



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2017 – 01:47 PM EST

PDB ID : 4AKH
Title : Dynein Motor Domain - AMPPNP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.60 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029077

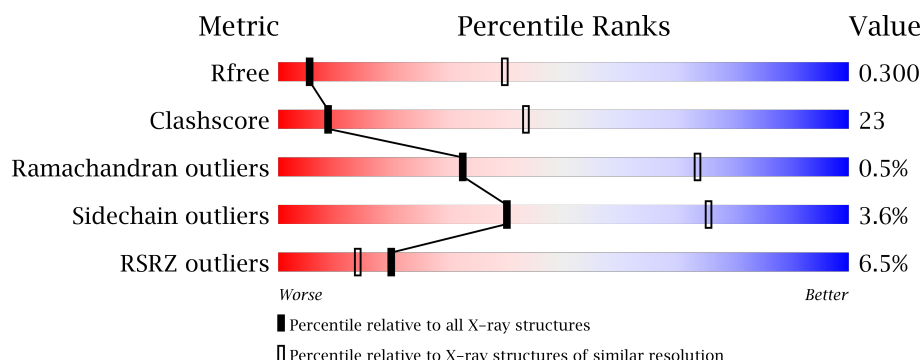
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2695	<div> <div>2%</div> <div>65%</div> <div>31%</div> <div>..</div> </div>
1	B	2695	<div> <div>10%</div> <div>67%</div> <div>30%</div> <div>..</div> </div>

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	ATP	B	5093	-	-	X	-
4	SO4	A	5095	-	-	X	-
4	SO4	B	5096	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41642 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.

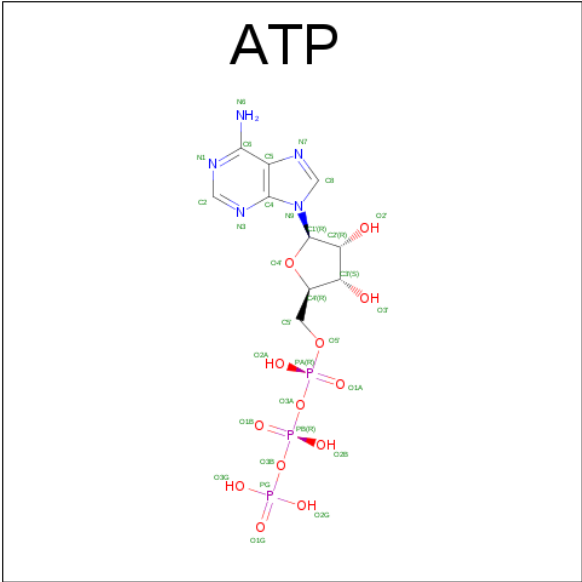
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			
1	B	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			

There are 8 discrepancies between the modelled and reference sequences:

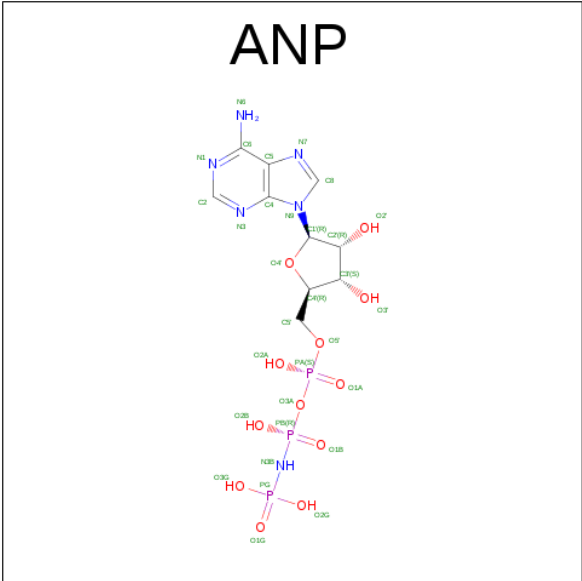
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	LINKER	UNP P36022
A	219	ASP	-	LINKER	UNP P36022
A	1630	ILE	LEU	CONFLICT	UNP P36022
A	3782	ASP	GLU	CONFLICT	UNP P36022
B	218	SER	-	LINKER	UNP P36022
B	219	ASP	-	LINKER	UNP P36022
B	1630	ILE	LEU	CONFLICT	UNP P36022
B	3782	ASP	GLU	CONFLICT	UNP P36022

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).

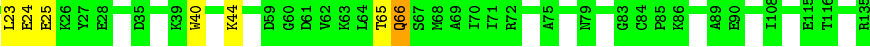


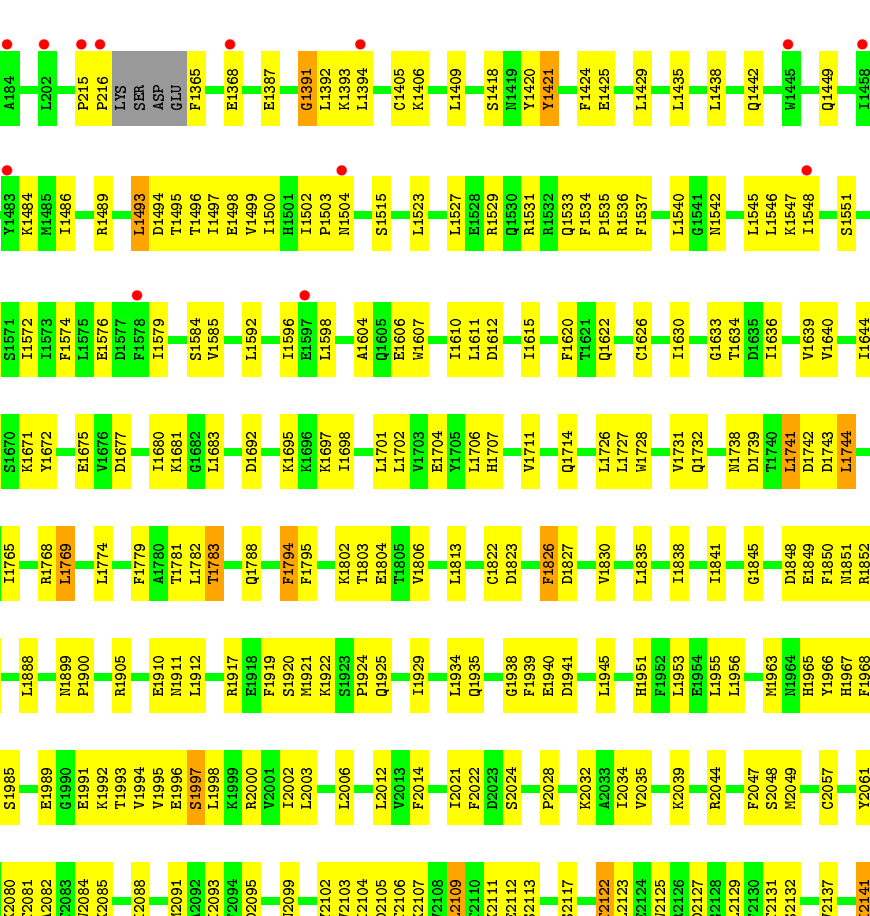
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

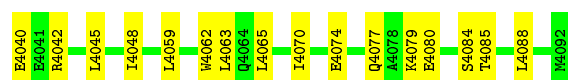
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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.

- Chain A: 

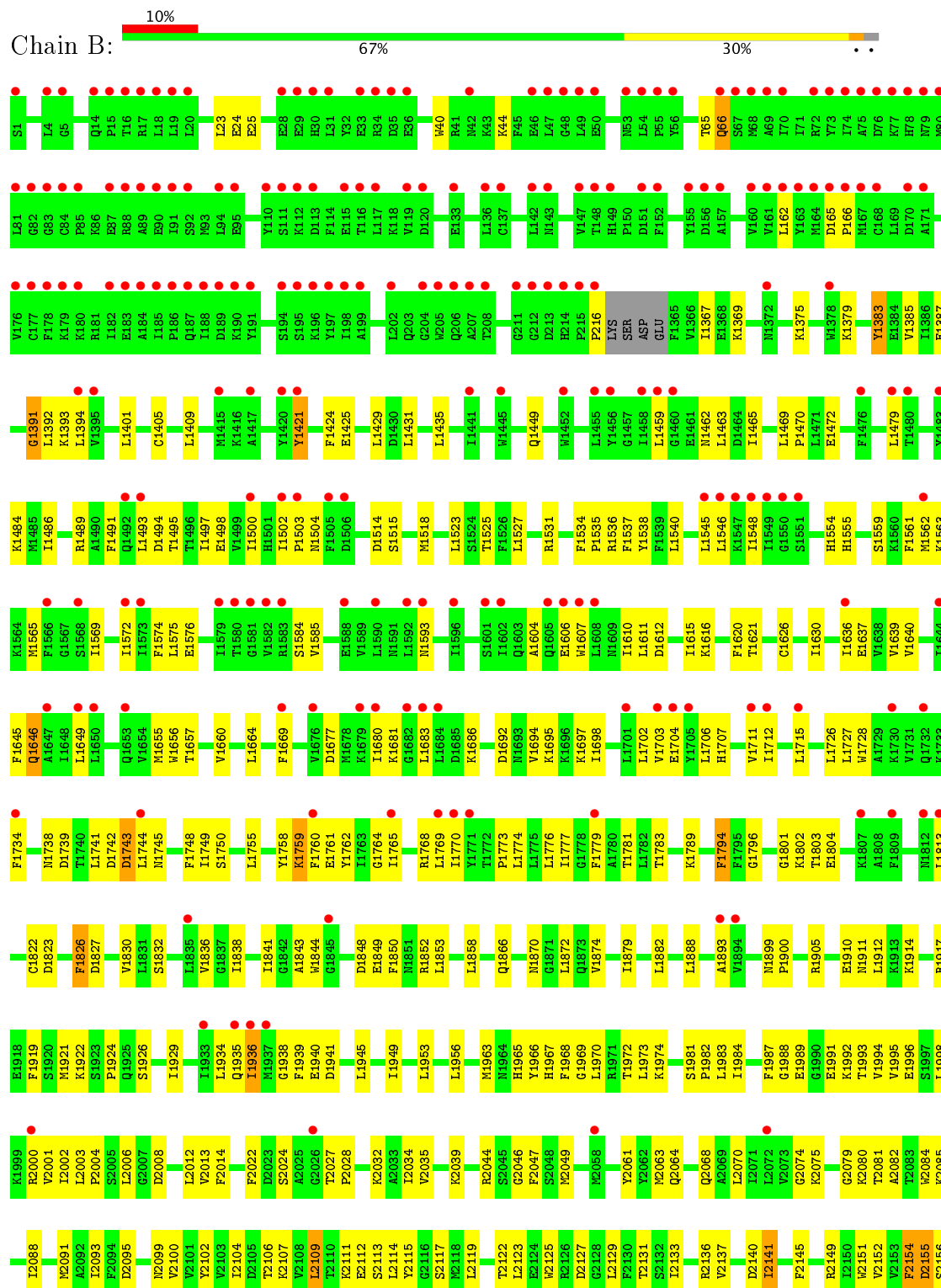


Item	Item	Item	Item	Item	Item	Item	Item	Item	Item
V2153	G2074	N1979	G1871	K1759	V1660	K1563	E1472	D165	S1
D2154	K2075	L1980	L1872	F1760	V1660	M1565	E1472	D165	P2
D2155	A2076	S1981	Q1873	F1761	V1660	M1565	T1473	P166	
E2161	G2077	P1982	V1874	L1762	L1664		L4779	I182	L19
E2169	C2078	L1983	I1879	G1764	F1669	I1569	L4779	E183	L20
V2160	K2080	S1985	I1879	I1765	S1670	E1570	Y1483	I184	L23
L2170	G2081	L1986	L1888	L1774	K1671	S1572	Y1483	L202	E24
L2171	A2082	G1989	N1889	R1768	Y1672	F1574	I1486	L202	E25
M2173	K2083	E1990	N1899	R1769	I1675	I1575	P215	P215	K26
K2174	W2084	E1991	P1900	L1774	V1676	E1576	P216	P216	Y27
L2175	K2085	L1993	R1905	L1774	D1677	D1577	LVS	LVS	E28
L2176	L2088	V1994	F1779	F1779	I1680	F1578	L493	ASP	D35
L2177	M2091	V1995	E1910	T1781	I1680	F1578	L493	ASP	D35
G2181	A2092	E1996	N1911	T1781	K1681	I1579	T1495	GIU	K39
E2182	L2093	S1997	L1912	L1782	G1682	S1584	T1496	F1365	W40
R2183	F2094	L1998	R1917	T1783	L1683	V1585	I1497	E1368	K44
L2184	K1999	E1918	E1918	Q1788	D1692	L1592	E1498	E1387	
P2185	R2000	F1919	F1919	F1794	K1695	I1596	V1499	E1387	D59
L2186	M2099	L2003	M1921	F1795	K1696	E1597	I1500	G1391	D61
L2187	Y2102	L2006	K1922	K1802	I1698	L1598	I1500	L1392	W62
L2193	V2103	L2012	S1923	E1803	L1701	A1604	I1500	L1392	A63
F2194	D2104	L2012	Q1925	E1804	L1702	A1605	I1500	L1394	L64
D2197	D2106	W2013	Q1925	T1805	W1703	E1606	I1500	C1405	Q66
L2198	K2107	F2014	I1929	V1806	E1704	W1607	I1523	K1406	S67
D2200	V2108	L2021	L1934	L1813	F1705	L1610	L1527	L1409	M68
H2201	L2109	L2022	Q1935	C1822	L1706	L1611	L1528	L1418	A69
T2202	K2111	D2023	Q1935	C1822	H1707	D1612	R1529	R171	I70
P2203	E2112	S2024	G1938	D1823	V1711	I1615	Q1530	N1419	H72
A2205	S2113	P2028	F1939	F1826	W1728	C1626	R1531	Y1420	R75
T2206	S2117	D1941	E1940	D1827	Q1714	F1620	R1532	Y1421	A75
L2207	K2032	L1945	L1945	V1830	L1726	Q1622	Q1533	F1424	M79
L2208	L2122	L2034	L1953	L1835	L1727	Q1622	F1534	E1425	G83
L2209	E2124	W2035	H1951	L1835	W1728	C1626	P1535	L1429	C84
F2215	W2125	K2039	F1952	L1838	W1731	I1630	R1536	L1435	P85
C2220	D2127	R2044	L1953	L1841	Q1732	G1633	F1537	L1438	A86
L2221	G2128	L2047	L1955	G1845	Q1732	G1633	L1540	L1438	A89
L2222	F2130	F2047	L1956	D1739	W1738	D1635	L1541	Q1442	E90
S2223	T2131	M2049	H1964	L1741	L1738	I1636	L1545	Q1442	I108
S2224	S2132	C2057	H1966	D1742	L1741	I1636	L1546	Y1445	
L2226	V2137	C2057	H1966	D1743	L1744	V1639	I1548	Q1449	E115
L2229	L2141	Y2061	L1968	L1852	L1744	V164			

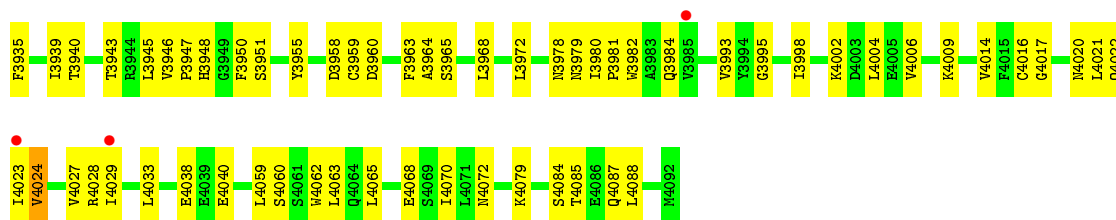




• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



H3858	I3774	Y3642	K3544	S3400	K3303	GLU	D2842	R2744	S2566	D2478	D2389	L2284	E2161
V3859	V3777	G3643	D3547	F3406	E3304	VAL	Q2845	I2745	Y2571	L2479	I2390	E2285	Y2162
T3862	V3778	S3645	L3548	F3409	R3305	LYS	G2846	D2746	E2572	L2482	V2391	V2288	V2169
A3865	A3779	I3646	K3549	D3409	W3306	GLU	A2748	A2748	Y2573	L2483	T2394	L2289	K2173
E3866	N3780	V3656	L3550	L3551	L3307	LEU	Y2849	Q2751	Y2574	L2484	T2395	L2290	K2174
E3869	N3784	F3657	K3425	K3425	N3308	VAL	L2853	Q2752	A2577	F2485	T2397	H2293	L2176
K3870	Y3785	L3658	V3426	V3426	T3310	THR		Q2753	L2578	E2488	F2404	L2294	T2177
F3871	F3786	LYS	L3428	L3428	K3311	GLU	L2856	G2754	E2590	I2489	F2404	L2295	L2178
K3872	T3787	SER	L3429	L3429	Q3312	PRO		H2755	E2590	I2490			
K3873	K3788	ARG	S3430	S3430	F3313	ILE	T2860	M2756	R2620	L2491	L2407	F2302	
K3874	R3792	GLU	F3431	F3431	E3319	T2860	L2865	M2757		L2492	L2408		
F3875	T3797	THR	K3564	K3564	L3320	I2861	L2866	L2758	T2623	K2493	I2409	L2305	G2181
M3876	T3797	ARG	R3440	R3440	I3321	I2862	L2867	L2759	T2623	L2494	S2410	D2306	E2182
C3877	K3799	ALA	L3566	L3566	G3322	D2863		G2760	R2627	I2496	I2411	D2307	R2183
H3878	L3803	ARG	F3458	F3458	N3323	I2863	E2870	A2761		K2412			
D3882	S3807	T3669	D3459	D3459	G3324	V2865	Q2871	K2766	Y2630	L2415			
K3883	K3808	R3670	F3460	F3460	I3325	V2866	E2872	L2769	T2635	P2420	L2310	L2186	
F3885	E3809	V3671	I3461	I3461	S3326	I2867	L2873	R2771	G2636	G2421	D2312	L2193	
A3886	S3810	I3674	S3463	S3463	S3327	L2868	V2878	K2779	P2637	G2422	T2314	F2194	E2195
P3887	L3811	L3677	I3465	I3465	S3328	L2869	K2883	L2779	R2638	K2424	L2317	T2196	D2197
L3888	K3812	K3681	K3580	K3580	Y3330	V2884		K2780	Q2639	T2425	L2318		
L3889	S3813	Y3683	A3473	A3473	F3334	R2986	H2886	Q2783	T2640	I2509	S2427		
Q3890	L3814	S3687	K3476	K3476	N3338	P2987	F2889	K2785	S2643	K2512	G2332	L2212	
R3894	P3815	K3687	K3584	K3584	E3341	S2988	T2890	K2786	R2653	Q2513	Q2335	L2213	
F3895	L3816	K3692	L3587	L3587	L3346	P2989	C2892	H2787	R2654	G2514	Q2336	W2214	
V3896	G3817	K3693	N3588	N3588	I3347	G2990	M2902	R2788	L2660	K2517	L2437		
F3897	I3819	F3694	D3483	D3483	V3348	L3002	L2908	F2789	V2661	P2519	V2441		
E3898	E3820	N3698	S3502	S3502	K3350	L3010	L2911	L2808		E2520			
N3899	N3821	M3699	K3591	K3591	R3351	V3017	R2916	R2812	V2677	V2524	Q2351	S2224	
I3900	L3822	K3700	K3592	K3592	L3352	R3018	N2915	T2813	L2681	T2525	E2352	S2225	
P3901	N3823	M3702	E2593	E2593	L3353	V3019	C2912	L2814	L2686	I2526	L2353	K2228	
T3906	S3832	K3714	N3596	N3596	F3356	K3023	N2916	L2816		R2528	Y2459	L2229	
W3911	G3836	L3726	E3598	E3598	A3357	L3024	Q2918	L2816	L2686		R2460	L2230	
G3912	K3837	S3727	E3605	E3605	V3358	LEU	D2918	S2820		V2532		L2252	
S3913	N3838	E3728	F3518	F3518	K3359	LYS	N2918	L2834	T2689	A2534	Q2362	L2262	
Q3914	I3840	S3729	V3519	V3519	D3361	VAL	W2920	N2821	L2689	I2463	A2362	L2265	
F3915	L3841	S3729	N3521	N3521	K3361	ASN	T2924	L2823	S2691	Y2464		L2262	
T3917	L3844	T3737	V3615	V3615	L3370	GLU					K2365		
G3918	Q3845	T3737	V3615	V3615	Y3371	LEU	L2936	E2829	V2707	T2467	F2368	L2265	
K3919	M3846	T3740	Y3618	Y3618	T3372	ASN	P2937		N2708	S2468	S2369	F2266	
W3923	S3847	L3744	G3622	G3622	E3375	LYS	M2938	T2833	L2712	K2469		H2274	
S3925	L3848	L3744	L3334	L3334	L3380	THR		L2835		G2470	L2380	L2275	
W3926	W3850	F3767	N3631	N3631	L3380	SER	T2941	L2835	L2728	T2471	L2380	L2276	
V3927	F3851	F3768	L3632	L3632	L3391	ILE	D2942	L2473		L2473	A2382		
K3852	K3852	V3769	N3538	N3538	L3391	SER	F2943	P2562	S2737			T2280	
T3853	Y3854	W3772	G3636	G3636	E3392	LEU	ILE	S2563		F2475	V2385	F2281	
F3930	F3854	N3773	F3641	F3641	N3393	VAL	PRO	L2840	H2741	G2564	M2386	N2282	
W3934	L3855	N3773				K3297		P2841		S2477		K2283	



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.56Å 118.13Å 201.02Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 70.46 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.60) 99.2 (70.46-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.302 0.236 , 0.300	Depositor DCC
R_{free} test set	4766 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	127.5	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 117.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41642	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, SO4, 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	0.53	0/21146	0.77	7/28618 (0.0%)
1	B	0.46	2/21146 (0.0%)	0.68	5/28618 (0.0%)
All	All	0.49	2/42292 (0.0%)	0.73	12/57236 (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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3306	TRP	CE3-CZ3	-6.25	1.27	1.38
1	B	3306	TRP	CE2-CZ2	-5.22	1.30	1.39

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2012	LEU	CA-CB-CG	7.99	133.67	115.30
1	A	1741	LEU	CB-CG-CD1	6.69	122.38	111.00
1	A	3792	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	1782	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	B	2460	ARG	NE-CZ-NH2	-5.52	117.54	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2119	LEU	Peptide
1	B	2620	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20206	952	0
1	B	20748	0	20206	909	0
2	A	31	0	12	8	0
2	B	31	0	12	17	0
3	A	31	0	13	7	0
3	B	31	0	13	7	0
4	A	10	0	0	3	0
4	B	10	0	0	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41642	0	40462	1861	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 23.

The worst 5 of 1861 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:216:PRO:CB	1:A:1365:PHE:CE1	2.05	1.38
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	1.67	1.28
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.25
1:A:1368:GLU:HG2	1:A:1424:PHE:CZ	1.69	1.24
1:B:2467:THR:HB	1:B:2473:LEU:CD1	1.66	1.23

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	2640/2695 (98%)	2518 (95%)	110 (4%)	12 (0%)	32	73
1	B	2640/2695 (98%)	2515 (95%)	111 (4%)	14 (0%)	32	73
All	All	5280/5390 (98%)	5033 (95%)	221 (4%)	26 (0%)	32	73

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	B	1391	GLY
1	B	3578	LEU
1	A	24	GLU
1	A	1633	GLY

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	2218/2453 (90%)	2138 (96%)	80 (4%)	40	75
1	B	2218/2453 (90%)	2137 (96%)	81 (4%)	39	74
All	All	4436/4906 (90%)	4275 (96%)	161 (4%)	40	75

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3940	THR

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Mol	Chain	Res	Type
1	B	1826	PHE
1	B	3899	ASP
1	A	3958	ASP
1	B	1421	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3962	GLN
1	B	1736	GLN
1	B	3783	ASN
1	A	3970	ASN
1	B	1501	HIS

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	ATP	A	5093	5	27,33,33	1.02	1 (3%)	25,52,52	1.66	2 (8%)
3	ANP	A	5094	-	29,33,33	2.99	5 (17%)	28,52,52	1.83	5 (17%)
4	SO4	A	5095	-	4,4,4	0.60	0	6,6,6	0.67	0
4	SO4	A	5096	-	4,4,4	0.53	0	6,6,6	0.22	0
2	ATP	B	5093	5	27,33,33	1.04	2 (7%)	25,52,52	1.61	2 (8%)
3	ANP	B	5094	-	29,33,33	3.05	6 (20%)	28,52,52	1.73	3 (10%)
4	SO4	B	5095	-	4,4,4	0.41	0	6,6,6	0.45	0
4	SO4	B	5096	-	4,4,4	0.43	0	6,6,6	0.19	0

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	ATP	A	5093	5	-	0/18/38/38	0/3/3/3
3	ANP	A	5094	-	-	0/13/38/38	0/3/3/3
4	SO4	A	5095	-	-	0/0/0/0	0/0/0/0
4	SO4	A	5096	-	-	0/0/0/0	0/0/0/0
2	ATP	B	5093	5	-	0/18/38/38	0/3/3/3
3	ANP	B	5094	-	-	1/13/38/38	0/3/3/3
4	SO4	B	5095	-	-	0/0/0/0	0/0/0/0
4	SO4	B	5096	-	-	0/0/0/0	0/0/0/0

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ANP	PG-O3G	-3.02	1.48	1.56
3	A	5094	ANP	PG-O3G	-2.97	1.48	1.56
2	B	5093	ATP	O4'-C1'	2.12	1.44	1.41
3	B	5094	ANP	PB-O1B	2.13	1.48	1.46
3	A	5094	ANP	C5-C4	3.04	1.47	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5094	ANP	N3-C2-N1	-6.24	123.42	128.86
3	B	5094	ANP	N3-C2-N1	-5.86	123.75	128.86
2	A	5093	ATP	N3-C2-N1	-5.84	123.77	128.86
2	B	5093	ATP	N3-C2-N1	-5.70	123.89	128.86
3	B	5094	ANP	PA-O3A-PB	-3.36	120.54	132.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5094	ANP	O1G-PG-N3B-PB

There are no ring outliers.

6 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	8	0
3	A	5094	ANP	7	0
4	A	5095	SO4	3	0
2	B	5093	ATP	17	0
3	B	5094	ANP	7	0
4	B	5096	SO4	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 [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	2650/2695 (98%)	0.11	67 (2%) 58 43	69, 151, 281, 423	0
1	B	2650/2695 (98%)	0.64	276 (10%) 7 6	92, 193, 357, 500	0
All	All	5300/5390 (98%)	0.38	343 (6%) 20 14	69, 172, 321, 500	0

The worst 5 of 343 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	ASP	24.8
1	B	164	MET	22.7
1	B	213	ASP	20.6
1	B	29	GLU	19.7
1	B	163	TYR	19.6

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 carbohydrates 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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	5095	5/5	0.96	0.25	0.94	84,98,104,105	0
2	ATP	A	5093	31/31	0.95	0.29	0.19	88,123,185,204	0
3	ANP	B	5094	31/31	0.89	0.29	-0.05	112,145,237,257	0
3	ANP	A	5094	31/31	0.94	0.27	-0.31	111,140,238,248	0
2	ATP	B	5093	31/31	0.92	0.24	-0.35	99,141,184,200	0
4	SO4	B	5096	5/5	0.95	0.14	-0.78	155,168,174,176	0
5	MG	A	5097	1/1	0.99	0.22	-1.10	62,62,62,62	0
4	SO4	B	5095	5/5	0.84	0.18	-1.17	152,154,166,167	0
4	SO4	A	5096	5/5	0.96	0.20	-1.50	115,130,143,145	0
5	MG	B	5097	1/1	0.97	0.18	-	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.