



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:45 PM EDT

PDB ID : 3LQR / pdb_00003lqr
Title : Structure of CED-4:CED-3 complex
Authors : Qi, S.; Pang, Y.; Shi, Y.; Yan, N.
Deposited on : 2010-02-09
Resolution : 3.90 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

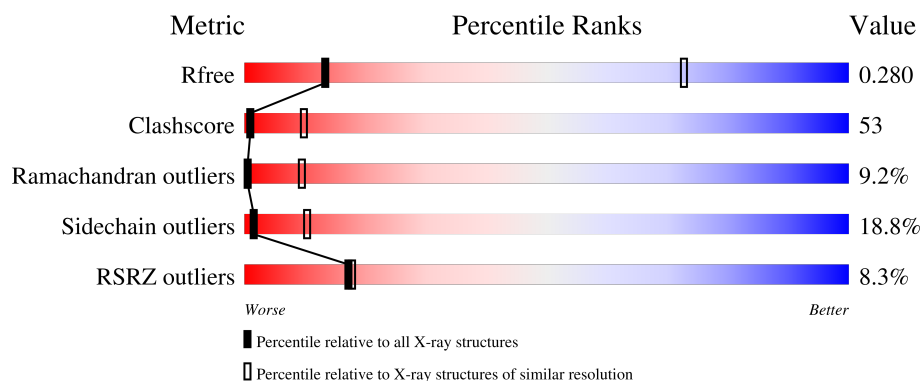
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	
1	B	549	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	A	602	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8124 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.

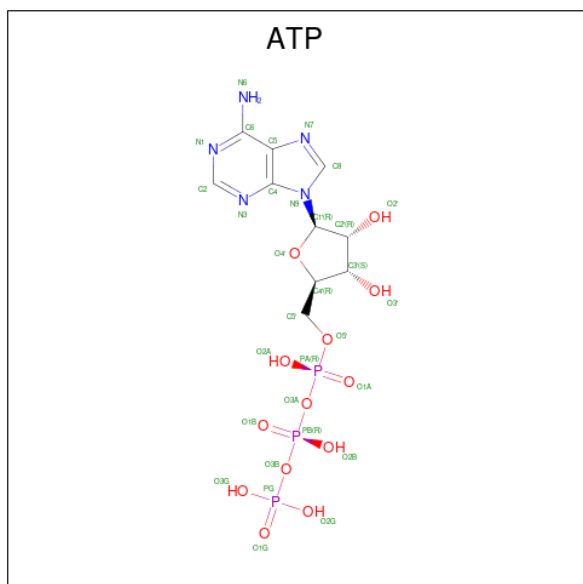
- Molecule 1 is a protein called Cell death protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			4039	2575	676	759	29			
1	B	501	Total	C	N	O	S	0	0	0
			4021	2565	673	754	29			

- 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		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

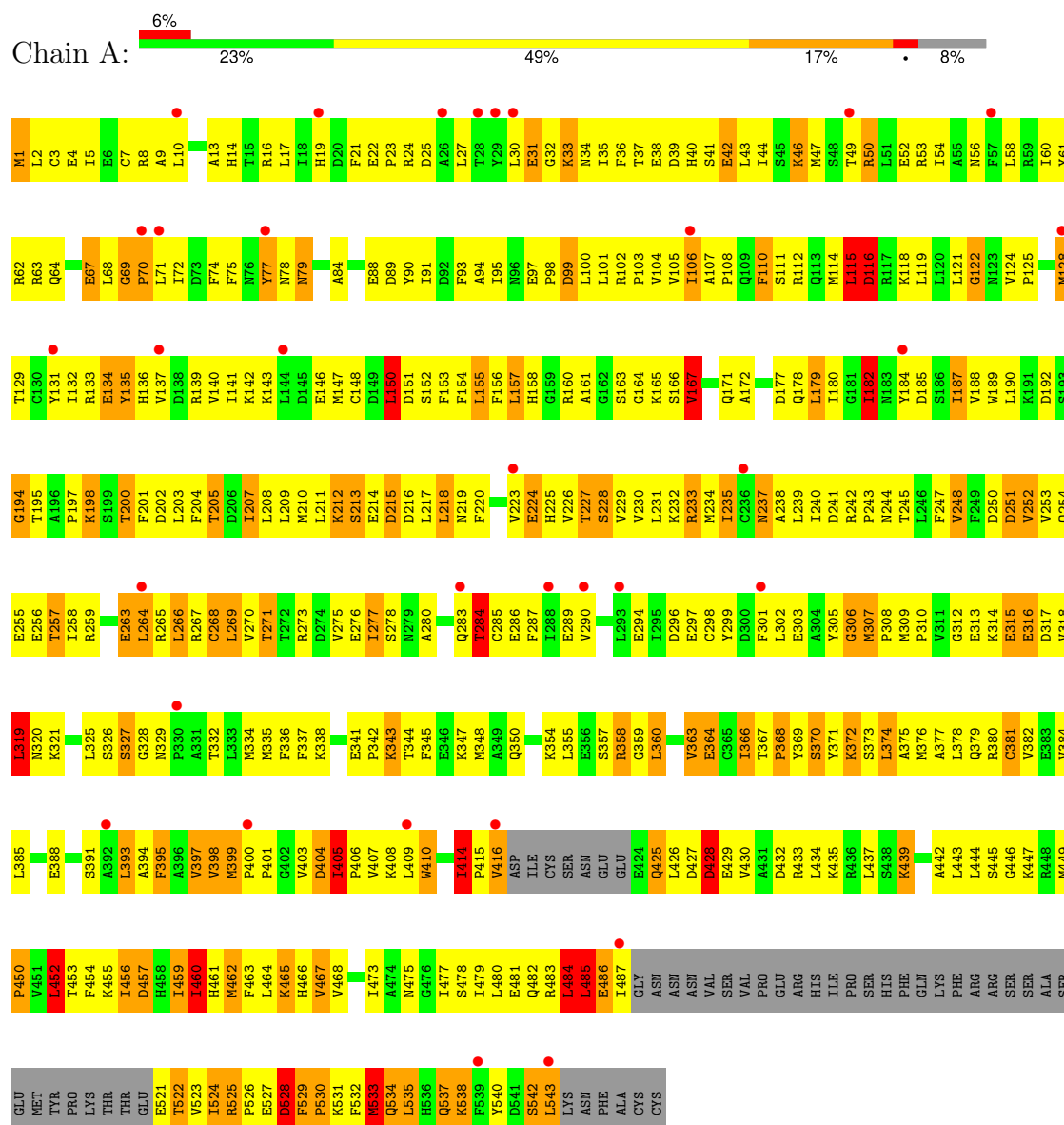


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cell death protein 4



• Molecule 1: Cell death protein 4





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	181.33Å 181.33Å 202.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.78 – 3.90 39.78 – 3.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (39.78-3.90) 96.5 (39.78-3.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.255 , 0.283 0.257 , 0.280	Depositor DCC
R_{free} test set	694 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	143.4	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 228.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8124	wwPDB-VP
Average B, all atoms (Å ²)	196.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/4113	1.01	21/5558 (0.4%)
1	B	0.56	0/4095	1.03	22/5534 (0.4%)
All	All	0.55	0/8208	1.02	43/11092 (0.4%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	MET	CA-C-N	9.57	129.66	119.90
1	A	307	MET	C-N-CA	9.57	129.66	119.90
1	B	307	MET	CA-C-N	9.14	129.22	119.90
1	B	307	MET	C-N-CA	9.14	129.22	119.90
1	A	217	LEU	N-CA-C	-7.46	104.17	113.28
1	B	217	LEU	N-CA-C	-7.07	104.65	113.28
1	B	107	ALA	CA-C-N	6.85	126.78	120.21
1	B	107	ALA	C-N-CA	6.85	126.78	120.21
1	A	428	ASP	N-CA-C	-6.76	105.18	113.50
1	A	268	CYS	N-CA-C	6.67	119.58	109.23
1	B	428	ASP	N-CA-C	-6.59	105.39	113.50
1	B	31	GLU	N-CA-C	-6.48	104.63	112.54
1	A	414	ILE	CA-C-N	6.11	126.07	120.03
1	A	414	ILE	C-N-CA	6.11	126.07	120.03
1	A	167	VAL	CB-CA-C	-6.10	103.91	112.14
1	B	268	CYS	N-CA-C	6.09	118.66	109.23
1	B	459	ILE	N-CA-C	-5.84	104.82	110.42
1	B	167	VAL	CB-CA-C	-5.77	104.36	112.14
1	B	414	ILE	CA-C-N	5.77	125.74	120.03
1	B	414	ILE	C-N-CA	5.77	125.74	120.03
1	A	525	ARG	CA-C-N	5.67	126.93	119.84
1	A	525	ARG	C-N-CA	5.67	126.93	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	GLN	N-CA-C	-5.63	104.52	111.33
1	A	31	GLU	N-CA-C	-5.57	105.36	111.82
1	A	528	ASP	N-CA-C	-5.56	105.37	111.82
1	B	537	GLN	N-CA-C	-5.51	104.67	111.33
1	B	528	ASP	N-CA-C	-5.49	105.40	111.71
1	B	405	ILE	CA-C-N	5.48	125.78	119.92
1	B	405	ILE	C-N-CA	5.48	125.78	119.92
1	B	525	ARG	CA-C-N	5.48	126.68	119.84
1	B	525	ARG	C-N-CA	5.48	126.68	119.84
1	A	405	ILE	CA-C-N	5.43	125.73	119.92
1	A	405	ILE	C-N-CA	5.43	125.73	119.92
1	A	535	LEU	N-CA-C	-5.37	105.42	111.28
1	B	140	VAL	CB-CA-C	-5.34	105.14	111.81
1	A	533	MET	N-CA-C	-5.25	106.64	112.57
1	B	405	ILE	N-CA-C	5.22	113.47	109.19
1	A	122	GLY	N-CA-C	-5.16	107.53	115.73
1	B	533	MET	N-CA-C	-5.11	106.79	112.57
1	A	405	ILE	N-CA-C	5.11	113.38	109.19
1	A	319	LEU	N-CA-C	-5.10	107.00	113.43
1	A	263	GLU	N-CA-C	-5.08	105.82	112.23
1	B	535	LEU	N-CA-C	-5.04	105.79	111.28

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	4039	0	4066	437	0
1	B	4021	0	4052	438	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	10	0
3	B	31	0	12	4	0
All	All	8124	0	8142	856	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 53.

All (856) 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:B:110:PHE:HA	1:B:113:GLN:HB2	1.34	1.08
1:B:4:GLU:O	1:B:8:ARG:HB2	1.59	1.01
1:B:484:LEU:HD11	1:B:533:MET:HG2	1.44	1.00
1:A:484:LEU:HD11	1:A:533:MET:HG2	1.45	0.99
1:A:534:GLN:HE21	1:A:534:GLN:HA	1.25	0.98
1:A:4:GLU:O	1:A:8:ARG:HB2	1.63	0.96
1:B:534:GLN:HE21	1:B:534:GLN:HA	1.27	0.96
1:B:468:VAL:HG23	1:B:473:ILE:HD11	1.48	0.96
1:A:342:PRO:HB3	1:B:448:ARG:HH11	1.31	0.94
1:A:468:VAL:HG23	1:A:473:ILE:HD11	1.50	0.94
1:A:1:MET:HE3	1:A:240:ILE:HG22	1.51	0.93
1:B:114:MET:SD	1:B:177:ASP:HA	2.07	0.93
1:A:533:MET:HE3	1:A:533:MET:O	1.71	0.90
1:A:164:GLY:HA2	3:A:602:ATP:O1A	1.72	0.89
1:B:540:TYR:O	1:B:543:LEU:HD23	1.72	0.89
1:B:533:MET:HE3	1:B:533:MET:O	1.71	0.89
1:A:128:MET:HE2	1:A:129:THR:H	1.37	0.88
1:B:101:LEU:HD11	1:B:106:ILE:HD12	1.53	0.88
1:B:128:MET:HE2	1:B:129:THR:H	1.37	0.87
1:A:540:TYR:O	1:A:543:LEU:HD23	1.74	0.86
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.43	0.84
1:A:78:ASN:OD1	1:B:37:THR:HG21	1.77	0.84
1:A:47:MET:HB2	1:A:53:ARG:HG3	1.62	0.82
1:A:299:TYR:HA	1:A:302:LEU:HD12	1.61	0.82
1:B:299:TYR:HA	1:B:302:LEU:HD12	1.60	0.81
1:A:155:LEU:HB3	1:A:269:LEU:HD23	1.63	0.81
1:B:47:MET:HB2	1:B:53:ARG:HG3	1.62	0.81
1:A:93:PHE:HB2	1:A:101:LEU:HD13	1.61	0.81
1:A:160:ARG:HB3	1:A:163:SER:HB3	1.61	0.80
1:A:189:TRP:HE3	1:A:248:VAL:HG21	1.46	0.80
1:A:524:ILE:HD12	1:A:525:ARG:H	1.46	0.79
1:B:155:LEU:HB3	1:B:269:LEU:HD23	1.64	0.79
1:B:443:LEU:O	1:B:460:ILE:HD12	1.83	0.79
1:A:44:ILE:O	1:A:53:ARG:HG2	1.83	0.79
1:A:305:TYR:O	1:A:307:MET:HG2	1.83	0.79
1:B:197:PRO:HD2	1:B:198:LYS:HG2	1.65	0.79
1:B:542:SER:C	1:B:543:LEU:HD22	2.07	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:ILE:HD12	1:B:525:ARG:H	1.48	0.78
1:A:197:PRO:HD2	1:A:198:LYS:HG2	1.66	0.77
1:A:247:PHE:CE1	1:A:266:LEU:HD13	2.19	0.77
1:A:75:PHE:HB2	1:A:84:ALA:HB2	1.67	0.77
1:B:527:GLU:HA	1:B:530:PRO:HG3	1.65	0.77
1:A:443:LEU:O	1:A:460:ILE:HD12	1.85	0.77
1:B:189:TRP:HE3	1:B:248:VAL:HG21	1.48	0.77
1:A:399:MET:SD	1:A:400:PRO:HD2	2.25	0.77
1:B:160:ARG:HB3	1:B:163:SER:HB3	1.65	0.77
1:A:233:ARG:HG3	1:A:233:ARG:HH11	1.49	0.77
1:B:305:TYR:O	1:B:307:MET:HG2	1.85	0.77
1:A:527:GLU:HA	1:A:530:PRO:HG3	1.65	0.77
1:B:264:LEU:HB3	1:B:266:LEU:HD21	1.66	0.76
1:A:156:PHE:HB2	1:A:287:PHE:HD2	1.50	0.76
1:B:241:ASP:C	1:B:243:PRO:HD3	2.10	0.76
1:A:408:LYS:HE2	1:A:427:ASP:HB2	1.68	0.75
1:A:313:GLU:O	1:A:316:GLU:HG3	1.86	0.75
1:A:112:ARG:NH1	1:A:115:LEU:HD12	2.01	0.75
1:B:75:PHE:HB2	1:B:84:ALA:HB2	1.68	0.75
1:B:247:PHE:CE1	1:B:266:LEU:HD13	2.21	0.75
1:A:264:LEU:HB3	1:A:266:LEU:HD21	1.68	0.74
1:A:542:SER:C	1:A:543:LEU:HD22	2.12	0.74
1:B:399:MET:SD	1:B:400:PRO:HD2	2.26	0.74
1:B:313:GLU:O	1:B:316:GLU:HG3	1.88	0.74
1:B:233:ARG:HH11	1:B:233:ARG:CG	2.01	0.73
1:A:189:TRP:CE3	1:A:248:VAL:HG21	2.24	0.73
1:A:208:LEU:HD23	1:A:235:ILE:HG12	1.71	0.73
1:B:331:ALA:HA	3:B:602:ATP:O2'	1.89	0.73
1:A:88:GLU:O	1:A:91:ILE:HG22	1.89	0.73
1:B:133:ARG:O	1:B:137:VAL:HG23	1.88	0.73
1:A:122:GLY:HA3	1:A:187:ILE:HG23	1.70	0.72
1:B:408:LYS:HE2	1:B:427:ASP:HB2	1.71	0.72
1:A:347:LYS:O	1:A:347:LYS:HD3	1.90	0.72
1:B:208:LEU:HD23	1:B:235:ILE:HG12	1.71	0.72
1:A:167:VAL:HG21	3:A:602:ATP:N7	2.05	0.72
1:B:44:ILE:O	1:B:53:ARG:HG2	1.90	0.72
1:B:216:ASP:HB3	1:B:219:ASN:HB3	1.72	0.71
1:A:452:LEU:HD23	1:A:452:LEU:H	1.55	0.71
1:B:156:PHE:HB2	1:B:287:PHE:HD2	1.56	0.71
1:A:216:ASP:HB3	1:A:219:ASN:HB3	1.73	0.71
1:B:7:CYS:SG	1:B:62:ARG:HD3	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASP:C	1:A:243:PRO:HD3	2.16	0.71
1:A:524:ILE:HD12	1:A:525:ARG:N	2.06	0.71
1:B:5:ILE:HD13	1:B:94:ALA:HB1	1.71	0.71
1:B:182:ILE:HD12	1:B:182:ILE:N	2.06	0.71
1:A:167:VAL:HG21	3:A:602:ATP:C8	2.25	0.71
1:B:312:GLY:H	1:B:315:GLU:CD	1.99	0.71
1:A:374:LEU:CD1	1:A:378:LEU:HG	2.21	0.71
1:B:122:GLY:HA3	1:B:187:ILE:HG23	1.71	0.71
1:A:7:CYS:SG	1:A:62:ARG:HD3	2.31	0.70
1:A:133:ARG:O	1:A:137:VAL:HG23	1.91	0.70
1:B:524:ILE:HD12	1:B:525:ARG:N	2.06	0.70
1:B:347:LYS:O	1:B:347:LYS:HD3	1.90	0.70
1:A:165:LYS:HZ2	1:A:273:ARG:HD3	1.56	0.70
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.05	0.70
1:B:88:GLU:O	1:B:91:ILE:HG22	1.91	0.70
1:A:480:LEU:HD23	1:A:481:GLU:OE2	1.91	0.70
1:B:534:GLN:HE21	1:B:534:GLN:CA	2.04	0.70
1:B:189:TRP:CE3	1:B:248:VAL:HG21	2.27	0.70
1:A:342:PRO:HB3	1:B:448:ARG:NH1	2.04	0.69
1:A:165:LYS:NZ	1:A:273:ARG:HD3	2.07	0.69
1:A:294:GLU:HB2	1:A:297:GLU:OE1	1.93	0.69
1:B:326:SER:O	1:B:328:GLY:N	2.25	0.69
1:B:374:LEU:CD1	1:B:378:LEU:HG	2.23	0.69
1:A:482:GLN:O	1:A:485:LEU:HD11	1.93	0.69
1:B:42:GLU:O	1:B:46:LYS:HG3	1.93	0.69
1:A:301:PHE:HE1	1:A:305:TYR:HE1	1.41	0.69
1:A:326:SER:O	1:A:328:GLY:N	2.26	0.69
1:A:1:MET:HE3	1:A:240:ILE:CG2	2.22	0.69
1:A:312:GLY:H	1:A:315:GLU:CD	2.01	0.68
1:B:301:PHE:HE1	1:B:305:TYR:HE1	1.41	0.68
1:B:294:GLU:HB2	1:B:297:GLU:OE1	1.93	0.68
1:B:480:LEU:HD23	1:B:481:GLU:OE2	1.93	0.68
1:B:406:PRO:HA	1:B:453:THR:HG22	1.74	0.68
1:B:110:PHE:CA	1:B:113:GLN:HB2	2.18	0.68
1:A:165:LYS:HG3	3:A:602:ATP:O2B	1.94	0.68
1:B:482:GLN:O	1:B:485:LEU:HD11	1.94	0.68
1:A:156:PHE:HB2	1:A:287:PHE:CD2	2.29	0.68
1:B:102:ARG:HG3	1:B:103:PRO:HD2	1.74	0.68
1:B:165:LYS:NZ	1:B:273:ARG:HD3	2.09	0.68
1:B:443:LEU:HB2	1:B:444:LEU:HD12	1.76	0.68
1:A:141:ILE:HG23	1:A:179:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PRO:HA	1:A:453:THR:HG22	1.76	0.67
1:B:447:LYS:NZ	1:B:450:PRO:HD2	2.08	0.67
1:A:443:LEU:HB2	1:A:444:LEU:HD12	1.76	0.67
1:A:98:PRO:O	1:A:99:ASP:HB2	1.95	0.67
1:B:35:ILE:HG22	1:B:35:ILE:O	1.95	0.67
1:B:452:LEU:HD23	1:B:452:LEU:H	1.60	0.67
1:B:415:PRO:O	1:B:416:VAL:HG23	1.94	0.66
1:A:341:GLU:HB2	1:A:342:PRO:HD3	1.76	0.66
1:A:182:ILE:N	1:A:182:ILE:HD12	2.10	0.66
1:B:203:LEU:HD22	1:B:204:PHE:CE1	2.30	0.66
1:A:255:GLU:CB	1:A:277:ILE:HG22	2.25	0.66
1:A:5:ILE:HD13	1:A:94:ALA:HB1	1.76	0.66
1:B:91:ILE:O	1:B:95:ILE:HG12	1.95	0.66
1:B:255:GLU:CB	1:B:277:ILE:HG22	2.26	0.65
1:A:447:LYS:NZ	1:A:450:PRO:HD2	2.11	0.65
1:A:394:ALA:O	1:A:397:VAL:HG23	1.96	0.65
1:A:72:ILE:HG23	1:A:84:ALA:HB1	1.79	0.65
1:B:165:LYS:HG3	3:B:602:ATP:O2B	1.97	0.65
1:B:203:LEU:HD22	1:B:204:PHE:CD1	2.31	0.65
1:B:259:ARG:O	1:B:263:GLU:HG3	1.97	0.65
1:B:319:LEU:HD23	1:B:320:ASN:N	2.12	0.65
1:B:341:GLU:HB2	1:B:342:PRO:HD3	1.77	0.65
1:B:318:VAL:HG12	1:B:318:VAL:O	1.96	0.65
1:A:218:LEU:HG	1:A:219:ASN:H	1.61	0.65
1:A:318:VAL:HG12	1:A:318:VAL:O	1.96	0.65
1:B:371:TYR:CD1	1:B:377:ALA:HB2	2.33	0.64
1:A:158:HIS:O	1:A:290:VAL:HG23	1.98	0.64
1:B:72:ILE:HG23	1:B:84:ALA:HB1	1.80	0.64
1:A:483:ARG:O	1:A:485:LEU:HD12	1.98	0.64
1:A:534:GLN:HA	1:A:534:GLN:NE2	2.06	0.64
1:A:203:LEU:HD22	1:A:204:PHE:CE1	2.33	0.64
1:B:468:VAL:CG2	1:B:473:ILE:HD11	2.25	0.64
1:B:156:PHE:HB2	1:B:287:PHE:CD2	2.33	0.63
1:A:37:THR:OG1	1:A:40:HIS:HD2	1.81	0.63
1:A:91:ILE:O	1:A:95:ILE:HG12	1.98	0.63
1:A:384:VAL:HG23	1:A:385:LEU:HD23	1.80	0.63
1:B:39:ASP:O	1:B:43:LEU:HB2	1.98	0.63
1:B:114:MET:HG2	1:B:180:ILE:HB	1.81	0.63
1:B:49:THR:HG22	1:B:50:ARG:N	2.14	0.63
1:B:108:PRO:O	1:B:109:GLN:HB2	1.98	0.63
1:A:40:HIS:ND1	1:A:60:ILE:HD13	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PRO:O	1:A:416:VAL:HG23	1.99	0.63
1:B:141:ILE:HG23	1:B:179:LEU:HD21	1.81	0.63
1:B:218:LEU:HG	1:B:219:ASN:H	1.63	0.63
1:B:447:LYS:CE	1:B:450:PRO:HD2	2.29	0.63
1:B:534:GLN:HA	1:B:534:GLN:NE2	2.08	0.63
1:A:42:GLU:O	1:A:46:LYS:HG3	1.97	0.62
1:B:527:GLU:CA	1:B:530:PRO:HG3	2.28	0.62
1:B:137:VAL:HG13	1:B:172:ALA:HB2	1.81	0.62
1:B:298:CYS:O	1:B:302:LEU:HG	2.00	0.62
1:B:40:HIS:ND1	1:B:60:ILE:HD13	2.13	0.62
1:B:77:TYR:CD1	1:B:77:TYR:O	2.53	0.62
1:A:477:ILE:O	1:A:480:LEU:HB3	1.99	0.62
1:B:114:MET:HE3	1:B:114:MET:O	2.00	0.62
1:B:447:LYS:HE3	1:B:450:PRO:HD2	1.80	0.62
1:A:366:ILE:HD12	1:A:366:ILE:H	1.64	0.62
1:A:259:ARG:O	1:A:263:GLU:HG3	2.00	0.62
1:A:329:ASN:HB2	1:A:459:ILE:HD13	1.81	0.62
1:A:443:LEU:HB2	1:A:444:LEU:CD1	2.30	0.62
1:A:371:TYR:CD1	1:A:377:ALA:HB2	2.35	0.62
1:B:485:LEU:HD12	1:B:486:GLU:HG3	1.81	0.62
1:B:405:ILE:HG12	1:B:410:TRP:CZ3	2.35	0.62
1:A:410:TRP:CZ3	1:A:454:PHE:HB2	2.35	0.61
1:A:203:LEU:HD22	1:A:204:PHE:CD1	2.35	0.61
1:A:298:CYS:O	1:A:302:LEU:HG	2.01	0.61
1:A:468:VAL:CG2	1:A:473:ILE:HD11	2.27	0.61
1:B:255:GLU:CA	1:B:277:ILE:HG22	2.30	0.61
1:A:447:LYS:HE3	1:A:450:PRO:HD2	1.82	0.61
1:A:527:GLU:CA	1:A:530:PRO:HG3	2.29	0.61
1:B:22:GLU:HB3	1:B:25:ASP:OD2	2.00	0.61
1:B:264:LEU:HB3	1:B:266:LEU:CD2	2.30	0.61
1:B:158:HIS:O	1:B:290:VAL:HG23	2.00	0.61
1:A:200:THR:HG21	1:A:256:GLU:HB3	1.82	0.61
1:A:22:GLU:HB2	1:B:63:ARG:NH1	2.16	0.61
1:A:255:GLU:CA	1:A:277:ILE:HG22	2.30	0.61
1:B:32:GLY:C	1:B:34:ASN:H	2.09	0.61
1:A:350:GLN:NE2	1:B:428:ASP:HB3	2.15	0.61
1:B:241:ASP:O	1:B:243:PRO:HD3	2.01	0.61
1:A:128:MET:HE2	1:A:129:THR:N	2.13	0.61
1:A:35:ILE:O	1:A:35:ILE:HG22	2.01	0.60
1:B:182:ILE:HD12	1:B:182:ILE:H	1.63	0.60
1:B:483:ARG:O	1:B:485:LEU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ASP:OD1	1:B:447:LYS:HD3	2.01	0.60
1:B:443:LEU:HB2	1:B:444:LEU:CD1	2.31	0.60
1:A:32:GLY:C	1:A:34:ASN:H	2.10	0.60
1:B:394:ALA:O	1:B:397:VAL:HG23	2.01	0.60
1:A:79:ASN:ND2	1:B:36:PHE:H	1.99	0.60
1:A:194:GLY:O	1:A:254:GLN:HG3	2.01	0.60
1:A:483:ARG:O	1:A:485:LEU:N	2.34	0.60
1:A:33:LYS:HD3	1:A:70:PRO:HB3	1.84	0.60
1:A:39:ASP:O	1:A:43:LEU:HB2	2.02	0.60
1:A:77:TYR:O	1:A:77:TYR:CD1	2.54	0.60
1:B:37:THR:OG1	1:B:40:HIS:HD2	1.85	0.60
1:B:200:THR:HG21	1:B:256:GLU:HB3	1.84	0.60
1:A:319:LEU:HD23	1:A:320:ASN:N	2.17	0.59
1:A:310:PRO:CB	1:A:316:GLU:HB3	2.33	0.59
1:A:443:LEU:HB3	1:A:460:ILE:HD11	1.83	0.59
1:B:121:LEU:O	1:B:210:MET:HE1	2.02	0.59
1:A:79:ASN:HD21	1:B:34:ASN:C	2.11	0.59
1:A:447:LYS:CE	1:A:450:PRO:HD2	2.32	0.59
1:B:109:GLN:C	1:B:111:SER:H	2.09	0.59
1:B:255:GLU:HA	1:B:277:ILE:HG22	1.84	0.59
1:A:37:THR:OG1	1:A:40:HIS:CD2	2.55	0.59
1:A:264:LEU:HB3	1:A:266:LEU:CD2	2.31	0.59
1:B:301:PHE:HE1	1:B:305:TYR:CE1	2.20	0.59
1:B:384:VAL:HG23	1:B:385:LEU:HD23	1.85	0.59
1:B:167:VAL:O	1:B:171:GLN:HG3	2.02	0.59
1:B:122:GLY:HA2	1:B:187:ILE:O	2.03	0.59
1:A:105:VAL:HG12	1:A:105:VAL:O	2.02	0.59
1:A:475:ASN:O	1:A:479:ILE:HG13	2.03	0.59
1:B:310:PRO:CB	1:B:316:GLU:HB3	2.33	0.59
1:B:483:ARG:O	1:B:485:LEU:HD12	2.02	0.59
1:A:49:THR:HB	1:A:52:GLU:OE1	2.03	0.59
1:B:342:PRO:O	1:B:343:LYS:CB	2.51	0.59
1:B:410:TRP:CZ3	1:B:454:PHE:HB2	2.38	0.59
1:B:480:LEU:HD22	1:B:540:TYR:HE2	1.68	0.59
1:B:484:LEU:HD11	1:B:533:MET:CG	2.26	0.59
1:B:49:THR:HG22	1:B:50:ARG:H	1.67	0.58
1:A:251:ASP:HA	1:A:271:THR:O	2.03	0.58
1:A:401:PRO:HA	1:A:456:ILE:HG23	1.85	0.58
1:B:443:LEU:HB3	1:B:460:ILE:HD11	1.84	0.58
1:A:301:PHE:HE1	1:A:305:TYR:CE1	2.21	0.58
1:A:426:LEU:HB3	1:A:428:ASP:OD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:HG22	1:A:50:ARG:N	2.18	0.58
1:B:459:ILE:C	1:B:461:HIS:H	2.11	0.58
1:B:477:ILE:O	1:B:480:LEU:HB3	2.03	0.58
1:A:178:GLN:O	1:A:182:ILE:HB	2.02	0.58
1:B:101:LEU:HD21	1:B:106:ILE:HD11	1.85	0.58
1:B:177:ASP:O	1:B:182:ILE:HD13	2.04	0.58
1:A:177:ASP:O	1:A:182:ILE:HD13	2.04	0.58
1:B:24:ARG:HA	1:B:27:LEU:HD12	1.85	0.58
1:B:136:HIS:O	1:B:140:VAL:HG23	2.04	0.58
1:B:128:MET:HE2	1:B:129:THR:N	2.13	0.58
1:B:10:LEU:HD22	1:B:58:LEU:HD21	1.86	0.57
1:B:135:TYR:CE1	1:B:139:ARG:HD2	2.39	0.57
1:B:233:ARG:CG	1:B:233:ARG:NH1	2.65	0.57
1:B:426:LEU:HB3	1:B:428:ASP:OD2	2.04	0.57
1:B:401:PRO:HA	1:B:456:ILE:HG23	1.86	0.57
1:A:414:ILE:HG21	1:A:430:VAL:HG22	1.86	0.57
1:B:178:GLN:O	1:B:182:ILE:HB	2.04	0.57
1:A:334:MET:HE3	1:A:334:MET:HA	1.86	0.57
1:B:366:ILE:HD12	1:B:366:ILE:H	1.70	0.57
1:A:241:ASP:O	1:A:243:PRO:HD3	2.04	0.57
1:A:376:MET:HE3	1:A:376:MET:HA	1.85	0.57
1:A:410:TRP:CH2	1:A:454:PHE:HB2	2.40	0.57
1:A:449:MET:HA	1:A:450:PRO:C	2.30	0.57
1:B:538:LYS:HD3	1:B:538:LYS:C	2.30	0.57
1:A:69:GLY:H	1:A:70:PRO:HD2	1.70	0.57
1:A:538:LYS:HD3	1:A:538:LYS:C	2.30	0.57
1:A:342:PRO:O	1:A:343:LYS:CB	2.52	0.57
1:A:366:ILE:HD12	1:A:366:ILE:N	2.19	0.57
1:B:248:VAL:CG1	1:B:269:LEU:HD12	2.35	0.57
1:B:251:ASP:HA	1:B:271:THR:O	2.04	0.57
1:A:135:TYR:CE1	1:A:139:ARG:HD2	2.40	0.57
1:B:153:PHE:CE2	1:B:267:ARG:HG2	2.40	0.57
1:A:9:ALA:HB2	1:A:90:TYR:CD2	2.40	0.56
1:A:327:SER:HB2	1:A:459:ILE:CG1	2.35	0.56
1:A:485:LEU:HD12	1:A:486:GLU:HG3	1.86	0.56
1:A:119:LEU:HB3	1:B:265:ARG:HH12	1.70	0.56
1:A:24:ARG:NE	1:A:53:ARG:HH11	2.03	0.56
1:A:192:ASP:OD2	1:A:252:VAL:HG22	2.05	0.56
1:A:405:ILE:HG12	1:A:410:TRP:CZ3	2.40	0.56
1:A:255:GLU:HA	1:A:277:ILE:HG22	1.87	0.56
1:B:327:SER:HB2	1:B:459:ILE:CG1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:HG2	1:A:68:LEU:N	2.21	0.56
1:A:182:ILE:HD12	1:A:182:ILE:H	1.68	0.56
1:B:533:MET:HE3	1:B:533:MET:C	2.29	0.56
1:A:314:LYS:HA	1:A:317:ASP:HB2	1.88	0.56
1:B:334:MET:HE3	1:B:334:MET:HA	1.88	0.56
1:A:400:PRO:HB2	1:A:403:VAL:HB	1.88	0.56
1:A:404:ASP:OD1	1:A:447:LYS:HD3	2.05	0.56
1:B:9:ALA:HB2	1:B:90:TYR:CD2	2.40	0.56
1:A:315:GLU:HB2	1:A:345:PHE:CE2	2.41	0.56
1:B:33:LYS:HD3	1:B:70:PRO:HB3	1.88	0.56
1:B:117:ARG:O	1:B:121:LEU:HG	2.05	0.56
1:B:369:TYR:HD1	1:B:370:SER:H	1.53	0.56
1:A:136:HIS:O	1:A:140:VAL:HG23	2.06	0.55
1:A:459:ILE:C	1:A:461:HIS:H	2.14	0.55
1:B:525:ARG:HD3	1:B:535:LEU:HD13	1.88	0.55
1:B:37:THR:O	1:B:40:HIS:HB2	2.06	0.55
1:B:72:ILE:HG21	1:B:88:GLU:HG2	1.88	0.55
1:B:153:PHE:HE2	1:B:267:ARG:HG2	1.71	0.55
1:A:19:HIS:HB3	1:B:1:MET:HB2	1.88	0.55
1:A:72:ILE:HG21	1:A:88:GLU:HG2	1.88	0.55
1:A:158:HIS:HB2	1:A:275:VAL:HG22	1.88	0.55
1:B:47:MET:HB2	1:B:53:ARG:CG	2.34	0.55
1:B:213:SER:C	1:B:215:ASP:N	2.64	0.55
1:A:167:VAL:O	1:A:171:GLN:HG3	2.06	0.55
1:A:354:LYS:O	1:A:358:ARG:HB2	2.06	0.55
1:B:37:THR:OG1	1:B:40:HIS:CD2	2.58	0.55
1:B:46:LYS:HE3	1:B:46:LYS:O	2.06	0.55
1:B:315:GLU:HB2	1:B:345:PHE:CE2	2.42	0.55
1:A:303:GLU:HG3	1:A:309:MET:HE1	1.88	0.55
1:B:449:MET:HA	1:B:450:PRO:C	2.31	0.55
1:A:47:MET:HE2	1:A:52:GLU:HB3	1.88	0.55
1:A:137:VAL:HG13	1:A:172:ALA:HB2	1.89	0.55
1:A:141:ILE:HG23	1:A:179:LEU:CD2	2.37	0.55
1:B:49:THR:HB	1:B:52:GLU:OE1	2.07	0.55
1:B:303:GLU:HG3	1:B:309:MET:HE1	1.89	0.55
1:B:314:LYS:HA	1:B:317:ASP:HB2	1.89	0.55
1:A:37:THR:O	1:A:40:HIS:HB2	2.07	0.55
1:A:223:VAL:O	1:A:226:VAL:HG23	2.06	0.55
1:B:115:LEU:O	1:B:116:ASP:C	2.49	0.55
1:B:342:PRO:HD2	1:B:347:LYS:HG3	1.89	0.55
1:A:460:ILE:HG23	1:A:460:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ARG:HD3	1:A:535:LEU:HD13	1.89	0.55
1:A:112:ARG:O	1:A:112:ARG:HD3	2.07	0.54
1:B:475:ASN:O	1:B:479:ILE:HG13	2.06	0.54
1:A:79:ASN:ND2	1:B:34:ASN:C	2.65	0.54
1:A:207:ILE:HG22	1:A:208:LEU:N	2.22	0.54
1:B:223:VAL:O	1:B:226:VAL:HG23	2.07	0.54
1:B:329:ASN:HB2	1:B:459:ILE:HD13	1.89	0.54
1:B:393:LEU:HD23	1:B:437:LEU:HD22	1.90	0.54
1:A:52:GLU:O	1:A:56:ASN:HB2	2.07	0.54
1:A:122:GLY:HA2	1:A:187:ILE:O	2.08	0.54
1:B:366:ILE:HD12	1:B:366:ILE:N	2.23	0.54
1:B:410:TRP:CH2	1:B:454:PHE:HB2	2.42	0.54
1:A:327:SER:O	1:A:459:ILE:HD11	2.08	0.54
1:A:533:MET:HE3	1:A:533:MET:C	2.31	0.54
1:A:153:PHE:CE2	1:A:267:ARG:HG2	2.43	0.54
1:A:350:GLN:CD	1:B:428:ASP:HB3	2.33	0.54
1:B:67:GLU:HG2	1:B:68:LEU:N	2.23	0.54
1:B:468:VAL:HG23	1:B:473:ILE:CD1	2.32	0.54
1:B:165:LYS:HZ2	1:B:273:ARG:HD3	1.73	0.54
1:B:166:SER:OG	1:B:250:ASP:OD1	2.20	0.54
1:A:22:GLU:HB3	1:A:25:ASP:OD2	2.07	0.54
1:A:47:MET:HB2	1:A:53:ARG:CG	2.36	0.54
1:B:327:SER:HB2	1:B:459:ILE:HG13	1.90	0.54
1:A:115:LEU:CD2	1:A:180:ILE:HB	2.39	0.53
1:B:167:VAL:HG21	3:B:602:ATP:N3	2.23	0.53
1:A:527:GLU:O	1:A:530:PRO:HD3	2.09	0.53
1:B:24:ARG:NE	1:B:53:ARG:HH11	2.06	0.53
1:B:534:GLN:NE2	1:B:537:GLN:HB2	2.23	0.53
1:A:188:VAL:HB	1:A:247:PHE:CD2	2.44	0.53
1:B:47:MET:HE2	1:B:52:GLU:HB3	1.91	0.53
1:A:480:LEU:HD22	1:A:540:TYR:HE2	1.72	0.53
1:B:228:SER:O	1:B:232:LYS:HG3	2.09	0.53
1:B:342:PRO:CD	1:B:347:LYS:HG3	2.38	0.53
1:B:429:GLU:HA	1:B:432:ASP:OD2	2.09	0.53
1:A:24:ARG:HA	1:A:27:LEU:HD12	1.90	0.53
1:A:380:ARG:C	1:A:382:VAL:H	2.15	0.53
1:B:189:TRP:HB2	1:B:248:VAL:HG23	1.91	0.53
1:B:391:SER:OG	1:B:415:PRO:HG2	2.09	0.53
1:B:4:GLU:O	1:B:8:ARG:CB	2.47	0.53
1:A:369:TYR:HD1	1:A:370:SER:H	1.55	0.53
1:A:484:LEU:C	1:A:485:LEU:HG	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:GLN:HE21	1:A:534:GLN:CA	2.04	0.53
1:B:178:GLN:HA	1:B:182:ILE:HD13	1.91	0.53
1:B:194:GLY:O	1:B:254:GLN:HG3	2.09	0.53
1:B:69:GLY:H	1:B:70:PRO:HD2	1.72	0.53
1:A:153:PHE:HE2	1:A:267:ARG:HG2	1.74	0.52
1:A:468:VAL:HG23	1:A:473:ILE:CD1	2.33	0.52
1:B:256:GLU:HA	1:B:259:ARG:HG3	1.90	0.52
1:A:121:LEU:O	1:A:210:MET:HE1	2.09	0.52
1:A:131:TYR:CD2	1:A:301:PHE:HA	2.44	0.52
1:A:534:GLN:NE2	1:A:537:GLN:HB2	2.23	0.52
1:B:478:SER:O	1:B:482:GLN:HG2	2.08	0.52
1:A:13:ALA:O	1:A:17:LEU:HD12	2.08	0.52
1:A:205:THR:HA	1:A:231:LEU:HD11	1.91	0.52
1:B:27:LEU:HD22	1:B:41:SER:HA	1.91	0.52
1:B:30:LEU:HD22	1:B:35:ILE:HB	1.90	0.52
1:B:52:GLU:O	1:B:56:ASN:HB2	2.08	0.52
1:B:10:LEU:HD13	1:B:58:LEU:CD2	2.40	0.52
1:A:178:GLN:HA	1:A:182:ILE:HD13	1.92	0.52
1:B:141:ILE:HG23	1:B:179:LEU:CD2	2.39	0.52
1:B:207:ILE:HG22	1:B:208:LEU:N	2.24	0.52
1:B:426:LEU:HB3	1:B:428:ASP:CG	2.34	0.52
1:A:364:GLU:HG3	1:A:372:LYS:HB3	1.92	0.52
1:A:27:LEU:HD22	1:A:41:SER:HA	1.92	0.52
1:A:327:SER:HB2	1:A:459:ILE:HG13	1.92	0.52
1:A:342:PRO:CD	1:A:347:LYS:HG3	2.40	0.52
1:A:310:PRO:HB3	1:A:316:GLU:HB3	1.92	0.52
1:A:69:GLY:C	1:A:71:LEU:H	2.18	0.52
1:A:429:GLU:HA	1:A:432:ASP:OD2	2.09	0.52
1:B:400:PRO:HB2	1:B:403:VAL:HB	1.92	0.52
1:A:165:LYS:NZ	3:A:602:ATP:O1G	2.43	0.52
1:A:380:ARG:C	1:A:382:VAL:N	2.67	0.52
1:A:426:LEU:HB3	1:A:428:ASP:CG	2.34	0.52
1:A:46:LYS:HE3	1:A:46:LYS:O	2.10	0.51
1:A:407:VAL:HG23	1:A:452:LEU:O	2.10	0.51
1:B:203:LEU:C	1:B:203:LEU:HD23	2.35	0.51
1:B:310:PRO:HB3	1:B:316:GLU:HB3	1.92	0.51
1:B:101:LEU:HD11	1:B:106:ILE:CD1	2.34	0.51
1:B:354:LYS:O	1:B:358:ARG:HB2	2.11	0.51
1:B:460:ILE:HG23	1:B:460:ILE:O	2.11	0.51
1:B:128:MET:CE	1:B:128:MET:HA	2.41	0.51
1:A:256:GLU:HA	1:A:259:ARG:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLY:C	1:B:71:LEU:H	2.19	0.51
1:B:165:LYS:HZ1	1:B:273:ARG:HD3	1.75	0.51
1:A:478:SER:O	1:A:482:GLN:HG2	2.10	0.51
1:B:35:ILE:O	1:B:35:ILE:CG2	2.58	0.51
1:B:426:LEU:HB3	1:B:428:ASP:OD1	2.11	0.51
1:A:93:PHE:O	1:A:101:LEU:HB2	2.11	0.51
1:A:391:SER:OG	1:A:415:PRO:HG2	2.10	0.51
1:A:345:PHE:HA	1:A:348:MET:HE3	1.93	0.51
1:B:360:LEU:HD23	1:B:374:LEU:HB3	1.93	0.51
1:A:49:THR:HG22	1:A:50:ARG:H	1.76	0.51
1:A:128:MET:HA	1:A:128:MET:CE	2.41	0.51
1:A:132:ILE:HG13	1:A:171:GLN:NE2	2.25	0.51
1:A:166:SER:OG	1:A:250:ASP:OD1	2.22	0.51
1:B:207:ILE:O	1:B:211:LEU:HG	2.11	0.51
1:A:10:LEU:HD22	1:A:58:LEU:HD21	1.93	0.51
1:A:69:GLY:H	1:A:70:PRO:CD	2.23	0.51
1:A:213:SER:C	1:A:215:ASP:N	2.66	0.51
1:B:142:LYS:HE2	1:B:146:GLU:OE2	2.11	0.51
1:B:182:ILE:H	1:B:182:ILE:CD1	2.24	0.51
1:B:367:THR:C	1:B:369:TYR:H	2.19	0.51
1:A:533:MET:HE2	1:A:534:GLN:NE2	2.26	0.50
1:B:213:SER:C	1:B:215:ASP:H	2.19	0.50
1:B:240:ILE:HG13	1:B:241:ASP:OD1	2.11	0.50
1:B:334:MET:HA	1:B:337:PHE:HD1	1.77	0.50
1:A:218:LEU:HG	1:A:219:ASN:N	2.26	0.50
1:A:368:PRO:HG3	1:B:279:ASN:O	2.11	0.50
1:B:35:ILE:O	1:B:36:PHE:CD2	2.65	0.50
1:B:527:GLU:O	1:B:530:PRO:HD3	2.12	0.50
1:A:248:VAL:CG1	1:A:269:LEU:HD12	2.42	0.50
1:A:532:PHE:HD1	1:A:532:PHE:O	1.95	0.50
1:B:40:HIS:O	1:B:43:LEU:HB3	2.11	0.50
1:B:484:LEU:C	1:B:485:LEU:HG	2.36	0.50
1:B:182:ILE:N	1:B:182:ILE:CD1	2.74	0.50
1:B:376:MET:HE3	1:B:376:MET:HA	1.92	0.50
1:A:4:GLU:OE2	1:A:267:ARG:NH2	2.44	0.50
1:B:345:PHE:HA	1:B:348:MET:HE3	1.94	0.50
1:B:364:GLU:HG3	1:B:372:LYS:HB3	1.94	0.50
1:A:327:SER:CB	1:A:457:ASP:HB3	2.42	0.50
1:A:434:LEU:HB3	1:A:454:PHE:CZ	2.47	0.50
1:B:207:ILE:CG2	1:B:208:LEU:N	2.74	0.49
1:B:401:PRO:HA	1:B:456:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ILE:HD11	1:B:248:VAL:CG2	2.42	0.49
1:A:40:HIS:O	1:A:43:LEU:HB3	2.12	0.49
1:A:44:ILE:HD11	1:A:60:ILE:HD12	1.93	0.49
1:A:529:PHE:N	1:A:530:PRO:HD3	2.27	0.49
1:B:158:HIS:HB2	1:B:275:VAL:HG22	1.94	0.49
1:B:321:LYS:O	1:B:325:LEU:HG	2.12	0.49
1:A:35:ILE:O	1:A:36:PHE:CD2	2.66	0.49
1:A:342:PRO:HD2	1:A:347:LYS:HG3	1.94	0.49
1:A:388:GLU:HB2	1:A:433:ARG:HH21	1.77	0.49
1:B:483:ARG:HD2	1:B:483:ARG:N	2.28	0.49
1:B:532:PHE:O	1:B:532:PHE:HD1	1.95	0.49
1:A:203:LEU:HD23	1:A:203:LEU:C	2.38	0.49
1:A:273:ARG:CZ	1:A:380:ARG:HH21	2.24	0.49
1:B:31:GLU:OE1	1:B:38:GLU:HG2	2.12	0.49
1:B:325:LEU:C	1:B:327:SER:H	2.21	0.49
1:A:367:THR:C	1:A:369:TYR:H	2.21	0.49
1:B:529:PHE:N	1:B:530:PRO:HD3	2.27	0.49
1:B:540:TYR:C	1:B:543:LEU:HD23	2.37	0.49
1:A:197:PRO:HD2	1:A:198:LYS:HE2	1.95	0.49
1:A:401:PRO:HA	1:A:456:ILE:O	2.13	0.49
1:B:197:PRO:HD2	1:B:198:LYS:HE2	1.95	0.49
1:B:407:VAL:HG23	1:B:452:LEU:O	2.12	0.49
1:B:414:ILE:HG21	1:B:430:VAL:HG22	1.94	0.49
1:A:233:ARG:CG	1:A:233:ARG:NH1	2.69	0.49
1:B:69:GLY:H	1:B:70:PRO:CD	2.25	0.49
1:B:109:GLN:C	1:B:111:SER:N	2.71	0.49
1:B:188:VAL:HB	1:B:247:PHE:CD2	2.47	0.49
1:A:115:LEU:O	1:A:116:ASP:C	2.55	0.49
1:A:360:LEU:HD23	1:A:374:LEU:HB3	1.95	0.49
1:A:484:LEU:HD11	1:A:533:MET:CG	2.29	0.49
1:A:10:LEU:HD13	1:A:58:LEU:CD2	2.42	0.49
1:A:155:LEU:HD23	1:A:286:GLU:O	2.12	0.49
1:A:230:VAL:HG12	1:A:234:MET:HE3	1.95	0.49
1:B:132:ILE:HG13	1:B:171:GLN:NE2	2.28	0.49
1:B:218:LEU:HG	1:B:219:ASN:N	2.27	0.48
1:B:405:ILE:HG12	1:B:410:TRP:CE3	2.48	0.48
1:A:4:GLU:OE2	1:A:244:ASN:ND2	2.46	0.48
1:A:142:LYS:HE2	1:A:146:GLU:OE2	2.13	0.48
1:A:393:LEU:CD1	1:A:464:LEU:HD21	2.43	0.48
1:A:540:TYR:C	1:A:543:LEU:HD23	2.38	0.48
1:B:115:LEU:CD2	1:B:116:ASP:H	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:THR:HG22	1:B:258:ILE:HD12	1.93	0.48
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.41	0.48
1:A:150:LEU:HD11	1:A:284:THR:HG21	1.95	0.48
1:A:426:LEU:HB3	1:A:428:ASP:OD1	2.12	0.48
1:B:388:GLU:HB2	1:B:433:ARG:HH21	1.77	0.48
1:B:342:PRO:HD2	1:B:347:LYS:CG	2.42	0.48
1:A:335:MET:HE2	1:A:363:VAL:CG1	2.43	0.48
1:B:13:ALA:O	1:B:17:LEU:HD12	2.14	0.48
1:A:321:LYS:O	1:A:325:LEU:HG	2.13	0.48
1:A:528:ASP:HB2	1:A:529:PHE:CE2	2.48	0.48
1:B:225:HIS:CD2	1:B:225:HIS:O	2.66	0.48
1:B:273:ARG:CZ	1:B:380:ARG:HH21	2.26	0.48
1:B:327:SER:CB	1:B:457:ASP:HB3	2.43	0.48
1:B:528:ASP:HB2	1:B:529:PHE:CE2	2.49	0.48
1:A:104:VAL:HG12	1:A:105:VAL:HG23	1.95	0.48
1:A:164:GLY:HA2	3:A:602:ATP:PA	2.52	0.48
1:A:395:PHE:O	1:A:398:VAL:HG22	2.14	0.48
1:B:264:LEU:O	1:B:266:LEU:HD23	2.13	0.48
1:B:398:VAL:HG23	1:B:398:VAL:O	2.14	0.48
1:A:167:VAL:HG23	3:A:602:ATP:O1A	2.13	0.48
1:B:205:THR:HA	1:B:231:LEU:HD11	1.95	0.48
1:B:230:VAL:HG12	1:B:234:MET:HE3	1.95	0.48
1:B:242:ARG:HB3	1:B:245:THR:OG1	2.14	0.48
1:B:334:MET:HE2	1:B:338:LYS:HD3	1.96	0.48
1:A:533:MET:H	1:A:533:MET:HG3	1.43	0.48
1:A:205:THR:O	1:A:209:LEU:HG	2.14	0.47
1:B:204:PHE:CD1	1:B:204:PHE:N	2.82	0.47
1:B:380:ARG:C	1:B:382:VAL:H	2.21	0.47
1:A:182:ILE:N	1:A:182:ILE:CD1	2.78	0.47
1:A:483:ARG:H	1:A:483:ARG:HD2	1.80	0.47
1:A:225:HIS:O	1:A:225:HIS:CD2	2.67	0.47
1:A:325:LEU:C	1:A:327:SER:H	2.21	0.47
1:A:326:SER:O	1:A:327:SER:C	2.57	0.47
1:A:483:ARG:HD2	1:A:483:ARG:N	2.29	0.47
1:A:242:ARG:HB3	1:A:245:THR:OG1	2.14	0.47
1:A:408:LYS:CE	1:A:427:ASP:HB2	2.41	0.47
1:B:101:LEU:HD21	1:B:106:ILE:CD1	2.44	0.47
1:B:327:SER:O	1:B:459:ILE:HD11	2.14	0.47
1:A:187:ILE:HD11	1:A:248:VAL:CG2	2.44	0.47
1:A:207:ILE:CG2	1:A:208:LEU:N	2.74	0.47
1:B:72:ILE:C	1:B:74:PHE:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:MET:C	1:B:114:MET:CE	2.87	0.47
1:B:131:TYR:CD2	1:B:301:PHE:HA	2.49	0.47
1:B:307:MET:HG3	1:B:337:PHE:CD2	2.49	0.47
1:B:434:LEU:HB3	1:B:454:PHE:CZ	2.50	0.47
1:A:143:LYS:O	1:A:147:MET:HG3	2.14	0.47
1:A:378:LEU:O	1:A:379:GLN:C	2.56	0.47
1:A:397:VAL:O	1:A:399:MET:N	2.48	0.47
1:A:455:LYS:HG2	1:A:456:ILE:N	2.30	0.47
1:B:89:ASP:O	1:B:93:PHE:HD2	1.98	0.47
1:B:134:GLU:O	1:B:135:TYR:C	2.57	0.47
1:B:533:MET:HE2	1:B:534:GLN:NE2	2.29	0.47
1:A:167:VAL:CG2	3:A:602:ATP:O1A	2.63	0.47
1:A:334:MET:HA	1:A:337:PHE:HD1	1.80	0.47
1:A:434:LEU:HB3	1:A:454:PHE:CE2	2.49	0.47
1:A:479:ILE:HG23	1:A:483:ARG:NH2	2.30	0.47
1:A:204:PHE:O	1:A:231:LEU:HD21	2.14	0.47
1:A:335:MET:HE3	1:A:373:SER:HA	1.96	0.47
1:A:35:ILE:O	1:A:35:ILE:CG2	2.61	0.46
1:A:156:PHE:CD1	1:A:287:PHE:CE2	3.03	0.46
1:A:158:HIS:CE1	1:A:289:GLU:HA	2.50	0.46
1:B:334:MET:HE3	1:B:337:PHE:CD1	2.51	0.46
1:B:380:ARG:C	1:B:382:VAL:N	2.72	0.46
1:A:72:ILE:C	1:A:74:PHE:H	2.22	0.46
1:B:84:ALA:O	1:B:88:GLU:HG2	2.15	0.46
1:B:397:VAL:O	1:B:399:MET:N	2.48	0.46
1:A:240:ILE:HG13	1:A:241:ASP:OD1	2.16	0.46
1:A:255:GLU:HB3	1:A:277:ILE:HG22	1.96	0.46
1:A:342:PRO:HD2	1:A:347:LYS:CG	2.46	0.46
1:A:374:LEU:O	1:A:375:ALA:C	2.58	0.46
1:B:479:ILE:HG23	1:B:483:ARG:NH2	2.30	0.46
1:A:188:VAL:HB	1:A:247:PHE:HD2	1.80	0.46
1:A:227:THR:HB	1:A:229:VAL:HG22	1.96	0.46
1:A:374:LEU:HD11	1:A:378:LEU:HG	1.98	0.46
1:A:405:ILE:HG12	1:A:410:TRP:CE3	2.51	0.46
1:A:525:ARG:HA	1:A:526:PRO:HD3	1.67	0.46
1:B:143:LYS:O	1:B:147:MET:HG3	2.14	0.46
1:B:212:LYS:HA	1:B:212:LYS:HD3	1.49	0.46
1:A:31:GLU:OE1	1:A:38:GLU:HG2	2.15	0.46
1:A:79:ASN:OD1	1:B:34:ASN:O	2.33	0.46
1:A:98:PRO:O	1:A:99:ASP:CB	2.63	0.46
1:A:160:ARG:HB3	1:A:163:SER:CB	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:HD22	1:B:270:VAL:H	1.80	0.46
1:B:335:MET:HE2	1:B:363:VAL:CG1	2.45	0.46
1:A:182:ILE:H	1:A:182:ILE:CD1	2.28	0.46
1:A:307:MET:HG3	1:A:337:PHE:CD2	2.51	0.46
1:B:192:ASP:OD2	1:B:252:VAL:HG22	2.15	0.46
1:A:107:ALA:N	1:A:108:PRO:CD	2.79	0.46
1:A:219:ASN:O	1:A:220:PHE:C	2.59	0.46
1:B:233:ARG:HD2	1:B:233:ARG:O	2.16	0.46
1:B:335:MET:HE3	1:B:373:SER:HA	1.97	0.46
1:A:23:PRO:HG2	1:A:53:ARG:HB3	1.98	0.46
1:A:50:ARG:O	1:A:54:ILE:HG13	2.16	0.46
1:A:93:PHE:CB	1:A:101:LEU:HD13	2.37	0.46
1:A:100:LEU:HG	1:A:104:VAL:HG21	1.97	0.46
1:A:134:GLU:O	1:A:135:TYR:C	2.57	0.46
1:A:164:GLY:CA	3:A:602:ATP:O1A	2.55	0.46
1:A:207:ILE:O	1:A:211:LEU:HG	2.16	0.46
1:A:212:LYS:HA	1:A:212:LYS:HD3	1.51	0.46
1:A:527:GLU:CD	1:A:527:GLU:N	2.74	0.46
1:A:99:ASP:C	1:A:101:LEU:H	2.22	0.46
1:B:326:SER:O	1:B:327:SER:C	2.59	0.46
1:A:307:MET:HG3	1:A:337:PHE:HD2	1.80	0.45
1:B:187:ILE:HD13	1:B:188:VAL:N	2.31	0.45
1:B:202:ASP:O	1:B:205:THR:HB	2.16	0.45
1:A:118:LYS:HD3	1:A:180:ILE:HG22	1.97	0.45
1:A:224:GLU:OE2	1:A:225:HIS:HB2	2.17	0.45
1:B:189:TRP:CD1	1:B:189:TRP:C	2.95	0.45
1:B:197:PRO:HD2	1:B:198:LYS:CG	2.42	0.45
1:B:247:PHE:HB2	1:B:268:CYS:HB3	1.97	0.45
1:B:466:HIS:ND1	1:B:466:HIS:N	2.63	0.45
1:B:483:ARG:HD2	1:B:483:ARG:H	1.81	0.45
1:A:30:LEU:HD22	1:A:35:ILE:HB	1.98	0.45
1:A:110:PHE:CD2	1:A:110:PHE:C	2.94	0.45
1:A:190:LEU:CD1	1:A:207:ILE:HG13	2.47	0.45
1:A:213:SER:C	1:A:215:ASP:H	2.23	0.45
1:A:393:LEU:HD23	1:A:437:LEU:HD22	1.98	0.45
1:A:89:ASP:O	1:A:93:PHE:HD2	2.00	0.45
1:B:114:MET:HE3	1:B:114:MET:C	2.41	0.45
1:B:216:ASP:HB3	1:B:219:ASN:CB	2.44	0.45
1:B:374:LEU:HD11	1:B:378:LEU:HG	1.99	0.45
1:A:204:PHE:CD1	1:A:204:PHE:N	2.85	0.45
1:A:528:ASP:C	1:A:530:PRO:HD3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:HD11	1:B:284:THR:HG21	1.99	0.45
1:B:201:PHE:C	1:B:201:PHE:CD2	2.95	0.45
1:B:527:GLU:N	1:B:527:GLU:CD	2.75	0.45
1:A:122:GLY:O	1:A:189:TRP:HB3	2.17	0.45
1:A:216:ASP:HB3	1:A:219:ASN:CB	2.44	0.45
1:B:112:ARG:O	1:B:117:ARG:HG2	2.17	0.45
1:A:79:ASN:HD22	1:B:36:PHE:H	1.62	0.45
1:A:115:LEU:O	1:A:118:LYS:N	2.49	0.45
1:B:164:GLY:HA2	3:B:602:ATP:O1A	2.17	0.45
1:B:533:MET:H	1:B:533:MET:HG3	1.43	0.45
1:A:61:TYR:HE2	1:A:68:LEU:HD23	1.82	0.45
1:A:398:VAL:HG23	1:A:398:VAL:O	2.16	0.45
1:B:204:PHE:O	1:B:231:LEU:HD21	2.17	0.45
1:B:385:LEU:HD23	1:B:385:LEU:N	2.32	0.45
1:B:434:LEU:HB3	1:B:454:PHE:CE2	2.52	0.45
1:A:7:CYS:HB2	1:A:243:PRO:HG2	1.98	0.45
1:B:102:ARG:O	1:B:104:VAL:HG23	2.17	0.45
1:B:197:PRO:HG2	1:B:198:LYS:HE2	1.99	0.45
1:B:255:GLU:HB3	1:B:277:ILE:HG22	1.98	0.45
1:A:197:PRO:HG2	1:A:198:LYS:HE2	1.98	0.44
1:A:202:ASP:O	1:A:205:THR:HB	2.17	0.44
1:A:354:LYS:HA	1:A:354:LYS:HD3	1.72	0.44
1:A:487:ILE:H	1:A:487:ILE:HG13	1.50	0.44
1:A:535:LEU:O	1:A:535:LEU:HD23	2.17	0.44
1:B:101:LEU:HD22	1:B:106:ILE:HG13	1.99	0.44
1:B:334:MET:HA	1:B:337:PHE:CD1	2.52	0.44
1:B:393:LEU:CD1	1:B:464:LEU:HD21	2.47	0.44
1:A:201:PHE:CD2	1:A:201:PHE:C	2.95	0.44
1:A:307:MET:HA	1:A:308:PRO:HD3	1.60	0.44
1:B:219:ASN:O	1:B:220:PHE:C	2.61	0.44
1:B:227:THR:HB	1:B:229:VAL:HG22	1.98	0.44
1:A:414:ILE:HA	1:A:415:PRO:HD3	1.78	0.44
1:A:456:ILE:HD13	1:A:461:HIS:HD2	1.83	0.44
1:B:21:PHE:HZ	1:B:57:PHE:CD2	2.35	0.44
1:B:115:LEU:HD23	1:B:116:ASP:H	1.81	0.44
1:A:23:PRO:HG2	1:A:53:ARG:CB	2.48	0.44
1:A:50:ARG:HE	1:A:50:ARG:HB3	1.50	0.44
1:A:131:TYR:CD1	1:A:131:TYR:C	2.96	0.44
1:B:72:ILE:HG21	1:B:88:GLU:CG	2.47	0.44
1:B:158:HIS:CE1	1:B:289:GLU:HA	2.51	0.44
1:B:307:MET:HG3	1:B:337:PHE:HD2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ASP:C	1:B:530:PRO:HD3	2.42	0.44
1:A:72:ILE:CG2	1:A:84:ALA:HB1	2.47	0.44
1:A:216:ASP:HA	1:A:218:LEU:HG	1.99	0.44
1:B:204:PHE:HD1	1:B:204:PHE:H	1.66	0.44
1:B:205:THR:O	1:B:209:LEU:HG	2.17	0.44
1:B:449:MET:HE3	1:B:450:PRO:HA	1.98	0.44
1:A:385:LEU:HD23	1:A:385:LEU:N	2.33	0.44
1:B:229:VAL:HG23	1:B:230:VAL:N	2.33	0.44
1:B:542:SER:O	1:B:543:LEU:HD22	2.16	0.44
1:A:257:THR:HG22	1:A:258:ILE:HD12	2.00	0.44
1:A:334:MET:HE3	1:A:337:PHE:CD1	2.53	0.44
1:A:381:CYS:C	1:A:384:VAL:HG22	2.43	0.44
1:B:155:LEU:HD23	1:B:286:GLU:O	2.17	0.44
1:B:408:LYS:CE	1:B:427:ASP:HB2	2.45	0.44
1:A:75:PHE:CB	1:A:84:ALA:HB2	2.43	0.44
1:A:542:SER:O	1:A:543:LEU:HD22	2.17	0.44
1:B:374:LEU:O	1:B:375:ALA:C	2.59	0.44
1:B:395:PHE:O	1:B:398:VAL:HG22	2.18	0.44
1:B:533:MET:C	1:B:533:MET:CE	2.91	0.44
1:A:111:SER:HB3	1:A:114:MET:HB2	1.99	0.43
1:A:264:LEU:O	1:A:266:LEU:HD23	2.18	0.43
1:A:449:MET:HE3	1:A:450:PRO:HA	1.99	0.43
1:B:68:LEU:HD21	1:B:71:LEU:HB3	1.98	0.43
1:B:163:SER:O	1:B:330:PRO:HG2	2.17	0.43
1:B:189:TRP:HB2	1:B:248:VAL:CG2	2.48	0.43
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.85	0.43
1:B:455:LYS:HG2	1:B:456:ILE:N	2.33	0.43
1:B:525:ARG:HH11	1:B:535:LEU:HD13	1.83	0.43
1:A:14:HIS:C	1:A:16:ARG:H	2.26	0.43
1:A:357:SER:O	1:A:358:ARG:HG3	2.18	0.43
1:B:49:THR:CG2	1:B:50:ARG:N	2.80	0.43
1:B:332:THR:HA	1:B:335:MET:SD	2.58	0.43
1:A:22:GLU:HA	1:A:23:PRO:HD3	1.83	0.43
1:A:25:ASP:HB3	1:A:78:ASN:HD21	1.82	0.43
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.84	0.43
1:B:131:TYR:C	1:B:131:TYR:CD1	2.96	0.43
1:B:313:GLU:C	1:B:315:GLU:H	2.26	0.43
1:A:84:ALA:O	1:A:88:GLU:HG2	2.18	0.43
1:A:466:HIS:ND1	1:A:466:HIS:N	2.65	0.43
1:B:77:TYR:CD1	1:B:77:TYR:C	2.96	0.43
1:B:128:MET:HE2	1:B:128:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:HG21	1:A:88:GLU:CG	2.46	0.43
1:A:128:MET:SD	1:B:282:SER:HB2	2.58	0.43
1:A:156:PHE:HD1	1:A:287:PHE:CE2	2.37	0.43
1:A:214:GLU:O	1:A:216:ASP:N	2.51	0.43
1:A:522:THR:O	1:A:523:VAL:HG23	2.18	0.43
1:B:35:ILE:CD1	1:B:70:PRO:HG2	2.48	0.43
1:B:310:PRO:HA	1:B:345:PHE:HZ	1.83	0.43
1:B:354:LYS:HA	1:B:354:LYS:HD3	1.74	0.43
1:A:79:ASN:ND2	1:B:36:PHE:N	2.66	0.43
1:A:148:CYS:HA	1:A:184:TYR:CZ	2.53	0.43
1:A:457:ASP:O	1:A:460:ILE:HG22	2.18	0.43
1:B:23:PRO:HG2	1:B:53:ARG:HB3	2.00	0.43
1:A:161:ALA:HB2	1:A:273:ARG:HD2	2.00	0.43
1:A:197:PRO:HD2	1:A:198:LYS:CG	2.43	0.43
1:B:148:CYS:HA	1:B:184:TYR:CZ	2.54	0.43
1:B:188:VAL:HG13	1:B:210:MET:HE2	2.01	0.43
1:B:465:LYS:HD3	1:B:466:HIS:HE1	1.84	0.43
1:B:483:ARG:H	1:B:483:ARG:CD	2.30	0.43
1:B:525:ARG:HA	1:B:526:PRO:HD3	1.68	0.43
1:A:2:LEU:O	1:A:3:CYS:HB3	2.19	0.43
1:A:336:PHE:O	1:A:337:PHE:C	2.59	0.43
1:B:451:VAL:O	1:B:453:THR:HG23	2.18	0.43
1:B:487:ILE:HG22	1:B:487:ILE:O	2.18	0.43
1:A:128:MET:CE	1:B:282:SER:HB2	2.48	0.43
1:A:233:ARG:HD2	1:A:233:ARG:O	2.19	0.43
1:B:142:LYS:O	1:B:146:GLU:HG3	2.19	0.43
1:B:188:VAL:HB	1:B:247:PHE:HD2	1.84	0.43
1:B:318:VAL:O	1:B:318:VAL:CG1	2.66	0.43
1:A:1:MET:HE3	1:A:240:ILE:CB	2.48	0.43
1:A:231:LEU:C	1:A:231:LEU:HD23	2.44	0.43
1:A:334:MET:HE2	1:A:338:LYS:HD3	2.00	0.43
1:A:318:VAL:O	1:A:318:VAL:CG1	2.66	0.42
1:A:435:LYS:NZ	1:A:446:GLY:HA3	2.34	0.42
1:B:102:ARG:O	1:B:104:VAL:N	2.52	0.42
1:B:351:LEU:N	1:B:351:LEU:HD23	2.33	0.42
1:B:522:THR:O	1:B:523:VAL:HG23	2.19	0.42
1:B:535:LEU:HD23	1:B:535:LEU:O	2.19	0.42
1:A:7:CYS:CB	1:A:243:PRO:HG2	2.49	0.42
1:A:158:HIS:CE1	1:A:289:GLU:HB2	2.54	0.42
1:A:259:ARG:HG2	1:A:280:ALA:HB1	2.01	0.42
1:B:39:ASP:O	1:B:43:LEU:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HH12	1:A:115:LEU:HD12	1.82	0.42
1:A:461:HIS:C	1:A:463:PHE:N	2.75	0.42
1:B:61:TYR:HE2	1:B:68:LEU:HD23	1.83	0.42
1:B:405:ILE:HA	1:B:406:PRO:HD3	1.82	0.42
1:A:313:GLU:C	1:A:315:GLU:H	2.27	0.42
3:A:602:ATP:O2G	3:A:602:ATP:O1B	2.37	0.42
1:B:310:PRO:HA	1:B:345:PHE:CZ	2.55	0.42
1:B:406:PRO:CA	1:B:453:THR:HG22	2.47	0.42
1:B:461:HIS:C	1:B:463:PHE:N	2.75	0.42
1:B:537:GLN:O	1:B:538:LYS:C	2.63	0.42
1:A:122:GLY:CA	1:A:187:ILE:O	2.67	0.42
1:A:479:ILE:HG23	1:A:483:ARG:HH22	1.84	0.42
1:B:14:HIS:C	1:B:16:ARG:H	2.27	0.42
1:B:29:TYR:CE2	1:B:33:LYS:HD2	2.54	0.42
1:A:247:PHE:HB2	1:A:268:CYS:HB3	2.02	0.42
1:A:99:ASP:C	1:A:101:LEU:N	2.77	0.42
1:B:357:SER:O	1:B:358:ARG:HG3	2.18	0.42
1:A:334:MET:HA	1:A:337:PHE:CD1	2.55	0.42
1:A:366:ILE:O	1:A:366:ILE:HG22	2.19	0.42
1:A:437:LEU:O	1:A:439:LYS:N	2.47	0.42
1:A:461:HIS:C	1:A:463:PHE:H	2.27	0.42
1:B:44:ILE:HD11	1:B:60:ILE:HD12	2.01	0.42
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.69	0.42
1:B:319:LEU:HD23	1:B:319:LEU:C	2.44	0.42
1:A:97:GLU:OE1	1:A:100:LEU:HD23	2.19	0.42
1:A:406:PRO:CA	1:A:453:THR:HG22	2.45	0.42
1:A:483:ARG:H	1:A:483:ARG:CD	2.32	0.42
1:A:310:PRO:HA	1:A:345:PHE:HZ	1.84	0.42
1:A:404:ASP:O	1:A:524:ILE:HD13	2.19	0.42
1:B:101:LEU:CD2	1:B:106:ILE:HG13	2.50	0.42
1:B:141:ILE:HD13	1:B:176:SER:HB3	2.02	0.42
1:B:307:MET:HA	1:B:308:PRO:HD3	1.61	0.42
1:B:327:SER:N	1:B:459:ILE:HG12	2.34	0.42
1:B:464:LEU:O	1:B:465:LYS:C	2.63	0.42
1:A:189:TRP:CD1	1:A:189:TRP:C	2.98	0.41
1:A:527:GLU:N	1:A:527:GLU:OE1	2.51	0.41
1:A:530:PRO:O	1:A:532:PHE:N	2.53	0.41
1:B:30:LEU:HB3	1:B:36:PHE:CD2	2.55	0.41
1:B:72:ILE:CG2	1:B:84:ALA:HB1	2.48	0.41
1:B:459:ILE:C	1:B:461:HIS:N	2.77	0.41
1:A:79:ASN:HD22	1:B:36:PHE:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:MET:HE2	1:A:128:MET:HA	2.01	0.41
1:B:158:HIS:CE1	1:B:289:GLU:HB2	2.55	0.41
1:B:367:THR:C	1:B:369:TYR:N	2.78	0.41
1:A:61:TYR:C	1:A:63:ARG:H	2.27	0.41
1:B:49:THR:CG2	1:B:50:ARG:H	2.32	0.41
1:B:122:GLY:O	1:B:189:TRP:HB3	2.20	0.41
1:B:161:ALA:HB2	1:B:273:ARG:HD2	2.02	0.41
1:B:265:ARG:C	1:B:266:LEU:HD23	2.45	0.41
1:B:342:PRO:O	1:B:343:LYS:HB2	2.21	0.41
1:B:458:HIS:O	1:B:461:HIS:HB3	2.21	0.41
1:A:71:LEU:HD11	1:A:75:PHE:HE1	1.85	0.41
1:A:77:TYR:CD1	1:A:77:TYR:C	2.98	0.41
1:A:269:LEU:HD22	1:A:270:VAL:H	1.85	0.41
1:A:343:LYS:HG2	1:A:343:LYS:O	2.21	0.41
1:A:348:MET:SD	1:A:348:MET:C	3.03	0.41
1:A:525:ARG:HH11	1:A:535:LEU:HD13	1.86	0.41
1:B:113:GLN:OE1	1:B:113:GLN:HA	2.19	0.41
1:A:189:TRP:HB2	1:A:248:VAL:HG23	2.03	0.41
1:A:443:LEU:C	1:A:444:LEU:HD12	2.46	0.41
1:A:533:MET:C	1:A:533:MET:CE	2.93	0.41
1:B:2:LEU:O	1:B:3:CYS:HB3	2.20	0.41
1:B:378:LEU:O	1:B:379:GLN:C	2.63	0.41
1:A:154:PHE:CE1	1:A:283:GLN:NE2	2.89	0.41
1:A:487:ILE:O	1:A:487:ILE:HG22	2.21	0.41
1:B:336:PHE:O	1:B:337:PHE:C	2.62	0.41
1:B:461:HIS:C	1:B:463:PHE:H	2.29	0.41
1:A:79:ASN:HD21	1:B:34:ASN:HA	1.85	0.41
1:A:237:ASN:O	1:A:239:LEU:N	2.53	0.41
1:B:23:PRO:HG2	1:B:53:ARG:CB	2.51	0.41
1:B:334:MET:HE2	1:B:338:LYS:CD	2.50	0.41
1:A:23:PRO:CG	1:A:53:ARG:O	2.69	0.41
1:A:102:ARG:HB2	1:A:103:PRO:HD3	2.02	0.41
1:A:204:PHE:HD1	1:A:204:PHE:H	1.69	0.41
1:A:283:GLN:O	1:A:285:CYS:N	2.54	0.41
1:A:305:TYR:O	1:A:306:GLY:C	2.62	0.41
1:B:122:GLY:CA	1:B:187:ILE:O	2.67	0.41
1:B:127:GLN:HA	1:B:170:SER:OG	2.21	0.41
1:B:393:LEU:HD12	1:B:464:LEU:HD21	2.03	0.41
1:A:32:GLY:C	1:A:34:ASN:N	2.75	0.41
1:A:228:SER:O	1:A:232:LYS:HG3	2.21	0.41
1:A:310:PRO:HA	1:A:345:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASP:HB3	1:B:78:ASN:HD21	1.86	0.41
1:B:443:LEU:C	1:B:444:LEU:HD12	2.45	0.41
1:B:479:ILE:HG23	1:B:483:ARG:HH22	1.86	0.41
1:B:541:ASP:O	1:B:543:LEU:N	2.48	0.41
1:A:35:ILE:CD1	1:A:70:PRO:HG2	2.51	0.41
1:A:393:LEU:CD1	1:A:393:LEU:C	2.94	0.41
1:B:216:ASP:HA	1:B:218:LEU:HG	2.02	0.41
1:B:224:GLU:OE2	1:B:225:HIS:HB2	2.20	0.41
1:B:327:SER:C	1:B:459:ILE:HD11	2.46	0.41
1:B:330:PRO:O	1:B:333:LEU:HB2	2.21	0.41
1:B:374:LEU:HD12	1:B:378:LEU:CD1	2.50	0.41
1:B:527:GLU:N	1:B:527:GLU:OE1	2.54	0.41
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.95	0.40
1:A:119:LEU:CB	1:B:265:ARG:HH12	2.32	0.40
1:A:265:ARG:C	1:A:266:LEU:HD23	2.46	0.40
1:A:276:GLU:C	1:A:278:SER:H	2.29	0.40
1:A:342:PRO:O	1:A:343:LYS:HB2	2.21	0.40
1:B:155:LEU:HD23	1:B:155:LEU:HA	1.78	0.40
1:A:68:LEU:HD21	1:A:71:LEU:HB3	2.04	0.40
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.81	0.40
1:A:374:LEU:HD12	1:A:378:LEU:CD1	2.51	0.40
1:B:69:GLY:N	1:B:70:PRO:CD	2.85	0.40
1:B:106:ILE:O	1:B:106:ILE:CG2	2.69	0.40
1:B:154:PHE:CE1	1:B:283:GLN:NE2	2.89	0.40
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.75	0.40
1:B:365:CYS:SG	1:B:366:ILE:N	2.92	0.40
1:B:444:LEU:HD12	1:B:444:LEU:N	2.36	0.40
1:B:477:ILE:HD11	1:B:543:LEU:HG	2.03	0.40
1:A:464:LEU:O	1:A:465:LYS:C	2.64	0.40
1:B:23:PRO:CG	1:B:53:ARG:O	2.69	0.40
1:B:131:TYR:C	1:B:132:ILE:HD12	2.46	0.40
1:B:248:VAL:HG13	1:B:269:LEU:HD12	2.03	0.40
1:A:143:LYS:O	1:A:147:MET:HE3	2.22	0.40
1:A:359:GLY:HA2	1:A:462:MET:HB3	2.03	0.40
1:A:537:GLN:O	1:A:538:LYS:C	2.64	0.40
1:B:47:MET:CB	1:B:53:ARG:HG3	2.44	0.40
1:B:61:TYR:C	1:B:63:ARG:H	2.28	0.40
1:B:179:LEU:HD12	1:B:179:LEU:HA	1.87	0.40
1:B:283:GLN:O	1:B:285:CYS:N	2.53	0.40
1:B:435:LYS:HZ2	1:B:446:GLY:HA3	1.87	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	497/549 (90%)	364 (73%)	87 (18%)	46 (9%)	0	9
1	B	495/549 (90%)	359 (72%)	91 (18%)	45 (9%)	0	9
All	All	992/1098 (90%)	723 (73%)	178 (18%)	91 (9%)	0	9

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	343	LYS
1	A	398	VAL
1	A	452	LEU
1	A	484	LEU
1	A	485	LEU
1	A	486	GLU
1	B	109	GLN
1	B	116	ASP
1	B	327	SER
1	B	343	LYS
1	B	398	VAL
1	B	452	LEU
1	B	484	LEU
1	B	485	LEU
1	B	486	GLU
1	A	99	ASP
1	A	115	LEU
1	A	116	ASP
1	A	134	GLU
1	A	215	ASP
1	A	238	ALA
1	A	284	THR
1	A	306	GLY
1	A	442	ALA

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Mol	Chain	Res	Type
1	A	460	ILE
1	A	465	LYS
1	B	104	VAL
1	B	115	LEU
1	B	134	GLU
1	B	215	ASP
1	B	238	ALA
1	B	284	THR
1	B	306	GLY
1	B	442	ALA
1	B	460	ILE
1	B	465	LYS
1	A	21	PHE
1	A	106	ILE
1	A	135	TYR
1	A	237	ASN
1	A	251	ASP
1	A	372	LYS
1	A	425	GLN
1	A	439	LYS
1	A	445	SER
1	A	522	THR
1	A	531	LYS
1	B	21	PHE
1	B	103	PRO
1	B	135	TYR
1	B	237	ASN
1	B	251	ASP
1	B	439	LYS
1	B	445	SER
1	B	531	LYS
1	A	33	LYS
1	A	150	LEU
1	A	152	SER
1	A	182	ILE
1	A	364	GLU
1	A	542	SER
1	B	33	LYS
1	B	152	SER
1	B	182	ILE
1	B	364	GLU
1	B	372	LYS

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Mol	Chain	Res	Type
1	B	522	THR
1	B	542	SER
1	A	70	PRO
1	A	212	LYS
1	A	358	ARG
1	A	530	PRO
1	B	70	PRO
1	B	150	LEU
1	B	212	LYS
1	B	530	PRO
1	A	69	GLY
1	A	213	SER
1	A	368	PRO
1	B	69	GLY
1	B	358	ARG
1	B	368	PRO
1	B	102	ARG
1	A	194	GLY
1	A	467	VAL
1	B	397	VAL
1	B	467	VAL
1	A	397	VAL
1	A	450	PRO
1	B	450	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	458/501 (91%)	374 (82%)	84 (18%)	2	11
1	B	456/501 (91%)	368 (81%)	88 (19%)	1	9
All	All	914/1002 (91%)	742 (81%)	172 (19%)	1	10

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	42	GLU
1	A	46	LYS
1	A	50	ARG
1	A	64	GLN
1	A	67	GLU
1	A	77	TYR
1	A	79	ASN
1	A	106	ILE
1	A	110	PHE
1	A	115	LEU
1	A	116	ASP
1	A	128	MET
1	A	150	LEU
1	A	151	ASP
1	A	155	LEU
1	A	157	LEU
1	A	167	VAL
1	A	179	LEU
1	A	182	ILE
1	A	185	ASP
1	A	187	ILE
1	A	195	THR
1	A	198	LYS
1	A	200	THR
1	A	205	THR
1	A	207	ILE
1	A	218	LEU
1	A	224	GLU
1	A	227	THR
1	A	228	SER
1	A	233	ARG
1	A	235	ILE
1	A	248	VAL
1	A	252	VAL
1	A	253	VAL
1	A	257	THR
1	A	264	LEU
1	A	266	LEU
1	A	269	LEU
1	A	271	THR
1	A	277	ILE
1	A	284	THR

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Mol	Chain	Res	Type
1	A	296	ASP
1	A	315	GLU
1	A	316	GLU
1	A	319	LEU
1	A	332	THR
1	A	344	THR
1	A	355	LEU
1	A	360	LEU
1	A	363	VAL
1	A	366	ILE
1	A	370	SER
1	A	374	LEU
1	A	381	CYS
1	A	393	LEU
1	A	395	PHE
1	A	399	MET
1	A	404	ASP
1	A	405	ILE
1	A	409	LEU
1	A	410	TRP
1	A	414	ILE
1	A	416	VAL
1	A	425	GLN
1	A	428	ASP
1	A	452	LEU
1	A	456	ILE
1	A	457	ASP
1	A	459	ILE
1	A	460	ILE
1	A	462	MET
1	A	467	VAL
1	A	484	LEU
1	A	485	LEU
1	A	521	GLU
1	A	524	ILE
1	A	528	ASP
1	A	529	PHE
1	A	533	MET
1	A	534	GLN
1	A	538	LYS
1	A	543	LEU
1	B	1	MET

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Mol	Chain	Res	Type
1	B	42	GLU
1	B	46	LYS
1	B	50	ARG
1	B	64	GLN
1	B	67	GLU
1	B	77	TYR
1	B	79	ASN
1	B	99	ASP
1	B	106	ILE
1	B	109	GLN
1	B	112	ARG
1	B	114	MET
1	B	115	LEU
1	B	116	ASP
1	B	121	LEU
1	B	128	MET
1	B	150	LEU
1	B	151	ASP
1	B	155	LEU
1	B	157	LEU
1	B	167	VAL
1	B	178	GLN
1	B	179	LEU
1	B	182	ILE
1	B	185	ASP
1	B	187	ILE
1	B	195	THR
1	B	198	LYS
1	B	200	THR
1	B	205	THR
1	B	207	ILE
1	B	218	LEU
1	B	224	GLU
1	B	227	THR
1	B	228	SER
1	B	233	ARG
1	B	248	VAL
1	B	252	VAL
1	B	253	VAL
1	B	257	THR
1	B	264	LEU
1	B	266	LEU

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Mol	Chain	Res	Type
1	B	269	LEU
1	B	271	THR
1	B	277	ILE
1	B	284	THR
1	B	296	ASP
1	B	315	GLU
1	B	316	GLU
1	B	319	LEU
1	B	332	THR
1	B	344	THR
1	B	355	LEU
1	B	360	LEU
1	B	363	VAL
1	B	366	ILE
1	B	370	SER
1	B	374	LEU
1	B	381	CYS
1	B	393	LEU
1	B	395	PHE
1	B	399	MET
1	B	404	ASP
1	B	405	ILE
1	B	409	LEU
1	B	410	TRP
1	B	414	ILE
1	B	416	VAL
1	B	428	ASP
1	B	452	LEU
1	B	456	ILE
1	B	457	ASP
1	B	459	ILE
1	B	460	ILE
1	B	462	MET
1	B	466	HIS
1	B	467	VAL
1	B	484	LEU
1	B	485	LEU
1	B	521	GLU
1	B	524	ILE
1	B	528	ASP
1	B	529	PHE
1	B	533	MET

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Mol	Chain	Res	Type
1	B	534	GLN
1	B	538	LYS
1	B	543	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	40	HIS
1	A	64	GLN
1	A	79	ASN
1	A	113	GLN
1	A	123	ASN
1	A	158	HIS
1	A	171	GLN
1	A	219	ASN
1	A	225	HIS
1	A	283	GLN
1	A	461	HIS
1	A	471	GLN
1	A	475	ASN
1	A	534	GLN
1	B	34	ASN
1	B	40	HIS
1	B	64	GLN
1	B	123	ASN
1	B	158	HIS
1	B	171	GLN
1	B	219	ASN
1	B	225	HIS
1	B	244	ASN
1	B	254	GLN
1	B	461	HIS
1	B	471	GLN
1	B	475	ASN
1	B	534	GLN
1	B	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	$\# Z > 2$
3	ATP	B	602	2	32,33,33	1.50	4 (12%)	48,52,52	2.18	12 (25%)
3	ATP	A	602	2	32,33,33	1.68	6 (18%)	48,52,52	1.94	10 (20%)

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	ATP	B	602	2	-	11/22/38/38	0/3/3/3
3	ATP	A	602	2	-	7/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ATP	C5-C4	5.53	1.49	1.39
3	A	602	ATP	C5-C4	5.26	1.48	1.39
3	A	602	ATP	PB-O3A	4.24	1.64	1.59
3	A	602	ATP	PA-O3A	3.43	1.63	1.59
3	A	602	ATP	C5-C6	3.03	1.49	1.41
3	B	602	ATP	C5-N7	-2.73	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ATP	C5-C6	2.64	1.48	1.41
3	A	602	ATP	C8-N7	2.49	1.36	1.31
3	B	602	ATP	C8-N7	2.27	1.36	1.31
3	A	602	ATP	C5-N7	-2.04	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	ATP	C5-C4-N3	-7.26	116.72	126.72
3	A	602	ATP	C5-C4-N3	-6.25	118.12	126.72
3	B	602	ATP	N3-C4-N9	5.79	137.02	127.17
3	B	602	ATP	O4'-C1'-N9	5.53	118.72	108.09
3	A	602	ATP	N3-C4-N9	4.95	135.58	127.17
3	B	602	ATP	C2-N3-C4	3.98	121.55	111.83
3	A	602	ATP	C2-N3-C4	3.87	121.29	111.83
3	A	602	ATP	C4-C5-N7	-3.40	106.70	110.58
3	A	602	ATP	O3B-PB-O1B	-3.33	100.67	110.70
3	A	602	ATP	N3-C2-N1	-3.30	123.58	128.58
3	B	602	ATP	N3-C2-N1	-3.01	124.02	128.58
3	B	602	ATP	C4-C5-N7	-2.95	107.21	110.58
3	B	602	ATP	C2'-C1'-N9	-2.93	106.03	113.30
3	B	602	ATP	C1'-N9-C8	-2.85	120.78	127.09
3	B	602	ATP	C4-N9-C1'	2.56	132.62	126.63
3	A	602	ATP	C5-N7-C8	2.51	107.39	103.45
3	B	602	ATP	O3G-PG-O3B	-2.43	96.48	104.64
3	A	602	ATP	O3G-PG-O2G	2.40	116.81	107.80
3	A	602	ATP	O2A-PA-O3A	2.20	113.22	107.27
3	B	602	ATP	O3A-PA-O1A	-2.16	104.21	110.70
3	A	602	ATP	O5'-C5'-C4'	-2.12	101.78	108.99
3	B	602	ATP	C5-N7-C8	2.07	106.70	103.45

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	ATP	C5'-O5'-PA-O2A
3	A	602	ATP	C5'-O5'-PA-O3A
3	A	602	ATP	O4'-C4'-C5'-O5'
3	B	602	ATP	C5'-O5'-PA-O1A
3	B	602	ATP	C5'-O5'-PA-O2A
3	B	602	ATP	C5'-O5'-PA-O3A
3	A	602	ATP	C3'-C4'-C5'-O5'

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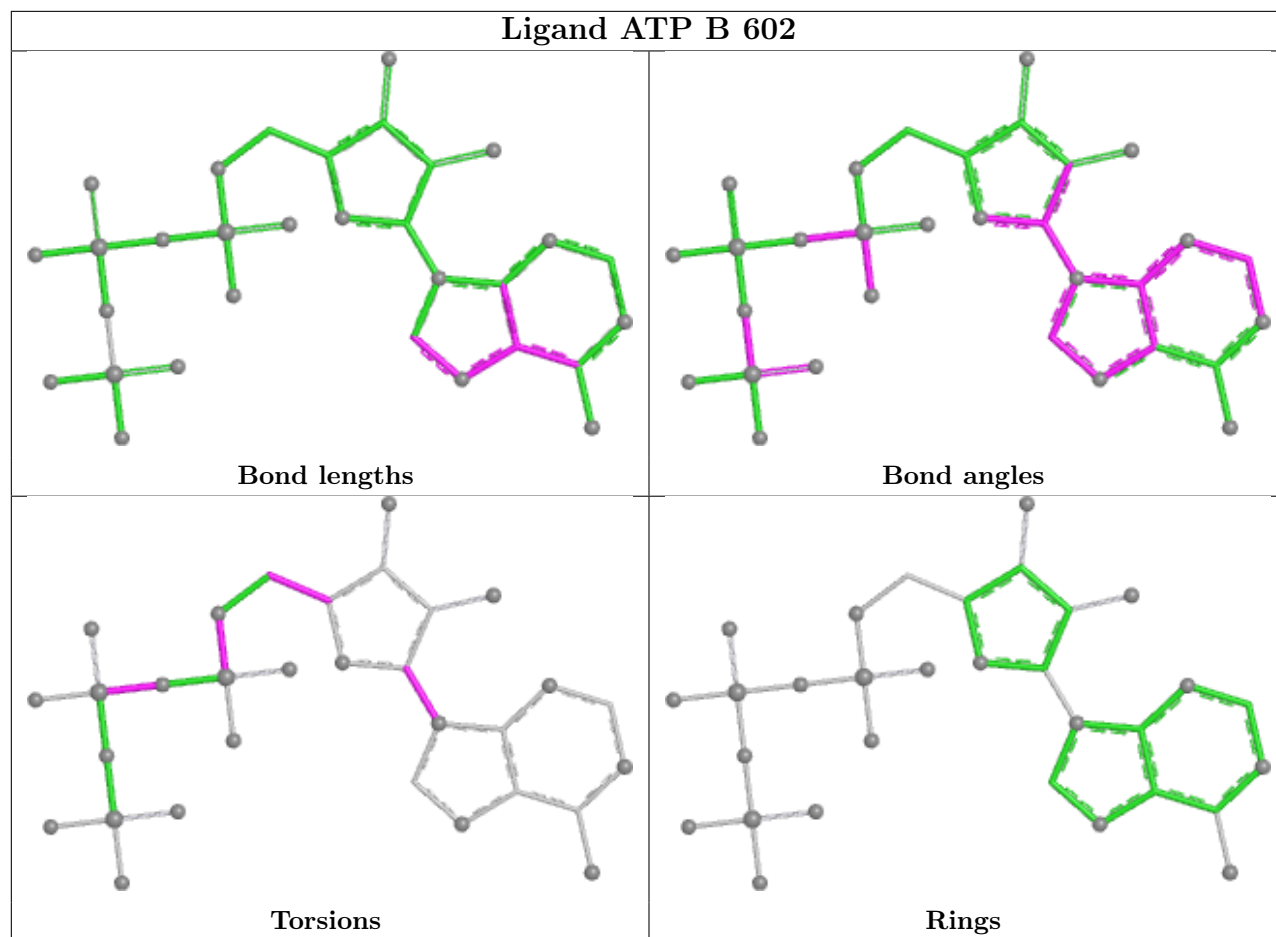
Mol	Chain	Res	Type	Atoms
3	B	602	ATP	O4'-C4'-C5'-O5'
3	B	602	ATP	C3'-C4'-C5'-O5'
3	A	602	ATP	PA-O3A-PB-O1B
3	B	602	ATP	PA-O3A-PB-O1B
3	B	602	ATP	C2'-C1'-N9-C8
3	A	602	ATP	C5'-O5'-PA-O1A
3	B	602	ATP	O4'-C1'-N9-C8
3	B	602	ATP	O4'-C1'-N9-C4
3	A	602	ATP	PA-O3A-PB-O2B
3	B	602	ATP	PA-O3A-PB-O2B
3	B	602	ATP	C2'-C1'-N9-C4

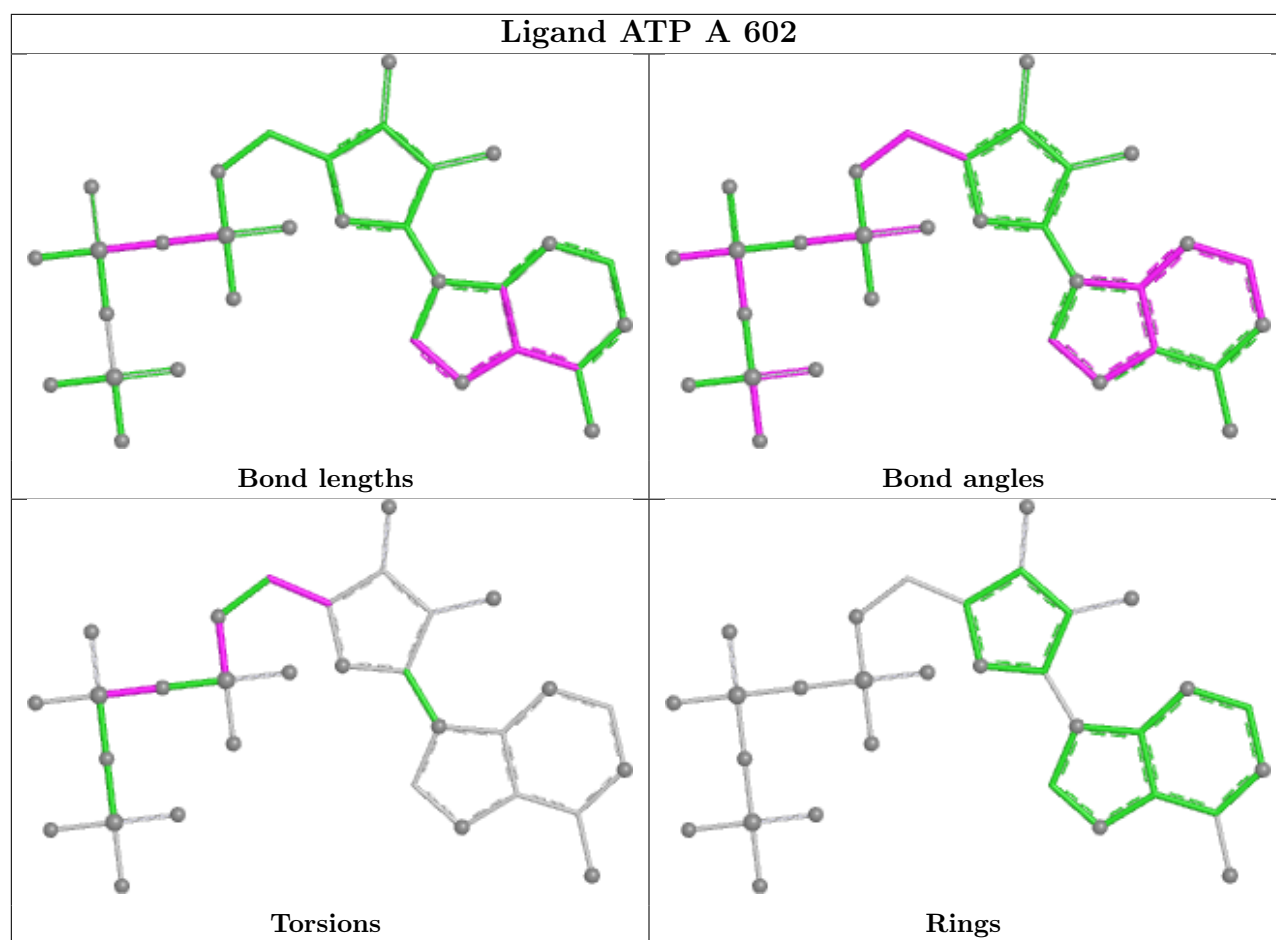
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	ATP	4	0
3	A	602	ATP	10	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 [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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	503/549 (91%)	0.71	33 (6%) 24 21	120, 188, 268, 332	0
1	B	501/549 (91%)	0.70	50 (9%) 12 15	121, 188, 270, 362	0
All	All	1004/1098 (91%)	0.70	83 (8%) 17 18	120, 188, 269, 362	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	402	GLY	6.8
1	A	49	THR	5.0
1	B	290	VAL	4.7
1	B	77	TYR	4.5
1	A	409	LEU	4.4
1	A	57	PHE	4.2
1	B	168	ILE	4.2
1	B	184	TYR	4.2
1	B	164	GLY	4.1
1	A	264	LEU	4.0
1	B	18	ILE	3.9
1	A	30	LEU	3.9
1	B	288	ILE	3.8
1	B	27	LEU	3.8
1	A	301	PHE	3.8
1	A	70	PRO	3.7
1	B	157	LEU	3.6
1	A	128	MET	3.6
1	A	293	LEU	3.5
1	B	26	ALA	3.4
1	B	274	ASP	3.3
1	B	38	GLU	3.3
1	B	136	HIS	3.3
1	A	10	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	51	LEU	3.2
1	A	71	LEU	3.2
1	A	29	TYR	3.2
1	B	36	PHE	3.1
1	A	392	ALA	3.0
1	A	487	ILE	2.9
1	B	29	TYR	2.9
1	B	543	LEU	2.9
1	B	140	VAL	2.8
1	B	283	GLN	2.8
1	B	180	ILE	2.7
1	A	223	VAL	2.7
1	B	336	PHE	2.7
1	A	288	ILE	2.7
1	B	435	LYS	2.7
1	A	137	VAL	2.6
1	A	28	THR	2.6
1	A	539	PHE	2.6
1	B	223	VAL	2.5
1	A	19	HIS	2.5
1	A	290	VAL	2.5
1	A	77	TYR	2.5
1	B	6	GLU	2.5
1	B	61	TYR	2.5
1	A	330	PRO	2.4
1	B	247	PHE	2.4
1	B	264	LEU	2.4
1	B	44	ILE	2.4
1	B	473	ILE	2.4
1	B	525	ARG	2.4
1	B	311	VAL	2.4
1	A	144	LEU	2.4
1	A	236	CYS	2.3
1	B	355	LEU	2.3
1	A	283	GLN	2.3
1	B	341	GLU	2.3
1	A	416	VAL	2.3
1	B	116	ASP	2.3
1	B	241	ASP	2.3
1	B	403	VAL	2.2
1	B	291	THR	2.2
1	B	211	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	539	PHE	2.2
1	B	338	LYS	2.2
1	A	131	TYR	2.2
1	A	184	TYR	2.2
1	A	400	PRO	2.2
1	B	530	PRO	2.2
1	A	26	ALA	2.2
1	B	208	LEU	2.2
1	B	285	CYS	2.2
1	B	332	THR	2.1
1	A	543	LEU	2.1
1	B	360	LEU	2.1
1	B	439	LYS	2.1
1	B	57	PHE	2.1
1	B	337	PHE	2.1
1	B	133	ARG	2.1
1	A	106	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

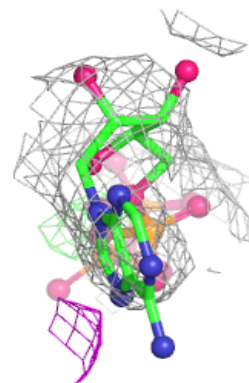
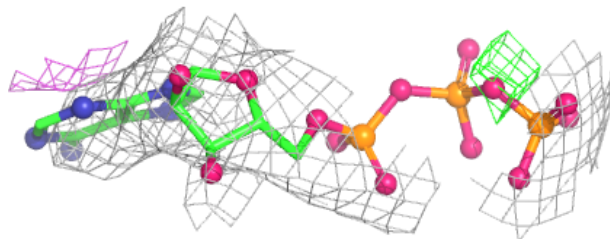
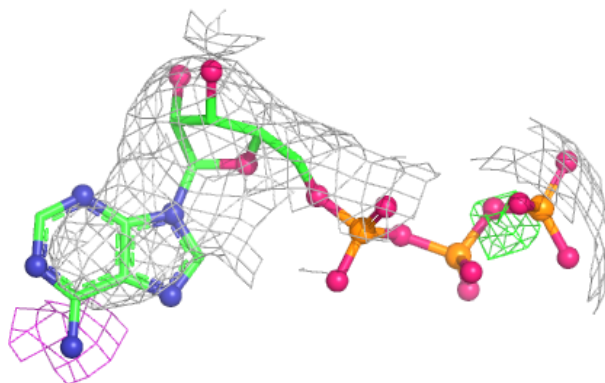
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	601	1/1	0.95	0.10	120,120,120,120	0
3	ATP	A	602	31/31	0.96	0.12	109,150,189,351	0
3	ATP	B	602	31/31	0.96	0.16	95,155,196,334	0
2	MG	B	601	1/1	0.97	0.09	104,104,104,104	0

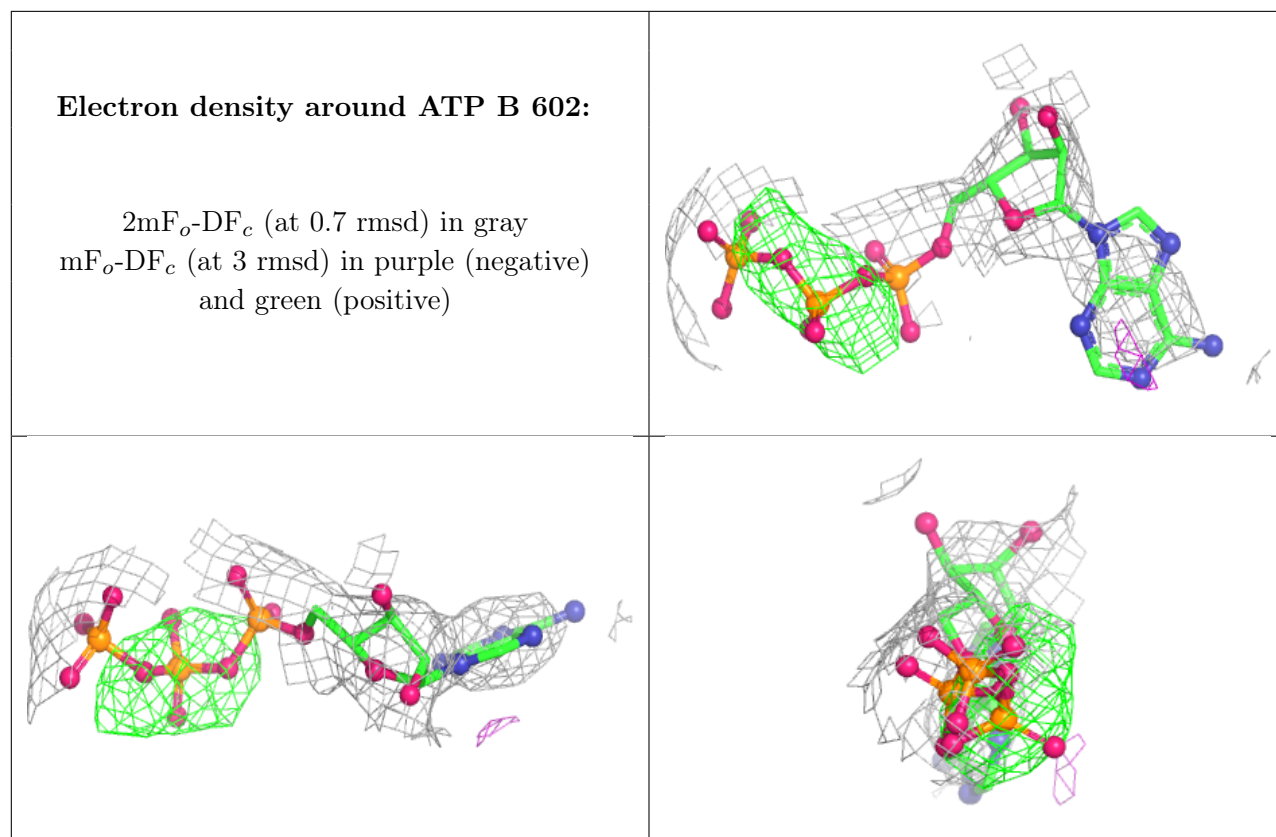
The following is a graphical depiction of the model fit to experimental electron density of all

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

Electron density around ATP A 602:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.