2	2.35	0.56
1:C:225:VAL:O	1:C:226:LYS:C	2.48	0.56
1:A:69:MET:HE1	1:A:107:VAL:HG13	1.88	0.56
1:B:149:MET:CB	1:B:154:ILE:HG22	2.35	0.56
1:B:213:GLN:HB2	1:B:239:ARG:CG	2.34	0.56
1:B:743:ILE:H	1:B:743:ILE:CD1	2.09	0.56
1:C:48:SER:HB2	1:C:87:THR:HG22	1.87	0.56
1:C:615:PHE:C	1:C:615:PHE:CD2	2.83	0.56
1:B:36:PRO:HD2	1:B:38:ILE:HD11	1.88	0.56
1:B:535:LEU:HD21	1:B:1023:PRO:HB2	1.87	0.56
1:C:736:ALA:C	1:C:738:ALA:H	2.12	0.56
1:A:204:ILE:CD1	1:A:773:VAL:HG11	2.35	0.56
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.40	0.56
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.20	0.56
1:B:921:LEU:HD21	1:B:1002:ALA:HA	1.87	0.56
1:A:63:GLN:O	1:A:64:VAL:C	2.48	0.56
1:B:589:LYS:HA	1:B:592:ASN:OD1	2.05	0.56
1:C:228:GLN:NE2	1:C:230:LEU:O	2.39	0.56
1:A:600:THR:O	1:A:601:LYS:HB2	2.06	0.56
1:A:747:ASN:HD21	1:C:237:GLN:NE2	2.04	0.56
1:B:73:ASP:HB2	1:B:106:GLN:HE22	1.71	0.56
1:B:356:TYR:HE2	1:B:365:THR:HG21	1.70	0.56
1:A:70:ASN:HB3	1:C:167:SER:HB3	1.88	0.56
1:A:527:TYR:CE2	1:A:972:LEU:HG	2.41	0.56
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.41	0.56
1:C:20:MET:O	1:C:377:LEU:HD12	2.06	0.56
1:C:100:ALA:HB2	1:C:295:THR:HG21	1.88	0.56
1:C:367:ILE:HD11	1:C:489:THR:HA	1.87	0.56
1:C:958:LYS:HB3	1:C:962:GLU:HB3	1.87	0.55
1:A:240:LEU:HD12	1:A:240:LEU:N	2.20	0.55
1:A:1029:VAL:O	1:A:1030:ARG:HB2	2.05	0.55
1:B:23:GLY:HA2	1:B:26:ALA:HB3	1.89	0.55
1:B:445:ILE:HD13	1:B:943:ILE:CG2	2.36	0.55
1:C:818:ARG:HA	1:C:824:SER:H	1.71	0.55
1:A:582:ALA:HB3	1:A:623:ASN:HB2	1.88	0.55
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.87	0.55
1:A:4:PHE:HB3	1:A:8:ARG:HH21	1.72	0.55
1:B:539:GLY:C	1:B:541:TYR:N	2.64	0.55
1:B:778:LYS:HD3	1:B:778:LYS:H	1.71	0.55
1:B:881:LEU:HD21	1:B:905:VAL:HG21	1.89	0.55
1:C:351:VAL:O	1:C:355:MET:HB2	2.07	0.55
1:B:366:LEU:O	1:B:369:THR:N	2.36	0.55
1:B:712:MET:HA	1:B:834:GLY:HA3	1.87	0.55
1:B:892:TYR:CB	1:B:897:ILE:HD11	2.37	0.55
2:C:3402:ERY:C30	2:C:3402:ERY:C14	2.84	0.55
1:B:680:PHE:CD1	1:B:859:TRP:HZ3	2.25	0.55
1:B:847:LEU:O	1:B:850:LYS:HG2	2.06	0.55
1:B:952:LEU:C	1:B:954:ASP:N	2.65	0.55
1:C:102:ILE:O	1:C:103:ALA:C	2.47	0.55
1:C:1032:ARG:HB3	1:C:1032:ARG:HH21	1.71	0.55
1:A:617:PHE:CE2	1:A:626:ILE:HD11	2.42	0.55
1:A:688:ALA:O	1:A:690:LEU:N	2.38	0.55
1:B:1023:PRO:O	1:B:1027:VAL:HG22	2.07	0.55
1:C:57:VAL:HG12	1:C:88:VAL:HG22	1.88	0.55
1:C:837:THR:O	1:C:841:MET:HG3	2.07	0.55
1:A:574:THR:HB	1:A:627:ALA:HB3	1.87	0.55
1:C:211:ASN:HA	1:C:240:LEU:HD23	1.89	0.55
1:A:156:ASP:OD1	1:A:182:TYR:HB2	2.07	0.55
1:B:415:ASN:ND2	1:B:434:SER:OG	2.36	0.55
1:B:709:HIS:N	1:B:710:PRO:HD3	2.22	0.55
1:B:987:MET:N	1:B:988:PRO:HD2	2.22	0.55
1:C:692:HIS:CE1	1:C:721:LEU:HD21	2.30	0.55
1:A:4:PHE:O	1:A:8:ARG:HG2	2.08	0.54
1:A:216:ALA:HA	1:B:751:GLY:HA2	1.89	0.54
1:B:13:TRP:HE3	1:B:13:TRP:HA	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768:VAL:HG23	1:C:63:GLN:NE2	2.22	0.54
1:A:219:LEU:HD22	1:B:781:MET:O	2.06	0.54
1:A:418:ARG:HA	1:A:421:ALA:HB3	1.90	0.54
1:A:456:MET:C	1:A:458:PHE:H	2.15	0.54
1:B:240:LEU:O	1:B:762:PHE:HB2	2.07	0.54
1:B:247:GLY:HA2	1:B:268:ILE:HD13	1.88	0.54
1:C:489:THR:N	1:C:490:PRO:HD2	2.22	0.54
1:A:832:ALA:O	1:A:833:PRO:C	2.49	0.54
1:B:927:PHE:CE1	1:B:931:LEU:HG	2.42	0.54
1:A:609:VAL:HG12	1:A:629:VAL:HB	1.89	0.54
1:A:703:LEU:HD11	1:A:718:PRO:HD3	1.88	0.54
1:B:59:ASP:HA	1:B:63:GLN:CG	2.37	0.54
1:B:219:LEU:HD23	1:B:230:LEU:HD11	1.88	0.54
1:B:971:ARG:HA	1:B:974:PRO:HG2	1.89	0.54
1:C:607:GLU:HB2	1:C:632:LYS:CG	2.36	0.54
1:C:632:LYS:O	1:C:634:TRP:N	2.39	0.54
1:A:126:GLY:HA3	1:B:116:PRO:HB3	1.89	0.54
1:A:543:VAL:C	1:A:545:TYR:N	2.65	0.54
1:B:250:LEU:HA	1:B:261:LEU:HB3	1.88	0.54
1:B:913:LEU:O	1:B:917:THR:HB	2.08	0.54
1:C:326:PRO:HG3	1:C:610:PHE:CD1	2.43	0.54
1:C:909:VAL:HA	1:C:931:LEU:HD11	1.88	0.54
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.89	0.54
1:B:274:ASN:OD1	1:B:276:ASP:HB2	2.08	0.54
1:B:404:LEU:C	1:B:406:VAL:H	2.16	0.54
1:B:569:GLN:HE21	1:B:668:LEU:HB2	1.71	0.54
1:C:819:TYR:N	1:C:824:SER:HB3	2.23	0.54
1:A:66:GLU:C	1:A:68:ASN:H	2.15	0.54
1:C:9:PRO:HG3	1:C:491:ALA:HB1	1.89	0.54
1:C:726:GLN:CD	1:C:812:GLY:HA3	2.33	0.54
1:A:302:THR:O	1:A:306:ILE:HG12	2.08	0.54
1:A:708:LYS:C	1:A:710:PRO:HD3	2.33	0.54
1:B:773:VAL:O	1:B:773:VAL:CG1	2.56	0.54
1:C:142:VAL:HG12	1:C:154:ILE:CG2	2.38	0.54
1:C:188:MET:HE2	1:C:773:VAL:HB	1.88	0.54
1:C:1018:ALA:O	1:C:1022:VAL:HG12	2.08	0.54
1:B:68:ASN:C	1:B:70:ASN:N	2.65	0.54
1:B:969:ARG:HH22	1:B:970:MET:HE3	1.73	0.54
1:C:203:VAL:HG13	1:C:262:LEU:HD11	1.89	0.54
1:A:133:SER:O	1:A:135:SER:N	2.32	0.54
1:B:580:ALA:O	1:B:581:GLY:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:ARG:HA	1:C:63:GLN:HE22	1.73	0.54
1:B:699:ARG:O	1:B:701:GLN:N	2.40	0.53
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.29	0.53
1:C:84:SER:C	1:C:86:GLY:N	2.65	0.53
1:C:782:LEU:HB3	1:C:783:PRO:HD2	1.90	0.53
1:C:938:SER:O	1:C:941:ASN:ND2	2.41	0.53
1:A:83:ASP:HB3	1:A:815:ARG:HG3	1.89	0.53
1:A:248:LYS:HA	1:A:261:LEU:HD22	1.90	0.53
1:A:417:GLU:HG3	1:A:420:MET:HE2	1.89	0.53
1:B:16:ALA:HB2	1:B:488:LEU:HG	1.90	0.53
1:B:115:MET:HA	1:B:115:MET:CE	2.37	0.53
1:B:158:VAL:HA	1:B:162:MET:HG2	1.90	0.53
1:B:892:TYR:O	1:B:894:SER:N	2.42	0.53
1:B:1017:LEU:O	1:B:1021:PHE:HD2	1.92	0.53
1:C:415:ASN:O	1:C:418:ARG:HG2	2.07	0.53
1:C:839:GLU:HA	1:C:842:GLU:CB	2.38	0.53
1:A:313:MET:HB2	1:A:317:PHE:CE1	2.44	0.53
1:A:740:GLY:HA3	1:A:794:ALA:H	1.73	0.53
1:A:754:TRP:CE3	1:A:780:ARG:HB2	2.44	0.53
1:A:191:ASN:C	1:A:193:LEU:N	2.67	0.53
1:A:376:LEU:C	1:A:378:GLY:H	2.14	0.53
1:A:783:PRO:C	1:A:785:ASP:H	2.17	0.53
1:B:138:MET:HE3	1:B:306:ILE:HD13	1.90	0.53
1:C:594:VAL:HG13	1:C:598:TYR:HE1	1.73	0.53
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.43	0.53
1:A:987:MET:N	1:A:988:PRO:CD	2.72	0.53
1:A:991:ILE:O	1:A:992:SER:HB3	2.07	0.53
1:B:152:GLU:O	1:B:182:TYR:HE1	1.90	0.53
1:B:428:LYS:O	1:B:432:ARG:HG3	2.07	0.53
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.90	0.53
1:C:265:VAL:O	1:C:265:VAL:CG2	2.50	0.53
1:C:371:ALA:HB2	1:C:488:LEU:HD23	1.90	0.53
1:C:444:GLY:O	1:C:448:VAL:HG23	2.08	0.53
1:C:894:SER:C	1:C:896:SER:H	2.16	0.53
1:B:393:LEU:HB2	1:B:469:GLN:HG2	1.89	0.53
1:B:452:VAL:O	1:B:453:PHE:HB2	2.08	0.53
1:B:580:ALA:O	1:B:582:ALA:N	2.41	0.53
1:B:654:ALA:C	1:B:656:SER:H	2.16	0.53
1:C:486:LEU:C	1:C:490:PRO:HG3	2.34	0.53
1:B:120:GLN:O	1:B:124:GLN:HG2	2.08	0.53
1:B:157:TYR:C	1:B:161:ASN:HD22	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:O	1:A:355:MET:HB2	2.08	0.53
1:A:578:LEU:HD21	1:A:587:THR:HA	1.91	0.53
1:A:597:TYR:CD1	1:A:597:TYR:C	2.86	0.53
1:B:252:LYS:HB3	1:B:260:VAL:HG12	1.91	0.53
1:B:339:GLU:OE1	1:B:339:GLU:HA	2.08	0.53
1:B:344:LEU:O	1:B:347:ALA:HB3	2.09	0.53
1:B:446:ALA:O	1:B:447:MET:C	2.52	0.53
1:B:528:THR:O	1:B:531:VAL:HG12	2.08	0.53
1:B:1005:THR:O	1:B:1005:THR:HG22	2.09	0.53
1:C:60:THR:HG22	1:C:61:VAL:HG23	1.89	0.53
1:C:164:ASP:O	1:C:168:ARG:HG3	2.09	0.53
1:C:655:PHE:HB3	1:C:663:VAL:CG2	2.38	0.53
1:C:761:ASP:HB3	1:C:769:LYS:O	2.09	0.53
1:A:35:TYR:CD1	1:A:671:ILE:HG22	2.44	0.53
1:A:164:ASP:HA	1:A:167:SER:HB2	1.91	0.53
1:A:242:SER:HB3	1:A:245:GLU:HB2	1.91	0.53
1:B:393:LEU:HD13	1:B:466:ILE:HG23	1.90	0.53
1:B:445:ILE:HG23	1:B:940:LYS:CG	2.29	0.53
1:B:762:PHE:C	1:B:763:ILE:HD12	2.34	0.53
1:B:888:LEU:HB2	1:B:898:PRO:HB3	1.90	0.53
1:C:851:LEU:HB3	1:C:852:PRO:HD2	1.91	0.53
1:A:128:SER:HB2	1:B:113:LEU:HD23	1.90	0.53
1:A:152:GLU:HG2	1:A:272:GLY:HA3	1.91	0.53
1:A:214:VAL:HG21	1:B:747:ASN:CG	2.34	0.53
1:B:399:VAL:HG11	1:B:989:LEU:HG	1.90	0.53
1:C:591:LEU:HD12	1:C:611:ALA:HB1	1.89	0.53
1:A:235:ILE:O	1:A:235:ILE:HG22	2.09	0.52
1:A:947:GLU:O	1:A:951:ASP:N	2.40	0.52
1:B:1:MET:HG2	1:B:439:GLN:HE22	1.74	0.52
1:B:564:LEU:HD23	1:B:565:PRO:HD2	1.90	0.52
1:B:986:VAL:CG2	1:B:1008:MET:HB2	2.38	0.52
1:C:350:LEU:HD21	1:C:984:LEU:HD22	1.90	0.52
1:C:400:LEU:HD21	1:C:1003:VAL:HG13	1.91	0.52
1:B:57:VAL:HG12	1:B:58:GLN:H	1.74	0.52
1:B:434:SER:O	1:B:438:ILE:HG22	2.10	0.52
1:B:518:ARG:HA	1:B:521:GLU:CD	2.34	0.52
1:C:172:VAL:HG22	1:C:306:ILE:HD11	1.91	0.52
1:C:466:ILE:HG13	1:C:563:PHE:HZ	1.73	0.52
1:C:997:SER:O	1:C:999:ALA:N	2.43	0.52
1:A:193:LEU:HB2	1:A:265:VAL:HG13	1.91	0.52
1:A:576:VAL:HG11	1:A:591:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HD2	1:B:772:TYR:HB2	1.91	0.52
1:B:409:ALA:HA	1:B:485:ALA:HB2	1.90	0.52
1:B:867:ARG:HG2	1:B:868:LEU:HD22	1.91	0.52
1:C:907:LEU:HD13	1:C:1018:ALA:HA	1.90	0.52
1:A:214:VAL:HG21	1:B:747:ASN:ND2	2.24	0.52
1:A:527:TYR:C	1:A:529:ASP:H	2.17	0.52
1:A:543:VAL:C	1:A:545:TYR:H	2.17	0.52
1:A:550:VAL:O	1:A:551:GLY:C	2.53	0.52
1:B:2:PRO:HB3	1:B:486:LEU:O	2.09	0.52
1:B:190:PRO:HB3	1:B:789:TRP:CD2	2.45	0.52
1:B:942:ALA:HA	1:B:1022:VAL:HG11	1.90	0.52
1:C:395:MET:C	1:C:397:GLY:H	2.17	0.52
1:C:445:ILE:O	1:C:449:LEU:N	2.39	0.52
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.92	0.52
1:C:831:ALA:HB2	1:C:840:ALA:CB	2.40	0.52
1:C:911:GLY:HA3	1:C:1010:GLY:HA2	1.91	0.52
1:B:5:PHE:O	1:B:9:PRO:HA	2.08	0.52
1:B:204:ILE:HG23	1:B:759:VAL:HG13	1.92	0.52
1:B:600:THR:C	1:B:602:GLU:H	2.17	0.52
1:C:208:LYS:HA	1:C:760:ASN:HD21	1.75	0.52
1:C:899:PHE:HD1	1:C:899:PHE:H	1.57	0.52
1:A:200:PRO:HA	1:A:203:VAL:HG23	1.92	0.52
1:A:406:VAL:HG12	1:A:407:ASP:N	2.24	0.52
1:A:584:GLN:H	1:A:622:GLN:HG2	1.74	0.52
1:B:13:TRP:HD1	1:C:895:TRP:HZ2	1.57	0.52
1:B:193:LEU:HD11	1:B:198:LEU:O	2.09	0.52
1:C:378:GLY:O	1:C:382:VAL:HG23	2.10	0.52
1:C:527:TYR:OH	1:C:1019:ILE:HG13	2.09	0.52
1:C:646:ALA:HA	1:C:649:MET:HB2	1.92	0.52
1:A:62:THR:HG23	1:A:88:VAL:CG1	2.40	0.52
1:B:115:MET:HA	1:B:118:LEU:HD13	1.92	0.52
1:B:335:ILE:O	1:B:336:SER:C	2.53	0.52
1:C:169:THR:O	1:C:172:VAL:HG23	2.10	0.52
1:C:453:PHE:C	1:C:455:PRO:HD2	2.34	0.52
1:B:972:LEU:HD21	1:B:1019:ILE:HG12	1.91	0.52
1:C:18:ILE:O	1:C:19:ILE:C	2.53	0.52
1:C:124:GLN:HB3	1:C:758:TYR:HE2	1.74	0.52
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.43	0.52
1:B:45:ILE:HB	1:B:90:ILE:HB	1.92	0.52
1:B:459:PHE:O	1:B:464:GLY:HA3	2.10	0.52
1:B:873:ALA:HB1	1:B:877:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:GLY:HA2	1:B:914:LEU:CB	2.40	0.52
1:C:380:PHE:HE1	1:C:395:MET:HE1	1.75	0.52
1:C:402:ILE:O	1:C:406:VAL:HG23	2.10	0.52
1:C:923:ASN:HD22	1:C:927:PHE:HD2	1.58	0.52
1:A:324:VAL:HG12	1:A:325:TYR:H	1.75	0.51
1:A:525:HIS:HA	1:A:528:THR:CG2	2.37	0.51
1:B:699:ARG:HA	1:B:702:LEU:HB2	1.92	0.51
1:B:729:ILE:CG1	1:B:730:ASP:H	2.23	0.51
1:B:1026:PHE:HB3	1:B:1030:ARG:HE	1.74	0.51
1:C:68:ASN:OD1	1:C:68:ASN:N	2.43	0.51
1:C:395:MET:O	1:C:398:MET:N	2.43	0.51
1:C:418:ARG:HD3	1:C:970:MET:HE2	1.91	0.51
1:C:527:TYR:OH	1:C:968:VAL:HG12	2.10	0.51
1:C:881:LEU:C	1:C:883:VAL:H	2.18	0.51
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.91	0.51
1:A:550:VAL:O	1:A:553:ALA:N	2.43	0.51
1:A:886:LEU:HD12	1:C:14:VAL:HG23	1.90	0.51
1:B:280:GLU:CB	1:B:284:GLN:O	2.58	0.51
1:B:482:VAL:O	1:B:486:LEU:HB2	2.10	0.51
1:C:34:GLN:O	1:C:391:ASN:HB2	2.09	0.51
1:A:945:ILE:HG13	1:A:971:ARG:CG	2.27	0.51
1:B:291:ILE:HG21	1:B:306:ILE:HD11	1.91	0.51
1:B:754:TRP:HH2	1:B:785:ASP:HB2	1.76	0.51
1:B:897:ILE:HG13	1:B:898:PRO:HD3	1.92	0.51
1:C:3:ASN:C	1:C:5:PHE:N	2.68	0.51
1:C:395:MET:C	1:C:397:GLY:N	2.69	0.51
1:B:349:ILE:C	1:B:351:VAL:N	2.69	0.51
1:C:176:GLN:HE22	1:C:620:ARG:HH12	1.58	0.51
1:C:210:GLN:O	1:C:240:LEU:CD2	2.58	0.51
1:A:204:ILE:HD11	1:A:773:VAL:HG11	1.93	0.51
1:B:776:GLU:HG2	1:B:777:ALA:H	1.75	0.51
1:C:731:ILE:HD13	1:C:746:ILE:HG21	1.92	0.51
1:C:947:GLU:C	1:C:949:ALA:N	2.68	0.51
1:A:139:VAL:CG1	1:A:327:TYR:HB3	2.39	0.51
1:A:886:LEU:HD13	1:C:14:VAL:HG23	1.91	0.51
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.25	0.51
1:B:13:TRP:O	1:B:16:ALA:HB3	2.11	0.51
1:B:418:ARG:HB3	1:B:418:ARG:HH11	1.76	0.51
1:C:146:ASP:C	1:C:148:THR:N	2.68	0.51
1:C:326:PRO:CB	1:C:610:PHE:HB2	2.40	0.51
1:C:681:ASP:CB	1:C:860:THR:CG2	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:CG	1:A:260:VAL:HG11	2.45	0.51
1:A:431:THR:O	1:A:435:MET:HB2	2.11	0.51
1:C:423:GLU:CB	1:C:426:PRO:HD2	2.41	0.51
1:A:167:SER:HA	1:A:175:VAL:HG21	1.93	0.51
1:A:282:ASN:ND2	1:A:609:VAL:H	2.08	0.51
1:A:584:GLN:N	1:A:622:GLN:HG2	2.25	0.51
1:B:428:LYS:CB	1:B:494:ALA:HB1	2.40	0.51
1:C:477:ALA:C	1:C:479:ALA:H	2.18	0.51
1:C:635:ALA:C	1:C:637:ARG:H	2.18	0.51
1:A:391:ASN:O	1:A:392:THR:C	2.54	0.51
1:A:585:GLU:OE2	1:C:227:GLY:HA2	2.10	0.51
1:A:601:LYS:O	1:A:602:GLU:HG2	2.11	0.51
1:A:671:ILE:CG1	1:A:674:LEU:HB3	2.41	0.51
1:C:176:GLN:HE21	1:C:620:ARG:HH11	1.55	0.51
1:C:326:PRO:HB3	1:C:610:PHE:HB2	1.93	0.51
1:C:352:PHE:HA	1:C:369:THR:HG21	1.93	0.51
1:C:465:ALA:O	1:C:469:GLN:HG2	2.10	0.51
1:C:712:MET:HB2	1:C:839:GLU:OE1	2.11	0.51
1:C:951:ASP:C	1:C:953:MET:H	2.19	0.51
1:A:261:LEU:CD1	1:A:263:ARG:HH11	2.24	0.51
1:B:68:ASN:O	1:B:70:ASN:ND2	2.44	0.51
1:B:160:ALA:HB1	1:B:767:ARG:HD3	1.93	0.51
1:B:213:GLN:HE21	1:B:239:ARG:HD2	1.76	0.51
1:B:683:GLU:O	1:B:857:TYR:HA	2.10	0.51
1:C:181:GLN:CG	1:C:769:LYS:HE2	2.41	0.51
1:C:239:ARG:HB2	1:C:763:ILE:CD1	2.41	0.51
1:C:404:LEU:HD21	1:C:449:LEU:CD1	2.41	0.51
1:C:801:PHE:CD1	1:C:804:PHE:CE1	2.99	0.51
1:A:455:PRO:HG2	1:A:880:SER:HB2	1.91	0.50
1:A:819:TYR:N	1:A:824:SER:HB3	2.25	0.50
1:B:552:MET:SD	1:B:909:VAL:HG23	2.50	0.50
1:B:764:ASP:HB3	1:B:769:LYS:HE3	1.93	0.50
1:B:833:PRO:C	1:B:835:LYS:H	2.18	0.50
1:B:899:PHE:O	1:B:899:PHE:CD1	2.64	0.50
1:B:900:SER:HA	1:B:903:LEU:HD12	1.92	0.50
1:C:485:ALA:HA	1:C:489:THR:OG1	2.11	0.50
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.92	0.50
1:A:92:LEU:H	1:A:92:LEU:HD12	1.75	0.50
1:A:185:ARG:HD3	1:A:272:GLY:O	2.10	0.50
1:A:780:ARG:HG2	1:A:780:ARG:NH1	2.25	0.50
1:B:46:SER:HA	1:B:88:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:TYR:HB3	1:B:57:VAL:HG23	1.92	0.50
1:B:213:GLN:HE21	1:B:239:ARG:CD	2.25	0.50
1:B:282:ASN:O	1:B:284:GLN:N	2.44	0.50
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.93	0.50
1:C:76:MET:SD	1:C:95:GLU:HG3	2.51	0.50
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.93	0.50
1:B:225:VAL:O	1:B:226:LYS:C	2.52	0.50
1:B:866:GLU:O	1:B:867:ARG:C	2.52	0.50
1:C:144:ASN:ND2	1:C:149:MET:N	2.57	0.50
1:C:189:ASN:ND2	1:C:192:GLU:H	2.09	0.50
1:C:463:THR:HA	1:C:466:ILE:HG12	1.93	0.50
1:B:59:ASP:HA	1:B:63:GLN:HG2	1.93	0.50
1:B:876:LEU:HD22	1:B:932:LEU:HD13	1.93	0.50
1:C:946:VAL:O	1:C:946:VAL:HG12	2.12	0.50
1:A:95:GLU:O	1:A:96:SER:C	2.55	0.50
1:A:877:TYR:O	1:A:881:LEU:HB2	2.12	0.50
1:B:356:TYR:C	1:B:358:PHE:H	2.17	0.50
1:C:47:ALA:HB2	1:C:127:VAL:HG12	1.92	0.50
1:C:382:VAL:HG11	1:C:476:SER:HB2	1.94	0.50
1:C:588:GLN:HG2	1:C:613:ASN:ND2	2.25	0.50
1:C:631:LEU:HB3	1:C:637:ARG:NH2	2.27	0.50
1:A:36:PRO:HG3	1:A:469:GLN:OE1	2.12	0.50
1:A:578:LEU:CD2	1:A:587:THR:HG23	2.42	0.50
1:A:612:VAL:CG2	1:A:626:ILE:HG22	2.37	0.50
1:A:659:LYS:CG	1:A:660:ASP:H	2.05	0.50
1:A:786:ILE:O	1:A:787:GLY:C	2.54	0.50
1:B:261:LEU:O	1:B:263:ARG:N	2.44	0.50
1:B:714:THR:HG21	1:B:832:ALA:H	1.75	0.50
1:B:891:LEU:HD12	1:B:892:TYR:CE1	2.46	0.50
1:C:32:VAL:O	1:C:33:ALA:C	2.54	0.50
1:C:894:SER:HG	1:C:897:ILE:HG12	1.73	0.50
1:B:213:GLN:HG3	1:C:56:THR:CG2	2.41	0.50
1:B:251:LEU:HB2	1:B:261:LEU:HA	1.94	0.50
1:B:699:ARG:HB3	1:B:699:ARG:HH11	1.77	0.50
1:B:814:PRO:O	1:B:815:ARG:HG2	2.12	0.50
1:C:239:ARG:HB2	1:C:763:ILE:HD13	1.92	0.50
1:C:477:ALA:HA	1:C:480:LEU:HB2	1.93	0.50
1:C:734:GLU:HA	1:C:737:GLN:HE21	1.76	0.50
1:C:912:ALA:C	1:C:914:LEU:N	2.69	0.50
1:C:912:ALA:O	1:C:914:LEU:N	2.44	0.50
1:C:920:GLY:O	1:C:921:LEU:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:ALA:O	1:A:679:GLY:N	2.31	0.50
1:A:904:VAL:HA	1:A:907:LEU:HD13	1.94	0.50
1:B:30:LEU:HD12	1:B:384:ALA:HB2	1.92	0.50
1:B:158:VAL:HB	1:B:289:LEU:HD21	1.93	0.50
1:B:391:ASN:HD21	1:B:393:LEU:HB2	1.77	0.50
1:B:414:GLU:CD	1:B:974:PRO:HG3	2.37	0.50
1:B:964:THR:O	1:B:968:VAL:HG23	2.11	0.50
1:A:159:ALA:HB2	1:A:177:LEU:HD22	1.93	0.50
1:A:552:MET:HE1	1:A:906:PRO:HA	1.94	0.50
1:A:841:MET:O	1:A:845:GLU:HG3	2.12	0.50
1:A:974:PRO:C	1:A:976:LEU:H	2.18	0.50
1:B:135:SER:HB2	1:B:676:THR:CG2	2.42	0.50
1:B:261:LEU:O	1:B:261:LEU:HD23	2.12	0.50
1:B:323:ILE:HD12	1:B:323:ILE:N	2.27	0.50
1:B:428:LYS:HB2	1:B:494:ALA:HB1	1.93	0.50
1:B:905:VAL:HG13	1:B:906:PRO:CD	2.40	0.50
1:B:990:VAL:HG13	1:B:1005:THR:OG1	2.10	0.50
1:A:193:LEU:HD12	1:A:265:VAL:HG11	1.93	0.49
1:A:201:VAL:HG21	1:A:745:ASP:OD2	2.12	0.49
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.12	0.49
1:A:1022:VAL:HA	1:A:1025:PHE:HD1	1.77	0.49
1:B:729:ILE:HG12	1:B:730:ASP:N	2.25	0.49
1:B:934:THR:C	1:B:936:GLY:N	2.58	0.49
1:B:967:ALA:C	1:B:969:ARG:N	2.68	0.49
1:A:311:ALA:O	1:A:312:LYS:HB2	2.11	0.49
1:A:583:THR:HG22	1:A:585:GLU:N	2.27	0.49
1:A:586:ARG:HA	1:A:589:LYS:HE3	1.94	0.49
1:A:590:VAL:O	1:A:594:VAL:HG23	2.12	0.49
1:B:115:MET:HE1	1:B:127:VAL:HG21	1.93	0.49
1:C:220:GLY:HA3	1:C:231:ASN:HD22	1.76	0.49
1:C:941:ASN:HD22	1:C:942:ALA:N	2.10	0.49
1:A:187:TRP:HZ2	1:A:275:TYR:HE1	1.60	0.49
1:A:644:VAL:HG11	1:A:667:ASN:OD1	2.12	0.49
1:A:979:SER:O	1:A:983:ILE:HG23	2.12	0.49
1:B:741:VAL:HG12	1:B:792:ARG:O	2.12	0.49
1:C:1:MET:HB2	1:C:2:PRO:CD	2.38	0.49
1:C:414:GLU:HA	1:C:417:GLU:HG2	1.95	0.49
1:C:527:TYR:C	1:C:529:ASP:H	2.19	0.49
1:A:232:ALA:HB1	1:B:725:PRO:O	2.12	0.49
1:B:183:ALA:HB2	1:B:273:GLU:HB3	1.94	0.49
1:B:967:ALA:C	1:B:969:ARG:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ILE:HG23	1:C:368:PRO:HD3	1.93	0.49
1:C:442:LEU:O	1:C:445:ILE:HG13	2.12	0.49
1:C:540:ARG:O	1:C:544:LEU:HB2	2.13	0.49
1:C:713:LEU:HD21	1:C:835:LYS:N	2.27	0.49
1:C:754:TRP:CZ3	1:C:780:ARG:HA	2.46	0.49
1:A:18:ILE:O	1:A:19:ILE:C	2.54	0.49
1:B:164:ASP:HB3	1:B:168:ARG:HH22	1.78	0.49
1:B:166:ILE:HD11	1:B:310:LEU:HG	1.94	0.49
1:B:204:ILE:O	1:B:205:THR:C	2.55	0.49
1:C:713:LEU:HD21	1:C:835:LYS:H	1.78	0.49
1:B:623:ASN:OD1	1:B:623:ASN:N	2.37	0.49
1:B:708:LYS:HG2	1:B:708:LYS:O	2.12	0.49
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.76	0.49
1:C:26:ALA:O	1:C:30:LEU:HD12	2.12	0.49
1:C:145:THR:C	1:C:147:GLY:H	2.19	0.49
1:A:1:MET:SD	1:A:487:ILE:CD1	3.01	0.49
1:A:930:GLY:C	1:A:932:LEU:H	2.21	0.49
1:B:95:GLU:O	1:B:98:THR:HG22	2.12	0.49
1:B:427:PRO:C	1:B:429:GLU:H	2.20	0.49
1:B:897:ILE:N	1:B:898:PRO:CD	2.76	0.49
1:C:618:ALA:CB	1:C:815:ARG:HH12	2.23	0.49
1:C:681:ASP:HB3	1:C:860:THR:HG22	1.94	0.49
1:C:686:ASP:CG	1:C:690:LEU:HB2	2.38	0.49
1:A:937:LEU:HD12	1:A:1011:MET:SD	2.53	0.49
1:B:587:THR:HB	1:B:613:ASN:HD21	1.78	0.49
1:C:410:ILE:O	1:C:411:VAL:C	2.55	0.49
1:C:456:MET:O	1:C:459:PHE:HB2	2.13	0.49
1:C:1030:ARG:C	1:C:1032:ARG:H	2.21	0.49
1:A:253:VAL:HG23	1:A:259:ARG:HG2	1.94	0.49
1:A:416:VAL:HG22	1:A:434:SER:OG	2.12	0.49
1:B:49:TYR:HB3	1:B:57:VAL:CG2	2.43	0.49
1:B:602:GLU:C	1:B:604:ASN:H	2.18	0.49
1:B:764:ASP:O	1:B:766:GLY:N	2.39	0.49
1:B:768:VAL:HG23	1:C:63:GLN:CD	2.38	0.49
1:B:831:ALA:CB	1:B:840:ALA:HB2	2.42	0.49
1:C:879:ILE:O	1:C:879:ILE:HG22	2.13	0.49
1:C:952:LEU:O	1:C:953:MET:HG3	2.13	0.49
1:A:561:SER:HA	1:A:923:ASN:HB3	1.95	0.49
1:B:16:ALA:O	1:B:374:VAL:HG23	2.13	0.49
1:B:1025:PHE:O	1:B:1029:VAL:HG12	2.13	0.49
1:C:33:ALA:HB1	1:C:34:GLN:HE21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.78	0.49
1:C:713:LEU:CD1	1:C:835:LYS:H	2.18	0.49
1:C:866:GLU:C	1:C:867:ARG:HG2	2.38	0.49
1:C:968:VAL:HG11	1:C:1023:PRO:HG3	1.94	0.49
1:B:154:ILE:O	1:B:157:TYR:N	2.46	0.48
1:C:75:LEU:HD11	1:C:92:LEU:HD23	1.95	0.48
1:C:354:VAL:O	1:C:355:MET:HE3	2.13	0.48
1:C:425:LEU:H	1:C:426:PRO:CD	2.26	0.48
1:C:575:MET:HE1	2:C:3402:ERY:H351	1.94	0.48
1:C:590:VAL:O	1:C:592:ASN:O	2.30	0.48
1:C:975:ILE:HG21	1:C:1019:ILE:HD13	1.95	0.48
1:A:173:GLY:N	1:A:293:LEU:O	2.43	0.48
1:A:316:PHE:CD2	1:A:316:PHE:N	2.82	0.48
1:A:467:TYR:CE1	1:A:925:VAL:HG13	2.47	0.48
1:A:649:MET:HA	1:A:653:ARG:HH22	1.76	0.48
1:B:776:GLU:HG2	1:B:777:ALA:N	2.28	0.48
1:C:792:ARG:HB2	1:C:798:MET:HE1	1.95	0.48
1:C:1032:ARG:HB3	1:C:1032:ARG:NH2	2.29	0.48
1:A:295:THR:HG22	1:A:295:THR:O	2.13	0.48
1:A:620:ARG:HG2	1:A:620:ARG:NH1	2.27	0.48
1:A:897:ILE:N	1:A:898:PRO:HD2	2.27	0.48
1:B:777:ALA:O	1:B:781:MET:HE2	2.14	0.48
1:B:946:VAL:HG21	1:B:1026:PHE:CE2	2.48	0.48
1:C:577:GLN:HE21	1:C:577:GLN:H	1.60	0.48
1:C:750:LEU:HD23	1:C:754:TRP:CD1	2.49	0.48
1:A:52:ALA:HB3	1:A:86:GLY:HA2	1.95	0.48
1:A:57:VAL:HG12	1:A:82:SER:HB3	1.96	0.48
1:A:660:ASP:O	1:A:661:ALA:HB2	2.12	0.48
1:A:947:GLU:O	1:A:951:ASP:HB2	2.13	0.48
1:C:681:ASP:HB2	1:C:860:THR:HG23	1.94	0.48
1:A:45:ILE:HG23	1:A:129:VAL:CG2	2.43	0.48
1:A:635:ALA:C	1:A:637:ARG:H	2.22	0.48
1:A:781:MET:HE3	1:C:228:GLN:CD	2.33	0.48
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.93	0.48
1:B:219:LEU:CD1	1:B:234:ILE:HG12	2.44	0.48
1:B:420:MET:HG2	1:B:426:PRO:HD3	1.95	0.48
1:B:744:ASN:O	1:B:748:THR:N	2.40	0.48
1:B:989:LEU:HD13	1:B:1000:GLN:O	2.13	0.48
1:C:911:GLY:CA	1:C:1010:GLY:HA2	2.43	0.48
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.76	0.48
1:A:210:GLN:CG	1:A:249:ILE:HG23	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:PHE:CZ	1:A:807:SER:HB3	2.49	0.48
1:A:991:ILE:O	1:A:992:SER:CB	2.61	0.48
1:B:448:VAL:O	1:B:452:VAL:HG23	2.13	0.48
1:B:453:PHE:CE2	1:B:474:ILE:HG21	2.48	0.48
1:B:616:GLY:HA3	1:B:624:THR:HG22	1.95	0.48
1:B:913:LEU:O	1:B:917:THR:CB	2.62	0.48
1:C:114:ALA:HA	1:C:117:LEU:HD12	1.95	0.48
1:C:191:ASN:O	1:C:192:GLU:C	2.56	0.48
1:C:204:ILE:HG22	1:C:205:THR:N	2.28	0.48
1:C:313:MET:O	1:C:317:PHE:CE1	2.66	0.48
1:C:637:ARG:CB	1:C:642:ASN:HB3	2.44	0.48
1:C:889:ALA:HB2	1:C:898:PRO:HG3	1.94	0.48
1:A:194:ASN:ND2	1:A:790:TYR:CD2	2.82	0.48
1:A:425:LEU:HB3	1:A:426:PRO:HD2	1.95	0.48
1:A:471:SER:O	1:A:475:VAL:CG1	2.59	0.48
1:B:55:LYS:CE	1:B:59:ASP:OD1	2.61	0.48
1:B:111:LEU:HD22	1:B:129:VAL:HG23	1.96	0.48
1:B:717:ARG:CD	1:B:717:ARG:N	2.77	0.48
1:C:188:MET:HA	1:C:266:ALA:HB2	1.96	0.48
1:C:353:LEU:C	1:C:355:MET:N	2.72	0.48
1:C:577:GLN:HA	1:C:624:THR:HA	1.96	0.48
1:C:586:ARG:O	1:C:590:VAL:HG23	2.14	0.48
1:C:896:SER:C	1:C:898:PRO:HD2	2.38	0.48
1:A:527:TYR:HE2	1:A:972:LEU:HG	1.78	0.48
1:A:733:GLN:HE22	1:A:743:ILE:HD12	1.78	0.48
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.44	0.48
1:A:225:VAL:O	1:A:226:LYS:C	2.56	0.48
1:A:896:SER:OG	1:A:897:ILE:N	2.47	0.48
1:B:115:MET:HA	1:B:115:MET:HE2	1.96	0.48
1:B:306:ILE:HG23	1:B:310:LEU:HD12	1.96	0.48
1:B:364:ALA:HB2	1:B:497:LEU:HG	1.94	0.48
1:B:524:THR:O	1:B:528:THR:N	2.40	0.48
1:C:255:GLN:C	1:C:257:GLY:N	2.71	0.48
1:C:367:ILE:HD13	1:C:492:LEU:HD22	1.95	0.48
1:C:527:TYR:CZ	1:C:1019:ILE:HG13	2.49	0.48
1:C:655:PHE:HB3	1:C:663:VAL:HG23	1.95	0.48
1:A:367:ILE:HA	1:A:370:ILE:HG22	1.96	0.48
1:B:188:MET:HB3	1:B:789:TRP:HH2	1.79	0.48
1:B:242:SER:C	1:B:244:GLU:N	2.72	0.48
1:B:640:GLU:H	1:B:643:LYS:HG2	1.79	0.48
1:B:940:LYS:HA	1:B:943:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:HD21	1:B:148:THR:N	2.10	0.47
1:B:372:VAL:HG13	1:B:405:LEU:HD21	1.96	0.47
1:B:452:VAL:HG11	1:B:932:LEU:O	2.14	0.47
1:C:33:ALA:HA	1:C:300:LEU:HD12	1.96	0.47
1:C:223:PRO:HA	1:C:224:PRO:HD3	1.75	0.47
1:C:824:SER:OG	1:C:825:MET:N	2.47	0.47
1:C:982:PHE:O	1:C:984:LEU:N	2.47	0.47
1:A:238:THR:OG1	1:A:239:ARG:N	2.47	0.47
1:A:298:ASN:C	1:A:300:LEU:H	2.22	0.47
1:A:449:LEU:O	1:A:453:PHE:HD1	1.97	0.47
1:A:685:ILE:HG22	1:A:686:ASP:N	2.29	0.47
1:A:901:VAL:HA	1:A:942:ALA:HB1	1.97	0.47
1:A:911:GLY:HA2	1:A:914:LEU:HB2	1.96	0.47
1:A:964:THR:HG21	1:A:1027:VAL:HG23	1.96	0.47
1:B:688:ALA:O	1:B:690:LEU:N	2.46	0.47
1:B:778:LYS:C	1:B:780:ARG:H	2.22	0.47
1:C:349:ILE:HG23	1:C:349:ILE:O	2.13	0.47
1:C:655:PHE:C	1:C:657:GLN:N	2.67	0.47
1:C:901:VAL:O	1:C:904:VAL:HG23	2.14	0.47
1:A:72:ILE:HD13	1:A:107:VAL:HA	1.95	0.47
1:B:350:LEU:O	1:B:984:LEU:HB3	2.13	0.47
1:B:713:LEU:HD13	1:B:843:LEU:HD13	1.95	0.47
1:C:941:ASN:HD22	1:C:941:ASN:C	2.23	0.47
1:A:189:ASN:ND2	1:A:779:TYR:OH	2.47	0.47
1:B:143:ILE:CD1	1:B:285:PRO:O	2.60	0.47
1:B:225:VAL:HG22	1:C:781:MET:HE3	1.95	0.47
1:B:542:LEU:HD11	1:B:1028:VAL:HG21	1.95	0.47
1:C:291:ILE:HD13	1:C:306:ILE:HD12	1.95	0.47
1:C:317:PHE:CD2	1:C:321:LEU:HD12	2.49	0.47
1:A:112:GLN:HE22	1:C:112:GLN:HG2	1.80	0.47
1:A:211:ASN:HB3	1:A:760:ASN:HD21	1.80	0.47
1:B:372:VAL:HB	1:B:373:PRO:CD	2.40	0.47
1:B:578:LEU:N	1:B:578:LEU:HD23	2.29	0.47
1:B:650:ARG:O	1:B:654:ALA:N	2.44	0.47
1:C:594:VAL:HG13	1:C:598:TYR:CE1	2.48	0.47
1:C:633:ASP:O	1:C:634:TRP:HB2	2.14	0.47
1:C:973:ARG:HG2	1:C:977:MET:HE3	1.96	0.47
1:A:206:ALA:C	1:A:208:LYS:N	2.73	0.47
1:A:894:SER:C	1:A:896:SER:H	2.20	0.47
1:B:463:THR:HA	1:B:466:ILE:HD12	1.97	0.47
1:B:843:LEU:HD23	1:B:847:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ASP:O	1:C:203:VAL:C	2.58	0.47
1:C:431:THR:O	1:C:434:SER:HB2	2.14	0.47
1:C:596:HIS:O	1:C:597:TYR:C	2.57	0.47
1:C:933:THR:O	1:C:937:LEU:HB2	2.14	0.47
1:A:250:LEU:CD2	1:A:259:ARG:HD2	2.45	0.47
1:A:542:LEU:HD23	1:A:1028:VAL:HG21	1.96	0.47
1:A:901:VAL:HG13	1:A:942:ALA:HB3	1.97	0.47
1:A:1021:PHE:CD1	1:A:1025:PHE:HE1	2.32	0.47
1:B:631:LEU:HB3	1:B:637:ARG:NH1	2.19	0.47
1:B:805:SER:OG	1:B:806:SER:N	2.47	0.47
1:C:4:PHE:O	1:C:8:ARG:NH1	2.48	0.47
1:C:34:GLN:NE2	1:C:299:ALA:HB3	2.11	0.47
1:C:62:THR:OG1	1:C:88:VAL:HG13	2.14	0.47
1:C:115:MET:HA	1:C:115:MET:HE2	1.97	0.47
1:A:69:MET:CE	1:A:107:VAL:HG13	2.44	0.47
1:A:198:LEU:HD22	1:A:202:ASP:HB3	1.96	0.47
1:A:636:ASP:OD2	1:A:636:ASP:N	2.48	0.47
1:A:655:PHE:O	1:A:657:GLN:N	2.43	0.47
1:A:726:GLN:NE2	1:C:235:ILE:HG13	2.30	0.47
1:A:961:ILE:O	1:A:965:LEU:HD23	2.15	0.47
1:B:314:GLU:N	1:B:315:PRO:CD	2.77	0.47
1:B:490:PRO:O	1:B:493:CYS:N	2.48	0.47
1:B:1022:VAL:HG23	1:B:1023:PRO:CD	2.44	0.47
1:C:9:PRO:C	1:C:11:PHE:H	2.21	0.47
1:C:655:PHE:O	1:C:657:GLN:N	2.48	0.47
1:A:108:GLN:HG3	1:B:112:GLN:OE1	2.15	0.47
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.95	0.47
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.96	0.47
1:A:780:ARG:O	1:A:780:ARG:HD2	2.14	0.47
1:B:45:ILE:HD13	1:B:65:ILE:CG2	2.45	0.47
1:B:445:ILE:HD12	1:B:940:LYS:CG	2.44	0.47
1:B:592:ASN:HA	1:B:595:THR:CG2	2.45	0.47
1:B:602:GLU:C	1:B:604:ASN:N	2.73	0.47
1:C:882:ILE:O	1:C:882:ILE:CG2	2.63	0.47
1:C:958:LYS:HB3	1:C:962:GLU:HB2	1.96	0.47
1:A:671:ILE:HG13	1:A:674:LEU:CB	2.45	0.47
1:B:262:LEU:C	1:B:264:ASP:N	2.72	0.47
1:B:946:VAL:C	1:B:948:PHE:H	2.22	0.47
1:C:353:LEU:O	1:C:355:MET:N	2.48	0.47
1:C:466:ILE:HG13	1:C:563:PHE:CZ	2.50	0.47
1:C:615:PHE:HE2	2:C:3402:ERY:H341	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:912:ALA:HB1	1:C:927:PHE:CE1	2.50	0.47
1:A:104:GLN:OE1	1:A:131:LYS:HG3	2.15	0.46
1:A:609:VAL:HG23	1:A:609:VAL:O	2.15	0.46
1:A:692:HIS:C	1:A:694:LYS:H	2.23	0.46
1:B:356:TYR:O	1:B:358:PHE:N	2.35	0.46
1:B:1031:ARG:HD2	1:B:1035:ARG:HH21	1.80	0.46
1:C:120:GLN:O	1:C:124:GLN:HG2	2.15	0.46
1:A:41:PRO:HD3	1:A:96:SER:O	2.15	0.46
1:B:23:GLY:H	1:B:381:ALA:HB2	1.79	0.46
1:B:194:ASN:HB2	1:B:790:TYR:HB2	1.96	0.46
1:B:326:PRO:HB3	1:B:610:PHE:HB2	1.97	0.46
1:B:452:VAL:O	1:B:453:PHE:CB	2.63	0.46
1:B:671:ILE:HB	1:B:672:VAL:H	1.50	0.46
1:B:681:ASP:CB	1:B:860:THR:CG2	2.93	0.46
1:C:34:GLN:HG2	1:C:35:TYR:H	1.79	0.46
1:A:261:LEU:HD13	1:A:263:ARG:HH11	1.79	0.46
1:A:376:LEU:O	1:A:378:GLY:N	2.39	0.46
1:B:200:PRO:HA	1:B:203:VAL:HG23	1.97	0.46
1:B:356:TYR:O	1:B:360:GLN:HG2	2.15	0.46
1:B:669:PRO:HB2	1:B:862:MET:SD	2.55	0.46
1:B:671:ILE:C	1:B:673:GLU:N	2.69	0.46
1:B:848:ALA:O	1:B:850:LYS:N	2.39	0.46
1:B:937:LEU:O	1:B:940:LYS:HB3	2.16	0.46
1:A:191:ASN:C	1:A:193:LEU:H	2.23	0.46
1:B:121:GLU:H	1:B:121:GLU:HG2	1.59	0.46
1:B:213:GLN:CB	1:B:239:ARG:HD2	2.43	0.46
1:C:379:THR:HB	1:C:398:MET:HE3	1.98	0.46
1:C:615:PHE:C	1:C:615:PHE:HD2	2.21	0.46
1:A:231:ASN:CB	1:B:622:GLN:HE22	2.28	0.46
1:A:316:PHE:N	1:A:316:PHE:HD2	2.14	0.46
1:A:395:MET:HA	1:A:395:MET:CE	2.40	0.46
1:A:890:ALA:HB1	1:C:11:PHE:HA	1.97	0.46
1:B:69:MET:HB3	1:B:92:LEU:HD11	1.96	0.46
1:B:355:MET:HE2	1:B:410:ILE:HD11	1.97	0.46
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.50	0.46
1:C:578:LEU:HD22	1:C:661:ALA:HB2	1.97	0.46
1:C:743:ILE:HA	1:C:746:ILE:HD12	1.97	0.46
1:C:912:ALA:HB1	1:C:927:PHE:HE1	1.80	0.46
1:A:1015:THR:C	1:A:1017:LEU:H	2.23	0.46
1:A:1022:VAL:HA	1:A:1025:PHE:CD1	2.50	0.46
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.98	0.46
1:B:408:ASP:OD2	1:B:445:ILE:HB	2.16	0.46
1:B:416:VAL:HG22	1:B:431:THR:HA	1.96	0.46
1:B:785:ASP:O	1:B:786:ILE:C	2.59	0.46
1:C:527:TYR:CE2	1:C:968:VAL:O	2.67	0.46
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.51	0.46
1:A:249:ILE:HB	1:A:262:LEU:HB2	1.98	0.46
1:A:426:PRO:CB	1:A:427:PRO:CD	2.94	0.46
1:A:444:GLY:HA3	1:A:891:LEU:HD22	1.97	0.46
1:A:516:PHE:CG	1:A:517:ASN:N	2.82	0.46
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.98	0.46
1:A:652:THR:HB	1:A:653:ARG:HH21	1.81	0.46
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.97	0.46
1:B:183:ALA:CB	1:B:273:GLU:HB3	2.45	0.46
1:B:398:MET:HG3	1:B:473:THR:CG2	2.46	0.46
1:B:729:ILE:CG1	1:B:730:ASP:N	2.79	0.46
1:C:49:TYR:N	1:C:122:VAL:HG23	2.31	0.46
1:C:563:PHE:CE2	1:C:564:LEU:HD12	2.51	0.46
1:C:680:PHE:CE1	1:C:844:MET:HE3	2.39	0.46
1:A:240:LEU:N	1:A:240:LEU:CD1	2.79	0.46
1:A:953:MET:HE3	1:A:963:ALA:HB3	1.97	0.46
1:B:45:ILE:HG12	1:B:129:VAL:HG22	1.97	0.46
1:C:298:ASN:O	1:C:299:ALA:C	2.58	0.46
1:C:346:GLU:O	1:C:350:LEU:HB2	2.16	0.46
1:C:683:GLU:HG3	1:C:819:TYR:CD2	2.51	0.46
1:C:1016:VAL:O	1:C:1018:ALA:N	2.42	0.46
1:B:13:TRP:CD1	1:C:895:TRP:HZ2	2.33	0.46
1:B:84:SER:HB3	1:B:814:PRO:HA	1.98	0.46
1:B:151:GLN:NE2	1:B:279:ALA:H	2.14	0.46
1:B:833:PRO:O	1:B:835:LYS:N	2.49	0.46
1:B:919:ARG:NH2	1:B:990:VAL:O	2.46	0.46
1:C:102:ILE:O	1:C:105:VAL:N	2.49	0.46
1:C:164:ASP:O	1:C:167:SER:HB2	2.16	0.46
1:C:592:ASN:HA	1:C:595:THR:OG1	2.16	0.46
1:C:878:ALA:C	1:C:880:SER:H	2.24	0.46
1:A:671:ILE:HG13	1:A:674:LEU:HB3	1.96	0.46
1:B:36:PRO:HD3	1:B:391:ASN:HD21	1.77	0.46
1:B:418:ARG:HB3	1:B:418:ARG:NH1	2.31	0.46
1:C:220:GLY:H	1:C:231:ASN:HD22	1.64	0.46
1:C:348:ILE:HG13	1:C:349:ILE:N	2.31	0.46
1:A:317:PHE:HB3	1:A:321:LEU:CB	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:O	1:A:356:TYR:N	2.48	0.45
1:A:391:ASN:H	1:A:394:THR:HG22	1.80	0.45
1:A:568:ASP:CG	1:A:637:ARG:HH12	2.24	0.45
1:B:414:GLU:OE2	1:B:974:PRO:HD3	2.16	0.45
1:B:464:GLY:O	1:B:468:ARG:HD3	2.16	0.45
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.98	0.45
1:C:357:LEU:HD23	1:C:358:PHE:CE2	2.51	0.45
1:C:367:ILE:HG21	1:C:497:LEU:HD23	1.98	0.45
1:A:189:ASN:ND2	1:A:779:TYR:CZ	2.84	0.45
1:A:228:GLN:O	1:B:583:THR:HG21	2.16	0.45
1:A:682:PHE:HE2	1:A:684:LEU:HD12	1.82	0.45
1:B:197:GLN:O	1:B:792:ARG:NH2	2.50	0.45
1:B:282:ASN:C	1:B:284:GLN:H	2.23	0.45
1:B:298:ASN:O	1:B:299:ALA:C	2.58	0.45
1:B:843:LEU:HD23	1:B:847:LEU:CD2	2.46	0.45
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.95	0.45
1:B:935:ILE:O	1:B:935:ILE:HG22	2.17	0.45
1:B:984:LEU:HA	1:B:987:MET:HB2	1.97	0.45
1:C:3:ASN:O	1:C:5:PHE:N	2.45	0.45
1:C:54:ALA:HB2	1:C:84:SER:CA	2.46	0.45
1:C:91:THR:HG21	2:C:3402:ERY:H272	1.98	0.45
1:C:330:THR:N	1:C:331:PRO:CD	2.79	0.45
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.41	0.45
1:C:898:PRO:HG2	1:C:899:PHE:CD1	2.51	0.45
1:A:307:ARG:NH2	1:A:328:ASP:OD2	2.49	0.45
1:A:579:PRO:O	1:A:580:ALA:C	2.59	0.45
1:A:1007:VAL:O	1:A:1008:MET:C	2.59	0.45
1:B:15:ILE:O	1:B:19:ILE:HG12	2.17	0.45
1:C:351:VAL:HG13	1:C:369:THR:HG22	1.99	0.45
1:C:373:PRO:O	1:C:377:LEU:HB2	2.15	0.45
1:C:733:GLN:OE1	1:C:733:GLN:HA	2.16	0.45
1:A:199:THR:HG22	1:A:791:VAL:HA	1.96	0.45
1:A:447:MET:CB	1:A:887:CYS:SG	2.91	0.45
1:B:198:LEU:HD23	1:B:792:ARG:HH22	1.81	0.45
1:B:639:GLY:HA2	1:B:643:LYS:NZ	2.31	0.45
1:B:938:SER:C	1:B:940:LYS:H	2.24	0.45
1:C:176:GLN:HE21	1:C:620:ARG:NH1	2.11	0.45
1:C:408:ASP:OD2	1:C:940:LYS:NZ	2.46	0.45
1:C:801:PHE:CD1	1:C:804:PHE:HE1	2.35	0.45
1:C:1015:THR:O	1:C:1019:ILE:HB	2.17	0.45
2:C:3402:ERY:H343	2:C:3402:ERY:H353	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:CD	1:A:763:ILE:HG13	2.47	0.45
1:A:714:THR:H	1:A:832:ALA:HB2	1.80	0.45
1:B:383:LEU:O	1:B:384:ALA:C	2.59	0.45
1:C:54:ALA:HB2	1:C:84:SER:CB	2.46	0.45
1:C:937:LEU:HD12	1:C:937:LEU:HA	1.88	0.45
1:A:216:ALA:O	1:A:217:GLY:O	2.35	0.45
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.52	0.45
1:A:800:PRO:O	1:A:803:ALA:HB3	2.17	0.45
1:A:901:VAL:HG13	1:A:942:ALA:CB	2.46	0.45
1:A:909:VAL:O	1:A:913:LEU:HD23	2.17	0.45
1:B:327:TYR:CG	1:B:327:TYR:O	2.70	0.45
1:B:671:ILE:C	1:B:673:GLU:H	2.25	0.45
1:C:6:ILE:O	1:C:9:PRO:HD3	2.16	0.45
1:C:27:ILE:HD11	1:C:380:PHE:CE2	2.52	0.45
1:C:251:LEU:CD1	1:C:262:LEU:HA	2.47	0.45
1:A:180:SER:O	1:A:181:GLN:CB	2.63	0.45
1:A:489:THR:HG22	1:A:490:PRO:HD3	1.98	0.45
1:A:708:LYS:C	1:A:709:HIS:HD2	2.24	0.45
1:B:6:ILE:HD11	1:B:490:PRO:HB2	1.98	0.45
1:B:409:ALA:HA	1:B:485:ALA:CB	2.47	0.45
1:B:934:THR:HA	1:B:937:LEU:HB2	1.98	0.45
1:C:314:GLU:N	1:C:315:PRO:HD2	2.32	0.45
1:C:463:THR:HA	1:C:466:ILE:CG1	2.46	0.45
1:C:734:GLU:HA	1:C:737:GLN:CG	2.46	0.45
1:C:736:ALA:C	1:C:738:ALA:N	2.75	0.45
1:C:801:PHE:O	1:C:803:ALA:N	2.38	0.45
1:C:986:VAL:O	1:C:986:VAL:CG1	2.64	0.45
1:A:974:PRO:C	1:A:976:LEU:N	2.75	0.45
1:B:27:ILE:HG22	1:B:380:PHE:CD2	2.51	0.45
1:B:399:VAL:O	1:B:402:ILE:CG2	2.59	0.45
1:B:892:TYR:OH	1:B:947:GLU:HB2	2.17	0.45
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.16	0.45
1:C:474:ILE:HG22	1:C:475:VAL:N	2.30	0.45
1:A:20:MET:O	1:A:21:LEU:C	2.59	0.45
1:A:200:PRO:HG2	1:A:749:THR:HG23	1.98	0.45
1:A:240:LEU:CD1	1:A:240:LEU:H	2.30	0.45
1:A:250:LEU:HD23	1:A:259:ARG:HD2	1.99	0.45
1:A:421:ALA:C	1:A:423:GLU:H	2.25	0.45
1:A:735:LYS:O	1:A:739:LEU:HD22	2.15	0.45
1:A:949:ALA:O	1:A:953:MET:HB2	2.16	0.45
1:B:57:VAL:HG12	1:B:82:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:HD12	1:B:288:GLY:O	2.17	0.45
1:B:232:ALA:HB1	1:C:725:PRO:O	2.17	0.45
1:B:306:ILE:CG2	1:B:310:LEU:HD12	2.47	0.45
1:B:343:THR:HA	1:B:346:GLU:HG2	1.99	0.45
1:B:356:TYR:C	1:B:358:PHE:N	2.75	0.45
1:C:176:GLN:NE2	1:C:620:ARG:HH12	2.09	0.45
1:C:672:VAL:HG13	1:C:673:GLU:H	1.77	0.45
1:A:61:VAL:HG21	1:A:122:VAL:HG21	1.98	0.45
1:A:596:HIS:O	1:A:597:TYR:C	2.58	0.45
1:B:356:TYR:O	1:B:360:GLN:N	2.50	0.45
1:B:358:PHE:CD1	1:B:977:MET:HB3	2.51	0.45
1:B:420:MET:SD	1:B:425:LEU:HA	2.57	0.45
1:B:484:VAL:HG12	1:B:489:THR:OG1	2.16	0.45
1:B:525:HIS:HA	1:B:528:THR:CG2	2.47	0.45
1:B:564:LEU:HG	1:B:925:VAL:HG11	1.98	0.45
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.52	0.45
1:C:491:ALA:C	1:C:493:CYS:H	2.24	0.45
1:C:528:THR:CG2	1:C:969:ARG:HG3	2.47	0.45
1:A:66:GLU:OE2	1:A:821:GLY:HA2	2.17	0.44
1:A:197:GLN:HA	1:A:798:MET:SD	2.57	0.44
1:A:367:ILE:CG1	1:A:368:PRO:HD3	2.46	0.44
1:B:230:LEU:HD21	1:C:809:TRP:CH2	2.53	0.44
1:C:463:THR:C	1:C:465:ALA:N	2.73	0.44
1:C:653:ARG:HG3	1:C:654:ALA:N	2.32	0.44
1:C:684:LEU:HD21	1:C:699:ARG:HA	1.99	0.44
1:C:721:LEU:CD1	1:C:825:MET:HE2	2.48	0.44
1:C:838:GLY:O	1:C:842:GLU:HB2	2.17	0.44
1:A:165:ALA:O	1:A:169:THR:HG23	2.17	0.44
1:A:527:TYR:C	1:A:529:ASP:N	2.74	0.44
1:A:594:VAL:O	1:A:595:THR:C	2.59	0.44
1:B:57:VAL:HG12	1:B:58:GLN:N	2.31	0.44
1:B:111:LEU:O	1:B:113:LEU:N	2.51	0.44
1:B:680:PHE:CD1	1:B:859:TRP:CZ3	3.05	0.44
1:B:712:MET:HA	1:B:834:GLY:CA	2.47	0.44
1:B:717:ARG:N	1:B:717:ARG:HD3	2.31	0.44
1:B:919:ARG:HG3	1:B:920:GLY:H	1.82	0.44
1:C:57:VAL:CG1	1:C:88:VAL:HG22	2.46	0.44
1:C:69:MET:CG	1:C:92:LEU:HD21	2.47	0.44
1:C:350:LEU:HD23	1:C:350:LEU:O	2.17	0.44
1:C:367:ILE:CD1	1:C:492:LEU:HD22	2.48	0.44
1:C:452:VAL:HG11	1:C:935:ILE:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:767:ARG:CG	1:C:767:ARG:NH1	2.77	0.44
1:A:355:MET:HB3	1:A:365:THR:HG22	2.00	0.44
1:B:343:THR:O	1:B:347:ALA:HB2	2.17	0.44
1:C:5:PHE:HD2	1:C:12:ALA:HB2	1.81	0.44
1:C:44:THR:HB	1:C:91:THR:HB	1.99	0.44
1:C:111:LEU:HD13	1:C:115:MET:HE3	2.00	0.44
1:C:191:ASN:O	1:C:194:ASN:N	2.48	0.44
1:C:428:LYS:O	1:C:428:LYS:HG2	2.17	0.44
1:A:96:SER:OG	1:A:97:GLY:N	2.48	0.44
1:A:207:ILE:CB	1:A:759:VAL:HG11	2.46	0.44
1:A:415:ASN:O	1:A:434:SER:HB2	2.17	0.44
1:B:34:GLN:OE1	1:B:35:TYR:CD1	2.71	0.44
1:B:35:TYR:HB3	1:B:38:ILE:HG13	1.99	0.44
1:B:87:THR:HG21	1:B:620:ARG:CZ	2.47	0.44
1:C:330:THR:N	1:C:331:PRO:HD2	2.33	0.44
1:C:467:TYR:OH	1:C:925:VAL:HG12	2.17	0.44
1:C:763:ILE:HD12	1:C:763:ILE:N	2.33	0.44
1:A:324:VAL:HG12	1:A:325:TYR:N	2.33	0.44
1:A:552:MET:HB2	1:A:910:ILE:HG23	1.99	0.44
1:B:778:LYS:C	1:B:780:ARG:N	2.75	0.44
1:B:945:ILE:HG13	1:B:946:VAL:HG23	2.00	0.44
1:B:972:LEU:N	1:B:974:PRO:HD2	2.32	0.44
1:C:72:ILE:HB	1:C:75:LEU:HD12	2.00	0.44
1:C:156:ASP:CG	1:C:182:TYR:CD2	2.96	0.44
1:C:189:ASN:C	1:C:189:ASN:HD22	2.26	0.44
1:C:544:LEU:O	1:C:548:ILE:HG13	2.17	0.44
1:C:830:GLN:OE1	1:C:832:ALA:HA	2.18	0.44
1:C:912:ALA:N	1:C:1010:GLY:HA2	2.33	0.44
1:A:355:MET:HG2	1:A:365:THR:HA	1.99	0.44
1:A:583:THR:O	1:A:587:THR:N	2.49	0.44
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.98	0.44
1:A:879:ILE:O	1:A:883:VAL:HG23	2.18	0.44
1:A:942:ALA:O	1:A:946:VAL:HB	2.17	0.44
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.99	0.44
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.99	0.44
1:C:449:LEU:HA	1:C:452:VAL:HG23	2.00	0.44
1:C:919:ARG:HG2	1:C:1005:THR:HG21	1.99	0.44
1:A:45:ILE:HD11	1:A:92:LEU:HD11	2.00	0.44
1:A:124:GLN:HG2	1:A:758:TYR:HE2	1.81	0.44
1:A:152:GLU:H	1:A:152:GLU:CD	2.25	0.44
1:A:682:PHE:HB2	1:A:859:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:ALA:C	1:B:709:HIS:H	2.25	0.44
1:B:859:TRP:HB3	1:B:863:SER:HB3	2.00	0.44
1:C:68:ASN:O	1:C:70:ASN:N	2.51	0.44
1:C:228:GLN:NE2	1:C:229:GLN:O	2.37	0.44
1:C:418:ARG:CD	1:C:970:MET:HE2	2.48	0.44
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.53	0.44
1:A:456:MET:HE3	1:A:471:SER:HB2	1.99	0.44
1:A:576:VAL:HG11	1:A:591:LEU:HD23	1.99	0.44
1:A:750:LEU:HD13	1:C:216:ALA:HB1	1.99	0.44
1:A:773:VAL:O	1:A:773:VAL:CG1	2.66	0.44
1:A:836:SER:O	1:A:837:THR:C	2.60	0.44
1:B:455:PRO:HG3	1:B:880:SER:HA	1.99	0.44
1:B:695:LEU:CD1	1:B:825:MET:HE3	2.47	0.44
1:B:897:ILE:O	1:B:901:VAL:HG23	2.18	0.44
1:C:467:TYR:O	1:C:470:PHE:N	2.51	0.44
1:C:684:LEU:HD22	1:C:702:LEU:HD23	2.00	0.44
1:C:885:PHE:CG	1:C:885:PHE:O	2.70	0.44
1:C:934:THR:C	1:C:936:GLY:H	2.25	0.44
1:A:353:LEU:C	1:A:354:VAL:O	2.59	0.44
1:A:375:VAL:O	1:A:379:THR:N	2.51	0.44
1:A:583:THR:HG22	1:A:585:GLU:H	1.82	0.44
1:A:634:TRP:CZ3	1:A:995:ALA:HA	2.52	0.44
1:B:151:GLN:O	1:B:153:ASP:N	2.43	0.44
1:C:210:GLN:HB2	1:C:249:ILE:HD12	1.99	0.44
1:C:564:LEU:HD13	1:C:671:ILE:HB	2.00	0.44
1:C:953:MET:HG3	1:C:963:ALA:HB2	2.00	0.44
2:C:3402:ERY:H321	2:C:3402:ERY:H8	1.78	0.44
1:A:515:TRP:O	1:A:516:PHE:HB2	2.18	0.43
1:A:552:MET:HE2	1:A:906:PRO:HA	1.97	0.43
1:A:993:THR:HG21	1:A:1000:GLN:OE1	2.18	0.43
1:B:78:MET:HE3	1:B:78:MET:HB2	1.91	0.43
1:B:111:LEU:HD22	1:B:129:VAL:HG21	1.99	0.43
1:B:404:LEU:C	1:B:406:VAL:N	2.76	0.43
1:B:560:PRO:CB	1:B:836:SER:HB2	2.42	0.43
1:B:574:THR:HA	1:B:665:ALA:HA	1.98	0.43
1:B:754:TRP:CH2	1:B:785:ASP:HB2	2.53	0.43
1:B:843:LEU:O	1:B:847:LEU:HD23	2.18	0.43
1:C:332:PHE:O	1:C:336:SER:HB2	2.17	0.43
1:C:897:ILE:N	1:C:898:PRO:CD	2.80	0.43
1:A:178:PHE:HB2	1:A:288:GLY:C	2.43	0.43
1:A:318:PRO:O	1:A:319:SER:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:ALA:O	1:B:705:GLU:HB3	2.17	0.43
1:B:864:TYR:CD1	1:B:864:TYR:C	2.96	0.43
1:B:950:LYS:O	1:B:954:ASP:HB3	2.18	0.43
1:C:181:GLN:HG2	1:C:769:LYS:HE2	2.00	0.43
1:C:255:GLN:O	1:C:256:ASP:C	2.60	0.43
1:C:395:MET:O	1:C:397:GLY:N	2.51	0.43
1:A:193:LEU:HD21	1:A:199:THR:HA	2.00	0.43
1:A:206:ALA:O	1:A:207:ILE:C	2.61	0.43
1:A:886:LEU:HD11	1:C:17:ILE:HB	1.99	0.43
1:B:14:VAL:O	1:B:15:ILE:C	2.61	0.43
1:B:26:ALA:HB1	1:B:384:ALA:HB2	2.00	0.43
1:B:262:LEU:O	1:B:265:VAL:N	2.51	0.43
1:B:293:LEU:HD22	1:B:294:ALA:N	2.33	0.43
1:B:355:MET:SD	1:B:369:THR:HG23	2.58	0.43
1:B:419:VAL:O	1:B:419:VAL:CG1	2.65	0.43
1:C:137:LEU:HD12	1:C:138:MET:HB3	2.01	0.43
1:C:145:THR:C	1:C:147:GLY:N	2.76	0.43
1:C:904:VAL:O	1:C:905:VAL:C	2.61	0.43
1:A:367:ILE:CD1	1:A:368:PRO:HD3	2.48	0.43
1:A:682:PHE:HD1	1:A:859:TRP:CH2	2.36	0.43
1:A:966:ASP:HA	1:A:969:ARG:HD2	1.99	0.43
1:B:25:LEU:O	1:B:28:LEU:HG	2.18	0.43
1:B:367:ILE:N	1:B:368:PRO:HD2	2.33	0.43
1:B:566:ASP:C	1:B:567:GLU:HG2	2.44	0.43
1:B:639:GLY:C	1:B:641:GLU:H	2.26	0.43
1:B:704:ALA:C	1:B:706:ALA:H	2.27	0.43
1:C:208:LYS:HA	1:C:760:ASN:ND2	2.32	0.43
1:C:314:GLU:N	1:C:315:PRO:CD	2.82	0.43
1:A:535:LEU:HB3	1:A:961:ILE:HD12	2.00	0.43
1:A:699:ARG:NH2	1:A:722:GLU:OE2	2.49	0.43
1:B:298:ASN:O	1:B:298:ASN:ND2	2.49	0.43
1:B:699:ARG:HB3	1:B:699:ARG:NH1	2.33	0.43
1:B:990:VAL:HG22	1:B:1004:GLY:C	2.43	0.43
1:C:72:ILE:HG22	1:C:94:PHE:HE2	1.83	0.43
1:C:80:SER:HA	1:C:90:ILE:HA	2.00	0.43
1:C:674:LEU:HD11	1:C:865:GLN:HB2	2.01	0.43
1:C:983:ILE:HD11	1:C:1011:MET:HG2	2.00	0.43
1:A:72:ILE:HG23	1:A:106:GLN:HB3	1.99	0.43
1:A:186:ILE:HG22	1:A:186:ILE:O	2.18	0.43
1:A:930:GLY:C	1:A:932:LEU:N	2.75	0.43
1:B:45:ILE:HD13	1:B:69:MET:HE3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ILE:HG22	1:B:350:LEU:HD23	2.00	0.43
1:B:901:VAL:HG22	1:B:1026:PHE:HZ	1.84	0.43
1:C:708:LYS:C	1:C:710:PRO:HD3	2.44	0.43
1:A:219:LEU:H	1:A:231:ASN:ND2	2.17	0.43
1:A:281:PHE:O	1:A:282:ASN:C	2.61	0.43
1:A:886:LEU:HD21	1:C:17:ILE:HG21	2.01	0.43
1:A:970:MET:O	1:A:971:ARG:HB2	2.19	0.43
1:B:58:GLN:C	1:B:60:THR:H	2.26	0.43
1:B:393:LEU:CB	1:B:469:GLN:HG2	2.49	0.43
1:B:651:ALA:HB1	1:B:655:PHE:CE2	2.53	0.43
1:B:964:THR:HG22	1:B:1023:PRO:HB3	2.01	0.43
1:C:77:TYR:N	1:C:77:TYR:CD2	2.87	0.43
1:C:84:SER:C	1:C:86:GLY:H	2.27	0.43
1:C:162:MET:HG2	1:C:313:MET:SD	2.59	0.43
1:C:214:VAL:HG23	1:C:236:ALA:HB3	2.00	0.43
1:A:997:SER:HB2	1:A:998:GLY:H	1.62	0.43
1:B:24:GLY:CA	1:B:27:ILE:HG23	2.48	0.43
1:B:219:LEU:HD12	1:B:234:ILE:HD11	2.00	0.43
1:B:961:ILE:O	1:B:965:LEU:HD23	2.18	0.43
1:B:967:ALA:O	1:B:969:ARG:N	2.52	0.43
1:C:34:GLN:CG	1:C:35:TYR:H	2.32	0.43
1:C:124:GLN:HB2	1:C:758:TYR:CE2	2.47	0.43
1:C:189:ASN:HA	1:C:190:PRO:HD3	1.84	0.43
1:C:199:THR:OG1	1:C:201:VAL:N	2.51	0.43
1:C:244:GLU:O	1:C:263:ARG:NH2	2.52	0.43
1:C:713:LEU:HD13	1:C:713:LEU:N	2.33	0.43
1:A:405:LEU:HD23	1:A:477:ALA:HB1	1.99	0.43
1:B:448:VAL:HG21	1:B:888:LEU:HD21	2.01	0.43
1:B:453:PHE:HA	1:B:456:MET:SD	2.59	0.43
1:B:566:ASP:O	1:B:567:GLU:HG2	2.18	0.43
1:B:1014:ALA:O	1:B:1018:ALA:HB2	2.19	0.43
1:A:575:MET:CE	1:A:577:GLN:HE21	2.29	0.43
1:A:584:GLN:H	1:A:622:GLN:HE21	1.66	0.43
1:A:1021:PHE:C	1:A:1023:PRO:HD2	2.43	0.43
1:B:226:LYS:HA	1:B:226:LYS:NZ	2.33	0.43
1:B:541:TYR:C	1:B:543:VAL:H	2.26	0.43
1:B:949:ALA:HB3	1:B:1030:ARG:HH22	1.84	0.43
1:C:605:ASN:CB	1:C:637:ARG:HD3	2.42	0.43
1:C:1016:VAL:C	1:C:1018:ALA:N	2.76	0.43
1:C:1030:ARG:HE	1:C:1030:ARG:HB3	1.52	0.43
1:A:53:ASP:O	1:A:54:ALA:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASN:HB3	1:A:192:GLU:HB2	2.00	0.42
1:A:199:THR:HG21	1:A:791:VAL:HA	2.00	0.42
1:A:457:ALA:O	1:A:458:PHE:HD2	2.02	0.42
1:A:536:ARG:H	1:A:536:ARG:HG2	1.56	0.42
1:B:118:LEU:O	1:B:119:PRO:C	2.62	0.42
1:B:240:LEU:HB3	1:B:245:GLU:HB2	2.00	0.42
1:B:520:PHE:O	1:B:523:SER:HB2	2.18	0.42
1:B:562:SER:O	1:B:924:ASP:HA	2.19	0.42
1:C:527:TYR:C	1:C:529:ASP:N	2.77	0.42
1:C:637:ARG:HB3	1:C:642:ASN:CB	2.48	0.42
1:A:146:ASP:OD2	1:A:146:ASP:N	2.52	0.42
1:A:364:ALA:O	1:A:367:ILE:HG13	2.20	0.42
1:A:961:ILE:HD11	1:A:1031:ARG:NH1	2.34	0.42
1:B:43:VAL:N	1:B:92:LEU:O	2.48	0.42
1:B:468:ARG:O	1:B:469:GLN:C	2.60	0.42
1:B:612:VAL:HG22	1:B:626:ILE:O	2.19	0.42
1:C:188:MET:HA	1:C:266:ALA:CB	2.49	0.42
1:C:204:ILE:O	1:C:205:THR:C	2.62	0.42
1:C:467:TYR:C	1:C:469:GLN:N	2.76	0.42
1:C:785:ASP:C	1:C:787:GLY:N	2.76	0.42
1:C:982:PHE:O	1:C:985:GLY:N	2.51	0.42
1:A:30:LEU:HD21	1:A:384:ALA:HB2	2.01	0.42
1:A:105:VAL:HG22	1:B:105:VAL:HG13	2.01	0.42
1:A:346:GLU:C	1:A:348:ILE:N	2.77	0.42
1:A:368:PRO:HA	1:A:371:ALA:HB3	2.00	0.42
1:A:843:LEU:O	1:A:846:GLN:N	2.51	0.42
1:A:876:LEU:HA	1:A:879:ILE:HD12	2.01	0.42
1:A:894:SER:HB2	1:A:896:SER:OG	2.19	0.42
1:C:641:GLU:CD	1:C:641:GLU:N	2.75	0.42
1:C:1008:MET:C	1:C:1010:GLY:H	2.27	0.42
1:A:35:TYR:CG	1:A:671:ILE:HG22	2.55	0.42
1:A:66:GLU:C	1:A:68:ASN:N	2.77	0.42
1:A:533:GLY:C	1:A:535:LEU:H	2.27	0.42
1:A:634:TRP:CD1	1:A:634:TRP:H	2.37	0.42
1:A:783:PRO:C	1:A:785:ASP:N	2.77	0.42
1:A:374:VAL:O	1:A:375:VAL:C	2.62	0.42
1:A:479:ALA:O	1:A:482:VAL:HG12	2.20	0.42
1:B:53:ASP:HB2	1:B:56:THR:OG1	2.20	0.42
1:B:58:GLN:O	1:B:59:ASP:HB2	2.19	0.42
1:B:95:GLU:O	1:B:96:SER:C	2.63	0.42
1:B:122:VAL:O	1:B:125:GLN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:TYR:CE1	1:B:1025:PHE:HZ	2.37	0.42
1:B:717:ARG:CG	1:B:717:ARG:NH1	2.73	0.42
1:C:165:ALA:O	1:C:169:THR:OG1	2.31	0.42
1:C:203:VAL:HG12	1:C:207:ILE:HD11	2.02	0.42
1:C:643:LYS:O	1:C:647:ILE:HG13	2.20	0.42
1:C:758:TYR:HD1	1:C:758:TYR:N	2.04	0.42
1:C:824:SER:O	1:C:825:MET:HB2	2.18	0.42
1:A:198:LEU:HD22	1:A:202:ASP:CB	2.50	0.42
1:A:354:VAL:HG12	1:A:355:MET:N	2.27	0.42
1:A:361:ASN:HB2	1:A:364:ALA:HB3	2.02	0.42
1:B:300:LEU:HD21	1:B:334:LYS:HG3	2.01	0.42
1:B:924:ASP:HB3	1:B:926:TYR:N	2.34	0.42
1:C:251:LEU:HD11	1:C:262:LEU:HA	2.01	0.42
1:C:324:VAL:O	1:C:326:PRO:HD2	2.20	0.42
1:B:380:PHE:O	1:B:383:LEU:N	2.53	0.42
1:B:697:GLN:O	1:B:699:ARG:O	2.38	0.42
1:B:733:GLN:HE22	1:B:743:ILE:CG2	2.32	0.42
1:C:534:ILE:H	1:C:534:ILE:HG13	1.74	0.42
1:C:545:TYR:CZ	1:C:1025:PHE:CZ	3.07	0.42
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.55	0.42
1:B:165:ALA:CB	1:B:313:MET:HE1	2.50	0.42
1:B:420:MET:SD	1:B:424:GLY:O	2.78	0.42
1:B:852:PRO:HB2	1:B:853:THR:H	1.52	0.42
1:B:1025:PHE:HA	1:B:1028:VAL:HG12	2.01	0.42
1:C:144:ASN:ND2	1:C:148:THR:N	2.67	0.42
1:C:334:LYS:O	1:C:335:ILE:C	2.62	0.42
1:C:379:THR:HB	1:C:398:MET:CE	2.50	0.42
1:C:415:ASN:O	1:C:419:VAL:HG22	2.19	0.42
1:C:818:ARG:HA	1:C:824:SER:N	2.33	0.42
1:C:905:VAL:HG22	1:C:935:ILE:HD11	2.02	0.42
1:A:282:ASN:HD21	1:A:609:VAL:H	1.68	0.42
1:A:323:ILE:HG12	1:A:325:TYR:HE1	1.85	0.42
1:A:889:ALA:HA	1:A:898:PRO:HG3	2.01	0.42
1:A:1029:VAL:O	1:A:1030:ARG:CB	2.67	0.42
1:B:3:ASN:C	1:B:4:PHE:O	2.58	0.42
1:B:452:VAL:HG12	1:B:932:LEU:HG	2.02	0.42
1:B:733:GLN:HE22	1:B:743:ILE:HG21	1.85	0.42
1:B:938:SER:C	1:B:940:LYS:N	2.78	0.42
1:B:959:GLY:O	1:B:960:LEU:C	2.63	0.42
1:B:986:VAL:HG23	1:B:1008:MET:HB2	2.00	0.42
1:B:1004:GLY:O	1:B:1006:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:PHE:HA	1:C:277:ILE:HG21	2.02	0.42
1:C:202:ASP:OD2	1:C:792:ARG:NH2	2.52	0.42
1:C:249:ILE:CG2	1:C:250:LEU:N	2.83	0.42
1:A:102:ILE:HA	1:A:105:VAL:HG23	2.02	0.42
1:A:412:VAL:O	1:A:416:VAL:HG23	2.20	0.42
1:A:978:THR:CG2	1:A:979:SER:N	2.83	0.42
1:B:20:MET:HG2	1:B:374:VAL:HA	2.02	0.42
1:B:136:PHE:HD1	1:B:136:PHE:H	1.65	0.42
1:B:150:THR:H	1:B:153:ASP:HB3	1.84	0.42
1:B:632:LYS:C	1:B:633:ASP:O	2.62	0.42
1:B:647:ILE:H	1:B:647:ILE:HG12	1.65	0.42
1:B:876:LEU:HD22	1:B:932:LEU:CD1	2.49	0.42
1:C:142:VAL:CG1	1:C:154:ILE:HG23	2.50	0.42
1:C:348:ILE:C	1:C:350:LEU:N	2.78	0.42
1:A:72:ILE:CD1	1:A:107:VAL:HA	2.50	0.41
1:A:446:ALA:HB2	1:A:482:VAL:HG21	2.01	0.41
1:A:682:PHE:C	1:A:682:PHE:CD2	2.98	0.41
1:B:57:VAL:HG21	1:B:86:GLY:HA2	2.01	0.41
1:B:151:GLN:HE22	1:B:278:ILE:HA	1.85	0.41
1:B:268:ILE:HD12	1:B:268:ILE:N	2.34	0.41
1:B:764:ASP:C	1:B:766:GLY:H	2.24	0.41
1:B:807:SER:C	1:B:808:ARG:HG3	2.45	0.41
1:B:924:ASP:HB3	1:B:926:TYR:H	1.84	0.41
1:C:248:LYS:HA	1:C:261:LEU:HD13	2.01	0.41
1:C:470:PHE:O	1:C:471:SER:C	2.63	0.41
1:C:680:PHE:CD2	1:C:680:PHE:N	2.88	0.41
1:C:739:LEU:HD12	1:C:739:LEU:HA	1.82	0.41
1:A:46:SER:HA	1:A:88:VAL:O	2.20	0.41
1:A:304:ALA:O	1:A:307:ARG:N	2.53	0.41
1:A:406:VAL:C	1:A:408:ASP:N	2.78	0.41
1:A:658:ILE:H	1:A:658:ILE:HG12	1.63	0.41
1:B:1008:MET:HE2	1:B:1008:MET:HB3	1.90	0.41
1:C:34:GLN:HB3	1:C:333:VAL:CG2	2.50	0.41
1:C:83:ASP:HA	1:C:815:ARG:HA	2.02	0.41
1:C:380:PHE:CE1	1:C:395:MET:HE1	2.55	0.41
1:C:450:SER:N	1:C:478:MET:HE1	2.35	0.41
1:C:615:PHE:CE2	2:C:3402:ERY:H341	2.55	0.41
1:A:119:PRO:C	1:A:121:GLU:H	2.28	0.41
1:A:901:VAL:HG11	1:A:943:ILE:HG13	2.01	0.41
1:B:9:PRO:HD2	1:C:893:GLU:OE1	2.20	0.41
1:B:23:GLY:C	1:B:25:LEU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ILE:HD11	1:B:118:LEU:HD21	2.02	0.41
1:B:572:PHE:HE2	1:B:631:LEU:HD21	1.84	0.41
1:B:602:GLU:OE2	1:B:650:ARG:NH2	2.54	0.41
1:B:613:ASN:HD22	1:B:613:ASN:C	2.26	0.41
1:B:696:THR:O	1:B:699:ARG:HB3	2.20	0.41
1:B:699:ARG:HG2	1:B:700:ASN:N	2.35	0.41
1:B:833:PRO:C	1:B:835:LYS:N	2.79	0.41
1:C:247:GLY:HA3	1:C:263:ARG:NE	2.35	0.41
1:C:303:ALA:O	1:C:304:ALA:C	2.63	0.41
1:A:31:PRO:HB2	1:A:389:SER:CB	2.48	0.41
1:A:193:LEU:HG	1:A:198:LEU:O	2.20	0.41
1:A:218:GLN:O	1:A:234:ILE:HD11	2.20	0.41
1:A:347:ALA:HA	1:A:350:LEU:HD23	2.02	0.41
1:A:533:GLY:C	1:A:534:ILE:HG13	2.45	0.41
1:A:892:TYR:CE1	1:A:947:GLU:OE2	2.73	0.41
1:A:943:ILE:O	1:A:947:GLU:HB2	2.20	0.41
1:B:218:GLN:HB2	1:B:232:ALA:O	2.20	0.41
1:B:782:LEU:HD23	1:B:782:LEU:H	1.84	0.41
1:B:845:GLU:HG3	1:B:857:TYR:OH	2.19	0.41
1:B:1021:PHE:O	1:B:1025:PHE:CD1	2.72	0.41
1:C:9:PRO:O	1:C:10:ILE:HB	2.20	0.41
1:C:111:LEU:CD1	1:C:115:MET:HE3	2.50	0.41
1:C:125:GLN:NE2	1:C:758:TYR:CZ	2.85	0.41
1:C:310:LEU:O	1:C:313:MET:HG2	2.20	0.41
1:C:545:TYR:CE1	1:C:1025:PHE:CZ	3.08	0.41
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.56	0.41
1:A:417:GLU:OE2	1:A:497:LEU:HD22	2.20	0.41
1:A:843:LEU:O	1:A:844:MET:C	2.62	0.41
1:B:14:VAL:HG21	1:C:886:LEU:O	2.21	0.41
1:B:219:LEU:HD13	1:B:234:ILE:HG12	2.02	0.41
1:B:355:MET:SD	1:B:368:PRO:HB2	2.60	0.41
1:B:696:THR:CG2	1:B:825:MET:HE1	2.50	0.41
1:B:911:GLY:HA3	1:B:1013:THR:CG2	2.49	0.41
1:C:137:LEU:CD1	1:C:138:MET:HB3	2.50	0.41
1:C:163:LYS:O	1:C:164:ASP:C	2.62	0.41
1:A:251:LEU:O	1:A:252:LYS:HB2	2.21	0.41
1:A:376:LEU:C	1:A:378:GLY:N	2.79	0.41
1:B:49:TYR:O	1:B:50:PRO:C	2.64	0.41
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.36	0.41
1:C:30:LEU:CD1	1:C:384:ALA:HB2	2.50	0.41
1:C:144:ASN:CB	1:C:154:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:ALA:HA	1:C:478:MET:HE3	2.02	0.41
1:C:602:GLU:O	1:C:604:ASN:N	2.54	0.41
1:A:239:ARG:HD3	1:A:763:ILE:HG13	2.03	0.41
1:B:61:VAL:HG23	1:B:118:LEU:HD23	2.03	0.41
1:B:330:THR:N	1:B:331:PRO:CD	2.84	0.41
1:B:420:MET:HG2	1:B:426:PRO:CD	2.50	0.41
1:C:5:PHE:CD2	1:C:12:ALA:HB2	2.55	0.41
1:C:206:ALA:O	1:C:207:ILE:C	2.64	0.41
1:C:226:LYS:HB3	1:C:227:GLY:H	1.74	0.41
1:C:413:VAL:O	1:C:413:VAL:HG22	2.20	0.41
1:C:431:THR:O	1:C:435:MET:HG2	2.21	0.41
1:C:463:THR:HG22	1:C:467:TYR:CD1	2.55	0.41
1:C:1017:LEU:HD23	1:C:1017:LEU:O	2.21	0.41
1:A:465:ALA:O	1:A:469:GLN:HG2	2.20	0.41
1:A:551:GLY:O	1:A:555:LEU:HB2	2.21	0.41
1:A:674:LEU:HD13	1:A:675:GLY:N	2.36	0.41
1:B:58:GLN:HB2	1:B:82:SER:HB3	2.02	0.41
1:B:189:ASN:HD22	1:B:190:PRO:HD2	1.85	0.41
1:B:851:LEU:N	1:B:852:PRO:HD3	2.35	0.41
1:C:9:PRO:C	1:C:11:PHE:N	2.79	0.41
1:C:164:ASP:CG	1:C:767:ARG:HH22	2.28	0.41
1:C:404:LEU:HD21	1:C:449:LEU:HD12	2.01	0.41
1:C:423:GLU:HB3	1:C:426:PRO:HG2	2.03	0.41
1:C:672:VAL:CG2	1:C:676:THR:H	2.31	0.41
1:A:294:ALA:HB3	1:A:297:ALA:CB	2.46	0.41
1:A:365:THR:O	1:A:368:PRO:HD2	2.21	0.41
1:A:644:VAL:O	1:A:645:GLU:C	2.64	0.41
1:A:701:GLN:O	1:A:702:LEU:C	2.62	0.41
1:B:18:ILE:HD12	1:C:886:LEU:HD13	2.02	0.41
1:B:46:SER:O	1:B:127:VAL:HA	2.20	0.41
1:B:57:VAL:CG1	1:B:82:SER:HB2	2.51	0.41
1:B:186:ILE:HB	1:B:773:VAL:HG23	2.02	0.41
1:B:239:ARG:NH2	1:B:761:ASP:HB2	2.36	0.41
1:B:262:LEU:O	1:B:266:ALA:N	2.44	0.41
1:B:462:SER:N	1:B:865:GLN:OE1	2.37	0.41
1:B:699:ARG:C	1:B:701:GLN:N	2.78	0.41
1:B:782:LEU:HB2	1:B:783:PRO:HD2	2.03	0.41
1:B:901:VAL:C	1:B:903:LEU:H	2.28	0.41
1:C:115:MET:CE	1:C:127:VAL:HG21	2.51	0.41
1:C:160:ALA:HA	1:C:767:ARG:NE	2.36	0.41
1:C:177:LEU:HD13	1:C:179:GLY:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:GLN:O	1:C:257:GLY:N	2.54	0.41
1:C:617:PHE:CZ	2:C:3402:ERY:H312	2.55	0.41
1:C:687:GLN:HE21	1:C:687:GLN:HB3	1.68	0.41
1:C:719:ASN:O	1:C:721:LEU:N	2.53	0.41
1:C:782:LEU:C	1:C:784:ASP:H	2.27	0.41
1:A:231:ASN:OD1	1:B:622:GLN:NE2	2.53	0.41
1:B:200:PRO:HD2	1:B:749:THR:CG2	2.51	0.41
1:B:213:GLN:CG	1:C:56:THR:CG2	2.96	0.41
1:B:310:LEU:HD22	1:B:323:ILE:HG21	2.03	0.41
1:C:251:LEU:HB2	1:C:260:VAL:O	2.20	0.41
1:C:961:ILE:O	1:C:961:ILE:HG22	2.20	0.41
1:A:53:ASP:HA	1:A:84:SER:HA	2.03	0.40
1:A:153:ASP:HA	1:A:182:TYR:CE1	2.56	0.40
1:A:438:ILE:O	1:A:439:GLN:C	2.65	0.40
1:A:456:MET:C	1:A:458:PHE:N	2.77	0.40
1:A:538:THR:HG23	1:A:540:ARG:NH2	2.37	0.40
1:A:904:VAL:HG12	1:A:938:SER:HB3	2.02	0.40
1:A:982:PHE:C	1:A:984:LEU:N	2.79	0.40
1:B:52:ALA:HB2	1:B:86:GLY:H	1.74	0.40
1:B:701:GLN:HE22	1:B:851:LEU:HB2	1.86	0.40
1:C:142:VAL:HG13	1:C:321:LEU:HD13	2.03	0.40
1:C:412:VAL:C	1:C:414:GLU:H	2.29	0.40
1:C:527:TYR:OH	1:C:968:VAL:CG1	2.69	0.40
1:C:655:PHE:HB3	1:C:663:VAL:HG21	2.03	0.40
1:A:62:THR:O	1:A:63:GLN:C	2.64	0.40
1:A:172:VAL:O	1:A:172:VAL:HG23	2.21	0.40
1:A:334:LYS:C	1:A:336:SER:H	2.29	0.40
1:A:695:LEU:HD23	1:A:825:MET:HE3	2.03	0.40
1:A:952:LEU:HD11	1:A:966:ASP:HB3	2.03	0.40
1:B:13:TRP:O	1:B:17:ILE:HG12	2.21	0.40
1:B:193:LEU:HD13	1:B:198:LEU:O	2.21	0.40
1:B:230:LEU:HD21	1:C:809:TRP:HH2	1.86	0.40
1:B:262:LEU:C	1:B:264:ASP:H	2.30	0.40
1:B:293:LEU:HD22	1:B:294:ALA:H	1.85	0.40
1:B:377:LEU:O	1:B:380:PHE:HB2	2.21	0.40
1:B:644:VAL:HA	1:B:647:ILE:HG13	2.03	0.40
1:C:945:ILE:C	1:C:947:GLU:N	2.79	0.40
1:A:184:MET:HB2	1:A:762:PHE:CE2	2.57	0.40
1:A:426:PRO:HB3	1:A:427:PRO:CD	2.51	0.40
1:A:686:ASP:OD1	1:A:690:LEU:HB2	2.21	0.40
1:B:115:MET:CE	1:B:127:VAL:HG21	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ILE:HD12	1:B:940:LYS:HG3	2.01	0.40
1:C:249:ILE:HG22	1:C:250:LEU:N	2.36	0.40
1:C:423:GLU:HB3	1:C:426:PRO:CD	2.49	0.40
1:C:944:LEU:O	1:C:971:ARG:HD2	2.20	0.40
1:C:1022:VAL:O	1:C:1022:VAL:HG22	2.21	0.40
1:A:61:VAL:O	1:A:62:THR:C	2.65	0.40
1:A:375:VAL:HG21	1:A:481:SER:HA	2.03	0.40
1:A:406:VAL:O	1:A:409:ALA:N	2.51	0.40
1:A:620:ARG:CG	1:A:620:ARG:NH1	2.78	0.40
1:A:897:ILE:O	1:A:900:SER:OG	2.29	0.40
1:B:158:VAL:HA	1:B:162:MET:HG3	2.00	0.40
1:B:231:ASN:ND2	1:B:232:ALA:N	2.70	0.40
1:B:443:VAL:O	1:B:447:MET:N	2.54	0.40
1:B:681:ASP:CB	1:B:860:THR:HG23	2.51	0.40
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.48	0.40
1:A:325:TYR:N	1:A:325:TYR:CD1	2.90	0.40
1:A:713:LEU:H	1:A:832:ALA:HB2	1.86	0.40
1:A:726:GLN:N	1:A:810:GLU:O	2.53	0.40
1:B:150:THR:HG22	1:B:151:GLN:H	1.86	0.40
1:B:231:ASN:HD22	1:B:232:ALA:N	2.20	0.40
1:B:240:LEU:HD13	1:B:245:GLU:HB3	2.02	0.40
1:B:240:LEU:HD22	1:B:245:GLU:HG2	2.03	0.40
1:B:416:VAL:HG21	1:B:431:THR:HG22	2.03	0.40
1:B:459:PHE:HB2	1:B:460:GLY:H	1.59	0.40
1:B:897:ILE:HA	1:B:900:SER:OG	2.21	0.40
1:B:935:ILE:HG12	1:B:935:ILE:H	1.58	0.40
1:C:33:ALA:HB2	1:C:298:ASN:ND2	2.36	0.40
1:C:343:THR:CG2	1:C:989:LEU:HD13	2.42	0.40
1:C:721:LEU:HD11	1:C:825:MET:HE2	2.04	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	1018/1053 (97%)	715 (70%)	198 (19%)	105 (10%)	0	2
1	B	1018/1053 (97%)	694 (68%)	214 (21%)	110 (11%)	0	2
1	C	1018/1053 (97%)	734 (72%)	207 (20%)	77 (8%)	1	6
All	All	3054/3159 (97%)	2143 (70%)	619 (20%)	292 (10%)	0	3

All (292) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	134	SER
1	A	160	ALA
1	A	170	SER
1	A	188	MET
1	A	212	ALA
1	A	256	ASP
1	A	293	LEU
1	A	319	SER
1	A	375	VAL
1	A	426	PRO
1	A	516	PHE
1	A	580	ALA
1	A	601	LYS
1	A	638	PRO
1	A	659	LYS
1	A	661	ALA
1	A	678	THR
1	A	775	SER
1	A	788	ASP
1	A	870	GLY
1	A	958	LYS
1	A	971	ARG
1	A	997	SER
1	A	998	GLY
1	A	1008	MET
1	B	2	PRO
1	B	54	ALA
1	B	69	MET
1	B	262	LEU
1	B	299	ALA
1	B	426	PRO
1	B	538	THR
1	B	580	ALA

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Mol	Chain	Res	Type
1	B	581	GLY
1	B	582	ALA
1	B	633	ASP
1	B	656	SER
1	B	671	ILE
1	B	676	THR
1	B	690	LEU
1	B	691	GLY
1	B	805	SER
1	B	806	SER
1	B	820	ASN
1	B	849	SER
1	B	893	GLU
1	B	918	PHE
1	B	921	LEU
1	B	935	ILE
1	B	1033	PHE
1	C	34	GLN
1	C	152	GLU
1	C	226	LYS
1	C	256	ASP
1	C	266	ALA
1	C	319	SER
1	C	427	PRO
1	C	633	ASP
1	C	673	GLU
1	C	713	LEU
1	C	720	GLY
1	C	806	SER
1	C	825	MET
1	C	832	ALA
1	C	836	SER
1	C	837	THR
1	C	921	LEU
1	C	958	LYS
1	C	965	LEU
1	A	64	VAL
1	A	181	GLN
1	A	213	GLN
1	A	217	GLY
1	A	220	GLY
1	A	221	GLY

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Mol	Chain	Res	Type
1	A	227	GLY
1	A	294	ALA
1	A	318	PRO
1	A	354	VAL
1	A	376	LEU
1	A	457	ALA
1	A	460	GLY
1	A	534	ILE
1	A	599	LEU
1	A	656	SER
1	A	670	ALA
1	A	675	GLY
1	A	784	ASP
1	A	787	GLY
1	A	917	THR
1	A	931	LEU
1	A	969	ARG
1	A	992	SER
1	A	1016	VAL
1	A	1017	LEU
1	A	1030	ARG
1	A	1035	ARG
1	B	22	ALA
1	B	84	SER
1	B	140	VAL
1	B	147	GLY
1	B	226	LYS
1	B	243	THR
1	B	263	ARG
1	B	283	GLY
1	B	358	PHE
1	B	360	GLN
1	B	424	GLY
1	B	453	PHE
1	B	486	LEU
1	B	490	PRO
1	B	558	ARG
1	B	601	LYS
1	B	618	ALA
1	B	638	PRO
1	B	658	ILE
1	B	669	PRO

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Mol	Chain	Res	Type
1	B	672	VAL
1	B	689	GLY
1	B	693	GLU
1	B	834	GLY
1	B	852	PRO
1	B	878	ALA
1	B	953	MET
1	B	1005	THR
1	C	4	PHE
1	C	221	GLY
1	C	285	PRO
1	C	411	VAL
1	C	577	GLN
1	C	601	LYS
1	C	602	GLU
1	C	618	ALA
1	C	733	GLN
1	C	802	SER
1	C	820	ASN
1	C	913	LEU
1	C	946	VAL
1	C	960	LEU
1	C	975	ILE
1	C	983	ILE
1	C	997	SER
1	C	998	GLY
1	C	1017	LEU
1	A	182	TYR
1	A	192	GLU
1	A	295	THR
1	A	374	VAL
1	A	377	LEU
1	A	378	GLY
1	A	427	PRO
1	A	517	ASN
1	A	636	ASP
1	A	689	GLY
1	A	714	THR
1	A	847	LEU
1	A	975	ILE
1	A	988	PRO
1	A	991	ILE

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Mol	Chain	Res	Type
1	B	52	ALA
1	B	223	PRO
1	B	258	SER
1	B	318	PRO
1	B	357	LEU
1	B	364	ALA
1	B	597	TYR
1	B	603	LYS
1	B	654	ALA
1	B	708	LYS
1	B	765	ARG
1	B	835	LYS
1	B	936	GLY
1	B	1018	ALA
1	B	1019	ILE
1	C	33	ALA
1	C	69	MET
1	C	81	ASN
1	C	146	ASP
1	C	224	PRO
1	C	230	LEU
1	C	354	VAL
1	C	477	ALA
1	C	555	LEU
1	C	656	SER
1	C	972	LEU
1	A	236	ALA
1	A	252	LYS
1	A	287	SER
1	A	335	ILE
1	A	357	LEU
1	A	392	THR
1	A	407	ASP
1	A	416	VAL
1	A	423	GLU
1	A	439	GLN
1	A	635	ALA
1	A	693	GLU
1	A	746	ILE
1	A	892	TYR
1	A	994	GLY
1	A	1007	VAL

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Mol	Chain	Res	Type
1	B	36	PRO
1	B	82	SER
1	B	112	GLN
1	B	127	VAL
1	B	350	LEU
1	B	428	LYS
1	B	491	ALA
1	B	655	PHE
1	B	733	GLN
1	B	766	GLY
1	B	776	GLU
1	B	959	GLY
1	C	54	ALA
1	C	80	SER
1	C	206	ALA
1	C	236	ALA
1	C	372	VAL
1	C	396	PHE
1	C	410	ILE
1	C	413	VAL
1	C	425	LEU
1	C	531	VAL
1	C	617	PHE
1	C	882	ILE
1	C	895	TRP
1	C	974	PRO
1	C	982	PHE
1	A	19	ILE
1	A	50	PRO
1	A	63	GLN
1	A	120	GLN
1	A	397	GLY
1	A	832	ALA
1	A	967	ALA
1	B	171	GLY
1	B	184	MET
1	B	228	GLN
1	B	254	ASN
1	B	297	ALA
1	B	346	GLU
1	B	446	ALA
1	B	539	GLY

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Mol	Chain	Res	Type
1	B	564	LEU
1	B	713	LEU
1	B	716	VAL
1	B	723	ASP
1	B	871	ASN
1	B	957	GLY
1	B	974	PRO
1	B	992	SER
1	C	187	TRP
1	C	335	ILE
1	C	422	GLU
1	C	528	THR
1	C	636	ASP
1	C	1006	GLY
1	A	340	VAL
1	A	361	ASN
1	A	422	GLU
1	A	452	VAL
1	A	515	TRP
1	B	73	ASP
1	B	126	GLY
1	B	326	PRO
1	B	438	ILE
1	B	557	VAL
1	B	614	GLY
1	B	939	ALA
1	C	349	ILE
1	C	751	GLY
1	A	207	ILE
1	A	543	VAL
1	A	833	PRO
1	B	119	PRO
1	B	783	PRO
1	B	968	VAL
1	C	315	PRO
1	A	107	VAL
1	B	227	GLY
1	B	786	ILE
1	C	658	ILE
1	C	671	ILE
1	A	461	GLY
1	B	224	PRO

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Mol	Chain	Res	Type
1	B	621	GLY
1	A	36	PRO
1	A	140	VAL
1	C	689	GLY
1	C	935	ILE
1	A	987	MET

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	833/859 (97%)	684 (82%)	149 (18%)	2	8
1	B	833/859 (97%)	671 (81%)	162 (19%)	1	6
1	C	833/859 (97%)	682 (82%)	151 (18%)	2	8
All	All	2499/2577 (97%)	2037 (82%)	462 (18%)	1	7

All (462) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	10	ILE
1	A	21	LEU
1	A	25	LEU
1	A	28	LEU
1	A	38	ILE
1	A	43	VAL
1	A	45	ILE
1	A	55	LYS
1	A	57	VAL
1	A	59	ASP
1	A	60	THR
1	A	62	THR
1	A	63	GLN
1	A	70	ASN
1	A	88	VAL

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Mol	Chain	Res	Type
1	A	105	VAL
1	A	110	LYS
1	A	113	LEU
1	A	130	GLU
1	A	146	ASP
1	A	148	THR
1	A	176	GLN
1	A	181	GLN
1	A	193	LEU
1	A	207	ILE
1	A	214	VAL
1	A	222	THR
1	A	225	VAL
1	A	235	ILE
1	A	239	ARG
1	A	255	GLN
1	A	256	ASP
1	A	260	VAL
1	A	269	GLU
1	A	270	LEU
1	A	277	ILE
1	A	280	GLU
1	A	295	THR
1	A	298	ASN
1	A	301	ASP
1	A	310	LEU
1	A	316	PHE
1	A	323	ILE
1	A	337	ILE
1	A	341	VAL
1	A	350	LEU
1	A	351	VAL
1	A	353	LEU
1	A	356	TYR
1	A	357	LEU
1	A	359	LEU
1	A	360	GLN
1	A	366	LEU
1	A	370	ILE
1	A	372	VAL
1	A	400	LEU
1	A	402	ILE

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Mol	Chain	Res	Type
1	A	404	LEU
1	A	406	VAL
1	A	410	ILE
1	A	418	ARG
1	A	443	VAL
1	A	447	MET
1	A	448	VAL
1	A	454	VAL
1	A	473	THR
1	A	475	VAL
1	A	482	VAL
1	A	489	THR
1	A	495	THR
1	A	496	MET
1	A	515	TRP
1	A	526	HIS
1	A	527	TYR
1	A	528	THR
1	A	530	SER
1	A	536	ARG
1	A	540	ARG
1	A	542	LEU
1	A	544	LEU
1	A	547	ILE
1	A	552	MET
1	A	562	SER
1	A	564	LEU
1	A	571	VAL
1	A	576	VAL
1	A	595	THR
1	A	612	VAL
1	A	620	ARG
1	A	626	ILE
1	A	629	VAL
1	A	630	SER
1	A	632	LYS
1	A	636	ASP
1	A	653	ARG
1	A	658	ILE
1	A	659	LYS
1	A	671	ILE
1	A	674	LEU

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Mol	Chain	Res	Type
1	A	687	GLN
1	A	702	LEU
1	A	711	ASP
1	A	712	MET
1	A	713	LEU
1	A	717	ARG
1	A	721	LEU
1	A	724	THR
1	A	739	LEU
1	A	741	VAL
1	A	746	ILE
1	A	750	LEU
1	A	764	ASP
1	A	773	VAL
1	A	780	ARG
1	A	791	VAL
1	A	795	ASP
1	A	806	SER
1	A	810	GLU
1	A	837	THR
1	A	842	GLU
1	A	843	LEU
1	A	844	MET
1	A	853	THR
1	A	867	ARG
1	A	881	LEU
1	A	882	ILE
1	A	886	LEU
1	A	918	PHE
1	A	928	GLN
1	A	929	VAL
1	A	934	THR
1	A	955	LYS
1	A	958	LYS
1	A	960	LEU
1	A	972	LEU
1	A	975	ILE
1	A	976	LEU
1	A	978	THR
1	A	980	LEU
1	A	982	PHE
1	A	983	ILE

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Mol	Chain	Res	Type
1	A	986	VAL
1	A	989	LEU
1	A	993	THR
1	A	997	SER
1	A	1007	VAL
1	A	1030	ARG
1	A	1035	ARG
1	B	10	ILE
1	B	13	TRP
1	B	18	ILE
1	B	21	LEU
1	B	28	LEU
1	B	34	GLN
1	B	38	ILE
1	B	53	ASP
1	B	57	VAL
1	B	60	THR
1	B	64	VAL
1	B	65	ILE
1	B	67	GLN
1	B	70	ASN
1	B	74	ASN
1	B	81	ASN
1	B	83	ASP
1	B	90	ILE
1	B	91	THR
1	B	92	LEU
1	B	93	THR
1	B	95	GLU
1	B	96	SER
1	B	104	GLN
1	B	108	GLN
1	B	109	ASN
1	B	115	MET
1	B	121	GLU
1	B	128	SER
1	B	136	PHE
1	B	137	LEU
1	B	145	THR
1	B	148	THR
1	B	150	THR
1	B	152	GLU

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Mol	Chain	Res	Type
1	B	154	ILE
1	B	155	SER
1	B	169	THR
1	B	176	GLN
1	B	182	TYR
1	B	185	ARG
1	B	186	ILE
1	B	188	MET
1	B	193	LEU
1	B	194	ASN
1	B	199	THR
1	B	203	VAL
1	B	207	ILE
1	B	226	LYS
1	B	230	LEU
1	B	231	ASN
1	B	235	ILE
1	B	243	THR
1	B	244	GLU
1	B	250	LEU
1	B	253	VAL
1	B	254	ASN
1	B	255	GLN
1	B	259	ARG
1	B	261	LEU
1	B	262	LEU
1	B	270	LEU
1	B	276	ASP
1	B	293	LEU
1	B	295	THR
1	B	298	ASN
1	B	300	LEU
1	B	302	THR
1	B	323	ILE
1	B	329	THR
1	B	330	THR
1	B	334	LYS
1	B	339	GLU
1	B	341	VAL
1	B	343	THR
1	B	345	VAL
1	B	348	ILE

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Mol	Chain	Res	Type
1	B	349	ILE
1	B	356	TYR
1	B	372	VAL
1	B	379	THR
1	B	394	THR
1	B	395	MET
1	B	399	VAL
1	B	402	ILE
1	B	404	LEU
1	B	406	VAL
1	B	410	ILE
1	B	414	GLU
1	B	435	MET
1	B	452	VAL
1	B	456	MET
1	B	459	PHE
1	B	463	THR
1	B	468	ARG
1	B	469	GLN
1	B	473	THR
1	B	478	MET
1	B	488	LEU
1	B	497	LEU
1	B	515	TRP
1	B	519	MET
1	B	528	THR
1	B	535	LEU
1	B	547	ILE
1	B	549	VAL
1	B	557	VAL
1	B	558	ARG
1	B	562	SER
1	B	564	LEU
1	B	571	VAL
1	B	578	LEU
1	B	587	THR
1	B	595	THR
1	B	599	LEU
1	B	601	LYS
1	B	606	VAL
1	B	623	ASN
1	B	629	VAL

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Mol	Chain	Res	Type
1	B	647	ILE
1	B	655	PHE
1	B	658	ILE
1	B	660	ASP
1	B	692	HIS
1	B	695	LEU
1	B	696	THR
1	B	702	LEU
1	B	714	THR
1	B	717	ARG
1	B	739	LEU
1	B	743	ILE
1	B	750	LEU
1	B	757	SER
1	B	758	TYR
1	B	773	VAL
1	B	778	LYS
1	B	779	TYR
1	B	782	LEU
1	B	795	ASP
1	B	799	VAL
1	B	808	ARG
1	B	818	ARG
1	B	826	GLU
1	B	844	MET
1	B	851	LEU
1	B	875	SER
1	B	876	LEU
1	B	891	LEU
1	B	897	ILE
1	B	900	SER
1	B	905	VAL
1	B	914	LEU
1	B	921	LEU
1	B	935	ILE
1	B	947	GLU
1	B	952	LEU
1	B	966	ASP
1	B	972	LEU
1	B	978	THR
1	B	989	LEU
1	B	991	ILE

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Mol	Chain	Res	Type
1	B	1034	SER
1	C	13	TRP
1	C	19	ILE
1	C	30	LEU
1	C	34	GLN
1	C	35	TYR
1	C	37	THR
1	C	38	ILE
1	C	44	THR
1	C	46	SER
1	C	55	LYS
1	C	56	THR
1	C	60	THR
1	C	64	VAL
1	C	68	ASN
1	C	82	SER
1	C	84	SER
1	C	89	GLN
1	C	91	THR
1	C	96	SER
1	C	108	GLN
1	C	109	ASN
1	C	111	LEU
1	C	115	MET
1	C	118	LEU
1	C	123	GLN
1	C	128	SER
1	C	129	VAL
1	C	137	LEU
1	C	150	THR
1	C	155	SER
1	C	158	VAL
1	C	164	ASP
1	C	166	ILE
1	C	177	LEU
1	C	189	ASN
1	C	195	LYS
1	C	204	ILE
1	C	207	ILE
1	C	226	LYS
1	C	228	GLN
1	C	239	ARG

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Mol	Chain	Res	Type
1	C	244	GLU
1	C	253	VAL
1	C	259	ARG
1	C	269	GLU
1	C	270	LEU
1	C	274	ASN
1	C	277	ILE
1	C	284	GLN
1	C	285	PRO
1	C	300	LEU
1	C	306	ILE
1	C	321	LEU
1	C	338	HIS
1	C	341	VAL
1	C	349	ILE
1	C	351	VAL
1	C	355	MET
1	C	367	ILE
1	C	370	ILE
1	C	372	VAL
1	C	374	VAL
1	C	377	LEU
1	C	394	THR
1	C	399	VAL
1	C	402	ILE
1	C	404	LEU
1	C	414	GLU
1	C	416	VAL
1	C	417	GLU
1	C	422	GLU
1	C	425	LEU
1	C	452	VAL
1	C	454	VAL
1	C	459	PHE
1	C	472	ILE
1	C	480	LEU
1	C	483	LEU
1	C	484	VAL
1	C	497	LEU
1	C	529	ASP
1	C	534	ILE
1	C	542	LEU

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Mol	Chain	Res	Type
1	C	544	LEU
1	C	547	ILE
1	C	555	LEU
1	C	567	GLU
1	C	571	VAL
1	C	573	MET
1	C	577	GLN
1	C	588	GLN
1	C	591	LEU
1	C	595	THR
1	C	596	HIS
1	C	636	ASP
1	C	641	GLU
1	C	644	VAL
1	C	658	ILE
1	C	664	PHE
1	C	668	LEU
1	C	671	ILE
1	C	685	ILE
1	C	687	GLN
1	C	693	GLU
1	C	695	LEU
1	C	696	THR
1	C	699	ARG
1	C	702	LEU
1	C	703	LEU
1	C	713	LEU
1	C	714	THR
1	C	716	VAL
1	C	722	GLU
1	C	724	THR
1	C	739	LEU
1	C	743	ILE
1	C	750	LEU
1	C	758	TYR
1	C	759	VAL
1	C	761	ASP
1	C	767	ARG
1	C	778	LYS
1	C	791	VAL
1	C	799	VAL
1	C	805	SER

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Mol	Chain	Res	Type
1	C	808	ARG
1	C	828	LEU
1	C	830	GLN
1	C	839	GLU
1	C	846	GLN
1	C	847	LEU
1	C	865	GLN
1	C	868	LEU
1	C	883	VAL
1	C	899	PHE
1	C	900	SER
1	C	903	LEU
1	C	909	VAL
1	C	914	LEU
1	C	931	LEU
1	C	935	ILE
1	C	941	ASN
1	C	945	ILE
1	C	952	LEU
1	C	960	LEU
1	C	982	PHE
1	C	983	ILE
1	C	984	LEU
1	C	993	THR
1	C	1007	VAL
1	C	1036	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	58	GLN
1	A	68	ASN
1	A	81	ASN
1	A	112	GLN
1	A	120	GLN
1	A	124	GLN
1	A	144	ASN
1	A	191	ASN
1	A	210	GLN
1	A	211	ASN
1	A	231	ASN

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Mol	Chain	Res	Type
1	A	254	ASN
1	A	274	ASN
1	A	282	ASN
1	A	298	ASN
1	A	439	GLN
1	A	577	GLN
1	A	584	GLN
1	A	622	GLN
1	A	623	ASN
1	A	709	HIS
1	A	719	ASN
1	A	726	GLN
1	A	865	GLN
1	A	928	GLN
1	A	1001	ASN
1	B	68	ASN
1	B	70	ASN
1	B	74	ASN
1	B	89	GLN
1	B	106	GLN
1	B	109	ASN
1	B	144	ASN
1	B	151	GLN
1	B	161	ASN
1	B	176	GLN
1	B	189	ASN
1	B	191	ASN
1	B	210	GLN
1	B	213	GLN
1	B	218	GLN
1	B	228	GLN
1	B	231	ASN
1	B	255	GLN
1	B	298	ASN
1	B	391	ASN
1	B	415	ASN
1	B	517	ASN
1	B	525	HIS
1	B	569	GLN
1	B	588	GLN
1	B	613	ASN
1	B	622	GLN

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Mol	Chain	Res	Type
1	B	700	ASN
1	B	709	HIS
1	B	726	GLN
1	B	733	GLN
1	B	830	GLN
1	B	846	GLN
1	B	871	ASN
1	B	872	GLN
1	B	923	ASN
1	C	3	ASN
1	C	34	GLN
1	C	58	GLN
1	C	63	GLN
1	C	89	GLN
1	C	104	GLN
1	C	144	ASN
1	C	176	GLN
1	C	189	ASN
1	C	197	GLN
1	C	211	ASN
1	C	231	ASN
1	C	237	GLN
1	C	274	ASN
1	C	284	GLN
1	C	525	HIS
1	C	577	GLN
1	C	700	ASN
1	C	737	GLN
1	C	923	ASN
1	C	941	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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
2	ERY	C	3402	-	53,53,53	1.04	1 (1%)	82,82,82	1.68	20 (24%)

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
2	ERY	C	3402	-	-	5/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3402	ERY	O2-C1	5.07	1.45	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3402	ERY	C20-O5-C16	4.28	126.23	117.51
2	C	3402	ERY	C29-N1-C24	3.89	124.37	113.15
2	C	3402	ERY	O2-C1-C2	3.63	119.29	111.53
2	C	3402	ERY	C15-C16-C17	3.58	113.78	107.64
2	C	3402	ERY	C13-O2-C1	-3.31	112.42	118.20
2	C	3402	ERY	O7-C5-C6	3.27	110.29	106.40
2	C	3402	ERY	O12-C11-C10	3.25	115.38	110.77
2	C	3402	ERY	C25-C24-N1	-3.14	106.77	115.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3402	ERY	C33-C8-C7	-3.13	104.06	109.88
2	C	3402	ERY	O7-C5-C4	-2.72	107.65	111.58
2	C	3402	ERY	O12-C11-C12	-2.66	101.69	106.57
2	C	3402	ERY	O2-C1-O1	-2.57	119.31	123.95
2	C	3402	ERY	O4-C18-C21	2.44	112.15	106.74
2	C	3402	ERY	C19-C16-C15	-2.20	106.80	110.64
2	C	3402	ERY	C34-C10-C11	-2.17	111.55	114.30
2	C	3402	ERY	C29-N1-C28	2.15	116.81	110.49
2	C	3402	ERY	O7-C22-C23	2.14	113.35	108.09
2	C	3402	ERY	C25-C24-C23	2.13	113.08	110.02
2	C	3402	ERY	O7-C22-O9	-2.07	105.23	110.69
2	C	3402	ERY	C7-C8-C9	-2.00	109.97	113.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

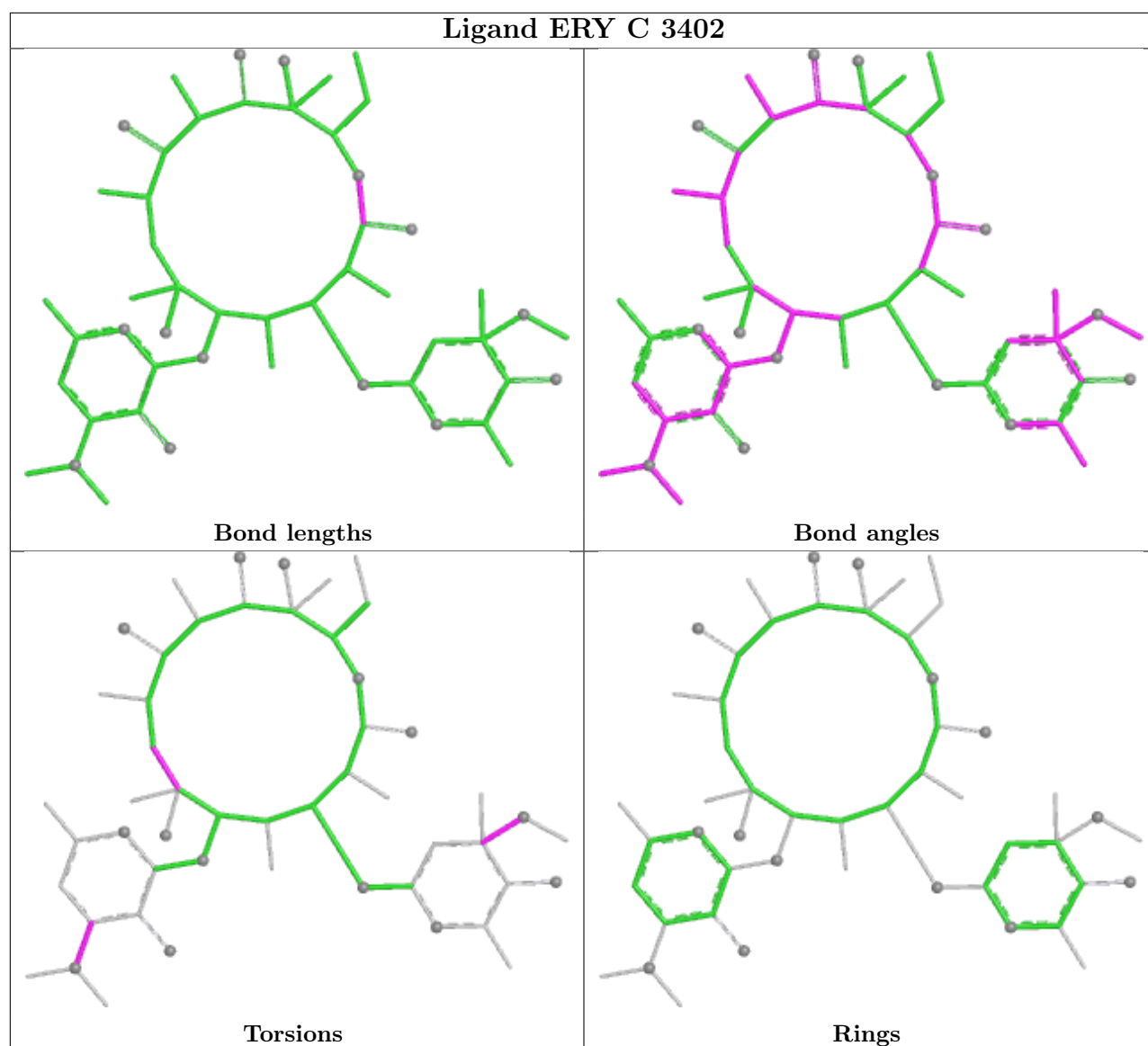
Mol	Chain	Res	Type	Atoms
2	C	3402	ERY	C32-C6-C7-C8
2	C	3402	ERY	C25-C24-N1-C28
2	C	3402	ERY	C23-C24-N1-C29
2	C	3402	ERY	C19-C16-O5-C20
2	C	3402	ERY	O10-C6-C7-C8

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3402	ERY	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	1022/1053 (97%)	0.08	12 (1%) 76 59	58, 111, 150, 192	0
1	B	1022/1053 (97%)	0.16	16 (1%) 70 52	69, 115, 154, 179	0
1	C	1022/1053 (97%)	0.10	17 (1%) 69 51	55, 109, 160, 188	0
All	All	3066/3159 (97%)	0.11	45 (1%) 72 53	55, 113, 155, 192	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	671	ILE	4.3
1	A	915	ALA	3.4
1	B	528	THR	3.2
1	B	420	MET	3.1
1	B	672	VAL	3.0
1	B	960	LEU	2.9
1	A	497	LEU	2.9
1	B	553	ALA	2.8
1	C	670	ALA	2.8
1	B	968	VAL	2.7
1	B	1019	ILE	2.7
1	C	676	THR	2.7
1	A	960	LEU	2.7
1	C	531	VAL	2.7
1	B	417	GLU	2.6
1	A	967	ALA	2.6
1	C	520	PHE	2.5
1	C	427	PRO	2.5
1	A	419	VAL	2.4
1	B	991	ILE	2.4
1	B	154	ILE	2.3
1	C	675	GLY	2.3
1	B	1026	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	713	LEU	2.3
1	A	32	VAL	2.3
1	A	1029	VAL	2.3
1	C	527	TYR	2.3
1	C	112	GLN	2.3
1	C	846	GLN	2.3
1	C	557	VAL	2.2
1	C	424	GLY	2.2
1	A	989	LEU	2.2
1	B	1017	LEU	2.2
1	A	1033	PHE	2.2
1	C	534	ILE	2.1
1	A	377	LEU	2.1
1	C	712	MET	2.1
1	B	868	LEU	2.1
1	A	145	THR	2.0
1	C	574	THR	2.0
1	B	775	SER	2.0
1	B	869	SER	2.0
1	A	54	ALA	2.0
1	C	53	ASP	2.0
1	C	469	GLN	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](#)

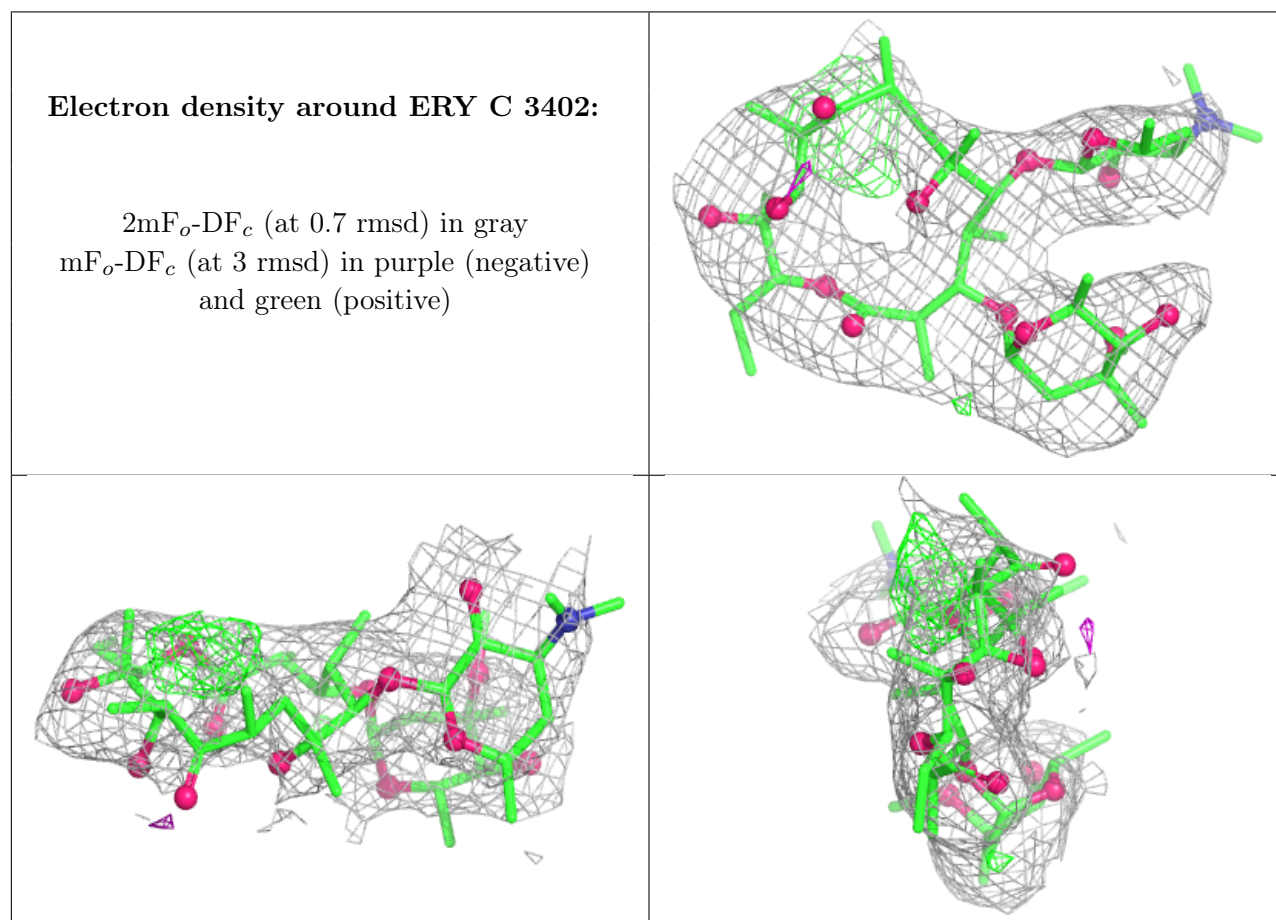
There are no oligosaccharides in this entry.

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
2	ERY	C	3402	51/51	0.88	0.15	58,68,74,79	51

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.