wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:57 PM GMT

PDB ID	:	3VKG
Title	:	X-ray structure of an MTBD truncation mutant of dynein motor domain
Authors	:	Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on	:	2011-11-16
Resolution	:	2.81 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

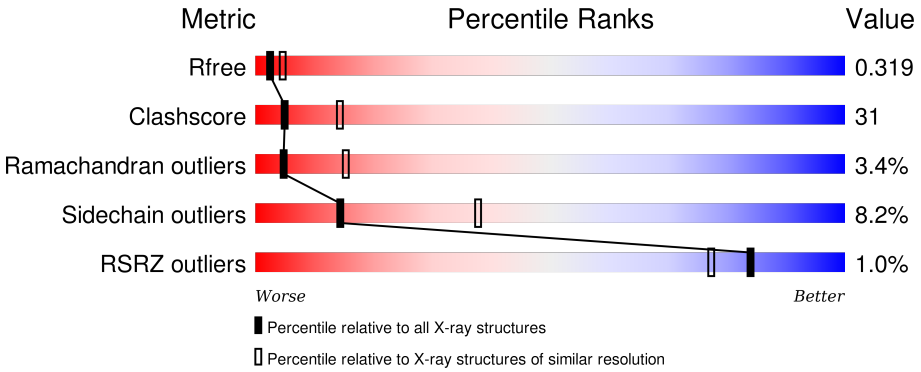
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.81 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}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	3245	% 44% 41% 5% 9%
1	B	3245	% 44% 38% 6% 12%

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	SPM	A	9016	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 45284 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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2954	Total	C	N	O	S	0	0	0
			22821	14585	3870	4270	96			
1	B	2853	Total	C	N	O	S	0	0	0
			22146	14131	3745	4174	96			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	EXPRESSION TAG	UNP P34036
A	1365	THR	-	EXPRESSION TAG	UNP P34036
A	1366	ARG	-	EXPRESSION TAG	UNP P34036
A	1367	HIS	-	EXPRESSION TAG	UNP P34036
A	1368	HIS	-	EXPRESSION TAG	UNP P34036
A	1369	HIS	-	EXPRESSION TAG	UNP P34036
A	1370	HIS	-	EXPRESSION TAG	UNP P34036
A	1371	HIS	-	EXPRESSION TAG	UNP P34036
A	1372	HIS	-	EXPRESSION TAG	UNP P34036
A	1373	GLY	-	EXPRESSION TAG	UNP P34036
A	1374	GLY	-	EXPRESSION TAG	UNP P34036
A	1375	GLY	-	EXPRESSION TAG	UNP P34036
A	1376	ASP	-	EXPRESSION TAG	UNP P34036
A	1377	TYR	-	EXPRESSION TAG	UNP P34036
A	1378	LYS	-	EXPRESSION TAG	UNP P34036
A	1379	ASP	-	EXPRESSION TAG	UNP P34036
A	1380	ASP	-	EXPRESSION TAG	UNP P34036
A	1381	ASP	-	EXPRESSION TAG	UNP P34036
A	1382	ASP	-	EXPRESSION TAG	UNP P34036
A	1383	LYS	-	EXPRESSION TAG	UNP P34036
A	1384	GLY	-	EXPRESSION TAG	UNP P34036
A	1385	GLY	-	EXPRESSION TAG	UNP P34036
A	1386	GLY	-	EXPRESSION TAG	UNP P34036
A	1387	LYS	-	EXPRESSION TAG	UNP P34036
A	3494	THR	-	LINKER	UNP P34036

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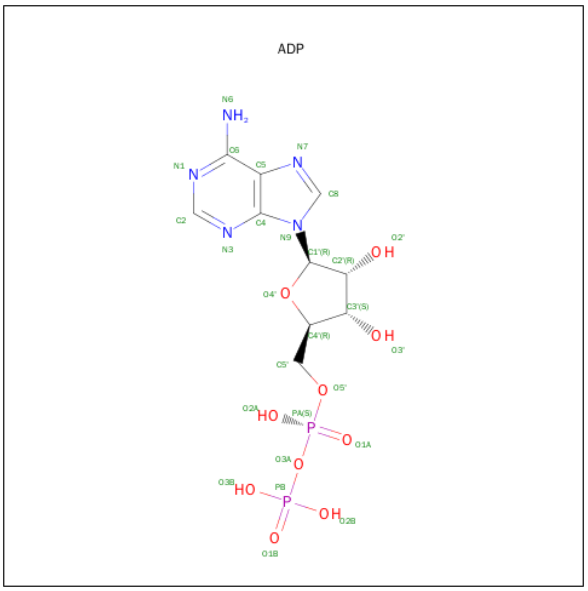
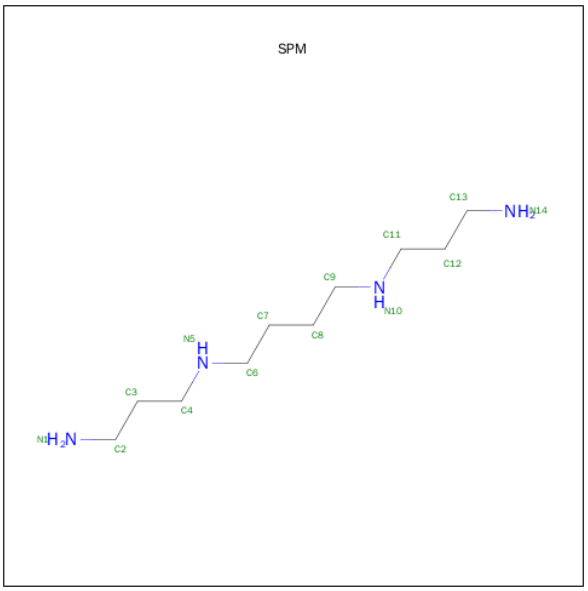
Chain	Residue	Modelled	Actual	Comment	Reference
A	3495	GLY	-	LINKER	UNP P34036
B	1364	MET	-	EXPRESSION TAG	UNP P34036
B	1365	THR	-	EXPRESSION TAG	UNP P34036
B	1366	ARG	-	EXPRESSION TAG	UNP P34036
B	1367	HIS	-	EXPRESSION TAG	UNP P34036
B	1368	HIS	-	EXPRESSION TAG	UNP P34036
B	1369	HIS	-	EXPRESSION TAG	UNP P34036
B	1370	HIS	-	EXPRESSION TAG	UNP P34036
B	1371	HIS	-	EXPRESSION TAG	UNP P34036
B	1372	HIS	-	EXPRESSION TAG	UNP P34036
B	1373	GLY	-	EXPRESSION TAG	UNP P34036
B	1374	GLY	-	EXPRESSION TAG	UNP P34036
B	1375	GLY	-	EXPRESSION TAG	UNP P34036
B	1376	ASP	-	EXPRESSION TAG	UNP P34036
B	1377	TYR	-	EXPRESSION TAG	UNP P34036
B	1378	LYS	-	EXPRESSION TAG	UNP P34036
B	1379	ASP	-	EXPRESSION TAG	UNP P34036
B	1380	ASP	-	EXPRESSION TAG	UNP P34036
B	1381	ASP	-	EXPRESSION TAG	UNP P34036
B	1382	ASP	-	EXPRESSION TAG	UNP P34036
B	1383	LYS	-	EXPRESSION TAG	UNP P34036
B	1384	GLY	-	EXPRESSION TAG	UNP P34036
B	1385	GLY	-	EXPRESSION TAG	UNP P34036
B	1386	GLY	-	EXPRESSION TAG	UNP P34036
B	1387	LYS	-	EXPRESSION TAG	UNP P34036
B	3494	THR	-	LINKER	UNP P34036
B	3495	GLY	-	LINKER	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 14 10 4	0	0
3	A	1	Total C N 14 10 4	0	0
3	B	1	Total C N 14 10 4	0	0
3	B	1	Total C N 14 10 4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

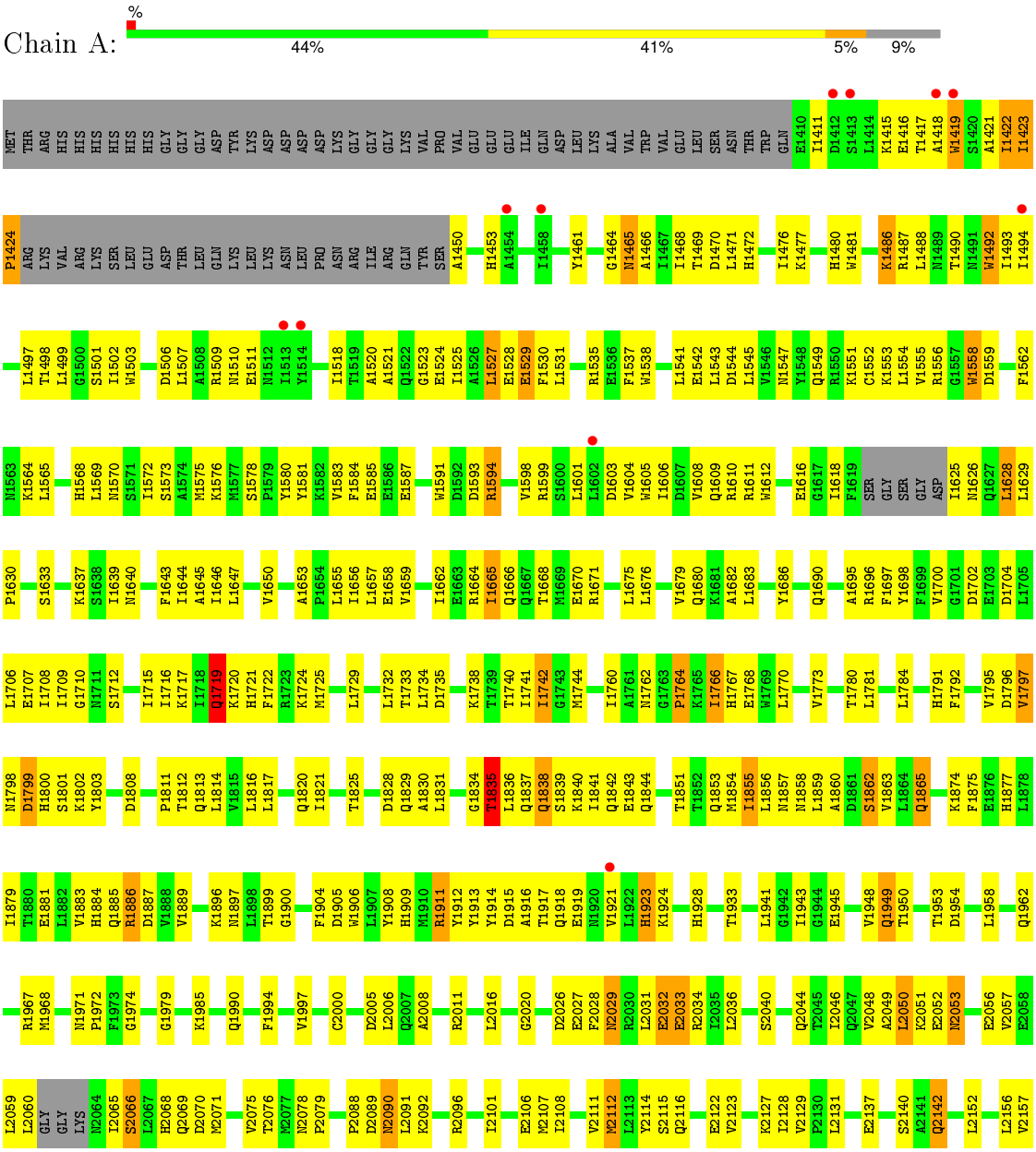
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O 23 23	0	0
5	B	19	Total O 19 19	0	0

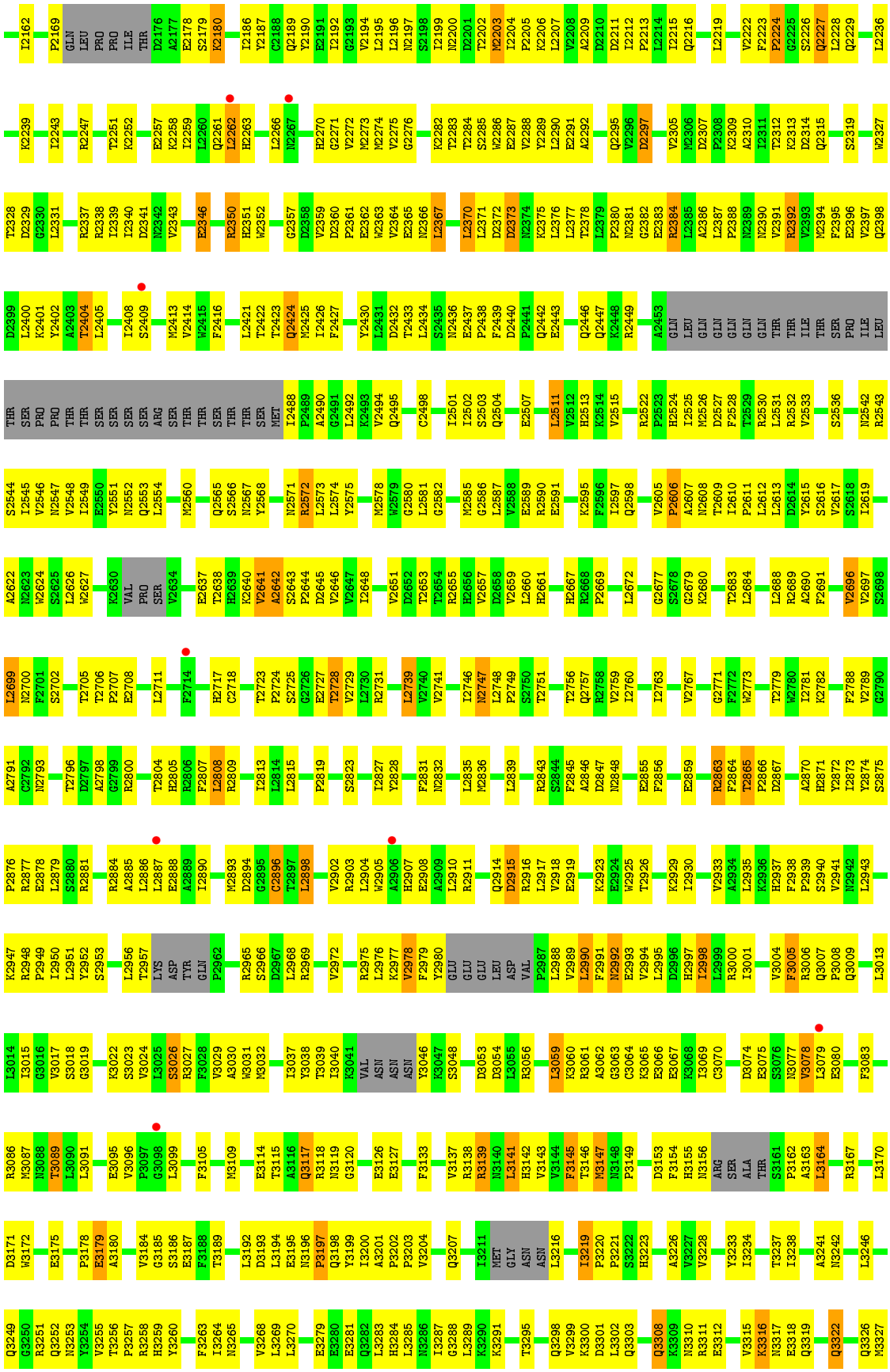
3 Residue-property plots (i)

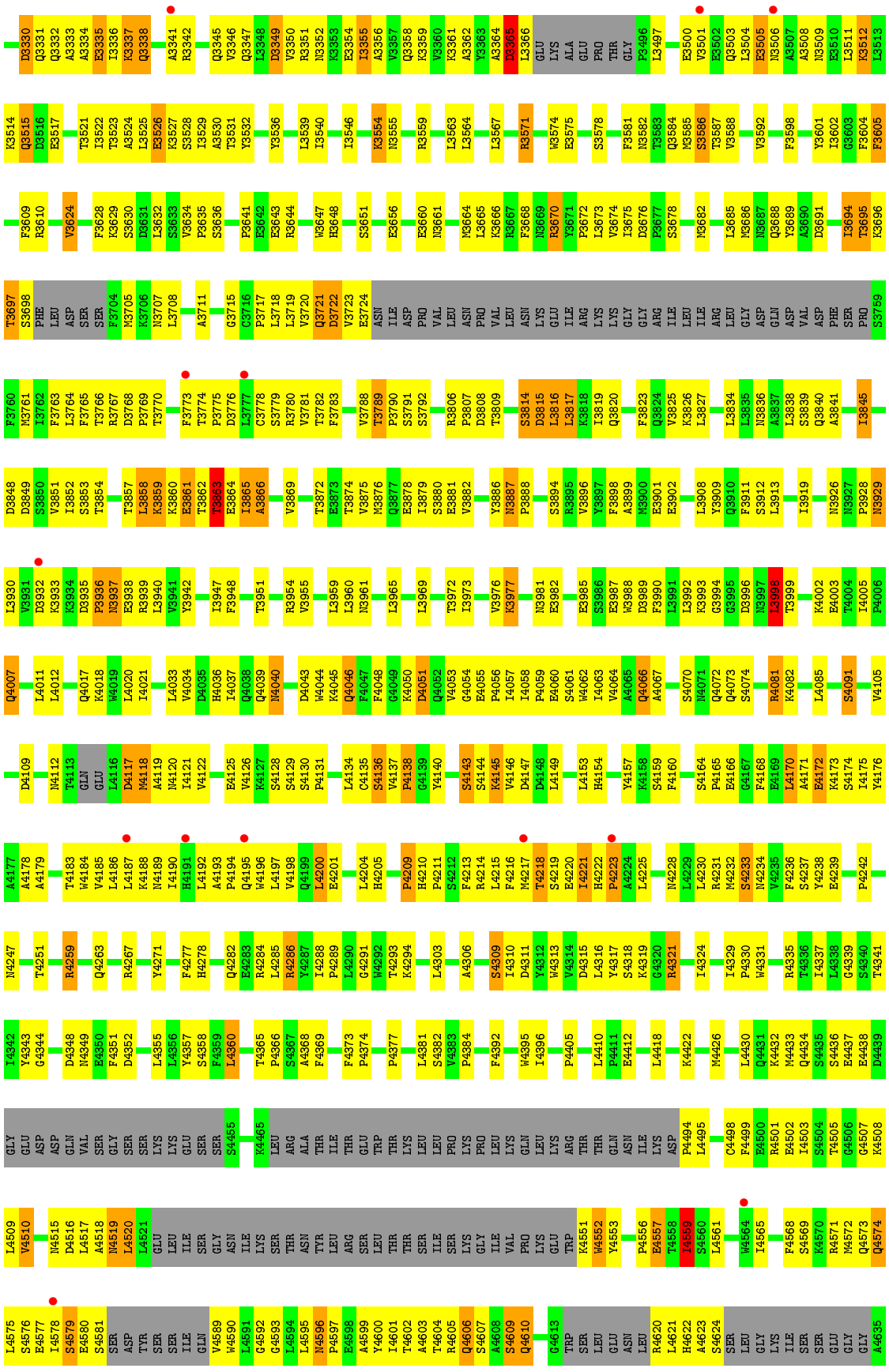
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

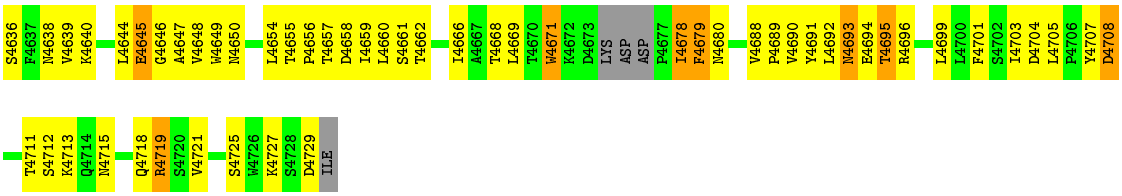
- Molecule 1: Dynein heavy chain, cytoplasmic

Chain A:



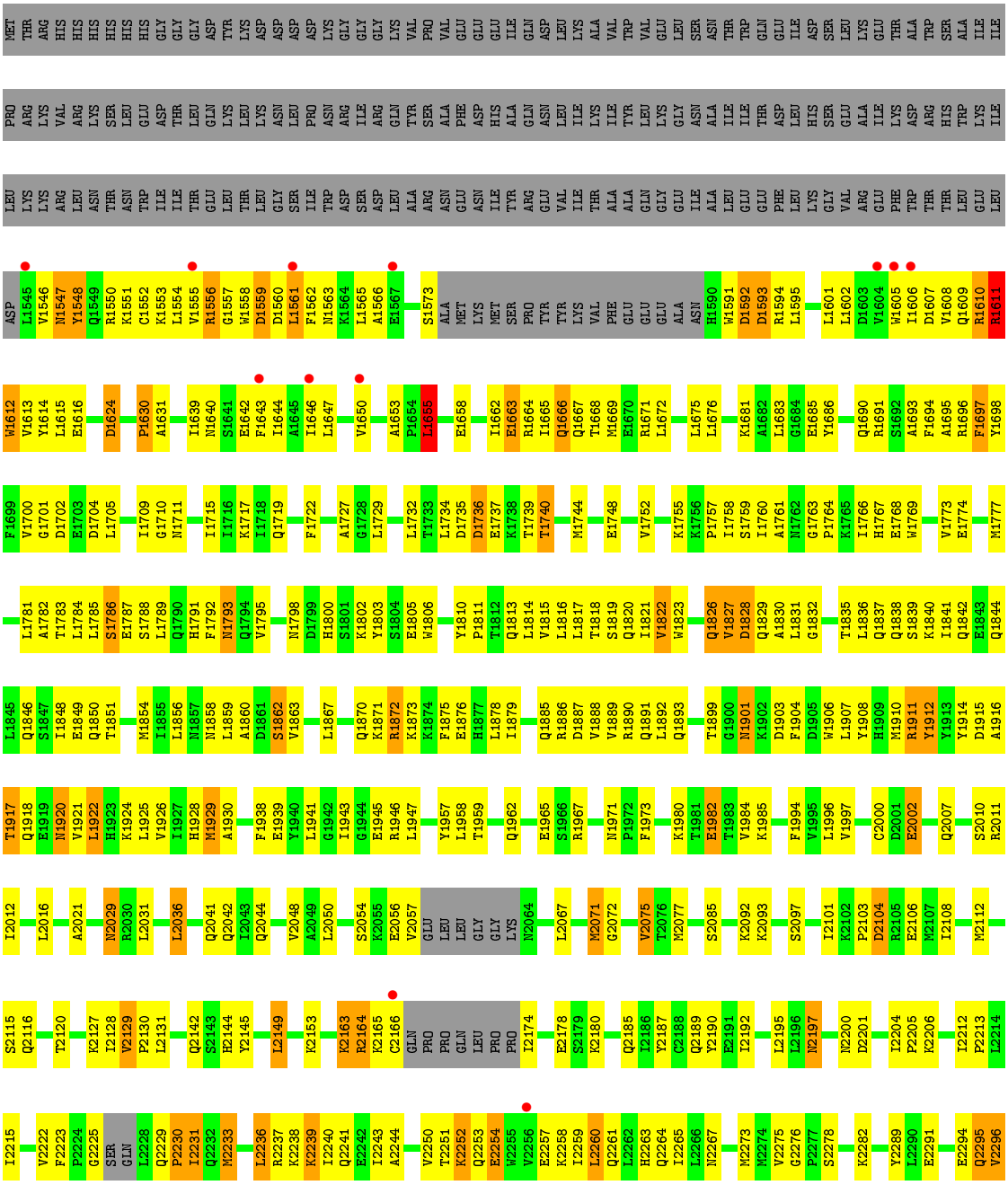


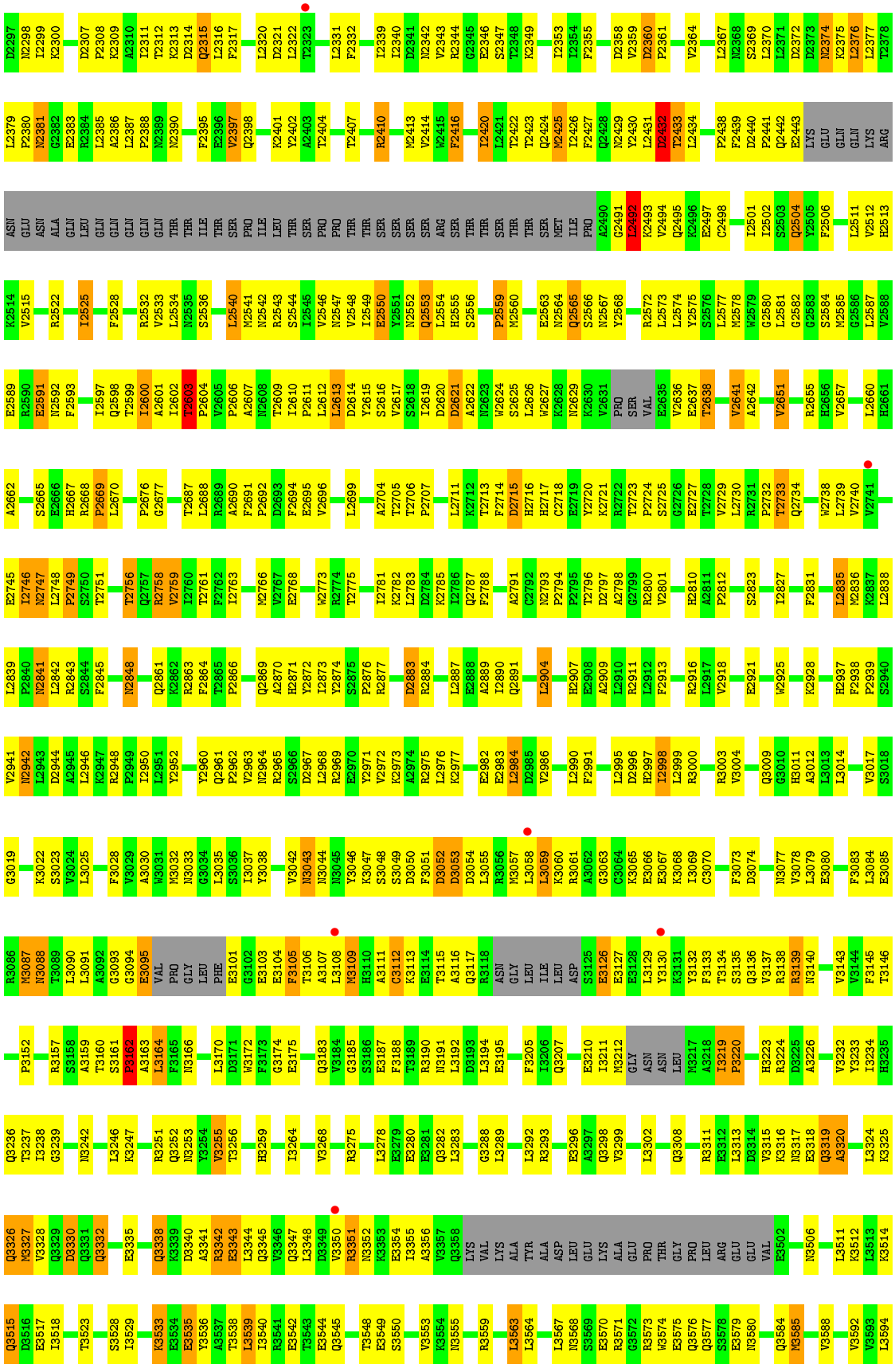




• Molecule 1: Dynein heavy chain, cytoplasmic

Chain B:




D2297 N2298 I2299 K2300 D2307 P2308 K2309 A2310 I2311 T2312 K2313 D2314 Q2315 L2316 F2317 L2320 D2321 L2322 T2323 L2331 F2332 I2339 I2340 D2341 N2342 V2343 R2344 G2345 E2346 S2347 T2348 K2349 I2353 I2354 F2355 D2358 V2359 D2360 P2361 V2364 L2367 N2368 S2369 L2370 L2371 D2372 D2373 N2374 K2375 L2376 L2377 T2378
L2379 P2380 N2381 G2382 E2383 R2384 L2385 A2386 L2387 P2388 N2389 N2390 F2395 E2396 V2397 Q2398 K2401 Y2402 A2403 T2404 T2407 R2410 M2413 V2414 W2415 F2416 I2420 L2421 T2422 T2423 Q2424 M2425 I2426 F2427 Q2428 N2429 Y2430 L2431 D2432 T2433 L2434 P2438 F2439 D2440 P2441 Q2442 E2443 LYS GLU GLN GLN LYS ARG
ASN GLU ASN ALA GLN LEU GLN GLN GLN GLN THR THR ILE THR SER PRO ILE LEU THR SER PRO PRO THR THR SER SER SER ARG SER THR THR THR SER THR THR SER MET ILE PRO A2490 G2491 L2492 K2493 V2494 Q2495 K2496 E2497 C2498 I2501 I2502 S2503 Q2504 Y2505 F2506 L2511 V2512 H2513
K2514 V2515 R2522 I2525 F2528 R2532 V2533 L2534 N2535 S2536 L2540 M2541 N2542 R2543 S2544 I2545 V2546 N2547 V2548 I2549 E2550 Y2551 N2552 Q2553 L2554 H2555 S2556 P2559 M2560 E2563 N2564 Q2565 S2566 N2567 Y2568 R2572 L2573 L2574 Y2575 S2576 L2577 M2578 W2579 G2580 L2581 G2582 G2583 S2584 M2585 G2586 L2587 V2588
E2589 R2590 E2591 N2592 F2593 I2597 Q2598 T2599 I2600 A2601 I2602 T2603 P2604 V2605 P2606 A2607 N2608 T2609 I2610 P2611 L2612 L2613 D2614 Y2615 S2616 V2617 S2618 I2619 D2620 D2621 A2622 N2623 W2624 S2625 L2626 W2627 K2628 N2629 K2630 V2631 PRO SER VAL E2635 V2636 E2637 T2638 V2641 A2642 V2651 R2655 H2656 V2657 L2660 H2661
A2662 S2665 E2666 H2667 R2668 P2669 L2670 P2676 G2677 T2687 L2688 R2689 A2690 F2691 P2692 D2693 F2694 E2695 V2696 L2699 A2704 T2705 T2706 P2707 L2711 K2712 T2713 F2714 D2715 H2716 H2717 C2718 E2719 Y2720 K2721 R2722 T2723 P2724 S2725 G2726 E2727 T2728 V2729 L2730 R2731 P2732 T2733 Q2734 W2738 L2739 V2740 V2741
E2745 I2746 N2747 L2748 P2749 S2750 T2751 T2756 Q2757 R2758 V2759 I2760 T2761 F2762 I2763 M2766 V2767 E2768 W2773 R2774 T2775 I2781 K2782 L2783 D2784 K2785 I2786 Q2787 F2788 A2791 C2792 N2793 P2794 P2795 T2796 D2797 A2798 G2799 R2800 V2801 H2810 A2811 P2812 S2823 I2827 F2831 L2835 M2836 K2837 L2838
L2839 P2840 N2841 L2842 R2843 S2844 F2845 N2848 Q2861 K2862 R2863 F2864 T2865 P2866 Q2869 A2870 H2871 Y2872 I2873 Y2874 S2875 P2876 R2877 D2883 R2884 L2887 E2888 A2889 I2890 Q2891 L2904 H2907 E2908 A2909 L2910 R2911 L2912 F2913 R2916 L2917 V2918 E2921 W2925 K2928 H2937 F2938 P2939 S2940
V2941 N2942 L2943 D2944 A2945 L2946 K2947 R2948 P2949 I2950 L2951 Y2952 Y2960 Q2961 P2962 V2963 N2964 R2965 S2966 D2967 L2968 R2969 E2970 Y2971 V2972 K2973 A2974 R2975 L2976 K2977 E2982 E2983 L2984 D2985 V2986 L2990 F2991 L2995 D2996 H2997 I2998 L2999 R3000 R3003 V3004 Q3009 G3010 H3011 A3012 L3013 L3014 V3017 S3018
G3019 K3022 S3023 V3024 L3025 F3028 V3029 A3030 W3031 M3032 N3033 G3034 L3035 S3036 I3037 Y3038 V3042 N3043 N3044 N3045 Y3046 K3047 S3048 S3049 D3050 F3051 D3052 D3053 D3054 L3055 R3056 M3057 L3058 L3059 K3060 R3061 A3062 G3063 C3064 K3065 E3066 E3067 K3068 I3069 C3070 F3073 D3074 N3077 V3078 L3079 E3080 F3083 L3084 E3085
R3086 M3087 N3088 T3089 L3090 L3091 A3092 G3093 G3094 E3095 VAL PRO GLY LEU PHE E3101 G3102 E3103 E3104 F3105 T3106 A3107 T3108 M3109 H3110 A3111 C3112 K3113 E3114 T3115 A3116 Q3117 R3118 ASN GLY LEU ILE LEU ASP S3125 E3126 E3127 E3128 L3129 Y3130 K3131 Y3132 F3133 T3134 S3135 Q3136 V3137 R3138 R3139 N3140 V3143 V3144 F3145 T3146
P3352 R3157 S3158 A3159 T3160 S3161 P3162 A3163 L3164 F3165 N3166 L3170 D3171 W3172 F3173 G3174 E3175 Q3183 V3184 G3185 S3186 E3187 F3188 T3189 R3190 N3191 L3192 D3193 L3194 E3195 F3205 I3206 Q3207 E3210 I3211 M3212 GLY ASN ASN LEU M3217 A3218 I3219 P3220 H3223 R3224 D3225 A3226 V3232 Y3233 I3234 H3235
Q3236 T3237 I3238 G3239 N3242 L3246 K3247 R3251 Q3252 N3253 Y3254 V3255 T3256 H3259 I3264 V3268 R3275 L3278 E3279 E3280 E3281 Q3282 L3283 G3288 L3289 L3292 R3293 E3296 A3297 Q3298 V3299 L3302 Q3308 R3311 E3312 L3313 D3314 V3315 K3316 N3317 E3318 Q3319 A3320 L3324 K3325
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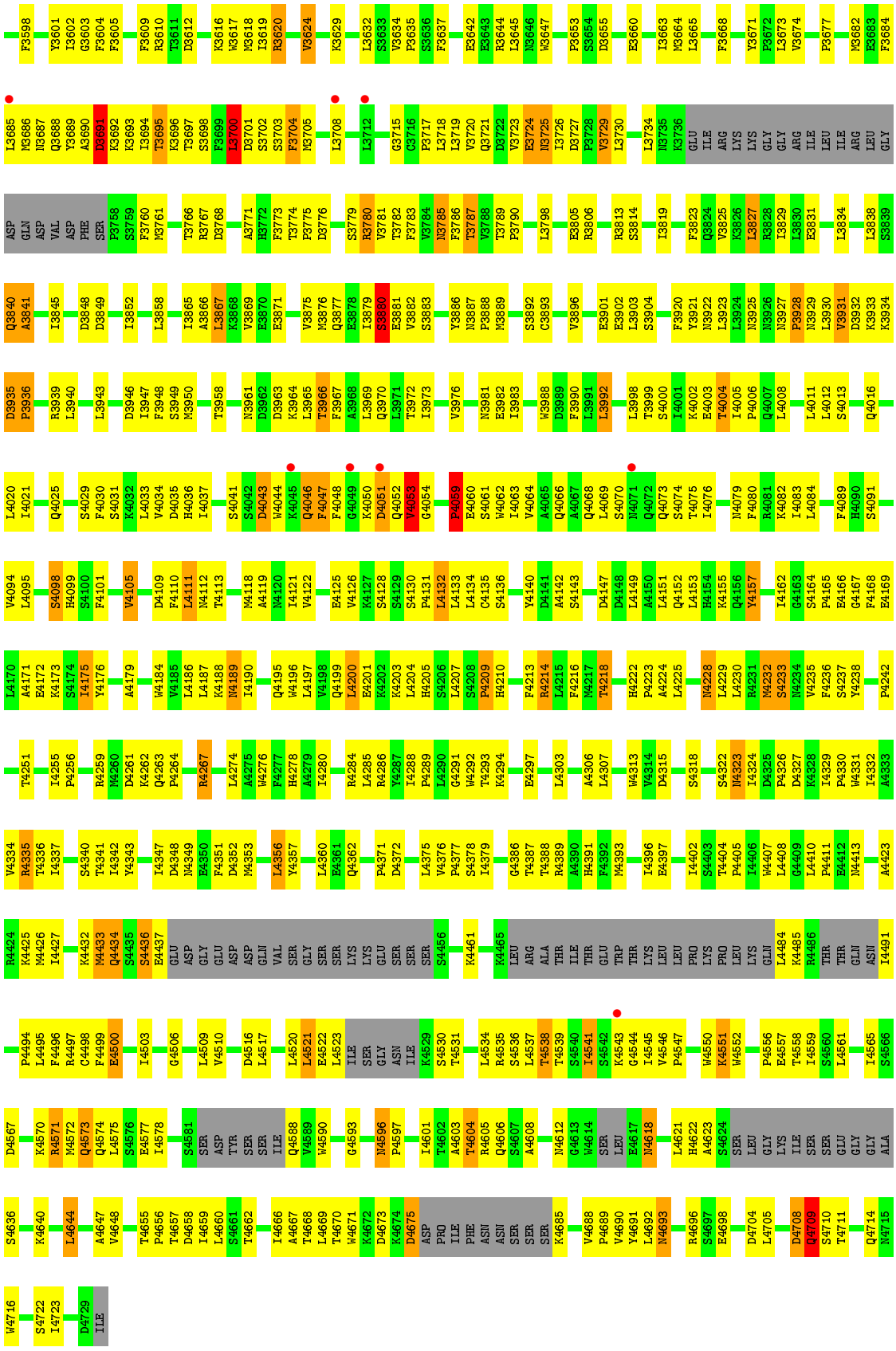
Q3515 D3516 E3517 I3518 T3523 S3528 I3529 K3533 E3534 E3535 Y3536 A3537 T3538 L3539 I3540 R3541 E3542 T3543 E3544 Q3545 T3548 E3549 S3550 V3553 K3554 N3555 R3559 L3563 L3564 L3567 N3568 S3569 E3570 R3571 G3572 R3573 W3574 E3575 Q3576 Q3577 S3578 E3579 N3580 Q3584 M3585 V3588 V3592 V3593 L3594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L4170 A4171 E4172 K4173 S4174 I4175 Y4176 A4179 W4184 V4185 L4186 L4187 K4188 N4189 I4190 Q4195 W4196 L4197 V4198 Q4199 L4200 E4201 K4202 K4203 L4204 H4205 S4206 L4207 S4208 P4209 H4210 F4213 R4214 L4215 F4216 M4217 T4218 H4222 P4223 A4224 L4225 N4228 L4229 L4230 R4231 M4232 S4233 N4234 V4235 F4236 S4237 Y4238 P4242
T4251 I4255 P4256 R4259 M4260 D4261 K4262 Q4263 P4264 R4267 L4274 A4275 W4276 F4277 H4278 A4279 T4280 R4284 L4285 R4286 Y4287 I4288 P4289 L4290 G4291 W4292 T4293 K4294 E4297 L4303 A4306 L4307 W4313 V4314 D4315 S4318 S4322 N4323 I4324 D4325 P4326 D4327 K4328 I4329 P4330 W4331 I4332 A4333
V4334 R4335 T4336 I4337 S4340 T4341 I4342 Y4343 I4347 D4348 N4349 E4350 F4351 D4352 M4353 L4356 Y4357 L4360 E4361 Q4362 P4371 D4372 L4375 V4376 P4377 S4378 I4379 G4386 T4387 T4388 R4389 A4390 H4391 F4392 M4393 I4396 E4397 I4402 S4403 T4404 P4405 I4406 W4407 L4408 G4409 L4410 P4411 E4412 N4413 A4423
R4424 K4425 M4426 I4427 K4432 M4433 Q4434 S4435 S4436 E4437 GLU ASP GLY GLU ASP ASP GLN VAL SER GLY SER SER LYS LYS GLU SER SER S4456 K4461 K4465 LEU ARG ALA THR ILE THR GLU TRP THR LYS LEU LEU PRO LYS PRO LEU LYS GLN L4484 K4485 R4486 THR THR GLN ASN I4491
P4494 L4495 F4496 R4497 C4498 F4499 E4500 I4503 G4506 L4509 V4510 D4516 L4517 L4520 L4521 E4522 L4523 ILE SER GLY ASN ILE K4529 S4530 T4531 L4534 R4535 S4536 L4537 T4538 T4539 S4540 I4541 S4542 K4543 G4544 I4545 V4546 P4547 W4550 K4551 W4552 P4556 E4557 T4558 I4559 S4560 L4561 I4565 S4566
D4567 K4570 R4571 M4572 Q4573 Q4574 L4575 S4576 E4577 I4578 S4581 SER ASP TYR SER SER ILE Q4588 V4589 W4590 G4593 N4596 P4597 I4601 T4602 A4603 T4604 R4605 Q4606 S4607 A4608 N4612 G4613 W4614 SER LEU E4617 N4618 L4621 H4622 A4623 S4624 SER LEU GLY LYS ILE SER SER GLU GLY GLY ALA
S4636 K4640 L4644 A4647 V4648 T4655 P4656 T4657 D4658 I4659 L4660 S4661 T4662 I4666 A4667 T4668 L4669 T4670 W4671 K4672 D4673 K4674 D4675 ASP PRO ILE PHE ASN ASN SER SER K4685 V4688 P4689 V4690 Y4691 L4692 N4693 R4696 S4697 E4698 D4704 L4705 D4708 Q4709 S4710 T4711 Q4714 N4715
W4716 S4722 I4723 D4729 ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	204.26Å 221.81Å 192.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.45 – 2.81 96.45 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (96.45-2.81) 98.1 (96.45-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.82Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.262 , 0.319 0.263 , 0.319	Depositor DCC
R_{free} test set	10413 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 209311 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	45284	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, SPM, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/23297	0.67	0/31692
1	B	0.47	0/22599	0.67	3/30724 (0.0%)
All	All	0.48	0/45896	0.67	3/62416 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2376	LEU	CA-CB-CG	6.25	129.68	115.30
1	B	4054	GLY	N-CA-C	-5.92	98.30	113.10
1	B	3219	ILE	C-N-CD	-5.09	109.41	120.60

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	22821	0	21998	1375	0
1	B	22146	0	21438	1397	0
2	A	108	0	48	14	0
2	B	108	0	48	9	0
3	A	28	0	52	2	0
3	B	28	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	23	0	0	1	0
5	B	19	0	0	1	0
All	All	45284	0	43636	2766	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 31.

The worst 5 of 2766 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:3330:ASP:HB3	1:A:3532:TYR:HE2	1.12	1.12
1:A:2902:VAL:HG21	1:A:2941:VAL:HG21	1.31	1.12
1:A:3766:THR:HG22	1:A:3768:ASP:H	1.14	1.09
1:A:2548:VAL:HG11	1:A:2565:GLN:HE21	1.20	1.06
1:B:1655:LEU:HD22	1:B:1655:LEU:H	1.20	1.05

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	2908/3245 (90%)	2474 (85%)	332 (11%)	102 (4%)	4 14
1	B	2813/3245 (87%)	2376 (84%)	347 (12%)	90 (3%)	5 16
All	All	5721/6490 (88%)	4850 (85%)	679 (12%)	192 (3%)	5 15

5 of 192 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1465	ASN
1	A	1583	VAL
1	A	1797	VAL
1	A	1835	THR
1	A	1839	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2408/2921 (82%)	2220 (92%)	188 (8%)	16	40
1	B	2369/2921 (81%)	2163 (91%)	206 (9%)	13	34
All	All	4777/5842 (82%)	4383 (92%)	394 (8%)	14	38

5 of 394 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4606	GLN
1	B	2029	ASN
1	B	4209	PRO
1	A	4655	THR
1	B	1736	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 210 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4278	HIS
1	B	1842	GLN
1	B	4199	GLN
1	A	4349	ASN
1	A	4718	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	ADP	A	9001	-	22,29,29	1.27	2 (9%)	27,45,45	2.28	7 (25%)
2	ADP	A	9002	4	22,29,29	1.43	3 (13%)	27,45,45	2.18	5 (18%)
2	ADP	A	9003	-	22,29,29	1.39	3 (13%)	27,45,45	2.32	7 (25%)
2	ADP	A	9004	-	22,29,29	1.25	2 (9%)	27,45,45	2.13	5 (18%)
3	SPM	A	9012	-	13,13,13	0.61	0	12,12,12	0.92	1 (8%)
3	SPM	A	9016	-	13,13,13	0.54	0	12,12,12	0.95	0
2	ADP	B	9007	4	22,29,29	1.16	2 (9%)	27,45,45	2.39	6 (22%)
2	ADP	B	9008	4	22,29,29	1.46	3 (13%)	27,45,45	2.14	5 (18%)
2	ADP	B	9009	-	22,29,29	1.35	2 (9%)	27,45,45	2.08	6 (22%)
2	ADP	B	9010	-	22,29,29	1.13	1 (4%)	27,45,45	2.28	4 (14%)
3	SPM	B	9018	-	13,13,13	0.58	0	12,12,12	0.90	0
3	SPM	B	9022	-	13,13,13	0.41	0	12,12,12	1.05	1 (8%)

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	ADP	A	9001	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	9002	4	-	0/12/32/32	0/3/3/3
2	ADP	A	9003	-	-	0/12/32/32	0/3/3/3
2	ADP	A	9004	-	-	0/12/32/32	0/3/3/3
3	SPM	A	9012	-	-	0/11/11/11	0/0/0/0
3	SPM	A	9016	-	-	0/11/11/11	0/0/0/0
2	ADP	B	9007	4	-	0/12/32/32	0/3/3/3
2	ADP	B	9008	4	-	0/12/32/32	0/3/3/3
2	ADP	B	9009	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9010	-	-	0/12/32/32	0/3/3/3
3	SPM	B	9018	-	-	0/11/11/11	0/0/0/0
3	SPM	B	9022	-	-	0/11/11/11	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9007	ADP	C5-N7	-2.11	1.32	1.39
2	A	9001	ADP	O4'-C4'	-2.08	1.40	1.45
2	A	9003	ADP	C4-N3	2.01	1.38	1.35
2	B	9008	ADP	O4'-C1'	2.34	1.44	1.41
2	A	9003	ADP	C2-N3	2.42	1.36	1.32

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	9007	ADP	N3-C2-N1	-10.14	121.13	128.89
2	A	9003	ADP	N3-C2-N1	-9.44	121.67	128.89
2	A	9001	ADP	N3-C2-N1	-9.18	121.86	128.89
2	A	9002	ADP	N3-C2-N1	-8.96	122.03	128.89
2	B	9008	ADP	N3-C2-N1	-8.78	122.17	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9001	ADP	1	0
2	A	9002	ADP	3	0
2	A	9003	ADP	4	0
2	A	9004	ADP	6	0
3	A	9012	SPM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9016	SPM	1	0
2	B	9007	ADP	2	0
2	B	9008	ADP	2	0
2	B	9009	ADP	2	0
2	B	9010	ADP	3	0
3	B	9018	SPM	2	0
3	B	9022	SPM	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	2954/3245 (91%)	-0.01	32 (1%)	82	75	17, 53, 78, 102	0
1	B	2853/3245 (87%)	-0.06	26 (0%)	85	79	24, 52, 75, 100	0
All	All	5807/6490 (89%)	-0.04	58 (0%)	84	77	17, 52, 77, 102	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1494	ILE	4.3
1	B	1643	PHE	3.9
1	B	1605	TRP	3.6
1	A	4191	HIS	3.4
1	B	3108	LEU	3.2

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	SPM	A	9016	14/14	0.83	0.25	2.10	43,50,54,55	0
3	SPM	A	9012	14/14	0.87	0.22	1.48	37,41,45,47	0
2	ADP	B	9008	27/27	0.93	0.23	1.45	41,51,53,54	0
4	MG	B	3	1/1	0.91	0.22	1.41	28,28,28,28	0
4	MG	A	1	1/1	0.98	0.22	1.02	44,44,44,44	0
2	ADP	A	9002	27/27	0.93	0.23	0.85	47,49,52,54	0
2	ADP	A	9001	27/27	0.96	0.21	0.82	32,38,42,44	0
3	SPM	B	9018	14/14	0.89	0.21	0.68	57,57,59,59	0
2	ADP	B	9009	27/27	0.96	0.20	0.60	39,45,48,51	0
3	SPM	B	9022	14/14	0.91	0.20	0.40	37,43,49,49	0
2	ADP	B	9007	27/27	0.96	0.20	0.21	38,47,50,52	0
2	ADP	A	9003	27/27	0.95	0.21	0.07	41,45,50,52	0
2	ADP	B	9010	27/27	0.97	0.18	-0.73	31,37,46,48	0
2	ADP	A	9004	27/27	0.96	0.15	-1.23	44,49,54,56	0
4	MG	B	2	1/1	0.87	0.14	-	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.