



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:35 am BST

PDB ID : 6VDE
Title : Full-length M. smegmatis Pol1
Authors : Shuman, S.; Goldgur, Y.; Ghosh, S.
Deposited on : 2019-12-24
Resolution : 2.71 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

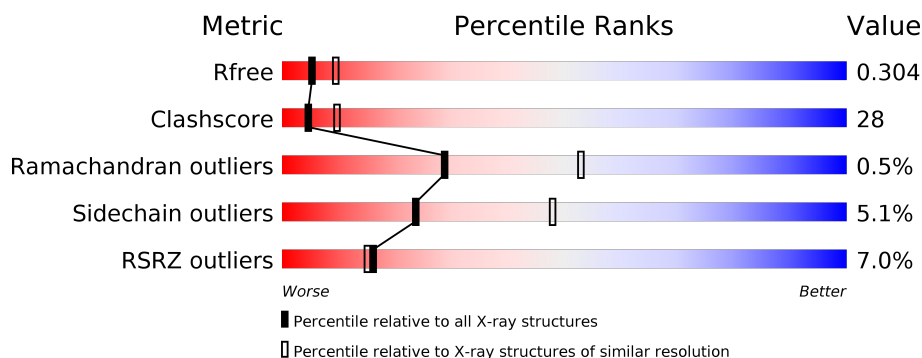
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 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	908	<div> <div>6%</div> <div> <div></div> <div>54%</div> <div>35%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	908	<div> <div>7%</div> <div> <div></div> <div>50%</div> <div>41%</div> <div>• • 5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13366 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 DNA polymerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	0	0
			6672	4181	1171	1304	16			
1	B	860	Total	C	N	O	S	0	0	0
			6672	4181	1171	1304	16			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Mn	0	0
			3	3		
2	A	3	Total	Mn	0	0
			3	3		

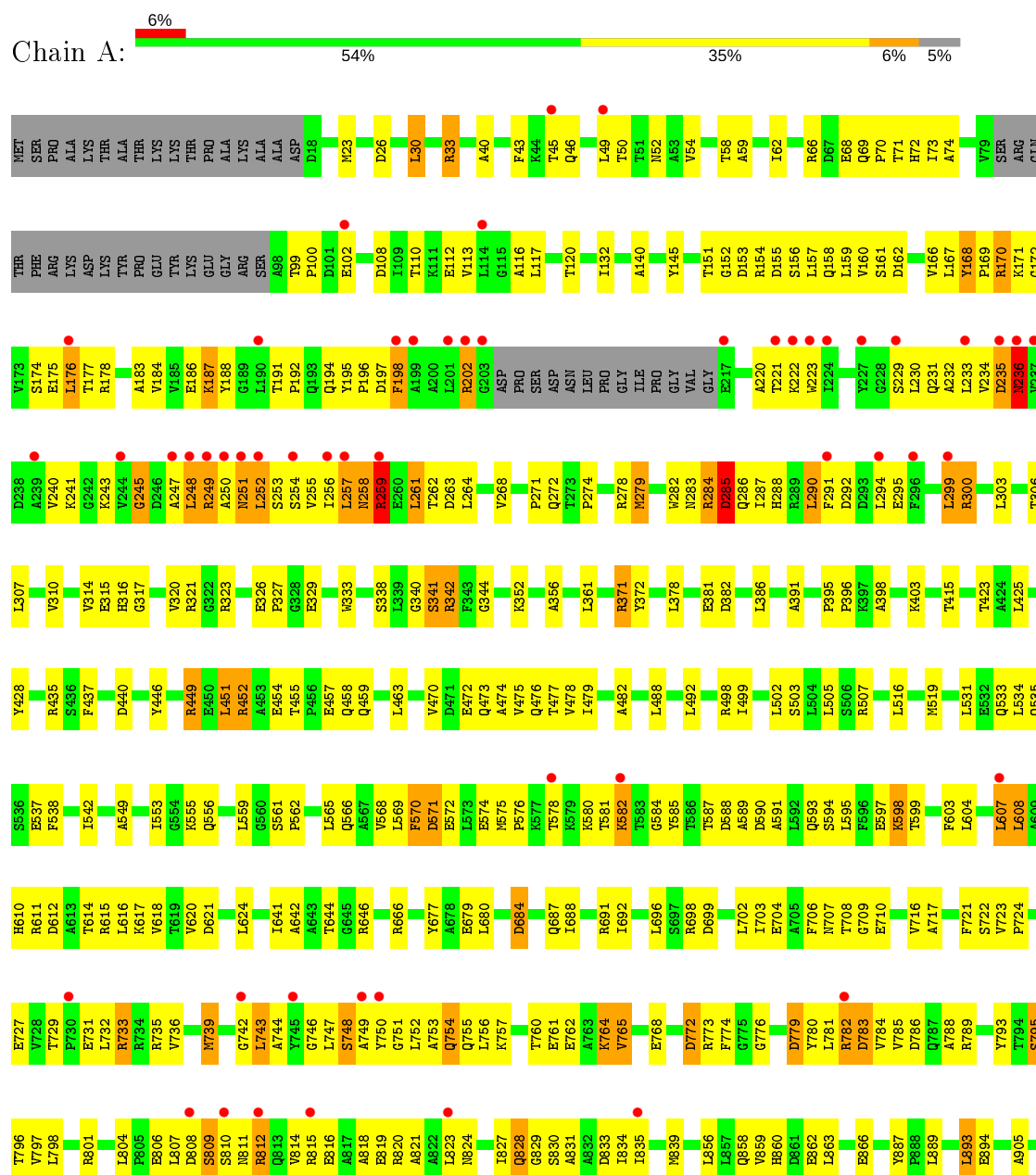
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	10	Total	O	0	0
			10	10		

3 Residue-property plots

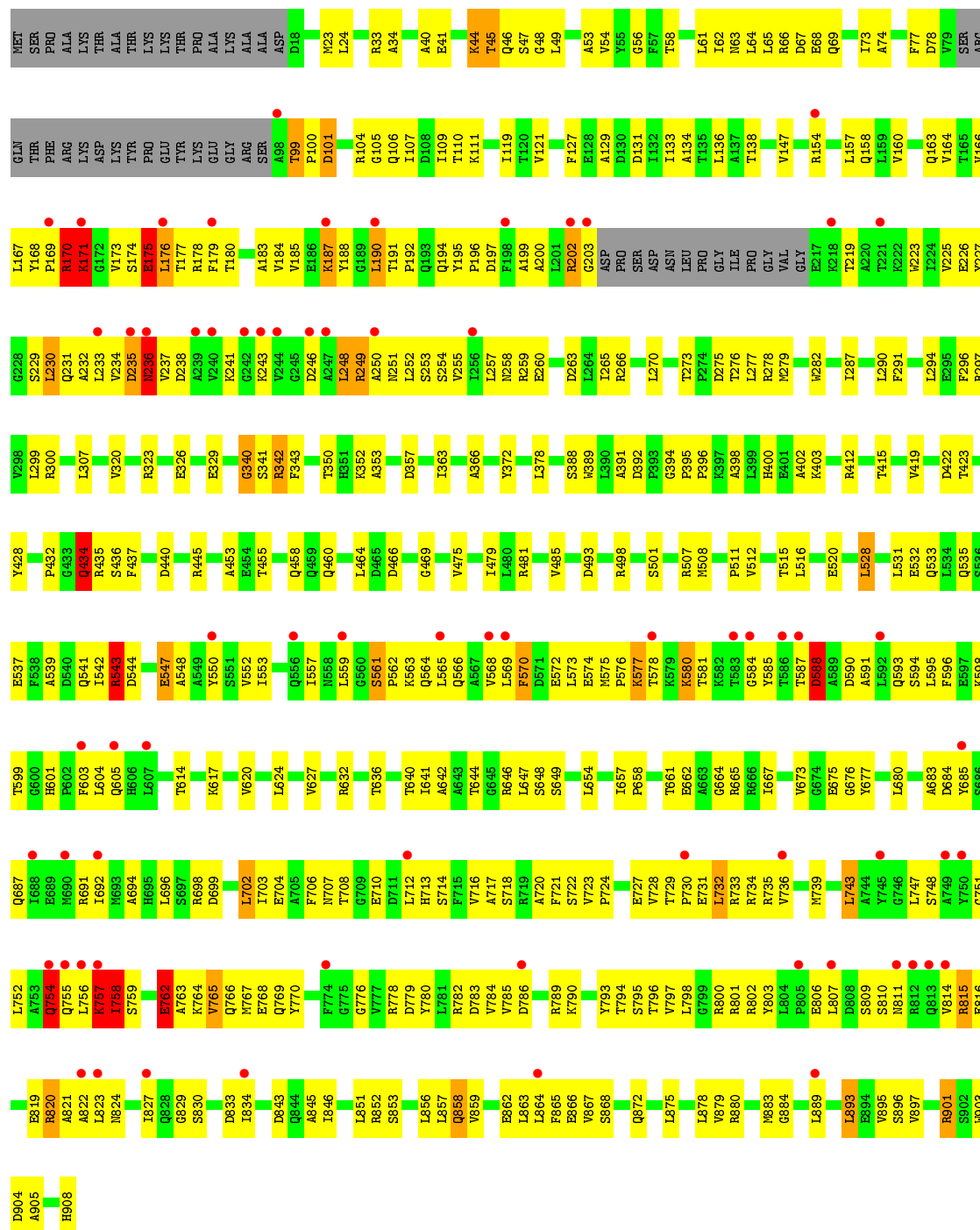
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: DNA polymerase I



H908

- Molecule 1: DNA polymerase I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.00 Å 80.94 Å 117.91 Å 98.68° 105.13° 109.36°	Depositor
Resolution (Å)	50.37 – 2.71 50.37 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.37-2.71) 90.5 (50.37-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.73 Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.234 , 0.304 0.235 , 0.304	Depositor DCC
R_{free} test set	2000 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13366	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.53	1/6783 (0.0%)	0.91	25/9208 (0.3%)
1	B	0.52	1/6783 (0.0%)	0.90	28/9208 (0.3%)
All	All	0.53	2/13566 (0.0%)	0.91	53/18416 (0.3%)

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	A	0	13
1	B	0	13
All	All	0	26

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	598	LYS	CD-CE	-5.90	1.36	1.51
1	B	434	GLN	CB-CG	5.33	1.67	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASP	CB-CG-OD1	-13.53	106.12	118.30
1	B	528	LEU	CB-CG-CD2	-11.86	90.85	111.00
1	B	176	LEU	CA-CB-CG	11.62	142.02	115.30
1	A	285	ASP	CB-CG-OD2	11.42	128.57	118.30
1	A	598	LYS	CD-CE-NZ	-10.32	87.96	111.70
1	B	588	ASP	CB-CG-OD1	-9.55	109.70	118.30
1	A	261	LEU	CA-CB-CG	9.42	136.96	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	588	ASP	CB-CG-OD2	8.73	126.16	118.30
1	B	732	LEU	CA-CB-CG	8.55	134.97	115.30
1	A	257	LEU	CA-CB-CG	8.39	134.60	115.30
1	B	190	LEU	CA-CB-CG	8.38	134.59	115.30
1	B	230	LEU	CA-CB-CG	8.38	134.57	115.30
1	B	434	GLN	CA-CB-CG	8.02	131.05	113.40
1	A	300	ARG	CG-CD-NE	7.95	128.50	111.80
1	B	758	ILE	CG1-CB-CG2	7.95	128.89	111.40
1	A	263	ASP	CB-CG-OD2	-7.85	111.24	118.30
1	A	321	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	806	GLU	CA-CB-CG	7.56	130.04	113.40
1	A	893	LEU	CA-CB-CG	7.26	132.00	115.30
1	B	171	LYS	CD-CE-NZ	7.18	128.22	111.70
1	A	452	ARG	NE-CZ-NH1	-6.99	116.80	120.30
1	A	299	LEU	CA-CB-CG	6.96	131.31	115.30
1	B	754	GLN	N-CA-CB	-6.83	98.30	110.60
1	A	299	LEU	CB-CG-CD1	6.59	122.21	111.00
1	A	176	LEU	CA-CB-CG	6.45	130.12	115.30
1	B	543	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	170	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	B	823	LEU	CA-CB-CG	6.17	129.50	115.30
1	A	236	ASN	CB-CA-C	-6.17	98.07	110.40
1	B	762	GLU	CA-CB-CG	6.17	126.97	113.40
1	B	171	LYS	CA-CB-CG	6.12	126.86	113.40
1	A	245	GLY	N-CA-C	6.09	128.33	113.10
1	B	893	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	547	GLU	N-CA-CB	-5.87	100.04	110.60
1	A	321	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	451	LEU	CA-CB-CG	5.76	128.54	115.30
1	A	321	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	171	LYS	CB-CG-CD	5.43	125.72	111.60
1	B	547	GLU	CA-CB-CG	5.39	125.27	113.40
1	A	321	ARG	CG-CD-NE	-5.34	100.58	111.80
1	B	553	ILE	CG1-CB-CG2	5.31	123.09	111.40
1	A	251	ASN	C-N-CA	-5.25	108.57	121.70
1	A	290	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	252	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	352	LYS	CA-CB-CG	5.17	124.78	113.40
1	A	263	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	285	ASP	CB-CA-C	5.12	120.65	110.40
1	A	300	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	B	466	ASP	CB-CG-OD2	-5.09	113.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	LYS	C-N-CA	5.07	132.95	122.30
1	B	171	LYS	CG-CD-CE	-5.07	96.70	111.90
1	B	378	LEU	CA-CB-CG	5.01	126.81	115.30
1	B	528	LEU	CB-CG-CD1	5.00	119.51	111.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	LEU	Peptide
1	A	235	ASP	Peptide
1	A	248	LEU	Peptide
1	A	258	ASN	Peptide
1	A	259	ARG	Peptide
1	A	284	ARG	Peptide
1	A	340	GLY	Peptide
1	A	45	THR	Peptide
1	A	570	PHE	Peptide
1	A	743	LEU	Peptide
1	A	754	GLN	Peptide
1	A	765	VAL	Peptide
1	A	859	VAL	Peptide
1	B	175	GLU	Peptide
1	B	235	ASP	Peptide
1	B	248	LEU	Peptide
1	B	340	GLY	Peptide
1	B	45	THR	Peptide
1	B	469	GLY	Peptide
1	B	587	THR	Peptide
1	B	754	GLN	Peptide
1	B	757	LYS	Peptide
1	B	758	ILE	Mainchain
1	B	765	VAL	Peptide
1	B	859	VAL	Peptide
1	B	99	THR	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	6672	0	6604	375	3
1	B	6672	0	6608	380	2
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	6	0	0	0	0
3	B	10	0	0	8	0
All	All	13366	0	13212	750	3

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 28.

All (750) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLU:OE2	1:A:735:ARG:NH2	1.59	1.33
1:A:288:HIS:CG	1:A:300:ARG:HH21	1.48	1.31
1:B:129:ALA:O	1:B:133:ILE:HD12	1.29	1.29
1:A:191:THR:HG23	1:A:194:GLN:OE1	1.18	1.26
1:A:288:HIS:HA	1:A:300:ARG:NH2	1.47	1.25
1:A:288:HIS:CA	1:A:300:ARG:HH22	1.55	1.20
1:A:99:THR:HG23	1:A:100:PRO:CD	1.79	1.13
1:A:288:HIS:CG	1:A:300:ARG:NH2	2.17	1.10
1:B:170:ARG:HH12	1:B:177:THR:HB	1.10	1.09
1:A:288:HIS:CA	1:A:300:ARG:NH2	2.14	1.09
1:A:746:GLY:HA3	1:A:820:ARG:HG2	1.39	1.04
1:A:261:LEU:HD23	1:A:262:THR:OG1	1.55	1.03
1:A:99:THR:HG23	1:A:100:PRO:HD3	1.39	1.02
1:A:333:TRP:CD1	1:A:371:ARG:NH1	2.27	1.02
1:B:170:ARG:NH1	1:B:177:THR:HB	1.73	1.01
1:B:255:VAL:HG13	1:B:258:ASN:HB2	1.43	1.00
1:B:45:THR:HG23	1:B:49:LEU:O	1.59	0.99
1:B:190:LEU:HD22	1:B:194:GLN:HE21	1.28	0.99
1:A:191:THR:O	1:A:194:GLN:NE2	1.94	0.99
1:B:810:SER:OG	1:B:815:ARG:NH2	1.94	0.97
1:A:797:VAL:HG23	1:A:830:SER:HB3	1.47	0.96
1:A:751:GLY:O	1:A:755:GLN:HG3	1.66	0.95
1:A:811:ASN:HB3	1:A:814:VAL:HG13	1.46	0.94
1:A:569:LEU:HD11	1:A:604:LEU:HD21	1.50	0.94
1:A:729:THR:H	1:A:733:ARG:HD3	1.33	0.92
1:A:764:LYS:O	1:A:764:LYS:HD2	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:LYS:NZ	1:A:765:VAL:HG22	1.84	0.91
1:B:575:MET:HG2	1:B:595:LEU:HD21	1.51	0.90
1:A:191:THR:CG2	1:A:194:GLN:OE1	2.15	0.88
1:A:811:ASN:HB3	1:A:814:VAL:CG1	2.02	0.88
1:B:528:LEU:HA	1:B:531:LEU:HB2	1.56	0.88
1:B:661:THR:HG23	1:B:664:GLY:H	1.36	0.88
1:B:764:LYS:HD3	1:B:764:LYS:O	1.74	0.88
1:B:231:GLN:HA	1:B:234:VAL:HG22	1.56	0.87
1:A:99:THR:HG23	1:A:100:PRO:HD2	1.56	0.86
1:A:175:GLU:HB2	1:A:176:LEU:HD12	1.57	0.86
1:B:24:LEU:HD22	1:B:133:ILE:HG23	1.56	0.85
1:A:288:HIS:HA	1:A:300:ARG:HH22	1.11	0.85
1:B:129:ALA:O	1:B:133:ILE:CD1	2.22	0.84
1:A:191:THR:HG23	1:A:194:GLN:CD	1.96	0.84
1:A:99:THR:CG2	1:A:100:PRO:CD	2.56	0.83
1:B:641:ILE:HD12	1:B:642:ALA:N	1.93	0.83
1:B:200:ALA:HB1	1:B:255:VAL:HG11	1.61	0.83
1:A:905:ALA:O	1:A:908:HIS:ND1	2.14	0.81
1:A:320:VAL:HG23	1:A:479:ILE:HG22	1.61	0.81
1:B:576:PRO:HG3	1:B:598:LYS:HE3	1.61	0.81
1:A:288:HIS:C	1:A:300:ARG:HH22	1.83	0.81
1:A:731:GLU:CD	1:A:735:ARG:NH2	2.34	0.81
1:B:550:TYR:OH	1:B:557:ILE:O	1.97	0.81
1:A:587:THR:O	1:A:611:ARG:NH2	2.14	0.81
1:B:432:PRO:HD2	1:B:802:ARG:HH11	1.44	0.80
1:A:856:LEU:HD11	1:A:866:GLU:HB2	1.63	0.80
1:B:797:VAL:HG23	1:B:830:SER:HB3	1.63	0.80
1:B:755:GLN:C	1:B:756:LEU:HD22	2.02	0.80
1:B:191:THR:HG23	1:B:194:GLN:OE1	1.83	0.79
1:B:641:ILE:HD12	1:B:642:ALA:H	1.46	0.79
1:B:901:ARG:HE	1:B:901:ARG:H	1.30	0.79
1:B:751:GLY:HA2	1:B:754:GLN:HG3	1.65	0.79
1:A:154:ARG:HG3	1:A:168:TYR:CE1	2.18	0.78
1:B:528:LEU:HD22	1:B:624:LEU:HD23	1.66	0.78
1:B:544:ASP:C	1:B:547:GLU:HG2	2.03	0.78
1:B:41:GLU:HA	1:B:44:LYS:HD3	1.64	0.78
1:A:23:MET:HB3	1:A:73:ILE:HD13	1.66	0.77
1:A:593:GLN:HG3	1:A:608:LEU:HD11	1.66	0.77
1:A:258:ASN:O	1:A:261:LEU:HD13	1.85	0.77
1:A:154:ARG:NH1	1:A:202:ARG:HH21	1.82	0.76
1:B:455:THR:CG2	1:B:458:GLN:HE21	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:NH2	1:A:168:TYR:CE2	2.52	0.76
1:A:590:ASP:HA	1:A:593:GLN:HB2	1.68	0.76
1:A:698:ARG:HA	1:A:703:ILE:HD11	1.66	0.76
1:A:171:LYS:HB2	1:A:174:SER:HB2	1.67	0.76
1:A:507:ARG:HH22	1:B:394:GLY:C	1.89	0.76
1:A:259:ARG:HA	1:A:261:LEU:HB3	1.66	0.75
1:B:455:THR:HG22	1:B:458:GLN:HE21	1.50	0.75
1:A:751:GLY:O	1:A:754:GLN:HB2	1.86	0.75
1:A:764:LYS:HZ2	1:A:765:VAL:HG22	1.49	0.75
1:A:168:TYR:O	1:A:177:THR:HG22	1.86	0.75
1:B:594:SER:O	1:B:598:LYS:HB3	1.87	0.75
1:A:342:ARG:HD2	1:A:398:ALA:HB2	1.67	0.75
1:B:111:LYS:HG2	1:B:121:VAL:HG11	1.68	0.75
1:B:575:MET:HG2	1:B:595:LEU:CD2	2.15	0.75
1:B:809:SER:OG	1:B:814:VAL:HB	1.86	0.75
1:B:45:THR:HG21	1:B:49:LEU:HB2	1.69	0.74
1:B:729:THR:OG1	1:B:732:LEU:HD23	1.87	0.74
1:A:316:HIS:HA	1:A:454:GLU:OE2	1.86	0.74
1:A:70:PRO:HG2	1:A:73:ILE:HD11	1.70	0.74
1:A:507:ARG:NH2	1:B:394:GLY:C	2.41	0.73
1:B:493:ASP:OD1	3:B:1102:HOH:O	2.05	0.73
1:B:632:ARG:NH2	1:B:866:GLU:OE2	2.20	0.73
1:B:588:ASP:H	1:B:591:ALA:HB3	1.51	0.73
1:A:571:ASP:OD1	1:A:574:GLU:OE1	2.08	0.72
1:B:657:ILE:HG23	1:B:667:ILE:HD11	1.70	0.72
1:A:729:THR:H	1:A:733:ARG:CD	2.04	0.71
1:B:251:ASN:HB2	1:B:254:SER:HB3	1.70	0.71
1:B:581:THR:OG1	1:B:584:GLY:N	2.18	0.71
1:B:576:PRO:HG2	1:B:595:LEU:HD11	1.72	0.71
1:A:155:ASP:HB3	1:A:262:THR:HG21	1.73	0.70
1:A:288:HIS:CD2	1:A:300:ARG:HH21	2.04	0.70
1:A:282:TRP:HZ3	1:A:307:LEU:HB3	1.56	0.70
1:A:99:THR:CG2	1:A:100:PRO:HD2	2.20	0.70
1:B:732:LEU:HA	1:B:735:ARG:HG2	1.73	0.70
1:B:528:LEU:HD23	1:B:531:LEU:HD12	1.71	0.70
1:B:708:THR:HG23	1:B:710:GLU:H	1.56	0.69
1:B:342:ARG:HD2	1:B:398:ALA:HB2	1.75	0.69
1:B:620:VAL:O	1:B:624:LEU:HD12	1.92	0.69
1:B:702:LEU:HD12	1:B:703:ILE:N	2.07	0.69
1:A:809:SER:OG	1:A:810:SER:N	2.24	0.69
1:B:573:LEU:HD11	1:B:575:MET:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:SER:O	1:A:834:ILE:HG13	1.93	0.69
1:B:544:ASP:HA	1:B:547:GLU:OE1	1.93	0.69
1:A:764:LYS:HZ1	1:A:765:VAL:HG22	1.58	0.69
1:A:815:ARG:O	1:A:819:GLU:N	2.25	0.69
1:B:190:LEU:HD22	1:B:194:GLN:NE2	2.04	0.68
1:B:576:PRO:HG3	1:B:598:LYS:CE	2.23	0.68
1:A:249:ARG:HA	1:A:252:LEU:HG	1.76	0.68
1:B:810:SER:CB	1:B:815:ARG:HH21	2.07	0.68
1:A:317:GLY:N	1:A:454:GLU:OE2	2.27	0.67
1:B:731:GLU:OE2	1:B:735:ARG:NH2	2.27	0.67
1:B:33:ARG:NH2	1:B:169:PRO:O	2.27	0.67
1:B:170:ARG:N	1:B:174:SER:OG	2.25	0.67
1:B:481:ARG:NE	3:B:1104:HOH:O	2.16	0.67
1:B:590:ASP:HA	1:B:593:GLN:HB3	1.76	0.67
1:A:288:HIS:CB	1:A:300:ARG:NH2	2.57	0.67
1:B:341:SER:O	1:B:366:ALA:HB2	1.94	0.67
1:B:575:MET:O	1:B:577:LYS:NZ	2.28	0.67
1:B:432:PRO:HD2	1:B:802:ARG:NH1	2.10	0.67
1:A:249:ARG:N	1:A:252:LEU:HD23	2.10	0.67
1:A:743:LEU:HD23	1:A:746:GLY:HA2	1.78	0.66
1:B:599:THR:HG23	1:B:601:HIS:H	1.61	0.66
1:A:248:LEU:O	1:A:250:ALA:N	2.29	0.66
1:B:856:LEU:HD11	1:B:866:GLU:HB2	1.78	0.66
1:B:568:VAL:HA	1:B:572:GLU:HB3	1.78	0.66
1:B:580:LYS:HD2	1:B:581:THR:N	2.11	0.66
1:B:751:GLY:O	1:B:754:GLN:HB2	1.96	0.66
1:A:316:HIS:CA	1:A:454:GLU:OE2	2.44	0.65
1:A:291:PHE:HB2	1:A:300:ARG:NH1	2.11	0.65
1:B:596:PHE:CE1	1:B:605:GLN:HB2	2.32	0.65
1:B:453:ALA:N	3:B:1103:HOH:O	2.13	0.65
1:A:43:PHE:HB2	1:A:52:ASN:HB3	1.79	0.65
1:B:561:SER:HG	1:B:564:GLN:HB2	1.62	0.65
1:B:722:SER:OG	1:B:723:VAL:N	2.30	0.65
1:A:555:LYS:HG2	1:A:556:GLN:H	1.63	0.64
1:A:743:LEU:CD2	1:A:746:GLY:HA2	2.28	0.64
1:A:288:HIS:HA	1:A:300:ARG:CZ	2.27	0.64
1:B:400:HIS:ND1	1:B:423:THR:OG1	2.27	0.64
1:B:46:GLN:CD	1:B:46:GLN:H	2.00	0.64
1:B:867:VAL:HG11	1:B:872:GLN:HG3	1.80	0.64
1:A:575:MET:HE3	1:A:576:PRO:HD2	1.80	0.64
1:A:288:HIS:ND1	1:A:300:ARG:NH2	2.39	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:SER:OG	1:A:749:ALA:N	2.25	0.64
1:A:314:VAL:HG21	1:A:449:ARG:HA	1.79	0.63
1:A:516:LEU:HA	1:A:519:MET:HE2	1.80	0.63
1:A:519:MET:SD	1:A:839:MET:HE1	2.38	0.63
1:B:565:LEU:O	1:B:569:LEU:N	2.27	0.63
1:B:704:GLU:HA	1:B:707:ASN:OD1	1.99	0.63
1:B:698:ARG:HA	1:B:703:ILE:HD11	1.79	0.63
1:B:758:ILE:HG23	1:B:759:SER:H	1.64	0.63
1:A:474:ALA:O	1:A:478:VAL:HG12	1.98	0.63
1:B:789:ARG:HH21	1:B:807:LEU:HD12	1.62	0.63
1:A:333:TRP:CG	1:A:371:ARG:NH1	2.67	0.62
1:A:120:THR:HG23	1:A:463:LEU:HA	1.79	0.62
1:A:646:ARG:NH1	1:A:828:GLN:OE1	2.32	0.62
1:A:722:SER:OG	1:A:723:VAL:N	2.30	0.62
1:B:573:LEU:HD12	1:B:573:LEU:C	2.19	0.62
1:B:762:GLU:O	1:B:766:GLN:N	2.32	0.62
1:B:758:ILE:HG23	1:B:759:SER:N	2.15	0.62
1:B:73:ILE:HG21	1:B:119:ILE:HD13	1.81	0.62
1:A:708:THR:OG1	1:A:710:GLU:OE1	2.16	0.62
1:B:297:ARG:HA	1:B:300:ARG:HB3	1.81	0.62
1:A:285:ASP:HA	1:A:288:HIS:HB2	1.81	0.62
1:A:565:LEU:CD2	1:A:607:LEU:HD11	2.30	0.62
1:B:764:LYS:O	1:B:767:MET:HB2	2.00	0.61
1:A:221:THR:HG23	1:A:222:LYS:HD2	1.82	0.61
1:A:175:GLU:H	1:A:175:GLU:CD	2.00	0.61
1:B:251:ASN:O	1:B:254:SER:OG	2.11	0.61
1:A:229:SER:HB2	1:A:232:ALA:HB3	1.82	0.61
1:A:782:ARG:O	1:A:786:ASP:N	2.22	0.61
1:A:50:THR:HG21	1:A:102:GLU:HB3	1.83	0.61
1:B:238:ASP:HB3	1:B:241:LYS:HD2	1.83	0.61
1:A:240:VAL:O	1:A:245:GLY:HA3	2.01	0.60
1:A:739:MET:HA	1:A:752:LEU:HD11	1.83	0.60
1:B:191:THR:HG22	1:B:194:GLN:HE22	1.66	0.60
1:A:46:GLN:NE2	1:A:295:GLU:OE1	2.35	0.60
1:B:641:ILE:HG12	1:B:648:SER:OG	2.00	0.60
1:B:575:MET:SD	1:B:604:LEU:HD11	2.42	0.60
1:A:733:ARG:O	1:A:736:VAL:HG22	2.02	0.60
1:B:290:LEU:O	1:B:294:LEU:HG	2.00	0.60
1:B:880:ARG:HH12	1:B:897:VAL:HG11	1.67	0.60
1:B:649:SER:HB2	1:B:654:LEU:H	1.66	0.60
1:B:323:ARG:NH1	1:B:329:GLU:OE2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:OG1	1:B:49:LEU:N	2.34	0.59
1:B:794:THR:HG21	1:B:822:ALA:HA	1.83	0.59
1:B:131:ASP:OD1	1:B:265:ILE:HG12	2.02	0.59
1:B:237:VAL:HG23	1:B:238:ASP:CG	2.22	0.59
1:B:561:SER:OG	1:B:564:GLN:HB2	2.02	0.59
1:B:507:ARG:HG2	1:B:507:ARG:HH11	1.68	0.59
1:A:716:VAL:HG23	1:A:774:PHE:CE2	2.37	0.59
1:B:105:GLY:O	1:B:109:ILE:HD13	2.02	0.59
1:B:170:ARG:NH1	1:B:177:THR:CB	2.60	0.59
1:B:758:ILE:CG2	1:B:759:SER:N	2.65	0.59
1:A:113:VAL:O	1:A:117:LEU:HD12	2.03	0.58
1:A:342:ARG:HB3	1:A:396:PRO:HB2	1.84	0.58
1:B:168:TYR:O	1:B:177:THR:HG22	2.03	0.58
1:A:170:ARG:H	1:A:170:ARG:HD3	1.67	0.58
1:A:247:ALA:O	1:A:251:ASN:HB2	2.04	0.58
1:B:685:TYR:HA	1:B:895:VAL:HG12	1.84	0.58
1:A:440:ASP:HA	1:A:451:LEU:HD22	1.85	0.58
1:B:642:ALA:HB3	1:B:644:THR:HG22	1.85	0.58
1:B:857:LEU:HD12	1:B:864:LEU:HD23	1.86	0.58
1:A:248:LEU:HB3	1:A:252:LEU:HD23	1.85	0.58
1:B:200:ALA:HB1	1:B:255:VAL:CG1	2.32	0.58
1:B:185:VAL:HG11	1:B:191:THR:HA	1.86	0.58
1:B:800:ARG:NH2	1:B:833:ASP:OD1	2.36	0.58
1:A:589:ALA:O	1:A:593:GLN:N	2.35	0.58
1:B:191:THR:CG2	1:B:194:GLN:HE22	2.17	0.58
1:B:810:SER:HA	1:B:814:VAL:HG21	1.85	0.58
1:A:684:ASP:OD2	1:A:862:GLU:HB3	2.03	0.58
1:A:757:LYS:O	1:A:757:LYS:HG2	2.02	0.58
1:B:782:ARG:O	1:B:786:ASP:N	2.26	0.57
1:B:785:VAL:HG11	1:B:819:GLU:OE1	2.04	0.57
1:B:830:SER:O	1:B:834:ILE:HG13	2.04	0.57
1:A:644:THR:O	1:A:829:GLY:HA2	2.04	0.57
1:A:677:TYR:CD2	1:A:866:GLU:HG2	2.39	0.57
1:B:278:ARG:NE	1:B:440:ASP:OD1	2.37	0.57
1:B:107:ILE:N	3:B:1105:HOH:O	2.22	0.57
1:A:816:GLU:HA	1:A:819:GLU:HB2	1.86	0.57
1:B:196:PRO:O	1:B:200:ALA:HB2	2.04	0.57
1:B:646:ARG:HG2	1:B:647:LEU:H	1.68	0.57
1:A:33:ARG:NH2	1:A:168:TYR:CZ	2.72	0.57
1:B:225:VAL:HG23	1:B:226:GLU:OE1	2.04	0.57
1:A:542:ILE:HD13	1:A:614:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:VAL:CG2	1:B:830:SER:HB3	2.33	0.57
1:A:315:GLU:HG2	1:A:316:HIS:CE1	2.39	0.56
1:A:455:THR:HB	1:A:457:GLU:OE1	2.05	0.56
1:B:528:LEU:HD11	1:B:627:VAL:HG11	1.87	0.56
1:A:262:THR:HG22	1:A:264:LEU:HG	1.87	0.56
1:A:779:ASP:O	1:A:783:ASP:N	2.31	0.56
1:A:797:VAL:HG23	1:A:830:SER:CB	2.30	0.56
1:A:729:THR:OG1	1:A:732:LEU:HB3	2.05	0.56
1:B:157:LEU:HD21	1:B:179:PHE:HD1	1.68	0.56
1:B:231:GLN:CA	1:B:234:VAL:HG22	2.33	0.56
1:B:237:VAL:HG23	1:B:238:ASP:N	2.21	0.56
1:B:185:VAL:CG1	1:B:191:THR:HA	2.35	0.56
1:A:780:TYR:CE1	1:A:784:VAL:HB	2.40	0.56
1:B:341:SER:N	3:B:1106:HOH:O	2.39	0.56
1:B:243:LYS:HG2	1:B:246:ASP:HB3	1.86	0.56
1:B:532:GLU:HA	1:B:535:GLN:HB2	1.88	0.56
1:B:713:HIS:HB3	1:B:736:VAL:HG23	1.87	0.56
1:A:704:GLU:OE2	1:A:707:ASN:ND2	2.38	0.56
1:A:116:ALA:HB1	1:A:287:ILE:HG23	1.88	0.56
1:A:747:LEU:HG	1:A:755:GLN:HE22	1.70	0.56
1:B:515:THR:HG23	1:B:843:ASP:OD2	2.06	0.56
1:B:712:LEU:O	1:B:716:VAL:HG23	2.06	0.56
1:B:685:TYR:HE1	1:B:893:LEU:HD13	1.70	0.56
1:A:452:ARG:HH22	1:A:459:GLN:HE22	1.52	0.56
1:B:237:VAL:HG23	1:B:238:ASP:OD2	2.06	0.56
1:A:108:ASP:O	1:A:112:GLU:HG3	2.06	0.55
1:A:566:GLN:O	1:A:570:PHE:HB2	2.07	0.55
1:B:147:VAL:HG13	1:B:164:VAL:HA	1.89	0.55
1:B:226:GLU:HB2	1:B:227:TYR:CD2	2.41	0.55
1:A:594:SER:HA	1:A:597:GLU:HG3	1.88	0.55
1:A:58:THR:O	1:A:62:ILE:HD12	2.07	0.55
1:B:574:GLU:OE2	1:B:577:LYS:NZ	2.38	0.55
1:B:65:LEU:O	1:B:69:GLN:NE2	2.38	0.55
1:B:173:VAL:HG12	1:B:173:VAL:O	2.06	0.55
1:B:588:ASP:O	1:B:591:ALA:N	2.40	0.55
1:A:198:PHE:CE1	1:A:221:THR:HB	2.42	0.55
1:A:261:LEU:HD23	1:A:262:THR:CB	2.35	0.55
1:B:184:VAL:O	1:B:188:TYR:HB2	2.06	0.55
1:B:248:LEU:O	1:B:250:ALA:N	2.40	0.55
1:A:291:PHE:HB2	1:A:300:ARG:HH12	1.72	0.55
1:A:33:ARG:HH12	1:A:170:ARG:HA	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:THR:H	1:B:733:ARG:HG3	1.71	0.55
1:A:699:ASP:HB3	1:A:702:LEU:HD12	1.88	0.55
1:A:905:ALA:O	1:A:908:HIS:CE1	2.59	0.55
1:B:175:GLU:HB2	1:B:176:LEU:HD12	1.89	0.55
1:B:350:THR:HG22	1:B:357:ASP:H	1.72	0.55
1:B:752:LEU:CD1	1:B:763:ALA:HB1	2.37	0.55
1:A:458:GLN:OE1	1:A:476:GLN:NE2	2.40	0.54
1:B:576:PRO:HG2	1:B:595:LEU:CD1	2.35	0.54
1:B:727:GLU:C	1:B:729:THR:HG23	2.28	0.54
1:A:717:ALA:HA	1:A:736:VAL:HG11	1.89	0.54
1:B:45:THR:HB	1:B:47:SER:H	1.72	0.54
1:B:528:LEU:O	1:B:532:GLU:HG2	2.08	0.54
1:A:157:LEU:O	1:A:160:VAL:HG12	2.08	0.54
1:A:566:GLN:HE22	1:A:585:TYR:N	2.06	0.54
1:B:184:VAL:HG13	1:B:185:VAL:HG13	1.88	0.54
1:A:259:ARG:C	1:A:261:LEU:N	2.59	0.54
1:B:73:ILE:HG12	1:B:119:ILE:HD12	1.90	0.54
1:B:47:SER:OG	1:B:47:SER:O	2.24	0.54
1:B:720:ALA:HB1	1:B:769:GLN:HE22	1.72	0.54
1:A:259:ARG:C	1:A:261:LEU:H	2.11	0.54
1:A:698:ARG:HG3	1:A:698:ARG:HH11	1.72	0.54
1:A:764:LYS:HZ1	1:A:765:VAL:CG2	2.20	0.54
1:A:507:ARG:NH2	1:B:395:PRO:N	2.56	0.54
1:B:45:THR:CG2	1:B:49:LEU:HB2	2.35	0.54
1:A:167:LEU:HD22	1:A:178:ARG:HG2	1.88	0.54
1:A:823:LEU:O	1:A:823:LEU:HD23	2.07	0.54
1:B:363:ILE:HD12	1:B:389:TRP:CZ3	2.43	0.54
1:B:880:ARG:HH22	1:B:897:VAL:HG12	1.72	0.54
1:A:229:SER:HB2	1:A:232:ALA:CB	2.38	0.54
1:B:728:VAL:HG12	1:B:733:ARG:HH21	1.72	0.54
1:B:845:ALA:HB1	1:B:878:LEU:HD21	1.90	0.54
1:A:779:ASP:O	1:A:783:ASP:HB2	2.08	0.53
1:A:795:SER:OG	1:A:796:THR:O	2.27	0.53
1:B:730:PRO:HA	1:B:733:ARG:HD2	1.89	0.53
1:A:282:TRP:CZ3	1:A:307:LEU:HB3	2.40	0.53
1:A:610:HIS:O	1:A:614:THR:HG23	2.08	0.53
1:B:252:LEU:HG	1:B:253:SER:N	2.23	0.53
1:A:581:THR:OG1	1:A:584:GLY:N	2.39	0.53
1:B:219:THR:HB	1:B:223:TRP:CZ2	2.43	0.53
1:B:45:THR:OG1	1:B:48:GLY:N	2.41	0.53
1:A:831:ALA:O	1:A:835:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:ARG:NH1	1:A:894:GLU:H	2.07	0.53
1:B:445:ARG:HH11	1:B:445:ARG:HG3	1.74	0.53
1:B:673:VAL:HB	1:B:680:LEU:HG	1.89	0.53
1:B:273:THR:HG23	1:B:275:ASP:H	1.73	0.53
1:B:516:LEU:O	1:B:520:GLU:HG3	2.09	0.53
1:B:780:TYR:O	1:B:784:VAL:HG12	2.08	0.53
1:B:764:LYS:CD	1:B:764:LYS:O	2.52	0.53
1:A:316:HIS:HB3	1:A:454:GLU:OE1	2.08	0.53
1:A:232:ALA:O	1:A:236:ASN:HB2	2.09	0.53
1:B:573:LEU:HD21	1:B:575:MET:HE3	1.91	0.53
1:A:220:ALA:HA	1:A:223:TRP:CD1	2.44	0.52
1:A:789:ARG:NH2	1:A:819:GLU:OE1	2.42	0.52
1:B:508:MET:O	1:B:512:VAL:HG23	2.09	0.52
1:A:159:LEU:HD11	1:A:264:LEU:HD12	1.91	0.52
1:A:158:GLN:HG3	1:A:159:LEU:HD12	1.90	0.52
1:A:341:SER:O	1:A:341:SER:OG	2.25	0.52
1:B:255:VAL:O	1:B:255:VAL:HG12	2.08	0.52
1:B:53:ALA:H	1:B:106:GLN:HE22	1.56	0.52
1:B:67:ASP:HB2	1:B:68:GLU:OE1	2.09	0.52
1:A:724:PRO:HA	1:A:727:GLU:OE2	2.09	0.52
1:A:747:LEU:HD21	1:A:751:GLY:HA3	1.91	0.52
1:A:764:LYS:C	1:A:764:LYS:HD2	2.29	0.52
1:B:816:GLU:O	1:B:820:ARG:N	2.19	0.52
1:B:273:THR:HG22	1:B:276:THR:HG23	1.91	0.52
1:B:61:LEU:HA	1:B:64:LEU:HD12	1.90	0.52
1:B:756:LEU:O	1:B:757:LYS:HB3	2.09	0.52
1:A:641:ILE:HG23	1:A:642:ALA:N	2.25	0.52
1:A:59:ALA:HB2	1:A:299:LEU:HD21	1.91	0.52
1:B:575:MET:SD	1:B:595:LEU:HD23	2.49	0.52
1:B:62:ILE:HD12	1:B:299:LEU:HD22	1.90	0.52
1:B:662:GLU:HA	1:B:665:ARG:HG2	1.92	0.52
1:B:533:GLN:O	1:B:537:GLU:HB2	2.09	0.52
1:B:237:VAL:HG23	1:B:238:ASP:H	1.75	0.52
1:A:234:VAL:O	1:A:235:ASP:HB2	2.10	0.52
1:A:699:ASP:HB2	1:A:776:GLY:HA3	1.92	0.52
1:A:768:GLU:O	1:A:772:ASP:HB2	2.09	0.52
1:A:806:GLU:OE2	1:A:806:GLU:N	2.42	0.52
1:B:821:ALA:HA	1:B:824:ASN:HB3	1.92	0.52
1:B:326:GLU:O	1:B:329:GLU:HG2	2.10	0.51
1:B:157:LEU:HD23	1:B:160:VAL:HG21	1.92	0.51
1:B:391:ALA:HA	1:B:415:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:PHE:O	1:B:300:ARG:N	2.44	0.51
1:B:552:VAL:HG11	1:B:603:PHE:HB2	1.92	0.51
1:A:249:ARG:H	1:A:252:LEU:HD23	1.76	0.51
1:A:446:TYR:CD2	1:A:492:LEU:HD21	2.45	0.51
1:A:807:LEU:HD23	1:A:818:ALA:HB1	1.92	0.51
1:B:562:PRO:O	1:B:566:GLN:HG3	2.10	0.51
1:A:616:LEU:O	1:A:620:VAL:HG12	2.10	0.51
1:A:372:TYR:CG	1:A:475:VAL:HG12	2.45	0.51
1:A:565:LEU:O	1:A:569:LEU:HB2	2.10	0.51
1:B:34:ALA:HB1	1:B:56:GLY:HA3	1.93	0.51
1:B:717:ALA:HB2	1:B:736:VAL:HG11	1.93	0.51
1:B:101:ASP:OD1	1:B:104:ARG:NH2	2.37	0.51
1:B:180:THR:H	1:B:183:ALA:HB3	1.75	0.51
1:B:747:LEU:HD21	1:B:751:GLY:C	2.31	0.51
1:B:793:TYR:CE1	1:B:801:ARG:HD2	2.46	0.51
1:A:241:LYS:HZ1	1:A:249:ARG:H	1.59	0.51
1:A:290:LEU:O	1:A:294:LEU:HG	2.11	0.51
1:B:436:SER:O	1:B:436:SER:OG	2.27	0.51
1:B:714:SER:O	1:B:718:SER:OG	2.24	0.51
1:B:45:THR:CG2	1:B:49:LEU:O	2.47	0.50
1:B:665:ARG:HB2	1:B:904:ASP:OD1	2.10	0.50
1:A:568:VAL:HA	1:A:572:GLU:HB2	1.93	0.50
1:A:779:ASP:C	1:A:781:LEU:N	2.63	0.50
1:B:99:THR:OG1	1:B:100:PRO:HD3	2.10	0.50
1:B:434:GLN:HG3	1:B:436:SER:H	1.75	0.50
1:B:577:LYS:N	1:B:577:LYS:HD2	2.27	0.50
1:B:63:ASN:OD1	1:B:66:ARG:NH2	2.44	0.50
1:A:727:GLU:HB3	1:A:732:LEU:HD21	1.92	0.50
1:A:816:GLU:O	1:A:820:ARG:N	2.31	0.50
1:B:183:ALA:O	1:B:187:LYS:HD3	2.11	0.50
1:A:195:TYR:N	1:A:196:PRO:HD2	2.27	0.50
1:B:233:LEU:HG	1:B:233:LEU:O	2.10	0.50
1:B:541:GLN:HA	1:B:544:ASP:HB2	1.93	0.50
1:B:73:ILE:CG2	1:B:279:MET:HG3	2.42	0.50
1:A:729:THR:O	1:A:731:GLU:N	2.45	0.50
1:A:140:ALA:HB1	1:A:145:TYR:HB2	1.93	0.50
1:A:457:GLU:OE1	1:A:457:GLU:N	2.44	0.50
1:B:729:THR:O	1:B:731:GLU:N	2.45	0.50
1:A:261:LEU:CD2	1:A:262:THR:OG1	2.45	0.50
1:B:435:ARG:HG2	1:B:641:ILE:O	2.11	0.50
1:B:227:TYR:CD1	1:B:236:ASN:OD1	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:LYS:O	1:B:757:LYS:HG2	2.12	0.49
1:A:473:GLN:O	1:A:477:THR:OG1	2.18	0.49
1:A:692:ILE:HG22	1:A:889:LEU:HD11	1.94	0.49
1:B:641:ILE:CD1	1:B:642:ALA:H	2.20	0.49
1:A:744:ALA:O	1:A:823:LEU:HD23	2.12	0.49
1:B:24:LEU:CD2	1:B:133:ILE:HG23	2.36	0.49
1:A:167:LEU:HD21	1:A:178:ARG:HH11	1.78	0.49
1:A:696:LEU:HD13	1:A:780:TYR:OH	2.12	0.49
1:B:238:ASP:HA	1:B:241:LYS:HB3	1.93	0.49
1:B:552:VAL:CG1	1:B:601:HIS:HE1	2.25	0.49
1:B:811:ASN:HB3	1:B:814:VAL:HG13	1.93	0.49
1:A:166:VAL:O	1:A:167:LEU:HD23	2.13	0.49
1:A:231:GLN:HE21	1:A:256:ILE:HD12	1.77	0.49
1:A:534:LEU:HD11	1:A:666:ARG:HG2	1.93	0.49
1:A:785:VAL:O	1:A:789:ARG:HG2	2.13	0.49
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.78	0.49
1:B:765:VAL:HA	1:B:768:GLU:H	1.77	0.49
1:A:99:THR:CG2	1:A:100:PRO:HD3	2.27	0.49
1:B:752:LEU:HD11	1:B:763:ALA:HB1	1.94	0.49
1:B:778:ARG:HG3	1:B:778:ARG:HH11	1.77	0.49
1:B:802:ARG:NH2	1:B:803:TYR:O	2.46	0.49
1:A:286:GLN:O	1:A:290:LEU:HD23	2.13	0.49
1:A:598:LYS:HD2	1:A:598:LYS:O	2.13	0.49
1:A:704:GLU:CD	1:A:707:ASN:HD21	2.16	0.49
1:B:158:GLN:HB2	1:B:266:ARG:HH22	1.78	0.49
1:B:548:ALA:O	1:B:552:VAL:HG23	2.13	0.49
1:A:187:LYS:HB2	1:A:188:TYR:CD2	2.48	0.49
1:A:271:PRO:HD2	1:A:272:GLN:OE1	2.13	0.49
1:A:197:ASP:HB3	1:A:230:LEU:HD12	1.95	0.48
1:B:259:ARG:O	1:B:263:ASP:HB2	2.13	0.48
1:A:535:GLN:HG3	1:A:617:LYS:HE2	1.95	0.48
1:A:575:MET:HE1	1:A:595:LEU:O	2.13	0.48
1:B:590:ASP:O	1:B:594:SER:HB3	2.13	0.48
1:A:498:ARG:HD3	1:A:499:ILE:HG23	1.95	0.48
1:A:288:HIS:CE1	1:A:300:ARG:HH21	2.28	0.48
1:A:326:GLU:HB2	1:A:327:PRO:HD2	1.95	0.48
1:A:446:TYR:CE2	1:A:492:LEU:HD21	2.48	0.48
1:A:533:GLN:NE2	1:A:537:GLU:OE1	2.42	0.48
1:B:507:ARG:O	1:B:511:PRO:HG2	2.13	0.48
1:A:507:ARG:HH22	1:B:394:GLY:CA	2.26	0.48
1:A:537:GLU:OE2	1:A:666:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLN:HG2	1:A:69:GLN:O	2.14	0.48
1:B:680:LEU:HD23	1:B:866:GLU:HA	1.94	0.48
1:A:159:LEU:HD11	1:A:264:LEU:CD1	2.44	0.48
1:B:756:LEU:N	1:B:756:LEU:HD22	2.27	0.48
1:B:784:VAL:HG13	1:B:785:VAL:HG23	1.94	0.48
1:B:184:VAL:HG11	1:B:192:PRO:HG3	1.96	0.48
1:B:229:SER:O	1:B:232:ALA:HB3	2.14	0.48
1:B:74:ALA:HB2	1:B:277:LEU:HD13	1.96	0.48
1:B:858:GLN:HG2	1:B:863:LEU:HD23	1.95	0.48
1:A:470:VAL:HG23	1:A:472:GLU:HG2	1.96	0.48
1:B:533:GLN:HA	1:B:533:GLN:OE1	2.14	0.48
1:B:780:TYR:CE1	1:B:784:VAL:HB	2.49	0.48
1:B:644:THR:O	1:B:829:GLY:HA2	2.14	0.48
1:A:531:LEU:HB3	1:A:624:LEU:HD21	1.95	0.48
1:A:704:GLU:HA	1:A:707:ASN:ND2	2.29	0.48
1:A:815:ARG:HG2	1:A:815:ARG:HH11	1.79	0.48
1:A:815:ARG:HA	1:A:818:ALA:HB3	1.96	0.48
1:B:624:LEU:O	1:B:627:VAL:HG12	2.14	0.48
1:B:713:HIS:HB3	1:B:736:VAL:CG2	2.44	0.48
1:A:748:SER:OG	1:A:750:TYR:N	2.47	0.47
1:B:677:TYR:CG	1:B:866:GLU:HG2	2.48	0.47
1:B:846:ILE:HG23	1:B:851:LEU:HB2	1.96	0.47
1:A:255:VAL:HG12	1:A:255:VAL:O	2.14	0.47
1:A:338:SER:OG	1:A:338:SER:O	2.31	0.47
1:A:395:PRO:HA	1:A:396:PRO:HD3	1.80	0.47
1:A:704:GLU:HA	1:A:707:ASN:HD21	1.79	0.47
1:A:789:ARG:HA	1:A:807:LEU:HD12	1.94	0.47
1:B:595:LEU:O	1:B:599:THR:N	2.37	0.47
1:A:197:ASP:OD1	1:A:259:ARG:NH1	2.47	0.47
1:A:591:ALA:O	1:A:595:LEU:HD13	2.15	0.47
1:B:46:GLN:NE2	1:B:46:GLN:H	2.12	0.47
1:B:320:VAL:HG23	1:B:479:ILE:HG22	1.96	0.47
1:A:132:ILE:HG22	1:A:268:VAL:HG11	1.96	0.47
1:A:708:THR:HG23	1:A:709:GLY:N	2.29	0.47
1:B:342:ARG:HB2	1:B:396:PRO:O	2.13	0.47
1:A:156:SER:O	1:A:166:VAL:HG21	2.14	0.47
1:B:692:ILE:HD11	1:B:827:ILE:HA	1.97	0.47
1:A:154:ARG:HG3	1:A:168:TYR:HE1	1.72	0.47
1:A:594:SER:HA	1:A:597:GLU:HB2	1.97	0.47
1:A:761:GLU:O	1:A:764:LYS:HB3	2.14	0.47
1:B:573:LEU:HD12	1:B:574:GLU:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:O	1:B:62:ILE:HG13	2.14	0.47
1:B:901:ARG:NE	1:B:901:ARG:H	2.04	0.47
1:A:158:GLN:CG	1:A:159:LEU:HD12	2.45	0.47
1:A:381:GLU:OE2	1:A:381:GLU:N	2.47	0.47
1:A:538:PHE:O	1:A:542:ILE:HG13	2.14	0.47
1:A:566:GLN:HE22	1:A:585:TYR:H	1.61	0.47
1:B:154:ARG:HB2	1:B:157:LEU:CD1	2.45	0.47
1:A:183:ALA:O	1:A:186:GLU:HG2	2.15	0.47
1:A:195:TYR:OH	1:A:202:ARG:NH2	2.48	0.47
1:A:733:ARG:HB2	1:A:733:ARG:HE	1.66	0.47
1:A:747:LEU:HD11	1:A:755:GLN:NE2	2.29	0.47
1:A:259:ARG:HA	1:A:261:LEU:CB	2.40	0.47
1:A:378:LEU:HG	1:A:382:ASP:HB2	1.97	0.47
1:A:581:THR:HG1	1:A:584:GLY:N	2.13	0.47
1:B:641:ILE:HD12	1:B:642:ALA:CB	2.44	0.47
1:B:767:MET:O	1:B:770:TYR:HB3	2.14	0.47
1:B:195:TYR:N	1:B:196:PRO:HD2	2.29	0.47
1:B:202:ARG:HD3	1:B:203:GLY:N	2.30	0.47
1:B:249:ARG:H	1:B:249:ARG:HG3	1.49	0.47
1:B:501:SER:HA	3:B:1107:HOH:O	2.15	0.47
1:B:574:GLU:HA	1:B:574:GLU:OE1	2.14	0.47
1:A:252:LEU:HD12	1:A:253:SER:N	2.30	0.46
1:A:116:ALA:HB1	1:A:287:ILE:CG2	2.45	0.46
1:A:316:HIS:CD2	1:A:454:GLU:OE1	2.68	0.46
1:B:718:SER:CB	1:B:724:PRO:HB3	2.45	0.46
1:A:196:PRO:HB2	1:A:259:ARG:HD3	1.96	0.46
1:A:145:TYR:OH	1:A:274:PRO:O	2.29	0.46
1:A:677:TYR:CG	1:A:866:GLU:HG2	2.50	0.46
1:A:391:ALA:HA	1:A:415:THR:O	2.16	0.46
1:B:573:LEU:CD1	1:B:575:MET:HB2	2.45	0.46
1:A:283:ASN:O	1:A:287:ILE:HG13	2.16	0.46
1:B:531:LEU:HD22	1:B:620:VAL:HG23	1.97	0.46
1:A:812:ARG:C	1:A:815:ARG:HH12	2.18	0.46
1:A:248:LEU:HB3	1:A:252:LEU:CD2	2.45	0.46
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.78	0.46
1:B:54:VAL:HG22	1:B:110:THR:HG23	1.98	0.46
1:B:419:VAL:HG12	3:B:1108:HOH:O	2.16	0.46
1:B:544:ASP:CA	1:B:547:GLU:HG2	2.45	0.46
1:A:283:ASN:O	1:A:285:ASP:N	2.48	0.46
1:A:117:LEU:HD21	1:A:303:LEU:HD11	1.98	0.46
1:A:352:LYS:O	1:A:356:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:THR:CG2	1:A:585:TYR:HB3	2.46	0.46
1:B:166:VAL:O	1:B:167:LEU:HD23	2.15	0.46
1:B:23:MET:HB3	1:B:73:ILE:HD12	1.97	0.46
1:B:729:THR:N	1:B:733:ARG:HE	2.14	0.46
1:A:33:ARG:HG2	1:A:172:GLY:O	2.16	0.45
1:A:184:VAL:HG11	1:A:192:PRO:HG3	1.98	0.45
1:A:284:ARG:O	1:A:284:ARG:HG2	2.15	0.45
1:A:574:GLU:OE2	1:A:575:MET:O	2.33	0.45
1:A:70:PRO:CG	1:A:73:ILE:HD11	2.42	0.45
1:A:748:SER:OG	1:A:750:TYR:CD1	2.58	0.45
1:B:779:ASP:O	1:B:783:ASP:HB2	2.16	0.45
1:B:889:LEU:HD12	1:B:893:LEU:HD23	1.97	0.45
1:A:644:THR:OG1	1:A:646:ARG:HG3	2.16	0.45
1:A:798:LEU:HD12	1:A:833:ASP:HB3	1.96	0.45
1:B:353:ALA:HB2	1:B:636:THR:HG22	1.98	0.45
1:B:793:TYR:CD1	1:B:801:ARG:HD2	2.51	0.45
1:A:333:TRP:CD1	1:A:371:ARG:CZ	2.96	0.45
1:A:40:ALA:HA	1:A:52:ASN:ND2	2.31	0.45
1:A:317:GLY:H	1:A:454:GLU:CD	2.19	0.45
1:A:425:LEU:O	1:A:428:TYR:HB3	2.16	0.45
1:A:451:LEU:HG	1:A:451:LEU:O	2.17	0.45
1:A:575:MET:HE2	1:A:575:MET:HB3	1.73	0.45
1:B:392:ASP:O	1:B:395:PRO:HD2	2.17	0.45
1:B:423:THR:CG2	1:B:485:VAL:HG23	2.46	0.45
1:B:575:MET:CG	1:B:595:LEU:HD21	2.35	0.45
1:A:72:HIS:HA	1:A:278:ARG:HA	1.99	0.45
1:A:753:ALA:HB2	1:A:760:THR:HA	1.98	0.45
1:B:796:THR:HG23	1:B:800:ARG:O	2.16	0.45
1:B:199:ALA:HA	1:B:202:ARG:HG3	1.98	0.45
1:B:578:THR:HG23	1:B:585:TYR:HB3	1.99	0.45
1:A:323:ARG:NH2	1:A:329:GLU:OE2	2.49	0.45
1:B:428:TYR:HB2	1:B:640:THR:HG22	1.98	0.45
1:B:552:VAL:CG1	1:B:603:PHE:HB2	2.47	0.45
1:B:797:VAL:HG23	1:B:830:SER:CB	2.41	0.45
1:B:884:GLY:HA2	1:B:893:LEU:HD12	1.99	0.45
1:A:423:THR:HG21	1:A:488:LEU:HD23	1.99	0.45
1:B:320:VAL:HG13	1:B:458:GLN:OE1	2.17	0.45
1:B:77:PHE:CE2	1:B:121:VAL:HG13	2.52	0.45
1:A:537:GLU:CD	1:A:666:ARG:HH12	2.19	0.45
1:A:555:LYS:HB3	1:A:555:LYS:HE2	1.63	0.45
1:B:809:SER:OG	1:B:814:VAL:CB	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:816:GLU:C	1:B:820:ARG:HE	2.20	0.45
1:A:249:ARG:HA	1:A:252:LEU:CG	2.47	0.44
1:A:320:VAL:HG23	1:A:479:ILE:CG2	2.40	0.44
1:A:249:ARG:HG2	1:A:252:LEU:HD21	1.99	0.44
1:A:687:GLN:O	1:A:691:ARG:HG3	2.17	0.44
1:A:243:LYS:HE3	1:A:243:LYS:HB3	1.78	0.44
1:A:555:LYS:HG2	1:A:556:GLN:N	2.28	0.44
1:A:160:VAL:HG13	1:A:192:PRO:HG3	1.99	0.44
1:A:361:LEU:HD21	1:A:386:LEU:HD21	1.98	0.44
1:A:717:ALA:CA	1:A:736:VAL:HG11	2.48	0.44
1:B:197:ASP:HB3	1:B:230:LEU:HB3	1.98	0.44
1:B:73:ILE:HG21	1:B:279:MET:HG3	1.99	0.44
1:B:343:PHE:N	1:B:343:PHE:CD1	2.85	0.44
1:A:615:ARG:HA	1:A:618:VAL:HG22	1.99	0.44
1:B:287:ILE:O	1:B:291:PHE:HB2	2.17	0.44
1:A:258:ASN:C	1:A:261:LEU:HB2	2.37	0.44
1:A:194:GLN:N	1:A:194:GLN:CD	2.71	0.44
1:A:254:SER:O	1:A:257:LEU:HB2	2.18	0.44
1:A:428:TYR:HA	1:A:437:PHE:CZ	2.53	0.44
1:B:147:VAL:N	1:B:163:GLN:O	2.50	0.44
1:B:550:TYR:OH	1:B:559:LEU:HG	2.18	0.44
1:A:323:ARG:NH1	1:A:329:GLU:OE2	2.49	0.44
1:B:191:THR:OG1	1:B:192:PRO:HD2	2.18	0.44
1:B:230:LEU:O	1:B:234:VAL:N	2.46	0.44
1:B:691:ARG:O	1:B:694:ALA:HB3	2.18	0.44
1:A:641:ILE:CG2	1:A:642:ALA:N	2.81	0.43
1:B:739:MET:O	1:B:743:LEU:HG	2.18	0.43
1:B:539:ALA:HB2	1:B:617:LYS:HE3	1.99	0.43
1:B:658:PRO:HB2	1:B:661:THR:HG22	2.00	0.43
1:B:729:THR:CB	1:B:732:LEU:HD23	2.48	0.43
1:A:572:GLU:N	1:A:572:GLU:OE2	2.52	0.43
1:A:68:GLU:O	1:A:69:GLN:C	2.57	0.43
1:A:291:PHE:CB	1:A:300:ARG:NH1	2.79	0.43
1:A:26:ASP:O	1:A:30:LEU:HD12	2.18	0.43
1:A:679:GLU:HG3	1:A:680:LEU:O	2.19	0.43
1:A:784:VAL:O	1:A:788:ALA:N	2.52	0.43
1:B:134:ALA:O	1:B:138:THR:HG23	2.18	0.43
1:B:191:THR:HG23	1:B:194:GLN:CD	2.38	0.43
1:B:184:VAL:HG11	1:B:192:PRO:HD3	2.00	0.43
1:B:24:LEU:HD21	1:B:136:LEU:HB3	2.01	0.43
1:B:535:GLN:HG3	1:B:624:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:MET:O	1:A:310:VAL:HG11	2.18	0.43
1:A:463:LEU:H	1:A:463:LEU:HD12	1.84	0.43
1:B:136:LEU:HD11	1:B:270:LEU:HD11	2.00	0.43
1:B:862:GLU:OE2	1:B:903:TRP:NE1	2.45	0.43
1:A:154:ARG:NH1	1:A:202:ARG:NH2	2.58	0.43
1:A:33:ARG:NH2	1:A:169:PRO:O	2.51	0.43
1:A:692:ILE:HG22	1:A:889:LEU:CD1	2.49	0.43
1:B:755:GLN:O	1:B:756:LEU:HD22	2.17	0.43
1:A:316:HIS:CB	1:A:454:GLU:OE2	2.67	0.43
1:A:559:LEU:HD22	1:A:607:LEU:HD12	2.00	0.43
1:A:535:GLN:NE2	1:A:621:ASP:OD1	2.51	0.43
1:B:278:ARG:HG3	1:B:440:ASP:OD2	2.19	0.43
1:B:790:LYS:O	1:B:790:LYS:HG2	2.17	0.43
1:A:804:LEU:HD13	1:A:818:ALA:HB1	2.01	0.43
1:B:691:ARG:HG2	1:B:706:PHE:CE1	2.54	0.43
1:B:696:LEU:HD23	1:B:780:TYR:OH	2.19	0.43
1:A:562:PRO:HA	1:A:565:LEU:HD12	2.01	0.43
1:A:588:ASP:O	1:A:591:ALA:N	2.49	0.43
1:A:742:GLY:O	1:A:747:LEU:HB3	2.19	0.43
1:A:49:LEU:HD13	1:A:49:LEU:HA	1.86	0.43
1:B:528:LEU:CD2	1:B:531:LEU:HD12	2.43	0.43
1:A:258:ASN:O	1:A:261:LEU:CD1	2.64	0.42
1:A:812:ARG:HA	1:A:815:ARG:HH12	1.83	0.42
1:B:259:ARG:HH12	1:B:263:ASP:CG	2.22	0.42
1:B:323:ARG:NE	3:B:1101:HOH:O	2.00	0.42
1:B:403:LYS:NZ	1:B:520:GLU:OE2	2.42	0.42
1:A:255:VAL:CG1	1:A:255:VAL:O	2.68	0.42
1:B:234:VAL:O	1:B:235:ASP:HB3	2.18	0.42
1:B:864:LEU:HD12	1:B:865:PHE:H	1.84	0.42
1:B:879:VAL:O	1:B:883:MET:HG3	2.20	0.42
1:A:187:LYS:H	1:A:187:LYS:HG2	1.71	0.42
1:A:300:ARG:O	1:A:303:LEU:HB3	2.18	0.42
1:A:531:LEU:HA	1:A:531:LEU:HD23	1.88	0.42
1:A:73:ILE:HG22	1:A:74:ALA:N	2.34	0.42
1:B:40:ALA:O	1:B:44:LYS:NZ	2.35	0.42
1:B:460:GLN:O	1:B:464:LEU:HG	2.19	0.42
1:B:542:ILE:HD13	1:B:614:THR:HG22	2.00	0.42
1:B:528:LEU:CD1	1:B:627:VAL:HG11	2.49	0.42
1:A:316:HIS:HD2	1:A:454:GLU:OE1	2.01	0.42
1:A:708:THR:HG23	1:A:709:GLY:H	1.85	0.42
1:A:756:LEU:HD23	1:A:756:LEU:HA	1.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HA	1:B:160:VAL:HG23	2.00	0.42
1:B:160:VAL:HG22	1:B:166:VAL:CG2	2.49	0.42
1:B:257:LEU:HG	1:B:260:GLU:HB2	2.01	0.42
1:B:683:ALA:HA	1:B:896:SER:O	2.19	0.42
1:B:732:LEU:HA	1:B:735:ARG:CG	2.44	0.42
1:A:54:VAL:HG22	1:A:110:THR:HG23	2.00	0.42
1:A:259:ARG:HB2	1:A:259:ARG:NH1	2.35	0.42
1:B:180:THR:N	1:B:183:ALA:HB3	2.34	0.42
1:A:797:VAL:HG12	1:A:887:TYR:CZ	2.55	0.42
1:B:687:GLN:O	1:B:691:ARG:HG3	2.20	0.42
1:B:789:ARG:HH21	1:B:807:LEU:HB2	1.83	0.42
1:B:853:SER:OG	1:B:868:SER:N	2.34	0.42
1:A:183:ALA:HA	1:A:186:GLU:OE1	2.19	0.42
1:A:576:PRO:HD2	1:A:599:THR:HG21	2.01	0.42
1:A:595:LEU:O	1:A:599:THR:OG1	2.28	0.42
1:A:747:LEU:CG	1:A:755:GLN:HE22	2.33	0.42
1:A:503:SER:OG	1:B:340:GLY:HA2	2.19	0.42
1:B:552:VAL:HG12	1:B:601:HIS:HE1	1.83	0.42
1:A:731:GLU:OE1	1:A:735:ARG:NH2	2.53	0.42
1:A:762:GLU:CD	1:A:762:GLU:C	2.77	0.42
1:B:127:PHE:HD2	1:B:265:ILE:HD11	1.84	0.42
1:B:434:GLN:HG2	1:B:437:PHE:CD2	2.55	0.42
1:B:372:TYR:CG	1:B:475:VAL:HG22	2.55	0.42
1:B:423:THR:HG21	1:B:485:VAL:HG23	2.02	0.42
1:A:553:ILE:HD13	1:A:568:VAL:HG13	2.02	0.42
1:A:688:ILE:HG13	1:A:893:LEU:CD2	2.49	0.42
1:B:403:LYS:HB3	1:B:403:LYS:HE2	1.77	0.42
1:B:498:ARG:CZ	1:B:498:ARG:HB2	2.50	0.42
1:B:702:LEU:CD1	1:B:703:ILE:HG13	2.50	0.42
1:A:569:LEU:HD13	1:A:575:MET:HG3	2.01	0.41
1:A:779:ASP:HA	1:A:781:LEU:HB3	2.01	0.41
1:A:823:LEU:HG	1:A:827:ILE:CD1	2.49	0.41
1:B:565:LEU:HA	1:B:568:VAL:HG22	2.02	0.41
1:B:699:ASP:HB2	1:B:776:GLY:HA3	2.02	0.41
1:A:252:LEU:HD12	1:A:253:SER:OG	2.19	0.41
1:A:314:VAL:HG21	1:A:449:ARG:CA	2.47	0.41
1:B:575:MET:CG	1:B:595:LEU:CD2	2.94	0.41
1:B:807:LEU:HD22	1:B:819:GLU:HG3	2.01	0.41
1:A:241:LYS:HZ1	1:A:249:ARG:N	2.18	0.41
1:A:403:LYS:HB3	1:A:403:LYS:HE2	1.59	0.41
1:A:549:ALA:HB1	1:A:603:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:LEU:CD2	1:A:751:GLY:HA3	2.50	0.41
1:B:170:ARG:H	1:B:174:SER:HG	1.62	0.41
1:B:642:ALA:CB	1:B:644:THR:HG22	2.48	0.41
1:A:344:GLY:O	1:A:482:ALA:HB1	2.21	0.41
1:B:63:ASN:OD1	1:B:66:ARG:CZ	2.68	0.41
1:B:68:GLU:O	1:B:69:GLN:C	2.59	0.41
1:B:875:LEU:O	1:B:875:LEU:HG	2.18	0.41
1:A:591:ALA:O	1:A:595:LEU:HB2	2.20	0.41
1:B:595:LEU:O	1:B:599:THR:HG22	2.21	0.41
1:B:798:LEU:HD23	1:B:798:LEU:HA	1.70	0.41
1:A:168:TYR:HB3	1:A:177:THR:CG2	2.50	0.41
1:A:818:ALA:O	1:A:821:ALA:HB3	2.20	0.41
1:B:147:VAL:CG1	1:B:164:VAL:HG22	2.50	0.41
1:B:702:LEU:HD12	1:B:703:ILE:HG13	2.03	0.41
1:B:810:SER:CB	1:B:815:ARG:NH2	2.75	0.41
1:B:685:TYR:CE1	1:B:893:LEU:HD13	2.53	0.41
1:B:566:GLN:HG2	1:B:570:PHE:HE1	1.86	0.41
1:A:66:ARG:HD3	1:A:306:THR:HG22	2.01	0.41
1:A:71:THR:OG1	1:A:72:HIS:ND1	2.49	0.41
1:A:729:THR:N	1:A:733:ARG:HD3	2.16	0.41
1:A:785:VAL:HA	1:A:788:ALA:HB3	2.02	0.41
1:B:154:ARG:HB2	1:B:157:LEU:HD11	2.03	0.41
1:B:543:ARG:O	1:B:547:GLU:HB3	2.20	0.41
1:A:582:LYS:N	1:A:582:LYS:HD2	2.34	0.41
1:B:434:GLN:OE1	1:B:436:SER:O	2.39	0.41
1:B:575:MET:CE	1:B:599:THR:HG21	2.51	0.41
1:B:747:LEU:HD23	1:B:748:SER:N	2.35	0.41
1:A:59:ALA:HA	1:A:299:LEU:HD22	2.03	0.41
1:A:815:ARG:HG2	1:A:815:ARG:NH1	2.36	0.41
1:B:199:ALA:HA	1:B:202:ARG:CG	2.51	0.41
1:B:402:ALA:N	1:B:422:ASP:OD2	2.35	0.41
1:B:445:ARG:NH1	1:B:445:ARG:HG3	2.34	0.41
1:A:151:THR:OG1	1:A:152:GLY:N	2.54	0.41
1:A:283:ASN:C	1:A:285:ASP:H	2.24	0.41
1:A:578:THR:HG23	1:A:585:TYR:HB3	2.02	0.41
1:B:363:ILE:HD12	1:B:389:TRP:CH2	2.56	0.41
1:B:573:LEU:HD12	1:B:574:GLU:N	2.36	0.41
1:B:795:SER:OG	1:B:796:THR:O	2.38	0.41
1:A:161:SER:OG	1:A:162:ASP:N	2.54	0.40
1:A:261:LEU:HD23	1:A:262:THR:N	2.37	0.40
1:A:262:THR:C	1:A:264:LEU:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:LEU:HA	1:A:604:LEU:HD23	1.86	0.40
1:A:789:ARG:HA	1:A:807:LEU:CD1	2.51	0.40
1:B:372:TYR:CD2	1:B:475:VAL:HG22	2.56	0.40
1:B:687:GLN:HG3	1:B:712:LEU:HD23	2.03	0.40
1:B:785:VAL:CG1	1:B:819:GLU:HG2	2.51	0.40
1:A:492:LEU:HA	1:A:492:LEU:HD23	1.77	0.40
1:A:594:SER:HA	1:A:597:GLU:CG	2.50	0.40
1:A:812:ARG:CA	1:A:815:ARG:HH12	2.35	0.40
1:B:498:ARG:NH1	1:B:498:ARG:HB2	2.35	0.40
1:B:66:ARG:HB3	1:B:307:LEU:HD21	2.02	0.40
1:B:676:GLY:O	1:B:852:ARG:NH2	2.54	0.40
1:B:905:ALA:O	1:B:908:HIS:ND1	2.54	0.40
1:A:300:ARG:HD2	1:A:300:ARG:HH11	1.68	0.40
1:A:198:PHE:O	1:A:198:PHE:HD2	2.05	0.40
1:A:262:THR:C	1:A:264:LEU:N	2.74	0.40
1:A:342:ARG:CB	1:A:396:PRO:HB2	2.51	0.40
1:A:452:ARG:HG3	1:A:452:ARG:NH1	2.36	0.40
1:A:839:MET:HG2	1:A:863:LEU:HD21	2.03	0.40
1:B:596:PHE:HB2	1:B:604:LEU:HB2	2.04	0.40
1:B:756:LEU:O	1:B:758:ILE:HG13	2.21	0.40
1:A:140:ALA:HB1	1:A:145:TYR:CB	2.51	0.40
1:A:691:ARG:HG2	1:A:706:PHE:CZ	2.56	0.40
1:A:793:TYR:CE1	1:A:801:ARG:HD2	2.56	0.40
1:A:824:ASN:ND2	1:A:828:GLN:HB2	2.36	0.40
1:B:257:LEU:HG	1:B:260:GLU:CB	2.51	0.40
1:B:353:ALA:HB1	1:B:520:GLU:HB3	2.04	0.40
1:B:675:GLU:HG2	1:B:676:GLY:H	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:GLU:CD	1:B:598:LYS:NZ[1_454]	1.66	0.54
1:A:762:GLU:OE1	1:B:598:LYS:NZ[1_454]	1.67	0.53
1:A:292:ASP:OD2	1:A:908:HIS:NE2[1_545]	2.16	0.04

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	854/908 (94%)	764 (90%)	85 (10%)	5 (1%)	25	48
1	B	854/908 (94%)	763 (89%)	87 (10%)	4 (0%)	29	53
All	All	1708/1816 (94%)	1527 (89%)	172 (10%)	9 (0%)	29	53

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	A	249	ARG
1	A	342	ARG
1	B	236	ASN
1	B	249	ARG
1	B	342	ARG
1	B	171	LYS
1	A	571	ASP
1	A	860	HIS

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	703/742 (95%)	663 (94%)	40 (6%)	20	43
1	B	703/742 (95%)	671 (95%)	32 (5%)	27	52
All	All	1406/1484 (95%)	1334 (95%)	72 (5%)	24	48

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	33	ARG
1	A	153	ASP
1	A	168	TYR
1	A	170	ARG
1	A	187	LYS
1	A	198	PHE
1	A	202	ARG
1	A	259	ARG
1	A	279	MET
1	A	285	ASP
1	A	341	SER
1	A	371	ARG
1	A	435	ARG
1	A	449	ARG
1	A	502	LEU
1	A	505	LEU
1	A	561	SER
1	A	580	LYS
1	A	582	LYS
1	A	607	LEU
1	A	608	LEU
1	A	612	ASP
1	A	684	ASP
1	A	721	PHE
1	A	733	ARG
1	A	739	MET
1	A	748	SER
1	A	764	LYS
1	A	772	ASP
1	A	773	ARG
1	A	779	ASP
1	A	782	ARG
1	A	783	ASP
1	A	795	SER
1	A	808	ASP
1	A	809	SER
1	A	812	ARG
1	A	828	GLN
1	A	858	GLN
1	B	44	LYS
1	B	78	ASP

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Mol	Chain	Res	Type
1	B	101	ASP
1	B	170	ARG
1	B	171	LYS
1	B	175	GLU
1	B	178	ARG
1	B	187	LYS
1	B	202	ARG
1	B	236	ASN
1	B	282	TRP
1	B	388	SER
1	B	412	ARG
1	B	434	GLN
1	B	543	ARG
1	B	561	SER
1	B	563	LYS
1	B	570	PHE
1	B	577	LYS
1	B	580	LYS
1	B	588	ASP
1	B	684	ASP
1	B	702	LEU
1	B	721	PHE
1	B	734	ARG
1	B	743	LEU
1	B	757	LYS
1	B	762	GLU
1	B	815	ARG
1	B	820	ARG
1	B	858	GLN
1	B	901	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	236	ASN
1	A	316	HIS
1	A	459	GLN
1	A	566	GLN
1	A	755	GLN
1	B	69	GLN
1	B	236	ASN

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Mol	Chain	Res	Type
1	B	434	GLN
1	B	458	GLN
1	B	476	GLN
1	B	639	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	860/908 (94%)	0.17	53 (6%)	20 20	62, 109, 171, 213	0
1	B	860/908 (94%)	0.34	68 (7%)	12 11	59, 116, 184, 215	0
All	All	1720/1816 (94%)	0.26	121 (7%)	16 15	59, 112, 180, 215	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	ALA	19.5
1	B	98	ALA	14.1
1	A	730	PRO	10.4
1	B	176	LEU	8.5
1	A	203	GLY	8.3
1	B	730	PRO	8.0
1	A	250	ALA	7.3
1	B	240	VAL	6.7
1	B	203	GLY	6.7
1	A	256	ILE	6.4
1	A	224	ILE	6.4
1	B	244	VAL	6.4
1	A	823	LEU	6.3
1	A	198	PHE	5.9
1	A	176	LEU	5.6
1	A	202	ARG	5.1
1	B	774	PHE	5.1
1	A	199	ALA	5.0
1	A	582	LYS	4.7
1	B	812	ARG	4.4
1	A	251	ASN	4.4
1	A	810	SER	4.3
1	B	750	TYR	4.3
1	B	823	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	257	LEU	4.2
1	B	756	LEU	4.2
1	B	603	PHE	4.2
1	B	559	LEU	4.2
1	B	607	LEU	4.0
1	B	813	GLN	3.9
1	B	822	ALA	3.9
1	A	294	LEU	3.8
1	B	246	ASP	3.8
1	A	750	TYR	3.7
1	A	237	VAL	3.7
1	A	45	THR	3.7
1	B	198	PHE	3.7
1	A	252	LEU	3.7
1	B	745	TYR	3.7
1	A	222	LYS	3.6
1	A	217	GLU	3.6
1	B	569	LEU	3.6
1	B	805	PRO	3.6
1	B	827	ILE	3.5
1	B	190	LEU	3.5
1	A	190	LEU	3.5
1	B	592	LEU	3.5
1	A	782	ARG	3.5
1	B	250	ALA	3.4
1	B	568	VAL	3.4
1	B	690	MET	3.2
1	A	291	PHE	3.2
1	B	556	GLN	3.2
1	A	745	TYR	3.1
1	B	749	ALA	3.1
1	B	712	LEU	3.1
1	B	550	TYR	3.1
1	A	259	ARG	3.1
1	B	202	ARG	3.1
1	B	754	GLN	3.0
1	A	248	LEU	3.0
1	B	755	GLN	2.9
1	B	692	ILE	2.9
1	A	236	ASN	2.9
1	A	742	GLY	2.9
1	A	227	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	233	LEU	2.8
1	A	812	ARG	2.8
1	A	249	ARG	2.8
1	A	808	ASP	2.8
1	A	239	ALA	2.8
1	B	834	ILE	2.7
1	A	229	SER	2.7
1	B	239	ALA	2.7
1	B	605	GLN	2.7
1	B	584	GLY	2.6
1	A	578	THR	2.6
1	A	235	ASP	2.6
1	B	685	TYR	2.5
1	B	243	LYS	2.5
1	B	578	THR	2.5
1	A	244	VAL	2.5
1	B	256	ILE	2.5
1	A	296	PHE	2.5
1	B	169	PRO	2.5
1	A	49	LEU	2.5
1	A	114	LEU	2.4
1	A	607	LEU	2.4
1	B	235	ASP	2.4
1	B	814	VAL	2.4
1	A	201	LEU	2.4
1	B	565	LEU	2.4
1	B	688	ILE	2.4
1	A	299	LEU	2.3
1	B	242	GLY	2.3
1	B	218	LYS	2.3
1	A	247	ALA	2.2
1	B	233	LEU	2.2
1	A	221	THR	2.2
1	A	815	ARG	2.2
1	B	221	THR	2.2
1	B	736	VAL	2.2
1	B	807	LEU	2.2
1	A	835	ILE	2.2
1	A	223	TRP	2.2
1	B	583	THR	2.1
1	B	187	LYS	2.1
1	B	587	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	254	SER	2.1
1	B	786	ASP	2.1
1	B	236	ASN	2.1
1	B	811	ASN	2.1
1	B	179	PHE	2.1
1	B	154	ARG	2.1
1	B	889	LEU	2.1
1	B	757	LYS	2.1
1	B	586	THR	2.1
1	A	102	GLU	2.0
1	B	864	LEU	2.0
1	A	749	ALA	2.0
1	B	171	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

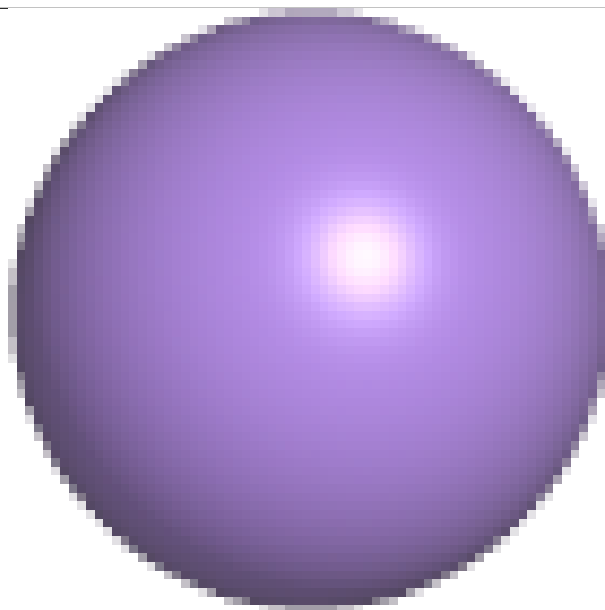
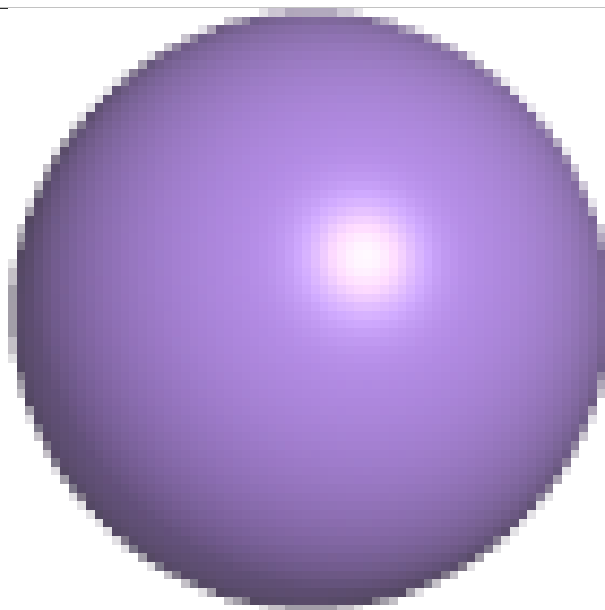
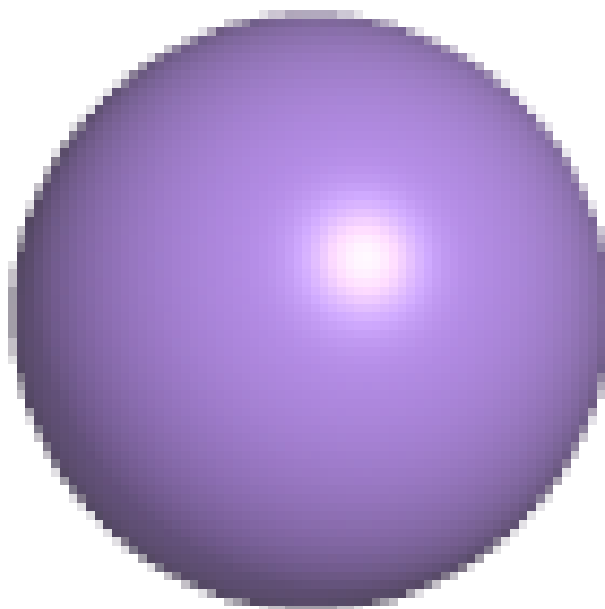
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	B	1002	1/1	0.29	0.35	197,197,197,197	0
2	MN	A	1001	1/1	0.54	0.32	314,314,314,314	0
2	MN	A	1002	1/1	0.64	0.29	164,164,164,164	1
2	MN	B	1001	1/1	0.65	0.35	266,266,266,266	1
2	MN	A	1003	1/1	0.92	0.46	150,150,150,150	0
2	MN	B	1003	1/1	0.92	0.31	95,95,95,95	0

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.

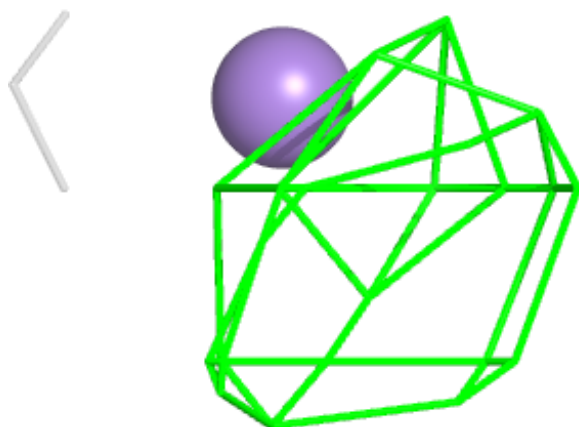
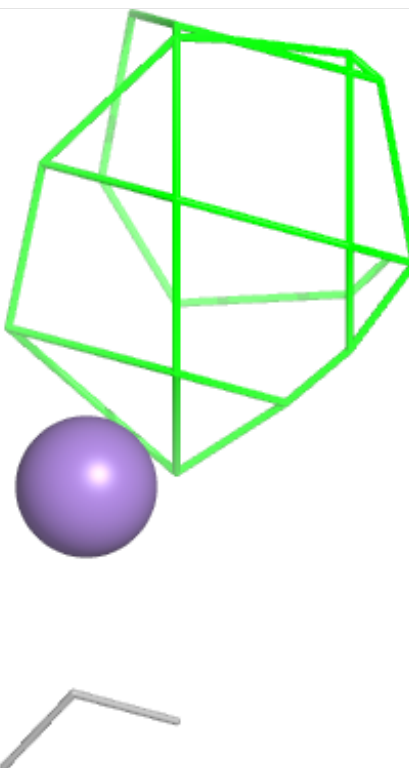
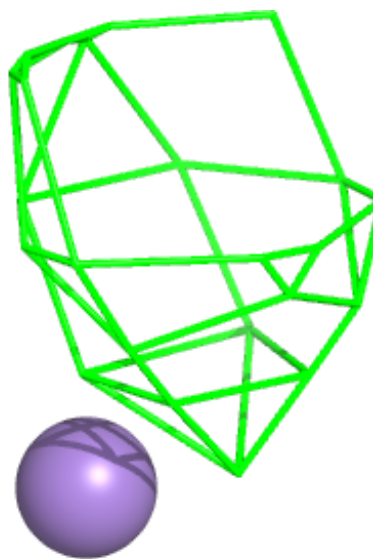
Electron density around MN B 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



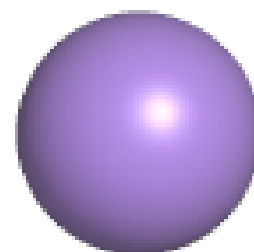
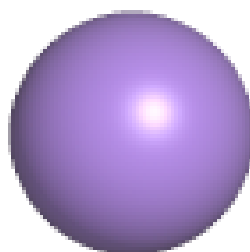
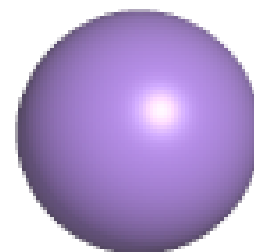
Electron density around MN A 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



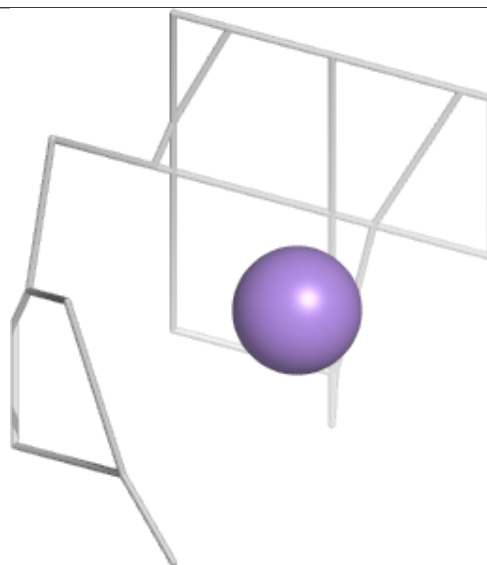
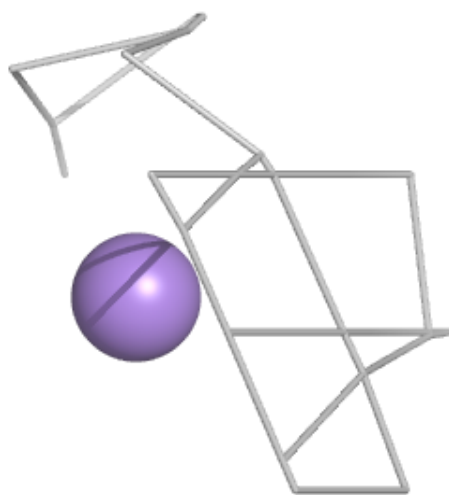
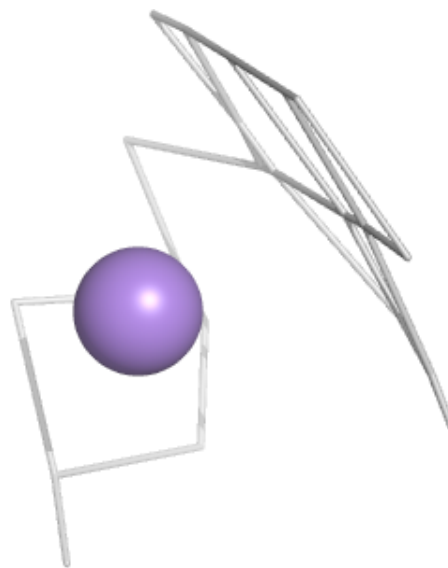
Electron density around MN A 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



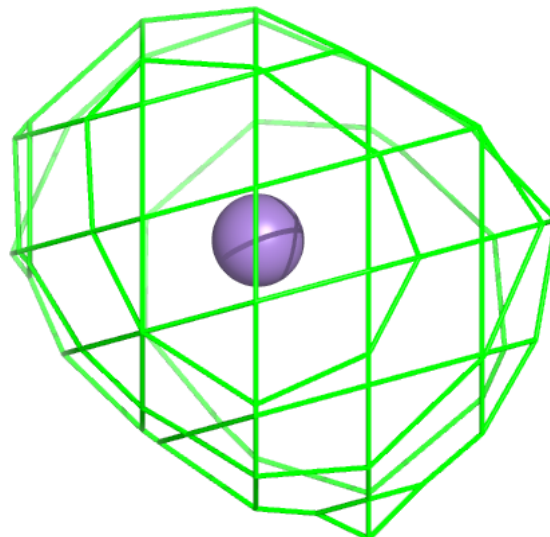
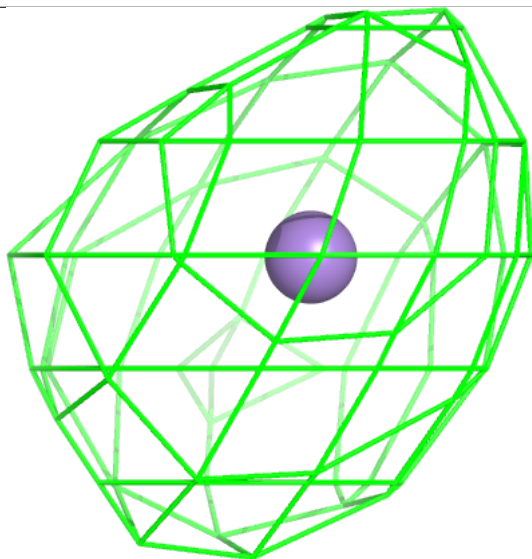
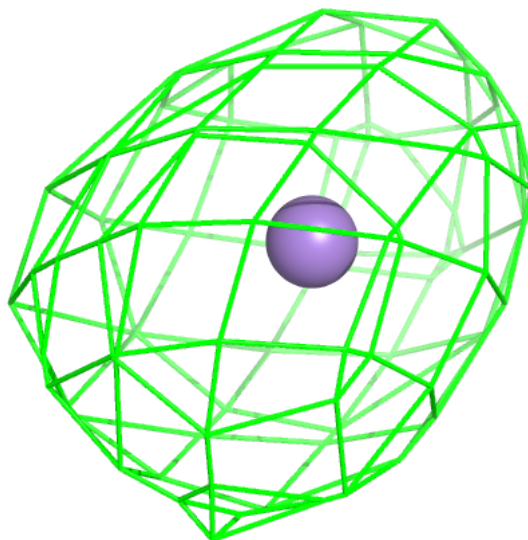
Electron density around MN B 1001:

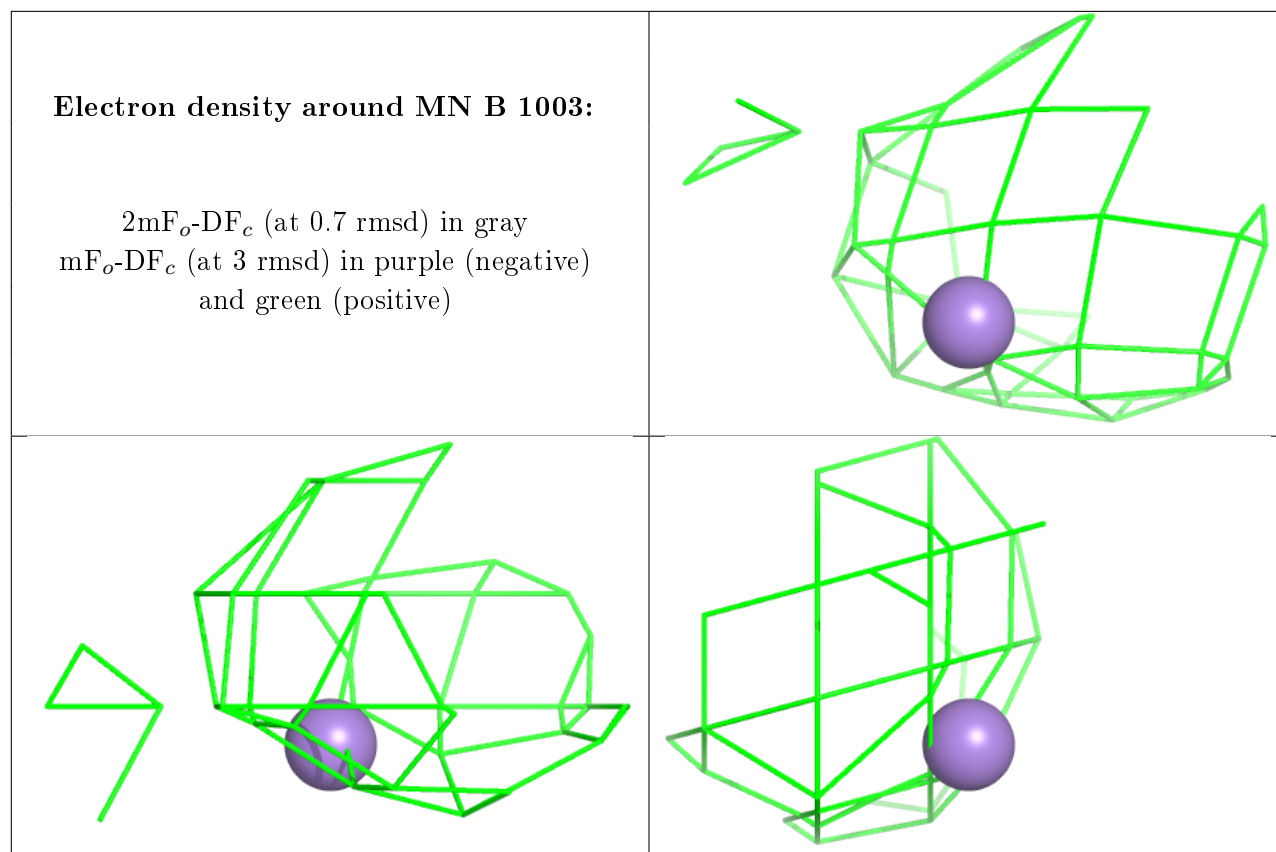
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN A 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.