



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:09 PM GMT

PDB ID : 3W9H
Title : Structural basis for the inhibition of bacterial multidrug exporters
Authors : Sakurai, K.; Nagata, C.; Nakashima, R.; Yamaguchi, A.
Deposited on : 2013-04-04
Resolution : 3.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

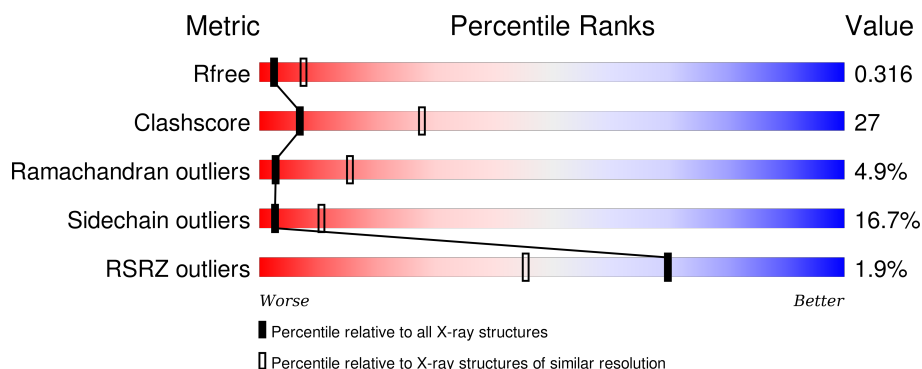
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



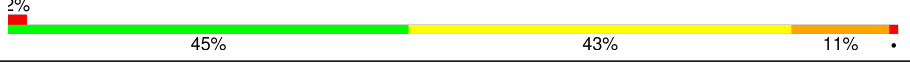
The reported resolution of this entry is 3.05 Å.

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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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

Mol	Chain	Length	Quality of chain
1	A	1033	 2% 52% 39% 9%
1	B	1033	 2% 45% 45% 9%
1	C	1033	 2% 45% 43% 11%

2 Entry composition [i](#)

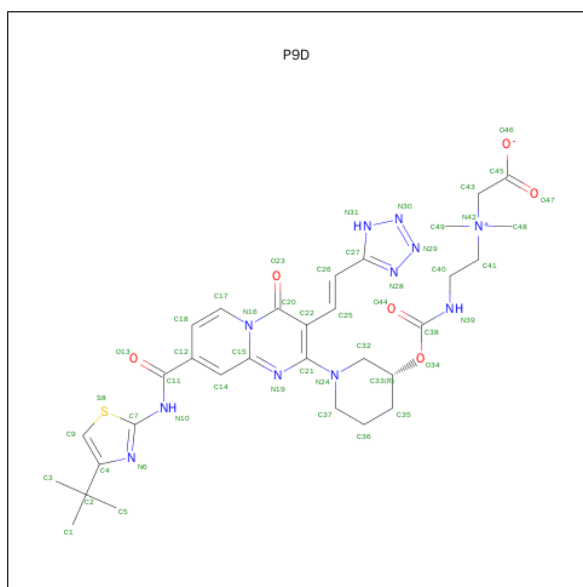
There are 3 unique types of molecules in this entry. The entry contains 23614 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1033	Total	C	N	O	S	0	0	0
			7850	5052	1295	1459	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7850	5052	1295	1459	44			
1	C	1033	Total	C	N	O	S	0	0	0
			7850	5052	1295	1459	44			

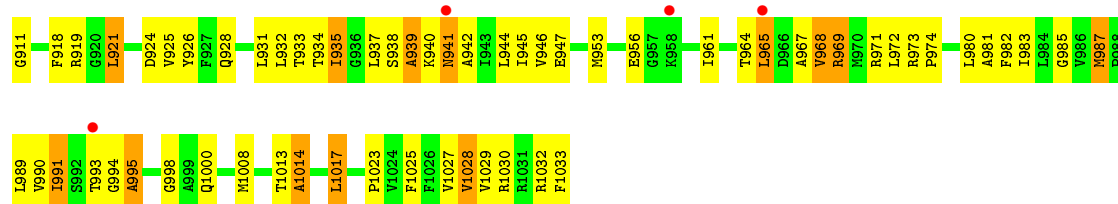
- Molecule 2 is [$\{2-[(\{[(3R)-1-\{8-[(4-TERT-BUTYL-1,3-THIAZOL-2-YL)CARBAMOYL]-4-OXO-3-[(E)-2-(1H-TETRAZOL-5-YL)ETHENYL]-4H-PYRIDO[1,2-A]PYRIMIDIN-2-YL\} PIPERIDIN-3-YL]OXY\}CARBONYL)AMINO\}ETHYL\} (DIMETHYL)AMMONIO\}ACETATE$ (three-letter code: P9D) (formula: $C_{31}H_{39}N_{11}O_6S$).



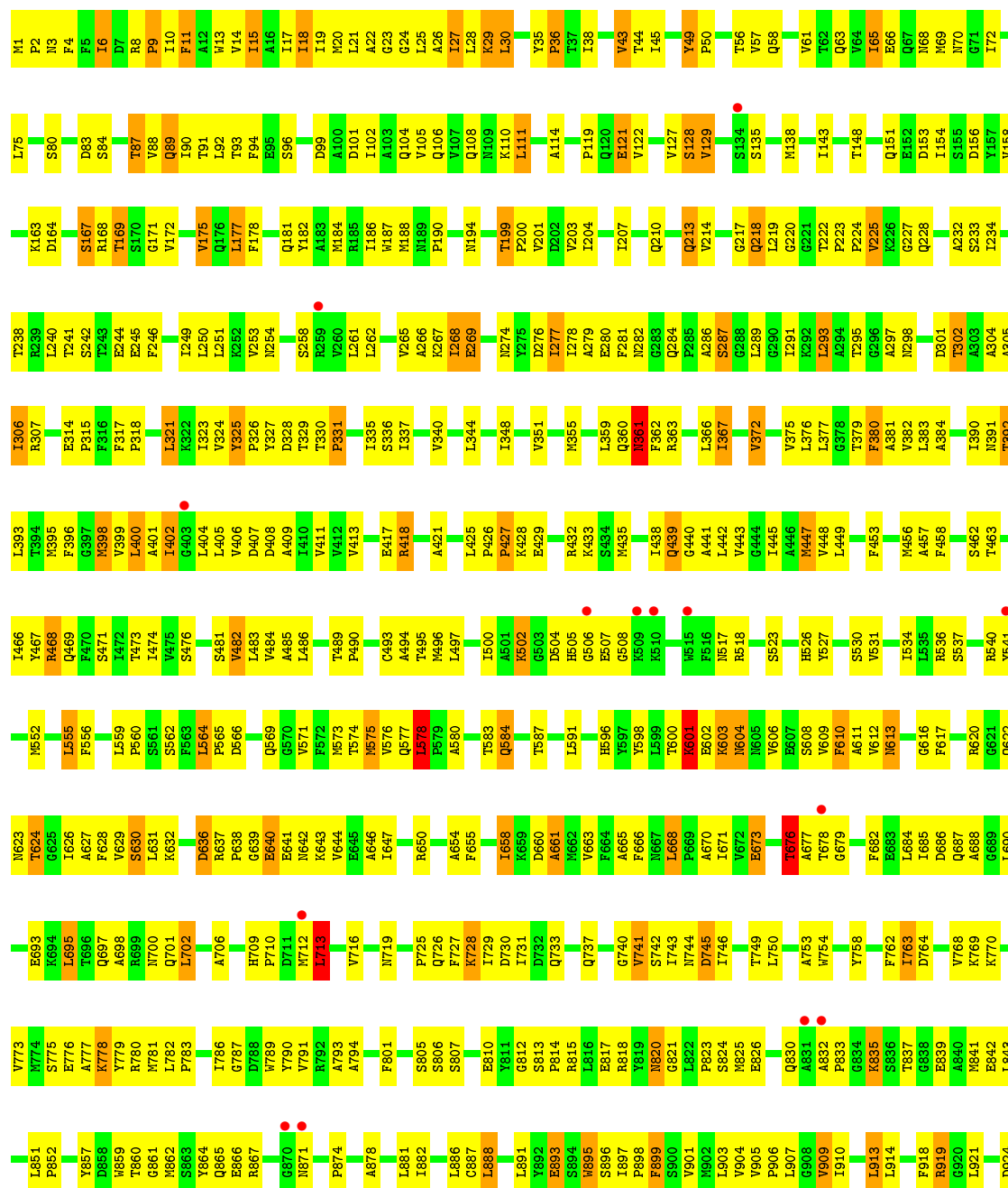
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			49	31	11	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	O 6	0	0
3	B	4	Total 4	O 4	0	0
3	C	5	Total 5	O 5	0	0



• 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	226.28 Å 134.16 Å 162.20 Å 90.00° 97.83° 90.00°	Depositor
Resolution (Å)	43.01 – 3.05 43.01 – 3.05	Depositor EDS
% Data completeness (in resolution range)	96.1 (43.01-3.05) 96.2 (43.01-3.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 3.06 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.231 , 0.317 0.229 , 0.316	Depositor DCC
R_{free} test set	4425 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	86.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	1 of 88240 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23614	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P9D

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	0.55	0/8000	0.81	8/10863 (0.1%)
1	B	0.54	0/8000	0.81	7/10863 (0.1%)
1	C	0.49	0/8000	0.75	2/10863 (0.0%)
All	All	0.53	0/24000	0.79	17/32589 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	LEU	CA-CB-CG	7.93	133.54	115.30
1	A	177	LEU	CA-CB-CG	7.50	132.56	115.30
1	B	578	LEU	CA-CB-CG	7.29	132.07	115.30
1	A	713	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	702	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	88	VAL	N-CA-C	-6.20	94.26	111.00
1	B	713	LEU	CA-CB-CG	6.15	129.45	115.30
1	A	289	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	177	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	168	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	250	LEU	CA-CB-CG	5.41	127.73	115.30
1	C	21	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	359	LEU	CA-CB-CG	5.29	127.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	767	ARG	CG-CD-NE	-5.21	100.85	111.80
1	B	601	LYS	CB-CA-C	5.18	120.77	110.40
1	C	544	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	996	GLY	Peptide

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	7850	0	8001	394	0
1	B	7850	0	8001	473	0
1	C	7850	0	8001	454	0
2	B	49	0	39	14	0
3	A	6	0	0	0	0
3	B	4	0	0	1	0
3	C	5	0	0	0	0
All	All	23614	0	24042	1270	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 27.

All (1270) 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:C:1011:MET:HE2	1:C:1011:MET:HA	1.17	1.09
1:B:901:VAL:O	1:B:904:VAL:HG12	1.50	1.08
1:A:235:ILE:HG22	1:B:728:LYS:HE3	1.16	1.08
1:C:1011:MET:CE	1:C:1011:MET:HA	1.85	1.06
1:A:142:VAL:HG13	1:A:321:LEU:HD21	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2000:P9D:H37	2:B:2000:P9D:H25	1.37	1.04
1:B:508:GLY:HA2	1:B:518:ARG:NH1	1.73	1.03
1:B:931:LEU:O	1:B:935:ILE:HG12	1.59	1.02
1:C:901:VAL:O	1:C:904:VAL:HG12	1.60	1.02
1:B:445:ILE:HD12	1:B:940:LYS:HB2	1.40	1.01
1:B:418:ARG:HH11	1:B:418:ARG:HB3	1.26	1.00
1:C:401:ALA:O	1:C:405:LEU:HD12	1.61	0.99
1:C:324:VAL:HG12	1:C:326:PRO:HD3	1.44	0.98
1:C:1026:PHE:O	1:C:1030:ARG:HB2	1.63	0.97
1:A:142:VAL:CG1	1:A:321:LEU:HD21	1.97	0.95
1:A:23:GLY:HA3	1:A:377:LEU:O	1.66	0.94
1:C:879:ILE:O	1:C:883:VAL:HG23	1.68	0.94
1:B:584:GLN:HB2	1:B:622:GLN:HG2	1.49	0.93
1:B:298:ASN:HB3	1:B:301:ASP:HB2	1.49	0.93
1:B:298:ASN:O	1:B:302:THR:HG23	1.68	0.93
1:B:888:LEU:HD11	1:B:943:ILE:HD11	1.51	0.92
1:B:731:ILE:CD1	1:B:746:ILE:HG21	2.00	0.92
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.50	0.92
1:B:742:SER:OG	1:B:745:ASP:HB2	1.71	0.90
1:B:686:ASP:HB3	1:B:823:PRO:HG2	1.51	0.90
1:A:142:VAL:HG13	1:A:321:LEU:CD2	2.02	0.90
1:A:911:GLY:HA3	1:A:1013:THR:OG1	1.71	0.90
1:B:668:LEU:HD23	1:B:668:LEU:H	1.33	0.90
1:C:731:ILE:HG21	1:C:746:ILE:HG21	1.51	0.89
1:A:261:LEU:HD12	1:A:263:ARG:NH1	1.87	0.88
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.53	0.88
1:B:965:LEU:O	1:B:969:ARG:HB2	1.73	0.88
1:A:168:ARG:HG2	1:B:69:MET:O	1.74	0.87
1:B:742:SER:HG	1:B:745:ASP:HB2	1.40	0.86
1:A:350:LEU:HD21	1:A:985:GLY:HA2	1.56	0.86
1:A:643:LYS:O	1:A:647:ILE:HG13	1.76	0.86
1:A:17:ILE:CG2	1:B:886:LEU:HD21	2.05	0.86
1:A:17:ILE:HG21	1:B:886:LEU:HD21	1.55	0.86
1:A:92:LEU:N	1:A:92:LEU:HD12	1.92	0.85
1:A:38:ILE:HD11	1:A:671:ILE:HD12	1.59	0.84
1:C:213:GLN:HE22	1:C:238:THR:HB	1.43	0.84
1:B:778:LYS:HD2	1:B:779:TYR:CZ	2.13	0.84
1:B:418:ARG:NH1	1:B:418:ARG:HB3	1.93	0.83
1:A:203:VAL:HG13	1:A:262:LEU:HD21	1.60	0.83
1:B:302:THR:O	1:B:306:ILE:HG22	1.79	0.83
1:C:1018:ALA:O	1:C:1022:VAL:HG22	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:VAL:HG21	1:C:310:LEU:HD21	1.59	0.82
1:B:966:ASP:O	1:B:970:MET:HG2	1.79	0.82
1:B:609:VAL:HG22	1:B:629:VAL:HG22	1.61	0.82
1:A:219:LEU:CD2	1:A:234:ILE:HD11	2.10	0.82
1:A:213:GLN:HE21	1:B:56:THR:HA	1.44	0.82
1:A:901:VAL:O	1:A:904:VAL:HG23	1.79	0.82
1:C:356:TYR:HD2	1:C:357:LEU:HD12	1.44	0.82
1:B:729:ILE:O	1:B:729:ILE:HG12	1.79	0.81
1:C:537:SER:HB2	1:C:540:ARG:HD2	1.61	0.81
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.62	0.81
1:A:239:ARG:HB2	1:A:763:ILE:HD12	1.62	0.81
1:B:186:ILE:HD12	1:B:186:ILE:N	1.95	0.81
1:B:731:ILE:HD11	1:B:746:ILE:HG21	1.64	0.80
1:B:990:VAL:HG13	1:B:1005:THR:HG22	1.63	0.80
1:B:439:GLN:HG3	1:B:440:GLY:H	1.45	0.80
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.64	0.80
1:B:603:LYS:O	1:B:604:ASN:HB2	1.82	0.80
1:A:626:ILE:HD13	1:A:627:ALA:N	1.97	0.80
1:A:144:ASN:HD21	1:A:148:THR:H	1.28	0.80
1:B:638:PRO:HD2	1:B:642:ASN:HD22	1.45	0.80
1:B:980:LEU:HD13	1:B:984:LEU:HD12	1.64	0.80
1:B:500:ILE:HG23	1:B:504:ASP:HB3	1.64	0.79
1:C:343:THR:HG21	1:C:989:LEU:HB3	1.63	0.79
1:A:485:ALA:O	1:A:490:PRO:HD3	1.82	0.79
1:B:620:ARG:HH12	2:B:2000:P9D:H43	1.48	0.79
1:B:428:LYS:HA	1:B:494:ALA:HB1	1.63	0.79
2:B:2000:P9D:C25	2:B:2000:P9D:H37	2.12	0.78
1:B:1013:THR:O	1:B:1017:LEU:HB3	1.82	0.78
1:C:38:ILE:HD11	1:C:671:ILE:HG21	1.66	0.78
1:C:324:VAL:CG1	1:C:326:PRO:HD3	2.14	0.78
1:C:184:MET:HB3	1:C:771:VAL:HG22	1.65	0.78
1:C:727:PHE:HE1	1:C:807:SER:HB2	1.48	0.78
1:C:344:LEU:HA	1:C:399:VAL:HG23	1.66	0.78
1:C:904:VAL:O	1:C:907:LEU:HG	1.84	0.78
1:C:547:ILE:HA	1:C:550:VAL:HG22	1.64	0.78
1:B:418:ARG:HE	1:B:970:MET:HB2	1.48	0.78
1:B:240:LEU:HD12	1:B:240:LEU:H	1.49	0.78
1:B:23:GLY:HA3	1:B:377:LEU:O	1.84	0.78
1:A:568:ASP:OD2	1:A:644:VAL:HG23	1.82	0.77
1:C:527:TYR:OH	1:C:968:VAL:HG22	1.84	0.77
1:A:939:ALA:HA	1:A:942:ALA:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:VAL:O	1:A:1032:ARG:HB3	1.84	0.77
1:B:127:VAL:HG12	1:B:128:SER:H	1.50	0.77
1:B:508:GLY:HA2	1:B:518:ARG:HH12	1.48	0.77
1:A:435:MET:O	1:A:439:GLN:HB2	1.84	0.77
1:A:626:ILE:C	1:A:626:ILE:HD13	2.05	0.76
1:B:640:GLU:O	1:B:646:ALA:HB2	1.85	0.76
1:A:878:ALA:O	1:A:882:ILE:HG12	1.83	0.76
1:B:620:ARG:NH1	2:B:2000:P9D:H43	2.00	0.76
1:B:655:PHE:HA	1:B:658:ILE:HD11	1.66	0.76
1:A:517:ASN:O	1:A:521:GLU:HG2	1.84	0.76
1:C:650:ARG:HG3	1:C:650:ARG:HH11	1.49	0.76
1:B:604:ASN:H	1:B:632:LYS:HZ2	1.34	0.76
1:A:261:LEU:HD12	1:A:263:ARG:HH12	1.49	0.76
1:B:277:ILE:HD13	1:B:612:VAL:HG13	1.69	0.75
1:C:727:PHE:CE1	1:C:807:SER:HB2	2.22	0.75
1:A:530:SER:O	1:A:534:ILE:HB	1.85	0.75
1:B:400:LEU:O	1:B:933:THR:HG21	1.87	0.75
1:B:441:ALA:O	1:B:445:ILE:HG12	1.86	0.75
1:A:944:LEU:HB3	1:A:971:ARG:HD3	1.68	0.75
1:C:894:SER:HB2	1:C:897:ILE:HD12	1.68	0.75
1:B:101:ASP:OD2	1:C:106:GLN:NE2	2.20	0.75
1:B:254:ASN:HB2	1:B:258:SER:OG	1.86	0.74
1:A:235:ILE:CG2	1:B:728:LYS:HE3	2.08	0.74
1:B:600:THR:HA	1:B:603:LYS:HE3	1.69	0.74
1:A:684:LEU:HD11	1:A:855:VAL:HG13	1.67	0.74
1:C:618:ALA:HB1	1:C:719:ASN:O	1.87	0.74
1:A:146:ASP:HB3	1:A:148:THR:HG23	1.69	0.74
1:A:762:PHE:CE2	1:A:764:ASP:HB2	2.23	0.74
1:B:240:LEU:HD12	1:B:240:LEU:N	2.01	0.74
1:A:425:LEU:HB3	1:A:426:PRO:HD2	1.70	0.74
1:C:171:GLY:HA3	1:C:302:THR:OG1	1.87	0.74
1:B:402:ILE:HA	1:B:405:LEU:HD12	1.70	0.74
1:B:220:GLY:HA2	1:C:781:MET:SD	2.27	0.73
1:C:974:PRO:O	1:C:978:THR:HG23	1.88	0.73
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.71	0.73
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.71	0.73
1:B:713:LEU:H	1:B:832:ALA:HB2	1.53	0.73
1:B:240:LEU:CD1	1:B:240:LEU:H	2.00	0.73
1:A:344:LEU:HD21	1:A:376:LEU:HD23	1.70	0.72
1:A:809:TRP:HH2	1:C:230:LEU:HD11	1.54	0.72
1:A:401:ALA:O	1:A:405:LEU:HG	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:THR:HA	1:B:837:THR:HG22	1.71	0.72
1:C:101:ASP:OD1	1:C:131:LYS:HE3	1.89	0.72
1:C:528:THR:CG2	1:C:969:ARG:HB3	2.20	0.72
1:B:508:GLY:HA2	1:B:518:ARG:HH11	1.55	0.72
1:B:663:VAL:HG12	1:B:663:VAL:O	1.89	0.71
1:B:924:ASP:O	1:B:928:GLN:HB2	1.90	0.71
1:A:144:ASN:ND2	1:A:148:THR:H	1.88	0.71
1:C:607:GLU:HB2	1:C:632:LYS:HG2	1.71	0.71
1:B:38:ILE:N	1:B:38:ILE:HD12	2.06	0.71
1:B:435:MET:SD	1:B:490:PRO:HB3	2.30	0.71
1:B:151:GLN:OE1	1:B:278:ILE:HA	1.90	0.71
1:B:860:THR:HA	1:B:864:TYR:HB2	1.73	0.71
1:B:186:ILE:HD12	1:B:186:ILE:H	1.55	0.71
1:B:241:THR:HG22	1:B:763:ILE:O	1.91	0.71
1:B:84:SER:OG	1:B:814:PRO:HA	1.91	0.70
1:C:150:THR:H	1:C:153:ASP:HB2	1.56	0.70
1:B:407:ASP:O	1:B:411:VAL:HG13	1.91	0.70
1:A:809:TRP:CH2	1:C:230:LEU:HD11	2.26	0.70
1:A:219:LEU:HD21	1:A:234:ILE:HD11	1.74	0.70
1:C:959:GLY:H	1:C:962:GLU:HB2	1.55	0.70
1:B:401:ALA:HB2	1:B:474:ILE:HD12	1.73	0.70
1:C:625:GLY:O	1:C:626:ILE:HD12	1.92	0.70
1:C:450:SER:O	1:C:452:VAL:N	2.25	0.69
1:C:947:GLU:O	1:C:951:ASP:HB2	1.92	0.69
1:B:186:ILE:HB	1:B:773:VAL:HG12	1.74	0.69
1:A:445:ILE:HG21	1:A:940:LYS:HE3	1.73	0.69
1:B:328:ASP:OD1	1:B:330:THR:HB	1.91	0.69
1:A:184:MET:HG2	1:A:246:PHE:CD1	2.27	0.69
1:C:1:MET:N	1:C:2:PRO:HD2	2.08	0.69
1:A:351:VAL:CG2	1:A:981:ALA:HB1	2.22	0.69
1:A:56:THR:O	1:A:60:THR:HB	1.93	0.69
1:B:228:GLN:HE22	1:C:781:MET:HB3	1.58	0.69
1:B:837:THR:O	1:B:841:MET:HG3	1.93	0.69
1:C:782:LEU:HD23	1:C:783:PRO:HD2	1.73	0.69
1:A:252:LYS:HG3	1:A:260:VAL:CG2	2.23	0.69
1:A:668:LEU:H	1:A:668:LEU:HD12	1.57	0.69
1:C:13:TRP:O	1:C:17:ILE:HG13	1.92	0.69
1:A:909:VAL:HA	1:A:931:LEU:HD21	1.75	0.69
1:A:676:THR:OG1	1:A:679:GLY:HA3	1.93	0.69
1:C:356:TYR:CD2	1:C:357:LEU:HD12	2.25	0.69
1:A:758:TYR:CZ	1:A:770:LYS:HG2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.28	0.68
1:C:681:ASP:HB3	1:C:860:THR:HG22	1.74	0.68
1:A:131:LYS:O	1:A:295:THR:HG22	1.93	0.68
1:A:222:THR:HG21	1:B:276:ASP:OD1	1.93	0.68
1:C:724:THR:HB	1:C:725:PRO:HD2	1.73	0.68
1:A:162:MET:HG2	1:A:313:MET:SD	2.33	0.68
1:B:650:ARG:O	1:B:654:ALA:HB2	1.93	0.68
1:A:790:TYR:CE2	1:A:800:PRO:HB3	2.29	0.67
1:C:688:ALA:HB3	1:C:690:LEU:HD13	1.75	0.67
1:C:485:ALA:HA	1:C:489:THR:HB	1.76	0.67
1:B:75:LEU:HD21	1:B:92:LEU:HB3	1.77	0.67
1:B:702:LEU:HG	1:B:702:LEU:O	1.92	0.67
1:B:685:ILE:HG22	1:B:687:GLN:HG2	1.76	0.67
1:B:493:CYS:O	1:B:497:LEU:HB2	1.95	0.67
2:B:2000:P9D:H43A	2:B:2000:P9D:H35	1.76	0.67
1:C:650:ARG:CG	1:C:650:ARG:HH11	2.08	0.66
1:A:44:THR:HG23	1:A:91:THR:HG23	1.76	0.66
1:C:447:MET:CE	1:C:447:MET:HA	2.25	0.66
1:C:144:ASN:ND2	1:C:320:GLY:O	2.28	0.66
1:A:81:ASN:OD1	1:A:815:ARG:HD2	1.94	0.66
1:B:610:PHE:CD2	2:B:2000:P9D:H18	2.30	0.66
1:C:344:LEU:O	1:C:348:ILE:HG12	1.94	0.66
1:B:778:LYS:HD2	1:B:779:TYR:CE2	2.31	0.66
1:B:335:ILE:HG21	1:B:995:ALA:HB1	1.77	0.66
1:C:685:ILE:HD11	1:C:858:ASP:HB2	1.78	0.66
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.76	0.66
1:B:11:PHE:O	1:B:14:VAL:HG22	1.95	0.66
1:B:639:GLY:O	1:B:641:GLU:N	2.28	0.66
1:A:261:LEU:CD1	1:A:263:ARG:HH12	2.09	0.66
1:C:157:TYR:O	1:C:161:ASN:HB2	1.96	0.66
1:B:727:PHE:CZ	1:B:807:SER:HB3	2.31	0.66
1:B:128:SER:HA	1:C:112:GLN:HE22	1.61	0.65
1:C:1022:VAL:HG23	1:C:1023:PRO:HD3	1.79	0.65
1:A:144:ASN:ND2	1:A:148:THR:N	2.44	0.65
1:B:336:SER:O	1:B:340:VAL:HG23	1.96	0.65
1:B:246:PHE:O	1:B:249:ILE:HG13	1.96	0.65
1:C:1028:VAL:O	1:C:1032:ARG:HB3	1.96	0.65
1:C:326:PRO:HG3	1:C:610:PHE:CD1	2.31	0.65
1:A:762:PHE:CE1	1:A:769:LYS:HB2	2.31	0.65
1:B:993:THR:HA	1:B:997:SER:HB3	1.77	0.65
1:B:340:VAL:CG1	1:B:399:VAL:HG11	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:GLN:HG3	1:A:438:ILE:H	1.61	0.65
1:A:57:VAL:HG12	1:A:88:VAL:CG2	2.24	0.65
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.26	0.65
1:B:127:VAL:HG12	1:B:128:SER:N	2.09	0.65
1:B:507:GLU:O	1:B:518:ARG:HD3	1.97	0.65
1:A:758:TYR:CE1	1:A:770:LYS:HG2	2.31	0.65
1:A:144:ASN:HD21	1:A:148:THR:N	1.95	0.65
1:C:731:ILE:HG21	1:C:746:ILE:CG2	2.27	0.64
1:C:1022:VAL:HG23	1:C:1023:PRO:CD	2.28	0.64
1:B:224:PRO:HA	1:C:781:MET:HE1	1.78	0.64
1:B:602:GLU:O	1:B:603:LYS:C	2.36	0.64
1:C:72:ILE:HD11	1:C:110:LYS:HG2	1.80	0.64
1:B:30:LEU:HD13	1:B:384:ALA:HB2	1.78	0.64
1:A:159:ALA:CB	1:A:181:GLN:HB2	2.27	0.64
1:B:445:ILE:HD12	1:B:940:LYS:CB	2.20	0.64
1:B:559:LEU:HD12	1:B:560:PRO:HD2	1.80	0.64
1:B:600:THR:O	1:B:602:GLU:N	2.31	0.64
1:B:344:LEU:HD23	1:B:402:ILE:CD1	2.28	0.64
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.78	0.64
1:C:176:GLN:NE2	1:C:620:ARG:HH11	1.96	0.64
1:A:364:ALA:HB1	1:A:497:LEU:HD23	1.80	0.64
1:A:781:MET:HE2	1:C:220:GLY:HA2	1.79	0.63
1:B:445:ILE:CD1	1:B:940:LYS:HB2	2.22	0.63
1:B:727:PHE:CE1	1:B:807:SER:HB3	2.33	0.63
1:A:781:MET:HB3	1:C:228:GLN:NE2	2.13	0.63
1:B:878:ALA:O	1:B:882:ILE:HG12	1.97	0.63
1:B:613:ASN:HD22	1:B:613:ASN:C	2.00	0.63
1:B:993:THR:HA	1:B:997:SER:CB	2.28	0.63
1:C:146:ASP:O	1:C:148:THR:N	2.31	0.63
1:B:167:SER:HA	1:B:175:VAL:HG21	1.80	0.63
1:C:310:LEU:HG	1:C:323:ILE:HD13	1.80	0.63
1:B:500:ILE:HG23	1:B:504:ASP:CB	2.27	0.63
1:B:376:LEU:HD21	1:B:405:LEU:HD13	1.80	0.63
1:B:668:LEU:CD2	1:B:668:LEU:H	2.07	0.63
1:C:690:LEU:HD21	1:C:855:VAL:HG23	1.78	0.63
1:B:203:VAL:O	1:B:207:ILE:HG13	1.98	0.63
1:B:485:ALA:HA	1:B:489:THR:OG1	1.99	0.63
1:B:14:VAL:HG23	1:B:15:ILE:H	1.63	0.63
1:A:644:VAL:CG1	1:A:667:ASN:HB2	2.27	0.63
1:B:10:ILE:HD12	1:C:895:TRP:CE3	2.33	0.63
1:A:797:GLN:HA	1:A:797:GLN:NE2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:616:GLY:HA2	1:C:626:ILE:HD13	1.81	0.63
1:B:108:GLN:OE1	1:C:112:GLN:HG3	1.98	0.62
1:A:416:VAL:HG11	1:A:431:THR:HG22	1.79	0.62
1:B:14:VAL:HG23	1:B:15:ILE:N	2.14	0.62
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.80	0.62
1:B:606:VAL:HA	1:B:631:LEU:HD23	1.80	0.62
1:A:252:LYS:HG3	1:A:260:VAL:HG21	1.81	0.62
1:A:211:ASN:HB2	1:A:240:LEU:HD22	1.82	0.62
1:B:327:TYR:CD2	2:B:2000:P9D:H9	2.35	0.62
1:A:326:PRO:HB2	1:A:610:PHE:HB2	1.80	0.62
1:B:910:ILE:O	1:B:914:LEU:HB2	2.00	0.62
1:B:317:PHE:CE2	1:B:323:ILE:HD11	2.35	0.62
1:A:261:LEU:CD1	1:A:263:ARG:NH1	2.62	0.62
1:C:340:VAL:HG11	1:C:395:MET:CB	2.30	0.62
1:A:448:VAL:HG23	1:A:887:CYS:HB2	1.80	0.62
1:C:688:ALA:HB3	1:C:690:LEU:CD1	2.30	0.62
1:C:714:THR:HG23	1:C:830:GLN:HB2	1.81	0.62
1:C:731:ILE:CG2	1:C:746:ILE:HG21	2.28	0.62
1:C:5:PHE:HB3	1:C:12:ALA:HB2	1.81	0.62
1:B:363:ARG:HB3	1:B:496:MET:O	1.99	0.62
1:C:192:GLU:O	1:C:196:PHE:CE2	2.53	0.62
1:A:474:ILE:HG22	1:A:475:VAL:N	2.14	0.61
1:A:911:GLY:CA	1:A:1013:THR:OG1	2.47	0.61
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.30	0.61
1:A:945:ILE:O	1:A:947:GLU:N	2.31	0.61
1:C:845:GLU:HG2	1:C:857:TYR:OH	2.00	0.61
1:C:156:ASP:OD1	1:C:182:TYR:HB2	1.99	0.61
1:B:504:ASP:O	1:B:506:GLY:N	2.32	0.61
1:C:251:LEU:CD1	1:C:262:LEU:HA	2.30	0.61
1:C:204:ILE:HG23	1:C:759:VAL:HG13	1.83	0.61
1:B:457:ALA:O	1:B:458:PHE:HD1	1.83	0.61
1:C:355:MET:HG2	1:C:410:ILE:HD11	1.83	0.61
1:C:664:PHE:HD1	1:C:715:SER:HG	1.48	0.61
1:B:111:LEU:HD11	1:B:127:VAL:HG11	1.82	0.61
1:A:16:ALA:O	1:A:20:MET:HG3	1.99	0.61
1:B:143:ILE:HD11	1:B:281:PHE:HB3	1.82	0.61
1:C:144:ASN:HB2	1:C:154:ILE:HD11	1.82	0.61
1:C:247:GLY:HA2	1:C:268:ILE:HG13	1.82	0.61
1:A:686:ASP:OD1	1:A:686:ASP:C	2.39	0.61
1:B:289:LEU:HB2	1:B:291:ILE:HD11	1.83	0.61
1:C:444:GLY:O	1:C:448:VAL:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:HD3	1:A:761:ASP:O	2.01	0.60
1:B:337:ILE:HG12	1:B:395:MET:SD	2.41	0.60
1:C:951:ASP:O	1:C:955:LYS:HB2	2.00	0.60
1:C:785:ASP:O	1:C:788:ASP:N	2.29	0.60
1:A:262:LEU:HD13	1:A:268:ILE:HD11	1.84	0.60
1:A:781:MET:HB3	1:C:228:GLN:HE22	1.67	0.60
1:B:4:PHE:CE2	1:B:8:ARG:HG3	2.36	0.60
1:A:57:VAL:CG1	1:A:88:VAL:CG2	2.79	0.60
1:B:960:LEU:HD22	1:B:1031:ARG:HH12	1.65	0.60
1:C:428:LYS:O	1:C:432:ARG:HG3	2.01	0.60
1:A:911:GLY:HA3	1:A:1013:THR:HG1	1.67	0.60
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.84	0.60
1:A:446:ALA:CB	1:A:482:VAL:HG21	2.31	0.60
1:C:103:ALA:O	1:C:107:VAL:HG23	2.01	0.60
1:C:72:ILE:HD11	1:C:110:LYS:CG	2.32	0.60
1:B:242:SER:OG	1:B:245:GLU:HB2	2.00	0.60
1:C:11:PHE:CE1	1:C:15:ILE:HD11	2.37	0.60
1:B:49:TYR:CE1	1:B:121:GLU:HG3	2.37	0.60
1:A:13:TRP:HA	1:A:13:TRP:CE3	2.36	0.60
1:B:919:ARG:HE	1:B:1005:THR:HG21	1.65	0.60
1:C:847:LEU:H	1:C:847:LEU:HD12	1.66	0.60
1:C:832:ALA:O	1:C:835:LYS:HG2	2.01	0.60
1:C:375:VAL:HG21	1:C:405:LEU:HD23	1.83	0.60
1:C:510:LYS:HG3	1:C:511:GLY:H	1.66	0.60
1:A:112:GLN:HG3	1:A:113:LEU:N	2.17	0.60
1:C:762:PHE:CZ	1:C:764:ASP:HB2	2.36	0.60
1:C:425:LEU:HD22	1:C:429:GLU:HB3	1.82	0.60
1:C:399:VAL:O	1:C:402:ILE:HB	2.02	0.59
1:B:1015:THR:O	1:B:1017:LEU:N	2.29	0.59
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.82	0.59
1:B:340:VAL:HG12	1:B:399:VAL:HG11	1.84	0.59
1:B:200:PRO:HG2	1:B:749:THR:HA	1.84	0.59
1:C:34:GLN:O	1:C:391:ASN:HB2	2.01	0.59
1:C:356:TYR:HB2	1:C:365:THR:HG21	1.84	0.59
1:C:777:ALA:HB1	1:C:781:MET:CE	2.33	0.59
1:B:14:VAL:HG21	1:C:890:ALA:HB2	1.83	0.59
1:B:418:ARG:HE	1:B:970:MET:CB	2.12	0.59
1:C:945:ILE:HD11	1:C:946:VAL:HG23	1.84	0.59
1:C:1011:MET:CE	1:C:1011:MET:CA	2.71	0.59
1:C:959:GLY:N	1:C:962:GLU:HB2	2.17	0.59
1:C:945:ILE:CD1	1:C:946:VAL:HG23	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:948:PHE:HB2	1:C:971:ARG:NH1	2.17	0.59
2:B:2000:P9D:C25	2:B:2000:P9D:C37	2.80	0.59
1:A:27:ILE:HD11	1:A:380:PHE:CD2	2.38	0.59
1:C:26:ALA:O	1:C:30:LEU:HD12	2.03	0.59
1:B:443:VAL:HG12	1:B:443:VAL:O	2.02	0.59
1:A:17:ILE:HG22	1:B:886:LEU:HD21	1.84	0.59
1:C:602:GLU:OE1	1:C:605:ASN:HB2	2.02	0.59
1:B:108:GLN:CD	1:C:112:GLN:HG3	2.23	0.59
1:C:1024:VAL:O	1:C:1028:VAL:HG23	2.03	0.59
1:A:945:ILE:C	1:A:947:GLU:H	2.06	0.58
1:C:782:LEU:O	1:C:785:ASP:HB2	2.02	0.58
1:C:492:LEU:O	1:C:496:MET:N	2.36	0.58
1:B:13:TRP:O	1:B:17:ILE:HG12	2.03	0.58
1:C:915:ALA:HB2	1:C:1009:GLY:HA3	1.85	0.58
1:A:1029:VAL:HG12	1:A:1029:VAL:O	2.03	0.58
1:A:965:LEU:O	1:A:969:ARG:HG2	2.02	0.58
1:B:281:PHE:CE2	1:B:608:SER:HB2	2.38	0.58
1:A:797:GLN:HA	1:A:797:GLN:HE21	1.69	0.58
1:A:735:LYS:O	1:A:739:LEU:HG	2.03	0.58
1:C:534:ILE:HG23	1:C:541:TYR:CE2	2.38	0.58
1:B:678:THR:HA	1:B:837:THR:CG2	2.34	0.58
1:A:728:LYS:HG3	1:A:729:ILE:N	2.17	0.58
1:B:616:GLY:HA3	1:B:624:THR:OG1	2.04	0.58
1:B:138:MET:SD	1:B:306:ILE:HD12	2.44	0.58
1:C:176:GLN:NE2	1:C:620:ARG:NH1	2.52	0.58
1:B:187:TRP:O	1:B:266:ALA:HB1	2.04	0.58
1:C:568:ASP:OD1	1:C:634:TRP:NE1	2.36	0.58
1:C:166:ILE:HG22	1:C:167:SER:N	2.19	0.58
1:B:603:LYS:O	1:B:604:ASN:CB	2.52	0.58
1:B:712:MET:HA	1:B:832:ALA:HB3	1.85	0.58
1:C:528:THR:HG21	1:C:969:ARG:HB3	1.86	0.57
1:A:684:LEU:HD11	1:A:855:VAL:CG1	2.32	0.57
1:C:559:LEU:HD12	1:C:560:PRO:HD2	1.85	0.57
1:A:817:GLU:OE1	1:A:825:MET:HA	2.04	0.57
1:B:602:GLU:O	1:B:603:LYS:O	2.22	0.57
1:A:4:PHE:CE2	1:A:8:ARG:HD3	2.39	0.57
1:A:235:ILE:HG22	1:B:728:LYS:CE	2.11	0.57
1:A:251:LEU:HD21	1:A:262:LEU:HD23	1.86	0.57
1:B:49:TYR:HE1	1:B:121:GLU:HG3	1.69	0.57
1:C:26:ALA:HA	1:C:29:LYS:HE2	1.86	0.57
1:B:153:ASP:HA	1:B:182:TYR:OH	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:PHE:CE2	1:A:564:LEU:HD12	2.39	0.57
1:B:68:ASN:OD1	1:B:114:ALA:HB2	2.04	0.57
1:A:355:MET:SD	1:A:410:ILE:HD11	2.44	0.57
1:B:328:ASP:O	1:B:330:THR:N	2.38	0.57
1:B:777:ALA:O	1:B:781:MET:HG2	2.04	0.57
1:C:987:MET:N	1:C:988:PRO:CD	2.67	0.57
1:C:695:LEU:CD2	1:C:825:MET:SD	2.93	0.57
1:C:36:PRO:O	1:C:38:ILE:HG23	2.04	0.57
1:C:241:THR:HG22	1:C:763:ILE:O	2.05	0.57
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.85	0.57
1:A:365:THR:O	1:A:368:PRO:HD2	2.04	0.57
1:B:695:LEU:HB3	1:B:825:MET:HE3	1.86	0.57
1:B:899:PHE:O	1:B:903:LEU:HG	2.05	0.57
1:A:343:THR:HA	1:A:346:GLU:HB2	1.86	0.57
1:B:764:ASP:HB3	1:B:769:LYS:HD2	1.86	0.57
1:B:536:ARG:HG3	1:B:537:SER:H	1.70	0.57
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.85	0.56
1:C:690:LEU:CD2	1:C:855:VAL:CG2	2.83	0.56
1:A:368:PRO:HD3	1:A:413:VAL:HG21	1.86	0.56
1:B:360:GLN:O	1:B:361:ASN:HB3	2.04	0.56
1:A:903:LEU:HD12	1:A:1025:PHE:HB3	1.87	0.56
1:A:534:ILE:HG13	1:A:541:TYR:CE1	2.40	0.56
1:B:485:ALA:O	1:B:490:PRO:HD3	2.05	0.56
1:C:681:ASP:HB3	1:C:860:THR:CG2	2.35	0.56
1:B:363:ARG:HD3	1:B:496:MET:O	2.05	0.56
1:C:774:MET:O	1:C:775:SER:CB	2.54	0.56
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.85	0.56
1:B:330:THR:HG22	1:B:331:PRO:HD3	1.86	0.56
1:B:298:ASN:CB	1:B:301:ASP:HB2	2.29	0.56
1:C:249:ILE:HB	1:C:262:LEU:HB2	1.87	0.56
1:A:131:LYS:O	1:A:131:LYS:HG3	2.04	0.56
1:C:243:THR:HG21	1:C:269:GLU:HA	1.86	0.56
1:C:200:PRO:HD2	1:C:749:THR:OG1	2.06	0.56
1:B:949:ALA:HB1	1:B:1026:PHE:CE2	2.40	0.56
1:A:485:ALA:O	1:A:490:PRO:CD	2.53	0.56
1:C:1021:PHE:O	1:C:1025:PHE:CD2	2.59	0.56
1:A:819:TYR:CE2	1:A:820:ASN:ND2	2.73	0.56
1:A:102:ILE:O	1:A:106:GLN:HG3	2.05	0.56
1:C:405:LEU:O	1:C:481:SER:HB2	2.05	0.56
1:A:310:LEU:HG	1:A:323:ILE:HD13	1.86	0.56
1:B:897:ILE:N	1:B:898:PRO:HD2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:LEU:HB3	1:B:825:MET:CE	2.36	0.56
1:B:706:ALA:CB	1:B:716:VAL:HG21	2.36	0.56
1:C:682:PHE:HB3	1:C:827:ILE:HG22	1.87	0.56
1:B:731:ILE:HD13	1:B:746:ILE:HD13	1.88	0.56
1:A:601:LYS:O	1:A:602:GLU:HG2	2.06	0.56
1:C:552:MET:HB2	1:C:910:ILE:HB	1.87	0.56
1:A:184:MET:HG2	1:A:246:PHE:CE1	2.41	0.56
1:B:11:PHE:CD1	1:C:890:ALA:HB1	2.41	0.56
1:B:210:GLN:O	1:B:240:LEU:HD11	2.06	0.55
1:B:111:LEU:HD11	1:B:127:VAL:CG1	2.37	0.55
1:C:773:VAL:O	1:C:773:VAL:HG23	2.05	0.55
1:A:896:SER:CB	1:A:1033:PHE:HB3	2.37	0.55
1:A:56:THR:HG23	1:C:213:GLN:HG2	1.87	0.55
1:B:578:LEU:CD2	1:B:587:THR:HG23	2.36	0.55
1:B:578:LEU:HD23	1:B:587:THR:HG23	1.87	0.55
1:C:1021:PHE:O	1:C:1024:VAL:HB	2.06	0.55
1:A:428:LYS:HB3	1:A:432:ARG:HH12	1.71	0.55
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.89	0.55
1:B:251:LEU:HD12	1:B:262:LEU:HA	1.87	0.55
1:B:223:PRO:HD3	1:C:275:TYR:HD1	1.72	0.55
1:C:143:ILE:HG23	1:C:286:ALA:HB2	1.88	0.55
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.37	0.55
1:A:234:ILE:HD12	1:B:727:PHE:HD2	1.71	0.55
1:B:219:LEU:HD11	1:C:727:PHE:HB2	1.88	0.55
1:A:339:GLU:O	1:A:343:THR:HG23	2.07	0.55
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.88	0.55
1:A:274:ASN:OD1	1:A:276:ASP:HB2	2.06	0.55
1:C:562:SER:O	1:C:924:ASP:HA	2.06	0.55
1:B:673:GLU:OE1	1:B:673:GLU:N	2.40	0.55
1:B:151:GLN:OE1	1:B:279:ALA:N	2.38	0.55
1:B:888:LEU:HB3	1:B:898:PRO:HB3	1.89	0.55
1:B:128:SER:HA	1:C:112:GLN:NE2	2.21	0.55
1:B:640:GLU:O	1:B:646:ALA:CB	2.55	0.55
1:B:38:ILE:H	1:B:38:ILE:HD12	1.70	0.55
1:A:492:LEU:O	1:A:496:MET:HB2	2.07	0.55
1:C:45:ILE:HD12	1:C:90:ILE:HB	1.88	0.55
2:B:2000:P9D:H25	2:B:2000:P9D:C37	2.24	0.55
1:A:38:ILE:HG12	1:A:38:ILE:O	2.07	0.55
1:C:671:ILE:O	1:C:671:ILE:HG13	2.06	0.55
1:B:399:VAL:HG23	1:B:399:VAL:O	2.07	0.55
1:C:685:ILE:HG22	1:C:686:ASP:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:680:PHE:O	1:C:828:LEU:HA	2.06	0.55
1:B:951:ASP:O	1:B:953:MET:N	2.40	0.55
1:A:968:VAL:HG21	1:A:1023:PRO:CG	2.29	0.55
1:B:578:LEU:HD21	1:B:587:THR:HA	1.89	0.55
1:A:760:ASN:O	1:A:771:VAL:HG23	2.07	0.55
1:B:200:PRO:CG	1:B:749:THR:HA	2.37	0.55
1:A:355:MET:SD	1:A:410:ILE:CD1	2.95	0.55
1:B:945:ILE:HG13	1:B:971:ARG:HG2	1.88	0.55
1:A:424:GLY:CA	1:A:502:LYS:HB2	2.37	0.55
1:B:325:TYR:CD1	1:B:325:TYR:N	2.74	0.54
1:C:897:ILE:O	1:C:901:VAL:HG23	2.06	0.54
1:C:531:VAL:HG11	1:C:968:VAL:HG11	1.88	0.54
1:C:1028:VAL:O	1:C:1032:ARG:CB	2.55	0.54
1:C:528:THR:HG22	1:C:969:ARG:HB3	1.89	0.54
1:B:396:PHE:O	1:B:400:LEU:HB2	2.08	0.54
1:C:618:ALA:HB2	1:C:719:ASN:OD1	2.07	0.54
1:A:425:LEU:HD12	1:A:425:LEU:H	1.72	0.54
1:C:219:LEU:HB3	1:C:230:LEU:HD21	1.88	0.54
1:C:183:ALA:N	1:C:271:GLY:O	2.37	0.54
1:C:736:ALA:HB1	1:C:741:VAL:HG21	1.89	0.54
1:B:728:LYS:HD2	1:B:730:ASP:HB2	1.88	0.54
1:A:216:ALA:O	1:A:234:ILE:HB	2.07	0.54
1:A:445:ILE:HA	1:A:448:VAL:HG12	1.88	0.54
1:B:775:SER:HB2	1:B:789:TRP:CZ2	2.41	0.54
1:C:143:ILE:CG2	1:C:286:ALA:HB2	2.37	0.54
1:C:831:ALA:HB2	1:C:840:ALA:HB2	1.90	0.54
1:A:197:GLN:O	1:A:792:ARG:NH1	2.41	0.54
1:A:344:LEU:O	1:A:348:ILE:HG12	2.07	0.54
1:C:192:GLU:O	1:C:196:PHE:HE2	1.90	0.54
1:C:952:LEU:HB3	1:C:958:LYS:HG3	1.88	0.54
1:B:611:ALA:HA	1:B:627:ALA:HA	1.90	0.54
1:A:934:THR:O	1:A:935:ILE:C	2.46	0.54
1:B:610:PHE:HB3	1:B:628:PHE:HB2	1.90	0.54
1:C:399:VAL:HG11	1:C:989:LEU:HD22	1.89	0.54
1:C:447:MET:HE2	1:C:447:MET:HA	1.88	0.54
1:C:228:GLN:OE1	1:C:228:GLN:HA	2.08	0.54
1:A:110:LYS:O	1:A:113:LEU:HB2	2.07	0.54
1:B:223:PRO:HD2	1:C:780:ARG:NH2	2.22	0.54
1:C:799:VAL:HG22	1:C:800:PRO:O	2.08	0.54
1:C:326:PRO:HG3	1:C:610:PHE:HD1	1.72	0.54
1:A:762:PHE:CZ	1:A:764:ASP:HB2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:HD22	1:B:417:GLU:HG3	1.89	0.54
1:A:375:VAL:HA	1:A:480:LEU:HD12	1.88	0.54
1:B:435:MET:HA	1:B:438:ILE:HG12	1.90	0.54
1:B:154:ILE:O	1:B:158:VAL:HG23	2.08	0.54
1:A:242:SER:OG	1:A:245:GLU:HG3	2.08	0.54
1:B:660:ASP:O	1:B:661:ALA:HB3	2.08	0.54
1:C:773:VAL:CG2	1:C:773:VAL:O	2.56	0.54
1:B:66:GLU:C	1:B:68:ASN:H	2.11	0.54
1:B:367:ILE:HG21	1:B:413:VAL:HG23	1.90	0.54
1:C:878:ALA:O	1:C:882:ILE:HG12	2.06	0.54
1:A:363:ARG:HG2	1:A:366:LEU:HD23	1.90	0.54
1:C:231:ASN:C	1:C:231:ASN:ND2	2.60	0.54
1:A:896:SER:HB3	1:A:1033:PHE:CD2	2.43	0.54
1:A:727:PHE:CE1	1:A:783:PRO:HB3	2.42	0.54
1:A:896:SER:HB2	1:A:1033:PHE:HB3	1.88	0.54
1:B:758:TYR:CE1	1:B:770:LYS:HG2	2.43	0.54
1:C:897:ILE:HD13	1:C:950:LYS:HD2	1.90	0.53
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.41	0.53
1:C:356:TYR:O	1:C:360:GLN:N	2.41	0.53
1:A:159:ALA:HB1	1:A:181:GLN:HB2	1.89	0.53
1:C:941:ASN:O	1:C:942:ALA:HB2	2.08	0.53
1:B:931:LEU:O	1:B:935:ILE:CG1	2.46	0.53
1:B:406:VAL:O	1:B:409:ALA:N	2.42	0.53
1:B:851:LEU:HB3	1:B:852:PRO:HD2	1.91	0.53
1:C:11:PHE:HE1	1:C:15:ILE:HD11	1.73	0.53
1:B:693:GLU:O	1:B:697:GLN:HG3	2.09	0.53
1:C:515:TRP:HE3	1:C:515:TRP:O	1.90	0.53
1:B:733:GLN:OE1	1:B:743:ILE:HD11	2.07	0.53
1:A:252:LYS:HG3	1:A:260:VAL:HG23	1.90	0.53
1:C:568:ASP:OD2	1:C:644:VAL:HG23	2.08	0.53
1:C:631:LEU:HD11	1:C:644:VAL:HG22	1.91	0.53
1:C:552:MET:HG2	1:C:913:LEU:CD1	2.38	0.53
1:B:604:ASN:H	1:B:632:LYS:NZ	2.04	0.53
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.43	0.53
1:C:782:LEU:N	1:C:785:ASP:OD2	2.41	0.53
1:B:274:ASN:OD1	1:B:276:ASP:HB2	2.08	0.53
1:C:176:GLN:HE22	1:C:620:ARG:HH11	1.56	0.53
1:A:339:GLU:HG3	1:A:995:ALA:HB3	1.89	0.53
1:B:80:SER:HB2	1:B:90:ILE:HG12	1.91	0.53
1:B:280:GLU:HB2	1:B:284:GLN:O	2.08	0.53
1:A:219:LEU:O	1:A:231:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:ILE:HG13	1:A:971:ARG:HG2	1.90	0.53
1:B:164:ASP:HA	1:B:167:SER:HB2	1.91	0.53
1:B:194:ASN:ND2	1:B:790:TYR:CD1	2.77	0.53
1:B:168:ARG:HB2	1:B:168:ARG:NH1	2.22	0.53
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.91	0.53
1:B:168:ARG:CB	1:B:168:ARG:HH11	2.21	0.53
1:C:499:PRO:O	1:C:500:ILE:HD13	2.09	0.53
1:C:939:ALA:O	1:C:943:ILE:HG12	2.09	0.53
1:A:146:ASP:CB	1:A:148:THR:HG23	2.38	0.53
1:B:712:MET:O	1:B:713:LEU:HB2	2.07	0.53
1:B:417:GLU:HA	1:B:417:GLU:OE2	2.08	0.53
1:A:78:MET:O	1:A:78:MET:HG2	2.09	0.53
1:B:213:GLN:HB2	1:B:238:THR:HA	1.91	0.53
1:C:1011:MET:O	1:C:1015:THR:OG1	2.25	0.53
1:C:880:SER:O	1:C:884:VAL:HG23	2.09	0.53
1:B:463:THR:HA	1:B:466:ILE:HD12	1.91	0.53
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.91	0.52
1:B:719:ASN:HB3	1:B:826:GLU:HB3	1.90	0.52
1:B:896:SER:O	1:B:899:PHE:HB2	2.09	0.52
1:A:34:GLN:NE2	1:A:332:PHE:HE2	2.07	0.52
1:B:610:PHE:O	1:B:628:PHE:N	2.22	0.52
1:C:910:ILE:HA	1:C:913:LEU:HD12	1.89	0.52
1:C:40:PRO:HB2	1:C:94:PHE:O	2.09	0.52
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.91	0.52
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.89	0.52
1:C:571:VAL:HG12	1:C:630:SER:HA	1.91	0.52
1:A:964:THR:O	1:A:968:VAL:HG12	2.08	0.52
1:A:510:LYS:HA	1:A:514:GLY:HA3	1.92	0.52
1:B:575:MET:HA	1:B:575:MET:HE2	1.90	0.52
1:A:373:PRO:O	1:A:377:LEU:HB2	2.10	0.52
1:C:847:LEU:H	1:C:847:LEU:CD1	2.23	0.52
1:B:706:ALA:HB3	1:B:716:VAL:HG21	1.92	0.52
1:B:367:ILE:HG21	1:B:413:VAL:CG2	2.38	0.52
2:B:2000:P9D:H43A	2:B:2000:P9D:C35	2.39	0.52
1:C:524:THR:O	1:C:528:THR:HG23	2.08	0.52
1:B:214:VAL:HG21	1:C:747:ASN:OD1	2.10	0.52
1:C:746:ILE:HD12	1:C:791:VAL:HG11	1.92	0.52
1:B:600:THR:C	1:B:602:GLU:N	2.60	0.52
1:A:781:MET:O	1:A:782:LEU:HD23	2.10	0.52
1:A:743:ILE:HA	1:A:746:ILE:HG13	1.91	0.52
1:C:213:GLN:NE2	1:C:238:THR:HB	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:THR:HA	1:B:665:ALA:HA	1.92	0.52
1:A:487:ILE:HG22	1:A:488:LEU:N	2.25	0.52
1:B:14:VAL:CG2	1:B:15:ILE:H	2.23	0.52
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.10	0.52
1:A:904:VAL:HG21	1:A:942:ALA:HB1	1.91	0.52
1:C:951:ASP:O	1:C:955:LYS:CB	2.58	0.52
1:A:341:VAL:O	1:A:345:VAL:HG23	2.09	0.52
1:B:348:ILE:HD11	1:B:372:VAL:CG1	2.40	0.52
1:A:168:ARG:CG	1:B:69:MET:O	2.54	0.51
1:B:623:ASN:OD1	1:B:624:THR:HG22	2.09	0.51
1:C:445:ILE:HG23	1:C:940:LYS:HB3	1.93	0.51
1:B:277:ILE:HD12	1:B:278:ILE:N	2.26	0.51
1:C:431:THR:O	1:C:433:LYS:N	2.43	0.51
1:B:138:MET:HB3	1:B:328:ASP:HA	1.92	0.51
1:C:690:LEU:CD2	1:C:855:VAL:HG23	2.40	0.51
1:C:636:ASP:C	1:C:638:PRO:HD3	2.30	0.51
1:C:808:ARG:HG3	1:C:809:TRP:N	2.24	0.51
1:B:199:THR:HB	1:B:201:VAL:HG23	1.92	0.51
1:A:142:VAL:HG12	1:A:154:ILE:HG21	1.92	0.51
1:B:186:ILE:CD1	1:B:186:ILE:H	2.21	0.51
1:B:851:LEU:HB3	1:B:852:PRO:CD	2.41	0.51
1:B:1010:GLY:O	1:B:1014:ALA:HB2	2.11	0.51
1:B:314:GLU:N	1:B:315:PRO:HD2	2.26	0.51
1:A:169:THR:O	1:A:170:SER:C	2.48	0.51
1:A:214:VAL:HG22	1:A:236:ALA:HB3	1.91	0.51
1:C:18:ILE:HG22	1:C:19:ILE:HD13	1.93	0.51
1:C:955:LYS:HA	1:C:955:LYS:HE3	1.92	0.51
1:A:449:LEU:HA	1:A:452:VAL:HG12	1.91	0.51
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.91	0.51
1:B:442:LEU:HA	1:B:445:ILE:HG12	1.93	0.51
1:C:356:TYR:O	1:C:358:PHE:N	2.43	0.51
1:B:28:LEU:O	1:B:29:LYS:HG3	2.09	0.51
1:A:141:GLY:O	1:A:142:VAL:HG23	2.10	0.51
1:C:370:ILE:O	1:C:370:ILE:HG22	2.11	0.51
1:A:92:LEU:N	1:A:92:LEU:CD1	2.66	0.51
1:C:307:ARG:HA	1:C:310:LEU:HB2	1.93	0.51
1:A:13:TRP:HA	1:A:13:TRP:HE3	1.74	0.51
1:C:26:ALA:HA	1:C:29:LYS:HG2	1.93	0.51
1:A:332:PHE:CE2	1:A:569:GLN:HG2	2.46	0.51
1:C:493:CYS:HB3	1:C:497:LEU:HD12	1.93	0.51
1:B:668:LEU:HD13	2:B:2000:P9D:H5B	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.41	0.51
1:C:396:PHE:CD2	1:C:1003:VAL:HG21	2.45	0.51
1:C:453:PHE:HZ	1:C:933:THR:HG23	1.76	0.51
1:B:225:VAL:HG21	1:C:778:LYS:HB3	1.92	0.51
1:A:252:LYS:O	1:A:260:VAL:HG23	2.11	0.51
1:C:101:ASP:OD1	1:C:131:LYS:CE	2.59	0.50
1:B:178:PHE:HB3	2:B:2000:P9D:H26	1.93	0.50
1:A:637:ARG:HA	1:A:642:ASN:HD22	1.77	0.50
1:A:897:ILE:N	1:A:898:PRO:HD2	2.26	0.50
1:C:980:LEU:HA	1:C:983:ILE:HB	1.93	0.50
1:C:355:MET:O	1:C:359:LEU:HB2	2.11	0.50
1:B:168:ARG:HB2	1:B:168:ARG:HH11	1.75	0.50
1:B:318:PRO:HD2	1:B:321:LEU:HD22	1.93	0.50
1:A:58:GLN:NE2	1:A:59:ASP:OD1	2.35	0.50
1:C:554:TYR:O	1:C:558:ARG:HB2	2.10	0.50
1:B:426:PRO:CB	1:B:427:PRO:HD2	2.41	0.50
1:B:650:ARG:O	1:B:654:ALA:CB	2.58	0.50
1:A:273:GLU:HG2	1:A:772:TYR:HE2	1.75	0.50
1:C:669:PRO:HD3	1:C:678:THR:N	2.27	0.50
1:B:127:VAL:CG1	1:B:128:SER:H	2.22	0.50
1:B:660:ASP:O	1:B:661:ALA:CB	2.59	0.50
1:A:30:LEU:HB3	1:A:390:ILE:HG12	1.94	0.50
1:B:602:GLU:OE1	1:B:647:ILE:HG23	2.12	0.50
1:A:375:VAL:HG13	1:A:480:LEU:HB3	1.94	0.50
1:A:181:GLN:OE1	1:A:767:ARG:NH2	2.45	0.50
1:C:216:ALA:HB2	1:C:236:ALA:HB2	1.94	0.50
1:B:818:ARG:NH1	1:B:821:GLY:O	2.36	0.50
1:C:190:PRO:O	1:C:194:ASN:HB3	2.12	0.50
1:C:707:ALA:O	1:C:710:PRO:HD3	2.12	0.50
1:A:38:ILE:H	1:A:38:ILE:HD13	1.76	0.50
1:A:971:ARG:O	1:A:974:PRO:HG2	2.12	0.50
1:C:1017:LEU:O	1:C:1021:PHE:HB2	2.12	0.50
1:C:741:VAL:HG23	1:C:742:SER:N	2.27	0.50
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.94	0.49
1:B:317:PHE:HE2	1:B:323:ILE:HD11	1.75	0.49
1:C:1012:VAL:HG12	1:C:1013:THR:HG23	1.94	0.49
1:B:927:PHE:CE2	1:B:931:LEU:HD11	2.46	0.49
1:C:973:ARG:O	1:C:977:MET:HG3	2.12	0.49
1:C:150:THR:HG23	1:C:153:ASP:HB2	1.93	0.49
1:A:361:ASN:O	1:A:365:THR:HG23	2.11	0.49
1:A:683:GLU:HG3	1:A:819:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:HZ	1:A:933:THR:HA	1.76	0.49
1:A:142:VAL:HG11	1:A:321:LEU:HD21	1.89	0.49
1:A:416:VAL:HG21	1:A:431:THR:HG22	1.94	0.49
1:A:683:GLU:HG2	1:A:860:THR:HG21	1.94	0.49
1:C:355:MET:HB3	1:C:365:THR:HG23	1.93	0.49
1:B:993:THR:CA	1:B:997:SER:HB3	2.42	0.49
1:C:753:ALA:HA	1:C:774:MET:O	2.12	0.49
1:C:139:VAL:O	1:C:139:VAL:HG12	2.11	0.49
1:B:613:ASN:C	1:B:613:ASN:ND2	2.66	0.49
1:C:552:MET:C	1:C:554:TYR:H	2.16	0.49
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.94	0.49
1:B:919:ARG:NE	1:B:1005:THR:HG21	2.27	0.49
1:C:1:MET:H3	1:C:2:PRO:HD2	1.77	0.49
1:C:808:ARG:HG3	1:C:809:TRP:H	1.78	0.49
1:B:571:VAL:HG12	1:B:630:SER:HA	1.94	0.49
1:A:415:ASN:O	1:A:415:ASN:ND2	2.45	0.49
1:A:150:THR:O	1:A:154:ILE:HG13	2.13	0.49
1:A:423:GLU:HB3	1:A:425:LEU:HD12	1.95	0.49
1:B:225:VAL:H	1:C:781:MET:HE1	1.78	0.49
1:A:331:PRO:O	1:A:335:ILE:HG12	2.13	0.49
1:A:640:GLU:O	1:A:646:ALA:CB	2.61	0.49
1:B:286:ALA:O	1:B:287:SER:HB2	2.13	0.49
1:C:563:PHE:HB2	1:C:866:GLU:HB2	1.95	0.49
1:B:375:VAL:HG21	1:B:481:SER:HA	1.94	0.49
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.95	0.49
1:C:359:LEU:HG	1:C:977:MET:CE	2.43	0.49
1:B:600:THR:O	1:B:601:LYS:C	2.51	0.49
1:A:416:VAL:CG1	1:A:431:THR:HG22	2.42	0.49
1:A:522:LYS:HE3	1:A:526:HIS:CE1	2.48	0.49
1:A:252:LYS:CG	1:A:260:VAL:HG21	2.43	0.49
1:A:781:MET:CE	1:C:220:GLY:HA2	2.43	0.49
1:B:527:TYR:O	1:B:530:SER:HB3	2.13	0.49
1:A:142:VAL:HG12	1:A:154:ILE:CG2	2.42	0.49
1:C:340:VAL:CG2	1:C:396:PHE:HE1	2.26	0.49
1:C:764:ASP:HB3	1:C:769:LYS:HZ2	1.78	0.49
1:A:423:GLU:HB3	1:A:425:LEU:CD1	2.42	0.49
1:A:214:VAL:HG23	1:A:215:ALA:N	2.28	0.49
1:B:268:ILE:O	1:B:268:ILE:HG22	2.13	0.49
1:A:987:MET:HA	1:A:990:VAL:HG22	1.94	0.49
1:C:335:ILE:HG23	1:C:336:SER:N	2.26	0.49
1:C:836:SER:HB2	1:C:922:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768:VAL:HB	1:C:60:THR:HG22	1.95	0.49
1:B:562:SER:HA	1:B:677:ALA:HB1	1.94	0.49
1:B:307:ARG:HH11	1:B:307:ARG:HG3	1.78	0.49
1:A:203:VAL:HG13	1:A:262:LEU:CD2	2.39	0.48
1:B:251:LEU:CD1	1:B:262:LEU:HA	2.42	0.48
1:B:643:LYS:O	1:B:647:ILE:HG13	2.12	0.48
1:C:758:TYR:CE2	1:C:770:LYS:HG3	2.48	0.48
1:B:731:ILE:HD11	1:B:746:ILE:CG2	2.41	0.48
1:A:14:VAL:HG11	1:B:886:LEU:O	2.13	0.48
1:C:456:MET:HG2	1:C:467:TYR:HB3	1.95	0.48
1:A:344:LEU:HD21	1:A:376:LEU:CD2	2.42	0.48
1:A:302:THR:O	1:A:306:ILE:HG13	2.13	0.48
1:B:523:SER:HA	1:B:526:HIS:HB2	1.94	0.48
1:B:888:LEU:CD1	1:B:943:ILE:HD11	2.32	0.48
1:A:193:LEU:HB3	1:A:198:LEU:O	2.14	0.48
1:C:978:THR:OG1	1:C:979:SER:N	2.46	0.48
1:C:785:ASP:O	1:C:786:ILE:C	2.50	0.48
1:C:367:ILE:HG22	1:C:489:THR:HG23	1.96	0.48
1:A:156:ASP:CG	1:A:182:TYR:CD2	2.86	0.48
1:A:925:VAL:HG12	1:A:926:TYR:N	2.27	0.48
1:C:894:SER:HB3	1:C:898:PRO:HD3	1.94	0.48
1:C:904:VAL:HG23	1:C:907:LEU:HD21	1.94	0.48
1:B:682:PHE:HE1	1:B:684:LEU:HD12	1.78	0.48
1:A:445:ILE:O	1:A:449:LEU:N	2.39	0.48
1:C:542:LEU:HA	1:C:545:TYR:HB3	1.95	0.48
1:B:960:LEU:HD22	1:B:1031:ARG:NH1	2.29	0.48
1:B:379:THR:O	1:B:381:ALA:N	2.46	0.48
1:C:754:TRP:CZ2	1:C:786:ILE:HD13	2.48	0.48
1:C:973:ARG:HB3	1:C:974:PRO:CD	2.43	0.48
1:A:428:LYS:HB3	1:A:432:ARG:NH1	2.29	0.48
1:B:523:SER:HA	1:B:526:HIS:CB	2.43	0.48
1:C:590:VAL:O	1:C:594:VAL:HG23	2.14	0.48
1:C:916:ALA:HB1	1:C:921:LEU:HB2	1.94	0.48
1:B:676:THR:HG23	1:B:679:GLY:HA3	1.95	0.48
1:A:213:GLN:HE21	1:B:56:THR:CA	2.22	0.48
1:B:655:PHE:CA	1:B:658:ILE:HD11	2.39	0.48
1:B:658:ILE:N	1:B:658:ILE:HD13	2.27	0.48
1:A:938:SER:C	1:A:940:LYS:H	2.17	0.48
1:B:30:LEU:HD13	1:B:384:ALA:CB	2.44	0.48
1:B:360:GLN:C	1:B:361:ASN:HD22	2.16	0.48
1:A:523:SER:HA	1:A:526:HIS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:VAL:HG21	1:B:591:LEU:HD23	1.95	0.48
1:B:1:MET:N	1:B:2:PRO:HD2	2.29	0.48
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.48	0.48
1:C:114:ALA:O	1:C:117:LEU:HB2	2.14	0.48
1:A:548:ILE:O	1:A:910:ILE:HD12	2.13	0.48
1:B:265:VAL:O	1:B:266:ALA:HB2	2.14	0.48
1:A:967:ALA:O	1:A:969:ARG:N	2.43	0.48
1:A:636:ASP:N	1:A:636:ASP:OD1	2.46	0.48
1:B:636:ASP:N	1:B:636:ASP:OD2	2.47	0.48
1:C:384:ALA:O	1:C:385:ALA:C	2.53	0.48
1:C:213:GLN:NE2	1:C:238:THR:HA	2.30	0.47
1:B:335:ILE:HG21	1:B:995:ALA:CB	2.42	0.47
1:B:14:VAL:CG2	1:B:15:ILE:N	2.77	0.47
1:B:443:VAL:O	1:B:443:VAL:CG1	2.61	0.47
1:A:34:GLN:O	1:A:391:ASN:HB2	2.13	0.47
1:A:886:LEU:O	1:C:14:VAL:HG11	2.14	0.47
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.96	0.47
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.96	0.47
1:B:45:ILE:O	1:B:89:GLN:HA	2.14	0.47
1:C:808:ARG:CG	1:C:809:TRP:N	2.76	0.47
1:C:314:GLU:HA	1:C:317:PHE:CD2	2.49	0.47
1:C:274:ASN:C	1:C:274:ASN:HD22	2.17	0.47
1:C:349:ILE:C	1:C:351:VAL:H	2.18	0.47
1:B:184:MET:HG3	1:B:186:ILE:HD11	1.96	0.47
1:B:99:ASP:OD1	1:B:101:ASP:HB2	2.14	0.47
1:B:11:PHE:CE1	1:C:890:ALA:HB1	2.49	0.47
1:A:223:PRO:HD2	1:B:780:ARG:NH1	2.30	0.47
1:C:699:ARG:HG3	1:C:827:ILE:HD11	1.96	0.47
1:A:424:GLY:HA3	1:A:502:LYS:HB2	1.96	0.47
1:A:808:ARG:HG3	1:A:808:ARG:HH11	1.78	0.47
1:B:697:GLN:O	1:B:698:ALA:C	2.51	0.47
1:B:709:HIS:N	1:B:710:PRO:HD3	2.29	0.47
1:A:590:VAL:O	1:A:593:GLU:HB2	2.14	0.47
1:B:728:LYS:C	1:B:728:LYS:HD3	2.35	0.47
1:A:681:ASP:HB3	1:A:860:THR:HG23	1.97	0.47
1:B:466:ILE:O	1:B:469:GLN:HB2	2.15	0.47
1:B:218:GLN:HB2	1:B:233:SER:HA	1.96	0.47
1:B:612:VAL:HB	1:B:626:ILE:HG22	1.95	0.47
1:C:971:ARG:HA	1:C:974:PRO:HG2	1.96	0.47
1:C:399:VAL:CG1	1:C:989:LEU:CD2	2.92	0.47
1:B:713:LEU:H	1:B:832:ALA:CB	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:PHE:O	1:C:491:ALA:HB2	2.14	0.47
1:A:13:TRP:CZ3	1:A:492:LEU:HD11	2.50	0.47
1:A:224:PRO:HA	1:B:781:MET:HE3	1.97	0.47
1:A:393:LEU:HD11	1:A:466:ILE:HG23	1.96	0.47
1:B:682:PHE:HE1	1:B:684:LEU:CD1	2.26	0.47
1:A:52:ALA:HB2	1:C:215:ALA:HB2	1.96	0.47
1:C:403:GLY:HA3	1:C:982:PHE:HA	1.96	0.47
1:C:587:THR:HG22	1:C:591:LEU:HD12	1.95	0.47
1:A:177:LEU:O	1:A:177:LEU:HD13	2.15	0.47
1:A:459:PHE:HB2	1:A:464:GLY:HA3	1.97	0.47
1:C:160:ALA:HB1	1:C:767:ARG:HD3	1.96	0.47
1:C:458:PHE:N	1:C:458:PHE:CD1	2.82	0.47
1:C:450:SER:O	1:C:451:ALA:C	2.53	0.47
1:A:994:GLY:O	1:A:995:ALA:C	2.53	0.47
1:C:960:LEU:HD21	1:C:1027:VAL:HA	1.96	0.47
1:A:155:SER:OG	1:A:179:GLY:HA3	2.15	0.47
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.97	0.47
1:A:10:ILE:O	1:A:14:VAL:HG23	2.14	0.47
1:A:463:THR:HG22	1:A:467:TYR:HE2	1.80	0.47
1:A:648:THR:O	1:A:651:ALA:HB3	2.15	0.47
1:A:63:GLN:O	1:A:67:GLN:HG3	2.14	0.47
1:C:597:TYR:CD1	1:C:597:TYR:C	2.88	0.47
1:C:555:LEU:HD22	1:C:917:THR:HG21	1.96	0.47
1:C:937:LEU:C	1:C:939:ALA:H	2.19	0.47
1:B:210:GLN:O	1:B:240:LEU:CD1	2.63	0.47
1:B:575:MET:HA	1:B:575:MET:CE	2.44	0.47
1:B:218:GLN:HA	1:B:234:ILE:HG13	1.97	0.47
1:A:621:GLY:HA3	1:A:624:THR:HG22	1.97	0.47
1:C:349:ILE:HA	1:C:349:ILE:HD13	1.81	0.46
1:C:192:GLU:HB3	1:C:265:VAL:HA	1.96	0.46
1:B:242:SER:HB2	1:B:244:GLU:OE2	2.14	0.46
1:A:801:PHE:HA	1:A:804:PHE:CZ	2.50	0.46
1:C:49:TYR:O	1:C:50:PRO:C	2.52	0.46
1:C:180:SER:OG	1:C:273:GLU:N	2.45	0.46
1:C:897:ILE:CD1	1:C:950:LYS:HD2	2.45	0.46
1:B:817:GLU:OE1	1:B:826:GLU:N	2.45	0.46
1:B:982:PHE:O	1:B:985:GLY:N	2.48	0.46
1:B:449:LEU:O	1:B:453:PHE:HD2	1.98	0.46
1:A:754:TRP:CH2	1:A:780:ARG:HA	2.50	0.46
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.97	0.46
1:B:733:GLN:OE1	1:B:743:ILE:CD1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:ND2	1:A:149:MET:H	2.14	0.46
1:B:638:PRO:HD2	1:B:642:ASN:ND2	2.22	0.46
1:C:847:LEU:N	1:C:847:LEU:HD12	2.29	0.46
1:B:891:LEU:HD12	1:B:891:LEU:O	2.16	0.46
1:B:442:LEU:O	1:B:445:ILE:HB	2.15	0.46
1:A:263:ARG:HG2	1:A:263:ARG:NH1	2.31	0.46
1:B:606:VAL:HG23	1:B:629:VAL:HG13	1.98	0.46
1:C:713:LEU:HG	1:C:843:LEU:HD23	1.97	0.46
1:A:230:LEU:HD22	1:B:782:LEU:HD23	1.97	0.46
1:A:314:GLU:N	1:A:315:PRO:HD2	2.30	0.46
1:C:402:ILE:HA	1:C:402:ILE:HD13	1.80	0.46
1:C:219:LEU:HG	1:C:234:ILE:HD11	1.98	0.46
1:B:163:LYS:O	1:B:167:SER:HB2	2.14	0.46
1:A:224:PRO:HA	1:B:781:MET:CE	2.45	0.46
1:C:699:ARG:HB3	1:C:699:ARG:HE	1.33	0.46
1:C:958:LYS:HB2	1:C:963:ALA:HB2	1.98	0.46
1:A:593:GLU:O	1:A:596:HIS:HB3	2.16	0.46
1:B:712:MET:O	1:B:713:LEU:HD13	2.16	0.46
1:B:702:LEU:HB2	1:B:851:LEU:HD11	1.97	0.46
1:B:188:MET:SD	1:B:200:PRO:HB3	2.56	0.46
1:C:314:GLU:HA	1:C:317:PHE:CE2	2.50	0.46
1:C:651:ALA:HA	1:C:654:ALA:HB3	1.97	0.46
1:C:61:VAL:CG2	1:C:122:VAL:HG21	2.45	0.46
1:C:282:ASN:O	1:C:284:GLN:N	2.49	0.46
1:C:136:PHE:HE2	1:C:617:PHE:CZ	2.34	0.46
1:A:662:MET:SD	1:A:664:PHE:HD1	2.39	0.46
1:A:263:ARG:HG2	1:A:263:ARG:HH11	1.80	0.46
1:C:351:VAL:HG12	1:C:355:MET:HE2	1.97	0.46
1:C:681:ASP:O	1:C:859:TRP:HE3	1.99	0.46
1:C:759:VAL:HG21	1:C:773:VAL:HG13	1.97	0.46
1:A:446:ALA:HB3	1:A:482:VAL:HG21	1.98	0.46
1:B:577:GLN:OE1	1:B:624:THR:HB	2.16	0.46
1:B:775:SER:HB2	1:B:789:TRP:CH2	2.51	0.46
1:C:52:ALA:HB3	1:C:57:VAL:HG23	1.98	0.46
1:C:415:ASN:HD22	1:C:434:SER:HB2	1.80	0.46
1:B:904:VAL:HA	1:B:907:LEU:HD13	1.97	0.46
1:A:213:GLN:CD	1:A:238:THR:HG22	2.35	0.46
1:C:400:LEU:C	1:C:402:ILE:H	2.19	0.46
1:C:347:ALA:HB1	1:C:402:ILE:HG21	1.98	0.46
1:C:485:ALA:HA	1:C:489:THR:CB	2.44	0.46
1:B:379:THR:C	1:B:381:ALA:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:SER:OG	1:C:806:SER:N	2.49	0.46
1:B:45:ILE:HG23	1:B:129:VAL:HG12	1.96	0.46
1:A:131:LYS:C	1:A:295:THR:HG22	2.35	0.46
1:A:437:GLN:HG3	1:A:438:ILE:N	2.30	0.46
1:A:727:PHE:CE2	1:A:807:SER:HB2	2.51	0.46
1:A:156:ASP:O	1:A:157:TYR:C	2.52	0.46
1:A:989:LEU:HD22	1:A:1000:GLN:HB3	1.96	0.46
1:A:697:GLN:O	1:A:700:ASN:N	2.49	0.46
1:B:35:TYR:OH	1:B:670:ALA:HB1	2.15	0.46
1:C:380:PHE:HA	1:C:383:LEU:HB2	1.98	0.46
1:B:104:GLN:O	1:B:108:GLN:HB3	2.16	0.45
1:C:330:THR:HA	1:C:333:VAL:HG23	1.98	0.45
1:C:937:LEU:HB3	1:C:1011:MET:CE	2.47	0.45
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.96	0.45
1:A:474:ILE:CG2	1:A:475:VAL:N	2.77	0.45
1:C:774:MET:O	1:C:775:SER:HB3	2.17	0.45
1:A:640:GLU:O	1:A:646:ALA:HB2	2.16	0.45
1:B:35:TYR:HB3	1:B:36:PRO:HD2	1.98	0.45
1:A:835:LYS:HB3	1:A:839:GLU:OE1	2.16	0.45
1:B:61:VAL:O	1:B:65:ILE:HG13	2.15	0.45
1:B:277:ILE:HG13	2:B:2000:P9D:N31	2.31	0.45
1:B:326:PRO:HG3	1:B:610:PHE:CD2	2.51	0.45
1:C:762:PHE:HB3	1:C:771:VAL:HG21	1.98	0.45
1:B:945:ILE:HG13	1:B:971:ARG:CG	2.46	0.45
1:B:348:ILE:HD11	1:B:372:VAL:HG12	1.97	0.45
1:B:1019:ILE:HG13	1:B:1020:PHE:H	1.81	0.45
1:B:817:GLU:OE1	1:B:825:MET:HA	2.16	0.45
1:C:300:LEU:HD12	1:C:333:VAL:HG11	1.98	0.45
1:A:527:TYR:CE2	1:A:972:LEU:HG	2.51	0.45
1:C:723:ASP:OD1	1:C:723:ASP:N	2.43	0.45
1:B:728:LYS:HD3	1:B:729:ILE:N	2.31	0.45
1:C:372:VAL:HA	1:C:405:LEU:HD21	1.97	0.45
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.98	0.45
1:A:967:ALA:C	1:A:969:ARG:H	2.18	0.45
1:A:356:TYR:O	1:A:360:GLN:N	2.42	0.45
1:C:972:LEU:HG	1:C:976:LEU:HD13	1.99	0.45
1:C:986:VAL:O	1:C:990:VAL:HG23	2.17	0.45
1:A:991:ILE:O	1:A:991:ILE:HG23	2.16	0.45
1:C:894:SER:O	1:C:895:TRP:HB2	2.15	0.45
1:A:792:ARG:HG2	1:A:793:ALA:O	2.17	0.45
1:B:281:PHE:O	1:B:282:ASN:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.52	0.45
1:A:886:LEU:HB3	1:C:14:VAL:HG22	1.99	0.45
1:C:589:LYS:HA	1:C:592:ASN:HD22	1.81	0.45
1:A:893:GLU:O	1:C:10:ILE:HG13	2.16	0.45
1:A:235:ILE:HD13	1:B:726:GLN:HB2	1.99	0.45
1:A:987:MET:HE2	1:A:990:VAL:HG21	1.98	0.45
1:A:1030:ARG:HD2	1:A:1030:ARG:HA	1.61	0.45
1:B:291:ILE:HD12	1:B:291:ILE:N	2.32	0.45
1:A:543:VAL:O	1:A:547:ILE:HD13	2.16	0.45
1:C:505:HIS:HD2	1:C:517:ASN:HD22	1.65	0.45
1:B:330:THR:HG22	1:B:331:PRO:CD	2.47	0.45
1:A:10:ILE:HG23	1:B:895:TRP:HD1	1.81	0.45
1:A:38:ILE:N	1:A:38:ILE:HD13	2.32	0.45
1:B:317:PHE:CZ	1:B:323:ILE:HD11	2.51	0.45
1:A:577:GLN:O	1:A:578:LEU:HD12	2.16	0.45
1:A:991:ILE:O	1:A:991:ILE:CG2	2.65	0.45
1:B:169:THR:O	1:B:172:VAL:HG13	2.17	0.45
1:B:391:ASN:O	1:B:392:THR:C	2.55	0.45
1:A:837:THR:O	1:A:841:MET:HG3	2.16	0.45
1:B:835:LYS:HG2	1:B:839:GLU:OE1	2.17	0.45
1:B:968:VAL:CG2	1:B:1023:PRO:HB3	2.47	0.45
1:B:344:LEU:HD22	1:B:376:LEU:HD11	1.99	0.45
1:A:378:GLY:O	1:A:382:VAL:HG23	2.17	0.45
1:B:127:VAL:CG1	1:B:128:SER:N	2.78	0.44
1:C:111:LEU:O	1:C:112:GLN:C	2.56	0.44
1:B:225:VAL:N	1:C:781:MET:HE1	2.32	0.44
1:B:359:LEU:HD23	1:B:973:ARG:NH1	2.32	0.44
1:A:34:GLN:HE21	1:A:332:PHE:HE2	1.64	0.44
1:A:578:LEU:HD11	1:A:590:VAL:HG21	1.99	0.44
1:B:600:THR:C	1:B:602:GLU:H	2.20	0.44
1:C:686:ASP:HB2	1:C:695:LEU:HD12	1.99	0.44
1:B:775:SER:HB3	1:B:780:ARG:HD3	1.98	0.44
1:C:155:SER:O	1:C:158:VAL:HG12	2.16	0.44
1:C:674:LEU:HD23	1:C:674:LEU:HA	1.64	0.44
1:A:941:ASN:HA	1:A:944:LEU:HB2	1.99	0.44
1:A:424:GLY:HA2	1:A:502:LYS:HB2	1.98	0.44
1:B:417:GLU:OE2	1:B:417:GLU:CA	2.65	0.44
1:B:156:ASP:HA	1:B:181:GLN:HA	1.99	0.44
1:A:293:LEU:HD11	1:A:297:ALA:O	2.17	0.44
1:A:5:PHE:HE1	1:A:11:PHE:CD1	2.36	0.44
1:B:43:VAL:HG13	1:B:94:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ILE:HB	1:B:613:ASN:HB3	1.98	0.44
1:C:894:SER:HB3	1:C:898:PRO:CD	2.47	0.44
1:A:261:LEU:O	1:A:264:ASP:HB2	2.18	0.44
1:C:414:GLU:OE2	1:C:974:PRO:HG3	2.17	0.44
1:A:644:VAL:HG11	1:A:667:ASN:CB	2.40	0.44
1:A:228:GLN:OE1	1:B:781:MET:HB3	2.17	0.44
1:C:282:ASN:C	1:C:284:GLN:H	2.21	0.44
1:B:700:ASN:O	1:B:701:GLN:C	2.55	0.44
1:B:690:LEU:HD23	1:B:690:LEU:HA	1.78	0.44
1:B:70:ASN:O	1:B:110:LYS:HE3	2.17	0.44
1:A:73:ASP:HB3	1:A:74:ASN:ND2	2.32	0.44
1:B:277:ILE:HD12	1:B:277:ILE:C	2.38	0.44
1:C:894:SER:CB	1:C:897:ILE:HD12	2.43	0.44
1:A:263:ARG:HA	1:A:268:ILE:CD1	2.48	0.44
1:A:356:TYR:O	1:A:358:PHE:N	2.49	0.44
1:A:705:GLU:HG2	1:A:847:LEU:HD22	1.99	0.44
1:C:393:LEU:HD21	1:C:926:TYR:OH	2.16	0.44
1:B:712:MET:O	1:B:713:LEU:CB	2.66	0.44
1:A:375:VAL:CG1	1:A:405:LEU:HD13	2.48	0.44
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.83	0.44
1:C:421:ALA:HB2	1:C:500:ILE:HG21	1.99	0.44
1:C:502:LYS:HG2	1:C:503:GLY:H	1.82	0.44
1:B:88:VAL:O	1:B:88:VAL:HG13	2.17	0.44
1:C:926:TYR:CD1	1:C:1003:VAL:CG2	3.01	0.44
1:C:399:VAL:HA	1:C:402:ILE:HG12	1.99	0.44
1:A:480:LEU:HD22	1:A:480:LEU:HA	1.73	0.44
1:A:416:VAL:HG22	1:A:431:THR:HA	1.99	0.44
1:C:380:PHE:O	1:C:383:LEU:N	2.51	0.44
1:C:400:LEU:HD21	1:C:933:THR:HG21	1.99	0.44
1:A:425:LEU:HB3	1:A:426:PRO:CD	2.44	0.44
1:A:578:LEU:HB2	1:A:623:ASN:O	2.18	0.44
1:C:556:PHE:O	1:C:558:ARG:N	2.52	0.43
1:B:69:MET:HE2	1:B:69:MET:HA	1.99	0.43
1:A:376:LEU:HD11	1:A:405:LEU:HD12	1.99	0.43
1:A:376:LEU:C	1:A:378:GLY:H	2.21	0.43
1:C:843:LEU:CD1	1:C:847:LEU:HD11	2.48	0.43
1:A:704:ALA:O	1:A:707:ALA:HB3	2.18	0.43
1:C:181:GLN:O	1:C:272:GLY:HA2	2.18	0.43
1:B:564:LEU:HA	1:B:565:PRO:HD2	1.74	0.43
1:B:905:VAL:HG13	1:B:935:ILE:HD12	2.00	0.43
1:A:684:LEU:HD12	1:A:856:GLY:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:THR:O	1:C:154:ILE:HG12	2.17	0.43
1:C:208:LYS:HG3	1:C:759:VAL:HG12	2.00	0.43
1:B:530:SER:O	1:B:534:ILE:HG13	2.18	0.43
1:A:254:ASN:HB2	1:A:258:SER:O	2.19	0.43
1:C:556:PHE:HB3	1:C:557:VAL:H	1.55	0.43
1:C:326:PRO:O	1:C:327:TYR:HB2	2.18	0.43
1:C:166:ILE:CG2	1:C:167:SER:N	2.81	0.43
1:C:688:ALA:HB2	1:C:854:GLY:HA3	2.01	0.43
1:B:18:ILE:O	1:B:21:LEU:N	2.50	0.43
1:C:291:ILE:HG21	1:C:306:ILE:CD1	2.45	0.43
1:C:416:VAL:HG22	1:C:434:SER:OG	2.18	0.43
1:B:1020:PHE:O	1:B:1024:VAL:HG23	2.18	0.43
1:B:893:GLU:O	1:B:893:GLU:HG3	2.19	0.43
1:A:869:SER:HB3	1:A:870:GLY:H	1.65	0.43
1:A:696:THR:O	1:A:699:ARG:HB3	2.17	0.43
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.49	0.43
1:C:484:VAL:CG1	1:C:485:ALA:N	2.81	0.43
1:B:14:VAL:O	1:B:17:ILE:N	2.52	0.43
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.99	0.43
1:B:318:PRO:HD2	1:B:321:LEU:HD13	2.01	0.43
1:A:719:ASN:HB2	1:A:828:LEU:HD13	2.01	0.43
1:A:924:ASP:O	1:A:928:GLN:HG3	2.19	0.43
1:B:324:VAL:C	1:B:325:TYR:CD1	2.91	0.43
1:C:907:LEU:HD12	1:C:908:GLY:N	2.33	0.43
1:B:743:ILE:O	1:B:746:ILE:HB	2.17	0.43
1:C:359:LEU:HG	1:C:977:MET:HE3	2.01	0.43
1:A:615:PHE:O	1:A:626:ILE:HG22	2.18	0.43
1:A:1030:ARG:C	1:A:1032:ARG:H	2.20	0.43
1:C:109:ASN:O	1:C:112:GLN:HB3	2.18	0.43
1:B:344:LEU:HD21	1:B:399:VAL:HG12	2.00	0.43
1:B:401:ALA:O	1:B:404:LEU:N	2.51	0.43
1:B:27:ILE:HG22	1:B:28:LEU:N	2.33	0.43
1:C:980:LEU:O	1:C:984:LEU:HD22	2.18	0.43
1:B:267:LYS:HE2	1:B:776:GLU:OE1	2.18	0.43
1:C:420:MET:SD	1:C:426:PRO:O	2.77	0.43
1:B:217:GLY:HA2	1:C:755:GLY:HA2	2.01	0.43
1:C:519:MET:O	1:C:523:SER:OG	2.30	0.43
1:A:702:LEU:HD22	1:A:702:LEU:O	2.19	0.43
1:C:310:LEU:HG	1:C:323:ILE:CD1	2.47	0.43
1:C:36:PRO:HG3	1:C:469:GLN:CD	2.38	0.43
1:A:687:GLN:NE2	1:A:856:GLY:HA3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:VAL:HG13	1:B:399:VAL:HG21	2.01	0.43
1:B:27:ILE:HD11	1:B:380:PHE:CD2	2.54	0.43
1:C:600:THR:OG1	1:C:601:LYS:N	2.52	0.43
1:B:482:VAL:O	1:B:486:LEU:HG	2.18	0.43
1:C:1020:PHE:O	1:C:1023:PRO:HD2	2.18	0.43
1:C:399:VAL:HG11	1:C:989:LEU:CD2	2.48	0.43
1:C:515:TRP:HE3	1:C:515:TRP:C	2.22	0.43
1:B:1010:GLY:O	1:B:1014:ALA:CB	2.67	0.43
1:C:458:PHE:N	1:C:458:PHE:HD1	2.15	0.43
1:B:974:PRO:O	1:B:975:ILE:C	2.57	0.43
1:B:325:TYR:HD1	1:B:325:TYR:N	2.16	0.43
1:B:598:TYR:O	1:B:606:VAL:HG11	2.18	0.43
1:A:231:ASN:HB2	1:B:583:THR:HG22	2.01	0.43
1:C:206:ALA:O	1:C:210:GLN:HG3	2.19	0.43
1:C:569:GLN:NE2	1:C:668:LEU:HD12	2.34	0.43
1:A:202:ASP:O	1:A:203:VAL:C	2.56	0.43
1:B:186:ILE:HG21	1:B:262:LEU:HD11	2.01	0.43
1:B:602:GLU:C	1:B:603:LYS:O	2.53	0.43
1:A:376:LEU:C	1:A:378:GLY:N	2.72	0.43
1:C:3:ASN:OD1	1:C:432:ARG:HG2	2.19	0.43
1:A:743:ILE:H	1:A:743:ILE:HD12	1.84	0.43
1:B:740:GLY:O	1:B:794:ALA:N	2.50	0.43
1:B:38:ILE:N	1:B:38:ILE:CD1	2.74	0.42
1:C:154:ILE:O	1:C:157:TYR:N	2.52	0.42
1:C:489:THR:HB	1:C:490:PRO:HD3	2.01	0.42
1:A:757:SER:O	1:A:772:TYR:HA	2.18	0.42
1:A:754:TRP:HH2	1:A:785:ASP:HB2	1.84	0.42
1:B:447:MET:HB3	1:B:887:CYS:SG	2.59	0.42
1:B:909:VAL:O	1:B:913:LEU:HG	2.18	0.42
1:C:658:ILE:HG13	1:C:658:ILE:H	1.58	0.42
1:C:396:PHE:HD2	1:C:1003:VAL:HG21	1.83	0.42
1:C:447:MET:HA	1:C:447:MET:HE3	2.01	0.42
1:A:683:GLU:HG2	1:A:860:THR:CG2	2.50	0.42
1:A:515:TRP:CD1	1:A:515:TRP:C	2.92	0.42
1:B:304:ALA:O	1:B:307:ARG:N	2.53	0.42
1:B:457:ALA:HB1	1:B:468:ARG:HG3	2.01	0.42
1:A:365:THR:C	1:A:367:ILE:H	2.23	0.42
1:C:4:PHE:O	1:C:8:ARG:HB2	2.19	0.42
1:C:1030:ARG:CA	1:C:1030:ARG:HE	2.32	0.42
1:A:146:ASP:HB3	1:A:148:THR:CG2	2.44	0.42
1:B:17:ILE:O	1:B:21:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:HA	1:C:31:PRO:HD2	1.61	0.42
1:A:228:GLN:OE1	1:B:781:MET:SD	2.78	0.42
1:C:441:ALA:O	1:C:445:ILE:HG13	2.20	0.42
1:B:531:VAL:HA	1:B:534:ILE:HD12	2.00	0.42
1:C:434:SER:O	1:C:438:ILE:HG12	2.20	0.42
1:B:83:ASP:OD1	1:B:87:THR:HG22	2.19	0.42
1:A:98:THR:HG22	1:A:99:ASP:N	2.34	0.42
1:B:927:PHE:HE2	1:B:931:LEU:HD11	1.85	0.42
1:C:145:THR:O	1:C:146:ASP:HB3	2.19	0.42
1:A:796:GLY:O	1:A:798:MET:N	2.52	0.42
1:C:900:SER:HA	1:C:903:LEU:HD12	2.02	0.42
1:B:861:GLY:O	1:B:862:MET:C	2.58	0.42
1:A:993:THR:HG22	1:A:994:GLY:N	2.34	0.42
1:A:836:SER:O	1:A:837:THR:C	2.58	0.42
1:A:841:MET:O	1:A:845:GLU:HG3	2.19	0.42
1:C:679:GLY:HA3	1:C:829:GLY:O	2.20	0.42
1:B:753:ALA:HB3	1:B:754:TRP:CD1	2.55	0.42
1:A:15:ILE:O	1:A:19:ILE:HG12	2.19	0.42
1:A:166:ILE:HD13	1:A:166:ILE:N	2.34	0.42
1:C:573:MET:HB2	1:C:666:PHE:CE1	2.55	0.42
1:C:731:ILE:HG13	1:C:731:ILE:H	1.67	0.42
1:C:355:MET:CG	1:C:410:ILE:HD11	2.48	0.42
1:C:985:GLY:O	1:C:988:PRO:HD2	2.19	0.42
1:B:2:PRO:O	1:B:6:ILE:N	2.50	0.42
1:C:578:LEU:HD13	1:C:587:THR:HG23	2.02	0.42
1:C:575:MET:HG2	1:C:666:PHE:HE2	1.84	0.42
1:C:907:LEU:O	1:C:910:ILE:HG22	2.19	0.42
1:C:987:MET:N	1:C:988:PRO:HD3	2.34	0.42
1:B:340:VAL:HG21	1:B:395:MET:HE3	2.01	0.42
1:C:685:ILE:HB	1:C:687:GLN:NE2	2.35	0.42
1:B:639:GLY:C	1:B:641:GLU:H	2.23	0.42
1:B:158:VAL:HG12	1:B:289:LEU:HD21	2.01	0.42
1:C:960:LEU:HD22	1:C:1027:VAL:HG22	2.02	0.42
1:B:569:GLN:HE22	1:B:670:ALA:HA	1.84	0.42
1:C:82:SER:HB3	1:C:88:VAL:HG13	2.01	0.42
1:C:24:GLY:O	1:C:27:ILE:HB	2.20	0.42
1:A:838:GLY:O	1:A:842:GLU:HG3	2.19	0.42
1:B:566:ASP:N	1:B:566:ASP:OD1	2.53	0.42
1:B:119:PRO:HB2	1:B:122:VAL:HG23	2.00	0.42
1:B:904:VAL:O	1:B:904:VAL:HG22	2.20	0.42
1:A:261:LEU:N	1:A:264:ASP:OD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:THR:O	1:C:531:VAL:HG12	2.20	0.42
1:A:448:VAL:HG23	1:A:887:CYS:CB	2.47	0.42
1:A:731:ILE:HD12	1:A:746:ILE:HG21	2.01	0.42
1:A:464:GLY:HA2	1:A:467:TYR:HD2	1.85	0.42
1:C:61:VAL:HG21	1:C:122:VAL:HG21	2.02	0.42
1:A:360:GLN:HG2	1:A:513:PHE:HD1	1.84	0.42
1:B:820:ASN:ND2	3:B:2102:HOH:O	2.34	0.42
1:C:743:ILE:HG13	1:C:743:ILE:H	1.24	0.42
1:A:788:ASP:OD2	1:A:788:ASP:N	2.52	0.42
1:A:620:ARG:HA	1:A:620:ARG:HD3	1.90	0.42
1:A:937:LEU:HA	1:A:937:LEU:HD23	1.77	0.42
1:C:356:TYR:HD2	1:C:357:LEU:CD1	2.24	0.42
1:A:973:ARG:N	1:A:974:PRO:HD2	2.35	0.42
1:B:360:GLN:O	1:B:361:ASN:CB	2.66	0.42
1:A:578:LEU:O	1:A:579:PRO:C	2.58	0.42
1:B:1025:PHE:O	1:B:1029:VAL:HG23	2.19	0.42
1:B:729:ILE:HD11	1:B:801:PHE:HD1	1.84	0.41
1:A:202:ASP:CG	1:A:792:ARG:HH22	2.23	0.41
1:B:1011:MET:O	1:B:1015:THR:HB	2.20	0.41
1:A:376:LEU:CD1	1:A:405:LEU:HD12	2.50	0.41
1:B:398:MET:HA	1:B:401:ALA:HB3	2.02	0.41
1:C:785:ASP:HA	1:C:788:ASP:OD2	2.21	0.41
1:C:634:TRP:C	1:C:636:ASP:H	2.24	0.41
1:B:267:LYS:O	1:B:268:ILE:HG12	2.20	0.41
1:B:151:GLN:OE1	1:B:278:ILE:CA	2.65	0.41
1:A:626:ILE:C	1:A:626:ILE:CD1	2.79	0.41
1:C:989:LEU:HD12	1:C:1000:GLN:O	2.20	0.41
1:B:427:PRO:HG2	1:B:428:LYS:H	1.85	0.41
1:A:795:ASP:O	1:A:796:GLY:C	2.57	0.41
1:A:1029:VAL:CG1	1:A:1029:VAL:O	2.67	0.41
1:A:7:ASP:O	1:A:8:ARG:HG3	2.20	0.41
1:B:223:PRO:HD2	1:C:780:ARG:HH22	1.84	0.41
1:A:898:PRO:C	1:A:900:SER:H	2.23	0.41
1:A:904:VAL:O	1:A:905:VAL:C	2.58	0.41
1:B:400:LEU:HD13	1:B:929:VAL:HG21	2.02	0.41
1:B:404:LEU:HD23	1:B:937:LEU:HD23	2.01	0.41
1:C:490:PRO:O	1:C:492:LEU:N	2.53	0.41
1:B:26:ALA:O	1:B:30:LEU:HB2	2.20	0.41
1:B:143:ILE:CD1	1:B:281:PHE:HB3	2.47	0.41
1:C:654:ALA:O	1:C:657:GLN:HG2	2.20	0.41
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:LYS:HG3	1:B:779:TYR:CD1	2.56	0.41
1:B:219:LEU:HD12	1:B:232:ALA:HB3	2.01	0.41
1:A:355:MET:SD	1:A:410:ILE:HD12	2.60	0.41
1:A:223:PRO:HD2	1:B:780:ARG:HH12	1.85	0.41
1:C:412:VAL:HG22	1:C:438:ILE:HD12	2.02	0.41
1:A:724:THR:CB	1:A:725:PRO:CD	2.98	0.41
1:B:9:PRO:HD2	1:C:893:GLU:HG3	2.02	0.41
1:C:166:ILE:O	1:C:168:ARG:N	2.53	0.41
1:B:986:VAL:HG12	1:B:990:VAL:HG23	2.01	0.41
1:C:563:PHE:O	1:C:924:ASP:HB2	2.21	0.41
1:A:514:GLY:O	1:A:515:TRP:C	2.58	0.41
1:A:314:GLU:HG2	1:A:317:PHE:CE2	2.55	0.41
1:B:555:LEU:O	1:B:556:PHE:HB3	2.20	0.41
1:A:853:THR:CG2	1:A:854:GLY:N	2.83	0.41
2:B:2000:P9D:H40A	2:B:2000:P9D:H48B	1.84	0.41
1:A:602:GLU:OE1	1:A:647:ILE:HG23	2.21	0.41
1:B:638:PRO:CD	1:B:642:ASN:HD22	2.24	0.41
1:B:426:PRO:CB	1:B:427:PRO:CD	2.99	0.41
1:C:38:ILE:HG13	1:C:39:ALA:N	2.34	0.41
1:B:104:GLN:HG3	1:B:129:VAL:HG23	2.02	0.41
1:B:712:MET:HE3	1:B:843:LEU:HD22	2.02	0.41
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.83	0.41
1:C:291:ILE:HD13	1:C:291:ILE:N	2.35	0.41
1:C:412:VAL:O	1:C:412:VAL:HG12	2.20	0.41
1:A:183:ALA:N	1:A:271:GLY:O	2.53	0.41
1:B:725:PRO:HA	1:B:810:GLU:O	2.20	0.41
1:B:946:VAL:HG12	1:B:946:VAL:O	2.19	0.41
1:A:884:VAL:O	1:A:884:VAL:CG1	2.68	0.41
1:B:344:LEU:HD23	1:B:402:ILE:HD12	2.01	0.41
1:C:545:TYR:CE1	1:C:1025:PHE:HZ	2.37	0.41
1:C:34:GLN:HG2	1:C:35:TYR:CE1	2.55	0.41
1:A:391:ASN:O	1:A:392:THR:C	2.59	0.41
1:B:534:ILE:HG23	1:B:541:TYR:CD2	2.55	0.41
1:C:591:LEU:HD22	1:C:611:ALA:HB1	2.03	0.41
1:A:444:GLY:HA3	1:A:891:LEU:HD13	2.02	0.41
1:A:121:GLU:N	1:A:121:GLU:OE1	2.39	0.41
1:B:22:ALA:C	1:B:24:GLY:H	2.24	0.41
1:B:632:LYS:O	1:B:637:ARG:NE	2.31	0.41
1:C:469:GLN:O	1:C:472:ILE:HG22	2.21	0.41
1:C:447:MET:CE	1:C:447:MET:CA	2.97	0.41
1:A:326:PRO:HG3	1:A:610:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:692:HIS:NE2	1:C:723:ASP:OD2	2.49	0.41
1:C:158:VAL:O	1:C:162:MET:HG3	2.21	0.41
1:C:457:ALA:C	1:C:459:PHE:H	2.24	0.41
1:C:223:PRO:HG2	1:C:223:PRO:O	2.21	0.41
1:A:932:LEU:HD23	1:A:932:LEU:HA	1.93	0.41
1:A:213:GLN:NE2	1:B:56:THR:HA	2.24	0.41
1:C:65:ILE:HD13	1:C:111:LEU:HD11	2.03	0.41
1:B:344:LEU:HD22	1:B:376:LEU:CD1	2.51	0.41
1:A:476:SER:O	1:A:480:LEU:HB2	2.20	0.41
1:B:406:VAL:O	1:B:407:ASP:C	2.59	0.41
1:A:759:VAL:O	1:A:760:ASN:HB3	2.20	0.41
1:C:110:LYS:HA	1:C:110:LYS:HD2	1.82	0.41
1:C:539:GLY:C	1:C:541:TYR:H	2.25	0.41
1:A:824:SER:OG	1:A:825:MET:N	2.52	0.41
1:A:332:PHE:CD2	1:A:569:GLN:HG2	2.56	0.41
1:C:916:ALA:O	1:C:919:ARG:N	2.52	0.41
1:C:383:LEU:HA	1:C:383:LEU:HD12	1.82	0.41
1:A:873:ALA:C	1:A:875:SER:N	2.74	0.41
1:B:783:PRO:O	1:B:786:ILE:HG12	2.21	0.41
1:A:983:ILE:HG23	1:A:1008:MET:HG3	2.03	0.41
1:C:21:LEU:HD12	1:C:22:ALA:H	1.86	0.41
1:C:177:LEU:HD22	1:C:178:PHE:N	2.36	0.41
1:A:249:ILE:O	1:A:261:LEU:HA	2.20	0.41
1:C:650:ARG:HB2	1:C:650:ARG:NH1	2.35	0.41
1:B:706:ALA:HB1	1:B:716:VAL:HG21	2.02	0.41
1:B:355:MET:CE	1:B:413:VAL:HG11	2.51	0.41
1:A:64:VAL:O	1:A:68:ASN:ND2	2.54	0.41
1:C:864:TYR:CD1	1:C:864:TYR:C	2.94	0.41
1:C:724:THR:HB	1:C:725:PRO:CD	2.48	0.40
1:B:684:LEU:O	1:B:824:SER:HA	2.21	0.40
1:A:989:LEU:HD22	1:A:1000:GLN:CB	2.51	0.40
1:B:555:LEU:HD23	1:B:555:LEU:HA	1.90	0.40
1:B:432:ARG:O	1:B:433:LYS:HB3	2.21	0.40
1:B:741:VAL:HG23	1:B:793:ALA:HB2	2.03	0.40
1:B:1032:ARG:HD2	1:B:1032:ARG:HA	1.83	0.40
1:A:573:MET:HG2	1:A:626:ILE:HD11	2.02	0.40
1:C:111:LEU:HD12	1:C:111:LEU:HA	1.74	0.40
1:C:695:LEU:HD22	1:C:825:MET:SD	2.61	0.40
1:C:72:ILE:HD11	1:C:110:LYS:HG3	2.03	0.40
1:C:100:ALA:HA	1:C:103:ALA:HB3	2.02	0.40
1:B:188:MET:HA	1:B:266:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:PHE:HB2	1:C:866:GLU:CG	2.51	0.40
1:C:597:TYR:CE2	1:C:654:ALA:HB1	2.56	0.40
1:C:54:ALA:HB1	1:C:816:LEU:HD12	2.04	0.40
1:A:795:ASP:O	1:A:797:GLN:N	2.55	0.40
1:C:458:PHE:H	1:C:458:PHE:HD1	1.70	0.40
1:A:714:THR:HB	1:A:830:GLN:HG3	2.03	0.40
1:A:192:GLU:O	1:A:195:LYS:HB3	2.22	0.40
1:A:6:ILE:HG12	1:A:494:ALA:HB2	2.03	0.40
1:C:894:SER:CB	1:C:897:ILE:HB	2.51	0.40
1:C:213:GLN:NE2	1:C:238:THR:CB	2.84	0.40
1:C:999:ALA:O	1:C:1000:GLN:C	2.59	0.40
1:C:453:PHE:O	1:C:456:MET:HB3	2.21	0.40
1:C:967:ALA:O	1:C:969:ARG:N	2.55	0.40
1:B:832:ALA:O	1:B:833:PRO:C	2.58	0.40
1:C:370:ILE:O	1:C:370:ILE:CG2	2.69	0.40
1:A:390:ILE:N	1:A:390:ILE:HD13	2.35	0.40
1:B:982:PHE:HA	1:B:982:PHE:HD2	1.78	0.40
1:B:391:ASN:O	1:B:393:LEU:N	2.54	0.40
1:C:459:PHE:HE2	1:C:872:GLN:HB2	1.86	0.40
1:B:102:ILE:O	1:B:106:GLN:HG3	2.21	0.40
1:C:877:TYR:OH	1:C:928:GLN:HG2	2.21	0.40
1:A:198:LEU:HA	1:A:792:ARG:HH12	1.86	0.40
1:C:1020:PHE:CD1	1:C:1020:PHE:N	2.90	0.40
1:B:489:THR:N	1:B:490:PRO:HD2	2.37	0.40
1:A:797:GLN:O	1:A:798:MET:HB2	2.21	0.40
1:B:682:PHE:HD2	1:B:859:TRP:CH2	2.40	0.40
1:A:314:GLU:O	1:A:316:PHE:N	2.54	0.40
1:C:805:SER:O	1:C:806:SER:HB3	2.22	0.40
1:B:564:LEU:HD13	1:B:671:ILE:HD12	2.04	0.40
1:A:870:GLY:O	1:A:871:ASN:C	2.60	0.40
1:A:121:GLU:O	1:A:125:GLN:HG2	2.22	0.40
1:C:21:LEU:HD12	1:C:22:ALA:N	2.37	0.40
1:A:961:ILE:HD12	1:A:961:ILE:H	1.86	0.40
1:B:867:ARG:HB3	1:B:867:ARG:HE	1.72	0.40
1:C:815:ARG:O	1:C:815:ARG:HG2	2.21	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	1031/1033 (100%)	818 (79%)	166 (16%)	47 (5%)	3	16
1	B	1031/1033 (100%)	812 (79%)	169 (16%)	50 (5%)	3	16
1	C	1031/1033 (100%)	770 (75%)	207 (20%)	54 (5%)	2	14
All	All	3093/3099 (100%)	2400 (78%)	542 (18%)	151 (5%)	3	15

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	LEU
1	A	439	GLN
1	A	463	THR
1	A	670	ALA
1	A	795	ASP
1	A	946	VAL
1	A	968	VAL
1	B	29	LYS
1	B	329	THR
1	B	361	ASN
1	B	439	GLN
1	B	502	LYS
1	B	505	HIS
1	B	640	GLU
1	B	713	LEU
1	B	893	GLU
1	B	952	LEU
1	B	953	MET
1	B	995	ALA
1	B	1016	VAL
1	C	146	ASP
1	C	147	GLY
1	C	422	GLU
1	C	451	ALA

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Mol	Chain	Res	Type
1	C	556	PHE
1	C	602	GLU
1	C	640	GLU
1	C	723	ASP
1	C	775	SER
1	C	895	TRP
1	C	942	ALA
1	C	997	SER
1	A	37	THR
1	A	364	ALA
1	A	422	GLU
1	A	504	ASP
1	A	601	LYS
1	A	796	GLY
1	A	797	GLN
1	A	820	ASN
1	A	825	MET
1	A	869	SER
1	A	871	ASN
1	A	995	ALA
1	A	1014	ALA
1	B	18	ILE
1	B	19	ILE
1	B	36	PRO
1	B	380	PHE
1	B	392	THR
1	B	421	ALA
1	B	427	PRO
1	B	471	SER
1	B	601	LYS
1	B	661	ALA
1	B	676	THR
1	B	909	VAL
1	B	958	LYS
1	B	975	ILE
1	B	1017	LEU
1	C	283	GLY
1	C	319	SER
1	C	357	LEU
1	C	358	PHE
1	C	432	ARG
1	C	486	LEU

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Mol	Chain	Res	Type
1	C	502	LYS
1	C	557	VAL
1	C	764	ASP
1	C	804	PHE
1	C	808	ARG
1	C	893	GLU
1	C	968	VAL
1	C	1016	VAL
1	A	321	LEU
1	A	539	GLY
1	A	661	ALA
1	A	720	GLY
1	A	939	ALA
1	B	9	PRO
1	B	305	ALA
1	B	555	LEU
1	B	580	ALA
1	B	604	ASN
1	B	820	ASN
1	B	1005	THR
1	C	112	GLN
1	C	194	ASN
1	C	427	PRO
1	C	491	ALA
1	C	519	MET
1	C	553	ALA
1	C	601	LYS
1	C	645	GLU
1	C	806	SER
1	C	820	ASN
1	C	938	SER
1	A	34	GLN
1	A	86	GLY
1	A	362	PHE
1	A	372	VAL
1	A	392	THR
1	A	659	LYS
1	A	837	THR
1	B	269	GLU
1	B	287	SER
1	B	398	MET
1	B	813	SER

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Mol	Chain	Res	Type
1	B	987	MET
1	C	34	GLN
1	C	173	GLY
1	C	270	LEU
1	C	450	SER
1	C	458	PHE
1	C	490	PRO
1	C	503	GLY
1	C	698	ALA
1	A	9	PRO
1	A	315	PRO
1	A	427	PRO
1	A	538	THR
1	A	596	HIS
1	A	660	ASP
1	A	921	LEU
1	A	953	MET
1	B	362	PHE
1	B	688	ALA
1	B	737	GLN
1	C	153	ASP
1	C	162	MET
1	C	953	MET
1	A	224	PRO
1	A	377	LEU
1	A	998	GLY
1	A	1017	LEU
1	C	746	ILE
1	A	935	ILE
1	B	787	GLY
1	C	741	VAL
1	C	786	ILE
1	A	36	PRO
1	B	50	PRO
1	C	139	VAL
1	A	508	GLY
1	B	227	GLY
1	B	812	GLY
1	B	874	PRO
1	C	783	PRO
1	B	15	ILE
1	C	2	PRO

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Mol	Chain	Res	Type
1	B	268	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	839/839 (100%)	710 (85%)	129 (15%)	3	13
1	B	839/839 (100%)	700 (83%)	139 (17%)	3	11
1	C	839/839 (100%)	687 (82%)	152 (18%)	2	9
All	All	2517/2517 (100%)	2097 (83%)	420 (17%)	3	10

All (420) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	13	TRP
1	A	25	LEU
1	A	30	LEU
1	A	37	THR
1	A	38	ILE
1	A	44	THR
1	A	49	TYR
1	A	67	GLN
1	A	93	THR
1	A	113	LEU
1	A	121	GLU
1	A	124	GLN
1	A	128	SER
1	A	135	SER
1	A	137	LEU
1	A	145	THR
1	A	150	THR
1	A	151	GLN
1	A	164	ASP
1	A	177	LEU

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Mol	Chain	Res	Type
1	A	198	LEU
1	A	199	THR
1	A	208	LYS
1	A	214	VAL
1	A	222	THR
1	A	226	LYS
1	A	230	LEU
1	A	235	ILE
1	A	237	GLN
1	A	238	THR
1	A	240	LEU
1	A	250	LEU
1	A	253	VAL
1	A	255	GLN
1	A	260	VAL
1	A	262	LEU
1	A	263	ARG
1	A	274	ASN
1	A	280	GLU
1	A	289	LEU
1	A	295	THR
1	A	300	LEU
1	A	310	LEU
1	A	312	LYS
1	A	321	LEU
1	A	339	GLU
1	A	341	VAL
1	A	350	LEU
1	A	351	VAL
1	A	356	TYR
1	A	377	LEU
1	A	428	LYS
1	A	452	VAL
1	A	463	THR
1	A	468	ARG
1	A	474	ILE
1	A	476	SER
1	A	480	LEU
1	A	486	LEU
1	A	489	THR
1	A	510	LYS
1	A	515	TRP

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Mol	Chain	Res	Type
1	A	516	PHE
1	A	524	THR
1	A	528	THR
1	A	537	SER
1	A	564	LEU
1	A	566	ASP
1	A	571	VAL
1	A	575	MET
1	A	578	LEU
1	A	588	GLN
1	A	589	LYS
1	A	603	LYS
1	A	604	ASN
1	A	624	THR
1	A	626	ILE
1	A	630	SER
1	A	636	ASP
1	A	659	LYS
1	A	662	MET
1	A	668	LEU
1	A	672	VAL
1	A	681	ASP
1	A	693	GLU
1	A	695	LEU
1	A	696	THR
1	A	699	ARG
1	A	702	LEU
1	A	708	LYS
1	A	713	LEU
1	A	717	ARG
1	A	724	THR
1	A	728	LYS
1	A	730	ASP
1	A	745	ASP
1	A	746	ILE
1	A	765	ARG
1	A	767	ARG
1	A	773	VAL
1	A	788	ASP
1	A	799	VAL
1	A	808	ARG
1	A	815	ARG

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Mol	Chain	Res	Type
1	A	825	MET
1	A	845	GLU
1	A	846	GLN
1	A	850	LYS
1	A	853	THR
1	A	867	ARG
1	A	868	LEU
1	A	894	SER
1	A	896	SER
1	A	904	VAL
1	A	918	PHE
1	A	919	ARG
1	A	921	LEU
1	A	941	ASN
1	A	956	GLU
1	A	965	LEU
1	A	969	ARG
1	A	980	LEU
1	A	982	PHE
1	A	987	MET
1	A	991	ILE
1	A	1017	LEU
1	A	1027	VAL
1	A	1028	VAL
1	B	3	ASN
1	B	6	ILE
1	B	11	PHE
1	B	20	MET
1	B	25	LEU
1	B	27	ILE
1	B	43	VAL
1	B	44	THR
1	B	49	TYR
1	B	57	VAL
1	B	58	GLN
1	B	63	GLN
1	B	65	ILE
1	B	72	ILE
1	B	87	THR
1	B	89	GLN
1	B	91	THR
1	B	93	THR

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Mol	Chain	Res	Type
1	B	96	SER
1	B	105	VAL
1	B	111	LEU
1	B	121	GLU
1	B	128	SER
1	B	129	VAL
1	B	135	SER
1	B	148	THR
1	B	167	SER
1	B	169	THR
1	B	175	VAL
1	B	177	LEU
1	B	199	THR
1	B	204	ILE
1	B	213	GLN
1	B	218	GLN
1	B	222	THR
1	B	225	VAL
1	B	253	VAL
1	B	261	LEU
1	B	269	GLU
1	B	277	ILE
1	B	295	THR
1	B	302	THR
1	B	306	ILE
1	B	321	LEU
1	B	325	TYR
1	B	331	PRO
1	B	351	VAL
1	B	361	ASN
1	B	366	LEU
1	B	367	ILE
1	B	372	VAL
1	B	382	VAL
1	B	383	LEU
1	B	390	ILE
1	B	400	LEU
1	B	402	ILE
1	B	418	ARG
1	B	425	LEU
1	B	429	GLU
1	B	447	MET

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Mol	Chain	Res	Type
1	B	448	VAL
1	B	462	SER
1	B	468	ARG
1	B	473	THR
1	B	476	SER
1	B	482	VAL
1	B	483	LEU
1	B	484	VAL
1	B	495	THR
1	B	502	LYS
1	B	517	ASN
1	B	540	ARG
1	B	552	MET
1	B	564	LEU
1	B	573	MET
1	B	575	MET
1	B	578	LEU
1	B	584	GLN
1	B	596	HIS
1	B	603	LYS
1	B	610	PHE
1	B	613	ASN
1	B	617	PHE
1	B	624	THR
1	B	630	SER
1	B	636	ASP
1	B	644	VAL
1	B	658	ILE
1	B	666	PHE
1	B	668	LEU
1	B	673	GLU
1	B	676	THR
1	B	695	LEU
1	B	702	LEU
1	B	728	LYS
1	B	741	VAL
1	B	744	ASN
1	B	745	ASP
1	B	750	LEU
1	B	762	PHE
1	B	763	ILE
1	B	778	LYS

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Mol	Chain	Res	Type
1	B	791	VAL
1	B	805	SER
1	B	806	SER
1	B	815	ARG
1	B	830	GLN
1	B	835	LYS
1	B	842	GLU
1	B	865	GLN
1	B	866	GLU
1	B	871	ASN
1	B	881	LEU
1	B	888	LEU
1	B	895	TRP
1	B	899	PHE
1	B	913	LEU
1	B	918	PHE
1	B	919	ARG
1	B	921	LEU
1	B	933	THR
1	B	943	ILE
1	B	950	LYS
1	B	952	LEU
1	B	954	ASP
1	B	961	ILE
1	B	972	LEU
1	B	978	THR
1	B	980	LEU
1	B	982	PHE
1	B	987	MET
1	B	991	ILE
1	B	1003	VAL
1	B	1007	VAL
1	B	1008	MET
1	B	1012	VAL
1	B	1030	ARG
1	B	1031	ARG
1	B	1033	PHE
1	C	4	PHE
1	C	11	PHE
1	C	18	ILE
1	C	19	ILE
1	C	21	LEU

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Mol	Chain	Res	Type
1	C	27	ILE
1	C	30	LEU
1	C	37	THR
1	C	49	TYR
1	C	62	THR
1	C	74	ASN
1	C	75	LEU
1	C	80	SER
1	C	82	SER
1	C	85	THR
1	C	88	VAL
1	C	90	ILE
1	C	95	GLU
1	C	96	SER
1	C	106	GLN
1	C	110	LYS
1	C	127	VAL
1	C	130	GLU
1	C	131	LYS
1	C	143	ILE
1	C	149	MET
1	C	150	THR
1	C	153	ASP
1	C	155	SER
1	C	158	VAL
1	C	164	ASP
1	C	166	ILE
1	C	169	THR
1	C	177	LEU
1	C	181	GLN
1	C	182	TYR
1	C	194	ASN
1	C	196	PHE
1	C	197	GLN
1	C	230	LEU
1	C	231	ASN
1	C	235	ILE
1	C	239	ARG
1	C	241	THR
1	C	244	GLU
1	C	255	GLN
1	C	256	ASP

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Mol	Chain	Res	Type
1	C	274	ASN
1	C	280	GLU
1	C	289	LEU
1	C	300	LEU
1	C	310	LEU
1	C	313	MET
1	C	324	VAL
1	C	337	ILE
1	C	341	VAL
1	C	345	VAL
1	C	349	ILE
1	C	350	LEU
1	C	354	VAL
1	C	361	ASN
1	C	372	VAL
1	C	379	THR
1	C	399	VAL
1	C	402	ILE
1	C	405	LEU
1	C	408	ASP
1	C	422	GLU
1	C	428	LYS
1	C	447	MET
1	C	456	MET
1	C	458	PHE
1	C	463	THR
1	C	474	ILE
1	C	482	VAL
1	C	484	VAL
1	C	488	LEU
1	C	510	LYS
1	C	512	PHE
1	C	515	TRP
1	C	523	SER
1	C	525	HIS
1	C	531	VAL
1	C	538	THR
1	C	556	PHE
1	C	567	GLU
1	C	571	VAL
1	C	574	THR
1	C	585	GLU

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Mol	Chain	Res	Type
1	C	586	ARG
1	C	589	LYS
1	C	591	LEU
1	C	596	HIS
1	C	597	TYR
1	C	603	LYS
1	C	617	PHE
1	C	624	THR
1	C	626	ILE
1	C	636	ASP
1	C	645	GLU
1	C	649	MET
1	C	650	ARG
1	C	668	LEU
1	C	672	VAL
1	C	690	LEU
1	C	696	THR
1	C	699	ARG
1	C	714	THR
1	C	715	SER
1	C	717	ARG
1	C	723	ASP
1	C	739	LEU
1	C	743	ILE
1	C	746	ILE
1	C	750	LEU
1	C	758	TYR
1	C	770	LYS
1	C	778	LYS
1	C	801	PHE
1	C	822	LEU
1	C	825	MET
1	C	826	GLU
1	C	827	ILE
1	C	835	LYS
1	C	836	SER
1	C	862	MET
1	C	864	TYR
1	C	868	LEU
1	C	876	LEU
1	C	879	ILE
1	C	884	VAL

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Mol	Chain	Res	Type
1	C	891	LEU
1	C	896	SER
1	C	917	THR
1	C	922	THR
1	C	933	THR
1	C	934	THR
1	C	945	ILE
1	C	950	LYS
1	C	955	LYS
1	C	960	LEU
1	C	966	ASP
1	C	968	VAL
1	C	993	THR
1	C	1008	MET
1	C	1011	MET
1	C	1012	VAL
1	C	1015	THR
1	C	1022	VAL
1	C	1030	ARG
1	C	1032	ARG
1	C	1033	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	74	ASN
1	A	144	ASN
1	A	151	GLN
1	A	437	GLN
1	A	517	ASN
1	A	526	HIS
1	A	588	GLN
1	A	592	ASN
1	A	604	ASN
1	A	605	ASN
1	A	642	ASN
1	A	797	GLN
1	A	820	ASN
1	B	112	GLN
1	B	228	GLN
1	B	361	ASN

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Mol	Chain	Res	Type
1	B	415	ASN
1	B	437	GLN
1	B	584	GLN
1	B	592	ASN
1	B	604	ASN
1	B	613	ASN
1	B	642	ASN
1	B	737	GLN
1	B	830	GLN
1	B	928	GLN
1	B	1001	ASN
1	C	68	ASN
1	C	89	GLN
1	C	120	GLN
1	C	124	GLN
1	C	144	ASN
1	C	176	GLN
1	C	213	GLN
1	C	231	ASN
1	C	361	ASN
1	C	439	GLN
1	C	505	HIS
1	C	569	GLN
1	C	584	GLN
1	C	592	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	P9D	B	2000	-	42,53,53	2.60	12 (28%)	50,77,77	2.34	16 (32%)

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	P9D	B	2000	-	-	0/33/49/49	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	P9D	C9-S8	-4.24	1.63	1.70
2	B	2000	P9D	C14-C12	2.01	1.40	1.37
2	B	2000	P9D	C21-N24	2.09	1.41	1.36
2	B	2000	P9D	C15-N19	2.20	1.37	1.34
2	B	2000	P9D	C20-C22	2.76	1.50	1.44
2	B	2000	P9D	N31-N30	3.69	1.40	1.34
2	B	2000	P9D	N28-N29	3.85	1.40	1.34
2	B	2000	P9D	C20-N16	4.06	1.45	1.37
2	B	2000	P9D	C22-C21	4.35	1.49	1.43
2	B	2000	P9D	C21-N19	5.03	1.37	1.31
2	B	2000	P9D	N30-N29	7.84	1.42	1.32
2	B	2000	P9D	O34-C38	8.71	1.50	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	P9D	C9-C4-C2	-6.77	120.80	129.15
2	B	2000	P9D	N31-N30-N29	-3.58	107.53	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	P9D	C22-C25-C26	-3.43	115.74	127.09
2	B	2000	P9D	O44-C38-N39	-3.28	119.90	124.97
2	B	2000	P9D	C22-C21-N24	-2.95	118.52	122.40
2	B	2000	P9D	O34-C38-O44	-2.94	119.97	124.51
2	B	2000	P9D	N28-N29-N30	-2.73	108.02	109.59
2	B	2000	P9D	C35-C36-C37	-2.38	107.79	110.97
2	B	2000	P9D	C36-C37-N24	-2.03	107.24	111.17
2	B	2000	P9D	O34-C33-C32	2.54	113.97	108.63
2	B	2000	P9D	C21-N19-C15	2.74	123.39	118.68
2	B	2000	P9D	N19-C21-N24	3.30	122.11	116.81
2	B	2000	P9D	C33-O34-C38	4.48	122.35	116.32
2	B	2000	P9D	O34-C38-N39	4.74	120.07	111.27
2	B	2000	P9D	N31-C27-N28	4.98	116.19	111.69
2	B	2000	P9D	C37-N24-C32	5.66	125.19	113.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2000	P9D	14	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1033/1033 (100%)	-0.20	22 (2%) 67 42	35, 100, 155, 204	0
1	B	1033/1033 (100%)	-0.16	17 (1%) 74 52	45, 101, 144, 190	0
1	C	1033/1033 (100%)	-0.05	19 (1%) 71 47	57, 110, 150, 183	0
All	All	3099/3099 (100%)	-0.14	58 (1%) 70 45	35, 104, 150, 204	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	424	GLY	5.5
1	A	511	GLY	4.1
1	C	676	THR	4.0
1	A	965	LEU	4.0
1	A	500	ILE	3.9
1	A	674	LEU	3.9
1	A	510	LYS	3.8
1	A	712	MET	3.7
1	C	510	LYS	3.6
1	B	678	THR	3.5
1	A	498	LYS	3.5
1	B	870	GLY	3.3
1	A	499	PRO	3.2
1	B	506	GLY	3.1
1	B	134	SER	3.0
1	C	604	ASN	3.0
1	A	512	PHE	2.9
1	B	259	ARG	2.8
1	C	606	VAL	2.8
1	A	958	LYS	2.6
1	C	994	GLY	2.6
1	B	712	MET	2.6
1	A	535	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	719	ASN	2.5
1	C	540	ARG	2.5
1	A	537	SER	2.4
1	C	501	ALA	2.4
1	B	509	LYS	2.4
1	C	508	GLY	2.4
1	C	675	GLY	2.4
1	A	541	TYR	2.4
1	C	145	THR	2.4
1	A	993	THR	2.3
1	B	515	TRP	2.3
1	A	640	GLU	2.3
1	A	497	LEU	2.3
1	A	501	ALA	2.2
1	A	941	ASN	2.2
1	C	634	TRP	2.2
1	C	979	SER	2.2
1	B	958	LYS	2.2
1	C	960	LEU	2.2
1	C	511	GLY	2.2
1	B	541	TYR	2.1
1	C	258	SER	2.1
1	A	538	THR	2.1
1	B	510	LYS	2.1
1	B	403	GLY	2.1
1	B	831	ALA	2.1
1	B	832	ALA	2.1
1	B	960	LEU	2.1
1	C	598	TYR	2.1
1	A	516	PHE	2.1
1	B	941	ASN	2.0
1	A	540	ARG	2.0
1	C	617	PHE	2.0
1	B	871	ASN	2.0
1	A	870	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	P9D	B	2000	49/49	0.95	0.22	0.76	74,90,135,145	0

6.5 Other polymers [i](#)

There are no such residues in this entry.