Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 11:15 PM EST

PDB ID	:	3VKG
Title	:	X-ray structure of an MTBD truncation mutant of dynein motor domain
Authors	:	Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on	:	2011-11-16
Resolution	:	2.81 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 (i) 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 (i)) were used in the production of this report:

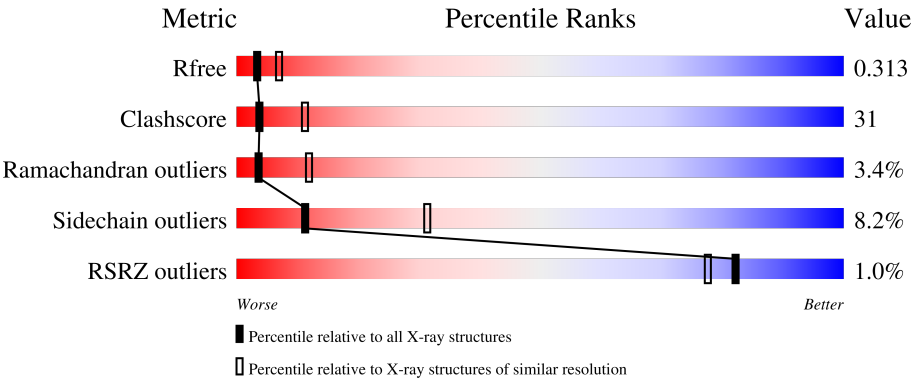
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 <=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	3245	% 44% 41% 5% 9%
1	B	3245	% 44% 38% 6% 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 45284 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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2954	Total	C	N	O	S	0	0	0
			22821	14585	3870	4270	96			
1	B	2853	Total	C	N	O	S	0	0	0
			22146	14131	3745	4174	96			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	expression tag	UNP P34036
A	1365	THR	-	expression tag	UNP P34036
A	1366	ARG	-	expression tag	UNP P34036
A	1367	HIS	-	expression tag	UNP P34036
A	1368	HIS	-	expression tag	UNP P34036
A	1369	HIS	-	expression tag	UNP P34036
A	1370	HIS	-	expression tag	UNP P34036
A	1371	HIS	-	expression tag	UNP P34036
A	1372	HIS	-	expression tag	UNP P34036
A	1373	GLY	-	expression tag	UNP P34036
A	1374	GLY	-	expression tag	UNP P34036
A	1375	GLY	-	expression tag	UNP P34036
A	1376	ASP	-	expression tag	UNP P34036
A	1377	TYR	-	expression tag	UNP P34036
A	1378	LYS	-	expression tag	UNP P34036
A	1379	ASP	-	expression tag	UNP P34036
A	1380	ASP	-	expression tag	UNP P34036
A	1381	ASP	-	expression tag	UNP P34036
A	1382	ASP	-	expression tag	UNP P34036
A	1383	LYS	-	expression tag	UNP P34036
A	1384	GLY	-	expression tag	UNP P34036
A	1385	GLY	-	expression tag	UNP P34036
A	1386	GLY	-	expression tag	UNP P34036
A	1387	LYS	-	expression tag	UNP P34036
A	3494	THR	-	linker	UNP P34036

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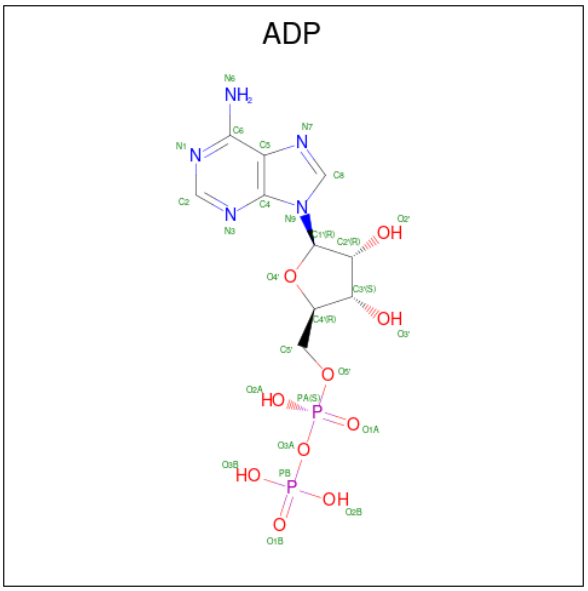
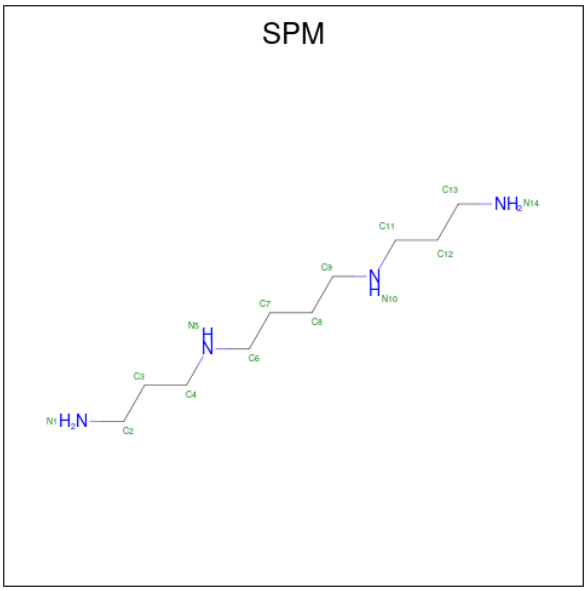
Chain	Residue	Modelled	Actual	Comment	Reference
A	3495	GLY	-	linker	UNP P34036
B	1364	MET	-	expression tag	UNP P34036
B	1365	THR	-	expression tag	UNP P34036
B	1366	ARG	-	expression tag	UNP P34036
B	1367	HIS	-	expression tag	UNP P34036
B	1368	HIS	-	expression tag	UNP P34036
B	1369	HIS	-	expression tag	UNP P34036
B	1370	HIS	-	expression tag	UNP P34036
B	1371	HIS	-	expression tag	UNP P34036
B	1372	HIS	-	expression tag	UNP P34036
B	1373	GLY	-	expression tag	UNP P34036
B	1374	GLY	-	expression tag	UNP P34036
B	1375	GLY	-	expression tag	UNP P34036
B	1376	ASP	-	expression tag	UNP P34036
B	1377	TYR	-	expression tag	UNP P34036
B	1378	LYS	-	expression tag	UNP P34036
B	1379	ASP	-	expression tag	UNP P34036
B	1380	ASP	-	expression tag	UNP P34036
B	1381	ASP	-	expression tag	UNP P34036
B	1382	ASP	-	expression tag	UNP P34036
B	1383	LYS	-	expression tag	UNP P34036
B	1384	GLY	-	expression tag	UNP P34036
B	1385	GLY	-	expression tag	UNP P34036
B	1386	GLY	-	expression tag	UNP P34036
B	1387	LYS	-	expression tag	UNP P34036
B	3494	THR	-	linker	UNP P34036
B	3495	GLY	-	linker	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 14 10 4	0	0
3	A	1	Total C N 14 10 4	0	0
3	B	1	Total C N 14 10 4	0	0
3	B	1	Total C N 14 10 4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	2	Total Mg 2 2	0	0

- Molecule 5 is water.

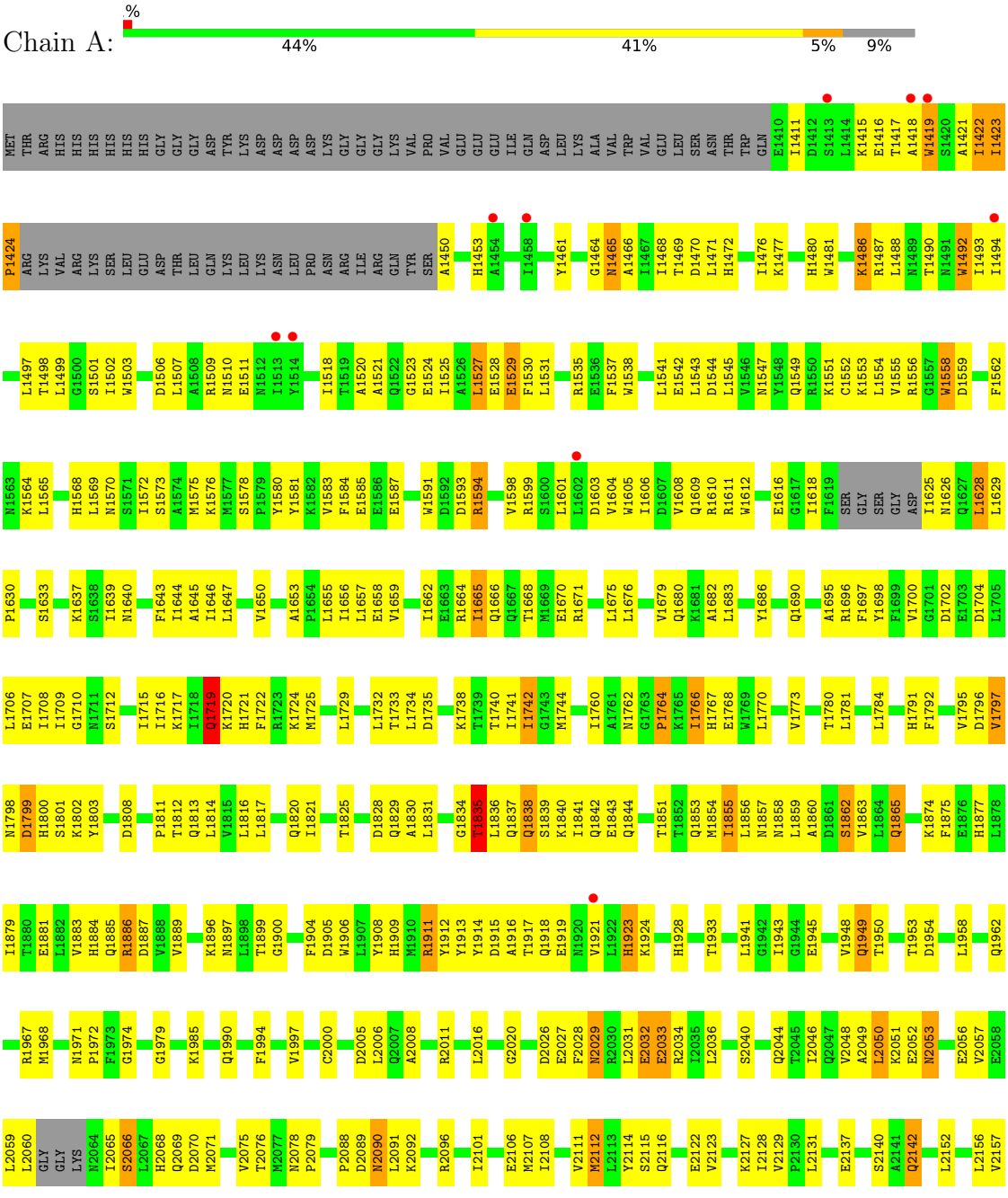
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O 23 23	0	0
5	B	19	Total O 19 19	0	0

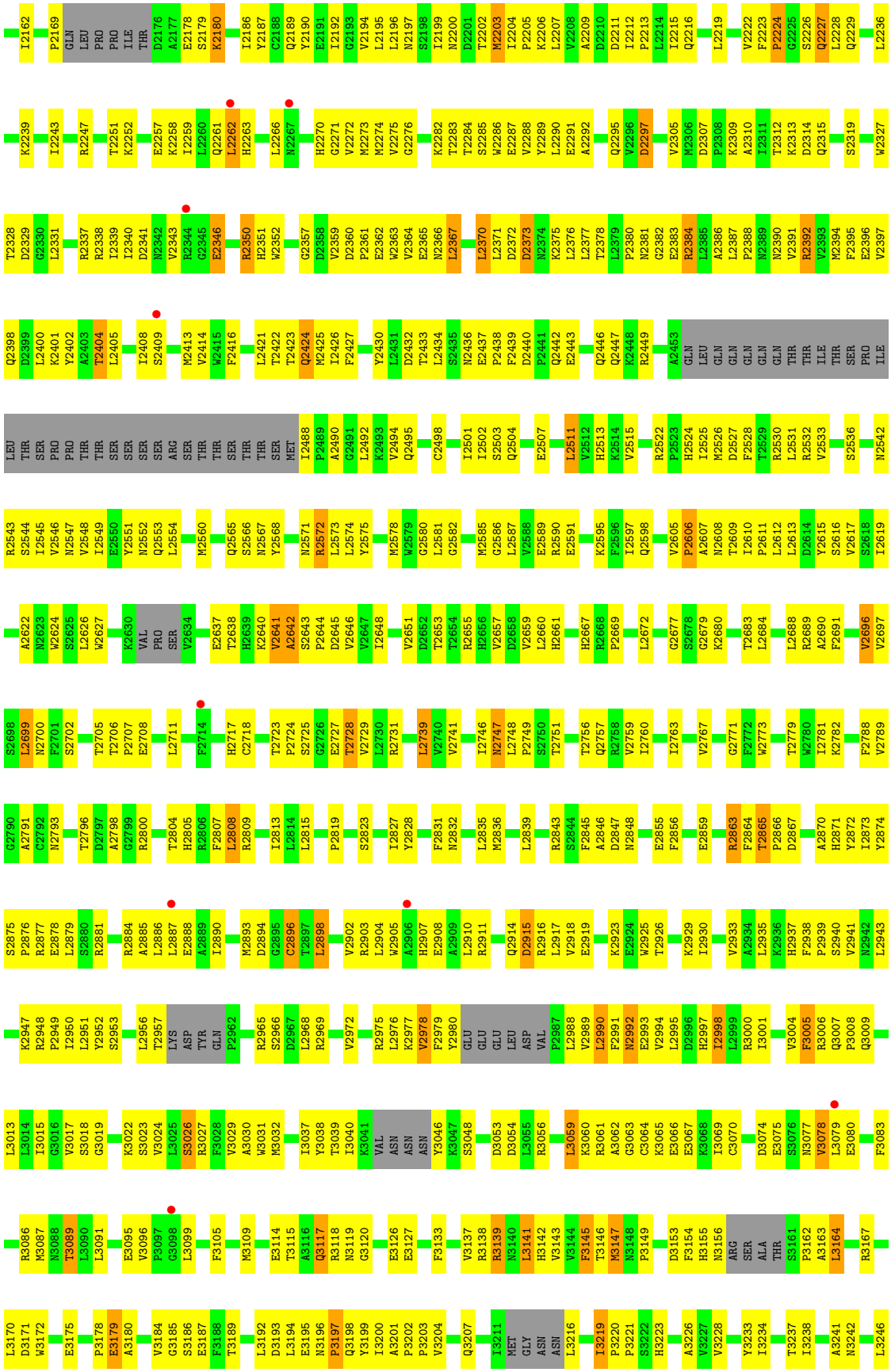
3 Residue-property plots (i)

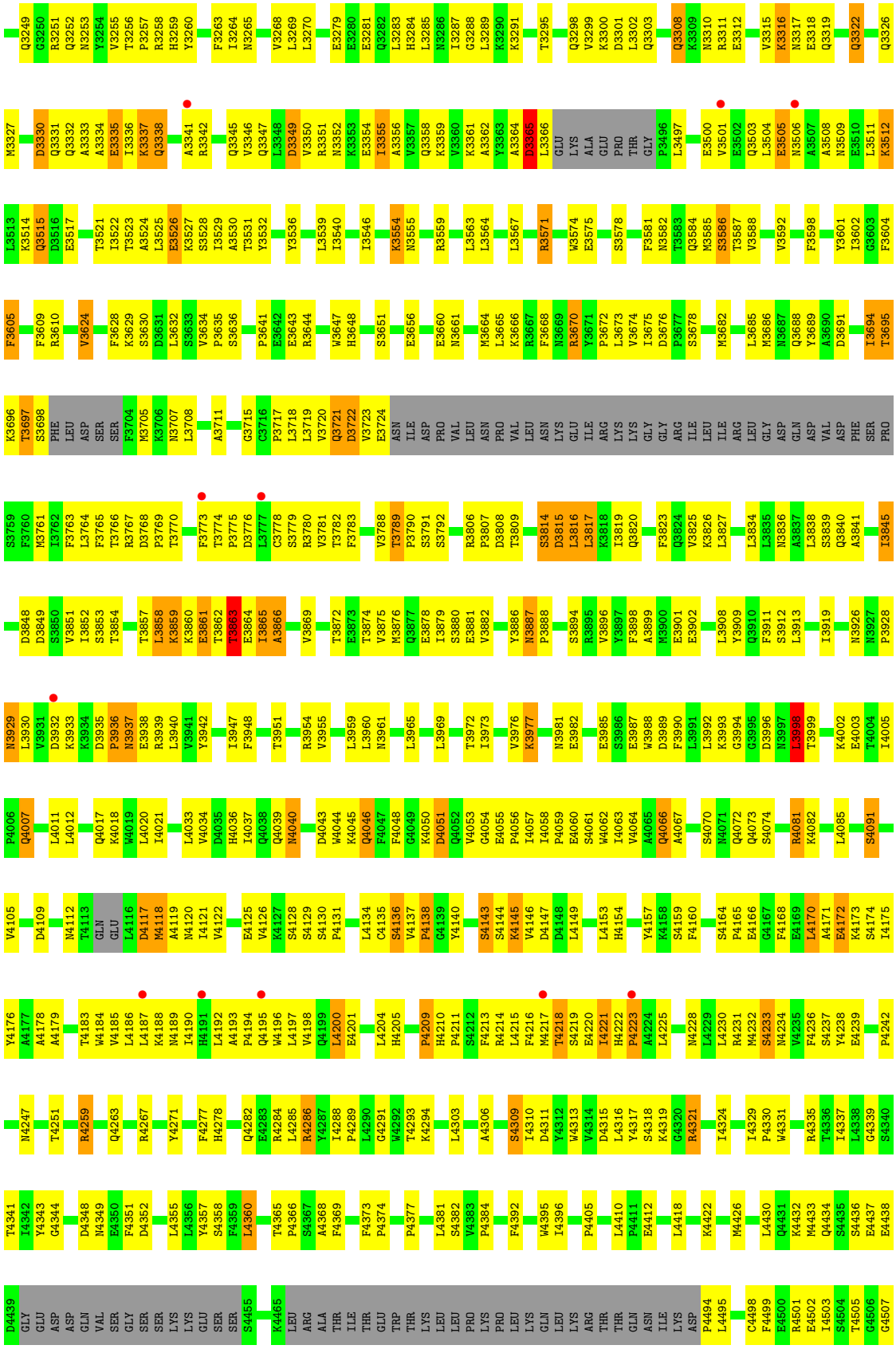
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

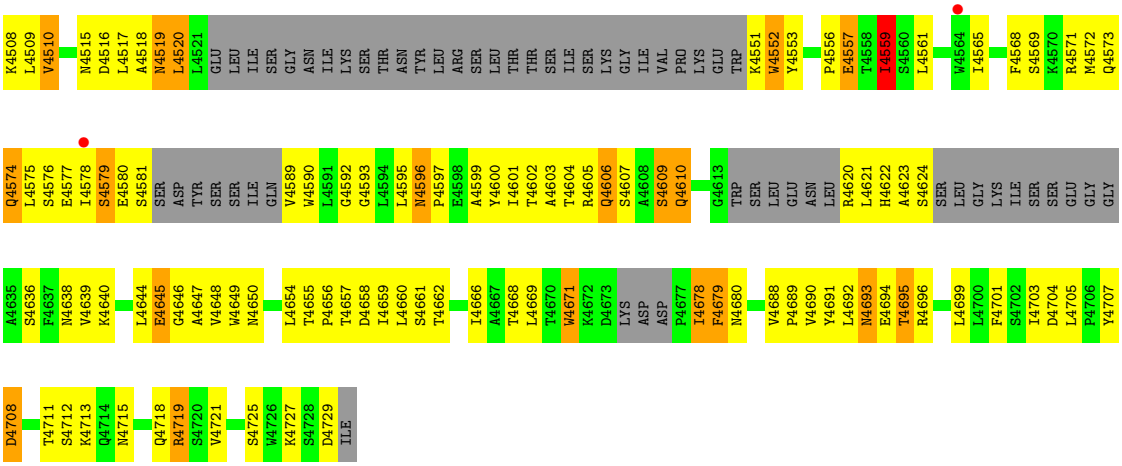
• Molecule 1: Dynein heavy chain, cytoplasmic

Chain A:



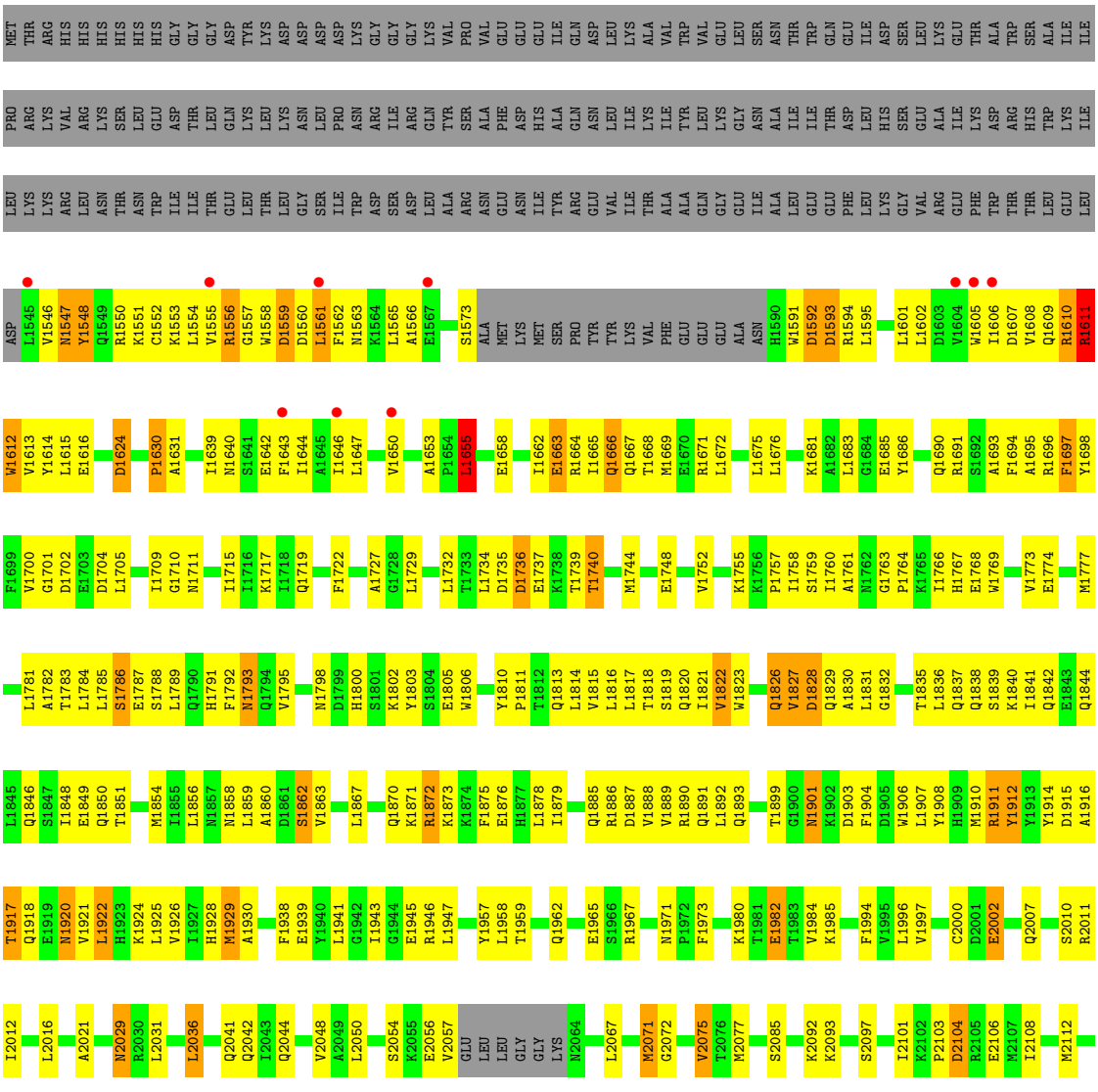


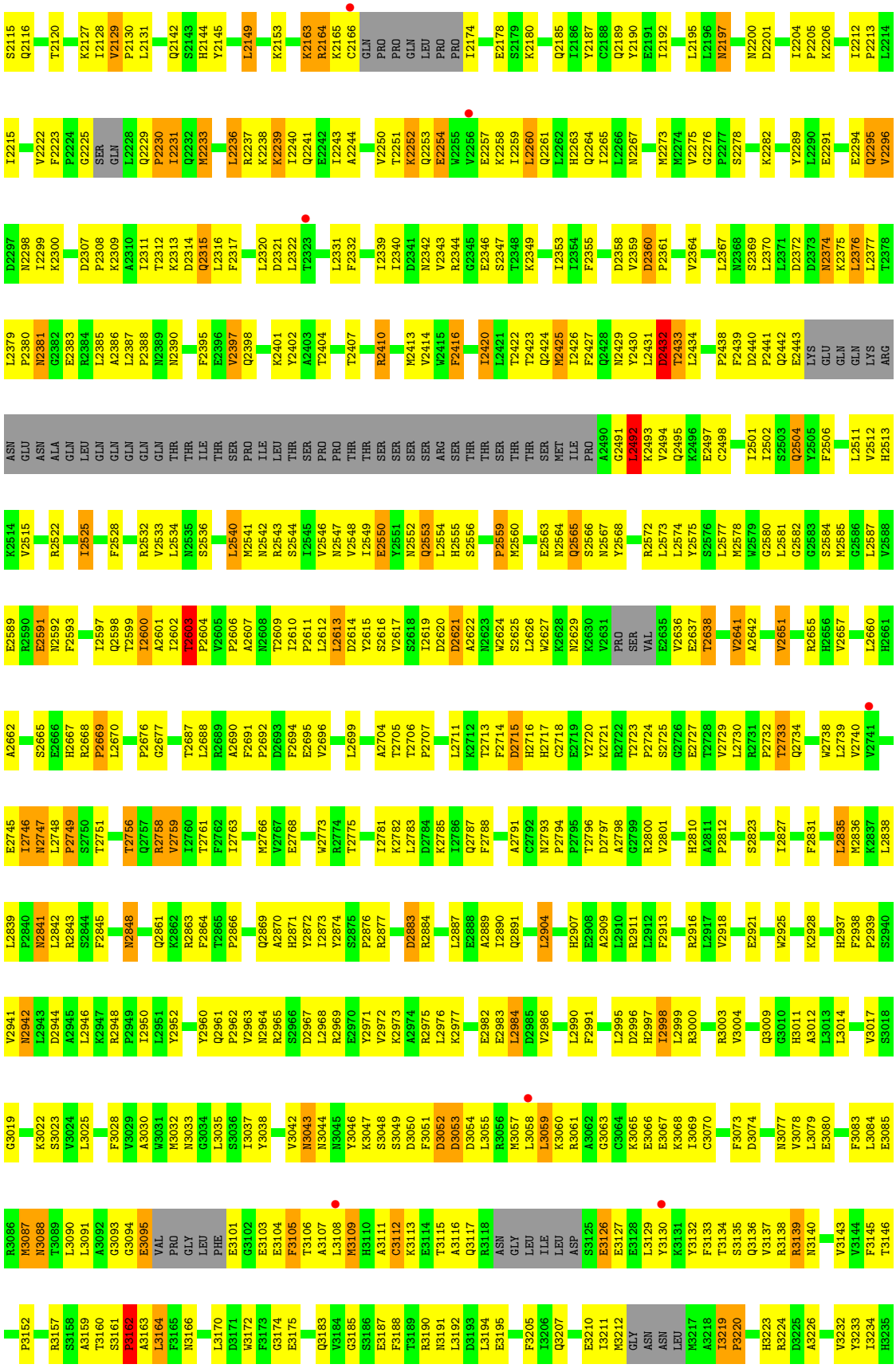


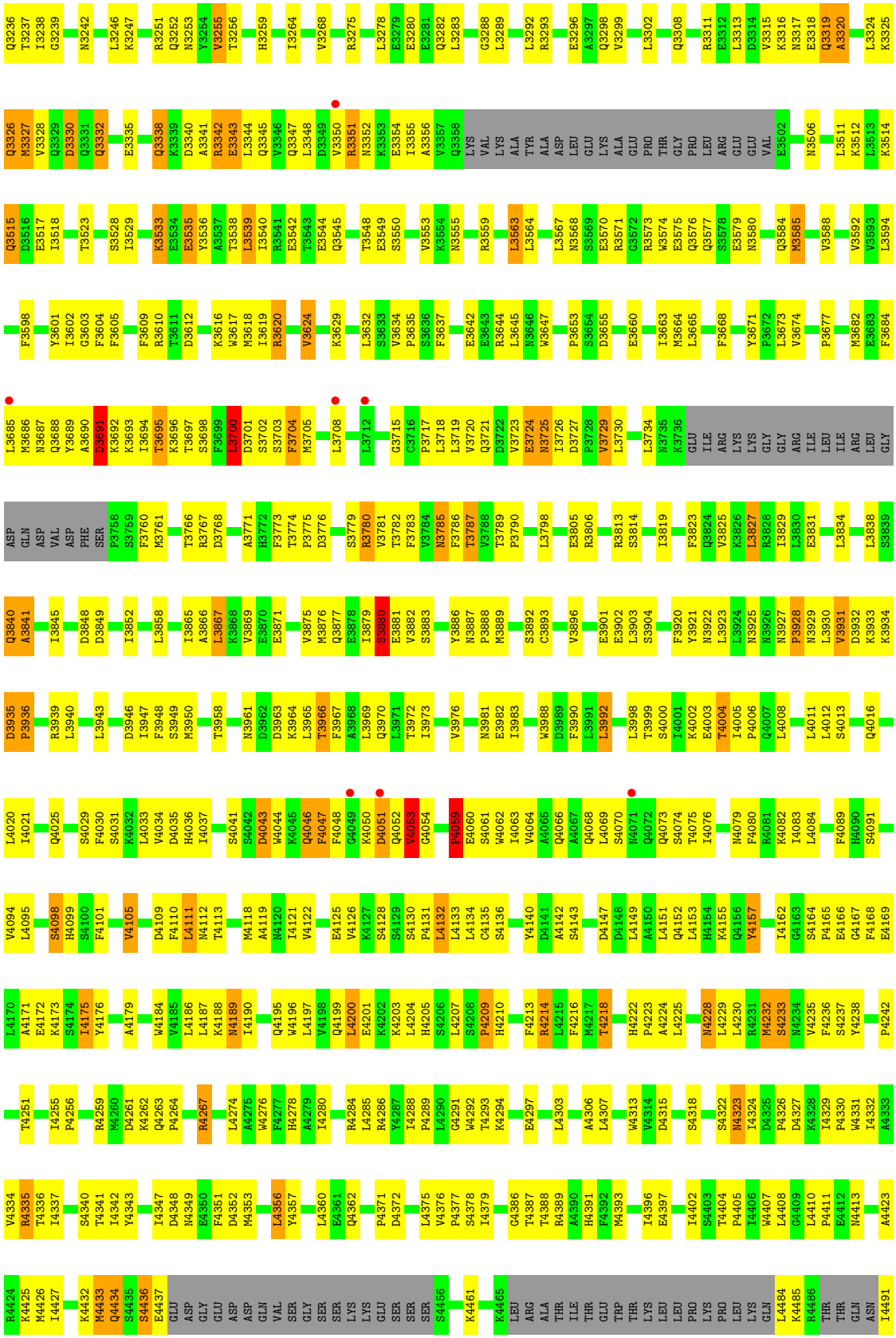


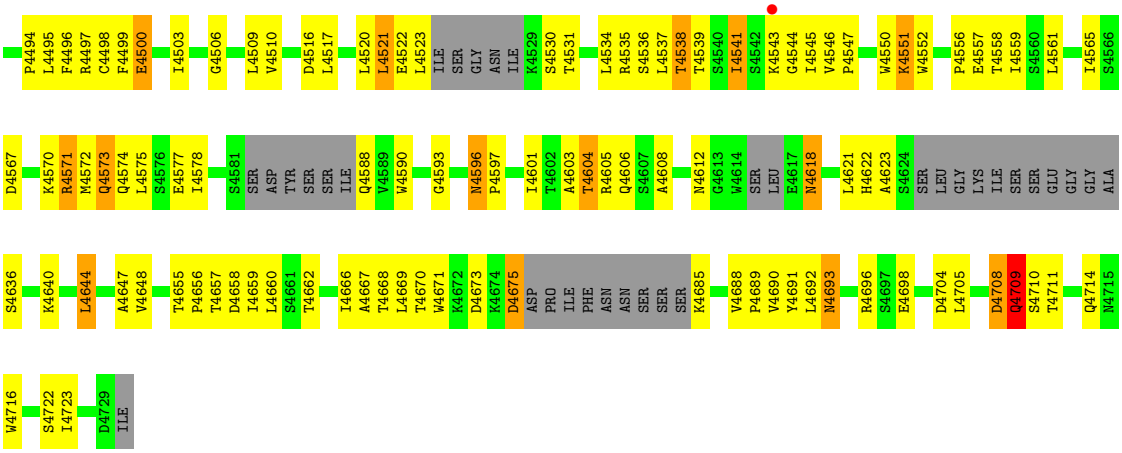
• Molecule 1: Dynein heavy chain, cytoplasmic

Chain B:








P4494 L4495 F4496 R4497 C4498 F4499 E4500 I4503 G4506 L4509 V4510 D4516 L4517 L4520 L4521 E4522 L4523 ILE SER GLY ASN ILE K4529 S4530 T4531 L4534 R4535 S4536 L4537 T4538 T4539 S4540 I4541 S4542 K4543 G4544 I4545 V4546 P4547 W4550 K4551 W4552 P4556 E4557 T4558 I4559 S4560 L4561 I4565 S4566
D4567 K4570 R4571 M4572 Q4573 Q4574 L4575 S4576 E4577 I4578 S4581 SER ASP TYR SER SER ILE Q4588 V4589 W4590 G4593 N4596 P4597 I4601 T4602 A4603 T4604 R4605 Q4606 S4607 A4608 N4612 G4613 W4614 SER LEU E4617 N4618 L4621 H4622 A4623 S4624 SER LEU GLY LYS ILE SER SER GLU GLY GLY ALA
S4636 K4640 L4644 A4647 V4648 T4655 P4656 T4657 D4658 I4659 L4660 S4661 T4662 I4666 A4667 T4668 L4669 T4670 W4671 K4672 D4673 K4674 D4675 ASP PRO ILE PHE ASN ASN SER SER SER K4685 V4688 P4689 V4690 Y4691 L4692 W4693 R4696 S4697 E4698 D4704 L4705 D4708 Q4709 S4710 T4711 Q4714 N4715
W4716 S4722 I4723 D4729 ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	204.26Å 221.81Å 192.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.45 – 2.81 96.45 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (96.45-2.81) 98.1 (96.45-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.82Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.262 , 0.319 0.255 , 0.313	Depositor DCC
R_{free} test set	10425 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	45284	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, ADP, SPM

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	0.50	0/23297	0.67	0/31692
1	B	0.47	0/22599	0.67	3/30724 (0.0%)
All	All	0.48	0/45896	0.67	3/62416 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2376	LEU	CA-CB-CG	6.25	129.68	115.30
1	B	4054	GLY	N-CA-C	-5.92	98.30	113.10
1	B	3219	ILE	C-N-CD	-5.09	109.41	120.60

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	22821	0	21998	1375	0
1	B	22146	0	21438	1397	0
2	A	108	0	48	14	0
2	B	108	0	48	9	0
3	A	28	0	52	2	0
3	B	28	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	23	0	0	1	0
5	B	19	0	0	1	0
All	All	45284	0	43636	2766	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 31.

All (2766) 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:3330:ASP:HB3	1:A:3532:TYR:HE2	1.12	1.12
1:A:2902:VAL:HG21	1:A:2941:VAL:HG21	1.31	1.12
1:A:3766:THR:HG22	1:A:3768:ASP:H	1.14	1.09
1:A:2548:VAL:HG11	1:A:2565:GLN:HE21	1.20	1.06
1:B:1655:LEU:H	1:B:1655:LEU:HD22	1.20	1.05
1:A:2000:CYS:HB3	1:A:2031:LEU:HD13	1.34	1.04
1:A:2641:VAL:HG12	1:A:2642:ALA:H	1.14	1.04
1:B:3700:LEU:HD13	1:B:3701:ASP:N	1.72	1.03
1:B:2129:VAL:HG22	1:B:2130:PRO:HD3	1.38	1.03
1:B:4136:SER:HB3	1:B:4238:TYR:HB2	1.40	1.03
1:B:4318:SER:HB3	1:B:4324:ILE:HD11	1.38	1.02
1:B:2381:ASN:HD21	1:B:2383:GLU:HB2	1.17	1.01
1:B:2603:THR:HG22	1:B:2604:PRO:HD2	1.41	1.01
1:A:2688:LEU:HD13	1:A:2696:VAL:HG11	1.44	0.99
1:A:2011:ARG:HB3	1:A:2011:ARG:HH11	1.27	0.99
1:B:4091:SER:H	3:B:9022:SPM:H132	1.25	0.99
1:A:3571:ARG:NH1	1:A:3571:ARG:HB3	1.78	0.99
1:B:4013:SER:H	1:B:4016:GLN:HE21	1.07	0.98
1:B:1653:ALA:HB1	1:B:1655:LEU:HD23	1.43	0.98
1:B:1813:GLN:HE22	1:B:1941:LEU:H	0.99	0.98
1:B:4222:HIS:CD2	1:B:4224:ALA:H	1.81	0.98
1:A:4349:ASN:ND2	1:A:4352:ASP:H	1.62	0.97
1:A:3817:LEU:HA	1:A:3820:GLN:HE21	1.26	0.97
1:B:2746:ILE:O	1:B:2749:PRO:HD2	1.64	0.97
1:B:3139:ARG:HG3	1:B:3139:ARG:HH11	1.30	0.97
1:B:1886:ARG:HH11	1:B:1890:ARG:NH1	1.61	0.97
1:B:4222:HIS:HD2	1:B:4224:ALA:H	0.97	0.96
1:A:3109:MET:SD	1:A:3126:GLU:HG2	2.05	0.96
1:B:2766:MET:HE2	1:B:2783:LEU:HD11	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1640:ASN:HD21	1:B:1644:ILE:HD11	1.31	0.95
1:B:4618:ASN:H	1:B:4618:ASN:HD22	1.11	0.95
1:A:4349:ASN:HD22	1:A:4352:ASP:H	0.98	0.94
1:A:2370:LEU:HD21	1:A:2387:LEU:HB2	1.50	0.94
1:A:1555:VAL:H	1:A:1609:GLN:HE22	1.16	0.94
1:A:1477:LYS:H	1:A:1480:HIS:HD2	0.94	0.94
1:A:4188:LYS:HA	1:A:4218:THR:HG22	1.47	0.93
1:B:4164:SER:HB3	1:B:4165:PRO:HD2	1.50	0.93
1:A:1477:LYS:H	1:A:1480:HIS:CD2	1.86	0.93
1:B:1605:TRP:HH2	1:B:1650:VAL:HG21	1.35	0.92
1:B:2000:CYS:HB3	1:B:2031:LEU:HD13	1.51	0.92
1:A:3330:ASP:HB3	1:A:3532:TYR:CE2	2.05	0.92
1:B:2515:VAL:HG11	1:B:2577:LEU:HD13	1.52	0.92
1:B:4484:LEU:HD21	1:B:4496:PHE:CE1	2.06	0.91
1:A:1859:LEU:HB3	1:A:1879:ILE:HD11	1.51	0.91
1:B:3724:GLU:OE2	1:B:3766:THR:HG23	1.70	0.91
1:A:1813:GLN:HE22	1:A:1941:LEU:H	1.17	0.91
1:B:4618:ASN:H	1:B:4618:ASN:ND2	1.69	0.91
1:A:3806:ARG:HG3	1:A:3882:VAL:HG11	1.52	0.91
1:B:3043:ASN:ND2	1:B:3046:TYR:HB2	1.84	0.90
1:B:4693:ASN:HD22	1:B:4693:ASN:H	1.19	0.90
1:A:1415:LYS:O	1:A:1498:THR:HB	1.70	0.90
1:B:4709:GLN:HE21	1:B:4709:GLN:N	1.67	0.90
1:B:1560:ASP:HA	1:B:1563:ASN:HB2	1.53	0.90
1:A:1611:ARG:HD3	1:A:1680:GLN:OE1	1.71	0.89
1:B:4657:THR:HG22	1:B:4658:ASP:H	1.35	0.89
1:B:4322:SER:C	1:B:4323:ASN:HD22	1.75	0.89
1:A:2641:VAL:CG1	1:A:2642:ALA:H	1.86	0.89
1:B:1813:GLN:NE2	1:B:1941:LEU:H	1.69	0.89
1:B:4709:GLN:HE21	1:B:4709:GLN:H	0.89	0.89
1:A:2247:ARG:HH22	1:A:2287:GLU:HB3	1.37	0.89
1:B:4251:THR:HG23	1:B:4303:LEU:HD21	1.54	0.89
1:A:3935:ASP:OD1	1:A:3936:PRO:HD2	1.72	0.88
1:A:2059:LEU:HG	1:A:2060:LEU:HD12	1.55	0.88
1:A:3936:PRO:HG2	1:A:3937:ASN:H	1.38	0.88
1:B:3105:PHE:O	1:B:3109:MET:HG3	1.74	0.88
1:B:1740:THR:HB	1:B:1759:SER:HA	1.56	0.88
1:A:3673:LEU:HD13	1:A:3783:PHE:CE1	2.08	0.88
1:A:2044:GLN:NE2	1:A:2090:ASN:HB2	1.88	0.88
1:B:3785:ASN:HD21	1:B:3787:THR:HG23	1.39	0.88
1:A:4210:HIS:ND1	1:A:4211:PRO:HD2	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3512:LYS:HA	1:B:3515:GLN:HE21	1.37	0.87
1:A:3636:SER:HA	1:A:3644:ARG:NH2	1.88	0.87
1:A:1547:ASN:HA	1:A:1553:LYS:HG2	1.57	0.87
1:B:1831:LEU:HD21	1:B:1892:LEU:HD23	1.57	0.86
1:A:1573:SER:HA	1:A:1576:LYS:HE2	1.57	0.86
1:B:4604:THR:HG23	1:B:4671:TRP:HE1	1.38	0.86
1:B:2638:THR:HG21	1:B:2838:LEU:HD21	1.56	0.85
1:A:1639:ILE:HD11	1:A:1675:LEU:HB3	1.57	0.85
1:B:2841:ASN:HD22	1:B:2841:ASN:H	1.25	0.85
1:A:3139:ARG:HH11	1:A:3139:ARG:HG3	1.42	0.85
1:A:3007:GLN:NE2	1:A:3008:PRO:HD2	1.92	0.84
1:B:1562:PHE:HA	1:B:1565:LEU:HB3	1.59	0.84
1:B:3700:LEU:HD13	1:B:3701:ASP:H	1.39	0.84
1:A:2405:LEU:HA	1:A:2408:ILE:HD11	1.58	0.84
1:A:3362:ALA:HB1	1:A:3497:LEU:HD11	1.59	0.84
1:A:3074:ASP:H	1:A:3077:ASN:ND2	1.74	0.84
1:A:2162:ILE:HD13	1:A:2197:ASN:HD22	1.40	0.83
1:A:2929:LYS:O	1:A:2933:VAL:HG23	1.76	0.83
1:A:3317:ASN:HB2	1:A:3546:ILE:HG21	1.61	0.83
1:B:3043:ASN:HD22	1:B:3046:TYR:HB2	1.40	0.83
1:B:4189:ASN:H	1:B:4218:THR:HG22	1.43	0.83
1:A:3864:GLU:HG3	1:A:3865:ILE:N	1.94	0.83
1:B:3602:ILE:HG22	1:B:3664:MET:HE1	1.61	0.83
1:B:4111:LEU:H	1:B:4111:LEU:HD12	1.43	0.83
1:B:4709:GLN:H	1:B:4709:GLN:NE2	1.74	0.83
1:B:2938:PHE:O	1:B:2941:VAL:HG12	1.78	0.83
1:B:3139:ARG:HG3	1:B:3139:ARG:NH1	1.89	0.83
1:B:2598:GLN:HG3	1:B:2612:LEU:HB2	1.60	0.83
1:B:3708:LEU:HD21	1:B:3730:LEU:HD21	1.60	0.83
1:B:3729:VAL:O	1:B:3729:VAL:HG22	1.77	0.82
1:A:4193:ALA:HB1	1:A:4196:TRP:HB3	1.61	0.82
1:A:2381:ASN:HD21	1:A:2383:GLU:HB2	1.44	0.82
1:A:3673:LEU:HD13	1:A:3783:PHE:HE1	1.44	0.82
1:B:3766:THR:HG22	1:B:3768:ASP:H	1.43	0.82
1:A:2439:PHE:H	1:A:2495:GLN:HE22	1.24	0.82
1:A:4636:SER:HB3	1:A:4669:LEU:O	1.79	0.82
1:B:4640:LYS:HB3	1:B:4666:ILE:HD12	1.60	0.82
1:A:1690:GLN:HE22	1:A:1766:ILE:HG21	1.42	0.82
1:A:2286:TRP:O	1:A:2290:LEU:HB2	1.79	0.82
1:A:2142:GLN:N	1:A:2142:GLN:HE21	1.77	0.81
1:B:3256:THR:H	1:B:3259:HIS:CD2	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3990:PHE:HD2	1:B:4084:LEU:HD22	1.45	0.81
1:B:1555:VAL:HG22	1:B:1609:GLN:HE21	1.44	0.81
1:B:2112:MET:O	1:B:2116:GLN:HG2	1.80	0.81
1:B:4119:ALA:HA	1:B:4149:LEU:HD11	1.62	0.81
1:A:3200:ILE:O	1:A:3202:PRO:HD3	1.80	0.81
1:B:1655:LEU:H	1:B:1655:LEU:CD2	1.92	0.81
1:A:3024:VAL:HG23	2:A:9004:ADP:O2A	1.79	0.81
1:A:3670:ARG:HD2	5:A:38:HOH:O	1.80	0.81
1:B:2375:LYS:HB3	1:B:2387:LEU:HB3	1.60	0.81
1:A:3665:LEU:HD13	1:A:3685:LEU:HD21	1.60	0.81
1:B:4604:THR:CG2	1:B:4671:TRP:HE1	1.94	0.81
1:B:2498:CYS:HA	1:B:2501:ILE:HD12	1.62	0.81
1:A:2552:ASN:ND2	1:A:2560:MET:H	1.78	0.81
1:B:2657:VAL:HG13	1:B:2687:THR:HG23	1.62	0.81
1:A:4349:ASN:ND2	1:A:4351:PHE:H	1.79	0.80
1:B:3126:GLU:O	1:B:3129:LEU:HB3	1.82	0.80
1:A:1477:LYS:N	1:A:1480:HIS:HD2	1.79	0.80
1:A:1813:GLN:NE2	1:A:1941:LEU:H	1.80	0.80
1:A:2552:ASN:HD21	1:A:2560:MET:H	1.25	0.80
1:B:2533:VAL:HB	1:B:2581:LEU:HD22	1.62	0.80
1:A:1766:ILE:HG23	1:A:1767:HIS:H	1.47	0.80
1:A:2391:VAL:O	1:A:2392:ARG:HD2	1.82	0.80
1:B:2309:LYS:NZ	1:B:2756:THR:HG21	1.95	0.80
1:B:3130:TYR:O	1:B:3134:THR:HG23	1.81	0.80
1:B:3972:THR:HG23	1:B:4105:VAL:HG21	1.63	0.79
1:B:1739:THR:O	1:B:1760:ILE:HG12	1.82	0.79
1:B:3355:ILE:HD12	1:B:3511:LEU:HD22	1.64	0.79
1:B:4013:SER:H	1:B:4016:GLN:NE2	1.79	0.79
1:A:4109:ASP:HA	1:A:4112:ASN:ND2	1.97	0.79
1:B:3017:VAL:HG23	1:B:3174:GLY:O	1.82	0.79
1:B:3930:LEU:HD11	1:B:3943:LEU:HD21	1.65	0.79
1:B:4574:GLN:HE22	1:B:4590:TRP:H	1.30	0.79
1:A:3352:ASN:ND2	1:A:3515:GLN:OE1	2.15	0.79
1:B:1553:LYS:O	1:B:1647:LEU:HD13	1.82	0.79
1:B:3139:ARG:HH11	1:B:3139:ARG:CG	1.96	0.79
1:B:3785:ASN:ND2	1:B:3787:THR:HG23	1.97	0.79
1:B:1735:ASP:OD2	1:B:1740:THR:HG23	1.84	0.78
1:B:3947:ILE:HG13	1:B:3948:PHE:H	1.45	0.78
1:A:3929:ASN:ND2	1:A:3942:TYR:HD1	1.81	0.78
1:B:2379:LEU:HD12	1:B:2383:GLU:HG2	1.64	0.78
1:A:2312:THR:OG1	1:A:2315:GLN:HG3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2706:THR:HA	1:B:2759:VAL:HG22	1.65	0.78
1:B:2835:LEU:HD11	1:B:2890:ILE:HD12	1.65	0.78
1:B:1813:GLN:HE22	1:B:1941:LEU:N	1.81	0.78
1:A:2684:LEU:HD22	1:A:2789:VAL:HG11	1.64	0.78
1:B:1886:ARG:NH1	1:B:1890:ARG:NH1	2.30	0.78
1:B:3768:ASP:HB3	1:B:3771:ALA:HB2	1.64	0.78
1:A:2044:GLN:O	1:A:2048:VAL:HG23	1.83	0.78
1:B:3970:GLN:HE22	1:B:4433:MET:HE2	1.49	0.78
1:B:1851:THR:O	1:B:1854:MET:HB3	1.84	0.78
1:A:4306:ALA:O	1:A:4310:ILE:HG12	1.83	0.78
1:A:3281:GLU:HB3	1:A:3581:PHE:HE1	1.48	0.77
1:B:1556:ARG:HD2	1:B:1556:ARG:O	1.84	0.77
1:A:2641:VAL:HG12	1:A:2642:ALA:N	1.94	0.77
1:B:4690:VAL:HG22	1:B:4723:ILE:HB	1.67	0.77
1:A:3075:GLU:O	1:A:3078:VAL:HG12	1.84	0.77
1:B:4020:LEU:HG	1:B:4034:VAL:HG22	1.66	0.77
1:A:3074:ASP:H	1:A:3077:ASN:HD22	1.31	0.77
1:A:1465:ASN:HA	1:A:1468:ILE:HD12	1.67	0.77
1:A:1842:GLN:OE1	1:A:1842:GLN:HA	1.85	0.77
1:A:3817:LEU:HA	1:A:3820:GLN:NE2	2.00	0.77
1:B:2238:LYS:HA	1:B:2241:GLN:HE21	1.50	0.77
1:B:3966:THR:HG22	1:B:4426:MET:HG3	1.66	0.77
1:B:3074:ASP:O	1:B:3077:ASN:HB2	1.85	0.76
1:A:3326:GLN:O	1:A:3330:ASP:HB2	1.84	0.76
1:A:4605:ARG:O	1:A:4609:SER:HB3	1.85	0.76
1:B:4188:LYS:HA	1:B:4218:THR:HG22	1.65	0.76
1:A:1875:PHE:O	1:A:1879:ILE:HG12	1.86	0.76
1:B:1565:LEU:HD23	1:B:1565:LEU:O	1.85	0.76
1:B:2745:GLU:HG3	1:B:2748:LEU:HG	1.66	0.76
1:B:4484:LEU:HD21	1:B:4496:PHE:HE1	1.46	0.76
1:A:3571:ARG:HB3	1:A:3571:ARG:HH11	1.48	0.76
1:B:1863:VAL:HG22	1:B:1872:ARG:HH11	1.49	0.76
1:A:2011:ARG:HB3	1:A:2011:ARG:NH1	2.00	0.75
1:A:2266:LEU:HD22	1:A:2392:ARG:HG2	1.67	0.75
1:A:3862:THR:HG23	1:A:3863:THR:N	2.01	0.75
1:A:2793:ASN:HD22	1:A:2800:ARG:HE	1.33	0.75
1:B:4393:MET:HE2	1:B:4396:ILE:HD12	1.68	0.75
1:A:2886:LEU:O	1:A:2890:ILE:HG12	1.87	0.75
1:B:3602:ILE:HD12	1:B:3610:ARG:HG2	1.66	0.75
1:B:1655:LEU:HB2	1:B:1658:GLU:HB2	1.68	0.75
1:B:4323:ASN:HD22	1:B:4323:ASN:N	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3723:VAL:HG22	1:A:3723:VAL:O	1.87	0.74
1:A:3862:THR:CG2	1:A:3863:THR:H	2.00	0.74
1:B:1546:VAL:HG11	1:B:1556:ARG:NH1	2.01	0.74
1:B:4313:TRP:HB3	1:B:4330:PRO:CG	2.17	0.74
1:B:3037:ILE:HD13	1:B:3070:CYS:HB3	1.70	0.74
1:B:4379:ILE:O	1:B:4379:ILE:HG12	1.86	0.74
1:A:3342:ARG:HH11	1:A:3345:GLN:HE22	1.36	0.74
1:A:3834:LEU:HA	1:A:3854:THR:HG21	1.67	0.74
1:A:4213:PHE:O	1:A:4214:ARG:HG2	1.86	0.74
1:A:4220:GLU:O	1:A:4222:HIS:N	2.21	0.74
1:B:1899:THR:HB	1:B:1903:ASP:HB2	1.68	0.74
1:B:3219:ILE:CB	1:B:3220:PRO:HD3	2.17	0.74
1:B:3139:ARG:HG3	1:B:3139:ARG:O	1.87	0.74
1:B:1777:MET:CE	1:B:1939:GLU:HA	2.17	0.74
1:B:4060:GLU:O	1:B:4064:VAL:HG23	1.87	0.74
1:B:2104:ASP:O	1:B:2108:ILE:HG13	1.87	0.74
1:B:3973:ILE:HG13	1:B:3988:TRP:CZ3	2.22	0.74
1:A:2525:ILE:HG12	1:A:2815:LEU:HD12	1.70	0.74
1:B:4484:LEU:HD23	1:B:4484:LEU:C	2.09	0.74
1:B:4693:ASN:H	1:B:4693:ASN:ND2	1.85	0.74
1:B:4657:THR:HG22	1:B:4658:ASP:N	2.02	0.73
1:A:2426:ILE:HD12	1:A:2530:ARG:NH1	2.02	0.73
1:B:2793:ASN:HD22	1:B:2800:ARG:NH2	1.86	0.73
1:B:3700:LEU:CD1	1:B:3701:ASP:N	2.50	0.73
1:A:4569:SER:O	1:A:4573:GLN:HG3	1.87	0.73
1:A:1967:ARG:NH2	1:A:2069:GLN:O	2.21	0.73
1:A:4405:PRO:HG2	1:A:4412:GLU:HA	1.69	0.73
1:A:4572:MET:O	1:A:4575:LEU:HB2	1.87	0.73
1:A:1766:ILE:HG23	1:A:1767:HIS:N	2.02	0.73
1:A:3253:ASN:HB2	1:A:3604:PHE:CE2	2.24	0.73
1:B:4657:THR:HG22	1:B:4659:ILE:H	1.53	0.73
1:B:2294:GLU:HG3	1:B:2299:ILE:O	1.88	0.73
1:B:3239:GLY:O	1:B:3242:ASN:HB2	1.88	0.73
1:B:3700:LEU:CD1	1:B:3701:ASP:H	2.02	0.73
1:A:3219:ILE:CB	1:A:3220:PRO:CD	2.67	0.73
1:A:4349:ASN:ND2	1:A:4352:ASP:N	2.36	0.73
1:B:3966:THR:CG2	1:B:4426:MET:HG3	2.19	0.73
1:B:4294:LYS:NZ	1:B:4348:ASP:OD1	2.22	0.72
1:A:2877:ARG:O	1:A:2881:ARG:HG3	1.89	0.72
1:A:3199:TYR:O	1:A:3200:ILE:HG13	1.89	0.72
1:A:3335:GLU:HG3	1:A:3529:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2606:PRO:HD3	1:B:2624:TRP:CD1	2.24	0.72
1:B:2887:LEU:O	1:B:2891:GLN:HG3	1.89	0.72
1:B:4213:PHE:O	1:B:4214:ARG:HG2	1.89	0.72
1:A:1797:VAL:HG12	1:A:1854:MET:HE1	1.72	0.72
1:A:1797:VAL:HG13	1:A:1855:ILE:HD11	1.69	0.72
1:B:2642:ALA:HB3	1:B:2884:ARG:CG	2.19	0.72
1:A:1666:GLN:O	1:A:1670:GLU:HG3	1.89	0.72
1:A:2890:ILE:HA	1:A:2893:MET:HE2	1.72	0.72
1:A:3789:THR:HG22	1:A:3792:SER:H	1.55	0.72
1:A:4657:THR:H	1:A:4719:ARG:HH22	1.38	0.72
1:B:4189:ASN:H	1:B:4218:THR:CG2	2.02	0.72
1:A:1811:PRO:HD2	1:A:1814:LEU:HD12	1.72	0.72
1:A:4197:LEU:HD22	1:A:4197:LEU:H	1.55	0.72
1:A:1972:PRO:HG2	1:A:2076:THR:HG22	1.72	0.72
1:A:4316:LEU:HD23	1:A:4317:TYR:HE2	1.55	0.72
1:B:3686:MET:CE	1:B:3696:LYS:HB2	2.19	0.72
1:B:3767:ARG:HD3	1:B:4205:HIS:CE1	2.24	0.72
1:B:4337:ILE:O	1:B:4341:THR:HB	1.89	0.72
1:A:1719:GLN:HA	1:A:1722:PHE:CD2	2.25	0.72
1:B:2717:HIS:O	1:B:2733:THR:HG22	1.89	0.72
1:A:3256:THR:H	1:A:3259:HIS:HD2	1.37	0.72
1:B:2438:PRO:HA	1:B:2495:GLN:HE22	1.55	0.72
1:B:3540:ILE:O	1:B:3544:GLU:HG3	1.88	0.72
1:B:4618:ASN:HD22	1:B:4618:ASN:N	1.85	0.72
1:A:2048:VAL:O	1:A:2052:GLU:HG3	1.90	0.71
1:B:1605:TRP:CH2	1:B:1650:VAL:HG21	2.22	0.71
1:A:1604:VAL:O	1:A:1608:VAL:HG23	1.90	0.71
1:A:2641:VAL:HB	1:A:2887:LEU:HD22	1.71	0.71
1:B:3112:CYS:SG	1:B:3133:PHE:HB2	2.29	0.71
1:B:4601:ILE:O	1:B:4604:THR:HG22	1.90	0.71
1:A:1704:ASP:HB3	1:A:1721:HIS:CE1	2.24	0.71
1:A:3015:ILE:HG22	1:A:3149:PRO:HG3	1.70	0.71
1:B:1630:PRO:HG2	1:B:1631:ALA:H	1.56	0.71
1:B:2642:ALA:HB3	1:B:2884:ARG:HG2	1.72	0.71
1:B:3695:THR:HB	1:B:3718:LEU:HD12	1.71	0.71
1:A:1817:LEU:O	1:A:1821:ILE:HG13	1.90	0.71
1:B:2611:PRO:HD2	1:B:2614:ASP:OD2	1.89	0.71
1:A:2422:THR:HG22	1:A:2424:GLN:H	1.56	0.71
1:A:3331:GLN:HG3	1:A:3532:TYR:CB	2.21	0.71
1:A:3766:THR:HG22	1:A:3768:ASP:N	1.97	0.71
1:A:2327:TRP:CZ3	1:A:2380:PRO:HD2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2641:VAL:HG12	1:B:2642:ALA:N	2.05	0.71
1:B:3059:LEU:HD23	1:B:3137:VAL:HG21	1.71	0.71
1:A:2259:ILE:HG23	1:A:2289:TYR:HB2	1.72	0.71
1:A:2877:ARG:HG3	2:A:9003:ADP:H4'	1.71	0.71
1:B:2370:LEU:HD12	1:B:2377:LEU:HB2	1.72	0.71
1:A:2199:ILE:O	1:A:2203:MET:HB2	1.91	0.71
1:B:1711:ASN:ND2	1:B:1717:LYS:HD3	2.06	0.71
1:B:1886:ARG:HD3	1:B:1890:ARG:CZ	2.20	0.71
1:A:2011:ARG:HH11	1:A:2011:ARG:CB	2.03	0.70
1:B:3207:GLN:HA	1:B:3210:GLU:HG3	1.74	0.70
1:B:1886:ARG:NH1	1:B:1890:ARG:HH12	1.89	0.70
1:A:1640:ASN:O	1:A:1644:ILE:HG12	1.91	0.70
1:B:2174:ILE:HD13	1:B:2180:LYS:HD2	1.73	0.70
1:B:2187:TYR:O	1:B:2190:TYR:HB3	1.92	0.70
1:B:2937:HIS:C	1:B:2939:PRO:HD3	2.11	0.70
1:A:2350:ARG:HG2	1:A:2350:ARG:HH11	1.56	0.70
1:A:2940:SER:HB3	1:B:4000:SER:O	1.91	0.70
1:B:4313:TRP:HB3	1:B:4330:PRO:HG2	1.73	0.70
1:B:4711:THR:OG1	1:B:4716:TRP:NE1	2.24	0.70
1:A:3862:THR:HG23	1:A:3863:THR:H	1.57	0.70
1:A:4242:PRO:HA	1:A:4286:ARG:NH1	2.07	0.70
1:B:2603:THR:CG2	1:B:2604:PRO:HD2	2.21	0.70
1:B:3351:ARG:O	1:B:3355:ILE:HG13	1.92	0.70
1:A:3038:TYR:OH	1:A:3054:ASP:HB3	1.92	0.70
1:A:3335:GLU:HG3	1:A:3529:ILE:CD1	2.22	0.70
1:B:1803:TYR:OH	1:B:1878:LEU:HD21	1.92	0.70
1:B:4685:LYS:HD3	1:B:4704:ASP:HB3	1.71	0.70
1:A:2263:HIS:HB2	1:A:2289:TYR:CE1	2.27	0.70
1:A:2338:ARG:HH11	1:A:2338:ARG:HG2	1.56	0.70
1:A:3333:ALA:HA	1:A:3336:ILE:HD12	1.74	0.70
1:A:4185:VAL:HB	1:A:4215:LEU:HD12	1.73	0.70
1:B:1671:ARG:O	1:B:1675:LEU:HG	1.92	0.70
1:B:4167:GLY:O	1:B:4171:ALA:HB2	1.92	0.70
1:B:4318:SER:CB	1:B:4324:ILE:HD11	2.20	0.70
1:A:2708:GLU:HA	1:A:2711:LEU:HD12	1.74	0.69
1:B:2863:ARG:HG3	1:B:2925:TRP:CE2	2.27	0.69
1:A:2203:MET:H	1:A:2205:PRO:HD2	1.55	0.69
1:B:2361:PRO:HD3	1:B:2402:TYR:O	1.91	0.69
1:A:3636:SER:HA	1:A:3644:ARG:HH21	1.55	0.69
1:B:3080:GLU:O	1:B:3083:PHE:HB2	1.91	0.69
1:B:4222:HIS:HD2	1:B:4224:ALA:N	1.81	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4011:LEU:HD11	1:B:4041:SER:HB2	1.73	0.69
1:B:1777:MET:HE1	1:B:1939:GLU:HA	1.75	0.69
1:B:3256:THR:H	1:B:3259:HIS:HD2	1.40	0.69
1:B:3886:TYR:O	1:B:3889:MET:HG3	1.92	0.69
1:A:3364:ALA:C	1:A:3366:LEU:H	1.95	0.69
1:B:1832:GLY:HA3	1:B:1836:LEU:HD13	1.75	0.69
1:B:3664:MET:O	1:B:3668:PHE:HB3	1.93	0.69
1:B:4389:ARG:HG2	1:B:4389:ARG:HH11	1.56	0.69
1:A:1851:THR:O	1:A:1854:MET:HB3	1.93	0.69
1:B:4331:TRP:O	1:B:4335:ARG:HB2	1.93	0.69
1:A:2725:SER:HB3	1:A:2727:GLU:HG3	1.75	0.68
1:A:4259:ARG:NH1	1:A:4311:ASP:OD2	2.26	0.68
1:B:1548:TYR:HE2	1:B:1613:VAL:HG22	1.59	0.68
1:A:2918:VAL:O	1:A:2918:VAL:HG12	1.94	0.68
1:A:3139:ARG:HG3	1:A:3139:ARG:NH1	2.07	0.68
1:B:3602:ILE:HG23	1:B:3610:ARG:HG2	1.72	0.68
1:B:4506:GLY:O	1:B:4510:VAL:HG23	1.92	0.68
1:B:4556:PRO:O	1:B:4559:ILE:HG22	1.92	0.68
1:A:2127:LYS:HE3	1:A:2222:VAL:O	1.93	0.68
1:B:3689:TYR:HB2	1:B:3694:ILE:HD12	1.76	0.68
1:B:4189:ASN:N	1:B:4189:ASN:HD22	1.90	0.68
1:A:3929:ASN:HD21	1:A:3942:TYR:HD1	1.42	0.68
1:B:3108:LEU:HD11	1:B:3133:PHE:CE2	2.28	0.68
1:B:4225:LEU:HD23	1:B:4230:LEU:HD21	1.76	0.68
1:B:4604:THR:HG23	1:B:4604:THR:O	1.92	0.68
1:A:3000:ARG:HD2	1:A:3171:ASP:OD2	1.94	0.68
1:B:3338:GLN:HA	1:B:3338:GLN:HE21	1.57	0.68
1:A:3180:ALA:O	1:A:3184:VAL:HG23	1.93	0.68
1:A:4368:ALA:HA	1:A:4373:PHE:CE1	2.28	0.68
1:B:2381:ASN:ND2	1:B:2383:GLU:HB2	2.00	0.68
1:B:2358:ASP:OD2	1:B:2756:THR:HB	1.93	0.68
1:A:1417:THR:HB	1:A:1422:ILE:HG22	1.76	0.68
1:A:1857:ASN:O	1:A:1860:ALA:HB3	1.93	0.68
1:A:1735:ASP:N	1:A:1742:ILE:HD11	2.08	0.68
1:A:2036:LEU:O	1:A:2040:SER:HB3	1.93	0.67
1:B:2308:PRO:HG3	1:B:2355:PHE:HB3	1.76	0.67
1:B:2591:GLU:HA	1:B:2613:LEU:HD12	1.76	0.67
1:A:2128:ILE:HD12	1:A:2131:LEU:HD23	1.77	0.67
1:A:2142:GLN:HE21	1:A:2142:GLN:CA	2.06	0.67
1:A:2381:ASN:ND2	1:A:2383:GLU:HB2	2.09	0.67
1:A:2501:ILE:HD13	1:A:2566:SER:HA	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1859:LEU:HB3	1:A:1879:ILE:CD1	2.24	0.67
1:A:4293:THR:HB	1:A:4352:ASP:OD1	1.93	0.67
1:B:1653:ALA:HB1	1:B:1655:LEU:CD2	2.22	0.67
1:A:4200:LEU:HD22	1:A:4204:LEU:CD1	2.25	0.67
1:B:2129:VAL:HG22	1:B:2130:PRO:CD	2.21	0.67
1:B:2332:PHE:CE1	1:B:2353:ILE:HG21	2.29	0.67
1:B:3690:ALA:O	1:B:3693:LYS:N	2.27	0.67
1:B:4351:PHE:CD2	1:B:4689:PRO:HG3	2.29	0.67
1:A:2607:ALA:C	1:A:2609:THR:H	1.97	0.67
1:A:3197:PRO:O	1:A:3198:GLN:HG3	1.94	0.67
1:A:3973:ILE:HG13	1:A:3988:TRP:CZ3	2.29	0.67
1:A:2911:ARG:HD3	1:A:2915:ASP:OD2	1.95	0.67
1:B:3512:LYS:HA	1:B:3515:GLN:NE2	2.09	0.67
1:A:3153:ASP:OD1	1:A:3156:ASN:ND2	2.28	0.67
1:A:3853:SER:OG	1:A:3854:THR:N	2.28	0.67
1:A:4121:ILE:O	1:A:4126:VAL:HG12	1.94	0.67
1:B:4133:LEU:HD23	1:B:4230:LEU:HD23	1.75	0.67
1:A:1554:LEU:HD22	1:A:1609:GLN:HG3	1.76	0.67
1:A:2290:LEU:HD11	1:A:2352:TRP:CD2	2.30	0.67
1:A:2378:THR:O	1:A:2378:THR:HG23	1.95	0.67
1:A:3163:ALA:HB1	1:A:3167:ARG:HG3	1.76	0.67
1:B:2793:ASN:ND2	1:B:2800:ARG:NH2	2.41	0.67
1:B:3827:LEU:HD12	1:B:3827:LEU:O	1.95	0.67
1:A:2284:THR:O	1:A:2288:VAL:HG23	1.94	0.67
1:A:2598:GLN:HG3	1:A:2612:LEU:HB2	1.76	0.67
1:A:4599:ALA:HA	1:A:4602:THR:HG22	1.76	0.67
1:B:1906:TRP:CZ2	1:B:1911:ARG:HG2	2.30	0.67
1:A:1704:ASP:O	1:A:1708:ILE:HG13	1.94	0.66
1:A:2247:ARG:NH2	1:A:2287:GLU:HB3	2.09	0.66
1:B:1811:PRO:O	1:B:1815:VAL:HG23	1.95	0.66
1:B:2375:LYS:HD3	1:B:2387:LEU:HD23	1.77	0.66
1:B:2612:LEU:HD11	1:B:2624:TRP:CH2	2.28	0.66
1:B:2797:ASP:HB2	1:B:2800:ARG:HG3	1.77	0.66
1:B:3042:VAL:HG11	1:B:3079:LEU:HG	1.76	0.66
1:B:4060:GLU:HA	1:B:4063:ILE:HD13	1.76	0.66
1:B:1546:VAL:CG1	1:B:1556:ARG:NH1	2.58	0.66
1:B:1554:LEU:HD22	1:B:1609:GLN:NE2	2.09	0.66
1:B:4494:PRO:HB3	1:B:4606:GLN:HB2	1.77	0.66
1:A:3919:ILE:HD13	1:A:3951:THR:HA	1.75	0.66
1:A:4384:PRO:HB3	1:A:4395:TRP:CD1	2.29	0.66
1:A:2372:ASP:OD1	1:A:2373:ASP:N	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3013:LEU:HD23	1:A:3170:LEU:HD12	1.77	0.66
1:A:3115:THR:HA	1:A:3118:ARG:NH1	2.10	0.66
1:A:3647:TRP:HD1	1:A:3688:GLN:OE1	1.79	0.66
1:B:2839:LEU:HD13	1:B:2842:LEU:HD12	1.78	0.66
1:B:2547:ASN:HB2	1:B:2568:TYR:OH	1.95	0.66
1:A:2504:GLN:O	1:A:2507:GLU:HG2	1.95	0.66
1:A:2610:ILE:HD12	1:A:2615:TYR:OH	1.96	0.66
1:A:4289:PRO:HB2	1:A:4696:ARG:HD2	1.78	0.66
1:A:1555:VAL:H	1:A:1609:GLN:NE2	1.91	0.66
1:A:2616:SER:HB3	1:A:2627:TRP:CE2	2.30	0.66
1:A:4005:ILE:H	1:A:4017:GLN:NE2	1.93	0.66
1:A:4623:ALA:HB2	1:A:4703:ILE:HD11	1.78	0.66
1:B:3514:LYS:HA	1:B:3517:GLU:HG3	1.77	0.66
1:B:4005:ILE:HG21	1:B:4008:LEU:HD12	1.78	0.66
1:A:3118:ARG:C	1:A:3120:GLY:H	1.98	0.66
1:B:1551:LYS:HE2	1:B:1616:GLU:OE1	1.95	0.66
1:B:1791:HIS:O	1:B:1795:VAL:HG23	1.95	0.66
1:B:3903:LEU:HD23	1:B:4433:MET:HE1	1.77	0.66
1:A:3689:TYR:HB2	1:A:3694:ILE:HD11	1.78	0.66
1:B:3682:MET:O	1:B:3686:MET:HG2	1.95	0.66
1:B:4596:ASN:C	1:B:4596:ASN:HD22	1.98	0.66
1:A:2090:ASN:HD22	1:A:2091:LEU:N	1.94	0.65
1:A:2200:ASN:HD22	1:A:2228:LEU:HD22	1.61	0.65
1:A:2405:LEU:HA	1:A:2408:ILE:CD1	2.26	0.65
1:B:2758:ARG:O	1:B:2761:THR:HG22	1.96	0.65
1:B:4169:GLU:HG3	1:B:4173:LYS:HZ2	1.60	0.65
1:A:3817:LEU:O	1:A:3820:GLN:HG2	1.96	0.65
1:A:4136:SER:O	1:A:4220:GLU:HA	1.96	0.65
1:B:1789:LEU:HD23	1:B:1818:THR:HG23	1.78	0.65
1:B:1915:ASP:OD1	1:B:1917:THR:HG23	1.96	0.65
1:A:1962:GLN:CB	1:A:4341:THR:HG21	2.26	0.65
1:B:3686:MET:HE1	1:B:3696:LYS:HB2	1.79	0.65
1:B:4135:CYS:O	1:B:4237:SER:HA	1.94	0.65
1:A:1628:LEU:HD22	1:A:1686:TYR:OH	1.96	0.65
1:B:2388:PRO:HB2	1:B:2390:ASN:OD1	1.97	0.65
1:A:2339:ILE:HA	1:A:2346:GLU:HG2	1.78	0.65
1:A:2488:ILE:O	1:A:2488:ILE:HG22	1.95	0.65
1:A:3062:ALA:HB2	1:A:3069:ILE:HD13	1.78	0.65
1:A:3203:PRO:HG2	1:B:3619:ILE:HD11	1.79	0.65
1:A:3256:THR:H	1:A:3259:HIS:CD2	2.14	0.65
1:B:1610:ARG:HH11	1:B:1610:ARG:HG3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4168:PHE:O	1:B:4171:ALA:HB3	1.97	0.65
1:A:3788:VAL:HG21	1:A:3913:LEU:HD22	1.77	0.65
1:B:4013:SER:N	1:B:4016:GLN:HE21	1.87	0.65
1:B:4534:LEU:O	1:B:4538:THR:HG23	1.96	0.65
1:A:2823:SER:O	1:A:2827:ILE:HG13	1.96	0.65
1:B:2311:ILE:HB	1:B:2315:GLN:HE21	1.60	0.65
1:B:3579:GLU:HA	1:B:3579:GLU:OE2	1.96	0.65
1:A:3086:ARG:HH11	1:A:3096:VAL:HG12	1.61	0.65
1:A:2617:VAL:HG13	1:A:2617:VAL:O	1.97	0.65
1:A:2684:LEU:CD2	1:A:2789:VAL:HG11	2.27	0.65
1:A:4109:ASP:HA	1:A:4112:ASN:HD22	1.59	0.65
1:A:2026:ASP:OD2	1:A:2027:GLU:HG3	1.97	0.65
1:A:2542:ASN:O	1:A:2546:VAL:HG23	1.97	0.65
1:A:4572:MET:HA	1:A:4575:LEU:HD12	1.77	0.65
1:B:4169:GLU:C	1:B:4171:ALA:H	2.00	0.65
1:B:4618:ASN:ND2	1:B:4618:ASN:N	2.41	0.65
1:B:4572:MET:O	1:B:4575:LEU:HB2	1.97	0.64
1:B:2651:VAL:O	1:B:2655:ARG:HG2	1.97	0.64
1:B:4386:GLY:HA3	1:B:4391:HIS:HB3	1.78	0.64
1:A:2641:VAL:CG1	1:A:2642:ALA:N	2.52	0.64
1:A:4660:LEU:HD12	1:A:4660:LEU:N	2.13	0.64
1:B:1788:SER:HA	1:B:1810:TYR:CZ	2.33	0.64
1:B:3038:TYR:OH	1:B:3054:ASP:HB3	1.97	0.64
1:B:4332:ILE:HD12	1:B:4332:ILE:H	1.60	0.64
1:B:4621:LEU:HD13	1:B:4671:TRP:CE2	2.32	0.64
1:A:2653:THR:O	1:A:2657:VAL:HG23	1.97	0.64
1:A:3023:SER:O	1:A:3027:ARG:HG3	1.96	0.64
1:A:3342:ARG:NH1	1:A:3345:GLN:HE22	1.94	0.64
1:A:4494:PRO:HD2	1:A:4610:GLN:HE22	1.62	0.64
1:B:2498:CYS:HA	1:B:2501:ILE:CD1	2.27	0.64
1:B:2877:ARG:HG2	2:B:9009:ADP:H4'	1.79	0.64
1:B:3947:ILE:HG13	1:B:3948:PHE:N	2.12	0.64
1:B:3981:ASN:ND2	1:B:4074:SER:OG	2.29	0.64
1:A:3056:ARG:HH11	1:A:3099:LEU:HD12	1.63	0.64
1:B:2029:ASN:HD22	1:B:2029:ASN:N	1.94	0.64
1:B:3219:ILE:CB	1:B:3220:PRO:CD	2.74	0.64
1:B:4323:ASN:N	1:B:4323:ASN:ND2	2.46	0.64
1:A:3352:ASN:O	1:A:3356:ALA:HB2	1.97	0.64
1:A:3862:THR:CG2	1:A:3863:THR:N	2.58	0.64
1:A:3872:THR:O	1:A:3876:MET:HG2	1.98	0.64
1:B:2441:PRO:C	1:B:2443:GLU:H	1.99	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4043:ASP:HB3	1:B:4059:PRO:HB3	1.78	0.64
1:B:4169:GLU:HG3	1:B:4173:LYS:NZ	2.13	0.64
1:A:2533:VAL:HB	1:A:2581:LEU:HD22	1.78	0.64
1:A:4147:ASP:OD2	1:A:4157:TYR:HE2	1.81	0.64
1:B:2501:ILE:HD13	1:B:2565:GLN:O	1.98	0.64
1:A:2052:GLU:O	1:A:2053:ASN:HB2	1.97	0.64
1:A:3834:LEU:CA	1:A:3854:THR:HG21	2.27	0.64
1:A:4574:GLN:O	1:A:4578:ILE:HG13	1.98	0.64
1:B:2129:VAL:CG2	1:B:2130:PRO:HD3	2.22	0.64
1:B:3603:GLY:HA3	1:B:3783:PHE:O	1.98	0.64
1:A:2359:VAL:HA	1:A:2363:TRP:HE1	1.63	0.64
1:A:3022:LYS:O	1:A:3026:SER:HB2	1.98	0.64
1:A:3061:ARG:NH1	1:A:3067:GLU:OE1	2.31	0.64
1:A:3724:GLU:OE2	1:A:3766:THR:HG23	1.98	0.64
1:A:4146:VAL:CG1	1:A:4157:TYR:OH	2.45	0.64
1:A:4623:ALA:CB	1:A:4703:ILE:HD11	2.28	0.64
1:B:2494:VAL:HG11	1:B:2548:VAL:HG11	1.79	0.64
1:B:2638:THR:O	1:B:2641:VAL:HG23	1.98	0.64
1:B:3701:ASP:OD1	1:B:3702:SER:N	2.30	0.64
1:B:4546:VAL:HA	1:B:4561:LEU:HD21	1.79	0.64
1:B:4648:VAL:HA	1:B:4662:THR:HG21	1.80	0.64
1:B:1601:LEU:HA	1:B:1666:GLN:OE1	1.99	0.63
1:B:1788:SER:HA	1:B:1810:TYR:CE2	2.32	0.63
1:B:2212:ILE:O	1:B:2215:ILE:HG22	1.97	0.63
1:A:2447:GLN:HE22	1:A:2492:LEU:CD2	2.11	0.63
1:B:1781:LEU:HG	1:B:1814:LEU:HD11	1.80	0.63
1:B:2668:ARG:HG2	1:B:2668:ARG:HH11	1.63	0.63
1:A:4277:PHE:CE1	1:A:4360:LEU:HD13	2.33	0.63
1:B:3344:LEU:HB3	1:B:3518:ILE:CD1	2.29	0.63
1:B:4267:ARG:HG2	1:B:4267:ARG:HH11	1.64	0.63
1:A:1551:LYS:NZ	1:A:1616:GLU:OE2	2.31	0.63
1:A:4620:ARG:HD3	1:A:4679:PHE:CD2	2.33	0.63
1:B:2841:ASN:HD22	1:B:2841:ASN:N	1.94	0.63
1:B:4132:LEU:HD13	1:B:4216:PHE:CE1	2.33	0.63
1:A:2044:GLN:HE22	1:A:2090:ASN:HB2	1.60	0.63
1:A:3584:GLN:O	1:A:3588:VAL:HG23	1.98	0.63
1:B:1655:LEU:HD22	1:B:1655:LEU:N	2.02	0.63
1:B:1763:GLY:H	1:B:1764:PRO:CD	2.12	0.63
1:B:2996:ASP:O	1:B:3000:ARG:HG3	1.98	0.63
1:A:2527:ASP:O	1:A:2532:ARG:NH1	2.30	0.63
1:A:4186:LEU:HA	1:A:4216:PHE:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1792:PHE:O	1:B:1795:VAL:HB	1.99	0.63
1:A:2243:ILE:HD12	1:A:2292:ALA:HB2	1.80	0.63
1:A:2340:ILE:HD11	1:A:2386:ALA:O	1.99	0.63
1:A:3145:PHE:CD1	1:A:3164:LEU:HD11	2.33	0.63
1:A:2890:ILE:HA	1:A:2893:MET:CE	2.28	0.63
1:A:3074:ASP:N	1:A:3077:ASN:HD22	1.96	0.63
1:A:4621:LEU:HD13	1:A:4671:TRP:CE2	2.33	0.63
1:B:1558:TRP:HZ3	1:B:1602:LEU:HB3	1.63	0.63
1:B:2231:ILE:HG23	1:B:2257:GLU:OE2	1.98	0.63
1:B:2999:LEU:O	1:B:3003:ARG:HG3	1.99	0.63
1:B:3976:VAL:HG23	1:B:3982:GLU:HA	1.79	0.63
1:A:3015:ILE:CG2	1:A:3149:PRO:HG3	2.28	0.63
1:A:3673:LEU:HA	1:A:3764:LEU:HB2	1.80	0.63
1:B:1640:ASN:ND2	1:B:1644:ILE:HD11	2.10	0.63
1:B:2598:GLN:CG	1:B:2612:LEU:HB2	2.29	0.63
1:B:2984:LEU:HD13	1:B:2986:VAL:CG2	2.28	0.63
1:B:3708:LEU:CD2	1:B:3730:LEU:HD21	2.29	0.63
1:B:4184:TRP:CD1	1:B:4214:ARG:HB2	2.34	0.63
1:B:4340:SER:HG	1:B:4357:TYR:HH	1.46	0.63
1:A:2548:VAL:HG11	1:A:2565:GLN:NE2	2.03	0.62
1:B:4091:SER:N	3:B:9022:SPM:H132	2.06	0.62
1:A:1862:SER:O	1:A:1865:GLN:HG2	1.98	0.62
1:A:2839:LEU:HD22	1:A:2896:CYS:HB2	1.79	0.62
1:B:3324:LEU:HD11	1:B:3539:LEU:HG	1.80	0.62
1:B:3963:ASP:HA	1:B:3966:THR:HG23	1.80	0.62
1:A:1464:GLY:O	1:A:1466:ALA:N	2.32	0.62
1:A:1537:PHE:CE2	1:A:1541:LEU:HD22	2.35	0.62
1:A:2239:LYS:HE2	1:A:2295:GLN:HB3	1.81	0.62
1:B:3934:LYS:O	1:B:3936:PRO:HD3	1.99	0.62
1:A:3285:LEU:HD13	1:A:3578:SER:HA	1.81	0.62
1:A:3839:SER:C	1:A:3841:ALA:H	2.03	0.62
1:B:3035:LEU:HD22	1:B:3068:LYS:HB3	1.79	0.62
1:B:4131:PRO:HD2	1:B:4233:SER:HB3	1.79	0.62
1:A:1418:ALA:O	1:A:1422:ILE:HG23	2.00	0.62
1:A:1525:ILE:O	1:A:1529:GLU:HB2	1.99	0.62
1:B:2861:GLN:HG3	1:B:2874:TYR:HB2	1.81	0.62
1:B:4484:LEU:HD21	1:B:4496:PHE:CZ	2.34	0.62
1:A:2439:PHE:H	1:A:2495:GLN:NE2	1.97	0.62
1:A:2968:LEU:O	1:A:2972:VAL:HG23	1.99	0.62
1:A:3673:LEU:HB2	1:A:3781:VAL:HG21	1.82	0.62
1:A:3928:PRO:HG2	1:A:3929:ASN:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4648:VAL:HG12	1:A:4662:THR:HG21	1.80	0.62
1:B:4076:ILE:HD13	1:B:4105:VAL:HG12	1.81	0.62
1:A:2525:ILE:HD11	1:A:2813:ILE:HG21	1.81	0.62
1:A:3643:GLU:OE2	1:A:3666:LYS:HE2	1.99	0.62
1:B:3849:ASP:HA	1:B:3852:ILE:HG22	1.81	0.62
1:A:1564:LYS:HD2	1:A:1568:HIS:CE1	2.34	0.62
1:A:1655:LEU:HB2	1:A:1658:GLU:HB2	1.82	0.62
1:A:2898:LEU:O	1:A:2898:LEU:HD22	2.00	0.62
1:A:3061:ARG:HG2	1:A:3061:ARG:HH11	1.64	0.62
1:A:4599:ALA:HA	1:A:4602:THR:CG2	2.29	0.62
1:A:2350:ARG:HG2	1:A:2350:ARG:NH1	2.13	0.62
1:A:4660:LEU:HD12	1:A:4660:LEU:H	1.63	0.62
1:B:1785:LEU:HA	1:B:1814:LEU:HD23	1.82	0.62
1:A:3817:LEU:HD21	1:A:3872:THR:HG21	1.82	0.62
1:B:2237:ARG:HH21	1:B:2260:LEU:HD23	1.65	0.62
1:B:3053:ASP:OD2	1:B:3053:ASP:N	2.32	0.62
1:A:2331:LEU:HD21	1:A:2773:TRP:CG	2.34	0.61
1:A:1543:LEU:O	1:A:1545:LEU:HD13	2.01	0.61
1:A:1834:GLY:O	1:A:1835:THR:HG23	2.00	0.61
1:A:2202:THR:O	1:A:2203:MET:HG3	2.01	0.61
1:A:2863:ARG:O	1:A:2863:ARG:HD3	1.99	0.61
1:A:2966:SER:HA	1:A:2969:ARG:HG2	1.82	0.61
1:A:4179:ALA:HA	1:A:4213:PHE:CD1	2.34	0.61
1:B:2439:PHE:HA	3:B:9018:SPM:H111	1.81	0.61
1:B:3030:ALA:CB	1:B:3037:ILE:HD11	2.31	0.61
1:B:4189:ASN:N	1:B:4189:ASN:ND2	2.47	0.61
1:A:3497:LEU:O	1:A:3501:VAL:HG23	2.00	0.61
1:B:2339:ILE:HG12	1:B:2346:GLU:HG2	1.82	0.61
1:B:2564:ASN:C	1:B:2566:SER:H	2.04	0.61
1:B:2942:ASN:ND2	1:B:2944:ASP:HB2	2.15	0.61
1:B:3104:GLU:O	1:B:3106:THR:N	2.34	0.61
1:B:3344:LEU:HB3	1:B:3518:ILE:HD13	1.82	0.61
1:A:2028:PHE:HB2	1:A:2075:VAL:HG13	1.82	0.61
1:A:3359:LYS:HE3	1:A:3505:GLU:OE1	1.99	0.61
1:A:3848:ASP:O	1:A:3851:VAL:HG12	2.00	0.61
1:A:4606:GLN:O	1:A:4610:GLN:N	2.30	0.61
1:B:1863:VAL:HG22	1:B:1872:ARG:NH1	2.15	0.61
1:B:2071:MET:HG3	1:B:2072:GLY:N	2.15	0.61
1:B:4484:LEU:HD22	1:B:4500:GLU:HG3	1.83	0.61
1:A:3253:ASN:HB2	1:A:3604:PHE:CD2	2.36	0.61
1:A:4153:LEU:O	1:A:4154:HIS:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4259:ARG:HD3	1:A:4271:TYR:OH	2.01	0.61
1:B:2441:PRO:O	1:B:2443:GLU:N	2.33	0.61
1:B:2969:ARG:O	1:B:2973:LYS:HB2	2.01	0.61
1:B:2971:TYR:CE2	1:B:2975:ARG:HG3	2.35	0.61
1:A:3256:THR:OG1	1:A:3779:SER:HB3	2.01	0.61
1:A:3860:LYS:O	1:A:3862:THR:N	2.34	0.61
1:B:1554:LEU:HD22	1:B:1609:GLN:HE22	1.65	0.61
1:B:2609:THR:O	1:B:2610:ILE:HG13	2.00	0.61
1:B:3278:LEU:HD12	1:B:3585:MET:HE3	1.83	0.61
1:B:4122:VAL:HG21	1:B:4149:LEU:HD21	1.83	0.61
1:A:4349:ASN:ND2	1:A:4351:PHE:N	2.49	0.61
1:B:3253:ASN:HB2	1:B:3604:PHE:CE2	2.34	0.61
1:B:4318:SER:HB3	1:B:4324:ILE:CD1	2.24	0.61
1:A:3179:GLU:OE1	1:A:3179:GLU:N	2.33	0.61
1:A:3342:ARG:HH11	1:A:3345:GLN:NE2	1.99	0.61
1:A:3359:LYS:HZ1	1:A:3505:GLU:HA	1.65	0.61
1:B:2342:ASN:ND2	1:B:2347:SER:H	1.99	0.61
1:B:3903:LEU:HD23	1:B:4433:MET:CE	2.31	0.61
1:A:2907:HIS:CE1	1:A:2911:ARG:HE	2.18	0.61
1:A:3864:GLU:CG	1:A:3865:ILE:N	2.63	0.61
1:B:2960:TYR:O	1:B:2961:GLN:HG3	2.00	0.61
1:B:4004:THR:OG1	1:B:4006:PRO:HD3	2.00	0.61
1:B:4389:ARG:HG2	1:B:4389:ARG:NH1	2.16	0.61
1:B:4636:SER:HA	1:B:4670:THR:HG22	1.82	0.61
1:A:2905:TRP:HZ3	1:A:2930:ILE:HG23	1.66	0.60
1:A:4693:ASN:C	1:A:4693:ASN:HD22	2.04	0.60
1:B:2254:GLU:HB2	1:B:2420:ILE:HG22	1.83	0.60
1:B:2714:PHE:C	1:B:2716:HIS:H	2.04	0.60
1:A:1877:HIS:HE1	1:A:1943:ILE:O	1.84	0.60
1:A:4091:SER:H	3:A:9016:SPM:H132	1.66	0.60
1:B:1821:ILE:HG23	1:B:1912:TYR:O	2.00	0.60
1:B:3965:LEU:HD23	1:B:4426:MET:HE1	1.82	0.60
1:A:2551:TYR:CD1	1:A:2619:ILE:HG13	2.36	0.60
1:A:2977:LYS:C	1:A:2979:PHE:H	2.04	0.60
1:A:4036:HIS:HD2	1:A:4044:TRP:HE1	1.49	0.60
1:B:3335:GLU:O	1:B:3338:GLN:HB3	2.01	0.60
1:A:1486:LYS:HG2	1:A:1487:ARG:N	2.15	0.60
1:A:2377:LEU:O	1:A:2384:ARG:HA	2.01	0.60
1:A:3086:ARG:HD2	1:A:3096:VAL:HG11	1.84	0.60
1:A:3969:LEU:O	1:A:3973:ILE:HG12	2.02	0.60
1:B:1624:ASP:OD2	1:B:1624:ASP:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1819:SER:O	1:B:1822:VAL:HG12	2.00	0.60
1:A:1886:ARG:HG3	1:A:1887:ASP:N	2.14	0.60
1:A:3678:SER:HB2	1:A:3913:LEU:HD23	1.82	0.60
1:A:4374:PRO:HB2	1:A:4377:PRO:HG3	1.83	0.60
1:B:1655:LEU:HG	1:B:1658:GLU:OE2	2.02	0.60
1:B:1962:GLN:HB3	1:B:4341:THR:HG21	1.84	0.60
1:B:2206:LYS:HE2	1:B:2413:MET:HB3	1.83	0.60
1:B:2344:ARG:O	1:B:2344:ARG:HG2	1.99	0.60
1:A:4242:PRO:HA	1:A:4286:ARG:HH11	1.66	0.60
1:B:2525:ILE:HD12	1:B:2525:ILE:N	2.16	0.60
1:B:3063:GLY:HA2	1:B:3136:GLN:HB2	1.83	0.60
1:B:3700:LEU:CG	1:B:3701:ASP:H	2.14	0.60
1:A:2200:ASN:HA	1:A:2204:ILE:CG2	2.32	0.60
1:B:3766:THR:HG22	1:B:3768:ASP:N	2.15	0.60
1:B:4053:VAL:O	1:B:4053:VAL:HG22	2.01	0.60
1:A:1470:ASP:HB3	1:A:1518:ILE:HD12	1.84	0.60
1:A:1612:TRP:CZ2	1:A:1616:GLU:HG3	2.36	0.60
1:A:1732:LEU:HB3	1:A:1741:ILE:HG23	1.83	0.60
1:A:2142:GLN:N	1:A:2142:GLN:NE2	2.50	0.60
1:A:2978:VAL:O	1:A:2978:VAL:HG12	2.02	0.60
1:B:3326:GLN:HG3	1:B:3326:GLN:O	2.01	0.60
1:B:4168:PHE:O	1:B:4172:GLU:HG3	2.02	0.60
1:A:1766:ILE:CG2	1:A:1767:HIS:H	2.15	0.60
1:B:2291:GLU:O	1:B:2295:GLN:HG2	2.01	0.60
1:B:2379:LEU:O	1:B:2381:ASN:N	2.35	0.60
1:A:1531:LEU:O	1:A:1535:ARG:HB2	2.02	0.59
1:A:2905:TRP:CZ3	1:A:2930:ILE:HG23	2.37	0.59
1:A:4033:LEU:HD13	1:A:4062:TRP:CZ2	2.36	0.59
1:B:2200:ASN:HD22	1:B:2204:ILE:HG13	1.66	0.59
1:B:2231:ILE:HG13	1:B:2231:ILE:O	2.01	0.59
1:B:3928:PRO:O	1:B:3931:VAL:HG23	2.02	0.59
1:A:2068:HIS:CE1	1:A:2070:ASP:HB2	2.37	0.59
1:A:2856:PHE:CE1	1:A:2930:ILE:HG13	2.37	0.59
1:A:3192:LEU:HD22	1:A:3268:VAL:HG22	1.83	0.59
1:A:3204:VAL:O	1:A:3207:GLN:HB3	2.02	0.59
1:A:3281:GLU:HB3	1:A:3581:PHE:CE1	2.35	0.59
1:B:3351:ARG:HG3	1:B:3355:ILE:CD1	2.33	0.59
1:A:1962:GLN:HB3	1:A:4341:THR:HG21	1.84	0.59
1:A:4122:VAL:HG21	1:A:4216:PHE:HZ	1.67	0.59
1:A:4349:ASN:HD22	1:A:4352:ASP:N	1.83	0.59
1:A:3355:ILE:HG21	1:A:3508:ALA:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3721:GLN:HE22	1:A:4205:HIS:CD2	2.20	0.59
1:A:3789:THR:HG23	1:A:3791:SER:H	1.68	0.59
1:A:4187:LEU:N	1:A:4187:LEU:HD12	2.17	0.59
1:B:3289:LEU:HD22	1:B:3293:ARG:NH2	2.17	0.59
1:B:3563:LEU:HD11	1:B:3845:ILE:HG13	1.85	0.59
1:A:1797:VAL:HG12	1:A:1854:MET:CE	2.32	0.59
1:A:4193:ALA:HB1	1:A:4196:TRP:CB	2.33	0.59
1:A:4329:ILE:HG23	1:A:4330:PRO:HD2	1.85	0.59
1:B:2578:MET:HB3	1:B:2597:ILE:HD12	1.82	0.59
1:B:2668:ARG:HG2	1:B:2668:ARG:NH1	2.16	0.59
1:B:2695:GLU:O	1:B:2739:LEU:HD12	2.02	0.59
1:B:3194:LEU:O	1:B:3223:HIS:HD2	1.84	0.59
1:A:2275:VAL:HG13	1:A:2397:VAL:HG23	1.84	0.59
1:A:3015:ILE:HG21	1:A:3172:TRP:CZ3	2.37	0.59
1:A:3588:VAL:O	1:A:3592:VAL:HG23	2.03	0.59
1:A:3641:PRO:HA	1:A:3644:ARG:NH1	2.16	0.59
1:A:3780:ARG:NH1	1:A:3780:ARG:HB2	2.17	0.59
1:B:2237:ARG:O	1:B:2241:GLN:NE2	2.35	0.59
1:B:2541:MET:O	1:B:2544:SER:HB2	2.02	0.59
1:B:3059:LEU:HD11	1:B:3090:LEU:HD22	1.85	0.59
1:B:4133:LEU:CD2	1:B:4230:LEU:HD23	2.32	0.59
1:A:2643:SER:O	1:A:2646:VAL:HG12	2.03	0.59
1:A:4121:ILE:HA	1:A:4125:GLU:HB3	1.84	0.59
1:B:2370:LEU:CD1	1:B:2377:LEU:HB2	2.32	0.59
1:B:2863:ARG:O	1:B:2863:ARG:HD3	2.02	0.59
1:A:2440:ASP:HB3	1:A:2443:GLU:HG3	1.85	0.59
1:A:3298:GLN:O	1:A:3301:ASP:HB2	2.03	0.59
1:A:3780:ARG:CB	1:A:3780:ARG:HH11	2.15	0.59
1:A:3965:LEU:HD23	1:A:4426:MET:HE1	1.83	0.59
1:B:3023:SER:HB2	2:B:9010:ADP:O1A	2.03	0.59
1:B:3966:THR:CB	1:B:4426:MET:HG3	2.32	0.59
1:B:4608:ALA:O	1:B:4612:ASN:HB3	2.03	0.59
1:A:1605:TRP:HH2	1:A:1650:VAL:HG21	1.68	0.59
1:A:1696:ARG:HD3	1:A:1725:MET:O	2.02	0.59
1:A:2270:HIS:HA	1:A:2392:ARG:HE	1.67	0.59
1:A:2525:ILE:HD12	1:A:2526:MET:N	2.17	0.59
1:A:3525:LEU:O	1:A:3529:ILE:HG22	2.02	0.59
1:B:3049:SER:O	1:B:3053:ASP:OD2	2.21	0.59
1:B:4165:PRO:HG2	1:B:4166:GLU:H	1.68	0.59
1:B:4294:LYS:NZ	1:B:4348:ASP:OD2	2.36	0.59
1:A:3086:ARG:HH11	1:A:3096:VAL:CG1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3928:PRO:C	1:A:3930:LEU:H	2.06	0.59
1:B:3923:LEU:HD22	1:B:3947:ILE:HG23	1.85	0.59
1:B:4657:THR:CG2	1:B:4658:ASP:H	2.13	0.59
1:A:1780:THR:O	1:A:1784:LEU:HB2	2.03	0.58
1:A:2338:ARG:HH11	1:A:2338:ARG:CG	2.15	0.58
1:A:2660:LEU:HD21	1:A:2672:LEU:HD21	1.85	0.58
1:A:3500:GLU:O	1:A:3503:GLN:HB3	2.03	0.58
1:A:4171:ALA:C	1:A:4173:LYS:H	2.05	0.58
1:B:3324:LEU:CD1	1:B:3539:LEU:HG	2.33	0.58
1:A:1742:ILE:HD13	1:A:1742:ILE:N	2.18	0.58
1:A:2065:ILE:HG22	1:A:2066:SER:N	2.18	0.58
1:A:3817:LEU:HD21	1:A:3872:THR:CG2	2.33	0.58
1:B:1548:TYR:HD1	1:B:1548:TYR:O	1.85	0.58
1:B:1840:LYS:O	1:B:1844:GLN:HG3	2.04	0.58
1:B:1890:ARG:O	1:B:1893:GLN:N	2.35	0.58
1:B:3073:PHE:CE1	1:B:3077:ASN:HB3	2.38	0.58
1:B:3299:VAL:HB	1:B:3564:LEU:HD21	1.85	0.58
1:B:3825:VAL:O	1:B:3829:ILE:HG12	2.03	0.58
1:A:1662:ILE:HB	1:A:1665:ILE:HG12	1.85	0.58
1:A:2200:ASN:ND2	1:A:2228:LEU:HD22	2.17	0.58
1:A:3571:ARG:HB3	1:A:3571:ARG:CZ	2.33	0.58
1:B:1912:TYR:CD2	1:B:1912:TYR:N	2.71	0.58
1:B:3095:GLU:HG3	1:B:3134:THR:HB	1.84	0.58
1:B:3348:LEU:HD12	1:B:3518:ILE:HD12	1.85	0.58
1:B:3715:GLY:HA2	1:B:3760:PHE:HB2	1.84	0.58
1:A:3069:ILE:O	1:A:3141:LEU:O	2.20	0.58
1:A:4603:ALA:O	1:A:4606:GLN:HG2	2.02	0.58
1:B:2613:LEU:HD22	1:B:2655:ARG:NH1	2.19	0.58
1:B:3351:ARG:HG3	1:B:3355:ILE:HD11	1.84	0.58
1:B:3927:ASN:HB3	1:B:3930:LEU:HD12	1.84	0.58
1:A:1523:GLY:HA3	1:A:1580:TYR:CE2	2.38	0.58
1:A:4337:ILE:O	1:A:4341:THR:HB	2.04	0.58
1:B:2823:SER:O	1:B:2827:ILE:HG13	2.03	0.58
1:B:4171:ALA:O	1:B:4175:ILE:HG13	2.03	0.58
1:A:1422:ILE:HG21	1:A:1499:LEU:HG	1.84	0.58
1:A:1884:HIS:HE1	1:A:1954:ASP:OD2	1.86	0.58
1:A:4046:GLN:NE2	1:A:4056:PRO:HA	2.19	0.58
1:A:3672:PRO:HG2	1:A:3763:PHE:HD1	1.67	0.58
1:A:4164:SER:HB2	1:A:4165:PRO:HD2	1.85	0.58
1:B:2984:LEU:HD13	1:B:2986:VAL:HG21	1.86	0.58
1:B:4134:LEU:HD23	1:B:4142:ALA:HB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1908:TYR:CE1	1:A:1958:LEU:HD22	2.39	0.58
1:A:4221:ILE:H	1:A:4221:ILE:HD12	1.69	0.58
1:A:4316:LEU:HD23	1:A:4317:TYR:CE2	2.35	0.58
1:A:4575:LEU:HA	1:A:4578:ILE:HD12	1.86	0.58
1:B:1562:PHE:HD2	1:B:1565:LEU:HD22	1.68	0.58
1:B:4313:TRP:HB3	1:B:4330:PRO:HG3	1.84	0.58
1:A:1733:THR:O	1:A:1742:ILE:HG12	2.04	0.58
1:A:2195:LEU:O	1:A:2199:ILE:HG12	2.04	0.58
1:A:3064:CYS:O	1:A:3066:GLU:HG3	2.03	0.58
1:A:3665:LEU:CD1	1:A:3685:LEU:HD21	2.32	0.58
1:A:4063:ILE:HG22	1:A:4063:ILE:O	2.03	0.58
1:B:1592:ASP:O	1:B:1595:LEU:N	2.37	0.58
1:B:3901:GLU:O	1:B:3901:GLU:HG2	2.02	0.58
1:B:3990:PHE:CD2	1:B:4084:LEU:HD22	2.33	0.58
1:A:1916:ALA:O	1:A:1918:GLN:N	2.31	0.58
1:A:3226:ALA:HB1	1:A:3624:VAL:HG13	1.85	0.58
1:A:3776:ASP:OD2	1:A:3780:ARG:NH2	2.36	0.58
1:A:4193:ALA:O	1:A:4197:LEU:HD22	2.03	0.58
1:B:3094:GLY:O	1:B:3137:VAL:HG11	2.04	0.58
1:B:3686:MET:HE2	1:B:3696:LYS:HB2	1.83	0.58
1:B:4294:LYS:NZ	1:B:4348:ASP:CG	2.58	0.58
1:B:4322:SER:HB2	1:B:4323:ASN:ND2	2.18	0.58
1:B:4543:LYS:HD2	1:B:4545:ILE:CD1	2.33	0.58
1:A:1812:THR:HG21	1:A:1943:ILE:HG23	1.87	0.57
1:A:3318:GLU:O	1:A:3322:GLN:HB2	2.04	0.57
1:B:1668:THR:O	1:B:1672:LEU:HG	2.04	0.57
1:B:1886:ARG:HD3	1:B:1890:ARG:NH2	2.20	0.57
1:B:2723:THR:HG22	1:B:2727:GLU:N	2.18	0.57
1:A:3242:ASN:OD1	1:A:3253:ASN:HB3	2.03	0.57
1:A:3288:GLY:HA3	1:A:3574:TRP:CZ3	2.39	0.57
1:B:1611:ARG:O	1:B:1612:TRP:C	2.43	0.57
1:B:1872:ARG:HH12	1:B:2164:ARG:HD3	1.70	0.57
1:B:2720:TYR:CE1	1:B:2730:LEU:HD13	2.39	0.57
1:B:4186:LEU:HD12	1:B:4187:LEU:N	2.20	0.57
1:B:3095:GLU:HG3	1:B:3134:THR:CG2	2.34	0.57
1:B:4076:ILE:HD13	1:B:4105:VAL:CG1	2.33	0.57
1:A:1792:PHE:HE1	1:A:1803:TYR:HE1	1.49	0.57
1:A:3602:ILE:HG23	1:A:3610:ARG:HG2	1.86	0.57
1:B:3061:ARG:HB2	1:B:3069:ILE:HD11	1.86	0.57
1:B:4349:ASN:OD1	1:B:4351:PHE:N	2.37	0.57
1:A:1417:THR:C	1:A:1498:THR:HG22	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1558:TRP:HH2	1:A:1605:TRP:CD1	2.23	0.57
1:A:2258:LYS:HD3	1:A:2261:GLN:OE1	2.04	0.57
1:A:3039:THR:HG22	1:A:3040:ILE:N	2.18	0.57
1:A:3219:ILE:CB	1:A:3220:PRO:HD3	2.35	0.57
1:A:3315:VAL:O	1:A:3319:GLN:HG3	2.03	0.57
1:A:3674:VAL:HG12	1:A:3676:ASP:HB2	1.86	0.57
1:B:2729:VAL:HG12	1:B:2782:LYS:HB3	1.86	0.57
1:B:3923:LEU:HD22	1:B:3947:ILE:CG2	2.34	0.57
1:A:1594:ARG:O	1:A:1598:VAL:HG23	2.04	0.57
1:A:2123:VAL:HG12	1:A:2127:LYS:HD2	1.87	0.57
1:A:2262:LEU:HD11	1:A:2416:PHE:HZ	1.70	0.57
1:A:2405:LEU:HA	1:A:2408:ILE:CG1	2.35	0.57
1:B:1614:TYR:CD2	1:B:1615:LEU:HD22	2.40	0.57
1:A:2212:ILE:H	1:A:2213:PRO:HD2	1.70	0.57
1:A:2284:THR:HG21	2:A:9002:ADP:N7	2.20	0.57
1:A:3806:ARG:HG3	1:A:3882:VAL:CG1	2.31	0.57
1:B:1739:THR:HB	1:B:1761:ALA:HB2	1.87	0.57
1:B:1925:LEU:HD12	1:B:1926:VAL:H	1.70	0.57
1:B:2564:ASN:O	1:B:2566:SER:N	2.36	0.57
1:B:3340:ASP:O	1:B:3343:GLU:HB2	2.05	0.57
1:B:3727:ASP:CB	1:B:3729:VAL:HG12	2.34	0.57
1:A:2440:ASP:OD1	1:A:2442:GLN:HB2	2.04	0.57
1:A:2902:VAL:CG2	1:A:2941:VAL:HG21	2.20	0.57
1:A:3695:THR:HB	1:A:3718:LEU:CD1	2.34	0.57
1:B:1886:ARG:HH11	1:B:1890:ARG:CZ	2.17	0.57
1:B:4261:ASP:OD1	1:B:4388:THR:HB	2.05	0.57
1:A:2375:LYS:HB3	1:A:2387:LEU:HB3	1.87	0.57
1:A:3682:MET:SD	1:A:3696:LYS:HD2	2.45	0.57
1:A:4339:GLY:O	1:A:4344:GLY:HA3	2.04	0.57
1:A:4657:THR:H	1:A:4719:ARG:NH2	2.01	0.57
1:B:1889:VAL:O	1:B:1893:GLN:HG3	2.05	0.57
1:A:2898:LEU:HD22	1:A:2941:VAL:CG2	2.35	0.57
1:A:3246:LEU:O	1:A:3249:GLN:O	2.21	0.57
1:A:3337:LYS:O	1:A:3341:ALA:N	2.35	0.57
1:A:4519:ASN:O	1:A:4520:LEU:C	2.42	0.57
1:B:1558:TRP:CZ3	1:B:1602:LEU:HB3	2.38	0.57
1:B:1980:LYS:O	1:B:1984:VAL:HG23	2.05	0.57
1:B:2128:ILE:HG23	1:B:2129:VAL:N	2.20	0.57
1:A:1770:LEU:O	1:A:1773:VAL:HG22	2.04	0.56
1:A:3817:LEU:CD2	1:A:3817:LEU:N	2.68	0.56
1:A:1796:ASP:O	1:A:1798:ASN:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1799:ASP:OD1	1:A:1802:LYS:N	2.37	0.56
1:A:1853:GLN:HA	1:A:1856:LEU:HD12	1.87	0.56
1:A:2422:THR:HB	1:A:2425:MET:HG3	1.87	0.56
1:A:2439:PHE:N	1:A:2495:GLN:HE22	1.99	0.56
1:A:3936:PRO:HG2	1:A:3937:ASN:N	2.16	0.56
1:A:4146:VAL:HG12	1:A:4157:TYR:OH	2.04	0.56
1:B:1729:LEU:HD11	1:B:1732:LEU:HD21	1.88	0.56
1:B:2309:LYS:HZ3	1:B:2756:THR:HG21	1.68	0.56
1:B:3061:ARG:HB3	1:B:3067:GLU:OE2	2.04	0.56
1:B:4362:GLN:HB2	1:B:4714:GLN:NE2	2.19	0.56
1:B:4570:LYS:O	1:B:4573:GLN:HB2	2.04	0.56
1:B:4657:THR:HG21	1:B:4659:ILE:HB	1.86	0.56
1:A:2140:SER:HB3	1:A:2142:GLN:HE22	1.70	0.56
1:A:2192:ILE:HG23	1:A:2223:PHE:CD1	2.40	0.56
1:A:2898:LEU:HD13	1:A:2941:VAL:HG23	1.86	0.56
1:A:3866:ALA:O	1:A:3869:VAL:HB	2.04	0.56
1:A:3928:PRO:O	1:A:3930:LEU:N	2.39	0.56
1:A:4368:ALA:HA	1:A:4373:PHE:CD1	2.39	0.56
1:A:4621:LEU:HD21	1:A:4669:LEU:HD23	1.86	0.56
1:B:2309:LYS:O	1:B:2758:ARG:HD2	2.05	0.56
1:B:2427:PHE:CE1	1:B:2534:LEU:HD21	2.40	0.56
1:B:2494:VAL:HG11	1:B:2548:VAL:CG1	2.35	0.56
1:B:3135:SER:HA	1:B:3138:ARG:HG2	1.88	0.56
1:B:3776:ASP:O	1:B:3780:ARG:HG2	2.05	0.56
1:B:4119:ALA:CA	1:B:4149:LEU:HD11	2.34	0.56
1:B:4121:ILE:HA	1:B:4125:GLU:HG3	1.86	0.56
1:B:4276:TRP:CE2	1:B:4375:LEU:HD22	2.41	0.56
1:B:4322:SER:CB	1:B:4323:ASN:HD22	2.19	0.56
1:A:1671:ARG:O	1:A:1675:LEU:HD13	2.05	0.56
1:A:1928:HIS:CD2	1:A:1933:THR:HG22	2.40	0.56
1:A:2864:PHE:O	1:A:2872:TYR:HB3	2.05	0.56
1:A:4137:VAL:CG2	1:A:4138:PRO:HD2	2.36	0.56
1:A:4278:HIS:HD2	1:A:4343:TYR:OH	1.88	0.56
1:B:2766:MET:HE2	1:B:2783:LEU:CD1	2.29	0.56
1:B:3921:TYR:CE2	1:B:3925:ASN:ND2	2.72	0.56
1:A:1800:HIS:HB2	1:A:1858:ASN:HD22	1.71	0.56
1:A:4247:ASN:HD21	1:A:4282:GLN:HE21	1.51	0.56
1:B:3091:LEU:HD11	1:B:3145:PHE:CE2	2.40	0.56
1:B:3635:PRO:HA	1:B:3663:ILE:HG13	1.86	0.56
1:B:3893:CYS:SG	1:B:3947:ILE:HG21	2.45	0.56
1:B:4278:HIS:HD2	1:B:4343:TYR:OH	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2257:GLU:O	1:A:2261:GLN:HG3	2.06	0.56
1:A:2574:LEU:HD22	1:A:2597:ILE:HG22	1.88	0.56
1:A:4188:LYS:HA	1:A:4218:THR:CG2	2.28	0.56
1:A:4190:ILE:HB	1:A:4197:LEU:HD11	1.88	0.56
1:B:3207:GLN:O	1:B:3210:GLU:HB2	2.06	0.56
1:B:3827:LEU:O	1:B:3831:GLU:HG3	2.05	0.56
1:B:4147:ASP:OD1	1:B:4157:TYR:OH	2.24	0.56
1:B:4264:PRO:HB3	1:B:4323:ASN:HA	1.87	0.56
1:B:4693:ASN:ND2	1:B:4693:ASN:N	2.47	0.56
1:A:2059:LEU:HG	1:A:2060:LEU:CD1	2.32	0.56
1:A:2528:PHE:CE1	1:A:2533:VAL:HG11	2.41	0.56
1:A:2536:SER:HB2	1:A:2580:GLY:O	2.06	0.56
1:A:3287:ILE:O	1:A:3291:LYS:HG2	2.06	0.56
1:A:4263:GLN:O	1:A:4267:ARG:NH1	2.38	0.56
1:B:2237:ARG:HE	1:B:2260:LEU:CD2	2.18	0.56
1:B:2265:ILE:HD12	1:B:2414:VAL:HG22	1.88	0.56
1:B:4537:LEU:O	1:B:4541:ILE:HG13	2.05	0.56
1:A:2571:ASN:OD1	1:A:2624:TRP:NE1	2.38	0.56
1:A:3331:GLN:HG3	1:A:3532:TYR:HB3	1.87	0.56
1:A:4600:TYR:O	1:A:4604:THR:HG23	2.06	0.56
1:B:2965:ARG:HD3	1:B:2995:LEU:HD12	1.87	0.56
1:A:4188:LYS:CA	1:A:4218:THR:HG22	2.28	0.56
1:A:4604:THR:HG1	1:A:4671:TRP:HZ3	1.53	0.56
1:B:1875:PHE:O	1:B:1879:ILE:HG13	2.05	0.56
1:B:2332:PHE:HE1	1:B:2353:ILE:HG21	1.71	0.56
1:B:2379:LEU:HD12	1:B:2383:GLU:CG	2.33	0.56
1:B:4423:ALA:O	1:B:4427:ILE:HG12	2.05	0.56
1:A:1531:LEU:HD11	1:A:1584:PHE:HB3	1.88	0.56
1:A:2612:LEU:HD11	1:A:2624:TRP:CH2	2.41	0.56
1:A:3268:VAL:HG12	1:A:3269:LEU:HD23	1.87	0.56
1:A:3270:LEU:HB3	1:A:3592:VAL:HG13	1.88	0.56
1:A:3664:MET:O	1:A:3668:PHE:HB3	2.05	0.56
1:A:4644:LEU:HD23	1:A:4647:ALA:C	2.27	0.56
1:B:1766:ILE:HG23	1:B:1767:HIS:N	2.21	0.56
1:B:3289:LEU:HD13	1:B:3293:ARG:HH21	1.71	0.56
1:B:4214:ARG:CG	1:B:4214:ARG:HH11	2.18	0.56
1:A:2855:GLU:O	1:A:2859:GLU:HG2	2.06	0.55
1:A:3661:ASN:HA	1:A:3664:MET:HE2	1.87	0.55
1:A:4121:ILE:HG21	1:A:4236:PHE:HZ	1.71	0.55
1:A:4166:GLU:O	1:A:4170:LEU:HG	2.06	0.55
1:A:4711:THR:CG2	1:A:4715:ASN:HB3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3019:GLY:HA2	2:B:9010:ADP:H5'2	1.89	0.55
1:B:3568:ASN:ND2	1:B:3571:ARG:HH12	2.04	0.55
1:B:4184:TRP:NE1	1:B:4214:ARG:HG3	2.20	0.55
1:A:2262:LEU:HG	1:A:2414:VAL:HG21	1.89	0.55
1:A:3788:VAL:HG21	1:A:3913:LEU:CD2	2.36	0.55
1:A:4620:ARG:NH1	1:A:4679:PHE:HB3	2.22	0.55
1:B:1863:VAL:HG21	1:B:2115:SER:O	2.05	0.55
1:B:2597:ILE:O	1:B:2600:ILE:HG22	2.05	0.55
1:B:3278:LEU:HD12	1:B:3585:MET:CE	2.36	0.55
1:A:1639:ILE:HG21	1:A:1676:LEU:HD21	1.87	0.55
1:A:2641:VAL:O	1:A:2643:SER:N	2.39	0.55
1:A:2856:PHE:HZ	1:A:2926:THR:HG23	1.72	0.55
1:A:3194:LEU:O	1:A:3223:HIS:HD2	1.89	0.55
1:B:4186:LEU:HA	1:B:4216:PHE:O	2.06	0.55
1:B:4280:ILE:CD1	1:B:4408:LEU:HD23	2.36	0.55
1:B:1831:LEU:HA	1:B:1841:ILE:HG23	1.88	0.55
1:B:2636:VAL:HG12	1:B:2637:GLU:N	2.22	0.55
1:B:3708:LEU:HD21	1:B:3730:LEU:CD2	2.35	0.55
1:B:4523:LEU:O	1:B:4523:LEU:HD23	2.06	0.55
1:A:2028:PHE:CB	1:A:2075:VAL:HG13	2.36	0.55
1:A:2595:LYS:HA	1:A:2598:GLN:HB2	1.89	0.55
1:A:2677:GLY:O	2:A:9003:ADP:H5'2	2.06	0.55
1:A:3528:SER:O	1:A:3532:TYR:HD1	1.90	0.55
1:B:1920:ASN:HD22	1:B:1921:VAL:N	2.04	0.55
1:B:1947:LEU:HD21	1:B:1982:GLU:HG2	1.88	0.55
1:A:1709:ILE:O	1:A:1712:SER:HB2	2.06	0.55
1:A:2949:PRO:HG2	1:A:2951:LEU:HD13	1.89	0.55
1:A:3001:ILE:O	1:A:3004:VAL:HB	2.06	0.55
1:A:3046:TYR:CD2	1:A:3079:LEU:HD12	2.42	0.55
1:A:3929:ASN:ND2	1:A:3942:TYR:CD1	2.70	0.55
1:B:1555:VAL:HG22	1:B:1609:GLN:NE2	2.19	0.55
1:B:2044:GLN:O	1:B:2048:VAL:HG23	2.06	0.55
1:B:2250:VAL:HB	1:B:2425:MET:CG	2.36	0.55
1:B:2250:VAL:HB	1:B:2425:MET:HG2	1.88	0.55
1:B:3211:ILE:O	1:B:3212:MET:HB2	2.07	0.55
1:B:4189:ASN:N	1:B:4218:THR:HG22	2.17	0.55
1:A:1662:ILE:HB	1:A:1665:ILE:CG1	2.36	0.55
1:A:1856:LEU:HD22	1:A:2114:TYR:HE2	1.71	0.55
1:A:2314:ASP:OD1	1:A:2319:SER:HB3	2.06	0.55
1:A:3359:LYS:NZ	1:A:3505:GLU:HA	2.22	0.55
1:B:1719:GLN:HA	1:B:1722:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3115:THR:C	1:B:3117:GLN:N	2.60	0.55
1:B:3966:THR:HB	1:B:4426:MET:HG3	1.87	0.55
1:B:4289:PRO:HA	1:B:4292:TRP:O	2.07	0.55
1:A:2090:ASN:ND2	1:A:2091:LEU:HG	2.22	0.55
1:A:3864:GLU:HG3	1:A:3865:ILE:H	1.70	0.55
1:A:4143:SER:HB2	1:A:4188:LYS:HD2	1.89	0.55
1:A:4157:TYR:OH	1:A:4186:LEU:HD22	2.07	0.55
1:B:1662:ILE:CG2	1:B:1663:GLU:N	2.70	0.55
1:B:2515:VAL:HG11	1:B:2577:LEU:CD1	2.33	0.55
1:B:2627:TRP:CE2	1:B:2655:ARG:HB3	2.40	0.55
1:B:3584:GLN:O	1:B:3588:VAL:HG23	2.06	0.55
1:B:3612:ASP:O	1:B:3616:LYS:HG3	2.07	0.55
1:B:4036:HIS:HD2	1:B:4044:TRP:HE1	1.54	0.55
1:A:2000:CYS:CB	1:A:2031:LEU:HD13	2.22	0.55
1:A:4693:ASN:ND2	1:A:4695:THR:OG1	2.40	0.55
1:B:1611:ARG:O	1:B:1614:TYR:N	2.40	0.55
1:B:1624:ASP:OD2	1:B:1710:GLY:O	2.25	0.55
1:B:1785:LEU:CA	1:B:1814:LEU:HD23	2.36	0.55
1:B:2128:ILE:O	1:B:2131:LEU:HB3	2.07	0.55
1:B:2233:MET:CE	1:B:2233:MET:HA	2.37	0.55
1:B:2506:PHE:HE1	1:B:2573:LEU:HD11	1.71	0.55
1:B:2669:PRO:HA	1:B:2788:PHE:O	2.06	0.55
1:B:3232:VAL:O	1:B:3236:GLN:HG3	2.06	0.55
1:B:3275:ARG:HG2	1:B:3585:MET:HE2	1.89	0.55
1:A:3816:LEU:HB3	1:A:3817:LEU:HD23	1.87	0.55
1:B:2197:ASN:O	1:B:2197:ASN:ND2	2.39	0.55
1:B:3238:ILE:HG12	1:B:3601:TYR:CG	2.42	0.55
1:B:4351:PHE:CE2	1:B:4689:PRO:HG3	2.42	0.55
1:A:1565:LEU:O	1:A:1569:LEU:HB2	2.06	0.54
1:A:3571:ARG:HH11	1:A:3571:ARG:CB	2.19	0.54
1:A:4118:MET:O	1:A:4122:VAL:HG12	2.08	0.54
1:B:1608:VAL:O	1:B:1609:GLN:C	2.46	0.54
1:B:2599:THR:O	1:B:2599:THR:HG22	2.06	0.54
1:B:3315:VAL:HG12	1:B:3316:LYS:N	2.21	0.54
1:B:4176:TYR:OH	1:B:4203:LYS:HG3	2.06	0.54
1:A:2204:ILE:HG23	1:A:2205:PRO:HD3	1.89	0.54
1:A:4134:LEU:HB3	1:A:4238:TYR:CE2	2.42	0.54
1:B:2714:PHE:O	1:B:2716:HIS:N	2.40	0.54
1:B:3704:PHE:CD2	1:B:3705:MET:N	2.75	0.54
1:B:4169:GLU:C	1:B:4171:ALA:N	2.61	0.54
1:A:2863:ARG:HG3	1:A:2925:TRP:CZ2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3511:LEU:O	1:A:3514:LYS:N	2.40	0.54
1:A:3981:ASN:HB3	1:A:4074:SER:OG	2.07	0.54
1:A:4134:LEU:HD23	1:A:4238:TYR:OH	2.07	0.54
1:B:1547:ASN:HD22	1:B:1547:ASN:C	2.11	0.54
1:B:1640:ASN:O	1:B:1644:ILE:HG12	2.07	0.54
1:B:2502:ILE:CG2	1:B:2573:LEU:HD13	2.38	0.54
1:B:2525:ILE:HD12	1:B:2525:ILE:H	1.72	0.54
1:B:2921:GLU:CD	1:B:2921:GLU:H	2.10	0.54
1:B:3028:PHE:O	1:B:3032:MET:HG2	2.06	0.54
1:B:3577:GLN:O	1:B:3580:ASN:HB2	2.06	0.54
1:A:2212:ILE:N	1:A:2213:PRO:HD2	2.22	0.54
1:A:2998:ILE:HG22	1:A:3029:VAL:CG2	2.38	0.54
1:A:3331:GLN:HG3	1:A:3532:TYR:HB2	1.89	0.54
1:A:3563:LEU:HD21	1:A:3845:ILE:HG22	1.89	0.54
1:B:4688:VAL:HG13	1:B:4722:SER:HA	1.89	0.54
1:A:2398:GLN:HE22	1:A:2805:HIS:HB2	1.72	0.54
1:A:2426:ILE:HD12	1:A:2530:ARG:HH11	1.71	0.54
1:A:2898:LEU:HD13	1:A:2941:VAL:CG2	2.38	0.54
1:A:3238:ILE:N	1:A:3238:ILE:HD12	2.23	0.54
1:A:3322:GLN:C	1:A:3322:GLN:HE21	2.10	0.54
1:B:2381:ASN:HD22	1:B:2381:ASN:C	2.10	0.54
1:B:2554:LEU:C	1:B:2556:SER:H	2.10	0.54
1:B:3170:LEU:HD23	1:B:3170:LEU:C	2.28	0.54
1:B:4157:TYR:HB3	1:B:4184:TRP:HB2	1.90	0.54
1:B:4413:ASN:ND2	1:B:4660:LEU:HD23	2.22	0.54
1:A:2187:TYR:O	1:A:2190:TYR:HB3	2.06	0.54
1:A:2498:CYS:O	1:A:2502:ILE:HG12	2.07	0.54
1:A:2819:PRO:HD2	1:A:2876:PRO:HG2	1.89	0.54
1:A:3238:ILE:HG12	1:A:3601:TYR:CG	2.43	0.54
1:A:3308:GLN:O	1:A:3311:ARG:N	2.36	0.54
1:A:4494:PRO:HD2	1:A:4610:GLN:NE2	2.22	0.54
1:A:4678:ILE:O	1:A:4680:ASN:N	2.39	0.54
1:B:2556:SER:O	1:B:2559:PRO:HD3	2.08	0.54
1:B:4200:LEU:O	1:B:4204:LEU:HB2	2.06	0.54
1:B:4657:THR:HG22	1:B:4659:ILE:N	2.22	0.54
1:B:3052:ASP:HA	1:B:3055:LEU:HB2	1.88	0.54
1:A:2667:HIS:HB2	3:A:9012:SPM:H121	1.90	0.54
1:A:3039:THR:CG2	1:A:3040:ILE:N	2.69	0.54
1:B:2372:ASP:HB3	1:B:2410:ARG:HD3	1.90	0.54
1:B:2642:ALA:HB3	1:B:2884:ARG:HG3	1.89	0.54
1:B:3298:GLN:O	1:B:3302:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4604:THR:CG2	1:B:4604:THR:O	2.56	0.54
1:A:2266:LEU:O	1:A:2392:ARG:NH1	2.41	0.54
1:B:1945:GLU:OE1	1:B:1945:GLU:HA	2.08	0.54
1:B:2572:ARG:NH1	1:B:2575:TYR:CE2	2.76	0.54
1:B:4332:ILE:O	1:B:4336:THR:HG23	2.08	0.54
1:A:2259:ILE:CG2	1:A:2289:TYR:HB2	2.38	0.54
1:A:2313:LYS:HE3	1:A:2366:ASN:ND2	2.22	0.54
1:B:1996:LEU:HD13	1:B:2016:LEU:HD21	1.89	0.54
1:B:3970:GLN:OE1	1:B:4433:MET:HE1	2.07	0.54
1:A:1527:LEU:O	1:A:1530:PHE:HB3	2.08	0.53
1:A:2204:ILE:N	1:A:2205:PRO:CD	2.72	0.53
1:A:2525:ILE:HD12	1:A:2526:MET:H	1.73	0.53
1:A:3312:GLU:O	1:A:3316:LYS:HB2	2.08	0.53
1:B:1606:ILE:HG23	1:B:1607:ASP:N	2.23	0.53
1:B:2273:MET:HG2	1:B:2395:PHE:HB2	1.90	0.53
1:B:3108:LEU:HD11	1:B:3133:PHE:CZ	2.43	0.53
1:B:4622:HIS:O	1:B:4669:LEU:HA	2.07	0.53
1:A:1949:GLN:NE2	1:A:1953:THR:HG21	2.23	0.53
1:A:3987:GLU:OE1	1:A:4081:ARG:NE	2.38	0.53
1:B:2401:LYS:HD3	1:B:2402:TYR:CE2	2.43	0.53
1:B:3973:ILE:HG13	1:B:3988:TRP:CE3	2.43	0.53
1:A:1702:ASP:O	1:A:1706:LEU:HG	2.07	0.53
1:A:2215:ILE:HG23	1:A:2216:GLN:N	2.24	0.53
1:A:2607:ALA:C	1:A:2609:THR:N	2.61	0.53
1:A:2828:TYR:CZ	1:A:2879:LEU:HB3	2.44	0.53
1:A:3069:ILE:HG22	1:A:3070:CYS:N	2.23	0.53
1:A:3086:ARG:NH1	1:A:3096:VAL:HG12	2.23	0.53
1:B:2282:LYS:HB2	2:B:9008:ADP:O3B	2.07	0.53
1:B:2720:TYR:HA	1:B:2729:VAL:O	2.09	0.53
1:B:3185:GLY:HA2	1:B:3264:ILE:CD1	2.37	0.53
1:A:1572:ILE:O	1:A:1575:MET:HG2	2.07	0.53
1:A:3056:ARG:NH1	1:A:3099:LEU:HD12	2.23	0.53
1:A:3338:GLN:HE21	1:A:3338:GLN:HA	1.72	0.53
1:A:3605:PHE:CD1	1:A:3605:PHE:N	2.74	0.53
1:A:4040:ASN:N	1:A:4040:ASN:ND2	2.55	0.53
1:A:4553:TYR:HD2	1:A:4595:LEU:HD22	1.73	0.53
1:B:2491:GLY:C	1:B:2493:LYS:N	2.62	0.53
1:B:2942:ASN:HD21	1:B:2944:ASP:HB2	1.71	0.53
1:B:3324:LEU:O	1:B:3328:VAL:HG12	2.08	0.53
1:B:4118:MET:O	1:B:4122:VAL:HG22	2.09	0.53
1:A:1419:TRP:NE1	1:A:1481:TRP:HZ2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1520:ALA:O	1:A:1524:GLU:HG3	2.09	0.53
1:A:2227:GLN:O	1:A:2229:GLN:NE2	2.37	0.53
1:A:2357:GLY:O	1:A:2397:VAL:HG12	2.08	0.53
1:A:2699:LEU:HD22	1:A:2741:VAL:CG1	2.38	0.53
1:A:3808:ASP:OD2	1:A:3809:THR:HG23	2.09	0.53
1:A:4043:ASP:HB3	1:A:4059:PRO:HB3	1.90	0.53
1:A:4418:LEU:HD11	1:A:4422:LYS:NZ	2.24	0.53
1:A:4621:LEU:CD2	1:A:4669:LEU:HD23	2.38	0.53
1:B:1691:ARG:NH2	1:B:1702:ASP:OD2	2.38	0.53
1:B:1755:LYS:O	1:B:1757:PRO:HD3	2.08	0.53
1:B:2339:ILE:HA	1:B:2346:GLU:HG2	1.90	0.53
1:B:4229:LEU:O	1:B:4233:SER:OG	2.27	0.53
1:A:3780:ARG:HB2	1:A:3780:ARG:HH11	1.73	0.53
1:A:3960:LEU:HA	1:A:4239:GLU:OE2	2.09	0.53
1:B:2602:ILE:O	1:B:2603:THR:O	2.27	0.53
1:B:2938:PHE:N	1:B:2939:PRO:HD3	2.24	0.53
1:B:3686:MET:HE2	1:B:3696:LYS:HD2	1.90	0.53
1:A:1840:LYS:O	1:A:1843:GLU:HB3	2.08	0.53
1:A:2918:VAL:HG22	1:A:3172:TRP:CE2	2.43	0.53
1:A:3027:ARG:O	1:A:3030:ALA:HB3	2.09	0.53
1:A:3069:ILE:N	1:A:3069:ILE:HD12	2.22	0.53
1:A:3335:GLU:CG	1:A:3529:ILE:HD11	2.38	0.53
1:A:3789:THR:HG22	1:A:3792:SER:OG	2.08	0.53
1:A:4067:ALA:O	1:A:4073:GLN:NE2	2.42	0.53
1:A:4137:VAL:HG23	1:A:4138:PRO:HD2	1.91	0.53
1:B:2617:VAL:HG22	1:B:2624:TRP:CZ3	2.44	0.53
1:B:3289:LEU:HD13	1:B:3293:ARG:NH2	2.23	0.53
1:B:4640:LYS:HB3	1:B:4666:ILE:CD1	2.37	0.53
1:B:4673:ASP:C	1:B:4675:ASP:H	2.11	0.53
1:A:3234:ILE:O	1:A:3238:ILE:HD13	2.09	0.53
1:A:3814:SER:O	1:A:3815:ASP:C	2.46	0.53
1:B:2165:LYS:O	1:B:2166:CYS:HB2	2.09	0.53
1:B:2554:LEU:O	1:B:2556:SER:N	2.40	0.53
1:B:3677:PRO:CD	1:B:3787:THR:HG22	2.39	0.53
1:A:1734:LEU:CD2	1:A:1741:ILE:HD13	2.39	0.53
1:A:3252:GLN:HE21	1:A:3253:ASN:H	1.57	0.53
1:A:3605:PHE:HB3	1:A:3609:PHE:HB2	1.91	0.53
1:B:2793:ASN:ND2	1:B:2800:ARG:HH21	2.07	0.53
1:B:3350:VAL:C	1:B:3352:ASN:N	2.59	0.53
1:A:1879:ILE:O	1:A:1883:VAL:HG23	2.08	0.53
1:A:4501:ARG:O	1:A:4505:THR:OG1	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2738:TRP:CH2	1:B:2785:LYS:HA	2.43	0.53
1:B:3529:ILE:O	1:B:3533:LYS:HB2	2.08	0.53
1:B:4647:ALA:O	1:B:4662:THR:CG2	2.56	0.53
1:A:1419:TRP:C	1:A:1421:ALA:N	2.61	0.52
1:A:1490:THR:HG21	1:A:1492:TRP:NE1	2.24	0.52
1:A:1506:ASP:CB	1:A:1509:ARG:HB3	2.40	0.52
1:A:2140:SER:HB3	1:A:2142:GLN:NE2	2.23	0.52
1:A:2206:LYS:HG2	1:A:2413:MET:O	2.10	0.52
1:A:2573:LEU:HD23	1:A:2573:LEU:C	2.30	0.52
1:A:2748:LEU:N	1:A:2749:PRO:CD	2.73	0.52
1:A:3807:PRO:O	1:A:3808:ASP:C	2.48	0.52
1:B:2578:MET:HB3	1:B:2597:ILE:CD1	2.40	0.52
1:B:3047:LYS:O	1:B:3050:ASP:HB2	2.09	0.52
1:B:4657:THR:CG2	1:B:4659:ILE:H	2.22	0.52
1:A:2524:HIS:CD2	1:A:2528:PHE:HB2	2.44	0.52
1:A:2798:ALA:O	1:A:2800:ARG:NH1	2.42	0.52
1:B:1562:PHE:O	1:B:1565:LEU:C	2.48	0.52
1:B:2128:ILE:HD13	1:B:2195:LEU:HD21	1.91	0.52
1:A:3117:GLN:HG2	1:A:3118:ARG:N	2.24	0.52
1:A:3346:VAL:O	1:A:3349:ASP:HB2	2.10	0.52
1:A:4170:LEU:N	1:A:4170:LEU:HD23	2.24	0.52
1:A:4183:THR:C	1:A:4184:TRP:HD1	2.12	0.52
1:A:4605:ARG:HG2	1:A:4605:ARG:HH11	1.74	0.52
1:B:1925:LEU:HD12	1:B:1926:VAL:N	2.23	0.52
1:B:2432:ASP:O	1:B:2434:LEU:N	2.42	0.52
1:A:1424:PRO:HB3	1:A:1469:THR:OG1	2.09	0.52
1:A:2378:THR:HA	1:A:2384:ARG:HA	1.91	0.52
1:A:2568:TYR:HB2	1:A:2622:ALA:HB1	1.90	0.52
1:A:3766:THR:HG22	1:A:3767:ARG:N	2.24	0.52
1:B:1646:ILE:HG21	1:B:1669:MET:HE1	1.92	0.52
1:B:1777:MET:HE3	1:B:1939:GLU:HA	1.90	0.52
1:B:1816:LEU:O	1:B:1820:GLN:HG3	2.10	0.52
1:B:2223:PHE:O	1:B:2225:GLY:N	2.43	0.52
1:B:4189:ASN:H	1:B:4189:ASN:HD22	1.54	0.52
1:B:4349:ASN:OD1	1:B:4352:ASP:N	2.30	0.52
1:A:2359:VAL:HG23	1:A:2397:VAL:HG11	1.90	0.52
1:A:2408:ILE:HG13	1:A:2409:SER:H	1.74	0.52
1:A:3337:LYS:H	1:A:3337:LYS:HD2	1.75	0.52
1:A:3896:VAL:O	1:A:3899:ALA:HB3	2.10	0.52
1:B:2976:LEU:HD11	1:B:2990:LEU:HD21	1.91	0.52
1:B:3313:LEU:HD13	1:B:3550:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2591:GLU:HG2	1:A:2613:LEU:HD22	1.91	0.52
1:A:2746:ILE:O	1:A:2749:PRO:HD2	2.10	0.52
1:A:2918:VAL:O	1:A:2919:GLU:HG2	2.10	0.52
1:A:3695:THR:HB	1:A:3718:LEU:HD11	1.92	0.52
1:B:1817:LEU:O	1:B:1821:ILE:HG13	2.10	0.52
1:B:3103:GLU:O	1:B:3106:THR:HG23	2.10	0.52
1:A:3063:GLY:HA3	1:A:3133:PHE:CE1	2.44	0.52
1:B:1828:ASP:OD2	1:B:1901:ASN:HB2	2.09	0.52
1:B:1901:ASN:H	1:B:1901:ASN:HD22	1.57	0.52
1:B:4094:VAL:O	1:B:4098:SER:OG	2.27	0.52
1:B:4186:LEU:HD12	1:B:4187:LEU:H	1.74	0.52
1:B:4688:VAL:HG11	1:B:4723:ILE:HG13	1.91	0.52
1:A:2273:MET:O	1:A:2413:MET:HG3	2.10	0.52
1:A:2511:LEU:CD2	1:A:2515:VAL:HG23	2.39	0.52
1:A:2522:ARG:NH1	1:A:2589:GLU:OE2	2.42	0.52
1:A:2700:ASN:HD22	1:A:3089:THR:HG22	1.75	0.52
1:A:3364:ALA:C	1:A:3366:LEU:N	2.62	0.52
1:A:3515:GLN:C	1:A:3517:GLU:N	2.61	0.52
1:A:4050:LYS:O	1:A:4051:ASP:C	2.48	0.52
1:A:4134:LEU:HD12	1:A:4217:MET:O	2.10	0.52
1:A:4669:LEU:N	1:A:4669:LEU:HD12	2.24	0.52
1:B:2582:GLY:HA2	1:B:2585:MET:CE	2.40	0.52
1:B:3047:LYS:C	1:B:3049:SER:H	2.13	0.52
1:B:3806:ARG:HD2	1:B:3882:VAL:HG11	1.91	0.52
1:B:4293:THR:HG22	1:B:4696:ARG:HD2	1.91	0.52
1:A:2274:MET:CE	1:A:2286:TRP:HB3	2.39	0.52
1:A:3998:LEU:CD1	1:A:4018:LYS:HD3	2.40	0.52
1:A:4285:LEU:O	1:A:4288:ILE:HG13	2.10	0.52
1:B:1802:LYS:O	1:B:1805:GLU:HB3	2.09	0.52
1:B:2231:ILE:HD11	1:B:2233:MET:HB2	1.92	0.52
1:B:2611:PRO:C	1:B:2613:LEU:N	2.62	0.52
1:B:3315:VAL:O	1:B:3316:LYS:C	2.48	0.52
1:B:3324:LEU:HD11	1:B:3539:LEU:HB3	1.91	0.52
1:A:2378:THR:O	1:A:2378:THR:CG2	2.57	0.52
1:A:2697:VAL:HG23	1:A:2739:LEU:HD21	1.92	0.52
1:A:2845:PHE:CZ	1:B:4002:LYS:HB2	2.45	0.52
1:A:2994:VAL:O	1:A:2998:ILE:HG12	2.10	0.52
1:A:4331:TRP:CD1	1:A:4366:PRO:HD3	2.45	0.52
1:A:4381:LEU:HD11	1:A:4395:TRP:CZ2	2.45	0.52
1:B:2314:ASP:O	1:B:2316:LEU:N	2.42	0.52
1:B:2991:PHE:HA	1:B:3183:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3161:SER:N	1:B:3162:PRO:HD3	2.25	0.52
1:A:1606:ILE:O	1:A:1610:ARG:HG3	2.10	0.51
1:A:1628:LEU:C	1:A:1630:PRO:HD3	2.29	0.51
1:A:1770:LEU:HA	1:A:1773:VAL:HG22	1.92	0.51
1:A:2672:LEU:O	1:A:2791:ALA:HA	2.10	0.51
1:A:3060:LYS:O	1:A:3064:CYS:HB2	2.10	0.51
1:A:3078:VAL:O	1:A:3078:VAL:HG13	2.11	0.51
1:B:1562:PHE:O	1:B:1566:ALA:N	2.43	0.51
1:B:2379:LEU:C	1:B:2381:ASN:H	2.13	0.51
1:A:1719:GLN:HA	1:A:1722:PHE:CE2	2.45	0.51
1:A:2239:LYS:CE	1:A:2295:GLN:HE21	2.24	0.51
1:A:2988:LEU:HD21	1:A:3024:VAL:HG11	1.91	0.51
1:A:3506:ASN:O	1:A:3509:ASN:HB2	2.09	0.51
1:A:3947:ILE:HG23	1:A:3948:PHE:N	2.24	0.51
1:B:1607:ASP:O	1:B:1611:ARG:HD3	2.11	0.51
1:B:1837:GLN:O	1:B:1838:GLN:C	2.48	0.51
1:B:1846:GLN:HA	1:B:1893:GLN:NE2	2.25	0.51
1:B:3598:PHE:O	1:B:3602:ILE:HB	2.10	0.51
1:A:1720:LYS:HE2	1:A:2384:ARG:CZ	2.41	0.51
1:A:2112:MET:O	1:A:2116:GLN:HG2	2.10	0.51
1:B:1971:ASN:HD22	1:B:2097:SER:HB3	1.76	0.51
1:B:2506:PHE:CD1	1:B:2512:VAL:HG21	2.45	0.51
1:B:4648:VAL:HG23	1:B:4655:THR:HB	1.92	0.51
1:A:1656:ILE:O	1:A:1659:VAL:HG22	2.10	0.51
1:A:2885:ALA:HB1	1:A:2908:GLU:OE1	2.10	0.51
1:B:2278:SER:H	1:B:2398:GLN:HE21	1.57	0.51
1:B:3328:VAL:O	1:B:3332:GLN:HG3	2.09	0.51
1:B:4214:ARG:HH11	1:B:4214:ARG:HG3	1.75	0.51
1:A:1549:GLN:HE21	1:A:1551:LYS:NZ	2.08	0.51
1:A:2380:PRO:C	1:A:2382:GLY:H	2.14	0.51
1:A:2568:TYR:HB2	1:A:2622:ALA:CB	2.40	0.51
1:A:2935:LEU:HD21	1:A:2943:LEU:HD23	1.91	0.51
1:A:3721:GLN:O	1:A:3722:ASP:C	2.49	0.51
1:A:3930:LEU:HD11	1:A:3939:ARG:HG2	1.93	0.51
1:A:4507:GLY:HA2	1:A:4510:VAL:HG23	1.93	0.51
1:B:2574:LEU:HD11	1:B:2601:ALA:HB1	1.91	0.51
1:B:4079:ASN:O	1:B:4082:LYS:HB2	2.10	0.51
1:A:1528:GLU:HB2	1:A:1584:PHE:CE1	2.45	0.51
1:A:2405:LEU:CD2	1:A:2408:ILE:HD11	2.41	0.51
1:A:3251:ARG:HH12	1:A:3675:ILE:HD13	1.74	0.51
1:A:3634:VAL:N	1:A:3635:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3697:THR:HG21	1:A:3718:LEU:HD21	1.92	0.51
1:A:4046:GLN:HE22	1:A:4056:PRO:HA	1.75	0.51
1:A:4134:LEU:HD23	1:A:4238:TYR:CZ	2.46	0.51
1:A:4499:PHE:O	1:A:4503:ILE:HG13	2.11	0.51
1:B:2874:TYR:CE1	1:B:2916:ARG:CZ	2.94	0.51
1:B:4128:SER:OG	1:B:4209:PRO:HG2	2.11	0.51
1:A:4622:HIS:O	1:A:4669:LEU:HA	2.10	0.51
1:B:2745:GLU:N	1:B:2791:ALA:O	2.44	0.51
1:B:3327:MET:SD	1:B:3535:GLU:HB3	2.50	0.51
1:B:3961:ASN:HA	1:B:3964:LYS:HE2	1.93	0.51
1:B:3981:ASN:OD1	1:B:4076:ILE:HD12	2.10	0.51
1:A:1554:LEU:HB3	1:A:1609:GLN:CD	2.31	0.51
1:A:1820:GLN:NE2	1:A:1881:GLU:OE1	2.44	0.51
1:A:2640:LYS:O	1:A:2641:VAL:O	2.29	0.51
1:A:3598:PHE:HZ	1:A:3660:GLU:HB3	1.76	0.51
1:A:4556:PRO:O	1:A:4559:ILE:HG22	2.11	0.51
1:A:4646:GLY:O	1:A:4719:ARG:NH1	2.44	0.51
1:A:4659:ILE:HG22	1:A:4661:SER:N	2.26	0.51
1:B:2315:GLN:HB3	1:B:2775:THR:HG21	1.93	0.51
1:B:2379:LEU:HD12	1:B:2383:GLU:CB	2.40	0.51
1:B:2540:LEU:HD12	1:B:2662:ALA:CB	2.41	0.51
1:B:2607:ALA:C	1:B:2609:THR:H	2.13	0.51
1:B:2615:TYR:HD1	1:B:2625:SER:O	1.94	0.51
1:B:3101:GLU:O	1:B:3104:GLU:HB2	2.11	0.51
1:B:3343:GLU:HG3	1:B:3347:GLN:HE22	1.75	0.51
1:A:3056:ARG:HG3	1:A:3099:LEU:HD11	1.91	0.51
1:A:3196:ASN:HB3	1:A:3223:HIS:CG	2.45	0.51
1:A:3302:LEU:HD12	1:A:3302:LEU:O	2.11	0.51
1:B:1639:ILE:HG21	1:B:1676:LEU:HD21	1.92	0.51
1:B:1958:LEU:O	1:B:1962:GLN:HB2	2.11	0.51
1:B:2522:ARG:HB3	1:B:2589:GLU:OE1	2.11	0.51
1:B:2714:PHE:C	1:B:2716:HIS:N	2.63	0.51
1:A:1554:LEU:HD22	1:A:1609:GLN:CG	2.41	0.51
1:A:1719:GLN:HA	1:A:1722:PHE:HD2	1.72	0.51
1:A:2005:ASP:HB3	1:A:2008:ALA:HB3	1.93	0.51
1:A:2404:THR:O	1:A:2408:ILE:HG12	2.11	0.51
1:A:3241:ALA:HB1	1:A:3605:PHE:CE2	2.46	0.51
1:B:1813:GLN:HG3	1:B:1814:LEU:HD12	1.94	0.51
1:B:3348:LEU:HD22	1:B:3511:LEU:HD11	1.93	0.51
1:B:4155:LYS:HE2	1:B:4184:TRP:CZ2	2.46	0.51
1:B:4280:ILE:HD13	1:B:4408:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2705:THR:O	1:A:2705:THR:HG22	2.09	0.50
1:A:3105:PHE:O	1:A:3109:MET:HG2	2.10	0.50
1:A:3118:ARG:C	1:A:3120:GLY:N	2.64	0.50
1:A:4196:TRP:CE3	1:A:4197:LEU:HD13	2.46	0.50
1:A:4576:SER:O	1:A:4578:ILE:N	2.44	0.50
1:B:2223:PHE:C	1:B:2225:GLY:N	2.63	0.50
1:B:3348:LEU:HD12	1:B:3518:ILE:CD1	2.41	0.50
1:B:3729:VAL:O	1:B:3729:VAL:CG2	2.49	0.50
1:B:4376:VAL:HG12	1:B:4379:ILE:HG22	1.93	0.50
1:B:4571:ARG:HD3	1:B:4593:GLY:O	2.11	0.50
1:A:2638:THR:O	1:A:2641:VAL:HG23	2.11	0.50
1:A:2989:VAL:O	1:A:2991:PHE:N	2.44	0.50
1:A:3186:SER:HA	1:A:3228:VAL:HG21	1.92	0.50
1:A:3694:ILE:HG22	1:A:3695:THR:H	1.76	0.50
1:A:3849:ASP:O	1:A:3853:SER:HB3	2.11	0.50
1:A:4117:ASP:OD1	1:A:4119:ALA:HB3	2.11	0.50
1:A:4157:TYR:HH	1:A:4186:LEU:HD22	1.76	0.50
1:B:2029:ASN:HD22	1:B:2029:ASN:H	1.59	0.50
1:B:2541:MET:SD	1:B:2573:LEU:HD12	2.51	0.50
1:B:2690:ALA:O	1:B:2691:PHE:CD1	2.64	0.50
1:B:2984:LEU:HD13	1:B:2986:VAL:HG22	1.93	0.50
1:B:3598:PHE:HZ	1:B:3660:GLU:HG2	1.76	0.50
1:B:4590:TRP:CE3	1:B:4593:GLY:HA3	2.46	0.50
1:A:2438:PRO:HA	1:A:2495:GLN:HE22	1.76	0.50
1:A:2747:ASN:HD22	1:A:2747:ASN:N	2.09	0.50
1:A:2832:ASN:HA	1:A:2835:LEU:HB3	1.92	0.50
1:A:3364:ALA:O	1:A:3366:LEU:N	2.45	0.50
1:A:3864:GLU:HG3	1:A:3865:ILE:HG13	1.92	0.50
1:A:4020:LEU:HD21	1:A:4037:ILE:HD12	1.94	0.50
1:A:4551:LYS:C	1:A:4553:TYR:H	2.14	0.50
1:B:3104:GLU:C	1:B:3106:THR:H	2.15	0.50
1:B:3292:LEU:HD13	1:B:3571:ARG:HA	1.93	0.50
1:B:3575:GLU:C	1:B:3577:GLN:H	2.15	0.50
1:B:3879:ILE:O	1:B:3881:GLU:N	2.44	0.50
1:B:4200:LEU:O	1:B:4200:LEU:HD23	2.11	0.50
1:A:3342:ARG:HD3	1:A:3522:ILE:HD11	1.93	0.50
1:A:3682:MET:O	1:A:3686:MET:HB2	2.12	0.50
1:A:4117:ASP:OD2	1:A:4119:ALA:HB3	2.12	0.50
1:A:4146:VAL:CG1	1:A:4157:TYR:HH	2.24	0.50
1:A:4645:GLU:O	1:A:4721:VAL:HG23	2.11	0.50
1:A:4654:LEU:HD11	1:A:4688:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2010:SER:HA	1:B:2042:GLN:HE22	1.77	0.50
1:B:2497:GLU:O	1:B:2501:ILE:HG13	2.12	0.50
1:B:2793:ASN:HD22	1:B:2800:ARG:CZ	2.23	0.50
1:B:3352:ASN:HA	1:B:3511:LEU:CD2	2.41	0.50
1:B:4169:GLU:OE1	1:B:4169:GLU:HA	2.11	0.50
1:B:4251:THR:CG2	1:B:4303:LEU:HD21	2.34	0.50
1:B:4341:THR:HG22	1:B:4342:ILE:HG13	1.93	0.50
1:B:4509:LEU:HD13	1:B:4552:TRP:CE2	2.46	0.50
1:A:1419:TRP:HZ2	1:A:1471:LEU:O	1.94	0.50
1:A:3260:TYR:O	1:A:3263:PHE:HB3	2.11	0.50
1:A:3697:THR:OG1	1:A:3698:SER:N	2.44	0.50
1:A:3860:LYS:C	1:A:3862:THR:N	2.64	0.50
1:A:3894:SER:O	1:A:3898:PHE:HD2	1.95	0.50
1:B:1863:VAL:HG23	1:B:1872:ARG:HD3	1.94	0.50
1:B:1907:LEU:O	1:B:1911:ARG:NH1	2.44	0.50
1:B:2000:CYS:C	1:B:2002:GLU:H	2.14	0.50
1:B:2422:THR:OG1	1:B:2424:GLN:HB2	2.11	0.50
1:B:3157:ARG:O	1:B:3160:THR:HB	2.11	0.50
1:B:3238:ILE:HD12	1:B:3238:ILE:N	2.27	0.50
1:B:3602:ILE:CD1	1:B:3610:ARG:HA	2.41	0.50
1:B:3893:CYS:HG	1:B:3920:PHE:HE1	1.57	0.50
1:B:4190:ILE:HB	1:B:4197:LEU:HD21	1.94	0.50
1:B:4573:GLN:O	1:B:4577:GLU:HG3	2.12	0.50
1:A:1525:ILE:HA	1:A:1528:GLU:HB3	1.94	0.50
1:B:2677:GLY:O	2:B:9009:ADP:H5'2	2.11	0.50
1:B:3871:GLU:O	1:B:3875:VAL:HG23	2.11	0.50
1:A:1985:LYS:HD2	1:A:1997:VAL:HG21	1.93	0.50
1:A:2338:ARG:CG	1:A:2338:ARG:NH1	2.71	0.50
1:A:2918:VAL:HG22	1:A:3172:TRP:CD2	2.46	0.50
1:A:3197:PRO:C	1:A:3198:GLN:HG3	2.32	0.50
1:A:3582:ASN:O	1:A:3586:SER:HB3	2.12	0.50
1:A:3775:PRO:O	1:A:3778:CYS:HB2	2.12	0.50
1:A:4436:SER:C	1:A:4438:GLU:H	2.15	0.50
1:B:3192:LEU:HD11	1:B:3268:VAL:HA	1.93	0.50
1:B:3536:TYR:O	1:B:3540:ILE:HD13	2.12	0.50
1:B:4122:VAL:HG11	1:B:4216:PHE:HZ	1.77	0.50
1:B:4259:ARG:NH2	1:B:4307:LEU:HB3	2.26	0.50
1:A:2421:LEU:HD11	2:A:9002:ADP:C5	2.46	0.50
1:A:3817:LEU:N	1:A:3817:LEU:HD22	2.27	0.50
1:B:1727:ALA:HB2	1:B:1994:PHE:CD1	2.46	0.50
1:B:2163:LYS:C	1:B:2165:LYS:H	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2612:LEU:O	1:B:2612:LEU:HD13	2.12	0.50
1:B:2836:MET:CE	1:B:2839:LEU:HD12	2.41	0.50
1:B:4176:TYR:O	1:B:4179:ALA:HB3	2.12	0.50
1:B:4274:LEU:HD12	1:B:4274:LEU:O	2.11	0.50
1:A:1885:GLN:O	1:A:1889:VAL:HG23	2.11	0.50
1:A:2046:ILE:O	1:A:2049:ALA:HB3	2.12	0.50
1:A:2273:MET:HG2	1:A:2395:PHE:CD1	2.47	0.50
1:A:2361:PRO:HD3	1:A:2402:TYR:O	2.12	0.50
1:A:3233:TYR:O	1:A:3237:THR:HG23	2.12	0.50
1:A:4168:PHE:O	1:A:4172:GLU:HG2	2.12	0.50
1:B:2427:PHE:HE1	1:B:2534:LEU:HD21	1.77	0.50
1:B:4132:LEU:HD23	1:B:4236:PHE:CE2	2.47	0.50
1:A:3074:ASP:O	1:A:3077:ASN:HB2	2.12	0.49
1:A:3359:LYS:CE	1:A:3505:GLU:HA	2.42	0.49
1:A:3694:ILE:HA	1:A:3717:PRO:O	2.12	0.49
1:A:3774:THR:O	1:A:3775:PRO:C	2.49	0.49
1:A:4131:PRO:HB2	1:A:4233:SER:HB3	1.94	0.49
1:B:1548:TYR:CD1	1:B:1548:TYR:C	2.86	0.49
1:B:1560:ASP:CA	1:B:1563:ASN:HB2	2.35	0.49
1:B:1739:THR:O	1:B:1760:ILE:CG1	2.56	0.49
1:B:3046:TYR:OH	1:B:3054:ASP:OD2	2.29	0.49
1:B:3109:MET:HA	1:B:3112:CYS:HB2	1.93	0.49
1:B:3805:GLU:HB3	1:B:3886:TYR:OH	2.12	0.49
1:B:3930:LEU:HD11	1:B:3943:LEU:CD2	2.39	0.49
1:B:4126:VAL:HG23	1:B:4214:ARG:HE	1.77	0.49
1:B:4693:ASN:HD22	1:B:4693:ASN:N	1.89	0.49
1:A:2026:ASP:OD2	1:A:2026:ASP:C	2.50	0.49
1:A:2056:GLU:HA	1:A:2065:ILE:O	2.12	0.49
1:A:2162:ILE:HG22	1:A:2194:VAL:HG13	1.94	0.49
1:A:2307:ASP:HB3	1:A:2310:ALA:CB	2.41	0.49
1:A:2688:LEU:CD1	1:A:2696:VAL:HG11	2.30	0.49
1:A:3091:LEU:HD21	1:A:3143:VAL:HB	1.94	0.49
1:B:1614:TYR:HD2	1:B:1615:LEU:HD22	1.78	0.49
1:B:1701:GLY:HA2	1:B:2011:ARG:NH1	2.27	0.49
1:B:3696:LYS:HZ1	1:B:3721:GLN:HE22	1.60	0.49
1:B:3696:LYS:NZ	1:B:3721:GLN:HE22	2.10	0.49
1:A:1690:GLN:HE22	1:A:1766:ILE:CG2	2.17	0.49
1:A:2751:THR:HG22	1:A:2757:GLN:HG3	1.94	0.49
1:A:4146:VAL:HG11	1:A:4157:TYR:OH	2.11	0.49
1:A:4349:ASN:HD21	1:A:4351:PHE:HB2	1.77	0.49
1:B:1655:LEU:HB2	1:B:1658:GLU:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2189:GLN:HE22	1:B:2225:GLY:HA3	1.77	0.49
1:B:3848:ASP:O	1:B:3849:ASP:HB2	2.12	0.49
1:A:2903:ARG:NH1	1:A:2950:ILE:HG23	2.27	0.49
1:A:3825:VAL:C	1:A:3827:LEU:H	2.15	0.49
1:A:4690:VAL:HG21	1:A:4701:PHE:CE1	2.47	0.49
1:B:2128:ILE:CG2	1:B:2129:VAL:N	2.75	0.49
1:B:2546:VAL:O	1:B:2550:GLU:HB2	2.12	0.49
1:B:2611:PRO:C	1:B:2613:LEU:H	2.15	0.49
1:B:3328:VAL:O	1:B:3328:VAL:HG22	2.12	0.49
1:B:3866:ALA:O	1:B:3869:VAL:HB	2.12	0.49
1:A:2020:GLY:HA2	1:A:2071:MET:HB3	1.95	0.49
1:A:2551:TYR:CE1	1:A:2619:ILE:HG23	2.48	0.49
1:A:3285:LEU:O	1:A:3289:LEU:HD12	2.12	0.49
1:A:3673:LEU:HD11	1:A:3773:PHE:CE2	2.47	0.49
1:A:3823:PHE:HA	1:A:3865:ILE:HD11	1.94	0.49
1:B:1859:LEU:O	1:B:1862:SER:HB2	2.13	0.49
1:B:1973:PHE:HA	1:B:2077:MET:O	2.11	0.49
1:B:2241:GLN:HA	1:B:2244:ALA:HB3	1.93	0.49
1:B:2493:LYS:O	1:B:2497:GLU:HG3	2.12	0.49
1:B:2525:ILE:H	1:B:2525:ILE:CD1	2.25	0.49
1:B:2863:ARG:O	1:B:2863:ARG:CD	2.60	0.49
1:B:3187:GLU:O	1:B:3190:ARG:HG2	2.12	0.49
1:B:3278:LEU:CD1	1:B:3585:MET:HE3	2.42	0.49
1:B:3288:GLY:HA3	1:B:3574:TRP:CZ3	2.47	0.49
1:B:3545:GLN:O	1:B:3548:THR:HB	2.11	0.49
1:B:4089:PHE:C	3:B:9022:SPM:H131	2.33	0.49
1:B:4411:PRO:HB2	1:B:4413:ASN:OD1	2.11	0.49
1:A:1836:LEU:O	1:A:1837:GLN:C	2.50	0.49
1:A:2524:HIS:HD2	1:A:2528:PHE:HB2	1.77	0.49
1:A:3823:PHE:CB	1:A:3865:ILE:HG12	2.42	0.49
1:A:4576:SER:O	1:A:4579:SER:N	2.45	0.49
1:A:4597:PRO:HG2	1:A:4692:LEU:HD11	1.93	0.49
1:B:2525:ILE:HD11	1:B:2584:SER:HB2	1.95	0.49
1:B:2564:ASN:C	1:B:2566:SER:N	2.66	0.49
1:B:3068:LYS:HA	1:B:3140:ASN:O	2.13	0.49
1:B:3598:PHE:CZ	1:B:3660:GLU:HG2	2.47	0.49
1:B:4091:SER:HA	1:B:4094:VAL:HG23	1.95	0.49
1:B:4099:HIS:CD2	1:B:4099:HIS:C	2.85	0.49
1:B:4109:ASP:CB	1:B:4112:ASN:HD22	2.25	0.49
1:B:4596:ASN:C	1:B:4596:ASN:ND2	2.66	0.49
1:A:1797:VAL:O	1:A:1854:MET:HE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4623:ALA:HB2	1:A:4703:ILE:CD1	2.43	0.49
1:B:1671:ARG:HG2	1:B:1675:LEU:HD11	1.94	0.49
1:B:2369:SER:HA	1:B:2372:ASP:OD2	2.12	0.49
1:B:3903:LEU:HD21	1:B:3967:PHE:CD1	2.48	0.49
1:B:4322:SER:CB	1:B:4323:ASN:ND2	2.75	0.49
1:A:2551:TYR:CD1	1:A:2619:ILE:CG1	2.95	0.49
1:A:2598:GLN:OE1	1:A:2611:PRO:HA	2.13	0.49
1:A:2669:PRO:HA	1:A:2788:PHE:O	2.13	0.49
1:A:2876:PRO:HB2	2:A:9003:ADP:O4'	2.12	0.49
1:A:3009:GLN:N	1:A:3138:ARG:O	2.43	0.49
1:A:3069:ILE:O	1:A:3142:HIS:HB2	2.13	0.49
1:A:3252:GLN:HE21	1:A:3253:ASN:N	2.10	0.49
1:A:3354:GLU:O	1:A:3356:ALA:N	2.46	0.49
1:A:4580:GLU:O	1:A:4581:SER:C	2.51	0.49
1:B:1592:ASP:CG	1:B:1593:ASP:N	2.65	0.49
1:B:1918:GLN:O	1:B:1924:LYS:HE2	2.13	0.49
1:B:2011:ARG:HH21	1:B:2012:ILE:HD11	1.77	0.49
1:B:3785:ASN:HD21	1:B:3787:THR:CG2	2.20	0.49
1:A:2243:ILE:HD13	1:A:2291:GLU:OE2	2.13	0.49
1:A:2839:LEU:CD2	1:A:2896:CYS:HB2	2.42	0.49
1:A:3928:PRO:C	1:A:3930:LEU:N	2.66	0.49
1:B:2205:PRO:HG3	1:B:2261:GLN:HG2	1.95	0.49
1:B:2309:LYS:HZ1	1:B:2756:THR:HG21	1.73	0.49
1:B:2381:ASN:ND2	1:B:2381:ASN:C	2.66	0.49
1:B:2866:PRO:HG3	1:B:2873:ILE:HG23	1.93	0.49
1:B:3697:THR:O	1:B:3720:VAL:HA	2.13	0.49
1:B:3819:ILE:HG23	1:B:3823:PHE:CE2	2.47	0.49
1:B:3903:LEU:N	1:B:4433:MET:HE3	2.27	0.49
1:B:4315:ASP:HA	1:B:4318:SER:OG	2.13	0.49
1:B:4597:PRO:HG2	1:B:4692:LEU:HD11	1.94	0.49
1:A:1813:GLN:HE22	1:A:1941:LEU:N	1.99	0.49
1:A:2090:ASN:HD22	1:A:2091:LEU:H	1.61	0.49
1:A:2607:ALA:O	1:A:2609:THR:N	2.45	0.49
1:A:2998:ILE:HG22	1:A:3029:VAL:HG23	1.94	0.49
1:A:3656:GLU:O	1:A:3660:GLU:HG3	2.13	0.49
1:A:3864:GLU:CG	1:A:3865:ILE:H	2.24	0.49
1:A:4128:SER:HB3	1:A:4211:PRO:O	2.13	0.49
1:A:4596:ASN:OD1	1:A:4599:ALA:HB2	2.12	0.49
1:B:1554:LEU:HD22	1:B:1609:GLN:CD	2.34	0.49
1:B:1608:VAL:HG22	1:B:1676:LEU:HD12	1.95	0.49
1:B:1642:GLU:OE1	1:B:1668:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1694:PHE:O	1:B:1697:PHE:HB2	2.12	0.49
1:B:1763:GLY:N	1:B:1764:PRO:CD	2.74	0.49
1:B:1842:GLN:HA	1:B:1842:GLN:NE2	2.28	0.49
1:B:1904:PHE:C	1:B:1906:TRP:N	2.66	0.49
1:B:2263:HIS:HB2	1:B:2289:TYR:CE1	2.47	0.49
1:B:2300:LYS:CB	1:B:2349:LYS:HG2	2.43	0.49
1:B:4644:LEU:HB2	1:B:4662:THR:HG23	1.95	0.49
1:A:1564:LYS:HD2	1:A:1568:HIS:NE2	2.28	0.48
1:A:1734:LEU:C	1:A:1742:ILE:HD11	2.33	0.48
1:A:2544:SER:OG	1:A:2572:ARG:NH1	2.46	0.48
1:B:2491:GLY:C	1:B:2493:LYS:H	2.16	0.48
1:B:2723:THR:HG21	1:B:2727:GLU:HB2	1.95	0.48
1:B:3091:LEU:HD11	1:B:3145:PHE:HE2	1.77	0.48
1:B:3947:ILE:HD11	1:B:3948:PHE:CE2	2.48	0.48
1:B:3972:THR:CG2	1:B:4105:VAL:HG21	2.38	0.48
1:B:4005:ILE:O	1:B:4005:ILE:HG22	2.13	0.48
1:B:4294:LYS:HZ1	1:B:4348:ASP:CG	2.13	0.48
1:A:1646:ILE:HD11	1:A:1668:THR:HG21	1.95	0.48
1:A:2548:VAL:HG13	1:A:2560:MET:HE3	1.93	0.48
1:A:3141:LEU:O	1:A:3142:HIS:HB2	2.13	0.48
1:A:3689:TYR:HB2	1:A:3694:ILE:CD1	2.42	0.48
1:A:3976:VAL:HB	1:A:3981:ASN:O	2.12	0.48
1:A:4507:GLY:HA2	1:A:4510:VAL:CG2	2.43	0.48
1:A:4592:GLY:HA3	1:A:4725:SER:O	2.13	0.48
1:B:3188:PHE:HB3	1:B:3264:ILE:HG21	1.94	0.48
1:B:3316:LYS:O	1:B:3317:ASN:C	2.52	0.48
1:B:4011:LEU:O	1:B:4012:LEU:HD23	2.13	0.48
1:B:4322:SER:HB2	1:B:4323:ASN:HD22	1.78	0.48
1:A:1629:LEU:HD11	1:A:1686:TYR:CG	2.49	0.48
1:A:1767:HIS:CG	1:A:1768:GLU:N	2.81	0.48
1:A:1808:ASP:OD2	1:A:1808:ASP:N	2.46	0.48
1:A:2169:PRO:HG2	1:A:2186:ILE:HG22	1.95	0.48
1:A:2586:GLY:HA2	1:A:2815:LEU:HD22	1.94	0.48
1:A:2643:SER:O	1:A:2645:ASP:N	2.47	0.48
1:A:3279:GLU:HG3	1:A:3585:MET:HE3	1.94	0.48
1:A:3634:VAL:HB	1:A:3635:PRO:HD3	1.93	0.48
1:B:2243:ILE:HD13	1:B:2291:GLU:HB2	1.95	0.48
1:B:2723:THR:CG2	1:B:2727:GLU:HB2	2.43	0.48
1:B:3017:VAL:HG22	1:B:3175:GLU:OE2	2.13	0.48
1:B:3689:TYR:O	1:B:3690:ALA:C	2.51	0.48
1:B:3781:VAL:CG1	1:B:3782:THR:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4075:THR:HG23	1:B:4076:ILE:N	2.27	0.48
1:A:2101:ILE:HG13	1:A:4348:ASP:HB2	1.96	0.48
1:A:2359:VAL:HA	1:A:2363:TRP:NE1	2.26	0.48
1:A:3355:ILE:CG2	1:A:3508:ALA:HB2	2.43	0.48
1:A:3598:PHE:O	1:A:3602:ILE:HB	2.12	0.48
1:A:3902:GLU:HB3	1:A:4433:MET:HB3	1.95	0.48
1:A:4122:VAL:CG2	1:A:4216:PHE:HZ	2.26	0.48
1:B:1611:ARG:HH11	1:B:1611:ARG:HG3	1.78	0.48
1:B:1715:ILE:HD12	1:B:1734:LEU:HD21	1.95	0.48
1:B:2050:LEU:HG	1:B:2067:LEU:HD21	1.95	0.48
1:B:2374:ASN:O	1:B:2376:LEU:N	2.47	0.48
1:B:3545:GLN:O	1:B:3548:THR:N	2.47	0.48
1:B:4432:LYS:C	1:B:4434:GLN:H	2.17	0.48
1:A:4063:ILE:HD13	1:A:4082:LYS:NZ	2.28	0.48
1:A:4157:TYR:OH	1:A:4186:LEU:HB2	2.12	0.48
1:A:4590:TRP:CD2	1:A:4593:GLY:HA3	2.48	0.48
1:B:1555:VAL:HG23	1:B:1555:VAL:O	2.14	0.48
1:B:1662:ILE:HG22	1:B:1663:GLU:N	2.28	0.48
1:B:2295:GLN:O	1:B:2296:VAL:C	2.51	0.48
1:B:2781:ILE:HD12	1:B:2781:ILE:N	2.28	0.48
1:B:2841:ASN:H	1:B:2841:ASN:ND2	2.03	0.48
1:B:3188:PHE:CB	1:B:3264:ILE:HG21	2.43	0.48
1:B:3774:THR:HB	1:B:3775:PRO:HD2	1.96	0.48
1:B:3939:ARG:O	1:B:3943:LEU:HG	2.13	0.48
1:A:1899:THR:HG22	1:A:1899:THR:O	2.14	0.48
1:A:1916:ALA:C	1:A:1918:GLN:H	2.16	0.48
1:A:3074:ASP:CB	1:A:3077:ASN:HD22	2.27	0.48
1:A:3858:LEU:O	1:A:3862:THR:HB	2.13	0.48
1:A:4436:SER:O	1:A:4438:GLU:N	2.47	0.48
1:B:1908:TYR:CE1	1:B:1958:LEU:HD22	2.48	0.48
1:B:3690:ALA:O	1:B:3691:ASP:C	2.52	0.48
1:B:4012:LEU:HA	1:B:4016:GLN:NE2	2.28	0.48
1:B:4176:TYR:OH	1:B:4203:LYS:CG	2.61	0.48
1:B:4603:ALA:C	1:B:4605:ARG:H	2.16	0.48
1:A:2275:VAL:HG22	1:A:2397:VAL:HG22	1.96	0.48
1:A:2359:VAL:CG2	1:A:2397:VAL:HG11	2.43	0.48
1:A:2935:LEU:HD21	1:A:2943:LEU:CD2	2.43	0.48
1:A:3185:GLY:O	1:A:3189:THR:HG23	2.13	0.48
1:B:1639:ILE:HG21	1:B:1676:LEU:CD2	2.44	0.48
1:B:2439:PHE:H	1:B:2495:GLN:HE22	1.61	0.48
1:B:2688:LEU:HD13	1:B:2696:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3704:PHE:CG	1:B:3705:MET:N	2.82	0.48
1:B:4669:LEU:HD12	1:B:4669:LEU:N	2.28	0.48
1:A:1679:VAL:O	1:A:1682:ALA:HB3	2.14	0.48
1:A:1974:GLY:O	1:A:2078:ASN:HA	2.14	0.48
1:A:2271:GLY:HA3	1:A:2371:LEU:HD22	1.96	0.48
1:A:2848:ASN:HD21	1:B:4002:LYS:HE3	1.79	0.48
1:A:2937:HIS:C	1:A:2939:PRO:HD3	2.34	0.48
1:A:2965:ARG:CZ	1:A:2992:ASN:ND2	2.76	0.48
1:A:3525:LEU:O	1:A:3526:GLU:C	2.51	0.48
1:A:4284:ARG:O	1:A:4291:GLY:HA3	2.13	0.48
1:B:1608:VAL:O	1:B:1611:ARG:N	2.47	0.48
1:B:1695:ALA:C	1:B:1697:PHE:H	2.17	0.48
1:B:1781:LEU:O	1:B:1814:LEU:HD21	2.14	0.48
1:B:3226:ALA:HB1	1:B:3624:VAL:CG1	2.43	0.48
1:B:3256:THR:HG21	1:B:3779:SER:HB3	1.95	0.48
1:B:3559:ARG:O	1:B:3563:LEU:HB2	2.14	0.48
1:A:1949:GLN:HE22	1:A:1953:THR:CG2	2.27	0.48
1:A:3332:GLN:O	1:A:3336:ILE:HG13	2.13	0.48
1:B:2205:PRO:CB	1:B:2265:ILE:HD11	2.43	0.48
1:B:2258:LYS:HD2	1:B:2414:VAL:CG1	2.44	0.48
1:B:2439:PHE:H	1:B:2495:GLN:NE2	2.12	0.48
1:B:2751:THR:HB	1:B:2756:THR:H	1.79	0.48
1:B:3538:THR:O	1:B:3542:GLU:HG3	2.14	0.48
1:A:1710:GLY:C	1:A:1712:SER:H	2.17	0.48
1:A:3283:LEU:HD23	1:A:3284:HIS:N	2.28	0.48
1:A:3334:ALA:O	1:A:3335:GLU:C	2.52	0.48
1:A:3809:THR:HB	1:A:3879:ILE:CD1	2.44	0.48
1:A:4251:THR:HG23	1:A:4303:LEU:HD22	1.95	0.48
1:A:4571:ARG:O	1:A:4574:GLN:HB3	2.14	0.48
1:B:1828:ASP:O	1:B:1830:ALA:N	2.46	0.48
1:B:1870:GLN:HG2	1:B:1943:ILE:CD1	2.44	0.48
1:B:1870:GLN:HG2	1:B:1943:ILE:HD11	1.95	0.48
1:B:2204:ILE:N	1:B:2205:PRO:CD	2.77	0.48
1:B:2621:ASP:O	1:B:2622:ALA:HB3	2.13	0.48
1:B:3033:ASN:HB2	1:B:3035:LEU:HG	1.94	0.48
1:B:3673:LEU:HB3	1:B:3781:VAL:HG11	1.94	0.48
1:B:4484:LEU:C	1:B:4484:LEU:CD2	2.81	0.48
1:A:1419:TRP:CE2	1:A:1481:TRP:HZ2	2.31	0.47
1:A:1800:HIS:CG	1:A:1858:ASN:HD22	2.32	0.47
1:A:2615:TYR:CE1	1:A:2626:LEU:HG	2.49	0.47
1:A:2976:LEU:HD22	1:A:2990:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3815:ASP:O	1:A:3819:ILE:N	2.47	0.47
1:B:4267:ARG:HG2	1:B:4267:ARG:NH1	2.28	0.47
1:A:1945:GLU:OE1	1:A:1945:GLU:HA	2.13	0.47
1:A:3571:ARG:HH11	1:A:3571:ARG:C	2.18	0.47
1:A:3605:PHE:H	1:A:3605:PHE:HD1	1.58	0.47
1:B:1828:ASP:O	1:B:1831:LEU:N	2.40	0.47
1:B:2869:GLN:HB2	1:B:2872:TYR:CD2	2.49	0.47
1:B:3892:SER:O	1:B:3896:VAL:HG23	2.14	0.47
1:B:4522:GLU:O	1:B:4523:LEU:C	2.51	0.47
1:A:1830:ALA:O	1:A:1841:ILE:HG23	2.14	0.47
1:A:2297:ASP:OD1	1:A:2297:ASP:N	2.46	0.47
1:A:2729:VAL:HB	1:A:2782:LYS:O	2.14	0.47
1:A:3064:CYS:C	1:A:3066:GLU:H	2.17	0.47
1:A:4044:TRP:HB3	1:A:4048:PHE:CE2	2.50	0.47
1:B:1547:ASN:HD21	1:B:1550:ARG:H	1.61	0.47
1:B:1841:ILE:O	1:B:1844:GLN:N	2.42	0.47
1:B:2295:GLN:O	1:B:2298:ASN:N	2.43	0.47
1:B:3095:GLU:HG3	1:B:3134:THR:CB	2.44	0.47
1:B:3132:TYR:O	1:B:3136:GLN:HG2	2.14	0.47
1:B:3539:LEU:HA	1:B:3539:LEU:HD12	1.70	0.47
1:A:1643:PHE:O	1:A:1647:LEU:HB2	2.14	0.47
1:A:1735:ASP:O	1:A:1738:LYS:N	2.36	0.47
1:A:1854:MET:O	1:A:1857:ASN:N	2.46	0.47
1:A:2032:GLU:O	1:A:2034:ARG:N	2.47	0.47
1:A:3851:VAL:CG1	1:A:3852:ILE:N	2.77	0.47
1:A:3865:ILE:O	1:A:3869:VAL:HG23	2.14	0.47
1:A:4225:LEU:HD13	1:A:4230:LEU:HD11	1.96	0.47
1:A:4293:THR:HG22	1:A:4294:LYS:HG3	1.95	0.47
1:A:4324:ILE:HD13	1:A:4329:ILE:HD11	1.95	0.47
1:B:2359:VAL:HG13	1:B:2364:VAL:HG21	1.96	0.47
1:B:2377:LEU:O	1:B:2385:LEU:N	2.40	0.47
1:B:3067:GLU:O	1:B:3069:ILE:HG13	2.14	0.47
1:B:4184:TRP:HE1	1:B:4214:ARG:HG3	1.78	0.47
1:A:1558:TRP:O	1:A:1562:PHE:HD2	1.98	0.47
1:A:2447:GLN:HE22	1:A:2492:LEU:HD22	1.79	0.47
1:A:3023:SER:HB2	2:A:9004:ADP:O1A	2.14	0.47
1:A:3347:GLN:O	1:A:3350:VAL:HG23	2.14	0.47
1:A:4117:ASP:OD1	1:A:4117:ASP:O	2.33	0.47
1:B:4052:GLN:O	1:B:4053:VAL:C	2.51	0.47
1:B:4284:ARG:O	1:B:4291:GLY:HA3	2.15	0.47
1:B:4284:ARG:NH2	1:B:4410:LEU:HD21	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4387:THR:H	1:B:4391:HIS:CD2	2.31	0.47
1:B:4484:LEU:HD23	1:B:4485:LYS:N	2.29	0.47
1:B:4636:SER:CA	1:B:4670:THR:HG22	2.44	0.47
1:A:1974:GLY:HA2	1:A:2079:PRO:HD3	1.96	0.47
1:A:2549:ILE:O	1:A:2553:GLN:HG3	2.15	0.47
1:A:3362:ALA:CB	1:A:3497:LEU:HD11	2.36	0.47
1:A:3911:PHE:CZ	1:A:3955:VAL:HG13	2.49	0.47
1:A:4153:LEU:O	1:A:4154:HIS:CB	2.62	0.47
1:B:2713:THR:HG22	1:B:2713:THR:O	2.14	0.47
1:B:2766:MET:HE1	1:B:2788:PHE:HZ	1.79	0.47
1:B:2975:ARG:HA	1:B:2975:ARG:HE	1.80	0.47
1:B:3205:PHE:CD1	1:B:3624:VAL:HG22	2.49	0.47
1:B:3768:ASP:CB	1:B:3771:ALA:HB2	2.39	0.47
1:B:4176:TYR:O	1:B:4179:ALA:N	2.47	0.47
1:B:4201:GLU:HG3	1:B:4228:ASN:HB3	1.96	0.47
1:B:4623:ALA:HA	1:B:4668:THR:O	2.15	0.47
1:A:1766:ILE:CG2	1:A:1767:HIS:N	2.71	0.47
1:A:2140:SER:HB2	1:A:2211:ASP:OD2	2.14	0.47
1:A:2152:LEU:O	1:A:2156:LEU:HG	2.14	0.47
1:A:2179:SER:O	1:A:2180:LYS:C	2.52	0.47
1:A:2272:VAL:O	1:A:2394:MET:HA	2.15	0.47
1:A:2283:THR:HB	2:A:9002:ADP:O1A	2.15	0.47
1:A:2433:THR:O	1:A:2437:GLU:HB2	2.14	0.47
1:A:2717:HIS:CB	1:A:2739:LEU:HD11	2.45	0.47
1:A:2873:ILE:HD12	1:A:2874:TYR:N	2.29	0.47
1:A:3201:ALA:HB1	1:A:3221:PRO:HD2	1.97	0.47
1:A:3279:GLU:HG3	1:A:3585:MET:CE	2.44	0.47
1:A:3694:ILE:HG23	1:A:3717:PRO:HB2	1.95	0.47
1:A:3711:ALA:O	1:A:3715:GLY:N	2.48	0.47
1:A:3860:LYS:C	1:A:3862:THR:H	2.18	0.47
1:A:3972:THR:HG23	1:A:4105:VAL:HG21	1.96	0.47
1:A:4003:GLU:HB3	1:A:4021:ILE:HD13	1.97	0.47
1:A:4351:PHE:CZ	1:A:4689:PRO:HB3	2.49	0.47
1:A:4639:VAL:HG12	1:A:4640:LYS:N	2.29	0.47
1:B:1610:ARG:HG3	1:B:1610:ARG:NH1	2.28	0.47
1:B:1643:PHE:CZ	1:B:1647:LEU:HD11	2.49	0.47
1:B:1888:VAL:O	1:B:1891:GLN:HB2	2.14	0.47
1:B:2101:ILE:O	1:B:2103:PRO:HD3	2.14	0.47
1:B:2212:ILE:N	1:B:2213:PRO:HD2	2.29	0.47
1:B:2997:HIS:C	1:B:2999:LEU:H	2.18	0.47
1:B:3042:VAL:HG11	1:B:3079:LEU:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3935:ASP:O	1:B:3939:ARG:HG3	2.15	0.47
1:B:4386:GLY:CA	1:B:4391:HIS:HB3	2.44	0.47
1:A:1909:HIS:O	1:A:1911:ARG:HD3	2.15	0.47
1:A:2836:MET:HG3	1:A:2846:ALA:HA	1.97	0.47
1:A:2863:ARG:HG3	1:A:2925:TRP:CE2	2.50	0.47
1:A:2917:LEU:HD12	1:A:2923:LYS:HA	1.97	0.47
1:A:3689:TYR:CB	1:A:3694:ILE:HD11	2.44	0.47
1:A:4020:LEU:CD1	1:A:4033:LEU:HD23	2.45	0.47
1:A:4060:GLU:O	1:A:4064:VAL:HG23	2.14	0.47
1:A:4418:LEU:HD11	1:A:4422:LYS:HZ1	1.79	0.47
1:A:4436:SER:C	1:A:4438:GLU:N	2.68	0.47
1:B:2969:ARG:HG3	1:B:2995:LEU:HD11	1.97	0.47
1:B:3030:ALA:HB3	1:B:3037:ILE:HD11	1.97	0.47
1:B:3247:LYS:O	1:B:3247:LYS:HG2	2.15	0.47
1:B:3317:ASN:O	1:B:3318:GLU:C	2.52	0.47
1:B:3677:PRO:HD3	1:B:3787:THR:HG22	1.97	0.47
1:B:4008:LEU:HD11	1:B:4034:VAL:HG13	1.95	0.47
1:B:4547:PRO:HG2	1:B:4550:TRP:CZ3	2.49	0.47
1:A:2898:LEU:O	1:A:2941:VAL:HG22	2.14	0.47
1:A:3022:LYS:HB2	2:A:9004:ADP:O3B	2.15	0.47
1:A:3258:ARG:HG2	1:A:3779:SER:HB2	1.95	0.47
1:B:2425:MET:HB3	2:B:9008:ADP:C2	2.50	0.47
1:B:2582:GLY:HA2	1:B:2585:MET:HE3	1.96	0.47
1:B:2843:ARG:HH11	1:B:2843:ARG:HG3	1.79	0.47
1:B:3095:GLU:CG	1:B:3134:THR:CG2	2.92	0.47
1:B:3237:THR:OG1	1:B:3238:ILE:HD12	2.15	0.47
1:A:2575:TYR:HA	1:A:2578:MET:CE	2.45	0.47
1:A:2728:THR:CG2	1:A:2779:THR:HG21	2.45	0.47
1:A:2991:PHE:CE1	1:A:2993:GLU:HB2	2.50	0.47
1:A:4589:VAL:O	1:A:4589:VAL:HG13	2.14	0.47
1:B:1792:PHE:CE2	1:B:1822:VAL:HG21	2.50	0.47
1:B:2201:ASP:O	1:B:2205:PRO:HG2	2.15	0.47
1:B:3348:LEU:HD23	1:B:3348:LEU:HA	1.78	0.47
1:B:3602:ILE:HD12	1:B:3610:ARG:HA	1.97	0.47
1:B:3782:THR:O	1:B:3782:THR:HG22	2.14	0.47
1:B:4050:LYS:O	1:B:4051:ASP:C	2.52	0.47
1:B:4590:TRP:HA	1:B:4640:LYS:O	2.15	0.47
1:A:2204:ILE:HA	1:A:2207:LEU:HG	1.96	0.46
1:A:2548:VAL:HG13	1:A:2560:MET:CE	2.45	0.46
1:A:2873:ILE:HD12	1:A:2873:ILE:C	2.36	0.46
1:A:3521:THR:O	1:A:3524:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3602:ILE:HD12	1:A:3610:ARG:HA	1.96	0.46
1:A:4507:GLY:O	1:A:4510:VAL:N	2.48	0.46
1:B:2533:VAL:HB	1:B:2581:LEU:CD2	2.39	0.46
1:B:2638:THR:HG21	1:B:2838:LEU:CD2	2.37	0.46
1:B:2907:HIS:CE1	1:B:2911:ARG:HE	2.33	0.46
1:B:3087:MET:O	1:B:3091:LEU:N	2.47	0.46
1:B:4371:PRO:O	1:B:4372:ASP:HB2	2.16	0.46
1:A:1722:PHE:C	1:A:1724:LYS:H	2.18	0.46
1:A:1948:VAL:O	1:A:1950:THR:N	2.49	0.46
1:A:2446:GLN:HA	1:A:2449:ARG:NH2	2.30	0.46
1:A:2511:LEU:HD23	1:A:2515:VAL:HG23	1.96	0.46
1:A:2706:THR:HB	1:A:2707:PRO:HD2	1.96	0.46
1:A:3515:GLN:C	1:A:3517:GLU:H	2.18	0.46
1:A:3880:SER:O	1:A:3881:GLU:C	2.54	0.46
1:A:4221:ILE:HG22	1:A:4221:ILE:O	2.14	0.46
1:B:2360:ASP:HB2	1:B:2361:PRO:HD2	1.97	0.46
1:B:2863:ARG:HG3	1:B:2925:TRP:CZ2	2.49	0.46
1:B:3107:ALA:C	1:B:3109:MET:H	2.18	0.46
1:B:4210:HIS:O	1:B:4213:PHE:HB3	2.16	0.46
1:B:4347:ILE:CG2	1:B:4353:MET:HG2	2.45	0.46
1:A:1722:PHE:C	1:A:1724:LYS:N	2.68	0.46
1:A:1831:LEU:HB3	1:A:1900:GLY:C	2.36	0.46
1:A:1967:ARG:HD3	1:A:2050:LEU:O	2.15	0.46
1:A:2283:THR:HA	1:A:2286:TRP:NE1	2.29	0.46
1:A:2525:ILE:HG21	1:A:2815:LEU:CD1	2.45	0.46
1:A:2551:TYR:HE1	1:A:2619:ILE:HG23	1.80	0.46
1:A:2723:THR:HB	1:A:2724:PRO:HD2	1.97	0.46
1:A:2911:ARG:NH1	1:A:2915:ASP:OD1	2.48	0.46
1:A:2948:ARG:HG2	1:A:2948:ARG:HH11	1.80	0.46
1:A:2989:VAL:HG23	2:A:9004:ADP:N1	2.30	0.46
1:B:1606:ILE:C	1:B:1608:VAL:N	2.68	0.46
1:B:3038:TYR:CD2	1:B:3058:LEU:HD13	2.50	0.46
1:B:3605:PHE:HB3	1:B:3609:PHE:CB	2.45	0.46
1:B:4130:SER:OG	1:B:4233:SER:HA	2.15	0.46
1:B:4263:GLN:HA	1:B:4264:PRO:C	2.35	0.46
1:B:4690:VAL:HG22	1:B:4723:ILE:CB	2.43	0.46
1:A:1422:ILE:HD12	1:A:1423:ILE:N	2.30	0.46
1:A:2717:HIS:HB2	1:A:2739:LEU:HD11	1.97	0.46
1:A:3335:GLU:O	1:A:3338:GLN:HB2	2.14	0.46
1:A:4210:HIS:ND1	1:A:4211:PRO:CD	2.71	0.46
1:B:2093:LYS:HB2	1:B:2093:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3725:ASN:N	1:B:3725:ASN:ND2	2.61	0.46
1:B:4068:GLN:C	1:B:4070:SER:H	2.19	0.46
1:A:3265:ASN:O	1:A:3269:LEU:HG	2.15	0.46
1:B:1691:ARG:HD3	1:B:1698:TYR:HA	1.98	0.46
1:B:1901:ASN:HD22	1:B:1901:ASN:N	2.13	0.46
1:B:2108:ILE:HD12	1:B:2149:LEU:HD11	1.97	0.46
1:B:2606:PRO:HB2	1:B:2615:TYR:CE2	2.51	0.46
1:B:3065:LYS:O	1:B:3066:GLU:HB2	2.16	0.46
1:B:3161:SER:O	1:B:3163:ALA:N	2.49	0.46
1:B:3544:GLU:O	1:B:3545:GLN:C	2.54	0.46
1:B:4636:SER:CB	1:B:4670:THR:HG22	2.46	0.46
1:A:1690:GLN:NE2	1:A:1766:ILE:HG21	2.20	0.46
1:A:2309:LYS:HE3	1:A:2756:THR:HG21	1.97	0.46
1:A:3083:PHE:CD2	1:A:3083:PHE:N	2.83	0.46
1:A:3854:THR:O	1:A:3857:THR:HB	2.15	0.46
1:B:1683:LEU:O	1:B:1686:TYR:HB3	2.16	0.46
1:B:2231:ILE:CD1	1:B:2233:MET:HB2	2.46	0.46
1:B:2381:ASN:ND2	1:B:2383:GLU:H	2.13	0.46
1:B:2705:THR:HB	1:B:2749:PRO:HG3	1.97	0.46
1:B:3879:ILE:C	1:B:3881:GLU:N	2.67	0.46
1:B:4327:ASP:N	1:B:4327:ASP:OD1	2.48	0.46
1:A:1528:GLU:HB2	1:A:1584:PHE:CZ	2.51	0.46
1:A:3338:GLN:O	1:A:3342:ARG:HG2	2.15	0.46
1:A:4432:LYS:C	1:A:4434:GLN:H	2.17	0.46
1:A:4649:TRP:C	1:A:4650:ASN:HD22	2.18	0.46
1:B:2029:ASN:N	1:B:2029:ASN:ND2	2.63	0.46
1:B:2948:ARG:HD2	1:B:2950:ILE:HG13	1.97	0.46
1:B:3674:VAL:HG13	1:B:3786:PHE:HD2	1.81	0.46
1:A:1653:ALA:HB1	1:A:1658:GLU:OE1	2.16	0.46
1:A:2610:ILE:HD13	1:A:2626:LEU:HD21	1.98	0.46
1:A:2969:ARG:HB3	1:A:2995:LEU:HD11	1.97	0.46
1:A:4639:VAL:O	1:A:4666:ILE:HA	2.16	0.46
1:B:1592:ASP:OD2	1:B:1592:ASP:C	2.54	0.46
1:B:1831:LEU:HA	1:B:1841:ILE:CG2	2.45	0.46
1:B:1872:ARG:NH1	1:B:2164:ARG:HD3	2.29	0.46
1:B:2239:LYS:O	1:B:2243:ILE:HG13	2.16	0.46
1:B:2332:PHE:CD1	1:B:2353:ILE:HG21	2.51	0.46
1:B:3061:ARG:NH2	1:B:3067:GLU:OE1	2.49	0.46
1:B:3275:ARG:HG2	1:B:3585:MET:CE	2.46	0.46
1:B:4073:GLN:HG2	1:B:4073:GLN:O	2.14	0.46
1:A:1921:VAL:HA	1:A:1924:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2432:ASP:O	1:A:2436:ASN:HB2	2.15	0.46
1:A:4117:ASP:OD1	1:A:4120:ASN:N	2.42	0.46
1:A:4335:ARG:NH2	1:A:4365:THR:HG22	2.31	0.46
1:B:1615:LEU:HD22	1:B:1615:LEU:N	2.31	0.46
1:B:1803:TYR:O	1:B:1806:TRP:HB3	2.15	0.46
1:B:1904:PHE:C	1:B:1906:TRP:H	2.19	0.46
1:B:2311:ILE:HB	1:B:2315:GLN:NE2	2.30	0.46
1:B:2611:PRO:O	1:B:2613:LEU:N	2.49	0.46
1:B:2745:GLU:HG2	1:B:2748:LEU:CD1	2.46	0.46
1:B:4588:GLN:O	1:B:4640:LYS:NZ	2.47	0.46
1:A:2053:ASN:N	1:A:2053:ASN:HD22	2.14	0.46
1:A:2223:PHE:N	1:A:2224:PRO:HD3	2.31	0.46
1:A:3790:PRO:HA	1:A:3898:PHE:CE2	2.51	0.46
1:A:4200:LEU:HD22	1:A:4204:LEU:HD12	1.98	0.46
1:B:3063:GLY:HA2	1:B:3136:GLN:CB	2.46	0.46
1:B:3344:LEU:HB3	1:B:3518:ILE:HD11	1.98	0.46
1:B:3946:ASP:O	1:B:3950:MET:HG3	2.16	0.46
1:B:4214:ARG:CG	1:B:4214:ARG:NH1	2.78	0.46
1:A:1690:GLN:NE2	1:A:1709:ILE:HG12	2.31	0.45
1:A:1796:ASP:O	1:A:1799:ASP:N	2.48	0.45
1:A:1820:GLN:HE22	1:A:1990:GLN:HE22	1.64	0.45
1:A:2202:THR:O	1:A:2203:MET:CG	2.63	0.45
1:A:2337:ARG:HH12	1:A:2383:GLU:CD	2.18	0.45
1:A:2865:THR:C	1:A:2867:ASP:N	2.70	0.45
1:A:3069:ILE:HG22	1:A:3070:CYS:H	1.80	0.45
1:A:3270:LEU:HB3	1:A:3592:VAL:CG1	2.46	0.45
1:A:4573:GLN:O	1:A:4574:GLN:C	2.54	0.45
1:B:1693:ALA:HB1	1:B:1767:HIS:CD2	2.50	0.45
1:B:1962:GLN:CB	1:B:4341:THR:HG21	2.46	0.45
1:B:2426:ILE:H	1:B:2426:ILE:HD12	1.81	0.45
1:B:2706:THR:HB	1:B:2707:PRO:HD2	1.96	0.45
1:B:2718:CYS:HA	1:B:2733:THR:H	1.81	0.45
1:B:2798:ALA:HB3	1:B:3159:ALA:HB2	1.98	0.45
1:B:3319:GLN:O	1:B:3320:ALA:C	2.55	0.45
1:A:1857:ASN:HA	1:A:1860:ALA:HB3	1.97	0.45
1:A:2028:PHE:O	1:A:2031:LEU:HB2	2.17	0.45
1:A:2648:ILE:HD11	1:A:2831:PHE:CE1	2.50	0.45
1:A:3074:ASP:N	1:A:3077:ASN:ND2	2.54	0.45
1:A:3199:TYR:C	1:A:3200:ILE:HG13	2.36	0.45
1:A:3511:LEU:O	1:A:3512:LYS:C	2.54	0.45
1:A:3720:VAL:O	1:A:3765:PHE:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4175:ILE:O	1:A:4178:ALA:HB3	2.16	0.45
1:A:4284:ARG:NH2	1:A:4410:LEU:HD21	2.31	0.45
1:A:4657:THR:OG1	1:A:4658:ASP:N	2.50	0.45
1:B:1695:ALA:C	1:B:1697:PHE:N	2.70	0.45
1:B:2918:VAL:HG22	1:B:3172:TRP:CE2	2.50	0.45
1:B:3588:VAL:O	1:B:3592:VAL:HG23	2.16	0.45
1:B:4329:ILE:HD12	1:B:4331:TRP:CZ2	2.51	0.45
1:B:4494:PRO:CB	1:B:4606:GLN:HB2	2.46	0.45
1:A:1770:LEU:O	1:A:1773:VAL:CG2	2.64	0.45
1:A:1912:TYR:CD2	1:A:1912:TYR:N	2.83	0.45
1:A:2263:HIS:ND1	1:A:2289:TYR:OH	2.43	0.45
1:A:2440:ASP:HB3	1:A:2443:GLU:CG	2.46	0.45
1:A:3836:ASN:O	1:A:3839:SER:HB2	2.16	0.45
1:A:3936:PRO:CG	1:A:3937:ASN:H	2.16	0.45
1:A:3961:ASN:N	1:A:4239:GLU:OE2	2.44	0.45
1:A:4277:PHE:CZ	1:A:4360:LEU:HD13	2.51	0.45
1:B:1606:ILE:CG2	1:B:1607:ASP:N	2.79	0.45
1:B:2738:TRP:CZ3	1:B:2785:LYS:HA	2.52	0.45
1:B:2800:ARG:HG2	1:B:2800:ARG:HH11	1.81	0.45
1:B:3598:PHE:CD2	1:B:3634:VAL:HG11	2.51	0.45
1:B:3629:LYS:NZ	1:B:3632:LEU:HD13	2.31	0.45
1:B:3665:LEU:HD13	1:B:3685:LEU:HD21	1.98	0.45
1:B:3876:MET:O	1:B:3880:SER:HB2	2.16	0.45
1:B:3882:VAL:HG23	1:B:3883:SER:N	2.31	0.45
1:B:4329:ILE:CG2	1:B:4330:PRO:HD2	2.46	0.45
1:A:1417:THR:O	1:A:1498:THR:HA	2.16	0.45
1:A:1499:LEU:HD13	1:A:1503:TRP:CH2	2.52	0.45
1:A:3567:LEU:O	1:A:3571:ARG:HB2	2.16	0.45
1:A:3723:VAL:O	1:A:3723:VAL:CG2	2.59	0.45
1:A:4134:LEU:HB3	1:A:4238:TYR:HE2	1.81	0.45
1:A:4165:PRO:HG2	1:A:4166:GLU:H	1.81	0.45
1:A:4557:GLU:O	1:A:4559:ILE:HG22	2.17	0.45
1:B:2312:THR:OG1	1:B:2315:GLN:HG3	2.17	0.45
1:B:2331:LEU:HD21	1:B:2773:TRP:CD1	2.51	0.45
1:B:3185:GLY:HA2	1:B:3264:ILE:HD11	1.97	0.45
1:B:4413:ASN:ND2	1:B:4660:LEU:CD2	2.79	0.45
1:A:1656:ILE:HG23	1:A:1657:LEU:N	2.32	0.45
1:A:1863:VAL:HG21	1:A:2115:SER:O	2.17	0.45
1:A:2367:LEU:HD22	1:A:2371:LEU:HG	1.99	0.45
1:A:3004:VAL:O	1:A:3006:ARG:N	2.50	0.45
1:A:4134:LEU:HD23	1:A:4238:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2294:GLU:OE2	1:B:2300:LYS:HA	2.17	0.45
1:B:3511:LEU:O	1:B:3515:GLN:NE2	2.49	0.45
1:B:4335:ARG:HG2	1:B:4360:LEU:HB3	1.98	0.45
1:B:4356:LEU:HD23	1:B:4356:LEU:HA	1.77	0.45
1:B:4673:ASP:C	1:B:4675:ASP:N	2.70	0.45
1:A:2090:ASN:HD21	1:A:2091:LEU:HG	1.81	0.45
1:A:2142:GLN:CA	1:A:2142:GLN:NE2	2.78	0.45
1:A:2189:GLN:NE2	1:A:2192:ILE:HD12	2.32	0.45
1:A:2283:THR:OG1	1:A:2396:GLU:OE1	2.29	0.45
1:A:2331:LEU:HD11	1:A:2773:TRP:CE3	2.51	0.45
1:A:2360:ASP:HB2	1:A:2361:PRO:HD2	1.98	0.45
1:A:2976:LEU:O	1:A:2980:TYR:CD1	2.70	0.45
1:B:1729:LEU:HD23	1:B:1729:LEU:C	2.36	0.45
1:B:2192:ILE:HG23	1:B:2223:PHE:CD1	2.52	0.45
1:B:2986:VAL:O	1:B:2986:VAL:HG23	2.17	0.45
1:B:4536:SER:O	1:B:4537:LEU:C	2.55	0.45
1:A:1781:LEU:HD23	1:A:1814:LEU:HD11	1.98	0.45
1:A:2307:ASP:HB3	1:A:2310:ALA:HB3	1.99	0.45
1:A:2879:LEU:HD23	1:A:2879:LEU:HA	1.86	0.45
1:A:2918:VAL:O	1:A:2918:VAL:CG1	2.64	0.45
1:A:3300:LYS:O	1:A:3303:GLN:HB2	2.17	0.45
1:A:4184:TRP:N	1:A:4184:TRP:CD1	2.84	0.45
1:B:1640:ASN:HD21	1:B:1644:ILE:CD1	2.16	0.45
1:B:2229:GLN:O	1:B:2230:PRO:O	2.34	0.45
1:B:2676:PRO:HD3	1:B:2793:ASN:OD1	2.16	0.45
1:B:3078:VAL:HG22	1:B:3078:VAL:O	2.16	0.45
1:B:3671:TYR:CD2	1:B:3734:LEU:HA	2.52	0.45
1:B:4499:PHE:CD1	1:B:4578:ILE:HD13	2.51	0.45
1:B:4636:SER:HB3	1:B:4670:THR:HG22	1.98	0.45
1:B:4647:ALA:O	1:B:4662:THR:HG21	2.16	0.45
1:B:4692:LEU:HD22	1:B:4698:GLU:OE1	2.16	0.45
1:A:1569:LEU:HD23	1:A:1569:LEU:HA	1.76	0.45
1:A:2266:LEU:CD2	1:A:2392:ARG:HG2	2.42	0.45
1:A:2567:ASN:O	1:A:2571:ASN:ND2	2.50	0.45
1:A:2651:VAL:O	1:A:2655:ARG:CB	2.65	0.45
1:A:3015:ILE:HD13	1:A:3147:MET:HG3	1.99	0.45
1:A:3024:VAL:HG23	2:A:9004:ADP:PA	2.56	0.45
1:A:3114:GLU:HG2	1:A:3118:ARG:NH2	2.31	0.45
1:A:3887:ASN:HB3	1:A:3888:PRO:HD3	1.98	0.45
1:A:4517:LEU:O	1:A:4518:ALA:C	2.55	0.45
1:A:4624:SER:HB2	1:A:4668:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4708:ASP:C	1:A:4708:ASP:OD1	2.54	0.45
1:B:2494:VAL:HG12	1:B:2498:CYS:SG	2.57	0.45
1:B:2669:PRO:HD2	1:B:2810:HIS:O	2.17	0.45
1:B:2723:THR:HG22	1:B:2727:GLU:H	1.80	0.45
1:B:3091:LEU:HD12	1:B:3164:LEU:HD22	1.99	0.45
1:B:3326:GLN:O	1:B:3330:ASP:HB2	2.15	0.45
1:A:2200:ASN:HA	1:A:2204:ILE:HG22	1.97	0.45
1:A:3064:CYS:O	1:A:3066:GLU:N	2.50	0.45
1:A:4551:LYS:O	1:A:4553:TYR:N	2.49	0.45
1:B:2441:PRO:C	1:B:2443:GLU:N	2.68	0.45
1:B:2998:ILE:O	1:B:2998:ILE:HG13	2.17	0.45
1:B:3760:PHE:CD1	1:B:3761:MET:N	2.85	0.45
1:B:3966:THR:HG22	1:B:4426:MET:HE3	1.98	0.45
1:A:1572:ILE:O	1:A:1576:LYS:HG3	2.16	0.45
1:A:1729:LEU:HD12	1:A:1744:MET:SD	2.57	0.45
1:A:1816:LEU:O	1:A:1820:GLN:HG3	2.16	0.45
1:A:1837:GLN:O	1:A:1838:GLN:C	2.54	0.45
1:A:2088:PRO:O	1:A:2089:ASP:C	2.55	0.45
1:A:2651:VAL:O	1:A:2655:ARG:HB2	2.17	0.45
1:A:4605:ARG:HA	1:A:4671:TRP:CE3	2.52	0.45
1:A:4707:TYR:OH	1:A:4713:LYS:HE2	2.18	0.45
1:B:1555:VAL:CG2	1:B:1609:GLN:HE21	2.21	0.45
1:B:2057:VAL:HG23	1:B:2057:VAL:O	2.17	0.45
1:B:2238:LYS:O	1:B:2241:GLN:HG2	2.17	0.45
1:B:2340:ILE:HD11	1:B:2386:ALA:O	2.17	0.45
1:B:2427:PHE:CE2	1:B:2513:HIS:CE1	3.05	0.45
1:B:2845:PHE:O	1:B:2848:ASN:HB2	2.17	0.45
1:B:3325:LYS:HA	1:B:3328:VAL:HG12	1.98	0.45
1:B:3343:GLU:OE1	1:B:3343:GLU:HA	2.16	0.45
1:B:3350:VAL:O	1:B:3351:ARG:C	2.54	0.45
1:B:4020:LEU:HD21	1:B:4037:ILE:HD12	1.98	0.45
1:B:4201:GLU:HG2	1:B:4232:MET:HE2	1.99	0.45
1:B:4322:SER:C	1:B:4323:ASN:ND2	2.57	0.45
1:A:1968:MET:HE3	1:A:2051:LYS:HZ1	1.82	0.44
1:A:2372:ASP:CG	1:A:2373:ASP:H	2.18	0.44
1:A:3251:ARG:NH2	1:A:3604:PHE:O	2.50	0.44
1:A:3327:MET:HE1	1:A:3539:LEU:HD22	1.98	0.44
1:A:3768:ASP:C	1:A:3768:ASP:OD2	2.56	0.44
1:A:3861:GLU:O	1:A:3864:GLU:HG2	2.17	0.44
1:A:3909:TYR:CE1	1:A:3959:LEU:HA	2.52	0.44
1:A:4135:CYS:SG	1:A:4225:LEU:CD1	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4601:ILE:HD13	1:A:4701:PHE:HD2	1.82	0.44
1:B:1715:ILE:O	1:B:1715:ILE:HG22	2.16	0.44
1:B:2320:LEU:HD23	1:B:2321:ASP:O	2.18	0.44
1:B:2416:PHE:N	1:B:2416:PHE:CD2	2.85	0.44
1:B:2617:VAL:HG22	1:B:2624:TRP:CE3	2.52	0.44
1:B:2745:GLU:HG2	1:B:2748:LEU:HD12	1.99	0.44
1:B:3164:LEU:C	1:B:3166:ASN:H	2.20	0.44
1:B:3251:ARG:NH2	1:B:3604:PHE:CZ	2.85	0.44
1:B:3343:GLU:C	1:B:3345:GLN:N	2.70	0.44
1:B:3594:LEU:HD11	1:B:3618:MET:HG2	1.99	0.44
1:B:4021:ILE:O	1:B:4025:GLN:HB3	2.17	0.44
1:B:4546:VAL:CG1	1:B:4551:LYS:HG3	2.46	0.44
1:A:1450:ALA:O	1:A:1453:HIS:HB2	2.16	0.44
1:A:2338:ARG:O	1:A:2346:GLU:OE2	2.34	0.44
1:A:2380:PRO:C	1:A:2382:GLY:N	2.69	0.44
1:A:2382:GLY:O	1:A:2384:ARG:HG3	2.17	0.44
1:A:2669:PRO:HG3	1:A:2767:VAL:HG21	2.00	0.44
1:A:2771:GLY:HA3	1:A:2781:ILE:O	2.17	0.44
1:A:3815:ASP:O	1:A:3816:LEU:C	2.55	0.44
1:A:4318:SER:O	1:A:4321:ARG:HD3	2.17	0.44
1:B:2050:LEU:HD11	1:B:2071:MET:HG2	1.98	0.44
1:B:2430:TYR:O	1:B:2431:LEU:C	2.54	0.44
1:B:2729:VAL:HB	1:B:2782:LYS:O	2.17	0.44
1:A:1856:LEU:O	1:A:1860:ALA:N	2.50	0.44
1:A:3632:LEU:O	1:A:3632:LEU:HD23	2.17	0.44
1:A:3901:GLU:O	1:A:3901:GLU:HG2	2.17	0.44
1:A:4659:ILE:HG22	1:A:4661:SER:H	1.82	0.44
1:A:4694:GLU:OE2	1:A:4727:LYS:NZ	2.50	0.44
1:B:2036:LEU:O	1:B:2036:LEU:HD23	2.16	0.44
1:B:2259:ILE:HG23	1:B:2289:TYR:HB2	1.98	0.44
1:B:2522:ARG:HD3	1:B:2585:MET:SD	2.57	0.44
1:B:2841:ASN:N	1:B:2841:ASN:ND2	2.64	0.44
1:B:3093:GLY:O	1:B:3138:ARG:HB3	2.17	0.44
1:B:3194:LEU:H	1:B:3224:ARG:NH2	2.15	0.44
1:B:3563:LEU:O	1:B:3567:LEU:HG	2.18	0.44
1:B:4025:GLN:O	1:B:4025:GLN:HG2	2.17	0.44
1:B:4109:ASP:HA	1:B:4112:ASN:ND2	2.32	0.44
1:B:4499:PHE:CE1	1:B:4578:ILE:HD13	2.52	0.44
1:A:2865:THR:C	1:A:2867:ASP:H	2.20	0.44
1:A:3118:ARG:O	1:A:3120:GLY:N	2.50	0.44
1:A:3270:LEU:HD12	1:A:3270:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3331:GLN:HE21	1:A:3532:TYR:HB3	1.82	0.44
1:A:3691:ASP:OD1	1:A:3691:ASP:C	2.56	0.44
1:A:3992:LEU:HD22	1:A:4430:LEU:HB2	1.99	0.44
1:A:4201:GLU:HG3	1:A:4228:ASN:HB2	1.98	0.44
1:A:4575:LEU:O	1:A:4578:ILE:HB	2.17	0.44
1:B:1630:PRO:HG2	1:B:1631:ALA:N	2.29	0.44
1:B:1904:PHE:O	1:B:1906:TRP:N	2.50	0.44
1:B:2492:LEU:HD12	1:B:2495:GLN:HB2	1.99	0.44
1:B:2501:ILE:HG21	1:B:2566:SER:HA	1.98	0.44
1:B:2606:PRO:HB3	1:B:2615:TYR:CZ	2.52	0.44
1:B:2641:VAL:O	1:B:2831:PHE:CE2	2.71	0.44
1:B:3343:GLU:C	1:B:3345:GLN:H	2.21	0.44
1:B:3352:ASN:CA	1:B:3511:LEU:HD21	2.47	0.44
1:B:3690:ALA:O	1:B:3692:LYS:N	2.50	0.44
1:B:4044:TRP:HB3	1:B:4048:PHE:CE2	2.52	0.44
1:B:4164:SER:HB3	1:B:4165:PRO:CD	2.33	0.44
1:A:2313:LYS:HE3	1:A:2366:ASN:HD21	1.81	0.44
1:A:2763:ILE:HG22	1:A:2807:PHE:HE2	1.82	0.44
1:A:3686:MET:CE	1:A:3719:LEU:HD13	2.48	0.44
1:A:4373:PHE:O	1:A:4382:SER:HB2	2.17	0.44
1:B:1782:ALA:HB2	1:B:1922:LEU:CD2	2.48	0.44
1:B:2265:ILE:CD1	1:B:2414:VAL:HG22	2.47	0.44
1:B:2732:PRO:O	1:B:2734:GLN:N	2.50	0.44
1:B:2937:HIS:O	1:B:2939:PRO:HD3	2.17	0.44
1:B:3073:PHE:CD2	1:B:3145:PHE:CE1	3.06	0.44
1:B:3563:LEU:HD22	1:B:3567:LEU:HD11	1.99	0.44
1:B:3635:PRO:C	1:B:3637:PHE:H	2.21	0.44
1:B:3717:PRO:HA	1:B:3761:MET:O	2.17	0.44
1:B:4517:LEU:O	1:B:4521:LEU:HB2	2.17	0.44
1:A:1468:ILE:HD11	1:A:1503:TRP:HE1	1.83	0.44
1:A:1538:TRP:HZ3	1:A:1656:ILE:HD13	1.82	0.44
1:A:2029:ASN:HD22	1:A:2029:ASN:N	2.14	0.44
1:A:2276:GLY:O	1:A:2398:GLN:HA	2.18	0.44
1:A:3017:VAL:HG21	1:A:3257:PRO:HD3	2.00	0.44
1:A:3056:ARG:HH11	1:A:3099:LEU:CD1	2.28	0.44
1:A:4174:SER:O	1:A:4178:ALA:HB2	2.17	0.44
1:A:4604:THR:OG1	1:A:4671:TRP:HZ3	2.00	0.44
1:A:4605:ARG:HA	1:A:4671:TRP:CZ3	2.53	0.44
1:B:1611:ARG:HH11	1:B:1611:ARG:CG	2.31	0.44
1:B:1655:LEU:CB	1:B:1658:GLU:HG3	2.47	0.44
1:B:2965:ARG:HG3	1:B:2965:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4099:HIS:HD2	1:B:4099:HIS:O	2.01	0.44
1:A:1612:TRP:O	1:A:1616:GLU:HB2	2.17	0.44
1:A:1796:ASP:C	1:A:1796:ASP:OD2	2.56	0.44
1:A:3031:TRP:CZ3	1:A:3032:MET:HG2	2.52	0.44
1:A:3114:GLU:HG3	1:A:3117:GLN:NE2	2.33	0.44
1:A:3977:LYS:HA	1:A:3982:GLU:HG3	1.99	0.44
1:A:4036:HIS:CD2	1:A:4044:TRP:HE1	2.34	0.44
1:B:1548:TYR:O	1:B:1548:TYR:CD1	2.67	0.44
1:B:1665:ILE:O	1:B:1667:GLN:N	2.51	0.44
1:B:1681:LYS:HE3	1:B:1685:GLU:OE2	2.17	0.44
1:B:2236:LEU:HD22	1:B:2240:ILE:HD11	2.00	0.44
1:B:2364:VAL:HG11	1:B:2407:THR:HB	1.99	0.44
1:B:2704:ALA:HB2	1:B:3085:GLU:OE2	2.18	0.44
1:B:3234:ILE:O	1:B:3238:ILE:HD13	2.17	0.44
1:B:3324:LEU:HD11	1:B:3539:LEU:CG	2.44	0.44
1:A:1419:TRP:C	1:A:1421:ALA:H	2.20	0.44
1:A:1578:SER:C	1:A:1580:TYR:H	2.21	0.44
1:A:2020:GLY:CA	1:A:2068:HIS:HB3	2.48	0.44
1:A:2282:LYS:O	1:A:2285:SER:HB2	2.17	0.44
1:A:2405:LEU:O	1:A:2408:ILE:HG13	2.18	0.44
1:A:2543:ARG:HD3	1:A:2661:HIS:CD2	2.53	0.44
1:A:4159:SER:OG	1:A:4160:PHE:N	2.51	0.44
1:A:4213:PHE:O	1:A:4214:ARG:CG	2.60	0.44
1:B:1783:THR:O	1:B:1784:LEU:C	2.55	0.44
1:B:2359:VAL:HG23	1:B:2397:VAL:HG21	1.99	0.44
1:B:3605:PHE:HB3	1:B:3609:PHE:HB3	2.00	0.44
1:B:3767:ARG:HD3	1:B:4205:HIS:NE2	2.32	0.44
1:B:4597:PRO:HG2	1:B:4692:LEU:CD1	2.48	0.44
1:A:2531:LEU:HD13	1:A:2809:ARG:NE	2.33	0.44
1:A:3061:ARG:CZ	1:A:3067:GLU:OE1	2.66	0.44
1:A:3555:ASN:O	1:A:3559:ARG:HB2	2.17	0.44
1:A:3768:ASP:HA	1:A:3769:PRO:HD2	1.82	0.44
1:A:3936:PRO:O	1:A:3938:GLU:N	2.51	0.44
1:A:3998:LEU:HD13	1:A:4018:LYS:HD3	2.00	0.44
1:A:4057:ILE:O	1:A:4057:ILE:CG2	2.65	0.44
1:A:4189:ASN:H	1:A:4218:THR:HG22	1.83	0.44
1:B:2189:GLN:NE2	1:B:2225:GLY:HA3	2.33	0.44
1:B:2797:ASP:HB2	1:B:2800:ARG:CG	2.47	0.44
1:B:4122:VAL:HG11	1:B:4216:PHE:CZ	2.53	0.44
1:A:1697:PHE:O	1:A:1700:VAL:HG22	2.18	0.43
1:A:2590:ARG:HG2	1:A:2613:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3858:LEU:O	1:A:3860:LYS:N	2.51	0.43
1:A:4392:PHE:O	1:A:4396:ILE:HG13	2.18	0.43
1:B:1557:GLY:O	1:B:1561:LEU:HB2	2.18	0.43
1:B:1592:ASP:O	1:B:1593:ASP:C	2.55	0.43
1:B:1700:VAL:CG1	1:B:1704:ASP:HB2	2.47	0.43
1:B:1748:GLU:O	1:B:1870:GLN:HG3	2.18	0.43
1:B:1788:SER:CA	1:B:1810:TYR:CZ	3.01	0.43
1:B:2236:LEU:HD22	1:B:2240:ILE:CD1	2.48	0.43
1:B:2549:ILE:O	1:B:2553:GLN:HB2	2.17	0.43
1:B:2641:VAL:HB	1:B:2887:LEU:HD22	1.98	0.43
1:B:2848:ASN:HD22	1:B:2848:ASN:HA	1.53	0.43
1:B:3644:ARG:O	1:B:3647:TRP:HB2	2.18	0.43
1:B:3949:SER:HA	1:B:4110:PHE:HE1	1.83	0.43
1:B:4256:PRO:HG2	1:B:4259:ARG:HB3	1.99	0.43
1:B:4572:MET:CE	1:B:4575:LEU:HD12	2.48	0.43
1:A:1490:THR:HG21	1:A:1492:TRP:CD1	2.53	0.43
1:A:1570:ASN:O	1:A:1573:SER:N	2.51	0.43
1:A:1968:MET:CE	1:A:2051:LYS:NZ	2.81	0.43
1:A:2057:VAL:CG1	1:A:2065:ILE:HB	2.48	0.43
1:A:2327:TRP:CH2	1:A:2380:PRO:HD2	2.52	0.43
1:A:3178:PRO:HB2	1:A:3179:GLU:OE1	2.18	0.43
1:A:3836:ASN:O	1:A:3839:SER:N	2.46	0.43
1:A:4644:LEU:HD23	1:A:4648:VAL:N	2.32	0.43
1:B:1823:TRP:CD1	1:B:1885:GLN:HB3	2.53	0.43
1:B:2129:VAL:CG2	1:B:2130:PRO:CD	2.89	0.43
1:B:2379:LEU:C	1:B:2381:ASN:N	2.71	0.43
1:B:2781:ILE:N	1:B:2781:ILE:CD1	2.81	0.43
1:B:3084:LEU:HD22	1:B:3161:SER:CB	2.48	0.43
1:B:3351:ARG:O	1:B:3355:ILE:CG1	2.64	0.43
1:B:4059:PRO:C	1:B:4061:SER:N	2.71	0.43
1:B:4644:LEU:HD13	1:B:4647:ALA:HB3	2.00	0.43
1:A:1472:HIS:CG	1:A:1472:HIS:O	2.70	0.43
1:A:1740:THR:O	1:A:1742:ILE:HD13	2.18	0.43
1:A:2239:LYS:HE3	1:A:2295:GLN:HE21	1.83	0.43
1:A:2977:LYS:C	1:A:2979:PHE:N	2.71	0.43
1:A:3506:ASN:HA	1:A:3509:ASN:HD22	1.82	0.43
1:A:3689:TYR:CE1	1:A:3761:MET:SD	3.11	0.43
1:A:3825:VAL:C	1:A:3827:LEU:N	2.71	0.43
1:A:4070:SER:C	1:A:4072:GLN:H	2.22	0.43
1:A:4293:THR:HG22	1:A:4294:LYS:CG	2.48	0.43
1:B:1871:LYS:O	1:B:1875:PHE:CD2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2491:GLY:O	1:B:2493:LYS:N	2.50	0.43
1:B:2606:PRO:CB	1:B:2615:TYR:CE2	3.00	0.43
1:B:3004:VAL:HG11	1:B:3012:ALA:HB2	2.00	0.43
1:B:3233:TYR:CD2	1:B:3620:ARG:HG3	2.53	0.43
1:B:3348:LEU:HD22	1:B:3511:LEU:CD1	2.48	0.43
1:B:3539:LEU:O	1:B:3540:ILE:C	2.55	0.43
1:B:3635:PRO:HA	1:B:3663:ILE:CD1	2.48	0.43
1:B:3972:THR:HG21	1:B:4101:PHE:CE2	2.53	0.43
1:B:4213:PHE:C	1:B:4214:ARG:HG2	2.37	0.43
1:B:4222:HIS:CD2	1:B:4223:PRO:N	2.86	0.43
1:B:4393:MET:O	1:B:4397:GLU:HG3	2.18	0.43
1:A:1419:TRP:CZ3	1:A:1502:ILE:HD12	2.54	0.43
1:A:1797:VAL:C	1:A:1854:MET:HE1	2.39	0.43
1:A:1854:MET:O	1:A:1856:LEU:N	2.51	0.43
1:A:2490:ALA:O	1:A:2494:VAL:HG23	2.19	0.43
1:A:2525:ILE:HD13	1:A:2526:MET:HG3	2.00	0.43
1:A:2547:ASN:O	1:A:2551:TYR:HB2	2.18	0.43
1:A:2627:TRP:HB3	1:A:2651:VAL:HG23	2.01	0.43
1:A:3632:LEU:HD23	1:A:3632:LEU:C	2.39	0.43
1:A:4003:GLU:HG3	1:B:2842:LEU:HD23	1.99	0.43
1:A:4495:LEU:O	1:A:4498:CYS:HB3	2.18	0.43
1:A:4503:ILE:HG13	1:A:4503:ILE:H	1.70	0.43
1:A:4656:PRO:HA	1:A:4719:ARG:NH2	2.34	0.43
1:A:4693:ASN:C	1:A:4693:ASN:ND2	2.71	0.43
1:B:2223:PHE:C	1:B:2225:GLY:H	2.20	0.43
1:B:2439:PHE:HA	3:B:9018:SPM:C11	2.48	0.43
1:B:2602:ILE:O	1:B:2603:THR:C	2.56	0.43
1:B:2952:TYR:CE1	1:B:2962:PRO:HD3	2.54	0.43
1:B:3813:ARG:CG	1:B:3814:SER:N	2.81	0.43
1:B:4118:MET:O	1:B:4119:ALA:C	2.56	0.43
1:B:4404:THR:HB	1:B:4405:PRO:HD2	2.00	0.43
1:A:1968:MET:HE3	1:A:2051:LYS:NZ	2.34	0.43
1:A:2212:ILE:N	1:A:2213:PRO:CD	2.80	0.43
1:A:2526:MET:HE1	1:A:2808:LEU:HD21	1.99	0.43
1:A:3875:VAL:O	1:A:3879:ILE:HG12	2.18	0.43
1:A:4117:ASP:OD1	1:A:4117:ASP:C	2.56	0.43
1:A:4221:ILE:HD12	1:A:4221:ILE:N	2.34	0.43
1:A:4719:ARG:HH11	1:A:4719:ARG:CG	2.32	0.43
1:B:1639:ILE:HD11	1:B:1675:LEU:HB3	2.00	0.43
1:B:1826:GLN:O	1:B:1827:VAL:C	2.57	0.43
1:B:1835:THR:O	1:B:1835:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1907:LEU:HD23	1:B:1907:LEU:HA	1.85	0.43
1:B:2205:PRO:HB3	1:B:2265:ILE:HD11	2.00	0.43
1:B:2314:ASP:O	1:B:2317:PHE:N	2.52	0.43
1:B:2696:VAL:HA	1:B:2740:VAL:O	2.18	0.43
1:B:3022:LYS:HB2	2:B:9010:ADP:O3B	2.18	0.43
1:B:3308:GLN:OE1	1:B:3311:ARG:NH2	2.38	0.43
1:B:4668:THR:C	1:B:4669:LEU:HD12	2.39	0.43
1:A:2275:VAL:HG12	1:A:2276:GLY:N	2.33	0.43
1:A:2427:PHE:O	1:A:2430:TYR:HB3	2.19	0.43
1:A:2679:GLY:O	1:A:2683:THR:OG1	2.34	0.43
1:A:3362:ALA:HA	1:A:3365:ASP:HB2	2.00	0.43
1:A:3672:PRO:HA	1:A:3782:THR:O	2.19	0.43
1:A:3993:LYS:O	1:A:3996:ASP:HB2	2.19	0.43
1:B:1736:ASP:OD2	1:B:1736:ASP:N	2.52	0.43
1:B:2187:TYR:O	1:B:2190:TYR:N	2.51	0.43
1:B:2432:ASP:O	1:B:2433:THR:C	2.57	0.43
1:B:2536:SER:HB2	1:B:2580:GLY:O	2.19	0.43
1:B:3057:MET:HA	1:B:3060:LYS:CB	2.48	0.43
1:B:3696:LYS:NZ	1:B:3721:GLN:NE2	2.67	0.43
1:B:3723:VAL:O	1:B:3725:ASN:N	2.52	0.43
1:B:3798:LEU:HD12	1:B:3798:LEU:O	2.18	0.43
1:B:3940:LEU:O	1:B:3940:LEU:HD13	2.19	0.43
1:B:3973:ILE:HD13	1:B:3983:ILE:HG13	2.01	0.43
1:A:1554:LEU:HD23	1:A:1647:LEU:HD21	2.00	0.43
1:A:1576:LYS:HG2	1:A:1581:TYR:CE1	2.53	0.43
1:A:1828:ASP:OD2	1:A:1913:TYR:HE1	2.01	0.43
1:A:2239:LYS:HA	1:A:2239:LYS:HD2	1.77	0.43
1:A:2447:GLN:HE22	1:A:2492:LEU:HD23	1.81	0.43
1:A:2890:ILE:HD12	1:A:2893:MET:HE1	2.00	0.43
1:A:2910:LEU:O	1:A:2914:GLN:HB3	2.19	0.43
1:A:3839:SER:C	1:A:3841:ALA:N	2.70	0.43
1:A:3936:PRO:CG	1:A:3937:ASN:N	2.78	0.43
1:A:4062:TRP:C	1:A:4064:VAL:H	2.22	0.43
1:A:4355:LEU:CD1	1:A:4718:GLN:HA	2.48	0.43
1:A:4553:TYR:C	1:A:4553:TYR:CD1	2.92	0.43
1:B:1769:TRP:O	1:B:1773:VAL:HG23	2.19	0.43
1:B:2092:LYS:HE2	1:B:4297:GLU:OE1	2.19	0.43
1:B:2542:ASN:O	1:B:2543:ARG:C	2.57	0.43
1:B:2723:THR:OG1	1:B:2724:PRO:HD2	2.18	0.43
1:B:4164:SER:CB	1:B:4165:PRO:HD2	2.33	0.43
1:B:4491:ILE:O	1:B:4491:ILE:CG1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4572:MET:HE2	1:B:4575:LEU:HD12	2.01	0.43
1:B:4704:ASP:O	1:B:4705:LEU:HD23	2.18	0.43
1:A:1480:HIS:CE1	1:A:1521:ALA:HA	2.54	0.43
1:A:2090:ASN:ND2	1:A:2091:LEU:N	2.64	0.43
1:A:2199:ILE:HG21	1:A:2219:LEU:HD11	2.01	0.43
1:A:3154:PHE:HD2	1:A:3155:HIS:NE2	2.17	0.43
1:A:3255:VAL:O	1:A:3255:VAL:HG13	2.18	0.43
1:A:3766:THR:HG22	1:A:3767:ARG:H	1.83	0.43
1:A:4192:LEU:O	1:A:4194:PRO:HD2	2.18	0.43
1:A:4719:ARG:HH11	1:A:4719:ARG:HG3	1.84	0.43
1:B:1554:LEU:HD22	1:B:1609:GLN:OE1	2.18	0.43
1:B:1786:SER:O	1:B:1787:GLU:C	2.57	0.43
1:B:1863:VAL:CG2	1:B:1872:ARG:HH11	2.26	0.43
1:B:2532:ARG:HG2	1:B:2532:ARG:HH11	1.83	0.43
1:B:2665:SER:O	1:B:2667:HIS:ND1	2.52	0.43
1:B:2759:VAL:O	1:B:2763:ILE:HG13	2.19	0.43
1:B:2869:GLN:HB2	1:B:2872:TYR:CG	2.54	0.43
1:B:3352:ASN:HA	1:B:3511:LEU:HD21	2.01	0.43
1:B:4571:ARG:CD	1:B:4593:GLY:O	2.67	0.43
1:A:1575:MET:O	1:A:1575:MET:HG3	2.19	0.43
1:A:1974:GLY:CA	1:A:2079:PRO:HD3	2.49	0.43
1:A:2106:GLU:HA	1:A:2129:VAL:HG21	1.99	0.43
1:A:2262:LEU:HD21	1:A:2274:MET:HG2	2.00	0.43
1:A:2551:TYR:HD1	1:A:2619:ILE:CG1	2.32	0.43
1:A:3540:ILE:HD13	1:A:3540:ILE:HA	1.93	0.43
1:A:4222:HIS:HA	1:A:4223:PRO:HD2	1.78	0.43
1:B:1826:GLN:O	1:B:1828:ASP:N	2.52	0.43
1:B:2322:LEU:HD23	1:B:2322:LEU:HA	1.84	0.43
1:B:2626:LEU:HB3	1:B:2629:ASN:ND2	2.33	0.43
1:B:3602:ILE:HD13	1:B:3602:ILE:HA	1.86	0.43
1:B:3653:PRO:HB2	1:B:3655:ASP:OD1	2.18	0.43
1:B:4063:ILE:HD12	1:B:4063:ILE:H	1.83	0.43
1:B:4189:ASN:HD22	1:B:4218:THR:CG2	2.32	0.43
1:B:4590:TRP:CZ3	1:B:4593:GLY:HA3	2.54	0.43
1:A:1555:VAL:HB	1:A:1558:TRP:CZ2	2.54	0.43
1:A:1662:ILE:O	1:A:1665:ILE:HG13	2.19	0.43
1:A:2274:MET:HE3	1:A:2286:TRP:HB3	2.00	0.43
1:A:2587:LEU:O	1:A:2591:GLU:HG3	2.18	0.43
1:A:3643:GLU:OE2	1:A:3666:LYS:CE	2.65	0.43
1:A:3648:HIS:O	1:A:3651:SER:N	2.51	0.43
1:A:4066:GLN:O	1:A:4066:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4369:PHE:CD2	1:A:4369:PHE:N	2.87	0.43
1:B:1737:GLU:HB2	1:B:1739:THR:HG23	2.01	0.43
1:B:1846:GLN:O	1:B:1850:GLN:HG2	2.19	0.43
1:B:1863:VAL:O	1:B:1872:ARG:NH1	2.51	0.43
1:B:2360:ASP:OD1	1:B:2360:ASP:C	2.57	0.43
1:B:3139:ARG:CG	1:B:3139:ARG:O	2.62	0.43
1:B:4020:LEU:HD11	1:B:4033:LEU:HG	2.01	0.43
1:B:4167:GLY:O	1:B:4171:ALA:CB	2.66	0.43
1:A:2582:GLY:HA2	1:A:2585:MET:CE	2.48	0.42
1:A:2875:SER:C	1:A:2877:ARG:H	2.22	0.42
1:A:3087:MET:HA	1:A:3087:MET:CE	2.49	0.42
1:A:3358:GLN:HB3	1:A:3504:LEU:HD11	2.01	0.42
1:A:3853:SER:O	1:A:3854:THR:C	2.57	0.42
1:A:3858:LEU:HA	1:A:3858:LEU:HD12	1.54	0.42
1:A:4011:LEU:C	1:A:4012:LEU:HD12	2.38	0.42
1:A:4668:THR:C	1:A:4669:LEU:HD12	2.39	0.42
1:B:2636:VAL:CG1	1:B:2637:GLU:N	2.81	0.42
1:B:3073:PHE:CD2	1:B:3145:PHE:HE1	2.37	0.42
1:B:3671:TYR:HD2	1:B:3734:LEU:HA	1.83	0.42
1:B:3727:ASP:CB	1:B:3729:VAL:CG1	2.97	0.42
1:A:1481:TRP:HB3	1:A:1494:ILE:HG13	1.99	0.42
1:A:2680:LYS:N	2:A:9003:ADP:O2B	2.50	0.42
1:A:2759:VAL:HG13	1:A:2760:ILE:HD13	2.01	0.42
1:A:2902:VAL:HG22	1:A:2938:PHE:CD2	2.54	0.42
1:A:2903:ARG:NH2	1:A:2947:LYS:O	2.52	0.42
1:A:3019:GLY:C	2:A:9004:ADP:H5'2	2.38	0.42
1:A:3061:ARG:NH1	1:A:3061:ARG:HG2	2.33	0.42
1:A:3083:PHE:N	1:A:3083:PHE:HD2	2.17	0.42
1:A:4020:LEU:CD2	1:A:4034:VAL:HG22	2.49	0.42
1:A:4568:PHE:CZ	1:A:4572:MET:SD	3.12	0.42
1:A:4694:GLU:O	1:A:4696:ARG:N	2.52	0.42
1:B:1630:PRO:O	1:B:1631:ALA:C	2.56	0.42
1:B:1655:LEU:HB2	1:B:1658:GLU:HG3	2.01	0.42
1:B:1798:ASN:HA	1:B:1854:MET:HE3	2.01	0.42
1:B:1871:LYS:O	1:B:1875:PHE:HD2	2.02	0.42
1:B:2229:GLN:C	1:B:2230:PRO:O	2.57	0.42
1:B:2502:ILE:HB	1:B:2573:LEU:HD13	2.01	0.42
1:B:2660:LEU:HD22	1:B:2670:LEU:HD13	2.01	0.42
1:B:3160:THR:C	1:B:3162:PRO:HD3	2.39	0.42
1:B:3238:ILE:HG22	1:B:3255:VAL:HG22	2.01	0.42
1:B:3324:LEU:HD12	1:B:3539:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3965:LEU:HD23	1:B:4426:MET:CE	2.49	0.42
1:A:1470:ASP:CB	1:A:1518:ILE:HD12	2.49	0.42
1:A:1576:LYS:HG2	1:A:1581:TYR:CZ	2.54	0.42
1:A:1601:LEU:HA	1:A:1666:GLN:OE1	2.18	0.42
1:A:1914:TYR:OH	1:A:1924:LYS:HD3	2.19	0.42
1:A:1950:THR:HG21	1:A:2108:ILE:HG13	2.01	0.42
1:A:2346:GLU:O	1:A:2351:HIS:HE1	2.02	0.42
1:A:2405:LEU:HD23	1:A:2408:ILE:HD11	2.00	0.42
1:A:2911:ARG:HD3	1:A:2911:ARG:HA	1.86	0.42
1:A:3074:ASP:OD1	1:A:3146:THR:OG1	2.31	0.42
1:A:3074:ASP:CA	1:A:3077:ASN:HD22	2.32	0.42
1:A:3295:THR:O	1:A:3299:VAL:HG23	2.19	0.42
1:A:3936:PRO:C	1:A:3938:GLU:H	2.23	0.42
1:A:4317:TYR:CD2	1:A:4317:TYR:N	2.88	0.42
1:B:1552:CYS:SG	1:B:1647:LEU:HD12	2.59	0.42
1:B:1558:TRP:CE2	1:B:1606:ILE:HG13	2.54	0.42
1:B:1608:VAL:HG12	1:B:1609:GLN:N	2.33	0.42
1:B:2863:ARG:HD2	1:B:2864:PHE:CE1	2.55	0.42
1:B:3949:SER:HA	1:B:4110:PHE:CE1	2.54	0.42
1:B:4596:ASN:ND2	1:B:4596:ASN:O	2.52	0.42
1:B:4666:ILE:HG13	1:B:4667:ALA:H	1.84	0.42
1:B:4709:GLN:N	1:B:4709:GLN:NE2	2.49	0.42
1:A:1791:HIS:O	1:A:1795:VAL:HG23	2.20	0.42
1:A:2728:THR:HG21	1:A:2779:THR:HG21	2.01	0.42
1:A:3023:SER:CB	1:A:3027:ARG:HH12	2.32	0.42
1:B:1910:MET:HA	1:B:1929:MET:HB2	2.01	0.42
1:B:4030:PHE:CD2	1:B:4030:PHE:N	2.88	0.42
1:B:4288:ILE:HG23	1:B:4289:PRO:HA	2.01	0.42
1:B:4484:LEU:CD2	1:B:4500:GLU:HG3	2.49	0.42
1:A:1578:SER:C	1:A:1580:TYR:N	2.72	0.42
1:A:1883:VAL:HG11	1:A:2111:VAL:HG22	2.01	0.42
1:A:2554:LEU:HD12	1:A:2554:LEU:HA	1.85	0.42
1:A:2718:CYS:HB3	1:A:2731:ARG:O	2.19	0.42
1:A:2997:HIS:O	1:A:3001:ILE:HG13	2.19	0.42
1:A:3179:GLU:HG3	1:A:3216:LEU:HD11	2.01	0.42
1:A:3602:ILE:HG23	1:A:3610:ARG:CG	2.49	0.42
1:A:4355:LEU:O	1:A:4358:SER:HB3	2.20	0.42
1:A:4622:HIS:HB2	1:A:4679:PHE:HE1	1.84	0.42
1:B:1671:ARG:HG3	1:B:1671:ARG:HH11	1.85	0.42
1:B:1828:ASP:C	1:B:1830:ALA:N	2.73	0.42
1:B:1856:LEU:O	1:B:1860:ALA:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2552:ASN:O	1:B:2554:LEU:N	2.53	0.42
1:B:3700:LEU:HD13	1:B:3701:ASP:CA	2.48	0.42
1:B:3701:ASP:OD1	1:B:3703:SER:N	2.47	0.42
1:B:3789:THR:HB	1:B:3790:PRO:HD2	2.00	0.42
1:B:4571:ARG:O	1:B:4572:MET:C	2.58	0.42
1:B:4621:LEU:HD13	1:B:4671:TRP:CD2	2.54	0.42
1:A:1417:THR:CB	1:A:1422:ILE:HG22	2.48	0.42
1:A:2598:GLN:OE1	1:A:2612:LEU:N	2.52	0.42
1:A:3185:GLY:HA2	1:A:3264:ILE:HD13	2.00	0.42
1:A:3536:TYR:O	1:A:3539:LEU:N	2.53	0.42
1:A:4604:THR:OG1	1:A:4671:TRP:CZ3	2.73	0.42
1:B:1920:ASN:HD22	1:B:1920:ASN:C	2.21	0.42
1:B:2252:LYS:HE2	1:B:2254:GLU:HG2	2.00	0.42
1:B:2909:ALA:O	1:B:2913:PHE:HB2	2.19	0.42
1:B:2918:VAL:HG22	1:B:3172:TRP:CZ2	2.55	0.42
1:B:3088:ASN:HD21	1:B:3163:ALA:HB2	1.84	0.42
1:B:3108:LEU:C	1:B:3109:MET:HG2	2.39	0.42
1:B:4165:PRO:HG2	1:B:4166:GLU:N	2.31	0.42
1:A:1549:GLN:HE21	1:A:1551:LYS:CE	2.33	0.42
1:A:1569:LEU:HD13	1:A:1599:ARG:NH2	2.34	0.42
1:A:2008:ALA:HA	1:A:2011:ARG:NH1	2.35	0.42
1:A:2972:VAL:O	1:A:2976:LEU:HB2	2.20	0.42
1:A:3858:LEU:C	1:A:3860:LYS:N	2.73	0.42
1:A:3859:LYS:C	1:A:3862:THR:HG22	2.39	0.42
1:A:3864:GLU:CG	1:A:3865:ILE:HG13	2.50	0.42
1:A:4117:ASP:CG	1:A:4119:ALA:HB3	2.40	0.42
1:A:4561:LEU:O	1:A:4565:ILE:HG13	2.19	0.42
1:A:4712:SER:OG	1:A:4715:ASN:HB2	2.19	0.42
1:B:1614:TYR:HD2	1:B:1615:LEU:CD2	2.33	0.42
1:B:1744:MET:HE3	1:B:1752:VAL:HG21	2.02	0.42
1:B:1763:GLY:H	1:B:1764:PRO:HD3	1.85	0.42
1:B:1830:ALA:O	1:B:1841:ILE:HG23	2.19	0.42
1:B:2540:LEU:HD12	1:B:2662:ALA:HB3	2.01	0.42
1:B:2963:VAL:HG12	1:B:2964:ASN:N	2.35	0.42
1:B:2972:VAL:HG12	1:B:2976:LEU:HD12	2.02	0.42
1:B:3338:GLN:O	1:B:3341:ALA:N	2.52	0.42
1:B:3719:LEU:HD23	1:B:3719:LEU:C	2.40	0.42
1:B:4207:LEU:O	1:B:4209:PRO:HD3	2.19	0.42
1:B:4255:ILE:O	1:B:4389:ARG:NE	2.46	0.42
1:A:1706:LEU:O	1:A:1707:GLU:C	2.58	0.42
1:A:1715:ILE:CG2	1:A:1719:GLN:HE22	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1735:ASP:OD2	1:A:1740:THR:HG23	2.19	0.42
1:A:1979:GLY:HA2	2:A:9001:ADP:O2A	2.20	0.42
1:A:2386:ALA:O	1:A:2388:PRO:HD3	2.19	0.42
1:A:2747:ASN:HD22	1:A:2747:ASN:H	1.68	0.42
1:A:2863:ARG:HG3	1:A:2925:TRP:CH2	2.54	0.42
1:A:3908:LEU:O	1:A:3908:LEU:HG	2.18	0.42
1:A:3990:PHE:O	1:A:3994:GLY:N	2.51	0.42
1:B:1606:ILE:C	1:B:1608:VAL:H	2.22	0.42
1:B:1655:LEU:CD2	1:B:1655:LEU:N	2.70	0.42
1:B:3104:GLU:C	1:B:3106:THR:N	2.73	0.42
1:B:3113:LYS:O	1:B:3116:ALA:HB3	2.20	0.42
1:A:2423:THR:HA	1:A:2530:ARG:HH11	1.85	0.42
1:A:2914:GLN:O	1:A:2916:ARG:N	2.52	0.42
1:A:3059:LEU:HD13	1:A:3137:VAL:HG21	2.02	0.42
1:A:3886:TYR:CE2	1:A:3940:LEU:HD13	2.55	0.42
1:A:4175:ILE:HA	1:A:4185:VAL:HG21	2.02	0.42
1:A:4502:GLU:O	1:A:4503:ILE:C	2.58	0.42
1:B:1788:SER:HB2	1:B:1810:TYR:CD1	2.54	0.42
1:B:1929:MET:O	1:B:1930:ALA:HB3	2.20	0.42
1:B:2307:ASP:HA	1:B:2308:PRO:HD3	1.89	0.42
1:B:2423:THR:HA	1:B:2426:ILE:HD13	2.02	0.42
1:B:2711:LEU:O	1:B:2714:PHE:HB2	2.19	0.42
1:B:2965:ARG:HG3	1:B:2965:ARG:NH1	2.34	0.42
1:B:3668:PHE:CD1	1:B:3668:PHE:O	2.73	0.42
1:B:4122:VAL:HG12	1:B:4132:LEU:HD11	2.02	0.42
1:B:4691:TYR:HA	1:B:4698:GLU:O	2.19	0.42
1:A:1416:GLU:O	1:A:1498:THR:HG21	2.20	0.42
1:A:1544:ASP:OD2	1:A:1556:ARG:NE	2.43	0.42
1:A:1545:LEU:HA	1:A:1554:LEU:O	2.19	0.42
1:A:1732:LEU:HD13	1:A:1741:ILE:HD12	2.02	0.42
1:A:2341:ASP:O	1:A:2343:VAL:N	2.52	0.42
1:A:3285:LEU:HD13	1:A:3578:SER:CA	2.49	0.42
1:A:3661:ASN:HA	1:A:3664:MET:CE	2.49	0.42
1:A:3838:LEU:O	1:A:3841:ALA:HB3	2.20	0.42
1:A:4187:LEU:HD13	1:A:4217:MET:HG2	2.02	0.42
1:A:4200:LEU:CD2	1:A:4204:LEU:HG	2.50	0.42
1:A:4576:SER:C	1:A:4578:ILE:N	2.71	0.42
1:A:4691:TYR:CD2	1:A:4696:ARG:HG2	2.54	0.42
1:B:1591:TRP:O	1:B:1595:LEU:HB2	2.19	0.42
1:B:1642:GLU:O	1:B:1646:ILE:HG12	2.20	0.42
1:B:1786:SER:O	1:B:1789:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2616:SER:O	1:B:2624:TRP:HE3	2.03	0.42
1:B:3702:SER:C	1:B:3704:PHE:N	2.74	0.42
1:B:4044:TRP:HZ2	1:B:4062:TRP:HB2	1.85	0.42
1:B:4285:LEU:O	1:B:4288:ILE:HG13	2.20	0.42
1:A:1603:ASP:O	1:A:1606:ILE:HG22	2.20	0.41
1:A:1825:THR:O	1:A:1829:GLN:HG3	2.20	0.41
1:A:1828:ASP:OD2	1:A:1913:TYR:CE1	2.73	0.41
1:A:1904:PHE:C	1:A:1906:TRP:N	2.73	0.41
1:A:2388:PRO:HB2	1:A:2390:ASN:OD1	2.20	0.41
1:A:3199:TYR:CG	1:A:3200:ILE:N	2.88	0.41
1:A:3767:ARG:NE	1:A:4205:HIS:CE1	2.88	0.41
1:A:4509:LEU:HD22	1:A:4552:TRP:HB2	2.02	0.41
1:A:4659:ILE:N	1:A:4659:ILE:HD12	2.35	0.41
1:A:4695:THR:O	1:A:4696:ARG:HB2	2.19	0.41
1:B:1547:ASN:HD22	1:B:1548:TYR:N	2.18	0.41
1:B:1665:ILE:C	1:B:1667:GLN:H	2.23	0.41
1:B:1711:ASN:ND2	1:B:1717:LYS:CD	2.80	0.41
1:B:1947:LEU:HB3	2:B:9007:ADP:N1	2.35	0.41
1:B:1947:LEU:HB3	2:B:9007:ADP:C6	2.55	0.41
1:B:1965:GLU:O	1:B:1967:ARG:NH1	2.52	0.41
1:B:2355:PHE:CE2	1:B:2367:LEU:HD21	2.55	0.41
1:B:2504:GLN:HE21	1:B:2504:GLN:HB2	1.65	0.41
1:B:2963:VAL:CG1	1:B:2968:LEU:HB2	2.49	0.41
1:B:3239:GLY:HA2	1:B:3255:VAL:HG21	2.02	0.41
1:B:3344:LEU:O	1:B:3348:LEU:HB2	2.19	0.41
1:B:3570:GLU:O	1:B:3573:ARG:N	2.53	0.41
1:B:4029:SER:HB2	1:B:4066:GLN:HE21	1.85	0.41
1:B:4043:ASP:O	1:B:4059:PRO:HG3	2.20	0.41
1:B:4143:SER:OG	1:B:4188:LYS:HE3	2.20	0.41
1:B:4162:ILE:HG13	1:B:4196:TRP:CZ3	2.55	0.41
1:A:1604:VAL:HG11	1:A:1670:GLU:HA	2.02	0.41
1:A:1655:LEU:HD12	1:A:1658:GLU:OE1	2.20	0.41
1:A:2434:LEU:HD11	1:A:2545:ILE:HD13	2.03	0.41
1:A:2689:ARG:O	1:A:2691:PHE:N	2.53	0.41
1:A:2807:PHE:O	1:A:2809:ARG:N	2.54	0.41
1:A:2907:HIS:O	1:A:2911:ARG:HG2	2.20	0.41
1:A:3202:PRO:HA	1:A:3203:PRO:HD3	1.93	0.41
1:A:3338:GLN:HE21	1:A:3338:GLN:CA	2.28	0.41
1:A:3689:TYR:O	1:A:3694:ILE:HG13	2.20	0.41
1:A:3721:GLN:HE21	1:A:3721:GLN:HB3	1.57	0.41
1:A:4058:ILE:HD13	1:A:4085:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1559:ASP:C	1:B:1561:LEU:H	2.24	0.41
1:B:1758:ILE:HD12	1:B:1773:VAL:HG22	2.02	0.41
1:B:1764:PRO:HB2	1:B:1768:GLU:CB	2.50	0.41
1:B:1926:VAL:HG12	1:B:1928:HIS:CD2	2.53	0.41
1:B:2016:LEU:HD23	1:B:2021:ALA:HB3	2.01	0.41
1:B:2085:SER:HB3	1:B:2092:LYS:CE	2.50	0.41
1:B:2112:MET:SD	1:B:2153:LYS:HG2	2.60	0.41
1:B:2359:VAL:HG12	1:B:2360:ASP:N	2.35	0.41
1:B:2540:LEU:HD12	1:B:2540:LEU:HA	1.95	0.41
1:B:2609:THR:O	1:B:2610:ILE:CG1	2.67	0.41
1:B:3773:PHE:CE2	1:B:3783:PHE:HE1	2.38	0.41
1:B:3840:GLN:O	1:B:3841:ALA:C	2.57	0.41
1:B:4262:LYS:CB	1:B:4267:ARG:HH12	2.33	0.41
1:B:4546:VAL:HG12	1:B:4551:LYS:HG3	2.02	0.41
1:A:1476:ILE:O	1:A:1476:ILE:HG22	2.19	0.41
1:A:2057:VAL:HG12	1:A:2065:ILE:HB	2.02	0.41
1:A:3017:VAL:HG22	1:A:3018:SER:N	2.35	0.41
1:A:3200:ILE:O	1:A:3202:PRO:CD	2.61	0.41
1:A:3351:ARG:HH11	1:A:3351:ARG:HG3	1.85	0.41
1:A:4219:SER:OG	1:A:4220:GLU:N	2.53	0.41
1:A:4515:ASN:O	1:A:4516:ASP:C	2.57	0.41
1:B:1562:PHE:CD2	1:B:1565:LEU:HD22	2.51	0.41
1:B:1844:GLN:O	1:B:1848:ILE:HG13	2.20	0.41
1:B:1846:GLN:HA	1:B:1893:GLN:HE22	1.83	0.41
1:B:2572:ARG:HA	1:B:2572:ARG:HD2	1.77	0.41
1:B:2694:PHE:HE1	1:B:2787:GLN:HE22	1.68	0.41
1:B:2889:ALA:CB	1:B:2904:LEU:HD11	2.50	0.41
1:B:3088:ASN:ND2	1:B:3163:ALA:HB2	2.36	0.41
1:B:3342:ARG:O	1:B:3345:GLN:HB3	2.21	0.41
1:B:3549:GLU:O	1:B:3553:VAL:HG23	2.20	0.41
1:B:3923:LEU:CD1	1:B:3946:ASP:HB2	2.50	0.41
1:B:3958:THR:HG23	1:B:4235:VAL:HB	2.02	0.41
1:A:1840:LYS:O	1:A:1843:GLU:N	2.52	0.41
1:A:2748:LEU:HD21	1:A:2800:ARG:NH1	2.35	0.41
1:A:4051:ASP:OD1	1:A:4658:ASP:CB	2.68	0.41
1:A:4171:ALA:C	1:A:4173:LYS:N	2.73	0.41
1:A:4315:ASP:O	1:A:4319:LYS:HB2	2.20	0.41
1:B:2144:HIS:HB2	1:B:2413:MET:CE	2.50	0.41
1:B:2506:PHE:CE1	1:B:2512:VAL:HG21	2.55	0.41
1:B:2620:ASP:O	1:B:2621:ASP:C	2.59	0.41
1:B:2889:ALA:HB1	1:B:2904:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2960:TYR:O	1:B:2961:GLN:CG	2.67	0.41
1:B:3011:HIS:CD2	1:B:3143:VAL:H	2.38	0.41
1:B:3296:GLU:OE1	1:B:3571:ARG:HD3	2.21	0.41
1:B:3324:LEU:O	1:B:3327:MET:HB3	2.20	0.41
1:B:3902:GLU:C	1:B:3904:SER:N	2.72	0.41
1:B:3902:GLU:C	1:B:4433:MET:HE3	2.41	0.41
1:A:1949:GLN:NE2	1:A:1953:THR:CG2	2.82	0.41
1:A:2052:GLU:O	1:A:2053:ASN:CB	2.67	0.41
1:A:2273:MET:O	1:A:2275:VAL:HG23	2.20	0.41
1:A:2400:LEU:O	1:A:2402:TYR:N	2.53	0.41
1:A:3027:ARG:HA	1:A:3037:ILE:CD1	2.51	0.41
1:A:3337:LYS:HB3	1:A:3525:LEU:HD11	2.03	0.41
1:A:3522:ILE:CG2	1:A:3523:THR:N	2.84	0.41
1:A:4002:LYS:HB2	1:B:2845:PHE:CZ	2.56	0.41
1:B:1558:TRP:HH2	1:B:1605:TRP:HB3	1.85	0.41
1:B:2572:ARG:NH1	1:B:2575:TYR:CD2	2.88	0.41
1:B:2670:LEU:HB3	1:B:2812:PRO:HG2	2.03	0.41
1:B:2984:LEU:HD22	1:B:2986:VAL:HG13	2.02	0.41
1:B:3136:GLN:O	1:B:3137:VAL:C	2.59	0.41
1:B:3602:ILE:HG12	1:B:3617:TRP:HH2	1.86	0.41
1:B:3780:ARG:HE	1:B:3780:ARG:HB3	1.58	0.41
1:B:4053:VAL:O	1:B:4053:VAL:CG2	2.68	0.41
1:B:4567:ASP:O	1:B:4571:ARG:HG2	2.20	0.41
1:B:4655:THR:HA	1:B:4656:PRO:HD3	1.89	0.41
1:A:1497:LEU:HD22	1:A:1501:SER:CB	2.50	0.41
1:A:1587:GLU:HG2	1:A:1591:TRP:CD1	2.56	0.41
1:A:1633:SER:O	1:A:1637:LYS:HG2	2.21	0.41
1:A:2376:LEU:HD11	1:A:2384:ARG:CB	2.50	0.41
1:A:2966:SER:HA	1:A:2969:ARG:CG	2.49	0.41
1:A:3023:SER:HB3	1:A:3027:ARG:NH1	2.34	0.41
1:A:3354:GLU:C	1:A:3356:ALA:N	2.72	0.41
1:A:3527:LYS:O	1:A:3530:ALA:N	2.53	0.41
1:A:3816:LEU:HB3	1:A:3817:LEU:CD2	2.50	0.41
1:A:4172:GLU:HG2	1:A:4172:GLU:H	1.60	0.41
1:A:4605:ARG:HG2	1:A:4605:ARG:NH1	2.35	0.41
1:B:1837:GLN:C	1:B:1839:SER:N	2.71	0.41
1:B:1873:LYS:HA	1:B:1876:GLU:OE2	2.21	0.41
1:B:2379:LEU:HB2	1:B:2383:GLU:CB	2.50	0.41
1:B:2522:ARG:HH21	1:B:2592:ASN:CB	2.33	0.41
1:B:2560:MET:CG	1:B:2564:ASN:HB2	2.50	0.41
1:B:2665:SER:O	1:B:2667:HIS:CE1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3698:SER:C	1:B:3700:LEU:H	2.24	0.41
1:B:3921:TYR:CD2	1:B:3925:ASN:ND2	2.85	0.41
1:B:3988:TRP:O	1:B:3992:LEU:HG	2.19	0.41
1:B:4030:PHE:HD1	1:B:4033:LEU:HD22	1.86	0.41
1:B:4242:PRO:HA	1:B:4286:ARG:NH2	2.36	0.41
1:B:4666:ILE:HG13	1:B:4667:ALA:N	2.35	0.41
1:A:1461:TYR:HE1	1:A:1503:TRP:HB3	1.86	0.41
1:A:1510:ASN:O	1:A:1511:GLU:C	2.57	0.41
1:A:2032:GLU:O	1:A:2033:GLU:C	2.59	0.41
1:A:2096:ARG:HH11	1:A:2096:ARG:HG3	1.84	0.41
1:A:2196:LEU:HD23	1:A:2196:LEU:HA	1.86	0.41
1:A:2525:ILE:CG2	1:A:2815:LEU:CD1	2.98	0.41
1:A:2689:ARG:C	1:A:2691:PHE:H	2.23	0.41
1:A:3338:GLN:HE22	1:A:3522:ILE:HG13	1.85	0.41
1:A:3554:LYS:HB3	1:A:3554:LYS:HE3	1.87	0.41
1:A:3564:LEU:HD23	1:A:3564:LEU:HA	1.82	0.41
1:A:4149:LEU:HD12	1:A:4149:LEU:HA	1.73	0.41
1:A:4201:GLU:HG2	1:A:4232:MET:CE	2.51	0.41
1:B:1552:CYS:HB2	1:B:1647:LEU:HD12	2.02	0.41
1:B:1665:ILE:C	1:B:1667:GLN:N	2.73	0.41
1:B:1696:ARG:HD2	1:B:1774:GLU:HG3	2.02	0.41
1:B:2239:LYS:HE2	1:B:2295:GLN:HB3	2.02	0.41
1:B:3014:LEU:O	1:B:3146:THR:HA	2.20	0.41
1:B:3354:GLU:O	1:B:3356:ALA:N	2.54	0.41
1:B:3635:PRO:HA	1:B:3663:ILE:CG1	2.50	0.41
1:B:3701:ASP:OD1	1:B:3701:ASP:C	2.58	0.41
1:B:4376:VAL:HG13	1:B:4407:TRP:HA	2.02	0.41
1:A:1542:GLU:HG2	1:A:1655:LEU:HD23	2.02	0.41
1:A:1625:ILE:HA	1:A:1628:LEU:HB2	2.02	0.41
1:A:1971:ASN:HA	1:A:2075:VAL:O	2.21	0.41
1:A:2424:GLN:HG2	1:A:2513:HIS:NE2	2.35	0.41
1:A:2617:VAL:O	1:A:2617:VAL:CG1	2.67	0.41
1:A:2699:LEU:HD22	1:A:2741:VAL:HG13	2.02	0.41
1:A:2884:ARG:O	1:A:2888:GLU:HG3	2.20	0.41
1:A:3194:LEU:O	1:A:3223:HIS:CD2	2.72	0.41
1:A:4130:SER:OG	1:A:4233:SER:HA	2.21	0.41
1:A:4136:SER:OG	1:A:4238:TYR:HB2	2.21	0.41
1:A:4553:TYR:CD2	1:A:4595:LEU:HD22	2.55	0.41
1:B:2998:ILE:CG2	1:B:3025:LEU:HD22	2.50	0.41
1:B:3127:GLU:O	1:B:3130:TYR:N	2.51	0.41
1:B:3673:LEU:HD23	1:B:3673:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4195:GLN:OE1	1:B:4195:GLN:HA	2.20	0.41
1:B:4484:LEU:HD22	1:B:4500:GLU:CG	2.50	0.41
1:B:4495:LEU:HA	1:B:4495:LEU:HD23	1.83	0.41
1:B:4535:ARG:O	1:B:4536:SER:C	2.59	0.41
1:A:1411:ILE:HD13	1:A:1411:ILE:HA	1.92	0.41
1:A:1715:ILE:O	1:A:1716:ILE:C	2.58	0.41
1:A:1715:ILE:O	1:A:1717:LYS:N	2.54	0.41
1:A:2372:ASP:O	1:A:2373:ASP:CG	2.59	0.41
1:A:2405:LEU:HD22	1:A:2408:ILE:HD11	2.03	0.41
1:A:2575:TYR:HA	1:A:2578:MET:HE3	2.03	0.41
1:A:2605:VAL:HG13	1:A:2606:PRO:HD2	2.03	0.41
1:A:2723:THR:N	1:A:2727:GLU:O	2.39	0.41
1:A:2952:TYR:O	1:A:2953:SER:HB2	2.20	0.41
1:A:3238:ILE:HG12	1:A:3601:TYR:HB3	2.03	0.41
1:A:3335:GLU:CD	1:A:3529:ILE:HD11	2.41	0.41
1:A:3839:SER:O	1:A:3841:ALA:N	2.53	0.41
1:A:3969:LEU:HD23	1:A:3969:LEU:HA	1.93	0.41
1:A:4186:LEU:HD12	1:A:4187:LEU:N	2.36	0.41
1:A:4704:ASP:O	1:A:4705:LEU:HD23	2.21	0.41
1:B:2127:LYS:HB3	1:B:2222:VAL:HG13	2.02	0.41
1:B:2142:GLN:HG3	1:B:2145:TYR:CZ	2.56	0.41
1:B:2178:GLU:HA	1:B:2178:GLU:OE1	2.20	0.41
1:B:2563:GLU:O	1:B:2567:ASN:ND2	2.54	0.41
1:B:2591:GLU:OE1	1:B:2611:PRO:HG2	2.20	0.41
1:B:2766:MET:HB3	1:B:2783:LEU:HD11	2.03	0.41
1:B:2768:GLU:HB2	1:B:2810:HIS:CE1	2.56	0.41
1:B:3111:ALA:O	1:B:3112:CYS:C	2.60	0.41
1:B:3185:GLY:HA2	1:B:3264:ILE:HD13	2.02	0.41
1:B:3238:ILE:HG22	1:B:3255:VAL:CG2	2.51	0.41
1:B:3246:LEU:HD22	1:B:3252:GLN:OE1	2.21	0.41
1:B:3320:ALA:O	1:B:3324:LEU:HD13	2.21	0.41
1:B:3324:LEU:CD1	1:B:3539:LEU:CG	2.98	0.41
1:B:3515:GLN:HE21	1:B:3515:GLN:HB2	1.49	0.41
1:B:3922:ASN:O	1:B:3923:LEU:C	2.58	0.41
1:B:4003:GLU:CG	1:B:4004:THR:N	2.84	0.41
1:B:4011:LEU:C	1:B:4012:LEU:HD23	2.41	0.41
1:B:4036:HIS:CD2	1:B:4044:TRP:HE1	2.36	0.41
1:B:4110:PHE:C	1:B:4112:ASN:H	2.23	0.41
1:B:4122:VAL:HG12	1:B:4132:LEU:CD1	2.50	0.41
1:B:4274:LEU:HD21	1:B:4306:ALA:HB3	2.03	0.41
1:B:4347:ILE:HG21	1:B:4353:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4402:ILE:O	1:B:4402:ILE:HG22	2.20	0.41
1:B:4434:GLN:HE21	1:B:4434:GLN:HB3	1.72	0.41
1:B:4520:LEU:O	1:B:4523:LEU:HB3	2.20	0.41
1:B:4536:SER:O	1:B:4539:THR:N	2.54	0.41
1:A:2865:THR:O	1:A:2867:ASP:N	2.54	0.41
1:A:3017:VAL:HB	1:A:3175:GLU:OE2	2.21	0.41
1:A:3062:ALA:HB2	1:A:3069:ILE:CD1	2.48	0.41
1:A:3087:MET:HA	1:A:3087:MET:HE2	2.02	0.41
1:A:3338:GLN:O	1:A:3342:ARG:N	2.54	0.41
1:A:3587:THR:HB	1:A:3628:PHE:HA	2.02	0.41
1:A:4055:GLU:HA	1:A:4056:PRO:HD3	1.96	0.41
1:B:1558:TRP:CZ3	1:B:1606:ILE:HB	2.56	0.41
1:B:2264:GLN:O	1:B:2267:ASN:HB3	2.21	0.41
1:B:2747:ASN:HB2	1:B:2801:VAL:O	2.21	0.41
1:B:3091:LEU:HA	1:B:3091:LEU:HD23	1.52	0.41
1:B:3108:LEU:HG	1:B:3108:LEU:O	2.21	0.41
1:B:3234:ILE:HG23	1:B:3617:TRP:NE1	2.35	0.41
1:B:3253:ASN:HB2	1:B:3604:PHE:CD2	2.56	0.41
1:B:3781:VAL:HG13	1:B:3782:THR:N	2.36	0.41
1:B:3969:LEU:HD23	1:B:3969:LEU:HA	1.91	0.41
1:B:4068:GLN:O	1:B:4070:SER:N	2.54	0.41
1:B:4080:PHE:HB2	1:B:4101:PHE:CE1	2.56	0.41
1:B:4461:LYS:CB	1:B:4565:ILE:HD13	2.51	0.41
1:B:4688:VAL:HA	1:B:4689:PRO:HD3	1.89	0.41
1:A:1715:ILE:HD12	1:A:1760:ILE:HD13	2.03	0.40
1:A:1879:ILE:HG21	1:A:2115:SER:HA	2.02	0.40
1:A:1967:ARG:HH22	1:A:2069:GLN:HA	1.86	0.40
1:A:2282:LYS:HG2	1:A:2416:PHE:CD2	2.56	0.40
1:A:2915:ASP:OD2	1:A:3000:ARG:HD3	2.21	0.40
1:A:3005:PHE:N	1:A:3005:PHE:CD1	2.89	0.40
1:A:3251:ARG:HH12	1:A:3675:ILE:CD1	2.33	0.40
1:A:3629:LYS:HB2	1:A:3632:LEU:HB2	2.04	0.40
1:A:3878:GLU:O	1:A:3882:VAL:HG23	2.21	0.40
1:A:3912:SER:HB3	1:A:4231:ARG:HG3	2.02	0.40
1:A:4689:PRO:HB2	1:A:4699:LEU:CD1	2.51	0.40
1:B:1793:ASN:C	1:B:1795:VAL:H	2.23	0.40
1:B:2075:VAL:O	1:B:2075:VAL:HG12	2.20	0.40
1:B:2869:GLN:O	1:B:2870:ALA:C	2.57	0.40
1:B:3091:LEU:CD1	1:B:3164:LEU:HD22	2.51	0.40
1:B:3697:THR:HG23	1:B:3720:VAL:HG13	2.03	0.40
1:A:2307:ASP:CG	1:A:2310:ALA:HB2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2376:LEU:HD11	1:A:2384:ARG:HB3	2.03	0.40
1:A:3139:ARG:HH11	1:A:3139:ARG:CG	2.19	0.40
1:A:4053:VAL:HG12	1:A:4054:GLY:N	2.36	0.40
1:A:4145:LYS:HE3	1:A:4238:TYR:CD1	2.57	0.40
1:A:4309:SER:O	1:A:4313:TRP:CD1	2.74	0.40
1:B:1739:THR:OG1	1:B:1740:THR:HG22	2.21	0.40
1:B:2528:PHE:HE1	1:B:2533:VAL:HG11	1.86	0.40
1:B:3112:CYS:HB3	1:B:3129:LEU:HD11	2.03	0.40
1:B:3865:ILE:O	1:B:3867:LEU:N	2.54	0.40
1:B:3921:TYR:CZ	1:B:3925:ASN:ND2	2.89	0.40
1:B:4033:LEU:HD13	1:B:4062:TRP:CZ2	2.57	0.40
1:B:4046:GLN:O	1:B:4047:PHE:C	2.59	0.40
1:B:4332:ILE:HA	1:B:4335:ARG:HH12	1.86	0.40
1:B:4541:ILE:O	1:B:4544:GLY:N	2.55	0.40
1:A:1554:LEU:HB3	1:A:1609:GLN:NE2	2.37	0.40
1:A:2116:GLN:HE21	1:A:2157:VAL:HA	1.86	0.40
1:A:2515:VAL:HG12	1:A:2581:LEU:HD12	2.04	0.40
1:A:2590:ARG:CD	1:A:2613:LEU:HD11	2.51	0.40
1:A:3351:ARG:HG3	1:A:3351:ARG:NH1	2.36	0.40
1:A:3602:ILE:HG23	1:A:3610:ARG:CD	2.52	0.40
1:B:1640:ASN:ND2	1:B:1644:ILE:CD1	2.82	0.40
1:B:1705:LEU:O	1:B:1709:ILE:HG13	2.21	0.40
1:B:1777:MET:HE3	1:B:1938:PHE:O	2.22	0.40
1:B:1821:ILE:HG21	1:B:1914:TYR:HB2	2.03	0.40
1:B:2241:GLN:HB2	1:B:2251:THR:HG21	2.04	0.40
1:B:2260:LEU:HD12	1:B:2260:LEU:HA	1.77	0.40
1:B:2344:ARG:O	1:B:2344:ARG:CG	2.67	0.40
1:B:2578:MET:HA	1:B:2593:PHE:HE2	1.86	0.40
1:B:3559:ARG:NE	1:B:3849:ASP:OD1	2.54	0.40
1:B:3700:LEU:HD22	1:B:3701:ASP:H	1.87	0.40
1:B:4189:ASN:HD22	1:B:4218:THR:HG23	1.87	0.40
1:B:4436:SER:O	1:B:4437:GLU:O	2.39	0.40
1:A:1507:LEU:O	1:A:1511:GLU:N	2.55	0.40
1:A:1800:HIS:HB2	1:A:1858:ASN:ND2	2.34	0.40
1:A:1812:THR:HA	1:A:1874:LYS:HD2	2.03	0.40
1:A:2544:SER:O	1:A:2548:VAL:HG23	2.21	0.40
1:B:1681:LYS:O	1:B:1685:GLU:HG3	2.21	0.40
1:B:2054:SER:OG	1:B:2056:GLU:O	2.40	0.40
1:B:2275:VAL:HG12	1:B:2276:GLY:N	2.35	0.40
1:B:2547:ASN:O	1:B:2619:ILE:HD11	2.21	0.40
1:B:3687:ASN:O	1:B:3689:TYR:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3887:ASN:N	1:B:3888:PRO:CD	2.84	0.40
1:B:4083:ILE:CD1	1:B:4098:SER:HA	2.52	0.40
1:B:4153:LEU:HB3	1:B:4155:LYS:HD3	2.04	0.40
1:B:4517:LEU:HD23	1:B:4517:LEU:HA	1.92	0.40
1:A:1618:ILE:CD1	1:A:1683:LEU:HD21	2.52	0.40
1:A:1698:TYR:O	1:A:2011:ARG:HG2	2.22	0.40
1:A:2273:MET:HG2	1:A:2395:PHE:CG	2.56	0.40
1:A:2364:VAL:O	1:A:2367:LEU:N	2.48	0.40
1:A:3064:CYS:C	1:A:3066:GLU:N	2.75	0.40
1:A:3571:ARG:O	1:A:3575:GLU:HG3	2.22	0.40
1:A:4044:TRP:HZ2	1:A:4062:TRP:CG	2.40	0.40
1:A:4187:LEU:HD11	1:A:4215:LEU:HD11	2.04	0.40
1:A:4349:ASN:HD21	1:A:4351:PHE:H	1.61	0.40
1:A:4357:TYR:HA	1:A:4360:LEU:HB2	2.03	0.40
1:A:4507:GLY:O	1:A:4508:LYS:C	2.59	0.40
1:A:4551:LYS:C	1:A:4553:TYR:N	2.74	0.40
1:A:4589:VAL:CG1	1:A:4638:ASN:O	2.69	0.40
1:B:1606:ILE:O	1:B:1608:VAL:N	2.54	0.40
1:B:1800:HIS:CE1	1:B:1858:ASN:CB	3.05	0.40
1:B:1916:ALA:HA	1:B:1924:LYS:CD	2.51	0.40
1:B:1985:LYS:HD3	1:B:1997:VAL:HG21	2.04	0.40
1:B:2241:GLN:CB	1:B:2251:THR:HG21	2.51	0.40
1:B:2552:ASN:O	1:B:2556:SER:N	2.54	0.40
1:B:2642:ALA:HB2	1:B:2883:ASP:HB3	2.03	0.40
1:B:2794:PRO:C	1:B:2796:THR:H	2.25	0.40
1:B:3191:ASN:HB2	5:B:26:HOH:O	2.20	0.40
1:B:3328:VAL:O	1:B:3332:GLN:CG	2.69	0.40
1:B:3834:LEU:HD22	1:B:3858:LEU:CD1	2.52	0.40
1:B:4497:ARG:HG3	1:B:4497:ARG:HH11	1.87	0.40
1:B:4604:THR:O	1:B:4671:TRP:NE1	2.55	0.40
1:B:4708:ASP:OD1	1:B:4710:SER:OG	2.38	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	2908/3245 (90%)	2474 (85%)	332 (11%)	102 (4%)	3	11
1	B	2813/3245 (87%)	2376 (84%)	347 (12%)	90 (3%)	4	13
All	All	5721/6490 (88%)	4850 (85%)	679 (12%)	192 (3%)	3	12

All (192) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1465	ASN
1	A	1583	VAL
1	A	1797	VAL
1	A	1835	THR
1	A	1839	SER
1	A	1919	GLU
1	A	2641	VAL
1	A	3697	THR
1	A	3722	ASP
1	A	3814	SER
1	A	3815	ASP
1	A	4045	LYS
1	A	4051	ASP
1	A	4221	ILE
1	A	4520	LEU
1	A	4557	GLU
1	B	1592	ASP
1	B	2296	VAL
1	B	2432	ASP
1	B	2442	GLN
1	B	2555	HIS
1	B	2559	PRO
1	B	2641	VAL
1	B	2982	GLU
1	B	2983	GLU
1	B	3105	PHE
1	B	3162	PRO
1	B	3220	PRO
1	B	4051	ASP
1	B	4053	VAL
1	B	4530	SER
1	A	1762	ASN
1	A	1764	PRO

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Mol	Chain	Res	Type
1	A	1838	GLN
1	A	2033	GLU
1	A	2203	MET
1	A	2384	ARG
1	A	2401	LYS
1	A	2608	ASN
1	A	2642	ALA
1	A	2871	HIS
1	A	2992	ASN
1	A	3005	PHE
1	A	3365	ASP
1	A	3816	LEU
1	A	3861	GLU
1	A	3866	ALA
1	A	3929	ASN
1	A	3937	ASN
1	A	4145	LYS
1	A	4209	PRO
1	A	4510	VAL
1	A	4519	ASN
1	A	4552	TRP
1	A	4559	ILE
1	A	4577	GLU
1	A	4679	PHE
1	A	4695	THR
1	B	1559	ASP
1	B	1611	ARG
1	B	1826	GLN
1	B	1829	GLN
1	B	2315	GLN
1	B	2433	THR
1	B	2553	GLN
1	B	2565	GLN
1	B	2600	ILE
1	B	2715	ASP
1	B	3164	LEU
1	B	3688	GLN
1	B	3691	ASP
1	B	3724	GLU
1	B	3729	VAL
1	B	3841	ALA
1	B	3932	ASP

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Mol	Chain	Res	Type
1	B	3933	LYS
1	B	3999	THR
1	B	4069	LEU
1	B	4378	SER
1	B	4541	ILE
1	B	4551	LYS
1	B	4708	ASP
1	B	4709	GLN
1	A	1585	GLU
1	A	1896	LYS
1	A	1917	THR
1	A	2373	ASP
1	A	2644	PRO
1	A	2690	ALA
1	A	2808	LEU
1	A	2915	ASP
1	A	2990	LEU
1	A	3065	LYS
1	A	3119	ASN
1	A	3355	ILE
1	A	3361	LYS
1	A	3865	ILE
1	A	3998	LEU
1	A	4223	PRO
1	A	4579	SER
1	B	1664	ARG
1	B	1827	VAL
1	B	1828	ASP
1	B	2230	PRO
1	B	2233	MET
1	B	2295	GLN
1	B	2343	VAL
1	B	2380	PRO
1	B	2733	THR
1	B	2747	ASN
1	B	2871	HIS
1	B	3044	ASN
1	B	3048	SER
1	B	3700	LEU
1	B	3704	PHE
1	B	3929	ASN
1	B	4047	PHE

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Mol	Chain	Res	Type
1	B	4175	ILE
1	B	4498	CYS
1	B	4571	ARG
1	A	1552	CYS
1	A	1558	TRP
1	A	1664	ARG
1	A	1695	ALA
1	A	1897	ASN
1	A	1949	GLN
1	A	2178	GLU
1	A	2209	ALA
1	A	2224	PRO
1	A	2365	GLU
1	A	3164	LEU
1	A	3840	GLN
1	A	3859	LYS
1	A	3863	THR
1	A	3936	PRO
1	A	4007	GLN
1	A	4138	PRO
1	A	4172	GLU
1	A	4437	GLU
1	B	1593	ASP
1	B	1612	TRP
1	B	1786	SER
1	B	1922	LEU
1	B	1929	MET
1	B	2164	ARG
1	B	2638	THR
1	B	3009	GLN
1	B	3684	PHE
1	B	3880	SER
1	B	4433	MET
1	A	1645	ALA
1	A	1855	ILE
1	A	1923	HIS
1	A	2843	ARG
1	A	2870	ALA
1	A	2978	VAL
1	A	3078	VAL
1	A	3162	PRO
1	A	3512	LYS

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Mol	Chain	Res	Type
1	A	3526	GLU
1	A	3705	MET
1	A	3826	LYS
1	A	3926	ASN
1	A	3999	THR
1	B	1655	LEU
1	B	1663	GLU
1	B	1666	GLN
1	B	2492	LEU
1	B	2603	THR
1	B	2692	PRO
1	B	3320	ALA
1	B	3576	GLN
1	B	4531	THR
1	A	1719	GLN
1	A	4143	SER
1	A	4144	SER
1	A	4708	ASP
1	B	1630	PRO
1	B	2511	LEU
1	B	2998	ILE
1	B	4059	PRO
1	B	4151	LEU
1	A	2606	PRO
1	B	3152	PRO
1	B	3931	VAL
1	B	3928	PRO
1	A	3219	ILE
1	A	4678	ILE
1	B	4377	PRO
1	A	1766	ILE
1	A	3197	PRO
1	B	2669	PRO

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	2408/2921 (82%)	2220 (92%)	188 (8%)	12	33
1	B	2369/2921 (81%)	2163 (91%)	206 (9%)	10	28
All	All	4777/5842 (82%)	4383 (92%)	394 (8%)	11	31

All (394) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1419	TRP
1	A	1422	ILE
1	A	1423	ILE
1	A	1424	PRO
1	A	1486	LYS
1	A	1488	LEU
1	A	1492	TRP
1	A	1493	ILE
1	A	1527	LEU
1	A	1529	GLU
1	A	1559	ASP
1	A	1593	ASP
1	A	1594	ARG
1	A	1626	ASN
1	A	1628	LEU
1	A	1665	ILE
1	A	1719	GLN
1	A	1742	ILE
1	A	1764	PRO
1	A	1799	ASP
1	A	1801	SER
1	A	1835	THR
1	A	1844	GLN
1	A	1862	SER
1	A	1865	GLN
1	A	1886	ARG
1	A	1905	ASP
1	A	1911	ARG
1	A	1915	ASP
1	A	1923	HIS
1	A	1994	PHE
1	A	2006	LEU
1	A	2016	LEU
1	A	2029	ASN
1	A	2032	GLU

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Mol	Chain	Res	Type
1	A	2050	LEU
1	A	2053	ASN
1	A	2066	SER
1	A	2090	ASN
1	A	2092	LYS
1	A	2107	MET
1	A	2112	MET
1	A	2122	GLU
1	A	2137	GLU
1	A	2142	GLN
1	A	2180	LYS
1	A	2226	SER
1	A	2227	GLN
1	A	2236	LEU
1	A	2251	THR
1	A	2252	LYS
1	A	2262	LEU
1	A	2297	ASP
1	A	2305	VAL
1	A	2328	THR
1	A	2329	ASP
1	A	2346	GLU
1	A	2350	ARG
1	A	2362	GLU
1	A	2367	LEU
1	A	2370	LEU
1	A	2392	ARG
1	A	2404	THR
1	A	2424	GLN
1	A	2503	SER
1	A	2511	LEU
1	A	2572	ARG
1	A	2637	GLU
1	A	2659	VAL
1	A	2696	VAL
1	A	2699	LEU
1	A	2702	SER
1	A	2728	THR
1	A	2739	LEU
1	A	2747	ASN
1	A	2796	THR
1	A	2804	THR

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Mol	Chain	Res	Type
1	A	2847	ASP
1	A	2863	ARG
1	A	2865	THR
1	A	2866	PRO
1	A	2878	GLU
1	A	2894	ASP
1	A	2896	CYS
1	A	2898	LEU
1	A	2904	LEU
1	A	2956	LEU
1	A	2957	THR
1	A	2975	ARG
1	A	2998	ILE
1	A	3026	SER
1	A	3048	SER
1	A	3053	ASP
1	A	3059	LEU
1	A	3080	GLU
1	A	3089	THR
1	A	3095	GLU
1	A	3117	GLN
1	A	3127	GLU
1	A	3139	ARG
1	A	3141	LEU
1	A	3145	PHE
1	A	3147	MET
1	A	3179	GLU
1	A	3187	GLU
1	A	3193	ASP
1	A	3195	GLU
1	A	3308	GLN
1	A	3310	ASN
1	A	3316	LYS
1	A	3322	GLN
1	A	3330	ASP
1	A	3335	GLU
1	A	3337	LYS
1	A	3338	GLN
1	A	3349	ASP
1	A	3365	ASP
1	A	3505	GLU
1	A	3515	GLN

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Mol	Chain	Res	Type
1	A	3531	THR
1	A	3554	LYS
1	A	3571	ARG
1	A	3586	SER
1	A	3605	PHE
1	A	3624	VAL
1	A	3630	SER
1	A	3670	ARG
1	A	3694	ILE
1	A	3695	THR
1	A	3707	ASN
1	A	3708	LEU
1	A	3721	GLN
1	A	3770	THR
1	A	3789	THR
1	A	3817	LEU
1	A	3845	ILE
1	A	3858	LEU
1	A	3863	THR
1	A	3874	THR
1	A	3887	ASN
1	A	3932	ASP
1	A	3933	LYS
1	A	3954	ARG
1	A	3977	LYS
1	A	3985	GLU
1	A	3989	ASP
1	A	3998	LEU
1	A	4007	GLN
1	A	4039	GLN
1	A	4040	ASN
1	A	4046	GLN
1	A	4061	SER
1	A	4066	GLN
1	A	4081	ARG
1	A	4091	SER
1	A	4117	ASP
1	A	4118	MET
1	A	4129	SER
1	A	4136	SER
1	A	4140	TYR
1	A	4170	LEU

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Mol	Chain	Res	Type
1	A	4176	TYR
1	A	4195	GLN
1	A	4198	VAL
1	A	4200	LEU
1	A	4209	PRO
1	A	4218	THR
1	A	4233	SER
1	A	4234	ASN
1	A	4237	SER
1	A	4259	ARG
1	A	4286	ARG
1	A	4309	SER
1	A	4321	ARG
1	A	4360	LEU
1	A	4559	ILE
1	A	4574	GLN
1	A	4596	ASN
1	A	4606	GLN
1	A	4607	SER
1	A	4609	SER
1	A	4610	GLN
1	A	4645	GLU
1	A	4655	THR
1	A	4671	TRP
1	A	4693	ASN
1	A	4719	ARG
1	A	4729	ASP
1	B	1547	ASN
1	B	1548	TYR
1	B	1556	ARG
1	B	1561	LEU
1	B	1573	SER
1	B	1594	ARG
1	B	1610	ARG
1	B	1611	ARG
1	B	1624	ASP
1	B	1655	LEU
1	B	1690	GLN
1	B	1697	PHE
1	B	1736	ASP
1	B	1740	THR
1	B	1793	ASN

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Mol	Chain	Res	Type
1	B	1822	VAL
1	B	1849	GLU
1	B	1862	SER
1	B	1867	LEU
1	B	1872	ARG
1	B	1887	ASP
1	B	1901	ASN
1	B	1911	ARG
1	B	1912	TYR
1	B	1917	THR
1	B	1920	ASN
1	B	1946	ARG
1	B	1957	TYR
1	B	1959	THR
1	B	1982	GLU
1	B	2002	GLU
1	B	2007	GLN
1	B	2029	ASN
1	B	2036	LEU
1	B	2041	GLN
1	B	2071	MET
1	B	2075	VAL
1	B	2104	ASP
1	B	2106	GLU
1	B	2120	THR
1	B	2129	VAL
1	B	2149	LEU
1	B	2163	LYS
1	B	2185	GLN
1	B	2197	ASN
1	B	2231	ILE
1	B	2236	LEU
1	B	2239	LYS
1	B	2252	LYS
1	B	2253	GLN
1	B	2254	GLU
1	B	2260	LEU
1	B	2313	LYS
1	B	2360	ASP
1	B	2374	ASN
1	B	2381	ASN
1	B	2397	VAL

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Mol	Chain	Res	Type
1	B	2404	THR
1	B	2410	ARG
1	B	2416	PHE
1	B	2420	ILE
1	B	2425	MET
1	B	2429	ASN
1	B	2432	ASP
1	B	2440	ASP
1	B	2492	LEU
1	B	2504	GLN
1	B	2525	ILE
1	B	2540	LEU
1	B	2550	GLU
1	B	2587	LEU
1	B	2591	GLU
1	B	2603	THR
1	B	2613	LEU
1	B	2621	ASP
1	B	2651	VAL
1	B	2699	LEU
1	B	2715	ASP
1	B	2721	LYS
1	B	2725	SER
1	B	2746	ILE
1	B	2749	PRO
1	B	2756	THR
1	B	2758	ARG
1	B	2759	VAL
1	B	2835	LEU
1	B	2841	ASN
1	B	2848	ASN
1	B	2876	PRO
1	B	2883	ASP
1	B	2904	LEU
1	B	2928	LYS
1	B	2942	ASN
1	B	2946	LEU
1	B	2967	ASP
1	B	2977	LYS
1	B	2984	LEU
1	B	3043	ASN
1	B	3051	PHE

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Mol	Chain	Res	Type
1	B	3052	ASP
1	B	3053	ASP
1	B	3059	LEU
1	B	3087	MET
1	B	3088	ASN
1	B	3095	GLU
1	B	3109	MET
1	B	3112	CYS
1	B	3126	GLU
1	B	3139	ARG
1	B	3162	PRO
1	B	3195	GLU
1	B	3255	VAL
1	B	3280	GLU
1	B	3282	GLN
1	B	3283	LEU
1	B	3319	GLN
1	B	3326	GLN
1	B	3327	MET
1	B	3330	ASP
1	B	3332	GLN
1	B	3338	GLN
1	B	3342	ARG
1	B	3343	GLU
1	B	3351	ARG
1	B	3506	ASN
1	B	3515	GLN
1	B	3523	THR
1	B	3528	SER
1	B	3533	LYS
1	B	3535	GLU
1	B	3539	LEU
1	B	3555	ASN
1	B	3563	LEU
1	B	3585	MET
1	B	3620	ARG
1	B	3624	VAL
1	B	3642	GLU
1	B	3645	LEU
1	B	3691	ASP
1	B	3695	THR
1	B	3700	LEU

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Mol	Chain	Res	Type
1	B	3725	ASN
1	B	3726	ILE
1	B	3780	ARG
1	B	3785	ASN
1	B	3787	THR
1	B	3827	LEU
1	B	3838	LEU
1	B	3840	GLN
1	B	3867	LEU
1	B	3877	GLN
1	B	3880	SER
1	B	3935	ASP
1	B	3936	PRO
1	B	3966	THR
1	B	3992	LEU
1	B	3998	LEU
1	B	4004	THR
1	B	4031	SER
1	B	4035	ASP
1	B	4043	ASP
1	B	4046	GLN
1	B	4053	VAL
1	B	4059	PRO
1	B	4095	LEU
1	B	4098	SER
1	B	4105	VAL
1	B	4111	LEU
1	B	4113	THR
1	B	4132	LEU
1	B	4140	TYR
1	B	4152	GLN
1	B	4157	TYR
1	B	4189	ASN
1	B	4199	GLN
1	B	4200	LEU
1	B	4209	PRO
1	B	4214	ARG
1	B	4218	THR
1	B	4228	ASN
1	B	4232	MET
1	B	4233	SER
1	B	4267	ARG

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Mol	Chain	Res	Type
1	B	4323	ASN
1	B	4326	PRO
1	B	4334	VAL
1	B	4335	ARG
1	B	4356	LEU
1	B	4425	LYS
1	B	4434	GLN
1	B	4436	SER
1	B	4500	GLU
1	B	4503	ILE
1	B	4516	ASP
1	B	4521	LEU
1	B	4538	THR
1	B	4557	GLU
1	B	4558	THR
1	B	4573	GLN
1	B	4596	ASN
1	B	4604	THR
1	B	4618	ASN
1	B	4644	LEU
1	B	4675	ASP
1	B	4693	ASN
1	B	4709	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (210) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1480	HIS
1	A	1522	GLN
1	A	1547	ASN
1	A	1549	GLN
1	A	1563	ASN
1	A	1609	GLN
1	A	1690	GLN
1	A	1719	GLN
1	A	1791	HIS
1	A	1798	ASN
1	A	1809	ASN
1	A	1813	GLN
1	A	1844	GLN
1	A	1857	ASN
1	A	1865	GLN

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Mol	Chain	Res	Type
1	A	1877	HIS
1	A	1884	HIS
1	A	1893	GLN
1	A	1918	GLN
1	A	1923	HIS
1	A	1928	HIS
1	A	1949	GLN
1	A	1971	ASN
1	A	1990	GLN
1	A	2029	ASN
1	A	2042	GLN
1	A	2044	GLN
1	A	2053	ASN
1	A	2090	ASN
1	A	2136	GLN
1	A	2138	GLN
1	A	2142	GLN
1	A	2167	GLN
1	A	2197	ASN
1	A	2200	ASN
1	A	2264	GLN
1	A	2269	ASN
1	A	2295	GLN
1	A	2351	HIS
1	A	2366	ASN
1	A	2368	ASN
1	A	2428	GLN
1	A	2447	GLN
1	A	2495	GLN
1	A	2524	HIS
1	A	2535	ASN
1	A	2552	ASN
1	A	2553	GLN
1	A	2555	HIS
1	A	2565	GLN
1	A	2700	ASN
1	A	2747	ASN
1	A	2793	ASN
1	A	2826	GLN
1	A	2848	ASN
1	A	2907	HIS
1	A	3007	GLN

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Mol	Chain	Res	Type
1	A	3033	ASN
1	A	3077	ASN
1	A	3117	GLN
1	A	3223	HIS
1	A	3236	GLN
1	A	3249	GLN
1	A	3252	GLN
1	A	3253	ASN
1	A	3259	HIS
1	A	3265	ASN
1	A	3277	GLN
1	A	3286	ASN
1	A	3303	GLN
1	A	3322	GLN
1	A	3331	GLN
1	A	3338	GLN
1	A	3345	GLN
1	A	3509	ASN
1	A	3555	ASN
1	A	3576	GLN
1	A	3582	ASN
1	A	3646	ASN
1	A	3687	ASN
1	A	3794	GLN
1	A	3820	GLN
1	A	3887	ASN
1	A	3929	ASN
1	A	4017	GLN
1	A	4025	GLN
1	A	4036	HIS
1	A	4040	ASN
1	A	4046	GLN
1	A	4079	ASN
1	A	4112	ASN
1	A	4205	HIS
1	A	4234	ASN
1	A	4263	GLN
1	A	4278	HIS
1	A	4282	GLN
1	A	4323	ASN
1	A	4349	ASN
1	A	4362	GLN

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Mol	Chain	Res	Type
1	A	4370	ASN
1	A	4606	GLN
1	A	4610	GLN
1	A	4638	ASN
1	A	4650	ASN
1	A	4693	ASN
1	A	4714	GLN
1	A	4718	GLN
1	B	1547	ASN
1	B	1549	GLN
1	B	1609	GLN
1	B	1640	ASN
1	B	1690	GLN
1	B	1711	ASN
1	B	1767	HIS
1	B	1793	ASN
1	B	1813	GLN
1	B	1820	GLN
1	B	1842	GLN
1	B	1844	GLN
1	B	1857	ASN
1	B	1885	GLN
1	B	1893	GLN
1	B	1901	ASN
1	B	1920	ASN
1	B	1971	ASN
1	B	1990	GLN
1	B	2029	ASN
1	B	2042	GLN
1	B	2044	GLN
1	B	2068	HIS
1	B	2110	GLN
1	B	2189	GLN
1	B	2200	ASN
1	B	2241	GLN
1	B	2264	GLN
1	B	2295	GLN
1	B	2315	GLN
1	B	2342	ASN
1	B	2351	HIS
1	B	2366	ASN
1	B	2374	ASN

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Mol	Chain	Res	Type
1	B	2381	ASN
1	B	2398	GLN
1	B	2495	GLN
1	B	2504	GLN
1	B	2567	ASN
1	B	2571	ASN
1	B	2629	ASN
1	B	2787	GLN
1	B	2793	ASN
1	B	2826	GLN
1	B	2832	ASN
1	B	2841	ASN
1	B	2861	GLN
1	B	2907	HIS
1	B	2992	ASN
1	B	3009	GLN
1	B	3011	HIS
1	B	3043	ASN
1	B	3140	ASN
1	B	3183	GLN
1	B	3223	HIS
1	B	3236	GLN
1	B	3259	HIS
1	B	3265	ASN
1	B	3272	ASN
1	B	3303	GLN
1	B	3331	GLN
1	B	3338	GLN
1	B	3515	GLN
1	B	3555	ASN
1	B	3566	ASN
1	B	3568	ASN
1	B	3577	GLN
1	B	3669	ASN
1	B	3721	GLN
1	B	3725	ASN
1	B	3731	ASN
1	B	3785	ASN
1	B	3794	GLN
1	B	3820	GLN
1	B	3840	GLN
1	B	3926	ASN

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Mol	Chain	Res	Type
1	B	3953	ASN
1	B	3981	ASN
1	B	4016	GLN
1	B	4025	GLN
1	B	4026	GLN
1	B	4036	HIS
1	B	4052	GLN
1	B	4066	GLN
1	B	4099	HIS
1	B	4112	ASN
1	B	4189	ASN
1	B	4199	GLN
1	B	4222	HIS
1	B	4263	GLN
1	B	4278	HIS
1	B	4323	ASN
1	B	4362	GLN
1	B	4391	HIS
1	B	4428	ASN
1	B	4573	GLN
1	B	4574	GLN
1	B	4596	ASN
1	B	4618	ASN
1	B	4651	ASN
1	B	4693	ASN
1	B	4709	GLN
1	B	4714	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	9002	4	24,29,29	1.39	3 (12%)	29,45,45	1.58	5 (17%)
2	ADP	B	9008	4	24,29,29	1.43	3 (12%)	29,45,45	1.51	6 (20%)
2	ADP	A	9001	-	24,29,29	1.25	3 (12%)	29,45,45	1.57	6 (20%)
3	SPM	B	9018	-	13,13,13	0.57	0	12,12,12	0.86	0
3	SPM	B	9022	-	13,13,13	0.41	0	12,12,12	0.96	0
2	ADP	A	9004	-	24,29,29	1.16	2 (8%)	29,45,45	1.55	5 (17%)
2	ADP	B	9009	-	24,29,29	1.34	2 (8%)	29,45,45	1.47	6 (20%)
3	SPM	A	9016	-	13,13,13	0.53	0	12,12,12	0.89	0
2	ADP	A	9003	-	24,29,29	1.36	3 (12%)	29,45,45	1.58	6 (20%)
3	SPM	A	9012	-	13,13,13	0.60	0	12,12,12	0.82	0
2	ADP	B	9007	4	24,29,29	1.07	3 (12%)	29,45,45	1.60	5 (17%)
2	ADP	B	9010	-	24,29,29	1.08	1 (4%)	29,45,45	1.52	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	9002	4	-	5/12/32/32	0/3/3/3
2	ADP	B	9008	4	-	4/12/32/32	0/3/3/3
2	ADP	A	9001	-	-	5/12/32/32	0/3/3/3
3	SPM	B	9018	-	-	8/11/11/11	-
3	SPM	B	9022	-	-	7/11/11/11	-
2	ADP	A	9004	-	-	3/12/32/32	0/3/3/3
2	ADP	B	9009	-	-	6/12/32/32	0/3/3/3
3	SPM	A	9016	-	-	11/11/11/11	-
2	ADP	A	9003	-	-	6/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SPM	A	9012	-	-	6/11/11/11	-
2	ADP	B	9007	4	-	5/12/32/32	0/3/3/3
2	ADP	B	9010	-	-	6/12/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9009	ADP	C5-C4	3.11	1.49	1.40
2	B	9008	ADP	C2-N3	3.02	1.37	1.32
2	B	9008	ADP	C5-C4	2.94	1.48	1.40
2	A	9002	ADP	C2-N3	2.91	1.36	1.32
2	A	9004	ADP	C5-C4	2.88	1.48	1.40
2	A	9001	ADP	C5-C4	2.81	1.48	1.40
2	A	9003	ADP	C5-C4	2.80	1.48	1.40
2	B	9009	ADP	C2-N3	2.74	1.36	1.32
2	A	9004	ADP	O4'-C1'	2.72	1.44	1.41
2	A	9003	ADP	C2-N3	2.72	1.36	1.32
2	A	9002	ADP	C5-C4	2.64	1.47	1.40
2	B	9007	ADP	C5-C4	2.47	1.47	1.40
2	A	9002	ADP	O4'-C1'	2.29	1.44	1.41
2	B	9010	ADP	C5-C4	2.25	1.46	1.40
2	B	9008	ADP	O4'-C1'	2.21	1.44	1.41
2	B	9007	ADP	C2-N3	2.15	1.35	1.32
2	A	9001	ADP	O4'-C4'	-2.14	1.40	1.45
2	A	9003	ADP	C4-N3	2.11	1.38	1.35
2	B	9007	ADP	C5-N7	-2.06	1.32	1.39
2	A	9001	ADP	C2-N3	2.02	1.35	1.32

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	9007	ADP	N3-C2-N1	-4.83	121.13	128.68
2	A	9003	ADP	N3-C2-N1	-4.49	121.67	128.68
2	A	9001	ADP	N3-C2-N1	-4.36	121.86	128.68
2	A	9002	ADP	N3-C2-N1	-4.25	122.03	128.68
2	B	9008	ADP	N3-C2-N1	-4.16	122.17	128.68
2	B	9010	ADP	N3-C2-N1	-4.14	122.21	128.68
2	B	9009	ADP	N3-C2-N1	-4.11	122.25	128.68
2	B	9010	ADP	C3'-C2'-C1'	4.09	107.13	100.98
2	A	9004	ADP	C3'-C2'-C1'	4.03	107.05	100.98
2	A	9004	ADP	N3-C2-N1	-3.96	122.48	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	9003	ADP	C3'-C2'-C1'	3.35	106.03	100.98
2	B	9007	ADP	C3'-C2'-C1'	3.33	105.99	100.98
2	A	9002	ADP	C3'-C2'-C1'	3.29	105.93	100.98
2	B	9008	ADP	C3'-C2'-C1'	3.06	105.59	100.98
2	B	9007	ADP	PA-O3A-PB	-2.95	122.71	132.83
2	B	9009	ADP	C3'-C2'-C1'	2.93	105.38	100.98
2	A	9001	ADP	C3'-C2'-C1'	2.90	105.34	100.98
2	A	9002	ADP	PA-O3A-PB	-2.90	122.89	132.83
2	A	9002	ADP	C4-C5-N7	-2.68	106.61	109.40
2	A	9003	ADP	C2'-C3'-C4'	2.61	107.70	102.64
2	A	9001	ADP	PA-O3A-PB	-2.57	124.01	132.83
2	B	9009	ADP	PA-O3A-PB	-2.51	124.22	132.83
2	A	9004	ADP	PA-O3A-PB	-2.50	124.26	132.83
2	B	9007	ADP	C2-N1-C6	2.48	123.00	118.75
2	B	9009	ADP	C4-C5-N7	-2.44	106.86	109.40
2	A	9003	ADP	PA-O3A-PB	-2.41	124.57	132.83
2	A	9004	ADP	C2-N1-C6	2.41	122.87	118.75
2	A	9003	ADP	C4-C5-N7	-2.38	106.92	109.40
2	B	9010	ADP	C2-N1-C6	2.35	122.78	118.75
2	A	9001	ADP	C2-N1-C6	2.35	122.77	118.75
2	B	9008	ADP	C2'-C3'-C4'	2.34	107.19	102.64
2	A	9001	ADP	C4-C5-N7	-2.34	106.96	109.40
2	A	9003	ADP	C2-N1-C6	2.30	122.69	118.75
2	B	9008	ADP	C4-C5-N7	-2.29	107.01	109.40
2	B	9009	ADP	C2'-C3'-C4'	2.29	107.08	102.64
2	B	9009	ADP	C2-N1-C6	2.23	122.56	118.75
2	B	9008	ADP	C2-N1-C6	2.22	122.55	118.75
2	A	9001	ADP	C2'-C3'-C4'	2.19	106.90	102.64
2	A	9004	ADP	C4-C5-N7	-2.11	107.20	109.40
2	A	9002	ADP	C2-N1-C6	2.10	122.34	118.75
2	B	9008	ADP	PA-O3A-PB	-2.08	125.68	132.83
2	B	9007	ADP	O3B-PB-O2B	2.05	115.48	107.64

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9001	ADP	C5'-O5'-PA-O1A
2	A	9001	ADP	C5'-O5'-PA-O2A
2	A	9002	ADP	C5'-O5'-PA-O3A
2	A	9003	ADP	C5'-O5'-PA-O1A
2	A	9003	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	B	9007	ADP	C5'-O5'-PA-O1A
2	B	9007	ADP	C5'-O5'-PA-O2A
2	B	9008	ADP	C5'-O5'-PA-O3A
2	B	9009	ADP	C5'-O5'-PA-O1A
2	B	9009	ADP	C5'-O5'-PA-O2A
2	B	9010	ADP	C5'-O5'-PA-O2A
3	A	9012	SPM	C2-C3-C4-N5
3	A	9016	SPM	C7-C8-C9-N10
3	B	9018	SPM	C2-C3-C4-N5
3	B	9022	SPM	C2-C3-C4-N5
3	A	9012	SPM	C12-C11-N10-C9
3	A	9016	SPM	C3-C4-N5-C6
3	A	9016	SPM	C7-C6-N5-C4
3	B	9018	SPM	N10-C11-C12-C13
3	A	9016	SPM	C2-C3-C4-N5
3	B	9022	SPM	C3-C4-N5-C6
3	A	9016	SPM	N10-C11-C12-C13
3	A	9012	SPM	N1-C2-C3-C4
3	B	9018	SPM	C11-C12-C13-N14
3	A	9016	SPM	C6-C7-C8-C9
3	A	9012	SPM	C7-C8-C9-N10
3	A	9012	SPM	N10-C11-C12-C13
2	A	9003	ADP	C5'-O5'-PA-O3A
2	B	9010	ADP	C5'-O5'-PA-O3A
3	A	9016	SPM	N1-C2-C3-C4
3	A	9016	SPM	C8-C9-N10-C11
3	A	9016	SPM	C12-C11-N10-C9
2	A	9001	ADP	PB-O3A-PA-O2A
2	A	9002	ADP	PB-O3A-PA-O2A
2	A	9003	ADP	PB-O3A-PA-O2A
2	A	9004	ADP	PB-O3A-PA-O2A
2	B	9007	ADP	PB-O3A-PA-O2A
2	B	9008	ADP	PB-O3A-PA-O2A
2	B	9009	ADP	PB-O3A-PA-O2A
2	B	9010	ADP	PB-O3A-PA-O2A
2	A	9002	ADP	C5'-O5'-PA-O1A
2	B	9008	ADP	C5'-O5'-PA-O1A
2	B	9010	ADP	C5'-O5'-PA-O1A
3	B	9018	SPM	C6-C7-C8-C9
3	A	9016	SPM	N5-C6-C7-C8
3	B	9022	SPM	N10-C11-C12-C13
3	A	9016	SPM	C11-C12-C13-N14

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Mol	Chain	Res	Type	Atoms
3	B	9018	SPM	N1-C2-C3-C4
3	B	9022	SPM	N1-C2-C3-C4
2	B	9007	ADP	O4'-C4'-C5'-O5'
2	A	9001	ADP	O4'-C4'-C5'-O5'
2	A	9004	ADP	O4'-C4'-C5'-O5'
2	B	9008	ADP	O4'-C4'-C5'-O5'
2	B	9010	ADP	O4'-C4'-C5'-O5'
3	B	9018	SPM	C7-C6-N5-C4
2	A	9002	ADP	O4'-C4'-C5'-O5'
2	B	9009	ADP	O4'-C4'-C5'-O5'
3	B	9022	SPM	C7-C6-N5-C4
3	B	9018	SPM	C12-C11-N10-C9
3	B	9022	SPM	C12-C11-N10-C9
2	A	9001	ADP	C5'-O5'-PA-O3A
2	B	9007	ADP	C5'-O5'-PA-O3A
2	B	9009	ADP	C5'-O5'-PA-O3A
3	B	9022	SPM	C11-C12-C13-N14
2	A	9003	ADP	O4'-C4'-C5'-O5'
2	A	9002	ADP	PB-O3A-PA-O1A
2	A	9003	ADP	PB-O3A-PA-O1A
2	A	9004	ADP	PB-O3A-PA-O1A
2	B	9009	ADP	PB-O3A-PA-O1A
2	B	9010	ADP	PB-O3A-PA-O1A
3	A	9012	SPM	C8-C9-N10-C11
3	B	9018	SPM	C3-C4-N5-C6

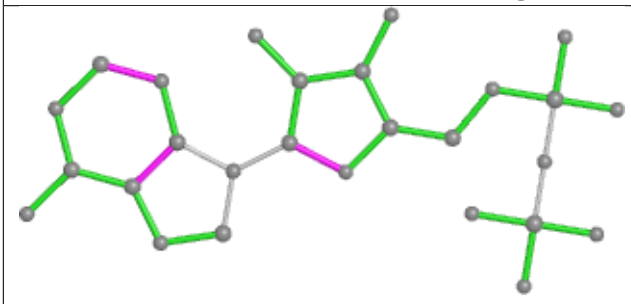
There are no ring outliers.

12 monomers are involved in 30 short contacts:

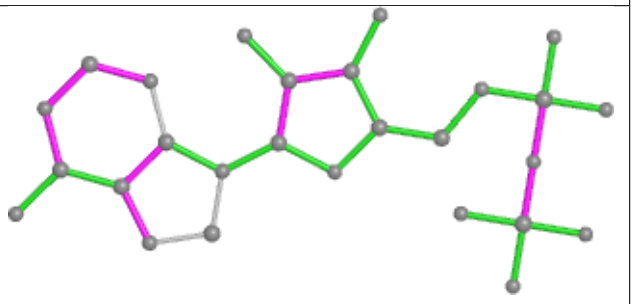
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9002	ADP	3	0
2	B	9008	ADP	2	0
2	A	9001	ADP	1	0
3	B	9018	SPM	2	0
3	B	9022	SPM	3	0
2	A	9004	ADP	6	0
2	B	9009	ADP	2	0
3	A	9016	SPM	1	0
2	A	9003	ADP	4	0
3	A	9012	SPM	1	0
2	B	9007	ADP	2	0
2	B	9010	ADP	3	0

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

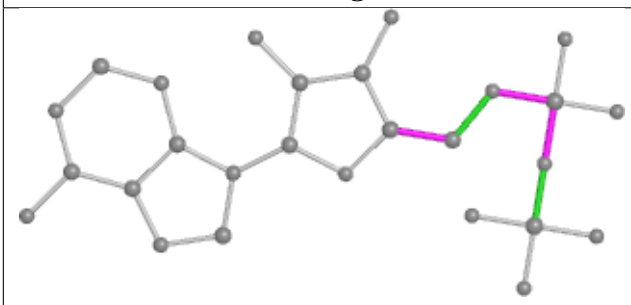
Ligand ADP A 9002



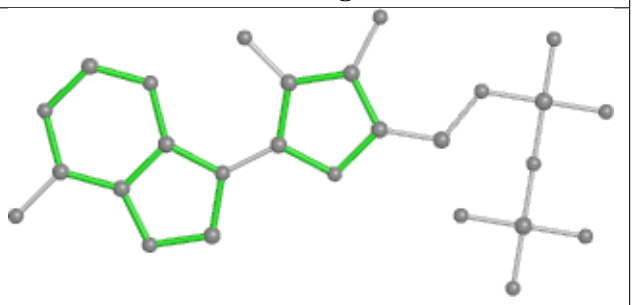
Bond lengths



Bond angles

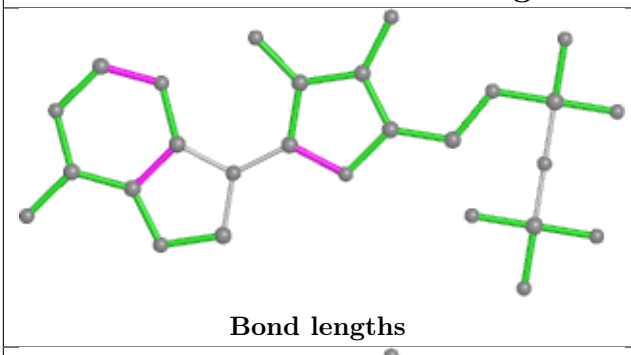


Torsions

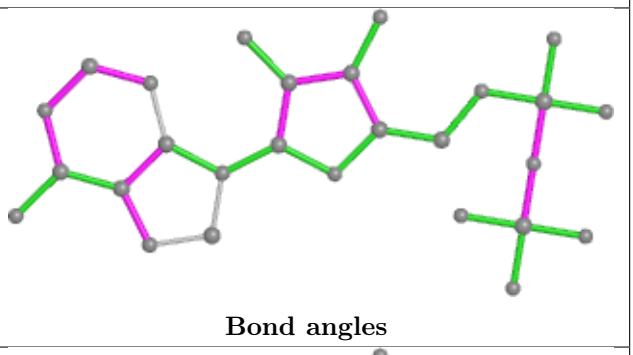


Rings

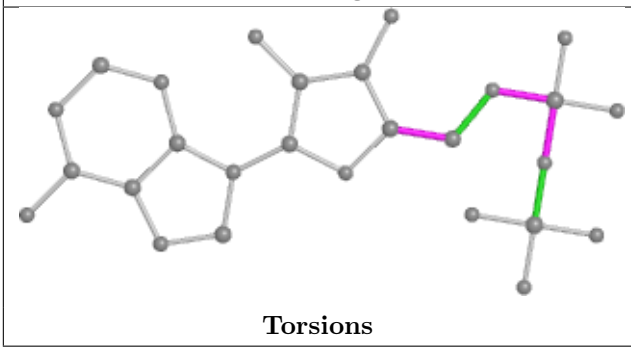
Ligand ADP B 9008



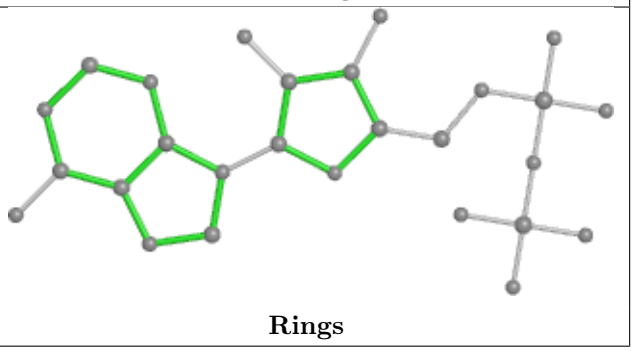
Bond lengths



Bond angles

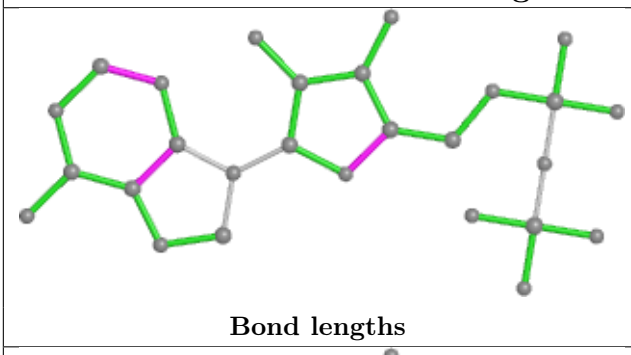


Torsions

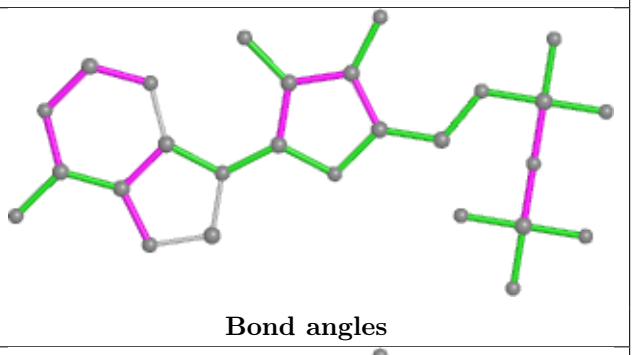


Rings

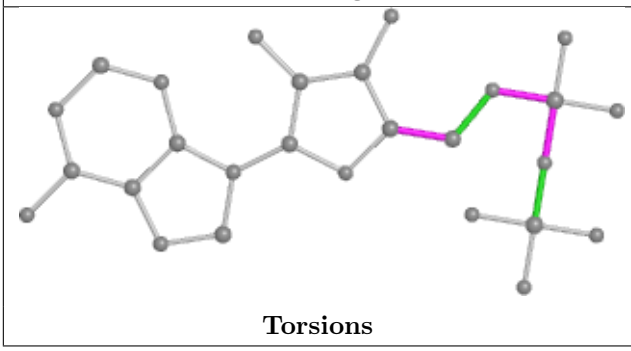
Ligand ADP A 9001



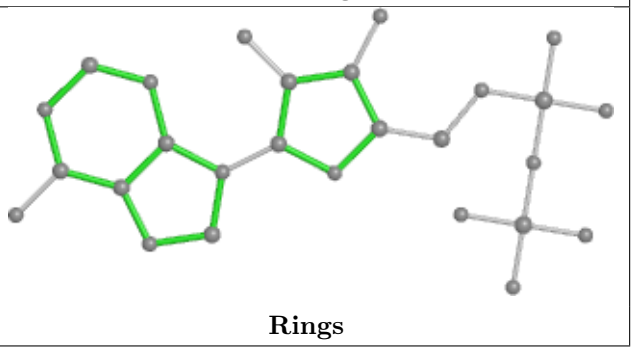
Bond lengths



Bond angles

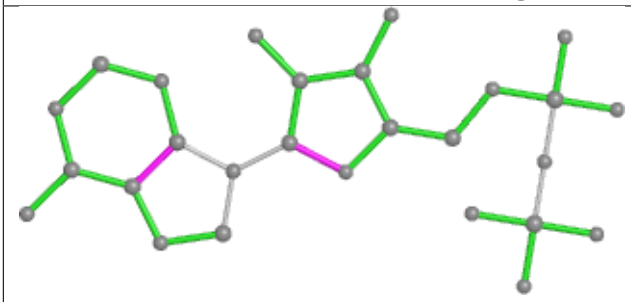


Torsions

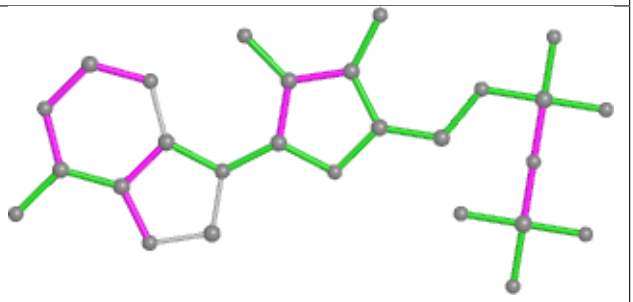


Rings

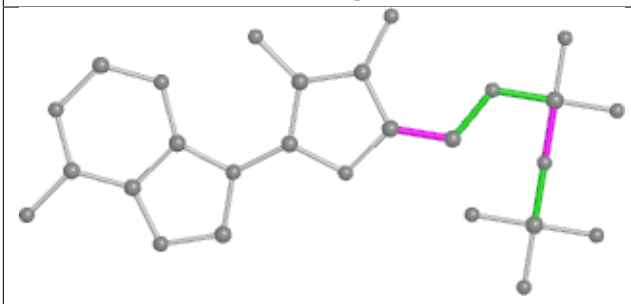
Ligand ADP A 9004



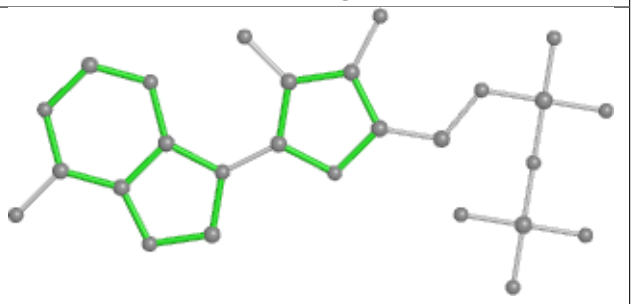
Bond lengths



Bond angles

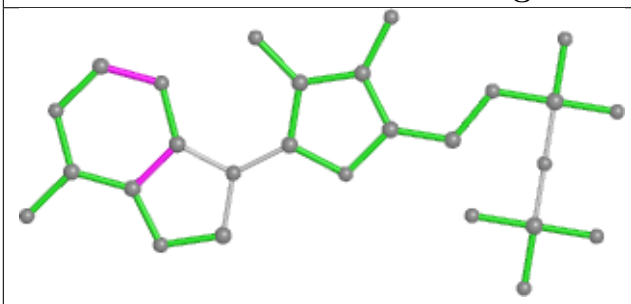


Torsions

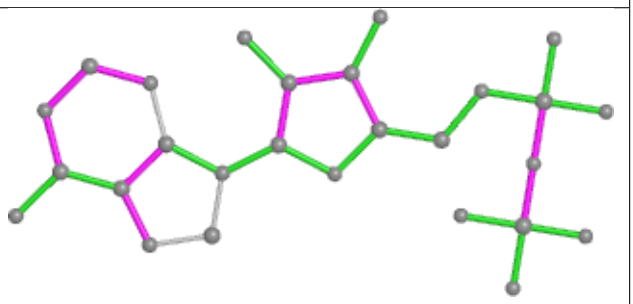


Rings

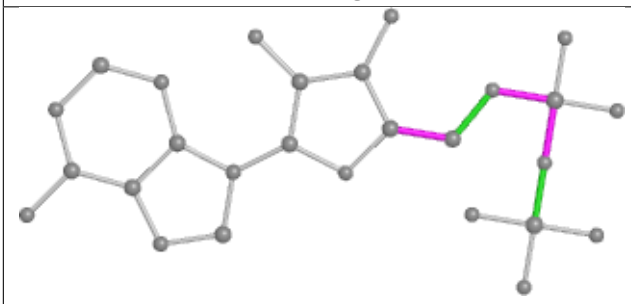
Ligand ADP B 9009



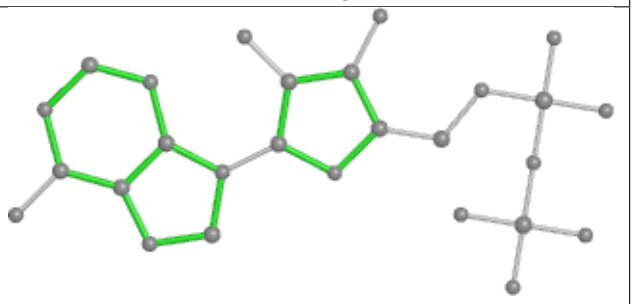
Bond lengths



Bond angles

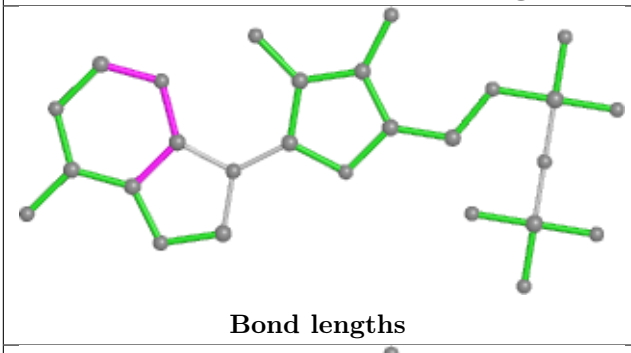


Torsions

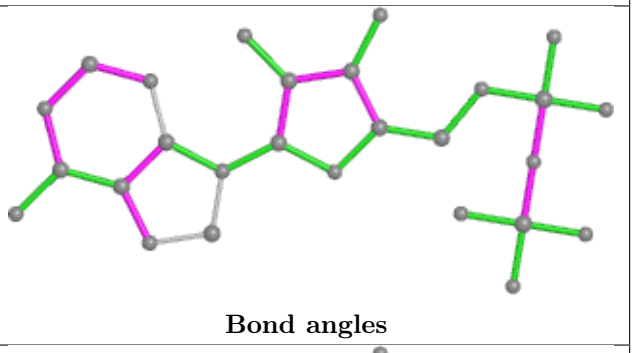


Rings

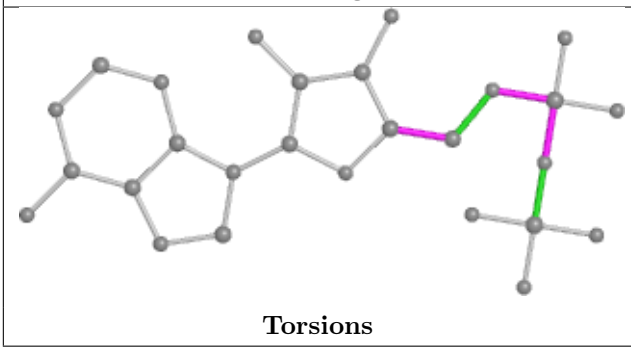
Ligand ADP A 9003



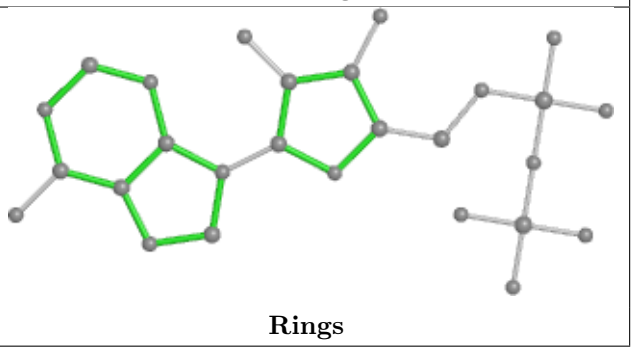
Bond lengths



Bond angles

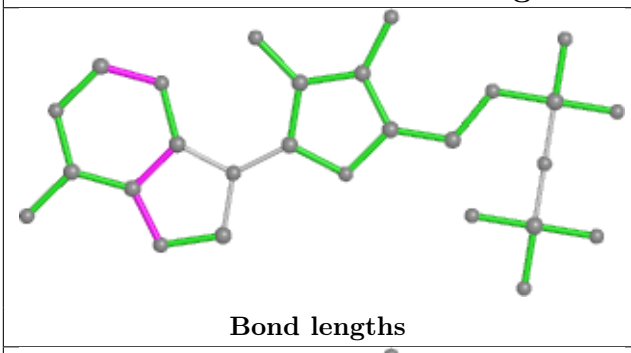


Torsions

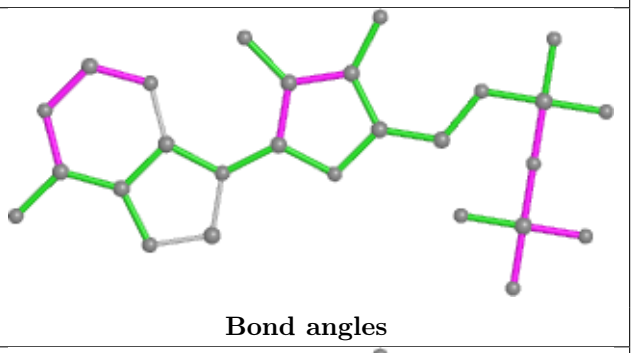


Rings

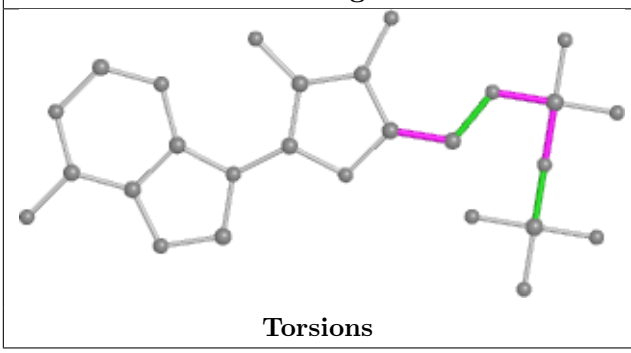
Ligand ADP B 9007



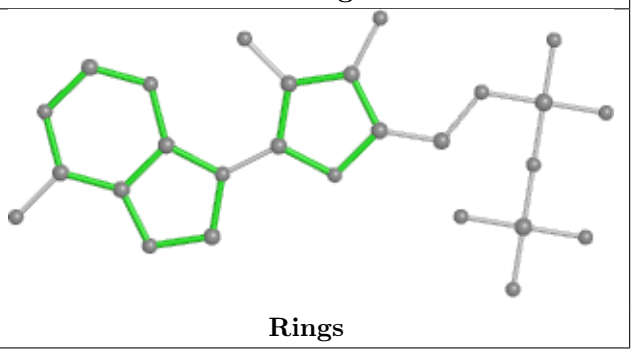
Bond lengths



Bond angles

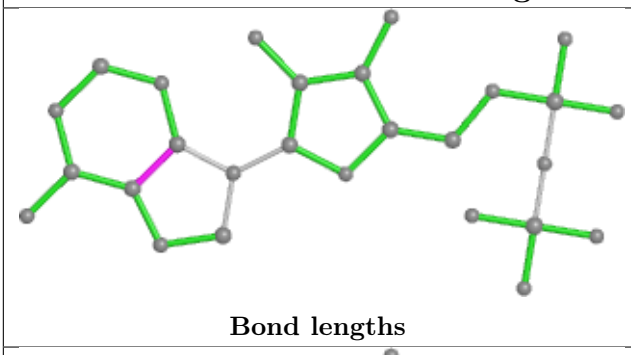


Torsions

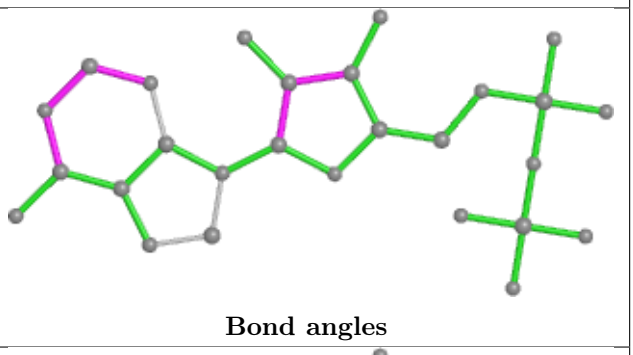


Rings

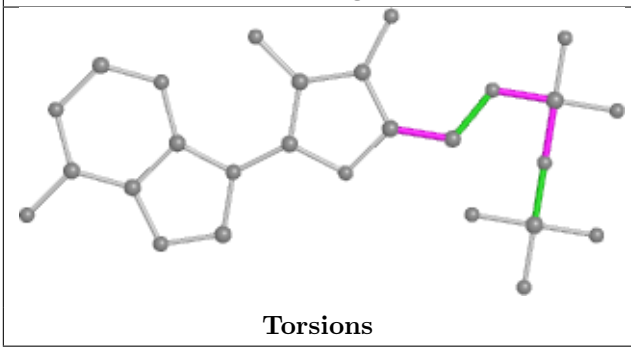
Ligand ADP B 9010



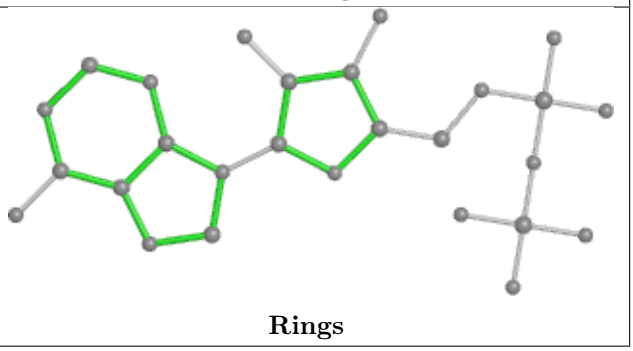
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	2954/3245 (91%)	-0.03	32 (1%)	80	75	17, 53, 78, 102	0
1	B	2853/3245 (87%)	-0.08	25 (0%)	84	80	24, 52, 75, 100	0
All	All	5807/6490 (89%)	-0.05	57 (0%)	82	77	17, 52, 77, 102	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1494	ILE	4.2
1	B	1643	PHE	3.8
1	B	1605	TRP	3.5
1	A	4191	HIS	3.2
1	B	1555	VAL	3.0
1	A	1513	ILE	3.0
1	A	2887	LEU	3.0
1	B	3108	LEU	3.0
1	B	3058	LEU	2.9
1	B	1604	VAL	2.9
1	A	3506	ASN	2.9
1	B	2323	THR	2.9
1	A	1413	SER	2.9
1	A	3079	LEU	2.9
1	A	4195	GLN	2.8
1	A	3501	VAL	2.8
1	A	4564	TRP	2.7
1	B	4543	LYS	2.7
1	A	3777	LEU	2.6
1	A	1419	TRP	2.6
1	B	4049	GLY	2.6
1	A	1454	ALA	2.6
1	B	4071	ASN	2.5
1	B	2166	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1602	LEU	2.5
1	B	4051	ASP	2.5
1	A	1458	ILE	2.4
1	A	2262	LEU	2.4
1	B	1650	VAL	2.4
1	A	2906	ALA	2.4
1	A	3932	ASP	2.4
1	A	4187	LEU	2.4
1	A	1418	ALA	2.3
1	A	1514	TYR	2.3
1	A	2409	SER	2.3
1	A	4223	PRO	2.3
1	A	4217	MET	2.3
1	A	2714	PHE	2.3
1	B	3712	LEU	2.3
1	B	1606	ILE	2.2
1	B	3350	VAL	2.2
1	B	1567	GLU	2.2
1	A	3773	PHE	2.2
1	B	3130	TYR	2.2
1	A	1921	VAL	2.2
1	B	1545	LEU	2.2
1	A	3341	ALA	2.2
1	B	2256	VAL	2.2
1	B	3708	LEU	2.2
1	B	1561	LEU	2.1
1	B	1646	ILE	2.1
1	B	2741	VAL	2.1
1	A	4578	ILE	2.1
1	B	3685	LEU	2.0
1	A	3098	GLY	2.0
1	A	2267	ASN	2.0
1	A	2344	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

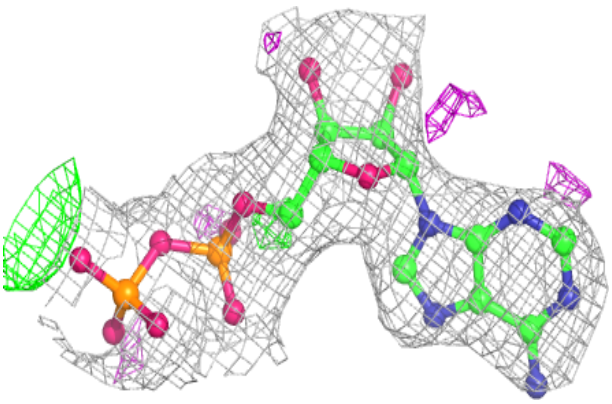
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

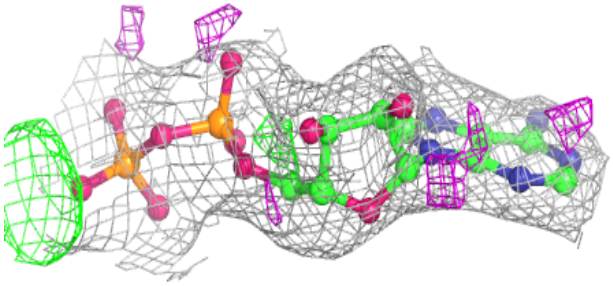
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SPM	A	9016	14/14	0.83	0.25	43,50,54,55	0
3	SPM	A	9012	14/14	0.87	0.22	37,41,45,47	0
4	MG	B	2	1/1	0.87	0.14	50,50,50,50	0
3	SPM	B	9018	14/14	0.89	0.21	57,57,59,59	0
3	SPM	B	9022	14/14	0.91	0.20	37,43,49,49	0
4	MG	B	3	1/1	0.91	0.22	28,28,28,28	0
2	ADP	A	9002	27/27	0.93	0.23	47,49,52,54	0
2	ADP	B	9008	27/27	0.93	0.23	41,51,53,54	0
2	ADP	A	9003	27/27	0.95	0.21	41,45,50,52	0
2	ADP	A	9001	27/27	0.96	0.21	32,38,42,44	0
2	ADP	B	9009	27/27	0.96	0.20	39,45,48,51	0
2	ADP	A	9004	27/27	0.96	0.15	44,49,54,56	0
2	ADP	B	9007	27/27	0.96	0.20	38,47,50,52	0
2	ADP	B	9010	27/27	0.97	0.18	31,37,46,48	0
4	MG	A	1	1/1	0.98	0.22	44,44,44,44	0

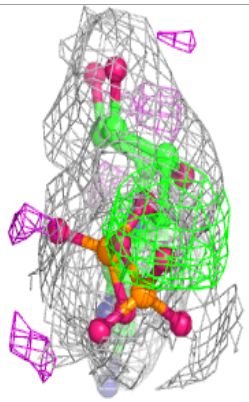
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 9002:

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

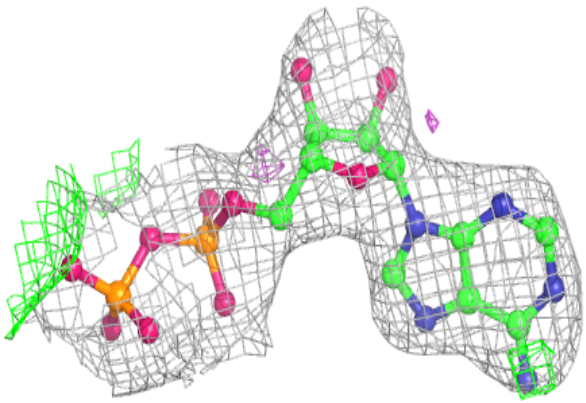


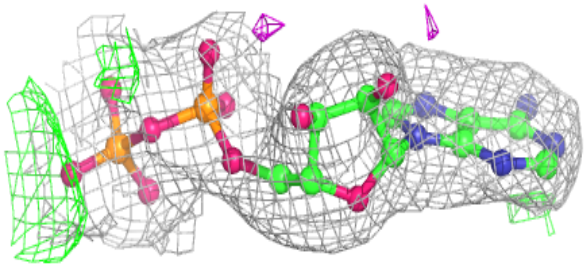


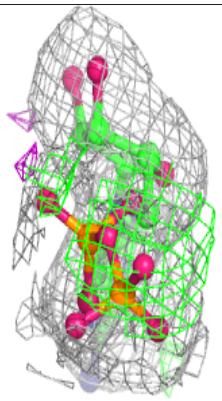


Electron density around ADP B 9008:

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

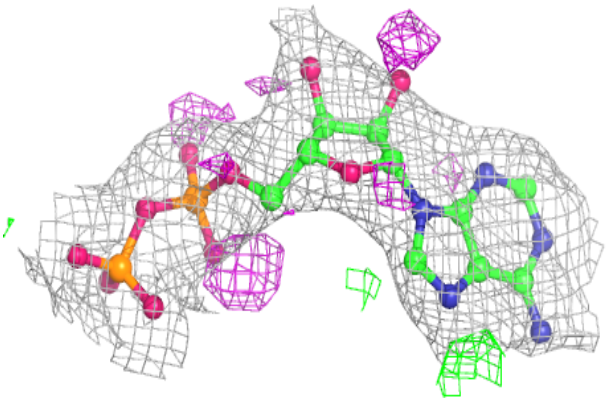


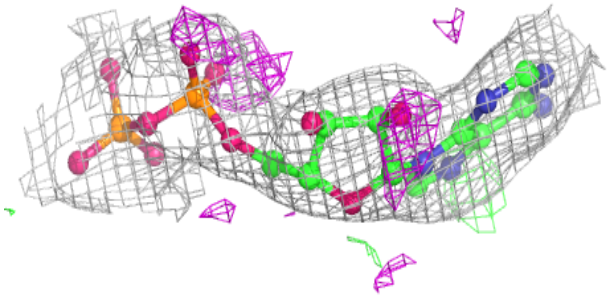


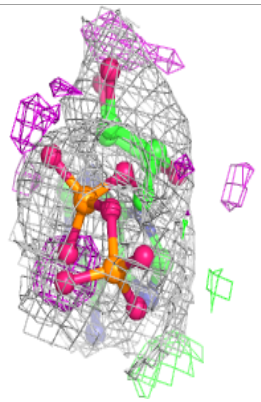


Electron density around ADP A 9003:

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

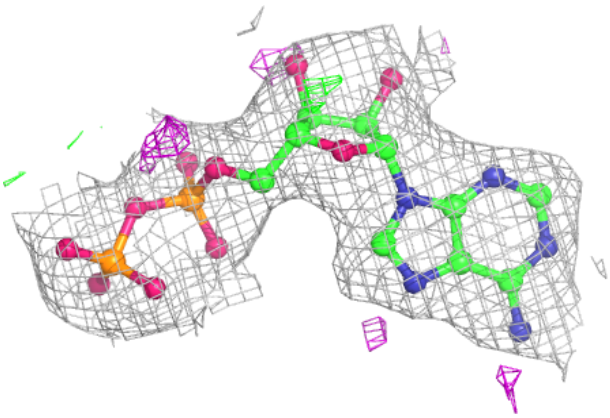


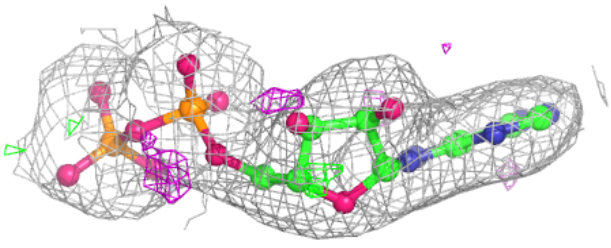


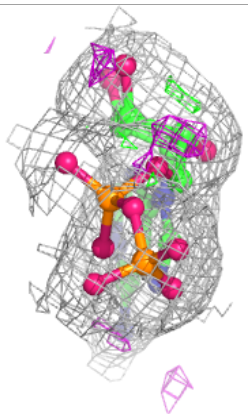


Electron density around ADP A 9001:

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

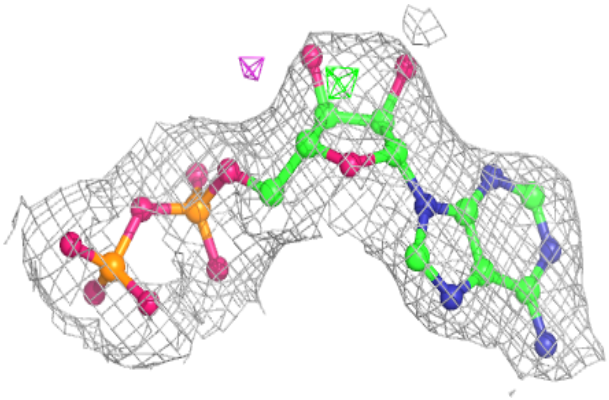


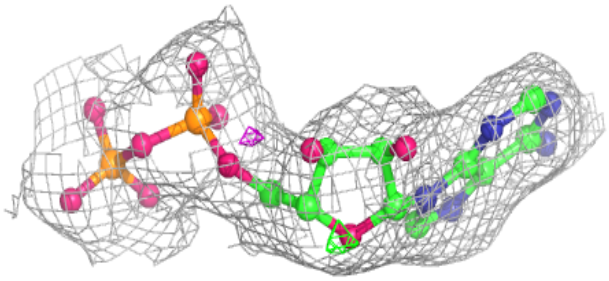


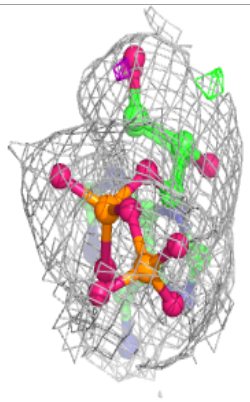


Electron density around ADP B 9009:

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

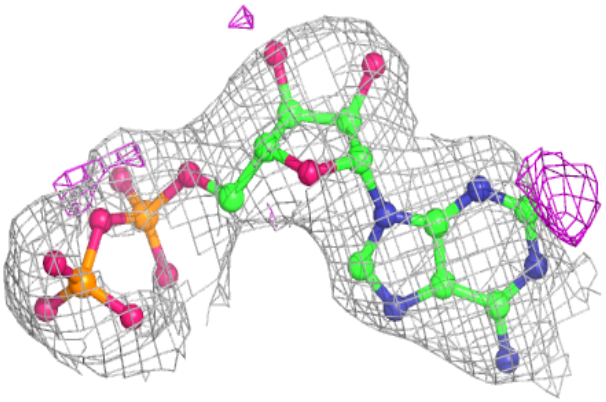


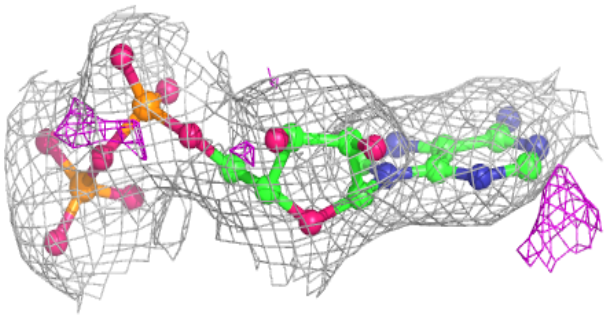


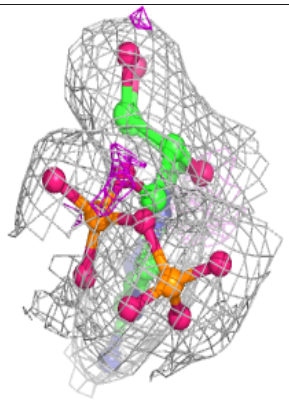


Electron density around ADP A 9004:

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

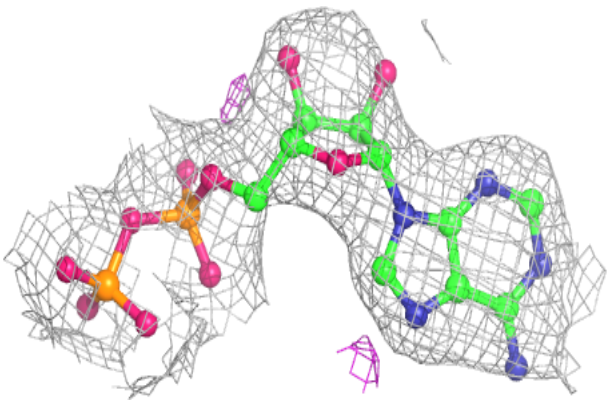


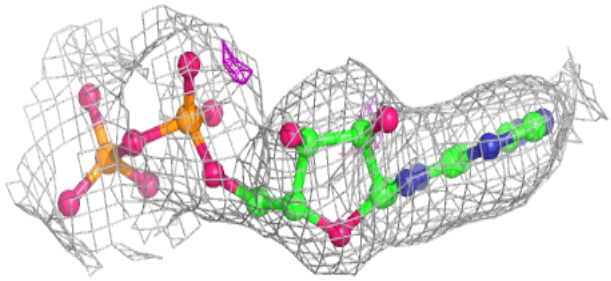


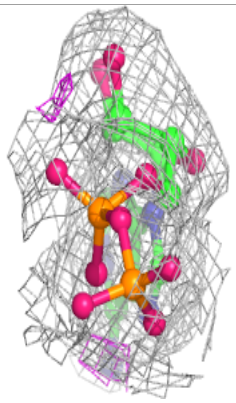


Electron density around ADP B 9007:

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

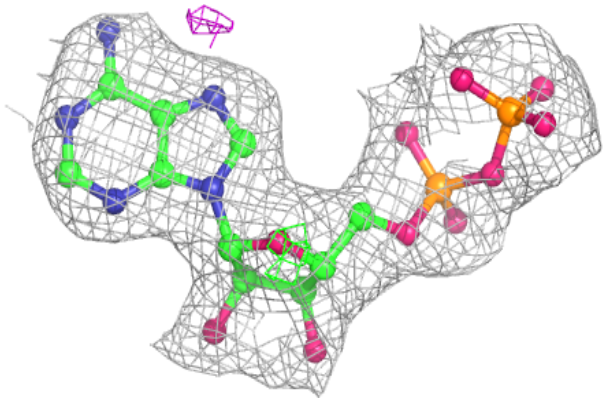


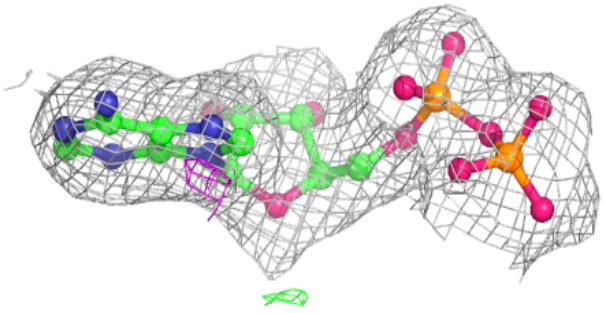


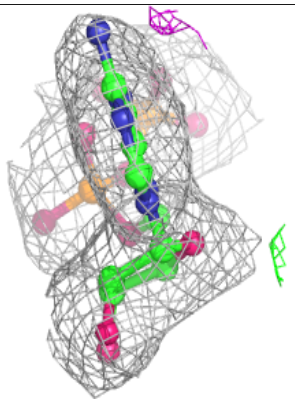


Electron density around ADP B 9010:

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







6.5 Other polymers (i)

There are no such residues in this entry.