



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:32 PM UTC

PDB ID : 3U44 / pdb_00003u44
Title : Crystal structure of AddAB-DNA complex
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Deposited on : 2011-10-07
Resolution : 3.20 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

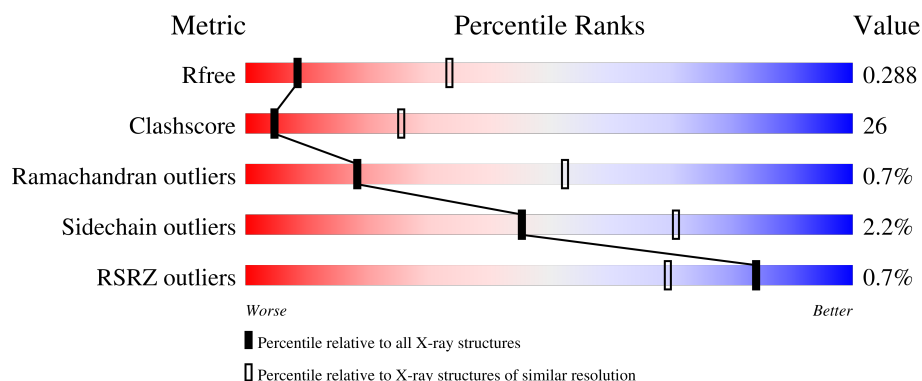
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	51% 39% 9%
2	B	1166	51% 44%
3	X	48	6% 69% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19156 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	1141	Total	C	N	O	S	0	0	0
			9261	5885	1583	1749	44			

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 (36-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	36	Total	C	N	O	P	0	0	0
			730	352	128	216	34			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is water.

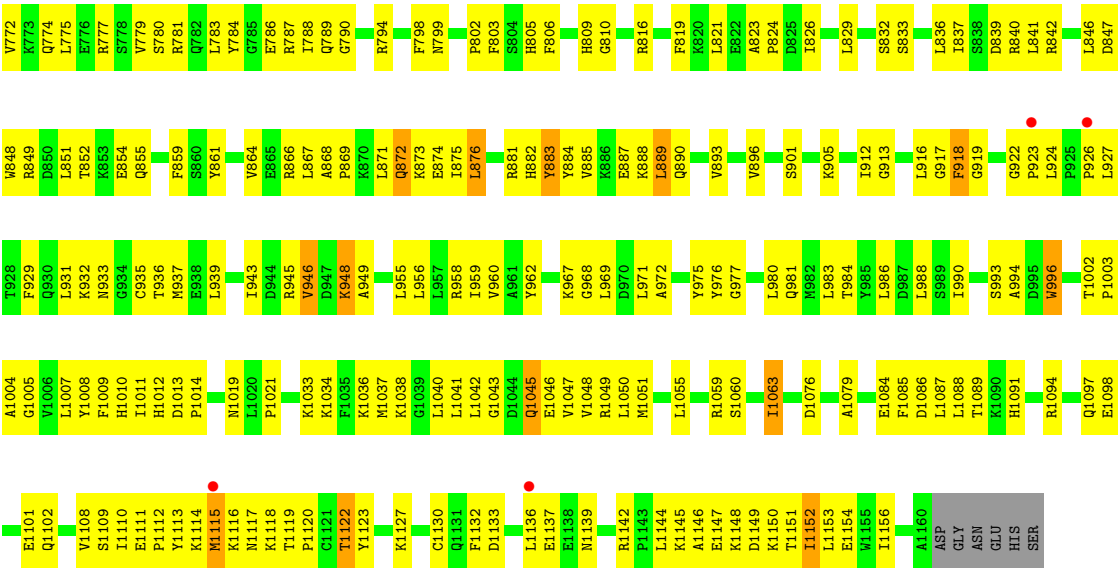
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	22	Total	O	0	0
			22	22		

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.

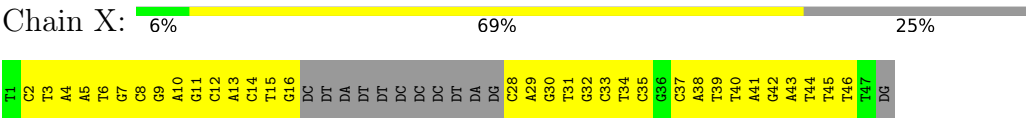
- Chain A: 51% 39% 9%

Chain A	Chain B	Chain C	Chain D	Chain E	Chain F	Chain G	Chain H	Chain I	Chain J	Chain K	Chain L	Chain M	Chain N	Chain O	Chain P	Chain Q	Chain R	Chain S	Chain T	Chain U	Chain V	Chain W	Chain X	Chain Y	Chain Z																																																																																																																																																																																																																																																																																																																																																																																																																																																															
I765	S684	P596	GLU	V181	V182	V183	V184	V187	V188	V189	V190	V191	V192	V198	V207	V208	V209	V213	V214	V215	V216	V217	V218	V219	V220	V221	V226	V227	V228	V229	V230	V231	V232	V233	V236	V237	V238	V239	V243	V244	V245	V246	V247	V248	V249	V250	V251	V252	V253	V254	V255	V256	V257	V258	V259	V260	V261	V262	V263	V264	V265	V266	V267	V268	V269	V270	V271	V272	V273	V274	V275	V276	V277	V278	V279	V280	V281	V282	V283	V284	V285	V286	V287	V288	V289	V290	V291	V292	V293	V294	V295	V296	V297	V298	V299	V300	V301	V302	V303	V304	V311	V312	V315	V316	V317	V318	V319	V320	V321	V324	V325	V326	V327	V328	V329	V332	V333	V334	V335	V338	V339	V340	V341	V342	V343	V344	V345	V346	V347	V348	V349	V350	V351	V352	V356	V360	V365	V366	V367	V368	V369	V370	V378	V379	V380	V381	V382	V383	V384	V387	V388	V389	V390	V391	V392	V393	V394	V395	V398	V401	V402	V403	V406	V407	V415	V416	V417	V418	V419	V422	V423	V424	V425	V428	V432	V433	V434	V435	V436	V437	V438	V439	V440	V441	V442	V443	V444	V445	V448	V449	V453	V454	V455	V456	V457	V458	V459	V460	V461	V462	V468	V469	V470	V471	V472	V473	V474	V475	V476	V477	V478	V479	V484	V488	V489	V490	V491	V492	V493	V494	V495	V496	V497	V498	V499	V500	V501	V502	V503	V506	V507	V508	V509	V510	V511	V512	V513	V514	V515	V516	V517	V518	V519	V520	V521	V522	V523	V524	V525	V526	V527	V528	V529	V530	V531	V532	V533	V534	V535	V536	V537	V538	V539	V540	V541	V542	V543	V544	V545	V546	V547	V548	V549	V550	V551	V552	V553	V554	V555	V556	V557	V558	V559	V560	V561	V562	V563	V564	V565	V566	V567	V568	V569	V570	V571	V572	V573	V574	V575	V576	V577	V578	V579	V580	V581	V582	V583	V584	V585	V586	V587	V588	V589	V590	V591	V592	V593	V594	V595	V596	V597	V598	V599	V600	V601	V602	V603	V604	V605	V606	V607	V608	V609	V610	V611	V616	V617	V618	V619	V620	V621	V622	V625	V628	V629	V632	V633	V636	V637	V638	V639	V640	V641	V642	V643	V644	V645	V646	V647	V648	V649	V650	V651	V652	V653	V654	V655	V656	V657	V658	V659	V660	V661	V662	V666	V667	V668	V669	V670	V671	V672	V673	V674	V675	V676	V677	V678	V679	V680	V681	V682	V683	V684	V685	V686	V687	V688	V689	V690	V691	V692	V693	V694	V695	V696	V697	V698	V699	V700	V701	V702	V703	V704	V705	V706	V707	V710	V711	V712	V713	V714	V715	V719	V723	V726	V727	V728	V729	V730	V731	V732	V736	V737	V738	V739	V740	V741	V742	V748	V751	V752	V753	V754	V755	V756	V757	V758	V759	V760	V761	V762	V763	V764	V765	V766	V767	V768	V769	V770	V771	V772	V773	V774	V775	V776	V777	V778	V779	V780	V781	V782	V783





• Molecule 3: DNA (36-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.23Å 138.96Å 102.97Å 90.00° 105.33° 90.00°	Depositor
Resolution (Å)	29.88 – 3.20 29.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.88-3.20) 99.0 (29.88-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_750)	Depositor
R, R_{free}	0.233 , 0.284 0.232 , 0.288	Depositor DCC
R_{free} test set	2206 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	72.0	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19156	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: SF4

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	0.27	0/9294	0.71	3/12535 (0.0%)
2	B	0.27	0/9448	0.72	8/12732 (0.1%)
3	X	0.14	0/816	0.67	0/1256
All	All	0.27	0/19558	0.71	11/26523 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	616	GLY	N-CA-C	-8.20	103.86	115.43
2	B	1013	ASP	CA-C-N	7.88	127.83	120.03
2	B	1013	ASP	C-N-CA	7.88	127.83	120.03
1	A	216	LEU	CA-C-N	6.49	125.98	119.24
1	A	216	LEU	C-N-CA	6.49	125.98	119.24
2	B	409	THR	N-CA-C	-5.77	106.22	113.20
2	B	80	GLY	N-CA-C	5.54	117.21	111.95
2	B	287	THR	CA-C-N	5.45	124.64	118.97
2	B	287	THR	C-N-CA	5.45	124.64	118.97
2	B	922	GLY	CA-C-N	5.15	125.19	119.32
2	B	922	GLY	C-N-CA	5.15	125.19	119.32

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	460	0
2	B	9261	0	9222	501	0
3	X	730	0	412	63	0
4	B	8	0	0	1	0
5	A	18	0	0	0	0
5	B	22	0	0	0	0
All	All	19156	0	18697	967	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 26.

All (967) 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:845:THR:HG22	1:A:847:PRO:HD2	1.30	1.12
1:A:172:ARG:H	2:B:888:LYS:HD3	1.20	1.04
2:B:864:VAL:HG11	2:B:890:GLN:HG2	1.38	1.01
2:B:972:ALA:HA	2:B:1152:ILE:HD12	1.43	1.01
1:A:243:LEU:HB3	1:A:301:LEU:HD21	1.45	0.99
3:X:30:DG:H2"	3:X:31:DT:H5"	1.43	0.97
2:B:929:PHE:HB2	2:B:937:MET:HB3	1.47	0.96
1:A:901:THR:HG22	1:A:902:ASP:H	1.31	0.95
2:B:347:ILE:HG22	2:B:605:PHE:HB2	1.47	0.94
1:A:379:LEU:HB3	1:A:422:LEU:CD2	1.99	0.93
1:A:705:SER:HB3	1:A:713:LEU:HD22	1.52	0.92
2:B:741:ASP:HA	2:B:744:TRP:HD1	1.37	0.90
1:A:1011:ARG:HD2	2:B:582:PRO:HB2	1.53	0.90
2:B:136:GLU:HG2	2:B:137:PRO:HD2	1.53	0.89
2:B:786:GLU:HG3	2:B:787:ARG:H	1.39	0.88
1:A:403:GLU:HA	1:A:432:ASN:HB2	1.56	0.86
2:B:916:LEU:HD21	2:B:924:LEU:HG	1.55	0.86
1:A:237:LEU:HD11	1:A:312:ALA:HB2	1.55	0.85
1:A:607:ILE:HG13	1:A:608:PRO:HD2	1.57	0.84
1:A:753:THR:HG22	1:A:754:ALA:H	1.42	0.84
2:B:912:ILE:HG13	2:B:913:GLY:H	1.42	0.83
2:B:641:SER:HB3	2:B:645:GLU:HB2	1.60	0.83
2:B:821:LEU:HD22	2:B:875:ILE:HD11	1.58	0.83
1:A:379:LEU:HB3	1:A:422:LEU:HD22	1.59	0.83
1:A:731:PRO:HG2	2:B:1136:LEU:HD23	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ILE:HB	2:B:205:ILE:HG22	1.61	0.82
3:X:33:DC:H2''	3:X:34:DT:H5''	1.62	0.82
2:B:315:MET:HE1	2:B:666:TYR:HD1	1.46	0.81
1:A:727:VAL:HA	1:A:730:MET:HE3	1.64	0.80
1:A:176:ASP:HA	1:A:179:PHE:CZ	2.17	0.80
1:A:48:ILE:HD13	1:A:57:VAL:HG22	1.63	0.79
1:A:326:ARG:HG2	2:B:1021:PRO:HG3	1.65	0.78
1:A:188:SER:HB3	1:A:198:LEU:HD11	1.65	0.78
2:B:931:LEU:HD12	2:B:932:LYS:O	1.85	0.77
1:A:562:LEU:HB3	1:A:580:ILE:HD12	1.67	0.77
1:A:243:LEU:HD22	1:A:301:LEU:HD11	1.66	0.76
1:A:979:ARG:HA	2:B:767:PHE:HZ	1.49	0.76
1:A:584:ASP:HB3	1:A:802:PRO:HG2	1.67	0.76
1:A:954:ILE:HG22	1:A:956:SER:H	1.51	0.75
1:A:869:VAL:O	1:A:873:ARG:HG2	1.85	0.75
2:B:501:LYS:HE3	2:B:560:ILE:O	1.87	0.75
1:A:814:ASN:HD22	3:X:45:DT:H5''	1.52	0.75
2:B:584:ALA:H	2:B:587:GLN:NE2	1.83	0.75
1:A:980:ARG:HG3	1:A:981:GLY:H	1.52	0.74
1:A:581:GLN:O	1:A:786:ASP:HB2	1.87	0.74
2:B:741:ASP:HA	2:B:744:TRP:CD1	2.21	0.74
3:X:30:DG:C2'	3:X:31:DT:H5''	2.17	0.74
2:B:532:ILE:HD12	2:B:532:ILE:H	1.49	0.74
1:A:874:ALA:HB3	1:A:878:LEU:HD11	1.69	0.74
2:B:348:LEU:HD11	2:B:598:MET:HE1	1.70	0.74
1:A:172:ARG:H	2:B:888:LYS:CD	1.98	0.74
1:A:753:THR:HG22	1:A:754:ALA:N	2.03	0.73
2:B:1076:ASP:OD1	3:X:8:DC:H4'	1.88	0.73
2:B:490:LYS:HA	2:B:493:LYS:HE2	1.69	0.73
1:A:529:LEU:HD11	1:A:890:GLN:NE2	2.04	0.72
2:B:205:ILE:HD11	2:B:231:ILE:HD12	1.70	0.72
2:B:298:GLU:HG2	2:B:299:ALA:N	2.04	0.72
1:A:490:PHE:CZ	1:A:927:HIS:HB2	2.25	0.72
1:A:771:ARG:HG3	1:A:772:GLY:H	1.53	0.72
2:B:139:ASP:HA	2:B:142:ARG:HE	1.55	0.71
2:B:393:VAL:HG21	2:B:485:LEU:HD21	1.71	0.71
2:B:1116:LYS:HG2	2:B:1146:ALA:HB2	1.69	0.71
3:X:2:DC:H2''	3:X:3:DT:H71	1.71	0.71
2:B:212:GLN:HA	2:B:258:THR:HG21	1.72	0.71
2:B:170:GLN:O	2:B:174:LYS:HD3	1.90	0.71
1:A:172:ARG:N	2:B:888:LYS:HD3	2.01	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:33:DC:H2''	3:X:34:DT:C5'	2.21	0.71
2:B:68:PHE:HB3	2:B:187:LEU:HD11	1.73	0.70
2:B:84:ARG:HD2	2:B:181:LEU:HD22	1.71	0.70
2:B:669:TYR:CE1	2:B:681:PRO:HG3	2.26	0.70
1:A:394:ALA:HB2	1:A:422:LEU:HD21	1.72	0.70
3:X:6:DT:H2''	3:X:7:DG:H5''	1.73	0.70
1:A:585:ILE:HG22	1:A:803:VAL:HB	1.73	0.70
2:B:977:GLY:HA2	2:B:980:LEU:HD21	1.73	0.70
1:A:335:LEU:HD13	1:A:845:THR:HG21	1.72	0.69
2:B:229:GLU:HG3	2:B:230:HIS:CD2	2.27	0.69
3:X:3:DT:H2''	3:X:4:DA:O5'	1.90	0.69
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.58	0.69
1:A:592:MET:HE2	1:A:792:THR:HG23	1.74	0.69
1:A:825:ASP:HB2	1:A:851:MET:HE3	1.75	0.69
2:B:495:ALA:HB1	2:B:500:GLU:HG3	1.75	0.69
1:A:1141:ILE:O	1:A:1143:PRO:HD3	1.92	0.69
1:A:674:MET:HE1	1:A:694:PHE:HD2	1.58	0.68
1:A:118:LYS:HB3	2:B:620:GLU:HG3	1.76	0.68
2:B:855:GLN:HB3	2:B:859:PHE:CE2	2.28	0.68
2:B:269:LEU:HB3	2:B:271:LEU:CD1	2.24	0.68
2:B:66:PHE:CE1	2:B:74:ARG:HG3	2.27	0.68
2:B:305:TYR:CZ	2:B:307:GLU:HB2	2.28	0.68
2:B:533:GLU:O	2:B:536:GLN:HG2	1.93	0.68
1:A:95:ARG:NH1	2:B:300:ARG:HG2	2.08	0.68
1:A:392:GLU:HA	1:A:395:ARG:HD2	1.74	0.68
2:B:215:PRO:O	2:B:219:ARG:HG2	1.94	0.68
1:A:901:THR:HG22	1:A:902:ASP:N	2.07	0.68
1:A:568:LYS:HB3	1:A:577:HIS:HB3	1.74	0.67
1:A:592:MET:N	1:A:593:PRO:HD3	2.09	0.67
2:B:777:ARG:NH1	2:B:781:ARG:HH21	1.93	0.67
3:X:2:DC:H2''	3:X:3:DT:C7	2.24	0.67
3:X:28:DC:H1'	3:X:29:DA:H5'	1.76	0.67
1:A:1139:LYS:HE2	1:A:1148:ALA:O	1.93	0.67
2:B:139:ASP:HA	2:B:142:ARG:NE	2.08	0.67
2:B:683:MET:HB2	2:B:687:ARG:HH12	1.59	0.67
1:A:555:ILE:HG12	1:A:881:ILE:HD12	1.77	0.67
1:A:1219:CYS:SG	1:A:1232:LEU:HB2	2.35	0.67
1:A:797:LYS:O	1:A:873:ARG:HD2	1.95	0.67
2:B:1045:GLN:HE21	2:B:1049:ARG:HH21	1.42	0.67
1:A:1000:TRP:CD2	2:B:336:ARG:HD3	2.29	0.67
1:A:1002:TYR:HB3	1:A:1005:GLN:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ILE:HD12	1:A:878:LEU:HD13	1.76	0.66
1:A:565:SER:OG	1:A:566:PRO:HD2	1.95	0.66
2:B:1115:MET:CB	2:B:1144:LEU:HB2	2.25	0.66
1:A:188:SER:CB	1:A:198:LEU:HD11	2.24	0.66
2:B:202:GLY:HA2	2:B:229:GLU:HB2	1.77	0.66
1:A:50:ALA:O	1:A:54:PRO:HG3	1.95	0.66
2:B:946:VAL:HG12	2:B:959:ILE:HG12	1.77	0.66
2:B:36:ILE:HG23	2:B:66:PHE:HD2	1.61	0.66
2:B:97:ARG:HH21	2:B:117:SER:HA	1.61	0.66
1:A:500:ILE:HD11	1:A:860:LEU:HD23	1.78	0.66
2:B:948:LYS:HG3	2:B:955:LEU:HD11	1.77	0.66
1:A:137:GLU:OE1	1:A:753:THR:HG23	1.96	0.65
1:A:444:TYR:O	1:A:449:ALA:HB3	1.95	0.65
2:B:298:GLU:HG2	2:B:299:ALA:H	1.59	0.65
1:A:379:LEU:HB3	1:A:422:LEU:HD21	1.75	0.65
1:A:980:ARG:HA	2:B:760:LYS:NZ	2.11	0.65
1:A:1148:ALA:HB1	1:A:1150:GLU:OE1	1.97	0.65
1:A:257:PHE:O	1:A:261:LEU:HB2	1.97	0.65
2:B:182:HIS:CE1	2:B:184:GLU:HG2	2.32	0.65
1:A:232:GLY:O	1:A:236:LYS:HB2	1.98	0.64
1:A:979:ARG:HA	2:B:767:PHE:CZ	2.31	0.64
1:A:1160:CYS:HB3	1:A:1171:LEU:HB3	1.78	0.64
1:A:146:LEU:HD13	1:A:178:GLN:HB2	1.78	0.64
1:A:826:LYS:HG3	1:A:827:GLU:H	1.63	0.64
1:A:1050:MET:SD	2:B:503:GLU:HG3	2.37	0.64
2:B:852:THR:OG1	2:B:854:GLU:HG2	1.96	0.64
2:B:958:ARG:HH21	2:B:1051:MET:HE3	1.60	0.64
1:A:27:LEU:HD11	1:A:454:PHE:CE1	2.33	0.64
2:B:226:VAL:HG22	2:B:269:LEU:HD21	1.79	0.64
3:X:32:DG:H2''	3:X:33:DC:O5'	1.97	0.64
2:B:551:PHE:HE1	2:B:555:MET:HE3	1.62	0.64
2:B:798:PHE:HD1	2:B:805:HIS:HD1	1.46	0.64
2:B:1007:LEU:HD11	2:B:1051:MET:CE	2.26	0.64
2:B:207:VAL:HG22	2:B:233:PHE:HA	1.80	0.64
1:A:1051:MET:HG2	1:A:1052:LYS:H	1.62	0.64
2:B:864:VAL:HG11	2:B:890:GLN:CG	2.22	0.63
1:A:213:ILE:HD11	1:A:274:PHE:HB3	1.81	0.63
1:A:1049:PHE:CD2	2:B:552:VAL:HG21	2.33	0.63
2:B:4:GLU:HB3	2:B:232:THR:HG22	1.80	0.63
2:B:562:LEU:HD12	2:B:563:ASP:N	2.12	0.63
2:B:840:ARG:NH1	2:B:866:ARG:HH22	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:10:DA:H2''	3:X:11:DG:C8	2.33	0.63
1:A:134:ASP:OD1	1:A:137:GLU:HG2	1.99	0.63
1:A:640:ILE:HB	1:A:641:PRO:HD3	1.78	0.63
1:A:1067:VAL:HG21	1:A:1103:ILE:HD13	1.80	0.63
2:B:140:ILE:HG22	2:B:166:SER:HB2	1.81	0.63
2:B:1037:MET:HB2	2:B:1063:ILE:HD12	1.79	0.63
3:X:15:DT:H2''	3:X:16:DG:C5'	2.28	0.63
1:A:874:ALA:CB	1:A:878:LEU:HD11	2.29	0.63
1:A:1007:VAL:O	1:A:1010:ILE:HG22	1.99	0.63
2:B:100:ILE:O	2:B:104:LYS:HB2	1.99	0.63
1:A:767:ARG:O	1:A:770:GLU:HG2	1.98	0.62
1:A:887:HIS:O	1:A:890:GLN:HG2	2.00	0.62
2:B:967:LYS:HG3	2:B:1038:LYS:HZ1	1.64	0.62
3:X:4:DA:H2''	3:X:5:DA:O5'	1.99	0.62
1:A:593:PRO:HG2	1:A:811:ARG:HH12	1.64	0.62
1:A:973:GLU:CD	1:A:973:GLU:H	2.06	0.62
2:B:769:ARG:HG3	2:B:771:GLU:HG2	1.81	0.62
3:X:28:DC:H2''	3:X:29:DA:H5'	1.82	0.62
1:A:983:PRO:HD3	2:B:747:TYR:CE2	2.35	0.62
2:B:386:PHE:HE1	2:B:412:LEU:HG	1.65	0.62
1:A:495:LEU:HD11	1:A:923:ALA:HB2	1.82	0.62
3:X:32:DG:H4'	3:X:32:DG:OP1	1.99	0.62
2:B:642:GLY:HA2	2:B:646:ARG:NE	2.14	0.61
2:B:1041:LEU:HD21	2:B:1051:MET:HE1	1.81	0.61
1:A:602:LEU:HB2	1:A:609:VAL:HG21	1.80	0.61
1:A:723:TYR:O	1:A:727:VAL:HG23	2.00	0.61
1:A:398:GLN:HB3	1:A:425:SER:HB3	1.83	0.61
1:A:926:ARG:HG2	1:A:942:ILE:HD13	1.81	0.61
1:A:748:ARG:O	1:A:751:GLU:HG2	2.00	0.61
1:A:165:VAL:O	1:A:169:THR:HG22	1.99	0.61
2:B:931:LEU:HB3	2:B:1097:GLN:OE1	2.00	0.61
1:A:600:GLU:O	1:A:603:ARG:HG2	2.01	0.61
2:B:96:LEU:O	2:B:100:ILE:HG23	2.00	0.61
2:B:916:LEU:HB3	2:B:943:ILE:HB	1.83	0.61
2:B:927:LEU:HD11	2:B:929:PHE:CE1	2.36	0.61
1:A:738:ALA:O	1:A:742:VAL:HG13	2.01	0.61
1:A:636:PRO:HD2	2:B:427:ASP:OD2	2.00	0.60
2:B:269:LEU:O	2:B:271:LEU:HD12	2.01	0.60
1:A:1209:GLU:HG2	1:A:1215:LYS:HA	1.82	0.60
2:B:849:ARG:HB2	2:B:905:LYS:HG2	1.82	0.60
1:A:587:ILE:HG22	1:A:805:PHE:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ALA:O	2:B:116:LYS:HG2	2.02	0.60
2:B:971:LEU:HD12	2:B:1149:ASP:HB3	1.82	0.60
2:B:1145:LYS:O	2:B:1147:GLU:HG2	2.01	0.60
3:X:28:DC:C2'	3:X:29:DA:H5'	2.32	0.60
1:A:659:SER:HB2	2:B:783:LEU:HD22	1.82	0.60
1:A:595:ALA:HA	1:A:790:LEU:HD21	1.84	0.60
1:A:867:LEU:HD21	1:A:920:ILE:HD11	1.82	0.60
2:B:635:ILE:O	2:B:635:ILE:HG22	2.01	0.60
2:B:187:LEU:HB3	2:B:216:GLN:HG2	1.82	0.60
1:A:942:ILE:HD12	1:A:943:SER:N	2.17	0.60
2:B:138:GLU:O	2:B:142:ARG:HG3	2.01	0.60
2:B:861:TYR:O	2:B:864:VAL:HG12	2.01	0.60
3:X:9:DG:H2''	3:X:10:DA:H5''	1.83	0.60
2:B:222:GLU:HA	2:B:225:MET:HE2	1.84	0.60
2:B:931:LEU:HG	2:B:935:CYS:HB3	1.83	0.60
1:A:576:THR:HB	1:A:578:ARG:HH22	1.67	0.59
1:A:282:PRO:HA	1:A:320:LYS:HD2	1.83	0.59
1:A:545:LEU:O	1:A:548:VAL:HG12	2.01	0.59
2:B:483:PRO:HB2	2:B:484:PRO:HD3	1.85	0.59
2:B:912:ILE:HG13	2:B:946:VAL:HG23	1.84	0.59
3:X:34:DT:H2''	3:X:35:DC:H5'	1.84	0.59
1:A:622:GLU:HA	1:A:723:TYR:OH	2.02	0.59
1:A:656:ASN:O	1:A:660:LEU:HB2	2.02	0.59
2:B:97:ARG:HH11	2:B:568:MET:HE3	1.66	0.59
2:B:1055:LEU:HD22	2:B:1060:SER:HB2	1.83	0.59
1:A:772:GLY:O	1:A:773:ASP:CG	2.45	0.59
2:B:1009:PHE:HD2	2:B:1037:MET:HE2	1.65	0.59
2:B:1152:ILE:O	2:B:1156:ILE:HG12	2.02	0.59
1:A:137:GLU:O	1:A:141:ILE:HG13	2.02	0.59
2:B:237:ALA:HA	2:B:252:PHE:CD1	2.38	0.59
2:B:917:GLY:HA3	2:B:923:PRO:HD2	1.84	0.59
1:A:82:GLU:OE2	1:A:98:LEU:HD21	2.03	0.59
1:A:1071:ILE:HG21	1:A:1112:PHE:CZ	2.38	0.59
1:A:379:LEU:HD13	1:A:422:LEU:HD22	1.85	0.59
2:B:912:ILE:HG13	2:B:913:GLY:N	2.16	0.58
1:A:95:ARG:HH12	2:B:300:ARG:HG2	1.66	0.58
1:A:1000:TRP:CE2	2:B:336:ARG:HG2	2.39	0.58
2:B:784:TYR:HB3	2:B:788:ILE:CD1	2.33	0.58
1:A:61:LEU:HB2	1:A:401:PHE:CD1	2.39	0.58
2:B:144:ALA:O	2:B:159:SER:HB2	2.03	0.58
2:B:876:LEU:HA	2:B:882:HIS:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:43:DA:H2''	3:X:44:DT:H5'	1.85	0.58
1:A:586:VAL:HG11	1:A:801:PHE:CD2	2.38	0.58
1:A:730:MET:C	2:B:731:ARG:HD3	2.29	0.58
2:B:336:ARG:NH2	2:B:717:VAL:HA	2.18	0.58
1:A:22:THR:HG22	1:A:23:GLY:N	2.19	0.58
1:A:41:VAL:HG12	1:A:45:ILE:HD11	1.84	0.58
1:A:1071:ILE:HG21	1:A:1112:PHE:HZ	1.66	0.58
2:B:650:GLU:O	2:B:654:ILE:HG23	2.04	0.58
2:B:497:THR:HA	2:B:559:GLU:HA	1.86	0.58
2:B:501:LYS:HE3	2:B:561:SER:HA	1.86	0.58
1:A:479:ARG:NH2	1:A:800:GLU:OE2	2.37	0.58
1:A:685:ASP:O	1:A:689:GLN:HG2	2.03	0.58
1:A:1136:LEU:O	1:A:1151:PRO:HA	2.04	0.58
1:A:1190:ALA:HB3	1:A:1191:PRO:HD3	1.85	0.58
2:B:491:ARG:O	2:B:494:LYS:HG2	2.04	0.58
2:B:1116:LYS:O	2:B:1117:ASN:HB2	2.04	0.58
1:A:170:THR:O	1:A:170:THR:HG23	2.03	0.58
1:A:731:PRO:HD3	2:B:731:ARG:NH1	2.19	0.58
2:B:747:TYR:O	2:B:751:MET:HG2	2.03	0.58
1:A:527:LEU:HA	1:A:880:LEU:O	2.05	0.57
2:B:486:PHE:CZ	2:B:490:LYS:HE2	2.39	0.57
1:A:753:THR:CG2	1:A:754:ALA:H	2.16	0.57
2:B:784:TYR:HB3	2:B:788:ILE:HD11	1.86	0.57
1:A:102:ASN:HB2	2:B:647:LEU:HD21	1.86	0.57
1:A:611:ALA:HB2	1:A:790:LEU:HB3	1.87	0.57
1:A:75:HIS:CD2	2:B:686:LYS:HD2	2.40	0.57
1:A:556:ALA:HB2	1:A:602:LEU:CD2	2.34	0.57
1:A:668:ALA:HB1	1:A:672:GLU:OE2	2.04	0.57
2:B:141:ARG:HG2	2:B:166:SER:OG	2.05	0.57
2:B:305:TYR:CE2	2:B:307:GLU:HB2	2.39	0.57
2:B:1114:LYS:HA	2:B:1118:LYS:O	2.04	0.57
1:A:982:GLU:HA	2:B:747:TYR:HE2	1.70	0.57
1:A:176:ASP:HA	1:A:179:PHE:CE2	2.40	0.57
1:A:978:ILE:HA	2:B:747:TYR:OH	2.05	0.57
1:A:560:ARG:HA	1:A:563:ILE:HG12	1.87	0.56
3:X:15:DT:H3	3:X:29:DA:H61	1.51	0.56
1:A:281:VAL:HB	1:A:282:PRO:HD3	1.88	0.56
2:B:204:HIS:HD2	2:B:230:HIS:HB2	1.69	0.56
2:B:315:MET:HE1	2:B:666:TYR:CD1	2.34	0.56
3:X:11:DG:H2''	3:X:12:DC:H5''	1.87	0.56
1:A:584:ASP:O	1:A:802:PRO:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:769:ARG:O	2:B:771:GLU:HG2	2.05	0.56
3:X:33:DC:C2'	3:X:34:DT:H5''	2.33	0.56
1:A:229:VAL:HG21	1:A:319:LEU:HD13	1.86	0.56
1:A:901:THR:O	1:A:902:ASP:HB2	2.05	0.56
1:A:1067:VAL:HG11	1:A:1108:ILE:HD13	1.87	0.56
2:B:222:GLU:HG3	2:B:265:LYS:HE2	1.87	0.56
1:A:1014:GLN:HE22	1:A:1142:TYR:HE2	1.53	0.56
1:A:1051:MET:HG2	1:A:1052:LYS:N	2.21	0.56
2:B:609:ALA:HB3	2:B:669:TYR:HB3	1.87	0.56
1:A:255:ASP:CG	1:A:256:ASN:H	2.13	0.56
2:B:97:ARG:O	2:B:101:GLU:HG2	2.06	0.56
2:B:786:GLU:HG3	2:B:787:ARG:N	2.16	0.56
2:B:872:GLN:O	2:B:875:ILE:HG23	2.06	0.56
3:X:10:DA:H2''	3:X:11:DG:H8	1.70	0.56
1:A:170:THR:HG22	1:A:176:ASP:OD2	2.06	0.56
1:A:594:TRP:HB3	1:A:598:ILE:CD1	2.35	0.56
1:A:901:THR:CG2	1:A:902:ASP:H	2.13	0.56
1:A:118:LYS:HD3	2:B:620:GLU:HB3	1.87	0.56
2:B:623:VAL:HG12	2:B:624:LEU:HD12	1.87	0.56
3:X:28:DC:C1'	3:X:29:DA:H5'	2.36	0.56
1:A:1073:LEU:HD12	1:A:1126:LYS:HD3	1.87	0.55
2:B:683:MET:CB	2:B:687:ARG:HH12	2.19	0.55
1:A:394:ALA:CB	1:A:422:LEU:HD21	2.36	0.55
2:B:102:GLU:HG3	2:B:103:HIS:ND1	2.21	0.55
2:B:158:LEU:HA	2:B:161:LYS:HD2	1.89	0.55
2:B:205:ILE:HG13	2:B:231:ILE:HG13	1.89	0.55
2:B:873:LYS:O	2:B:874:GLU:HG2	2.05	0.55
1:A:140:LEU:HD22	1:A:755:PHE:CZ	2.42	0.55
1:A:146:LEU:HG	1:A:352:TYR:CE1	2.41	0.55
2:B:1086:ASP:HA	2:B:1089:THR:HG22	1.87	0.55
1:A:161:PHE:O	1:A:165:VAL:HG23	2.07	0.55
1:A:1004:HIS:O	1:A:1007:VAL:HG12	2.06	0.55
2:B:1148:LYS:HB2	2:B:1151:THR:HG23	1.88	0.55
2:B:769:ARG:HG3	2:B:771:GLU:CG	2.36	0.55
2:B:881:ARG:O	2:B:885:VAL:HG23	2.06	0.55
1:A:494:GLN:HA	1:A:904:LEU:HA	1.88	0.55
2:B:541:TRP:O	2:B:544:VAL:HG22	2.06	0.55
1:A:592:MET:HE1	1:A:791:MET:HA	1.88	0.55
1:A:1047:PRO:HB3	1:A:1049:PHE:CE2	2.42	0.55
1:A:1221:LEU:HB2	1:A:1230:LEU:CD2	2.37	0.55
1:A:356:PHE:CZ	1:A:360:LYS:HE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:LEU:HD22	2:B:846:LEU:HD22	1.87	0.55
3:X:11:DG:H2''	3:X:12:DC:C5'	2.37	0.55
3:X:41:DA:H2'	3:X:42:DG:C8	2.42	0.55
2:B:326:GLY:HA2	2:B:329:ARG:NH1	2.22	0.55
2:B:840:ARG:HH11	2:B:866:ARG:HH22	1.55	0.54
2:B:563:ASP:O	2:B:567:GLN:HG3	2.06	0.54
1:A:607:ILE:CG1	1:A:608:PRO:HD2	2.32	0.54
2:B:477:THR:HA	2:B:480:TRP:NE1	2.21	0.54
1:A:133:ALA:HB1	1:A:137:GLU:HG3	1.90	0.54
1:A:339:LYS:HB3	1:A:340:PRO:HD3	1.90	0.54
1:A:731:PRO:HG2	2:B:1136:LEU:CD2	2.33	0.54
1:A:800:GLU:O	1:A:801:PHE:CD1	2.60	0.54
2:B:19:ILE:HG23	2:B:51:LEU:HD23	1.89	0.54
2:B:614:LEU:HB3	2:B:615:PRO:CD	2.38	0.54
2:B:707:VAL:HG12	2:B:708:SER:H	1.73	0.54
2:B:1045:GLN:NE2	2:B:1049:ARG:HH21	2.04	0.54
3:X:41:DA:H2''	3:X:42:DG:C5'	2.38	0.54
1:A:282:PRO:HG3	1:A:324:PHE:HB3	1.89	0.54
1:A:991:ASP:HA	2:B:745:SER:HB3	1.88	0.54
2:B:419:LYS:HG3	2:B:420:ALA:N	2.22	0.54
1:A:16:TRP:CZ2	1:A:20:VAL:HG21	2.42	0.54
1:A:924:LEU:HD11	1:A:949:PHE:CE1	2.42	0.54
2:B:956:LEU:HD23	2:B:1002:THR:HG23	1.89	0.54
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.22	0.54
2:B:110:TYR:OH	2:B:161:LYS:HE2	2.08	0.54
2:B:642:GLY:HA2	2:B:646:ARG:CZ	2.38	0.54
1:A:171:ASP:O	1:A:172:ARG:CB	2.56	0.54
1:A:581:GLN:C	1:A:583:ARG:H	2.16	0.54
1:A:974:ARG:O	1:A:978:ILE:HG13	2.08	0.54
2:B:158:LEU:HD12	2:B:628:ASP:OD2	2.08	0.54
2:B:735:ARG:O	2:B:736:GLU:HB2	2.06	0.54
1:A:501:GLY:C	1:A:503:VAL:H	2.15	0.54
2:B:110:TYR:OH	2:B:623:VAL:HG13	2.08	0.54
2:B:321:ARG:HA	2:B:358:MET:SD	2.48	0.54
2:B:932:LYS:O	2:B:933:ASN:OD1	2.26	0.54
1:A:213:ILE:HD11	1:A:274:PHE:CB	2.37	0.53
1:A:507:GLU:HA	1:A:507:GLU:OE1	2.07	0.53
1:A:809:LEU:O	1:A:917:LEU:HG	2.07	0.53
2:B:190:LEU:O	2:B:194:ILE:HG13	2.09	0.53
2:B:660:SER:OG	2:B:661:PRO:HD3	2.08	0.53
1:A:580:ILE:HG22	1:A:582:TYR:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:559:GLU:N	2:B:559:GLU:OE1	2.41	0.53
1:A:184:VAL:HG22	1:A:824:LEU:HD21	1.91	0.53
1:A:1112:PHE:HD1	1:A:1121:ILE:HD11	1.73	0.53
2:B:66:PHE:HE1	2:B:74:ARG:HG3	1.72	0.53
2:B:1051:MET:HE2	2:B:1063:ILE:HG12	1.91	0.53
1:A:321:THR:HA	1:A:325:THR:HG23	1.89	0.53
2:B:747:TYR:CE2	2:B:751:MET:HG3	2.42	0.53
1:A:140:LEU:HD22	1:A:755:PHE:HZ	1.73	0.53
1:A:555:ILE:HG23	1:A:805:PHE:CD2	2.44	0.53
1:A:1194:LYS:O	1:A:1198:GLU:HB2	2.09	0.53
2:B:131:LYS:HZ3	2:B:169:TYR:HE1	1.55	0.53
2:B:525:ALA:HB3	2:B:534:ALA:HB2	1.89	0.53
1:A:127:ASP:HA	2:B:116:LYS:HD3	1.90	0.53
2:B:846:LEU:HD23	2:B:847:ASP:N	2.24	0.53
2:B:848:TRP:O	2:B:851:LEU:HB2	2.09	0.53
1:A:93:HIS:O	1:A:97:GLN:HG2	2.08	0.53
2:B:494:LYS:HG3	2:B:495:ALA:N	2.24	0.53
1:A:569:VAL:O	1:A:577:HIS:HA	2.09	0.53
2:B:958:ARG:HB3	2:B:1004:ALA:HB3	1.91	0.53
3:X:37:DC:H2''	3:X:38:DA:H5'	1.91	0.53
1:A:213:ILE:HD12	1:A:214:GLU:N	2.24	0.52
2:B:1047:VAL:O	2:B:1051:MET:HG3	2.08	0.52
2:B:536:GLN:HB2	2:B:578:PHE:CZ	2.44	0.52
2:B:470:MET:O	2:B:474:LEU:HD13	2.10	0.52
2:B:945:ARG:HH21	2:B:960:VAL:HG21	1.74	0.52
1:A:237:LEU:HD22	1:A:264:ILE:HD12	1.91	0.52
2:B:612:GLY:HA2	2:B:617:ARG:CZ	2.40	0.52
2:B:772:VAL:HG21	2:B:1110:ILE:HG13	1.90	0.52
1:A:731:PRO:CG	2:B:1136:LEU:HD23	2.37	0.52
1:A:1000:TRP:CG	2:B:336:ARG:HD3	2.43	0.52
2:B:34:PRO:HG2	2:B:199:ASP:O	2.09	0.52
2:B:593:MET:HE2	2:B:654:ILE:HG22	1.90	0.52
1:A:1047:PRO:HD3	2:B:506:TYR:CE1	2.45	0.52
2:B:981:GLN:O	2:B:984:THR:HG22	2.10	0.52
2:B:1033:LYS:O	2:B:1036:LYS:HB2	2.09	0.52
1:A:529:LEU:HD21	1:A:884:CYS:SG	2.49	0.52
2:B:72:ALA:O	2:B:76:LEU:HG	2.10	0.52
2:B:745:SER:O	2:B:749:VAL:HG23	2.10	0.52
1:A:806:VAL:CG2	1:A:880:LEU:HD23	2.40	0.52
2:B:495:ALA:O	2:B:501:LYS:HE2	2.10	0.52
2:B:772:VAL:HG12	2:B:1108:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:871:LEU:HD23	2:B:872:GLN:CB	2.40	0.52
1:A:484:ILE:HD11	1:A:876:GLU:O	2.10	0.51
2:B:225:MET:HE1	2:B:265:LYS:HG3	1.92	0.51
2:B:672:ALA:O	2:B:679:LEU:HD12	2.10	0.51
2:B:986:LEU:HD21	2:B:1003:PRO:HB3	1.92	0.51
1:A:594:TRP:HB3	1:A:598:ILE:HD13	1.91	0.51
2:B:182:HIS:HE1	2:B:184:GLU:HG2	1.73	0.51
2:B:787:ARG:HA	2:B:936:THR:OG1	2.10	0.51
2:B:832:SER:O	2:B:836:LEU:HB2	2.10	0.51
1:A:763:ARG:O	1:A:767:ARG:HG2	2.10	0.51
2:B:137:PRO:HG3	2:B:169:TYR:CD1	2.45	0.51
2:B:1086:ASP:HA	2:B:1089:THR:CG2	2.40	0.51
1:A:109:LEU:HD23	1:A:416:GLN:HG2	1.93	0.51
1:A:490:PHE:HZ	1:A:927:HIS:HB2	1.76	0.51
1:A:62:VAL:HB	1:A:106:ILE:HG12	1.93	0.51
1:A:697:HIS:HB3	1:A:701:TRP:CZ2	2.46	0.51
1:A:832:THR:C	1:A:848:LEU:HD12	2.35	0.51
1:A:908:PHE:O	1:A:911:TYR:HB3	2.11	0.51
1:A:698:LEU:O	1:A:702:ARG:HG2	2.11	0.51
1:A:715:TRP:CE2	2:B:361:GLU:HB3	2.46	0.51
1:A:739:ASN:O	1:A:742:VAL:HG22	2.10	0.51
2:B:794:ARG:HG3	2:B:809:HIS:CD2	2.46	0.51
1:A:173:HIS:HD2	1:A:175:LEU:H	1.58	0.51
1:A:1013:LYS:HE3	1:A:1030:SER:HB3	1.93	0.51
2:B:531:ILE:N	2:B:531:ILE:HD12	2.26	0.51
2:B:718:ASN:HB3	2:B:721:VAL:HG22	1.93	0.51
2:B:1150:LYS:O	2:B:1154:GLU:OE1	2.28	0.51
1:A:190:SER:HB3	1:A:448:LEU:HD23	1.93	0.51
1:A:939:HIS:HA	1:A:942:ILE:HG12	1.93	0.51
1:A:107:SER:HB2	1:A:111:SER:HB3	1.93	0.51
2:B:635:ILE:O	2:B:635:ILE:CG2	2.58	0.51
1:A:657:GLU:HB3	1:A:687:LEU:HD13	1.92	0.50
2:B:200:ILE:C	2:B:200:ILE:HD12	2.37	0.50
1:A:618:PHE:CG	1:A:769:GLN:HG2	2.47	0.50
1:A:826:LYS:HG3	1:A:827:GLU:N	2.27	0.50
2:B:806:PHE:HB2	2:B:1108:VAL:HG12	1.91	0.50
2:B:1091:HIS:HA	2:B:1094:ARG:HH11	1.76	0.50
1:A:137:GLU:CD	1:A:753:THR:HG23	2.36	0.50
1:A:810:GLY:HA3	1:A:883:SER:H	1.77	0.50
1:A:1112:PHE:CD1	1:A:1121:ILE:HD11	2.46	0.50
2:B:1115:MET:CG	2:B:1144:LEU:HB2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:29:DA:H2''	3:X:30:DG:OP2	2.11	0.50
1:A:555:ILE:HD11	1:A:807:ALA:HB2	1.93	0.50
1:A:576:THR:HG22	1:A:577:HIS:N	2.26	0.50
1:A:759:PHE:HE2	1:A:763:ARG:CZ	2.24	0.50
1:A:1002:TYR:HD2	1:A:1005:GLN:HA	1.76	0.50
1:A:1209:GLU:HA	1:A:1214:THR:O	2.11	0.50
2:B:319:ASN:OD1	2:B:321:ARG:HB2	2.12	0.50
1:A:586:VAL:HG11	1:A:801:PHE:HD2	1.75	0.50
2:B:44:THR:HB	2:B:70:ARG:NH1	2.27	0.50
2:B:212:GLN:NE2	2:B:258:THR:HG23	2.27	0.50
2:B:326:GLY:HA2	2:B:329:ARG:HH11	1.77	0.50
1:A:41:VAL:O	1:A:45:ILE:HG13	2.12	0.50
1:A:190:SER:CB	1:A:448:LEU:HD23	2.42	0.50
2:B:441:ASP:HB3	2:B:445:LYS:HD3	1.94	0.50
2:B:1046:GLU:HG2	2:B:1050:LEU:HD13	1.94	0.50
1:A:300:ALA:O	1:A:304:GLU:HB3	2.12	0.50
2:B:197:ALA:O	2:B:200:ILE:HG13	2.12	0.50
3:X:11:DG:C2'	3:X:12:DC:H5''	2.42	0.50
1:A:169:THR:OG1	1:A:174:ASP:HA	2.12	0.49
1:A:366:ILE:HB	1:A:370:ASP:HB2	1.94	0.49
1:A:530:ILE:HD11	1:A:554:ALA:HB2	1.93	0.49
1:A:730:MET:HB2	1:A:731:PRO:HD2	1.94	0.49
2:B:269:LEU:C	2:B:270:ASN:OD1	2.54	0.49
2:B:1116:LYS:CG	2:B:1146:ALA:HB2	2.37	0.49
3:X:13:DA:H8	3:X:13:DA:H5'	1.77	0.49
1:A:367:ASP:CG	1:A:368:PHE:H	2.19	0.49
1:A:671:TYR:O	1:A:674:MET:HB3	2.11	0.49
1:A:825:ASP:CB	1:A:851:MET:HE3	2.40	0.49
2:B:7:VAL:HG12	2:B:235:LEU:HB2	1.94	0.49
2:B:901:SER:O	2:B:905:LYS:HG3	2.11	0.49
2:B:1147:GLU:HB3	2:B:1151:THR:OG1	2.12	0.49
1:A:556:ALA:HB2	1:A:602:LEU:HD23	1.94	0.49
1:A:595:ALA:O	1:A:599:MET:HG3	2.12	0.49
2:B:543:ALA:HB1	2:B:576:LEU:HD22	1.94	0.49
2:B:837:ILE:O	2:B:841:LEU:HG	2.13	0.49
2:B:958:ARG:NH2	2:B:1051:MET:HE3	2.27	0.49
1:A:335:LEU:HD13	1:A:845:THR:CG2	2.40	0.49
2:B:181:LEU:CD2	2:B:186:TYR:HE1	2.25	0.49
2:B:913:GLY:H	2:B:946:VAL:HG23	1.77	0.49
3:X:14:DC:H2''	3:X:15:DT:O4'	2.12	0.49
1:A:560:ARG:O	1:A:563:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ARG:HD2	2:B:568:MET:HE3	1.95	0.49
1:A:560:ARG:HA	1:A:563:ILE:CG1	2.42	0.49
1:A:703:ALA:O	1:A:706:LYS:HB3	2.11	0.49
3:X:3:DT:H71	3:X:3:DT:OP2	2.13	0.49
1:A:567:PHE:HD2	1:A:580:ILE:HD11	1.77	0.49
1:A:654:ASP:HB2	1:A:657:GLU:HG3	1.94	0.49
2:B:136:GLU:HG2	2:B:137:PRO:CD	2.35	0.49
2:B:692:PHE:HB3	2:B:695:HIS:CG	2.47	0.49
2:B:976:TYR:CE2	2:B:1144:LEU:HB3	2.48	0.49
1:A:167:ARG:HG2	1:A:835:ILE:HB	1.95	0.49
1:A:218:PHE:CE2	1:A:847:PRO:HG3	2.48	0.49
1:A:773:ASP:OD1	1:A:773:ASP:C	2.55	0.49
2:B:551:PHE:CE1	2:B:555:MET:HE3	2.46	0.49
2:B:896:VAL:HG21	2:B:1011:ILE:HG23	1.93	0.49
1:A:24:GLN:HE21	1:A:470:ARG:CB	2.26	0.49
1:A:595:ALA:N	1:A:596:PRO:HD2	2.28	0.49
1:A:638:GLN:CD	2:B:816:ARG:HH21	2.20	0.49
2:B:97:ARG:O	2:B:100:ILE:HG12	2.13	0.49
2:B:614:LEU:HB3	2:B:615:PRO:HD3	1.93	0.49
1:A:173:HIS:C	1:A:173:HIS:CD2	2.91	0.49
1:A:230:LEU:HD12	1:A:271:GLN:HG2	1.94	0.49
1:A:1139:LYS:HE3	1:A:1146:HIS:C	2.38	0.49
2:B:366:TYR:CD2	2:B:717:VAL:HG21	2.47	0.49
2:B:847:ASP:OD1	2:B:848:TRP:N	2.46	0.49
2:B:819:PHE:CE1	2:B:875:ILE:HG22	2.48	0.48
1:A:268:ILE:HA	1:A:271:GLN:HG3	1.95	0.48
2:B:395:LYS:C	2:B:397:ASN:H	2.21	0.48
2:B:481:ILE:O	2:B:484:PRO:HD2	2.13	0.48
2:B:823:ALA:N	2:B:824:PRO:CD	2.76	0.48
1:A:360:LYS:HB3	1:A:365:ILE:HG13	1.94	0.48
2:B:158:LEU:C	2:B:158:LEU:HD23	2.39	0.48
2:B:933:ASN:OD1	2:B:933:ASN:O	2.31	0.48
1:A:311:GLY:O	1:A:315:LEU:HG	2.12	0.48
1:A:479:ARG:HH21	1:A:800:GLU:CD	2.21	0.48
2:B:265:LYS:O	2:B:269:LEU:HB2	2.12	0.48
2:B:441:ASP:O	2:B:445:LYS:HG2	2.13	0.48
2:B:949:ALA:O	2:B:956:LEU:HB2	2.13	0.48
2:B:984:THR:O	2:B:988:LEU:HD13	2.13	0.48
2:B:1112:PRO:HG3	4:B:1167:SF4:S4	2.54	0.48
1:A:127:ASP:O	1:A:130:PHE:HB3	2.13	0.48
1:A:216:LEU:HD13	1:A:218:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ALA:O	1:A:389:GLU:HB2	2.13	0.48
1:A:567:PHE:CD2	1:A:580:ILE:HD11	2.48	0.48
1:A:826:LYS:CG	1:A:827:GLU:H	2.26	0.48
2:B:489:GLN:O	2:B:493:LYS:HG2	2.14	0.48
2:B:962:TYR:HB3	2:B:1011:ILE:HD11	1.95	0.48
1:A:462:THR:HG23	1:A:468:THR:HG21	1.94	0.48
1:A:500:ILE:CG2	1:A:501:GLY:N	2.76	0.48
2:B:713:LEU:O	2:B:716:VAL:HG22	2.13	0.48
2:B:1059:ARG:NH2	3:X:37:DC:O2	2.47	0.48
1:A:63:VAL:HA	1:A:107:SER:O	2.13	0.48
1:A:163:GLU:O	1:A:167:ARG:HB2	2.14	0.48
2:B:717:VAL:CG2	2:B:721:VAL:HG21	2.44	0.48
1:A:417:GLU:HB2	1:A:453:LEU:HD21	1.95	0.48
1:A:527:LEU:C	1:A:527:LEU:HD23	2.38	0.48
1:A:563:ILE:HG13	1:A:564:SER:H	1.78	0.48
2:B:1133:ASP:HB3	2:B:1136:LEU:HD12	1.95	0.48
1:A:732:GLY:O	1:A:736:ARG:HG3	2.14	0.48
3:X:13:DA:H5'	3:X:13:DA:C8	2.49	0.48
1:A:495:LEU:CD1	1:A:923:ALA:HB2	2.44	0.47
1:A:834:TYR:O	1:A:842:SER:HA	2.14	0.47
1:A:1131:PRO:HG2	2:B:64:GLN:OE1	2.13	0.47
2:B:287:THR:HG21	2:B:290:LEU:HD12	1.96	0.47
2:B:343:LYS:HA	2:B:587:GLN:O	2.14	0.47
2:B:887:GLU:HA	2:B:890:GLN:CG	2.43	0.47
3:X:42:DG:H2''	3:X:43:DA:H5''	1.96	0.47
1:A:237:LEU:CD1	1:A:312:ALA:HB2	2.37	0.47
1:A:576:THR:HG22	1:A:577:HIS:H	1.80	0.47
1:A:1046:ARG:HG2	2:B:506:TYR:OH	2.14	0.47
2:B:883:TYR:CD1	2:B:883:TYR:C	2.92	0.47
2:B:1043:GLY:HA2	2:B:1079:ALA:HB1	1.96	0.47
2:B:1046:GLU:HG2	2:B:1050:LEU:CD1	2.44	0.47
3:X:32:DG:H2''	3:X:33:DC:C5'	2.45	0.47
1:A:233:ALA:O	1:A:237:LEU:HD13	2.14	0.47
1:A:1152:LEU:HD23	1:A:1152:LEU:H	1.79	0.47
2:B:204:HIS:CD2	2:B:230:HIS:HB2	2.49	0.47
2:B:474:LEU:O	2:B:478:ARG:HG2	2.14	0.47
2:B:673:ASP:OD1	2:B:674:ALA:N	2.44	0.47
2:B:916:LEU:C	2:B:916:LEU:HD23	2.39	0.47
1:A:1141:ILE:HD12	1:A:1141:ILE:N	2.30	0.47
1:A:1221:LEU:HB2	1:A:1230:LEU:HD21	1.95	0.47
2:B:477:THR:O	2:B:481:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:927:LEU:C	2:B:927:LEU:HD12	2.40	0.47
2:B:996:TRP:CD1	2:B:996:TRP:C	2.92	0.47
1:A:19:ILE:HG13	1:A:39:VAL:HG13	1.96	0.47
1:A:239:ARG:O	1:A:243:LEU:HG	2.15	0.47
1:A:328:PRO:O	1:A:332:LEU:HG	2.15	0.47
3:X:9:DG:C2'	3:X:10:DA:H5''	2.43	0.47
1:A:730:MET:HA	2:B:731:ARG:HH11	1.80	0.47
1:A:849:ILE:O	1:A:853:LYS:HD3	2.14	0.47
2:B:371:PHE:HB2	2:B:587:GLN:NE2	2.30	0.47
2:B:826:ILE:O	2:B:829:LEU:HB3	2.13	0.47
1:A:120:TYR:HB2	1:A:378:ILE:HD13	1.97	0.47
1:A:1085:THR:O	1:A:1089:LEU:HG	2.14	0.47
2:B:14:LYS:HE2	2:B:236:THR:HA	1.97	0.47
2:B:141:ARG:HH12	2:B:163:HIS:CD2	2.33	0.47
2:B:378:MET:HE1	2:B:540:ALA:HA	1.97	0.47
2:B:555:MET:HE1	2:B:568:MET:SD	2.55	0.47
2:B:1007:LEU:HD11	2:B:1051:MET:HE3	1.93	0.47
3:X:39:DT:H2''	3:X:40:DT:OP2	2.15	0.47
1:A:19:ILE:CG1	1:A:39:VAL:HG13	2.44	0.47
2:B:912:ILE:HG12	2:B:946:VAL:O	2.13	0.47
2:B:917:GLY:CA	2:B:923:PRO:HD2	2.45	0.47
1:A:599:MET:HG2	1:A:609:VAL:HG11	1.97	0.47
1:A:727:VAL:CG1	1:A:736:ARG:HB3	2.45	0.47
2:B:403:VAL:O	2:B:407:VAL:HG23	2.15	0.47
2:B:488:LEU:HD22	2:B:508:TYR:CG	2.50	0.47
3:X:37:DC:H2''	3:X:38:DA:C5'	2.45	0.47
1:A:326:ARG:HH12	2:B:1019:ASN:HA	1.80	0.47
1:A:507:GLU:O	1:A:508:GLN:HG2	2.15	0.47
1:A:596:PRO:HA	1:A:599:MET:HE2	1.97	0.47
1:A:633:ILE:HD13	1:A:701:TRP:HB3	1.96	0.47
2:B:371:PHE:CE1	2:B:580:LEU:HD21	2.50	0.47
2:B:783:LEU:HD11	2:B:810:GLY:O	2.15	0.47
2:B:919:GLY:HA2	2:B:926:PRO:CA	2.45	0.47
2:B:754:GLN:HG2	2:B:755:ASP:N	2.30	0.46
1:A:338:MET:O	1:A:342:ILE:HG12	2.16	0.46
1:A:454:PHE:C	1:A:454:PHE:CD2	2.93	0.46
1:A:796:SER:HB3	1:A:873:ARG:HG3	1.97	0.46
1:A:1064:MET:HE1	1:A:1108:ILE:HG13	1.97	0.46
2:B:229:GLU:O	2:B:230:HIS:HD2	1.97	0.46
2:B:314:VAL:O	2:B:697:GLU:HB2	2.15	0.46
2:B:790:GLY:O	2:B:939:LEU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1098:GLU:O	2:B:1102:GLN:HG3	2.15	0.46
1:A:177:LEU:O	1:A:181:VAL:HG23	2.15	0.46
1:A:209:GLU:OE2	1:A:333:LYS:HE3	2.14	0.46
2:B:8:GLY:N	2:B:14:LYS:HE3	2.30	0.46
2:B:554:MET:HA	2:B:554:MET:HE2	1.96	0.46
2:B:833:SER:O	2:B:837:ILE:HG12	2.14	0.46
1:A:530:ILE:HD11	1:A:554:ALA:CB	2.46	0.46
1:A:1045:ARG:O	2:B:545:ILE:HD13	2.15	0.46
1:A:529:LEU:HD22	1:A:887:HIS:CE1	2.51	0.46
2:B:52:ALA:O	2:B:58:GLY:HA2	2.16	0.46
2:B:152:TYR:O	2:B:155:GLU:HB2	2.15	0.46
1:A:531:ASP:C	1:A:956:SER:HB3	2.39	0.46
1:A:560:ARG:NH2	1:A:605:GLN:HG3	2.31	0.46
1:A:583:ARG:HB3	1:A:786:ASP:HA	1.96	0.46
1:A:926:ARG:CG	1:A:942:ILE:HD13	2.45	0.46
1:A:1173:TYR:O	1:A:1174:LYS:HD3	2.15	0.46
2:B:25:GLU:OE2	2:B:204:HIS:ND1	2.49	0.46
2:B:819:PHE:CZ	2:B:875:ILE:HG22	2.51	0.46
2:B:871:LEU:HD23	2:B:871:LEU:C	2.41	0.46
2:B:1012:HIS:NE2	2:B:1034:LYS:HE3	2.31	0.46
2:B:213:PHE:CE2	2:B:221:LEU:HD11	2.51	0.46
3:X:38:DA:H2"	3:X:39:DT:C6	2.51	0.46
1:A:218:PHE:CD1	1:A:218:PHE:C	2.94	0.46
1:A:657:GLU:O	1:A:661:ILE:HG13	2.15	0.46
1:A:382:GLU:HB2	1:A:388:ARG:HD3	1.97	0.46
1:A:439:VAL:HG23	1:A:454:PHE:CD2	2.51	0.46
2:B:7:VAL:HG23	2:B:277:GLU:OE1	2.15	0.46
2:B:514:VAL:HB	2:B:515:PRO:HD3	1.96	0.46
2:B:779:VAL:HG13	2:B:780:SER:H	1.80	0.46
1:A:526:GLU:HG2	1:A:950:ALA:HB3	1.98	0.46
1:A:628:SER:O	1:A:632:VAL:HG23	2.15	0.46
1:A:848:LEU:HD21	1:A:852:LYS:NZ	2.31	0.46
2:B:434:ILE:HD12	2:B:816:ARG:HH11	1.81	0.46
2:B:918:PHE:C	2:B:918:PHE:CD2	2.93	0.46
1:A:140:LEU:HD23	1:A:140:LEU:O	2.16	0.45
1:A:417:GLU:CG	1:A:453:LEU:HD21	2.47	0.45
1:A:556:ALA:O	1:A:559:ILE:HB	2.16	0.45
1:A:715:TRP:NE1	1:A:719:ARG:HH21	2.14	0.45
1:A:980:ARG:HG3	1:A:981:GLY:N	2.25	0.45
2:B:927:LEU:HD11	2:B:929:PHE:HE1	1.81	0.45
2:B:969:LEU:HD23	2:B:1040:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:975:TYR:CB	2:B:1152:ILE:HD13	2.46	0.45
1:A:42:GLU:HA	1:A:45:ILE:HD12	1.98	0.45
1:A:818:LEU:HD21	1:A:855:MET:SD	2.56	0.45
1:A:1136:LEU:O	1:A:1152:LEU:HD23	2.16	0.45
1:A:726:TYR:CD2	2:B:765:SER:HB3	2.51	0.45
1:A:1051:MET:CG	1:A:1052:LYS:H	2.27	0.45
2:B:821:LEU:HD22	2:B:875:ILE:CD1	2.40	0.45
1:A:622:GLU:HG2	1:A:727:VAL:HG11	1.97	0.45
1:A:729:GLY:O	2:B:731:ARG:HD2	2.17	0.45
1:A:1000:TRP:CG	1:A:1001:THR:N	2.84	0.45
2:B:22:ILE:O	2:B:26:LEU:HG	2.17	0.45
2:B:836:LEU:HD22	2:B:866:ARG:NH1	2.32	0.45
1:A:24:GLN:HE21	1:A:470:ARG:HB3	1.81	0.45
1:A:445:ARG:HH22	1:A:502:GLU:CD	2.24	0.45
1:A:551:GLU:OE1	1:A:883:SER:HB3	2.17	0.45
1:A:803:VAL:HG22	1:A:877:LYS:HB3	1.99	0.45
1:A:890:GLN:HG3	1:A:891:LEU:HD12	1.98	0.45
1:A:1056:THR:HG23	1:A:1059:GLU:H	1.81	0.45
2:B:86:PHE:HE2	2:B:183:SER:HA	1.81	0.45
2:B:722:ALA:O	2:B:726:THR:HG23	2.17	0.45
1:A:103:ARG:CZ	2:B:644:ARG:HB2	2.46	0.45
1:A:221:TYR:CZ	1:A:854:LYS:HD2	2.52	0.45
1:A:683:ARG:NH2	1:A:688:TYR:HE2	2.13	0.45
2:B:355:TYR:O	2:B:359:VAL:HG23	2.16	0.45
2:B:948:LYS:HG2	2:B:949:ALA:N	2.32	0.45
2:B:1147:GLU:CB	2:B:1152:ILE:HG13	2.47	0.45
1:A:939:HIS:HA	1:A:942:ILE:CG1	2.47	0.45
2:B:15:THR:O	2:B:19:ILE:HG13	2.17	0.45
2:B:109:VAL:HG23	2:B:160:GLU:HB3	1.98	0.45
2:B:137:PRO:HG3	2:B:169:TYR:CE1	2.51	0.45
2:B:485:LEU:HD13	2:B:508:TYR:OH	2.16	0.45
2:B:912:ILE:HG23	2:B:948:LYS:HB3	1.98	0.45
1:A:226:ILE:HG12	1:A:319:LEU:HD11	1.99	0.45
1:A:586:VAL:HG23	1:A:789:ARG:O	2.16	0.45
1:A:687:LEU:O	1:A:691:LEU:HG	2.17	0.45
2:B:156:ARG:HG2	2:B:160:GLU:OE1	2.16	0.45
2:B:194:ILE:HB	2:B:195:PRO:HD3	1.98	0.45
1:A:506:ASP:O	1:A:510:GLU:HG3	2.16	0.45
1:A:507:GLU:C	1:A:509:ALA:H	2.24	0.45
2:B:851:LEU:HD23	2:B:851:LEU:HA	1.80	0.45
2:B:1119:THR:HB	2:B:1120:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:ARG:HA	2:B:300:ARG:HD3	1.77	0.45
2:B:482:VAL:HB	2:B:483:PRO:HD3	1.98	0.45
2:B:839:ASP:O	2:B:842:ARG:HG2	2.17	0.45
2:B:1010:HIS:CE1	2:B:1012:HIS:CD2	3.05	0.45
2:B:1086:ASP:C	2:B:1089:THR:HG22	2.42	0.45
1:A:47:LYS:O	1:A:55:ILE:HG12	2.17	0.44
1:A:591:SER:CB	1:A:593:PRO:HD3	2.47	0.44
1:A:636:PRO:HD3	1:A:702:ARG:NH1	2.32	0.44
2:B:726:THR:HG22	2:B:743:TRP:HE3	1.82	0.44
2:B:1084:GLU:HG2	2:B:1153:LEU:HD21	1.98	0.44
2:B:1122:THR:OG1	2:B:1123:TYR:N	2.50	0.44
1:A:379:LEU:CB	1:A:422:LEU:HD22	2.38	0.44
1:A:587:ILE:HG22	1:A:805:PHE:CB	2.47	0.44
1:A:599:MET:HG2	1:A:609:VAL:CG1	2.47	0.44
1:A:866:VAL:O	1:A:869:VAL:HG22	2.17	0.44
2:B:968:GLY:HA3	2:B:1008:TYR:CG	2.52	0.44
1:A:845:THR:CG2	1:A:847:PRO:HD2	2.22	0.44
2:B:64:GLN:HB2	2:B:66:PHE:CE2	2.53	0.44
2:B:84:ARG:HD2	2:B:181:LEU:HD13	1.99	0.44
2:B:829:LEU:CD2	2:B:889:LEU:HD23	2.47	0.44
2:B:871:LEU:HD23	2:B:872:GLN:HB3	1.99	0.44
1:A:592:MET:SD	1:A:595:ALA:HB2	2.57	0.44
1:A:740:LEU:HD12	1:A:740:LEU:HA	1.89	0.44
1:A:945:HIS:HA	1:A:946:PRO:HD3	1.81	0.44
2:B:333:ALA:O	2:B:337:GLU:HB2	2.18	0.44
2:B:336:ARG:HH22	2:B:717:VAL:HA	1.83	0.44
2:B:492:MET:HE1	2:B:501:LYS:HB3	1.98	0.44
2:B:552:VAL:O	2:B:556:GLY:HA3	2.18	0.44
2:B:918:PHE:CE2	2:B:988:LEU:HD21	2.52	0.44
3:X:41:DA:OP1	3:X:41:DA:H4'	2.15	0.44
1:A:1210:GLN:O	1:A:1213:LYS:HE3	2.17	0.44
2:B:100:ILE:HD12	2:B:114:SER:O	2.17	0.44
2:B:378:MET:CE	2:B:540:ALA:HA	2.48	0.44
2:B:1084:GLU:O	2:B:1087:LEU:HB3	2.17	0.44
3:X:11:DG:H1'	3:X:12:DC:H5''	1.99	0.44
1:A:133:ALA:HB1	1:A:137:GLU:CG	2.47	0.44
1:A:490:PHE:HE1	1:A:942:ILE:O	2.00	0.44
1:A:846:LEU:HB3	1:A:847:PRO:HD3	1.99	0.44
2:B:381:HIS:HE2	2:B:537:HIS:HA	1.81	0.44
2:B:1012:HIS:N	2:B:1012:HIS:HD1	2.16	0.44
1:A:163:GLU:HB3	1:A:167:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:LEU:HD11	1:A:852:LYS:HG2	1.99	0.44
1:A:874:ALA:CB	1:A:878:LEU:CD1	2.94	0.44
2:B:36:ILE:HG23	2:B:66:PHE:CD2	2.47	0.44
2:B:221:LEU:O	2:B:225:MET:HG3	2.18	0.44
2:B:275:TYR:O	2:B:276:LYS:HD2	2.17	0.44
2:B:509:LEU:O	2:B:514:VAL:HG23	2.18	0.44
2:B:875:ILE:HD12	2:B:876:LEU:N	2.32	0.44
1:A:915:THR:HG22	1:A:917:LEU:H	1.82	0.44
2:B:299:ALA:O	2:B:302:ALA:HB2	2.18	0.44
2:B:404:PHE:CZ	2:B:430:GLU:HA	2.53	0.44
2:B:931:LEU:HG	2:B:935:CYS:CB	2.46	0.44
2:B:939:LEU:HD12	2:B:939:LEU:O	2.18	0.44
3:X:41:DA:H2''	3:X:42:DG:H5'	1.98	0.44
3:X:41:DA:C8	3:X:41:DA:H5''	2.53	0.44
1:A:162:PHE:CD1	2:B:884:TYR:CE1	3.06	0.44
1:A:506:ASP:O	1:A:509:ALA:HB3	2.18	0.44
1:A:1079:ILE:O	1:A:1083:GLU:HG3	2.17	0.44
2:B:702:ASN:O	2:B:704:PRO:HD3	2.18	0.44
2:B:868:ALA:N	2:B:869:PRO:HD2	2.32	0.44
2:B:1042:LEU:C	2:B:1079:ALA:HB1	2.43	0.44
1:A:501:GLY:C	1:A:503:VAL:N	2.76	0.43
1:A:556:ALA:HA	1:A:559:ILE:HD12	2.00	0.43
2:B:117:SER:O	2:B:120:THR:HG22	2.18	0.43
2:B:541:TRP:NE1	2:B:545:ILE:HD11	2.33	0.43
1:A:26:ILE:HA	1:A:470:ARG:O	2.17	0.43
2:B:757:LEU:O	2:B:760:LYS:HB3	2.18	0.43
1:A:188:SER:CB	1:A:198:LEU:CD1	2.95	0.43
1:A:662:ARG:HD2	1:A:666:LYS:HA	1.99	0.43
2:B:110:TYR:HE1	2:B:161:LYS:HB3	1.83	0.43
2:B:153:ARG:NH2	2:B:156:ARG:HD2	2.33	0.43
2:B:873:LYS:C	2:B:874:GLU:HG2	2.43	0.43
1:A:1138:ALA:HA	1:A:1152:LEU:HD22	2.00	0.43
2:B:22:ILE:HG23	2:B:35:ILE:HG21	2.00	0.43
2:B:505:LEU:O	2:B:508:TYR:HB3	2.18	0.43
2:B:990:ILE:O	2:B:993:SER:HB3	2.17	0.43
3:X:3:DT:C2'	3:X:4:DA:C8	3.02	0.43
3:X:42:DG:H1'	3:X:43:DA:H5''	2.01	0.43
2:B:84:ARG:NH1	2:B:178:ASP:O	2.51	0.43
2:B:629:ARG:O	2:B:633:LYS:HG3	2.18	0.43
1:A:41:VAL:HG12	1:A:45:ILE:CD1	2.49	0.43
1:A:228:MET:HE1	1:A:911:TYR:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLU:O	1:A:321:THR:HG23	2.18	0.43
2:B:187:LEU:HD21	2:B:217:GLU:HG2	2.00	0.43
2:B:419:LYS:O	2:B:420:ALA:C	2.62	0.43
2:B:726:THR:O	2:B:730:LEU:HG	2.18	0.43
2:B:799:ASN:O	2:B:1142:ARG:NH2	2.51	0.43
2:B:933:ASN:O	2:B:933:ASN:CG	2.62	0.43
1:A:1134:LEU:HD11	1:A:1210:GLN:OE1	2.19	0.43
2:B:317:ALA:HB2	2:B:700:LEU:HB2	2.01	0.43
2:B:466:GLN:HG2	2:B:467:GLU:N	2.33	0.43
2:B:1113:TYR:O	2:B:1120:PRO:HD3	2.18	0.43
3:X:30:DG:C3'	3:X:31:DT:H5''	2.45	0.43
1:A:162:PHE:HD1	2:B:884:TYR:CE1	2.37	0.43
1:A:546:GLU:HA	1:A:549:GLN:OE1	2.18	0.43
1:A:562:LEU:HB3	1:A:580:ILE:CD1	2.44	0.43
1:A:993:LYS:HD3	2:B:713:LEU:HD21	2.01	0.43
2:B:1132:PHE:CE2	2:B:1139:ASN:HB3	2.53	0.43
1:A:715:TRP:CZ2	2:B:361:GLU:HB3	2.54	0.43
2:B:346:ALA:O	2:B:604:THR:HA	2.19	0.43
2:B:400:TYR:CE1	2:B:434:ILE:HG12	2.53	0.43
2:B:580:LEU:C	2:B:580:LEU:HD23	2.43	0.43
2:B:918:PHE:HZ	2:B:939:LEU:CD1	2.32	0.43
2:B:1115:MET:HB2	2:B:1144:LEU:HB2	1.97	0.43
1:A:1064:MET:SD	1:A:1103:ILE:HG23	2.59	0.43
2:B:415:LEU:HD11	2:B:513:ASP:OD2	2.19	0.43
2:B:608:GLY:C	2:B:610:ASN:H	2.27	0.43
2:B:829:LEU:HD22	2:B:889:LEU:HD23	1.99	0.43
2:B:854:GLU:CG	2:B:855:GLN:N	2.82	0.43
1:A:15:GLN:O	1:A:19:ILE:HG13	2.18	0.42
1:A:16:TRP:HZ3	1:A:46:ARG:HH22	1.67	0.42
1:A:1143:PRO:O	1:A:1144:ASP:C	2.62	0.42
1:A:1220:ALA:C	1:A:1221:LEU:HD12	2.44	0.42
2:B:383:LEU:HD13	2:B:514:VAL:HG11	2.01	0.42
2:B:912:ILE:CG1	2:B:913:GLY:H	2.23	0.42
3:X:41:DA:H5''	3:X:41:DA:H8	1.84	0.42
1:A:678:LEU:O	1:A:688:TYR:HE1	2.02	0.42
1:A:819:ASN:HB3	3:X:2:DC:H4'	2.00	0.42
1:A:840:ARG:NE	2:B:1014:PRO:O	2.52	0.42
2:B:774:GLN:CD	2:B:774:GLN:H	2.27	0.42
2:B:945:ARG:O	2:B:959:ILE:HG23	2.19	0.42
2:B:1110:ILE:C	2:B:1111:GLU:HG3	2.43	0.42
1:A:22:THR:CG2	1:A:23:GLY:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:HA	1:A:176:ASP:HB2	2.01	0.42
1:A:339:LYS:O	1:A:343:GLU:HG3	2.19	0.42
1:A:529:LEU:HD11	1:A:890:GLN:HE21	1.81	0.42
1:A:588:LEU:HB2	1:A:806:VAL:HG12	1.99	0.42
2:B:758:GLN:O	2:B:761:LYS:HB2	2.19	0.42
3:X:44:DT:H2"	3:X:45:DT:OP2	2.19	0.42
1:A:73:MET:O	1:A:77:ILE:HG13	2.19	0.42
1:A:120:TYR:HB3	1:A:123:LEU:HD12	2.01	0.42
1:A:176:ASP:OD1	1:A:179:PHE:HZ	2.02	0.42
1:A:515:ALA:HB1	1:A:517:TYR:HD2	1.84	0.42
2:B:207:VAL:HG21	2:B:233:PHE:CD2	2.54	0.42
2:B:418:PRO:O	2:B:422:VAL:HG23	2.19	0.42
2:B:465:ASP:O	2:B:469:GLU:HG2	2.19	0.42
2:B:867:LEU:C	2:B:869:PRO:HD2	2.45	0.42
2:B:1091:HIS:HA	2:B:1094:ARG:HE	1.85	0.42
1:A:901:THR:O	1:A:902:ASP:CB	2.66	0.42
2:B:507:ARG:O	2:B:511:GLU:OE1	2.37	0.42
2:B:872:GLN:O	2:B:873:LYS:C	2.61	0.42
2:B:1148:LYS:O	2:B:1149:ASP:C	2.62	0.42
3:X:46:DT:H6	3:X:46:DT:H2'	1.59	0.42
1:A:125:ASP:HB2	2:B:112:LYS:NZ	2.35	0.42
1:A:495:LEU:HA	1:A:910:ARG:HD3	2.01	0.42
1:A:697:HIS:HB3	1:A:701:TRP:CE2	2.55	0.42
1:A:723:TYR:CD2	1:A:740:LEU:HD21	2.54	0.42
1:A:762:LEU:O	1:A:766:GLU:HG3	2.19	0.42
1:A:846:LEU:HD12	1:A:846:LEU:HA	1.80	0.42
1:A:1162:TYR:O	1:A:1168:LEU:HD12	2.19	0.42
2:B:72:ALA:HA	2:B:190:LEU:HD13	2.00	0.42
2:B:207:VAL:HG21	2:B:233:PHE:HD2	1.84	0.42
2:B:265:LYS:HD2	2:B:268:GLU:OE2	2.19	0.42
2:B:465:ASP:OD1	2:B:465:ASP:N	2.51	0.42
2:B:552:VAL:HA	2:B:556:GLY:HA2	2.02	0.42
2:B:983:LEU:HD13	2:B:1088:LEU:HB3	2.01	0.42
1:A:255:ASP:O	1:A:258:LEU:HD12	2.19	0.42
1:A:592:MET:N	1:A:593:PRO:CD	2.78	0.42
1:A:1170:LEU:HD23	1:A:1171:LEU:N	2.34	0.42
2:B:207:VAL:CG2	2:B:233:PHE:HA	2.49	0.42
2:B:802:PRO:HB2	2:B:1109:SER:O	2.19	0.42
1:A:602:LEU:HB2	1:A:609:VAL:CG2	2.48	0.42
1:A:862:GLU:O	1:A:866:VAL:HG23	2.20	0.42
1:A:926:ARG:HG2	1:A:942:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:ALA:O	2:B:178:ASP:HB3	2.20	0.42
2:B:714:MET:O	2:B:717:VAL:HG13	2.20	0.42
2:B:1041:LEU:HD22	2:B:1051:MET:SD	2.59	0.42
3:X:45:DT:H6	3:X:45:DT:H2'	1.60	0.42
1:A:407:ASP:HA	1:A:436:VAL:HG13	2.01	0.42
1:A:805:PHE:HA	1:A:879:PHE:HB2	2.02	0.42
1:A:1221:LEU:HB2	1:A:1230:LEU:HD23	2.01	0.42
2:B:404:PHE:HZ	2:B:429:LEU:HG	1.84	0.42
2:B:511:GLU:OE1	2:B:511:GLU:N	2.52	0.42
2:B:798:PHE:HD1	2:B:805:HIS:ND1	2.13	0.42
2:B:1127:LYS:HA	2:B:1130:CYS:SG	2.60	0.42
1:A:500:ILE:HG22	1:A:501:GLY:N	2.35	0.42
1:A:654:ASP:O	1:A:658:LEU:HG	2.20	0.42
2:B:76:LEU:C	2:B:78:HIS:N	2.78	0.42
2:B:194:ILE:N	2:B:195:PRO:CD	2.83	0.42
2:B:689:GLU:O	2:B:693:PRO:HA	2.20	0.42
2:B:777:ARG:HH22	2:B:933:ASN:ND2	2.18	0.42
1:A:16:TRP:HZ3	1:A:46:ARG:NH2	2.18	0.41
1:A:237:LEU:HD11	1:A:312:ALA:CB	2.40	0.41
1:A:389:GLU:HA	1:A:390:PRO:HD3	1.94	0.41
2:B:303:ILE:O	2:B:303:ILE:HG13	2.19	0.41
2:B:548:LEU:O	2:B:552:VAL:HG13	2.19	0.41
2:B:932:LYS:O	2:B:933:ASN:CG	2.63	0.41
2:B:1005:GLY:HA2	2:B:1085:PHE:CZ	2.55	0.41
1:A:183:GLN:HG3	1:A:824:LEU:HD12	2.02	0.41
1:A:589:LEU:O	1:A:792:THR:HA	2.20	0.41
2:B:323:GLU:O	2:B:327:ILE:HG13	2.21	0.41
2:B:772:VAL:CG1	2:B:1108:VAL:HG23	2.49	0.41
2:B:1086:ASP:CA	2:B:1089:THR:HG22	2.50	0.41
1:A:587:ILE:HG13	1:A:790:LEU:HA	2.03	0.41
1:A:761:PHE:O	1:A:764:PHE:HB3	2.21	0.41
1:A:791:MET:HE1	1:A:799:LEU:HD12	2.01	0.41
1:A:1212:ALA:HA	2:B:30:PRO:HB3	2.03	0.41
2:B:157:VAL:O	2:B:161:LYS:HG3	2.19	0.41
2:B:469:GLU:HG2	2:B:469:GLU:H	1.70	0.41
2:B:770:ASN:ND2	2:B:1130:CYS:O	2.54	0.41
2:B:803:PHE:HD1	2:B:1108:VAL:O	2.03	0.41
2:B:988:LEU:CD1	2:B:988:LEU:H	2.34	0.41
3:X:13:DA:C2	3:X:14:DC:C2	3.07	0.41
3:X:42:DG:C2'	3:X:43:DA:H5''	2.50	0.41
1:A:37:THR:O	1:A:41:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HB2	1:A:401:PHE:CE1	2.54	0.41
1:A:367:ASP:CG	1:A:368:PHE:N	2.77	0.41
2:B:581:ILE:HA	2:B:582:PRO:HD3	1.91	0.41
2:B:975:TYR:HB2	2:B:1152:ILE:HD13	2.02	0.41
2:B:1042:LEU:HD23	2:B:1043:GLY:N	2.36	0.41
1:A:625:VAL:O	1:A:629:VAL:HG23	2.19	0.41
1:A:806:VAL:HG23	1:A:806:VAL:O	2.20	0.41
2:B:1045:GLN:NE2	2:B:1049:ARG:NH2	2.68	0.41
1:A:476:LYS:HD3	1:A:478:PHE:HE1	1.85	0.41
1:A:489:ASN:ND2	1:A:510:GLU:HB3	2.35	0.41
1:A:819:ASN:HB3	3:X:2:DC:H5''	2.02	0.41
1:A:983:PRO:CD	2:B:747:TYR:CE2	3.03	0.41
1:A:1084:GLN:O	1:A:1088:ARG:HG3	2.20	0.41
2:B:239:LYS:N	2:B:240:PRO:HD3	2.36	0.41
2:B:316:GLN:HG3	2:B:671:ILE:HG12	2.01	0.41
2:B:468:ILE:HG23	2:B:472:ASN:OD1	2.21	0.41
2:B:501:LYS:CE	2:B:561:SER:HA	2.50	0.41
2:B:564:LEU:O	2:B:568:MET:HG3	2.21	0.41
2:B:1148:LYS:O	2:B:1151:THR:N	2.52	0.41
3:X:42:DG:H2''	3:X:43:DA:C5'	2.50	0.41
1:A:70:ALA:HB1	1:A:106:ILE:HG22	2.02	0.41
1:A:726:TYR:CE2	2:B:765:SER:HB3	2.55	0.41
2:B:654:ILE:HG13	2:B:655:TYR:N	2.36	0.41
2:B:753:GLU:HB3	2:B:754:GLN:H	1.49	0.41
2:B:968:GLY:HA3	2:B:1008:TYR:CD2	2.55	0.41
1:A:321:THR:HA	1:A:325:THR:CG2	2.51	0.41
2:B:222:GLU:OE1	2:B:222:GLU:N	2.53	0.41
2:B:238:ASP:O	2:B:239:LYS:C	2.64	0.41
2:B:300:ARG:N	2:B:301:PRO:CD	2.83	0.41
2:B:309:GLN:HG3	2:B:695:HIS:CD2	2.56	0.41
2:B:975:TYR:HB2	2:B:1152:ILE:HG21	2.02	0.41
2:B:1042:LEU:C	2:B:1042:LEU:HD23	2.46	0.41
1:A:16:TRP:CH2	1:A:20:VAL:HG21	2.56	0.41
1:A:191:HIS:HA	1:A:192:PRO:HD3	1.93	0.41
1:A:213:ILE:HD12	1:A:213:ILE:C	2.46	0.41
1:A:582:TYR:O	1:A:585:ILE:HG13	2.21	0.41
1:A:771:ARG:HG3	1:A:772:GLY:N	2.30	0.41
1:A:836:HIS:CD2	1:A:839:LEU:HD13	2.56	0.41
1:A:1051:MET:CG	1:A:1052:LYS:N	2.84	0.41
1:A:1143:PRO:O	1:A:1146:HIS:CE1	2.74	0.41
2:B:532:ILE:H	2:B:532:ILE:CD1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:ILE:HD11	2:B:564:LEU:HD23	2.02	0.41
2:B:572:GLY:O	2:B:576:LEU:HG	2.21	0.41
2:B:1101:GLU:HG3	2:B:1102:GLN:N	2.36	0.41
3:X:30:DG:H2''	3:X:31:DT:C6	2.56	0.41
3:X:32:DG:OP1	3:X:32:DG:C4'	2.68	0.41
1:A:428:GLU:OE2	1:A:460:ARG:HD2	2.21	0.41
1:A:599:MET:HA	1:A:609:VAL:HG21	2.03	0.41
1:A:707:ASN:OD1	1:A:707:ASN:O	2.39	0.41
1:A:282:PRO:HA	1:A:320:LYS:CD	2.49	0.40
1:A:826:LYS:CG	1:A:827:GLU:N	2.84	0.40
1:A:982:GLU:HB3	2:B:751:MET:CB	2.52	0.40
1:A:1050:MET:HE3	1:A:1050:MET:HB3	1.70	0.40
1:A:1095:LEU:HD21	1:A:1103:ILE:CD1	2.51	0.40
2:B:342:TYR:HB2	2:B:586:ASP:OD1	2.21	0.40
1:A:207:VAL:HG22	1:A:208:SER:N	2.36	0.40
1:A:529:LEU:HD22	1:A:887:HIS:ND1	2.35	0.40
2:B:182:HIS:O	2:B:185:ASP:HB2	2.20	0.40
2:B:559:GLU:O	2:B:560:ILE:HB	2.20	0.40
2:B:887:GLU:HA	2:B:890:GLN:CD	2.46	0.40
2:B:1041:LEU:O	2:B:1085:PHE:HE1	2.04	0.40
2:B:1137:GLU:C	2:B:1139:ASN:H	2.30	0.40
2:B:1153:LEU:HD12	2:B:1153:LEU:HA	1.90	0.40
1:A:63:VAL:CG2	1:A:406:VAL:HG22	2.51	0.40
1:A:424:THR:HG21	1:A:433:LEU:HD13	2.03	0.40
1:A:569:VAL:HG12	1:A:570:TYR:N	2.35	0.40
1:A:796:SER:O	1:A:799:LEU:HB2	2.21	0.40
2:B:422:VAL:O	2:B:426:VAL:HG23	2.20	0.40
2:B:889:LEU:O	2:B:893:VAL:HG23	2.21	0.40
2:B:1045:GLN:HE21	2:B:1049:ARG:NH2	2.12	0.40
1:A:214:GLU:HA	1:A:219:TYR:CD2	2.56	0.40
1:A:618:PHE:CE1	1:A:765:ILE:HG23	2.57	0.40
1:A:415:VAL:O	1:A:419:ILE:HG13	2.21	0.40
1:A:854:LYS:O	1:A:857:ARG:HG2	2.21	0.40
2:B:212:GLN:NE2	2:B:254:MET:C	2.79	0.40
2:B:218:PHE:O	2:B:222:GLU:OE1	2.40	0.40
2:B:269:LEU:HD22	2:B:271:LEU:HD11	2.03	0.40
2:B:336:ARG:HH22	2:B:717:VAL:CA	2.34	0.40
2:B:1142:ARG:O	2:B:1142:ARG:HG3	2.21	0.40
3:X:6:DT:H2''	3:X:7:DG:C5'	2.48	0.40
3:X:8:DC:H2''	3:X:9:DG:H5'	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1096/1232 (89%)	1024 (93%)	63 (6%)	9 (1%)	16	50
2	B	1137/1166 (98%)	1053 (93%)	77 (7%)	7 (1%)	21	56
All	All	2233/2398 (93%)	2077 (93%)	140 (6%)	16 (1%)	18	52

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	284	VAL
1	A	172	ARG
1	A	567	PHE
1	A	887	HIS
2	B	641	SER
2	B	996	TRP
2	B	1122	THR
1	A	566	PRO
1	A	1052	LYS
2	B	254	MET
1	A	903	TRP
1	A	1144	ASP
2	B	872	GLN
2	B	560	ILE
2	B	994	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	977/1062 (92%)	963 (99%)	14 (1%)	59	77
2	B	1007/1029 (98%)	978 (97%)	29 (3%)	37	67
All	All	1984/2091 (95%)	1941 (98%)	43 (2%)	45	71

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	187	TYR
1	A	329	GLU
1	A	365	ILE
1	A	445	ARG
1	A	500	ILE
1	A	548	VAL
1	A	551	GLU
1	A	587	ILE
1	A	598	ILE
1	A	654	ASP
1	A	903	TRP
1	A	1095	LEU
1	A	1140	GLU
2	B	60	MET
2	B	78	HIS
2	B	128	THR
2	B	269	LEU
2	B	298	GLU
2	B	353	GLU
2	B	532	ILE
2	B	538	GLN
2	B	554	MET
2	B	590	VAL
2	B	635	ILE
2	B	639	LEU
2	B	644	ARG
2	B	654	ILE
2	B	678	THR
2	B	707	VAL
2	B	775	LEU
2	B	789	GLN
2	B	876	LEU
2	B	883	TYR
2	B	889	LEU

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Mol	Chain	Res	Type
2	B	918	PHE
2	B	946	VAL
2	B	948	LYS
2	B	1045	GLN
2	B	1048	VAL
2	B	1063	ILE
2	B	1115	MET
2	B	1152	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	75	HIS
1	A	173	HIS
1	A	707	ASN
1	A	735	GLN
1	A	890	GLN
1	A	1014	GLN
2	B	212	GLN
2	B	230	HIS
2	B	351	GLN
2	B	587	GLN
2	B	809	HIS
2	B	981	GLN
2	B	1045	GLN
2	B	1102	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	B	1167	2	0,12,12	-	-	-		

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
4	SF4	B	1167	2	-	-	0/6/5/5

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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1167	SF4	1	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%)	0.04	10 (0%) 81 64	40, 70, 114, 133	0
2	B	1141/1166 (97%)	0.05	6 (0%) 87 76	40, 72, 108, 148	0
3	X	36/48 (75%)	0.71	0 100 100	80, 119, 147, 158	0
All	All	2299/2446 (93%)	0.06	16 (0%) 84 69	40, 71, 113, 158	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	898	ALA	3.6
2	B	502	ALA	3.2
1	A	171	ASP	2.8
2	B	923	PRO	2.7
1	A	302	LEU	2.6
1	A	285	SER	2.5
1	A	1185	GLY	2.5
1	A	244	THR	2.3
2	B	1115	MET	2.2
2	B	1136	LEU	2.2
1	A	984	VAL	2.2
1	A	523	THR	2.1
1	A	1138	ALA	2.1
2	B	598	MET	2.1
2	B	926	PRO	2.1
1	A	994	ALA	2.1

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
4	SF4	B	1167	8/8	0.96	0.07	69,77,84,112	8

6.5 Other polymers [i](#)

There are no such residues in this entry.