



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:59 AM GMT

PDB ID : 3QMZ
Title : Crystal structure of the cytoplasmic dynein heavy chain motor domain
Authors : Cho, C.; Carter, A.P.; Jin, L.; Vale, R.D.
Deposited on : 2011-02-07
Resolution : 6.00 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 (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

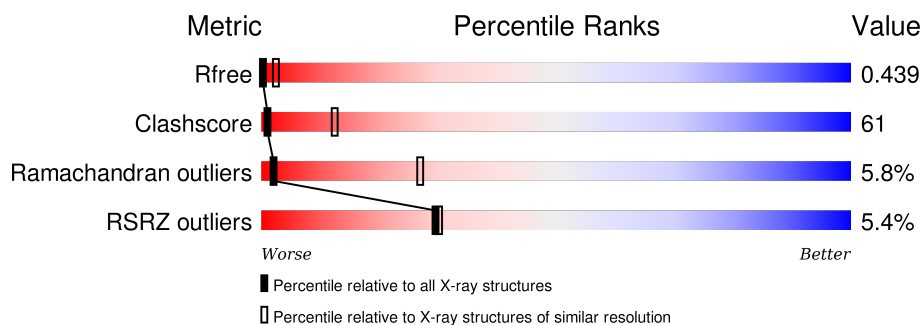
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
RSRZ outliers	91569	1001 (8.30-3.66)

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	2486	<div> <div>3%</div> <div>53% 19% 10% • 14%</div> </div>
1	B	2486	<div> <div>4%</div> <div>53% 19% 10% • 14%</div> </div>
2	S	219	<div> <div>20%</div> <div>92% 5% ..</div> </div>
2	T	219	<div> <div>14%</div> <div>91% 6% •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23302 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 Cytoplasmic dynein heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	2136	Total	C	N	O	0	0	0
			10585	6313	2136	2136			
1	B	2136	Total	C	N	O	0	0	0
			10586	6314	2136	2136			

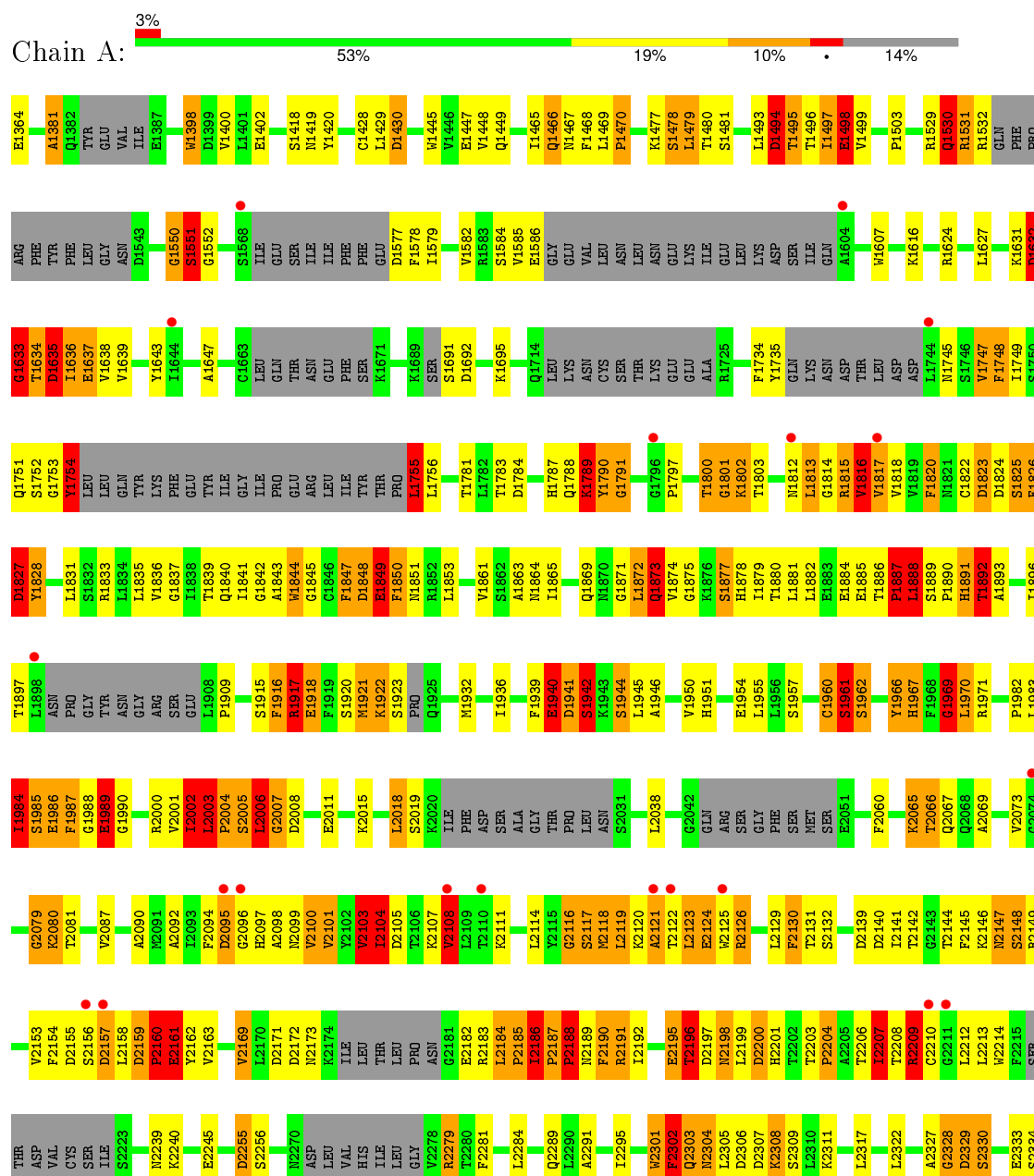
- Molecule 2 is a protein called Glutathione-S-transferase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	T	216	Total	C	N	O	0	0	0
			1066	634	216	216			
2	S	216	Total	C	N	O	0	0	0
			1065	633	216	216			

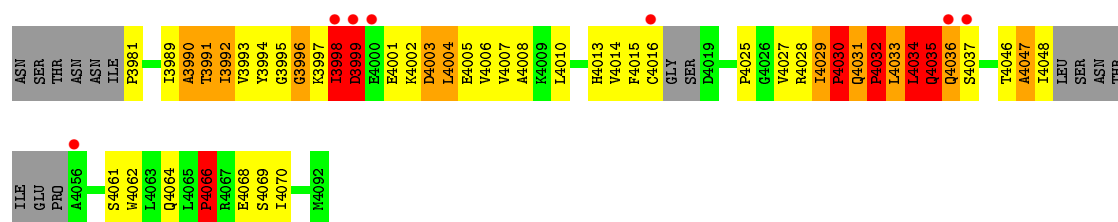
3 Residue-property plots

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.

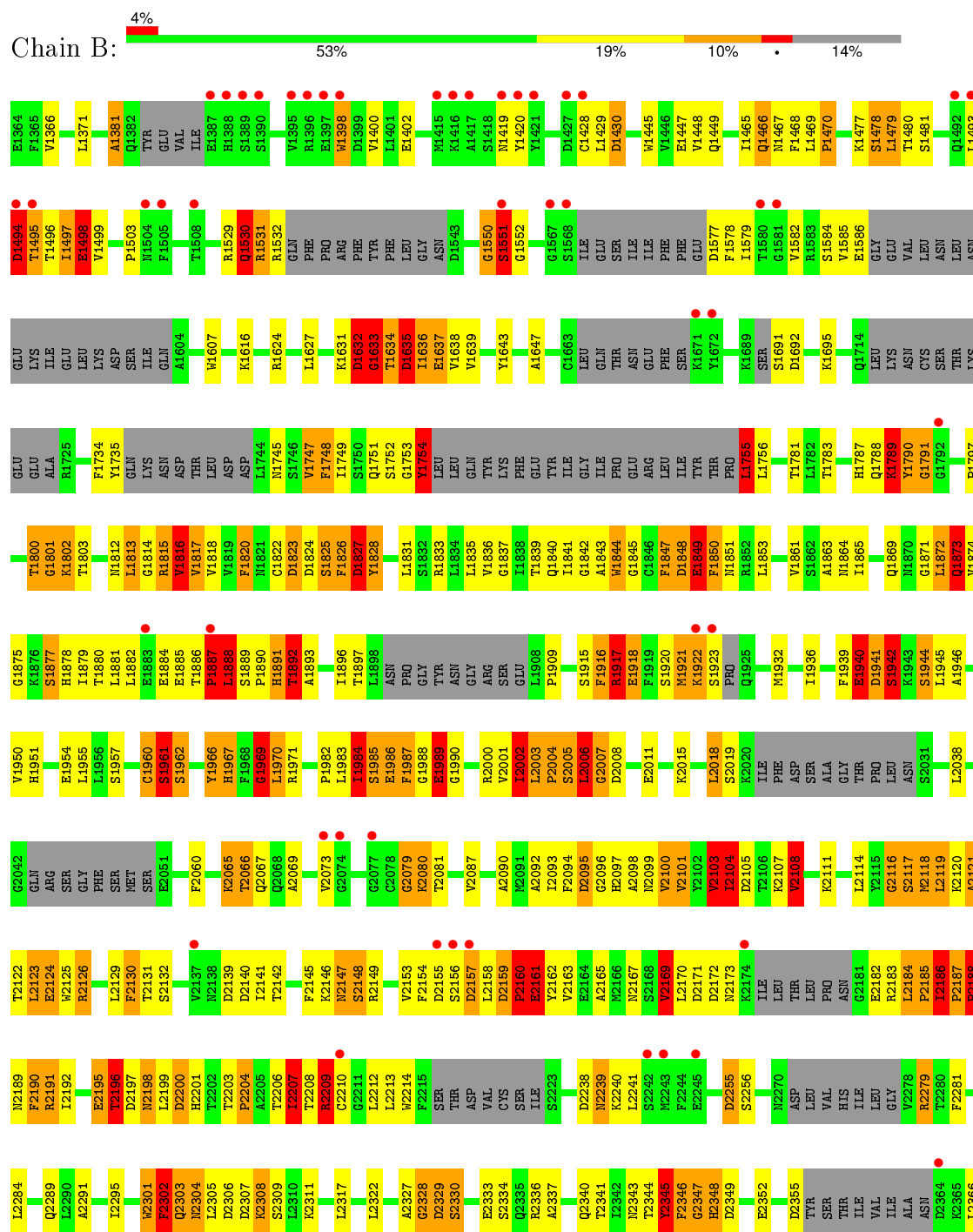
• Molecule 1: Cytoplasmic dynein heavy chain



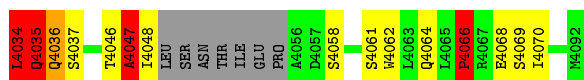




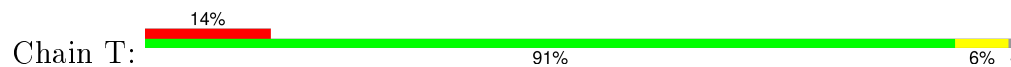
• Molecule 1: Cytoplasmic dynein heavy chain



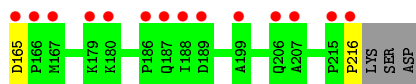
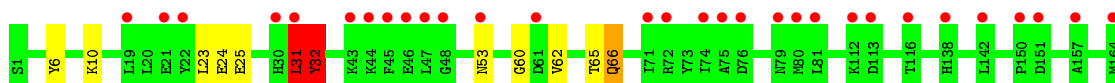
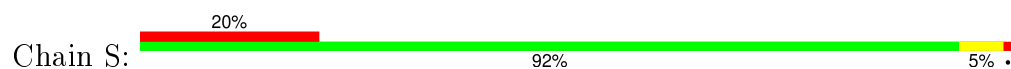
PHE	K3857	N3761	Q3680	H3517	E3434	V3358	VAL	D2868	Q2612	E2527	S2367
SER	H3858	W3762	E3681	F3518	G3435	K3859	VAL	T2869	S2613	R2528	F2368
LYS	V3859	N3765	E3682	V3519	Y3360	D3361	ASN	E2870	E2614	R2529	S2369
TYR	E3860	GLU	Y3682	T3520	I3452	Y3362	ILE	Q2871	Y2615	V2532	S2370
PHE	E3861	GLU	Y3683	ASN	I3453	E3862	LEU	E2872	F2617	A2533	F2371
PHE	E3862	PHE	C3684	LYS	D3454	H3863	ILE	K2873	S2618	A2534	C2372
ASN	E3863	PHE	Q3685	GLU	G3455	Y3864	HIS	Y2874	P2619	C2535	C2373
ASP	A3864	VAL	Q3686	S3524	E3456	R3365	PHE	W2875	P2620	I2536	E2374
GLU	A3865	ASP	S3687	S3524	F3457	V3369	ASP	W2876	R2627	T2461	E2375
GLU	E3866	GLU	S3688	R3545	F3458	L3370	ARG	D2725	T2462	T2462	P2376
ASP	E3867	GLU	A3689	R3545	D3459	V3371	ASN	E2726	Y2463	Y2463	S2377
GLU	W3772	GLU	A3689	I3549	P3460	T3372	PHE	E2727	D2540	V2465	V2378
GLU	S3781	S3781	K3707	R3565	I3461	L3373	GLN	LEU	THR	THR	V2379
ASN	E3782	E3782	F3708	R3565	I3462	L3373	GLN	GLU	THR	THR	L2380
ASN	N3783	N3783	D3709	E3568	S3463	K3376	MET	VAL	SER	E2381	E2381
ASN	N3784	N3784	I3710	E3568	R3464	K3377	LYS	E2728	L2544	L2544	A2382
ASN	T3787	T3787	E3711	E3569	I3465	K3378	LYS	V2732	GLY	GLY	H2383
GLU	W3788	W3788	S3712	L3570	I3466	K3379	VAL	V2733	Q2639	Q2639	H2384
GLU	A3789	A3789	E3713	N3571	F3470	V3379	GLY	I2734	T2640	S2547	V2385
GLU	S3790	S3790	Q3714	N3572	ASN	L3380	VAL	Q2751	L2641	T2551	L2386
GLU	E3791	E3791	T3715	SER	ASN	E3881	ASN	TYR	F2485	F2485	R2387
GLU	W3792	W3792	L3716	GLN	HIS	C3382	PRO	L2753	C2486	C2486	P2388
GLU	T3793	T3793	E3717	GLY	ALA	G3383	ARG	R2552	L2552	L2552	L2389
GLU	A3794	A3794	S3718	ASN	GLY	LEU	SER	A2554	ASP	ASP	I2390
GLU	D3795	D3795	Q3719	LEU	R3476	ASP	LEU	A2555	ASP	V2391	V2391
GLU	S3800	S3800	T3720	GLU	I3477	LYS	GLY	I2556	I2479	I2392	I2392
GLU	E3801	E3801	E3721	GLU	T3478	ASP	ASN	R2654	LEU	P2393	P2393
GLU	S3802	S3802	I3722	ASN	F3479	ASP	ASN	T2655	F2485	T2394	T2394
GLU	A3803	A3803	E3723	GLY	R3480	V3389	LYS	C2912	L2655	L2655	I2395
GLU	S3804	S3804	E3724	GLY	I3481	S3400	ASN	I2913	F2656	F2656	I2396
GLU	K3805	K3805	S3725	GLY	C3482	Q3401	GLU	I2914	ASP	GLY	I2397
GLU	S3806	S3806	V3726	GLY	D3483	ASP	LEU	N2915	ARG	GLU	T2398
GLU	K3807	K3807	E3727	GLY	E3484	ALA	ASN	N2916	VAL	ILE	K2399
GLU	S3808	S3808	S3728	GLY	R3485	ASP	GLY	N2917	GLY	ASN	K2399
GLU	E3809	E3809	Q3729	GLY	E3486	ALA	LEU	TRP	V2574	V2574	L2407
GLU	S3810	S3810	I3730	GLY	V3487	V3404	THR	ASP	A2575	A2575	S2410
GLU	P3811	P3811	E3731	GLY	VAL	F3405	THR	ASP	L2576	L2576	K2411
GLY	E3812	E3812	S3732	GLY	SER	F3406	LEU	ASP	F2577	F2577	S2410
GLY	N3813	N3813	V3733	GLY	VAL	L3407	PRO	ASP	F2578	F2578	K2411
GLY	E3814	E3814	E3734	GLY	GLY	L3408	PRO	L2681	F2579	F2579	P2419
GLY	S3815	S3815	S3735	GLY	ASP	D3409	ALA	L2581	K2580	K2580	P2420
GLY	E3816	E3816	I3736	GLY	PHE	P3410	ALA	S2820	V2582	V2582	P2420
GLY	N3817	N3817	T3737	GLY	GLY	S3411	PRO	P2583	L2686	L2686	M2428
GLY	S3818	S3818	E3738	GLY	GLY	S3412	PRO	C2687	C2687	C2687	M2429
GLY	E3819	E3819	D3739	GLY	F3495	H3413	GLU	N2688	V2502	V2502	M2430
GLY	N3820	N3820	T3740	GLY	F3496	Y3421	GLU	I2689	L2504	L2504	A2431
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GLY	S3824	S3824	D3744	GLY	S3499	Y3421	GLU	S2693	K2512	K2512	S2435
GLY	E3825	E3825	S3745	GLY	S3499	Y3422	GLU	S2694	Q2513	Q2513	S2436
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GLY	S3830	S3830	D3750	GLY	S3499	Y3427	GLU	S2699	P2518	P2518	I2444
GLY	E3831	E3831	V3751	GLY	S3499	Y3428	GLU	S2700	P2519	P2519	I2445
GLY	N3832	N3832	T3752	GLY	S3499	Y3429	GLU	S2701	P2520	P2520	G2446
GLY	S3833	S3833	E3753	GLY	S3499	Y3430	GLU	S2702	P2521	P2521	G2447
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GLY	N3835	N3835	S3755	GLY	S3499	Y3432	GLU	S2704	P2523	P2523	G2449
GLY	S3836	S3836	E3756	GLY	S3499	Y3433	GLU	S2705	P2524	P2524	G2450
GLY	E3837	E3837	S3757	GLY	S3499	Y3434	GLU	S2706	P2525	P2525	G2451
GLY	N3838	N3838	K3758	GLY	S3499	Y3435	GLU	S2707	P2526	P2526	G2452
GLY	S3839	S3839	E3759	GLY	S3499	Y3436	GLU	S2708	P2527	P2527	G2453
GLY	E3840	E3840	D3760	GLY	S3499	Y3437	GLU	S2709	P2528	P2528	G2454
GLY	N3841	N3841	S3760	GLY	S3499	Y3438	GLU	S2710	P2529	P2529	G2455
GLY	S3842	S3842	E3761	GLY	S3499	Y3439	GLU	S2711	P2530	P2530	G2456
GLY	E3843	E3843	K3762	GLY	S3499	Y3440	GLU	S2712	P2531	P2531	G2457
GLY	N3844	N3844	S3763	GLY	S3499	Y3441	GLU	S2713	P2532	P2532	G2458
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GLY	E3846	E3846	K3765	GLY	S3499	Y3443	GLU	S2715	P2534	P2534	G2460
GLY	N3847	N3847	S3766	GLY	S3499	Y3444	GLU	S2716	P2535	P2535	G2461
GLY	S3848	S3848	E3767	GLY	S3499	Y3445	GLU	S2717	P2536	P2536	G2462
GLY	E3849	E3849	K3768	GLY	S3499	Y3446	GLU	S2718	P2537	P2537	G2463
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GLY	E3882	E3882	K3799	GLY	S3499	Y3479	GLU	S2751	P2570	P2570	G2496
GLY	N3883	N3883	S3800	GLY	S3499	Y3480	GLU	S2752	P2571	P2571	G2497
GLY	S3884	S3884	E3801	GLY	S3499	Y3481	GLU	S2753	P2572	P2572	G2498
GLY	E3885	E3885	K3802	GLY	S3499	Y3482	GLU	S2754	P2573	P2573	G2499
GLY	N3886	N3886	S3803	GLY	S3499	Y3483	GLU	S2755	P2574	P2574	G2500
GLY	S3887	S3887	E3804	GLY	S3499	Y3484	GLU	S2756	P2575	P2575	G2501
GLY	E3888	E3888	K3805	GLY	S3499	Y3485	GLU	S2757	P2576	P2576	G2502
GLY	N3889	N3889	S3806	GLY	S3499	Y3486	GLU	S2758	P2577	P2577	G2503
GLY	S3890	S3890	E3807	GLY	S3499	Y3487	GLU	S2759	P2578	P2578	G2504
GLY	E3891	E3891	K3808								



• Molecule 2: Glutathione-S-transferase



• Molecule 2: Glutathione-S-transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	174.08Å 118.92Å 200.51Å 90.00° 90.27° 90.00°	Depositor
Resolution (Å)	50.00 – 6.00 50.13 – 6.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-6.00) 99.9 (50.13-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.38 (at 6.15Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.430 , 0.430 0.445 , 0.439	Depositor DCC
R_{free} test set	1079 reflections (5.47%)	DCC
Wilson B-factor (Å ²)	259.8	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 749.2	EDS
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 20819 reflections	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	23302	wwPDB-VP
Average B, all atoms (Å ²)	222.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.63	201/10536 (1.9%)	2.24	571/14615 (3.9%)
1	B	1.63	201/10537 (1.9%)	2.24	572/14617 (3.9%)
2	S	1.94	2/1064 (0.2%)	0.86	3/1479 (0.2%)
2	T	0.39	0/1065	0.78	6/1481 (0.4%)
All	All	1.61	404/23202 (1.7%)	2.15	1152/32192 (3.6%)

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	3	136
1	B	3	136
2	S	0	3
All	All	6	275

The worst 5 of 404 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	32	TYR	N-CA	49.28	2.44	1.46
2	S	32	TYR	CA-C	37.84	2.51	1.52
1	B	4047	ALA	C-N	-30.16	0.64	1.34
1	A	4047	ALA	C-N	-30.14	0.64	1.34
1	A	3426	THR	C-N	-25.27	0.76	1.34

The worst 5 of 1152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1466	GLN	O-C-N	-31.44	72.39	122.70
1	A	1466	GLN	O-C-N	-31.43	72.42	122.70
1	B	2436	SER	O-C-N	-28.51	77.09	122.70
1	A	2436	SER	O-C-N	-28.49	77.12	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1466	GLN	CA-C-N	-28.26	55.02	117.20

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1888	LEU	CA
1	A	2375	ILE	CA
1	A	3641	PHE	CA
1	B	1888	LEU	CA
1	B	2375	ILE	CA

5 of 275 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1381	ALA	Mainchain
1	A	1430	ASP	Mainchain
1	A	1479	LEU	Mainchain
1	A	1494	ASP	Mainchain,Peptide
1	A	1530	GLN	Peptide

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	10585	0	4454	1006	3
1	B	10586	0	4455	994	3
2	S	1065	0	464	9	0
2	T	1066	0	465	22	0
All	All	23302	0	9838	2013	3

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 61.

The worst 5 of 2013 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:1364:GLU:CA	2:T:216:PRO:HA	1.19	1.65
1:A:1932:MET:CB	1:A:1946:ALA:HB1	1.24	1.64
1:B:2060:PHE:CB	1:B:2087:VAL:CB	1.78	1.62
1:A:2060:PHE:CB	1:A:2087:VAL:CB	1.78	1.57
1:A:3666:ALA:HB2	1:A:3668:ARG:CB	1.32	1.57

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2245:GLU:N	1:B:2241:LEU:CB[1_554]	1.43	0.77
1:A:2245:GLU:CA	1:B:2241:LEU:CB[1_554]	1.81	0.39
1:A:2245:GLU:CB	1:B:2241:LEU:CB[1_554]	2.05	0.15

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	2039/2486 (82%)	1605 (79%)	307 (15%)	127 (6%)	2	25
1	B	2039/2486 (82%)	1605 (79%)	308 (15%)	126 (6%)	2	25
2	S	214/219 (98%)	194 (91%)	16 (8%)	4 (2%)	10	52
2	T	214/219 (98%)	190 (89%)	20 (9%)	4 (2%)	10	52
All	All	4506/5410 (83%)	3594 (80%)	651 (14%)	261 (6%)	2	27

5 of 261 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1470	PRO
1	A	1494	ASP
1	A	1498	GLU
1	A	1635	ASP

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Mol	Chain	Res	Type
1	A	1637	GLU

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

There are no ligands in this entry.

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	2136/2486 (85%)	0.02	86 (4%) 42 40	183, 210, 384, 480	0
1	B	2136/2486 (85%)	0.13	93 (4%) 38 36	183, 210, 384, 480	0
2	S	216/219 (98%)	1.06	44 (20%) 1 6	209, 233, 253, 268	0
2	T	216/219 (98%)	0.74	31 (14%) 3 9	201, 219, 248, 273	0
All	All	4704/5410 (86%)	0.15	254 (5%) 29 30	183, 210, 376, 480	0

The worst 5 of 254 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	80	MET	7.5
1	B	2156	SER	6.1
1	B	1397	GLU	5.9
1	B	3899	ASP	5.7
2	T	52	PRO	5.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.