Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 06:46 PM EST

PDB ID	:	4RH7
Title	:	Crystal structure of human cytoplasmic dynein 2 motor domain in complex with ADP.Vi
Authors	:	Schmidt, H.; Zalyte, R.; Urnavicius, L.; Carter, A.P.
Deposited on	:	2014-10-01
Resolution	:	3.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

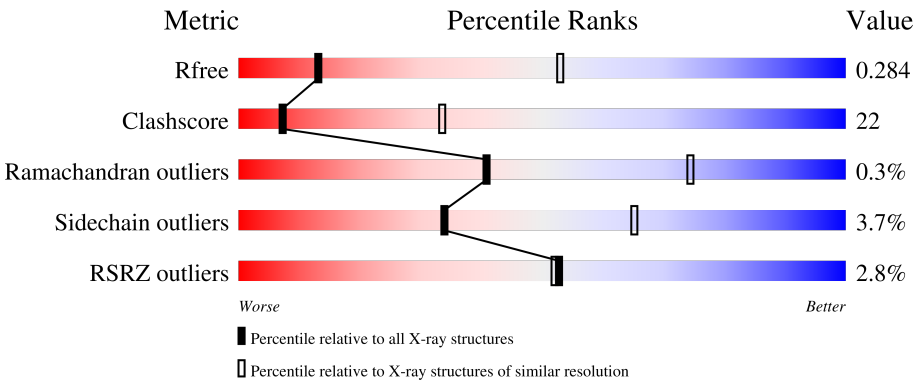
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.41 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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

Mol	Chain	Length	Quality of chain
1	A	3450	2% 59% 27% • 13%

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
2	AOV	A	4401	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22816 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.

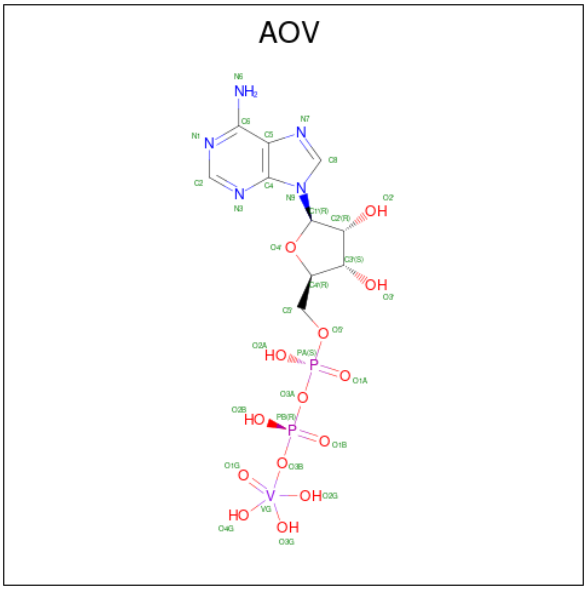
- Molecule 1 is a protein called Green fluorescent protein/Cytoplasmic dynein 2 heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	3005	22697	14414	3922	4263	98	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1089	GLY	-	linker	UNP Q8NCM8
A	1090	SER	-	linker	UNP Q8NCM8
A	1413	ARG	LYS	variant	UNP Q8NCM8
A	2871	GLN	ARG	variant	UNP Q8NCM8
A	3680	VAL	ALA	variant	UNP Q8NCM8
A	4308	VAL	-	expression tag	UNP Q8NCM8

- Molecule 2 is ADP ORTHOVANADATE (three-letter code: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$).

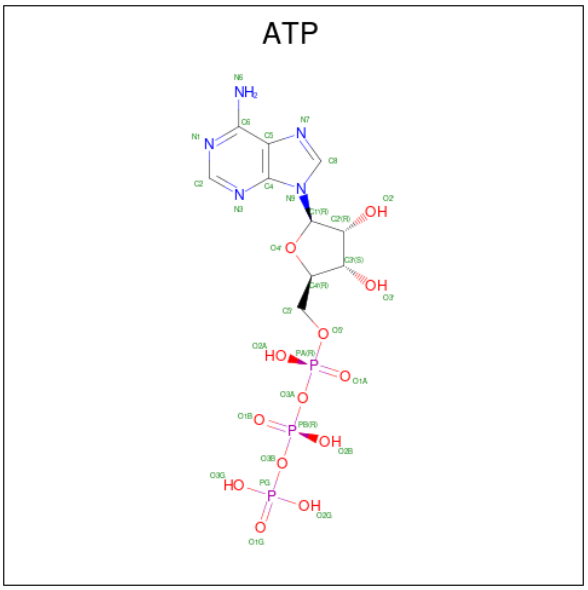


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	V		
2	A	1	32	10	5	14	2	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

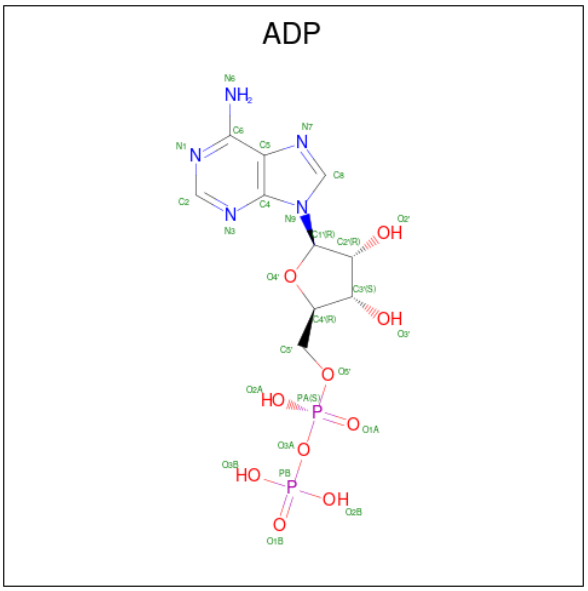
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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



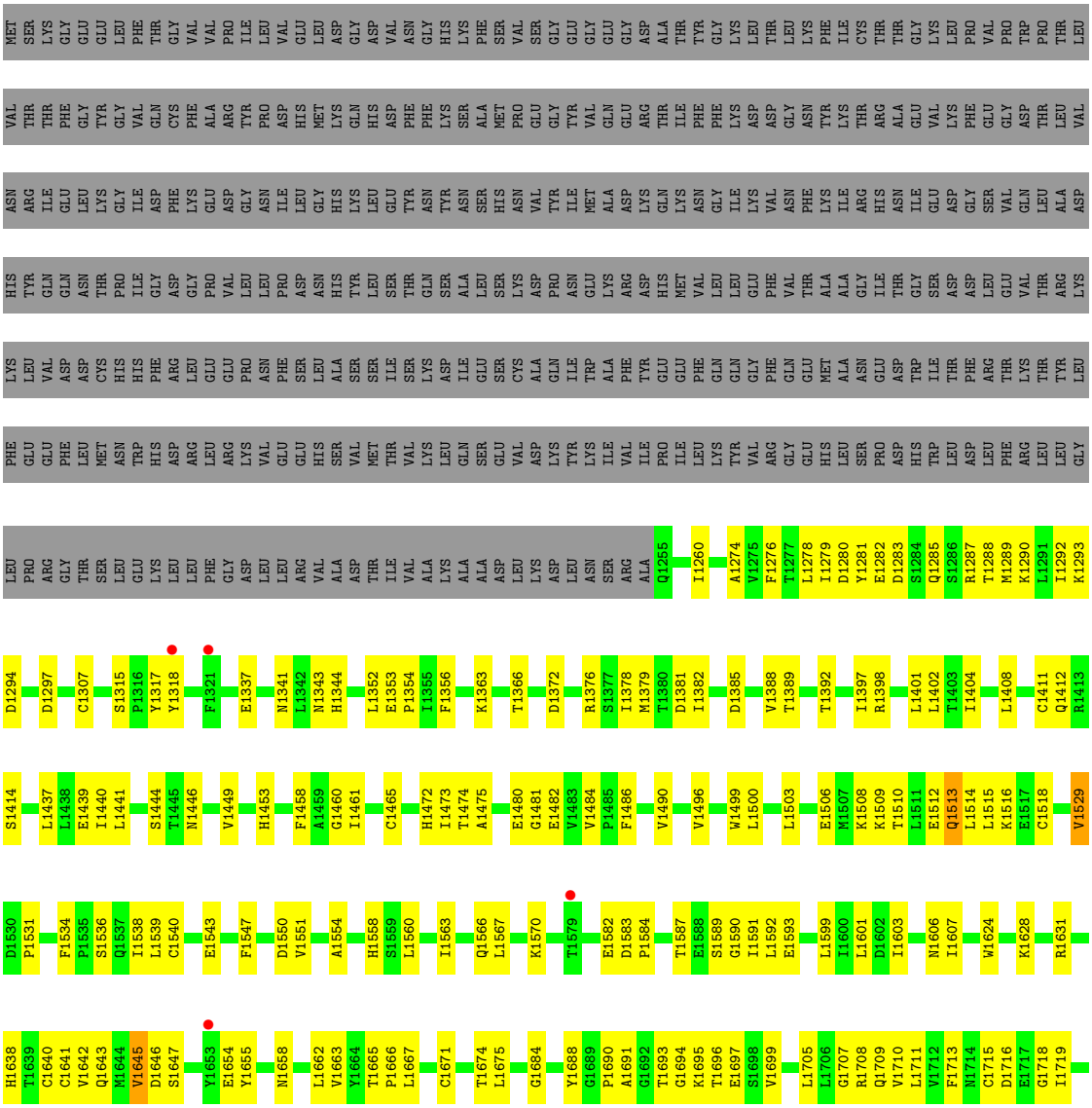
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

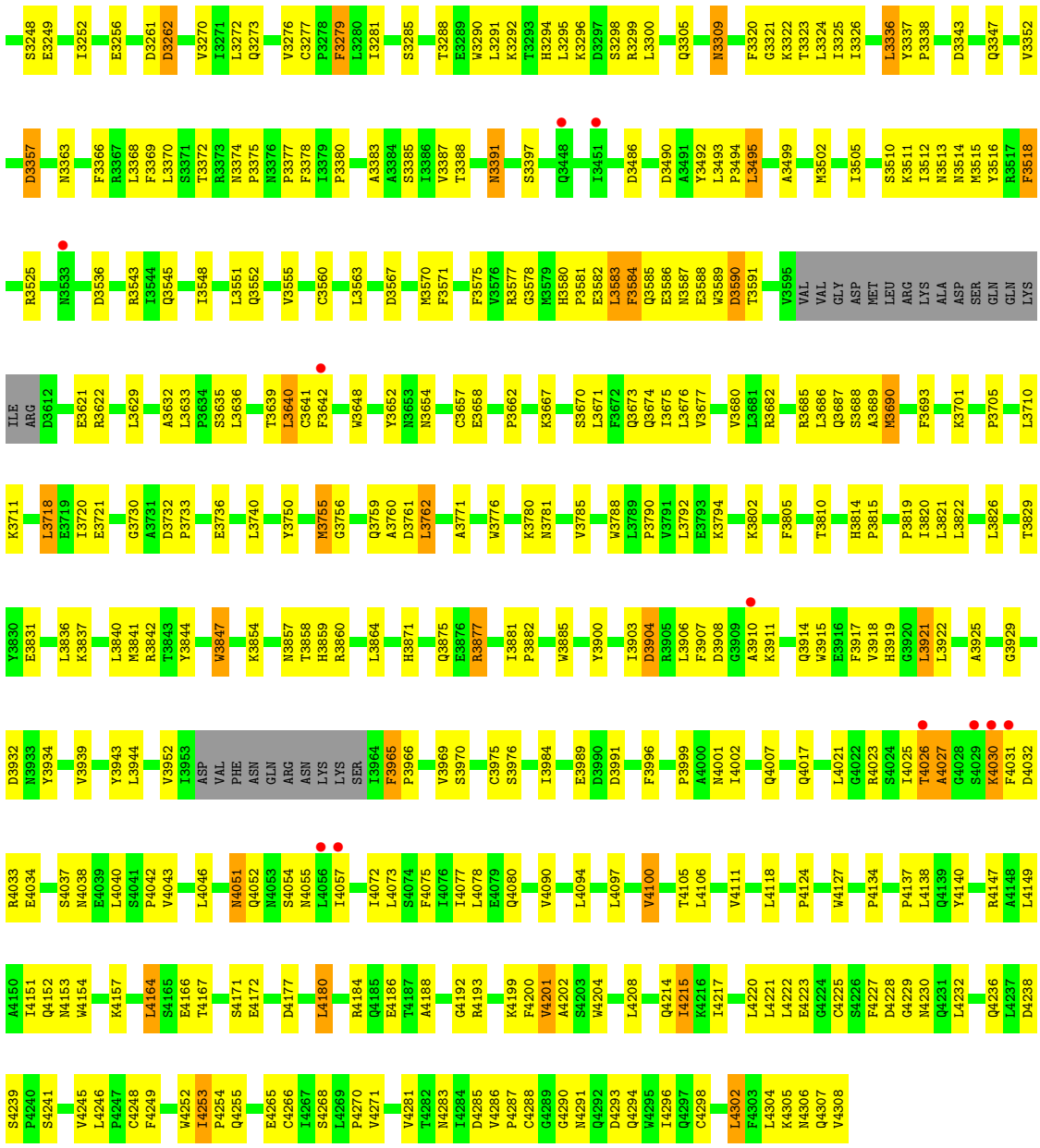
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Green fluorescent protein/Cytoplasmic dynein 2 heavy chain 1

Chain A:



S3136 V3137 G3138 Q3139 K3140 V3141 S3142 E3143 L3144 K3145
M2943 Q2944 D2945 A2946 S2947 E2948 Q2949 K2950 T2951 E2952 L2953
LYS GLU GLU LYS LYS LYS ASN SER V2847 D2848 P2849 D2850 F2851 L2852
L2723 L2730 Y2739 L2744 E2745 P2746 L2749 P2750 V2764 F2765 N2766 Y2767 F2768 T2769 Y2770 M2782 D2783 K2802 C2803 Q2804 V2805 L2806 G2810 W2811 S2812 M2816 I2819 P2820 E2821 M2822 L2823 E2826 THR GLY GLY GLY GLU LYS TYR ASN ASP LYS LYS ARG
L2625 D2626 I2627 L2628 L2629 E2632 V2633 L2634 E2635 R2639 R2642 V2643 L2644 S2645 S2650 L2651 L2652 L2653 R2656 S2657 G2658 V2659 G2660 R2661 R2662 T2663 I2664 T2665 V2668 L2676 R2683 G2684 Y2685 Q2689 F2690 Q2699 E2704 A2705 Q2706 Q2707 L2711 L2712 F2717 V2718 H2719 P2720
A2531 R2532 R2533 L2534 F2535 R2536 E2544 L2545 F2548 D2549 I2550 I2551 L2552 T2553 Q2557 W2560 I2564 L2565 D2566 D2570 Y2573 V2574 T2575 W2576 G2577 A2578 R2579 H2580 G2583 ALA ARG ALA A2587 Q2590 P2591 L2592 P2593 P2594 H2595 G2596 K2597 K2601 L2602 D2606 L2607 V2527 V2610 L2615
S2429 I2430 D2431 Y2432 R2435 I2441 Y2442 G2443 A2444 Y2445 L2446 E2447 P2448 V2449 L2450 N2453 I2459 W2460 G2461 S2462 K2465 L2468 L2469 M2473 V2486 T2495 P2496 C2497 I2498 W2502 V2503 L2504 D2510 L2511 E2512 N2517 H2518 P2519 L2520 D2521 Y2522 V2523 L2524 V2527 A2528 Y2529 E2530
Y2346 R2347 P2348 C2351 E2352 R2353 L2354 V2355 L2356 Y2357 L2358 K2359 D2360 I2361 N2362 L2363 P2364 K2365 L2366 D2367 V2375 L2378 L2382 T2383 Y2384 D2389 E2390 N2391 L2392 E2393 G2396 L2397 E2398 N2399 I2400 Q2401 I2402 M2406 R2411 R2414 H2415 K2416 R2420 F2421 I2424 V2425 R2426 L2427 C2428
D2248 L2249 D2253 F2254 S2255 N2256 G2257 L2258 P2261 V2262 I2263 Q2264 T2265 P2266 D2267 M2268 Q2269 R2270 Y2274 F2275 K2276 P2277 K2284 F2287 I2288 P2292 E2293 G2294 C2295 G2296 K2297 L2301 Q2307 S2310 T2311 Q2312 C2318 S2319 A2320 Q2321 T2322 L2327 L2328 C2335 I2338 V2345
V2163 V2164 E2165 T2166 S2167 L2168 V2169 G2170 T2171 V2172 M2173 N2174 G2175 H2178 H2185 D2186 E2187 F2188 I2189 I2190 N2191 L2192 I2193 L2196 N2199 L2200 N2201 R2205 F2208 T2209 V2212 F2213 H2214 W2215 A2216 S2219 F2223 H2224 Y2230 R2235 G2236 R2237 L2238 A2239 T2240 Y2241 V2242 E2247
S2049 S2050 W2051 I2052 D2055 E2064 S2065 L2066 N2067 L2070 D2071 D2072 N2073 R2074 L2075 L2076 T2077 M2078 P2079 E2082 R2083 F2092 E2095 A2105 R2109 M2112 I2113 F2114 L2115 S2116 L2130 R2131 N2132 Q2133 P2134 A2135 E2136 Y2137 R2138 E2142 A2152 L2153 Q2154 W2155 V2156 L2157 Y2162
L1939 L1943 K1944 I1955 P1956 A1962 L1963 E1964 L1965 M1973 I1977 P1980 S1981 G1982 A1983 S1986 T1987 L1988 W1989 R1993 A1994 A1995 L1996 C1997 K1998 T1999 G2000 K2001 V2002 V2003 K2004 Q2005 Y2006 T2007 K2011 L2019 W2029 S2030 D2031 T2035 A2038 V2041 P2045 V2048
H1819 P1820 D1821 N1822 E1823 L1824 I1825 V1828 I1829 S1832 F1835 F1849 L1855 Q1859 Q1860 H1861 Y1862 D1863 W1864 G1865 L1866 R1867 A1868 L1869 L1879 Q1882 E1894 S1895 H1896 I1897 Q1900 A1901 L1902 T1906 M1907 S1908 K1909 F1910 C1915 F1918 V1925 F1926 I1929 E1938
S1723 F1728 V1729 G1730 L1731 V1732 W1737 G1738 C1739 F1740 D1741 E1742 F1743 N1744 R1745 L1746 E1747 E1748 S1749 V1750 L1751 S1752 I1758 V1781 N1784 I1787 F1788 I1789 T1790 M1791 N1792 G1795 K1796 G1797 Y1798 G1799 G1800 R1801 Q1802 K1803 L1804 P1805 D1806 Q1810 L1811 F1812 R1813 P1814 V1815 A1816 M1817 S1818


S3248 E3249 I3252 E3256 D3261 D3262 V3270 I3271 L3272 Q3273 V3276 C3277 P3278 F3279 L3280 I3281 S3285 T3288 E3289 W3290 L3291 K3292 T3293 H3294 L3295 K3296 D3297 S3298 R3299 L3300 Q3305 N3309 F3320 G3321 K3322 T3323 L3324 I3325 I3326 L3336 Y3337 P3338 D3343 Q3347 V3352
D3357 N3363 F3366 R3367 L3368 F3369 L3370 S3371 T3372 R3373 N3374 P3375 N3376 P3377 F3378 I3379 P3380 A3383 A3384 S3385 I3386 V3387 T3388 N3391 S3397 Q3448 I3451 D3486 D3490 A3491 Y3492 L3493 P3494 L3495 A3499 M3502 I3505 S3510 K3511 I3512 N3513 N3514 M3515 Y3516 R3517 F3518
R3525 N3533 D3536 R3543 I3544 Q3545 I3548 L3551 Q3552 V3555 C3560 L3563 D3567 M3570 F3571 F3575 V3576 R3577 G3578 M3579 H3580 P3581 E3582 L3583 F3584 Q3585 E3586 N3587 E3588 W3589 D3590 T3591 V3595 VAL VAL GLY ASP MET LEU ARG LYS ALA ASP SER GLN GLN LYS
ILE ARG D3612 E3621 R3622 L3629 A3632 L3633 P3634 S3635 L3636 T3639 L3640 C3641 F3642 W3648 Y3652 N3653 N3654 C3657 E3658 P3662 K3667 S3670 L3671 F3672 Q3673 Q3674 I3675 L3676 V3677 V3680 L3681 R3682 R3685 L3686 Q3687 S3688 A3689 M3690 F3693 K3701 P3705 L3710
K3711 L3718 E3719 I3720 E3721 G3730 A3731 D3732 P3733 E3736 L3740 Y3750 M3755 G3756 Q3759 A3760 D3761 L3762 A3771 W3776 K3780 N3781 V3785 W3788 L3789 P3790 V3791 L3792 E3793 K3794 K3802 F3805 T3810 H3814 P3815 P3819 I3820 L3821 L3822 L3826 T3829
Y3830 E3831 L3836 K3837 L3840 M3841 R3842 T3843 Y3844 W3847 K3854 N3857 T3858 H3859 R3860 L3864 H3871 Q3875 E3876 R3877 I3881 P3882 W3885 Y3900 I3903 D3904 R3905 L3906 F3907 D3908 G3909 A3910 K3911 Q3914 W3915 E3916 F3917 V3918 H3919 G3920 L3921 L3922 A3925 G3929
D3932 N3933 Y3934 V3939 Y3943 L3944 V3952 I3953 ASP VAL PHE ASN GLN ARG ASN LYS LYS SER I3964 F3965 P3966 V3969 S3970 C3975 S3976 I3984 E3989 D3990 D3991 F3996 P3999 A4000 N4001 I4002 Q4007 Q4017 L4021 G4022 R4023 S4024 I4025 T4026 A4027 G4028 S4029 K4030 F4031 D4032
R4033 E4034 S4037 N4038 E4039 L4040 S4041 P4042 V4043 L4046 N4051 Q4052 N4053 S4054 N4055 L4056 I4057 I4072 L4073 S4074 F4075 I4076 I4077 L4078 E4079 Q4080 V4090 L4094 L4097 V4100 T4105 L4106 V4111 L4118 P4124 W4127 P4134 P4137 L4138 Q4139 Y4140 R4147 A4148 L4149
A4150 I4151 Q4152 N4153 W4154 K4157 L4164 S4165 E4166 T4167 S4171 E4172 D4177 L4180 R4184 Q4185 E4186 T4187 A4188 G4192 R4193 K4199 F4200 V4201 A4202 S4203 W4204 L4208 Q4214 I4215 K4216 I4217 L4220 L4221 L4222 E4223 G4224 C4225 S4226 F4227 D4228 G4229 N4230 Q4231 L4232 Q4236 L4237 D4238
S4239 P4240 S4241 V4245 L4246 P4247 C4248 F4249 W4252 I4253 P4254 Q4255 E4265 C4266 I4267 S4268 L4269 P4270 V4271 V4281 T4282 N4283 I4284 D4285 V4286 P4287 C4288 G4289 G4290 N4291 Q4292 D4293 Q4294 W4295 I4296 Q4297 C4298 L4302 F4303 L4304 K4305 N4306 Q4307 V4308

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	136.03Å 487.15Å 276.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.60 – 3.41 56.54 – 3.41	Depositor EDS
% Data completeness (in resolution range)	62.2 (56.60-3.41) 62.2 (56.54-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.237 , 0.285 0.239 , 0.284	Depositor DCC
R_{free} test set	3915 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	108.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 110.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22816	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, AOV, 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	0.61	2/23147 (0.0%)	0.78	5/31474 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2275	PHE	CB-CG	-5.18	1.42	1.51
1	A	2826	GLU	CD-OE2	5.06	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2426	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	2275	PHE	CB-CA-C	-5.82	98.76	110.40
1	A	1915	CYS	CA-CB-SG	5.68	124.22	114.00
1	A	4253	ILE	CB-CA-C	-5.50	100.59	111.60
1	A	2426	ARG	NE-CZ-NH2	5.42	123.01	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2238	LEU	Peptide
1	A	2247	GLU	Peptide
1	A	2275	PHE	Peptide
1	A	2310	SER	Peptide
1	A	2416	LYS	Peptide
1	A	2659	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22697	0	21503	995	0
2	A	32	0	12	12	0
3	A	2	0	0	0	0
4	A	31	0	12	4	0
5	A	54	0	24	10	0
All	All	22816	0	21551	996	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 22.

All (996) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3581:PRO:HA	1:A:3584:PHE:CE1	1.16	1.63
1:A:2284:LYS:CE	1:A:2401:GLN:HG3	1.33	1.55
1:A:2284:LYS:HE3	1:A:2401:GLN:CG	1.49	1.40
1:A:3291:LEU:O	1:A:3294:HIS:CE1	1.75	1.39
1:A:3581:PRO:CA	1:A:3584:PHE:CE1	2.04	1.38
1:A:2284:LYS:CD	1:A:2353:ARG:HH22	1.37	1.37
1:A:2659:VAL:CG2	1:A:2811:TRP:HE1	1.45	1.30
1:A:2847:VAL:CG1	1:A:2849:PRO:HD2	1.61	1.30
1:A:3291:LEU:O	1:A:3294:HIS:ND1	1.63	1.29
1:A:2284:LYS:HD2	1:A:2353:ARG:NH2	1.47	1.27
1:A:2473:MET:HE2	1:A:2502:TRP:CD2	1.70	1.26
1:A:3238:PHE:HZ	1:A:3243:PHE:CD1	1.51	1.25
1:A:4030:LYS:HG3	1:A:4034:GLU:OE1	1.34	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2660:GLY:HA3	5:A:4406:ADP:O1A	1.34	1.21
1:A:2592:LEU:HD21	1:A:2707:GLN:OE1	1.37	1.19
1:A:4054:SER:HB3	1:A:4057:ILE:CD1	1.71	1.19
1:A:2284:LYS:HG3	1:A:2401:GLN:OE1	1.38	1.18
1:A:3238:PHE:CZ	1:A:3243:PHE:CD1	2.32	1.18
1:A:4054:SER:CB	1:A:4057:ILE:HD12	1.73	1.17
1:A:1690:PRO:HA	1:A:1798:TYR:OH	1.47	1.15
1:A:2004:LYS:HG3	1:A:2006:TYR:CE1	1.82	1.14
1:A:2659:VAL:CB	1:A:2811:TRP:HE1	1.61	1.13
1:A:2131:ARG:HA	1:A:2138:ARG:NH2	1.66	1.11
1:A:4100:VAL:HG12	1:A:4105:THR:HG21	1.31	1.10
1:A:4100:VAL:HG12	1:A:4105:THR:CG2	1.83	1.08
1:A:2473:MET:CE	1:A:2502:TRP:CE2	2.14	1.08
1:A:2847:VAL:HG12	1:A:2849:PRO:CD	1.83	1.08
1:A:4171:SER:HB2	1:A:4308:VAL:O	1.54	1.08
1:A:2661:ARG:O	1:A:2665:THR:HG23	1.55	1.06
1:A:3581:PRO:HA	1:A:3584:PHE:CZ	1.89	1.06
1:A:4100:VAL:HA	1:A:4105:THR:HG22	1.36	1.06
1:A:1867:ARG:NH1	2:A:4401:AOV:O3B	1.89	1.05
1:A:3580:HIS:O	1:A:3584:PHE:CZ	2.08	1.05
1:A:1716:ASP:CG	1:A:1745:ARG:NH2	2.10	1.05
1:A:2659:VAL:CG2	1:A:2811:TRP:NE1	2.20	1.03
1:A:2607:LEU:HD23	1:A:2634:LEU:CD1	1.86	1.03
1:A:3291:LEU:HD12	1:A:3294:HIS:CE1	1.95	1.02
1:A:4100:VAL:HA	1:A:4105:THR:CG2	1.90	1.02
1:A:2607:LEU:CD2	1:A:2634:LEU:HD12	1.89	1.01
1:A:2607:LEU:HD23	1:A:2634:LEU:HD12	1.01	1.01
1:A:2653:LEU:HB3	1:A:2661:ARG:HG2	1.44	1.00
1:A:2473:MET:HE2	1:A:2502:TRP:CE2	1.47	0.98
1:A:2284:LYS:HE3	1:A:2401:GLN:CB	1.93	0.98
1:A:3581:PRO:CA	1:A:3584:PHE:HE1	1.56	0.97
1:A:2284:LYS:CE	1:A:2353:ARG:HH22	1.76	0.96
1:A:2811:TRP:HB2	1:A:2816:MET:CE	1.96	0.96
1:A:2359:LYS:O	1:A:2360:ASP:OD1	1.83	0.96
1:A:2284:LYS:CE	1:A:2401:GLN:CG	2.23	0.96
1:A:2847:VAL:HG12	1:A:2849:PRO:HD2	0.97	0.95
1:A:3511:LYS:NZ	1:A:4021:LEU:O	1.98	0.94
1:A:2284:LYS:HD2	1:A:2353:ARG:HH22	0.79	0.93
1:A:2659:VAL:HG23	1:A:2811:TRP:HE1	1.33	0.93
1:A:4054:SER:HB3	1:A:4057:ILE:HD12	0.94	0.92
1:A:1584:PRO:HB2	1:A:1587:THR:CG2	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4100:VAL:CG1	1:A:4105:THR:HG21	1.98	0.92
1:A:4171:SER:CB	1:A:4308:VAL:O	2.16	0.92
1:A:3581:PRO:CB	1:A:3584:PHE:HE1	1.82	0.92
1:A:1896:HIS:CD2	1:A:1929:ILE:HG23	2.05	0.92
1:A:3238:PHE:HZ	1:A:3243:PHE:HD1	0.98	0.91
1:A:1716:ASP:OD2	1:A:1745:ARG:NH2	2.03	0.91
1:A:2847:VAL:CG1	1:A:2849:PRO:CD	2.42	0.91
1:A:2659:VAL:HB	1:A:2811:TRP:HE1	1.33	0.91
1:A:2284:LYS:CD	1:A:2401:GLN:HG3	2.01	0.90
1:A:1662:LEU:HD11	1:A:1697:GLU:HB3	1.54	0.90
1:A:2284:LYS:HE2	1:A:2401:GLN:HG3	1.51	0.90
1:A:1584:PRO:HB2	1:A:1587:THR:HG22	1.55	0.89
1:A:4057:ILE:HD13	1:A:4149:LEU:HD23	1.54	0.89
1:A:3581:PRO:HA	1:A:3584:PHE:HE1	1.08	0.88
1:A:1674:THR:HG22	1:A:3925:ALA:HA	1.54	0.88
1:A:3291:LEU:C	1:A:3294:HIS:CE1	2.46	0.88
1:A:1716:ASP:OD1	1:A:1745:ARG:NH2	2.06	0.88
1:A:2004:LYS:CG	1:A:2006:TYR:CE1	2.56	0.88
1:A:2659:VAL:HB	1:A:2811:TRP:NE1	1.88	0.88
1:A:1796:LYS:HD3	1:A:1797:GLY:N	1.88	0.87
1:A:1690:PRO:CA	1:A:1798:TYR:OH	2.22	0.87
1:A:2284:LYS:CD	1:A:2353:ARG:NH2	2.19	0.87
1:A:2284:LYS:HE3	1:A:2401:GLN:HG3	0.88	0.87
1:A:2660:GLY:CA	5:A:4406:ADP:O1A	2.22	0.87
1:A:3377:PRO:CB	1:A:3378:PHE:HB2	2.05	0.86
1:A:4100:VAL:CA	1:A:4105:THR:CG2	2.53	0.86
1:A:4030:LYS:HB2	1:A:4034:GLU:HG3	1.57	0.85
1:A:2284:LYS:CE	1:A:2353:ARG:NH2	2.36	0.85
1:A:2660:GLY:O	1:A:2664:ILE:HD13	1.76	0.85
1:A:2284:LYS:HG3	1:A:2401:GLN:CD	1.97	0.84
1:A:2592:LEU:CD2	1:A:2707:GLN:OE1	2.24	0.84
1:A:2510:ASP:O	1:A:2522:TYR:OH	1.96	0.83
1:A:4171:SER:C	1:A:4308:VAL:O	2.16	0.83
1:A:2659:VAL:HG23	1:A:2811:TRP:NE1	1.87	0.83
1:A:2284:LYS:HD2	1:A:2353:ARG:CZ	2.07	0.83
1:A:1716:ASP:OD1	1:A:1745:ARG:CZ	2.27	0.82
1:A:2004:LYS:HG3	1:A:2006:TYR:HE1	1.41	0.82
1:A:2811:TRP:HB2	1:A:2816:MET:HE2	1.61	0.82
1:A:4057:ILE:HD13	1:A:4149:LEU:CD2	2.09	0.82
1:A:2658:GLY:HA3	1:A:2870:SER:HB3	1.62	0.81
1:A:3291:LEU:HA	1:A:3294:HIS:CE1	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2055:ASP:OD1	1:A:2420:ARG:NH2	2.14	0.81
1:A:1716:ASP:OD2	1:A:2065:SER:HA	1.80	0.81
1:A:4171:SER:CB	1:A:4305:LYS:CB	2.59	0.80
1:A:1554:ALA:HA	1:A:1560:LEU:HD12	1.63	0.80
1:A:2288:ILE:HD11	1:A:2425:VAL:HG21	1.63	0.80
1:A:3238:PHE:CZ	1:A:3243:PHE:HD1	1.85	0.80
1:A:4171:SER:HB3	1:A:4305:LYS:CB	2.12	0.80
1:A:4057:ILE:CD1	1:A:4149:LEU:CD2	2.60	0.80
1:A:3291:LEU:HD12	1:A:3294:HIS:HE1	1.46	0.79
1:A:2575:THR:HG21	1:A:2645:SER:OG	1.80	0.79
1:A:3857:ASN:HB2	1:A:3975:CYS:SG	2.21	0.79
1:A:1715:CYS:SG	1:A:1743:PHE:HA	2.22	0.79
1:A:4100:VAL:CG1	1:A:4105:THR:CG2	2.57	0.79
1:A:3377:PRO:HB2	1:A:3378:PHE:HB2	1.65	0.78
1:A:3640:LEU:HG	1:A:3642:PHE:CE2	2.18	0.78
1:A:2263:ILE:HD13	1:A:2441:ILE:HA	1.65	0.78
1:A:3640:LEU:HG	1:A:3642:PHE:CZ	2.20	0.77
1:A:3581:PRO:HA	1:A:3584:PHE:CD1	2.11	0.77
1:A:1513:GLN:HG3	1:A:1514:LEU:N	2.00	0.76
1:A:2847:VAL:HG13	1:A:2849:PRO:HD2	1.66	0.76
1:A:2658:GLY:HA3	1:A:2870:SER:CB	2.16	0.76
1:A:3291:LEU:C	1:A:3294:HIS:ND1	2.40	0.76
1:A:3512:ILE:HG23	1:A:4021:LEU:CD2	2.16	0.76
1:A:4171:SER:CA	1:A:4308:VAL:O	2.33	0.76
1:A:4304:LEU:HD12	1:A:4305:LYS:N	2.00	0.76
1:A:4030:LYS:CG	1:A:4034:GLU:OE1	2.28	0.75
1:A:2811:TRP:HB2	1:A:2816:MET:HE3	1.66	0.75
1:A:2821:GLU:HB2	1:A:2852:LEU:HD13	1.68	0.75
1:A:3291:LEU:CA	1:A:3294:HIS:CE1	2.70	0.75
1:A:2473:MET:HE2	1:A:2502:TRP:CE3	1.91	0.74
1:A:3760:ALA:HA	1:A:3788:TRP:CH2	2.22	0.74
1:A:2810:GLY:O	1:A:2811:TRP:HD1	1.70	0.74
1:A:4208:LEU:O	1:A:4214:GLN:NE2	2.20	0.74
1:A:2685:TYR:HB2	1:A:2718:VAL:HG21	1.68	0.73
1:A:2135:ALA:HA	1:A:2138:ARG:CB	1.71	0.73
1:A:4057:ILE:CD1	1:A:4152:GLN:HE22	2.01	0.73
1:A:1583:ASP:N	1:A:1584:PRO:HD2	2.02	0.73
1:A:1696:THR:OG1	2:A:4401:AOV:O2B	2.05	0.73
1:A:2659:VAL:CB	1:A:2811:TRP:NE1	2.41	0.73
1:A:1896:HIS:HA	1:A:1929:ILE:HD13	1.69	0.73
1:A:2205:ARG:NH2	1:A:2429:SER:OG	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2653:LEU:CB	1:A:2661:ARG:HG2	2.17	0.72
1:A:3587:ASN:OD1	1:A:3590:ASP:OD2	2.07	0.72
1:A:1752:SER:OG	1:A:3755:MET:O	2.06	0.72
1:A:1283:ASP:HB3	1:A:1353:GLU:OE2	1.89	0.72
1:A:1693:THR:HG23	1:A:1817:MET:O	1.89	0.72
1:A:1460:GLY:HA3	1:A:1655:TYR:HD2	1.54	0.72
1:A:2135:ALA:N	1:A:2138:ARG:HG3	1.73	0.71
1:A:1801:ARG:NH1	1:A:2064:GLU:OE1	2.23	0.71
1:A:1279:ILE:HD12	1:A:1293:LYS:HG3	1.71	0.71
1:A:1514:LEU:CD1	1:A:1534:PHE:CE1	2.74	0.71
1:A:1690:PRO:HD2	1:A:1818:SER:HA	1.72	0.71
1:A:2661:ARG:O	1:A:2665:THR:CG2	2.37	0.71
1:A:3642:PHE:HA	1:A:3648:TRP:NE1	2.06	0.70
1:A:3881:ILE:HG23	1:A:3882:PRO:HA	1.72	0.70
1:A:3512:ILE:HD12	1:A:3513:ASN:HB2	1.72	0.70
1:A:4100:VAL:HG12	1:A:4105:THR:HG23	1.72	0.70
1:A:2607:LEU:CD2	1:A:2634:LEU:CD1	2.61	0.70
1:A:3966:PRO:HB2	1:A:3969:VAL:HG12	1.73	0.70
1:A:2004:LYS:CG	1:A:2006:TYR:HE1	2.00	0.70
1:A:2658:GLY:CA	1:A:2870:SER:HB3	2.21	0.70
1:A:4100:VAL:CB	1:A:4105:THR:CG2	2.70	0.70
1:A:2135:ALA:HA	1:A:2138:ARG:HB2	1.72	0.69
1:A:1587:THR:OG1	1:A:1590:GLY:HA3	1.93	0.69
1:A:3847:TRP:HH2	1:A:3900:TYR:HB2	1.56	0.69
1:A:4097:LEU:HD13	1:A:4111:VAL:CG1	2.23	0.69
1:A:2867:ALA:HA	1:A:2871:GLN:OE1	1.93	0.69
1:A:1900:GLN:N	1:A:1900:GLN:OE1	2.22	0.68
1:A:4236:GLN:O	1:A:4239:SER:OG	2.10	0.68
1:A:3291:LEU:C	1:A:3294:HIS:HD1	1.95	0.68
1:A:2274:TYR:CE2	1:A:2428:CYS:HB3	2.28	0.68
1:A:2284:LYS:CG	1:A:2401:GLN:HG3	2.22	0.68
1:A:4057:ILE:HD11	1:A:4152:GLN:HE22	1.57	0.68
1:A:1397:ILE:HD12	1:A:1398:ARG:N	2.09	0.67
1:A:1665:THR:OG1	1:A:1666:PRO:HD2	1.94	0.67
1:A:2719:HIS:ND1	1:A:2720:PRO:HD2	2.09	0.67
1:A:1752:SER:CB	1:A:3755:MET:O	2.43	0.67
1:A:4046:LEU:HD11	1:A:4138:LEU:HD13	1.77	0.67
1:A:4222:LEU:HD23	1:A:4223:GLU:N	2.09	0.67
1:A:1540:CYS:SG	1:A:1599:LEU:HD12	2.35	0.67
1:A:3837:LYS:HB2	1:A:3984:ILE:HG23	1.75	0.67
1:A:3877:ARG:CZ	1:A:3943:TYR:OH	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2131:ARG:HA	1:A:2138:ARG:CZ	2.24	0.67
1:A:1514:LEU:HD12	1:A:1534:PHE:HE1	1.58	0.67
1:A:2390:GLU:O	1:A:2391:ASN:CB	2.43	0.67
1:A:1514:LEU:HD12	1:A:1534:PHE:CE1	2.30	0.66
1:A:2473:MET:HE1	1:A:2502:TRP:CE2	2.12	0.66
1:A:3099:TYR:O	1:A:3103:LEU:N	2.29	0.66
1:A:4154:TRP:NE1	1:A:4172:GLU:OE2	2.28	0.66
1:A:3814:HIS:ND1	1:A:3815:PRO:O	2.21	0.66
1:A:2450:LEU:HD11	1:A:2460:TRP:HB3	1.78	0.66
1:A:2242:VAL:O	1:A:2269:GLN:NE2	2.28	0.66
1:A:2284:LYS:HG3	1:A:2401:GLN:CG	2.25	0.66
1:A:2265:THR:HB	1:A:2266:PRO:CD	2.26	0.66
1:A:2518:HIS:N	1:A:2519:PRO:HA	2.10	0.66
1:A:4171:SER:O	1:A:4308:VAL:O	2.13	0.66
1:A:2109:ARG:NH2	2:A:4401:AOV:O3G	2.28	0.66
1:A:2295:CYS:SG	1:A:2430:ILE:HG13	2.35	0.66
1:A:1624:TRP:CD2	1:A:3917:PHE:HB3	2.31	0.66
1:A:3847:TRP:HH2	1:A:3900:TYR:CB	2.09	0.66
1:A:4051:ASN:OD1	1:A:4051:ASN:N	2.29	0.66
1:A:1662:LEU:HD11	1:A:1697:GLU:CB	2.25	0.65
1:A:2135:ALA:H	1:A:2138:ARG:HG3	1.56	0.65
1:A:3374:ASN:ND2	1:A:3377:PRO:HD2	2.10	0.65
1:A:2212:VAL:HA	1:A:2215:TRP:HE3	1.62	0.65
1:A:4030:LYS:HB2	1:A:4034:GLU:CG	2.25	0.65
1:A:4215:ILE:HB	1:A:4217:ILE:HD11	1.77	0.65
1:A:2816:MET:HB2	1:A:2856:LEU:HD21	1.78	0.65
1:A:2292:PRO:O	1:A:2295:CYS:HB2	1.96	0.65
1:A:4307:GLN:HG3	1:A:4307:GLN:O	1.97	0.65
1:A:2131:ARG:CA	1:A:2138:ARG:NH2	2.52	0.65
1:A:1693:THR:CG2	1:A:1817:MET:O	2.44	0.65
1:A:2004:LYS:HE3	1:A:2006:TYR:CZ	2.32	0.65
1:A:4057:ILE:CD1	1:A:4149:LEU:HD22	2.27	0.65
1:A:2168:LEU:O	1:A:2169:VAL:C	2.34	0.65
1:A:2354:LEU:HD23	1:A:2355:VAL:N	2.12	0.65
1:A:1696:THR:OG1	1:A:1741:ASP:OD1	2.15	0.64
1:A:2362:ASN:HD21	1:A:2406:MET:HB2	1.62	0.64
1:A:1584:PRO:HB2	1:A:1587:THR:HG21	1.77	0.64
1:A:2651:LEU:HD23	1:A:2653:LEU:HD21	1.78	0.64
1:A:2135:ALA:N	1:A:2138:ARG:CG	2.38	0.64
1:A:2442:TYR:O	1:A:2446:LEU:HB2	1.97	0.64
1:A:2473:MET:CE	1:A:2502:TRP:CD2	2.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2656:ARG:NH1	1:A:2783:ASP:OD1	2.31	0.64
1:A:1938:GLU:N	1:A:1938:GLU:OE2	2.31	0.64
1:A:2653:LEU:HB3	1:A:2661:ARG:CG	2.25	0.63
1:A:3273:GLN:OE1	1:A:3276:VAL:N	2.31	0.63
1:A:4025:ILE:HD12	1:A:4025:ILE:N	2.14	0.63
1:A:1482:GLU:OE1	1:A:1658:ASN:ND2	2.32	0.63
1:A:3871:HIS:NE2	1:A:3875:GLN:OE1	2.32	0.63
1:A:1752:SER:HB3	1:A:3755:MET:O	1.99	0.63
1:A:3762:LEU:C	1:A:3762:LEU:HD12	2.18	0.63
1:A:2261:PRO:O	1:A:2445:TYR:OH	2.08	0.62
1:A:1279:ILE:HD12	1:A:1293:LYS:CG	2.28	0.62
1:A:1499:TRP:CZ3	1:A:1503:LEU:HD11	2.34	0.62
1:A:2264:GLN:HA	1:A:2268:MET:HG3	1.80	0.62
1:A:4220:LEU:HB2	1:A:4245:VAL:HG13	1.80	0.62
1:A:3080:LYS:CB	1:A:3087:ALA:HB2	2.30	0.62
1:A:3374:ASN:HB2	1:A:3820:ILE:HD11	1.82	0.62
1:A:1715:CYS:O	1:A:1716:ASP:OD1	2.18	0.62
1:A:3836:LEU:HD23	1:A:3991:ASP:CB	2.30	0.62
1:A:4052:GLN:HA	1:A:4055:ASN:OD1	1.98	0.62
1:A:2660:GLY:HA3	5:A:4406:ADP:PA	2.38	0.62
1:A:2664:ILE:HD12	1:A:2664:ILE:N	2.14	0.62
1:A:2699:GLN:NE2	1:A:2704:GLU:OE1	2.33	0.62
1:A:3511:LYS:CE	1:A:4021:LEU:O	2.48	0.61
1:A:2375:VAL:HA	1:A:2378:LEU:HD12	1.82	0.61
1:A:1472:HIS:ND1	1:A:1490:VAL:O	2.33	0.61
1:A:2239:ALA:O	1:A:2240:THR:HG23	2.00	0.61
1:A:1645:VAL:HG12	1:A:1646:ASP:H	1.66	0.61
1:A:2597:LYS:HB2	1:A:2645:SER:HB3	1.82	0.61
1:A:4057:ILE:HG23	1:A:4152:GLN:OE1	2.01	0.61
1:A:4281:VAL:HG21	1:A:4304:LEU:HD23	1.81	0.61
1:A:2335:CYS:HG	1:A:2347:ARG:C	2.04	0.61
1:A:3238:PHE:CZ	1:A:3243:PHE:CG	2.86	0.61
1:A:3755:MET:HG3	1:A:3785:VAL:HG21	1.83	0.61
1:A:1509:LYS:NZ	1:A:1512:GLU:OE1	2.34	0.61
1:A:3238:PHE:CZ	1:A:3243:PHE:HB2	2.36	0.61
1:A:3377:PRO:HB2	1:A:3378:PHE:CB	2.29	0.61
1:A:4030:LYS:HG3	1:A:4034:GLU:CD	2.16	0.61
1:A:2517:ASN:CB	1:A:2519:PRO:HB3	2.31	0.60
1:A:4265:GLU:O	1:A:4288:CYS:CB	2.49	0.60
1:A:2265:THR:HB	1:A:2266:PRO:HD2	1.83	0.60
1:A:2517:ASN:HB3	1:A:2519:PRO:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3374:ASN:HD22	1:A:3377:PRO:HD2	1.66	0.60
1:A:3904:ASP:O	1:A:3908:ASP:N	2.34	0.60
1:A:2284:LYS:CG	1:A:2401:GLN:CG	2.79	0.60
1:A:2288:ILE:HD11	1:A:2425:VAL:CG2	2.32	0.60
1:A:3292:LYS:O	1:A:3295:LEU:HB2	2.01	0.60
1:A:2284:LYS:NZ	1:A:2353:ARG:NH2	2.49	0.60
1:A:1795:GLY:HA3	1:A:1798:TYR:HD1	1.66	0.60
1:A:4217:ILE:HD12	1:A:4217:ILE:N	2.17	0.60
1:A:1583:ASP:N	1:A:1584:PRO:CD	2.64	0.60
1:A:2816:MET:CB	1:A:2856:LEU:HD21	2.32	0.59
1:A:1662:LEU:HB3	2:A:4401:AOV:C6	2.31	0.59
1:A:3837:LYS:O	1:A:3841:MET:N	2.30	0.59
1:A:2363:LEU:N	1:A:2364:PRO:HD2	2.17	0.59
1:A:2659:VAL:HG22	1:A:2659:VAL:O	2.01	0.59
1:A:3372:THR:HG22	1:A:3374:ASN:H	1.67	0.59
1:A:2548:PHE:HA	1:A:2551:ILE:HD12	1.84	0.59
1:A:3245:CYS:SG	1:A:3249:GLU:HB2	2.43	0.59
1:A:4100:VAL:CA	1:A:4105:THR:HG21	2.30	0.59
1:A:1943:LEU:HA	1:A:1995:ALA:HB2	1.85	0.59
1:A:2011:LYS:NZ	1:A:2367:ASP:OD2	2.33	0.59
1:A:2284:LYS:HD2	1:A:2353:ARG:NH1	2.17	0.59
1:A:4281:VAL:HG21	1:A:4304:LEU:CD2	2.32	0.59
1:A:2135:ALA:CA	1:A:2138:ARG:HB2	2.30	0.59
1:A:2353:ARG:HG2	1:A:2354:LEU:N	2.16	0.59
1:A:2847:VAL:CG1	1:A:2849:PRO:CG	2.80	0.59
1:A:1747:GLU:HB3	1:A:1750:VAL:HG23	1.84	0.59
1:A:3512:ILE:CG2	1:A:4021:LEU:CD2	2.80	0.59
1:A:3844:TYR:HA	1:A:3847:TRP:HB2	1.85	0.58
1:A:3585:GLN:O	1:A:3585:GLN:NE2	2.36	0.58
1:A:4306:ASN:O	1:A:4307:GLN:HB3	2.03	0.58
1:A:2335:CYS:SG	1:A:2347:ARG:O	2.58	0.58
1:A:1554:ALA:CA	1:A:1560:LEU:HD12	2.32	0.58
1:A:2357:TYR:C	1:A:2358:LEU:HD23	2.24	0.58
1:A:3711:LYS:HG2	1:A:3740:LEU:HD13	1.85	0.58
1:A:1973:MET:SD	1:A:2074:ARG:NH1	2.77	0.58
1:A:2162:TYR:HB2	1:A:2199:ASN:O	2.03	0.58
1:A:2185:HIS:CE1	1:A:2189:ILE:HD11	2.39	0.58
1:A:3591:THR:HG21	1:A:3632:ALA:HB1	1.85	0.58
1:A:1584:PRO:CB	1:A:1587:THR:HG22	2.31	0.58
1:A:3781:ASN:H	1:A:3810:THR:HB	1.67	0.58
1:A:1796:LYS:HD3	1:A:1797:GLY:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2544:GLU:OE1	1:A:2544:GLU:N	2.37	0.58
1:A:2676:LEU:O	1:A:2676:LEU:HD23	2.04	0.58
1:A:3877:ARG:NH1	1:A:3943:TYR:OH	2.37	0.58
1:A:1986:SER:OG	4:A:4403:ATP:O2B	2.16	0.57
1:A:1496:VAL:HA	1:A:1499:TRP:NE1	2.18	0.57
1:A:2625:LEU:HB3	1:A:2627:ILE:HD13	1.85	0.57
1:A:2858:ILE:O	1:A:2861:SER:OG	2.16	0.57
1:A:2366:LEU:HD11	1:A:2415:HIS:HB3	1.85	0.57
1:A:1437:LEU:CD2	1:A:1441:LEU:HD12	2.34	0.57
1:A:2462:SER:O	1:A:2465:LYS:N	2.37	0.57
1:A:3621:GLU:HG3	1:A:3622:ARG:N	2.19	0.57
1:A:3492:TYR:O	1:A:3495:LEU:HB3	2.05	0.57
1:A:2095:GLU:OE2	4:A:4403:ATP:O3G	2.23	0.57
1:A:3067:LEU:O	1:A:3071:LYS:N	2.38	0.57
1:A:1397:ILE:HD12	1:A:1398:ARG:H	1.69	0.57
1:A:1514:LEU:CD1	1:A:1534:PHE:HE1	2.16	0.57
1:A:2739:TYR:HB3	1:A:2744:LEU:HD21	1.87	0.57
1:A:3525:ARG:NH2	1:A:3721:GLU:OE1	2.38	0.57
1:A:1440:ILE:HD11	1:A:1453:HIS:CG	2.40	0.56
1:A:4220:LEU:HB3	1:A:4302:LEU:HD21	1.84	0.56
1:A:3921:LEU:HD23	1:A:3922:LEU:N	2.19	0.56
1:A:4054:SER:HB3	1:A:4057:ILE:CG1	2.34	0.56
1:A:1534:PHE:HB2	1:A:1539:LEU:HD11	1.86	0.56
1:A:2130:LEU:O	1:A:2138:ARG:NE	2.38	0.56
1:A:2643:VAL:HG11	1:A:2651:LEU:CD1	2.36	0.56
1:A:3245:CYS:SG	1:A:3249:GLU:CB	2.93	0.56
1:A:3640:LEU:HD12	1:A:3642:PHE:CE1	2.40	0.56
1:A:3642:PHE:HA	1:A:3648:TRP:CD1	2.40	0.56
1:A:1908:SER:N	1:A:1964:GLU:OE2	2.39	0.56
1:A:3291:LEU:O	1:A:3294:HIS:HE1	1.74	0.56
1:A:3864:LEU:HD23	1:A:3903:ILE:HD12	1.87	0.56
1:A:4164:LEU:HD13	1:A:4214:GLN:O	2.05	0.56
1:A:4204:TRP:CZ2	1:A:4248:CYS:SG	2.99	0.56
1:A:3249:GLU:N	1:A:3249:GLU:OE1	2.39	0.56
1:A:3577:ARG:O	1:A:3584:PHE:HZ	1.89	0.56
1:A:3580:HIS:O	1:A:3584:PHE:CE2	2.55	0.56
1:A:3591:THR:CG2	1:A:3632:ALA:HB1	2.36	0.56
1:A:1353:GLU:HB3	1:A:1354:PRO:HD3	1.87	0.56
1:A:2565:LEU:HG	1:A:2566:ASP:O	2.06	0.56
1:A:4100:VAL:CB	1:A:4105:THR:HG23	2.35	0.56
1:A:2382:LEU:HD21	1:A:2402:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2810:GLY:O	1:A:2811:TRP:CD1	2.58	0.55
1:A:1282:GLU:HA	1:A:1287:ARG:O	2.06	0.55
1:A:1813:ARG:HD3	1:A:1814:PRO:HD2	1.89	0.55
1:A:1824:LEU:O	1:A:1828:VAL:HG23	2.06	0.55
1:A:2402:ILE:HD12	1:A:2402:ILE:N	2.21	0.55
1:A:2664:ILE:O	1:A:2668:VAL:HG23	2.05	0.55
1:A:4220:LEU:O	1:A:4221:LEU:HD23	2.06	0.55
1:A:3581:PRO:HB3	1:A:3584:PHE:HE1	1.69	0.55
1:A:1260:ILE:HD12	1:A:1317:TYR:HB2	1.87	0.55
1:A:1667:LEU:HD22	1:A:1819:HIS:O	2.06	0.55
1:A:4137:PRO:O	1:A:4140:TYR:HB3	2.07	0.55
1:A:2536:ARG:HG2	1:A:2545:LEU:HD22	1.88	0.55
1:A:3239:ASP:O	1:A:3242:ARG:HG2	2.06	0.55
1:A:3570:MET:SD	1:A:4017:GLN:HB3	2.47	0.55
1:A:2767:TYR:CE2	1:A:2771:ARG:HD2	2.42	0.55
1:A:3294:HIS:CE1	1:A:3295:LEU:HG	2.42	0.55
1:A:1694:GLY:HA3	2:A:4401:AOV:H8	1.89	0.55
1:A:2592:LEU:HD22	1:A:2645:SER:O	2.05	0.55
1:A:1408:LEU:HA	1:A:1411:CYS:SG	2.46	0.55
1:A:1716:ASP:CG	1:A:1745:ARG:HH22	1.97	0.55
1:A:2348:PRO:HB3	1:A:2354:LEU:HB2	1.88	0.55
1:A:2390:GLU:O	1:A:2391:ASN:HB3	2.07	0.55
1:A:3718:LEU:HD13	1:A:3720:ILE:HB	1.89	0.55
1:A:1439:GLU:HB2	1:A:1440:ILE:HD12	1.87	0.55
1:A:1835:PHE:CE2	1:A:1894:GLU:HB3	2.42	0.55
1:A:2659:VAL:HG21	1:A:2811:TRP:NE1	2.20	0.55
1:A:3238:PHE:CE1	1:A:3243:PHE:HB2	2.41	0.55
1:A:1996:LEU:O	1:A:2000:GLY:N	2.36	0.54
1:A:2230:TYR:OH	1:A:2266:PRO:O	2.24	0.54
1:A:3991:ASP:N	1:A:3991:ASP:OD1	2.40	0.54
1:A:4051:ASN:O	1:A:4055:ASN:N	2.40	0.54
1:A:1925:VAL:HG23	1:A:1926:PHE:HD1	1.72	0.54
1:A:2167:SER:O	1:A:2168:LEU:C	2.43	0.54
1:A:1810:GLN:HG3	1:A:3732:ASP:HB2	1.90	0.54
1:A:3658:GLU:OE1	1:A:3658:GLU:N	2.41	0.54
1:A:3291:LEU:C	1:A:3294:HIS:HE1	2.08	0.54
1:A:1711:LEU:HD12	1:A:1731:LEU:HD21	1.89	0.54
1:A:3512:ILE:CG2	1:A:4021:LEU:HD21	2.38	0.54
1:A:2536:ARG:NH1	1:A:2549:ASP:OD2	2.41	0.54
1:A:4025:ILE:HG22	1:A:4027:ALA:N	2.24	0.54
1:A:1645:VAL:HG12	1:A:1646:ASP:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2134:PRO:O	1:A:2135:ALA:HB3	2.08	0.53
1:A:3854:LYS:O	1:A:3857:ASN:HB3	2.07	0.53
1:A:1663:VAL:CG2	1:A:1829:ILE:HD11	2.38	0.53
1:A:3296:LYS:C	1:A:3298:SER:H	2.10	0.53
1:A:3750:TYR:HA	1:A:3776:TRP:O	2.08	0.53
1:A:4057:ILE:HD12	1:A:4149:LEU:CD2	2.35	0.53
1:A:2663:THR:OG1	5:A:4406:ADP:H5'1	2.09	0.53
1:A:4051:ASN:O	1:A:4055:ASN:OD1	2.27	0.53
1:A:4308:VAL:O	1:A:4308:VAL:HG12	2.08	0.53
1:A:1411:CYS:O	1:A:1414:SER:OG	2.19	0.53
1:A:1879:LEU:HD12	1:A:1897:ILE:HG23	1.90	0.53
1:A:2135:ALA:CA	1:A:2138:ARG:CB	2.56	0.53
1:A:2396:GLY:C	1:A:2397:LEU:HD22	2.28	0.53
1:A:2450:LEU:O	1:A:2453:ASN:O	2.27	0.53
1:A:3740:LEU:HD12	1:A:3740:LEU:O	2.07	0.53
1:A:4147:ARG:O	1:A:4151:ILE:HG12	2.08	0.53
1:A:4265:GLU:O	1:A:4288:CYS:N	2.35	0.53
1:A:1709:GLN:O	1:A:1709:GLN:HG3	2.09	0.53
1:A:2689:GLN:HG3	1:A:2690:PHE:N	2.24	0.53
1:A:4199:LYS:CD	1:A:4255:GLN:HG2	2.39	0.53
1:A:1376:ARG:O	1:A:1379:MET:HB3	2.08	0.53
1:A:2041:VAL:CG2	1:A:2050:SER:CB	2.87	0.53
1:A:2249:LEU:HB2	1:A:2448:PRO:HG3	1.91	0.53
1:A:1590:GLY:C	1:A:1591:ILE:HG13	2.29	0.53
1:A:2660:GLY:HA2	5:A:4406:ADP:PB	2.49	0.53
1:A:3299:ARG:HH21	1:A:3322:LYS:HD3	1.73	0.53
1:A:3577:ARG:HA	1:A:3584:PHE:HE2	1.72	0.53
1:A:2639:ARG:O	1:A:2642:ARG:HG2	2.09	0.52
1:A:3864:LEU:CD2	1:A:3903:ILE:HG21	2.39	0.52
1:A:1343:ASN:OD1	1:A:1344:HIS:N	2.42	0.52
1:A:1472:HIS:HA	1:A:1490:VAL:O	2.10	0.52
1:A:1624:TRP:CZ2	1:A:3906:LEU:HD13	2.44	0.52
1:A:3212:THR:HG23	1:A:3213:TYR:CD2	2.44	0.52
1:A:3262:ASP:OD1	1:A:3262:ASP:N	2.42	0.52
1:A:1993:ARG:HB2	1:A:2003:VAL:HG11	1.92	0.52
1:A:2004:LYS:HE2	1:A:2006:TYR:OH	2.09	0.52
1:A:2175:GLY:CA	1:A:2196:LEU:HD23	2.39	0.52
1:A:2389:ASP:N	1:A:2393:GLU:O	2.43	0.52
1:A:2848:ASP:N	1:A:2849:PRO:HD2	2.24	0.52
1:A:3296:LYS:HA	1:A:3300:LEU:HD21	1.92	0.52
1:A:4052:GLN:HA	1:A:4055:ASN:CG	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4188:ALA:O	1:A:4192:GLY:N	2.42	0.52
1:A:2650:SER:HB2	1:A:2803:CYS:HB3	1.91	0.52
1:A:3238:PHE:CA	1:A:3242:ARG:HH21	2.23	0.52
1:A:4199:LYS:CE	1:A:4255:GLN:HG2	2.39	0.52
1:A:1691:ALA:HB1	1:A:2105:ALA:HA	1.91	0.52
1:A:1908:SER:HB2	1:A:2113:ILE:HA	1.91	0.52
1:A:3324:LEU:HG	1:A:3325:ILE:N	2.25	0.52
1:A:3675:ILE:HD11	1:A:3693:PHE:HB2	1.92	0.52
1:A:4265:GLU:O	1:A:4288:CYS:HB3	2.09	0.52
1:A:1861:HIS:HB2	1:A:2112:MET:SD	2.50	0.52
1:A:2131:ARG:HA	1:A:2138:ARG:HH22	1.64	0.52
1:A:2254:PHE:O	1:A:2595:HIS:HE1	1.92	0.52
1:A:4046:LEU:CD1	1:A:4138:LEU:HD22	2.40	0.52
1:A:1631:ARG:O	1:A:1642:VAL:HG13	2.10	0.52
1:A:1811:LEU:HD12	1:A:1811:LEU:N	2.25	0.52
1:A:1896:HIS:CD2	1:A:1929:ILE:CG2	2.88	0.52
1:A:2254:PHE:O	1:A:2595:HIS:CE1	2.63	0.52
1:A:2486:VAL:HB	1:A:4106:LEU:HD21	1.91	0.52
1:A:2774:GLN:N	1:A:2774:GLN:OE1	2.42	0.52
1:A:3218:PRO:HD2	1:A:3221:LEU:HD12	1.92	0.52
1:A:3635:SER:O	1:A:3639:THR:HG23	2.09	0.52
1:A:4026:THR:O	1:A:4027:ALA:HB3	2.10	0.52
1:A:4204:TRP:CE2	1:A:4248:CYS:SG	3.03	0.52
1:A:1398:ARG:O	1:A:1402:LEU:HG	2.09	0.52
1:A:1408:LEU:O	1:A:1411:CYS:SG	2.67	0.52
1:A:2577:GLY:HA3	1:A:2602:LEU:HD11	1.92	0.52
1:A:2465:LYS:O	1:A:2468:LEU:HB3	2.10	0.51
1:A:2823:LEU:HD13	1:A:2826:GLU:OE1	2.09	0.51
1:A:3877:ARG:HB2	1:A:3885:TRP:CD1	2.46	0.51
1:A:3965:PHE:HB3	1:A:3966:PRO:CD	2.40	0.51
1:A:1285:GLN:O	1:A:1287:ARG:HG3	2.10	0.51
1:A:2133:GLN:O	1:A:2138:ARG:HD2	2.11	0.51
1:A:3380:PRO:HD2	1:A:3383:ALA:HB3	1.92	0.51
1:A:4100:VAL:CG1	1:A:4105:THR:HG23	2.35	0.51
1:A:2263:ILE:HD11	1:A:2444:ALA:HB3	1.93	0.51
1:A:3640:LEU:CD1	1:A:3648:TRP:CZ2	2.93	0.51
1:A:4052:GLN:HA	1:A:4055:ASN:ND2	2.26	0.51
1:A:1800:GLY:C	1:A:1801:ARG:HG3	2.29	0.51
1:A:1993:ARG:HG3	1:A:1994:ALA:N	2.25	0.51
1:A:3240:LEU:HA	1:A:3243:PHE:HB3	1.92	0.51
1:A:2592:LEU:HD11	1:A:2707:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3577:ARG:NH2	1:A:3577:ARG:HB3	2.26	0.51
1:A:1628:LYS:HB2	1:A:3917:PHE:CZ	2.46	0.51
1:A:1806:ASP:OD2	1:A:3730:GLY:N	2.43	0.51
1:A:2284:LYS:NZ	1:A:2401:GLN:N	2.59	0.51
1:A:2811:TRP:CE2	1:A:2869:PRO:HB3	2.46	0.51
1:A:3325:ILE:HA	1:A:3369:PHE:O	2.11	0.51
1:A:3515:MET:HA	1:A:3822:LEU:HD13	1.93	0.51
1:A:2847:VAL:HG13	1:A:2849:PRO:CD	2.30	0.50
1:A:3586:GLU:O	1:A:3587:ASN:HB3	2.11	0.50
1:A:3640:LEU:HD12	1:A:3648:TRP:CZ2	2.46	0.50
1:A:1472:HIS:C	1:A:1473:ILE:HD12	2.31	0.50
1:A:1804:LEU:HD12	1:A:1805:PRO:HD2	1.92	0.50
1:A:2187:GLU:HG2	1:A:2191:ASN:OD1	2.11	0.50
1:A:3577:ARG:HB3	1:A:3577:ARG:CZ	2.42	0.50
1:A:1697:GLU:OE2	1:A:2072:ASP:HB3	2.12	0.50
1:A:1973:MET:HG3	1:A:2070:LEU:HD23	1.94	0.50
1:A:1458:PHE:HB3	1:A:1461:ILE:CD1	2.42	0.50
1:A:1728:PHE:CZ	1:A:1758:ILE:HD11	2.47	0.50
1:A:1802:GLN:N	1:A:1802:GLN:OE1	2.45	0.50
1:A:2294:GLY:O	1:A:2496:PRO:HG2	2.11	0.50
1:A:3514:ASN:O	1:A:3515:MET:HB2	2.11	0.50
1:A:3881:ILE:CG2	1:A:3882:PRO:HA	2.41	0.50
1:A:3932:ASP:OD1	1:A:3932:ASP:N	2.45	0.50
1:A:3910:ALA:O	1:A:3911:LYS:HG3	2.12	0.50
1:A:1337:GLU:O	1:A:1341:ASN:ND2	2.45	0.50
1:A:2004:LYS:CE	1:A:2006:TYR:CZ	2.95	0.50
1:A:3291:LEU:HA	1:A:3294:HIS:ND1	2.27	0.50
1:A:4227:PHE:CD2	1:A:4232:LEU:CD2	2.94	0.50
1:A:1499:TRP:CE3	1:A:1503:LEU:HD11	2.47	0.49
1:A:2078:MET:HG3	1:A:2082:GLU:HB3	1.94	0.49
1:A:2284:LYS:CG	1:A:2401:GLN:OE1	2.33	0.49
1:A:2659:VAL:HG21	1:A:2811:TRP:CD1	2.47	0.49
1:A:4171:SER:HB2	1:A:4305:LYS:CB	2.39	0.49
1:A:1388:VAL:HG13	1:A:1389:THR:N	2.27	0.49
1:A:2318:CYS:HB2	1:A:2360:ASP:O	2.12	0.49
1:A:2363:LEU:N	1:A:2363:LEU:HD22	2.27	0.49
1:A:2769:THR:HA	1:A:2772:ILE:HD12	1.94	0.49
1:A:1582:GLU:C	1:A:1584:PRO:HD2	2.33	0.49
1:A:3291:LEU:CA	1:A:3294:HIS:ND1	2.75	0.49
1:A:2045:PRO:O	1:A:2048:VAL:HG22	2.13	0.49
1:A:2173:MET:HB3	1:A:2426:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3922:LEU:C	1:A:3922:LEU:HD13	2.32	0.49
1:A:4038:ASN:O	1:A:4042:PRO:HD3	2.13	0.49
1:A:1825:ILE:O	1:A:1829:ILE:HG12	2.12	0.49
1:A:2362:ASN:HB2	1:A:2363:LEU:HD22	1.94	0.49
1:A:1547:PHE:CE1	1:A:1606:ASN:HB3	2.48	0.49
1:A:1862:TYR:CD2	1:A:1864:TRP:CH2	3.01	0.49
1:A:2473:MET:CE	1:A:2502:TRP:CE3	2.79	0.49
1:A:2512:GLU:OE2	1:A:2579:ARG:HG3	2.12	0.49
1:A:1879:LEU:O	1:A:1882:GLN:N	2.43	0.49
1:A:1896:HIS:O	1:A:1900:GLN:OE1	2.30	0.49
1:A:2284:LYS:CE	1:A:2401:GLN:CA	2.91	0.49
1:A:2683:ARG:NH2	1:A:3305:GLN:O	2.46	0.49
1:A:3587:ASN:OD1	1:A:3590:ASP:CG	2.51	0.49
1:A:3674:GLN:O	1:A:3677:VAL:HB	2.13	0.49
1:A:2175:GLY:HA2	1:A:2196:LEU:HD23	1.93	0.49
1:A:2320:ALA:HA	1:A:2364:PRO:HA	1.95	0.49
1:A:3847:TRP:CH2	1:A:3900:TYR:HB2	2.41	0.49
1:A:1695:LYS:NZ	2:A:4401:AOV:O1G	2.44	0.49
1:A:2223:PHE:CE2	1:A:2224:HIS:HB2	2.47	0.49
1:A:2625:LEU:HD22	1:A:2627:ILE:HD13	1.94	0.49
1:A:3636:LEU:HA	1:A:3639:THR:OG1	2.12	0.49
1:A:4253:ILE:HG22	1:A:4254:PRO:HD2	1.95	0.49
1:A:2051:TRP:C	1:A:2052:ILE:HD13	2.34	0.49
1:A:2530:GLU:O	1:A:2531:ALA:C	2.51	0.49
1:A:2819:ILE:HB	1:A:2820:PRO:HD3	1.95	0.49
1:A:3300:LEU:HA	1:A:3323:THR:O	2.13	0.49
1:A:1514:LEU:HD11	1:A:1534:PHE:CE1	2.47	0.48
1:A:1696:THR:HA	1:A:1790:THR:HG21	1.95	0.48
1:A:2274:TYR:HE2	1:A:2428:CYS:HB3	1.76	0.48
1:A:3536:ASP:O	1:A:3543:ARG:NH1	2.46	0.48
1:A:3577:ARG:HA	1:A:3584:PHE:CE2	2.48	0.48
1:A:2579:ARG:C	1:A:2580:HIS:CD2	2.87	0.48
1:A:4171:SER:OG	1:A:4308:VAL:HG12	2.13	0.48
1:A:2041:VAL:HG21	1:A:2050:SER:CB	2.43	0.48
1:A:2284:LYS:HZ1	1:A:2401:GLN:N	2.11	0.48
1:A:2459:ILE:HD12	1:A:2519:PRO:HD2	1.95	0.48
1:A:2749:LEU:N	1:A:2750:PRO:CD	2.76	0.48
1:A:1516:LYS:HD3	1:A:1638:HIS:HB3	1.94	0.48
1:A:1939:LEU:O	1:A:1939:LEU:HD23	2.14	0.48
1:A:2396:GLY:O	1:A:2397:LEU:HD22	2.13	0.48
1:A:4030:LYS:HB2	1:A:4034:GLU:CD	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4222:LEU:HD22	1:A:4225:CYS:O	2.13	0.48
1:A:1276:PHE:HE1	1:A:1388:VAL:HA	1.79	0.48
1:A:1280:ASP:HA	1:A:1289:MET:O	2.13	0.48
1:A:2723:LEU:N	1:A:2723:LEU:HD22	2.29	0.48
1:A:1378:ILE:O	1:A:1382:ILE:HD12	2.13	0.48
1:A:2529:TYR:O	1:A:2533:ARG:HG2	2.13	0.48
1:A:3291:LEU:O	1:A:3295:LEU:HG	2.14	0.48
1:A:3829:THR:HG22	1:A:3831:GLU:HG3	1.96	0.48
1:A:4043:VAL:HG21	1:A:4118:LEU:CD2	2.44	0.48
1:A:1749:SER:O	1:A:3756:GLY:CA	2.61	0.48
1:A:3374:ASN:HB2	1:A:3820:ILE:CG1	2.44	0.48
1:A:4046:LEU:HD12	1:A:4138:LEU:HD22	1.96	0.48
1:A:1792:ASN:HB3	1:A:1798:TYR:CE2	2.49	0.48
1:A:1795:GLY:HA3	1:A:1798:TYR:CD1	2.48	0.48
1:A:1943:LEU:HA	1:A:1995:ALA:CB	2.44	0.48
1:A:2284:LYS:HD2	1:A:2353:ARG:HH12	1.79	0.48
1:A:3296:LYS:HD2	1:A:3296:LYS:O	2.14	0.48
1:A:3347:GLN:HG3	1:A:3352:VAL:CG2	2.44	0.48
1:A:3238:PHE:HA	1:A:3242:ARG:HH21	1.79	0.47
1:A:3245:CYS:SG	1:A:3249:GLU:HB3	2.53	0.47
1:A:4188:ALA:HB1	1:A:4193:ARG:O	2.14	0.47
1:A:1716:ASP:OD2	1:A:2065:SER:CA	2.57	0.47
1:A:1879:LEU:HD23	1:A:1879:LEU:N	2.29	0.47
1:A:2168:LEU:O	1:A:2171:THR:OG1	2.26	0.47
1:A:2345:VAL:HG21	1:A:2398:GLU:HB2	1.96	0.47
1:A:2625:LEU:HD22	1:A:2627:ILE:CD1	2.44	0.47
1:A:3219:GLU:N	1:A:3219:GLU:OE1	2.47	0.47
1:A:3238:PHE:N	1:A:3242:ARG:HH21	2.12	0.47
1:A:3256:GLU:OE1	1:A:3290:TRP:NE1	2.47	0.47
1:A:1987:THR:O	1:A:1988:LEU:C	2.49	0.47
1:A:2235:ARG:HB3	1:A:2237:ARG:CG	2.44	0.47
1:A:2848:ASP:N	1:A:2849:PRO:CD	2.77	0.47
1:A:3629:LEU:HD22	1:A:3680:VAL:HG21	1.95	0.47
1:A:3966:PRO:HB2	1:A:3969:VAL:CG1	2.43	0.47
1:A:4270:PRO:HA	1:A:4283:ASN:HB3	1.97	0.47
1:A:1902:LEU:HD21	1:A:1918:PHE:HZ	1.78	0.47
1:A:2208:PHE:O	1:A:2209:THR:C	2.51	0.47
1:A:2238:LEU:HD22	1:A:2238:LEU:N	2.28	0.47
1:A:2230:TYR:N	1:A:2239:ALA:HB1	2.28	0.47
1:A:2632:GLU:OE2	1:A:2812:SER:N	2.48	0.47
1:A:2643:VAL:HG11	1:A:2651:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2659:VAL:CG2	1:A:2811:TRP:CD1	2.95	0.47
1:A:2704:GLU:O	1:A:2705:ALA:HB3	2.14	0.47
1:A:3640:LEU:CD1	1:A:3642:PHE:CE1	2.96	0.47
1:A:3877:ARG:HH22	1:A:3996:PHE:HA	1.80	0.47
1:A:4072:ILE:HG23	1:A:4073:LEU:N	2.30	0.47
1:A:4077:ILE:O	1:A:4080:GLN:HB3	2.15	0.47
1:A:1643:GLN:HG3	1:A:1647:SER:O	2.14	0.47
1:A:1742:GLU:OE2	2:A:4401:AOV:O2G	2.32	0.47
1:A:2495:THR:H	1:A:2498:ILE:HG12	1.80	0.47
1:A:3321:GLY:HA3	1:A:3363:ASN:OD1	2.13	0.47
1:A:4033:ARG:O	1:A:4037:SER:N	2.46	0.47
1:A:1746:LEU:HB3	1:A:1751:LEU:HD21	1.96	0.47
1:A:1792:ASN:OD1	2:A:4401:AOV:O2G	2.32	0.47
1:A:1993:ARG:HB2	1:A:2003:VAL:HG21	1.95	0.47
1:A:3197:LEU:C	1:A:3197:LEU:HD12	2.35	0.47
1:A:1280:ASP:OD1	1:A:1290:LYS:HE3	2.14	0.47
1:A:1815:VAL:HA	1:A:3929:GLY:HA2	1.97	0.47
1:A:2319:SER:N	1:A:2322:THR:OG1	2.42	0.47
1:A:2764:VAL:O	1:A:2767:TYR:HB3	2.14	0.47
1:A:3291:LEU:CD1	1:A:3294:HIS:HE1	2.23	0.47
1:A:1732:VAL:HB	1:A:1781:VAL:HG23	1.96	0.47
1:A:1440:ILE:HD11	1:A:1453:HIS:CD2	2.49	0.47
1:A:2447:GLU:HB3	1:A:2448:PRO:HD3	1.97	0.47
1:A:2469:LEU:HD22	1:A:2560:TRP:HZ2	1.80	0.47
1:A:2639:ARG:O	1:A:2643:VAL:HG23	2.14	0.47
1:A:3357:ASP:N	1:A:3357:ASP:OD1	2.48	0.47
2:A:4401:AOV:O2B	2:A:4401:AOV:O4G	2.33	0.47
1:A:1508:LYS:O	1:A:1512:GLU:HB2	2.15	0.46
1:A:1529:VAL:C	1:A:1531:PRO:HD3	2.36	0.46
1:A:2004:LYS:CG	1:A:2006:TYR:CZ	2.98	0.46
1:A:2019:LEU:O	1:A:2035:THR:HG21	2.14	0.46
1:A:2076:LEU:HD12	1:A:2077:THR:N	2.31	0.46
1:A:2166:THR:OG1	1:A:2171:THR:HG23	2.15	0.46
1:A:2256:ASN:OD1	1:A:2257:GLY:N	2.48	0.46
1:A:2297:LYS:HZ3	5:A:4405:ADP:PB	2.38	0.46
1:A:3771:ALA:HA	1:A:3805:PHE:CD1	2.50	0.46
1:A:1444:SER:HB3	1:A:1496:VAL:HG22	1.96	0.46
1:A:2607:LEU:O	1:A:2610:VAL:N	2.48	0.46
1:A:3337:TYR:N	1:A:3338:PRO:HD2	2.31	0.46
1:A:3560:CYS:HA	1:A:3563:LEU:HG	1.98	0.46
1:A:1534:PHE:CB	1:A:1539:LEU:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2502:TRP:HE1	1:A:2531:ALA:HB2	1.81	0.46
1:A:3864:LEU:HD21	1:A:3903:ILE:HG21	1.97	0.46
1:A:1363:LYS:O	1:A:1366:THR:OG1	2.33	0.46
1:A:2287:PHE:HA	1:A:2426:ARG:O	2.15	0.46
1:A:3347:GLN:HG3	1:A:3352:VAL:HG22	1.96	0.46
1:A:3560:CYS:HB3	1:A:3705:PRO:HG3	1.97	0.46
1:A:1411:CYS:SG	1:A:1412:GLN:N	2.89	0.46
1:A:2284:LYS:HE3	1:A:2353:ARG:NH2	2.29	0.46
1:A:2664:ILE:N	1:A:2664:ILE:CD1	2.78	0.46
1:A:1518:CYS:HB2	1:A:1534:PHE:CZ	2.51	0.46
1:A:1747:GLU:O	1:A:1750:VAL:HB	2.15	0.46
1:A:3587:ASN:OD1	1:A:3590:ASP:HB2	2.16	0.46
1:A:3780:LYS:HA	1:A:3810:THR:HB	1.96	0.46
1:A:4229:GLY:O	1:A:4230:ASN:HB2	2.16	0.46
1:A:1446:ASN:HB3	1:A:1449:VAL:HB	1.98	0.46
1:A:1624:TRP:HB3	1:A:3917:PHE:CB	2.46	0.46
1:A:1719:ILE:HG22	1:A:1723:SER:HB3	1.96	0.46
1:A:2004:LYS:HG2	1:A:2006:TYR:CE1	2.47	0.46
1:A:2077:THR:HA	1:A:2083:ARG:HG2	1.97	0.46
1:A:2155:TRP:CZ3	1:A:2208:PHE:HB2	2.51	0.46
1:A:2213:PHE:HB3	1:A:2219:SER:HA	1.98	0.46
1:A:3563:LEU:HD11	1:A:3571:PHE:CD2	2.50	0.46
1:A:2041:VAL:HG23	1:A:2050:SER:CB	2.45	0.46
1:A:2360:ASP:HB3	1:A:2363:LEU:HD23	1.97	0.46
1:A:3216:ALA:O	1:A:3391:ASN:ND2	2.48	0.46
1:A:3621:GLU:HG3	1:A:3622:ARG:H	1.81	0.46
1:A:4057:ILE:CG2	1:A:4152:GLN:OE1	2.63	0.46
1:A:2307:GLN:HA	1:A:2307:GLN:OE1	2.16	0.46
1:A:3505:ILE:HG21	1:A:3575:PHE:HA	1.98	0.46
1:A:4177:ASP:O	1:A:4180:LEU:HB2	2.16	0.46
1:A:4199:LYS:HD2	1:A:4255:GLN:HG2	1.96	0.46
1:A:1401:LEU:HA	1:A:1404:ILE:HD12	1.96	0.46
1:A:1499:TRP:HZ3	1:A:1503:LEU:HD11	1.80	0.46
1:A:1982:GLY:HA3	1:A:2169:VAL:HG21	1.98	0.46
1:A:2134:PRO:HB2	1:A:2136:GLU:HG3	1.98	0.46
1:A:2223:PHE:CG	1:A:2224:HIS:N	2.84	0.46
1:A:3325:ILE:HG22	1:A:3326:ILE:N	2.30	0.46
1:A:4177:ASP:OD1	1:A:4177:ASP:N	2.49	0.46
1:A:2805:VAL:O	1:A:2806:LEU:HD23	2.17	0.45
1:A:3701:LYS:HE2	1:A:3989:GLU:OE1	2.16	0.45
1:A:2130:LEU:HD13	1:A:2142:GLU:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2292:PRO:HG2	1:A:2432:TYR:HE1	1.82	0.45
1:A:2392:LEU:N	1:A:2392:LEU:HD12	2.31	0.45
1:A:3292:LYS:O	1:A:3296:LYS:N	2.49	0.45
1:A:3499:ALA:HA	1:A:3502:MET:HE2	1.98	0.45
1:A:3512:ILE:HG23	1:A:4021:LEU:HD23	1.97	0.45
1:A:3685:ARG:O	1:A:3686:LEU:C	2.53	0.45
1:A:3819:PRO:HA	1:A:3822:LEU:HD12	1.98	0.45
1:A:2311:THR:OG1	1:A:2312:GLN:N	2.50	0.45
1:A:2447:GLU:N	1:A:2448:PRO:CD	2.78	0.45
1:A:2650:SER:O	1:A:2803:CYS:HB2	2.16	0.45
1:A:3299:ARG:NH2	1:A:3320:PHE:O	2.48	0.45
1:A:3970:SER:O	1:A:3970:SER:OG	2.34	0.45
1:A:4090:VAL:HG12	1:A:4094:LEU:HD12	1.97	0.45
1:A:1654:GLU:HB3	1:A:1707:GLY:O	2.17	0.45
1:A:1955:ILE:CG2	1:A:1956:PRO:HD2	2.46	0.45
1:A:2164:VAL:O	1:A:2166:THR:HG23	2.16	0.45
1:A:3261:ASP:OD1	1:A:3262:ASP:N	2.50	0.45
1:A:3272:LEU:C	1:A:3272:LEU:HD23	2.37	0.45
1:A:3721:GLU:HG3	1:A:3826:LEU:HD11	1.98	0.45
1:A:2235:ARG:HB3	1:A:2237:ARG:HG2	1.98	0.45
1:A:2327:LEU:O	1:A:2328:LEU:C	2.53	0.45
1:A:2460:TRP:HE1	1:A:2519:PRO:HB2	1.80	0.45
1:A:2593:PRO:HG2	1:A:2597:LYS:HA	1.99	0.45
1:A:2749:LEU:HB3	1:A:2750:PRO:HD3	1.98	0.45
1:A:3279:PHE:HA	1:A:3370:LEU:HD12	1.99	0.45
1:A:4184:ARG:HG3	1:A:4252:TRP:CD2	2.52	0.45
1:A:4227:PHE:HD2	1:A:4232:LEU:CD2	2.28	0.45
1:A:1601:LEU:HD21	1:A:1832:SER:HB3	1.99	0.45
1:A:3577:ARG:O	1:A:3584:PHE:CZ	2.69	0.45
1:A:4025:ILE:N	1:A:4025:ILE:CD1	2.79	0.45
1:A:4097:LEU:HD13	1:A:4111:VAL:HG12	1.98	0.45
1:A:1741:ASP:O	1:A:1742:GLU:CB	2.64	0.45
1:A:2495:THR:HB	1:A:2496:PRO:HD2	1.99	0.45
1:A:2870:SER:OG	1:A:3385:SER:HB2	2.17	0.45
1:A:4025:ILE:HG22	1:A:4027:ALA:H	1.81	0.45
1:A:1274:ALA:HB1	1:A:1388:VAL:CG1	2.47	0.45
1:A:1624:TRP:CE3	1:A:3917:PHE:HB3	2.51	0.45
1:A:1663:VAL:N	2:A:4401:AOV:N1	2.64	0.45
1:A:1708:ARG:NH1	1:A:1784:ASN:O	2.49	0.45
1:A:2651:LEU:HD12	1:A:2651:LEU:N	2.32	0.45
1:A:4134:PRO:HG2	1:A:4140:TYR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1381:ASP:O	1:A:1385:ASP:HB3	2.17	0.45
1:A:1906:THR:HG21	1:A:1918:PHE:CZ	2.52	0.45
1:A:2007:THR:HG21	1:A:2384:TYR:CE2	2.52	0.45
1:A:4201:VAL:HG12	1:A:4202:ALA:H	1.81	0.45
1:A:1560:LEU:HD23	1:A:1560:LEU:HA	1.80	0.45
1:A:1787:ILE:O	1:A:1788:PHE:CD1	2.70	0.45
1:A:1820:PRO:O	1:A:1822:ASN:OD1	2.35	0.45
1:A:3368:LEU:HD23	1:A:3369:PHE:N	2.32	0.45
1:A:3580:HIS:C	1:A:3584:PHE:CZ	2.86	0.45
1:A:4057:ILE:CD1	1:A:4152:GLN:NE2	2.77	0.45
1:A:1315:SER:O	1:A:1318:TYR:HB3	2.17	0.44
1:A:1372:ASP:OD1	1:A:1376:ARG:NH1	2.49	0.44
1:A:1749:SER:O	1:A:3756:GLY:HA3	2.17	0.44
1:A:2004:LYS:HG2	1:A:2006:TYR:OH	2.17	0.44
1:A:2041:VAL:HG23	1:A:2050:SER:OG	2.17	0.44
1:A:2382:LEU:CD2	1:A:2402:ILE:HD13	2.47	0.44
1:A:2411:ARG:CB	1:A:2414:ARG:CZ	2.94	0.44
1:A:3200:LEU:N	1:A:3201:PRO:CD	2.80	0.44
1:A:3640:LEU:CG	1:A:3642:PHE:CZ	2.98	0.44
1:A:3732:ASP:HA	1:A:3733:PRO:HD3	1.81	0.44
1:A:3847:TRP:HH2	1:A:3900:TYR:CG	2.35	0.44
1:A:1547:PHE:O	1:A:1551:VAL:HG23	2.17	0.44
1:A:1550:ASP:O	1:A:1554:ALA:N	2.49	0.44
1:A:2004:LYS:CE	1:A:2006:TYR:OH	2.64	0.44
1:A:2517:ASN:HB3	1:A:2519:PRO:CB	2.47	0.44
1:A:3864:LEU:HD21	1:A:3903:ILE:CG2	2.47	0.44
1:A:4001:ASN:ND2	1:A:4241:SER:HA	2.33	0.44
1:A:4057:ILE:HG12	1:A:4152:GLN:OE1	2.17	0.44
1:A:4134:PRO:CG	1:A:4140:TYR:HA	2.48	0.44
1:A:1278:LEU:HD12	1:A:1278:LEU:N	2.32	0.44
1:A:1444:SER:CB	1:A:1496:VAL:HG22	2.47	0.44
1:A:1591:ILE:HB	1:A:1592:LEU:HD12	1.98	0.44
1:A:1671:CYS:O	1:A:1675:LEU:HG	2.16	0.44
1:A:1699:VAL:HG11	1:A:1788:PHE:CD2	2.52	0.44
1:A:1719:ILE:HG13	1:A:2079:PRO:HB3	2.00	0.44
1:A:2213:PHE:HA	1:A:2216:ALA:HB3	1.99	0.44
1:A:2503:VAL:HG13	1:A:2504:LEU:CD1	2.48	0.44
1:A:2711:LEU:O	1:A:2712:LEU:HD23	2.17	0.44
1:A:1862:TYR:CD2	1:A:1864:TRP:HH2	2.36	0.44
1:A:2002:VAL:HG12	1:A:2003:VAL:N	2.30	0.44
1:A:1401:LEU:HB2	1:A:1402:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:THR:O	1:A:1474:THR:HG22	2.16	0.44
1:A:2168:LEU:O	1:A:2171:THR:N	2.50	0.44
1:A:2821:GLU:HB2	1:A:2852:LEU:CD1	2.44	0.44
1:A:3193:ILE:HG22	1:A:3197:LEU:HD23	1.99	0.44
1:A:3291:LEU:CA	1:A:3294:HIS:HE1	2.25	0.44
1:A:3577:ARG:HD2	1:A:3589:TRP:CH2	2.53	0.44
1:A:3755:MET:N	1:A:3755:MET:CE	2.81	0.44
1:A:4286:VAL:HG13	1:A:4287:PRO:HD2	2.00	0.44
1:A:4288:CYS:SG	1:A:4290:GLY:CA	3.06	0.44
1:A:2629:LEU:N	1:A:2629:LEU:HD12	2.32	0.44
1:A:2643:VAL:CG1	1:A:2651:LEU:HD11	2.48	0.44
1:A:3755:MET:CG	1:A:3785:VAL:HG21	2.47	0.44
1:A:4040:LEU:HD22	1:A:4118:LEU:HD23	1.99	0.44
1:A:4266:CYS:HB3	1:A:4285:ASP:HB3	1.98	0.44
1:A:1624:TRP:CG	1:A:3917:PHE:HB3	2.52	0.44
1:A:1810:GLN:HG3	1:A:3732:ASP:CB	2.48	0.44
1:A:2730:LEU:HB3	1:A:2802:LYS:HG3	2.00	0.44
1:A:3587:ASN:OD1	1:A:3590:ASP:CB	2.66	0.44
1:A:3654:ASN:O	1:A:3682:ARG:NH1	2.50	0.44
1:A:3965:PHE:CB	1:A:3966:PRO:CD	2.94	0.44
1:A:1276:PHE:CD2	1:A:1292:ILE:HD12	2.53	0.44
1:A:1713:PHE:HB2	1:A:1740:PHE:CD1	2.52	0.44
1:A:2000:GLY:O	1:A:2001:LYS:C	2.54	0.44
1:A:2284:LYS:HE3	1:A:2401:GLN:CA	2.46	0.44
1:A:2717:PHE:CD1	1:A:2723:LEU:HD21	2.53	0.44
1:A:3837:LYS:HB2	1:A:3984:ILE:CG2	2.45	0.44
1:A:4307:GLN:O	1:A:4308:VAL:HG23	2.18	0.44
1:A:2038:ALA:HA	1:A:2041:VAL:HG12	2.00	0.43
1:A:3217:ALA:O	1:A:3222:ARG:NE	2.51	0.43
1:A:3244:LEU:HD22	1:A:3244:LEU:HA	1.85	0.43
1:A:3285:SER:O	1:A:3288:THR:OG1	2.26	0.43
1:A:3999:PRO:HG2	1:A:4002:ILE:HG12	2.00	0.43
1:A:4227:PHE:HD2	1:A:4232:LEU:HD21	1.84	0.43
1:A:1506:GLU:OE2	1:A:1510:THR:OG1	2.36	0.43
1:A:2579:ARG:O	1:A:2580:HIS:CD2	2.71	0.43
1:A:1274:ALA:HB1	1:A:1388:VAL:HG11	2.00	0.43
1:A:1397:ILE:O	1:A:1398:ARG:C	2.56	0.43
1:A:1500:LEU:HA	1:A:1503:LEU:HG	2.00	0.43
1:A:1699:VAL:CG1	1:A:1788:PHE:CD2	3.01	0.43
1:A:2765:PHE:O	1:A:2768:PHE:HB3	2.18	0.43
1:A:3273:GLN:OE1	1:A:3276:VAL:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3581:PRO:CA	1:A:3584:PHE:CZ	2.73	0.43
1:A:3802:LYS:O	1:A:3805:PHE:HB3	2.18	0.43
1:A:4202:ALA:HA	1:A:4249:PHE:O	2.19	0.43
1:A:1458:PHE:HB3	1:A:1461:ILE:HD12	1.98	0.43
1:A:1859:GLN:HB2	1:A:1862:TYR:CD2	2.53	0.43
1:A:1973:MET:HG3	1:A:2070:LEU:CD2	2.49	0.43
1:A:2052:ILE:HB	1:A:2092:PHE:CE1	2.53	0.43
1:A:3185:ARG:O	1:A:3189:GLN:NE2	2.51	0.43
1:A:3673:GLN:HA	1:A:3676:LEU:HD12	2.01	0.43
1:A:4030:LYS:O	1:A:4034:GLU:HB2	2.18	0.43
1:A:4100:VAL:HB	1:A:4105:THR:HG23	1.99	0.43
1:A:4124:PRO:HD2	1:A:4127:TRP:CE3	2.53	0.43
1:A:4147:ARG:HG2	1:A:4172:GLU:O	2.19	0.43
1:A:1558:HIS:HB3	1:A:1560:LEU:HG	1.99	0.43
1:A:1603:ILE:O	1:A:1606:ASN:HB2	2.19	0.43
1:A:2004:LYS:HB3	1:A:2050:SER:HA	2.00	0.43
1:A:2114:PHE:C	1:A:2115:LEU:HD12	2.39	0.43
1:A:2284:LYS:CE	1:A:2401:GLN:CB	2.77	0.43
1:A:3654:ASN:O	1:A:3657:CYS:HB3	2.19	0.43
1:A:4201:VAL:HG23	1:A:4253:ILE:CD1	2.48	0.43
1:A:1294:ASP:O	1:A:1297:ASP:HB3	2.19	0.43
1:A:1518:CYS:HB2	1:A:1534:PHE:CE1	2.53	0.43
1:A:1855:LEU:C	1:A:1855:LEU:HD12	2.39	0.43
1:A:2805:VAL:C	1:A:2806:LEU:HD23	2.39	0.43
1:A:3281:ILE:HD12	1:A:3391:ASN:HB3	1.99	0.43
1:A:3374:ASN:ND2	1:A:3377:PRO:CD	2.78	0.43
1:A:3686:LEU:HD22	1:A:3690:MET:SD	2.59	0.43
1:A:4100:VAL:N	1:A:4105:THR:HG21	2.34	0.43
1:A:1281:TYR:O	1:A:1288:THR:HA	2.19	0.43
1:A:2201:ASN:OD1	1:A:2201:ASN:N	2.51	0.43
1:A:1475:ALA:HB1	1:A:1484:VAL:O	2.19	0.43
1:A:2590:GLN:HG3	1:A:2591:PRO:HD3	2.01	0.43
1:A:4227:PHE:CD1	1:A:4227:PHE:C	2.92	0.43
1:A:2288:ILE:HD12	1:A:2426:ARG:O	2.19	0.43
1:A:2296:GLY:CA	5:A:4405:ADP:O1A	2.67	0.43
1:A:2312:GLN:HB2	1:A:2351:CYS:SG	2.59	0.43
1:A:2357:TYR:O	1:A:2358:LEU:HD23	2.19	0.43
1:A:2745:GLU:N	1:A:2746:PRO:HD2	2.34	0.43
1:A:3510:SER:HA	1:A:3516:TYR:HB2	2.00	0.43
1:A:3230:THR:HG23	1:A:3235:LEU:O	2.19	0.42
1:A:3239:ASP:OD1	1:A:3239:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3493:LEU:N	1:A:3494:PRO:CD	2.82	0.42
1:A:3577:ARG:HD2	1:A:3589:TRP:CZ3	2.54	0.42
1:A:2652:LEU:HD22	1:A:2805:VAL:HG13	2.01	0.42
1:A:2851:PHE:CE2	1:A:3201:PRO:HB2	2.54	0.42
1:A:3238:PHE:CZ	1:A:3243:PHE:CB	3.01	0.42
1:A:3336:LEU:CD2	1:A:3336:LEU:N	2.82	0.42
1:A:3512:ILE:HG23	1:A:4021:LEU:HD21	1.95	0.42
1:A:4057:ILE:HD12	1:A:4149:LEU:HD22	1.98	0.42
1:A:4288:CYS:SG	1:A:4290:GLY:C	2.97	0.42
1:A:2167:SER:O	1:A:2170:GLY:N	2.52	0.42
1:A:2200:LEU:HD12	1:A:2205:ARG:HA	2.01	0.42
1:A:2301:LEU:HD13	1:A:2357:TYR:CE1	2.55	0.42
1:A:2503:VAL:HG13	1:A:2504:LEU:HD13	2.01	0.42
1:A:2606:ASP:O	1:A:2610:VAL:HG23	2.19	0.42
1:A:2664:ILE:HD12	1:A:2664:ILE:H	1.83	0.42
1:A:1515:LEU:HD13	1:A:1538:ILE:HG23	2.01	0.42
1:A:2029:TRP:HE1	1:A:2031:ASP:HA	1.84	0.42
1:A:2163:VAL:HG23	1:A:2164:VAL:HG23	1.99	0.42
1:A:2212:VAL:HA	1:A:2215:TRP:CE3	2.48	0.42
1:A:4072:ILE:HB	1:A:4186:GLU:HG3	2.00	0.42
1:A:4075:PHE:O	1:A:4078:LEU:HB2	2.20	0.42
1:A:4227:PHE:CD2	1:A:4232:LEU:HD21	2.54	0.42
1:A:1593:GLU:OE1	1:A:1593:GLU:N	2.47	0.42
1:A:3321:GLY:HA2	1:A:3366:PHE:HB2	2.02	0.42
1:A:3374:ASN:HB2	1:A:3820:ILE:CD1	2.47	0.42
1:A:3545:GLN:HA	1:A:3548:ILE:HG22	2.01	0.42
1:A:1684:GLY:O	1:A:1812:PHE:HA	2.19	0.42
1:A:1731:LEU:HD23	1:A:1731:LEU:HA	1.91	0.42
1:A:1862:TYR:HB3	1:A:1864:TRP:CH2	2.54	0.42
1:A:2193:ILE:HG21	1:A:2209:THR:HG22	2.02	0.42
1:A:1514:LEU:HD11	1:A:1534:PHE:CD1	2.54	0.42
1:A:2041:VAL:HG21	1:A:2050:SER:HB2	2.01	0.42
1:A:2135:ALA:C	1:A:2138:ARG:H	2.23	0.42
1:A:2276:LYS:N	1:A:2277:PRO:HD2	2.35	0.42
1:A:3277:CYS:SG	1:A:3368:LEU:CD2	3.07	0.42
1:A:4134:PRO:HG2	1:A:4140:TYR:CA	2.50	0.42
1:A:2652:LEU:C	1:A:2652:LEU:HD23	2.40	0.42
1:A:2662:ARG:NH1	1:A:2662:ARG:HG2	2.35	0.42
1:A:3248:SER:O	1:A:3252:ILE:HG13	2.20	0.42
1:A:3299:ARG:HE	1:A:3322:LYS:HD2	1.84	0.42
1:A:3518:PHE:CD1	1:A:3518:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3583:LEU:H	1:A:3583:LEU:HG	1.68	0.42
1:A:3788:TRP:O	1:A:3788:TRP:HD1	2.03	0.42
1:A:3860:ARG:HB3	1:A:3907:PHE:CD2	2.55	0.42
1:A:4271:VAL:HA	1:A:4302:LEU:O	2.19	0.42
1:A:1866:LEU:HD12	2:A:4401:AOV:O4'	2.20	0.42
1:A:2296:GLY:HA2	5:A:4405:ADP:O1A	2.20	0.42
1:A:2517:ASN:HB2	1:A:2519:PRO:HB3	1.99	0.42
1:A:4281:VAL:CG2	1:A:4304:LEU:HD23	2.48	0.42
1:A:1481:GLY:O	1:A:1591:ILE:HD13	2.20	0.42
1:A:1693:THR:HG21	1:A:1817:MET:HB2	2.01	0.42
1:A:2076:LEU:HD12	1:A:2077:THR:H	1.85	0.42
1:A:3512:ILE:HD12	1:A:3513:ASN:CB	2.46	0.42
1:A:1688:TYR:CD1	1:A:1688:TYR:C	2.93	0.41
1:A:1906:THR:HG22	1:A:1910:PHE:CE1	2.55	0.41
1:A:3847:TRP:CH2	1:A:3900:TYR:CG	3.08	0.41
1:A:3919:HIS:HB2	1:A:3944:LEU:HB3	2.03	0.41
1:A:3965:PHE:HB3	1:A:3966:PRO:HD3	2.02	0.41
1:A:4030:LYS:O	1:A:4034:GLU:N	2.44	0.41
1:A:1624:TRP:HZ2	1:A:3906:LEU:HD13	1.85	0.41
1:A:1962:ALA:O	1:A:1965:LEU:HB3	2.19	0.41
1:A:1986:SER:HB3	1:A:2095:GLU:OE2	2.19	0.41
1:A:3309:ASN:OD1	1:A:3309:ASN:N	2.53	0.41
1:A:3567:ASP:O	1:A:3570:MET:HB2	2.19	0.41
1:A:3836:LEU:O	1:A:3840:LEU:HD13	2.19	0.41
1:A:2153:LEU:HD22	1:A:2157:LEU:HD11	2.03	0.41
1:A:2230:TYR:O	1:A:2239:ALA:HA	2.20	0.41
1:A:2276:LYS:N	1:A:2277:PRO:CD	2.83	0.41
1:A:2460:TRP:CH2	1:A:2523:VAL:HG11	2.55	0.41
1:A:3836:LEU:HD23	1:A:3991:ASP:HB3	2.00	0.41
1:A:3915:TRP:O	1:A:3918:VAL:HB	2.20	0.41
1:A:3934:TYR:CD1	1:A:3934:TYR:C	2.93	0.41
1:A:1496:VAL:HA	1:A:1499:TRP:HE1	1.84	0.41
1:A:1691:ALA:HA	2:A:4401:AOV:O1G	2.20	0.41
1:A:1982:GLY:HA2	4:A:4403:ATP:C5'	2.50	0.41
1:A:2186:ASP:HB3	1:A:2238:LEU:HD21	2.01	0.41
1:A:3214:LEU:HD12	1:A:3214:LEU:N	2.35	0.41
1:A:1289:MET:CE	1:A:1379:MET:HG2	2.51	0.41
1:A:1514:LEU:HD23	1:A:1538:ILE:CD1	2.50	0.41
1:A:2296:GLY:HA2	5:A:4405:ADP:H5'1	2.03	0.41
1:A:3551:LEU:HD13	1:A:3555:VAL:HG23	2.02	0.41
1:A:3790:PRO:O	1:A:3794:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1440:ILE:HD11	1:A:1453:HIS:CB	2.51	0.41
1:A:1563:ILE:O	1:A:1566:GLN:HB3	2.20	0.41
1:A:3270:VAL:O	1:A:3273:GLN:HB3	2.19	0.41
1:A:1849:PHE:CE2	1:A:1869:LEU:HB2	2.56	0.41
1:A:3238:PHE:CG	1:A:3238:PHE:O	2.72	0.41
1:A:3249:GLU:HA	1:A:3252:ILE:HD12	2.03	0.41
1:A:3648:TRP:CZ3	1:A:3662:PRO:HG3	2.56	0.41
1:A:1690:PRO:CD	1:A:1818:SER:HA	2.48	0.41
1:A:2223:PHE:CD2	1:A:2224:HIS:HB2	2.55	0.41
1:A:2335:CYS:SG	1:A:2348:PRO:HA	2.60	0.41
1:A:2534:LEU:HD12	1:A:2534:LEU:N	2.36	0.41
1:A:4153:ASN:O	1:A:4157:LYS:HG2	2.21	0.41
1:A:4166:GLU:HG2	1:A:4167:THR:N	2.36	0.41
1:A:1352:LEU:O	1:A:1356:PHE:N	2.47	0.41
1:A:1388:VAL:CG1	1:A:1389:THR:N	2.84	0.41
1:A:1480:GLU:H	1:A:1480:GLU:CD	2.25	0.41
1:A:1486:PHE:CD1	1:A:1506:GLU:OE1	2.74	0.41
1:A:1591:ILE:O	1:A:1592:LEU:HB2	2.21	0.41
1:A:1640:CYS:SG	1:A:1641:CYS:N	2.94	0.41
1:A:1718:GLY:HA2	1:A:1746:LEU:HD12	2.03	0.41
1:A:1729:VAL:O	1:A:1732:VAL:HG22	2.21	0.41
1:A:1925:VAL:HG23	1:A:1926:PHE:CD1	2.53	0.41
1:A:2067:ASN:O	1:A:2071:ASP:HB2	2.20	0.41
1:A:2152:ALA:O	1:A:2156:VAL:HG23	2.21	0.41
1:A:2421:PHE:HA	1:A:2424:ILE:HD12	2.02	0.41
1:A:2524:LEU:HD12	1:A:2564:ILE:HG21	2.03	0.41
1:A:2573:TYR:CZ	1:A:2601:LYS:HG3	2.56	0.41
1:A:3502:MET:HE1	1:A:3551:LEU:HD12	2.03	0.41
1:A:3505:ILE:HD11	1:A:3578:GLY:HA3	2.03	0.41
1:A:3759:GLN:O	1:A:3762:LEU:HG	2.21	0.41
1:A:4072:ILE:O	1:A:4075:PHE:HB3	2.21	0.41
1:A:4238:ASP:OD1	1:A:4239:SER:N	2.54	0.41
1:A:4291:ASN:OD1	1:A:4294:GLN:HB2	2.21	0.41
1:A:1906:THR:CG2	1:A:1910:PHE:CE1	3.04	0.41
1:A:2230:TYR:OH	1:A:2270:ARG:N	2.53	0.41
1:A:2338:ILE:HD11	1:A:2345:VAL:HG13	2.03	0.41
1:A:2689:GLN:CG	1:A:2690:PHE:N	2.83	0.41
1:A:3552:GLN:O	1:A:3555:VAL:HB	2.21	0.41
1:A:1591:ILE:HG22	1:A:1592:LEU:N	2.36	0.40
1:A:1624:TRP:CD1	1:A:3914:GLN:HB2	2.56	0.40
1:A:1693:THR:HG21	1:A:1817:MET:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1710:VAL:HA	1:A:1737:TRP:O	2.20	0.40
1:A:1789:ILE:O	1:A:1789:ILE:HG13	2.21	0.40
1:A:1980:PRO:O	1:A:1983:ALA:HB2	2.21	0.40
1:A:2156:VAL:HG13	1:A:2200:LEU:HD21	2.04	0.40
1:A:2523:VAL:O	1:A:2527:VAL:HG23	2.21	0.40
1:A:2739:TYR:CB	1:A:2744:LEU:HD21	2.51	0.40
1:A:3202:LYS:O	1:A:3206:LEU:HG	2.21	0.40
1:A:3230:THR:CG2	1:A:3235:LEU:O	2.70	0.40
1:A:3387:VAL:HG12	1:A:3388:THR:N	2.36	0.40
1:A:3512:ILE:CG2	1:A:4021:LEU:HD23	2.52	0.40
1:A:3640:LEU:CD1	1:A:3642:PHE:CZ	3.04	0.40
1:A:3686:LEU:O	1:A:3689:ALA:HB3	2.21	0.40
1:A:1539:LEU:O	1:A:1543:GLU:HG2	2.21	0.40
1:A:2296:GLY:C	5:A:4405:ADP:O1A	2.60	0.40
1:A:2399:ASN:C	1:A:2400:ILE:HD12	2.41	0.40
1:A:2553:THR:HG22	1:A:2557:GLN:NE2	2.36	0.40
1:A:3670:SER:OG	1:A:3673:GLN:HG3	2.22	0.40
1:A:3675:ILE:HD11	1:A:3693:PHE:CB	2.49	0.40
1:A:3687:GLN:HB3	1:A:4007:GLN:OE1	2.22	0.40
1:A:4075:PHE:CD1	1:A:4075:PHE:C	2.94	0.40
1:A:1741:ASP:O	1:A:1742:GLU:HB2	2.21	0.40
1:A:1982:GLY:HA2	4:A:4403:ATP:H5'1	2.04	0.40
1:A:2174:ASN:HA	1:A:2426:ARG:HD2	2.03	0.40
1:A:2766:ASN:O	1:A:2769:THR:HB	2.21	0.40
1:A:3710:LEU:CD1	1:A:3736:GLU:CD	2.89	0.40
1:A:4288:CYS:HG	1:A:4290:GLY:C	2.24	0.40
1:A:1986:SER:HA	1:A:1989:TRP:NE1	2.37	0.40
1:A:2453:ASN:ND2	1:A:2512:GLU:HA	2.36	0.40
1:A:2664:ILE:CD1	1:A:2664:ILE:H	2.34	0.40
1:A:3858:THR:HG23	1:A:3859:HIS:N	2.36	0.40
1:A:4200:PHE:HB2	1:A:4252:TRP:CZ3	2.57	0.40
1:A:1567:LEU:HB3	1:A:1607:ILE:HD11	2.04	0.40
1:A:2175:GLY:HA3	1:A:2196:LEU:CD2	2.51	0.40
1:A:2659:VAL:O	1:A:2659:VAL:HG13	2.21	0.40
1:A:3277:CYS:SG	1:A:3368:LEU:HD23	2.61	0.40
1:A:3486:ASP:O	1:A:3490:ASP:N	2.42	0.40
1:A:3588:GLU:HA	1:A:3633:LEU:HD11	2.03	0.40
1:A:3755:MET:HB2	1:A:3780:LYS:O	2.21	0.40
1:A:3939:VAL:HG22	1:A:4296:ILE:HG22	2.04	0.40
1:A:4073:LEU:O	1:A:4077:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2995/3450 (87%)	2834 (95%)	153 (5%)	8 (0%)	41 74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1820	PRO
1	A	3965	PHE
1	A	1589	SER
1	A	1645	VAL
1	A	3375	PRO
1	A	4027	ALA
1	A	1529	VAL
1	A	3952	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2286/3065 (75%)	2201 (96%)	85 (4%)	34 65

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1307	CYS
1	A	1392	THR
1	A	1465	CYS

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Mol	Chain	Res	Type
1	A	1513	GLN
1	A	1536	SER
1	A	1570	LYS
1	A	1705	LEU
1	A	1737	TRP
1	A	1739	CYS
1	A	1744	ASN
1	A	1787	ILE
1	A	1796	LYS
1	A	1944	LYS
1	A	1977	ILE
1	A	1997	CYS
1	A	1999	THR
1	A	2050	SER
1	A	2064	GLU
1	A	2116	SER
1	A	2178	HIS
1	A	2248	ASP
1	A	2253	ASP
1	A	2258	LEU
1	A	2322	THR
1	A	2435	ARG
1	A	2521	ASP
1	A	2570	ASP
1	A	2615	LEU
1	A	2627	ILE
1	A	2635	GLU
1	A	2661	ARG
1	A	2782	MET
1	A	2821	GLU
1	A	2875	PHE
1	A	3239	ASP
1	A	3262	ASP
1	A	3279	PHE
1	A	3309	ASN
1	A	3336	LEU
1	A	3343	ASP
1	A	3357	ASP
1	A	3391	ASN
1	A	3397	SER
1	A	3495	LEU
1	A	3518	PHE

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Mol	Chain	Res	Type
1	A	3582	GLU
1	A	3583	LEU
1	A	3584	PHE
1	A	3590	ASP
1	A	3640	LEU
1	A	3641	CYS
1	A	3652	TYR
1	A	3667	LYS
1	A	3671	LEU
1	A	3688	SER
1	A	3690	MET
1	A	3718	LEU
1	A	3755	MET
1	A	3761	ASP
1	A	3762	LEU
1	A	3792	LEU
1	A	3821	LEU
1	A	3842	ARG
1	A	3847	TRP
1	A	3877	ARG
1	A	3904	ASP
1	A	3921	LEU
1	A	3976	SER
1	A	4023	ARG
1	A	4026	THR
1	A	4030	LYS
1	A	4031	PHE
1	A	4032	ASP
1	A	4051	ASN
1	A	4100	VAL
1	A	4164	LEU
1	A	4180	LEU
1	A	4201	VAL
1	A	4215	ILE
1	A	4228	ASP
1	A	4246	LEU
1	A	4268	SER
1	A	4293	ASP
1	A	4298	CYS
1	A	4302	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1792	ASN
1	A	1810	GLN
1	A	2140	ASN
1	A	2178	HIS
1	A	2269	GLN
1	A	2362	ASN
1	A	2391	ASN
1	A	2580	HIS
1	A	2595	HIS
1	A	2777	HIS
1	A	3738	GLN
1	A	3742	ASN
1	A	4214	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AOV	A	4401	3	27,34,34	5.35	3 (11%)	26,56,56	1.55	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ADP	A	4406	-	24,29,29	1.12	1 (4%)	29,45,45	1.65	7 (24%)
5	ADP	A	4405	-	24,29,29	1.07	1 (4%)	29,45,45	1.67	7 (24%)
4	ATP	A	4403	3	26,33,33	0.88	1 (3%)	31,52,52	1.99	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AOV	A	4401	3	-	0/12/39/39	0/3/3/3
5	ADP	A	4406	-	-	0/12/32/32	0/3/3/3
5	ADP	A	4405	-	-	3/12/32/32	0/3/3/3
4	ATP	A	4403	3	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4401	AOV	O1G-VG	27.32	2.10	1.61
5	A	4406	ADP	PB-O1B	3.16	1.60	1.50
2	A	4401	AOV	C5-C4	2.50	1.47	1.40
2	A	4401	AOV	C2-N3	2.37	1.35	1.32
5	A	4405	ADP	C4-N3	-2.31	1.32	1.35
4	A	4403	ATP	C2-N3	2.07	1.35	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	4403	ATP	PA-O3A-PB	-6.39	110.88	132.83
4	A	4403	ATP	PB-O3B-PG	-6.11	111.86	132.83
2	A	4401	AOV	PA-O3A-PB	-4.77	116.47	132.83
5	A	4405	ADP	C4-C5-N7	-4.16	105.06	109.40
2	A	4401	AOV	C4-C5-N7	-3.87	105.36	109.40
5	A	4406	ADP	N3-C2-N1	-3.77	122.78	128.68
4	A	4403	ATP	N3-C2-N1	-3.74	122.83	128.68
5	A	4405	ADP	C3'-C2'-C1'	3.60	106.40	100.98
5	A	4405	ADP	PA-O3A-PB	-3.59	120.50	132.83
2	A	4401	AOV	N3-C2-N1	-3.45	123.28	128.68
5	A	4406	ADP	PA-O3A-PB	-3.17	121.94	132.83
5	A	4406	ADP	O3B-PB-O2B	2.85	118.52	107.64
5	A	4406	ADP	C3'-C2'-C1'	2.67	105.00	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	4403	ATP	C4-C5-N7	-2.58	106.71	109.40
5	A	4406	ADP	C4-C5-N7	-2.54	106.75	109.40
5	A	4406	ADP	O2A-PA-O1A	2.46	124.41	112.24
5	A	4406	ADP	O4'-C4'-C3'	2.27	109.60	105.11
5	A	4405	ADP	N3-C2-N1	-2.23	125.19	128.68
5	A	4405	ADP	O2A-PA-O1A	2.20	123.10	112.24
5	A	4405	ADP	O2B-PB-O3A	2.13	111.76	104.64
4	A	4403	ATP	O4'-C4'-C3'	2.05	109.17	105.11
5	A	4405	ADP	C5-C6-N6	2.01	123.41	120.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	4405	ADP	C5'-O5'-PA-O2A
5	A	4405	ADP	C5'-O5'-PA-O3A
5	A	4405	ADP	O4'-C4'-C5'-O5'

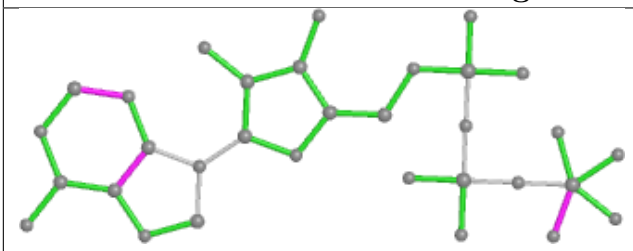
There are no ring outliers.

4 monomers are involved in 26 short contacts:

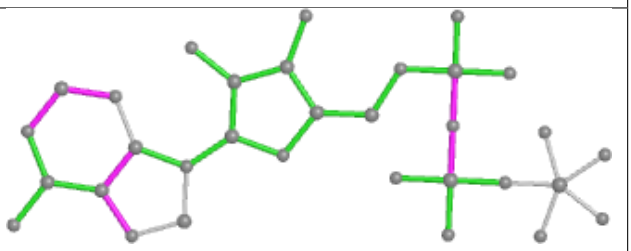
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4401	AOV	12	0
5	A	4406	ADP	5	0
5	A	4405	ADP	5	0
4	A	4403	ATP	4	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

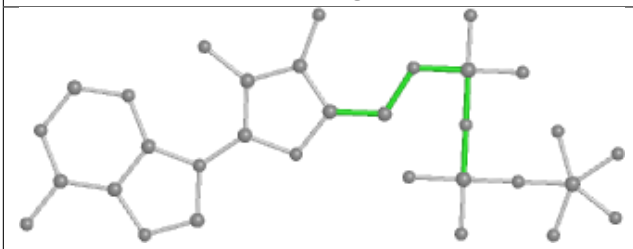
Ligand AOV A 4401



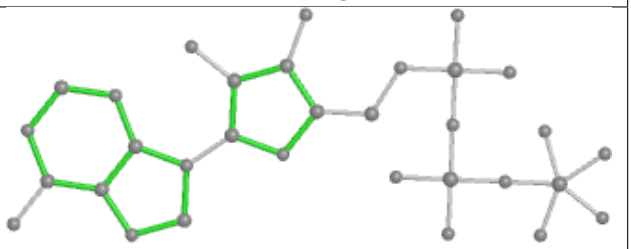
Bond lengths



Bond angles

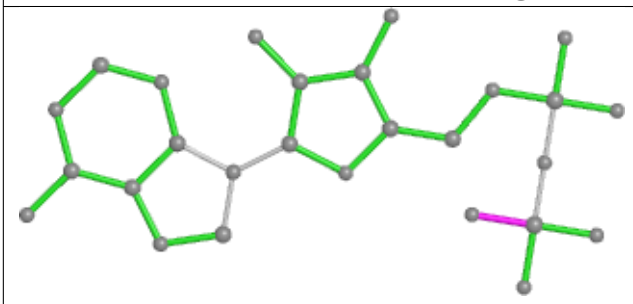


Torsions

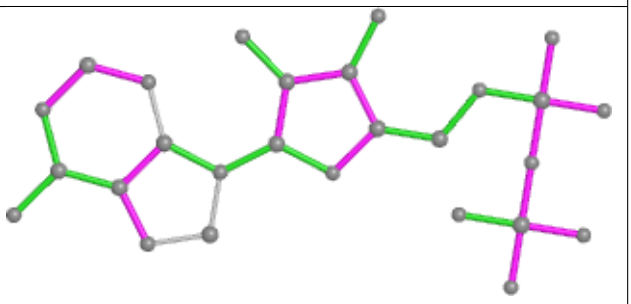


Rings

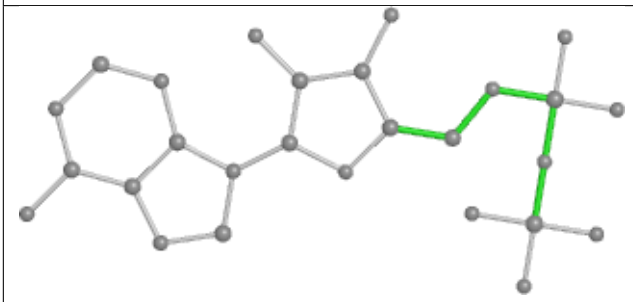
Ligand ADP A 4406



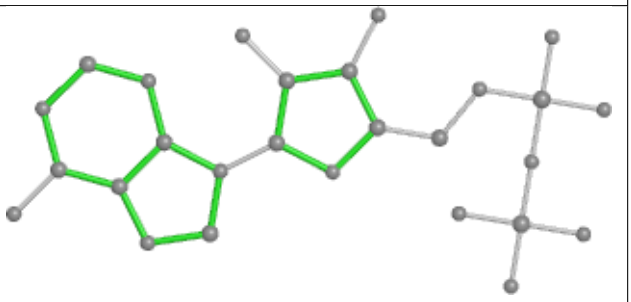
Bond lengths



Bond angles

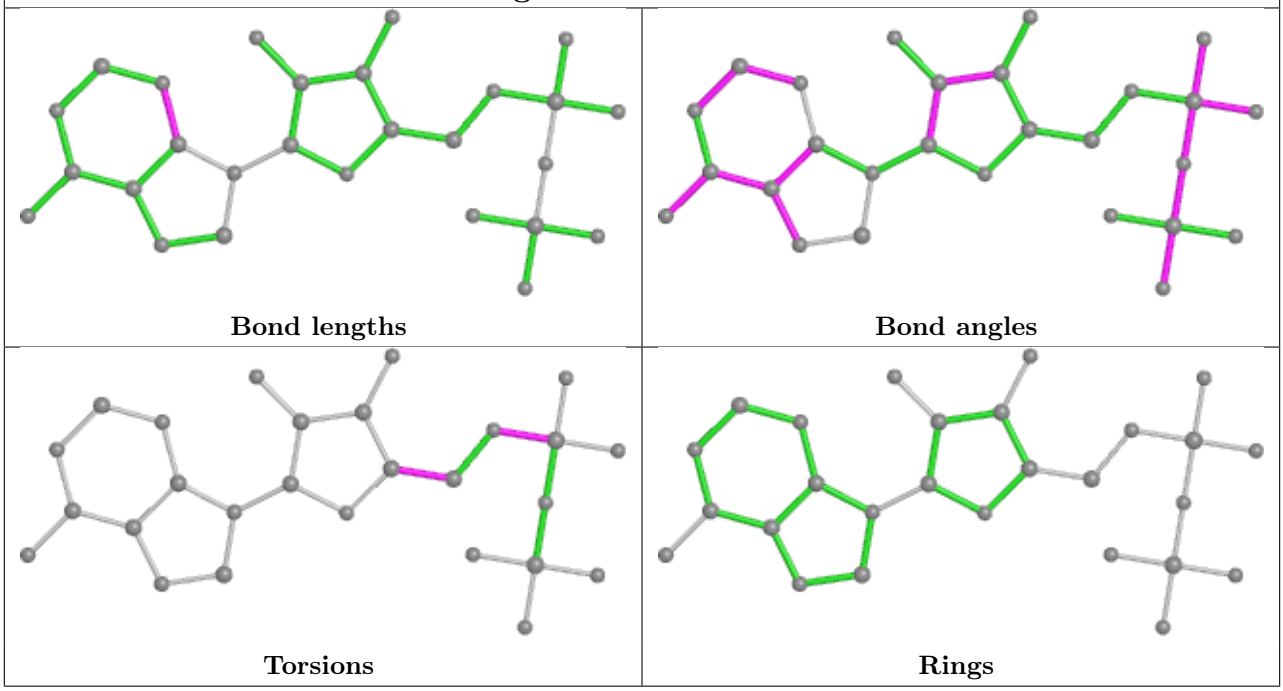


Torsions

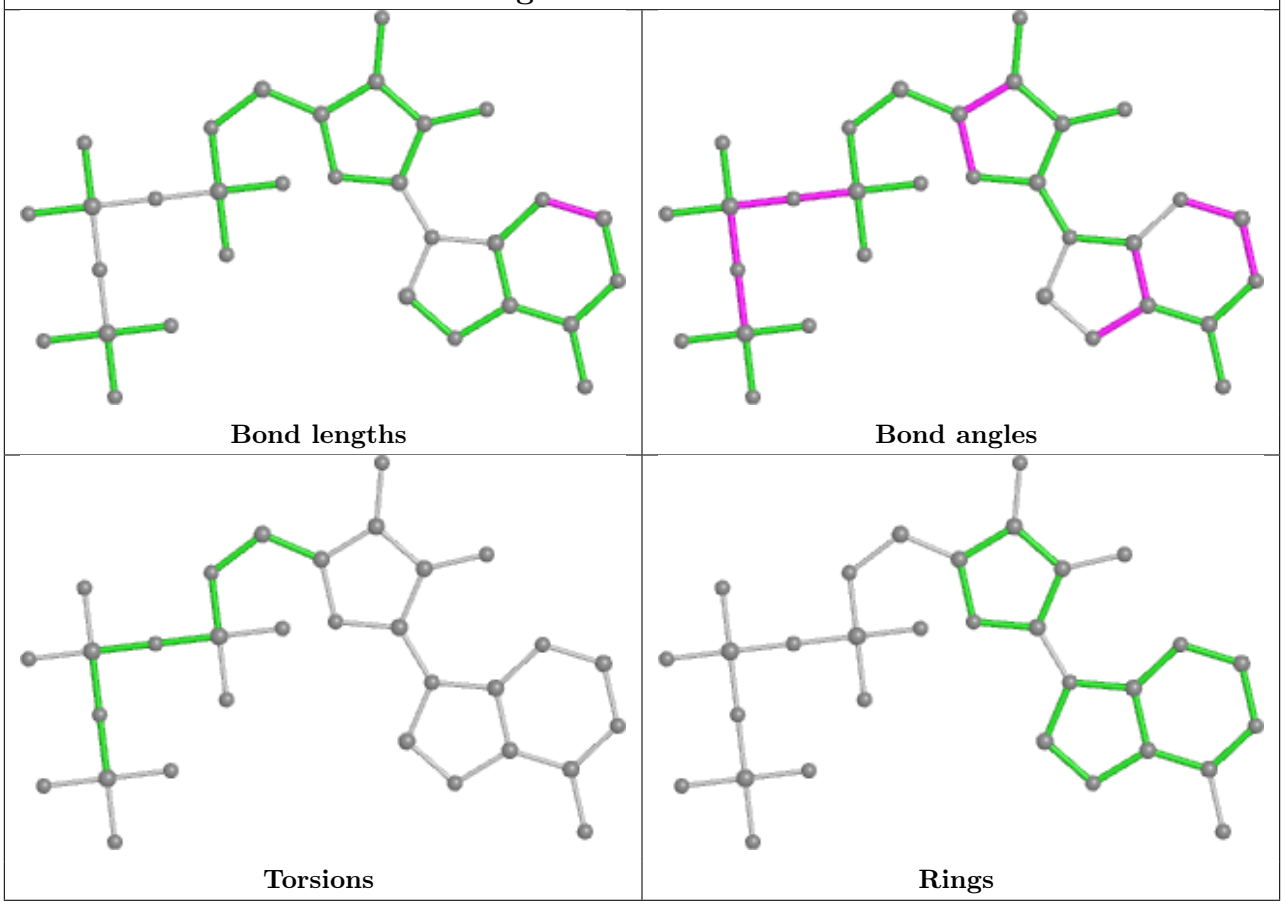


Rings

Ligand ADP A 4405



Ligand ATP A 4403



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	3005/3450 (87%)	-0.31	85 (2%) 53 52	39, 110, 274, 477	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3130	LEU	8.1
1	A	2975	ASP	5.9
1	A	3136	SER	5.5
1	A	2942	SER	4.7
1	A	2946	ALA	4.5
1	A	3134	LEU	4.4
1	A	2949	GLN	4.1
1	A	2945	ASP	4.0
1	A	3138	GLY	3.9
1	A	3133	LEU	3.9
1	A	2915	ASN	3.8
1	A	2953	LEU	3.7
1	A	3139	GLN	3.7
1	A	3123	THR	3.7
1	A	3135	ASN	3.7
1	A	2918	ALA	3.6
1	A	3131	GLU	3.6
1	A	2909	ALA	3.5
1	A	2964	VAL	3.5
1	A	2947	SER	3.5
1	A	2911	VAL	3.4
1	A	2907	ALA	3.3
1	A	2937	GLN	3.2
1	A	3238	PHE	3.2
1	A	3142	SER	3.2
1	A	2956	LEU	3.2
1	A	3137	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1579	THR	3.1
1	A	3019	GLY	3.1
1	A	2938	MET	3.1
1	A	2951	THR	3.0
1	A	4030	LYS	3.0
1	A	3156	ALA	2.9
1	A	3533	ASN	2.8
1	A	4056	LEU	2.8
1	A	3128	ARG	2.8
1	A	3144	LEU	2.8
1	A	1318	TYR	2.7
1	A	3642	PHE	2.7
1	A	2935	ALA	2.7
1	A	3451	ILE	2.7
1	A	3910	ALA	2.7
1	A	4029	SER	2.6
1	A	2902	SER	2.6
1	A	2912	ASP	2.6
1	A	4031	PHE	2.6
1	A	2906	GLU	2.6
1	A	3187	ASN	2.6
1	A	3132	GLU	2.6
1	A	4026	THR	2.6
1	A	3143	GLU	2.5
1	A	3154	GLU	2.5
1	A	1321	PHE	2.5
1	A	3125	ASP	2.5
1	A	3025	GLY	2.5
1	A	1653	TYR	2.5
1	A	2944	GLN	2.5
1	A	3159	GLU	2.4
1	A	3129	LYS	2.4
1	A	3121	LYS	2.4
1	A	3153	SER	2.4
1	A	3127	LYS	2.4
1	A	3155	ALA	2.3
1	A	3448	GLN	2.3
1	A	3141	VAL	2.3
1	A	2962	GLU	2.3
1	A	3037	PHE	2.3
1	A	3168	THR	2.2
1	A	2900	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	3126	ARG	2.2
1	A	3119	ASN	2.2
1	A	2943	MET	2.2
1	A	2939	ILE	2.2
1	A	2950	LYS	2.2
1	A	2941	VAL	2.2
1	A	2952	GLU	2.1
1	A	2979	LYS	2.1
1	A	2919	GLY	2.1
1	A	2933	ASP	2.1
1	A	3076	PRO	2.1
1	A	2965	VAL	2.0
1	A	2893	ARG	2.0
1	A	4057	ILE	2.0
1	A	2922	SER	2.0
1	A	3145	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

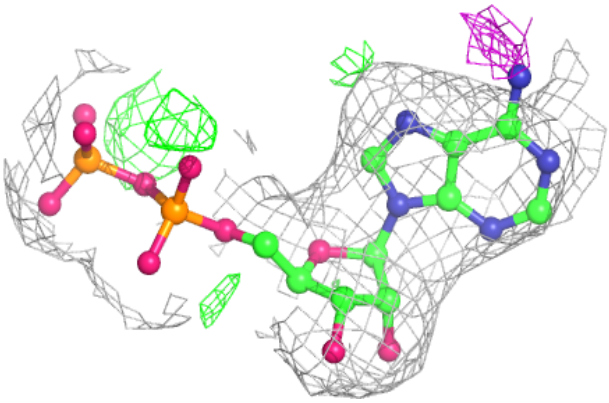
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

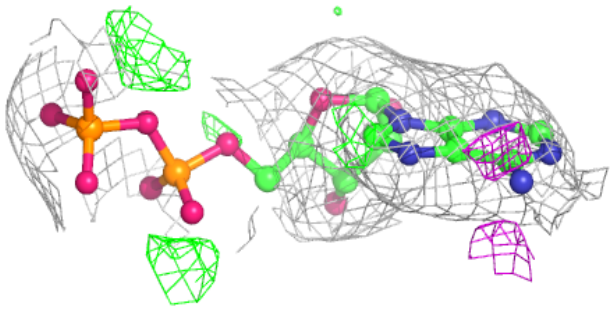
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ADP	A	4406	27/27	0.95	0.20	66,85,103,111	0
5	ADP	A	4405	27/27	0.97	0.18	42,46,57,61	0
4	ATP	A	4403	31/31	0.97	0.18	49,80,97,108	0
2	AOV	A	4401	32/32	0.98	0.20	41,69,88,93	0
3	MG	A	4402	1/1	0.99	0.21	31,31,31,31	0
3	MG	A	4404	1/1	1.00	0.22	22,22,22,22	0

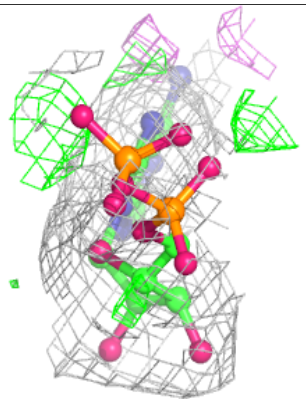
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 4406:

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

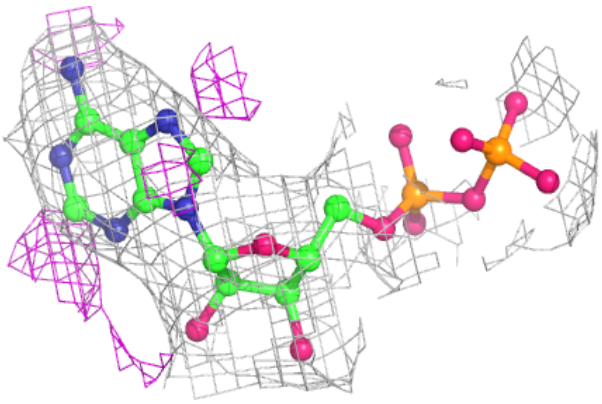


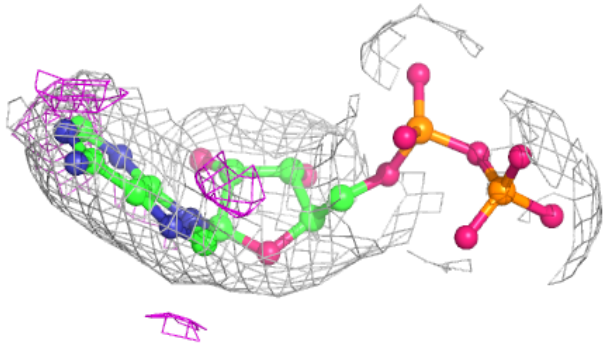


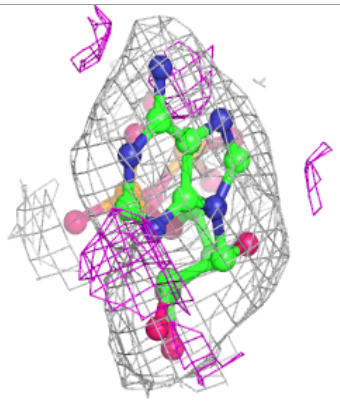


Electron density around ADP A 4405:

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

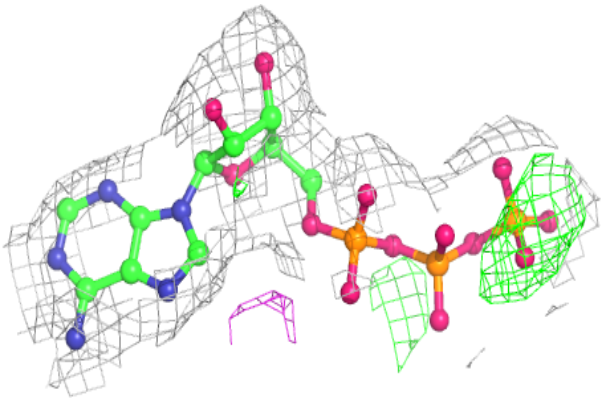


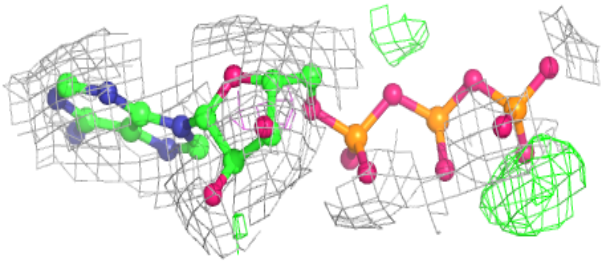


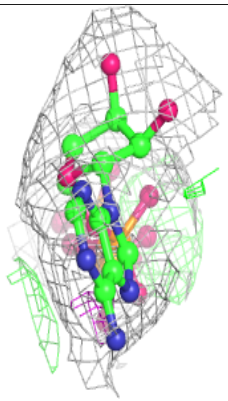


Electron density around ATP A 4403:

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

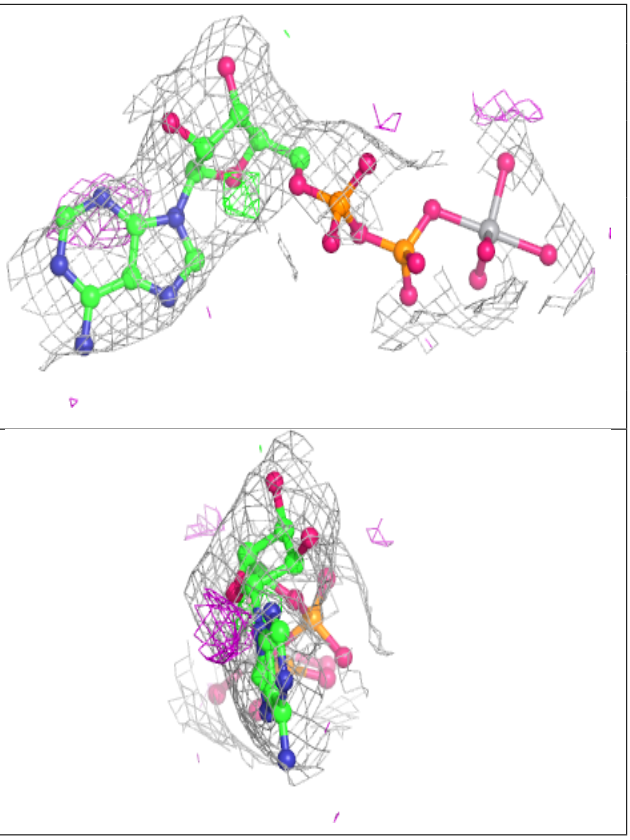






Electron density around AOV A 4401:

$2mF_o$-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.