



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:15 AM UTC

PDB ID : 2A5Y / pdb_00002a5y
Title : Structure of a CED-4/CED-9 complex
Authors : Yan, N.; Liu, Q.; Hao, Q.; Gu, L.; Shi, Y.
Deposited on : 2005-07-01
Resolution : 2.60 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

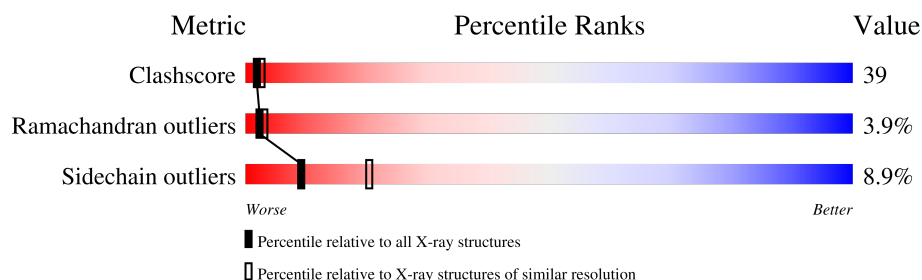
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	204	41% 39% • • 15%
2	B	549	36% 46% 9% 9%
2	C	549	30% 31% 6% • 32%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8730 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 Apoptosis regulator ced-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1417	900	246	262	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	SER	CYS	engineered mutation	UNP P41958
A	135	SER	CYS	engineered mutation	UNP P41958
A	164	SER	CYS	engineered mutation	UNP P41958

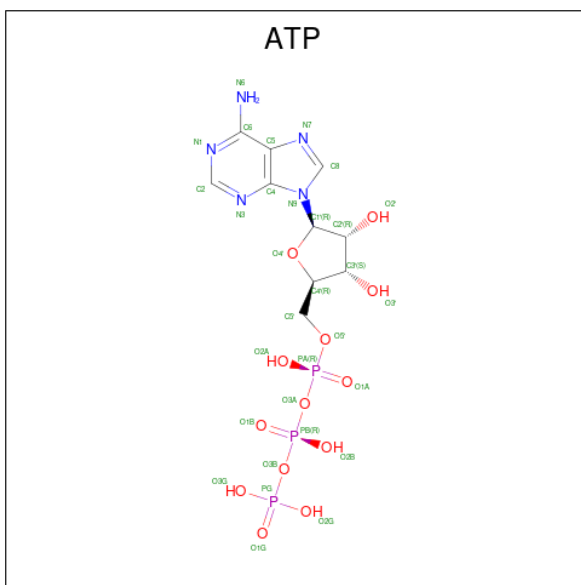
- Molecule 2 is a protein called ced-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	501	Total	C	N	O	S	0	0	0
			4028	2568	674	757	29			
2	C	373	Total	C	N	O	S	0	0	0
			2961	1885	493	558	25			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 5 is water.

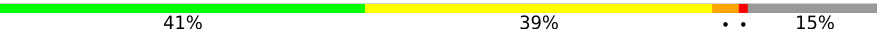
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	32	Total O 32 32	0	0
5	B	145	Total O 145 145	0	0
5	C	83	Total O 83 83	0	0

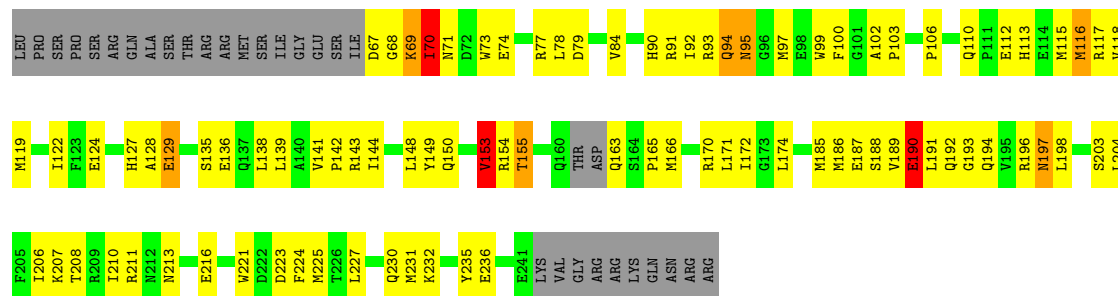
3 Residue-property plots

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

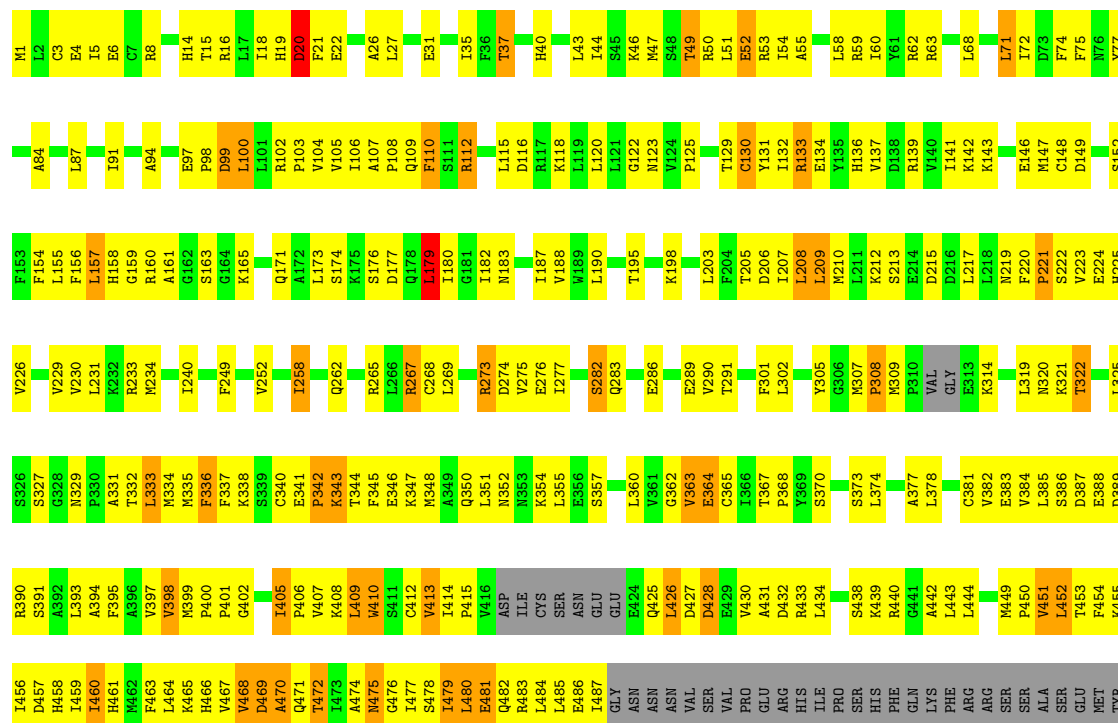
- Molecule 1: Apoptosis regulator ced-9

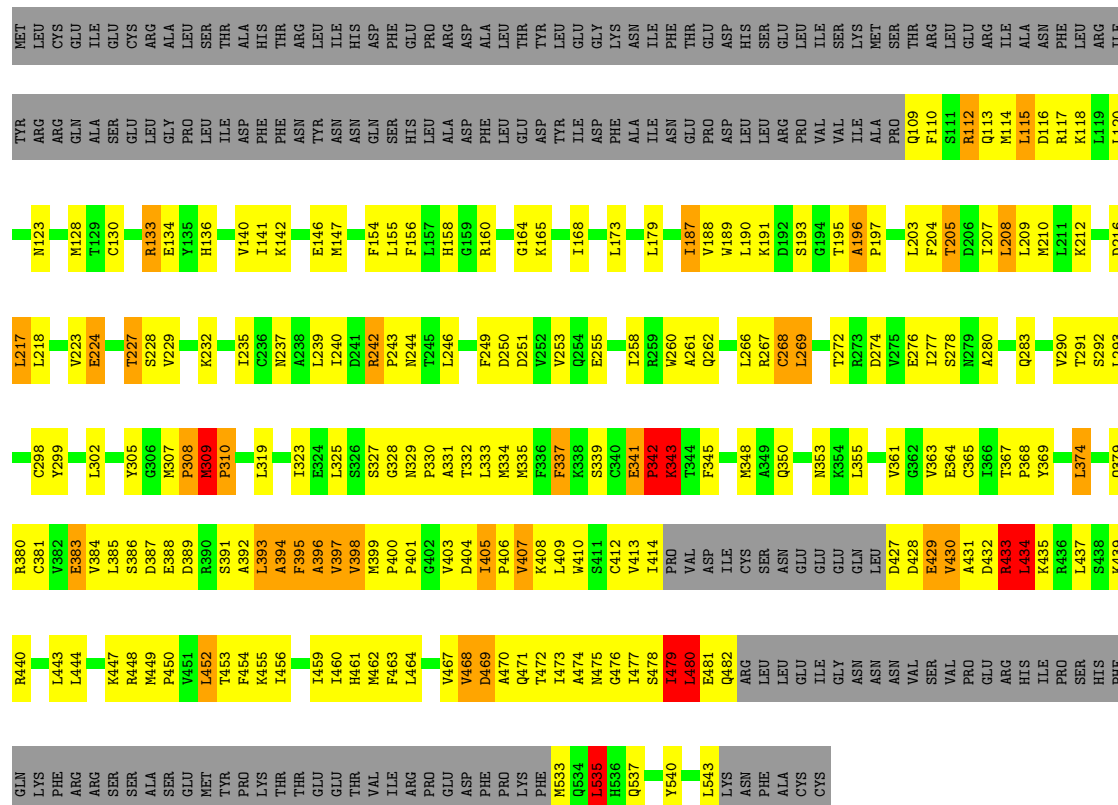
Chain A: 



- Molecule 2: ced-4

Chain B: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.90Å 128.90Å 209.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8730	wwPDB-VP
Average B, all atoms (Å ²)	82.0	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, ATP

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	0.55	0/1450	1.14	9/1950 (0.5%)
2	B	0.46	0/4101	1.07	25/5540 (0.5%)
2	C	0.44	0/3010	1.06	23/4061 (0.6%)
All	All	0.47	0/8561	1.08	57/11551 (0.5%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	GLY	N-CA-C	20.45	141.59	111.12
2	C	535	LEU	N-CA-C	-11.70	98.39	112.89
2	B	479	ILE	N-CA-C	-10.99	102.44	113.10
2	B	105	VAL	N-CA-C	10.65	120.43	110.74
2	B	480	LEU	N-CA-C	-10.23	100.93	113.41
2	C	309	MET	CA-C-N	10.19	130.28	119.89
2	C	309	MET	C-N-CA	10.19	130.28	119.89
2	B	428	ASP	N-CA-C	-8.59	102.06	112.54
2	B	100	LEU	N-CA-C	-8.46	103.39	114.31
1	A	69	LYS	N-CA-C	8.40	128.70	110.80
2	B	282	SER	N-CA-C	-8.03	102.74	114.39
2	B	360	LEU	N-CA-C	-7.99	104.01	114.31
1	A	153	VAL	N-CA-C	7.88	121.86	112.80
2	C	429	GLU	N-CA-C	-7.76	104.74	112.97
2	B	268	CYS	N-CA-C	7.68	121.63	109.50
2	B	222	SER	N-CA-C	-7.25	99.54	110.28
2	C	205	THR	N-CA-C	-7.23	103.48	111.36
2	B	322	THR	N-CA-C	-7.17	103.16	110.97
2	C	269	LEU	N-CA-C	-7.14	97.57	109.07
1	A	70	ILE	N-CA-C	7.12	124.15	109.34
2	C	476	GLY	N-CA-C	-6.92	105.79	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	ILE	N-CA-C	6.91	116.92	110.42
2	B	538	LYS	N-CA-C	-6.55	104.39	112.38
2	B	430	VAL	N-CA-C	-6.47	104.18	110.72
2	C	268	CYS	N-CA-C	6.45	119.69	109.50
2	B	458	HIS	N-CA-C	6.26	117.77	111.07
2	C	134	GLU	CB-CA-C	6.20	121.03	110.74
2	C	434	LEU	N-CA-C	-6.07	106.20	113.97
2	B	205	THR	N-CA-C	-6.00	104.31	111.69
1	A	68	GLY	CA-C-O	5.93	127.77	121.31
2	B	27	LEU	N-CA-C	5.84	117.33	110.97
2	C	310	PRO	N-CA-C	5.76	120.27	111.11
2	B	343	LYS	N-CA-C	-5.71	104.17	113.19
2	C	133	ARG	CA-C-N	5.62	129.25	120.82
2	C	133	ARG	C-N-CA	5.62	129.25	120.82
2	B	31	GLU	N-CA-C	-5.61	105.25	111.36
2	B	273	ARG	N-CA-C	-5.55	107.06	113.88
2	C	242	ARG	CA-C-N	5.48	125.68	120.31
2	C	242	ARG	C-N-CA	5.48	125.68	120.31
2	B	221	PRO	N-CA-C	5.42	119.59	111.14
2	B	20	ASP	N-CA-C	5.40	118.94	111.71
2	B	37	THR	N-CA-C	-5.39	102.47	110.46
2	B	35	ILE	N-CA-C	-5.37	107.55	111.90
1	A	210	ILE	N-CA-C	-5.34	105.08	112.50
2	B	267	ARG	N-CA-C	-5.30	100.08	108.73
2	B	535	LEU	N-CA-C	-5.26	105.54	111.28
2	C	480	LEU	N-CA-C	-5.18	108.23	114.75
1	A	68	GLY	CA-C-N	5.14	131.37	121.54
1	A	68	GLY	C-N-CA	5.14	131.37	121.54
2	C	196	ALA	CA-C-N	5.11	124.28	118.97
2	C	196	ALA	C-N-CA	5.11	124.28	118.97
2	C	433	ARG	N-CA-C	-5.10	106.89	113.01
1	A	190	GLU	N-CA-C	-5.02	100.10	110.80
2	C	405	ILE	CA-C-N	5.01	124.77	119.76
2	C	405	ILE	C-N-CA	5.01	124.77	119.76
2	C	341	GLU	CA-C-N	5.01	139.02	127.00
2	C	341	GLU	C-N-CA	5.01	139.02	127.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1417	0	1365	96	0
2	B	4028	0	4052	349	0
2	C	2961	0	2998	247	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	B	31	0	12	4	0
4	C	31	0	12	4	0
5	A	32	0	0	7	0
5	B	145	0	0	22	0
5	C	83	0	0	17	0
All	All	8730	0	8439	666	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (666) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:332:THR:HA	2:C:335:MET:HE3	1.21	1.20
2:C:123:ASN:HD21	2:C:210:MET:HE2	1.00	1.13
1:A:166:MET:HE1	1:A:171:LEU:HB2	1.30	1.11
2:B:302:LEU:HA	2:B:337:PHE:HZ	1.05	1.11
2:C:433:ARG:HH11	2:C:433:ARG:HB2	1.17	1.05
2:C:307:MET:HG3	2:C:308:PRO:HD2	1.36	1.04
2:C:123:ASN:ND2	2:C:210:MET:HE2	1.73	1.02
2:B:49:THR:HG22	2:B:52:GLU:H	1.22	1.01
2:B:302:LEU:HA	2:B:337:PHE:CZ	1.96	0.99
2:B:262:GLN:HE21	2:B:283:GLN:HB2	1.24	0.99
2:C:406:PRO:HD2	2:C:409:LEU:HD12	1.46	0.97
2:C:473:ILE:HD11	2:C:543:LEU:HD22	1.47	0.96
2:B:402:GLY:HA2	2:B:455:LYS:HE3	1.48	0.95
2:C:472:THR:HG22	5:C:574:HOH:O	1.68	0.93
2:B:262:GLN:HE22	2:B:282:SER:H	0.97	0.92
2:B:46:LYS:HE2	5:B:686:HOH:O	1.69	0.90
2:B:367:THR:HB	2:B:368:PRO:HD2	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HA	1:A:194:GLN:HE22	1.38	0.89
2:B:37:THR:H	2:B:40:HIS:HD2	1.21	0.88
2:C:400:PRO:HG2	2:C:403:VAL:HG21	1.55	0.87
1:A:74:GLU:OE2	2:B:49:THR:HG21	1.73	0.87
2:B:18:ILE:HD12	2:B:51:LEU:HD22	1.55	0.86
1:A:166:MET:HE1	1:A:171:LEU:CB	2.06	0.86
2:B:459:ILE:HD12	2:B:460:ILE:N	1.89	0.85
1:A:110:GLN:H	1:A:113:HIS:CD2	1.94	0.85
2:B:532:PHE:HE1	2:B:535:LEU:HB2	1.42	0.85
2:C:404:ASP:HB3	2:C:453:THR:HG21	1.59	0.84
2:B:395:PHE:HD1	2:B:415:PRO:HD3	1.42	0.84
2:B:388:GLU:HB2	2:B:433:ARG:HE	1.41	0.84
2:B:37:THR:H	2:B:40:HIS:CD2	1.96	0.83
2:B:341:GLU:HB2	2:B:342:PRO:HD3	1.58	0.83
2:C:332:THR:CA	2:C:335:MET:HE3	2.08	0.83
2:B:344:THR:HB	5:B:662:HOH:O	1.80	0.82
2:C:482:GLN:HG3	5:C:587:HOH:O	1.78	0.82
2:B:529:PHE:C	2:B:531:LYS:H	1.88	0.81
2:C:399:MET:HE1	2:C:405:ILE:HG21	1.62	0.81
1:A:208:THR:HG21	2:B:217:LEU:H	1.44	0.81
1:A:90:HIS:CD2	1:A:117:ARG:HD3	2.16	0.80
2:B:59:ARG:O	2:B:63:ARG:HG2	1.82	0.80
2:B:469:ASP:O	2:B:471:GLN:N	2.15	0.80
2:B:262:GLN:NE2	2:B:282:SER:H	1.78	0.80
2:B:409:LEU:HD23	2:B:530:PRO:HB3	1.65	0.79
2:C:474:ALA:HA	2:C:477:ILE:HD12	1.64	0.79
2:B:233:ARG:NH2	2:C:210:MET:HE3	1.97	0.79
2:B:68:LEU:HD12	2:B:91:ILE:HD11	1.64	0.79
2:B:219:ASN:HB2	5:B:599:HOH:O	1.83	0.79
2:B:456:ILE:HD13	5:B:574:HOH:O	1.83	0.78
1:A:150:GLN:O	1:A:154:ARG:HG3	1.83	0.78
1:A:204:LEU:HD13	2:B:209:LEU:HD22	1.64	0.78
2:C:123:ASN:HD21	2:C:210:MET:CE	1.89	0.78
1:A:190:GLU:HB3	1:A:191:LEU:HD12	1.66	0.77
2:B:347:LYS:HB2	5:B:662:HOH:O	1.82	0.77
2:B:143:LYS:HB3	2:B:147:MET:HE2	1.67	0.77
2:B:163:SER:HB2	2:B:290:VAL:HG12	1.66	0.77
1:A:166:MET:CE	1:A:171:LEU:HB2	2.13	0.77
1:A:196:ARG:HH11	1:A:196:ARG:HB2	1.49	0.77
1:A:153:VAL:HG11	1:A:174:LEU:HD23	1.67	0.76
2:C:464:LEU:HA	2:C:467:VAL:HG12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:369:TYR:HB2	4:C:551:ATP:H3'	1.68	0.75
2:C:332:THR:HA	2:C:335:MET:CE	2.10	0.75
2:C:405:ILE:C	2:C:453:THR:HG23	2.11	0.75
2:B:262:GLN:NE2	2:B:283:GLN:HB2	2.01	0.75
2:B:438:SER:HB3	5:B:687:HOH:O	1.84	0.75
2:B:100:LEU:C	2:B:103:PRO:HD2	2.12	0.75
2:C:302:LEU:HD13	2:C:319:LEU:HD11	1.69	0.74
1:A:124:GLU:O	1:A:128:ALA:HB2	1.88	0.74
2:C:400:PRO:O	2:C:403:VAL:HG22	1.87	0.74
1:A:189:VAL:HA	1:A:192:GLN:HG3	1.69	0.74
2:C:133:ARG:HG2	2:C:136:HIS:HD2	1.53	0.74
2:B:393:LEU:HD13	2:B:464:LEU:HD21	1.69	0.74
2:B:407:VAL:CG2	2:B:452:LEU:HD21	2.18	0.74
2:B:283:GLN:HA	5:B:620:HOH:O	1.87	0.73
2:B:449:MET:HB2	2:B:450:PRO:HA	1.70	0.73
1:A:138:LEU:HD22	1:A:144:ILE:HD11	1.68	0.73
1:A:186:MET:HE2	1:A:186:MET:HA	1.70	0.73
2:B:104:VAL:O	2:B:108:PRO:HG2	1.88	0.73
2:B:14:HIS:CE1	2:B:18:ILE:HD11	2.24	0.72
2:C:414:ILE:HG13	2:C:430:VAL:HG13	1.71	0.72
2:C:433:ARG:HB2	2:C:433:ARG:NH1	1.98	0.72
1:A:115:MET:CB	1:A:225:MET:HE1	2.19	0.72
1:A:196:ARG:NH2	2:B:125:PRO:HG3	2.05	0.72
2:C:227:THR:HG22	2:C:229:VAL:H	1.55	0.72
2:C:432:ASP:HA	2:C:435:LYS:HB3	1.70	0.72
2:C:473:ILE:O	2:C:477:ILE:HG13	1.89	0.71
2:C:443:LEU:H	2:C:443:LEU:HD12	1.55	0.71
2:B:410:TRP:HD1	2:B:414:ILE:HD13	1.56	0.71
2:B:460:ILE:HD13	2:B:460:ILE:O	1.90	0.71
2:B:395:PHE:HE2	2:B:472:THR:HG22	1.55	0.70
2:B:443:LEU:O	2:B:444:LEU:HD12	1.89	0.70
2:B:44:ILE:O	2:B:53:ARG:HG2	1.90	0.70
2:B:487:ILE:O	2:B:531:LYS:HD3	1.92	0.70
2:C:331:ALA:HA	4:C:551:ATP:O3'	1.91	0.70
2:B:18:ILE:HG23	2:B:51:LEU:HD21	1.73	0.69
2:C:302:LEU:HD22	2:C:307:MET:HG2	1.72	0.69
2:C:393:LEU:HD23	2:C:394:ALA:N	2.07	0.69
2:B:262:GLN:HE22	2:B:282:SER:N	1.80	0.69
2:B:335:MET:HE1	2:B:373:SER:HA	1.72	0.69
2:B:529:PHE:O	2:B:531:LYS:N	2.25	0.69
2:B:58:LEU:O	2:B:62:ARG:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:TRP:HZ3	2:B:454:PHE:O	1.77	0.68
2:B:262:GLN:HE22	2:B:283:GLN:H	1.41	0.68
2:B:406:PRO:HD3	2:B:524:ILE:CD1	2.23	0.68
2:B:386:SER:HB3	2:B:389:ASP:OD2	1.94	0.68
2:C:400:PRO:HG2	2:C:403:VAL:CG2	2.23	0.68
2:B:147:MET:HE1	2:B:155:LEU:HG	1.74	0.68
2:C:480:LEU:HD21	2:C:533:MET:HE1	1.75	0.68
2:B:16:ARG:HG3	2:B:16:ARG:HH11	1.58	0.68
2:B:400:PRO:HD3	2:B:540:TYR:CE1	2.29	0.68
2:C:333:LEU:O	2:C:337:PHE:CD1	2.47	0.68
2:B:341:GLU:OE1	2:B:347:LYS:HE3	1.92	0.68
2:C:255:GLU:CG	2:C:280:ALA:HB2	2.23	0.67
2:C:331:ALA:O	2:C:335:MET:HG3	1.94	0.67
2:B:374:LEU:O	2:B:374:LEU:HD13	1.94	0.67
2:B:75:PHE:HB2	2:B:84:ALA:HB2	1.75	0.67
2:B:142:LYS:HG2	5:B:636:HOH:O	1.95	0.67
2:C:461:HIS:HB2	5:C:611:HOH:O	1.95	0.67
2:B:476:GLY:O	2:B:479:ILE:HG22	1.96	0.66
1:A:115:MET:HB2	1:A:225:MET:HE1	1.76	0.66
2:B:5:ILE:HA	5:B:603:HOH:O	1.94	0.66
2:B:190:LEU:HD12	2:B:207:ILE:HG13	1.77	0.66
2:B:338:LYS:HB3	2:B:365:CYS:SG	2.36	0.66
2:B:262:GLN:NE2	2:B:283:GLN:H	1.92	0.66
2:B:98:PRO:C	2:B:100:LEU:H	2.03	0.66
2:C:302:LEU:HG	2:C:337:PHE:CZ	2.31	0.66
2:B:532:PHE:CE1	2:B:535:LEU:HB2	2.30	0.66
2:C:307:MET:CG	2:C:308:PRO:HD2	2.21	0.65
2:B:143:LYS:HE2	5:B:562:HOH:O	1.96	0.65
2:B:343:LYS:N	2:B:343:LYS:HD3	2.11	0.65
2:C:227:THR:HG22	2:C:229:VAL:N	2.11	0.65
2:B:394:ALA:O	2:B:397:VAL:HG23	1.97	0.65
2:B:230:VAL:HG21	2:C:209:LEU:HD13	1.78	0.65
2:B:407:VAL:HG21	2:B:452:LEU:HD21	1.78	0.65
2:B:452:LEU:HD23	2:B:452:LEU:O	1.97	0.65
2:C:209:LEU:HD23	2:C:212:LYS:CE	2.26	0.65
2:C:393:LEU:C	2:C:395:PHE:H	2.05	0.65
2:B:398:VAL:HG23	2:B:398:VAL:O	1.96	0.64
2:B:16:ARG:HH12	2:B:109:GLN:HG2	1.63	0.64
1:A:106:PRO:HG3	2:B:116:ASP:O	1.98	0.64
1:A:196:ARG:HB2	1:A:196:ARG:NH1	2.12	0.64
1:A:93:ARG:C	1:A:95:ASN:H	2.04	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:PHE:CE2	2:B:472:THR:HG22	2.32	0.64
2:C:479:ILE:HD12	2:C:479:ILE:N	2.13	0.64
2:C:473:ILE:CD1	2:C:543:LEU:HD22	2.27	0.64
2:B:37:THR:N	2:B:40:HIS:HD2	1.93	0.63
2:B:321:LYS:O	2:B:325:LEU:HG	1.98	0.63
2:B:469:ASP:C	2:B:471:GLN:H	2.05	0.63
2:C:361:VAL:HG23	5:C:618:HOH:O	1.97	0.63
2:B:68:LEU:HD12	2:B:91:ILE:CD1	2.28	0.63
2:B:449:MET:HB2	2:B:450:PRO:CA	2.28	0.63
2:C:232:LYS:HE2	2:C:260:TRP:CD2	2.33	0.63
2:C:434:LEU:HD21	2:C:454:PHE:CG	2.34	0.63
1:A:171:LEU:HD12	1:A:206:ILE:HD13	1.81	0.63
2:C:400:PRO:CG	2:C:403:VAL:HG21	2.27	0.63
2:C:308:PRO:O	2:C:309:MET:HB2	1.97	0.63
2:B:382:VAL:HA	2:B:385:LEU:HD12	1.81	0.63
1:A:77:ARG:HG2	5:A:271:HOH:O	1.97	0.62
2:C:227:THR:CG2	2:C:229:VAL:H	2.12	0.62
1:A:189:VAL:HG22	1:A:192:GLN:OE1	1.99	0.62
2:C:479:ILE:HG22	2:C:479:ILE:O	1.98	0.62
1:A:204:LEU:CD1	2:B:209:LEU:HD22	2.29	0.62
2:B:529:PHE:C	2:B:531:LYS:N	2.58	0.62
2:C:433:ARG:HH11	2:C:433:ARG:CB	2.04	0.62
1:A:153:VAL:CG1	1:A:174:LEU:HD23	2.29	0.62
2:B:395:PHE:HD1	2:B:415:PRO:CD	2.11	0.62
2:C:307:MET:HG3	2:C:308:PRO:CD	2.23	0.62
2:C:302:LEU:CD2	2:C:307:MET:HG2	2.30	0.62
2:C:399:MET:CE	2:C:405:ILE:HD13	2.30	0.62
2:C:448:ARG:HB3	2:C:452:LEU:CD2	2.30	0.62
2:B:347:LYS:O	2:B:350:GLN:HB2	1.99	0.62
2:C:244:ASN:HA	2:C:267:ARG:NH1	2.14	0.62
2:B:165:LYS:NZ	4:B:551:ATP:O1G	2.31	0.62
2:B:381:CYS:O	2:B:384:VAL:HG22	2.00	0.61
2:B:395:PHE:CD1	2:B:415:PRO:HD3	2.29	0.61
2:C:443:LEU:HD12	2:C:443:LEU:N	2.15	0.61
5:A:260:HOH:O	2:B:49:THR:HG23	1.99	0.61
2:C:342:PRO:O	2:C:343:LYS:CB	2.47	0.61
2:C:154:PHE:HB3	2:C:156:PHE:CE1	2.34	0.61
2:C:239:LEU:HD11	2:C:266:LEU:HD21	1.83	0.61
2:B:108:PRO:HB2	2:B:109:GLN:NE2	2.14	0.61
2:B:336:PHE:HE1	2:B:355:LEU:HD11	1.65	0.61
2:C:262:GLN:HE22	2:C:283:GLN:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:GLN:HG3	5:B:627:HOH:O	2.00	0.61
2:C:384:VAL:HG12	2:C:384:VAL:O	1.99	0.61
2:B:484:LEU:HD23	2:B:485:LEU:H	1.65	0.61
2:C:253:VAL:HB	5:C:566:HOH:O	2.00	0.60
2:C:393:LEU:HB2	2:C:437:LEU:CD1	2.31	0.60
2:C:397:VAL:HG13	2:C:398:VAL:H	1.66	0.60
2:C:399:MET:CE	2:C:405:ILE:HG21	2.29	0.60
1:A:97:MET:HE2	1:A:186:MET:HB3	1.84	0.60
2:B:157:LEU:O	2:B:165:LYS:HD2	2.01	0.60
1:A:185:MET:HE2	1:A:194:GLN:HB2	1.83	0.60
2:B:132:ILE:O	2:B:134:GLU:N	2.34	0.60
2:B:223:VAL:HG12	2:B:223:VAL:O	2.01	0.60
2:B:475:ASN:O	2:B:479:ILE:HB	2.02	0.60
2:C:142:LYS:O	2:C:146:GLU:HG2	2.02	0.60
2:B:223:VAL:HG13	2:B:226:VAL:HB	1.83	0.60
2:B:393:LEU:CD1	2:B:464:LEU:HD21	2.31	0.60
2:C:477:ILE:O	2:C:480:LEU:HD22	2.01	0.60
2:B:347:LYS:CB	5:B:662:HOH:O	2.47	0.60
2:B:367:THR:HB	2:B:368:PRO:CD	2.27	0.60
2:B:384:VAL:O	2:B:440:ARG:NH1	2.35	0.60
1:A:143:ARG:NH2	2:B:206:ASP:OD2	2.35	0.59
2:B:331:ALA:O	2:B:335:MET:HG3	2.01	0.59
2:B:451:VAL:O	2:B:453:THR:HG23	2.02	0.59
2:C:460:ILE:O	2:C:463:PHE:HB3	2.01	0.59
2:B:406:PRO:HD3	2:B:524:ILE:HD11	1.84	0.59
2:C:401:PRO:HB3	5:C:611:HOH:O	2.02	0.59
2:C:456:ILE:HG12	5:C:611:HOH:O	2.01	0.59
2:B:407:VAL:HG23	2:B:452:LEU:HD21	1.83	0.59
1:A:110:GLN:H	1:A:113:HIS:HD2	1.45	0.59
1:A:74:GLU:HB3	2:B:51:LEU:HD12	1.85	0.59
1:A:143:ARG:HA	1:A:194:GLN:NE2	2.12	0.59
2:B:479:ILE:O	2:B:483:ARG:HD3	2.03	0.58
2:B:276:GLU:OE1	2:B:440:ARG:HD2	2.03	0.58
2:B:410:TRP:CD1	2:B:414:ILE:HD13	2.38	0.58
2:B:527:GLU:C	2:B:530:PRO:HD2	2.29	0.58
2:B:405:ILE:HD12	2:B:409:LEU:HD12	1.84	0.58
2:C:400:PRO:HG2	2:C:405:ILE:HD11	1.84	0.58
1:A:208:THR:HG21	2:B:217:LEU:N	2.14	0.58
2:B:529:PHE:N	2:B:530:PRO:HD2	2.17	0.58
1:A:165:PRO:HD2	1:A:213:ASN:OD1	2.04	0.58
2:C:435:LYS:HA	2:C:454:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:CG2	5:A:279:HOH:O	2.52	0.58
1:A:84:VAL:HG23	5:A:279:HOH:O	2.03	0.58
2:C:393:LEU:HB2	2:C:437:LEU:HD13	1.85	0.58
2:B:526:PRO:O	2:B:530:PRO:HD2	2.04	0.57
2:B:59:ARG:HD2	5:B:555:HOH:O	2.03	0.57
2:B:122:GLY:O	2:B:123:ASN:HB2	2.04	0.57
2:B:407:VAL:O	2:B:410:TRP:N	2.37	0.57
2:B:484:LEU:HD23	2:B:485:LEU:N	2.19	0.57
2:B:341:GLU:HB2	2:B:342:PRO:CD	2.34	0.57
2:C:197:PRO:HD2	5:C:582:HOH:O	2.05	0.57
2:B:130:CYS:HB3	2:B:305:TYR:CE1	2.40	0.56
2:B:347:LYS:O	2:B:351:LEU:HD23	2.05	0.56
2:B:434:LEU:HD22	2:B:444:LEU:HD23	1.86	0.56
2:B:461:HIS:HD2	5:B:574:HOH:O	1.88	0.56
2:B:475:ASN:N	2:B:475:ASN:HD22	2.04	0.56
2:C:223:VAL:HG12	2:C:224:GLU:O	2.06	0.56
2:C:329:ASN:HA	5:C:572:HOH:O	2.05	0.56
2:C:428:ASP:HA	2:C:431:ALA:HB3	1.87	0.56
2:B:72:ILE:HD13	2:B:87:LEU:HB2	1.87	0.56
1:A:196:ARG:HH21	2:B:125:PRO:HG3	1.71	0.56
2:B:428:ASP:O	2:B:431:ALA:HB3	2.05	0.56
1:A:112:GLU:HA	1:A:225:MET:CE	2.35	0.56
2:B:388:GLU:HB2	2:B:433:ARG:NE	2.19	0.56
2:B:289:GLU:HG3	2:B:291:THR:HG23	1.87	0.56
2:C:147:MET:HE1	2:C:155:LEU:HD23	1.88	0.56
1:A:112:GLU:HA	1:A:225:MET:HE3	1.88	0.56
2:C:141:ILE:HG23	2:C:179:LEU:HD13	1.87	0.56
2:C:155:LEU:HD12	2:C:269:LEU:CD1	2.36	0.56
2:B:98:PRO:C	2:B:100:LEU:N	2.64	0.55
2:B:302:LEU:HD23	2:B:337:PHE:CE1	2.41	0.55
2:C:480:LEU:HD23	2:C:481:GLU:N	2.20	0.55
2:B:399:MET:HG3	2:B:400:PRO:HD2	1.88	0.55
1:A:119:MET:HE1	1:A:231:MET:SD	2.46	0.55
1:A:166:MET:HE1	1:A:171:LEU:CA	2.36	0.55
2:B:207:ILE:HD11	2:B:249:PHE:CE2	2.41	0.55
2:B:538:LYS:O	2:B:538:LYS:HD3	2.06	0.55
2:B:158:HIS:CD2	2:B:158:HIS:H	2.24	0.55
2:C:468:VAL:O	2:C:469:ASP:C	2.49	0.55
2:B:534:GLN:OE1	2:B:537:GLN:HG3	2.07	0.55
2:C:459:ILE:HG23	2:C:460:ILE:N	2.20	0.55
1:A:208:THR:HG22	1:A:211:ARG:HH21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ARG:HG3	2:B:16:ARG:NH1	2.22	0.55
2:B:341:GLU:CB	2:B:342:PRO:HD3	2.34	0.55
2:C:209:LEU:HD23	2:C:212:LYS:HE2	1.88	0.55
1:A:207:LYS:HE3	5:A:254:HOH:O	2.07	0.54
2:B:475:ASN:HD22	2:B:475:ASN:H	1.53	0.54
2:C:298:CYS:O	2:C:302:LEU:HD12	2.07	0.54
2:C:205:THR:HG23	2:C:223:VAL:CG2	2.37	0.54
2:C:367:THR:HB	2:C:368:PRO:CD	2.37	0.54
2:B:282:SER:HB3	2:C:128:MET:HE3	1.90	0.54
2:B:19:HIS:HD2	2:B:20:ASP:OD2	1.91	0.54
2:B:94:ALA:O	2:B:98:PRO:HG3	2.07	0.54
2:B:98:PRO:O	2:B:100:LEU:N	2.41	0.54
2:C:209:LEU:HD23	2:C:212:LYS:HE3	1.89	0.54
2:C:274:ASP:OD1	2:C:440:ARG:HG2	2.07	0.54
2:C:291:THR:HG22	2:C:292:SER:H	1.71	0.54
2:C:456:ILE:HG23	5:C:611:HOH:O	2.07	0.54
2:B:18:ILE:HG23	2:B:51:LEU:CD2	2.36	0.54
2:B:43:LEU:HG	5:B:693:HOH:O	2.08	0.54
2:B:345:PHE:HA	2:B:348:MET:HE3	1.89	0.54
1:A:149:TYR:O	1:A:153:VAL:HG23	2.06	0.54
2:B:154:PHE:HB3	2:B:156:PHE:CE1	2.42	0.54
2:C:173:LEU:HD23	2:C:179:LEU:HD23	1.88	0.54
2:C:427:ASP:HB3	2:C:430:VAL:HB	1.89	0.54
2:C:480:LEU:HD23	2:C:480:LEU:C	2.33	0.54
2:B:469:ASP:C	2:B:471:GLN:N	2.61	0.54
2:C:443:LEU:O	2:C:444:LEU:HD12	2.07	0.54
2:C:237:ASN:O	2:C:240:ILE:HG22	2.07	0.54
2:B:118:LYS:HD3	5:B:695:HOH:O	2.08	0.54
2:B:347:LYS:O	2:B:347:LYS:HD3	2.08	0.54
2:B:325:LEU:O	2:B:459:ILE:HG23	2.08	0.53
2:B:55:ALA:O	2:B:59:ARG:HG3	2.08	0.53
2:C:203:LEU:HD11	2:C:249:PHE:HE2	1.72	0.53
2:C:291:THR:HG22	2:C:292:SER:N	2.23	0.53
2:C:292:SER:HB3	2:C:327:SER:O	2.07	0.53
2:C:364:GLU:O	2:C:365:CYS:HB3	2.07	0.53
2:C:468:VAL:O	2:C:468:VAL:HG13	2.08	0.53
2:B:4:GLU:CD	2:B:267:ARG:HH22	2.16	0.53
2:B:347:LYS:NZ	2:B:351:LEU:HD21	2.24	0.53
2:C:205:THR:HG23	2:C:223:VAL:HG21	1.90	0.53
2:C:255:GLU:CD	2:C:280:ALA:HB2	2.34	0.53
2:C:342:PRO:O	2:C:343:LYS:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:GLN:O	2:B:110:PHE:HB2	2.09	0.53
2:B:302:LEU:O	2:B:307:MET:HB2	2.09	0.53
2:B:482:GLN:HE21	2:B:482:GLN:HA	1.74	0.53
2:C:464:LEU:O	2:C:468:VAL:HG12	2.09	0.53
2:B:141:ILE:HD13	2:B:176:SER:HB2	1.89	0.53
2:B:187:ILE:HG12	2:B:188:VAL:N	2.23	0.53
2:B:521:GLU:HG3	2:B:523:VAL:HG12	1.90	0.53
2:C:337:PHE:N	2:C:337:PHE:HD1	2.06	0.53
2:B:112:ARG:NH2	2:B:174:SER:O	2.34	0.53
2:C:337:PHE:CD1	2:C:337:PHE:N	2.76	0.53
2:B:102:ARG:HG2	2:B:182:ILE:CG2	2.40	0.53
1:A:118:VAL:O	1:A:122:ILE:HG12	2.10	0.52
2:B:343:LYS:HD3	2:B:343:LYS:H	1.73	0.52
2:C:203:LEU:HD12	2:C:204:PHE:CE1	2.44	0.52
2:C:478:SER:HB2	2:C:479:ILE:HD12	1.89	0.52
2:B:459:ILE:HD12	2:B:460:ILE:H	1.69	0.52
2:B:378:LEU:O	2:B:382:VAL:HG23	2.09	0.52
2:B:468:VAL:O	2:B:469:ASP:C	2.51	0.52
2:C:393:LEU:CD1	2:C:443:LEU:HD22	2.40	0.52
1:A:153:VAL:HG12	1:A:153:VAL:O	2.09	0.52
2:B:480:LEU:C	2:B:482:GLN:H	2.16	0.52
2:B:37:THR:HG23	2:B:40:HIS:CD2	2.45	0.52
2:B:354:LYS:HA	2:B:357:SER:OG	2.10	0.52
2:B:302:LEU:HD23	2:B:337:PHE:CZ	2.44	0.52
2:B:478:SER:HA	2:B:481:GLU:HB2	1.92	0.52
1:A:171:LEU:HD21	1:A:221:TRP:CH2	2.44	0.52
2:B:439:LYS:HE2	2:C:341:GLU:OE1	2.10	0.52
2:C:308:PRO:HB2	2:C:345:PHE:CZ	2.44	0.52
2:B:408:LYS:HE3	2:B:527:GLU:OE2	2.10	0.52
1:A:99:TRP:CE3	1:A:102:ALA:HB2	2.45	0.52
2:B:307:MET:HE3	2:B:348:MET:HE2	1.92	0.52
2:B:327:SER:OG	2:B:457:ASP:HB3	2.09	0.52
2:B:425:GLN:OE1	2:C:350:GLN:HG3	2.10	0.52
2:C:133:ARG:HG2	2:C:136:HIS:CD2	2.41	0.52
2:B:334:MET:HE3	2:B:334:MET:HA	1.91	0.52
2:C:396:ALA:O	2:C:399:MET:HB2	2.10	0.52
2:C:479:ILE:HD12	2:C:479:ILE:H	1.74	0.52
2:B:147:MET:HE1	2:B:155:LEU:CG	2.39	0.51
1:A:141:VAL:HG13	1:A:142:PRO:HD2	1.92	0.51
2:B:471:GLN:O	2:B:475:ASN:ND2	2.43	0.51
1:A:67:ASP:O	2:B:53:ARG:NH2	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:398:VAL:HG22	2:C:473:ILE:HG13	1.93	0.51
1:A:93:ARG:C	1:A:95:ASN:N	2.69	0.51
1:A:97:MET:CE	1:A:186:MET:HB3	2.40	0.51
2:C:228:SER:HB3	2:C:260:TRP:CH2	2.46	0.51
2:B:526:PRO:HD2	2:B:529:PHE:CD1	2.46	0.51
2:C:203:LEU:HD13	2:C:203:LEU:C	2.36	0.51
1:A:70:ILE:HD11	2:B:18:ILE:HG22	1.93	0.51
2:C:112:ARG:NH1	2:C:115:LEU:HD12	2.26	0.51
2:C:155:LEU:C	2:C:155:LEU:HD13	2.36	0.51
2:C:397:VAL:HG13	2:C:398:VAL:HG23	1.92	0.51
2:C:405:ILE:N	2:C:453:THR:HG23	2.26	0.51
2:B:190:LEU:CD1	2:B:207:ILE:HG13	2.40	0.51
2:C:406:PRO:HG2	2:C:409:LEU:HG	1.93	0.51
2:C:477:ILE:O	2:C:480:LEU:HB3	2.11	0.51
1:A:192:GLN:O	1:A:194:GLN:N	2.44	0.50
2:C:429:GLU:O	2:C:429:GLU:HG3	2.11	0.50
2:B:158:HIS:CE1	2:B:289:GLU:HB3	2.46	0.50
2:B:344:THR:HG22	2:B:346:GLU:H	1.76	0.50
2:C:389:ASP:HA	2:C:392:ALA:HB3	1.93	0.50
2:B:351:LEU:O	2:B:352:ASN:C	2.53	0.50
2:C:395:PHE:C	2:C:397:VAL:H	2.18	0.50
2:C:406:PRO:HD2	2:C:409:LEU:CD1	2.31	0.50
2:B:47:MET:HB3	2:B:52:GLU:HB3	1.93	0.50
2:B:137:VAL:O	2:B:141:ILE:HG13	2.11	0.50
2:C:133:ARG:CG	2:C:136:HIS:HD2	2.23	0.50
2:C:193:SER:OG	2:C:251:ASP:OD2	2.29	0.50
2:B:173:LEU:HD13	2:B:187:ILE:CD1	2.42	0.50
2:B:344:THR:C	2:B:346:GLU:N	2.69	0.50
2:B:426:LEU:HB3	5:B:668:HOH:O	2.12	0.50
2:B:262:GLN:NE2	2:B:283:GLN:N	2.56	0.50
2:C:109:GLN:O	2:C:113:GLN:HG3	2.12	0.50
2:C:278:SER:C	2:C:280:ALA:H	2.20	0.50
2:B:139:ARG:NH2	2:B:143:LYS:HE3	2.27	0.49
2:B:537:GLN:C	2:B:539:PHE:N	2.68	0.49
2:C:395:PHE:O	2:C:397:VAL:N	2.46	0.49
2:C:242:ARG:N	2:C:243:PRO:HD3	2.28	0.49
2:C:319:LEU:O	2:C:323:ILE:HG13	2.11	0.49
1:A:208:THR:CG2	2:B:217:LEU:H	2.20	0.49
2:B:363:VAL:HG13	2:B:363:VAL:O	2.12	0.49
2:B:457:ASP:O	2:B:460:ILE:HG22	2.12	0.49
2:C:397:VAL:O	2:C:399:MET:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:464:LEU:HA	2:C:467:VAL:CG1	2.37	0.49
2:B:97:GLU:N	2:B:98:PRO:HD3	2.27	0.49
2:B:405:ILE:HG23	2:B:410:TRP:CZ3	2.47	0.49
2:C:405:ILE:N	2:C:453:THR:CG2	2.75	0.49
2:B:152:SER:OG	2:B:283:GLN:NE2	2.46	0.49
5:B:553:HOH:O	2:C:117:ARG:HD2	2.12	0.49
2:B:344:THR:C	2:B:346:GLU:H	2.19	0.49
2:C:160:ARG:HH11	2:C:459:ILE:HG21	1.78	0.49
2:C:393:LEU:O	2:C:395:PHE:N	2.43	0.49
2:B:68:LEU:O	2:B:72:ILE:HG12	2.13	0.49
2:C:397:VAL:HG13	2:C:398:VAL:N	2.25	0.49
2:C:477:ILE:HG22	2:C:478:SER:N	2.26	0.49
2:B:461:HIS:CD2	5:B:574:HOH:O	2.64	0.49
2:C:136:HIS:O	2:C:140:VAL:HG23	2.12	0.49
2:B:477:ILE:CD1	2:B:543:LEU:HG	2.43	0.48
1:A:191:LEU:HD12	1:A:191:LEU:N	2.27	0.48
2:C:158:HIS:HA	2:C:272:THR:O	2.12	0.48
2:C:203:LEU:HD11	2:C:249:PHE:CE2	2.48	0.48
1:A:116:MET:HE2	1:A:224:PHE:CZ	2.48	0.48
2:B:362:GLY:C	2:B:364:GLU:H	2.21	0.48
1:A:153:VAL:C	1:A:155:THR:H	2.20	0.48
2:C:459:ILE:CG2	2:C:460:ILE:N	2.77	0.48
2:B:537:GLN:HG2	2:B:541:ASP:OD1	2.13	0.48
1:A:100:PHE:CD2	2:B:368:PRO:HA	2.48	0.48
2:B:198:LYS:HD2	5:B:694:HOH:O	2.12	0.48
2:C:299:TYR:CZ	2:C:319:LEU:HD23	2.48	0.48
1:A:203:SER:O	1:A:207:LYS:HB2	2.14	0.48
2:B:541:ASP:O	2:B:543:LEU:N	2.45	0.48
2:B:322:THR:CA	2:B:352:ASN:HD21	2.27	0.48
2:B:410:TRP:CZ3	2:B:454:PHE:O	2.61	0.48
2:B:413:VAL:HG23	2:B:414:ILE:HD12	1.96	0.48
2:C:274:ASP:O	2:C:277:ILE:HG12	2.14	0.48
2:C:427:ASP:O	2:C:431:ALA:HB2	2.13	0.48
2:C:475:ASN:N	2:C:475:ASN:HD22	2.12	0.48
1:A:185:MET:CE	1:A:194:GLN:HB2	2.42	0.48
2:B:410:TRP:C	2:B:412:CYS:H	2.21	0.48
2:C:410:TRP:O	2:C:413:VAL:HG22	2.14	0.48
2:B:18:ILE:C	2:B:50:ARG:HH22	2.19	0.47
2:B:100:LEU:O	2:B:103:PRO:HD2	2.14	0.47
2:B:160:ARG:HB2	2:B:442:ALA:HB3	1.96	0.47
2:B:527:GLU:O	2:B:530:PRO:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:191:LYS:HA	2:C:250:ASP:HB3	1.96	0.47
2:C:407:VAL:HG11	2:C:431:ALA:HB2	1.95	0.47
2:B:444:LEU:HB3	5:B:687:HOH:O	2.14	0.47
2:C:187:ILE:HG12	2:C:188:VAL:N	2.28	0.47
2:B:26:ALA:HB2	2:B:74:PHE:CZ	2.49	0.47
2:B:102:ARG:HG2	2:B:182:ILE:HG23	1.95	0.47
2:B:307:MET:HA	2:B:308:PRO:HD3	1.81	0.47
2:B:434:LEU:HD22	2:B:444:LEU:CD2	2.43	0.47
2:C:255:GLU:HG3	2:C:280:ALA:HB2	1.97	0.47
2:C:384:VAL:HG12	2:C:440:ARG:HH12	1.80	0.47
2:B:173:LEU:HD13	2:B:187:ILE:HD12	1.96	0.47
2:C:447:LYS:N	2:C:453:THR:O	2.47	0.47
2:C:481:GLU:N	5:C:587:HOH:O	2.47	0.47
2:B:451:VAL:O	2:B:451:VAL:CG2	2.63	0.47
2:C:469:ASP:O	2:C:471:GLN:N	2.48	0.47
1:A:208:THR:HG21	2:B:217:LEU:HB2	1.96	0.47
2:B:485:LEU:HD12	2:B:486:GLU:N	2.29	0.47
2:C:325:LEU:O	2:C:462:MET:HE2	2.14	0.47
2:C:386:SER:O	2:C:389:ASP:N	2.47	0.47
2:C:393:LEU:C	2:C:395:PHE:N	2.72	0.47
1:A:138:LEU:HD22	1:A:144:ILE:CD1	2.42	0.47
1:A:192:GLN:C	1:A:194:GLN:H	2.23	0.47
1:A:78:LEU:O	1:A:79:ASP:C	2.57	0.47
1:A:186:MET:C	1:A:188:SER:H	2.22	0.47
2:B:485:LEU:HD12	2:B:485:LEU:C	2.40	0.47
2:C:374:LEU:HD23	2:C:374:LEU:HA	1.78	0.47
2:B:98:PRO:O	2:B:99:ASP:OD1	2.32	0.47
2:B:409:LEU:CD2	2:B:530:PRO:HB3	2.42	0.47
2:B:468:VAL:O	2:B:470:ALA:N	2.48	0.47
4:B:551:ATP:H5'2	4:B:551:ATP:H2'	1.55	0.47
2:C:389:ASP:C	2:C:391:SER:H	2.23	0.47
2:B:157:LEU:HD22	2:B:290:VAL:HG23	1.96	0.46
2:B:273:ARG:HD3	2:B:381:CYS:SG	2.54	0.46
2:B:536:HIS:O	2:B:540:TYR:HD1	1.97	0.46
2:C:189:TRP:CD1	2:C:189:TRP:C	2.93	0.46
1:A:92:ILE:HD13	1:A:99:TRP:HB2	1.97	0.46
2:B:355:LEU:HD21	2:B:363:VAL:CG1	2.45	0.46
2:B:374:LEU:HD13	2:B:378:LEU:HG	1.96	0.46
2:B:477:ILE:HD12	2:B:543:LEU:HG	1.97	0.46
2:C:239:LEU:HD11	2:C:266:LEU:CD2	2.45	0.46
2:C:328:GLY:O	2:C:330:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:435:LYS:HA	2:C:454:PHE:HE2	1.79	0.46
2:C:165:LYS:HG2	2:C:290:VAL:HG21	1.97	0.46
1:A:197:ASN:HD22	1:A:197:ASN:H	1.63	0.46
2:B:307:MET:CE	2:B:348:MET:HE2	2.46	0.46
2:C:112:ARG:O	2:C:112:ARG:HD3	2.16	0.46
1:A:122:ILE:HD12	1:A:235:TYR:CD2	2.51	0.46
1:A:91:ARG:HH21	1:A:124:GLU:CD	2.22	0.46
2:B:410:TRP:CZ3	2:B:454:PHE:HB2	2.51	0.46
2:B:410:TRP:C	2:B:412:CYS:N	2.71	0.46
2:B:467:VAL:HG12	2:B:467:VAL:O	2.15	0.46
2:C:112:ARG:NH1	2:C:116:ASP:OD1	2.49	0.46
2:C:160:ARG:HB3	5:C:576:HOH:O	2.16	0.46
2:C:480:LEU:HD11	2:C:540:TYR:CE1	2.50	0.46
2:B:212:LYS:HE2	5:C:554:HOH:O	2.15	0.46
2:C:475:ASN:O	2:C:479:ILE:HD13	2.16	0.46
2:B:342:PRO:CD	2:B:347:LYS:HG3	2.45	0.45
1:A:115:MET:HB3	1:A:225:MET:HE1	1.94	0.45
1:A:223:ASP:O	1:A:227:LEU:HD13	2.17	0.45
2:B:523:VAL:HG22	2:B:524:ILE:H	1.82	0.45
2:C:386:SER:C	2:C:388:GLU:N	2.71	0.45
2:C:395:PHE:C	2:C:397:VAL:N	2.74	0.45
1:A:71:ASN:HB3	1:A:73:TRP:CZ3	2.50	0.45
1:A:127:HIS:C	1:A:129:GLU:H	2.24	0.45
1:A:163:GLN:N	5:A:267:HOH:O	2.48	0.45
2:B:220:PHE:CD1	2:B:221:PRO:HD2	2.51	0.45
1:A:92:ILE:HG23	1:A:97:MET:HB2	1.99	0.45
2:B:456:ILE:HG23	2:B:456:ILE:O	2.15	0.45
1:A:232:LYS:O	1:A:236:GLU:HG3	2.16	0.45
2:B:115:LEU:CD1	2:B:177:ASP:HA	2.47	0.45
2:B:224:GLU:HG2	2:B:225:HIS:CD2	2.51	0.45
2:B:469:ASP:O	2:B:472:THR:N	2.48	0.45
1:A:122:ILE:HD12	1:A:235:TYR:CG	2.52	0.45
2:B:322:THR:N	2:B:352:ASN:HD21	2.15	0.45
2:B:336:PHE:CE1	2:B:355:LEU:HD11	2.50	0.45
2:B:426:LEU:N	2:B:426:LEU:HD23	2.31	0.45
2:B:529:PHE:H	2:B:530:PRO:HD2	1.81	0.45
2:B:131:TYR:HD1	2:B:301:PHE:HD1	1.65	0.45
2:B:182:ILE:HD12	2:B:182:ILE:N	2.32	0.45
2:C:302:LEU:HG	2:C:337:PHE:HZ	1.82	0.45
2:B:443:LEU:C	2:B:444:LEU:HD12	2.42	0.45
2:B:21:PHE:CD2	2:B:22:GLU:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ALA:O	2:B:374:LEU:HD21	2.16	0.45
2:B:163:SER:HB2	2:B:290:VAL:CG1	2.43	0.45
2:C:141:ILE:HG23	2:C:179:LEU:CD1	2.47	0.45
2:C:224:GLU:CD	2:C:224:GLU:H	2.24	0.45
2:C:474:ALA:O	2:C:477:ILE:HB	2.17	0.45
2:B:179:LEU:HA	2:B:183:ASN:HB2	1.99	0.45
2:B:347:LYS:HZ2	2:B:351:LEU:HD21	1.82	0.45
2:C:154:PHE:HZ	2:C:261:ALA:HB3	1.82	0.45
2:C:448:ARG:HB3	2:C:452:LEU:HG	1.98	0.45
2:C:479:ILE:N	2:C:479:ILE:CD1	2.80	0.45
2:B:4:GLU:OE2	2:B:267:ARG:NH2	2.50	0.44
2:B:102:ARG:N	2:B:103:PRO:CD	2.80	0.44
2:C:133:ARG:NE	2:C:136:HIS:CD2	2.85	0.44
2:C:244:ASN:HA	2:C:267:ARG:HH11	1.81	0.44
2:B:331:ALA:HA	4:B:551:ATP:O3'	2.17	0.44
2:B:333:LEU:O	2:B:336:PHE:HB2	2.17	0.44
2:B:463:PHE:O	2:B:467:VAL:HG23	2.16	0.44
2:B:474:ALA:HA	2:B:477:ILE:HG22	1.99	0.44
2:C:196:ALA:HB1	2:C:197:PRO:CD	2.47	0.44
2:C:274:ASP:OD1	2:C:440:ARG:HA	2.17	0.44
2:C:403:VAL:O	2:C:403:VAL:HG23	2.16	0.44
2:B:159:GLY:N	2:B:165:LYS:HD3	2.32	0.44
2:B:308:PRO:C	2:B:309:MET:HG3	2.42	0.44
2:B:407:VAL:O	2:B:408:LYS:C	2.59	0.44
2:C:379:GLN:O	2:C:383:GLU:HG3	2.17	0.44
2:C:467:VAL:HG13	2:C:468:VAL:N	2.32	0.44
2:B:97:GLU:O	2:B:100:LEU:HB2	2.18	0.44
2:B:274:ASP:O	2:B:277:ILE:HG12	2.18	0.44
2:B:393:LEU:HD22	2:B:393:LEU:O	2.17	0.44
1:A:189:VAL:HG22	1:A:192:GLN:CD	2.42	0.44
2:B:165:LYS:NZ	4:B:551:ATP:O2B	2.46	0.44
2:C:386:SER:O	2:C:388:GLU:N	2.50	0.44
2:B:223:VAL:CG1	2:B:226:VAL:HB	2.47	0.44
2:B:393:LEU:HD22	2:B:464:LEU:HD11	1.99	0.44
2:B:405:ILE:HD11	2:B:409:LEU:HB3	1.99	0.44
2:C:187:ILE:HG12	2:C:188:VAL:H	1.83	0.44
2:B:374:LEU:O	2:B:377:ALA:HB3	2.17	0.44
2:C:164:GLY:O	2:C:168:ILE:HG13	2.18	0.44
2:C:480:LEU:N	5:C:587:HOH:O	2.50	0.44
2:B:50:ARG:O	2:B:54:ILE:HG13	2.17	0.43
2:B:123:ASN:HD22	2:B:210:MET:CE	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:276:GLU:C	2:C:278:SER:H	2.26	0.43
2:C:355:LEU:HD21	2:C:363:VAL:HG13	2.00	0.43
2:B:1:MET:HE2	2:B:240:ILE:HD12	1.99	0.43
2:B:3:CYS:SG	2:B:6:GLU:HG3	2.58	0.43
2:B:131:TYR:CD1	2:B:301:PHE:HD1	2.36	0.43
2:B:152:SER:HB3	2:B:265:ARG:O	2.17	0.43
2:B:233:ARG:CZ	2:C:210:MET:HE3	2.48	0.43
2:B:407:VAL:HG23	2:B:452:LEU:CD2	2.46	0.43
2:B:523:VAL:HG22	2:B:524:ILE:N	2.32	0.43
2:C:428:ASP:C	2:C:430:VAL:H	2.25	0.43
2:B:400:PRO:HD3	2:B:540:TYR:CZ	2.53	0.43
2:B:102:ARG:NH1	2:B:149:ASP:OD1	2.49	0.43
2:C:118:LYS:HE2	5:C:629:HOH:O	2.17	0.43
2:C:367:THR:HB	2:C:368:PRO:HD2	2.00	0.43
2:C:473:ILE:HG23	2:C:474:ALA:N	2.33	0.43
1:A:77:ARG:HH22	1:A:112:GLU:CD	2.26	0.43
1:A:192:GLN:C	1:A:194:GLN:N	2.77	0.43
2:B:342:PRO:HG2	2:B:347:LYS:HG3	1.99	0.43
2:C:154:PHE:CE2	2:C:258:ILE:HG23	2.52	0.43
1:A:128:ALA:O	1:A:129:GLU:C	2.62	0.43
2:B:425:GLN:HE21	2:C:353:ASN:HD22	1.67	0.43
2:C:196:ALA:C	5:C:562:HOH:O	2.60	0.43
2:C:276:GLU:C	2:C:278:SER:N	2.75	0.43
1:A:171:LEU:CD1	1:A:206:ILE:HD13	2.47	0.43
2:B:75:PHE:CB	2:B:84:ALA:HB2	2.44	0.43
2:B:374:LEU:CD1	2:B:378:LEU:HG	2.49	0.43
2:C:276:GLU:OE2	2:C:439:LYS:HE3	2.18	0.43
2:C:368:PRO:HD2	4:C:551:ATP:O2'	2.19	0.43
2:B:535:LEU:HD23	2:B:535:LEU:O	2.18	0.42
2:C:302:LEU:CD1	2:C:319:LEU:HD11	2.45	0.42
2:C:345:PHE:HA	2:C:348:MET:HB2	2.00	0.42
2:C:405:ILE:O	2:C:453:THR:HG23	2.19	0.42
2:B:319:LEU:C	2:B:319:LEU:HD23	2.44	0.42
2:B:329:ASN:OD1	2:B:332:THR:N	2.45	0.42
2:C:403:VAL:HG23	2:C:405:ILE:HG13	2.01	0.42
2:C:432:ASP:HA	2:C:435:LYS:CB	2.45	0.42
2:B:335:MET:HE1	2:B:373:SER:CA	2.46	0.42
1:A:143:ARG:NH1	5:A:282:HOH:O	2.51	0.42
1:A:170:ARG:HG3	1:A:170:ARG:HH11	1.83	0.42
2:B:319:LEU:HD23	2:B:320:ASN:N	2.34	0.42
2:B:451:VAL:O	2:B:451:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:PRO:O	2:B:99:ASP:CG	2.61	0.42
2:B:188:VAL:HG13	2:B:210:MET:HG2	2.01	0.42
2:B:405:ILE:CD1	2:B:409:LEU:HB3	2.49	0.42
2:B:401:PRO:HA	2:B:456:ILE:O	2.20	0.42
2:B:457:ASP:OD2	2:B:457:ASP:N	2.52	0.42
2:C:110:PHE:O	2:C:114:MET:HG2	2.20	0.42
2:C:203:LEU:HD12	2:C:204:PHE:CD1	2.55	0.42
2:B:143:LYS:NZ	2:B:286:GLU:HG3	2.34	0.42
2:B:336:PHE:CD1	2:B:363:VAL:HG21	2.55	0.42
2:B:387:ASP:OD1	2:B:390:ARG:NH2	2.53	0.42
2:C:334:MET:HE3	4:C:551:ATP:H8	1.83	0.42
1:A:135:SER:O	1:A:139:LEU:HG	2.20	0.42
2:B:207:ILE:HD11	2:B:249:PHE:HE2	1.83	0.42
2:B:354:LYS:HA	2:B:354:LYS:HD3	1.87	0.42
2:B:427:ASP:HB2	5:B:616:HOH:O	2.18	0.42
2:B:480:LEU:C	2:B:482:GLN:N	2.78	0.42
2:C:432:ASP:C	2:C:434:LEU:H	2.27	0.42
1:A:100:PHE:CG	2:B:368:PRO:HB3	2.55	0.42
2:B:234:MET:HG2	2:C:217:LEU:CD1	2.50	0.42
2:C:112:ARG:HD3	2:C:112:ARG:C	2.45	0.42
2:C:414:ILE:HG21	2:C:430:VAL:HG22	2.02	0.42
1:A:189:VAL:HG11	2:B:370:SER:O	2.20	0.41
2:C:309:MET:HA	2:C:310:PRO:HD3	1.79	0.41
2:C:385:LEU:HD23	2:C:440:ARG:NH2	2.35	0.41
2:C:412:CYS:O	2:C:412:CYS:SG	2.78	0.41
2:B:115:LEU:HD11	2:B:177:ASP:HA	2.02	0.41
2:B:351:LEU:O	2:B:354:LYS:N	2.53	0.41
1:A:102:ALA:HA	1:A:103:PRO:HD3	1.98	0.41
1:A:211:ARG:NH2	2:B:215:ASP:O	2.53	0.41
2:B:208:LEU:CD1	2:B:220:PHE:CZ	3.04	0.41
2:B:481:GLU:HA	2:B:484:LEU:HD22	2.02	0.41
2:C:133:ARG:NH1	2:C:293:LEU:HD23	2.36	0.41
2:B:44:ILE:HD11	2:B:60:ILE:HD12	2.02	0.41
2:B:173:LEU:HD22	2:B:180:ILE:HD11	2.03	0.41
2:C:472:THR:O	5:C:574:HOH:O	2.22	0.41
2:B:22:GLU:O	2:B:22:GLU:HG3	2.20	0.41
2:B:133:ARG:NE	2:B:136:HIS:CD2	2.89	0.41
2:B:533:MET:HE3	2:B:540:TYR:CD2	2.55	0.41
1:A:116:MET:HE1	1:A:172:ILE:HG12	2.01	0.41
1:A:204:LEU:HD21	2:B:213:SER:HB2	2.02	0.41
2:B:400:PRO:HA	2:B:401:PRO:HD2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:455:LYS:HE2	2:C:455:LYS:HB3	1.84	0.41
2:C:479:ILE:H	2:C:479:ILE:CD1	2.33	0.41
2:B:18:ILE:HD12	2:B:51:LEU:CD2	2.39	0.41
2:B:340:CYS:SG	2:B:348:MET:HA	2.61	0.41
2:B:410:TRP:CZ3	2:B:454:PHE:C	2.99	0.41
2:C:272:THR:HG21	2:C:277:ILE:HD11	2.01	0.41
2:C:535:LEU:HD22	2:C:535:LEU:N	2.35	0.41
1:A:141:VAL:HG12	1:A:143:ARG:H	1.86	0.41
2:B:71:LEU:HD22	2:B:75:PHE:CE1	2.56	0.41
2:B:107:ALA:O	2:B:108:PRO:C	2.62	0.41
2:B:252:VAL:HG11	2:B:258:ILE:CD1	2.52	0.41
2:B:335:MET:CE	2:B:373:SER:HA	2.46	0.41
2:C:391:SER:HA	2:C:394:ALA:HB3	2.03	0.41
2:C:448:ARG:CB	2:C:452:LEU:HG	2.51	0.41
2:C:535:LEU:N	2:C:535:LEU:CD2	2.84	0.41
1:A:141:VAL:CG1	1:A:142:PRO:HD2	2.51	0.40
2:B:26:ALA:HA	2:B:74:PHE:CE1	2.56	0.40
2:B:49:THR:HB	2:B:52:GLU:CD	2.46	0.40
2:B:133:ARG:NE	2:B:136:HIS:HD2	2.19	0.40
2:B:521:GLU:CG	2:B:523:VAL:HG12	2.51	0.40
2:B:405:ILE:HG13	2:B:409:LEU:HB3	2.03	0.40
2:C:130:CYS:HB3	2:C:305:TYR:OH	2.21	0.40
2:C:208:LEU:HB2	2:C:235:ILE:CD1	2.50	0.40
2:C:533:MET:N	2:C:535:LEU:HD23	2.36	0.40
2:B:26:ALA:HB2	2:B:74:PHE:CE2	2.56	0.40
2:B:208:LEU:CD2	2:B:212:LYS:HD2	2.51	0.40
2:B:481:GLU:C	2:B:484:LEU:HD22	2.47	0.40
2:B:539:PHE:N	2:B:539:PHE:CD1	2.89	0.40
2:C:242:ARG:HE	2:C:242:ARG:HB3	1.78	0.40
2:C:333:LEU:HD23	2:C:333:LEU:HA	1.96	0.40
2:C:432:ASP:C	2:C:434:LEU:N	2.78	0.40
2:C:187:ILE:HG12	2:C:246:LEU:O	2.21	0.40
2:C:190:LEU:HD12	2:C:207:ILE:CD1	2.52	0.40
2:C:262:GLN:NE2	2:C:283:GLN:H	2.16	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	169/204 (83%)	144 (85%)	18 (11%)	7 (4%)	2	3
2	B	493/549 (90%)	430 (87%)	46 (9%)	17 (3%)	3	4
2	C	367/549 (67%)	315 (86%)	36 (10%)	16 (4%)	2	2
All	All	1029/1302 (79%)	889 (86%)	100 (10%)	40 (4%)	2	3

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	470	ALA
2	C	342	PRO
2	C	343	LYS
2	C	450	PRO
2	C	470	ALA
1	A	69	LYS
1	A	70	ILE
1	A	129	GLU
1	A	190	GLU
1	A	193	GLY
2	B	99	ASP
2	B	133	ARG
2	B	314	LYS
2	B	363	VAL
2	B	465	LYS
2	B	469	ASP
2	C	394	ALA
2	C	396	ALA
2	C	469	ASP
2	B	130	CYS
2	B	148	CYS
2	B	179	LEU
2	C	383	GLU
1	A	94	GLN

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Mol	Chain	Res	Type
1	A	187	GLU
2	B	110	PHE
2	B	308	PRO
2	B	466	HIS
2	B	527	GLU
2	C	309	MET
2	C	398	VAL
2	C	479	ILE
2	B	530	PRO
2	C	308	PRO
2	C	387	ASP
2	C	430	VAL
2	C	468	VAL
2	C	449	MET
2	B	398	VAL
2	B	342	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/179 (84%)	140 (93%)	11 (7%)	13	29
2	B	457/501 (91%)	416 (91%)	41 (9%)	9	20
2	C	338/501 (68%)	306 (90%)	32 (10%)	8	18
All	All	946/1181 (80%)	862 (91%)	84 (9%)	9	20

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	95	ASN
1	A	116	MET
1	A	136	GLU
1	A	148	LEU
1	A	153	VAL

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Mol	Chain	Res	Type
1	A	155	THR
1	A	197	ASN
1	A	198	LEU
1	A	216	GLU
1	A	230	GLN
2	B	8	ARG
2	B	15	THR
2	B	20	ASP
2	B	49	THR
2	B	52	GLU
2	B	71	LEU
2	B	77	TYR
2	B	112	ARG
2	B	120	LEU
2	B	129	THR
2	B	146	GLU
2	B	157	LEU
2	B	179	LEU
2	B	195	THR
2	B	203	LEU
2	B	208	LEU
2	B	209	LEU
2	B	229	VAL
2	B	231	LEU
2	B	258	ILE
2	B	269	LEU
2	B	275	VAL
2	B	333	LEU
2	B	336	PHE
2	B	364	GLU
2	B	383	GLU
2	B	391	SER
2	B	405	ILE
2	B	409	LEU
2	B	410	TRP
2	B	413	VAL
2	B	426	LEU
2	B	432	ASP
2	B	451	VAL
2	B	452	LEU
2	B	460	ILE
2	B	468	VAL

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Mol	Chain	Res	Type
2	B	472	THR
2	B	475	ASN
2	B	481	GLU
2	B	534	GLN
2	C	112	ARG
2	C	115	LEU
2	C	120	LEU
2	C	187	ILE
2	C	195	THR
2	C	208	LEU
2	C	216	ASP
2	C	217	LEU
2	C	218	LEU
2	C	224	GLU
2	C	227	THR
2	C	268	CYS
2	C	309	MET
2	C	337	PHE
2	C	339	SER
2	C	342	PRO
2	C	343	LYS
2	C	374	LEU
2	C	380	ARG
2	C	381	CYS
2	C	393	LEU
2	C	395	PHE
2	C	397	VAL
2	C	407	VAL
2	C	408	LYS
2	C	433	ARG
2	C	434	LEU
2	C	452	LEU
2	C	479	ILE
2	C	480	LEU
2	C	535	LEU
2	C	537	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	113	HIS

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Mol	Chain	Res	Type
1	A	194	GLN
1	A	197	ASN
1	A	213	ASN
1	A	217	HIS
1	A	230	GLN
2	B	19	HIS
2	B	34	ASN
2	B	40	HIS
2	B	64	GLN
2	B	109	GLN
2	B	123	ASN
2	B	127	GLN
2	B	136	HIS
2	B	158	HIS
2	B	219	ASN
2	B	225	HIS
2	B	244	ASN
2	B	254	GLN
2	B	262	GLN
2	B	283	GLN
2	B	475	ASN
2	B	482	GLN
2	B	536	HIS
2	C	123	ASN
2	C	127	GLN
2	C	136	HIS
2	C	183	ASN
2	C	219	ASN
2	C	254	GLN
2	C	320	ASN
2	C	353	ASN
2	C	458	HIS
2	C	466	HIS
2	C	475	ASN
2	C	482	GLN
2	C	534	GLN
2	C	537	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
4	ATP	C	551	3	32,33,33	1.96	9 (28%)	48,52,52	1.68	5 (10%)
4	ATP	B	551	3	32,33,33	2.23	11 (34%)	48,52,52	1.60	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	C	551	3	-	4/22/38/38	0/3/3/3
4	ATP	B	551	3	-	3/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	551	ATP	O4'-C1'	5.58	1.54	1.42
4	C	551	ATP	PB-O3B	5.20	1.65	1.59
4	B	551	ATP	PB-O3A	4.85	1.64	1.59
4	B	551	ATP	PB-O3B	4.38	1.64	1.59
4	C	551	ATP	C8-N7	4.30	1.39	1.31
4	C	551	ATP	C8-N9	4.30	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	551	ATP	C4-N3	3.87	1.41	1.34
4	B	551	ATP	C8-N9	3.46	1.43	1.37
4	C	551	ATP	C5-C4	2.95	1.44	1.39
4	B	551	ATP	C2-N3	2.86	1.39	1.33
4	B	551	ATP	O3'-C3'	2.83	1.50	1.43
4	B	551	ATP	C8-N7	2.76	1.37	1.31
4	C	551	ATP	O4'-C4'	2.72	1.51	1.45
4	C	551	ATP	C2-N3	2.70	1.38	1.33
4	C	551	ATP	O3'-C3'	2.68	1.49	1.43
4	B	551	ATP	C5-N7	2.63	1.43	1.39
4	C	551	ATP	C2-N1	2.51	1.38	1.33
4	C	551	ATP	O4'-C1'	2.44	1.47	1.42
4	B	551	ATP	C2-N1	2.33	1.38	1.33
4	B	551	ATP	PA-O3A	-2.14	1.57	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	551	ATP	O3A-PA-O1A	-6.91	89.91	110.70
4	B	551	ATP	O3A-PA-O1A	-4.58	96.92	110.70
4	C	551	ATP	O4'-C1'-C2'	-3.33	99.50	106.62
4	B	551	ATP	C2'-C3'-C4'	-3.07	96.68	102.61
4	B	551	ATP	O2B-PB-O3A	3.06	115.54	107.27
4	B	551	ATP	O5'-C5'-C4'	2.80	118.53	108.99
4	B	551	ATP	O2A-PA-O1A	2.77	125.31	112.44
4	C	551	ATP	O2A-PA-O1A	2.75	125.25	112.44
4	B	551	ATP	O4'-C4'-C3'	-2.69	99.81	105.15
4	B	551	ATP	O3B-PB-O1B	-2.69	102.62	110.70
4	C	551	ATP	O3G-PG-O2G	2.61	117.60	107.80
4	B	551	ATP	O3G-PG-O2G	2.58	117.48	107.80
4	C	551	ATP	C5'-C4'-C3'	-2.41	106.55	115.21
4	B	551	ATP	C5'-C4'-C3'	-2.18	107.35	115.21
4	B	551	ATP	O4'-C1'-C2'	-2.04	102.25	106.62
4	B	551	ATP	O3B-PG-O1G	-2.01	100.49	111.04

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	551	ATP	C4'-C5'-O5'-PA
4	C	551	ATP	C5'-O5'-PA-O2A
4	C	551	ATP	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
4	C	551	ATP	O4'-C1'-N9-C4
4	C	551	ATP	C5'-O5'-PA-O3A
4	B	551	ATP	PA-O3A-PB-O1B
4	B	551	ATP	PA-O3A-PB-O2B

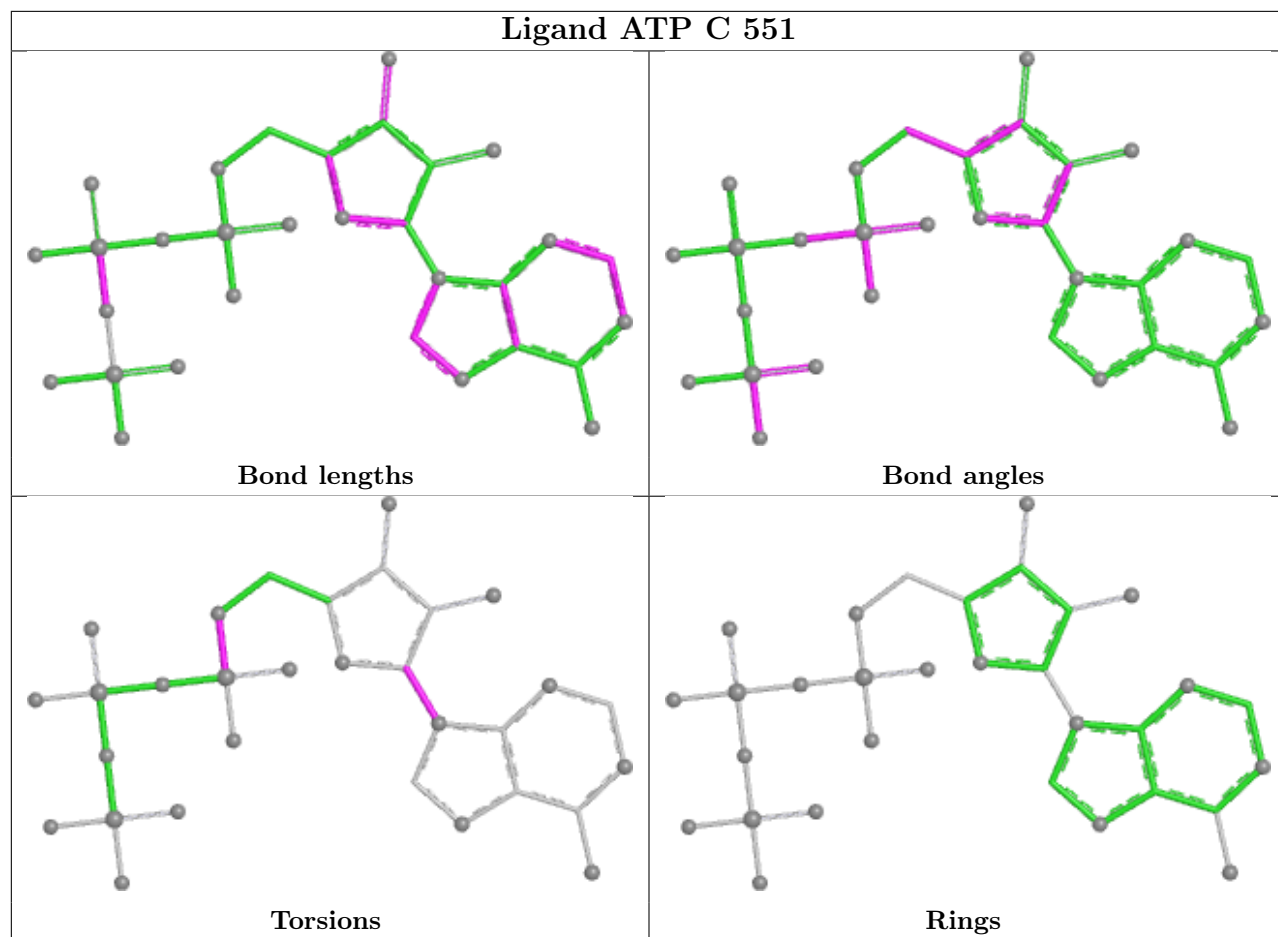
There are no ring outliers.

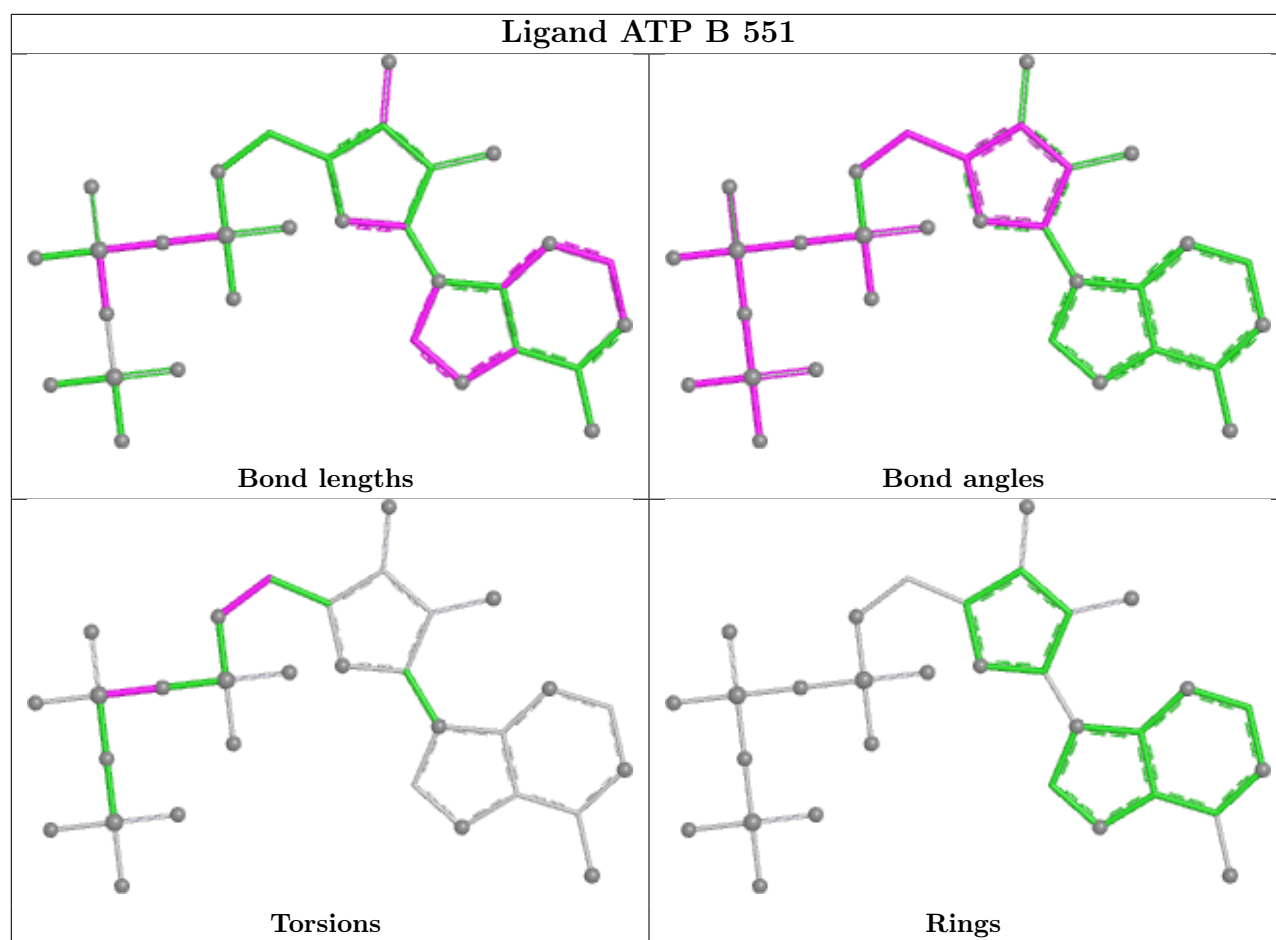
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	551	ATP	4	0
4	B	551	ATP	4	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.

Ligand ATP C 551





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 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.