



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:34 PM UTC

PDB ID : 3U4Q / pdb_00003u4q
Title : Structure of AddAB-DNA complex at 2.8 angstroms
Authors : Saikrishnan, K.; Krajewski, W.; Wigley, D.
Deposited on : 2011-10-10
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

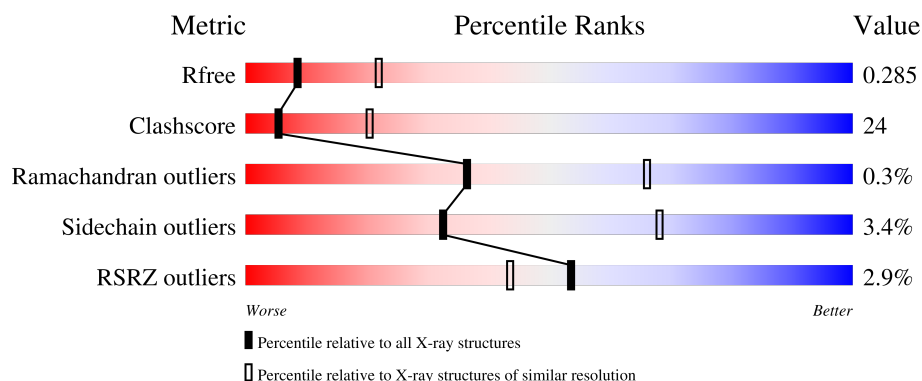
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

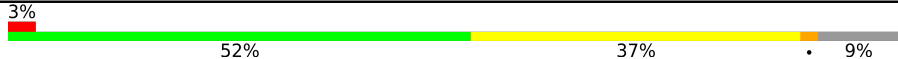
The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1232	
2	B	1166	
3	X	48	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19058 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 ATP-dependent helicase/nuclease subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1122	Total	C	N	O	S	0	0	0
			9117	5821	1548	1721	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	780	GLY	ALA	conflict	UNP P23478
A	1172	ALA	ASP	engineered mutation	UNP P23478

- Molecule 2 is a protein called ATP-dependent helicase/deoxyribonuclease subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1132	Total	C	N	O	S	0	0	0
			9188	5839	1571	1736	42			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	843	ASP	GLU	conflict	UNP P23477
B	844	GLU	GLN	conflict	UNP P23477
B	961	ALA	ASP	engineered mutation	UNP P23477

- Molecule 3 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	27	Total	C	N	O	P	0	0	0
			555	265	98	165	27			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	X	1	Total	C	O	0	0
			4	2	2		

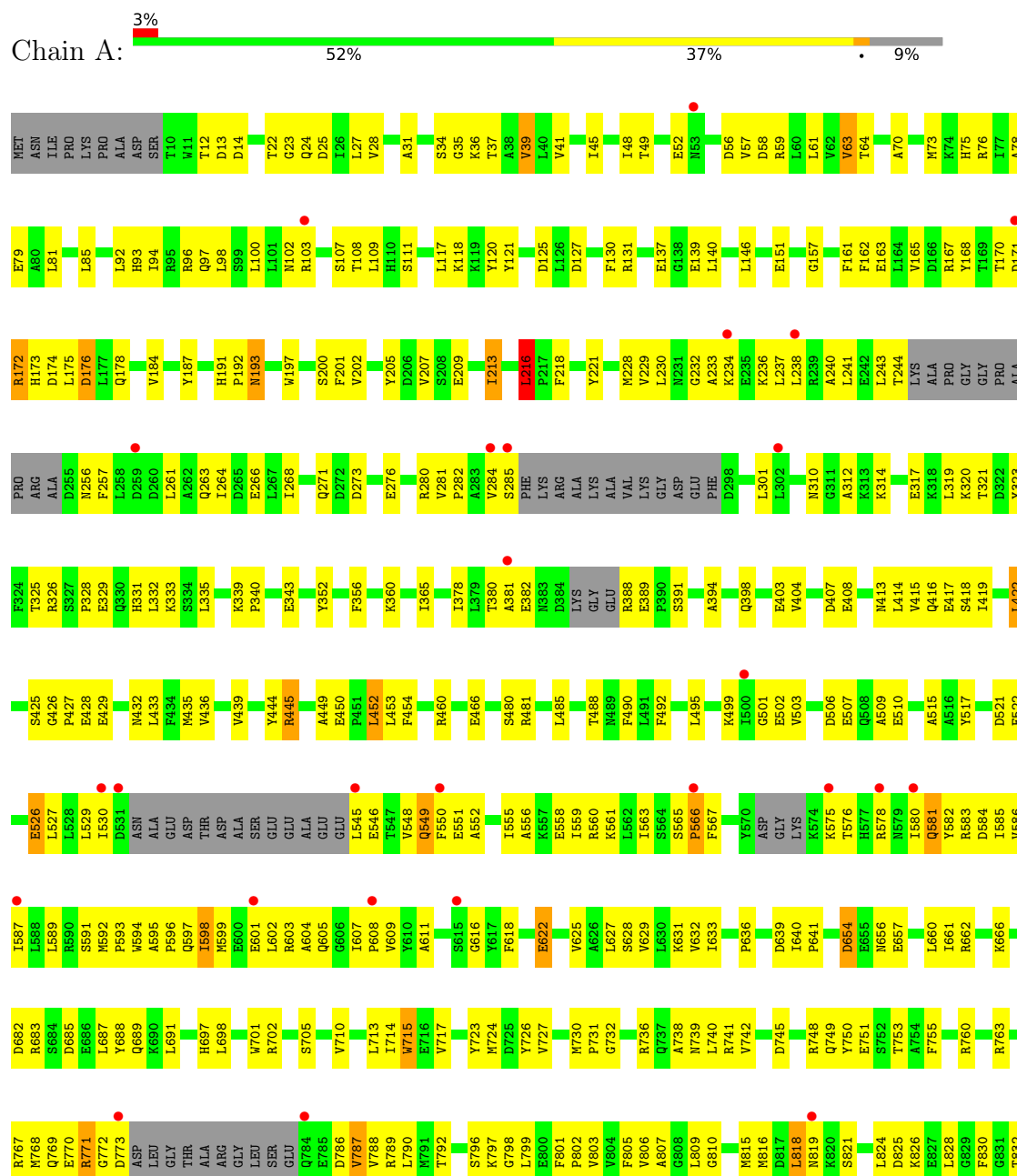
- Molecule 6 is water.

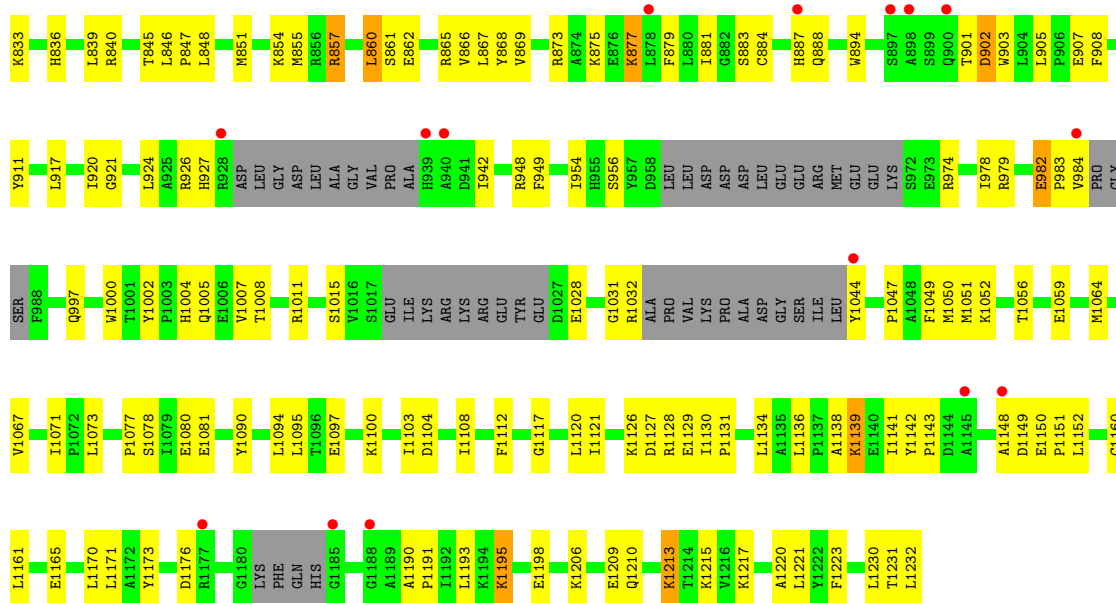
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total 89	O 89	0	0
6	B	99	Total 99	O 99	0	0
6	X	1	Total 1	O 1	0	0

3 Residue-property plots

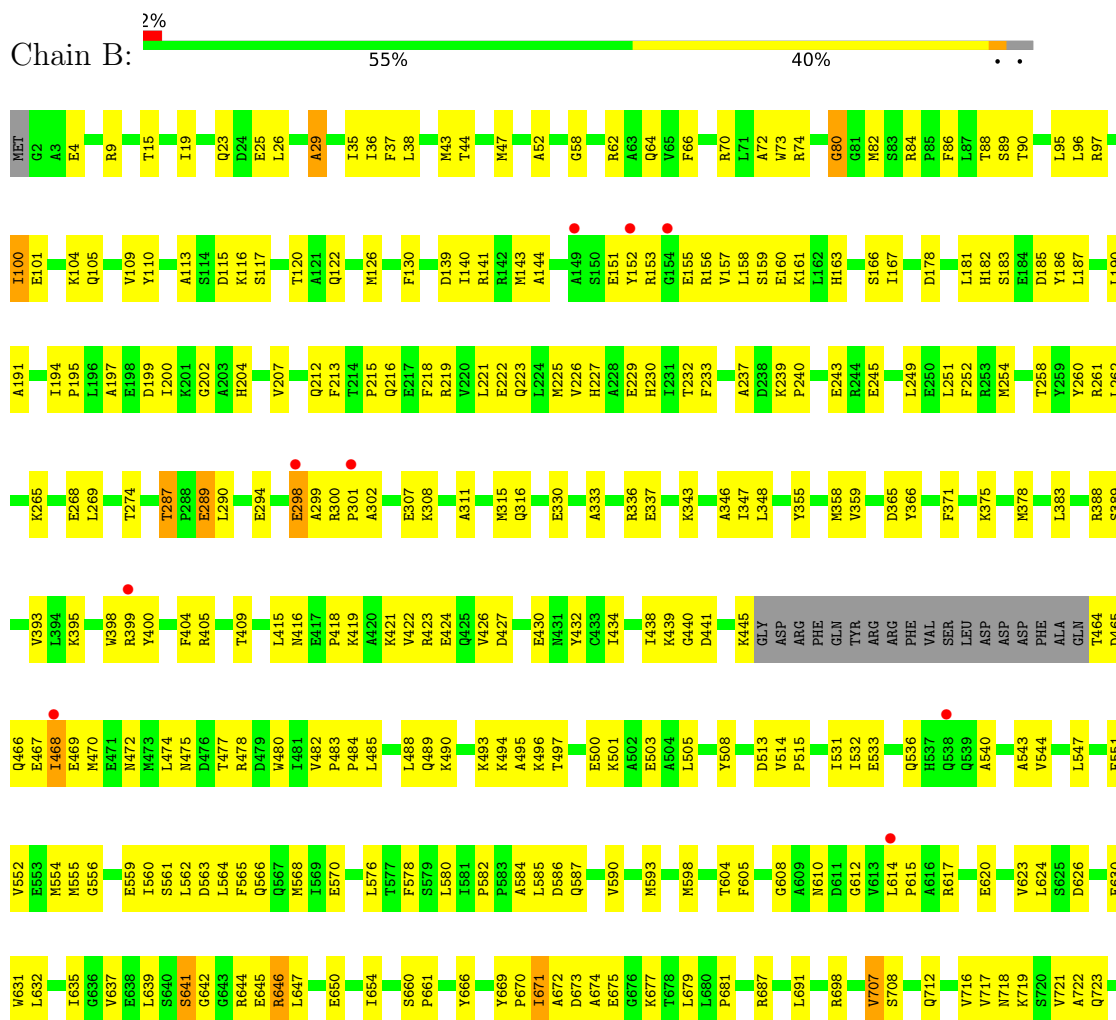
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

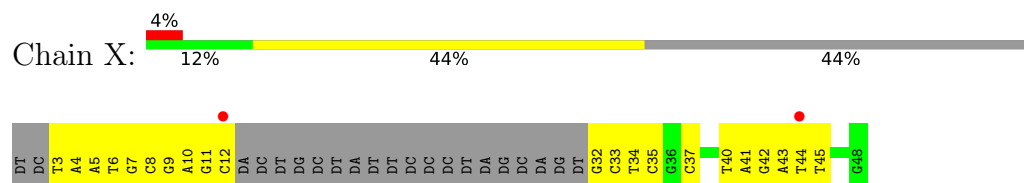
- Molecule 1: ATP-dependent helicase/nuclease subunit A





• Molecule 2: ATP-dependent helicase/deoxyribonuclease subunit B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.56Å 139.71Å 103.09Å 90.00° 105.54° 90.00°	Depositor
Resolution (Å)	29.92 – 2.80 29.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.92-2.80) 95.5 (29.92-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_750)	Depositor
R, R_{free}	0.233 , 0.286 0.229 , 0.285	Depositor DCC
R_{free} test set	3363 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19058	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: EDO, SO4

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	0.28	0/9294	0.71	5/12535 (0.0%)
2	B	0.28	0/9372	0.71	9/12628 (0.1%)
3	X	0.15	0/620	0.65	0/953
All	All	0.27	0/19286	0.70	14/26116 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	616	GLY	N-CA-C	-8.44	103.53	115.43
2	B	409	THR	N-CA-C	-6.87	104.88	113.20
1	A	216	LEU	CA-C-N	6.77	126.28	119.24
1	A	216	LEU	C-N-CA	6.77	126.28	119.24
2	B	922	GLY	CA-C-N	5.73	125.20	119.24
2	B	922	GLY	C-N-CA	5.73	125.20	119.24
1	A	193	ASN	CA-C-N	5.65	125.12	119.24
1	A	193	ASN	C-N-CA	5.65	125.12	119.24
2	B	287	THR	CA-C-N	5.39	124.57	118.97
2	B	287	THR	C-N-CA	5.39	124.57	118.97
2	B	80	GLY	N-CA-C	5.29	116.97	111.95
2	B	29	ALA	CA-C-N	5.05	124.84	119.28
2	B	29	ALA	C-N-CA	5.05	124.84	119.28
2	B	941	GLY	N-CA-C	5.02	118.47	111.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9117	0	9063	464	0
2	B	9188	0	9149	445	0
3	X	555	0	308	37	0
4	B	5	0	0	0	0
5	X	4	0	6	2	0
6	A	89	0	0	1	0
6	B	99	0	0	1	0
6	X	1	0	0	0	0
All	All	19058	0	18526	895	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 24.

All (895) 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)
2:B:864:VAL:HG11	2:B:890:GLN:HG2	1.35	1.08
2:B:916:LEU:HD21	2:B:924:LEU:HG	1.34	1.05
2:B:917:GLY:HA3	2:B:923:PRO:HD2	1.39	1.04
1:A:585:ILE:HD11	1:A:788:VAL:HG22	1.39	1.03
1:A:237:LEU:HD11	1:A:312:ALA:HB2	1.37	1.01
1:A:797:LYS:HG2	1:A:798:GLY:H	1.25	1.00
1:A:1195:LYS:HA	1:A:1198:GLU:HB2	1.47	0.96
2:B:501:LYS:HE3	2:B:561:SER:HA	1.44	0.96
1:A:1011:ARG:HD2	2:B:582:PRO:HB2	1.52	0.92
2:B:212:GLN:HA	2:B:258:THR:HG21	1.52	0.92
1:A:753:THR:HG23	1:A:755:PHE:H	1.34	0.91
3:X:41:DA:H2''	3:X:42:DG:H5'	1.54	0.89
1:A:607:ILE:HD11	1:A:788:VAL:HG23	1.54	0.89
2:B:732:LEU:HD21	2:B:737:TYR:CD2	2.07	0.88
1:A:205:TYR:HA	1:A:335:LEU:HD21	1.56	0.88
2:B:614:LEU:HB3	2:B:615:PRO:HD3	1.56	0.86
1:A:575:LYS:HG3	1:A:576:THR:H	1.41	0.86
2:B:821:LEU:HD22	2:B:875:ILE:HD11	1.54	0.86
1:A:582:TYR:HB3	1:A:607:ILE:HD13	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD22	1:A:103:ARG:HH21	1.39	0.85
2:B:929:PHE:HB2	2:B:937:MET:HB3	1.60	0.83
1:A:58:ASP:HB3	1:A:103:ARG:HH22	1.44	0.83
2:B:836:LEU:HD21	2:B:866:ARG:HH21	1.42	0.83
1:A:750:TYR:O	1:A:753:THR:HG22	1.77	0.83
1:A:587:ILE:HG22	1:A:805:PHE:HB2	1.60	0.83
1:A:603:ARG:HG2	1:A:608:PRO:HA	1.61	0.82
2:B:972:ALA:HA	2:B:1152:ILE:HD12	1.59	0.82
2:B:769:ARG:HA	2:B:1136:LEU:HD21	1.60	0.81
1:A:1148:ALA:HB1	1:A:1150:GLU:OE1	1.79	0.81
1:A:869:VAL:O	1:A:873:ARG:HG2	1.80	0.80
1:A:797:LYS:HG2	1:A:798:GLY:N	1.96	0.80
1:A:954:ILE:HG22	1:A:956:SER:H	1.46	0.80
2:B:347:ILE:HG22	2:B:605:PHE:HB2	1.64	0.80
1:A:521:ASP:O	1:A:522:GLU:HG2	1.81	0.80
1:A:715:TRP:HE1	2:B:358:MET:HE1	1.44	0.80
1:A:926:ARG:HD2	1:A:942:ILE:HG21	1.64	0.80
1:A:403:GLU:HA	1:A:432:ASN:HB2	1.62	0.80
1:A:806:VAL:HG12	1:A:809:LEU:HD21	1.64	0.79
2:B:967:LYS:HA	2:B:1038:LYS:HD3	1.61	0.79
1:A:243:LEU:HB3	1:A:301:LEU:HD21	1.64	0.78
1:A:797:LYS:CG	1:A:798:GLY:H	1.94	0.78
2:B:95:LEU:HB2	2:B:554:MET:HE2	1.64	0.78
1:A:603:ARG:HD3	1:A:609:VAL:H	1.48	0.77
3:X:43:DA:H2''	3:X:44:DT:H5'	1.64	0.77
2:B:1045:GLN:HE21	2:B:1049:ARG:HH21	1.32	0.77
3:X:4:DA:H2''	3:X:5:DA:O5'	1.81	0.77
2:B:43:MET:HE2	2:B:47:MET:HE2	1.65	0.77
2:B:497:THR:HG22	2:B:559:GLU:HG2	1.67	0.77
3:X:6:DT:H2''	3:X:7:DG:H5''	1.67	0.77
3:X:43:DA:H2''	3:X:44:DT:C5'	2.13	0.77
2:B:1009:PHE:HD2	2:B:1037:MET:HE2	1.50	0.76
1:A:48:ILE:HD13	1:A:57:VAL:HG22	1.67	0.76
2:B:97:ARG:HA	2:B:100:ILE:HG12	1.66	0.76
2:B:495:ALA:HB1	2:B:500:GLU:HG3	1.68	0.76
1:A:28:VAL:HB	1:A:436:VAL:HG12	1.68	0.75
1:A:170:THR:HG22	1:A:176:ASP:OD1	1.87	0.75
2:B:719:LYS:HE3	2:B:755:ASP:OD2	1.85	0.75
3:X:3:DT:H2''	3:X:4:DA:C8	2.22	0.75
3:X:7:DG:H5''	3:X:7:DG:H8	1.52	0.74
1:A:127:ASP:HA	2:B:116:LYS:HD3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LEU:HD11	1:A:826:LYS:HD2	1.70	0.73
2:B:15:THR:HG23	2:B:47:MET:HE1	1.68	0.73
1:A:213:ILE:HD12	1:A:332:LEU:HD21	1.70	0.73
1:A:380:THR:HG22	1:A:422:LEU:HD21	1.68	0.73
2:B:916:LEU:HD21	2:B:924:LEU:CG	2.15	0.73
1:A:229:VAL:HG21	1:A:319:LEU:HD13	1.71	0.73
2:B:792:VAL:O	2:B:796:GLU:HG2	1.87	0.73
2:B:536:GLN:HB2	2:B:578:PHE:CE1	2.23	0.73
2:B:912:ILE:HD11	2:B:957:LEU:HD22	1.69	0.73
1:A:797:LYS:O	1:A:873:ARG:HD2	1.88	0.73
1:A:1071:ILE:HG21	1:A:1112:PHE:CZ	2.23	0.73
2:B:393:VAL:HG21	2:B:485:LEU:HD21	1.70	0.73
2:B:971:LEU:HD12	2:B:1149:ASP:HB3	1.73	0.71
1:A:171:ASP:O	1:A:172:ARG:HB3	1.91	0.71
1:A:563:ILE:HD13	1:A:582:TYR:CE1	2.25	0.71
2:B:917:GLY:CA	2:B:923:PRO:HD2	2.20	0.71
1:A:607:ILE:CD1	1:A:788:VAL:HG23	2.21	0.71
1:A:845:THR:HG22	1:A:848:LEU:HB2	1.73	0.70
2:B:631:TRP:CE2	2:B:635:ILE:HD11	2.26	0.70
1:A:901:THR:O	1:A:902:ASP:HB2	1.92	0.70
2:B:141:ARG:HG2	2:B:166:SER:OG	1.92	0.70
2:B:1055:LEU:HD22	2:B:1060:SER:HB2	1.72	0.70
1:A:636:PRO:HD2	2:B:427:ASP:OD2	1.92	0.69
1:A:1120:LEU:O	1:A:1126:LYS:HD3	1.92	0.69
2:B:36:ILE:HG23	2:B:66:PHE:HD2	1.57	0.69
2:B:97:ARG:HH21	2:B:117:SER:HA	1.57	0.69
2:B:555:MET:HE1	2:B:568:MET:SD	2.32	0.69
1:A:175:LEU:HD12	1:A:178:GLN:HE21	1.57	0.69
2:B:888:LYS:HE3	2:B:892:ILE:HG13	1.74	0.69
1:A:170:THR:O	1:A:170:THR:HG23	1.92	0.69
1:A:317:GLU:OE1	1:A:320:LYS:HE3	1.93	0.69
1:A:171:ASP:HB3	2:B:888:LYS:CD	2.23	0.69
1:A:825:ASP:HB2	1:A:851:MET:HE3	1.75	0.69
2:B:873:LYS:O	2:B:874:GLU:HG2	1.92	0.68
1:A:560:ARG:HA	1:A:563:ILE:HD12	1.74	0.68
1:A:581:GLN:O	1:A:786:ASP:HB3	1.94	0.68
3:X:45:DT:H5"	5:X:49:EDO:H11	1.76	0.68
1:A:1139:LYS:NZ	1:A:1149:ASP:HA	2.08	0.68
1:A:586:VAL:HG11	1:A:801:PHE:CD1	2.29	0.67
2:B:805:HIS:HE1	2:B:1103:ILE:HD13	1.60	0.67
2:B:916:LEU:HD22	2:B:943:ILE:HD13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:793:SER:HA	2:B:796:GLU:HG3	1.75	0.67
2:B:931:LEU:HD13	2:B:932:LYS:N	2.08	0.67
1:A:191:HIS:CD2	1:A:193:ASN:H	2.12	0.67
1:A:398:GLN:HB3	1:A:425:SER:HB3	1.77	0.67
1:A:772:GLY:O	1:A:773:ASP:HB2	1.92	0.67
2:B:144:ALA:O	2:B:159:SER:HB2	1.93	0.67
1:A:1139:LYS:HZ1	1:A:1149:ASP:HA	1.60	0.67
2:B:465:ASP:O	2:B:469:GLU:HG2	1.95	0.67
1:A:241:LEU:HD11	1:A:261:LEU:HD22	1.75	0.67
2:B:641:SER:HB3	2:B:645:GLU:HB2	1.77	0.67
1:A:146:LEU:HD13	1:A:178:GLN:HB2	1.75	0.67
2:B:784:TYR:HB3	2:B:788:ILE:HD11	1.77	0.67
2:B:883:TYR:CE2	2:B:886:LYS:HD2	2.30	0.67
1:A:575:LYS:HG3	1:A:576:THR:N	2.08	0.66
2:B:97:ARG:O	2:B:101:GLU:HG2	1.96	0.66
3:X:43:DA:H2''	3:X:44:DT:O5'	1.95	0.66
2:B:799:ASN:O	2:B:1113:TYR:HE2	1.79	0.66
2:B:871:LEU:HD21	2:B:876:LEU:HD22	1.78	0.66
1:A:592:MET:N	1:A:593:PRO:HD3	2.11	0.66
2:B:584:ALA:H	2:B:587:GLN:NE2	1.94	0.66
2:B:819:PHE:CE1	2:B:875:ILE:HG22	2.30	0.66
2:B:1007:LEU:HD21	2:B:1041:LEU:HD21	1.77	0.65
1:A:1051:MET:HG2	1:A:1052:LYS:H	1.61	0.65
1:A:1209:GLU:HG2	1:A:1215:LYS:HA	1.77	0.65
2:B:66:PHE:CE1	2:B:74:ARG:HG3	2.32	0.65
1:A:738:ALA:O	1:A:742:VAL:HG13	1.96	0.65
1:A:1141:ILE:O	1:A:1143:PRO:HD3	1.96	0.65
1:A:151:GLU:OE1	2:B:879:SER:HB2	1.96	0.65
1:A:381:ALA:O	1:A:389:GLU:HB2	1.96	0.65
1:A:499:LYS:HE2	1:A:907:GLU:OE2	1.96	0.65
2:B:718:ASN:HB3	2:B:721:VAL:HG22	1.79	0.65
1:A:997:GLN:NE2	2:B:716:VAL:HG23	2.12	0.65
1:A:1134:LEU:HD21	1:A:1206:LYS:HD2	1.77	0.65
2:B:468:ILE:HG23	2:B:469:GLU:H	1.61	0.65
1:A:100:LEU:HD22	1:A:103:ARG:NH2	2.10	0.65
1:A:413:ASN:OD1	1:A:416:GLN:N	2.29	0.65
2:B:650:GLU:O	2:B:654:ILE:HG13	1.96	0.65
1:A:565:SER:OG	1:A:566:PRO:HD2	1.96	0.65
1:A:585:ILE:HG22	1:A:803:VAL:HB	1.79	0.65
1:A:1049:PHE:CD2	2:B:552:VAL:HG21	2.32	0.65
1:A:563:ILE:HD13	1:A:582:TYR:HE1	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASP:HB3	1:A:103:ARG:NH2	2.13	0.64
2:B:222:GLU:HA	2:B:225:MET:HE2	1.78	0.64
3:X:43:DA:H1'	3:X:44:DT:OP1	1.97	0.64
1:A:102:ASN:HA	2:B:617:ARG:NH1	2.12	0.64
1:A:102:ASN:HB2	2:B:647:LEU:HD21	1.80	0.64
1:A:321:THR:HA	1:A:325:THR:HG23	1.80	0.64
2:B:1113:TYR:CD1	2:B:1144:LEU:HD21	2.33	0.64
2:B:840:ARG:O	2:B:844:GLU:HG2	1.98	0.64
2:B:872:GLN:O	2:B:875:ILE:HG23	1.98	0.64
2:B:948:LYS:HG3	2:B:955:LEU:HD11	1.79	0.63
2:B:972:ALA:HA	2:B:1152:ILE:CD1	2.26	0.63
1:A:887:HIS:CD2	1:A:888:GLN:HG3	2.34	0.63
1:A:552:ALA:HB3	1:A:601:GLU:OE2	1.99	0.63
1:A:978:ILE:HA	2:B:747:TYR:OH	1.98	0.63
2:B:623:VAL:HG12	2:B:624:LEU:HD12	1.81	0.63
2:B:799:ASN:O	2:B:1113:TYR:CE2	2.51	0.63
1:A:580:ILE:HG22	1:A:582:TYR:H	1.63	0.63
2:B:15:THR:CG2	2:B:47:MET:HE1	2.28	0.63
1:A:515:ALA:HB1	1:A:517:TYR:HD2	1.64	0.63
1:A:867:LEU:HD21	1:A:920:ILE:HD11	1.81	0.63
1:A:657:GLU:HB3	1:A:687:LEU:HD13	1.81	0.63
2:B:298:GLU:CD	2:B:298:GLU:H	2.07	0.63
1:A:594:TRP:HB3	1:A:598:ILE:HD12	1.81	0.62
1:A:640:ILE:HB	1:A:641:PRO:HD3	1.80	0.62
1:A:1067:VAL:HG21	1:A:1103:ILE:HD13	1.80	0.62
2:B:84:ARG:HH12	2:B:178:ASP:C	2.07	0.62
2:B:158:LEU:O	2:B:161:LYS:HG3	1.98	0.62
2:B:464:THR:O	2:B:468:ILE:HG22	1.98	0.62
1:A:213:ILE:HD11	1:A:332:LEU:HD11	1.81	0.62
1:A:58:ASP:HB2	1:A:103:ARG:HH12	1.64	0.62
1:A:232:GLY:O	1:A:236:LYS:HB2	1.98	0.62
1:A:730:MET:HA	2:B:731:ARG:HH11	1.65	0.62
2:B:181:LEU:HD21	2:B:186:TYR:CE1	2.35	0.62
3:X:41:DA:H2''	3:X:42:DG:C5'	2.28	0.62
3:X:4:DA:H2'	3:X:5:DA:H8	1.65	0.62
1:A:233:ALA:O	1:A:237:LEU:HD13	2.00	0.61
1:A:594:TRP:HB3	1:A:598:ILE:CD1	2.29	0.61
1:A:727:VAL:HA	1:A:730:MET:HE3	1.81	0.61
2:B:261:ARG:O	2:B:265:LYS:HG2	2.00	0.61
2:B:533:GLU:O	2:B:536:GLN:HG2	1.99	0.61
2:B:1042:LEU:HD23	2:B:1047:VAL:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:ILE:HD11	2:B:564:LEU:HD23	1.81	0.61
2:B:918:PHE:C	2:B:918:PHE:CD2	2.75	0.61
1:A:559:ILE:O	1:A:563:ILE:HG13	1.99	0.61
2:B:490:LYS:HA	2:B:493:LYS:HE2	1.82	0.61
1:A:118:LYS:HB3	2:B:620:GLU:HG3	1.81	0.61
2:B:113:ALA:O	2:B:116:LYS:HG2	2.00	0.61
2:B:1090:LYS:HE3	2:B:1094:ARG:HH22	1.65	0.61
1:A:901:THR:O	1:A:902:ASP:CB	2.47	0.61
2:B:896:VAL:HG21	2:B:1011:ILE:HG23	1.80	0.61
2:B:669:TYR:CE1	2:B:681:PRO:HG3	2.36	0.61
1:A:1213:LYS:HZ3	1:A:1213:LYS:HB2	1.66	0.61
1:A:171:ASP:HB3	2:B:888:LYS:HD3	1.83	0.60
1:A:845:THR:HG23	1:A:847:PRO:HD2	1.83	0.60
1:A:92:LEU:HG	1:A:96:ARG:NH2	2.17	0.60
1:A:582:TYR:CD1	1:A:607:ILE:HD13	2.36	0.60
1:A:760:ARG:HH22	2:B:399:ARG:NH2	1.99	0.60
1:A:942:ILE:HD12	1:A:942:ILE:H	1.66	0.60
2:B:877:LEU:HD23	2:B:883:TYR:CE2	2.36	0.60
1:A:1071:ILE:HG21	1:A:1112:PHE:HZ	1.66	0.60
2:B:864:VAL:HG11	2:B:890:GLN:CG	2.23	0.60
2:B:593:MET:HE1	2:B:614:LEU:HD11	1.82	0.60
3:X:7:DG:H5''	3:X:7:DG:C8	2.35	0.60
1:A:205:TYR:HA	1:A:335:LEU:CD2	2.30	0.60
2:B:732:LEU:HD21	2:B:737:TYR:CG	2.37	0.60
2:B:1041:LEU:HD22	2:B:1051:MET:HE1	1.84	0.60
3:X:6:DT:H2''	3:X:7:DG:C5'	2.32	0.60
2:B:207:VAL:HG22	2:B:233:PHE:HA	1.82	0.59
1:A:723:TYR:O	1:A:727:VAL:HG23	2.01	0.59
1:A:1002:TYR:HB3	1:A:1005:GLN:HB2	1.85	0.59
1:A:171:ASP:HB3	2:B:888:LYS:CE	2.32	0.59
1:A:1213:LYS:HB2	1:A:1213:LYS:NZ	2.16	0.59
2:B:942:ARG:HG3	2:B:942:ARG:O	2.02	0.59
2:B:769:ARG:CA	2:B:1136:LEU:HD21	2.32	0.59
2:B:784:TYR:HB3	2:B:788:ILE:CD1	2.31	0.59
1:A:41:VAL:HG12	1:A:45:ILE:HD11	1.83	0.59
1:A:466:GLU:HG2	1:A:466:GLU:O	2.01	0.59
2:B:829:LEU:CD2	2:B:889:LEU:HD13	2.32	0.59
2:B:886:LYS:O	2:B:890:GLN:HG3	2.02	0.59
1:A:802:PRO:HA	1:A:875:LYS:HB2	1.84	0.59
3:X:34:DT:C2'	3:X:35:DC:H5''	2.33	0.59
1:A:58:ASP:CB	1:A:103:ARG:HH12	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:HG23	1:A:173:HIS:HB3	1.82	0.59
1:A:560:ARG:HG2	1:A:563:ILE:HD12	1.84	0.59
1:A:22:THR:HG22	1:A:23:GLY:H	1.66	0.59
1:A:268:ILE:HA	1:A:271:GLN:HG3	1.84	0.59
1:A:243:LEU:HD22	1:A:301:LEU:HD11	1.85	0.58
2:B:300:ARG:N	2:B:301:PRO:HD2	2.18	0.58
2:B:829:LEU:HD13	2:B:871:LEU:HD22	1.86	0.58
2:B:474:LEU:O	2:B:478:ARG:HG2	2.02	0.58
1:A:221:TYR:CZ	1:A:854:LYS:HD2	2.39	0.58
2:B:977:GLY:HA2	2:B:980:LEU:HD21	1.85	0.58
1:A:1028:GLU:OE2	2:B:375:LYS:HE2	2.04	0.58
2:B:551:PHE:HE1	2:B:555:MET:HE3	1.68	0.58
1:A:582:TYR:CB	1:A:607:ILE:HD13	2.30	0.58
2:B:543:ALA:HB1	2:B:576:LEU:HD22	1.86	0.58
1:A:12:THR:HG22	1:A:14:ASP:H	1.68	0.58
2:B:996:TRP:CD1	2:B:996:TRP:C	2.82	0.58
3:X:41:DA:H2'	3:X:42:DG:C8	2.38	0.58
1:A:549:GLN:H	1:A:549:GLN:HE21	1.52	0.57
1:A:608:PRO:HG2	1:A:787:VAL:CG2	2.33	0.57
1:A:1077:PRO:HG3	6:A:1257:HOH:O	2.04	0.57
2:B:430:GLU:O	2:B:434:ILE:HG13	2.04	0.57
2:B:829:LEU:HD22	2:B:889:LEU:HD13	1.84	0.57
1:A:560:ARG:NH2	1:A:605:GLN:HG3	2.19	0.57
2:B:287:THR:HG21	2:B:290:LEU:HD12	1.86	0.57
2:B:395:LYS:HD2	2:B:566:GLN:OE1	2.05	0.57
1:A:639:ASP:HB2	2:B:814:LYS:H	1.69	0.57
1:A:924:LEU:HD11	1:A:949:PHE:CE2	2.39	0.57
2:B:37:PHE:CZ	2:B:47:MET:HE3	2.40	0.57
2:B:495:ALA:HB1	2:B:500:GLU:CG	2.32	0.57
1:A:598:ILE:HG23	1:A:602:LEU:HD12	1.84	0.57
1:A:979:ARG:HA	2:B:767:PHE:HZ	1.68	0.57
1:A:428:GLU:OE2	1:A:460:ARG:HD2	2.05	0.57
1:A:587:ILE:HG22	1:A:805:PHE:CB	2.33	0.57
2:B:769:ARG:O	2:B:771:GLU:HG3	2.04	0.57
2:B:1090:LYS:HG3	2:B:1094:ARG:NH2	2.20	0.57
1:A:546:GLU:HA	1:A:549:GLN:NE2	2.20	0.57
1:A:280:ARG:O	1:A:284:VAL:HG12	2.05	0.56
2:B:229:GLU:HG2	2:B:230:HIS:CD2	2.40	0.56
1:A:526:GLU:OE2	1:A:877:LYS:HE3	2.04	0.56
1:A:1139:LYS:CE	1:A:1149:ASP:HA	2.35	0.56
2:B:315:MET:HE2	2:B:666:TYR:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:868:ALA:HB3	2:B:869:PRO:HD3	1.87	0.56
2:B:887:GLU:HA	2:B:890:GLN:NE2	2.20	0.56
2:B:958:ARG:HB3	2:B:1004:ALA:HB3	1.87	0.56
1:A:146:LEU:HG	1:A:352:TYR:CE1	2.41	0.56
1:A:216:LEU:HD13	1:A:218:PHE:CE2	2.40	0.56
2:B:562:LEU:HD12	2:B:563:ASP:N	2.20	0.56
2:B:747:TYR:CE2	2:B:751:MET:HG3	2.40	0.56
2:B:931:LEU:HB3	2:B:935:CYS:HB2	1.88	0.56
1:A:548:VAL:HG11	1:A:597:GLN:NE2	2.21	0.56
2:B:378:MET:HG2	2:B:578:PHE:CZ	2.40	0.56
1:A:732:GLY:O	1:A:736:ARG:HG3	2.06	0.56
2:B:258:THR:O	2:B:262:LEU:HD13	2.06	0.56
2:B:722:ALA:O	2:B:726:THR:HG22	2.05	0.56
2:B:777:ARG:O	2:B:781:ARG:HG2	2.06	0.56
1:A:499:LYS:HD2	1:A:857:ARG:CZ	2.35	0.56
1:A:723:TYR:CD2	1:A:740:LEU:HD21	2.41	0.56
1:A:979:ARG:HG3	2:B:767:PHE:CZ	2.40	0.56
1:A:1215:LYS:HD3	1:A:1217:LYS:HZ1	1.71	0.56
2:B:887:GLU:HA	2:B:890:GLN:CD	2.30	0.56
1:A:58:ASP:CB	1:A:103:ARG:HH22	2.15	0.56
1:A:213:ILE:CD1	1:A:332:LEU:HD21	2.35	0.56
1:A:263:GLN:O	1:A:266:GLU:HB3	2.06	0.56
2:B:1113:TYR:CE1	2:B:1144:LEU:HD21	2.40	0.56
1:A:27:LEU:HD11	1:A:454:PHE:CE1	2.41	0.56
2:B:1114:LYS:HB2	2:B:1143:PRO:HA	1.88	0.56
1:A:209:GLU:OE2	1:A:333:LYS:HE3	2.07	0.55
1:A:563:ILE:CD1	1:A:582:TYR:HE1	2.18	0.55
1:A:979:ARG:HA	2:B:767:PHE:CZ	2.41	0.55
2:B:497:THR:HA	2:B:559:GLU:HA	1.87	0.55
1:A:685:ASP:HB3	1:A:688:TYR:HB3	1.89	0.55
1:A:1004:HIS:O	1:A:1007:VAL:HG12	2.06	0.55
2:B:109:VAL:HG23	2:B:160:GLU:HB3	1.87	0.55
2:B:140:ILE:HG22	2:B:166:SER:HB2	1.88	0.55
2:B:415:LEU:HD11	2:B:513:ASP:OD2	2.05	0.55
2:B:551:PHE:CE1	2:B:555:MET:HE3	2.41	0.55
1:A:450:GLU:HG2	1:A:826:LYS:NZ	2.20	0.55
1:A:715:TRP:NE1	2:B:358:MET:HE1	2.19	0.55
2:B:732:LEU:CD2	2:B:737:TYR:CD2	2.86	0.55
3:X:3:DT:O4	3:X:41:DA:N1	2.40	0.55
3:X:12:DC:H42	3:X:32:DG:H1	1.52	0.55
1:A:583:ARG:HH11	1:A:786:ASP:CG	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1230:LEU:HD23	1:A:1230:LEU:H	1.71	0.55
1:A:109:LEU:HD23	1:A:416:GLN:HG2	1.89	0.55
1:A:583:ARG:HD3	1:A:786:ASP:OD1	2.07	0.55
2:B:672:ALA:O	2:B:679:LEU:HD12	2.07	0.55
2:B:832:SER:HB2	2:B:867:LEU:HD21	1.88	0.55
2:B:989:SER:O	2:B:993:SER:HB2	2.07	0.55
1:A:555:ILE:O	1:A:559:ILE:HG13	2.07	0.55
1:A:582:TYR:CG	1:A:607:ILE:HG21	2.42	0.55
1:A:48:ILE:HG22	1:A:49:THR:HG23	1.89	0.55
1:A:563:ILE:CD1	1:A:582:TYR:CE1	2.89	0.55
1:A:739:ASN:O	1:A:742:VAL:HG22	2.06	0.55
1:A:490:PHE:CZ	1:A:927:HIS:HB2	2.41	0.54
1:A:1190:ALA:HB3	1:A:1191:PRO:HD3	1.89	0.54
2:B:868:ALA:HB1	2:B:876:LEU:HD23	1.89	0.54
1:A:527:LEU:C	1:A:527:LEU:HD23	2.33	0.54
1:A:555:ILE:HD11	1:A:807:ALA:HB2	1.90	0.54
1:A:575:LYS:CG	1:A:576:THR:H	2.16	0.54
2:B:110:TYR:OH	2:B:623:VAL:HG13	2.06	0.54
1:A:983:PRO:HD3	2:B:747:TYR:CE2	2.43	0.54
2:B:152:TYR:O	2:B:155:GLU:HB2	2.07	0.54
2:B:733:TRP:HB2	2:B:739:ILE:HD13	1.88	0.54
1:A:380:THR:CG2	1:A:422:LEU:HD21	2.37	0.54
1:A:1049:PHE:CD1	1:A:1050:MET:HG3	2.42	0.54
1:A:1015:SER:O	1:A:1032:ARG:HD2	2.08	0.54
2:B:97:ARG:HD2	2:B:568:MET:HE2	1.89	0.54
1:A:603:ARG:CG	1:A:608:PRO:HA	2.35	0.54
1:A:36:LYS:O	1:A:39:VAL:HG22	2.07	0.54
1:A:184:VAL:HG22	1:A:824:LEU:HD21	1.90	0.54
1:A:507:GLU:HA	1:A:507:GLU:OE1	2.07	0.54
1:A:1160:CYS:HB3	1:A:1171:LEU:HB3	1.89	0.54
1:A:582:TYR:CG	1:A:607:ILE:HD13	2.43	0.54
1:A:770:GLU:HG3	1:A:771:ARG:HG2	1.89	0.54
2:B:29:ALA:HB3	2:B:62:ARG:NH1	2.23	0.54
1:A:161:PHE:O	1:A:165:VAL:HG23	2.08	0.53
2:B:612:GLY:HA2	2:B:617:ARG:NE	2.23	0.53
1:A:628:SER:O	1:A:632:VAL:HG23	2.08	0.53
2:B:889:LEU:O	2:B:893:VAL:HG23	2.08	0.53
1:A:861:SER:O	1:A:865:ARG:HG3	2.08	0.53
2:B:968:GLY:HA3	2:B:1008:TYR:CD2	2.43	0.53
2:B:468:ILE:HG23	2:B:469:GLU:N	2.23	0.53
1:A:529:LEU:HD21	1:A:884:CYS:SG	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:584:ALA:H	2:B:587:GLN:CD	2.16	0.53
2:B:741:ASP:HA	2:B:744:TRP:HD1	1.73	0.53
1:A:563:ILE:HG21	1:A:582:TYR:OH	2.09	0.53
1:A:118:LYS:HD3	2:B:620:GLU:O	2.09	0.53
1:A:282:PRO:HA	1:A:320:LYS:CD	2.39	0.53
1:A:284:VAL:HG13	1:A:285:SER:N	2.24	0.53
1:A:501:GLY:C	1:A:503:VAL:H	2.17	0.53
1:A:599:MET:O	1:A:603:ARG:HG3	2.09	0.53
2:B:956:LEU:O	2:B:957:LEU:HD23	2.08	0.53
1:A:12:THR:HG22	1:A:13:ASP:N	2.23	0.53
1:A:730:MET:C	2:B:731:ARG:HD3	2.34	0.53
2:B:631:TRP:O	2:B:635:ILE:HD12	2.09	0.53
2:B:1045:GLN:HE21	2:B:1049:ARG:NH2	2.04	0.53
2:B:1043:GLY:HA2	2:B:1079:ALA:HB1	1.91	0.52
1:A:723:TYR:HD2	1:A:740:LEU:HD21	1.73	0.52
2:B:97:ARG:NH2	2:B:117:SER:HA	2.24	0.52
2:B:719:LYS:HE3	2:B:755:ASP:CG	2.34	0.52
2:B:868:ALA:O	2:B:871:LEU:HG	2.08	0.52
3:X:9:DG:H2''	3:X:10:DA:O4'	2.09	0.52
1:A:745:ASP:O	1:A:749:GLN:HG3	2.08	0.52
2:B:1034:LYS:HE2	2:B:1034:LYS:HA	1.92	0.52
1:A:522:GLU:HG3	1:A:567:PHE:CE2	2.44	0.52
1:A:618:PHE:CG	1:A:769:GLN:HG2	2.44	0.52
1:A:1000:TRP:CE2	2:B:336:ARG:HG3	2.44	0.52
2:B:903:HIS:CE1	2:B:1037:MET:HE3	2.44	0.52
3:X:45:DT:H5''	5:X:49:EDO:C1	2.39	0.52
1:A:237:LEU:HD22	1:A:264:ILE:HD12	1.92	0.52
1:A:530:ILE:HD12	1:A:551:GLU:HA	1.92	0.52
1:A:1008:THR:HG22	2:B:586:ASP:HB3	1.91	0.52
1:A:1047:PRO:HB3	1:A:1049:PHE:CE2	2.45	0.52
2:B:355:TYR:O	2:B:359:VAL:HG23	2.09	0.52
2:B:191:ALA:O	2:B:223:GLN:HG2	2.10	0.52
1:A:93:HIS:O	1:A:97:GLN:HG2	2.10	0.52
1:A:552:ALA:HB2	1:A:598:ILE:HG13	1.92	0.52
2:B:980:LEU:HD13	2:B:1096:PHE:HE1	1.75	0.52
3:X:42:DG:H2''	3:X:43:DA:O4'	2.10	0.52
2:B:946:VAL:HG12	2:B:959:ILE:HG13	1.92	0.52
2:B:477:THR:HA	2:B:480:TRP:NE1	2.25	0.52
2:B:836:LEU:O	2:B:836:LEU:HD23	2.10	0.52
3:X:33:DC:H6	3:X:33:DC:C5'	2.22	0.52
1:A:1073:LEU:HD11	1:A:1128:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:ALA:O	2:B:337:GLU:HB2	2.10	0.51
1:A:1161:LEU:HD23	1:A:1170:LEU:HA	1.92	0.51
2:B:4:GLU:HB3	2:B:232:THR:HG22	1.91	0.51
1:A:444:TYR:O	1:A:449:ALA:HB3	2.09	0.51
2:B:912:ILE:CD1	2:B:957:LEU:HD22	2.39	0.51
1:A:887:HIS:CG	1:A:888:GLN:H	2.29	0.51
2:B:202:GLY:HA2	2:B:229:GLU:HB2	1.93	0.51
1:A:107:SER:HB2	1:A:111:SER:HB3	1.93	0.51
1:A:567:PHE:HD1	1:A:567:PHE:O	1.94	0.51
1:A:727:VAL:HA	1:A:730:MET:CE	2.41	0.51
1:A:1220:ALA:C	1:A:1221:LEU:HD12	2.36	0.51
2:B:215:PRO:O	2:B:219:ARG:HG2	2.10	0.51
2:B:389:SER:O	2:B:393:VAL:HG23	2.10	0.51
2:B:632:LEU:HB3	2:B:637:VAL:HG13	1.92	0.51
1:A:1050:MET:SD	2:B:503:GLU:HG2	2.51	0.51
2:B:316:GLN:HG3	2:B:671:ILE:HG12	1.93	0.51
2:B:822:GLU:O	2:B:826:ILE:HG12	2.10	0.51
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.76	0.51
1:A:171:ASP:HB3	2:B:888:LYS:HE2	1.92	0.51
1:A:284:VAL:O	1:A:285:SER:C	2.54	0.51
1:A:578:ARG:HH12	1:A:583:ARG:HH22	1.59	0.51
1:A:730:MET:HB2	1:A:731:PRO:HD2	1.91	0.51
1:A:323:TYR:O	1:A:331:HIS:HE1	1.94	0.51
1:A:339:LYS:O	1:A:343:GLU:HG3	2.11	0.51
1:A:1049:PHE:CE1	1:A:1050:MET:HG3	2.45	0.51
2:B:875:ILE:HD12	2:B:876:LEU:N	2.26	0.51
1:A:64:THR:O	1:A:108:THR:HA	2.10	0.51
1:A:596:PRO:HA	1:A:599:MET:HE3	1.93	0.51
2:B:829:LEU:HD13	2:B:871:LEU:CD2	2.42	0.51
2:B:832:SER:CB	2:B:867:LEU:HD21	2.41	0.51
2:B:980:LEU:HD13	2:B:1096:PHE:CE1	2.45	0.51
3:X:8:DC:H2''	3:X:9:DG:C8	2.45	0.51
3:X:9:DG:H2'	3:X:10:DA:C8	2.46	0.51
1:A:595:ALA:N	1:A:596:PRO:HD2	2.26	0.50
2:B:772:VAL:HG12	2:B:1108:VAL:HG23	1.93	0.50
2:B:439:LYS:HG2	2:B:440:GLY:N	2.26	0.50
2:B:1084:GLU:HG2	2:B:1153:LEU:HD21	1.92	0.50
1:A:92:LEU:HG	1:A:96:ARG:HH21	1.76	0.50
1:A:413:ASN:OD1	1:A:413:ASN:C	2.53	0.50
1:A:506:ASP:O	1:A:510:GLU:HG3	2.10	0.50
2:B:642:GLY:O	2:B:646:ARG:CZ	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:LEU:O	2:B:269:LEU:HD23	2.11	0.50
2:B:805:HIS:CE1	2:B:1103:ILE:HD13	2.42	0.50
1:A:41:VAL:O	1:A:45:ILE:HG13	2.11	0.50
2:B:751:MET:HA	2:B:756:ARG:HG3	1.94	0.50
2:B:805:HIS:CD2	2:B:809:HIS:HB2	2.46	0.50
2:B:913:GLY:H	2:B:946:VAL:HG23	1.77	0.50
1:A:22:THR:HG22	1:A:23:GLY:N	2.27	0.50
2:B:770:ASN:H	2:B:1136:LEU:HD21	1.76	0.50
1:A:974:ARG:O	1:A:978:ILE:HG13	2.10	0.50
1:A:1095:LEU:HD21	1:A:1103:ILE:HD11	1.93	0.50
2:B:1112:PRO:HB2	2:B:1141:TYR:CE1	2.47	0.50
3:X:11:DG:H1'	3:X:12:DC:H5'	1.92	0.50
1:A:587:ILE:HG13	1:A:790:LEU:HD13	1.94	0.50
1:A:877:LYS:HD2	1:A:879:PHE:CE1	2.46	0.50
2:B:207:VAL:HG21	2:B:233:PHE:HD2	1.77	0.50
1:A:1094:LEU:CD2	2:B:80:GLY:HA2	2.41	0.50
2:B:806:PHE:HB2	2:B:1108:VAL:HG12	1.94	0.50
2:B:96:LEU:O	2:B:100:ILE:HG23	2.12	0.49
2:B:981:GLN:O	2:B:984:THR:HG22	2.12	0.49
1:A:589:LEU:O	1:A:792:THR:HA	2.12	0.49
2:B:441:ASP:O	2:B:445:LYS:HG3	2.12	0.49
2:B:918:PHE:HZ	2:B:939:LEU:CD1	2.24	0.49
2:B:943:ILE:HG21	2:B:946:VAL:HG13	1.94	0.49
2:B:1047:VAL:HG12	2:B:1051:MET:HE2	1.94	0.49
1:A:102:ASN:HA	2:B:617:ARG:HH11	1.77	0.49
1:A:360:LYS:HB3	1:A:365:ILE:O	2.13	0.49
1:A:530:ILE:CD1	1:A:551:GLU:HA	2.42	0.49
1:A:586:VAL:HG23	1:A:789:ARG:O	2.11	0.49
2:B:221:LEU:O	2:B:225:MET:HG3	2.12	0.49
2:B:398:TRP:HB2	2:B:440:GLY:HA2	1.93	0.49
1:A:727:VAL:HG22	1:A:730:MET:HE3	1.94	0.49
1:A:581:GLN:H	1:A:581:GLN:NE2	2.11	0.49
2:B:626:ASP:O	2:B:630:GLU:HB2	2.11	0.49
2:B:1112:PRO:HB2	2:B:1141:TYR:HE1	1.77	0.49
3:X:10:DA:H2'	3:X:11:DG:C8	2.47	0.49
1:A:595:ALA:HA	1:A:790:LEU:HD21	1.95	0.49
2:B:772:VAL:CG1	2:B:1108:VAL:HG23	2.42	0.49
2:B:912:ILE:HG12	2:B:948:LYS:CB	2.43	0.49
1:A:657:GLU:O	1:A:661:ILE:HG13	2.12	0.49
2:B:470:MET:O	2:B:474:LEU:HD13	2.13	0.49
1:A:836:HIS:CD2	1:A:839:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:SER:OG	1:A:1081:GLU:HG3	2.13	0.49
1:A:1221:LEU:HB2	1:A:1230:LEU:HD21	1.94	0.49
1:A:1094:LEU:HD21	2:B:80:GLY:HA2	1.95	0.49
2:B:86:PHE:HE2	2:B:183:SER:HA	1.78	0.49
2:B:745:SER:O	2:B:749:VAL:HG23	2.13	0.49
2:B:754:GLN:HG2	2:B:755:ASP:N	2.28	0.49
2:B:994:ALA:HA	2:B:999:MET:O	2.12	0.49
1:A:731:PRO:HD3	2:B:731:ARG:NH1	2.27	0.49
1:A:836:HIS:NE2	1:A:839:LEU:HD13	2.27	0.49
2:B:44:THR:HB	2:B:70:ARG:NH1	2.28	0.49
2:B:181:LEU:HD11	2:B:186:TYR:CE2	2.48	0.49
2:B:343:LYS:HA	2:B:587:GLN:O	2.13	0.49
2:B:383:LEU:HD13	2:B:514:VAL:HG11	1.95	0.49
2:B:488:LEU:HD13	2:B:508:TYR:HB2	1.95	0.49
2:B:931:LEU:HB3	2:B:935:CYS:CB	2.43	0.49
1:A:171:ASP:O	1:A:172:ARG:CB	2.61	0.48
1:A:321:THR:HA	1:A:325:THR:CG2	2.42	0.48
1:A:685:ASP:O	1:A:689:GLN:HG2	2.14	0.48
1:A:763:ARG:O	1:A:767:ARG:HG2	2.13	0.48
2:B:52:ALA:O	2:B:58:GLY:HA2	2.12	0.48
2:B:151:GLU:HA	2:B:151:GLU:OE2	2.12	0.48
2:B:881:ARG:O	2:B:885:VAL:HG23	2.14	0.48
3:X:4:DA:H2'	3:X:5:DA:C8	2.45	0.48
3:X:40:DT:H2''	3:X:41:DA:C8	2.49	0.48
1:A:581:GLN:C	1:A:583:ARG:H	2.22	0.48
2:B:163:HIS:CE1	2:B:167:ILE:HD11	2.48	0.48
2:B:614:LEU:HB3	2:B:615:PRO:CD	2.36	0.48
2:B:986:LEU:HD21	2:B:1003:PRO:HB3	1.94	0.48
1:A:727:VAL:CG1	1:A:736:ARG:HB3	2.44	0.48
2:B:115:ASP:OD1	2:B:115:ASP:C	2.56	0.48
2:B:299:ALA:O	2:B:302:ALA:HB2	2.13	0.48
1:A:592:MET:N	1:A:593:PRO:CD	2.75	0.48
2:B:212:GLN:CD	2:B:254:MET:HE3	2.38	0.48
1:A:37:THR:O	1:A:41:VAL:HG23	2.13	0.48
1:A:41:VAL:HG12	1:A:45:ILE:CD1	2.43	0.48
1:A:633:ILE:HD13	1:A:701:TRP:HB3	1.95	0.48
2:B:868:ALA:HA	2:B:871:LEU:HD23	1.96	0.48
1:A:127:ASP:O	1:A:130:PHE:HB3	2.14	0.48
1:A:439:VAL:HG23	1:A:454:PHE:CD2	2.49	0.48
1:A:499:LYS:HD2	1:A:857:ARG:NH1	2.28	0.48
2:B:404:PHE:CZ	2:B:430:GLU:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:687:ARG:O	2:B:691:LEU:HD13	2.13	0.48
2:B:927:LEU:HD12	2:B:927:LEU:O	2.13	0.48
1:A:49:THR:HG22	1:A:94:ILE:HG12	1.96	0.48
1:A:163:GLU:O	1:A:167:ARG:HB2	2.14	0.48
1:A:339:LYS:HB3	1:A:340:PRO:HD3	1.95	0.48
2:B:466:GLN:HG2	2:B:467:GLU:N	2.27	0.48
2:B:912:ILE:HG12	2:B:948:LYS:HB3	1.95	0.48
1:A:75:HIS:O	1:A:79:GLU:HG3	2.13	0.48
2:B:840:ARG:NH1	2:B:859:PHE:HA	2.29	0.48
2:B:918:PHE:HZ	2:B:939:LEU:HD11	1.78	0.48
1:A:317:GLU:OE1	1:A:317:GLU:HA	2.13	0.48
1:A:582:TYR:CD2	1:A:607:ILE:HG21	2.49	0.48
1:A:1056:THR:HG22	1:A:1059:GLU:OE2	2.14	0.48
2:B:336:ARG:HH12	2:B:717:VAL:HG12	1.79	0.48
2:B:635:ILE:O	2:B:635:ILE:HG22	2.14	0.48
2:B:1036:LYS:NZ	2:B:1064:ASN:HA	2.28	0.48
3:X:41:DA:H2'	3:X:42:DG:H8	1.79	0.48
1:A:281:VAL:HB	1:A:282:PRO:HD3	1.96	0.47
1:A:698:LEU:O	1:A:702:ARG:HG2	2.14	0.47
2:B:472:ASN:C	2:B:475:ASN:OD1	2.57	0.47
2:B:876:LEU:HA	2:B:882:HIS:HB3	1.96	0.47
2:B:924:LEU:HB3	2:B:925:PRO:HD2	1.95	0.47
1:A:120:TYR:HB2	1:A:378:ILE:HD13	1.97	0.47
1:A:125:ASP:HA	2:B:116:LYS:HZ1	1.78	0.47
1:A:454:PHE:CD2	1:A:454:PHE:C	2.92	0.47
1:A:942:ILE:HD12	1:A:942:ILE:N	2.29	0.47
2:B:151:GLU:OE2	2:B:156:ARG:NH1	2.48	0.47
2:B:488:LEU:HD22	2:B:508:TYR:CG	2.49	0.47
2:B:1005:GLY:HA2	2:B:1085:PHE:CZ	2.49	0.47
1:A:172:ARG:HH12	2:B:964:SER:HB2	1.79	0.47
1:A:243:LEU:HD13	1:A:301:LEU:HG	1.96	0.47
1:A:603:ARG:HG2	1:A:608:PRO:CA	2.40	0.47
1:A:1138:ALA:HA	1:A:1152:LEU:HD22	1.96	0.47
2:B:36:ILE:HG23	2:B:66:PHE:CD2	2.45	0.47
2:B:97:ARG:HA	2:B:100:ILE:CG1	2.42	0.47
2:B:157:VAL:O	2:B:161:LYS:HG2	2.14	0.47
2:B:892:ILE:HG12	2:B:1013:ASP:HB2	1.96	0.47
3:X:9:DG:N2	3:X:35:DC:N3	2.62	0.47
1:A:603:ARG:CD	1:A:609:VAL:H	2.23	0.47
1:A:772:GLY:O	1:A:773:ASP:CB	2.62	0.47
2:B:187:LEU:HB3	2:B:216:GLN:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:34:DT:H2'	3:X:35:DC:H5''	1.97	0.47
1:A:175:LEU:O	1:A:178:GLN:HG2	2.15	0.47
2:B:182:HIS:O	2:B:183:SER:C	2.58	0.47
2:B:769:ARG:HA	2:B:1136:LEU:CD2	2.39	0.47
2:B:861:TYR:O	2:B:864:VAL:HG12	2.14	0.47
2:B:918:PHE:HB2	2:B:943:ILE:HD12	1.96	0.47
1:A:157:GLY:HA2	1:A:162:PHE:CE2	2.50	0.47
1:A:234:LYS:HG3	1:A:261:LEU:HD11	1.97	0.47
2:B:141:ARG:HH12	2:B:163:HIS:CD2	2.32	0.47
2:B:707:VAL:HG12	2:B:708:SER:H	1.78	0.47
2:B:821:LEU:HD13	2:B:872:GLN:HG2	1.97	0.47
2:B:963:LYS:HE2	2:B:1008:TYR:CD1	2.50	0.47
2:B:980:LEU:O	2:B:984:THR:HG22	2.14	0.47
2:B:1068:LYS:HA	3:X:10:DA:OP1	2.15	0.47
3:X:41:DA:H2''	3:X:42:DG:O4'	2.14	0.47
1:A:488:THR:O	1:A:492:PHE:HD1	1.98	0.47
1:A:862:GLU:O	1:A:866:VAL:HG23	2.14	0.47
1:A:228:MET:HE1	1:A:911:TYR:CG	2.49	0.47
2:B:195:PRO:HA	2:B:227:HIS:CD2	2.49	0.47
2:B:562:LEU:HA	2:B:565:PHE:HB3	1.97	0.47
1:A:887:HIS:CG	1:A:888:GLN:N	2.83	0.47
2:B:307:GLU:HG3	2:B:308:LYS:H	1.80	0.47
1:A:627:LEU:O	1:A:631:LYS:HG3	2.15	0.46
1:A:887:HIS:NE2	1:A:888:GLN:HG3	2.30	0.46
2:B:73:TRP:CD1	2:B:82:MET:HE1	2.50	0.46
2:B:122:GLN:HG2	2:B:623:VAL:HG23	1.97	0.46
1:A:326:ARG:HB3	2:B:1021:PRO:HG3	1.97	0.46
1:A:450:GLU:OE2	1:A:452:LEU:HB2	2.15	0.46
1:A:583:ARG:HB3	1:A:786:ASP:HA	1.97	0.46
1:A:726:TYR:CD1	1:A:730:MET:HE2	2.50	0.46
1:A:803:VAL:HG22	1:A:877:LYS:HB2	1.96	0.46
1:A:1067:VAL:HG11	1:A:1108:ILE:HD13	1.96	0.46
2:B:251:LEU:HD22	2:B:298:GLU:HG3	1.96	0.46
2:B:976:TYR:CD1	2:B:1144:LEU:HD22	2.50	0.46
1:A:70:ALA:O	1:A:73:MET:HB3	2.15	0.46
1:A:96:ARG:HG2	2:B:249:LEU:HD11	1.97	0.46
1:A:450:GLU:HG2	1:A:826:LYS:HZ2	1.81	0.46
1:A:550:PHE:N	1:A:550:PHE:CD1	2.83	0.46
1:A:578:ARG:NE	1:A:581:GLN:OE1	2.48	0.46
1:A:639:ASP:CB	2:B:814:LYS:H	2.29	0.46
1:A:63:VAL:HA	1:A:107:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:O	1:A:241:LEU:HB2	2.15	0.46
1:A:982:GLU:HA	2:B:747:TYR:HE2	1.79	0.46
2:B:330:GLU:CD	2:B:698:ARG:HH12	2.24	0.46
2:B:976:TYR:CE1	2:B:1144:LEU:HD22	2.50	0.46
3:X:44:DT:H2"	3:X:45:DT:OP2	2.15	0.46
1:A:567:PHE:O	1:A:567:PHE:CD1	2.69	0.46
1:A:821:SER:HA	1:A:833:LYS:NZ	2.30	0.46
1:A:854:LYS:O	1:A:857:ARG:HG2	2.15	0.46
2:B:723:GLN:HE21	2:B:759:SER:HB3	1.81	0.46
2:B:931:LEU:HG	2:B:1101:GLU:HB3	1.98	0.46
1:A:560:ARG:HA	1:A:563:ILE:CD1	2.42	0.46
1:A:598:ILE:CG2	1:A:602:LEU:HD12	2.46	0.46
1:A:815:MET:HE1	1:A:860:LEU:HD13	1.97	0.46
1:A:1134:LEU:HD11	1:A:1210:GLN:OE1	2.16	0.46
2:B:927:LEU:HD12	2:B:927:LEU:C	2.41	0.46
2:B:1136:LEU:C	2:B:1136:LEU:HD23	2.41	0.46
2:B:1151:THR:O	2:B:1154:GLU:HB3	2.15	0.46
1:A:429:GLU:CD	1:A:429:GLU:H	2.24	0.46
2:B:418:PRO:O	2:B:422:VAL:HG23	2.16	0.46
2:B:877:LEU:CD2	2:B:883:TYR:CZ	2.98	0.46
2:B:918:PHE:HB2	2:B:943:ILE:CD1	2.45	0.46
1:A:713:LEU:O	1:A:717:VAL:HG23	2.15	0.46
2:B:371:PHE:CE1	2:B:580:LEU:HD21	2.51	0.46
2:B:389:SER:OG	2:B:405:ARG:HD2	2.15	0.46
2:B:770:ASN:N	2:B:1136:LEU:HD21	2.31	0.46
1:A:768:MET:O	1:A:773:ASP:N	2.48	0.46
2:B:113:ALA:HA	2:B:116:LYS:HE3	1.97	0.46
2:B:888:LYS:HE3	2:B:892:ILE:CG1	2.45	0.46
1:A:1007:VAL:HG22	2:B:585:LEU:HB2	1.98	0.45
1:A:175:LEU:HD12	1:A:178:GLN:NE2	2.28	0.45
1:A:836:HIS:HD2	1:A:839:LEU:H	1.63	0.45
2:B:931:LEU:HD12	2:B:935:CYS:SG	2.56	0.45
1:A:417:GLU:HB2	1:A:453:LEU:HD21	1.96	0.45
2:B:482:VAL:HB	2:B:483:PRO:HD3	1.96	0.45
1:A:567:PHE:HB3	1:A:580:ILE:HD11	1.99	0.45
1:A:748:ARG:O	1:A:751:GLU:HG2	2.16	0.45
1:A:1136:LEU:O	1:A:1151:PRO:HA	2.16	0.45
2:B:489:GLN:O	2:B:493:LYS:HG2	2.16	0.45
1:A:240:ALA:HB1	1:A:257:PHE:CE2	2.51	0.45
1:A:622:GLU:HG2	1:A:727:VAL:HG11	1.98	0.45
1:A:284:VAL:HG13	1:A:285:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ARG:HH22	1:A:502:GLU:CD	2.25	0.45
1:A:654:ASP:HB2	1:A:657:GLU:HG3	1.99	0.45
1:A:810:GLY:HA3	1:A:883:SER:H	1.80	0.45
1:A:1136:LEU:O	1:A:1152:LEU:HD23	2.17	0.45
1:A:1223:PHE:HE1	1:A:1230:LEU:CD2	2.30	0.45
2:B:197:ALA:O	2:B:200:ILE:HG13	2.17	0.45
2:B:207:VAL:HG21	2:B:233:PHE:CD2	2.52	0.45
2:B:552:VAL:HA	2:B:556:GLY:HA2	1.97	0.45
2:B:614:LEU:CB	2:B:615:PRO:HD3	2.36	0.45
2:B:1114:LYS:HB3	2:B:1144:LEU:H	1.82	0.45
1:A:61:LEU:HB3	1:A:404:VAL:HG22	1.98	0.45
2:B:245:GLU:HG2	2:B:260:TYR:CD2	2.52	0.45
2:B:378:MET:HG2	2:B:578:PHE:CE2	2.52	0.45
2:B:822:GLU:HB3	2:B:824:PRO:HD2	1.97	0.45
2:B:903:HIS:ND1	2:B:1037:MET:HE3	2.31	0.45
2:B:1148:LYS:O	2:B:1149:ASP:C	2.59	0.45
1:A:558:GLU:HA	1:A:561:LYS:HB3	1.99	0.45
1:A:591:SER:CB	1:A:593:PRO:HD3	2.47	0.45
1:A:740:LEU:HD12	1:A:740:LEU:HA	1.83	0.45
1:A:825:ASP:CB	1:A:851:MET:HE3	2.44	0.45
1:A:840:ARG:O	2:B:1016:ILE:HG12	2.16	0.45
1:A:1139:LYS:HA	1:A:1142:TYR:O	2.16	0.45
2:B:213:PHE:CE2	2:B:221:LEU:HD11	2.52	0.45
2:B:366:TYR:CD2	2:B:717:VAL:HG21	2.51	0.45
1:A:415:VAL:O	1:A:419:ILE:HG13	2.17	0.45
1:A:599:MET:HG2	1:A:609:VAL:CG1	2.47	0.45
1:A:662:ARG:HD2	1:A:666:LYS:HA	1.98	0.45
1:A:1015:SER:N	1:A:1031:GLY:O	2.47	0.45
2:B:673:ASP:OD2	2:B:675:GLU:HG2	2.17	0.45
2:B:726:THR:HG23	2:B:763:PHE:CE2	2.52	0.45
1:A:599:MET:SD	1:A:611:ALA:HB3	2.57	0.45
1:A:1044:TYR:CG	1:A:1044:TYR:O	2.70	0.45
2:B:1111:GLU:O	2:B:1142:ARG:NE	2.50	0.45
1:A:328:PRO:O	1:A:332:LEU:HG	2.18	0.44
1:A:687:LEU:O	1:A:691:LEU:HG	2.17	0.44
1:A:818:LEU:N	1:A:818:LEU:HD23	2.32	0.44
2:B:1090:LYS:HD2	2:B:1090:LYS:HA	1.78	0.44
1:A:394:ALA:O	1:A:398:GLN:HG3	2.17	0.44
2:B:239:LYS:N	2:B:240:PRO:HD3	2.33	0.44
2:B:514:VAL:HB	2:B:515:PRO:HD3	1.98	0.44
2:B:560:ILE:HD11	2:B:564:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ASP:O	1:A:802:PRO:HD2	2.17	0.44
1:A:846:LEU:HD12	1:A:846:LEU:HA	1.78	0.44
2:B:432:TYR:HE1	2:B:438:ILE:HD11	1.82	0.44
2:B:919:GLY:HA2	2:B:926:PRO:HA	2.00	0.44
2:B:959:ILE:N	2:B:959:ILE:HD12	2.32	0.44
1:A:157:GLY:HA2	1:A:162:PHE:HE2	1.82	0.44
1:A:1131:PRO:HG2	2:B:64:GLN:OE1	2.17	0.44
2:B:226:VAL:CG2	2:B:269:LEU:HD11	2.47	0.44
1:A:608:PRO:HG2	1:A:787:VAL:HG21	1.99	0.44
2:B:833:SER:O	2:B:837:ILE:HG12	2.17	0.44
1:A:31:ALA:O	1:A:34:SER:HB3	2.17	0.44
1:A:273:ASP:CG	1:A:276:GLU:HB2	2.43	0.44
1:A:710:VAL:O	1:A:714:ILE:HG13	2.17	0.44
1:A:832:THR:C	1:A:848:LEU:HD12	2.42	0.44
1:A:1007:VAL:CG2	2:B:585:LEU:HD12	2.48	0.44
2:B:88:THR:HG22	2:B:90:THR:H	1.82	0.44
2:B:490:LYS:O	2:B:494:LYS:HB2	2.18	0.44
2:B:875:ILE:HD12	2:B:875:ILE:C	2.43	0.44
2:B:1090:LYS:HG3	2:B:1094:ARG:CZ	2.47	0.44
1:A:229:VAL:HG23	1:A:230:LEU:N	2.32	0.44
1:A:625:VAL:O	1:A:629:VAL:HG23	2.16	0.44
1:A:1176:ASP:HB2	1:A:1223:PHE:HE2	1.83	0.44
2:B:805:HIS:CD2	2:B:805:HIS:C	2.95	0.44
2:B:871:LEU:C	2:B:871:LEU:HD12	2.43	0.44
1:A:35:GLY:O	1:A:39:VAL:HG13	2.18	0.44
1:A:85:LEU:HD21	2:B:300:ARG:HG2	2.00	0.44
1:A:1176:ASP:HB2	1:A:1223:PHE:CE2	2.53	0.44
2:B:673:ASP:HB3	2:B:677:LYS:N	2.32	0.44
2:B:1154:GLU:O	2:B:1157:LYS:HB2	2.18	0.44
1:A:789:ARG:CZ	1:A:801:PHE:HE2	2.31	0.43
1:A:894:TRP:CE2	1:A:921:GLY:HA3	2.53	0.43
1:A:78:ALA:O	1:A:81:LEU:N	2.50	0.43
1:A:282:PRO:HA	1:A:320:LYS:HD2	1.99	0.43
2:B:346:ALA:O	2:B:604:THR:HA	2.19	0.43
2:B:415:LEU:O	2:B:416:ASN:CG	2.61	0.43
1:A:417:GLU:CG	1:A:453:LEU:HD21	2.49	0.43
2:B:199:ASP:OD1	2:B:199:ASP:C	2.61	0.43
2:B:885:VAL:O	2:B:889:LEU:HG	2.18	0.43
1:A:201:PHE:CE2	1:A:830:PHE:HB2	2.52	0.43
1:A:566:PRO:O	1:A:567:PHE:C	2.60	0.43
1:A:607:ILE:HD11	1:A:788:VAL:CG2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:HIS:CE1	2:B:230:HIS:CD2	3.07	0.43
2:B:642:GLY:HA2	2:B:646:ARG:NE	2.34	0.43
2:B:1149:ASP:O	2:B:1153:LEU:HB2	2.18	0.43
1:A:836:HIS:CD2	1:A:839:LEU:H	2.37	0.43
2:B:400:TYR:O	2:B:404:PHE:HD1	2.02	0.43
1:A:256:ASN:OD1	1:A:257:PHE:N	2.51	0.43
1:A:818:LEU:HD21	1:A:855:MET:HG2	2.01	0.43
1:A:1193:LEU:HD13	1:A:1223:PHE:CZ	2.53	0.43
2:B:421:LYS:HD3	2:B:424:GLU:OE1	2.19	0.43
2:B:803:PHE:HZ	2:B:1129:VAL:HG12	1.82	0.43
1:A:78:ALA:O	1:A:79:GLU:C	2.61	0.43
2:B:72:ALA:HA	2:B:190:LEU:HD13	2.00	0.43
2:B:126:MET:HE3	2:B:130:PHE:CE2	2.54	0.43
2:B:468:ILE:O	2:B:469:GLU:C	2.61	0.43
2:B:660:SER:OG	2:B:661:PRO:HD3	2.18	0.43
2:B:916:LEU:HD21	2:B:924:LEU:CD1	2.47	0.43
1:A:197:TRP:O	1:A:200:SER:HB3	2.19	0.43
1:A:356:PHE:CZ	1:A:360:LYS:HE2	2.53	0.43
2:B:25:GLU:HG2	2:B:35:ILE:HD11	2.01	0.43
2:B:100:ILE:O	2:B:104:LYS:HB2	2.18	0.43
2:B:105:GLN:CD	2:B:105:GLN:H	2.26	0.43
2:B:871:LEU:HD12	2:B:871:LEU:O	2.18	0.43
2:B:1036:LYS:HZ3	2:B:1064:ASN:HA	1.83	0.43
1:A:92:LEU:O	1:A:96:ARG:HG3	2.19	0.43
1:A:207:VAL:CG2	1:A:335:LEU:HD22	2.49	0.43
1:A:230:LEU:HD12	1:A:271:GLN:HG2	2.00	0.43
1:A:1136:LEU:HD21	1:A:1206:LYS:CD	2.49	0.43
2:B:298:GLU:O	2:B:299:ALA:C	2.60	0.43
2:B:608:GLY:C	2:B:610:ASN:H	2.26	0.43
2:B:948:LYS:HG2	2:B:949:ALA:N	2.32	0.43
1:A:228:MET:HE1	1:A:911:TYR:CD1	2.53	0.43
1:A:555:ILE:HG12	1:A:881:ILE:HG13	2.01	0.43
1:A:1000:TRP:NE1	2:B:336:ARG:HG3	2.34	0.43
2:B:348:LEU:HD11	2:B:598:MET:HE1	2.01	0.43
2:B:496:LYS:N	2:B:500:GLU:OE2	2.51	0.43
1:A:506:ASP:O	1:A:509:ALA:HB3	2.19	0.42
1:A:578:ARG:HH12	1:A:583:ARG:NH2	2.17	0.42
1:A:796:SER:O	1:A:799:LEU:HB2	2.20	0.42
1:A:840:ARG:NH1	2:B:1015:MET:HG2	2.34	0.42
2:B:265:LYS:HA	2:B:268:GLU:HG2	2.00	0.42
2:B:610:ASN:HD21	2:B:670:PRO:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:918:PHE:CZ	2:B:939:LEU:CD1	3.01	0.42
2:B:1007:LEU:CD1	2:B:1063:ILE:HD11	2.49	0.42
1:A:507:GLU:C	1:A:509:ALA:H	2.27	0.42
1:A:753:THR:HG23	1:A:755:PHE:N	2.17	0.42
1:A:1231:THR:O	1:A:1232:LEU:HD23	2.19	0.42
2:B:66:PHE:HE1	2:B:74:ARG:HG3	1.79	0.42
1:A:172:ARG:HH12	2:B:964:SER:CB	2.33	0.42
1:A:418:SER:O	1:A:422:LEU:HB2	2.20	0.42
1:A:480:SER:HB3	1:A:485:LEU:HD21	2.02	0.42
1:A:582:TYR:CD1	1:A:607:ILE:CD1	3.01	0.42
1:A:816:MET:HG3	3:X:44:DT:O2	2.19	0.42
2:B:300:ARG:N	2:B:301:PRO:CD	2.82	0.42
2:B:805:HIS:HD2	2:B:809:HIS:HB2	1.84	0.42
3:X:34:DT:C3'	3:X:35:DC:H5''	2.49	0.42
1:A:481:ARG:NH1	1:A:517:TYR:HD1	2.18	0.42
1:A:560:ARG:HH22	1:A:605:GLN:HG3	1.84	0.42
1:A:1090:TYR:CE1	1:A:1097:GLU:HA	2.54	0.42
1:A:1117:GLY:O	1:A:1121:ILE:HG12	2.19	0.42
2:B:218:PHE:CE1	2:B:262:LEU:HD12	2.55	0.42
2:B:483:PRO:HB2	2:B:484:PRO:HD3	2.00	0.42
2:B:673:ASP:CG	2:B:674:ALA:N	2.77	0.42
2:B:734:THR:HG21	2:B:766:LEU:HD11	2.00	0.42
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.89	0.42
2:B:230:HIS:HB3	6:B:1257:HOH:O	2.20	0.42
2:B:237:ALA:HA	2:B:252:PHE:CD1	2.54	0.42
1:A:168:TYR:OH	1:A:832:THR:HG21	2.20	0.42
1:A:310:ASN:O	1:A:314:LYS:HG2	2.19	0.42
1:A:556:ALA:HA	1:A:559:ILE:HD12	2.01	0.42
1:A:581:GLN:O	1:A:582:TYR:HB2	2.20	0.42
2:B:505:LEU:O	2:B:508:TYR:HB3	2.19	0.42
1:A:170:THR:O	1:A:173:HIS:HB3	2.20	0.42
1:A:545:LEU:O	1:A:548:VAL:HG12	2.19	0.42
1:A:767:ARG:HD2	1:A:770:GLU:OE2	2.20	0.42
1:A:908:PHE:O	1:A:911:TYR:HB3	2.19	0.42
2:B:97:ARG:O	2:B:100:ILE:HG13	2.19	0.42
2:B:181:LEU:HD23	2:B:182:HIS:N	2.34	0.42
2:B:289:GLU:H	2:B:289:GLU:HG2	1.66	0.42
2:B:918:PHE:CZ	2:B:939:LEU:HD12	2.55	0.42
2:B:932:LYS:O	2:B:933:ASN:CG	2.63	0.42
1:A:221:TYR:CD2	1:A:854:LYS:HB2	2.55	0.42
1:A:601:GLU:HA	1:A:604:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:819:PHE:CZ	2:B:875:ILE:HG22	2.55	0.42
1:A:117:LEU:O	1:A:121:TYR:HB3	2.20	0.42
2:B:552:VAL:O	2:B:556:GLY:HA3	2.20	0.42
1:A:56:ASP:HB2	1:A:58:ASP:OD1	2.20	0.42
1:A:381:ALA:N	1:A:391:SER:HB3	2.35	0.42
1:A:656:ASN:O	1:A:660:LEU:HB2	2.19	0.42
1:A:866:VAL:O	1:A:869:VAL:HG22	2.20	0.42
2:B:182:HIS:H	2:B:185:ASP:HB2	1.84	0.42
3:X:7:DG:H1	3:X:37:DC:H42	1.67	0.42
1:A:139:GLU:HB3	1:A:771:ARG:NH2	2.35	0.41
1:A:426:GLY:HA2	1:A:427:PRO:HD3	1.91	0.41
1:A:683:ARG:O	1:A:689:GLN:NE2	2.54	0.41
1:A:1049:PHE:CE1	2:B:503:GLU:HG3	2.55	0.41
2:B:790:GLY:O	2:B:939:LEU:HA	2.20	0.41
2:B:826:ILE:O	2:B:829:LEU:HB3	2.19	0.41
1:A:213:ILE:N	1:A:213:ILE:HD13	2.35	0.41
1:A:238:LEU:HD23	1:A:241:LEU:HD12	2.01	0.41
1:A:317:GLU:O	1:A:321:THR:HG23	2.20	0.41
1:A:599:MET:HG3	1:A:790:LEU:HD23	2.02	0.41
1:A:816:MET:HA	1:A:819:ASN:ND2	2.35	0.41
1:A:1080:GLU:CD	1:A:1080:GLU:H	2.28	0.41
2:B:497:THR:OG1	2:B:500:GLU:HG2	2.20	0.41
2:B:726:THR:O	2:B:730:LEU:HG	2.20	0.41
1:A:27:LEU:HD13	1:A:435:MET:HG3	2.03	0.41
1:A:241:LEU:O	1:A:244:THR:HG23	2.19	0.41
1:A:607:ILE:HD12	1:A:788:VAL:H	1.85	0.41
2:B:19:ILE:O	2:B:23:GLN:HG3	2.20	0.41
1:A:81:LEU:HB3	1:A:98:LEU:HD13	2.02	0.41
1:A:382:GLU:OE1	1:A:388:ARG:CZ	2.69	0.41
1:A:603:ARG:HG2	1:A:609:VAL:N	2.35	0.41
1:A:828:LEU:HD22	1:A:828:LEU:N	2.36	0.41
1:A:1129:GLU:O	1:A:1131:PRO:HD3	2.20	0.41
1:A:529:LEU:C	1:A:529:LEU:HD23	2.46	0.41
1:A:948:ARG:HD3	1:A:948:ARG:HA	1.89	0.41
2:B:38:LEU:O	2:B:207:VAL:HA	2.20	0.41
2:B:158:LEU:C	2:B:158:LEU:HD23	2.45	0.41
2:B:388:ARG:HD2	2:B:570:GLU:OE1	2.20	0.41
2:B:477:THR:HA	2:B:480:TRP:HE1	1.84	0.41
2:B:868:ALA:HA	2:B:871:LEU:CD2	2.50	0.41
1:A:803:VAL:HG22	1:A:877:LYS:CB	2.50	0.41
2:B:660:SER:N	2:B:661:PRO:CD	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:823:ALA:N	2:B:824:PRO:CD	2.82	0.41
1:A:1136:LEU:HD21	1:A:1206:LYS:HD2	2.02	0.41
2:B:9:ARG:HD3	2:B:294:GLU:OE1	2.21	0.41
2:B:117:SER:O	2:B:120:THR:HG22	2.20	0.41
2:B:153:ARG:NH2	2:B:156:ARG:HD2	2.35	0.41
2:B:422:VAL:O	2:B:426:VAL:HG23	2.20	0.41
2:B:927:LEU:HD21	2:B:939:LEU:HD11	2.01	0.41
1:A:407:ASP:OD1	1:A:408:GLU:N	2.51	0.41
2:B:143:MET:HE3	2:B:637:VAL:HG11	2.03	0.41
2:B:289:GLU:HG3	2:B:311:ALA:HB3	2.03	0.41
2:B:308:LYS:HE2	2:B:308:LYS:HB3	1.87	0.41
1:A:131:ARG:NH2	1:A:365:ILE:HD11	2.36	0.41
1:A:191:HIS:CG	1:A:192:PRO:HD2	2.56	0.41
1:A:587:ILE:O	1:A:790:LEU:HD12	2.21	0.41
1:A:724:MET:HE1	1:A:741:ARG:HB3	2.01	0.41
1:A:1064:MET:HE1	1:A:1104:ASP:H	1.86	0.41
2:B:531:ILE:HD12	2:B:532:ILE:N	2.36	0.41
2:B:757:LEU:HD12	2:B:758:GLN:N	2.35	0.41
2:B:786:GLU:HG3	2:B:787:ARG:H	1.86	0.41
2:B:800:ALA:HA	2:B:1113:TYR:HE2	1.85	0.41
2:B:808:SER:O	2:B:812:HIS:HA	2.20	0.41
2:B:982:MET:HG3	2:B:1008:TYR:CZ	2.56	0.41
1:A:191:HIS:HA	1:A:192:PRO:HD3	1.98	0.41
1:A:202:VAL:HG11	1:A:343:GLU:HG2	2.02	0.41
1:A:492:PHE:CZ	1:A:868:TYR:HA	2.56	0.41
1:A:894:TRP:HZ2	1:A:917:LEU:HG	1.85	0.41
2:B:371:PHE:HB2	2:B:587:GLN:NE2	2.36	0.41
1:A:495:LEU:HD23	1:A:905:LEU:HD12	2.03	0.40
1:A:697:HIS:HB3	1:A:701:TRP:CZ2	2.56	0.40
1:A:1127:ASP:C	1:A:1130:ILE:HD11	2.45	0.40
2:B:88:THR:HG22	2:B:89:SER:N	2.35	0.40
2:B:514:VAL:N	2:B:515:PRO:CD	2.84	0.40
2:B:544:VAL:O	2:B:547:LEU:HB3	2.22	0.40
2:B:747:TYR:O	2:B:751:MET:HG2	2.22	0.40
1:A:25:ASP:CG	1:A:433:LEU:HB3	2.46	0.40
1:A:137:GLU:HA	1:A:140:LEU:HB2	2.02	0.40
1:A:167:ARG:HB2	1:A:167:ARG:HE	1.72	0.40
1:A:559:ILE:HG22	1:A:563:ILE:HD11	2.03	0.40
1:A:705:SER:HB3	1:A:713:LEU:HD22	2.02	0.40
1:A:715:TRP:CH2	2:B:365:ASP:OD1	2.75	0.40
2:B:194:ILE:HB	2:B:195:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:PHE:N	1:A:550:PHE:HD1	2.19	0.40
1:A:1221:LEU:HB2	1:A:1230:LEU:CD2	2.51	0.40
2:B:254:MET:O	2:B:258:THR:HG23	2.22	0.40
2:B:883:TYR:HD2	2:B:883:TYR:HA	1.65	0.40
2:B:1137:GLU:C	2:B:1139:ASN:H	2.29	0.40
2:B:139:ASP:O	2:B:143:MET:HG3	2.22	0.40
2:B:671:ILE:HA	2:B:671:ILE:HD13	1.86	0.40
2:B:873:LYS:C	2:B:874:GLU:HG2	2.46	0.40
1:A:592:MET:HG2	1:A:792:THR:CG2	2.51	0.40
2:B:298:GLU:CD	2:B:298:GLU:N	2.77	0.40
2:B:378:MET:CE	2:B:540:ALA:HA	2.51	0.40
2:B:419:LYS:HB3	2:B:423:ARG:HH12	1.86	0.40
2:B:819:PHE:HZ	2:B:878:SER:HB3	1.87	0.40
2:B:832:SER:O	2:B:836:LEU:HB2	2.22	0.40
2:B:956:LEU:HD23	2:B:1002:THR:OG1	2.22	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	1096/1232 (89%)	1035 (94%)	57 (5%)	4 (0%)	30	60
2	B	1126/1166 (97%)	1061 (94%)	63 (6%)	2 (0%)	43	72
All	All	2222/2398 (93%)	2096 (94%)	120 (5%)	6 (0%)	36	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	902	ASP
2	B	641	SER

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Mol	Chain	Res	Type
2	B	994	ALA
1	A	172	ARG
1	A	566	PRO

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	977/1062 (92%)	940 (96%)	37 (4%)	29	64
2	B	998/1029 (97%)	968 (97%)	30 (3%)	36	72
All	All	1975/2091 (94%)	1908 (97%)	67 (3%)	32	68

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	39	VAL
1	A	59	ARG
1	A	63	VAL
1	A	76	ARG
1	A	174	ASP
1	A	176	ASP
1	A	187	TYR
1	A	213	ILE
1	A	216	LEU
1	A	329	GLU
1	A	422	LEU
1	A	445	ARG
1	A	452	LEU
1	A	526	GLU
1	A	549	GLN
1	A	581	GLN
1	A	598	ILE
1	A	622	GLU
1	A	654	ASP

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Mol	Chain	Res	Type
1	A	682	ASP
1	A	715	TRP
1	A	771	ARG
1	A	787	VAL
1	A	818	LEU
1	A	857	ARG
1	A	860	LEU
1	A	877	LYS
1	A	903	TRP
1	A	982	GLU
1	A	984	VAL
1	A	1100	LYS
1	A	1139	LYS
1	A	1165	GLU
1	A	1173	TYR
1	A	1195	LYS
1	A	1213	LYS
2	B	26	LEU
2	B	100	ILE
2	B	243	GLU
2	B	274	THR
2	B	289	GLU
2	B	298	GLU
2	B	468	ILE
2	B	590	VAL
2	B	639	LEU
2	B	644	ARG
2	B	646	ARG
2	B	671	ILE
2	B	707	VAL
2	B	712	GLN
2	B	757	LEU
2	B	775	LEU
2	B	786	GLU
2	B	796	GLU
2	B	844	GLU
2	B	867	LEU
2	B	876	LEU
2	B	883	TYR
2	B	918	PHE
2	B	948	LYS
2	B	1017	GLN

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Mol	Chain	Res	Type
2	B	1045	GLN
2	B	1063	ILE
2	B	1070	ASP
2	B	1086	ASP
2	B	1141	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	75	HIS
1	A	93	HIS
1	A	178	GLN
1	A	191	HIS
1	A	310	ASN
1	A	331	HIS
1	A	421	GLN
1	A	549	GLN
1	A	769	GLN
1	A	997	GLN
1	A	1087	HIS
2	B	163	HIS
2	B	179	GLN
2	B	230	HIS
2	B	351	GLN
2	B	587	GLN
2	B	695	HIS
2	B	702	ASN
2	B	723	GLN
2	B	890	GLN
2	B	992	HIS
2	B	1045	GLN
2	B	1064	ASN
2	B	1097	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	$\# Z > 2$
4	SO4	B	1167	-	4,4,4	0.23	0	6,6,6	0.10	0
5	EDO	X	49	-	3,3,3	0.61	0	2,2,2	0.75	0

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
5	EDO	X	49	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	X	49	EDO	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1122/1232 (91%)	0.29	41 (3%) 45 36	34, 58, 100, 118	0
2	B	1132/1166 (97%)	0.23	24 (2%) 63 54	30, 58, 91, 131	0
3	X	27/48 (56%)	1.15	2 (7%) 20 15	61, 107, 130, 139	0
All	All	2281/2446 (93%)	0.27	67 (2%) 53 43	30, 58, 97, 139	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	897	SER	4.7
2	B	1160	ALA	4.3
1	A	530	ILE	4.2
2	B	538	GLN	4.1
1	A	580	ILE	4.0
1	A	984	VAL	3.6
2	B	149	ALA	3.4
2	B	399	ARG	3.3
1	A	615	SER	3.3
2	B	154	GLY	3.2
1	A	773	ASP	3.1
1	A	1185	GLY	3.1
1	A	608	PRO	3.0
2	B	934	GLY	3.0
2	B	301	PRO	3.0
1	A	285	SER	2.9
1	A	53	ASN	2.9
1	A	928	ARG	2.7
1	A	1177	ARG	2.7
1	A	575	LYS	2.6
1	A	1044	TYR	2.6
1	A	531	ASP	2.6
1	A	171	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	152	TYR	2.6
2	B	871	LEU	2.6
2	B	1156	ILE	2.5
2	B	614	LEU	2.5
2	B	1146	ALA	2.4
1	A	545	LEU	2.4
2	B	821	LEU	2.4
2	B	769	ARG	2.3
1	A	381	ALA	2.3
3	X	44	DT	2.3
1	A	302	LEU	2.3
1	A	887	HIS	2.3
1	A	878	LEU	2.3
1	A	238	LEU	2.3
2	B	966	ASP	2.3
2	B	1114	LYS	2.3
1	A	939	HIS	2.3
2	B	468	ILE	2.3
1	A	284	VAL	2.3
1	A	784	GLN	2.2
1	A	1148	ALA	2.2
1	A	587	ILE	2.2
2	B	804	SER	2.2
1	A	898	ALA	2.2
1	A	500	ILE	2.2
1	A	259	ASP	2.2
1	A	1145	ALA	2.2
1	A	550	PHE	2.1
3	X	12	DC	2.1
2	B	995	ASP	2.1
1	A	578	ARG	2.1
1	A	940	ALA	2.1
2	B	1135	SER	2.1
1	A	900	GLN	2.1
1	A	234	LYS	2.1
2	B	931	LEU	2.0
1	A	1188	GLY	2.0
1	A	601	GLU	2.0
2	B	298	GLU	2.0
2	B	921	LYS	2.0
1	A	566	PRO	2.0
2	B	926	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	103	ARG	2.0
1	A	819	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	X	49	4/4	0.59	0.17	68,79,86,89	0
4	SO4	B	1167	5/5	0.95	0.14	38,40,45,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.