



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:40 am BST

PDB ID : 4W8F
Title : Crystal structure of the dynein motor domain in the AMPPNP-bound state
Authors : Cheng, H.-C.; Bhabha, G.; Zhang, N.; Vale, R.D.
Deposited on : 2014-08-24
Resolution : 3.54 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

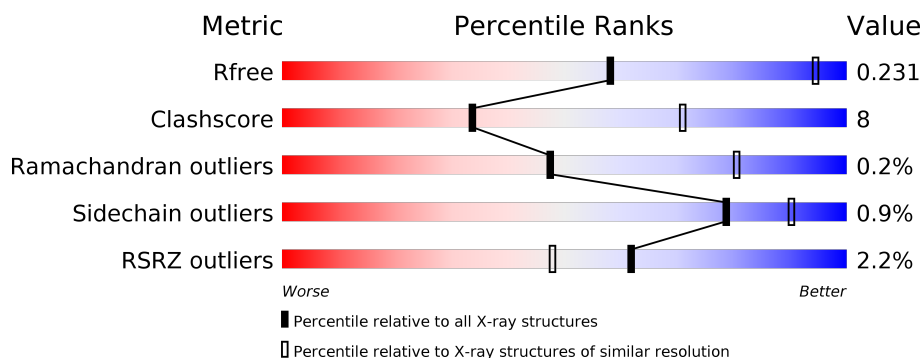
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2661	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>••</div> </div> </div>
1	B	2661	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>•</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 84822 atoms, of which 42429 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 lysozyme chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	2608	Total	C	H	N	O	S	0	0	0
			42239	13515	21166	3504	3957	97			
1	B	2609	Total	C	H	N	O	S	0	0	0
			42236	13509	21166	3505	3959	97			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1363	GLY	-	expression tag	UNP P36022
A	1849	GLN	GLU	engineered mutation	UNP P36022
A	3120	GLY	-	linker	UNP P36022
A	3121	SER	-	linker	UNP P36022
A	3122	GLY	-	linker	UNP P36022
A	3123	SER	-	linker	UNP P36022
A	3124	GLY	-	linker	UNP P36022
A	3125	SER	-	linker	UNP P36022
A	3136	GLY	ARG	conflict	UNP P00720
A	3178	THR	CYS	conflict	UNP P00720
A	3221	ALA	CYS	conflict	UNP P00720
A	3261	ARG	ILE	conflict	UNP P00720
A	3286	GLY	-	linker	UNP P00720
A	3287	SER	-	linker	UNP P00720
A	3288	GLY	-	linker	UNP P00720
A	3289	SER	-	linker	UNP P00720
A	3290	GLY	-	linker	UNP P00720
A	3291	SER	-	linker	UNP P00720
A	3742	ASP	ASN	conflict	UNP P36022
A	3895	VAL	PHE	conflict	UNP P36022
A	4072	ASP	ASN	conflict	UNP P36022
A	4093	GLY	-	linker	UNP P36022
A	4094	SER	-	linker	UNP P36022
A	4095	GLY	-	linker	UNP P36022
A	4096	SER	-	linker	UNP P36022

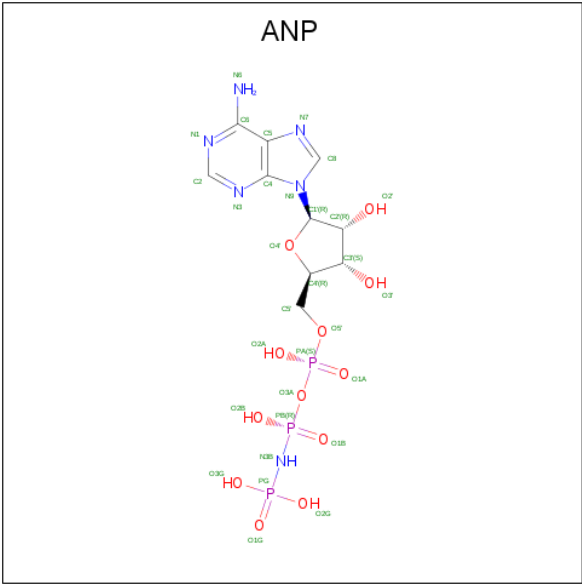
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Chain	Residue	Modelled	Actual	Comment	Reference
A	4097	GLY	-	linker	UNP P36022
A	4098	SER	-	linker	UNP P36022
A	4099	HIS	-	expression tag	UNP P36022
A	4100	HIS	-	expression tag	UNP P36022
A	4101	HIS	-	expression tag	UNP P36022
A	4102	HIS	-	expression tag	UNP P36022
A	4103	HIS	-	expression tag	UNP P36022
A	4104	HIS	-	expression tag	UNP P36022
B	1363	GLY	-	expression tag	UNP P36022
B	1849	GLN	GLU	engineered mutation	UNP P36022
B	3120	GLY	-	linker	UNP P36022
B	3121	SER	-	linker	UNP P36022
B	3122	GLY	-	linker	UNP P36022
B	3123	SER	-	linker	UNP P36022
B	3124	GLY	-	linker	UNP P36022
B	3125	SER	-	linker	UNP P36022
B	3136	GLY	ARG	conflict	UNP P00720
B	3178	THR	CYS	conflict	UNP P00720
B	3221	ALA	CYS	conflict	UNP P00720
B	3261	ARG	ILE	conflict	UNP P00720
B	3286	GLY	-	linker	UNP P00720
B	3287	SER	-	linker	UNP P00720
B	3288	GLY	-	linker	UNP P00720
B	3289	SER	-	linker	UNP P00720
B	3290	GLY	-	linker	UNP P00720
B	3291	SER	-	linker	UNP P00720
B	3742	ASP	ASN	conflict	UNP P36022
B	3895	VAL	PHE	conflict	UNP P36022
B	4072	ASP	ASN	conflict	UNP P36022
B	4093	GLY	-	linker	UNP P36022
B	4094	SER	-	linker	UNP P36022
B	4095	GLY	-	linker	UNP P36022
B	4096	SER	-	linker	UNP P36022
B	4097	GLY	-	linker	UNP P36022
B	4098	SER	-	linker	UNP P36022
B	4099	HIS	-	expression tag	UNP P36022
B	4100	HIS	-	expression tag	UNP P36022
B	4101	HIS	-	expression tag	UNP P36022
B	4102	HIS	-	expression tag	UNP P36022
B	4103	HIS	-	expression tag	UNP P36022
B	4104	HIS	-	expression tag	UNP P36022

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	A	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		

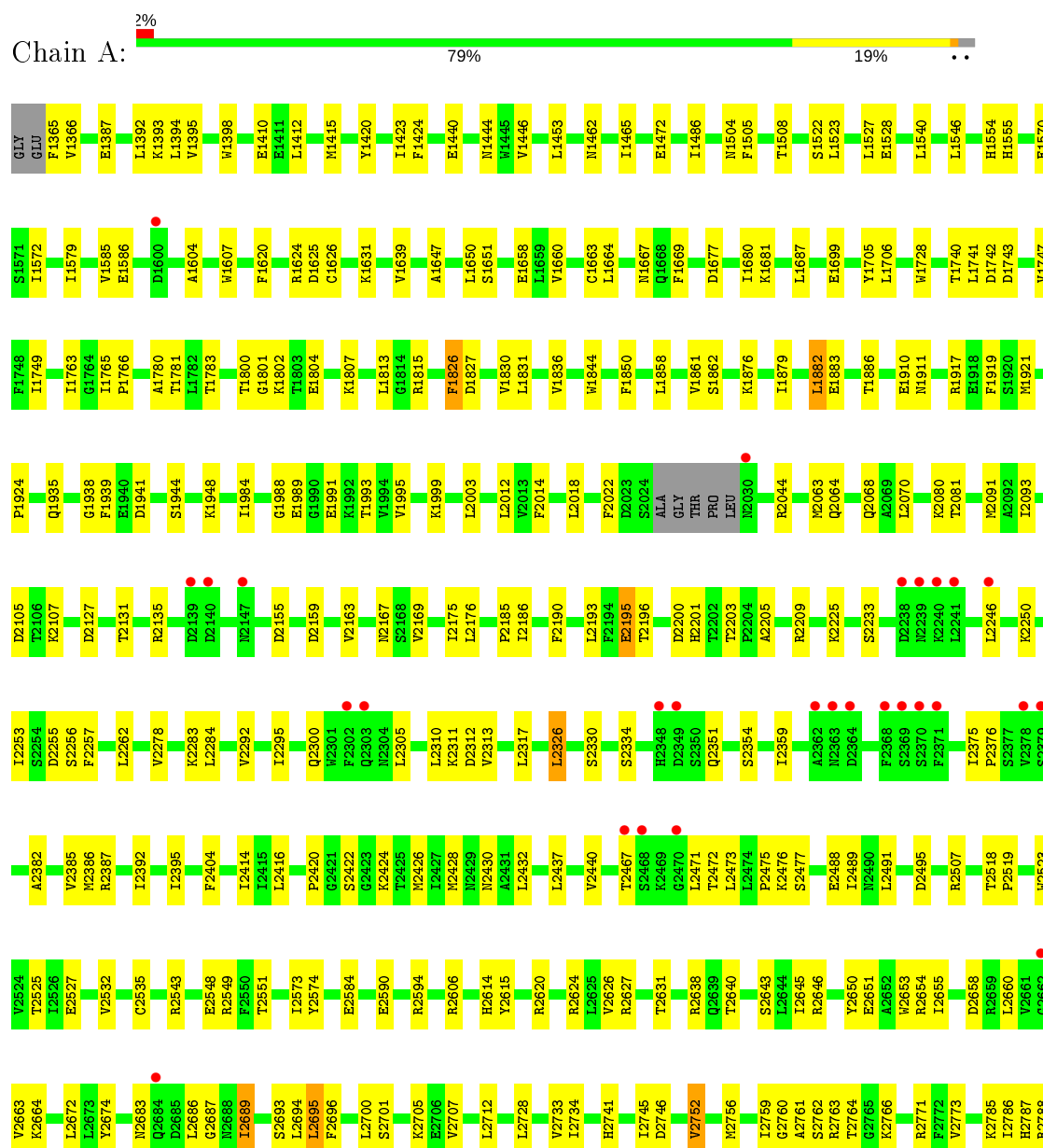
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

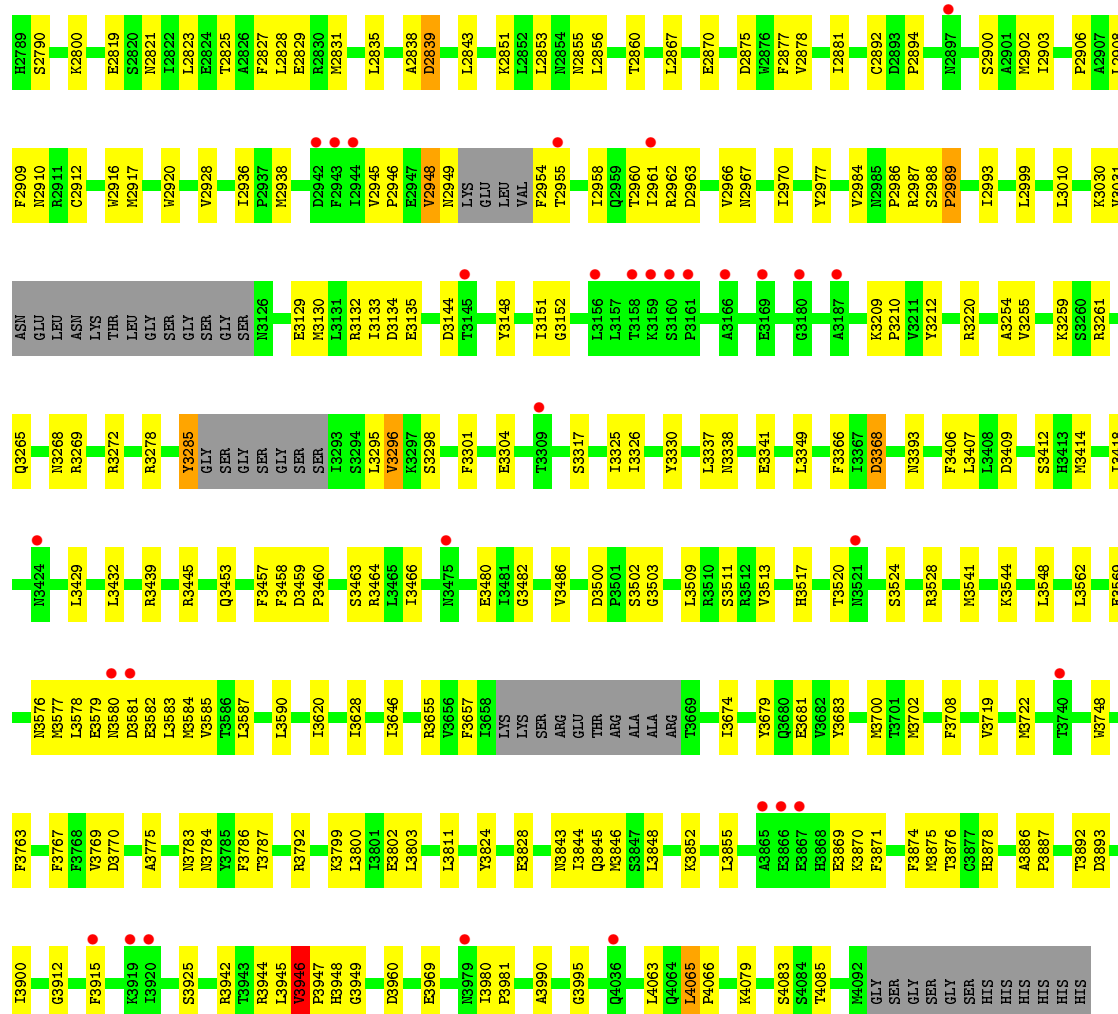
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

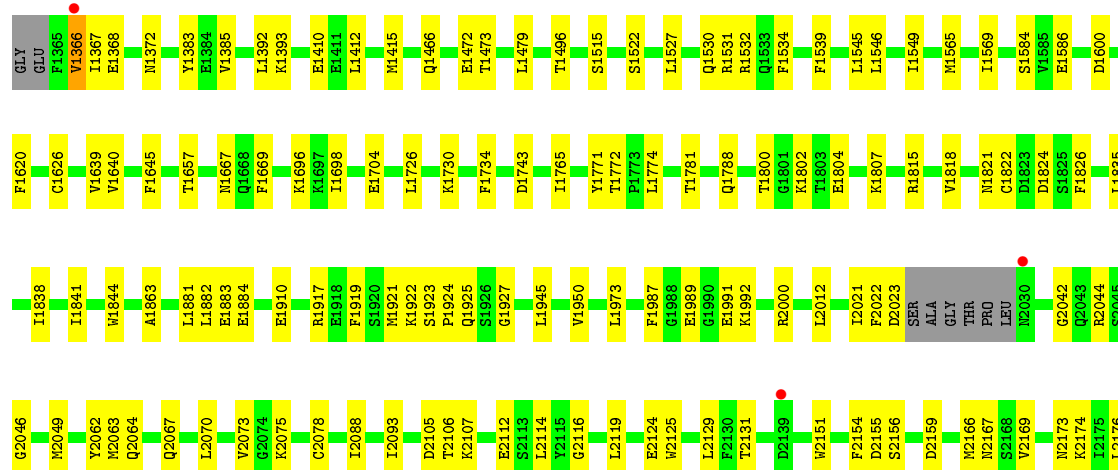
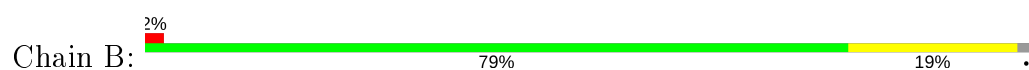
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Dynein heavy chain lysozyme chimera





• Molecule 1: Dynein heavy chain lysozyme chimera



H4092	S9925	E3728	L3583	V8477	L3307	R3132	VAL	L2828	R2646	L482	S2354	T2177
GLY	F9930	S3729	K3584	T3478	Q3318	I3133	PRO	E829	R2660	E488	D2355	L2178
GLY			V3585	V3479			GLU	N2832		I2489		I2186
GLY	R3942	T3740	T3586	E3480	I3325	R3138	ASN	T2833	V2663	N2490	N2363	R2191
GLY	L3945	D3743	L3587	ILE	H3336	R3143	LYS	L2834	K2664	L2491	K2364	I2192
SER	L3946		N3588	ASP	L3337	R3146	GLU	L2835	K2665		K2365	L2193
HIS	L3947		N3589	HIS		E3146	LEU	A2836	K2666	D2495	F2368	
HIS	P3947		L3590	E3485	E3341		VAL	D2837		R2507		T2196
HIS	H9948	Y3746	K3591	E3486	R3342	T3158	T2955	A2838	N2683	T2518	E2374	D2197
HIS	G3949	V3769	E3592	D3487	R3442	K3159	E2956	D2839	Q2684	P2519	I2375	
HIS		D3770	E3593	V3488	A3357	S3160	P2957	L2840	D2685		P2376	R2209
HIS	D3960		I3597	S3489	F3358	P3161	L2958	V2878			S2377	G2210
		N3783		F3492	K3359	S3162	Q2959		N2688	V2523		G2211
	V3966	N3784	F3629	H3497	F3366	A3165	T2960	L2885		V2524	L2380	
	E3969	K3788	S3630	H3497	F3367	A3166	T2961	L2885	S2693	T2525	E2381	F2215
	K3789	A3789	K3634	D3500	D3368	A3173	R2962	D2893	L2694	C2535	A2382	
					F3369		D2963	P2894	L2695	N2536		S2223
	I3801		I3646	G3503	L3370		V2966	T2896	L2699		V2385	Y2234
		S3810	R3655	F3508	L3371	N3177	N2967	N2897	L2700	P2541	M2386	
	L3811		F3656	F3508	T3372	T3178	K2898	K2898	S2701		P2387	N2239
	G3836		I3657	S3511	L3373	N3179	N2975	S2899	D2702	R2549	D2389	K2240
	G3837		K3658	R3512	D3374		P2976	S2900	D2703		I2390	L2241
			K3659	V3513		I3202	Y2977	S2901	F2704	R2582		
	L3840		SER		Y3389	N3205		K2902	K2705		T2394	L2246
		L3844	ARG	H3517	N3393	A3206	K2981	L2903	E2706	P2562	T2397	K2250
	Q4017		GLU		F3406	K3207	V2984	S2905	V2733	S2566	I2398	D2255
	P4019		THR	K3522	D3409	L3208	N2985	P2906	L2712	Y2574	Y2405	N2259
	N4020		ARG	E3523		K3209	S2988	L2907		T2575		L2262
	V4024		ALA	S3524	P3210	P3210	P2989	L2908	S2737	K2576	R2412	L2263
		L3855	ALA	R3528	D3216	D3216	L2999	R2911		I2578	P2420	N2264
	Q4031		ARG					C2912	E2741			L2285
	P4032			M3541	R3219		L3021			E2584	M2426	T2286
	Q4036		I3674	K3544	A3254	A3254	N3025	N2915	I2745	R2585	A2431	
			L3675	L3548	R3278		E3026	N2917	K2750	R2586		R2299
	R4042		L3676				S3027	G2918		E2614	L2437	F2302
	L4045		L3677	Y3555	A3284	A3284	V3028	D2919	K2756	Y2615		
	L4059			L3559	Y3285	Y3285	L3028	V2920	G2760		I2443	D2312
	W4062		E3681	L3562	G3286	G3286	K3030	D2921	R2763	R2624	A2457	T2315
	L4063		V3682	L3562	S3287	S3287	N3032	T2924	T2764	L2625		
	Q4064		Y3683	L3566	S3289	S3289	E3033	T2924		V2626	T2467	S2330
	L4065		D3691	L3566	V3286	V3286	LEU	S2926	I2786	R2627	K2468	
	P4066		K3692	E3569	K3297	K3297	ASN	Q2827	E2787		K2469	G2470
		E3898			S3298	S3298	LYS	V2928	E2789	Y2630	L2471	S2334
	R4075	P3901	K3698	G3575	L3299	L3299	THR		K2790	T2635	T2472	L2342
	K4079	T3906	N3576	N3576	T3300	T3300	GLY	I2936	S2790	G2636	L2473	
			M3577	M3577	F3301	F3301	SER	F2940	P2637	P2637		Y2345
	S4083	F3315	L3578	L3578	E3302	E3302	GLY	T2941	K2476	R2638		F2346
	S4084	F3916	E3579	E3579	K3303	K3303	SER	T2942	S2477	Q2639		
	T4085	G3917	N3580	N3580	E3304	E3304	GLY	F2943				S2350
	E4086	G3918	D3581	D3581	R3305	R3305	SER	A2826	T2827		D2478	
			R3475	R3475	N3306	N3306		I2944		S2643		Q2351

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.73Å 154.38Å 177.55Å 90.00° 96.59° 90.00°	Depositor
Resolution (Å)	49.40 – 3.54 49.40 – 3.54	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.40-3.54) 92.3 (49.40-3.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1769)	Depositor
R, R_{free}	0.228 , 0.262 0.234 , 0.231	Depositor DCC
R_{free} test set	4148 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	84822	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

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	0.32	0/21492	0.58	5/29041 (0.0%)
1	B	0.32	0/21487	0.57	2/29028 (0.0%)
All	All	0.32	0/42979	0.57	7/58069 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3575	GLY	N-CA-C	-6.92	95.81	113.10
1	A	3296	VAL	N-CA-C	-6.30	93.98	111.00
1	B	3587	LEU	CA-CB-CG	6.22	129.60	115.30
1	A	1882	LEU	CB-CG-CD2	5.96	121.13	111.00
1	A	1882	LEU	CA-CB-CG	5.91	128.90	115.30
1	A	2695	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	4065	LEU	CB-CG-CD2	-5.03	102.45	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3946	VAL	Peptide
1	B	3946	VAL	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	21073	21166	21167	354	0
1	B	21070	21166	21167	361	0
2	A	124	49	52	8	0
2	B	124	48	52	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	42393	42429	42438	721	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 8.

All (721) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3692:LYS:N	1:B:3898:GLU:OE2	1.95	0.99
1:A:2946:PRO:HG3	1:A:2958:ILE:HG23	1.51	0.89
1:A:3134:ASP:OD2	1:A:3269:ARG:NE	2.08	0.86
1:A:2387:ARG:NH2	1:A:2875:ASP:OD2	2.10	0.84
1:A:3945:LEU:HD13	1:A:4065:LEU:HD21	1.62	0.82
1:A:3655:ARG:NH1	1:A:3681:GLU:OE1	2.12	0.81
1:B:3470:PHE:HB3	1:B:3475:ASN:HA	1.65	0.79
1:A:2107:LYS:NZ	1:A:2159:ASP:OD2	2.16	0.78
1:B:3461:ILE:CG2	1:B:3479:VAL:HG13	2.14	0.77
1:B:3925:SER:OG	1:B:3969:GLU:OE2	2.02	0.77
1:A:2762:SER:N	1:A:2988:SER:OG	2.17	0.76
2:B:5001:ANP:N3B	2:B:5001:ANP:O2A	2.16	0.75
1:A:1948:LYS:NZ	1:A:1991:GLU:OE2	2.20	0.75
1:B:2155:ASP:OD1	1:B:2507:ARG:NH2	2.20	0.75
1:B:3569:GLU:O	1:B:3580:ASN:ND2	2.20	0.75
1:A:1472:GLU:OE2	1:A:1472:GLU:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2763:ARG:NH1	1:B:3511:SER:O	2.20	0.74
1:B:2064:GLN:O	1:B:2191:ARG:NH1	2.21	0.73
1:B:3444:ILE:HA	1:B:3492:PHE:CE2	2.24	0.73
1:A:2760:GLY:O	1:A:2764:THR:OG1	2.05	0.73
1:B:2921:ASP:OD1	1:B:2922:THR:N	2.21	0.72
1:B:2688:ASN:OD1	1:B:2693:SER:OG	2.04	0.72
1:A:1939:PHE:HB2	1:A:1989:GLU:HB3	1.71	0.72
1:B:2825:THR:O	1:B:2828:LEU:N	2.24	0.71
1:B:2584:GLU:OE2	1:B:2638:ARG:NH1	2.24	0.71
2:A:5003:ANP:O1B	2:A:5003:ANP:O3G	2.09	0.69
1:A:2819:GLU:OE2	1:A:2892:CYS:N	2.23	0.69
1:B:3287:SER:H	1:B:3299:LEU:HD22	1.57	0.69
1:A:2900:SER:HA	1:A:2903:ILE:HB	1.76	0.68
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.75	0.67
1:B:1472:GLU:OE1	1:B:1472:GLU:N	2.27	0.67
1:B:3287:SER:HB3	1:B:3584:MET:O	1.94	0.67
1:A:2064:GLN:NE2	1:A:2091:MET:SD	2.67	0.67
1:A:2420:PRO:HB3	1:A:2906:PRO:HB2	1.76	0.67
1:A:2762:SER:H	1:A:2988:SER:HG	1.42	0.66
1:A:1740:THR:OG1	1:A:1741:LEU:N	2.26	0.66
1:A:2763:ARG:NH1	1:A:3511:SER:O	2.29	0.66
1:B:2549:ARG:NE	2:B:5002:ANP:O3G	2.26	0.66
1:B:3287:SER:HA	1:B:3588:ASN:CA	2.26	0.66
1:A:3030:LYS:NZ	1:A:3031:VAL:O	2.28	0.65
1:A:3925:SER:OG	1:A:3969:GLU:OE2	2.14	0.65
1:B:3287:SER:HA	1:B:3588:ASN:HA	1.77	0.65
1:A:2745:ILE:HG12	1:A:2756:MET:HE1	1.78	0.65
1:B:1657:THR:HG21	1:B:1734:PHE:H	1.62	0.65
1:B:2760:GLY:O	1:B:2764:THR:OG1	2.13	0.64
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.79	0.64
2:A:5003:ANP:O2B	2:A:5003:ANP:O2A	2.15	0.64
1:A:2955:THR:OG1	1:A:2967:ASN:OD1	2.16	0.64
1:B:3584:MET:O	1:B:3587:LEU:N	2.30	0.64
1:B:2695:LEU:HD23	1:B:2706:GLU:HB3	1.80	0.63
1:B:3836:GLY:N	1:B:3869:GLU:OE1	2.32	0.63
1:B:3296:VAL:HA	1:B:3299:LEU:CD2	2.29	0.63
1:B:2385:VAL:HG21	1:B:2578:ILE:HD11	1.81	0.63
1:B:1466:GLN:HB2	1:B:1473:THR:HG21	1.81	0.63
1:A:2167:ASN:HB2	1:A:2209:ARG:NH1	2.14	0.62
1:B:2405:TYR:OH	1:B:2431:ALA:O	2.12	0.62
1:B:3569:GLU:HB3	1:B:3583:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2920:TRP:CD1	1:A:2989:PRO:CG	2.82	0.62
1:B:2900:SER:HA	1:B:2903:ILE:HB	1.81	0.62
1:A:1910:GLU:OE2	1:A:3792:ARG:NH2	2.21	0.62
1:A:2825:THR:O	1:A:2828:LEU:N	2.33	0.62
1:B:2893:ASP:O	1:B:2899:SER:OG	2.12	0.62
1:B:3216:ASP:OD2	1:B:3219:ARG:NH1	2.30	0.62
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.81	0.62
1:B:2908:LEU:O	1:B:2912:CYS:N	2.33	0.62
1:A:1941:ASP:HB3	1:A:1944:SER:HB3	1.82	0.62
1:B:3840:LEU:HD11	1:B:3876:THR:HG23	1.82	0.61
1:B:4079:LYS:O	1:B:4083:SER:OG	2.09	0.61
1:B:1383:TYR:HD2	1:B:1496:THR:HG1	1.48	0.61
1:A:2761:ALA:O	1:A:2766:LYS:NZ	2.31	0.61
1:A:2987:ARG:HG2	1:A:2988:SER:N	2.15	0.61
1:A:2422:SER:OG	1:A:2424:LYS:NZ	2.32	0.61
1:A:3869:GLU:HG2	1:A:3870:LYS:H	1.65	0.61
1:A:2787:HIS:N	1:A:2790:SER:OG	2.33	0.60
1:B:2472:THR:OG1	1:B:2523:TRP:O	2.17	0.60
1:A:1882:LEU:HD23	1:A:1882:LEU:O	2.01	0.60
1:A:2155:ASP:OD1	1:A:2507:ARG:NH2	2.35	0.60
1:B:3287:SER:N	1:B:3299:LEU:HD22	2.16	0.60
1:B:1922:LYS:HB2	1:B:1924:PRO:HD3	1.83	0.60
1:B:2491:LEU:HD13	1:B:2829:GLU:HG2	1.82	0.60
2:B:5003:ANP:O1G	2:B:5003:ANP:O2B	2.20	0.60
1:B:1917:ARG:NH2	1:B:3960:ASP:OD1	2.33	0.59
1:A:2428:MET:SD	1:A:2532:VAL:HG11	2.41	0.59
1:B:3296:VAL:HG11	1:B:3581:ASP:OD1	2.02	0.59
1:A:2473:LEU:HD23	1:A:2525:THR:HB	1.85	0.59
1:B:2420:PRO:HA	2:B:5003:ANP:HNB1	1.67	0.59
1:B:3287:SER:HB2	1:B:3587:LEU:CD2	2.33	0.59
1:B:3303:LYS:NZ	1:B:3590:LEU:HD11	2.17	0.59
1:B:3728:GLU:OE1	1:B:4075:ARG:NH1	2.35	0.59
1:A:2620:ARG:HH11	1:A:2910:ASN:HB3	1.68	0.59
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.42	0.59
1:B:3287:SER:HB3	1:B:3588:ASN:N	2.18	0.59
1:A:3368:ASP:OD2	1:A:3548:LEU:HD23	2.03	0.58
1:A:1802:LYS:HG2	1:A:1921:MET:HG3	1.85	0.58
1:B:3444:ILE:HA	1:B:3492:PHE:CZ	2.38	0.58
1:A:3144:ASP:OD1	1:A:3148:TYR:N	2.37	0.58
1:A:2694:LEU:HD12	1:A:2695:LEU:N	2.18	0.58
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3459:ASP:OD2	1:B:3461:ILE:HD11	2.03	0.58
1:B:3461:ILE:HG22	1:B:3479:VAL:HG13	1.85	0.58
1:A:2760:GLY:HA2	1:A:2917:MET:HB2	1.86	0.58
1:A:3464:ARG:NH2	1:A:3480:GLU:OE1	2.37	0.57
1:B:1586:GLU:HG3	1:B:1765:ILE:H	1.68	0.57
1:B:3303:LYS:HD2	1:B:3591:LYS:HZ1	1.68	0.57
1:A:2903:ILE:HG23	1:A:2909:PHE:CE2	2.38	0.57
1:A:2127:ASP:OD1	1:A:2135:ARG:NH1	2.38	0.57
1:A:2624:ARG:NH2	1:A:2912:CYS:O	2.37	0.57
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.69	0.57
1:B:1774:LEU:HD22	1:B:1924:PRO:HD2	1.86	0.57
1:B:3393:ASN:ND2	1:B:3517:HIS:O	2.38	0.57
1:A:1995:VAL:HG12	1:A:1999:LYS:NZ	2.18	0.57
1:A:3520:THR:HG21	1:A:3646:ILE:HG12	1.87	0.57
1:B:2920:TRP:O	1:B:2924:THR:OG1	2.20	0.57
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.87	0.57
1:A:1862:SER:OG	1:A:1911:ASN:OD1	2.22	0.56
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.35	0.56
1:A:1988:GLY:O	1:A:1993:THR:OG1	2.23	0.56
1:A:2414:ILE:HB	1:A:2532:VAL:HG13	1.87	0.56
1:A:3254:ALA:HB2	1:A:3278:ARG:HG3	1.87	0.56
1:B:3470:PHE:CB	1:B:3475:ASN:HA	2.34	0.56
1:B:1532:ARG:NH2	1:B:1884:GLU:OE2	2.33	0.56
1:B:3660:LYS:NZ	1:B:3677:LEU:HD22	2.20	0.56
1:B:2701:SER:OG	1:B:2705:LYS:NZ	2.30	0.56
1:B:3318:GLN:HG3	1:B:3359:LYS:HG3	1.86	0.56
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	2.06	0.56
1:A:2700:LEU:HD12	1:A:2701:SER:N	2.21	0.56
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.87	0.56
1:A:2700:LEU:HD21	1:A:2712:LEU:HD12	1.88	0.55
2:A:5004:ANP:O3G	2:A:5004:ANP:O2B	2.24	0.55
1:B:2169:VAL:HG13	1:B:2186:ILE:HD13	1.88	0.55
1:B:2893:ASP:OD2	1:B:2896:ASN:HB2	2.07	0.55
1:A:1939:PHE:CB	1:A:1989:GLU:HB3	2.37	0.55
1:B:1987:PHE:CZ	1:B:1992:LYS:HG2	2.42	0.55
1:B:3655:ARG:NH1	1:B:3681:GLU:OE1	2.40	0.55
1:A:2785:LYS:HD3	1:A:3482:GLY:O	2.06	0.55
1:B:1991:GLU:OE2	1:B:2023:ASP:HA	2.07	0.55
1:B:2903:ILE:HA	1:B:2909:PHE:CZ	2.42	0.55
1:A:2200:ASP:OD1	1:A:2201:HIS:N	2.40	0.54
1:A:2903:ILE:HG23	1:A:2909:PHE:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2614:HIS:HA	1:B:2909:PHE:CE2	2.43	0.54
1:B:2836:ALA:HA	1:B:2911:ARG:HG3	1.88	0.54
1:A:1741:LEU:HG	1:A:1742:ASP:H	1.71	0.54
1:B:2342:ILE:HG23	1:B:2346:PHE:CE2	2.41	0.54
1:A:2733:VAL:HG11	1:A:2928:VAL:HA	1.88	0.54
1:A:3409:ASP:N	1:A:3409:ASP:OD1	2.39	0.54
1:A:3524:SER:OG	1:A:3528:ARG:NH2	2.40	0.54
1:B:3461:ILE:HG21	1:B:3479:VAL:HG13	1.88	0.54
1:A:1586:GLU:HG3	1:A:1765:ILE:H	1.71	0.54
1:B:3289:SER:CB	1:B:3299:LEU:HB3	2.38	0.54
1:B:3296:VAL:HA	1:B:3299:LEU:HG	1.90	0.54
1:A:3132:ARG:NH2	1:A:3581:ASP:OD1	2.41	0.53
1:B:1479:LEU:HD11	1:B:1515:SER:HB3	1.89	0.53
1:B:2063:MET:HB3	1:B:2070:LEU:HD11	1.89	0.53
1:A:1410:GLU:OE1	1:A:3439:ARG:NH1	2.42	0.53
1:A:3458:PHE:CE1	1:A:3466:ILE:HD11	2.43	0.53
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	2.38	0.53
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	2.08	0.53
1:B:3801:ILE:HD13	1:B:3811:LEU:HD23	1.91	0.53
1:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.91	0.53
1:A:2977:TYR:HE1	1:A:2987:ARG:HD3	1.74	0.53
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.29	0.53
1:B:2620:ARG:HD2	1:B:2910:ASN:HB3	1.91	0.53
1:B:3845:GLN:OE1	1:B:3878:HIS:N	2.41	0.53
1:A:2762:SER:O	1:A:2988:SER:OG	2.25	0.53
1:A:2851:LYS:O	1:A:2855:ASN:ND2	2.40	0.53
1:A:2958:ILE:HG13	1:A:2963:ASP:HB2	1.90	0.53
1:B:2955:THR:HG21	1:B:2966:VAL:HG21	1.89	0.53
1:A:1882:LEU:O	1:A:1883:GLU:HB2	2.08	0.52
1:A:2902:MET:O	1:A:2908:LEU:HD22	2.10	0.52
1:B:3288:GLY:N	1:B:3299:LEU:HB2	2.24	0.52
1:B:3296:VAL:O	1:B:3299:LEU:HG	2.09	0.52
1:B:3301:PHE:HE1	1:B:3305:ARG:NE	2.07	0.52
1:A:3134:ASP:OD1	1:A:3135:GLU:N	2.42	0.52
1:B:2624:ARG:NH2	1:B:2912:CYS:O	2.41	0.52
1:B:3522:LYS:C	1:B:3524:SER:H	2.13	0.52
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.91	0.52
1:A:2856:LEU:O	1:A:2860:THR:OG1	2.18	0.52
1:A:3942:ARG:NH1	1:A:3949:GLY:HA2	2.24	0.52
1:A:3946:VAL:O	1:A:3948:HIS:N	2.42	0.52
1:B:2894:PRO:HB3	1:B:2903:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3302:GLU:OE2	1:B:3591:LYS:HE2	2.08	0.52
1:B:3480:GLU:HB3	1:B:3485:GLU:CA	2.39	0.52
1:B:3480:GLU:HB3	1:B:3485:GLU:HA	1.91	0.52
1:B:2958:ILE:CG2	1:B:2963:ASP:HB3	2.40	0.52
1:B:3474:GLY:O	1:B:3475:ASN:CG	2.48	0.52
1:B:3683:TYR:HB2	1:B:3702:MET:HE1	1.92	0.52
1:B:3021:LEU:HD13	1:B:3307:LEU:HB3	1.92	0.52
1:A:2310:LEU:HD12	1:A:2311:LYS:N	2.25	0.52
1:B:2078:CYS:SG	1:B:2215:PHE:HB3	2.49	0.52
1:B:3930:PHE:CG	1:B:4045:LEU:HD13	2.45	0.52
1:A:2386:MET:HE1	1:A:2627:ARG:HG2	1.92	0.52
1:A:4079:LYS:O	1:A:4083:SER:OG	2.21	0.52
1:B:2125:TRP:CZ2	1:B:2178:LEU:HD12	2.44	0.52
1:B:2070:LEU:HB2	1:B:2193:LEU:HD23	1.92	0.51
1:B:2646:ARG:HE	1:B:2695:LEU:HD21	1.75	0.51
1:B:3500:ASP:OD2	1:B:3503:GLY:N	2.43	0.51
1:B:2330:SER:HB3	1:B:2334:SER:HB2	1.92	0.51
1:A:1647:ALA:O	1:A:1651:SER:OG	2.20	0.51
1:A:2253:ILE:O	1:A:2256:SER:OG	2.23	0.51
1:A:2955:THR:HG22	1:A:2970:ILE:HD12	1.92	0.51
1:A:3464:ARG:NE	1:A:3480:GLU:HB2	2.25	0.51
1:A:3946:VAL:O	1:A:3948:HIS:O	2.29	0.51
1:B:3287:SER:OG	1:B:3299:LEU:HD13	2.11	0.51
1:B:2646:ARG:NH2	1:B:2695:LEU:HD11	2.26	0.51
1:B:3289:SER:HB3	1:B:3299:LEU:HB3	1.92	0.51
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.92	0.51
1:B:2042:GLY:O	1:B:2046:GLY:N	2.43	0.51
1:B:2954:PHE:N	1:B:2967:ASN:HD21	2.08	0.51
1:B:2707:VAL:HG21	1:B:2712:LEU:HD13	1.92	0.51
1:A:2196:THR:HA	1:A:2549:ARG:NH1	2.26	0.51
1:A:3133:ILE:HG23	1:A:3585:VAL:HG11	1.92	0.51
1:A:2169:VAL:HG13	1:A:2186:ILE:HD13	1.93	0.50
1:B:1989:GLU:N	1:B:1989:GLU:OE1	2.44	0.50
1:B:2639:GLN:OE1	1:B:2643:SER:OG	2.21	0.50
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.45	0.50
1:B:1531:ARG:NH1	1:B:1545:LEU:HD22	2.26	0.50
1:B:2822:ILE:HD11	1:B:2898:LYS:HB3	1.94	0.50
1:A:3562:LEU:HB3	1:A:3590:LEU:HD12	1.94	0.50
1:B:3306:TRP:CH2	1:B:3559:LEU:HD21	2.46	0.50
1:B:3470:PHE:HB3	1:B:3475:ASN:CA	2.38	0.50
1:B:2574:TYR:HB3	1:B:2626:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3255:VAL:HG12	1:A:3259:LYS:NZ	2.27	0.50
1:B:3366:PHE:CE1	1:B:3370:LEU:HD12	2.46	0.50
1:B:3460:PRO:O	1:B:3463:SER:HB3	2.12	0.50
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.94	0.50
1:B:3132:ARG:NH1	1:B:3577:MET:O	2.45	0.50
1:B:3584:MET:O	1:B:3587:LEU:HB3	2.12	0.50
1:A:3132:ARG:NH1	1:A:3577:MET:O	2.44	0.50
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	2.42	0.50
1:B:2021:ILE:HG22	1:B:2022:PHE:H	1.75	0.50
1:A:2472:THR:OG1	1:A:2523:TRP:O	2.29	0.50
1:B:1534:PHE:HE2	1:B:1565:MET:CE	2.24	0.50
1:A:3845:GLN:OE1	1:A:3878:HIS:N	2.43	0.49
1:B:1802:LYS:NZ	2:B:5001:ANP:O2G	2.36	0.49
1:A:2163:VAL:O	1:A:2167:ASN:N	2.45	0.49
1:A:3296:VAL:HG12	1:A:3298:SER:H	1.76	0.49
1:B:3461:ILE:HB	1:B:3479:VAL:HG22	1.94	0.49
1:A:2920:TRP:CZ2	1:A:2993:ILE:HD11	2.47	0.49
1:B:1815:ARG:NH1	1:B:1844:TRP:HE1	2.11	0.49
1:B:2635:THR:HG23	1:B:2704:PHE:HB2	1.94	0.49
1:B:3287:SER:HA	1:B:3588:ASN:CB	2.42	0.49
1:A:2491:LEU:HD13	1:A:2829:GLU:HG2	1.94	0.49
1:B:3284:ALA:O	1:B:3285:TYR:HB2	2.12	0.49
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	1.93	0.49
1:B:3743:ASP:HA	1:B:3746:TYR:CD1	2.47	0.49
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.94	0.49
1:B:2000:ARG:NH1	1:B:2062:TYR:CG	2.81	0.49
1:B:2576:LYS:HG2	1:B:2586:ARG:NH1	2.28	0.49
1:B:4065:LEU:HB2	1:B:4066:PRO:HD2	1.95	0.49
1:B:2902:MET:HA	1:B:2908:LEU:HD22	1.95	0.49
1:A:1624:ARG:NH1	1:A:1625:ASP:OD1	2.45	0.49
1:B:3946:VAL:HG12	1:B:3947:PRO:HD3	1.94	0.49
1:A:2606:ARG:NH1	1:A:2672:LEU:HB2	2.28	0.49
1:A:2788:ARG:HG3	1:A:3459:ASP:HB3	1.94	0.49
1:B:1704:GLU:OE2	1:B:1771:TYR:CE1	2.66	0.49
1:B:3337:LEU:HB3	1:B:3341:GLU:HB2	1.94	0.49
1:A:2954:PHE:CE2	1:A:2970:ILE:HG21	2.48	0.48
1:A:3429:LEU:O	1:A:3453:GLN:N	2.45	0.48
1:A:3466:ILE:HD13	1:A:3509:LEU:CD1	2.43	0.48
1:B:3288:GLY:H	1:B:3299:LEU:HB2	1.77	0.48
1:B:3318:GLN:CG	1:B:3359:LYS:HG3	2.43	0.48
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2650:TYR:HE1	1:A:2654:ARG:HE	1.61	0.48
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.49	0.48
1:B:3288:GLY:HA2	1:B:3591:LYS:HG3	1.95	0.48
1:B:3844:ILE:HD11	1:B:3855:LEU:HD23	1.95	0.48
1:A:2382:ALA:O	1:A:2385:VAL:HG12	2.13	0.48
1:A:2993:ILE:HD13	2:A:5004:ANP:N3	2.28	0.48
1:B:1366:VAL:HG22	1:B:3488:VAL:HG11	1.95	0.48
1:B:3524:SER:O	1:B:3528:ARG:HG2	2.13	0.48
1:B:3729:SER:OG	1:B:4086:GLU:OE1	2.29	0.48
1:A:2920:TRP:CD1	1:A:2989:PRO:HB2	2.48	0.48
1:B:2265:ILE:CD1	1:B:2346:PHE:CE2	2.96	0.48
1:B:3691:ASP:HA	1:B:3898:GLU:OE2	2.14	0.48
1:B:2112:GLU:O	1:B:2116:GLY:N	2.47	0.48
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.94	0.48
1:B:2903:ILE:HG23	1:B:2909:PHE:CE2	2.49	0.48
1:B:3030:LYS:O	1:B:3031:VAL:HG22	2.13	0.48
1:B:3303:LYS:HZ3	1:B:3590:LEU:CD1	2.26	0.48
1:A:2386:MET:SD	1:A:2752:VAL:HG21	2.53	0.48
1:B:2733:VAL:HG11	1:B:2928:VAL:HA	1.96	0.48
1:A:3942:ARG:HA	1:A:3945:LEU:HD12	1.96	0.48
1:A:3942:ARG:HH11	1:A:3949:GLY:HA2	1.79	0.48
1:B:2107:LYS:NZ	1:B:2159:ASP:OD2	2.39	0.48
1:B:2476:LYS:HD3	1:B:2482:LEU:HB2	1.95	0.48
1:A:3212:TYR:O	1:A:3220:ARG:NE	2.47	0.48
1:A:3130:MET:HG3	1:A:3285:TYR:CE2	2.49	0.48
1:A:3945:LEU:HD11	1:A:4063:LEU:HD23	1.96	0.48
1:B:2265:ILE:HD11	1:B:2346:PHE:CE2	2.48	0.48
1:B:3254:ALA:HB2	1:B:3278:ARG:HG3	1.95	0.48
1:A:2695:LEU:HD12	1:A:2696:PHE:H	1.79	0.48
1:A:2762:SER:CA	1:A:2988:SER:OG	2.61	0.48
1:A:3786:PHE:CD1	1:A:3893:ASP:HB2	2.49	0.48
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.96	0.48
1:A:3500:ASP:OD2	1:A:3502:SER:HB2	2.13	0.47
1:A:1999:LYS:HB2	1:A:2003:LEU:HD12	1.94	0.47
1:A:2283:LYS:HD3	1:A:2326:LEU:HA	1.95	0.47
1:B:1910:GLU:HB2	1:B:3846:MET:HA	1.96	0.47
1:B:2167:ASN:HB2	1:B:2209:ARG:NH1	2.28	0.47
1:B:2699:LEU:CD1	1:B:2750:LYS:HZ1	2.27	0.47
1:B:3945:LEU:HD13	1:B:4065:LEU:HD21	1.95	0.47
1:A:2070:LEU:HB2	1:A:2193:LEU:HD23	1.95	0.47
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2075:LYS:O	1:B:2078:CYS:HB2	2.13	0.47
1:B:3555:TYR:HB3	1:B:3597:ILE:HG12	1.97	0.47
1:B:4018:SER:O	1:B:4020:ASN:N	2.48	0.47
1:A:3799:LYS:HD3	1:A:3802:GLU:OE2	2.15	0.47
1:B:1821:ASN:ND2	1:B:1824:ASP:OD2	2.39	0.47
1:B:3287:SER:CB	1:B:3587:LEU:HB3	2.45	0.47
1:B:3656:VAL:HG11	1:B:3674:ILE:HD12	1.95	0.47
1:A:1423:ILE:HD12	1:A:1424:PHE:CD1	2.49	0.47
1:B:2088:ILE:HD11	1:B:2151:TRP:CD2	2.49	0.47
1:A:2761:ALA:C	1:A:2766:LYS:HZ1	2.15	0.47
1:A:2786:ILE:HD11	1:A:2821:ASN:HA	1.97	0.47
1:A:3460:PRO:O	1:A:3463:SER:HB3	2.14	0.47
1:B:2169:VAL:HG22	1:B:2186:ILE:HD11	1.95	0.47
1:B:3480:GLU:HB3	1:B:3485:GLU:N	2.29	0.47
1:B:4018:SER:C	1:B:4020:ASN:H	2.18	0.47
1:A:2584:GLU:CD	1:A:2638:ARG:HH22	2.18	0.47
1:A:2853:LEU:HD11	1:A:2870:GLU:HG3	1.97	0.47
1:A:3683:TYR:HB2	1:A:3702:MET:HE1	1.97	0.47
1:B:3986:ARG:NE	1:B:4016:CYS:HB2	2.29	0.47
1:A:1486:ILE:HG23	1:A:1505:PHE:CE2	2.50	0.47
1:A:2385:VAL:HG13	1:A:2386:MET:HE3	1.97	0.47
1:A:2491:LEU:HD13	1:A:2829:GLU:CG	2.45	0.47
1:B:1927:GLY:HA2	1:B:1950:VAL:HG21	1.96	0.47
1:B:2741:HIS:CG	1:B:2917:MET:SD	3.07	0.47
1:A:3584:MET:O	1:A:3587:LEU:HG	2.15	0.47
1:B:2286:THR:HA	1:B:2412:ARG:HD2	1.97	0.47
1:B:3578:LEU:HD12	1:B:3579:GLU:N	2.30	0.47
1:B:3769:VAL:HG12	1:B:3770:ASP:N	2.30	0.47
1:A:2475:PRO:HB3	1:A:2527:GLU:HB2	1.97	0.47
1:A:3584:MET:HA	1:A:3587:LEU:HG	1.97	0.47
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.30	0.46
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.96	0.46
1:B:3342:ARG:CZ	1:B:3389:TYR:HE1	2.28	0.46
1:B:3287:SER:HB2	1:B:3587:LEU:HB3	1.96	0.46
1:A:1800:THR:OG1	1:A:1801:GLY:N	2.48	0.46
1:A:2936:ILE:HG22	1:A:2962:ARG:NH1	2.30	0.46
1:A:3393:ASN:ND2	1:A:3517:HIS:O	2.48	0.46
1:B:1539:PHE:CZ	1:B:1841:ILE:HD12	2.50	0.46
1:B:2646:ARG:CZ	1:B:2695:LEU:HD11	2.45	0.46
1:A:3409:ASP:OD2	1:A:3412:SER:HA	2.15	0.46
1:A:3787:THR:HG23	1:A:3892:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3296:VAL:HA	1:B:3299:LEU:CG	2.45	0.46
1:B:3409:ASP:N	1:B:3409:ASP:OD1	2.49	0.46
1:B:2552:ARG:NH2	2:B:5002:ANP:O2G	2.48	0.46
1:A:2081:THR:OG1	1:A:2195:GLU:OE1	2.33	0.46
1:B:2315:THR:HG21	1:B:2350:SER:HB3	1.98	0.46
1:B:2838:ALA:HB3	1:B:2878:VAL:CG1	2.45	0.46
1:B:2903:ILE:HG12	1:B:2909:PHE:HZ	1.80	0.46
1:B:2944:ILE:HD11	1:B:3357:ALA:H	1.80	0.46
1:A:1395:VAL:HG21	1:A:1398:TRP:CZ2	2.51	0.46
1:A:2127:ASP:OD2	1:A:2135:ARG:HD2	2.16	0.46
1:A:2693:SER:HA	1:A:2696:PHE:CZ	2.50	0.46
1:A:3722:MET:SD	1:A:3748:TRP:HB2	2.56	0.46
1:A:3843:ASN:H	1:A:3876:THR:HB	1.80	0.46
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.98	0.46
1:A:2312:ASP:HB3	1:A:2351:GLN:HG3	1.96	0.46
1:A:3130:MET:HG3	1:A:3285:TYR:CD2	2.50	0.46
1:A:4065:LEU:HB2	1:A:4066:PRO:HD2	1.97	0.46
1:B:2700:LEU:HD12	1:B:2701:SER:N	2.31	0.46
1:A:2246:LEU:HG	1:A:2250:LYS:HE3	1.97	0.46
1:B:2114:LEU:O	1:B:2129:LEU:N	2.49	0.46
1:B:2663:VAL:O	1:B:2666:LYS:N	2.49	0.46
1:B:2699:LEU:HD13	1:B:2750:LYS:NZ	2.31	0.46
1:B:3287:SER:HB2	1:B:3587:LEU:HD22	1.98	0.46
1:A:1365:PHE:CE2	1:A:1420:TYR:HB3	2.51	0.46
1:A:1677:ASP:OD2	1:A:1681:LYS:HE3	2.16	0.46
1:A:2385:VAL:HG13	1:A:2386:MET:CE	2.46	0.46
1:A:3800:LEU:HD21	1:A:3874:PHE:CG	2.51	0.46
1:B:3289:SER:N	1:B:3299:LEU:CB	2.79	0.46
1:B:2999:LEU:HD11	1:B:3325:ILE:HG12	1.98	0.46
1:A:1831:LEU:HD12	1:A:1861:VAL:HG22	1.99	0.45
1:B:3945:LEU:CD1	1:B:4065:LEU:HD21	2.46	0.45
1:A:1850:PHE:CE2	1:A:1858:LEU:HD11	2.51	0.45
1:A:2428:MET:CE	1:A:2532:VAL:HG11	2.45	0.45
1:A:2823:LEU:HD11	1:A:3460:PRO:CD	2.45	0.45
1:B:2166:MET:HE1	1:B:2192:ILE:HD13	1.98	0.45
1:B:3475:ASN:HD21	1:B:3489:SER:N	2.14	0.45
1:A:1876:LYS:HE2	1:A:1879:ILE:HG22	1.99	0.45
1:A:3844:ILE:HD11	1:A:3855:LEU:HD23	1.98	0.45
1:B:1412:LEU:HD23	1:B:1415:MET:SD	2.57	0.45
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.57	0.45
1:B:3655:ARG:HA	1:B:3658:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1398:TRP:CZ2	1:A:1446:VAL:HA	2.51	0.45
1:A:2068:GLN:NE2	1:A:2190:PHE:O	2.48	0.45
1:A:2317:LEU:HD21	1:A:2359:ILE:HD12	1.97	0.45
1:B:2903:ILE:HG12	1:B:2909:PHE:CZ	2.52	0.45
1:B:2940:PHE:CG	1:B:2941:THR:N	2.84	0.45
1:B:3462:ILE:HG23	1:B:3465:LEU:HD23	1.98	0.45
1:A:1763:ILE:HG22	1:A:1766:PRO:HD3	1.97	0.45
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.82	0.45
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.52	0.45
1:A:2653:TRP:HB3	1:A:2654:ARG:NH1	2.31	0.45
1:A:2856:LEU:HD21	1:A:2877:PHE:HB2	1.99	0.45
1:A:3578:LEU:HD12	1:A:3579:GLU:N	2.32	0.45
1:B:1772:THR:OG1	1:B:1925:GLN:HG3	2.16	0.45
1:B:2699:LEU:HD13	1:B:2750:LYS:HE3	1.98	0.45
1:B:3303:LYS:NZ	1:B:3590:LEU:CD1	2.80	0.45
1:A:2330:SER:HB3	1:A:2334:SER:HB2	1.99	0.45
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.99	0.45
1:B:2420:PRO:HB3	1:B:2906:PRO:HB2	1.99	0.45
1:B:2956:GLU:HB3	1:B:2957:PRO:HD2	1.98	0.45
1:B:3562:LEU:HB3	1:B:3590:LEU:HD12	1.99	0.45
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.82	0.45
1:A:2225:LYS:HD3	1:A:2284:LEU:HD12	1.99	0.45
1:A:2233:SER:HB3	1:A:2292:VAL:HG11	1.98	0.45
1:B:3915:PHE:CZ	1:B:4042:ARG:HB3	2.52	0.45
1:A:2640:THR:HG23	1:A:2643:SER:H	1.81	0.45
1:A:2615:TYR:CE1	1:A:2660:LEU:HD23	2.52	0.45
1:A:3990:ALA:O	1:A:3995:GLY:HA3	2.17	0.45
1:B:1527:LEU:HD22	1:B:1545:LEU:HD23	1.98	0.45
1:B:3296:VAL:HA	1:B:3299:LEU:HD21	1.96	0.45
1:B:3676:TRP:CE3	1:B:3677:LEU:HD23	2.52	0.45
1:B:3946:VAL:O	1:B:3948:HIS:O	2.34	0.45
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.99	0.45
1:A:1650:LEU:HD21	1:A:1747:VAL:HG11	1.98	0.45
1:A:2955:THR:HG21	1:A:2966:VAL:HG23	1.98	0.45
1:B:2958:ILE:HB	1:B:2963:ASP:HB2	1.99	0.45
1:B:3657:PHE:CZ	1:B:3674:ILE:HD11	2.51	0.45
1:B:3708:PHE:HE1	1:B:3719:VAL:HG11	1.82	0.45
1:A:1836:VAL:HG13	1:A:1886:THR:HG21	1.99	0.44
1:A:2574:TYR:HB3	1:A:2626:VAL:HG11	1.99	0.44
1:A:2653:TRP:CD1	1:A:2694:LEU:HD21	2.52	0.44
1:A:3620:ILE:H	1:A:3620:ILE:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.31	0.44
1:B:2787:HIS:N	1:B:2790:SER:OG	2.50	0.44
1:A:2620:ARG:HH11	1:A:2910:ASN:CB	2.30	0.44
1:A:2838:ALA:HB3	1:A:2878:VAL:CG1	2.48	0.44
1:B:3901:PRO:HB2	1:B:3906:THR:HG23	1.99	0.44
1:A:2375:ILE:HD11	1:A:2395:ILE:HG13	1.99	0.44
1:A:2543:ARG:NH2	1:A:2906:PRO:HD2	2.32	0.44
1:B:1863:ALA:HB3	1:B:1882:LEU:HD11	1.99	0.44
1:B:2380:LEU:HD13	1:B:2390:ILE:HD11	1.99	0.44
1:B:2699:LEU:HD13	1:B:2750:LYS:HZ1	1.83	0.44
1:B:2898:LYS:HD2	1:B:2898:LYS:N	2.33	0.44
1:A:1392:LEU:CD1	1:A:1394:LEU:HD23	2.46	0.44
1:A:1504:ASN:O	1:A:1508:THR:OG1	2.25	0.44
1:A:1917:ARG:NH2	1:A:3960:ASP:OD1	2.43	0.44
1:B:2926:SER:OG	1:B:2955:THR:HG22	2.17	0.44
1:A:3824:TYR:CZ	1:A:3828:GLU:HG3	2.53	0.44
1:A:2948:VAL:HG22	1:A:2949:ASN:N	2.33	0.44
1:A:2987:ARG:CG	1:A:2988:SER:N	2.79	0.44
1:B:1600:ASP:OD1	1:B:1600:ASP:N	2.50	0.44
1:B:3302:GLU:OE2	1:B:3591:LYS:CE	2.64	0.44
1:A:2651:GLU:O	1:A:2655:ILE:HG12	2.18	0.44
1:A:2800:LYS:HG3	1:A:2843:LEU:HG	1.99	0.44
1:A:3946:VAL:HG12	1:A:3947:PRO:HD3	1.99	0.44
1:B:1883:GLU:OE2	1:B:1883:GLU:N	2.51	0.44
1:B:2473:LEU:HD23	1:B:2525:THR:HB	1.98	0.44
1:B:2663:VAL:HG13	1:B:2664:LYS:H	1.82	0.44
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.53	0.44
1:A:1780:ALA:HA	1:A:1783:THR:HG22	1.99	0.44
1:A:2278:VAL:O	1:A:2283:LYS:HE2	2.17	0.44
1:A:2760:GLY:HA3	1:A:2766:LYS:HD3	2.00	0.44
1:A:2759:ILE:HG21	1:A:2916:TRP:CZ3	2.53	0.44
1:B:2042:GLY:HA3	1:B:2049:MET:CE	2.48	0.44
1:B:2312:ASP:HB3	1:B:2351:GLN:HG3	2.00	0.44
1:B:3284:ALA:O	1:B:3285:TYR:CB	2.64	0.44
1:B:3288:GLY:O	1:B:3302:GLU:OE2	2.35	0.44
1:B:3474:GLY:O	1:B:3475:ASN:ND2	2.51	0.44
1:B:3133:ILE:HG23	1:B:3585:VAL:HG11	1.99	0.44
1:A:1815:ARG:NH1	1:A:1844:TRP:NE1	2.66	0.44
1:A:1802:LYS:HE2	2:A:5001:ANP:O1B	2.18	0.44
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	2.48	0.44
1:A:1995:VAL:HG22	1:A:2022:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2392:ILE:CG2	1:A:2573:ILE:HD12	2.47	0.43
1:B:2476:LYS:HD3	1:B:2482:LEU:HD22	1.99	0.43
1:B:2839:ASP:HB3	1:B:2878:VAL:HG22	1.99	0.43
1:A:2175:ILE:HG12	1:A:2185:PRO:HA	2.00	0.43
1:A:2938:MET:HB2	1:A:2962:ARG:HH21	1.83	0.43
1:B:1530:GLN:HG2	1:B:1549:ILE:HD11	2.00	0.43
1:B:1696:LYS:HB2	1:B:1765:ILE:HD12	1.99	0.43
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.83	0.43
1:B:2386:MET:HB2	1:B:2627:ARG:NE	2.33	0.43
1:B:2834:LEU:HB2	1:B:2840:ILE:HD11	2.00	0.43
1:B:2936:ILE:CG2	1:B:2962:ARG:HD3	2.48	0.43
1:B:3810:SER:HB3	1:B:3837:GLY:HA2	1.99	0.43
1:A:1472:GLU:OE1	1:A:1522:SER:OG	2.33	0.43
1:A:2404:PHE:CZ	1:A:2416:LEU:HD11	2.53	0.43
1:A:2894:PRO:HA	1:A:2903:ILE:HD11	1.99	0.43
1:A:3708:PHE:HE1	1:A:3719:VAL:HG11	1.83	0.43
1:B:1385:VAL:CG1	1:B:1393:LYS:HB3	2.48	0.43
1:B:2355:ASP:O	1:B:2399:LYS:NZ	2.34	0.43
1:B:2737:SER:O	1:B:2741:HIS:ND1	2.51	0.43
1:B:3942:ARG:HG3	1:B:3945:LEU:HD12	2.00	0.43
1:A:3432:LEU:HD21	1:A:3457:PHE:CD1	2.52	0.43
1:A:3769:VAL:HG12	1:A:3770:ASP:N	2.33	0.43
1:A:3783:ASN:OD1	1:A:3784:ASN:N	2.51	0.43
1:B:3288:GLY:HA3	1:B:3299:LEU:O	2.18	0.43
1:A:1631:LYS:HE2	1:A:1658:GLU:OE1	2.19	0.43
1:A:2733:VAL:HG12	1:A:2734:ILE:N	2.33	0.43
1:A:3942:ARG:HG3	1:A:3945:LEU:HD12	1.99	0.43
1:B:2196:THR:HA	1:B:2549:ARG:NH1	2.33	0.43
1:B:2234:TYR:CE2	1:B:2250:LYS:HB2	2.53	0.43
1:B:1410:GLU:OE1	1:B:3439:ARG:NH1	2.52	0.43
1:A:2674:TYR:CZ	1:A:2689:ILE:HG22	2.53	0.43
1:A:3338:ASN:HB2	1:A:3341:GLU:HG2	2.01	0.43
1:B:2246:LEU:HG	1:B:2250:LYS:HE3	2.01	0.43
1:B:2976:PHE:HZ	1:B:3336:HIS:HE1	1.67	0.43
1:B:3946:VAL:O	1:B:3948:HIS:N	2.51	0.43
1:A:2920:TRP:CD1	1:A:2989:PRO:CB	3.01	0.43
1:A:3337:LEU:HB3	1:A:3341:GLU:HB2	2.00	0.43
1:A:1440:GLU:O	1:A:1444:ASN:ND2	2.46	0.43
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	3.01	0.43
1:A:2548:GLU:HA	1:A:2551:THR:OG1	2.18	0.43
1:A:2584:GLU:OE1	1:A:2584:GLU:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2999:LEU:HD11	1:A:3325:ILE:HG12	2.01	0.43
1:B:2106:THR:OG1	1:B:2156:SER:HB2	2.19	0.43
1:B:3444:ILE:HG21	1:B:3487:ASP:OD2	2.19	0.43
1:B:2426:MET:HG3	2:B:5003:ANP:H5'1	2.00	0.43
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.84	0.43
1:A:2386:MET:HE1	1:A:2627:ARG:CG	2.48	0.43
1:A:3129:GLU:HB2	1:A:3295:LEU:HB3	2.01	0.43
1:B:3441:GLU:HA	1:B:3444:ILE:HG22	2.00	0.43
1:A:1800:THR:HA	1:A:1924:PRO:HG3	2.00	0.43
1:A:3579:GLU:O	1:A:3582:GLU:N	2.52	0.43
1:A:3980:ILE:N	1:A:3981:PRO:CD	2.82	0.43
1:B:2490:ASN:ND2	1:B:2536:ASN:O	2.52	0.43
2:B:5004:ANP:O1B	2:B:5004:ANP:O3G	2.37	0.43
1:A:1527:LEU:HD21	1:A:1546:LEU:HD21	2.00	0.42
1:A:2645:ILE:HD11	1:A:2686:LEU:HG	2.01	0.42
1:A:2728:LEU:HD12	1:A:2771:ARG:HH22	1.83	0.42
1:A:2827:PHE:CD1	1:A:2827:PHE:N	2.87	0.42
1:A:3628:ILE:HD11	1:A:3679:TYR:CZ	2.54	0.42
1:A:3763:PHE:O	1:A:3767:PHE:N	2.52	0.42
1:B:2106:THR:HG22	1:B:2154:PHE:CD1	2.53	0.42
1:B:2197:ASP:N	1:B:2197:ASP:OD1	2.50	0.42
1:B:2223:SER:HB3	1:B:2259:MET:HG2	2.01	0.42
1:B:2518:THR:HB	1:B:2519:PRO:HD3	2.01	0.42
1:A:1935:GLN:O	1:A:1938:GLY:HA2	2.18	0.42
1:A:2695:LEU:O	1:A:2696:PHE:C	2.58	0.42
1:A:2839:ASP:HB3	1:A:2878:VAL:HG22	2.02	0.42
1:A:3261:ARG:NH1	1:A:3265:GLN:HG3	2.34	0.42
1:B:1367:ILE:HG23	1:B:1415:MET:CE	2.48	0.42
1:B:1800:THR:HA	1:B:1923:SER:HB3	2.02	0.42
1:B:1772:THR:HB	1:B:1925:GLN:CD	2.40	0.42
1:B:3025:ASN:O	1:B:3028:VAL:HG22	2.19	0.42
1:A:2695:LEU:HD12	1:A:2696:PHE:N	2.34	0.42
1:B:1667:ASN:HA	1:B:1669:PHE:CE2	2.53	0.42
1:B:2264:ASN:HB3	1:B:2345:TYR:CE2	2.54	0.42
1:B:3306:TRP:HH2	1:B:3559:LEU:HD21	1.84	0.42
1:A:1462:ASN:HB3	1:A:1465:ILE:HG22	2.02	0.42
1:A:1572:ILE:HD11	1:A:1579:ILE:HD13	2.01	0.42
1:A:1667:ASN:HA	1:A:1669:PHE:CE2	2.55	0.42
1:A:2426:MET:O	1:A:2430:ASN:HB2	2.19	0.42
1:A:2518:THR:N	1:A:2519:PRO:CD	2.82	0.42
1:A:2518:THR:N	1:A:2519:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2786:ILE:HG21	1:A:2827:PHE:CE2	2.54	0.42
1:A:2894:PRO:HA	1:A:2903:ILE:CD1	2.49	0.42
1:B:2787:HIS:CD2	1:B:2789:HIS:HB2	2.54	0.42
1:B:2943:PHE:O	1:B:2944:ILE:C	2.58	0.42
1:B:3206:ALA:HA	1:B:3209:LYS:HB3	2.01	0.42
1:A:2426:MET:HG2	2:A:5003:ANP:O1A	2.19	0.42
1:A:2428:MET:SD	1:A:2532:VAL:CG1	3.07	0.42
1:A:2762:SER:C	1:A:2764:THR:H	2.22	0.42
1:A:3581:ASP:O	1:A:3584:MET:HG2	2.19	0.42
1:B:2956:GLU:HB3	1:B:2957:PRO:CD	2.49	0.42
1:B:2977:TYR:CD1	1:B:2981:LYS:HG3	2.54	0.42
1:A:2988:SER:HA	1:A:2989:PRO:HD3	1.91	0.42
1:B:1640:VAL:HG11	1:B:1698:ILE:HG12	2.02	0.42
1:B:1822:CYS:HA	1:B:1826:PHE:HE1	1.84	0.42
1:B:3475:ASN:HD21	1:B:3489:SER:H	1.67	0.42
1:B:2173:ASN:O	1:B:2174:LYS:HG2	2.19	0.42
1:B:2476:LYS:HG3	1:B:2478:ASP:H	1.85	0.42
1:B:2940:PHE:CD2	1:B:3318:GLN:OE1	2.73	0.42
1:B:3372:THR:HG22	1:B:3374:ASP:H	1.85	0.42
1:B:3478:THR:OG1	1:B:3479:VAL:N	2.52	0.42
1:A:1680:ILE:HD13	1:A:1706:LEU:HD23	2.01	0.42
1:A:1804:GLU:OE1	1:A:1807:LYS:NZ	2.38	0.42
1:A:2305:LEU:HD23	1:A:2310:LEU:HB3	2.01	0.42
1:A:3569:GLU:HB3	1:A:3583:LEU:HD22	2.02	0.42
1:B:1368:GLU:O	1:B:1372:ASN:ND2	2.53	0.42
1:B:3368:ASP:OD2	1:B:3548:LEU:HD23	2.18	0.42
1:A:1749:ILE:HD13	1:A:1813:LEU:HD23	2.02	0.42
1:A:1815:ARG:NH1	1:A:1844:TRP:HE1	2.18	0.42
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	2.02	0.42
1:A:2476:LYS:HG2	1:A:2477:SER:N	2.35	0.42
1:A:2936:ILE:HG22	1:A:2962:ARG:CZ	2.50	0.42
1:B:1726:LEU:HD11	1:B:1730:LYS:NZ	2.35	0.42
1:B:2576:LYS:HG2	1:B:2586:ARG:HH12	1.85	0.42
1:B:2919:ASP:OD1	1:B:2985:ASN:ND2	2.52	0.42
1:B:3202:ILE:HG23	1:B:3208:LEU:HB2	2.01	0.42
1:A:1687:LEU:HD11	1:A:1699:GLU:HG3	2.01	0.42
1:A:3500:ASP:OD2	1:A:3503:GLY:N	2.53	0.42
1:A:3946:VAL:O	1:A:3947:PRO:C	2.58	0.42
1:A:2080:LYS:NZ	2:A:5002:ANP:O1G	2.47	0.42
1:B:2614:HIS:HB3	1:B:2909:PHE:CZ	2.55	0.42
1:A:1412:LEU:HD23	1:A:1415:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2432:LEU:HB3	1:A:2440:VAL:HG22	2.01	0.41
1:B:3296:VAL:C	1:B:3299:LEU:HG	2.40	0.41
1:B:3700:MET:HB3	1:B:4085:THR:HG21	2.02	0.41
1:A:1995:VAL:HG22	1:A:2022:PHE:CE1	2.55	0.41
1:A:2169:VAL:HG22	1:A:2186:ILE:HD11	2.01	0.41
1:A:2707:VAL:HG21	1:A:2712:LEU:HD13	2.03	0.41
1:A:2936:ILE:HG22	1:A:2962:ARG:NH2	2.36	0.41
1:A:3285:TYR:C	1:A:3295:LEU:HD21	2.40	0.41
1:B:1392:LEU:HD22	1:B:1393:LYS:N	2.36	0.41
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.54	0.41
1:B:2615:TYR:CE1	1:B:2660:LEU:HD23	2.55	0.41
1:B:2827:PHE:N	1:B:2827:PHE:CD1	2.88	0.41
1:B:2834:LEU:HD21	1:B:2885:LEU:HD21	2.02	0.41
1:B:3030:LYS:HG3	1:B:3297:LYS:CD	2.50	0.41
1:B:3476:ARG:HD3	1:B:3486:VAL:HG11	2.01	0.41
1:B:3789:ALA:HA	1:B:3877:CYS:HB3	2.02	0.41
1:B:3691:ASP:CA	1:B:3898:GLU:OE2	2.68	0.41
1:B:4024:VAL:HB	1:B:4062:TRP:CD1	2.55	0.41
1:A:2375:ILE:HG23	1:A:2376:PRO:HD2	2.02	0.41
1:A:2920:TRP:HD1	1:A:2989:PRO:HB2	1.85	0.41
1:A:3407:LEU:HD12	1:A:3407:LEU:N	2.35	0.41
1:A:3767:PHE:HD2	1:A:3769:VAL:HG23	1.86	0.41
1:B:1881:LEU:O	1:B:1881:LEU:HD12	2.20	0.41
1:B:2067:GLN:HG3	1:B:2211:GLY:HA3	2.01	0.41
1:B:2695:LEU:HD12	1:B:2695:LEU:N	2.35	0.41
1:B:2541:PRO:HD2	1:B:2904:SER:HB2	2.01	0.41
1:B:2977:TYR:HD1	1:B:2981:LYS:HG3	1.85	0.41
1:A:2014:PHE:O	1:A:2018:LEU:HB2	2.21	0.41
1:A:2696:PHE:HB3	1:A:2707:VAL:H	1.84	0.41
1:A:3130:MET:O	1:A:3285:TYR:HE2	2.03	0.41
1:B:3431:PHE:CE2	1:B:3452:ILE:HG21	2.55	0.41
1:A:1554:HIS:O	1:A:1555:HIS:HB2	2.19	0.41
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	2.36	0.41
1:A:2654:ARG:HD3	1:A:2658:ASP:OD2	2.20	0.41
1:A:3912:GLY:HA2	1:A:3915:PHE:CE2	2.55	0.41
1:A:2080:LYS:NZ	2:A:5002:ANP:O1B	2.45	0.41
1:B:2388:PRO:HG3	1:B:2878:VAL:CG1	2.50	0.41
1:B:2541:PRO:HB2	1:B:2904:SER:CB	2.51	0.41
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.35	0.41
1:B:3209:LYS:N	1:B:3210:PRO:HD2	2.35	0.41
1:B:3788:MET:O	1:B:3788:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4059:LEU:O	1:B:4063:LEU:HB2	2.20	0.41
1:A:1989:GLU:N	1:A:1989:GLU:OE1	2.54	0.41
1:A:3209:LYS:N	1:A:3210:PRO:HD2	2.36	0.41
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	2.03	0.41
1:A:3576:ASN:HB3	1:A:3580:ASN:HB2	2.02	0.41
1:A:3775:ALA:HB2	1:A:3803:LEU:HD22	2.03	0.41
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	2.03	0.41
1:A:3900:ILE:HG23	1:A:3944:ARG:CZ	2.51	0.41
1:B:3869:GLU:HG2	1:B:3870:LYS:H	1.85	0.41
1:A:2823:LEU:HD11	1:A:3460:PRO:HD2	2.01	0.41
1:A:2920:TRP:CD1	1:A:2989:PRO:HG3	2.56	0.41
1:A:2945:VAL:HG13	1:A:2946:PRO:HD2	2.02	0.41
1:B:1412:LEU:HA	1:B:1415:MET:SD	2.61	0.41
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.99	0.41
1:B:3470:PHE:HD2	1:B:3475:ASN:H	1.69	0.41
1:B:4031:GLN:HB3	1:B:4032:PRO:HD2	2.03	0.41
1:A:1395:VAL:CG2	1:A:1398:TRP:CE2	3.04	0.41
1:A:1984:ILE:HG23	1:A:1989:GLU:CD	2.40	0.41
1:A:2746:ASP:HA	1:A:2773:VAL:HG11	2.02	0.41
1:A:2838:ALA:HB3	1:A:2878:VAL:HG13	2.01	0.41
1:A:3326:ILE:HA	1:A:3349:LEU:HD21	2.02	0.41
1:B:1804:GLU:HA	1:B:1807:LYS:HE2	2.03	0.41
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	2.02	0.41
1:B:2467:THR:O	1:B:2471:LEU:N	2.54	0.41
1:B:3555:TYR:HE1	1:B:3593:GLU:OE2	2.04	0.41
1:B:3629:PHE:CE2	1:B:3646:ILE:HG22	2.55	0.41
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.36	0.41
1:A:2920:TRP:HD1	1:A:2989:PRO:CB	2.34	0.41
1:A:3151:ILE:HG12	1:A:3152:GLY:N	2.36	0.41
1:A:3844:ILE:HD11	1:A:3855:LEU:CD2	2.51	0.41
1:B:1472:GLU:OE2	1:B:1522:SER:OG	2.25	0.41
1:B:2119:LEU:HD12	1:B:2124:GLU:OE2	2.20	0.41
1:B:2829:GLU:O	1:B:2832:ASN:HB2	2.20	0.41
1:B:3508:PHE:O	1:B:3512:ARG:HG2	2.21	0.41
1:B:3659:LYS:O	1:B:3660:LYS:CB	2.68	0.41
1:B:3783:ASN:OD1	1:B:3784:ASN:N	2.53	0.41
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	2.03	0.41
1:A:1660:VAL:HA	1:A:1663:CYS:HB3	2.03	0.41
1:A:2631:THR:HG21	1:A:2752:VAL:HG23	2.03	0.41
1:A:3330:TYR:HB3	1:A:3366:PHE:CE1	2.56	0.41
1:A:3787:THR:HG22	1:A:3875:MET:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1788:GLN:OE1	1:B:3966:VAL:HG21	2.21	0.41
1:B:3942:ARG:NH1	1:B:3949:GLY:HA2	2.36	0.41
1:B:3980:ILE:N	1:B:3981:PRO:CD	2.84	0.41
1:A:1826:PHE:HE2	1:A:1831:LEU:HG	1.85	0.41
1:A:2253:ILE:HD11	1:A:2295:ILE:HG21	2.03	0.41
1:A:3272:ARG:HB3	1:A:3285:TYR:CD1	2.56	0.41
1:A:3301:PHE:O	1:A:3304:GLU:HB3	2.21	0.41
1:B:2394:THR:H	1:B:2397:THR:HB	1.85	0.41
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	2.03	0.41
1:B:3412:SER:HB3	1:B:3497:HIS:NE2	2.36	0.41
1:A:2877:PHE:CZ	1:A:2881:ILE:HD11	2.56	0.40
1:A:3414:MET:O	1:A:3418:ILE:HG12	2.20	0.40
1:B:1835:LEU:HD23	1:B:1838:ILE:HD11	2.03	0.40
1:B:1945:LEU:HD21	1:B:1991:GLU:CB	2.51	0.40
1:B:2044:ARG:HH21	1:B:2093:ILE:HD11	1.86	0.40
1:B:2562:PRO:CB	1:B:2566:SER:HB2	2.51	0.40
1:B:2578:ILE:HD12	1:B:2630:TYR:HB2	2.03	0.40
1:B:3687:SER:HA	1:B:3698:MET:HE1	2.03	0.40
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.56	0.40
1:A:2310:LEU:O	1:A:2313:VAL:N	2.54	0.40
1:A:2467:THR:O	1:A:2471:LEU:N	2.55	0.40
1:A:2614:HIS:CB	1:A:2909:PHE:CE2	3.04	0.40
1:A:2614:HIS:HA	1:A:2909:PHE:CE2	2.56	0.40
1:A:2654:ARG:HH21	1:A:2695:LEU:HD23	1.86	0.40
1:A:2663:VAL:HG13	1:A:2664:LYS:H	1.87	0.40
1:B:2070:LEU:HB2	1:B:2193:LEU:CD2	2.50	0.40
1:B:2073:VAL:HA	1:B:2196:THR:O	2.20	0.40
1:B:2382:ALA:HB1	1:B:2630:TYR:CE1	2.56	0.40
1:B:2637:PRO:HD3	1:B:2703:ASP:HB3	2.03	0.40
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	2.03	0.40
1:A:2831:MET:HB3	1:A:2835:LEU:HD13	2.03	0.40
1:A:2920:TRP:HZ2	1:A:2993:ILE:HD11	1.84	0.40
1:B:2741:HIS:NE2	1:B:2917:MET:HB3	2.36	0.40
1:B:3630:SER:O	1:B:3634:LYS:HG2	2.21	0.40
1:A:1540:LEU:HA	1:A:1540:LEU:HD23	1.96	0.40
1:A:2645:ILE:HD11	1:A:2686:LEU:CG	2.50	0.40
1:A:2786:ILE:HG21	1:A:2827:PHE:CZ	2.57	0.40
1:A:3800:LEU:HD21	1:A:3874:PHE:CD2	2.55	0.40
1:B:2443:ILE:HD11	1:B:2457:ALA:HB3	2.03	0.40
1:A:2590:GLU:OE2	1:A:2594:ARG:HD2	2.22	0.40
1:A:2646:ARG:NH1	1:A:2687:GLY:H	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2686:LEU:HD23	1:A:2689:ILE:HD12	2.02	0.40
1:A:2701:SER:HB3	1:A:2705:LYS:HE3	2.04	0.40
1:A:2707:VAL:HG21	1:A:2712:LEU:CD1	2.51	0.40
1:A:2741:HIS:O	1:A:2745:ILE:HG13	2.21	0.40
1:A:2860:THR:HG21	1:A:2867:LEU:CD1	2.52	0.40
1:A:3445:ARG:NH2	1:A:3486:VAL:HG12	2.36	0.40
1:A:3657:PHE:CE2	1:A:3674:ILE:HD11	2.56	0.40
1:A:3946:VAL:HG12	1:A:3947:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2596/2661 (98%)	2473 (95%)	118 (4%)	5 (0%)	47	80
1	B	2597/2661 (98%)	2476 (95%)	116 (4%)	5 (0%)	47	80
All	All	5193/5322 (98%)	4949 (95%)	234 (4%)	10 (0%)	47	80

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1366	VAL
1	A	3946	VAL
1	B	1366	VAL
1	B	3031	VAL
1	B	3946	VAL
1	A	2948	VAL
1	B	2956	GLU
1	A	2989	PRO
1	A	2752	VAL
1	B	3993	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2367/2406 (98%)	2347 (99%)	20 (1%)	81	92
1	B	2366/2406 (98%)	2345 (99%)	21 (1%)	78	90
All	All	4733/4812 (98%)	4692 (99%)	41 (1%)	78	90

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1453	LEU
1	A	1523	LEU
1	A	1528	GLU
1	A	1705	TYR
1	A	1826	PHE
1	A	2012	LEU
1	A	2105	ASP
1	A	2195	GLU
1	A	2255	ASP
1	A	2300	GLN
1	A	2326	LEU
1	A	2354	SER
1	A	2683	ASN
1	A	2689	ILE
1	A	2839	ASP
1	A	3268	ASN
1	A	3285	TYR
1	A	3368	ASP
1	A	3811	LEU
1	A	3871	PHE
1	B	1818	VAL
1	B	1973	LEU
1	B	2012	LEU
1	B	2105	ASP
1	B	2255	ASP
1	B	2354	SER
1	B	2536	ASN

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Mol	Chain	Res	Type
1	B	2683	ASN
1	B	2712	LEU
1	B	2786	ILE
1	B	2910	ASN
1	B	2915	ASN
1	B	2975	ASN
1	B	3026	GLU
1	B	3205	ASN
1	B	3287	SER
1	B	3412	SER
1	B	3471	ASN
1	B	3475	ASN
1	B	3487	ASP
1	B	3588	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3962	GLN
1	B	2201	HIS
1	B	2444	ASN
1	B	3318	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 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	ANP	B	5001	-	29,33,33	2.14	6 (20%)	31,52,52	1.32	2 (6%)
2	ANP	A	5004	-	29,33,33	1.81	5 (17%)	31,52,52	1.30	3 (9%)
2	ANP	B	5004	-	29,33,33	1.63	5 (17%)	31,52,52	1.19	2 (6%)
2	ANP	A	5001	-	29,33,33	1.11	3 (10%)	31,52,52	1.07	2 (6%)
2	ANP	A	5002	3	29,33,33	1.01	3 (10%)	31,52,52	1.10	2 (6%)
2	ANP	B	5002	3	29,33,33	1.82	5 (17%)	31,52,52	1.26	3 (9%)
2	ANP	B	5003	-	29,33,33	1.80	5 (17%)	31,52,52	1.05	2 (6%)
2	ANP	A	5003	-	29,33,33	2.07	5 (17%)	31,52,52	1.21	3 (9%)

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	ANP	B	5001	-	-	7/14/38/38	0/3/3/3
2	ANP	A	5004	-	-	8/14/38/38	0/3/3/3
2	ANP	B	5004	-	-	5/14/38/38	0/3/3/3
2	ANP	A	5001	-	-	4/14/38/38	0/3/3/3
2	ANP	A	5002	3	-	5/14/38/38	0/3/3/3
2	ANP	B	5002	3	-	3/14/38/38	0/3/3/3
2	ANP	B	5003	-	-	5/14/38/38	0/3/3/3
2	ANP	A	5003	-	-	7/14/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	ANP	PG-O1G	7.80	1.58	1.46
2	B	5002	ANP	PG-O1G	7.77	1.58	1.46
2	B	5003	ANP	PG-O1G	7.72	1.58	1.46
2	A	5004	ANP	PG-O1G	7.71	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5003	ANP	PG-O1G	7.35	1.57	1.46
2	B	5004	ANP	PB-O1B	6.32	1.56	1.46
2	A	5003	ANP	PB-O1B	6.16	1.55	1.46
2	B	5001	ANP	PB-O1B	6.10	1.55	1.46
2	B	5002	ANP	PG-O3G	-2.94	1.48	1.56
2	A	5003	ANP	PB-O2B	-2.69	1.49	1.56
2	A	5001	ANP	PB-O3A	-2.68	1.55	1.59
2	B	5004	ANP	PB-O2B	-2.67	1.49	1.56
2	A	5004	ANP	PG-O3G	-2.63	1.49	1.56
2	B	5004	ANP	PB-O3A	-2.59	1.55	1.59
2	B	5003	ANP	PG-O3G	-2.59	1.49	1.56
2	A	5003	ANP	PG-O2G	-2.58	1.49	1.56
2	B	5001	ANP	PB-O3A	-2.56	1.55	1.59
2	B	5001	ANP	PB-O2B	-2.54	1.49	1.56
2	A	5004	ANP	PB-O3A	-2.52	1.55	1.59
2	B	5001	ANP	PG-O3G	-2.51	1.50	1.56
2	A	5001	ANP	PG-O1G	2.48	1.50	1.46
2	B	5004	ANP	PG-N3B	2.42	1.69	1.63
2	A	5001	ANP	PG-N3B	2.35	1.69	1.63
2	A	5004	ANP	PG-N3B	2.34	1.69	1.63
2	A	5002	ANP	PG-N3B	2.34	1.69	1.63
2	B	5003	ANP	PG-N3B	2.32	1.69	1.63
2	B	5004	ANP	PG-O1G	2.29	1.49	1.46
2	B	5001	ANP	PG-N3B	2.29	1.69	1.63
2	B	5002	ANP	PB-O3A	-2.27	1.56	1.59
2	A	5004	ANP	PB-O1B	2.23	1.49	1.46
2	B	5003	ANP	PB-O1B	2.18	1.49	1.46
2	A	5002	ANP	PG-O1G	2.15	1.49	1.46
2	B	5002	ANP	PB-O1B	2.15	1.49	1.46
2	A	5003	ANP	PG-N3B	2.14	1.69	1.63
2	B	5002	ANP	PG-N3B	2.14	1.69	1.63
2	B	5003	ANP	PB-O3A	-2.05	1.56	1.59
2	A	5002	ANP	PB-O1B	2.04	1.49	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	ANP	PA-O3A-PB	-5.09	114.69	132.62
2	B	5002	ANP	PA-O3A-PB	-4.73	115.97	132.62
2	A	5004	ANP	PA-O3A-PB	-4.64	116.27	132.62
2	B	5004	ANP	PA-O3A-PB	-4.24	117.70	132.62
2	A	5003	ANP	PA-O3A-PB	-4.01	118.51	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	ANP	PA-O3A-PB	-3.95	118.69	132.62
2	A	5002	ANP	PA-O3A-PB	-3.18	121.43	132.62
2	B	5003	ANP	PA-O3A-PB	-3.17	121.46	132.62
2	A	5004	ANP	C3'-C2'-C1'	2.51	104.75	100.98
2	B	5001	ANP	C5-C6-N6	2.35	123.92	120.35
2	B	5002	ANP	C5-C6-N6	2.34	123.91	120.35
2	A	5003	ANP	C5-C6-N6	2.28	123.82	120.35
2	A	5001	ANP	C5-C6-N6	2.26	123.79	120.35
2	B	5003	ANP	C5-C6-N6	2.25	123.77	120.35
2	A	5004	ANP	C5-C6-N6	2.24	123.75	120.35
2	A	5002	ANP	C5-C6-N6	2.23	123.74	120.35
2	B	5004	ANP	C5-C6-N6	2.22	123.73	120.35
2	A	5003	ANP	O1G-PG-N3B	-2.11	108.67	111.77
2	B	5002	ANP	O3A-PB-N3B	2.04	112.26	106.59

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5001	ANP	C5'-O5'-PA-O1A
2	B	5001	ANP	C5'-O5'-PA-O2A
2	A	5004	ANP	PB-N3B-PG-O1G
2	A	5004	ANP	PG-N3B-PB-O1B
2	A	5004	ANP	PA-O3A-PB-O1B
2	A	5004	ANP	PA-O3A-PB-O2B
2	B	5004	ANP	PB-N3B-PG-O1G
2	B	5004	ANP	PG-N3B-PB-O3A
2	A	5001	ANP	PG-N3B-PB-O1B
2	A	5001	ANP	PA-O3A-PB-O1B
2	A	5002	ANP	PB-N3B-PG-O1G
2	A	5002	ANP	PG-N3B-PB-O1B
2	A	5002	ANP	PG-N3B-PB-O3A
2	B	5002	ANP	PG-N3B-PB-O3A
2	B	5002	ANP	O4'-C4'-C5'-O5'
2	B	5003	ANP	PG-N3B-PB-O3A
2	B	5003	ANP	C5'-O5'-PA-O1A
2	B	5003	ANP	C3'-C4'-C5'-O5'
2	A	5003	ANP	PB-N3B-PG-O1G
2	A	5003	ANP	PA-O3A-PB-O1B
2	A	5003	ANP	PA-O3A-PB-O2B
2	A	5003	ANP	C3'-C4'-C5'-O5'
2	B	5001	ANP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	5001	ANP	C3'-C4'-C5'-O5'
2	A	5004	ANP	O4'-C4'-C5'-O5'
2	A	5004	ANP	C3'-C4'-C5'-O5'
2	B	5004	ANP	O4'-C4'-C5'-O5'
2	B	5004	ANP	C3'-C4'-C5'-O5'
2	A	5001	ANP	O4'-C4'-C5'-O5'
2	B	5002	ANP	C3'-C4'-C5'-O5'
2	A	5003	ANP	O4'-C4'-C5'-O5'
2	B	5003	ANP	O4'-C4'-C5'-O5'
2	A	5001	ANP	C3'-C4'-C5'-O5'
2	A	5004	ANP	C5'-O5'-PA-O3A
2	A	5004	ANP	C4'-C5'-O5'-PA
2	A	5003	ANP	C5'-O5'-PA-O2A
2	A	5002	ANP	C4'-C5'-O5'-PA
2	B	5001	ANP	PB-O3A-PA-O1A
2	B	5001	ANP	PB-O3A-PA-O2A
2	B	5003	ANP	PG-N3B-PB-O1B
2	B	5001	ANP	C5'-O5'-PA-O3A
2	A	5003	ANP	C5'-O5'-PA-O3A
2	B	5004	ANP	C5'-O5'-PA-O1A
2	A	5002	ANP	O4'-C4'-C5'-O5'

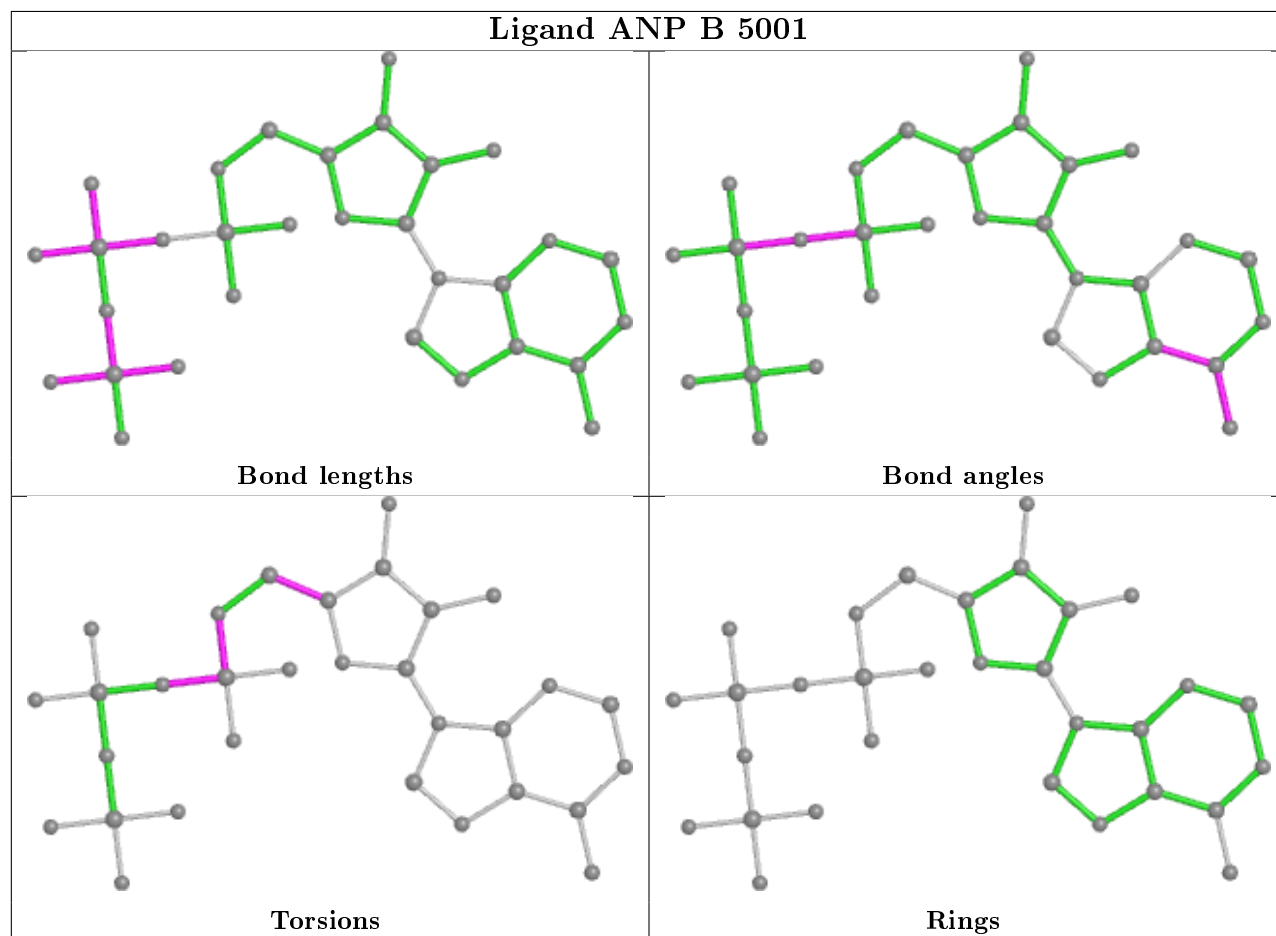
There are no ring outliers.

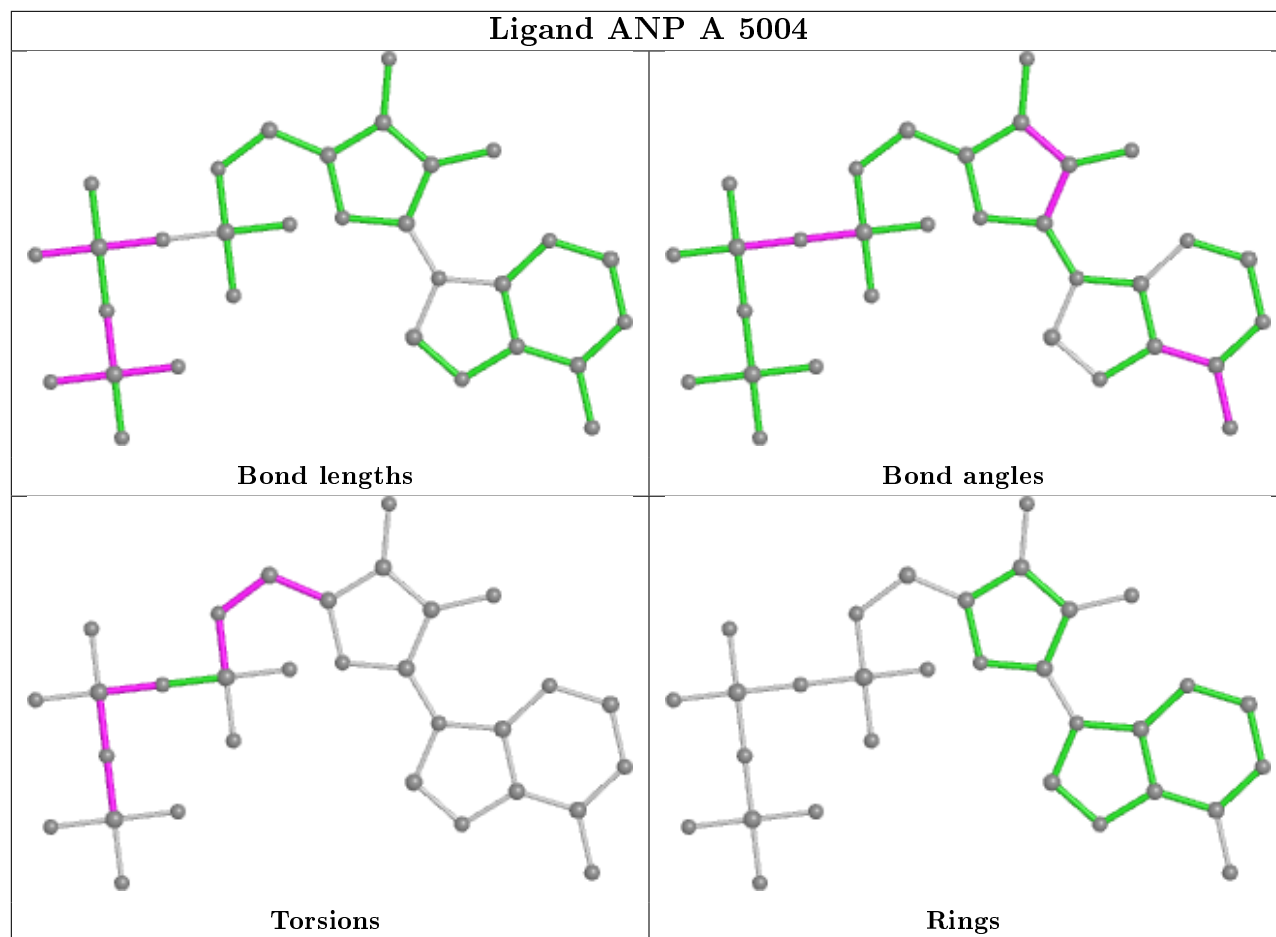
8 monomers are involved in 16 short contacts:

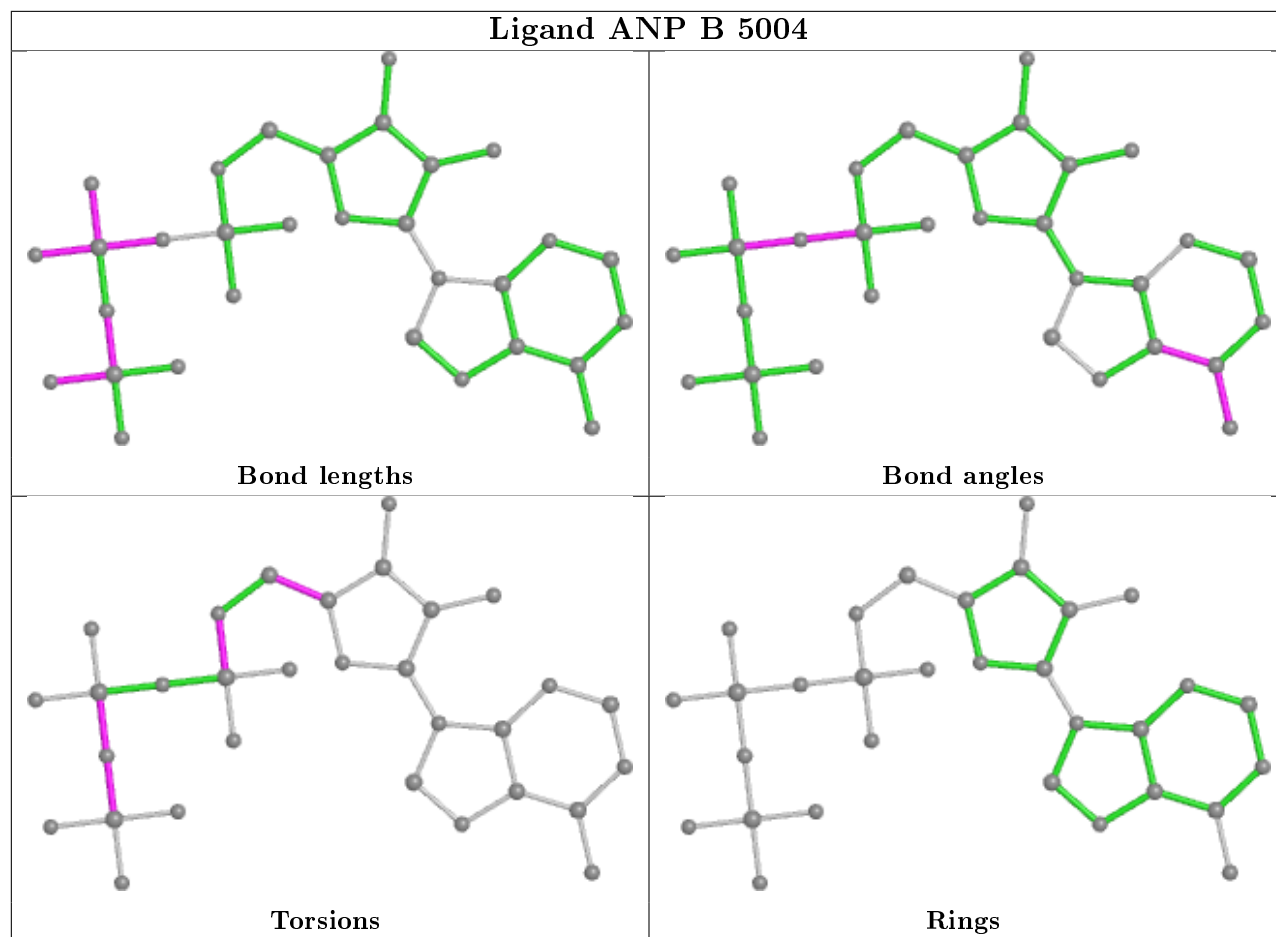
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5001	ANP	2	0
2	A	5004	ANP	2	0
2	B	5004	ANP	1	0
2	A	5001	ANP	1	0
2	A	5002	ANP	2	0
2	B	5002	ANP	2	0
2	B	5003	ANP	3	0
2	A	5003	ANP	3	0

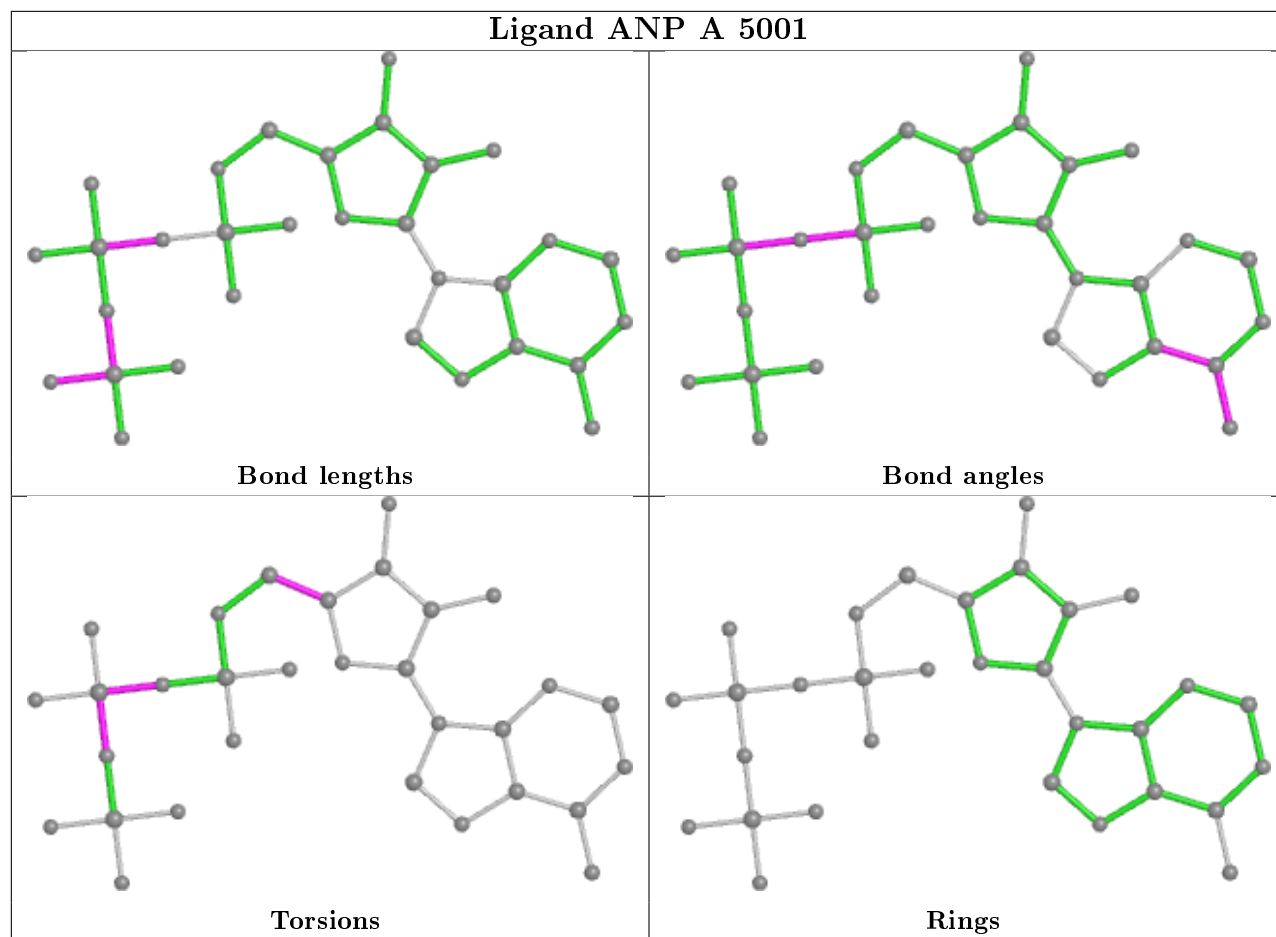
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

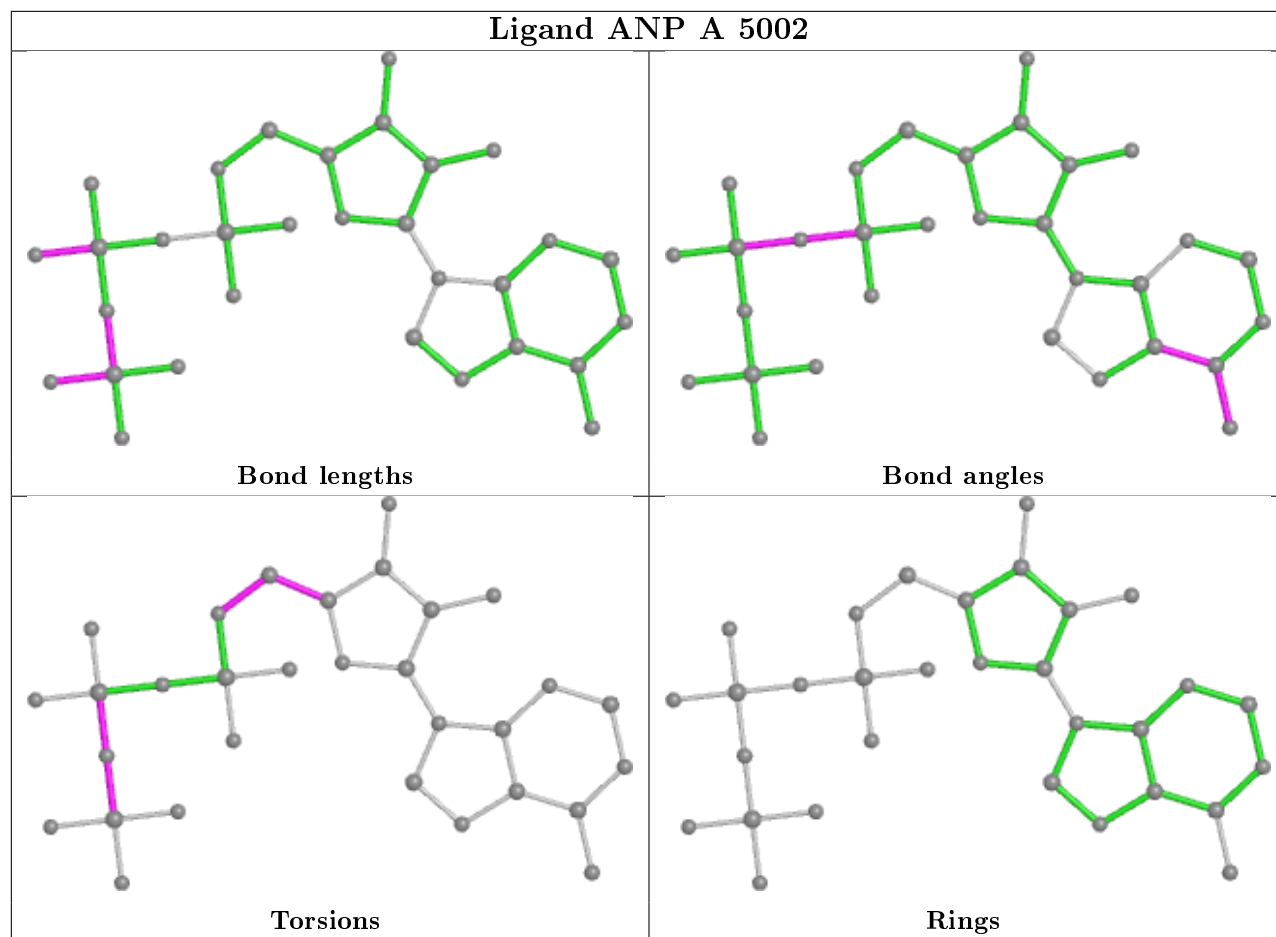
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

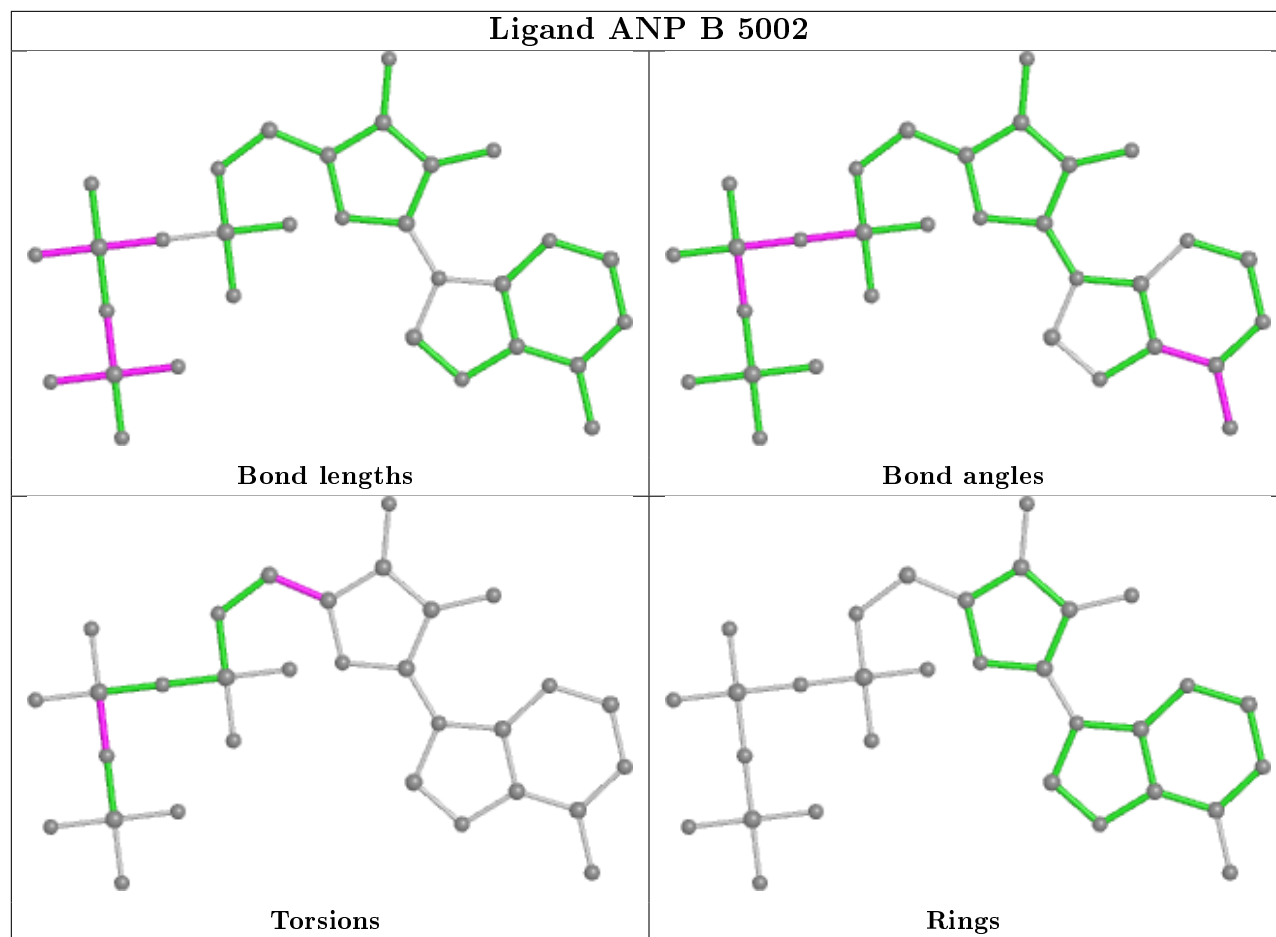


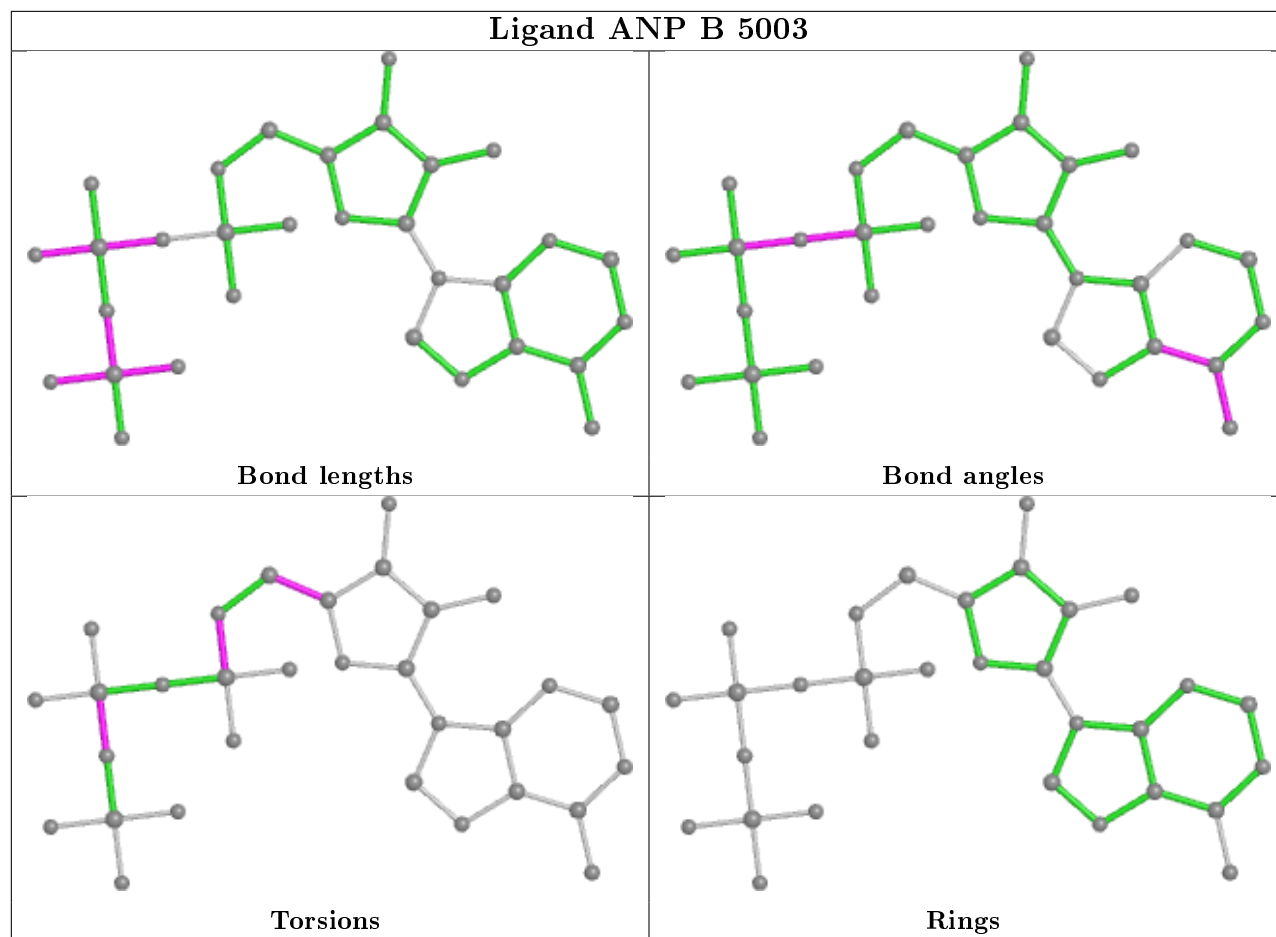


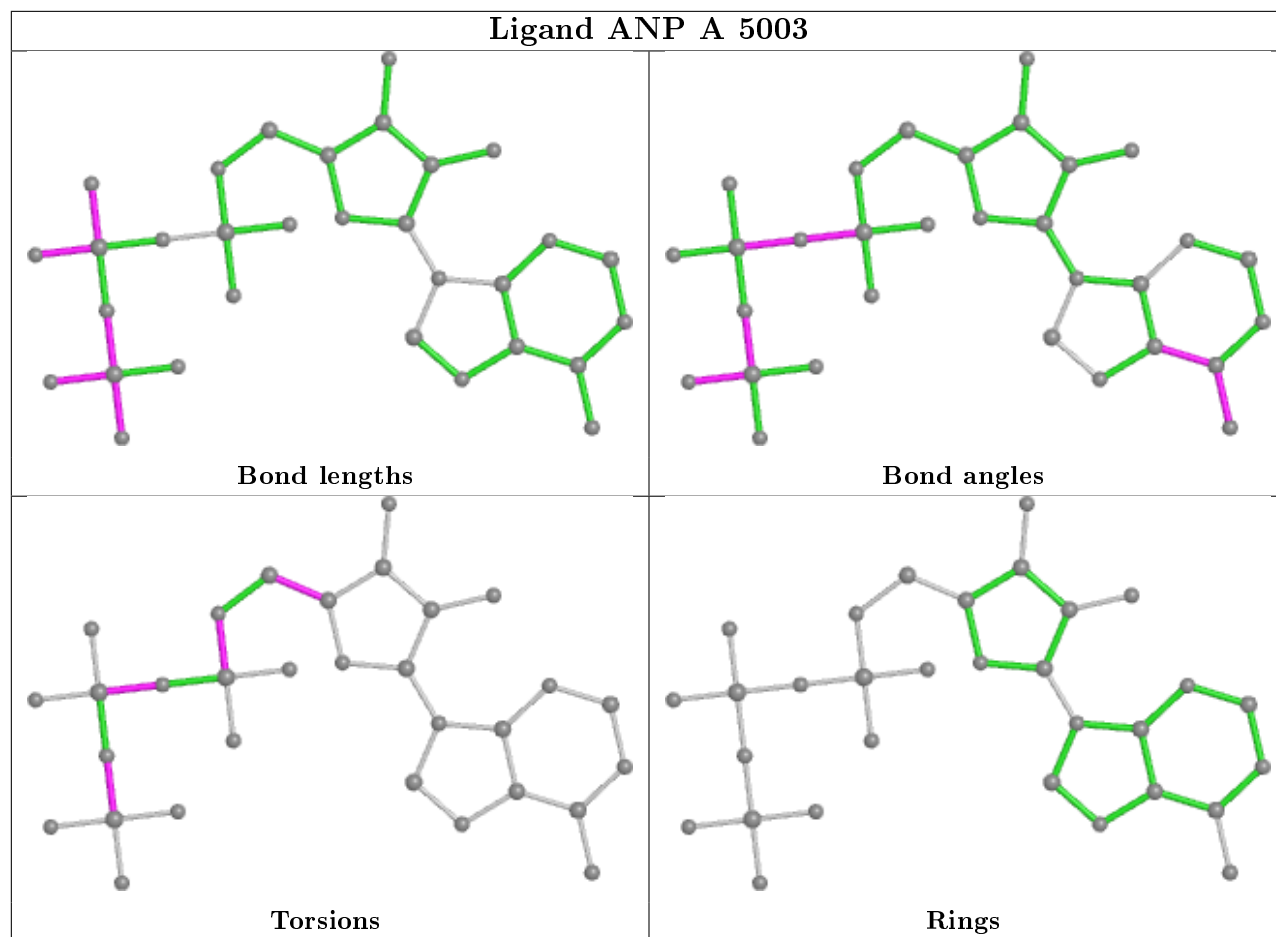












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	2608/2661 (98%)	-0.10	59 (2%)	60	46	20, 50, 119, 275	0
1	B	2609/2661 (98%)	-0.09	58 (2%)	62	48	23, 54, 121, 247	0
All	All	5217/5322 (98%)	-0.10	117 (2%)	62	48	20, 52, 120, 275	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3166	ALA	6.8
1	B	2364	ASP	6.5
1	A	2363	ASN	6.5
1	B	3159	LYS	5.5
1	B	2363	ASN	5.5
1	A	3979	ASN	4.8
1	A	2364	ASP	4.7
1	A	3580	ASN	4.6
1	A	2030	ASN	4.4
1	B	3160	SER	4.3
1	A	3867	GLU	4.2
1	A	3920	ILE	4.2
1	A	3159	LYS	4.2
1	B	2299	ARG	4.1
1	B	3179	ASN	4.0
1	B	2030	ASN	3.8
1	B	3979	ASN	3.8
1	B	3161	PRO	3.7
1	B	3177	ASN	3.6
1	A	2238	ASP	3.6
1	B	2239	ASN	3.5
1	A	2303	GLN	3.5
1	B	2984	VAL	3.5
1	B	2240	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	3165	ALA	3.5
1	B	3740	THR	3.4
1	B	2897	ASN	3.3
1	A	3156	LEU	3.3
1	A	3581	ASP	3.3
1	A	2239	ASN	3.3
1	B	3980	ILE	3.3
1	A	2468	SER	3.2
1	B	3288	GLY	3.2
1	B	2302	PHE	3.2
1	B	2902	MET	3.2
1	A	3180	GLY	3.2
1	B	2684	GLN	3.2
1	B	3865	ALA	3.1
1	A	2943	PHE	3.1
1	A	2955	THR	3.1
1	A	2379	SER	3.1
1	A	2371	PHE	3.0
1	B	3162	SER	3.0
1	A	2140	ASP	2.9
1	A	2362	ALA	2.9
1	B	2896	ASN	2.9
1	B	2904	SER	2.9
1	B	3575	GLY	2.9
1	A	3166	ALA	2.8
1	A	2470	GLY	2.8
1	B	3580	ASN	2.8
1	A	2348	HIS	2.8
1	B	2685	ASP	2.8
1	A	3865	ALA	2.7
1	A	2147	ASN	2.7
1	A	3866	GLU	2.7
1	A	2246	LEU	2.6
1	B	2985	ASN	2.6
1	A	2684	GLN	2.6
1	A	1600	ASP	2.5
1	A	2368	PHE	2.5
1	A	2241	LEU	2.5
1	B	1366	VAL	2.5
1	A	3161	PRO	2.5
1	B	2368	PHE	2.5
1	B	3918	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2897	ASN	2.4
1	B	4036	GLN	2.4
1	A	3158	THR	2.4
1	B	3146	GLU	2.4
1	B	2139	ASP	2.3
1	A	3521	ASN	2.3
1	A	2942	ASP	2.3
1	A	3145	THR	2.3
1	A	2139	ASP	2.3
1	B	4018	SER	2.3
1	A	2349	ASP	2.3
1	B	3138	ARG	2.3
1	A	3919	LYS	2.3
1	B	3837	GLY	2.3
1	A	3187	ALA	2.3
1	B	2943	PHE	2.2
1	A	4036	GLN	2.2
1	A	2370	SER	2.2
1	B	3867	GLU	2.2
1	B	2377	SER	2.2
1	A	2240	LYS	2.2
1	B	2388	PRO	2.2
1	A	3740	THR	2.2
1	A	2467	THR	2.2
1	B	2241	LEU	2.2
1	B	3917	THR	2.2
1	A	2378	VAL	2.2
1	A	2302	PHE	2.2
1	A	2961	ILE	2.2
1	B	2246	LEU	2.1
1	B	3143	LYS	2.1
1	B	3205	ASN	2.1
1	B	2374	GLU	2.1
1	A	3160	SER	2.1
1	B	2469	LYS	2.1
1	A	2662	GLY	2.1
1	B	2365	LYS	2.1
1	A	3309	THR	2.1
1	B	3173	ALA	2.1
1	B	3158	THR	2.1
1	A	2369	SER	2.1
1	B	2468	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	3475	ASN	2.1
1	B	3287	SER	2.0
1	A	3915	PHE	2.0
1	A	3169	GLU	2.0
1	B	3555	TYR	2.0
1	B	2375	ILE	2.0
1	A	2944	ILE	2.0
1	B	2919	ASP	2.0
1	A	3424	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

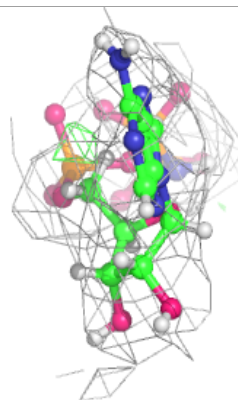
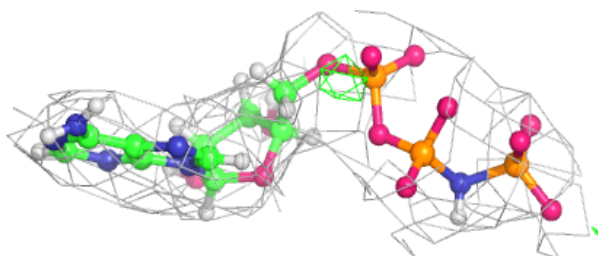
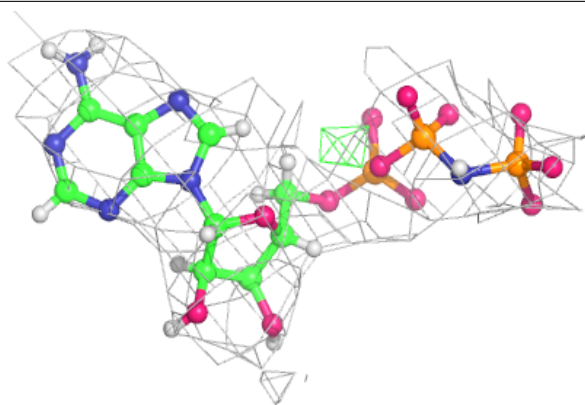
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ANP	A	5004	31/31	0.91	0.27	49,72,160,227	0
2	ANP	A	5002	31/31	0.91	0.28	36,66,98,149	0
2	ANP	A	5003	31/31	0.91	0.28	21,52,121,134	0
2	ANP	B	5003	31/31	0.92	0.34	43,75,101,161	0
2	ANP	B	5002	31/31	0.93	0.25	28,67,122,162	0
2	ANP	B	5004	31/31	0.94	0.24	47,78,162,183	0
2	ANP	A	5001	31/31	0.94	0.24	23,51,183,503	0
2	ANP	B	5001	31/31	0.94	0.24	31,57,180,372	0
3	MG	B	5005	1/1	0.97	0.26	54,54,54,54	0
3	MG	A	5005	1/1	0.98	0.36	50,50,50,50	0

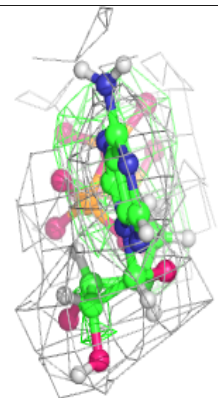
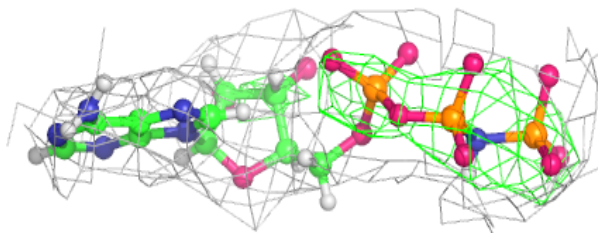
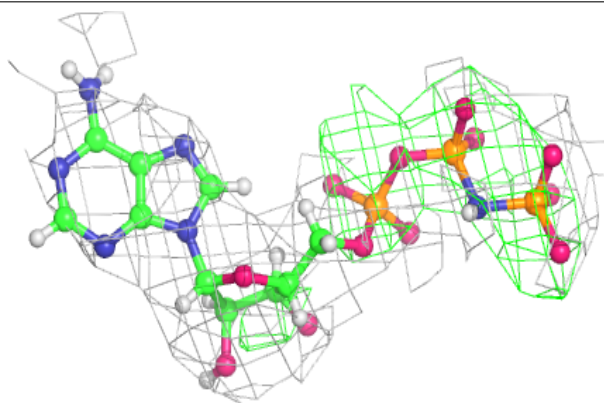
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 5004:

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

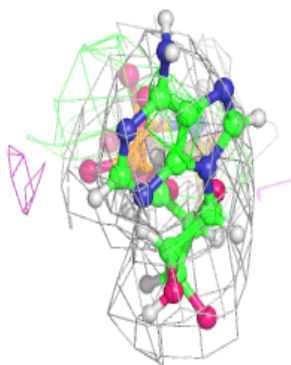
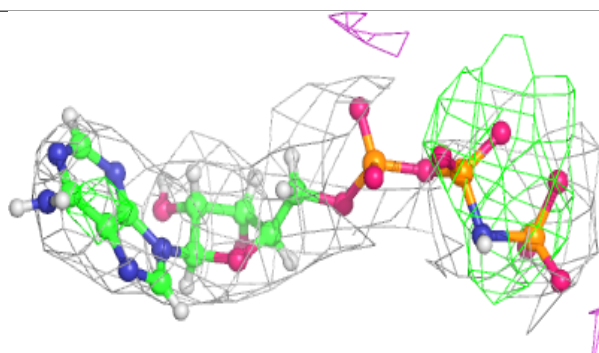
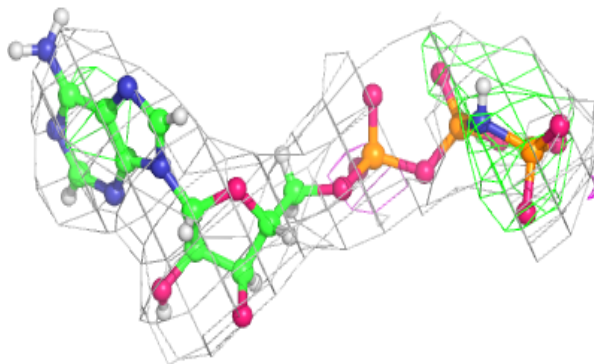
**Electron density around ANP A 5002:**

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

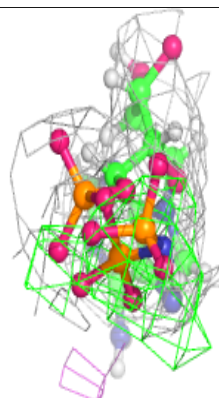
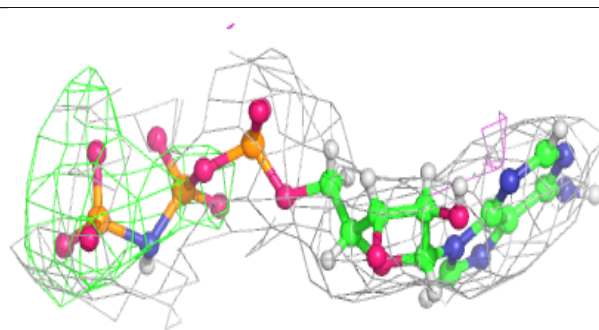
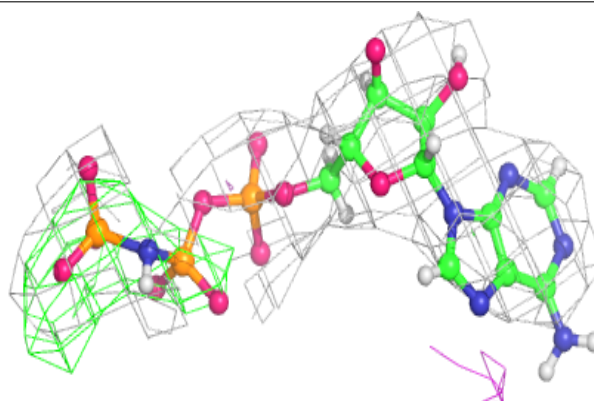


Electron density around ANP A 5003:

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

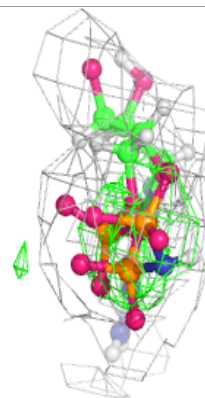
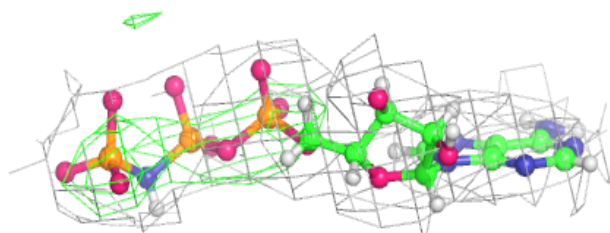
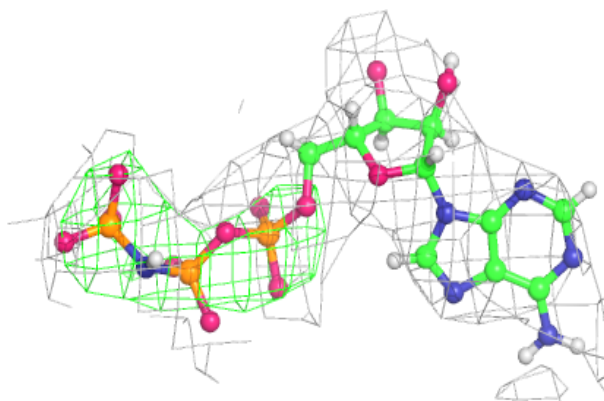
**Electron density around ANP B 5003:**

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

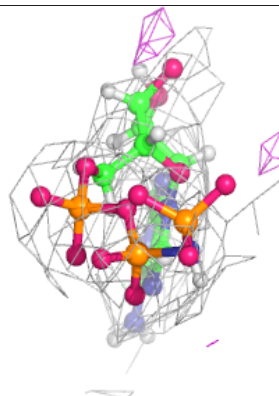
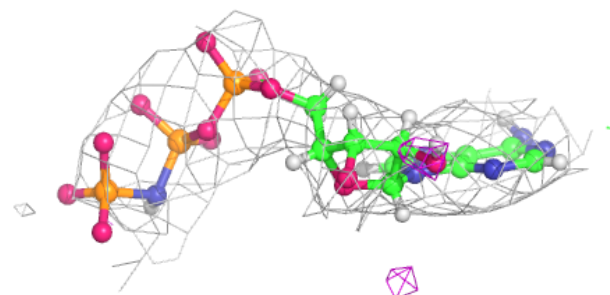
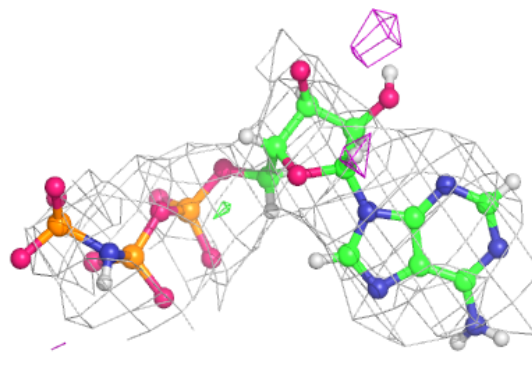


Electron density around ANP B 5002:

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

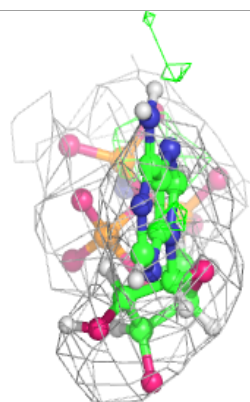
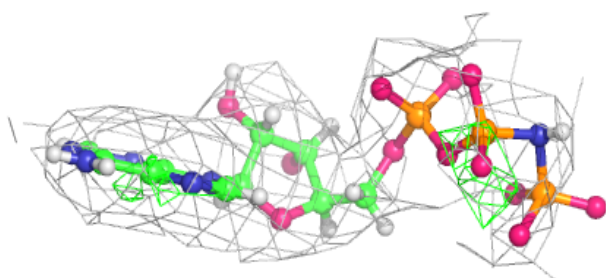
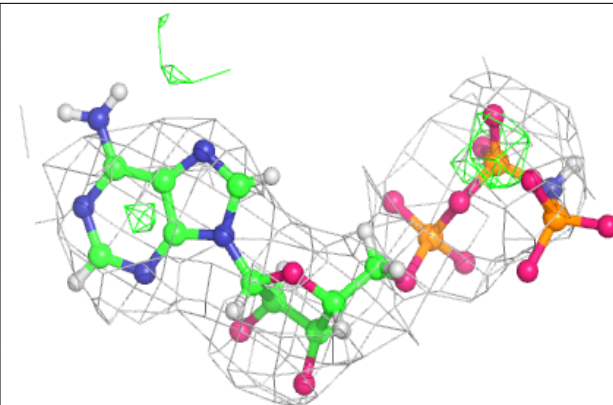
**Electron density around ANP B 5004:**

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

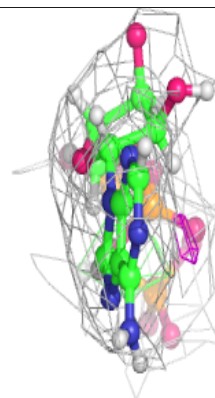
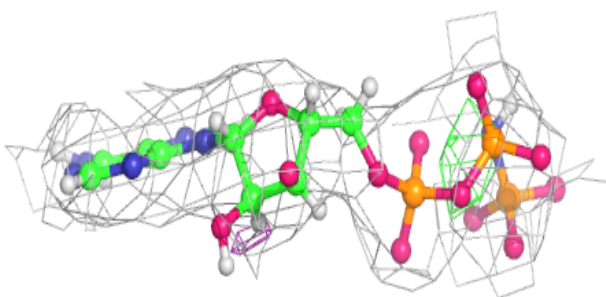
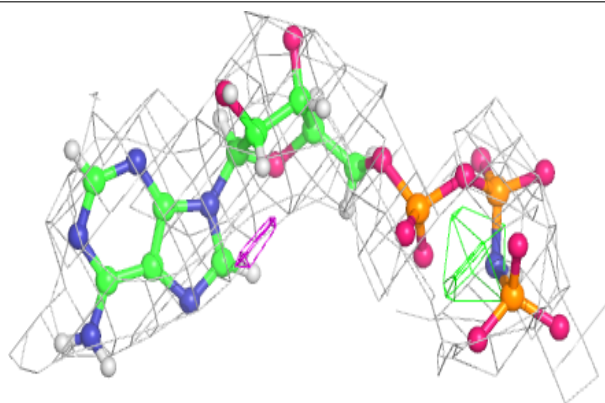


Electron density around ANP A 5001:

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

**Electron density around ANP B 5001:**

$2mF_o-DF_c$ (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.