Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:53 PM GMT

PDB ID	:	1CZ7
Title	:	THE CRYSTAL STRUCTURE OF A MINUS-END DIRECTED MICROTUBULE MOTOR PROTEIN NCD REVEALS VARIABLE DIMER CONFORMATIONS
Authors	:	Kozielski, F.K.; De Bonis, S.; Burmeister, W.; Cohen-Addad, C.; Wade, R.
Deposited on	:	1999-09-01
Resolution	:	2.90 Å(reported)

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

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

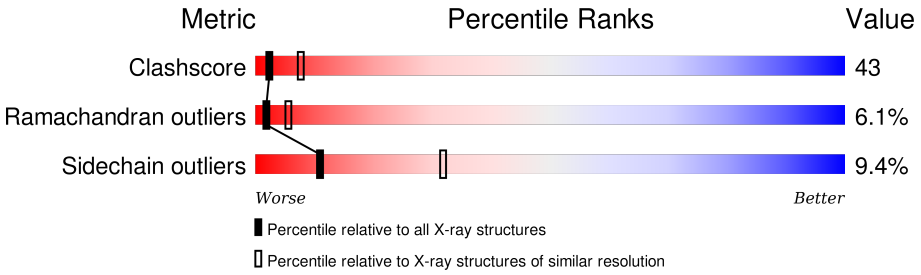
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	406	37% 39% 8% 16%
1	B	406	36% 39% 7% 17%
1	C	406	38% 45% 6% 10%
1	D	406	34% 45% 11% • 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11439 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.

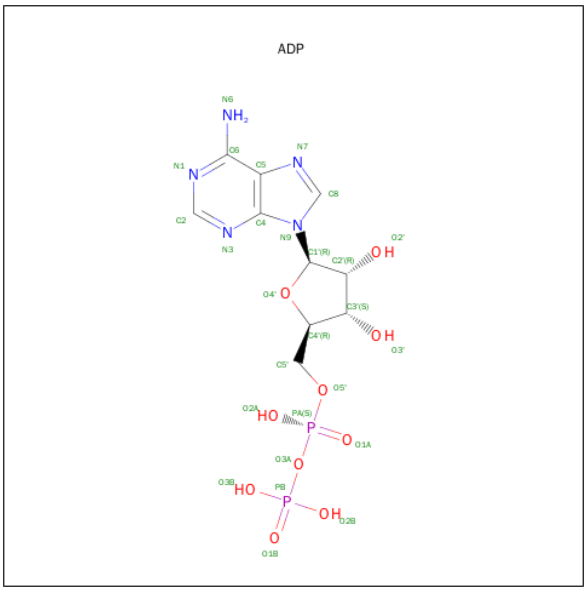
- Molecule 1 is a protein called MICROTUBULE MOTOR PROTEIN NCD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2711	1691	472	529	19			
1	B	337	Total	C	N	O	S	0	0	0
			2682	1674	467	523	18			
1	C	364	Total	C	N	O	S	0	0	0
			2888	1798	509	562	19			
1	D	365	Total	C	N	O	S	0	0	0
			2898	1803	510	565	20			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	32	Total	O	0	0
			32	32		
4	C	18	Total	O	0	0
			18	18		
4	D	50	Total	O	0	0
			50	50		

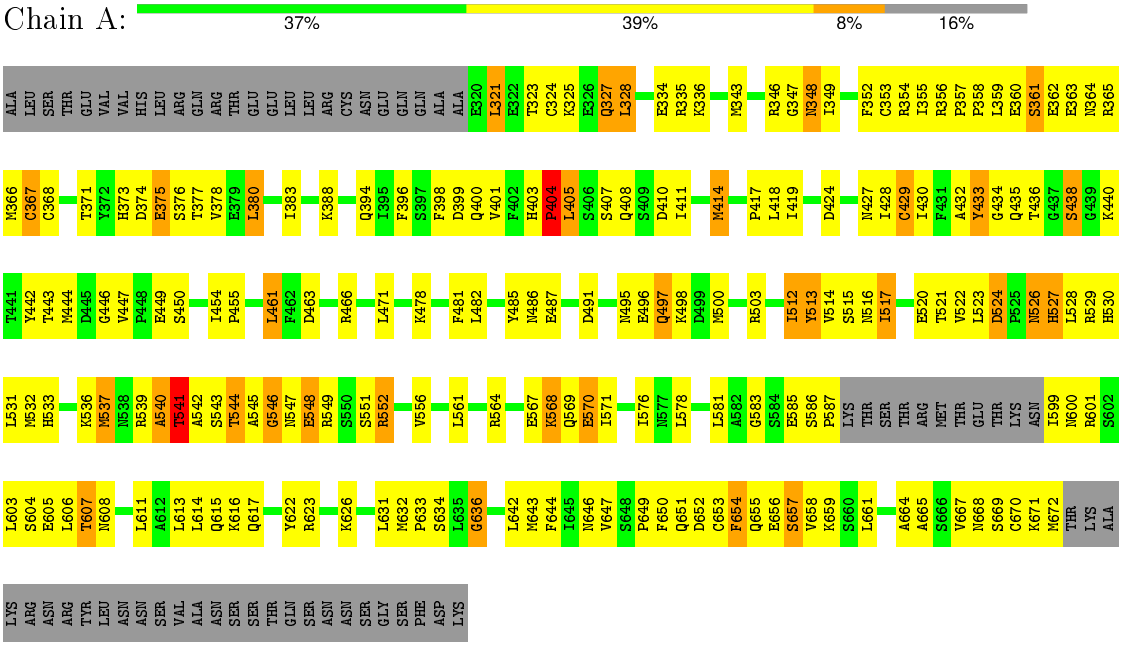
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

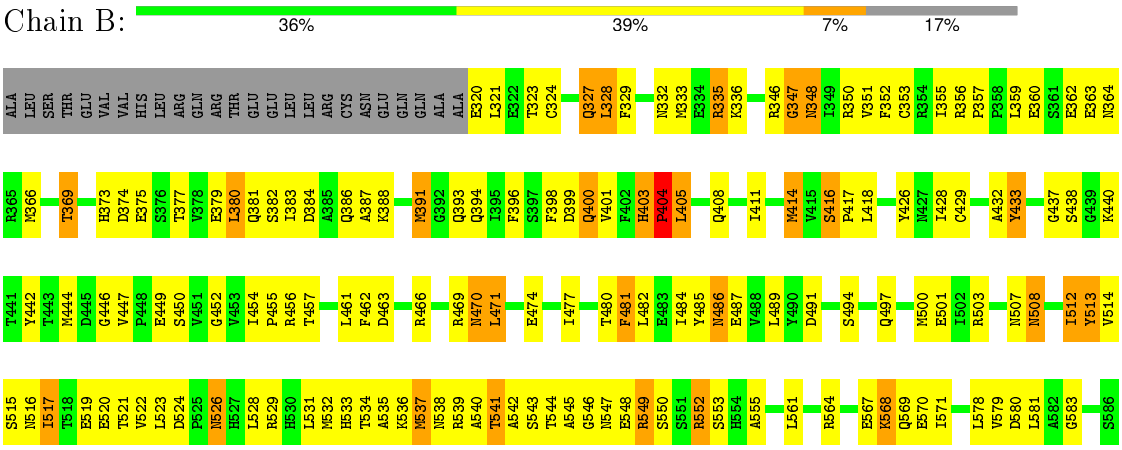
- Molecule 1: MICROTUBULE MOTOR PROTEIN NCD

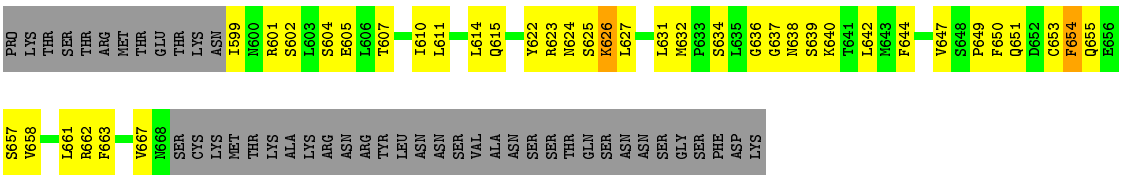
Chain A:



- Molecule 1: MICROTUBULE MOTOR PROTEIN NCD

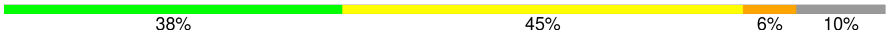
Chain B:

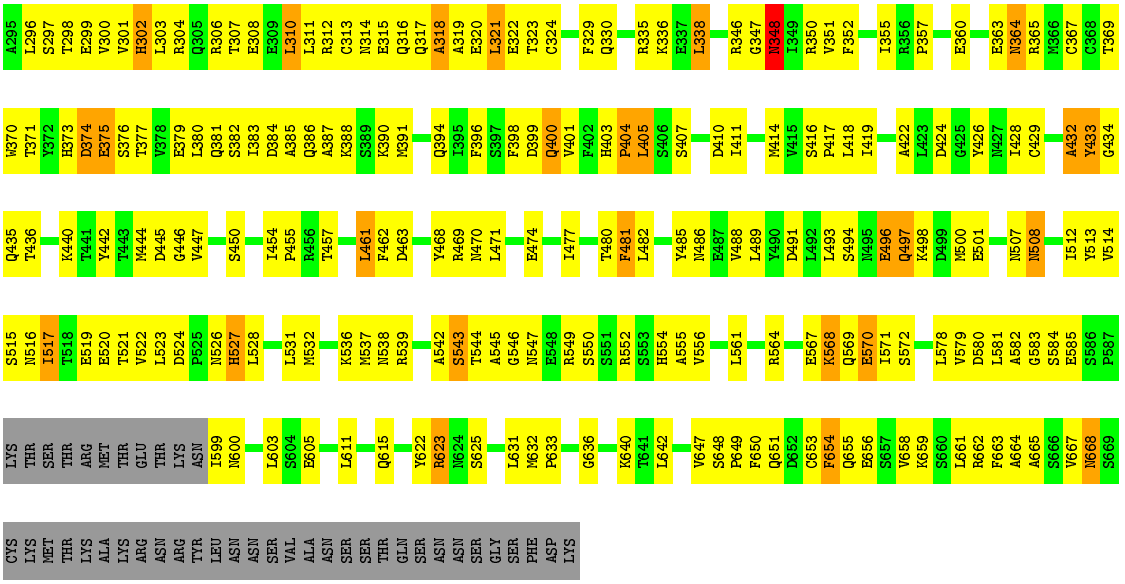




• Molecule 1: MICROTUBULE MOTOR PROTEIN NCD

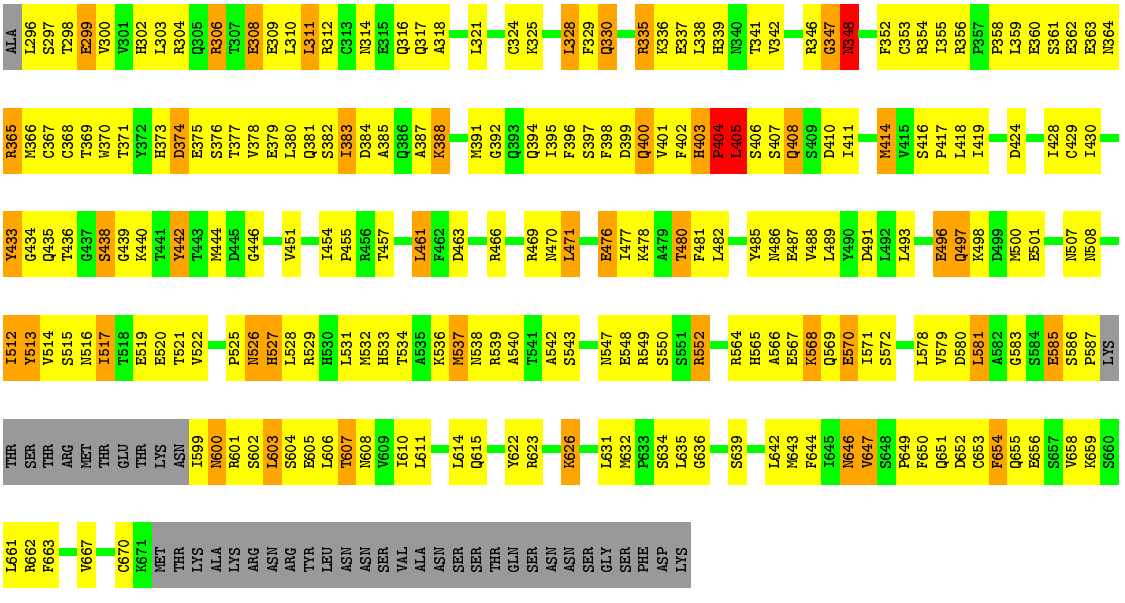
Chain C:





• Molecule 1: MICROTUBULE MOTOR PROTEIN NCD

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	116.19Å 148.83Å 261.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90	Depositor
% Data completeness (in resolution range)	96.5 (40.00-2.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11439	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

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

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	0.76	3/2757 (0.1%)	0.87	1/3722 (0.0%)
1	B	0.55	0/2727	0.72	0/3680
1	C	0.50	0/2933	0.71	2/3960 (0.1%)
1	D	0.72	1/2943 (0.0%)	0.84	1/3973 (0.0%)
All	All	0.64	4/11360 (0.0%)	0.79	4/15335 (0.0%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	579	VAL	CB-CG2	-6.29	1.39	1.52
1	A	367	CYS	CB-SG	5.54	1.91	1.82
1	A	429	CYS	CB-SG	-5.24	1.73	1.81
1	A	556	VAL	CB-CG1	-5.23	1.41	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	405	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	354	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	C	432	ALA	N-CA-C	-5.30	96.70	111.00
1	C	310	LEU	CA-CB-CG	-5.07	103.65	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	442	TYR	Sidechain

5.2 Too-close contacts (i)

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	2711	0	2664	233	0
1	B	2682	0	2644	215	0
1	C	2888	0	2849	236	0
1	D	2898	0	2855	294	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	4	0
3	B	27	0	12	5	0
3	C	27	0	12	5	0
3	D	27	0	12	3	0
4	A	48	0	0	17	1
4	B	32	0	0	13	0
4	C	18	0	0	17	0
4	D	50	0	0	30	0
All	All	11439	0	11060	960	1

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 43.

All (960) 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:D:476:GLU:HA	4:D:110:HOH:O	1.31	1.30
1:B:394:GLN:HA	4:B:33:HOH:O	1.29	1.28
1:B:357:PRO:HB3	1:B:404:PRO:HB3	1.27	1.15
1:D:599:ILE:HG22	1:D:600:ASN:H	1.15	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:ARG:HB3	4:B:44:HOH:O	1.53	1.06
1:B:380:LEU:O	1:B:394:GLN:HB2	1.58	1.01
1:A:347:GLY:O	1:A:348:ASN:HB2	1.58	1.00
1:B:381:GLN:HB3	1:B:388:LYS:HD3	1.42	1.00
1:B:380:LEU:HD23	1:B:394:GLN:HB3	1.42	1.00
1:D:486:ASN:N	4:D:113:HOH:O	1.94	0.99
1:A:418:LEU:HD11	1:A:642:LEU:HD13	1.40	0.99
1:A:436:THR:OG1	1:A:585:GLU:OE2	1.80	0.98
1:A:358:PRO:O	4:A:79:HOH:O	1.80	0.98
1:C:542:ALA:H	1:C:550:SER:HB2	1.27	0.98
1:C:542:ALA:HA	1:C:545:ALA:HB3	1.46	0.97
1:D:347:GLY:O	1:D:348:ASN:HB2	1.62	0.97
1:B:614:LEU:HD11	1:B:667:VAL:HG13	1.48	0.96
1:A:367:CYS:SG	4:A:94:HOH:O	2.23	0.95
1:A:498:LYS:HB2	4:A:52:HOH:O	1.66	0.95
1:A:367:CYS:N	4:A:94:HOH:O	2.00	0.93
1:B:357:PRO:HD3	1:B:404:PRO:HA	1.49	0.93
1:B:347:GLY:O	1:B:348:ASN:HB2	1.68	0.92
1:C:491:ASP:HB2	1:C:500:MET:CE	2.00	0.91
1:A:435:GLN:O	1:A:438:SER:OG	1.87	0.91
1:B:440:LYS:HE3	3:B:801:ADP:O3B	1.69	0.91
1:A:346:ARG:HH11	1:A:346:ARG:HG3	1.37	0.90
1:C:347:GLY:O	1:C:348:ASN:HB2	1.69	0.90
1:A:542:ALA:HB2	4:A:140:HOH:O	1.71	0.90
1:B:394:GLN:CA	4:B:33:HOH:O	1.96	0.89
1:A:586:SER:HB3	1:A:587:PRO:HD2	1.55	0.88
1:A:564:ARG:NH2	4:A:48:HOH:O	2.05	0.88
1:C:554:HIS:HE1	4:C:69:HOH:O	1.56	0.88
1:D:569:GLN:CB	4:D:148:HOH:O	2.22	0.88
1:A:440:LYS:NZ	1:A:583:GLY:HA2	1.89	0.87
1:C:418:LEU:HD11	1:C:642:LEU:HD13	1.55	0.87
1:D:615:GLN:HG2	1:D:670:CYS:SG	2.15	0.87
1:D:569:GLN:HB2	4:D:148:HOH:O	1.74	0.86
1:C:396:PHE:HD2	1:C:665:ALA:HB2	1.40	0.86
1:D:382:SER:HB2	1:D:651:GLN:HE22	1.39	0.86
1:D:570:GLU:N	4:D:148:HOH:O	2.08	0.86
1:C:317:GLN:NE2	1:D:318:ALA:HB2	1.90	0.85
1:A:547:ASN:O	1:A:549:ARG:N	2.11	0.84
1:D:650:PHE:HB3	4:D:121:HOH:O	1.78	0.83
1:D:388:LYS:HA	1:D:391:MET:HE2	1.60	0.83
1:C:522:VAL:HG21	1:C:528:LEU:HD22	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ILE:HG23	1:A:601:ARG:H	1.39	0.83
1:C:491:ASP:HB2	1:C:500:MET:HE1	1.58	0.83
1:D:501:GLU:CD	4:D:116:HOH:O	2.16	0.83
1:A:366:MET:O	1:A:651:GLN:N	2.11	0.83
3:C:802:ADP:O3A	4:C:37:HOH:O	1.95	0.82
1:B:357:PRO:CB	1:B:404:PRO:HB3	2.08	0.82
1:A:528:LEU:HG	1:A:532:MET:CE	2.09	0.82
1:B:449:GLU:O	4:B:41:HOH:O	1.96	0.81
1:B:542:ALA:HB3	1:B:549:ARG:HB2	1.60	0.81
1:C:319:ALA:HA	1:C:322:GLU:HG3	1.62	0.81
1:B:381:GLN:HB3	1:B:388:LYS:CD	2.11	0.81
1:B:440:LYS:NZ	1:B:583:GLY:HA2	1.97	0.80
1:B:388:LYS:HA	1:B:391:MET:SD	2.22	0.80
1:A:522:VAL:HG11	1:A:528:LEU:HD22	1.64	0.80
1:C:488:VAL:HA	4:C:49:HOH:O	1.82	0.80
1:B:398:PHE:HZ	1:B:661:LEU:HD22	1.47	0.80
1:D:380:LEU:HD23	1:D:394:GLN:HB3	1.64	0.79
1:D:418:LEU:CD1	1:D:642:LEU:HD13	2.13	0.79
1:C:369:THR:HB	1:C:381:GLN:HB2	1.65	0.79
1:C:623:ARG:HG3	1:C:623:ARG:HH11	1.47	0.79
1:B:380:LEU:CD2	1:B:394:GLN:HB3	2.13	0.79
1:D:440:LYS:HE3	3:D:803:ADP:O3B	1.83	0.79
1:B:539:ARG:HG2	1:B:541:THR:HG23	1.65	0.78
1:D:488:VAL:N	4:D:113:HOH:O	2.16	0.78
1:D:543:SER:HA	1:D:547:ASN:OD1	1.83	0.78
1:D:356:ARG:HG2	1:D:647:VAL:O	1.84	0.78
1:D:400:GLN:HG3	1:D:401:VAL:N	1.99	0.78
1:C:599:ILE:HG22	1:C:600:ASN:H	1.48	0.78
1:A:358:PRO:HB3	1:A:650:PHE:CZ	2.18	0.78
1:D:418:LEU:HD11	1:D:642:LEU:HD13	1.65	0.77
1:D:528:LEU:HG	1:D:532:MET:CE	2.14	0.77
1:D:599:ILE:HG22	1:D:600:ASN:N	1.97	0.77
1:D:528:LEU:HG	1:D:532:MET:HE2	1.65	0.77
1:C:445:ASP:OD1	4:C:107:HOH:O	2.01	0.77
1:A:418:LEU:CD1	1:A:642:LEU:HD13	2.15	0.77
1:C:440:LYS:HE3	3:C:802:ADP:O3B	1.85	0.77
1:C:317:GLN:HE22	1:D:318:ALA:HB2	1.46	0.76
1:B:650:PHE:HB2	1:B:653:CYS:SG	2.26	0.76
1:B:614:LEU:CD1	1:B:667:VAL:HG13	2.15	0.76
1:D:602:SER:HB2	4:D:70:HOH:O	1.87	0.75
1:D:566:ALA:N	4:D:74:HOH:O	1.79	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:ALA:HB3	1:C:549:ARG:HB3	1.67	0.75
1:C:418:LEU:CD1	1:C:642:LEU:HD13	2.17	0.75
1:B:394:GLN:N	4:B:33:HOH:O	2.16	0.74
1:D:454:ILE:HG23	1:D:578:LEU:HD13	1.69	0.74
1:A:537:MET:O	1:A:540:ALA:N	2.18	0.74
1:C:314:ASN:HB2	1:D:314:ASN:HD21	1.52	0.74
1:D:522:VAL:HG11	1:D:528:LEU:HD22	1.68	0.74
1:B:522:VAL:HG13	1:B:528:LEU:HB2	1.68	0.74
1:A:400:GLN:HG3	1:A:401:VAL:N	2.00	0.74
1:D:537:MET:C	1:D:539:ARG:H	1.90	0.73
1:C:585:GLU:HA	1:C:656:GLU:OE1	1.87	0.73
1:C:599:ILE:HG22	1:C:600:ASN:N	2.04	0.73
1:D:388:LYS:O	1:D:391:MET:HG2	1.88	0.73
1:C:542:ALA:N	1:C:550:SER:HB2	2.02	0.73
1:B:522:VAL:CG1	1:B:528:LEU:HB2	2.18	0.73
1:A:564:ARG:HG2	1:A:571:ILE:HG22	1.71	0.73
1:C:461:LEU:HD21	1:C:561:LEU:HD21	1.69	0.73
1:C:663:PHE:O	1:C:667:VAL:HG23	1.88	0.73
1:C:396:PHE:CD2	1:C:665:ALA:HB2	2.23	0.72
1:C:457:THR:O	1:C:461:LEU:HB2	1.87	0.72
1:C:622:TYR:CD1	1:C:632:MET:HG3	2.24	0.72
1:A:528:LEU:HG	1:A:532:MET:HE2	1.71	0.72
1:A:652:ASP:O	4:A:133:HOH:O	2.07	0.72
1:D:623:ARG:HH11	1:D:623:ARG:HG3	1.55	0.72
1:D:335:ARG:HH21	1:D:336:LYS:HA	1.55	0.72
1:C:520:GLU:HG3	1:C:531:LEU:HD21	1.72	0.71
1:A:522:VAL:HG21	1:A:528:LEU:HD22	1.71	0.71
1:D:515:SER:O	1:D:516:ASN:HB2	1.90	0.71
1:D:352:PHE:CZ	1:D:414:MET:HG3	2.26	0.71
1:D:486:ASN:C	4:D:113:HOH:O	2.27	0.71
1:D:358:PRO:O	4:D:80:HOH:O	2.09	0.71
1:A:517:ILE:H	1:A:517:ILE:HD12	1.56	0.71
1:A:418:LEU:HD11	1:A:642:LEU:CD1	2.20	0.71
1:C:486:ASN:N	4:C:111:HOH:O	2.00	0.71
1:A:358:PRO:HB3	1:A:650:PHE:CE2	2.26	0.70
1:C:346:ARG:HH11	1:C:346:ARG:HG3	1.56	0.70
1:D:651:GLN:N	4:D:121:HOH:O	2.23	0.70
1:A:547:ASN:C	1:A:549:ARG:H	1.93	0.70
1:B:537:MET:CE	1:B:537:MET:HA	2.21	0.70
1:D:614:LEU:HD11	1:D:667:VAL:HG13	1.73	0.70
1:B:528:LEU:HG	1:B:532:MET:HE2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ARG:HG3	1:B:623:ARG:HH11	1.57	0.69
1:A:542:ALA:CB	4:A:140:HOH:O	2.33	0.69
1:D:435:GLN:O	1:D:438:SER:OG	2.08	0.69
1:C:537:MET:C	1:C:539:ARG:H	1.95	0.69
1:A:357:PRO:HD3	1:A:404:PRO:HA	1.73	0.69
1:A:599:ILE:CG2	1:A:601:ARG:H	2.05	0.69
1:D:537:MET:HA	1:D:537:MET:CE	2.23	0.69
1:A:454:ILE:HB	1:A:455:PRO:HD3	1.74	0.69
1:A:321:LEU:HD23	1:A:321:LEU:C	2.13	0.69
1:C:528:LEU:HG	1:C:532:MET:HE3	1.75	0.69
1:D:403:HIS:O	1:D:405:LEU:N	2.25	0.69
1:D:433:TYR:CD2	1:D:433:TYR:C	2.66	0.69
1:D:367:CYS:HA	1:D:650:PHE:HA	1.74	0.68
1:C:440:LYS:NZ	1:C:583:GLY:HA2	2.08	0.68
1:C:387:ALA:O	1:C:391:MET:HG2	1.93	0.68
1:A:440:LYS:HZ3	1:A:583:GLY:HA2	1.59	0.68
1:C:528:LEU:HG	1:C:532:MET:CE	2.24	0.68
1:C:351:VAL:CG2	1:C:667:VAL:HG11	2.24	0.68
1:A:438:SER:HB2	1:A:646:ASN:HB2	1.75	0.68
1:D:548:GLU:OE2	1:D:552:ARG:HG3	1.92	0.68
1:D:380:LEU:O	1:D:394:GLN:HB2	1.93	0.68
1:C:623:ARG:CG	1:C:623:ARG:HH11	2.07	0.68
1:B:457:THR:O	1:B:461:LEU:HB2	1.92	0.68
1:C:400:GLN:HG3	1:C:401:VAL:N	2.07	0.68
1:D:543:SER:HA	1:D:547:ASN:CG	2.14	0.68
1:C:599:ILE:CG2	1:C:600:ASN:H	2.06	0.68
1:D:552:ARG:HH21	1:D:585:GLU:HG2	1.58	0.68
1:A:346:ARG:NH1	1:A:346:ARG:HG3	2.05	0.67
1:A:670:CYS:C	1:A:672:MET:H	1.97	0.67
1:D:522:VAL:HG13	1:D:528:LEU:HB2	1.77	0.67
1:A:586:SER:CB	1:A:587:PRO:HD2	2.25	0.67
1:C:306:ARG:HG3	1:C:310:LEU:HD12	1.77	0.67
1:B:541:THR:CB	1:B:550:SER:HB2	2.24	0.67
1:B:384:ASP:OD2	1:B:386:GLN:HB3	1.94	0.67
1:D:328:LEU:HD12	1:D:328:LEU:C	2.14	0.67
1:C:522:VAL:CG1	1:C:528:LEU:HB2	2.25	0.67
1:A:396:PHE:HA	4:A:100:HOH:O	1.94	0.67
1:D:358:PRO:HB3	1:D:650:PHE:CZ	2.30	0.67
1:C:321:LEU:HD13	1:D:321:LEU:HD13	1.76	0.67
1:C:307:THR:O	1:C:311:LEU:HB2	1.95	0.67
1:C:373:HIS:O	1:C:377:THR:HB	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:LEU:O	1:C:615:GLN:HG3	1.95	0.67
1:C:623:ARG:NH1	1:C:623:ARG:HG3	2.07	0.67
1:A:491:ASP:HB2	1:A:500:MET:CE	2.25	0.67
1:C:555:ALA:HB3	1:C:580:ASP:HB3	1.76	0.67
1:D:380:LEU:CD2	1:D:394:GLN:HB3	2.25	0.67
1:C:385:ALA:HA	1:C:388:LYS:HZ3	1.59	0.67
1:B:418:LEU:HD11	1:B:642:LEU:HD13	1.76	0.66
1:D:583:GLY:N	4:D:152:HOH:O	2.29	0.66
1:B:500:MET:CE	1:B:517:ILE:HA	2.25	0.66
1:B:393:GLN:C	4:B:33:HOH:O	2.34	0.66
1:A:321:LEU:HD12	1:B:321:LEU:CD2	2.25	0.66
1:A:485:TYR:CE1	1:A:549:ARG:HD2	2.31	0.66
1:B:393:GLN:OE1	1:B:393:GLN:HA	1.95	0.66
1:D:352:PHE:CZ	1:D:414:MET:CG	2.79	0.66
1:A:403:HIS:O	1:A:405:LEU:N	2.29	0.66
1:A:367:CYS:CB	4:A:94:HOH:O	2.41	0.66
1:D:383:ILE:HG22	1:D:383:ILE:O	1.95	0.65
1:A:542:ALA:HB1	4:A:142:HOH:O	1.97	0.65
1:B:555:ALA:HB3	1:B:580:ASP:HB3	1.78	0.65
1:A:485:TYR:HE1	1:A:549:ARG:HA	1.62	0.65
1:D:522:VAL:HG21	1:D:528:LEU:HD22	1.79	0.65
1:C:364:ASN:HD22	1:C:364:ASN:N	1.94	0.65
1:B:400:GLN:HG3	1:B:401:VAL:N	2.08	0.65
1:C:582:ALA:HB3	4:C:69:HOH:O	1.96	0.65
1:A:523:LEU:O	1:A:524:ASP:HB3	1.96	0.65
1:B:500:MET:HE1	1:B:517:ILE:HA	1.79	0.65
1:B:352:PHE:CD2	1:B:400:GLN:HB3	2.31	0.65
1:D:359:LEU:HA	4:D:90:HOH:O	1.96	0.65
1:C:486:ASN:ND2	1:C:599:ILE:HG13	2.12	0.65
1:C:650:PHE:HB2	1:C:653:CYS:SG	2.37	0.65
1:D:418:LEU:HD11	1:D:642:LEU:CD1	2.27	0.65
1:B:662:ARG:HG2	1:B:662:ARG:HH11	1.60	0.65
1:C:489:LEU:N	4:C:49:HOH:O	2.24	0.64
1:B:373:HIS:O	1:B:374:ASP:HB3	1.97	0.64
1:A:440:LYS:HE3	3:A:800:ADP:O3B	1.97	0.64
1:D:438:SER:HB2	1:D:646:ASN:HB2	1.79	0.64
1:B:522:VAL:HG11	1:B:528:LEU:HD22	1.79	0.64
1:B:346:ARG:HH11	1:B:346:ARG:HG3	1.63	0.64
1:D:356:ARG:HD2	1:D:438:SER:O	1.97	0.64
1:A:373:HIS:O	1:A:377:THR:HB	1.98	0.64
1:A:498:LYS:CB	4:A:52:HOH:O	2.34	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:LEU:HD13	1:D:321:LEU:CD1	2.28	0.64
1:D:436:THR:HG23	3:D:803:ADP:O1B	1.98	0.64
1:D:328:LEU:HD12	1:D:328:LEU:O	1.98	0.64
1:C:302:HIS:HD2	1:C:303:LEU:HD23	1.62	0.64
1:C:485:TYR:HB3	4:C:111:HOH:O	1.98	0.63
1:A:522:VAL:HG13	1:A:528:LEU:HB2	1.80	0.63
1:C:363:GLU:C	1:C:364:ASN:HD22	2.00	0.63
1:C:522:VAL:HG13	1:C:528:LEU:HB2	1.78	0.63
1:D:338:LEU:O	1:D:341:THR:N	2.32	0.63
1:D:487:GLU:N	4:D:113:HOH:O	2.30	0.63
1:B:528:LEU:HG	1:B:532:MET:CE	2.28	0.63
1:A:321:LEU:HD23	1:A:321:LEU:O	1.97	0.63
1:A:373:HIS:O	1:A:374:ASP:HB3	1.98	0.63
1:C:398:PHE:HZ	1:C:661:LEU:HD22	1.63	0.63
1:B:447:VAL:HG23	1:B:450:SER:H	1.63	0.63
1:A:335:ARG:NH2	1:A:424:ASP:OD2	2.32	0.63
1:D:537:MET:O	1:D:539:ARG:N	2.32	0.63
1:D:408:GLN:HG3	1:D:451:VAL:O	1.98	0.62
1:A:407:SER:N	1:A:410:ASP:OD2	2.32	0.62
1:C:387:ALA:HB1	1:C:391:MET:CE	2.29	0.62
1:D:381:GLN:HG2	1:D:391:MET:SD	2.39	0.62
1:D:336:LYS:HG2	1:D:337:GLU:N	2.13	0.62
1:A:478:LYS:HE2	1:A:521:THR:HG22	1.82	0.62
1:C:316:GLN:O	1:C:320:GLU:HB2	2.00	0.62
1:D:614:LEU:CD1	1:D:667:VAL:HG13	2.28	0.62
1:D:567:GLU:O	1:D:568:LYS:HB2	2.00	0.62
1:B:537:MET:HE2	1:B:537:MET:HA	1.82	0.62
1:A:367:CYS:CA	4:A:94:HOH:O	2.43	0.62
1:D:358:PRO:HB3	1:D:650:PHE:HZ	1.64	0.62
1:C:515:SER:O	1:C:516:ASN:HB2	2.00	0.62
1:D:520:GLU:HG3	1:D:531:LEU:HD21	1.82	0.62
1:C:554:HIS:CE1	4:C:69:HOH:O	2.40	0.62
1:C:603:LEU:HD22	4:C:69:HOH:O	1.99	0.62
1:B:485:TYR:HE1	1:B:549:ARG:HA	1.65	0.62
1:B:539:ARG:O	1:B:541:THR:N	2.33	0.62
1:D:366:MET:O	1:D:651:GLN:N	2.20	0.61
1:B:547:ASN:C	1:B:549:ARG:H	2.02	0.61
1:D:310:LEU:O	1:D:312:ARG:N	2.33	0.61
1:D:615:GLN:CG	1:D:670:CYS:SG	2.88	0.61
1:B:452:GLY:O	1:B:455:PRO:HD2	2.00	0.61
1:A:376:SER:HA	1:A:401:VAL:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ILE:H	1:A:411:ILE:HD12	1.65	0.61
1:A:514:VAL:O	1:A:517:ILE:HD11	2.00	0.61
1:A:500:MET:CE	1:A:517:ILE:HA	2.30	0.61
1:D:482:LEU:HD12	1:D:482:LEU:C	2.21	0.61
1:D:382:SER:C	1:D:384:ASP:H	2.04	0.61
1:C:482:LEU:C	1:C:482:LEU:HD12	2.21	0.61
1:C:665:ALA:O	1:C:668:ASN:ND2	2.34	0.61
1:D:501:GLU:OE2	4:D:116:HOH:O	2.16	0.61
1:D:383:ILE:CG2	1:D:383:ILE:O	2.48	0.61
1:A:436:THR:H	1:A:585:GLU:CD	2.04	0.61
1:C:352:PHE:HD2	1:C:400:GLN:HB3	1.66	0.61
1:C:379:GLU:HG3	1:C:394:GLN:O	2.01	0.61
1:B:388:LYS:NZ	1:B:388:LYS:HB3	2.16	0.60
1:D:356:ARG:O	1:D:649:PRO:HG3	2.01	0.60
1:D:536:LYS:O	1:D:539:ARG:HB3	2.01	0.60
1:C:346:ARG:NH1	1:C:346:ARG:HG3	2.16	0.60
1:C:352:PHE:CD2	1:C:400:GLN:HB3	2.36	0.60
1:A:323:THR:O	1:A:327:GLN:HB2	2.01	0.60
1:C:542:ALA:HB3	1:C:549:ARG:CB	2.32	0.60
1:C:381:GLN:HB3	4:C:82:HOH:O	1.99	0.60
1:A:517:ILE:H	1:A:517:ILE:CD1	2.12	0.60
1:D:381:GLN:HB3	1:D:391:MET:HE3	1.83	0.60
1:A:440:LYS:HE3	3:A:800:ADP:PB	2.41	0.60
1:B:523:LEU:O	1:B:524:ASP:HB3	2.00	0.60
1:D:477:ILE:N	4:D:110:HOH:O	2.30	0.60
1:A:500:MET:CE	1:A:517:ILE:HG23	2.31	0.60
1:B:520:GLU:HG3	1:B:531:LEU:HD21	1.84	0.60
1:A:520:GLU:HG3	1:A:531:LEU:HD21	1.83	0.60
1:D:569:GLN:HB3	4:D:148:HOH:O	1.96	0.60
1:B:357:PRO:HD3	1:B:404:PRO:CA	2.28	0.59
1:A:528:LEU:HG	1:A:532:MET:HE3	1.82	0.59
1:A:569:GLN:O	1:A:570:GLU:O	2.19	0.59
1:A:537:MET:CE	1:A:537:MET:HA	2.32	0.59
1:D:296:LEU:O	1:D:298:THR:N	2.35	0.59
1:A:324:CYS:O	1:A:328:LEU:N	2.35	0.59
1:A:517:ILE:N	1:A:517:ILE:HD12	2.17	0.59
1:C:315:GLU:O	1:C:318:ALA:HB3	2.01	0.59
1:D:537:MET:C	1:D:539:ARG:N	2.55	0.59
1:D:370:TRP:CZ3	1:D:380:LEU:HB3	2.37	0.59
1:C:310:LEU:O	1:C:311:LEU:C	2.40	0.59
1:D:370:TRP:CZ3	1:D:380:LEU:CB	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:ALA:HB1	1:C:391:MET:HE1	1.83	0.59
1:A:353:CYS:HB3	1:A:401:VAL:HG13	1.84	0.59
1:D:387:ALA:O	1:D:391:MET:HB3	2.03	0.59
1:A:352:PHE:CE1	1:A:414:MET:HG2	2.38	0.59
1:B:491:ASP:HB2	1:B:500:MET:HE1	1.85	0.59
1:A:349:ILE:HG22	1:A:349:ILE:O	2.03	0.59
1:D:380:LEU:HD23	1:D:394:GLN:CB	2.32	0.58
1:A:414:MET:CE	1:A:414:MET:HA	2.33	0.58
1:C:351:VAL:HG21	1:C:667:VAL:HG11	1.85	0.58
1:B:537:MET:C	1:B:539:ARG:H	2.06	0.58
1:C:599:ILE:CG2	1:C:600:ASN:N	2.66	0.58
1:B:369:THR:HB	1:B:381:GLN:HB2	1.84	0.58
1:C:403:HIS:O	1:C:405:LEU:N	2.37	0.58
1:D:414:MET:HA	1:D:414:MET:CE	2.33	0.58
1:C:481:PHE:CD1	1:C:481:PHE:N	2.70	0.58
1:D:623:ARG:HG3	1:D:623:ARG:NH1	2.17	0.58
1:C:350:ARG:HG3	4:C:87:HOH:O	2.04	0.58
1:D:658:VAL:O	1:D:662:ARG:HG3	2.04	0.58
1:B:364:ASN:N	1:B:364:ASN:HD22	2.00	0.58
1:A:586:SER:HB3	1:A:587:PRO:CD	2.30	0.58
1:D:599:ILE:CG2	1:D:600:ASN:H	1.97	0.58
1:D:382:SER:O	1:D:388:LYS:HD3	2.03	0.58
1:B:541:THR:HB	1:B:550:SER:HB2	1.85	0.58
1:A:435:GLN:HA	1:A:585:GLU:OE1	2.04	0.57
1:D:454:ILE:HG23	1:D:578:LEU:CD1	2.33	0.57
1:A:491:ASP:HB2	1:A:500:MET:HE1	1.86	0.57
1:D:489:LEU:HD11	1:D:626:LYS:HG3	1.86	0.57
1:C:537:MET:C	1:C:539:ARG:N	2.58	0.57
1:C:373:HIS:O	1:C:374:ASP:HB3	2.03	0.57
1:B:491:ASP:HB2	1:B:500:MET:CE	2.35	0.57
1:B:373:HIS:O	1:B:377:THR:HB	2.05	0.57
1:D:370:TRP:HZ3	1:D:380:LEU:HB3	1.70	0.57
1:D:434:GLY:O	1:D:440:LYS:NZ	2.37	0.57
1:C:360:GLU:OE1	1:C:360:GLU:N	2.36	0.57
1:B:614:LEU:HD13	1:B:667:VAL:O	2.05	0.57
1:B:380:LEU:HD23	1:B:394:GLN:CB	2.26	0.57
1:A:432:ALA:HB2	1:A:444:MET:HG2	1.86	0.57
1:B:480:THR:CG2	1:B:519:GLU:HG3	2.35	0.57
1:A:522:VAL:CG1	1:A:528:LEU:HB2	2.35	0.57
1:C:454:ILE:HG12	1:C:578:LEU:HD13	1.87	0.57
1:D:500:MET:CE	1:D:517:ILE:HG23	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:THR:OG1	1:D:521:THR:O	2.21	0.57
1:A:358:PRO:HB3	1:A:650:PHE:HZ	1.67	0.56
1:D:654:PHE:O	1:D:658:VAL:HG13	2.05	0.56
1:A:547:ASN:C	1:A:549:ARG:N	2.56	0.56
1:C:436:THR:HG23	3:C:802:ADP:O1B	2.05	0.56
1:D:366:MET:O	4:D:121:HOH:O	2.18	0.56
1:C:440:LYS:HE3	3:C:802:ADP:PB	2.45	0.56
1:D:398:PHE:HZ	1:D:661:LEU:HD22	1.69	0.56
1:B:416:SER:OG	1:B:417:PRO:HD3	2.05	0.56
1:D:367:CYS:HA	1:D:649:PRO:O	2.05	0.56
1:D:537:MET:HA	1:D:537:MET:HE2	1.87	0.56
1:A:396:PHE:HD2	1:A:665:ALA:HB2	1.70	0.56
1:D:527:HIS:NE2	1:D:531:LEU:HD11	2.21	0.56
1:C:454:ILE:HG23	1:C:578:LEU:HD13	1.86	0.56
1:D:457:THR:O	1:D:461:LEU:HB2	2.04	0.56
1:B:602:SER:HB2	4:B:68:HOH:O	2.05	0.56
1:A:427:ASN:HB3	1:A:634:SER:OG	2.05	0.56
1:D:543:SER:HA	1:D:547:ASN:CB	2.35	0.56
1:B:650:PHE:O	4:B:81:HOH:O	2.17	0.56
1:A:408:GLN:HA	1:A:408:GLN:OE1	2.06	0.56
1:C:317:GLN:O	1:C:321:LEU:HB2	2.06	0.56
1:A:486:ASN:HD21	1:A:599:ILE:HD13	1.70	0.56
1:D:522:VAL:CG1	1:D:528:LEU:HD22	2.36	0.56
1:C:569:GLN:O	1:C:570:GLU:O	2.24	0.56
1:D:607:THR:HG22	1:D:608:ASN:N	2.21	0.56
1:C:480:THR:HG22	1:C:519:GLU:HG3	1.86	0.56
1:A:436:THR:N	1:A:585:GLU:OE1	2.34	0.56
1:C:480:THR:CG2	1:C:519:GLU:HG3	2.35	0.56
1:C:655:GLN:O	1:C:658:VAL:HG22	2.05	0.56
1:C:314:ASN:HB2	1:D:314:ASN:ND2	2.20	0.56
1:C:364:ASN:N	1:C:364:ASN:ND2	2.52	0.56
1:B:380:LEU:O	1:B:381:GLN:HG3	2.06	0.56
1:C:545:ALA:C	1:C:547:ASN:H	2.09	0.56
1:D:352:PHE:CD2	1:D:400:GLN:HB3	2.40	0.56
1:D:634:SER:O	1:D:635:LEU:HD23	2.06	0.56
1:A:436:THR:HG23	3:A:800:ADP:O1B	2.05	0.55
1:B:522:VAL:HG22	1:B:528:LEU:HD13	1.88	0.55
1:D:355:ILE:HG22	1:D:404:PRO:HD3	1.88	0.55
1:A:436:THR:CB	1:A:585:GLU:OE2	2.54	0.55
1:D:376:SER:HA	1:D:401:VAL:HG23	1.88	0.55
1:A:328:LEU:O	1:A:328:LEU:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:556:VAL:HG22	1:C:579:VAL:HG22	1.88	0.55
1:B:366:MET:O	1:B:651:GLN:N	2.29	0.55
1:D:565:HIS:O	1:D:569:GLN:N	2.39	0.55
1:D:369:THR:HA	4:D:96:HOH:O	2.06	0.55
3:C:802:ADP:PA	4:C:37:HOH:O	2.61	0.55
1:C:444:MET:O	1:C:454:ILE:HG13	2.06	0.55
1:B:329:PHE:CE2	1:B:568:LYS:HE2	2.41	0.55
1:B:567:GLU:O	1:B:568:LYS:HB2	2.05	0.55
1:D:500:MET:CE	1:D:517:ILE:HA	2.37	0.55
1:A:435:GLN:OE1	1:A:656:GLU:HB2	2.06	0.55
1:D:652:ASP:OD1	4:D:121:HOH:O	2.18	0.55
1:A:522:VAL:CG1	1:A:528:LEU:HD22	2.34	0.55
1:B:444:MET:O	1:B:454:ILE:HG13	2.07	0.55
1:D:586:SER:HB3	1:D:587:PRO:HD2	1.87	0.55
1:B:543:SER:HA	1:B:547:ASN:HA	1.88	0.55
1:C:488:VAL:HB	4:C:111:HOH:O	2.07	0.55
1:D:369:THR:O	1:D:380:LEU:HA	2.07	0.55
1:C:469:ARG:NH1	1:C:474:GLU:OE2	2.40	0.55
1:C:411:ILE:H	1:C:411:ILE:HD12	1.71	0.54
1:B:393:GLN:O	1:B:394:GLN:HG2	2.06	0.54
1:C:537:MET:O	1:C:539:ARG:N	2.40	0.54
1:C:336:LYS:HE3	1:C:424:ASP:HB3	1.89	0.54
1:D:411:ILE:HG23	1:D:644:PHE:CZ	2.43	0.54
1:C:301:VAL:O	1:C:303:LEU:N	2.41	0.54
1:D:564:ARG:HG2	1:D:571:ILE:HG22	1.89	0.54
1:B:544:THR:HG23	1:B:545:ALA:H	1.72	0.54
1:A:545:ALA:O	1:A:546:GLY:C	2.46	0.54
1:D:622:TYR:CD1	1:D:632:MET:HG3	2.43	0.54
1:A:360:GLU:N	1:A:360:GLU:OE1	2.40	0.54
1:D:385:ALA:N	4:D:83:HOH:O	2.40	0.54
1:D:650:PHE:HB2	1:D:653:CYS:SG	2.47	0.54
1:C:398:PHE:CE2	1:C:664:ALA:HB1	2.42	0.54
1:D:397:SER:N	4:D:25:HOH:O	1.73	0.54
1:D:399:ASP:O	1:D:400:GLN:HB2	2.08	0.54
1:B:482:LEU:HD12	1:B:482:LEU:C	2.28	0.54
1:A:515:SER:O	1:A:516:ASN:HB2	2.08	0.54
1:D:522:VAL:CG1	1:D:528:LEU:HB2	2.37	0.54
1:C:324:CYS:SG	1:D:325:LYS:HG2	2.48	0.54
1:A:432:ALA:O	1:A:581:LEU:HB2	2.07	0.54
1:B:414:MET:HA	1:B:414:MET:CE	2.37	0.54
1:D:308:GLU:O	1:D:312:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ILE:HG12	1:B:647:VAL:HG23	1.90	0.54
1:C:564:ARG:HG2	1:C:571:ILE:HG22	1.90	0.54
1:A:530:HIS:O	1:A:533:HIS:N	2.41	0.54
1:D:599:ILE:O	1:D:601:ARG:N	2.41	0.54
1:B:347:GLY:O	1:B:348:ASN:CB	2.51	0.54
1:A:321:LEU:HD12	1:B:321:LEU:HD21	1.88	0.54
1:D:346:ARG:HG3	1:D:346:ARG:HH11	1.73	0.54
1:A:542:ALA:C	1:A:544:THR:N	2.61	0.53
1:D:491:ASP:OD1	1:D:493:LEU:N	2.26	0.53
1:A:435:GLN:CA	1:A:585:GLU:OE1	2.56	0.53
1:D:433:TYR:HD2	1:D:433:TYR:C	2.11	0.53
1:A:364:ASN:HD22	1:A:364:ASN:N	2.04	0.53
1:B:607:THR:HG23	1:B:663:PHE:CE1	2.44	0.53
1:B:333:MET:O	1:B:336:LYS:HB3	2.09	0.53
1:D:396:PHE:HA	4:D:25:HOH:O	2.09	0.53
1:D:346:ARG:NH1	1:D:346:ARG:HG3	2.24	0.53
1:A:428:ILE:HG22	1:A:429:CYS:N	2.24	0.53
1:B:522:VAL:HG21	1:B:528:LEU:HD22	1.90	0.53
1:D:364:ASN:N	1:D:364:ASN:HD22	2.07	0.53
1:B:622:TYR:CD1	1:B:632:MET:HG3	2.44	0.53
1:A:432:ALA:HB1	1:A:440:LYS:HB3	1.91	0.53
1:D:611:LEU:O	1:D:615:GLN:HG3	2.08	0.53
1:D:352:PHE:CZ	1:D:414:MET:HG2	2.43	0.53
1:A:500:MET:HE1	1:A:517:ILE:CG2	2.39	0.53
1:A:352:PHE:CE1	1:A:414:MET:CG	2.92	0.53
1:A:526:ASN:O	1:A:529:ARG:N	2.42	0.53
1:A:599:ILE:HG23	1:A:601:ARG:N	2.18	0.53
1:A:440:LYS:HZ1	1:A:583:GLY:HA2	1.74	0.53
1:D:537:MET:HA	1:D:537:MET:HE3	1.90	0.53
1:C:329:PHE:HD2	1:C:330:GLN:OE1	1.92	0.53
1:B:442:TYR:O	1:B:446:GLY:HA2	2.08	0.53
1:B:379:GLU:HG3	1:B:394:GLN:O	2.09	0.52
1:D:565:HIS:O	1:D:569:GLN:O	2.27	0.52
1:D:347:GLY:O	1:D:348:ASN:CB	2.43	0.52
1:A:542:ALA:C	1:A:544:THR:H	2.11	0.52
1:D:653:CYS:O	1:D:656:GLU:N	2.37	0.52
1:D:500:MET:HE1	1:D:517:ILE:CG2	2.39	0.52
1:A:599:ILE:HG22	1:A:601:ARG:HB2	1.92	0.52
1:A:355:ILE:HG12	1:A:647:VAL:HG23	1.91	0.52
1:B:384:ASP:OD1	1:B:387:ALA:HB2	2.10	0.52
1:D:300:VAL:HG12	1:D:304:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ILE:HG23	1:B:644:PHE:CZ	2.44	0.52
1:D:356:ARG:HG3	1:D:649:PRO:HD3	1.90	0.52
1:D:382:SER:O	1:D:384:ASP:N	2.43	0.52
1:B:533:HIS:CE1	4:B:138:HOH:O	2.63	0.52
1:A:500:MET:HE1	1:A:517:ILE:HG23	1.90	0.52
1:D:500:MET:HE1	1:D:517:ILE:HG23	1.91	0.52
1:C:514:VAL:O	1:C:517:ILE:HD11	2.09	0.52
1:C:622:TYR:CG	1:C:632:MET:HG3	2.45	0.52
1:D:514:VAL:O	1:D:517:ILE:HD11	2.10	0.52
1:C:347:GLY:O	1:C:348:ASN:CB	2.51	0.52
1:B:418:LEU:CD1	1:B:642:LEU:HD13	2.39	0.52
1:C:665:ALA:HA	1:C:668:ASN:ND2	2.25	0.51
1:B:485:TYR:HD1	1:B:549:ARG:NH1	2.08	0.51
1:B:547:ASN:C	1:B:549:ARG:N	2.63	0.51
1:D:444:MET:O	1:D:454:ILE:HG13	2.10	0.51
1:B:454:ILE:HB	1:B:455:PRO:HD3	1.92	0.51
1:C:407:SER:N	1:C:410:ASP:OD2	2.41	0.51
1:C:507:ASN:O	1:C:508:ASN:HB2	2.09	0.51
1:C:542:ALA:CA	1:C:545:ALA:HB3	2.32	0.51
1:C:517:ILE:HD12	1:C:517:ILE:N	2.25	0.51
1:D:599:ILE:C	1:D:601:ARG:H	2.13	0.51
1:D:663:PHE:O	1:D:667:VAL:HG23	2.11	0.51
1:A:599:ILE:HG23	1:A:600:ASN:N	2.24	0.51
1:B:507:ASN:O	1:B:508:ASN:HB2	2.09	0.51
1:B:388:LYS:HZ3	1:B:388:LYS:HB3	1.76	0.51
1:C:380:LEU:C	1:C:381:GLN:HG3	2.31	0.51
1:C:445:ASP:CG	4:C:107:HOH:O	2.47	0.51
1:A:622:TYR:CD1	1:A:632:MET:HG3	2.45	0.51
1:D:526:ASN:O	1:D:529:ARG:N	2.43	0.51
1:A:352:PHE:CE2	1:A:399:ASP:HB2	2.45	0.51
1:D:407:SER:N	1:D:410:ASP:OD2	2.44	0.51
1:B:379:GLU:HG3	1:B:394:GLN:C	2.30	0.51
1:A:363:GLU:C	1:A:364:ASN:HD22	2.14	0.51
1:B:408:GLN:HB2	1:B:456:ARG:HH21	1.76	0.51
1:D:368:CYS:SG	1:D:654:PHE:HD1	2.33	0.51
1:B:544:THR:HG23	1:B:545:ALA:N	2.26	0.51
1:B:484:ILE:HD12	1:B:627:LEU:HD13	1.93	0.51
1:A:334:GLU:OE1	1:B:335:ARG:HD2	2.11	0.51
1:B:548:GLU:O	1:B:552:ARG:HB2	2.10	0.51
1:A:653:CYS:O	1:A:654:PHE:C	2.49	0.51
1:A:547:ASN:CG	1:A:547:ASN:O	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:TYR:CD2	1:D:434:GLY:N	2.79	0.51
1:B:461:LEU:HD21	1:B:561:LEU:HD21	1.92	0.51
1:B:517:ILE:N	1:B:517:ILE:HD12	2.25	0.51
1:D:354:ARG:O	1:D:646:ASN:HA	2.11	0.51
1:B:539:ARG:HG2	1:B:541:THR:CG2	2.39	0.51
1:C:296:LEU:HD21	1:D:296:LEU:HD22	1.93	0.51
1:D:370:TRP:CZ3	1:D:380:LEU:HB2	2.45	0.50
1:B:623:ARG:HG3	1:B:623:ARG:NH1	2.21	0.50
1:B:514:VAL:O	1:B:517:ILE:HD11	2.11	0.50
1:D:411:ILE:H	1:D:411:ILE:HD12	1.76	0.50
1:D:631:LEU:O	1:D:632:MET:C	2.50	0.50
1:B:542:ALA:HB3	1:B:549:ARG:CB	2.38	0.50
1:D:310:LEU:C	1:D:312:ARG:N	2.63	0.50
1:C:433:TYR:C	1:C:433:TYR:CD2	2.84	0.50
1:C:442:TYR:O	1:C:446:GLY:HA2	2.11	0.50
1:B:440:LYS:HE3	3:B:801:ADP:PB	2.52	0.50
1:D:436:THR:OG1	1:D:585:GLU:OE2	2.29	0.50
1:D:296:LEU:C	1:D:296:LEU:HD23	2.31	0.50
1:B:552:ARG:HD2	1:B:599:ILE:N	2.26	0.50
1:B:403:HIS:HB2	1:B:404:PRO:HD2	1.93	0.50
1:A:585:GLU:HA	1:A:656:GLU:OE1	2.11	0.50
1:A:567:GLU:O	1:A:568:LYS:HB2	2.12	0.50
1:C:496:GLU:HG2	1:C:496:GLU:O	2.12	0.50
1:B:611:LEU:O	1:B:615:GLN:HG3	2.12	0.50
1:A:536:LYS:O	1:A:539:ARG:HB3	2.12	0.50
1:B:543:SER:HB2	1:B:547:ASN:ND2	2.26	0.50
1:B:380:LEU:C	1:B:381:GLN:HG3	2.32	0.50
1:A:498:LYS:N	4:A:52:HOH:O	2.42	0.50
1:C:319:ALA:C	1:C:321:LEU:N	2.65	0.50
1:C:367:CYS:HA	1:C:650:PHE:HA	1.93	0.50
1:D:478:LYS:HE2	1:D:521:THR:HG22	1.94	0.50
1:B:481:PHE:N	1:B:481:PHE:CD1	2.79	0.50
1:A:435:GLN:OE1	1:A:656:GLU:CB	2.59	0.50
1:B:522:VAL:HG11	1:B:528:LEU:HB2	1.93	0.50
1:C:388:LYS:NZ	1:C:388:LYS:HB3	2.26	0.50
1:D:299:GLU:O	1:D:302:HIS:N	2.45	0.50
1:D:408:GLN:HA	1:D:408:GLN:OE1	2.12	0.50
1:C:564:ARG:HG2	1:C:571:ILE:CG2	2.42	0.50
1:B:437:GLY:N	3:B:801:ADP:O1B	2.40	0.50
1:D:485:TYR:CD1	1:D:549:ARG:NH1	2.79	0.50
1:B:384:ASP:HB3	1:B:387:ALA:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ILE:H	1:B:517:ILE:HD12	1.77	0.49
1:B:604:SER:O	1:B:607:THR:HB	2.12	0.49
1:A:433:TYR:C	1:A:433:TYR:CD2	2.84	0.49
1:B:533:HIS:O	1:B:534:THR:C	2.48	0.49
1:C:369:THR:CB	1:C:381:GLN:HB2	2.40	0.49
1:A:503:ARG:HD3	1:A:513:TYR:CE2	2.47	0.49
1:B:657:SER:O	1:B:661:LEU:HG	2.12	0.49
1:B:522:VAL:CG2	1:B:528:LEU:HD13	2.42	0.49
1:B:364:ASN:N	1:B:364:ASN:ND2	2.60	0.49
1:C:485:TYR:CE1	1:C:549:ARG:HD2	2.47	0.49
1:C:662:ARG:HH11	1:C:662:ARG:HG2	1.77	0.49
1:C:654:PHE:O	1:C:658:VAL:HG13	2.12	0.49
1:B:662:ARG:HG2	1:B:662:ARG:NH1	2.24	0.49
1:C:432:ALA:HB2	1:C:444:MET:HG2	1.95	0.49
1:B:433:TYR:C	1:B:433:TYR:CD2	2.86	0.49
1:B:537:MET:C	1:B:539:ARG:N	2.65	0.49
1:D:454:ILE:HB	1:D:455:PRO:HD3	1.94	0.49
1:C:481:PHE:HD1	1:C:481:PHE:N	2.09	0.49
1:A:503:ARG:HD3	1:A:513:TYR:HE2	1.78	0.49
1:A:548:GLU:O	1:A:552:ARG:HB2	2.12	0.49
1:B:469:ARG:HD3	1:B:474:GLU:OE1	2.12	0.49
1:A:536:LYS:NZ	1:A:539:ARG:HH11	2.11	0.49
1:C:351:VAL:HG23	1:C:667:VAL:HG11	1.94	0.49
1:B:363:GLU:C	1:B:364:ASN:HD22	2.16	0.49
1:B:469:ARG:NH1	1:B:474:GLU:OE2	2.46	0.49
1:A:346:ARG:CG	1:A:346:ARG:NH1	2.70	0.49
1:C:380:LEU:O	1:C:381:GLN:HG3	2.13	0.49
1:C:537:MET:HA	1:C:537:MET:CE	2.43	0.49
1:D:653:CYS:O	1:D:654:PHE:C	2.51	0.49
1:A:522:VAL:CG2	1:A:528:LEU:HD22	2.39	0.49
1:B:521:THR:OG1	1:B:521:THR:O	2.28	0.49
1:A:357:PRO:HD3	1:A:404:PRO:CA	2.42	0.48
1:B:432:ALA:O	1:B:581:LEU:HB2	2.12	0.48
1:B:411:ILE:HD12	1:B:411:ILE:H	1.78	0.48
1:D:606:LEU:HD13	1:D:606:LEU:C	2.33	0.48
1:A:383:ILE:CG2	1:A:383:ILE:O	2.60	0.48
1:B:539:ARG:NH2	4:B:67:HOH:O	2.46	0.48
1:D:583:GLY:HA3	1:D:585:GLU:OE2	2.14	0.48
1:C:370:TRP:CZ2	1:C:649:PRO:HA	2.48	0.48
1:C:299:GLU:O	1:C:300:VAL:C	2.52	0.48
1:D:603:LEU:O	1:D:603:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:LEU:HD12	1:D:642:LEU:HD13	1.94	0.48
1:A:352:PHE:HE2	1:A:399:ASP:HB2	1.78	0.48
1:C:651:GLN:O	1:C:654:PHE:CB	2.61	0.48
1:B:346:ARG:NH1	1:B:346:ARG:HG3	2.25	0.48
1:B:454:ILE:HG23	1:B:578:LEU:HD13	1.95	0.48
1:C:508:ASN:ND2	4:C:58:HOH:O	2.45	0.48
1:B:429:CYS:SG	1:B:634:SER:HB3	2.53	0.48
1:D:430:ILE:HD13	1:D:430:ILE:N	2.28	0.48
1:B:328:LEU:HD12	1:B:328:LEU:O	2.14	0.48
1:A:527:HIS:O	1:A:527:HIS:HD2	1.96	0.48
1:B:537:MET:O	1:B:539:ARG:N	2.46	0.48
1:D:602:SER:O	1:D:605:GLU:N	2.46	0.48
1:B:515:SER:O	1:B:516:ASN:HB2	2.14	0.48
1:C:485:TYR:HE1	1:C:549:ARG:HA	1.77	0.48
1:B:440:LYS:HZ3	1:B:583:GLY:HA2	1.77	0.48
1:A:365:ARG:NH1	1:A:650:PHE:CD1	2.82	0.48
1:D:654:PHE:CD2	1:D:655:GLN:N	2.82	0.48
1:C:316:GLN:O	1:C:320:GLU:CB	2.61	0.48
1:D:527:HIS:CD2	1:D:527:HIS:O	2.66	0.48
1:B:428:ILE:HG22	1:B:429:CYS:N	2.28	0.48
1:A:485:TYR:CD1	1:A:549:ARG:HD2	2.48	0.48
1:A:599:ILE:HG22	1:A:601:ARG:CB	2.43	0.48
1:D:486:ASN:O	1:D:487:GLU:HB2	2.13	0.48
1:C:522:VAL:HG11	1:C:528:LEU:HB2	1.96	0.48
1:D:542:ALA:HB3	1:D:549:ARG:HB3	1.96	0.48
1:A:653:CYS:O	1:A:655:GLN:N	2.47	0.48
1:A:564:ARG:HG2	1:A:571:ILE:CG2	2.41	0.48
1:B:452:GLY:C	1:B:455:PRO:HD2	2.33	0.48
1:A:623:ARG:HH11	1:A:623:ARG:HG3	1.78	0.48
1:D:370:TRP:HE1	1:D:649:PRO:CB	2.27	0.48
1:A:605:GLU:HA	1:A:608:ASN:HD22	1.79	0.48
1:C:469:ARG:HD3	1:C:474:GLU:OE1	2.14	0.47
1:B:355:ILE:HG12	1:B:647:VAL:CG2	2.43	0.47
1:A:486:ASN:O	1:A:487:GLU:HB2	2.14	0.47
1:B:398:PHE:CZ	1:B:661:LEU:HD22	2.38	0.47
1:D:522:VAL:HG11	1:D:528:LEU:CD2	2.42	0.47
1:A:613:LEU:O	1:A:616:LYS:N	2.36	0.47
1:A:447:VAL:HG23	1:A:450:SER:H	1.80	0.47
1:A:367:CYS:O	1:A:651:GLN:HB2	2.15	0.47
1:C:651:GLN:O	1:C:654:PHE:HB3	2.14	0.47
1:A:347:GLY:O	1:A:348:ASN:CB	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:ASP:O	1:D:400:GLN:CB	2.61	0.47
1:D:310:LEU:C	1:D:312:ARG:H	2.17	0.47
1:C:324:CYS:SG	1:D:324:CYS:SG	3.09	0.47
1:A:651:GLN:O	1:A:654:PHE:HB3	2.15	0.47
1:B:399:ASP:O	1:B:400:GLN:HB2	2.14	0.47
1:C:303:LEU:HD12	1:D:303:LEU:HB2	1.96	0.47
1:C:350:ARG:CG	4:C:87:HOH:O	2.60	0.47
1:D:378:VAL:HG22	1:D:379:GLU:N	2.30	0.47
1:A:537:MET:C	1:A:539:ARG:N	2.67	0.47
1:D:548:GLU:O	1:D:552:ARG:HB2	2.14	0.47
1:D:491:ASP:OD1	1:D:491:ASP:C	2.50	0.47
1:D:365:ARG:O	4:D:95:HOH:O	2.20	0.47
1:B:396:PHE:CG	1:B:661:LEU:HB3	2.50	0.47
1:B:360:GLU:OE1	1:B:360:GLU:N	2.46	0.47
1:D:496:GLU:O	1:D:496:GLU:HG2	2.15	0.47
1:B:320:GLU:OE2	1:B:323:THR:HB	2.15	0.47
1:A:670:CYS:O	1:A:672:MET:N	2.47	0.47
1:A:606:LEU:HD13	1:A:606:LEU:C	2.35	0.47
1:D:485:TYR:CE1	1:D:549:ARG:HD2	2.50	0.47
1:A:656:GLU:O	1:A:659:LYS:N	2.48	0.47
1:C:500:MET:CE	1:C:517:ILE:HA	2.45	0.47
1:B:352:PHE:CZ	1:B:414:MET:HG3	2.50	0.47
1:D:359:LEU:HB2	1:D:362:GLU:OE1	2.15	0.47
1:B:426:TYR:CD2	1:B:638:ASN:HB3	2.50	0.47
1:D:370:TRP:N	4:D:96:HOH:O	1.98	0.47
1:C:454:ILE:HG23	1:C:578:LEU:CD1	2.45	0.47
1:D:373:HIS:O	1:D:374:ASP:HB3	2.14	0.47
1:A:614:LEU:CD1	1:A:667:VAL:HG13	2.45	0.47
1:D:480:THR:HG22	1:D:519:GLU:HG3	1.95	0.47
1:C:486:ASN:HD21	1:C:599:ILE:HG13	1.81	0.46
1:B:353:CYS:HB2	1:B:398:PHE:CD2	2.50	0.46
1:C:370:TRP:HZ2	1:C:649:PRO:HA	1.81	0.46
1:C:567:GLU:O	1:C:568:LYS:HB2	2.15	0.46
1:A:527:HIS:CD2	1:A:527:HIS:O	2.68	0.46
1:A:623:ARG:HG3	1:A:623:ARG:NH1	2.30	0.46
1:C:447:VAL:HG23	1:C:450:SER:H	1.79	0.46
1:D:488:VAL:HB	4:D:113:HOH:O	2.15	0.46
1:C:321:LEU:O	1:C:322:GLU:C	2.52	0.46
1:A:547:ASN:HD21	1:A:551:SER:HB3	1.80	0.46
1:C:536:LYS:O	1:C:539:ARG:HB3	2.16	0.46
1:C:556:VAL:O	1:C:556:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:SER:H	1:D:391:MET:HE1	1.80	0.46
1:D:382:SER:C	1:D:384:ASP:N	2.69	0.46
1:A:522:VAL:HG22	1:A:528:LEU:HD13	1.96	0.46
1:A:517:ILE:N	1:A:517:ILE:CD1	2.78	0.46
1:D:360:GLU:OE1	1:D:360:GLU:N	2.48	0.46
1:C:462:PHE:CZ	1:C:477:ILE:HD12	2.50	0.46
1:D:416:SER:OG	1:D:417:PRO:HD3	2.15	0.46
1:A:442:TYR:O	1:A:446:GLY:HA2	2.15	0.46
1:C:514:VAL:HG12	1:C:517:ILE:HG13	1.97	0.46
1:C:387:ALA:O	1:C:390:LYS:N	2.48	0.46
1:A:321:LEU:HD21	1:A:325:LYS:HD2	1.96	0.46
1:A:336:LYS:HE3	1:A:424:ASP:O	2.14	0.46
1:A:433:TYR:CD2	1:A:434:GLY:N	2.84	0.46
1:A:536:LYS:HZ1	1:A:539:ARG:NH1	2.14	0.46
1:B:382:SER:C	1:B:384:ASP:H	2.18	0.46
1:C:385:ALA:HA	1:C:388:LYS:NZ	2.28	0.46
1:A:364:ASN:ND2	1:A:364:ASN:N	2.64	0.46
1:B:526:ASN:O	1:B:529:ARG:N	2.49	0.46
1:D:382:SER:H	1:D:391:MET:CE	2.29	0.46
1:A:536:LYS:NZ	1:A:539:ARG:NH1	2.63	0.46
1:D:522:VAL:CG2	1:D:528:LEU:HD22	2.44	0.46
1:D:328:LEU:CD1	1:D:328:LEU:C	2.82	0.46
1:D:296:LEU:C	1:D:298:THR:H	2.17	0.46
1:C:435:GLN:OE1	1:C:656:GLU:CB	2.63	0.46
1:D:491:ASP:HB2	1:D:500:MET:HE1	1.97	0.46
1:B:359:LEU:N	1:B:362:GLU:OE1	2.41	0.46
1:D:337:GLU:OE1	1:D:337:GLU:HA	2.16	0.46
1:D:296:LEU:C	1:D:298:THR:N	2.70	0.46
1:C:454:ILE:CG1	1:C:578:LEU:HD13	2.46	0.46
1:D:373:HIS:CD2	1:D:395:ILE:HD11	2.51	0.46
1:A:631:LEU:O	1:A:632:MET:C	2.55	0.46
1:B:350:ARG:NE	4:B:88:HOH:O	2.49	0.46
1:D:533:HIS:O	1:D:534:THR:C	2.52	0.46
1:A:543:SER:HA	1:A:547:ASN:HB2	1.96	0.46
1:C:433:TYR:HB2	1:C:581:LEU:HD12	1.98	0.46
1:A:432:ALA:CB	1:A:440:LYS:HB3	2.46	0.45
1:B:541:THR:HG21	1:B:550:SER:CB	2.46	0.45
1:B:353:CYS:HB2	1:B:398:PHE:CE2	2.52	0.45
1:D:352:PHE:CE2	1:D:400:GLN:HB3	2.51	0.45
1:C:296:LEU:HD23	1:C:297:SER:N	2.31	0.45
1:A:607:THR:HG22	1:A:608:ASN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:LEU:HD21	1:D:296:LEU:CD2	2.46	0.45
1:A:599:ILE:CG2	1:A:601:ARG:HB2	2.45	0.45
1:D:536:LYS:NZ	1:D:539:ARG:NH1	2.64	0.45
1:A:343:MET:HE3	1:A:417:PRO:HB3	1.98	0.45
1:B:403:HIS:O	1:B:405:LEU:N	2.49	0.45
1:B:501:GLU:O	1:B:514:VAL:HA	2.17	0.45
1:C:428:ILE:HG22	1:C:429:CYS:N	2.32	0.45
1:A:615:GLN:O	1:A:617:GLN:N	2.49	0.45
1:C:416:SER:OG	1:C:417:PRO:HD3	2.16	0.45
1:B:437:GLY:H	3:B:801:ADP:PB	2.38	0.45
1:B:534:THR:O	1:B:537:MET:N	2.49	0.45
1:D:580:ASP:OD1	1:D:580:ASP:C	2.55	0.45
1:D:547:ASN:C	1:D:549:ARG:H	2.20	0.45
1:B:438:SER:N	3:B:801:ADP:O2B	2.50	0.45
1:D:643:MET:CE	1:D:663:PHE:HE2	2.30	0.45
1:A:611:LEU:O	1:A:615:GLN:HG3	2.16	0.45
1:B:470:ASN:OD1	4:B:46:HOH:O	2.21	0.45
1:D:380:LEU:O	1:D:394:GLN:CB	2.64	0.45
1:C:387:ALA:HB1	1:C:391:MET:HE3	1.98	0.45
1:D:403:HIS:N	1:D:406:SER:OG	2.50	0.45
1:A:440:LYS:HE3	3:A:800:ADP:O2B	2.17	0.45
1:C:500:MET:CE	1:C:517:ILE:HG23	2.47	0.45
1:D:398:PHE:C	1:D:400:GLN:H	2.20	0.45
1:D:355:ILE:CG2	1:D:404:PRO:HD3	2.45	0.45
1:B:352:PHE:CZ	1:B:414:MET:CG	3.00	0.45
1:C:304:ARG:O	1:C:308:GLU:HG2	2.16	0.45
1:D:485:TYR:CD1	1:D:549:ARG:HD2	2.52	0.45
1:D:549:ARG:HG3	1:D:550:SER:N	2.32	0.45
1:A:357:PRO:HB3	1:A:404:PRO:HB3	1.99	0.45
1:A:522:VAL:HG11	1:A:528:LEU:CD2	2.41	0.45
1:B:487:GLU:O	1:B:626:LYS:NZ	2.47	0.45
1:A:398:PHE:CE2	1:A:664:ALA:CB	3.00	0.45
1:C:383:ILE:O	1:C:383:ILE:CG2	2.64	0.45
1:A:541:THR:C	1:A:543:SER:H	2.21	0.45
1:A:352:PHE:CZ	1:A:414:MET:CG	3.00	0.45
1:D:360:GLU:O	1:D:363:GLU:HG3	2.17	0.45
1:C:302:HIS:CD2	1:C:303:LEU:HD23	2.49	0.45
1:B:380:LEU:HD21	1:B:658:VAL:HG12	1.99	0.44
1:B:388:LYS:NZ	1:B:388:LYS:CB	2.80	0.44
1:C:632:MET:N	1:C:633:PRO:HD2	2.32	0.44
1:D:512:ILE:HG23	1:D:513:TYR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:TYR:HD2	1:D:486:ASN:HB2	1.82	0.44
1:A:396:PHE:CA	4:A:100:HOH:O	2.61	0.44
1:B:352:PHE:CE2	1:B:400:GLN:HB3	2.52	0.44
1:A:374:ASP:OD2	1:A:375:GLU:N	2.50	0.44
1:B:324:CYS:O	1:B:327:GLN:N	2.47	0.44
1:C:567:GLU:HG2	1:C:567:GLU:O	2.17	0.44
1:A:539:ARG:C	1:A:541:THR:N	2.67	0.44
1:D:339:HIS:CD2	1:D:339:HIS:C	2.90	0.44
1:B:486:ASN:ND2	1:B:599:ILE:HG13	2.32	0.44
1:B:394:GLN:HE21	1:B:654:PHE:HZ	1.64	0.44
1:A:440:LYS:O	1:A:443:THR:N	2.50	0.44
1:C:367:CYS:HA	1:C:649:PRO:O	2.17	0.44
1:C:388:LYS:HZ3	1:C:388:LYS:HB3	1.83	0.44
1:A:632:MET:HB3	1:A:633:PRO:CD	2.48	0.44
1:C:523:LEU:O	1:C:524:ASP:HB3	2.17	0.44
1:B:579:VAL:HG21	1:B:631:LEU:HD11	1.98	0.44
1:B:383:ILE:O	1:B:383:ILE:CG2	2.66	0.44
1:D:656:GLU:O	1:D:659:LYS:N	2.50	0.44
1:B:485:TYR:CD1	1:B:549:ARG:NH1	2.85	0.44
1:B:517:ILE:H	1:B:517:ILE:CD1	2.31	0.44
1:D:377:THR:HA	1:D:397:SER:HA	2.00	0.44
1:C:376:SER:HA	1:C:401:VAL:HG23	1.99	0.44
1:A:482:LEU:C	1:A:482:LEU:HD12	2.38	0.44
1:B:605:GLU:HG3	1:B:625:SER:HB3	1.99	0.44
1:C:640:LYS:N	1:C:640:LYS:HD2	2.33	0.44
1:B:564:ARG:HG2	1:B:571:ILE:HG22	1.99	0.44
1:C:501:GLU:O	1:C:514:VAL:HA	2.18	0.44
1:B:486:ASN:ND2	1:B:599:ILE:CG1	2.80	0.44
1:A:430:ILE:HD13	1:A:430:ILE:N	2.32	0.43
1:A:380:LEU:HD21	1:A:658:VAL:HG12	2.00	0.43
1:A:537:MET:C	1:A:539:ARG:H	2.20	0.43
1:A:670:CYS:C	1:A:672:MET:N	2.65	0.43
1:B:599:ILE:HG22	1:B:601:ARG:H	1.83	0.43
1:D:512:ILE:HD12	1:D:512:ILE:HA	1.73	0.43
1:C:357:PRO:HB3	1:C:404:PRO:HB3	2.00	0.43
1:A:359:LEU:HB2	1:A:362:GLU:OE1	2.17	0.43
1:C:658:VAL:HG23	1:C:659:LYS:N	2.33	0.43
1:A:449:GLU:CD	1:A:449:GLU:H	2.22	0.43
1:D:400:GLN:HG2	1:D:402:PHE:CE1	2.53	0.43
1:D:528:LEU:HG	1:D:532:MET:HE3	1.98	0.43
1:A:399:ASP:O	1:A:400:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:MET:HE1	1:D:517:ILE:HA	1.99	0.43
1:A:512:ILE:HD12	1:A:512:ILE:HA	1.78	0.43
1:D:329:PHE:C	1:D:329:PHE:CD2	2.91	0.43
1:A:356:ARG:O	1:A:649:PRO:HG3	2.18	0.43
1:C:313:CYS:O	1:C:317:GLN:HG3	2.19	0.43
1:D:363:GLU:C	1:D:364:ASN:HD22	2.21	0.43
1:C:301:VAL:O	1:C:302:HIS:C	2.57	0.43
1:D:308:GLU:O	1:D:309:GLU:C	2.57	0.43
1:B:486:ASN:HD21	1:B:599:ILE:HD11	1.83	0.43
1:D:496:GLU:O	1:D:497:GLN:C	2.57	0.43
1:A:461:LEU:HD11	1:A:561:LEU:HD11	2.01	0.43
1:C:517:ILE:HD12	1:C:517:ILE:H	1.82	0.43
1:D:643:MET:HE2	1:D:663:PHE:HE2	1.84	0.43
1:A:543:SER:HA	1:A:547:ASN:OD1	2.19	0.43
1:C:382:SER:C	1:C:384:ASP:H	2.21	0.43
1:C:454:ILE:HB	1:C:455:PRO:HD3	2.00	0.43
1:B:329:PHE:CD2	1:B:568:LYS:HE2	2.54	0.43
1:A:481:PHE:N	1:A:481:PHE:CD1	2.87	0.43
1:B:553:SER:O	4:B:67:HOH:O	2.21	0.43
1:D:436:THR:CG2	3:D:803:ADP:O1B	2.67	0.43
1:A:656:GLU:O	1:A:657:SER:C	2.57	0.43
1:A:536:LYS:HA	1:A:536:LYS:HD2	1.74	0.43
1:D:433:TYR:HB2	1:D:581:LEU:HD12	2.00	0.43
1:D:353:CYS:HB2	1:D:398:PHE:CE2	2.54	0.43
1:A:622:TYR:CG	1:A:632:MET:HG3	2.54	0.43
1:C:355:ILE:HG12	1:C:647:VAL:HG23	2.01	0.43
1:D:442:TYR:O	1:D:446:GLY:HA2	2.19	0.43
1:D:381:GLN:HB3	1:D:388:LYS:HD2	2.00	0.43
1:B:542:ALA:HB3	1:B:546:GLY:O	2.19	0.43
1:B:398:PHE:CD1	1:B:398:PHE:N	2.86	0.43
1:A:321:LEU:HD12	1:B:321:LEU:HD23	2.00	0.43
1:C:399:ASP:O	1:C:400:GLN:HB2	2.19	0.42
1:D:419:ILE:HD12	1:D:457:THR:HG23	2.01	0.42
1:C:493:LEU:HA	1:C:493:LEU:HD23	1.88	0.42
1:D:330:GLN:HE21	1:D:330:GLN:HB2	1.43	0.42
1:C:543:SER:N	1:C:550:SER:HB3	2.34	0.42
1:D:614:LEU:HB2	1:D:670:CYS:SG	2.59	0.42
1:B:352:PHE:HD2	1:B:400:GLN:HB3	1.77	0.42
1:B:432:ALA:HB2	1:B:444:MET:HG2	1.99	0.42
1:B:480:THR:HG22	1:B:519:GLU:HG3	2.01	0.42
1:A:548:GLU:OE2	1:A:552:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLN:HG2	4:A:53:HOH:O	2.20	0.42
1:A:367:CYS:HA	1:A:650:PHE:HA	2.02	0.42
1:C:517:ILE:H	1:C:517:ILE:CD1	2.32	0.42
1:C:435:GLN:OE1	1:C:656:GLU:HB3	2.20	0.42
1:C:653:CYS:O	1:C:654:PHE:C	2.56	0.42
1:C:374:ASP:OD2	1:C:375:GLU:N	2.53	0.42
1:D:411:ILE:HG23	1:D:644:PHE:CE2	2.54	0.42
1:A:361:SER:C	1:A:362:GLU:HG3	2.38	0.42
1:C:310:LEU:O	1:C:312:ARG:N	2.51	0.42
1:A:352:PHE:CZ	1:A:414:MET:HG2	2.55	0.42
1:C:382:SER:CB	1:C:651:GLN:HE22	2.33	0.42
1:A:512:ILE:HG23	1:A:513:TYR:N	2.34	0.42
1:B:469:ARG:C	1:B:471:LEU:H	2.23	0.42
1:C:491:ASP:HB2	1:C:500:MET:SD	2.60	0.42
1:D:548:GLU:O	1:D:548:GLU:HG3	2.19	0.42
1:B:384:ASP:C	1:B:386:GLN:N	2.71	0.42
1:A:324:CYS:SG	1:B:324:CYS:SG	3.13	0.42
1:D:514:VAL:HG12	1:D:517:ILE:HG13	1.99	0.42
1:A:667:VAL:HG12	1:A:668:ASN:N	2.34	0.42
1:A:398:PHE:CE2	1:A:664:ALA:HB1	2.55	0.42
1:D:341:THR:O	1:D:342:VAL:C	2.57	0.42
1:B:356:ARG:O	1:B:649:PRO:HD3	2.19	0.42
1:D:385:ALA:HA	1:D:388:LYS:HE2	2.02	0.42
1:A:537:MET:HE2	1:A:537:MET:HA	2.01	0.42
1:C:296:LEU:O	1:C:300:VAL:HG23	2.20	0.42
1:B:622:TYR:CG	1:B:632:MET:HG3	2.55	0.42
1:A:604:SER:O	1:A:607:THR:HB	2.20	0.42
1:D:580:ASP:O	1:D:580:ASP:OD1	2.36	0.42
1:C:321:LEU:HD22	1:D:321:LEU:HB2	2.02	0.42
1:C:419:ILE:HD12	1:C:457:THR:HG23	2.02	0.42
1:B:382:SER:C	1:B:384:ASP:N	2.73	0.42
1:C:304:ARG:HH21	1:D:299:GLU:CD	2.22	0.42
1:C:296:LEU:C	1:C:298:THR:N	2.73	0.42
1:D:622:TYR:CG	1:D:632:MET:HG3	2.55	0.42
1:C:496:GLU:O	1:C:497:GLN:C	2.57	0.42
1:B:328:LEU:HD13	1:B:328:LEU:HA	1.82	0.42
1:B:537:MET:HA	1:B:537:MET:HE3	2.00	0.42
1:D:604:SER:O	1:D:607:THR:HB	2.20	0.42
1:D:335:ARG:HH22	1:D:424:ASP:CG	2.23	0.42
1:B:491:ASP:HB2	1:B:500:MET:SD	2.59	0.42
1:D:364:ASN:ND2	1:D:364:ASN:N	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:ASP:HB2	1:D:500:MET:CE	2.49	0.42
1:C:329:PHE:CD1	1:C:568:LYS:HE2	2.55	0.42
1:C:497:GLN:NE2	1:C:498:LYS:O	2.53	0.42
1:A:357:PRO:HA	1:A:358:PRO:HD3	1.82	0.42
1:A:367:CYS:HB3	1:A:368:CYS:H	1.51	0.42
1:C:528:LEU:O	1:C:528:LEU:HD12	2.20	0.42
1:B:351:VAL:HG12	1:B:398:PHE:HD2	1.85	0.42
1:D:373:HIS:O	1:D:377:THR:HB	2.20	0.42
1:D:429:CYS:C	1:D:430:ILE:HD13	2.39	0.42
1:C:521:THR:O	1:C:523:LEU:HD12	2.19	0.42
1:C:355:ILE:HG22	1:C:404:PRO:HG3	2.02	0.42
1:A:495:ASN:C	1:A:497:GLN:H	2.24	0.42
1:A:636:GLY:HA3	4:A:92:HOH:O	2.20	0.42
1:D:388:LYS:HA	1:D:391:MET:CE	2.42	0.41
1:B:503:ARG:HD3	1:B:513:TYR:CE2	2.54	0.41
1:D:379:GLU:HA	1:D:394:GLN:O	2.20	0.41
1:C:318:ALA:O	1:C:321:LEU:N	2.45	0.41
1:D:335:ARG:C	1:D:335:ARG:HE	2.24	0.41
1:D:469:ARG:C	1:D:471:LEU:H	2.23	0.41
1:D:549:ARG:O	1:D:550:SER:C	2.59	0.41
1:D:566:ALA:O	1:D:567:GLU:C	2.59	0.41
1:A:352:PHE:CZ	1:A:414:MET:HG3	2.55	0.41
1:C:384:ASP:HB3	1:C:387:ALA:HB3	2.03	0.41
1:D:403:HIS:N	1:D:406:SER:HG	2.18	0.41
1:D:359:LEU:HD23	4:D:90:HOH:O	2.19	0.41
1:C:324:CYS:HG	1:D:324:CYS:HG	1.56	0.41
1:D:316:GLN:O	1:D:317:GLN:C	2.57	0.41
1:D:487:GLU:O	1:D:626:LYS:NZ	2.52	0.41
1:D:360:GLU:OE1	4:D:90:HOH:O	2.22	0.41
1:C:329:PHE:CE1	1:C:568:LYS:HE2	2.54	0.41
1:D:497:GLN:NE2	1:D:498:LYS:O	2.53	0.41
1:D:428:ILE:N	1:D:428:ILE:HD13	2.34	0.41
1:D:599:ILE:C	1:D:601:ARG:N	2.73	0.41
1:B:549:ARG:HB3	1:B:550:SER:H	1.64	0.41
1:C:398:PHE:CD1	1:C:398:PHE:N	2.88	0.41
1:C:398:PHE:CE2	1:C:664:ALA:CB	3.03	0.41
1:C:426:TYR:CD2	1:C:640:LYS:HE2	2.56	0.41
1:A:380:LEU:HD23	1:A:394:GLN:HB3	2.02	0.41
1:A:658:VAL:HG23	1:A:659:LYS:N	2.36	0.41
1:C:311:LEU:HA	1:C:311:LEU:HD12	1.66	0.41
1:C:310:LEU:C	1:C:312:ARG:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:ALA:CB	1:B:546:GLY:O	2.69	0.41
1:C:631:LEU:C	1:C:633:PRO:HD2	2.41	0.41
1:D:403:HIS:C	1:D:405:LEU:H	2.23	0.41
1:D:338:LEU:HA	1:D:338:LEU:HD23	1.81	0.41
1:B:324:CYS:O	1:B:327:GLN:HB2	2.20	0.41
1:D:373:HIS:CD2	1:D:395:ILE:CD1	3.04	0.41
1:B:486:ASN:O	1:B:487:GLU:HB2	2.21	0.41
1:B:489:LEU:HD11	1:B:626:LYS:HG3	2.03	0.41
1:B:654:PHE:CD2	1:B:655:GLN:N	2.89	0.41
1:D:536:LYS:HZ1	1:D:539:ARG:NH1	2.19	0.41
1:C:419:ILE:O	1:C:422:ALA:HB3	2.21	0.41
1:C:527:HIS:NE2	1:C:531:LEU:HD11	2.36	0.41
1:A:411:ILE:HG23	1:A:644:PHE:CZ	2.56	0.41
1:B:541:THR:O	1:B:544:THR:HG22	2.21	0.41
1:A:400:GLN:HG3	1:A:401:VAL:H	1.79	0.41
1:C:653:CYS:O	1:C:656:GLU:N	2.50	0.41
1:A:454:ILE:HG12	1:A:578:LEU:HD13	2.01	0.41
1:D:304:ARG:O	1:D:308:GLU:OE1	2.38	0.41
1:C:568:LYS:O	1:C:569:GLN:HB2	2.21	0.41
1:A:661:LEU:O	1:A:664:ALA:N	2.54	0.41
1:A:388:LYS:HG3	1:A:388:LYS:O	2.20	0.41
1:A:355:ILE:HG22	1:A:404:PRO:CG	2.51	0.41
1:D:515:SER:O	1:D:516:ASN:CB	2.62	0.41
1:D:403:HIS:HB2	1:D:404:PRO:HD2	2.03	0.41
1:B:469:ARG:HB2	1:B:469:ARG:HE	1.71	0.40
1:C:584:SER:HA	1:C:603:LEU:HD21	2.03	0.40
1:C:319:ALA:C	1:C:321:LEU:H	2.24	0.40
1:B:533:HIS:O	1:B:536:LYS:N	2.53	0.40
1:D:536:LYS:HD2	1:D:536:LYS:HA	1.82	0.40
1:C:527:HIS:CD2	1:C:527:HIS:O	2.74	0.40
1:C:301:VAL:O	1:C:304:ARG:N	2.54	0.40
1:D:310:LEU:O	1:D:311:LEU:C	2.59	0.40
1:B:462:PHE:CZ	1:B:477:ILE:HD12	2.56	0.40
1:C:418:LEU:HA	1:C:418:LEU:HD23	1.83	0.40
1:B:534:THR:O	1:B:535:ALA:C	2.59	0.40
1:D:359:LEU:O	1:D:360:GLU:C	2.57	0.40
1:B:568:LYS:O	1:B:569:GLN:HB2	2.21	0.40
1:C:433:TYR:CD2	1:C:434:GLY:N	2.89	0.40
1:C:306:ARG:HG3	1:C:310:LEU:CD1	2.46	0.40
1:B:512:ILE:HG23	1:B:513:TYR:N	2.36	0.40
1:C:605:GLU:HG3	1:C:625:SER:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:ARG:HD2	1:D:306:ARG:HA	1.91	0.40
1:A:430:ILE:HD12	1:A:642:LEU:HB2	2.02	0.40
1:C:312:ARG:HA	1:C:315:GLU:OE2	2.22	0.40
1:C:382:SER:C	1:C:384:ASP:N	2.75	0.40
1:C:536:LYS:HA	1:C:536:LYS:HD2	1.89	0.40
1:B:461:LEU:HD11	1:B:561:LEU:HD11	2.04	0.40
1:A:428:ILE:CG2	1:A:429:CYS:N	2.85	0.40
1:D:481:PHE:CD1	1:D:481:PHE:N	2.89	0.40
1:D:605:GLU:HA	1:D:608:ASN:HD22	1.86	0.40
1:C:338:LEU:HD23	1:D:342:VAL:HG21	2.03	0.40
1:A:521:THR:OG1	1:A:521:THR:O	2.33	0.40
1:A:359:LEU:N	1:A:362:GLU:OE1	2.48	0.40
1:A:419:ILE:HD12	1:A:576:ILE:HD13	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:ASN:O	4:A:118:HOH:O[4_566]	2.02	0.18

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	338/406 (83%)	273 (81%)	47 (14%)	18 (5%)	2	8
1	B	333/406 (82%)	264 (79%)	48 (14%)	21 (6%)	2	5
1	C	360/406 (89%)	283 (79%)	56 (16%)	21 (6%)	2	6
1	D	361/406 (89%)	282 (78%)	54 (15%)	25 (7%)	1	4
All	All	1392/1624 (86%)	1102 (79%)	205 (15%)	85 (6%)	2	5

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	PRO
1	A	541	THR
1	A	544	THR
1	A	548	GLU
1	A	568	LYS
1	A	570	GLU
1	A	636	GLY
1	A	654	PHE
1	B	497	GLN
1	B	508	ASN
1	B	540	ALA
1	B	568	LYS
1	C	318	ALA
1	C	404	PRO
1	C	568	LYS
1	C	570	GLU
1	D	404	PRO
1	D	568	LYS
1	D	585	GLU
1	A	348	ASN
1	A	375	GLU
1	A	497	GLN
1	A	546	GLY
1	A	671	LYS
1	B	348	ASN
1	B	391	MET
1	B	404	PRO
1	B	470	ASN
1	B	538	ASN
1	B	570	GLU
1	B	636	GLY
1	B	654	PHE
1	C	302	HIS
1	C	348	ASN
1	C	497	GLN
1	C	508	ASN
1	C	526	ASN
1	C	538	ASN
1	C	636	GLY
1	C	654	PHE
1	D	297	SER
1	D	311	LEU
1	D	348	ASN

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Mol	Chain	Res	Type
1	D	375	GLU
1	D	383	ILE
1	D	497	GLN
1	D	538	ASN
1	D	570	GLU
1	D	600	ASN
1	D	654	PHE
1	A	496	GLU
1	A	526	ASN
1	A	540	ALA
1	B	375	GLU
1	B	541	THR
1	C	323	THR
1	C	468	TYR
1	C	527	HIS
1	D	526	ASN
1	A	527	HIS
1	B	400	GLN
1	C	375	GLU
1	C	470	ASN
1	C	543	SER
1	D	392	GLY
1	D	400	GLN
1	D	470	ASN
1	D	496	GLU
1	D	508	ASN
1	B	526	ASN
1	B	639	SER
1	C	400	GLN
1	D	527	HIS
1	B	347	GLY
1	B	610	ILE
1	B	637	GLY
1	C	496	GLU
1	D	540	ALA
1	D	581	LEU
1	C	546	GLY
1	D	439	GLY
1	D	347	GLY
1	A	524	ASP
1	D	636	GLY
1	B	416	SER

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	308/368 (84%)	280 (91%)	28 (9%)	12 34
1	B	305/368 (83%)	279 (92%)	26 (8%)	13 37
1	C	326/368 (89%)	300 (92%)	26 (8%)	15 40
1	D	328/368 (89%)	289 (88%)	39 (12%)	6 19
All	All	1267/1472 (86%)	1148 (91%)	119 (9%)	11 32

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	LEU
1	A	327	GLN
1	A	328	LEU
1	A	361	SER
1	A	371	THR
1	A	378	VAL
1	A	380	LEU
1	A	404	PRO
1	A	405	LEU
1	A	414	MET
1	A	433	TYR
1	A	438	SER
1	A	461	LEU
1	A	463	ASP
1	A	466	ARG
1	A	471	LEU
1	A	512	ILE
1	A	513	TYR
1	A	517	ILE
1	A	537	MET
1	A	541	THR
1	A	552	ARG
1	A	603	LEU
1	A	607	THR

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Mol	Chain	Res	Type
1	A	626	LYS
1	A	643	MET
1	A	657	SER
1	A	669	SER
1	B	327	GLN
1	B	328	LEU
1	B	332	ASN
1	B	335	ARG
1	B	369	THR
1	B	380	LEU
1	B	403	HIS
1	B	404	PRO
1	B	405	LEU
1	B	414	MET
1	B	433	TYR
1	B	463	ASP
1	B	466	ARG
1	B	471	LEU
1	B	481	PHE
1	B	486	ASN
1	B	494	SER
1	B	512	ILE
1	B	513	TYR
1	B	517	ILE
1	B	537	MET
1	B	549	ARG
1	B	552	ARG
1	B	624	ASN
1	B	626	LYS
1	B	640	LYS
1	C	321	LEU
1	C	335	ARG
1	C	338	LEU
1	C	348	ASN
1	C	364	ASN
1	C	365	ARG
1	C	371	THR
1	C	374	ASP
1	C	386	GLN
1	C	405	LEU
1	C	414	MET
1	C	433	TYR

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Mol	Chain	Res	Type
1	C	461	LEU
1	C	463	ASP
1	C	471	LEU
1	C	481	PHE
1	C	494	SER
1	C	512	ILE
1	C	513	TYR
1	C	517	ILE
1	C	544	THR
1	C	552	ARG
1	C	572	SER
1	C	623	ARG
1	C	648	SER
1	C	668	ASN
1	D	299	GLU
1	D	306	ARG
1	D	308	GLU
1	D	328	LEU
1	D	330	GLN
1	D	335	ARG
1	D	348	ASN
1	D	361	SER
1	D	365	ARG
1	D	371	THR
1	D	374	ASP
1	D	388	LYS
1	D	403	HIS
1	D	404	PRO
1	D	405	LEU
1	D	408	GLN
1	D	414	MET
1	D	433	TYR
1	D	438	SER
1	D	461	LEU
1	D	463	ASP
1	D	466	ARG
1	D	471	LEU
1	D	476	GLU
1	D	480	THR
1	D	512	ILE
1	D	513	TYR
1	D	517	ILE

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Mol	Chain	Res	Type
1	D	525	PRO
1	D	537	MET
1	D	552	ARG
1	D	572	SER
1	D	603	LEU
1	D	607	THR
1	D	610	ILE
1	D	626	LYS
1	D	639	SER
1	D	646	ASN
1	D	647	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	364	ASN
1	A	470	ASN
1	A	486	ASN
1	A	497	GLN
1	A	507	ASN
1	A	608	ASN
1	A	615	GLN
1	A	624	ASN
1	A	668	ASN
1	B	327	GLN
1	B	330	GLN
1	B	364	ASN
1	B	470	ASN
1	B	486	ASN
1	B	507	ASN
1	B	533	HIS
1	B	547	ASN
1	B	577	ASN
1	B	608	ASN
1	C	302	HIS
1	C	314	ASN
1	C	317	GLN
1	C	364	ASN
1	C	381	GLN
1	C	386	GLN
1	C	470	ASN

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Mol	Chain	Res	Type
1	C	486	ASN
1	C	497	GLN
1	C	507	ASN
1	C	608	ASN
1	C	629	HIS
1	C	668	ASN
1	D	314	ASN
1	D	316	GLN
1	D	330	GLN
1	D	339	HIS
1	D	364	ASN
1	D	386	GLN
1	D	470	ASN
1	D	486	ASN
1	D	507	ASN
1	D	577	ASN
1	D	600	ASN
1	D	608	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	ADP	A	800	2	22,29,29	1.76	3 (13%)	27,45,45	3.64	10 (37%)
3	ADP	B	801	2	22,29,29	1.76	3 (13%)	27,45,45	3.65	10 (37%)
3	ADP	C	802	2	22,29,29	1.75	3 (13%)	27,45,45	3.65	10 (37%)
3	ADP	D	803	2	22,29,29	1.77	3 (13%)	27,45,45	3.64	10 (37%)

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
3	ADP	A	800	2	-	0/12/32/32	0/3/3/3
3	ADP	B	801	2	-	0/12/32/32	0/3/3/3
3	ADP	C	802	2	-	0/12/32/32	0/3/3/3
3	ADP	D	803	2	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	803	ADP	C5-N7	-2.30	1.31	1.39
3	A	800	ADP	C5-N7	-2.28	1.31	1.39
3	C	802	ADP	C5-N7	-2.28	1.31	1.39
3	B	801	ADP	C5-N7	-2.28	1.31	1.39
3	B	801	ADP	C5'-C4'	2.00	1.58	1.51
3	A	800	ADP	C5'-C4'	2.01	1.58	1.51
3	C	802	ADP	C5'-C4'	2.01	1.58	1.51
3	D	803	ADP	C5'-C4'	2.02	1.58	1.51
3	C	802	ADP	O4'-C1'	6.13	1.49	1.41
3	A	800	ADP	O4'-C1'	6.18	1.49	1.41
3	B	801	ADP	O4'-C1'	6.19	1.49	1.41
3	D	803	ADP	O4'-C1'	6.23	1.49	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	802	ADP	N3-C2-N1	-13.09	118.87	128.89
3	B	801	ADP	N3-C2-N1	-13.08	118.88	128.89
3	D	803	ADP	N3-C2-N1	-13.02	118.92	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	800	ADP	N3-C2-N1	-12.98	118.96	128.89
3	C	802	ADP	O4'-C4'-C5'	2.01	116.49	109.32
3	B	801	ADP	O4'-C4'-C5'	2.01	116.50	109.32
3	A	800	ADP	O4'-C4'-C5'	2.01	116.50	109.32
3	D	803	ADP	O4'-C4'-C5'	2.01	116.52	109.32
3	A	800	ADP	C2-N1-C6	2.02	122.37	118.77
3	C	802	ADP	C2-N1-C6	2.02	122.38	118.77
3	D	803	ADP	C2-N1-C6	2.03	122.39	118.77
3	A	800	ADP	C2'-C3'-C4'	2.04	106.81	102.61
3	D	803	ADP	C2'-C3'-C4'	2.05	106.83	102.61
3	C	802	ADP	C2'-C3'-C4'	2.06	106.85	102.61
3	B	801	ADP	C2-N1-C6	2.07	122.46	118.77
3	B	801	ADP	C2'-C3'-C4'	2.08	106.89	102.61
3	C	802	ADP	O2B-PB-O1B	2.09	117.31	110.58
3	A	800	ADP	O2B-PB-O1B	2.11	117.38	110.58
3	D	803	ADP	O2B-PB-O1B	2.12	117.39	110.58
3	B	801	ADP	O2B-PB-O1B	2.12	117.40	110.58
3	A	800	ADP	PA-O3A-PB	3.21	143.44	132.67
3	C	802	ADP	PA-O3A-PB	3.22	143.45	132.67
3	B	801	ADP	PA-O3A-PB	3.24	143.52	132.67
3	D	803	ADP	PA-O3A-PB	3.24	143.54	132.67
3	B	801	ADP	O5'-C5'-C4'	4.51	125.73	109.12
3	D	803	ADP	O5'-C5'-C4'	4.51	125.74	109.12
3	A	800	ADP	O5'-C5'-C4'	4.51	125.74	109.12
3	C	802	ADP	O5'-C5'-C4'	4.52	125.78	109.12
3	C	802	ADP	C4-C5-N7	4.72	113.82	109.48
3	B	801	ADP	C4-C5-N7	4.76	113.86	109.48
3	A	800	ADP	C4-C5-N7	4.79	113.89	109.48
3	D	803	ADP	C4-C5-N7	4.86	113.95	109.48
3	C	802	ADP	O3A-PA-O5'	5.72	118.11	102.94
3	A	800	ADP	O3A-PA-O5'	5.72	118.12	102.94
3	B	801	ADP	O3A-PA-O5'	5.73	118.14	102.94
3	D	803	ADP	O3A-PA-O5'	5.74	118.16	102.94
3	D	803	ADP	O4'-C1'-N9	7.87	124.57	108.10
3	C	802	ADP	O4'-C1'-N9	7.87	124.57	108.10
3	A	800	ADP	O4'-C1'-N9	7.90	124.63	108.10
3	B	801	ADP	O4'-C1'-N9	7.90	124.63	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	ADP	4	0
3	B	801	ADP	5	0
3	C	802	ADP	5	0
3	D	803	ADP	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.