



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:47 AM UTC

PDB ID : 1CZ7 / pdb_00001cz7
Title : THE CRYSTAL STRUCTURE OF A MINUS-END DIRECTED MICRO-TUBULE MOTOR PROTEIN NCD REVEALS VARIABLE DIMER CONFORMATIONS
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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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

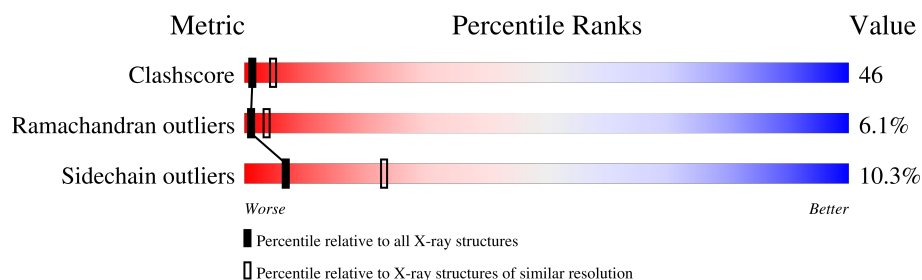
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	406	35% 37% 11% • 16%
1	B	406	33% 38% 11% • 17%
1	C	406	33% 44% 11% 10%
1	D	406	30% 46% 14% • 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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is water.

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

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	1.02	2/2757 (0.1%)	1.24	21/3722 (0.6%)
1	B	0.68	1/2727 (0.0%)	1.07	15/3680 (0.4%)
1	C	0.65	2/2933 (0.1%)	1.07	15/3960 (0.4%)
1	D	0.95	3/2943 (0.1%)	1.21	21/3973 (0.5%)
All	All	0.84	8/11360 (0.1%)	1.15	72/15335 (0.5%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	ILE	CA-CB	-11.33	1.48	1.54
1	B	537	MET	SD-CE	8.11	1.99	1.79
1	C	532	MET	SD-CE	6.58	1.96	1.79
1	A	556	VAL	C-O	-6.08	1.17	1.24
1	D	454	ILE	CA-CB	-5.86	1.51	1.54
1	D	500	MET	SD-CE	-5.68	1.65	1.79
1	C	454	ILE	CA-CB	-5.37	1.51	1.54
1	D	451	VAL	CA-CB	-5.24	1.49	1.54

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	SER	N-CA-C	-9.00	102.21	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	395	ILE	N-CA-C	8.44	119.93	108.11
1	D	579	VAL	N-CA-C	8.21	120.79	108.23
1	A	539	ARG	N-CA-C	-8.02	103.48	113.18
1	C	432	ALA	N-CA-C	-8.01	96.70	109.59
1	C	356	ARG	CA-C-N	7.80	125.28	119.66
1	C	356	ARG	C-N-CA	7.80	125.28	119.66
1	A	635	LEU	N-CA-C	-7.47	102.09	113.89
1	C	322	GLU	N-CA-C	-7.29	102.12	111.02
1	C	668	ASN	N-CA-C	-7.22	104.45	113.18
1	A	368	CYS	N-CA-C	-7.05	98.92	108.86
1	A	328	LEU	N-CA-C	-7.02	103.68	111.82
1	A	357	PRO	CA-C-N	6.94	126.90	120.03
1	A	357	PRO	C-N-CA	6.94	126.90	120.03
1	C	544	THR	N-CA-C	-6.89	104.74	113.01
1	B	518	THR	N-CA-C	-6.83	100.17	110.28
1	C	453	VAL	N-CA-C	6.71	117.21	110.23
1	B	335	ARG	N-CA-C	-6.56	104.05	111.07
1	D	399	ASP	N-CA-C	-6.45	105.51	113.19
1	C	635	LEU	N-CA-C	-6.32	103.91	113.89
1	D	518	THR	N-CA-C	-6.28	100.27	110.20
1	A	432	ALA	N-CA-C	-6.23	99.08	109.24
1	D	407	SER	N-CA-C	6.18	118.02	110.41
1	B	653	CYS	N-CA-C	-6.12	105.95	113.41
1	D	635	LEU	N-CA-C	-6.08	104.29	113.89
1	C	556	VAL	N-CA-C	6.07	116.10	106.88
1	B	650	PHE	N-CA-C	6.02	119.30	109.24
1	D	432	ALA	N-CA-C	-5.98	99.45	109.07
1	A	321	LEU	N-CA-C	-5.97	105.84	113.01
1	D	495	ASN	N-CA-C	-5.92	105.36	113.30
1	A	650	PHE	N-CA-C	5.92	118.77	108.76
1	B	635	LEU	N-CA-C	-5.92	105.80	114.39
1	A	517	ILE	CB-CA-C	-5.92	102.86	111.68
1	C	581	LEU	N-CA-C	5.90	117.91	110.24
1	A	324	CYS	N-CA-C	-5.83	103.71	111.24
1	D	578	LEU	N-CA-C	5.83	118.95	108.17
1	B	454	ILE	CB-CA-C	-5.83	108.17	114.35
1	A	491	ASP	N-CA-C	-5.77	101.30	109.96
1	C	320	GLU	N-CA-C	-5.76	105.96	112.87
1	D	359	LEU	N-CA-C	5.76	119.35	110.42
1	C	304	ARG	N-CA-C	-5.74	105.11	111.71
1	A	356	ARG	CA-C-N	5.68	126.23	120.38
1	A	356	ARG	C-N-CA	5.68	126.23	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	393	GLN	N-CA-C	5.68	117.62	107.80
1	A	641	THR	N-CA-C	5.55	118.14	108.76
1	B	329	PHE	N-CA-C	-5.54	105.24	111.28
1	C	579	VAL	N-CA-C	5.53	115.56	107.37
1	A	487	GLU	N-CA-C	-5.48	104.57	111.92
1	C	495	ASN	N-CA-C	-5.43	106.32	113.17
1	B	579	VAL	N-CA-C	5.40	115.56	107.51
1	C	529	ARG	N-CA-C	-5.38	105.49	111.36
1	D	559	LEU	N-CA-C	-5.38	99.52	108.34
1	A	408	GLN	N-CA-C	-5.35	105.53	111.36
1	D	375	GLU	N-CA-C	5.35	122.19	110.80
1	B	567	GLU	N-CA-C	-5.32	104.07	111.52
1	D	567	GLU	N-CA-C	-5.30	104.08	111.39
1	D	376	SER	N-CA-C	-5.28	106.35	114.16
1	D	408	GLN	N-CA-C	-5.24	105.48	111.14
1	B	432	ALA	N-CA-C	-5.23	100.72	109.24
1	D	320	GLU	N-CA-C	-5.23	105.18	112.45
1	D	529	ARG	N-CA-C	-5.21	105.60	111.28
1	D	669	SER	N-CA-C	-5.17	106.23	112.54
1	A	429	CYS	CB-CA-C	-5.16	103.62	110.79
1	D	415	VAL	N-CA-C	5.13	116.55	111.67
1	D	342	VAL	N-CA-C	-5.13	104.90	110.23
1	D	454	ILE	CB-CA-C	-5.12	108.83	113.70
1	B	529	ARG	N-CA-C	-5.10	105.72	111.28
1	B	389	SER	N-CA-C	-5.09	107.02	113.18
1	A	375	GLU	N-CA-C	5.08	121.63	110.80
1	B	581	LEU	N-CA-C	5.07	117.07	110.43
1	B	415	VAL	N-CA-C	5.02	116.12	111.45
1	A	407	SER	N-CA-C	5.01	116.58	110.41

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

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	251	0
1	B	2682	0	2644	235	0
1	C	2888	0	2849	258	0
1	D	2898	0	2855	308	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	18	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	1035	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 46.

All (1035) 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
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:A:528:LEU:HG	1:A:532:MET:HE2	1.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:491:ASP:HB2	1:C:500:MET:HE1	1.48	0.95
1:C:387:ALA:HB1	1:C:391:MET:HE3	1.49	0.94
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:D:643:MET:HE3	1:D:663:PHE:HE2	1.35	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:D:528:LEU:HG	1:D:532:MET:HE2	1.52	0.90
1:A:346:ARG:HG3	1:A:346:ARG:HH11	1.37	0.90
1:B:537:MET:HE2	1:B:537:MET:HA	1.52	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:D:501:GLU:CD	4:D:116:HOH:O	2.16	0.87
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:D:388:LYS:HA	1:D:391:MET:HE3	1.56	0.85
1:A:547:ASN:O	1:A:549:ARG:N	2.11	0.84
1:B:528:LEU:HG	1:B:532:MET:HE2	1.58	0.84
1:D:414:MET:HE3	1:D:414:MET:HA	1.58	0.84
1:D:650:PHE:HB3	4:D:121:HOH:O	1.78	0.83
1:A:414:MET:HA	1:A:414:MET:HE3	1.58	0.83
1:A:599:ILE:HG23	1:A:601:ARG:H	1.39	0.83
1:C:522:VAL:HG21	1:C:528:LEU:HD22	1.59	0.83
1:A:366:MET:O	1:A:651:GLN:N	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:643:MET:HE3	1:D:663:PHE:CE2	2.16	0.81
1:A:376:SER:OG	4:A:98:HOH:O	1.98	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:414:MET:HE3	1:B:414:MET:HA	1.63	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:D:537:MET:C	1:D:539:ARG:H	1.90	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:356:ARG:HG2	1:D:647:VAL:O	1.84	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:C:537:MET:HA	1:C:537:MET:HE2	1.66	0.78
1:D:400:GLN:HG3	1:D:401:VAL:N	1.99	0.78
1:A:537:MET:HE2	1:A:537:MET:HA	1.66	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: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:D:528:LEU:HG	1:D:532:MET:CE	2.14	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:486:ASN:C	4:D:113:HOH:O	2.27	0.76
1:D:602:SER:HB2	4:D:70:HOH:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ASN:C	1:A:549:ARG:H	1.93	0.75
1:D:566:ALA:N	4:D:74:HOH:O	1.79	0.75
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:D:382:SER:H	1:D:391:MET:HE1	1.51	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:A:440:LYS:HZ3	1:A:583:GLY:HA2	1.50	0.74
1:D:599:ILE:HG22	1:D:600:ASN:N	1.97	0.74
1:A:400:GLN:HG3	1:A:401:VAL:N	2.00	0.74
1:B:522:VAL:HG13	1:B:528:LEU:HB2	1.68	0.74
1:D:522:VAL:HG11	1:D:528:LEU:HD22	1.68	0.74
1:C:537:MET:C	1:C:539:ARG:H	1.95	0.74
1:A:321:LEU:C	1:A:321:LEU:HD23	2.13	0.74
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:D:433:TYR:C	1:D:433:TYR:CD2	2.66	0.73
1:B:522:VAL:CG1	1:B:528:LEU:HB2	2.18	0.73
1:C:542:ALA:N	1:C:550:SER:HB2	2.02	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:D:328:LEU:HD12	1:D:328:LEU:C	2.14	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:D:543:SER:HA	1:D:547:ASN:CG	2.14	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:652:ASP:O	4:A:133:HOH:O	2.07	0.72
1:A:670:CYS:C	1:A:672:MET:H	1.97	0.72
1:D:623:ARG:HG3	1:D:623:ARG:HH11	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:A:517:ILE:HD12	1:A:517:ILE:H	1.56	0.71
1:D:358:PRO:O	4:D:80:HOH:O	2.09	0.71
1:A:418:LEU:HD11	1:A:642:LEU:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:GLN:C	4:B:33:HOH:O	2.34	0.71
1:C:486:ASN:N	4:C:111:HOH:O	2.00	0.71
1:D:435:GLN:O	1:D:438:SER:OG	2.08	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:B:537:MET:HA	1:B:537:MET:CE	2.21	0.70
1:D:614:LEU:HD11	1:D:667:VAL:HG13	1.73	0.70
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:A:643:MET:HE3	1:A:663:PHE:HE2	1.58	0.69
1:A:357:PRO:HD3	1:A:404:PRO:HA	1.73	0.69
1:A:454:ILE:HB	1:A:455:PRO:HD3	1.74	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:D:403:HIS:O	1:D:405:LEU:N	2.25	0.69
1:C:387:ALA:O	1:C:391:MET:HG2	1.93	0.68
1:C:440:LYS:NZ	1:C:583:GLY:HA2	2.08	0.68
1:D:367:CYS:HA	1:D:650:PHE:HA	1.74	0.68
1:C:351:VAL:CG2	1:C:667:VAL:HG11	2.24	0.68
1:C:528:LEU:HG	1:C:532:MET:CE	2.24	0.68
1:A:438:SER:HB2	1:A:646:ASN:HB2	1.75	0.68
1:C:363:GLU:C	1:C:364:ASN:HD22	2.00	0.68
1:D:548:GLU:OE2	1:D:552:ARG:HG3	1.92	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:C:623:ARG:HH11	1:C:623:ARG:CG	2.07	0.68
1:D:380:LEU:O	1:D:394:GLN:HB2	1.93	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:C:414:MET:HE3	1:C:414:MET:HA	1.76	0.67
1:A:346:ARG:HG3	1:A:346:ARG:NH1	2.05	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:B:541:THR:CB	1:B:550:SER:HB2	2.24	0.67
1:C:306:ARG:HG3	1:C:310:LEU:HD12	1.77	0.67
1:B:384:ASP:OD2	1:B:386:GLN:HB3	1.94	0.67
1:A:396:PHE:HA	4:A:100:HOH:O	1.94	0.67
1:C:522:VAL:CG1	1:C:528:LEU:HB2	2.25	0.67
1:C:321:LEU:HD13	1:D:321:LEU:HD13	1.76	0.67
1:D:358:PRO:HB3	1:D:650:PHE:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:611:LEU:O	1:C:615:GLN:HG3	1.95	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:C:623:ARG:HG3	1:C:623:ARG:NH1	2.07	0.67
1:D:380:LEU:CD2	1:D:394:GLN:HB3	2.25	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:C:385:ALA:HA	1:C:388:LYS:HZ3	1.60	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:547:ASN:C	1:B:549:ARG:H	2.02	0.66
1:D:482:LEU:C	1:D:482:LEU:HD12	2.21	0.66
1:B:393:GLN:HA	1:B:393:GLN:OE1	1.95	0.66
1:A:403:HIS:O	1:A:405:LEU:N	2.29	0.66
1:D:352:PHE:CZ	1:D:414:MET:CG	2.79	0.66
1:A:367:CYS:CB	4:A:94:HOH:O	2.41	0.66
1:C:482:LEU:C	1:C:482:LEU:HD12	2.21	0.66
1:D:383:ILE:HG22	1:D:383:ILE:O	1.95	0.65
1:A:436:THR:H	1:A:585:GLU:CD	2.04	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:B:400:GLN:HG3	1:B:401:VAL:N	2.08	0.65
1:C:364:ASN:HD22	1:C:364:ASN:N	1.94	0.65
1:D:522:VAL:HG21	1:D:528:LEU:HD22	1.79	0.65
1:A:523:LEU:O	1:A:524:ASP:HB3	1.96	0.65
1:C:582:ALA:HB3	4:C:69:HOH:O	1.96	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:B:373:HIS:O	1:B:374:ASP:HB3	1.97	0.64
1:C:489:LEU:N	4:C:49:HOH:O	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:SER:C	1:D:384:ASP:H	2.04	0.64
1:B:346:ARG:HG3	1:B:346:ARG:HH11	1.63	0.64
1:A:373:HIS:O	1:A:377:THR:HB	1.98	0.64
1:C:310:LEU:O	1:C:311:LEU:C	2.40	0.64
1:D:356:ARG:HD2	1:D:438:SER:O	1.97	0.64
1:B:500:MET:HE1	1:B:517:ILE:HA	1.80	0.64
1:A:491:ASP:HB2	1:A:500:MET:HE1	1.80	0.64
1:A:498:LYS:CB	4:A:52:HOH:O	2.34	0.64
1:C:321:LEU:HD13	1:D:321:LEU:CD1	2.28	0.64
1:C:302:HIS:HD2	1:C:303:LEU:HD23	1.62	0.64
1:D:328:LEU:HD12	1:D:328:LEU:O	1.98	0.64
1:D:436:THR:HG23	3:D:803:ADP:O1B	1.98	0.64
1:A:366:MET:HE2	1:A:366:MET:HA	1.80	0.63
1:A:522:VAL:HG13	1:A:528:LEU:HB2	1.80	0.63
1:C:485:TYR:HB3	4:C:111:HOH:O	1.98	0.63
1:C:522:VAL:HG13	1:C:528:LEU:HB2	1.78	0.63
1:B:537:MET:C	1:B:539:ARG:H	2.06	0.63
1:D:338:LEU:O	1:D:341:THR:N	2.32	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:D:487:GLU:N	4:D:113:HOH:O	2.30	0.63
1:A:335:ARG:NH2	1:A:424:ASP:OD2	2.32	0.63
1:B:447:VAL:HG23	1:B:450:SER:H	1.63	0.63
1:D:537:MET:O	1:D:539:ARG:N	2.32	0.63
1:A:407:SER:N	1:A:410:ASP:OD2	2.32	0.62
1:D:408:GLN:HG3	1:D:451:VAL:O	1.98	0.62
1:D:537:MET:HA	1:D:537:MET:HE2	1.81	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:381:GLN:HG2	1:D:391:MET:SD	2.39	0.62
1:B:643:MET:HE3	1:B:663:PHE:HE2	1.63	0.62
1:D:567:GLU:O	1:D:568:LYS:HB2	2.00	0.62
1:D:614:LEU:CD1	1:D:667:VAL:HG13	2.28	0.62
1:A:367:CYS:CA	4:A:94:HOH:O	2.43	0.62
1:B:528:LEU:HG	1:B:532:MET:CE	2.28	0.62
1:C:515:SER:O	1:C:516:ASN:HB2	2.00	0.62
1:D:358:PRO:HB3	1:D:650:PHE:HZ	1.64	0.62
1:D:520:GLU:HG3	1:D:531:LEU:HD21	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:310:LEU:O	1:D:312:ARG:N	2.33	0.61
1:D:366:MET:O	1:D:651:GLN:N	2.20	0.61
1:B:452:GLY:O	1:B:455:PRO:HD2	2.00	0.61
1:D:336:LYS:HG2	1:D:337:GLU:N	2.13	0.61
1:D:615:GLN:CG	1:D:670:CYS:SG	2.88	0.61
1:A:376:SER:HA	1:A:401:VAL:HG23	1.81	0.61
1:A:411:ILE:H	1:A:411:ILE:HD12	1.65	0.61
1:A:547:ASN:C	1:A:549:ARG:N	2.56	0.61
1:A:500:MET:CE	1:A:517:ILE:HA	2.30	0.61
1:A:514:VAL:O	1:A:517:ILE:HD11	2.00	0.61
1:B:491:ASP:HB2	1:B:500:MET:HE1	1.83	0.61
1:C:528:LEU:HG	1:C:532:MET:HE2	1.83	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:O	1:D:383:ILE:CG2	2.48	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:A:323:THR:O	1:A:327:GLN:HB2	2.01	0.60
1:B:388:LYS:NZ	1:B:388:LYS:HB3	2.16	0.60
1:C:346:ARG:HG3	1:C:346:ARG:NH1	2.16	0.60
1:C:352:PHE:CD2	1:C:400:GLN:HB3	2.36	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:A:517:ILE:H	1:A:517:ILE:CD1	2.12	0.60
1:C:381:GLN:HB3	4:C:82:HOH:O	1.99	0.60
1:C:542:ALA:HB3	1:C:549:ARG:CB	2.32	0.60
1:C:545:ALA:C	1:C:547:ASN:H	2.09	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:C:387:ALA:HB1	1:C:391:MET:CE	2.29	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:D:477:ILE:N	4:D:110:HOH:O	2.30	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:A:569:GLN:O	1:A:570:GLU:O	2.19	0.59
1:B:357:PRO:HD3	1:B:404:PRO:CA	2.28	0.59
1:A:324:CYS:O	1:A:328:LEU:N	2.35	0.59
1:A:537:MET:HA	1:A:537:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:LEU:O	1:D:298:THR:N	2.35	0.59
1:A:517:ILE:HD12	1:A:517:ILE:N	2.17	0.59
1:C:315:GLU:O	1:C:318:ALA:HB3	2.01	0.59
1:C:512:ILE:HD13	1:C:632:MET:HE2	1.83	0.59
1:D:370:TRP:CZ3	1:D:380:LEU:HB3	2.37	0.59
1:D:370:TRP:CZ3	1:D:380:LEU:CB	2.86	0.59
1:A:353:CYS:HB3	1:A:401:VAL:HG13	1.84	0.59
1:A:545:ALA:O	1:A:546:GLY:C	2.46	0.59
1:D:433:TYR:C	1:D:433:TYR:HD2	2.11	0.59
1:A:349:ILE:HG22	1:A:349:ILE:O	2.03	0.59
1:A:352:PHE:CE1	1:A:414:MET:HG2	2.38	0.59
1:D:387:ALA:O	1:D:391:MET:HB3	2.03	0.59
1:B:482:LEU:HD12	1:B:482:LEU:C	2.28	0.58
1:C:351:VAL:HG21	1:C:667:VAL:HG11	1.85	0.58
1:D:380:LEU:HD23	1:D:394:GLN:CB	2.32	0.58
1:C:599:ILE:CG2	1:C:600:ASN:N	2.66	0.58
1:A:542:ALA:C	1:A:544:THR:N	2.61	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:C:481:PHE:N	1:C:481:PHE:CD1	2.70	0.58
1:C:350:ARG:HG3	4:C:87:HOH:O	2.04	0.58
1:C:537:MET:C	1:C:539:ARG:N	2.58	0.58
1:D:623:ARG:HG3	1:D:623:ARG:NH1	2.17	0.58
1:B:364:ASN:N	1:B:364:ASN:HD22	2.00	0.58
1:D:658:VAL:O	1:D:662:ARG:HG3	2.04	0.58
1:A:586:SER:HB3	1:A:587:PRO:CD	2.30	0.58
1:B:541:THR:HB	1:B:550:SER:HB2	1.85	0.58
1:D:382:SER:O	1:D:388:LYS:HD3	2.03	0.58
1:D:599:ILE:CG2	1:D:600:ASN:H	1.97	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:B:373:HIS:O	1:B:377:THR:HB	2.05	0.57
1:B:491:ASP:HB2	1:B:500:MET:CE	2.35	0.57
1:C:373:HIS:O	1:C:374:ASP:HB3	2.03	0.57
1:D:489:LEU:HD11	1:D:626:LYS:HG3	1.86	0.57
1:C:360:GLU:N	1:C:360:GLU:OE1	2.36	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:B:614:LEU:HD13	1:B:667:VAL:O	2.05	0.57
1:A:432:ALA:HB2	1:A:444:MET:HG2	1.86	0.57
1:B:380:LEU:HD23	1:B:394:GLN:CB	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:THR:CG2	1:B:519:GLU:HG3	2.35	0.57
1:C:445:ASP:CG	4:C:107:HOH:O	2.47	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
1:A:542:ALA:C	1:A:544:THR:H	2.11	0.57
1:A:358:PRO:HB3	1:A:650:PHE:HZ	1.67	0.56
1:C:436:THR:HG23	3:C:802:ADP:O1B	2.05	0.56
1:D:654:PHE:O	1:D:658:VAL:HG13	2.05	0.56
1:B:416:SER:OG	1:B:417:PRO:HD3	2.05	0.56
1:C:440:LYS:HE3	3:C:802:ADP:PB	2.45	0.56
1:D:366:MET:O	4:D:121:HOH:O	2.18	0.56
1:D:398:PHE:HZ	1:D:661:LEU:HD22	1.69	0.56
1:A:396:PHE:HD2	1:A:665:ALA:HB2	1.70	0.56
1:A:414:MET:HA	1:A:414:MET:CE	2.33	0.56
1:A:427:ASN:HB3	1:A:634:SER:OG	2.05	0.56
1:B:602:SER:HB2	4:B:68:HOH:O	2.05	0.56
1:C:454:ILE:HG23	1:C:578:LEU:HD13	1.86	0.56
1:D:367:CYS:HA	1:D:649:PRO:O	2.05	0.56
1:D:457:THR:O	1:D:461:LEU:HB2	2.04	0.56
1:D:527:HIS:NE2	1:D:531:LEU:HD11	2.21	0.56
1:B:650:PHE:O	4:B:81:HOH:O	2.17	0.56
1:D:543:SER:HA	1:D:547:ASN:CB	2.35	0.56
1:A:486:ASN:HD21	1:A:599:ILE:HD13	1.70	0.56
1:C:317:GLN:O	1:C:321:LEU:HB2	2.06	0.56
1:C:569:GLN:O	1:C:570:GLU:O	2.24	0.56
1:D:522:VAL:CG1	1:D:528:LEU:HD22	2.36	0.56
1:D:599:ILE:C	1:D:601:ARG:H	2.13	0.56
1:B:547:ASN:C	1:B:549:ARG:N	2.63	0.56
1:C:480:THR:HG22	1:C:519:GLU:HG3	1.86	0.56
1:D:607:THR:HG22	1:D:608:ASN:N	2.21	0.56
1:A:436:THR:N	1:A:585:GLU:OE1	2.34	0.56
1:A:458:VAL:HG21	1:A:532:MET:HE1	1.87	0.56
1:C:380:LEU:C	1:C:381:GLN:HG3	2.31	0.56
1:C:480:THR:CG2	1:C:519:GLU:HG3	2.35	0.56
1:D:414:MET:HA	1:D:414:MET:CE	2.33	0.56
1:C:655:GLN:O	1:C:658:VAL:HG22	2.05	0.56
1:D:382:SER:N	1:D:391:MET:HE1	2.18	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:A:363:GLU:C	1:A:364:ASN:HD22	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:O	1:B:381:GLN:HG3	2.06	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:A:547:ASN:O	1:A:547:ASN:CG	2.48	0.55
1:B:379:GLU:HG3	1:B:394:GLN:C	2.30	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:A:653:CYS:O	1:A:654:PHE:C	2.49	0.55
1:D:376:SER:HA	1:D:401:VAL:HG23	1.88	0.55
1:A:328:LEU:HD12	1:A:328:LEU:O	2.06	0.55
1:B:366:MET:O	1:B:651:GLN:N	2.29	0.55
1:C:556:VAL:HG22	1:C:579:VAL:HG22	1.88	0.55
1:B:329:PHE:CE2	1:B:568:LYS:HE2	2.41	0.55
1:C:444:MET:O	1:C:454:ILE:HG13	2.06	0.55
3:C:802:ADP:PA	4:C:37:HOH:O	2.61	0.55
1:D:369:THR:HA	4:D:96:HOH:O	2.06	0.55
1:D:565:HIS:O	1:D:569:GLN:N	2.39	0.55
1:D:631:LEU:O	1:D:632:MET:C	2.50	0.55
1:B:567:GLU:O	1:B:568:LYS:HB2	2.05	0.55
1:C:433:TYR:CD2	1:C:433:TYR:C	2.84	0.55
1:D:310:LEU:C	1:D:312:ARG:N	2.63	0.55
1:D:537:MET:C	1:D:539:ARG:N	2.55	0.55
1:D:296:LEU:C	1:D:296:LEU:HD23	2.31	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: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:D:652:ASP:OD1	4:D:121:HOH:O	2.18	0.55
1:B:543:SER:HA	1:B:547:ASN:HA	1.88	0.55
1:A:408:GLN:OE1	1:A:408:GLN:HA	2.06	0.55
1:C:488:VAL:HB	4:C:111:HOH:O	2.07	0.55
1:A:643:MET:HE3	1:A:663:PHE:CE2	2.40	0.55
1:B:380:LEU:C	1:B:381:GLN:HG3	2.32	0.55
1:C:469:ARG:NH1	1:C:474:GLU:OE2	2.40	0.55
1:D:369:THR:O	1:D:380:LEU:HA	2.07	0.55
1:C:411:ILE:HD12	1:C:411:ILE:H	1.71	0.54
1:B:393:GLN:O	1:B:394:GLN:HG2	2.06	0.54
1:B:363:GLU:C	1:B:364:ASN:HD22	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LYS:HE3	1:C:424:ASP:HB3	1.89	0.54
1:C:537:MET:O	1:C:539:ARG:N	2.40	0.54
1:D:411:ILE:HG23	1:D:644:PHE:CZ	2.43	0.54
1:A:433:TYR:C	1:A:433:TYR:CD2	2.84	0.54
1:B:533:HIS:O	1:B:534:THR:C	2.48	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:A:360:GLU:N	1:A:360:GLU:OE1	2.40	0.54
1:B:544:THR:HG23	1:B:545:ALA:H	1.72	0.54
1:D:622:TYR:CD1	1:D:632:MET:HG3	2.43	0.54
1:C:398:PHE:CE2	1:C:664:ALA:HB1	2.42	0.54
1:D:385:ALA:N	4:D:83:HOH:O	2.40	0.54
1:D:397:SER:N	4:D:25:HOH:O	1.73	0.54
1:D:650:PHE:HB2	1:D:653:CYS:SG	2.47	0.54
1:A:515:SER:O	1:A:516:ASN:HB2	2.08	0.54
1:D:399:ASP:O	1:D:400:GLN:HB2	2.08	0.54
1:C:324:CYS:SG	1:D:325:LYS:HG2	2.48	0.54
1:D:522:VAL:CG1	1:D:528:LEU:HB2	2.37	0.54
1:A:432:ALA:O	1:A:581:LEU:HB2	2.07	0.54
1:A:530:HIS:O	1:A:533:HIS:N	2.41	0.54
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:D:308:GLU:O	1:D:312:ARG:HD2	2.08	0.54
1:D:606:LEU:HD13	1:D:606:LEU:C	2.33	0.54
1:A:321:LEU:HD12	1:B:321:LEU:HD21	1.88	0.54
1:B:347:GLY:O	1:B:348:ASN:CB	2.51	0.54
1:D:346:ARG:HG3	1:D:346:ARG:HH11	1.73	0.54
1:D:599:ILE:O	1:D:601:ARG:N	2.41	0.54
1:D:491:ASP:OD1	1:D:493:LEU:N	2.26	0.53
1:A:364:ASN:HD22	1:A:364:ASN:N	2.04	0.53
1:A:435:GLN:CA	1:A:585:GLU:OE1	2.56	0.53
1:B:333:MET:O	1:B:336:LYS:HB3	2.09	0.53
1:B:607:THR:HG23	1:B:663:PHE:CE1	2.44	0.53
1:D:653:CYS:O	1:D:654:PHE:C	2.51	0.53
1:B:433:TYR:C	1:B:433:TYR:CD2	2.86	0.53
1:D:396:PHE:HA	4:D:25:HOH:O	2.09	0.53
1:A:428:ILE:HG22	1:A:429:CYS:N	2.24	0.53
1:C:299:GLU:O	1:C:300:VAL:C	2.52	0.53
1:D:346:ARG:HG3	1:D:346:ARG:NH1	2.24	0.53
1:B:522:VAL:HG21	1:B:528:LEU:HD22	1.90	0.53
1:B:622:TYR:CD1	1:B:632:MET:HG3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ASN:HD22	1:D:364:ASN:N	2.07	0.53
1:A:432:ALA:HB1	1:A:440:LYS:HB3	1.91	0.53
1:D:352:PHE:CZ	1:D:414:MET:HG2	2.43	0.53
1:D:611:LEU:O	1:D:615:GLN:HG3	2.08	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:B:442:TYR:O	1:B:446:GLY:HA2	2.08	0.53
1:C:329:PHE:HD2	1:C:330:GLN:OE1	1.92	0.53
1:B:379:GLU:HG3	1:B:394:GLN:O	2.09	0.52
1:B:452:GLY:C	1:B:455:PRO:HD2	2.33	0.52
1:D:565:HIS:O	1:D:569:GLN:O	2.27	0.52
1:B:512:ILE:HD13	1:B:632:MET:HE2	1.90	0.52
1:D:347:GLY:O	1:D:348:ASN:CB	2.43	0.52
1:D:653:CYS:O	1:D:656:GLU:N	2.37	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:B:411:ILE:HG23	1:B:644:PHE:CZ	2.44	0.52
1:D:300:VAL:HG12	1:D:304:ARG:NH1	2.24	0.52
1:D:310:LEU:C	1:D:312:ARG:H	2.17	0.52
1:D:356:ARG:HG3	1:D:649:PRO:HD3	1.90	0.52
1:B:533:HIS:CE1	4:B:138:HOH:O	2.63	0.52
1:D:296:LEU:C	1:D:298:THR:H	2.17	0.52
1:D:382:SER:O	1:D:384:ASP:N	2.43	0.52
1:A:537:MET:C	1:A:539:ARG:N	2.67	0.52
1:B:382:SER:C	1:B:384:ASP:H	2.18	0.52
1:D:491:ASP:OD1	1:D:491:ASP:C	2.50	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:D:521:THR:O	1:D:521:THR:OG1	2.21	0.52
1:A:536:LYS:HZ1	1:A:539:ARG:NH1	2.07	0.52
1:B:418:LEU:CD1	1:B:642:LEU:HD13	2.39	0.52
1:C:347:GLY:O	1:C:348:ASN:CB	2.51	0.52
1:B:454:ILE:HB	1:B:455:PRO:HD3	1.92	0.51
1:B:485:TYR:HD1	1:B:549:ARG:NH1	2.08	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:665:ALA:HA	1:C:668:ASN:ND2	2.25	0.51
1:D:444:MET:O	1:D:454:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:ILE:HD12	1:C:517:ILE:N	2.25	0.51
1:C:542:ALA:CA	1:C:545:ALA:HB3	2.32	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:D:663:PHE:O	1:D:667:VAL:HG23	2.11	0.51
1:A:606:LEU:HD13	1:A:606:LEU:C	2.35	0.51
1:A:622:TYR:CD1	1:A:632:MET:HG3	2.45	0.51
1:B:388:LYS:HB3	1:B:388:LYS:HZ3	1.76	0.51
1:D:500:MET:HE1	1:D:517:ILE:CG2	2.40	0.51
1:D:526:ASN:O	1:D:529:ARG:N	2.43	0.51
1:B:414:MET:HA	1:B:414:MET:CE	2.37	0.51
1:C:321:LEU:O	1:C:322:GLU:C	2.52	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:408:GLN:HB2	1:B:456:ARG:HH21	1.76	0.51
1:D:382:SER:C	1:D:384:ASP:N	2.69	0.51
1:A:334:GLU:OE1	1:B:335:ARG:HD2	2.11	0.51
1:B:484:ILE:HD12	1:B:627:LEU:HD13	1.93	0.51
1:B:544:THR:HG23	1:B:545:ALA:N	2.26	0.51
1:B:548:GLU:O	1:B:552:ARG:HB2	2.10	0.51
1:D:368:CYS:SG	1:D:654:PHE:HD1	2.33	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:433:TYR:CD2	1:D:434:GLY:N	2.79	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:354:ARG:O	1:D:646:ASN:HA	2.11	0.51
1:B:514:VAL:O	1:B:517:ILE:HD11	2.11	0.50
1:B:623:ARG:HG3	1:B:623:ARG:NH1	2.21	0.50
1:D:296:LEU:C	1:D:298:THR:N	2.70	0.50
1:D:328:LEU:C	1:D:328:LEU:CD1	2.82	0.50
1:D:370:TRP:CZ3	1:D:380:LEU:HB2	2.45	0.50
1:D:411:ILE:HD12	1:D:411:ILE:H	1.76	0.50
1:D:533:HIS:O	1:D:534:THR:C	2.52	0.50
1:A:631:LEU:O	1:A:632:MET:C	2.55	0.50
1:B:537:MET:C	1:B:539:ARG:N	2.65	0.50
1:B:542:ALA:HB3	1:B:549:ARG:CB	2.38	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:B:552:ARG:HD2	1:B:599:ILE:N	2.26	0.50
1:D:436:THR:OG1	1:D:585:GLU:OE2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:MET:HE1	1:D:517:ILE:HG23	1.93	0.50
1:A:567:GLU:O	1:A:568:LYS:HB2	2.12	0.50
1:A:585:GLU:HA	1:A:656:GLU:OE1	2.11	0.50
1:B:403:HIS:HB2	1:B:404:PRO:HD2	1.93	0.50
1:B:611:LEU:O	1:B:615:GLN:HG3	2.12	0.50
1:C:496:GLU:O	1:C:496:GLU:HG2	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:C:500:MET:HE2	1:C:517:ILE:HG23	1.92	0.50
1:A:498:LYS:N	4:A:52:HOH:O	2.42	0.50
1:B:481:PHE:N	1:B:481:PHE:CD1	2.79	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: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:C:564:ARG:HG2	1:C:571:ILE:CG2	2.42	0.50
1:D:299:GLU:O	1:D:302:HIS:N	2.45	0.50
1:D:408:GLN:OE1	1:D:408:GLN:HA	2.12	0.50
1:D:547:ASN:C	1:D:549:ARG:H	2.20	0.50
1:D:580:ASP:OD1	1:D:580:ASP:C	2.55	0.50
1:B:437:GLY:N	3:B:801:ADP:O1B	2.40	0.50
1:B:384:ASP:HB3	1:B:387:ALA:HB3	1.92	0.50
1:D:398:PHE:C	1:D:400:GLN:H	2.20	0.50
1:D:485:TYR:CD1	1:D:549:ARG:NH1	2.79	0.50
1:B:517:ILE:HD12	1:B:517:ILE:H	1.77	0.49
1:B:604:SER:O	1:B:607:THR:HB	2.12	0.49
1:A:503:ARG:HD3	1:A:513:TYR:CE2	2.47	0.49
1:A:539:ARG:C	1:A:541:THR:N	2.67	0.49
1:C:369:THR:CB	1:C:381:GLN:HB2	2.40	0.49
1:B:364:ASN:N	1:B:364:ASN:ND2	2.60	0.49
1:B:522:VAL:CG2	1:B:528:LEU:HD13	2.42	0.49
1:B:657:SER:O	1:B:661:LEU:HG	2.12	0.49
1:A:541:THR:C	1:A:543:SER:H	2.21	0.49
1:C:485:TYR:CE1	1:C:549:ARG:HD2	2.47	0.49
1:C:662:ARG:HG2	1:C:662:ARG:HH11	1.77	0.49
1:B:662:ARG:HG2	1:B:662:ARG:NH1	2.24	0.49
1:C:324:CYS:SG	1:D:324:CYS:SG	3.09	0.49
1:C:432:ALA:HB2	1:C:444:MET:HG2	1.95	0.49
1:C:654:PHE:O	1:C:658:VAL:HG13	2.12	0.49
1:A:503:ARG:HD3	1:A:513:TYR:HE2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:GLU:O	1:A:552:ARG:HB2	2.12	0.49
1:C:481:PHE:N	1:C:481:PHE:HD1	2.09	0.49
1:D:454:ILE:HB	1:D:455:PRO:HD3	1.94	0.49
1:A:536:LYS:NZ	1:A:539:ARG:HH11	2.11	0.49
1:B:469:ARG:HD3	1:B:474:GLU:OE1	2.12	0.49
1:C:351:VAL:HG23	1:C:667:VAL:HG11	1.94	0.49
1:A:346:ARG:NH1	1:A:346:ARG:CG	2.70	0.49
1:B:469:ARG:NH1	1:B:474:GLU:OE2	2.46	0.49
1:C:380:LEU:O	1:C:381:GLN:HG3	2.13	0.49
1:A:522:VAL:CG2	1:A:528:LEU:HD22	2.39	0.49
1:D:339:HIS:C	1:D:339:HIS:CD2	2.90	0.49
1:A:357:PRO:HD3	1:A:404:PRO:CA	2.42	0.48
1:A:383:ILE:CG2	1:A:383:ILE:O	2.60	0.48
1:B:411:ILE:HD12	1:B:411:ILE:H	1.78	0.48
1:B:432:ALA:O	1:B:581:LEU:HB2	2.12	0.48
1:A:482:LEU:C	1:A:482:LEU:HD12	2.38	0.48
1:B:539:ARG:NH2	4:B:67:HOH:O	2.46	0.48
1:C:370:TRP:CZ2	1:C:649:PRO:HA	2.48	0.48
1:D:388:LYS:HG3	1:D:391:MET:HE3	1.94	0.48
1:D:583:GLY:HA3	1:D:585:GLU:OE2	2.14	0.48
1:D:603:LEU:O	1:D:603:LEU:HD12	2.13	0.48
1:A:352:PHE:HE2	1:A:399:ASP:HB2	1.78	0.48
1:A:527:HIS:HD2	1:A:527:HIS:O	1.96	0.48
1:B:328:LEU:HD12	1:B:328:LEU:O	2.14	0.48
1:B:346:ARG:HG3	1:B:346:ARG:NH1	2.25	0.48
1:B:429:CYS:SG	1:B:634:SER:HB3	2.53	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:C:651:GLN:O	1:C:654:PHE:CB	2.61	0.48
1:D:418:LEU:HD12	1:D:642:LEU:HD13	1.94	0.48
1:D:430:ILE:N	1:D:430:ILE:HD13	2.28	0.48
1:A:670:CYS:C	1:A:672:MET:N	2.65	0.48
1:B:515:SER:O	1:B:516:ASN:HB2	2.14	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:A:449:GLU:H	1:A:449:GLU:CD	2.22	0.48
1:A:537:MET:C	1:A:539:ARG:H	2.20	0.48
1:B:440:LYS:HZ3	1:B:583:GLY:HA2	1.77	0.48
1:C:485:TYR:HE1	1:C:549:ARG:HA	1.77	0.48
1:A:365:ARG:NH1	1:A:650:PHE:CD1	2.82	0.48
1:B:428:ILE:HG22	1:B:429:CYS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:GLN:O	1:C:320:GLU:CB	2.61	0.48
1:D:329:PHE:C	1:D:329:PHE:CD2	2.91	0.48
1:D:527:HIS:CD2	1:D:527:HIS:O	2.66	0.48
1:D:654:PHE:CD2	1:D:655:GLN:N	2.82	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:B:521:THR:O	1:B:521:THR:OG1	2.28	0.48
1:C:301:VAL:O	1:C:302:HIS:C	2.57	0.48
1:C:319:ALA:C	1:C:321:LEU:N	2.65	0.48
1:C:522:VAL:HG11	1:C:528:LEU:HB2	1.96	0.48
1:D:308:GLU:O	1:D:309:GLU:C	2.57	0.48
1:D:486:ASN:O	1:D:487:GLU:HB2	2.13	0.48
1:A:564:ARG:HG2	1:A:571:ILE:CG2	2.41	0.48
1:A:623:ARG:HG3	1:A:623:ARG:HH11	1.78	0.48
1:A:653:CYS:O	1:A:655:GLN:N	2.47	0.48
1:C:382:SER:C	1:C:384:ASP:H	2.21	0.48
1:D:542:ALA:HB3	1:D:549:ARG:HB3	1.96	0.48
1:A:605:GLU:HA	1:A:608:ASN:HD22	1.79	0.48
1:B:387:ALA:C	1:B:391:MET:HE3	2.39	0.48
1:D:370:TRP:HE1	1:D:649:PRO:CB	2.27	0.48
1:B:355:ILE:HG12	1:B:647:VAL:CG2	2.43	0.47
1:C:469:ARG:HD3	1:C:474:GLU:OE1	2.14	0.47
1:A:447:VAL:HG23	1:A:450:SER:H	1.80	0.47
1:A:486:ASN:O	1:A:487:GLU:HB2	2.14	0.47
1:A:500:MET:HE1	1:A:517:ILE:CG2	2.44	0.47
1:A:613:LEU:O	1:A:616:LYS:N	2.36	0.47
1:A:656:GLU:O	1:A:657:SER:C	2.57	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: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
1:D:399:ASP:O	1:D:400:GLN:CB	2.61	0.47
1:D:429:CYS:C	1:D:430:ILE:HD13	2.39	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:363:GLU:C	1:D:364:ASN:HD22	2.21	0.47
1:D:469:ARG:C	1:D:471:LEU:H	2.23	0.47
1:D:496:GLU:O	1:D:497:GLN:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:653:CYS:O	1:C:654:PHE:C	2.56	0.47
1:D:365:ARG:O	4:D:95:HOH:O	2.20	0.47
1:D:491:ASP:HB2	1:D:500:MET:HE1	1.95	0.47
1:D:548:GLU:O	1:D:552:ARG:HB2	2.14	0.47
1:A:361:SER:C	1:A:362:GLU:HG3	2.38	0.47
1:B:320:GLU:OE2	1:B:323:THR:HB	2.15	0.47
1:B:360:GLU:OE1	1:B:360:GLU:N	2.46	0.47
1:B:396:PHE:CG	1:B:661:LEU:HB3	2.50	0.47
1:B:469:ARG:C	1:B:471:LEU:H	2.23	0.47
1:D:496:GLU:O	1:D:496:GLU:HG2	2.15	0.47
1:A:324:CYS:SG	1:B:324:CYS:SG	3.13	0.47
1:A:670:CYS:O	1:A:672:MET:N	2.47	0.47
1:D:341:THR:O	1:D:342:VAL:C	2.57	0.47
1:A:656:GLU:O	1:A:659:LYS:N	2.48	0.47
1:B:352:PHE:CZ	1:B:414:MET:HG3	2.50	0.47
1:B:384:ASP:C	1:B:386:GLN:N	2.71	0.47
1:B:426:TYR:CD2	1:B:638:ASN:HB3	2.50	0.47
1:C:500:MET:CE	1:C:517:ILE:HA	2.45	0.47
1:D:359:LEU:HB2	1:D:362:GLU:OE1	2.15	0.47
1:D:485:TYR:CE1	1:D:549:ARG:HD2	2.50	0.47
1:A:614:LEU:CD1	1:A:667:VAL:HG13	2.45	0.47
1:C:304:ARG:HH21	1:D:299:GLU:CD	2.22	0.47
1:C:454:ILE:HG23	1:C:578:LEU:CD1	2.45	0.47
1:C:496:GLU:O	1:C:497:GLN:C	2.57	0.47
1:D:370:TRP:N	4:D:96:HOH:O	1.98	0.47
1:D:373:HIS:O	1:D:374:ASP:HB3	2.14	0.47
1:D:480:THR:HG22	1:D:519:GLU:HG3	1.95	0.47
1:A:527:HIS:O	1:A:527:HIS:CD2	2.68	0.46
1:A:623:ARG:HG3	1:A:623:ARG:NH1	2.30	0.46
1:B:353:CYS:HB2	1:B:398:PHE:CD2	2.50	0.46
1:B:382:SER:C	1:B:384:ASP:N	2.73	0.46
1:C:370:TRP:HZ2	1:C:649:PRO:HA	1.81	0.46
1:C:447:VAL:HG23	1:C:450:SER:H	1.79	0.46
1:C:486:ASN:HD21	1:C:599:ILE:HG13	1.81	0.46
1:C:537:MET:HA	1:C:537:MET:CE	2.43	0.46
1:C:567:GLU:O	1:C:568:LYS:HB2	2.15	0.46
1:D:335:ARG:HH22	1:D:424:ASP:CG	2.23	0.46
1:A:495:ASN:C	1:A:497:GLN:H	2.24	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:488:VAL:HB	4:D:113:HOH:O	2.15	0.46
1:D:537:MET:HA	1:D:537:MET:HE3	1.97	0.46
1:A:442:TYR:O	1:A:446:GLY:HA2	2.15	0.46
1:A:517:ILE:CD1	1:A:517:ILE:N	2.78	0.46
1:A:522:VAL:HG22	1:A:528:LEU:HD13	1.96	0.46
1:C:462:PHE:CZ	1:C:477:ILE:HD12	2.50	0.46
1:D:316:GLN:O	1:D:317:GLN:C	2.57	0.46
1:D:335:ARG:C	1:D:335:ARG:HE	2.24	0.46
1:D:360:GLU:N	1:D:360:GLU:OE1	2.48	0.46
1:D:416:SER:OG	1:D:417:PRO:HD3	2.15	0.46
1:D:599:ILE:C	1:D:601:ARG:N	2.73	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:C:387:ALA:O	1:C:390:LYS:N	2.48	0.46
1:C:514:VAL:HG12	1:C:517:ILE:HG13	1.97	0.46
1:D:549:ARG:O	1:D:550:SER:C	2.59	0.46
1:D:566:ALA:O	1:D:567:GLU:C	2.59	0.46
1:A:364:ASN:N	1:A:364:ASN:ND2	2.64	0.46
1:B:526:ASN:O	1:B:529:ARG:N	2.49	0.46
1:C:385:ALA:HA	1:C:388:LYS:NZ	2.28	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:B:359:LEU:N	1:B:362:GLU:OE1	2.41	0.46
1:C:310:LEU:C	1:C:312:ARG:N	2.73	0.46
1:C:435:GLN:OE1	1:C:656:GLU:CB	2.63	0.46
1:A:500:MET:HE1	1:A:517:ILE:HG23	1.96	0.46
1:B:350:ARG:NE	4:B:88:HOH:O	2.49	0.46
1:C:454:ILE:CG1	1:C:578:LEU:HD13	2.46	0.46
1:C:631:LEU:C	1:C:633:PRO:HD2	2.41	0.46
1:D:337:GLU:HA	1:D:337:GLU:OE1	2.16	0.46
1:D:373:HIS:CD2	1:D:395:ILE:HD11	2.51	0.46
1:D:403:HIS:C	1:D:405:LEU:H	2.23	0.46
1:A:543:SER:HA	1:A:547:ASN:HB2	1.96	0.46
1:B:366:MET:HA	1:B:366:MET:HE2	1.97	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:A:607:THR:HG22	1:A:608:ASN:N	2.31	0.45
1:B:353:CYS:HB2	1:B:398:PHE:CE2	2.52	0.45
1:B:541:THR:HG21	1:B:550:SER:CB	2.46	0.45
1:C:296:LEU:HD23	1:C:297:SER:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:LYS:HZ3	1:C:388:LYS:HB3	1.81	0.45
1:D:352:PHE:CE2	1:D:400:GLN:HB3	2.51	0.45
1:A:536:LYS:HZ1	1:A:539:ARG:HH11	1.64	0.45
1:C:296:LEU:HD21	1:D:296:LEU:CD2	2.46	0.45
1:C:319:ALA:C	1:C:321:LEU:H	2.24	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:615:GLN:O	1:A:617:GLN:N	2.49	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:B:534:THR:O	1:B:535:ALA:C	2.59	0.45
1:C:416:SER:OG	1:C:417:PRO:HD3	2.16	0.45
1:C:428:ILE:HG22	1:C:429:CYS:N	2.32	0.45
1:D:310:LEU:O	1:D:311:LEU:C	2.59	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:359:LEU:O	1:D:360:GLU:C	2.57	0.45
1:A:611:LEU:O	1:A:615:GLN:HG3	2.16	0.45
1:B:438:SER:N	3:B:801:ADP:O2B	2.50	0.45
1:B:470:ASN:OD1	4:B:46:HOH:O	2.21	0.45
1:D:378:VAL:HG22	1:D:379:GLU:N	2.30	0.45
1:D:380:LEU:O	1:D:394:GLN:CB	2.64	0.45
1:D:398:PHE:C	1:D:400:GLN:N	2.73	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: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:C:500:MET:CE	1:C:517:ILE:HG23	2.47	0.45
1:D:355:ILE:CG2	1:D:404:PRO:HD3	2.45	0.45
1:A:357:PRO:HB3	1:A:404:PRO:HB3	1.99	0.45
1:A:398:PHE:CE2	1:A:664:ALA:CB	3.00	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:C:383:ILE:O	1:C:383:ILE:CG2	2.64	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:352:PHE:CZ	1:A:414:MET:CG	3.00	0.45
1:C:302:HIS:CD2	1:C:303:LEU:HD23	2.49	0.45
1:D:360:GLU:O	1:D:363:GLU:HG3	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:MET:N	1:C:633:PRO:HD2	2.32	0.44
1:D:415:VAL:O	1:D:416:SER:C	2.60	0.44
1:D:427:ASN:C	1:D:428:ILE:HD13	2.43	0.44
1:D:512:ILE:HG23	1:D:513:TYR:N	2.32	0.44
1:A:374:ASP:OD2	1:A:375:GLU:N	2.50	0.44
1:A:396:PHE:CA	4:A:100:HOH:O	2.61	0.44
1:B:324:CYS:O	1:B:327:GLN:N	2.47	0.44
1:B:352:PHE:CE2	1:B:400:GLN:HB3	2.52	0.44
1:C:567:GLU:O	1:C:567:GLU:HG2	2.17	0.44
1:C:631:LEU:O	1:C:632:MET:C	2.61	0.44
1:D:303:LEU:O	1:D:304:ARG:C	2.60	0.44
1:D:485:TYR:HD2	1:D:486:ASN:HB2	1.82	0.44
1:C:296:LEU:HD23	1:C:296:LEU:C	2.42	0.44
1:B:486:ASN:ND2	1:B:599:ILE:HG13	2.32	0.44
1:A:440:LYS:O	1:A:443:THR:N	2.50	0.44
1:A:632:MET:HB3	1:A:633:PRO:CD	2.48	0.44
1:B:383:ILE:O	1:B:383:ILE:CG2	2.66	0.44
1:B:394:GLN:HE21	1:B:654:PHE:HZ	1.64	0.44
1:B:579:VAL:HG21	1:B:631:LEU:HD11	1.98	0.44
1:C:367:CYS:HA	1:C:649:PRO:O	2.17	0.44
1:C:523:LEU:O	1:C:524:ASP:HB3	2.17	0.44
1:C:643:MET:HE3	1:C:663:PHE:CE2	2.53	0.44
1:A:398:PHE:C	1:A:400:GLN:H	2.26	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:D:656:GLU:O	1:D:659:LYS:N	2.50	0.44
1:B:605:GLU:HG3	1:B:625:SER:HB3	1.99	0.44
1:C:376:SER:HA	1:C:401:VAL:HG23	1.99	0.44
1:C:469:ARG:C	1:C:471:LEU:H	2.26	0.44
1:D:381:GLN:HB3	1:D:391:MET:HE1	1.98	0.44
1:B:415:VAL:C	1:B:417:PRO:CD	2.91	0.44
1:B:564:ARG:HG2	1:B:571:ILE:HG22	1.99	0.44
1:C:640:LYS:N	1:C:640:LYS:HD2	2.33	0.44
1:B:361:SER:C	1:B:362:GLU:HG3	2.43	0.44
1:B:486:ASN:ND2	1:B:599:ILE:CG1	2.80	0.44
1:C:296:LEU:C	1:C:298:THR:N	2.73	0.44
1:C:501:GLU:O	1:C:514:VAL:HA	2.18	0.44
1:A:359:LEU:HB2	1:A:362:GLU:OE1	2.17	0.43
1:A:380:LEU:HD21	1:A:658:VAL:HG12	2.00	0.43
1:A:430:ILE:HD13	1:A:430:ILE:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:ILE:HG22	1:B:601:ARG:H	1.83	0.43
1:C:357:PRO:HB3	1:C:404:PRO:HB3	2.00	0.43
1:C:482:LEU:C	1:C:482:LEU:CD1	2.89	0.43
1:D:304:ARG:O	1:D:308:GLU:CD	2.60	0.43
1:D:512:ILE:HD12	1:D:512:ILE:HA	1.73	0.43
1:D:400:GLN:HG2	1:D:402:PHE:CE1	2.53	0.43
1:A:356:ARG:O	1:A:649:PRO:HG3	2.18	0.43
1:A:512:ILE:HD12	1:A:512:ILE:HA	1.78	0.43
1:D:547:ASN:C	1:D:549:ARG:N	2.75	0.43
1:A:461:LEU:HD11	1:A:561:LEU:HD11	2.01	0.43
1:B:486:ASN:HD21	1:B:599:ILE:HD11	1.83	0.43
1:C:313:CYS:O	1:C:317:GLN:HG3	2.19	0.43
1:C:458:VAL:HG21	1:C:532:MET:HE1	1.99	0.43
1:A:481:PHE:N	1:A:481:PHE:CD1	2.87	0.43
1:A:543:SER:HA	1:A:547:ASN:OD1	2.19	0.43
1:B:329:PHE:CD2	1:B:568:LYS:HE2	2.54	0.43
1:B:602:SER:O	1:B:603:LEU:C	2.61	0.43
1:C:454:ILE:HB	1:C:455:PRO:HD3	2.00	0.43
1:C:517:ILE:HD12	1:C:517:ILE:H	1.82	0.43
1:D:403:HIS:C	1:D:405:LEU:N	2.77	0.43
1:A:399:ASP:O	1:A:400:GLN:HB2	2.18	0.43
1:A:615:GLN:C	1:A:617:GLN:N	2.74	0.43
1:B:553:SER:O	4:B:67:HOH:O	2.21	0.43
1:B:653:CYS:O	1:B:654:PHE:C	2.62	0.43
1:A:661:LEU:O	1:A:662:ARG:C	2.60	0.43
1:D:436:THR:CG2	3:D:803:ADP:O1B	2.67	0.43
1:D:500:MET:HE1	1:D:517:ILE:HA	1.99	0.43
1:A:536:LYS:HA	1:A:536:LYS:HD2	1.74	0.43
1:A:622:TYR:CG	1:A:632:MET:HG3	2.54	0.43
1:B:539:ARG:O	1:B:540:ALA:C	2.62	0.43
1:C:355:ILE:HG12	1:C:647:VAL:HG23	2.01	0.43
1:C:438:SER:HB2	1:C:646:ASN:C	2.43	0.43
1:C:658:VAL:HG23	1:C:659:LYS:N	2.33	0.43
1:D:353:CYS:HB2	1:D:398:PHE:CE2	2.54	0.43
1:D:433:TYR:HB2	1:D:581:LEU:HD12	2.00	0.43
1:D:442:TYR:O	1:D:446:GLY:HA2	2.19	0.43
1:A:321:LEU:HD12	1:B:321:LEU:HD23	2.00	0.43
1:B:398:PHE:CD1	1:B:398:PHE:N	2.86	0.43
1:B:542:ALA:HB3	1:B:546:GLY:O	2.19	0.43
1:D:381:GLN:HB3	1:D:388:LYS:HD2	2.00	0.43
1:C:399:ASP:O	1:C:400:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:LEU:HD23	1:C:493:LEU:HA	1.88	0.42
1:D:330:GLN:HE21	1:D:330:GLN:HB2	1.43	0.42
1:D:419:ILE:HD12	1:D:457:THR:HG23	2.01	0.42
1:A:469:ARG:C	1:A:471:LEU:H	2.28	0.42
1:A:497:GLN:HG2	4:A:53:HOH:O	2.20	0.42
1:A:548:GLU:OE2	1:A:552:ARG:HG3	2.19	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:435:GLN:O	1:B:436:THR:C	2.62	0.42
1:B:480:THR:HG22	1:B:519:GLU:HG3	2.01	0.42
1:C:543:SER:N	1:C:550:SER:HB3	2.34	0.42
1:D:536:LYS:HZ2	1:D:539:ARG:NH1	2.17	0.42
1:D:614:LEU:HB2	1:D:670:CYS:SG	2.59	0.42
1:A:367:CYS:HA	1:A:650:PHE:HA	2.02	0.42
1:B:542:ALA:O	1:B:546:GLY:C	2.62	0.42
1:C:374:ASP:OD2	1:C:375:GLU:N	2.53	0.42
1:C:382:SER:C	1:C:384:ASP:N	2.75	0.42
1:C:435:GLN:OE1	1:C:656:GLU:HB3	2.20	0.42
1:C:517:ILE:H	1:C:517:ILE:CD1	2.32	0.42
1:C:533:HIS:O	1:C:534:THR:C	2.59	0.42
1:D:411:ILE:HG23	1:D:644:PHE:CE2	2.54	0.42
1:D:602:SER:O	1:D:603:LEU:C	2.63	0.42
1:A:352:PHE:CZ	1:A:414:MET:HG2	2.55	0.42
1:A:512:ILE:HG23	1:A:513:TYR:N	2.34	0.42
1:C:310:LEU:O	1:C:312:ARG:N	2.51	0.42
1:C:382:SER:CB	1:C:651:GLN:HE22	2.33	0.42
1:C:539:ARG:O	1:C:540:ALA:C	2.62	0.42
1:A:398:PHE:CE2	1:A:664:ALA:HB1	2.55	0.42
1:A:667:VAL:HG12	1:A:668:ASN:N	2.34	0.42
1:C:491:ASP:HB2	1:C:500:MET:SD	2.60	0.42
1:D:330:GLN:O	1:D:331:SER:C	2.62	0.42
1:D:514:VAL:HG12	1:D:517:ILE:HG13	1.99	0.42
1:D:548:GLU:O	1:D:548:GLU:HG3	2.19	0.42
1:B:356:ARG:O	1:B:649:PRO:HD3	2.19	0.42
1:D:299:GLU:O	1:D:300:VAL:C	2.61	0.42
1:A:604:SER:O	1:A:607:THR:HB	2.20	0.42
1:B:622:TYR:CG	1:B:632:MET:HG3	2.55	0.42
1:C:296:LEU:O	1:C:300:VAL:HG23	2.20	0.42
1:D:385:ALA:HA	1:D:388:LYS:HE2	2.02	0.42
1:D:580:ASP:OD1	1:D:580:ASP:O	2.36	0.42
1:B:328:LEU:HD13	1:B:328:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:LEU:HD22	1:D:321:LEU:HB2	2.02	0.42
1:C:365:ARG:O	1:C:366:MET:HE2	2.20	0.42
1:C:419:ILE:HD12	1:C:457:THR:HG23	2.02	0.42
1:D:622:TYR:CG	1:D:632:MET:HG3	2.55	0.42
1:A:602:SER:O	1:A:603:LEU:C	2.63	0.42
1:B:393:GLN:C	1:B:394:GLN:HG2	2.45	0.42
1:B:491:ASP:HB2	1:B:500:MET:SD	2.59	0.42
1:B:543:SER:HA	1:B:547:ASN:CG	2.44	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:C:545:ALA:C	1:C:547:ASN:N	2.74	0.42
1:D:364:ASN:N	1:D:364:ASN:ND2	2.67	0.42
1:D:604:SER:O	1:D:607:THR:HB	2.20	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:A:636:GLY:HA3	4:A:92:HOH:O	2.20	0.42
1:B:351:VAL:HG12	1:B:398:PHE:HD2	1.85	0.42
1:B:415:VAL:C	1:B:417:PRO:HD2	2.44	0.42
1:C:312:ARG:O	1:C:313:CYS:C	2.61	0.42
1:C:355:ILE:HG22	1:C:404:PRO:HG3	2.02	0.42
1:C:521:THR:O	1:C:523:LEU:HD12	2.19	0.42
1:C:528:LEU:HD12	1:C:528:LEU:O	2.20	0.42
1:D:373:HIS:O	1:D:377:THR:HB	2.20	0.42
1:D:527:HIS:CD2	1:D:527:HIS:C	2.98	0.42
1:D:534:THR:O	1:D:535:ALA:C	2.62	0.42
1:B:503:ARG:HD3	1:B:513:TYR:CE2	2.54	0.41
1:C:606:LEU:C	1:C:606:LEU:HD13	2.45	0.41
1:A:500:MET:HE2	1:A:517:ILE:HG23	2.01	0.41
1:C:318:ALA:O	1:C:321:LEU:N	2.45	0.41
1:C:322:GLU:O	1:C:323:THR:C	2.63	0.41
1:D:379:GLU:HA	1:D:394:GLN:O	2.20	0.41
1:A:352:PHE:CZ	1:A:414:MET:HG3	2.55	0.41
1:A:382:SER:CB	1:A:391:MET:HE1	2.50	0.41
1:B:526:ASN:O	1:B:527:HIS:C	2.63	0.41
1:B:609:VAL:O	1:B:610:ILE:C	2.62	0.41
1:C:384:ASP:HB3	1:C:387:ALA:HB3	2.03	0.41
1:C:398:PHE:C	1:C:400:GLN:H	2.29	0.41
1:D:359:LEU:HD23	4:D:90:HOH:O	2.19	0.41
1:D:403:HIS:N	1:D:406:SER:HG	2.18	0.41
1:A:403:HIS:C	1:A:405:LEU:H	2.28	0.41
1:C:329:PHE:CE1	1:C:568:LYS:HE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:GLU:OE1	4:D:90:HOH:O	2.22	0.41
1:D:428:ILE:HD13	1:D:428:ILE:N	2.34	0.41
1:D:487:GLU:O	1:D:626:LYS:NZ	2.52	0.41
1:D:497:GLN:NE2	1:D:498:LYS:O	2.53	0.41
1:B:332:ASN:O	1:B:333:MET:C	2.63	0.41
1:B:549:ARG:HB3	1:B:550:SER:H	1.64	0.41
1:B:643:MET:HE3	1:B:663:PHE:CE2	2.50	0.41
1:D:491:ASP:HB2	1:D:500:MET:CE	2.49	0.41
1:D:670:CYS:O	1:D:671:LYS:C	2.63	0.41
1:C:398:PHE:CE2	1:C:664:ALA:CB	3.03	0.41
1:C:398:PHE:CD1	1:C:398:PHE:N	2.88	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:B:324:CYS:O	1:B:327:GLN:HB2	2.20	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:542:ALA:CB	1:B:546:GLY:O	2.69	0.41
1:C:311:LEU:HD12	1:C:311:LEU:HA	1.66	0.41
1:D:338:LEU:HD23	1:D:338:LEU:HA	1.81	0.41
1:D:373:HIS:CD2	1:D:395:ILE:CD1	3.04	0.41
1:A:335:ARG:HH22	1:A:424:ASP:CG	2.28	0.41
1:A:411:ILE:HG23	1:A:644:PHE:CZ	2.56	0.41
1:B:654:PHE:CD2	1:B:655:GLN:N	2.89	0.41
1:C:419:ILE:O	1:C:422:ALA:HB3	2.21	0.41
1:C:526:ASN:O	1:C:527:HIS:C	2.63	0.41
1:C:527:HIS:NE2	1:C:531:LEU:HD11	2.36	0.41
1:D:325:LYS:O	1:D:326:GLU:C	2.64	0.41
1:A:388:LYS:O	1:A:388:LYS:HG3	2.20	0.41
1:A:400:GLN:HG3	1:A:401:VAL:H	1.79	0.41
1:A:429:CYS:C	1:A:430:ILE:HD13	2.45	0.41
1:A:454:ILE:HG12	1:A:578:LEU:HD13	2.01	0.41
1:A:661:LEU:O	1:A:664:ALA:N	2.54	0.41
1:B:541:THR:O	1:B:544:THR:HG22	2.21	0.41
1:C:366:MET:HE2	1:C:366:MET:HA	2.03	0.41
1:C:568:LYS:O	1:C:569:GLN:HB2	2.21	0.41
1:C:653:CYS:O	1:C:656:GLU:N	2.50	0.41
1:D:303:LEU:C	1:D:305:GLN:N	2.78	0.41
1:D:304:ARG:O	1:D:308:GLU:OE1	2.38	0.41
1:A:355:ILE:HG22	1:A:404:PRO:CG	2.51	0.41
1:B:486:ASN:CG	1:B:599:ILE:HG13	2.45	0.41
1:C:491:ASP:CB	1:C:500:MET:HE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:HIS:HB2	1:D:404:PRO:HD2	2.03	0.41
1:D:515:SER:O	1:D:516:ASN:CB	2.62	0.41
1:B:462:PHE:CZ	1:B:477:ILE:HD12	2.56	0.40
1:B:469:ARG:HE	1:B:469:ARG:HB2	1.71	0.40
1:B:533:HIS:O	1:B:536:LYS:N	2.53	0.40
1:C:301:VAL:O	1:C:304:ARG:N	2.54	0.40
1:C:527:HIS:O	1:C:527:HIS:CD2	2.74	0.40
1:C:584:SER:HA	1:C:603:LEU:HD21	2.03	0.40
1:D:536:LYS:HD2	1:D:536:LYS:HA	1.82	0.40
1:A:524:ASP:O	1:A:525:PRO:C	2.64	0.40
1:B:398:PHE:C	1:B:400:GLN:H	2.28	0.40
1:B:568:LYS:O	1:B:569:GLN:HB2	2.21	0.40
1:C:418:LEU:HA	1:C:418:LEU:HD23	1.83	0.40
1:C:433:TYR:CD2	1:C:434:GLY:N	2.89	0.40
1:A:599:ILE:C	1:A:601:ARG:N	2.80	0.40
1:B:512:ILE:HG23	1:B:513:TYR:N	2.36	0.40
1:C:306:ARG:HG3	1:C:310:LEU:CD1	2.46	0.40
1:C:605:GLU:HG3	1:C:625:SER:HB2	2.04	0.40
1:D:306:ARG:HD2	1:D:306:ARG:HA	1.91	0.40
1:A:428:ILE:CG2	1:A:429:CYS:N	2.85	0.40
1:A:430:ILE:HD12	1:A:642:LEU:HB2	2.02	0.40
1:A:527:HIS:CD2	1:A:527:HIS:C	2.98	0.40
1:B:461:LEU:HD11	1:B:561:LEU:HD11	2.04	0.40
1:C:312:ARG:HA	1:C:315:GLU:OE2	2.22	0.40
1:C:361:SER:C	1:C:362:GLU:HG3	2.46	0.40
1:C:536:LYS:HD2	1:C:536:LYS:HA	1.89	0.40
1:D:481:PHE:CD1	1:D:481:PHE:N	2.89	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
1:A:485:TYR:CD2	1:A:485:TYR:C	2.99	0.40
1:A:521:THR:O	1:A:521:THR:OG1	2.33	0.40
1:A:538:ASN:C	1:A:540:ALA:N	2.78	0.40
1:C:338:LEU:HD23	1:D:342:VAL:HG21	2.03	0.40
1:C:495:ASN:C	1:C:497:GLN:H	2.29	0.40
1:D:605:GLU:HA	1:D:608:ASN:HD22	1.86	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/406 (83%)	273 (81%)	47 (14%)	18 (5%)	1	5
1	B	333/406 (82%)	264 (79%)	48 (14%)	21 (6%)	1	3
1	C	360/406 (89%)	283 (79%)	56 (16%)	21 (6%)	1	4
1	D	361/406 (89%)	282 (78%)	54 (15%)	25 (7%)	1	2
All	All	1392/1624 (86%)	1102 (79%)	205 (15%)	85 (6%)	1	4

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	282 (92%)	26 (8%)	10	31
1	B	305/368 (83%)	279 (92%)	26 (8%)	10	31
1	C	326/368 (89%)	292 (90%)	34 (10%)	7	23
1	D	328/368 (89%)	283 (86%)	45 (14%)	3	12
All	All	1267/1472 (86%)	1136 (90%)	131 (10%)	7	23

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	LEU
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	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	600	ASN
1	A	603	LEU
1	A	607	THR
1	A	610	ILE
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	364	ASN
1	B	369	THR
1	B	380	LEU
1	B	388	LYS
1	B	393	GLN
1	B	404	PRO
1	B	405	LEU
1	B	414	MET
1	B	433	TYR
1	B	463	ASP
1	B	471	LEU
1	B	481	PHE
1	B	494	SER

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Mol	Chain	Res	Type
1	B	512	ILE
1	B	513	TYR
1	B	517	ILE
1	B	531	LEU
1	B	537	MET
1	B	552	ARG
1	B	607	THR
1	B	624	ASN
1	B	642	LEU
1	C	314	ASN
1	C	321	LEU
1	C	335	ARG
1	C	338	LEU
1	C	364	ASN
1	C	371	THR
1	C	374	ASP
1	C	383	ILE
1	C	388	LYS
1	C	404	PRO
1	C	405	LEU
1	C	414	MET
1	C	433	TYR
1	C	461	LEU
1	C	463	ASP
1	C	471	LEU
1	C	481	PHE
1	C	482	LEU
1	C	494	SER
1	C	512	ILE
1	C	513	TYR
1	C	517	ILE
1	C	525	PRO
1	C	531	LEU
1	C	537	MET
1	C	544	THR
1	C	552	ARG
1	C	572	SER
1	C	607	THR
1	C	623	ARG
1	C	624	ASN
1	C	642	LEU
1	C	648	SER

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Mol	Chain	Res	Type
1	C	668	ASN
1	D	299	GLU
1	D	301	VAL
1	D	308	GLU
1	D	325	LYS
1	D	328	LEU
1	D	330	GLN
1	D	332	ASN
1	D	335	ARG
1	D	361	SER
1	D	371	THR
1	D	374	ASP
1	D	388	LYS
1	D	400	GLN
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	454	ILE
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	486	ASN
1	D	512	ILE
1	D	513	TYR
1	D	517	ILE
1	D	525	PRO
1	D	537	MET
1	D	552	ARG
1	D	557	THR
1	D	572	SER
1	D	580	ASP
1	D	585	GLU
1	D	603	LEU
1	D	607	THR
1	D	610	ILE
1	D	624	ASN

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Mol	Chain	Res	Type
1	D	639	SER
1	D	646	ASN
1	D	647	VAL
1	D	658	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	364	ASN
1	A	400	GLN
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	629	HIS
1	A	646	ASN
1	A	668	ASN
1	B	364	ASN
1	B	400	GLN
1	B	470	ASN
1	B	486	ASN
1	B	495	ASN
1	B	507	ASN
1	B	533	HIS
1	B	547	ASN
1	B	577	ASN
1	B	608	ASN
1	B	668	ASN
1	C	302	HIS
1	C	317	GLN
1	C	330	GLN
1	C	332	ASN
1	C	364	ASN
1	C	381	GLN
1	C	386	GLN
1	C	403	HIS
1	C	470	ASN
1	C	486	ASN

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Mol	Chain	Res	Type
1	C	495	ASN
1	C	497	GLN
1	C	507	ASN
1	C	516	ASN
1	C	608	ASN
1	C	615	GLN
1	C	629	HIS
1	C	646	ASN
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	400	GLN
1	D	470	ASN
1	D	486	ASN
1	D	497	GLN
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 oligosaccharides 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	28,29,29	2.52	6 (21%)	43,45,45	2.72	14 (32%)
3	ADP	B	801	2	28,29,29	2.52	7 (25%)	43,45,45	2.73	14 (32%)
3	ADP	C	802	2	28,29,29	2.52	6 (21%)	43,45,45	2.72	14 (32%)
3	ADP	D	803	2	28,29,29	2.52	6 (21%)	43,45,45	2.72	14 (32%)

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	-	6/16/32/32	0/3/3/3
3	ADP	B	801	2	-	6/16/32/32	0/3/3/3
3	ADP	C	802	2	-	6/16/32/32	0/3/3/3
3	ADP	D	803	2	-	6/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	ADP	PA-O3A	10.77	1.71	1.59
3	D	803	ADP	PA-O3A	10.76	1.71	1.59
3	B	801	ADP	PA-O3A	10.74	1.71	1.59
3	A	800	ADP	PA-O3A	10.74	1.71	1.59
3	D	803	ADP	C5-N7	-4.10	1.31	1.39
3	A	800	ADP	C5-N7	-4.06	1.31	1.39
3	C	802	ADP	C5-N7	-4.06	1.31	1.39
3	B	801	ADP	C5-N7	-4.05	1.31	1.39
3	D	803	ADP	O4'-C1'	3.06	1.49	1.42
3	B	801	ADP	O4'-C1'	3.04	1.49	1.42
3	A	800	ADP	O4'-C1'	3.04	1.49	1.42
3	C	802	ADP	O4'-C1'	3.01	1.49	1.42
3	A	800	ADP	C1'-N9	2.73	1.53	1.46
3	C	802	ADP	C1'-N9	2.73	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	803	ADP	C1'-N9	2.72	1.53	1.46
3	B	801	ADP	C1'-N9	2.71	1.53	1.46
3	D	803	ADP	C5'-C4'	2.20	1.58	1.51
3	C	802	ADP	C5'-C4'	2.19	1.58	1.51
3	A	800	ADP	C5'-C4'	2.19	1.58	1.51
3	B	801	ADP	C5'-C4'	2.18	1.58	1.51
3	A	800	ADP	C4-N9	-2.11	1.33	1.37
3	B	801	ADP	O4'-C4'	2.07	1.49	1.45
3	B	801	ADP	C4-N9	-2.05	1.33	1.37
3	D	803	ADP	C4-N9	-2.02	1.33	1.37
3	C	802	ADP	C4-N9	-2.00	1.33	1.37

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	ADP	O4'-C1'-N9	8.61	124.63	108.09
3	A	800	ADP	O4'-C1'-N9	8.61	124.63	108.09
3	C	802	ADP	O4'-C1'-N9	8.58	124.57	108.09
3	D	803	ADP	O4'-C1'-N9	8.58	124.57	108.09
3	C	802	ADP	N3-C2-N1	-6.41	118.87	128.58
3	B	801	ADP	N3-C2-N1	-6.41	118.88	128.58
3	D	803	ADP	N3-C2-N1	-6.38	118.92	128.58
3	A	800	ADP	N3-C2-N1	-6.36	118.96	128.58
3	B	801	ADP	C5-C4-N3	-6.24	118.13	126.72
3	A	800	ADP	C5-C4-N3	-6.23	118.13	126.72
3	C	802	ADP	C5-C4-N3	-6.22	118.15	126.72
3	D	803	ADP	C5-C4-N3	-6.19	118.20	126.72
3	B	801	ADP	N3-C4-N9	5.71	136.88	127.17
3	A	800	ADP	N3-C4-N9	5.71	136.88	127.17
3	D	803	ADP	N3-C4-N9	5.70	136.87	127.17
3	C	802	ADP	N3-C4-N9	5.70	136.85	127.17
3	C	802	ADP	O5'-C5'-C4'	4.93	125.78	108.99
3	A	800	ADP	O5'-C5'-C4'	4.92	125.74	108.99
3	D	803	ADP	O5'-C5'-C4'	4.92	125.74	108.99
3	B	801	ADP	O5'-C5'-C4'	4.91	125.73	108.99
3	C	802	ADP	C2-N3-C4	4.32	122.38	111.83
3	B	801	ADP	C2-N3-C4	4.31	122.37	111.83
3	A	800	ADP	C2-N3-C4	4.31	122.35	111.83
3	D	803	ADP	C2-N3-C4	4.30	122.34	111.83
3	D	803	ADP	C6-C5-N7	-3.41	125.52	132.09
3	A	800	ADP	C6-C5-N7	-3.40	125.54	132.09
3	B	801	ADP	C6-C5-N7	-3.38	125.58	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	ADP	C6-C5-N7	-3.34	125.64	132.09
3	D	803	ADP	C4-C5-N7	2.94	113.95	110.58
3	B	801	ADP	C3'-C2'-C1'	2.93	107.00	101.46
3	A	800	ADP	C3'-C2'-C1'	2.92	106.99	101.46
3	C	802	ADP	C3'-C2'-C1'	2.92	106.99	101.46
3	D	803	ADP	C3'-C2'-C1'	2.91	106.97	101.46
3	A	800	ADP	C4-C5-N7	2.89	113.89	110.58
3	B	801	ADP	C4-C5-N7	2.87	113.86	110.58
3	C	802	ADP	C4-C5-N7	2.84	113.82	110.58
3	A	800	ADP	C6-C5-C4	2.47	120.55	117.18
3	B	801	ADP	C6-C5-C4	2.46	120.54	117.18
3	C	802	ADP	C6-C5-C4	2.44	120.51	117.18
3	D	803	ADP	C6-C5-C4	2.44	120.51	117.18
3	B	801	ADP	C2-N1-C6	2.27	122.46	118.73
3	D	803	ADP	O4'-C4'-C5'	2.24	116.52	109.33
3	A	800	ADP	O4'-C4'-C5'	2.24	116.50	109.33
3	B	801	ADP	O4'-C4'-C5'	2.24	116.50	109.33
3	C	802	ADP	O4'-C4'-C5'	2.23	116.49	109.33
3	D	803	ADP	C2-N1-C6	2.23	122.39	118.73
3	C	802	ADP	C2-N1-C6	2.22	122.38	118.73
3	A	800	ADP	C2-N1-C6	2.22	122.37	118.73
3	B	801	ADP	C2'-C3'-C4'	2.22	106.89	102.61
3	C	802	ADP	O2A-PA-O1A	2.20	122.67	112.44
3	B	801	ADP	O2A-PA-O1A	2.20	122.66	112.44
3	C	802	ADP	C2'-C3'-C4'	2.19	106.85	102.61
3	D	803	ADP	O2A-PA-O1A	2.19	122.63	112.44
3	D	803	ADP	C2'-C3'-C4'	2.19	106.83	102.61
3	A	800	ADP	O2A-PA-O1A	2.19	122.61	112.44
3	A	800	ADP	C2'-C3'-C4'	2.18	106.81	102.61

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	ADP	PA-O3A-PB-O2B
3	B	801	ADP	PA-O3A-PB-O2B
3	C	802	ADP	PA-O3A-PB-O2B
3	D	803	ADP	PA-O3A-PB-O2B
3	A	800	ADP	C3'-C4'-C5'-O5'
3	B	801	ADP	C3'-C4'-C5'-O5'
3	C	802	ADP	C3'-C4'-C5'-O5'
3	D	803	ADP	C3'-C4'-C5'-O5'

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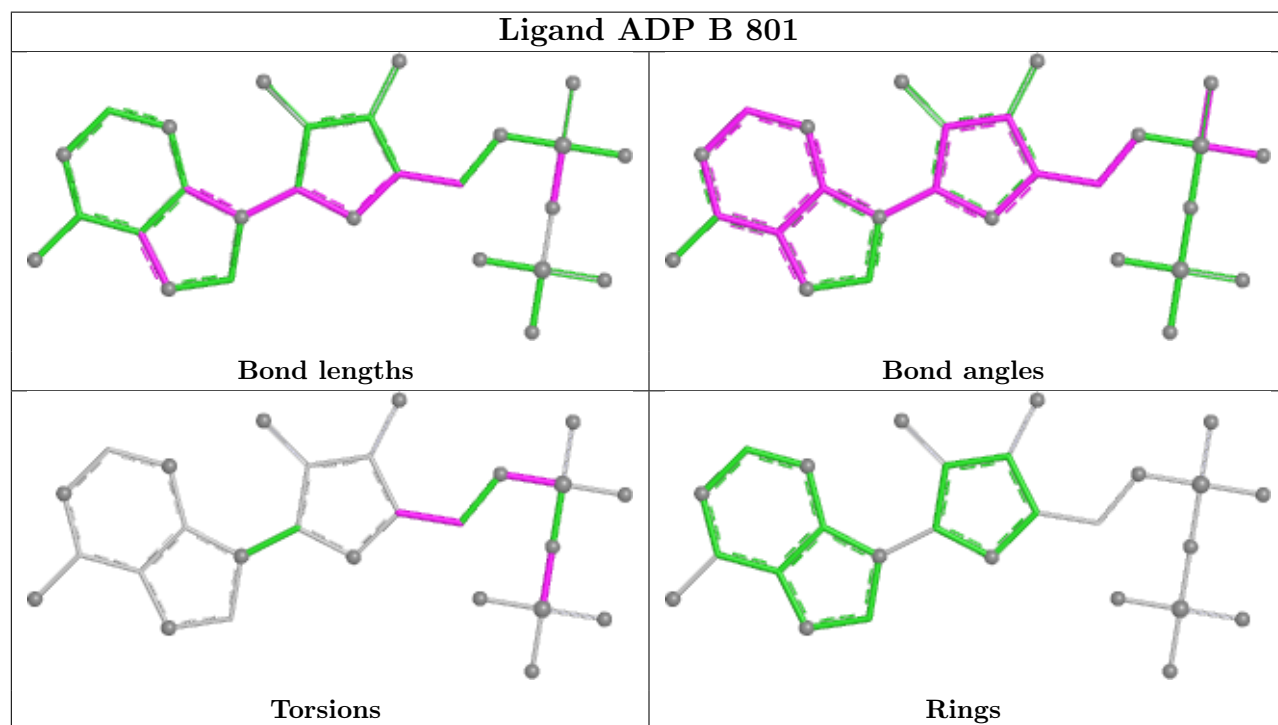
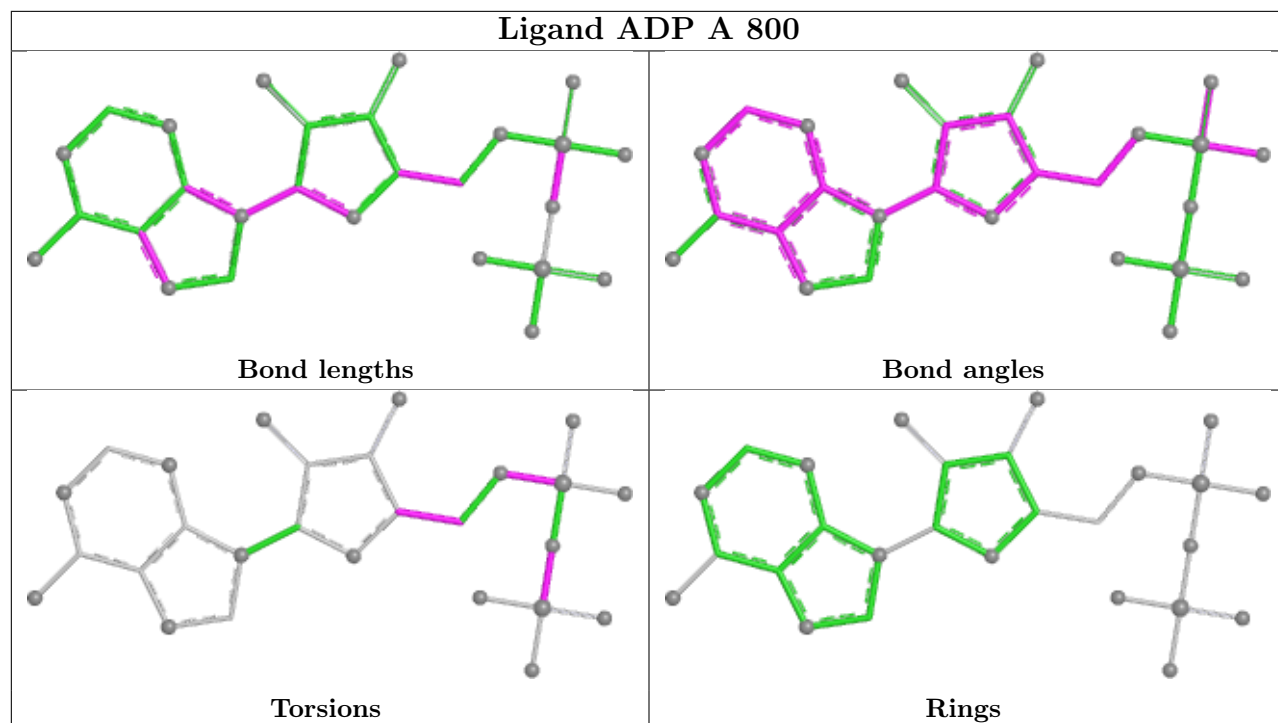
Mol	Chain	Res	Type	Atoms
3	A	800	ADP	O4'-C4'-C5'-O5'
3	B	801	ADP	O4'-C4'-C5'-O5'
3	C	802	ADP	O4'-C4'-C5'-O5'
3	D	803	ADP	O4'-C4'-C5'-O5'
3	A	800	ADP	C5'-O5'-PA-O1A
3	B	801	ADP	C5'-O5'-PA-O1A
3	C	802	ADP	C5'-O5'-PA-O1A
3	D	803	ADP	C5'-O5'-PA-O1A
3	A	800	ADP	PA-O3A-PB-O1B
3	B	801	ADP	PA-O3A-PB-O1B
3	C	802	ADP	PA-O3A-PB-O1B
3	D	803	ADP	PA-O3A-PB-O1B
3	A	800	ADP	PA-O3A-PB-O3B
3	B	801	ADP	PA-O3A-PB-O3B
3	C	802	ADP	PA-O3A-PB-O3B
3	D	803	ADP	PA-O3A-PB-O3B

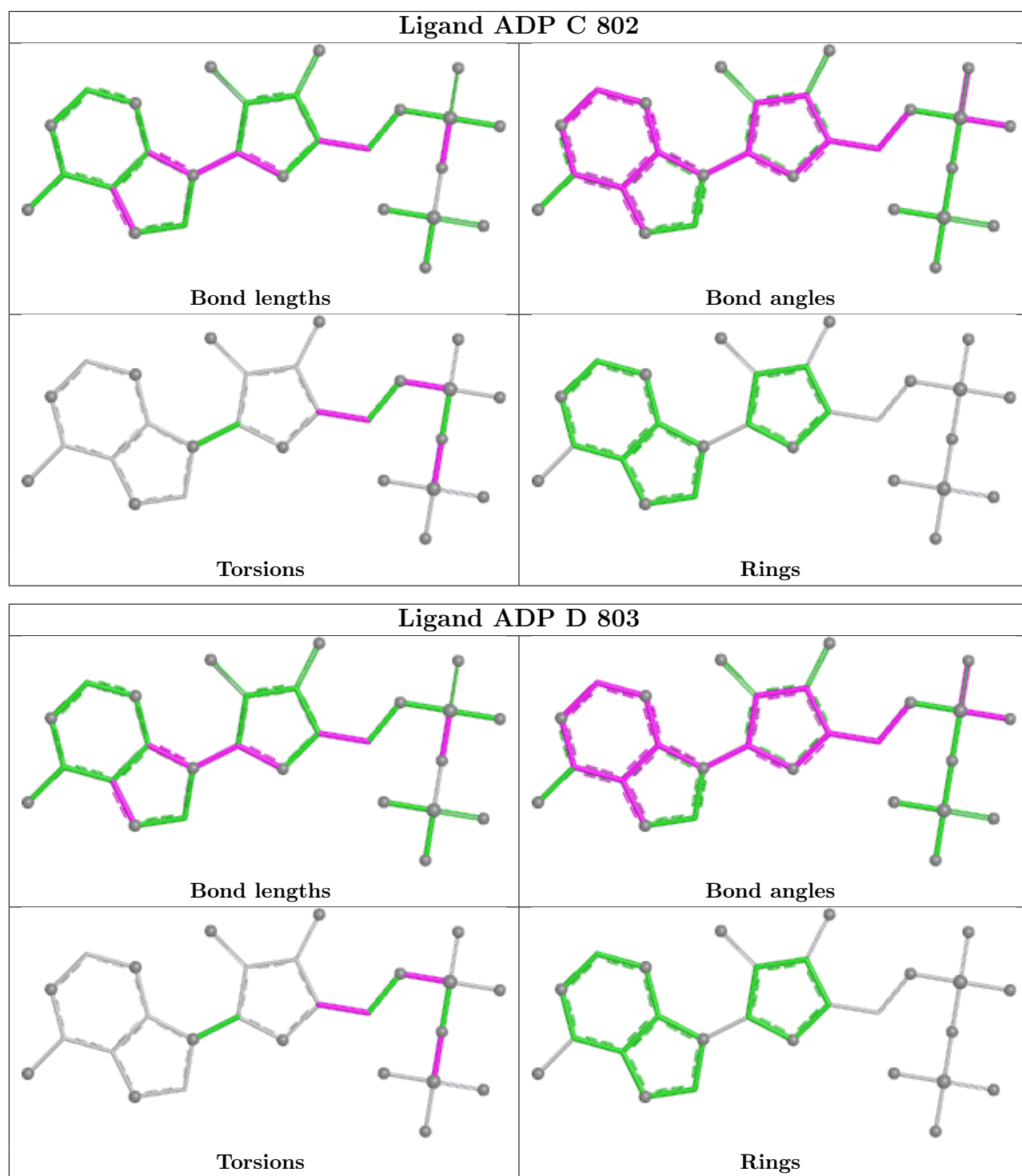
There are no ring outliers.

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

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 than 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.





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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.