



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:19 PM UTC

PDB ID : 4W8F / pdb_00004w8f
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

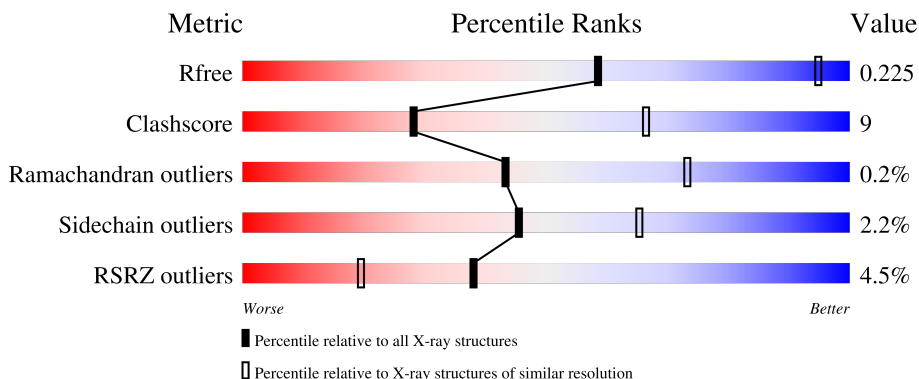
1 Overall quality at a glance

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}	180053	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	5% 76% 20% ..
1	B	2661	4% 77% 19% ..

2 Entry composition [i](#)

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

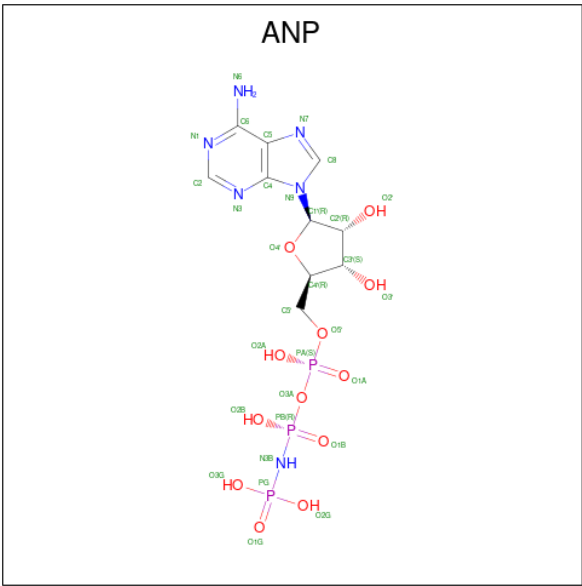
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Chain	Residue	Modelled	Actual	Comment	Reference
A	4097	GLY	-	linker	UNP P36022
A	4098	SER	-	linker	UNP P36022
A	4099	HIS	-	expression tag	UNP P36022
A	4100	HIS	-	expression tag	UNP P36022
A	4101	HIS	-	expression tag	UNP P36022
A	4102	HIS	-	expression 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 (CCD ID:

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		

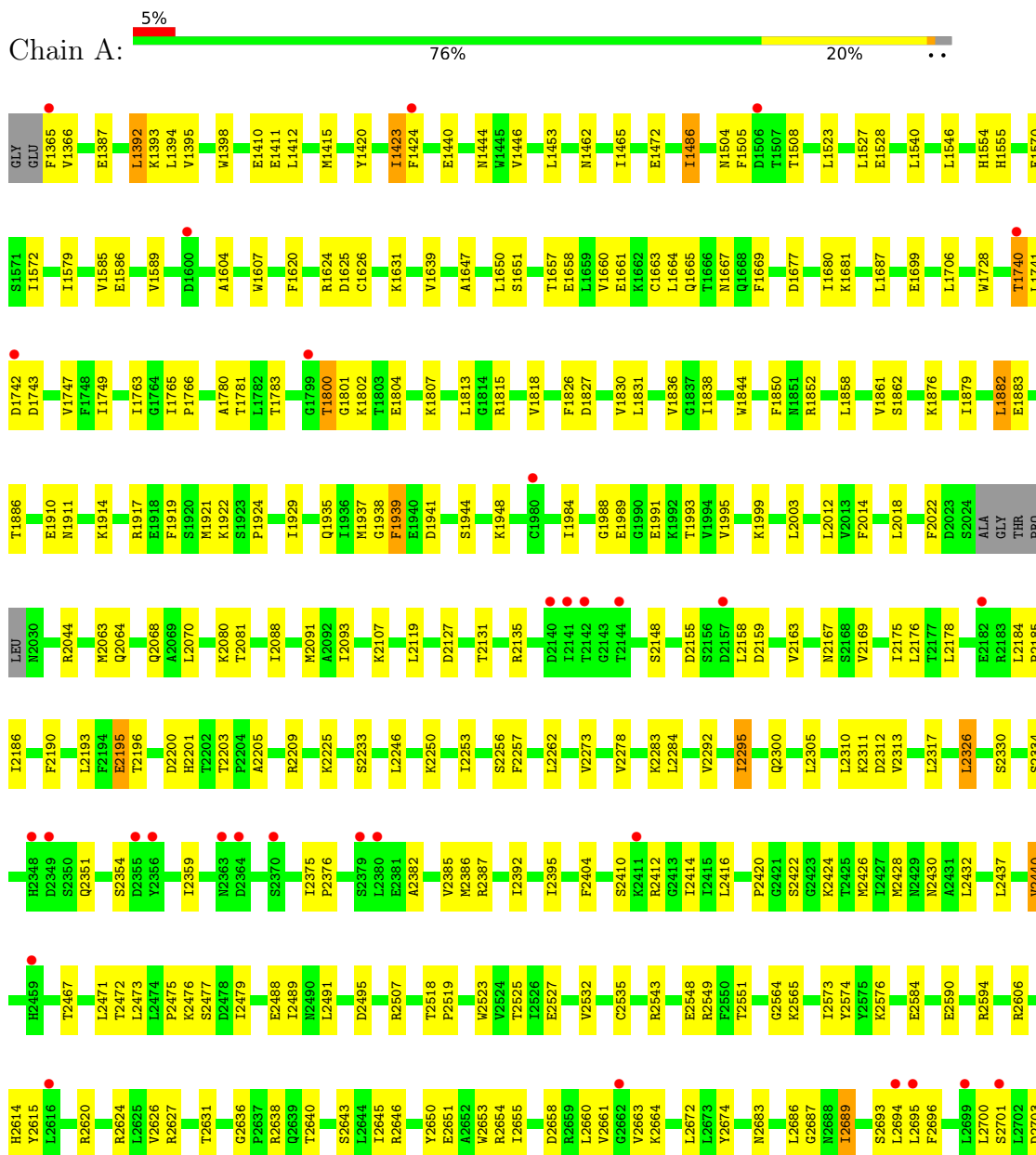
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

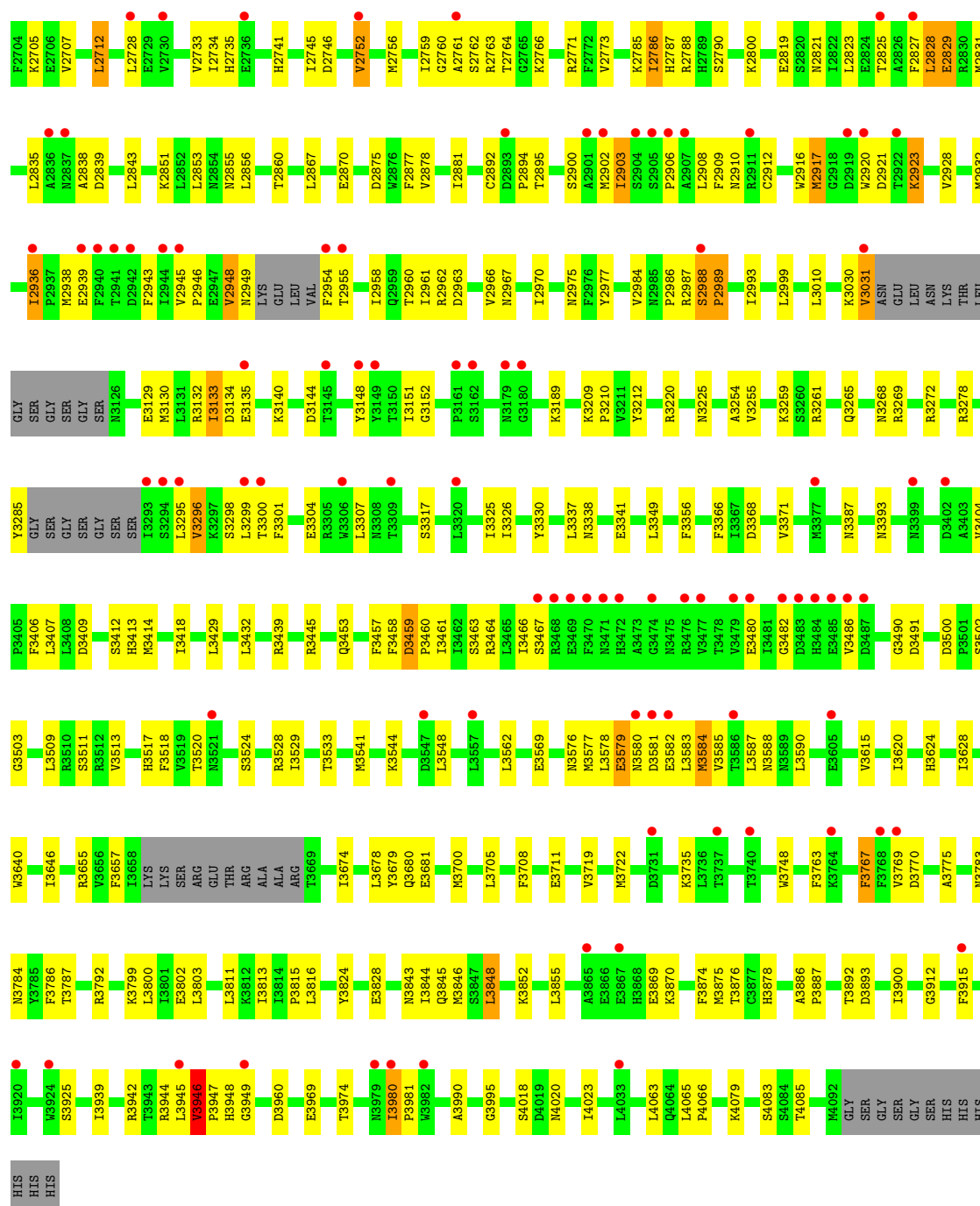
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

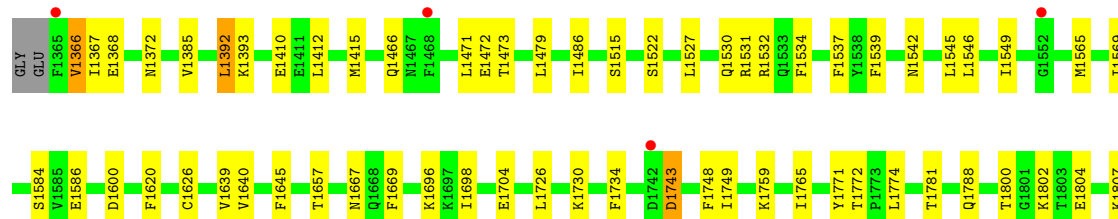
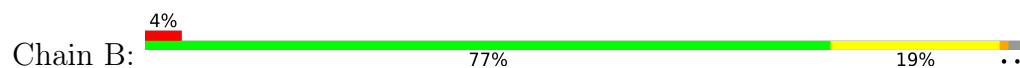
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

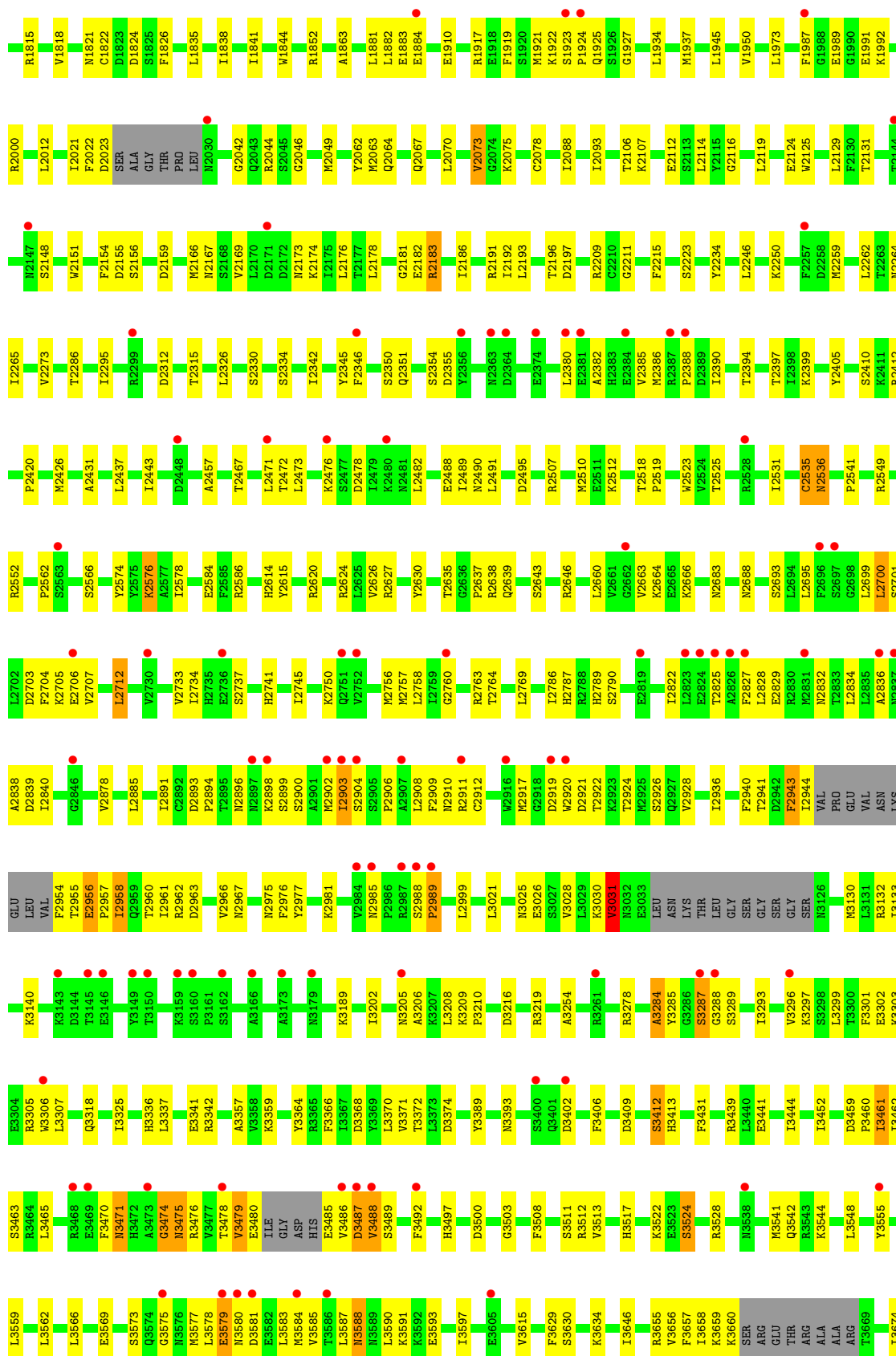
- Molecule 1: Dynein heavy chain lysozyme chimera

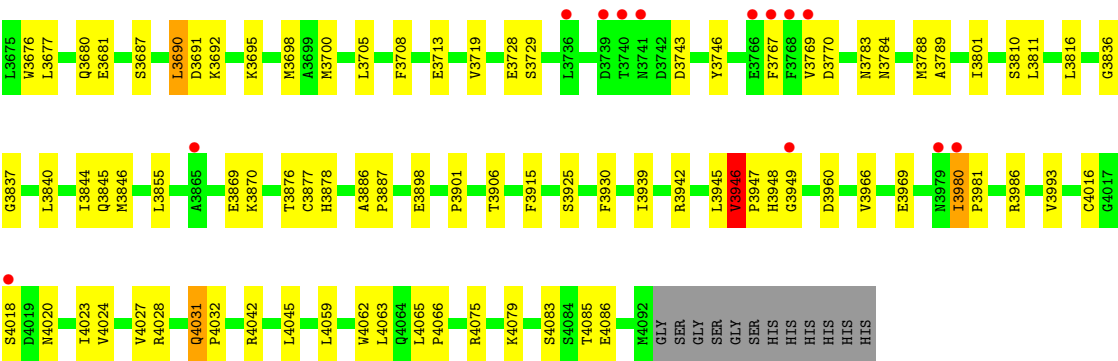




● Molecule 1: Dynein heavy chain lysozyme chimera







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) 92.2 (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 0.232 , 0.225	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)	0.35 , 40.2	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	0.43	0/21492	0.87	41/29041 (0.1%)
1	B	0.43	0/21487	0.87	27/29028 (0.1%)
All	All	0.43	0/42979	0.87	68/58069 (0.1%)

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 (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3296	VAL	N-CA-C	-10.07	93.98	107.88
1	B	3479	VAL	N-CA-C	9.49	123.05	113.47
1	B	3575	GLY	N-CA-C	-8.95	95.81	111.46
1	A	2703	ASP	N-CA-C	8.66	123.58	112.92
1	A	2988	SER	CA-C-N	8.41	130.35	119.84
1	A	2988	SER	C-N-CA	8.41	130.35	119.84
1	A	2565	LYS	N-CA-C	-7.90	101.97	111.69
1	B	3524	SER	N-CA-C	-7.88	103.45	113.23
1	B	3284	ALA	N-CA-C	-7.72	99.86	110.35
1	A	2988	SER	N-CA-C	7.32	119.98	110.40
1	B	3413	HIS	N-CA-C	-7.00	104.55	113.23
1	A	2936	ILE	CA-C-N	7.00	127.14	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2936	ILE	C-N-CA	7.00	127.14	119.87
1	B	3479	VAL	N-CA-CB	-6.99	104.01	112.33
1	B	3573	SER	N-CA-C	-6.87	102.01	111.28
1	A	1939	PHE	N-CA-C	6.86	121.01	109.76
1	A	2923	LYS	N-CA-C	-6.63	103.04	112.13
1	A	2829	GLU	N-CA-C	6.33	119.12	111.40
1	B	2943	PHE	N-CA-C	6.29	118.21	111.36
1	A	3133	ILE	N-CA-C	6.27	116.42	110.53
1	B	3471	ASN	N-CA-C	6.26	119.79	110.52
1	B	3402	ASP	N-CA-C	-6.22	105.33	113.17
1	A	3491	ASP	N-CA-C	-6.09	105.61	113.16
1	B	1743	ASP	N-CA-C	6.08	119.53	111.75
1	A	3767	PHE	N-CA-C	-6.07	104.78	111.82
1	A	1740	THR	N-CA-C	6.02	116.23	108.34
1	A	1800	THR	N-CA-C	-5.97	100.83	109.31
1	A	3467	SER	N-CA-C	-5.88	102.36	110.35
1	B	4027	VAL	N-CA-C	5.80	116.15	107.51
1	A	2479	ILE	N-CA-C	5.78	115.96	110.53
1	A	2903	ILE	N-CA-C	5.77	115.99	110.74
1	A	2917	MET	N-CA-C	-5.76	101.65	109.95
1	B	3542	GLN	N-CA-C	-5.76	105.08	111.36
1	B	1542	ASN	N-CA-C	5.72	118.00	111.02
1	A	2564	GLY	N-CA-C	-5.71	106.61	114.67
1	A	3459	ASP	CA-C-N	5.65	126.90	119.84
1	A	3459	ASP	C-N-CA	5.65	126.90	119.84
1	A	2184	LEU	CA-C-N	-5.63	114.46	120.03
1	A	2184	LEU	C-N-CA	-5.63	114.46	120.03
1	A	3356	PHE	N-CA-C	-5.60	102.99	110.55
1	B	2183	ARG	N-CA-C	5.53	117.93	111.02
1	A	3711	GLU	N-CA-C	5.51	117.96	110.35
1	B	1471	LEU	N-CA-C	5.50	118.11	111.40
1	A	2636	GLY	CA-C-N	5.41	125.41	120.21
1	A	2636	GLY	C-N-CA	5.41	125.41	120.21
1	A	1937	MET	N-CA-C	-5.40	106.53	113.01
1	A	2943	PHE	N-CA-C	-5.38	105.50	111.36
1	A	3735	LYS	N-CA-C	-5.38	101.69	109.59
1	B	3474	GLY	CA-C-N	5.33	131.72	121.54
1	B	3474	GLY	C-N-CA	5.33	131.72	121.54
1	B	2700	LEU	N-CA-C	-5.29	105.52	111.28
1	B	2989	PRO	N-CA-C	5.29	118.78	110.80
1	B	2535	CYS	N-CA-C	5.28	115.33	107.88
1	B	3946	VAL	N-CA-C	-5.22	97.61	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3413	HIS	N-CA-C	-5.20	106.93	113.28
1	B	2181	GLY	N-CA-C	5.20	123.60	114.76
1	A	3404	VAL	N-CA-C	5.19	114.04	108.95
1	B	2958	ILE	N-CA-C	5.13	115.44	107.28
1	B	4031	GLN	CA-C-N	5.13	125.14	119.90
1	B	4031	GLN	C-N-CA	5.13	125.14	119.90
1	A	3387	ASN	N-CA-C	5.11	116.88	110.24
1	A	3588	ASN	N-CA-C	-5.11	105.79	111.36
1	A	3848	LEU	N-CA-C	5.10	118.28	111.75
1	B	3767	PHE	N-CA-C	-5.10	105.91	111.82
1	A	2895	THR	N-CA-C	5.05	117.68	111.82
1	A	2939	GLU	N-CA-C	5.05	116.96	109.69
1	A	3299	LEU	N-CA-C	-5.04	105.97	111.82
1	A	3490	GLY	N-CA-C	-5.00	107.63	114.64

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	372	0
1	B	21070	21166	21167	377	0
2	A	124	49	52	7	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	755	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 9.

All (755) 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:O2A	2:B:5001:ANP:N3B	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:N	1:A:1472:GLU:OE2	2.20	0.74
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:N	1:B:1472:GLU:OE1	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: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:A:2762:SER:H	1:A:2988:SER:HG	1.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3287:SER:HA	1:B:3588:ASN:HA	1.77	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:O2A	2:A:5003:ANP:O2B	2.15	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
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:B:1367:ILE:HG23	1:B:1415:MET:HE3	1.81	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: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:A:2955:THR:OG1	1:A:2967:ASN:OD1	2.16	0.60
1:B:2472:THR:OG1	1:B:2523:TRP:O	2.17	0.60
1:A:1882:LEU:O	1:A:1882:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3296:VAL:HG11	1:B:3581:ASP:OD1	2.02	0.59
1:B:2920:TRP:O	1:B:2924:THR:OG1	2.20	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:B:3303:LYS:HD2	1:B:3591:LYS:HZ1	1.67	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
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:A:2903:ILE:HG23	1:A:2909:PHE:CE2	2.38	0.57
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.29	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:B:3522:LYS:C	1:B:3524:SER:H	2.13	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:3406:PHE:HB2	1:B:3513:VAL:HG11	1.87	0.57
1:B:3474:GLY:O	1:B:3475:ASN:CG	2.48	0.56
1:A:1862:SER:OG	1:A:1911:ASN:OD1	2.22	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:1802:LYS:NZ	2:B:5001:ANP:O2G	2.36	0.56
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.35	0.56
1:B:3470:PHE:CB	1:B:3475:ASN:HA	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O2B	2:A:5004:ANP:O3G	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
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:OD1	1:A:3409:ASP:N	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:A:2977:TYR:HE1	1:A:2987:ARG:HD3	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2699:LEU:CD1	1:B:2750:LYS:HZ1	2.22	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:2385:VAL:HG13	1:A:2386:MET:HE3	1.92	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: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
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: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: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:A:2584:GLU:CD	1:A:2638:ARG:HH22	2.18	0.51
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:2761:ALA:C	1:A:2766:LYS:HZ1	2.16	0.51
1:B:2699:LEU:HD13	1:B:2750:LYS:HZ1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2646:ARG:NH2	1:B:2695:LEU:HD11	2.26	0.51
1:B:4018:SER:C	1:B:4020:ASN:H	2.18	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
1:A:3255:VAL:HG12	1:A:3259:LYS:NZ	2.27	0.50
1:B:1472:GLU:OE2	1:B:1522:SER:OG	2.25	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:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.93	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	1.93	0.49
1:B:3284:ALA:O	1:B:3285:TYR:HB2	2.12	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
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:2386:MET:HE1	1:A:2627:ARG:HG2	1.96	0.48
1:A:3942:ARG:HA	1:A:3945:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3130:MET:HG3	1:A:3285:TYR:CE2	2.49	0.48
1:A:3212:TYR:O	1:A:3220:ARG:NE	2.47	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:B:1934:LEU:HD23	1:B:1937:MET:HE3	1.96	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: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
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:A:2695:LEU:O	1:A:2696:PHE:C	2.58	0.47
1:B:2088:ILE:HD11	1:B:2151:TRP:CD2	2.49	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:A:2762:SER:C	1:A:2764:THR:H	2.22	0.47
1:A:2853:LEU:HD11	1:A:2870:GLU:HG3	1.97	0.47
1:B:1772:THR:HB	1:B:1925:GLN:CD	2.40	0.47
1:B:2943:PHE:O	1:B:2944:ILE:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3130:MET:HE2	1:A:3225:ASN:HD22	1.81	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:3287:SER:HB2	1:B:3587:LEU:HB3	1.96	0.46
1:B:3296:VAL:C	1:B:3299:LEU:HG	2.40	0.46
1:B:3342:ARG:CZ	1:B:3389:TYR:HE1	2.28	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:A:3946:VAL:O	1:A:3947:PRO:C	2.58	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
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:A:2932:MET:HE1	1:A:2993:ILE:HG23	1.97	0.46
1:A:3285:TYR:C	1:A:3295:LEU:HD21	2.40	0.46
1:B:2552:ARG:NH2	2:B:5002:ANP:O2G	2.48	0.46
1:A:1984:ILE:HG23	1:A:1989:GLU:CD	2.40	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:A:2081:THR:OG1	1:A:2195:GLU:OE1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2999:LEU:HD11	1:B:3325:ILE:HG12	1.98	0.46
1:B:3289:SER:N	1:B:3299:LEU:CB	2.79	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:2510:MET:HE3	1:B:2531:ILE:HB	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3690:LEU:O	1:B:3695:LYS:NZ	2.45	0.45
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.99	0.45
1:A:2330:SER:HB3	1:A:2334:SER:HB2	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:2615:TYR:CE1	1:A:2660:LEU:HD23	2.52	0.45
1:A:2640:THR:HG23	1:A:2643:SER:H	1.81	0.45
1:A:3529:ILE:O	1:A:3533:THR:OG1	2.25	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:2410:SER:C	1:B:2412:ARG:H	2.25	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:HD12	1:A:3620:ILE:H	1.82	0.44
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:B:3307:LEU:C	1:B:3307:LEU:HD12	2.42	0.44
1:A:2410:SER:C	1:A:2412:ARG:H	2.26	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:2898:LYS:HD2	1:B:2898:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2745:ILE:HG12	1:A:2756:MET:HE1	2.00	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:2759:ILE:HG21	1:A:2916:TRP:CZ3	2.53	0.44
1:A:2760:GLY:HA3	1:A:2766:LYS:HD3	2.00	0.44
1:A:3680:GLN:CD	1:A:3769:VAL:HG22	2.43	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:3133:ILE:HG23	1:B:3585:VAL:HG11	1.99	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:3475:ASN:C	1:B:3475:ASN:HD22	2.25	0.44
1:A:1802:LYS:HE2	2:A:5001:ANP:O1B	2.18	0.44
1:A:1815:ARG:NH1	1:A:1844:TRP:NE1	2.66	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
1:A:2392:ILE:CG2	1:A:2573:ILE:HD12	2.47	0.43
1:A:3307:LEU:HD12	1:A:3307:LEU:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2386:MET:HB2	1:B:2627:ARG:NE	2.33	0.43
1:B:2437:LEU:HD12	1:B:2437:LEU:H	1.83	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: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:3624:HIS:ND1	1:A:3679:TYR:OH	2.47	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:2182:GLU:C	1:B:2183:ARG:HG2	2.43	0.43
1:B:2758:LEU:HD22	1:B:2917:MET:HE2	1.98	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:1410:GLU:OE1	1:B:3439:ARG:NH1	2.52	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: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:1922:LYS:C	1:B:1924:PRO:HD3	2.44	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:B:3492:PHE:CD1	1:B:3492:PHE:C	2.97	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
1:A:2999:LEU:HD11	1:A:3325:ILE:HG12	2.01	0.43
1:B:1748:PHE:C	1:B:1749:ILE:HD12	2.44	0.43
1:B:2106:THR:OG1	1:B:2156:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2426:MET:HG3	2:B:5003:ANP:H5'1	2.00	0.43
1:B:3444:ILE:HG21	1:B:3487:ASP:OD2	2.19	0.43
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.84	0.43
1:A:2785:LYS:HZ3	1:A:3480:GLU:HB3	1.83	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:2921:ASP:C	1:A:2923:LYS:H	2.27	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:OD1	1:B:2197:ASP:N	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:B:3680:GLN:CD	1:B:3769:VAL:HG22	2.44	0.42
1:B:4020:ASN:CG	1:B:4028:ARG:HH11	2.27	0.42
1:A:1935:GLN:O	1:A:1938:GLY:HA2	2.18	0.42
1:A:2416:LEU:CD1	1:A:2428:MET:HE3	2.48	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:1800:THR:HA	1:B:1923:SER:HB3	2.02	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:A:3678:LEU:HD23	1:A:3678:LEU:C	2.44	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:2694:LEU:O	1:A:2695:LEU:C	2.63	0.42
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: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: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:1367:ILE:HG23	1:B:1415:MET:CE	2.48	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:2166:MET:HE1	1:B:2192:ILE:HD13	2.02	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:A:3529:ILE:HD12	1:A:3529:ILE:C	2.45	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:2757:MET:HE2	1:B:2891:ILE:HD13	2.02	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:2080:LYS:NZ	2:A:5002:ANP:O1G	2.47	0.42
1:A:3500:ASP:OD2	1:A:3503:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:2432:LEU:HB3	1:A:2440:VAL:HG22	2.01	0.41
1:B:3364:TYR:CD1	1:B:3364:TYR:C	2.98	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: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:CD1	1:B:2827:PHE:N	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:3691:ASP:CA	1:B:3898:GLU:OE2	2.68	0.41
1:B:3789:ALA:HA	1:B:3877:CYS:HB3	2.02	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:2416:LEU:HD11	1:A:2428:MET:HE3	2.01	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:2541:PRO:HD2	1:B:2904:SER:HB2	2.01	0.41
1:B:2695:LEU:N	1:B:2695:LEU:HD12	2.35	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:3414:MET:HE3	1:A:3518:PHE:CD2	2.55	0.41
1:A:3912:GLY:HA2	1:A:3915:PHE:CE2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3209:LYS:N	1:B:3210:PRO:HD2	2.35	0.41
1:B:3687:SER:HA	1:B:3698:MET:HE1	2.03	0.41
1:B:3788:MET:O	1:B:3788:MET:HG3	2.20	0.41
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:2945:VAL:O	1:A:2946:PRO:C	2.62	0.41
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	2.03	0.41
1:A:3209:LYS:N	1:A:3210:PRO:HD2	2.36	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:A:4018:SER:C	1:A:4020:ASN:H	2.29	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: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: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: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: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
1:A:3844:ILE:HD11	1:A:3855:LEU:CD2	2.51	0.41
1:B:1788:GLN:OE1	1:B:3966:VAL:HG21	2.21	0.41
1:B:2119:LEU:HD12	1:B:2124:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:3640:TRP:CD1	1:A:3640:TRP:H	2.38	0.40
1:A:3815:PRO:C	1:A:3816:LEU:HD12	2.46	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: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:A:2745:ILE:HA	1:A:2756:MET:HE1	2.03	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:1537:PHE:CE1	1:B:1565:MET:HE1	2.56	0.40
1:B:2741:HIS:NE2	1:B:2917:MET:HB3	2.36	0.40
1:B:3130:MET:HE3	1:B:3285:TYR:CE2	2.57	0.40
1:B:3630:SER:O	1:B:3634:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1411:GLU:HG2	1:A:1415:MET:HE3	2.02	0.40
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	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
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:3587:LEU:C	1:A:3587:LEU:HD12	2.46	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%)	43	73
1	B	2597/2661 (98%)	2476 (95%)	116 (4%)	5 (0%)	43	73
All	All	5193/5322 (98%)	4949 (95%)	234 (4%)	10 (0%)	43	73

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1366	VAL

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Mol	Chain	Res	Type
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%)	2311 (98%)	56 (2%)	43	64
1	B	2366/2406 (98%)	2319 (98%)	47 (2%)	48	67
All	All	4733/4812 (98%)	4630 (98%)	103 (2%)	45	65

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1392	LEU
1	A	1423	ILE
1	A	1453	LEU
1	A	1486	ILE
1	A	1523	LEU
1	A	1528	GLU
1	A	1589	VAL
1	A	1657	THR
1	A	1661	GLU
1	A	1665	GLN
1	A	1818	VAL
1	A	1838	ILE
1	A	1852	ARG
1	A	1882	LEU

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Mol	Chain	Res	Type
1	A	1914	LYS
1	A	1922	LYS
1	A	1929	ILE
1	A	2012	LEU
1	A	2088	ILE
1	A	2119	LEU
1	A	2148	SER
1	A	2158	LEU
1	A	2178	LEU
1	A	2195	GLU
1	A	2273	VAL
1	A	2295	ILE
1	A	2300	GLN
1	A	2326	LEU
1	A	2354	SER
1	A	2440	VAL
1	A	2576	LYS
1	A	2661	VAL
1	A	2683	ASN
1	A	2689	ILE
1	A	2712	LEU
1	A	2735	HIS
1	A	2786	ILE
1	A	2828	LEU
1	A	2975	ASN
1	A	3031	VAL
1	A	3140	LYS
1	A	3189	LYS
1	A	3268	ASN
1	A	3300	THR
1	A	3371	VAL
1	A	3461	ILE
1	A	3579	GLU
1	A	3584	MET
1	A	3615	VAL
1	A	3705	LEU
1	A	3811	LEU
1	A	3813	ILE
1	A	3939	ILE
1	A	3974	THR
1	A	3980	ILE
1	A	4023	ILE

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Mol	Chain	Res	Type
1	B	1392	LEU
1	B	1486	ILE
1	B	1759	LYS
1	B	1818	VAL
1	B	1852	ARG
1	B	1973	LEU
1	B	2012	LEU
1	B	2073	VAL
1	B	2148	SER
1	B	2273	VAL
1	B	2295	ILE
1	B	2326	LEU
1	B	2354	SER
1	B	2512	LYS
1	B	2536	ASN
1	B	2576	LYS
1	B	2683	ASN
1	B	2712	LEU
1	B	2734	ILE
1	B	2769	LEU
1	B	2786	ILE
1	B	2903	ILE
1	B	2975	ASN
1	B	3026	GLU
1	B	3031	VAL
1	B	3140	LYS
1	B	3189	LYS
1	B	3205	ASN
1	B	3287	SER
1	B	3293	ILE
1	B	3371	VAL
1	B	3412	SER
1	B	3461	ILE
1	B	3471	ASN
1	B	3475	ASN
1	B	3487	ASP
1	B	3488	VAL
1	B	3579	GLU
1	B	3588	ASN
1	B	3615	VAL
1	B	3690	LEU
1	B	3705	LEU

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Mol	Chain	Res	Type
1	B	3713	GLU
1	B	3816	LEU
1	B	3939	ILE
1	B	3980	ILE
1	B	4023	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1533	GLN
1	A	1745	ASN
1	A	1821	ASN
1	A	2099	ASN
1	A	2264	ASN
1	A	2300	GLN
1	A	2340	GLN
1	A	2348	HIS
1	A	2383	HIS
1	A	2453	HIS
1	A	2530	HIS
1	A	2601	ASN
1	A	2777	ASN
1	A	2789	HIS
1	A	2971	HIS
1	A	3011	GLN
1	A	3318	GLN
1	A	3420	ASN
1	A	3552	ASN
1	A	3648	GLN
1	A	3780	ASN
1	A	3826	GLN
1	A	3988	HIS
1	A	4031	GLN
1	B	1444	ASN
1	B	1707	HIS
1	B	1811	GLN
1	B	1899	ASN
1	B	2201	HIS
1	B	2264	ASN
1	B	2453	HIS
1	B	2530	HIS
1	B	2927	GLN

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Mol	Chain	Res	Type
1	B	2975	ASN
1	B	3318	GLN
1	B	3588	ASN
1	B	3624	HIS
1	B	3741	ASN
1	B	3780	ASN
1	B	3826	GLN
1	B	4077	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 oligosaccharides 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	5004	-	33,33,33	1.51	5 (15%)	45,52,52	0.65	0
2	ANP	B	5002	3	33,33,33	1.71	5 (15%)	45,52,52	0.71	1 (2%)
2	ANP	B	5003	-	33,33,33	1.68	5 (15%)	45,52,52	0.67	0
2	ANP	A	5002	3	33,33,33	0.85	3 (9%)	45,52,52	0.67	0
2	ANP	B	5001	-	33,33,33	2.04	6 (18%)	45,52,52	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	A	5001	-	33,33,33	1.01	3 (9%)	45,52,52	0.58	0
2	ANP	A	5004	-	33,33,33	1.70	5 (15%)	45,52,52	0.68	0
2	ANP	A	5003	-	33,33,33	1.97	5 (15%)	45,52,52	0.73	1 (2%)

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	5004	-	-	4/18/38/38	0/3/3/3
2	ANP	B	5002	3	-	4/18/38/38	0/3/3/3
2	ANP	B	5003	-	-	7/18/38/38	0/3/3/3
2	ANP	A	5002	3	-	4/18/38/38	0/3/3/3
2	ANP	B	5001	-	-	7/18/38/38	0/3/3/3
2	ANP	A	5001	-	-	4/18/38/38	0/3/3/3
2	ANP	A	5004	-	-	8/18/38/38	0/3/3/3
2	ANP	A	5003	-	-	10/18/38/38	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	8.17	1.58	1.46
2	B	5002	ANP	PG-O1G	8.14	1.58	1.46
2	B	5003	ANP	PG-O1G	8.08	1.58	1.46
2	A	5004	ANP	PG-O1G	8.08	1.58	1.46
2	A	5003	ANP	PG-O1G	7.70	1.57	1.46
2	B	5004	ANP	PB-O1B	6.61	1.56	1.46
2	A	5003	ANP	PB-O1B	6.45	1.55	1.46
2	B	5001	ANP	PB-O1B	6.38	1.55	1.46
2	B	5002	ANP	PG-O3G	-3.00	1.48	1.56
2	A	5003	ANP	PB-O2B	-2.75	1.49	1.56
2	B	5004	ANP	PB-O2B	-2.73	1.49	1.56
2	A	5001	ANP	PB-O3A	-2.73	1.55	1.59
2	A	5004	ANP	PG-O3G	-2.69	1.49	1.56
2	B	5003	ANP	PG-O3G	-2.64	1.49	1.56
2	A	5003	ANP	PG-O2G	-2.64	1.49	1.56
2	B	5004	ANP	PB-O3A	-2.63	1.55	1.59
2	B	5001	ANP	PB-O3A	-2.60	1.55	1.59
2	B	5001	ANP	PB-O2B	-2.59	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	ANP	PG-O1G	2.57	1.50	1.46
2	B	5001	ANP	PG-O3G	-2.57	1.50	1.56
2	A	5004	ANP	PB-O3A	-2.56	1.55	1.59
2	B	5004	ANP	PG-N3B	2.42	1.69	1.63
2	B	5004	ANP	PG-O1G	2.37	1.49	1.46
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	A	5004	ANP	PB-O1B	2.32	1.49	1.46
2	B	5002	ANP	PB-O3A	-2.31	1.56	1.59
2	B	5001	ANP	PG-N3B	2.29	1.69	1.63
2	B	5003	ANP	PB-O1B	2.26	1.49	1.46
2	A	5002	ANP	PG-O1G	2.23	1.49	1.46
2	B	5002	ANP	PB-O1B	2.23	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	A	5002	ANP	PB-O1B	2.11	1.49	1.46
2	B	5003	ANP	PB-O3A	-2.08	1.56	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 (48) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	B	5001	ANP	C5'-O5'-PA-O2A
2	B	5001	ANP	C5'-O5'-PA-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	5004	ANP	PB-N3B-PG-O1G
2	B	5004	ANP	PG-N3B-PB-O3A
2	A	5003	ANP	O4'-C4'-C5'-O5'
2	B	5001	ANP	O4'-C4'-C5'-O5'
2	B	5001	ANP	C3'-C4'-C5'-O5'
2	B	5003	ANP	C3'-C4'-C5'-O5'
2	A	5001	ANP	O4'-C4'-C5'-O5'
2	A	5004	ANP	O4'-C4'-C5'-O5'
2	B	5002	ANP	C3'-C4'-C5'-O5'
2	B	5003	ANP	O4'-C4'-C5'-O5'
2	B	5004	ANP	O4'-C4'-C5'-O5'
2	A	5004	ANP	C3'-C4'-C5'-O5'
2	B	5004	ANP	C3'-C4'-C5'-O5'
2	A	5003	ANP	C2'-C1'-N9-C4
2	A	5003	ANP	C2'-C1'-N9-C8
2	A	5001	ANP	C3'-C4'-C5'-O5'
2	B	5003	ANP	C2'-C1'-N9-C4
2	B	5003	ANP	C2'-C1'-N9-C8
2	A	5003	ANP	C5'-O5'-PA-O3A
2	A	5004	ANP	C5'-O5'-PA-O3A
2	A	5004	ANP	C4'-C5'-O5'-PA
2	B	5001	ANP	PB-O3A-PA-O1A
2	A	5002	ANP	C4'-C5'-O5'-PA
2	B	5001	ANP	PB-O3A-PA-O2A
2	B	5003	ANP	PG-N3B-PB-O1B
2	A	5001	ANP	PA-O3A-PB-O1B
2	A	5003	ANP	PA-O3A-PB-O1B
2	A	5004	ANP	PA-O3A-PB-O1B
2	B	5002	ANP	PA-O3A-PB-O1B
2	A	5003	ANP	PB-O3A-PA-O1A

There are no ring outliers.

8 monomers are involved in 15 short contacts:

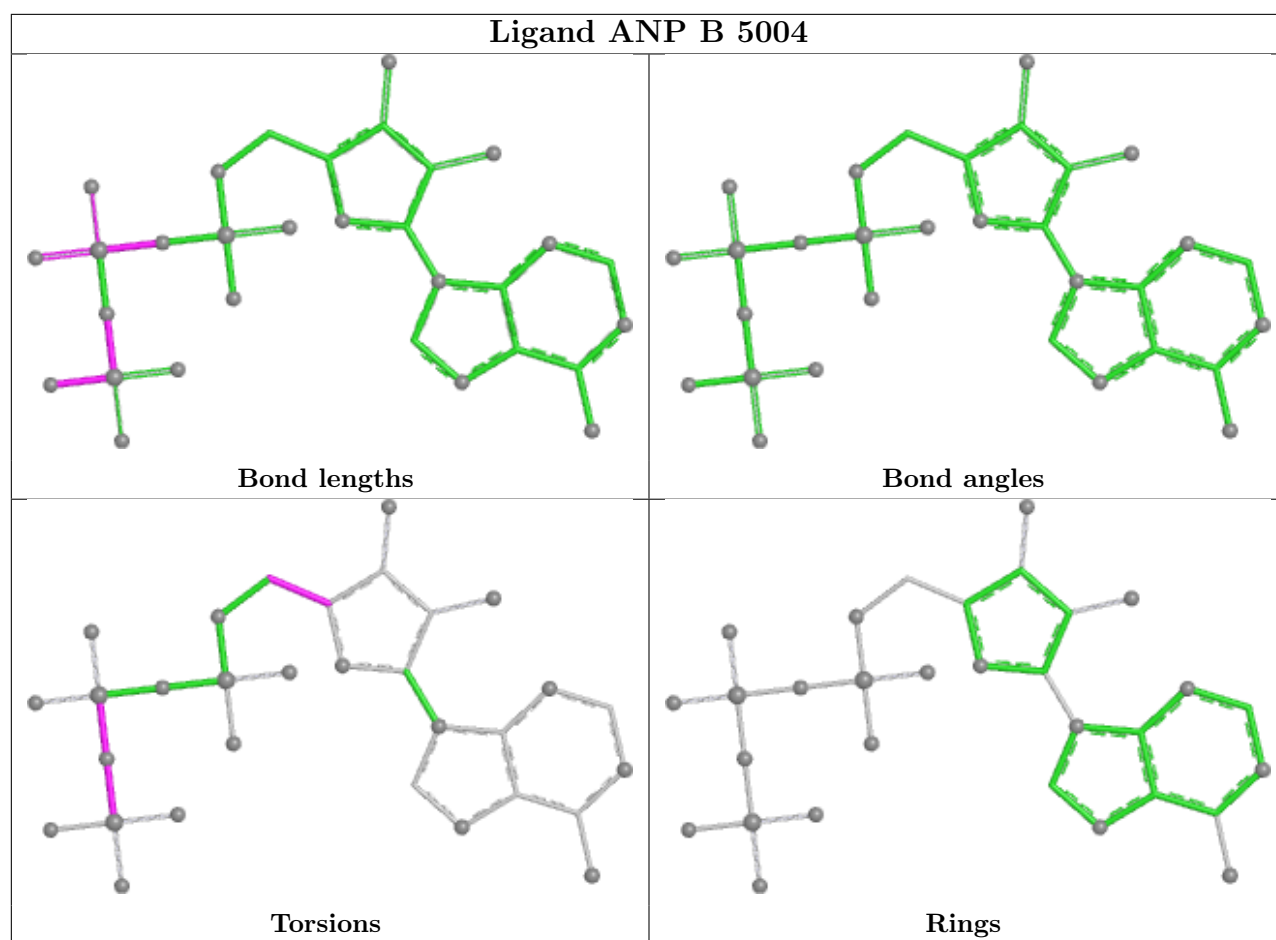
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5004	ANP	1	0

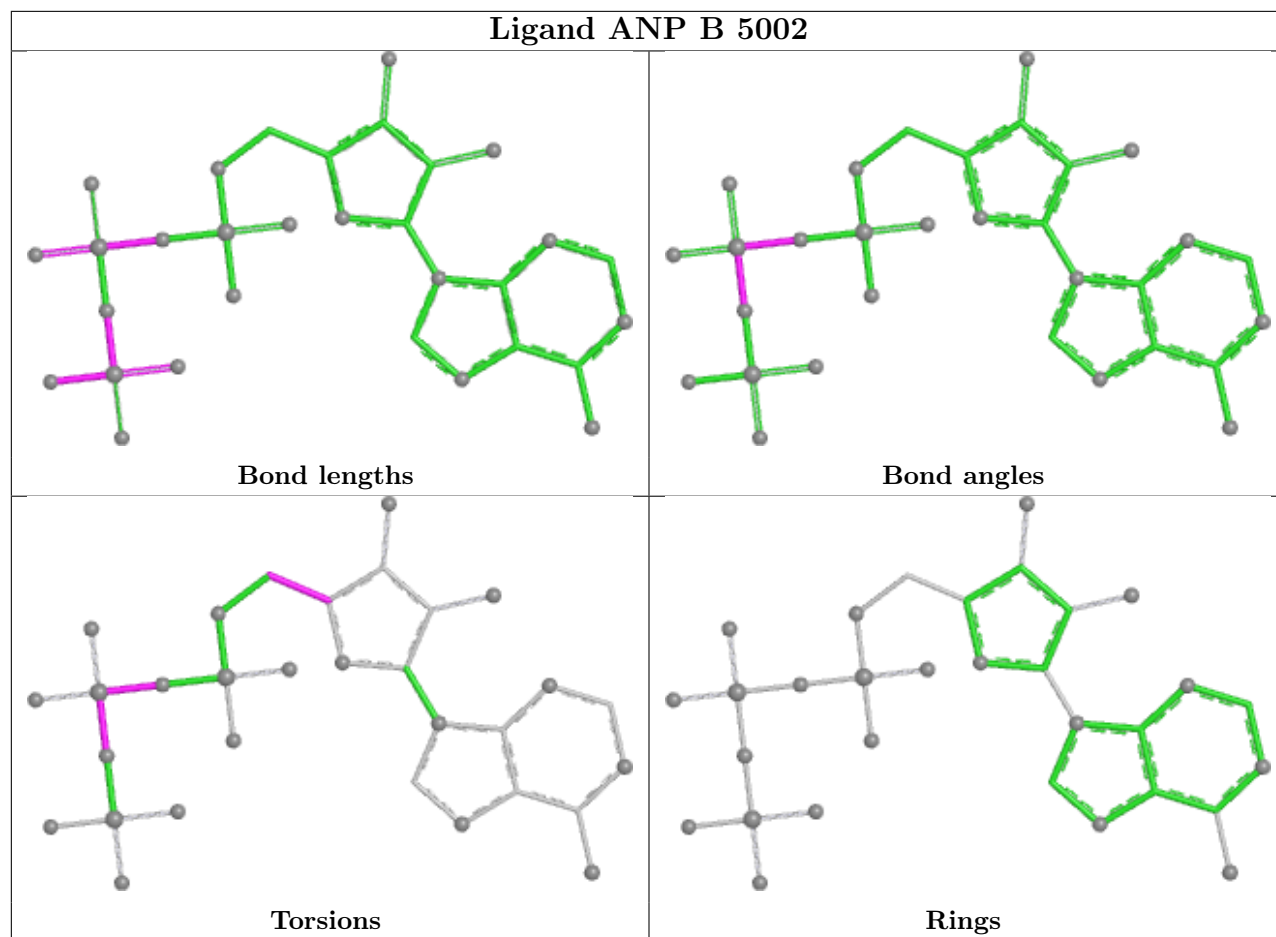
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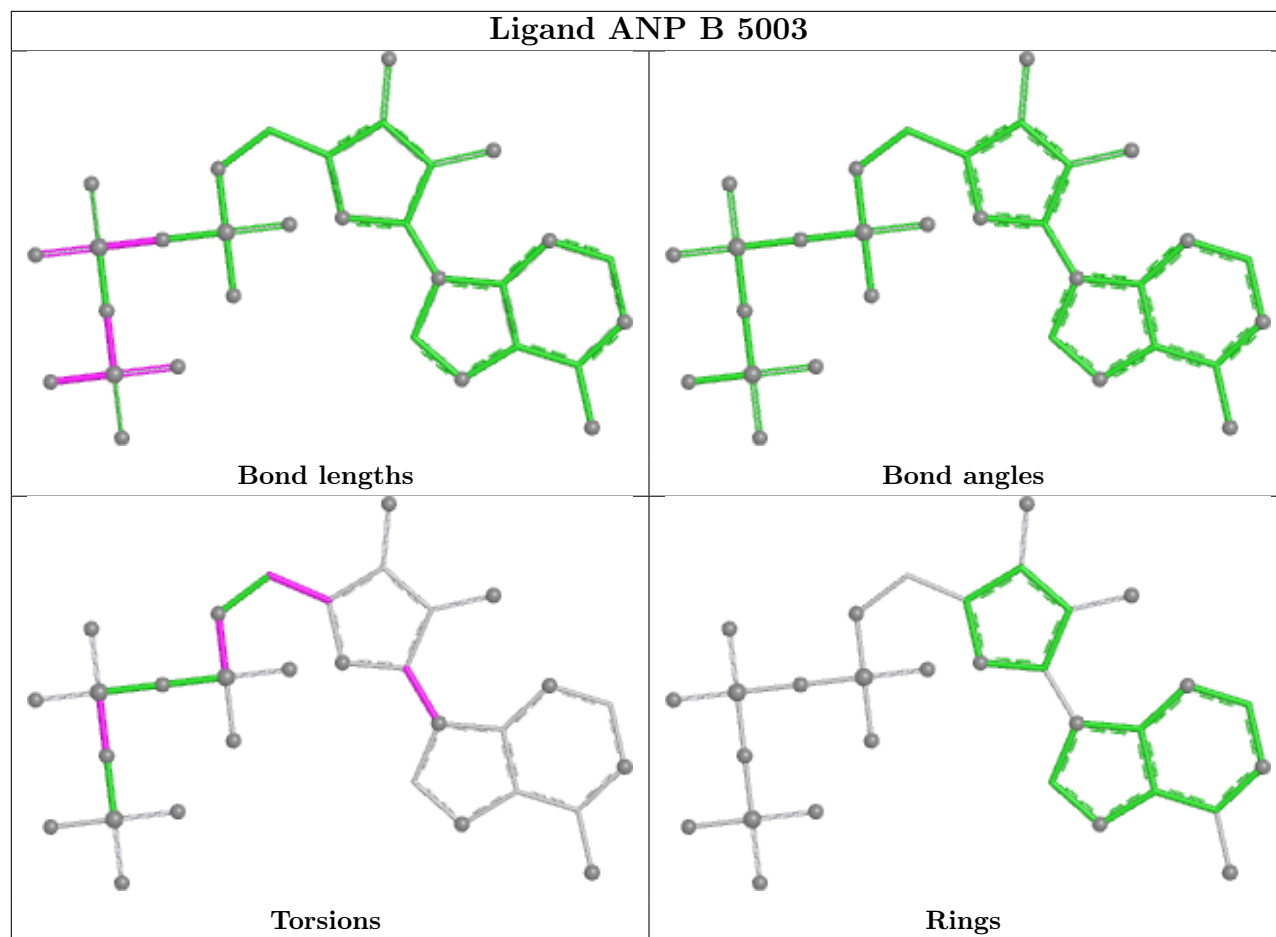
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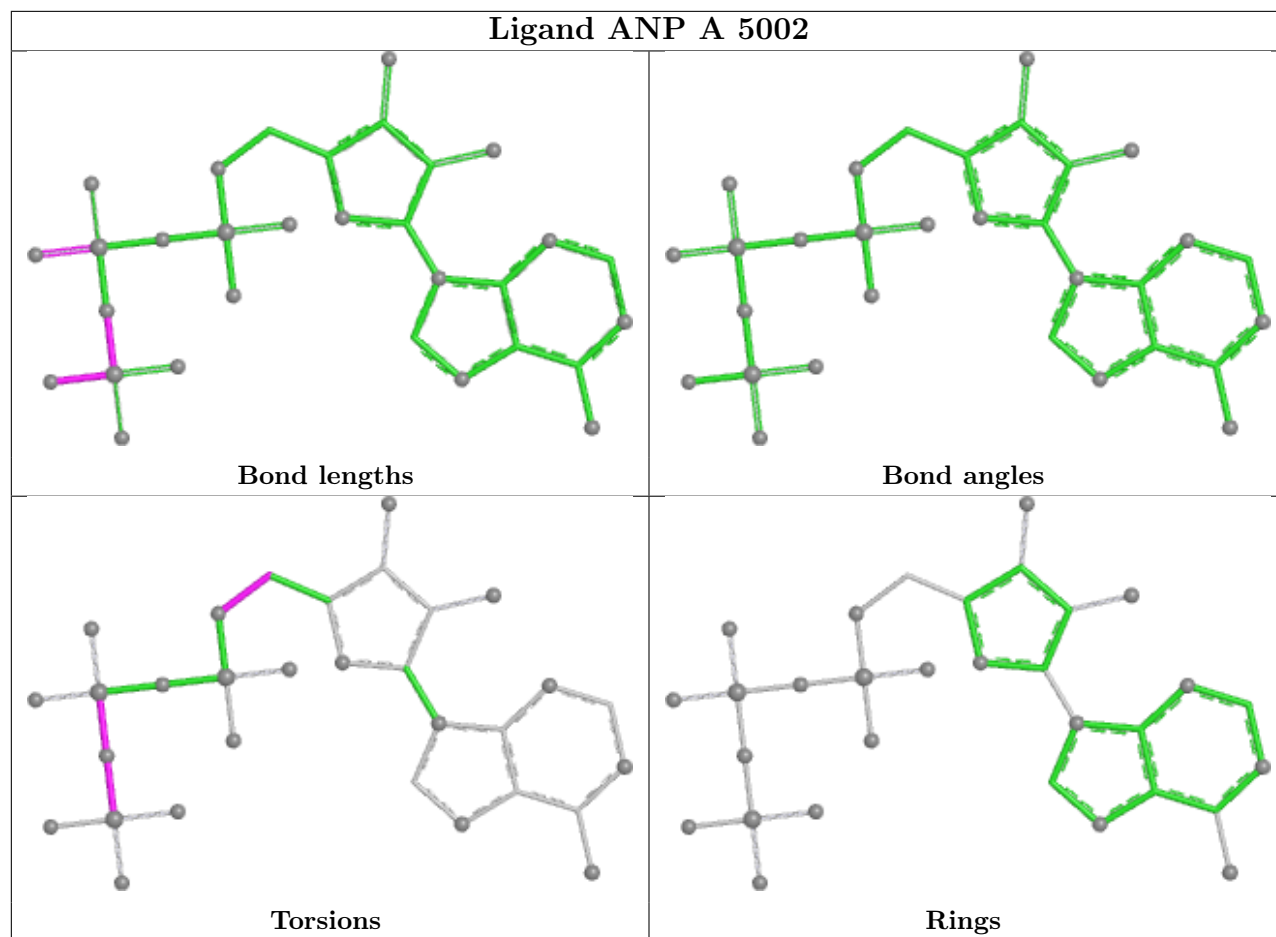
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5002	ANP	2	0
2	B	5003	ANP	3	0
2	A	5002	ANP	1	0
2	B	5001	ANP	2	0
2	A	5001	ANP	1	0
2	A	5004	ANP	2	0
2	A	5003	ANP	3	0

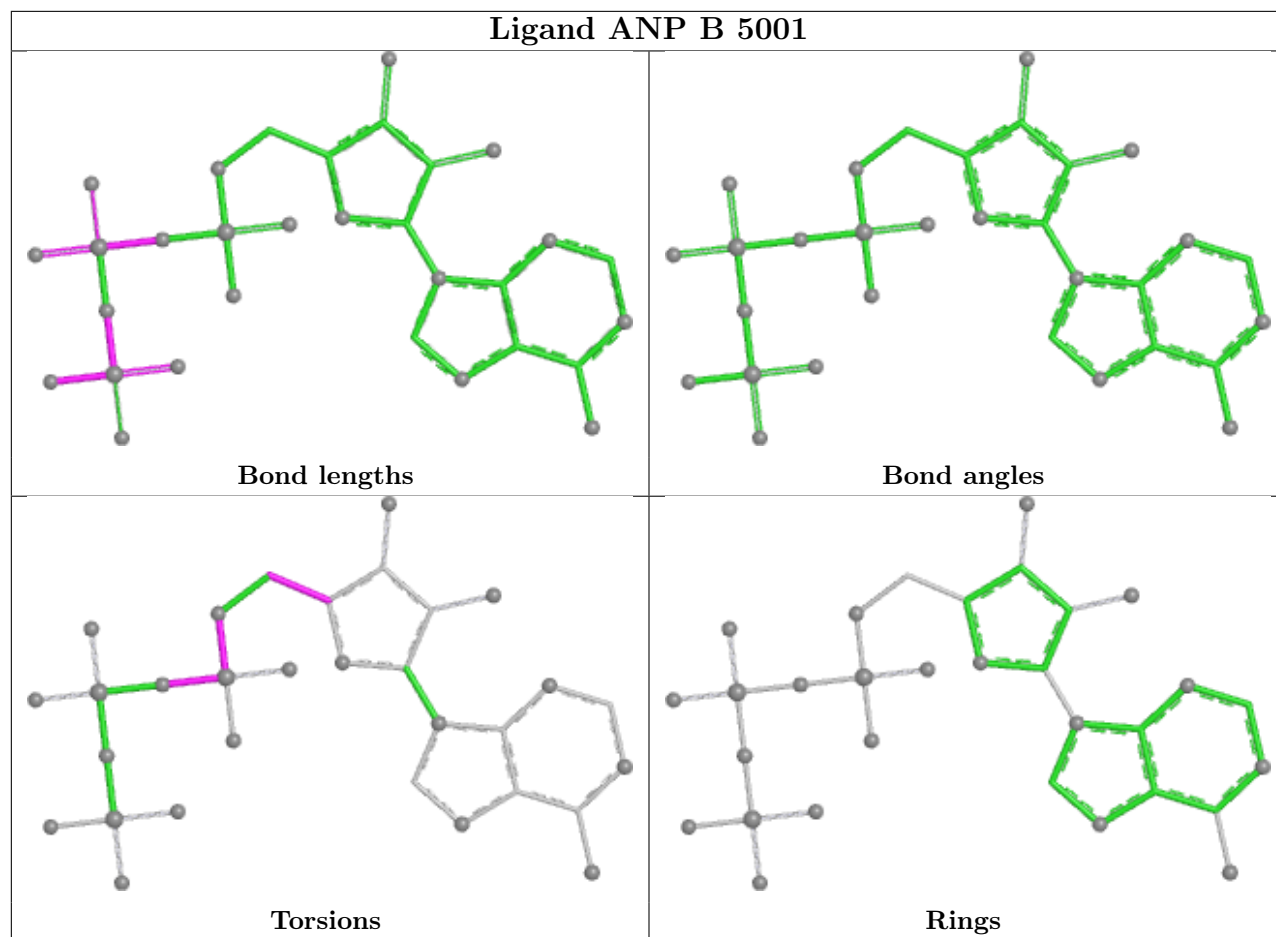
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

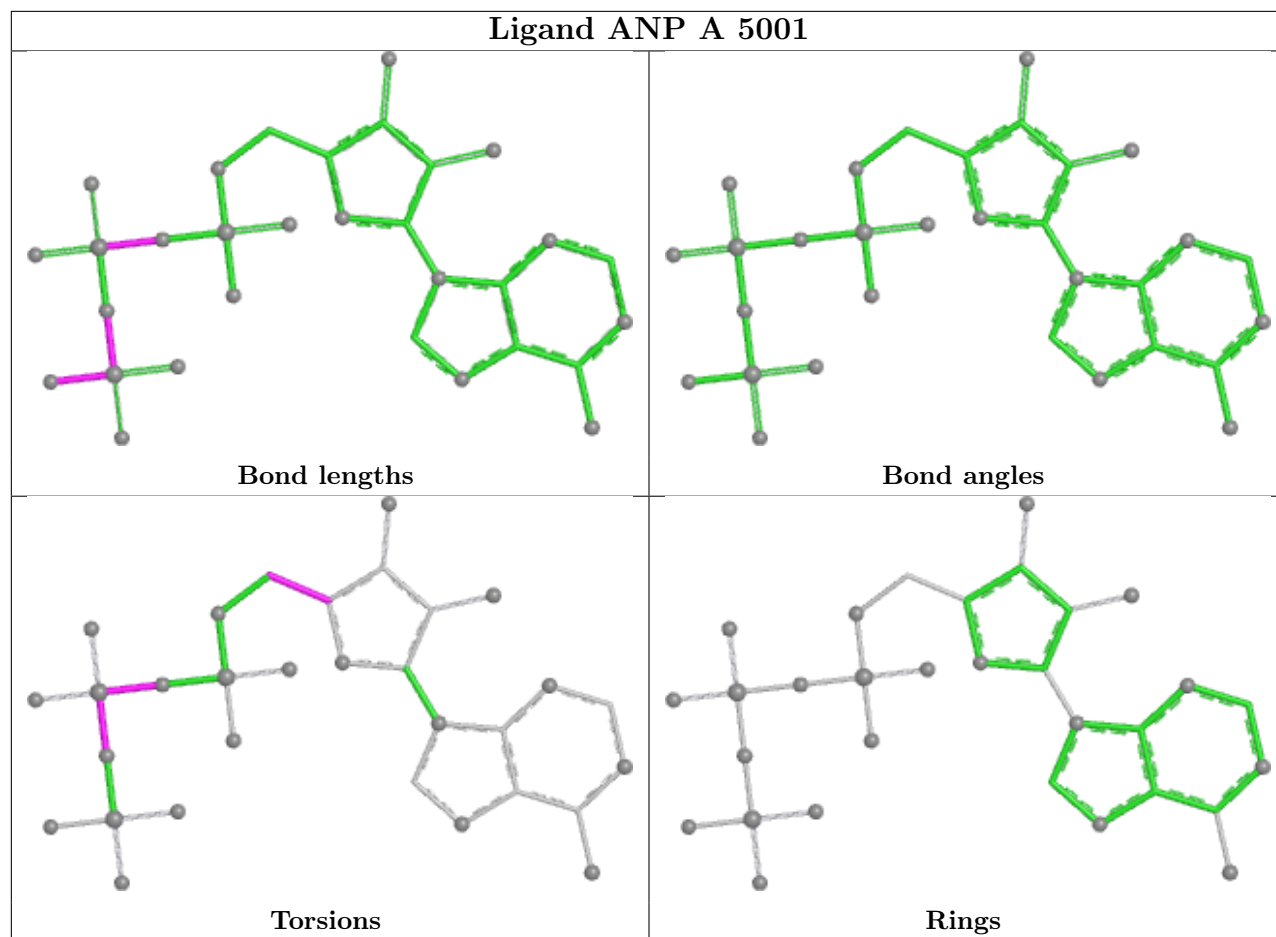


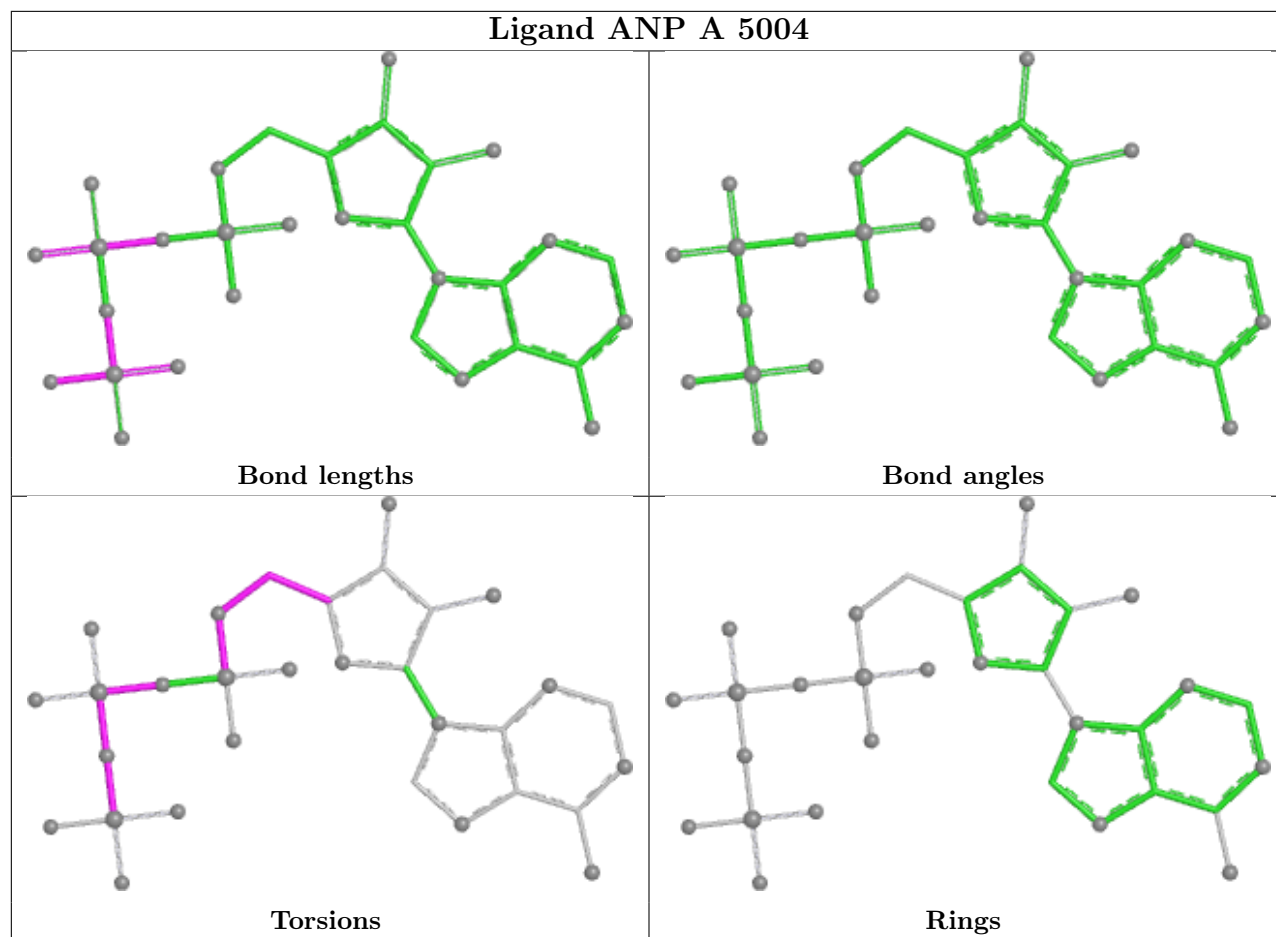


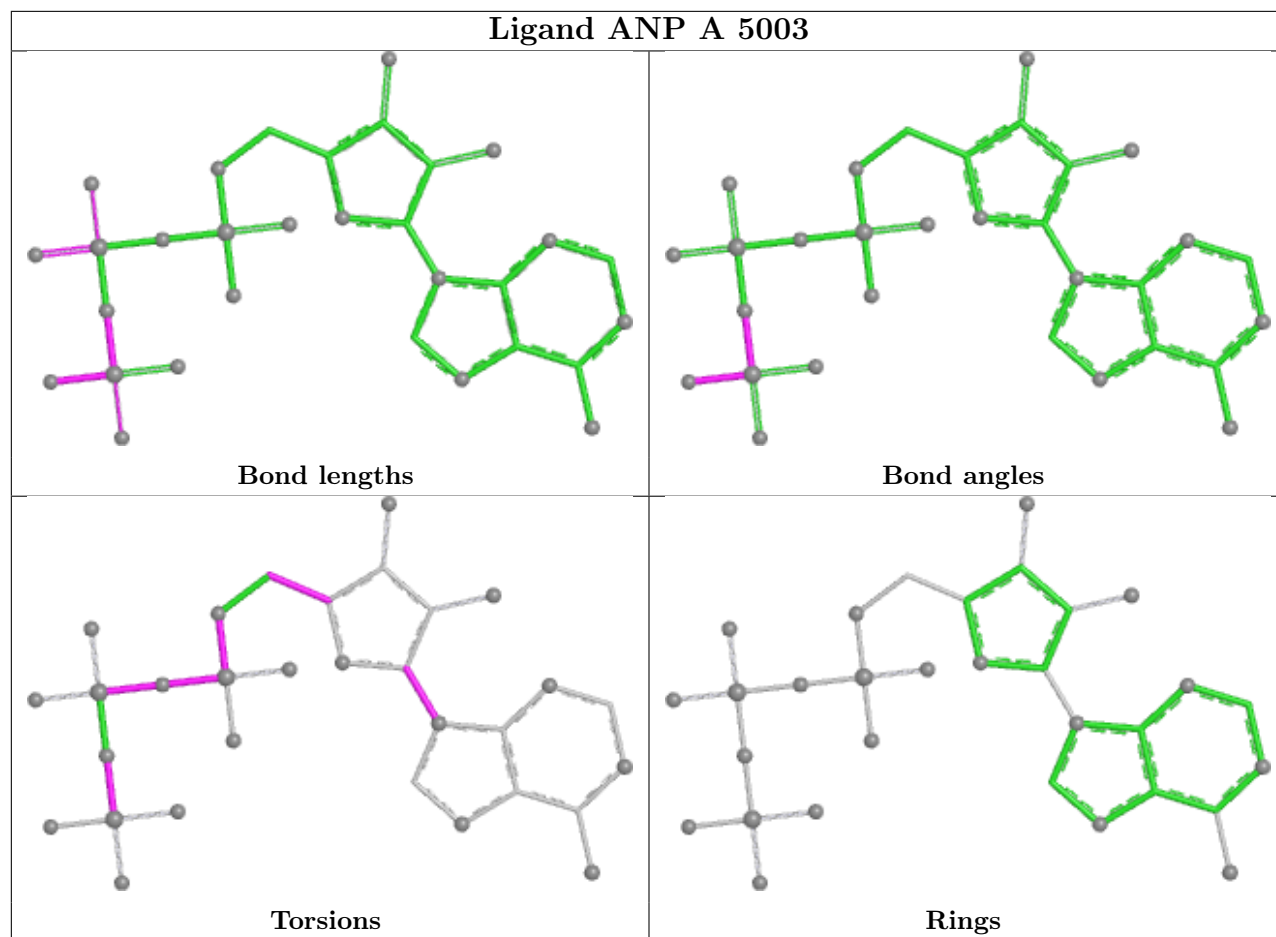












5.7 Other polymers [i](#)

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%)	0.30	123 (4%)	36	18	22, 55, 129, 303	0
1	B	2609/2661 (98%)	0.29	113 (4%)	40	20	25, 59, 132, 274	0
All	All	5217/5322 (98%)	0.30	236 (4%)	38	19	22, 57, 131, 303	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3482	GLY	5.2
1	A	3865	ALA	5.2
1	A	2911	ARG	5.1
1	B	2916	TRP	4.9
1	B	2904	SER	4.9
1	A	1742	ASP	4.7
1	A	3294	SER	4.7
1	A	3768	PHE	4.7
1	A	2920	TRP	4.6
1	A	3480	GLU	4.4
1	A	2730	VAL	4.4
1	A	3731	ASP	4.4
1	A	3580	ASN	4.3
1	B	2902	MET	4.2
1	B	2388	PRO	4.1
1	A	3487	ASP	4.1
1	B	2736	GLU	4.1
1	B	1552	GLY	4.0
1	A	3471	ASN	4.0
1	A	2902	MET	4.0
1	B	3288	GLY	4.0
1	A	2662	GLY	3.9
1	B	3581	ASP	3.9
1	A	3484	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	3306	TRP	3.7
1	B	3400	SER	3.7
1	B	3575	GLY	3.7
1	A	2736	GLU	3.7
1	B	2363	ASN	3.7
1	A	2939	GLU	3.6
1	B	3768	PHE	3.6
1	A	2827	PHE	3.6
1	A	3586	THR	3.6
1	A	2356	TYR	3.5
1	B	3767	PHE	3.5
1	A	3581	ASP	3.5
1	B	2356	TYR	3.5
1	B	3145	THR	3.5
1	B	2696	PHE	3.5
1	B	2919	ASP	3.5
1	A	2955	THR	3.5
1	A	3300	THR	3.5
1	A	3979	ASN	3.5
1	A	3740	THR	3.5
1	B	1742	ASP	3.4
1	A	2901	ALA	3.4
1	B	3296	VAL	3.4
1	B	3205	ASN	3.4
1	B	3740	THR	3.3
1	A	2695	LEU	3.3
1	B	3580	ASN	3.3
1	A	2363	ASN	3.3
1	B	2824	GLU	3.3
1	A	3402	ASP	3.2
1	B	2751	GLN	3.2
1	B	3146	GLU	3.2
1	A	2907	ALA	3.2
1	B	2837	ASN	3.2
1	B	2471	LEU	3.2
1	B	3980	ILE	3.2
1	A	3485	GLU	3.2
1	B	3736	LEU	3.1
1	B	2662	GLY	3.1
1	B	2911	ARG	3.1
1	B	3166	ALA	3.0
1	A	3867	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	3402	ASP	3.0
1	B	3739	ASP	3.0
1	A	2988	SER	3.0
1	B	2528	ARG	3.0
1	A	2142	THR	3.0
1	B	3586	THR	3.0
1	A	3031	VAL	3.0
1	A	3145	THR	3.0
1	B	3159	LYS	3.0
1	A	2904	SER	3.0
1	B	3306	TRP	3.0
1	A	2919	ASP	3.0
1	B	2827	PHE	3.0
1	A	3486	VAL	3.0
1	B	2299	ARG	3.0
1	A	2355	ASP	3.0
1	A	2936	ILE	2.9
1	A	2348	HIS	2.9
1	A	3468	ARG	2.9
1	A	3769	VAL	2.9
1	B	3478	THR	2.9
1	A	3399	ASN	2.9
1	B	1924	PRO	2.9
1	A	3483	ASP	2.9
1	A	2411	LYS	2.9
1	A	1506	ASP	2.8
1	A	3477	VAL	2.8
1	A	3920	ILE	2.8
1	A	2837	ASN	2.8
1	B	2920	TRP	2.8
1	A	3470	PHE	2.8
1	A	1799	GLY	2.8
1	B	2825	THR	2.8
1	A	3295	LEU	2.7
1	A	1980	CYS	2.7
1	B	3538	ASN	2.7
1	B	3769	VAL	2.7
1	A	2364	ASP	2.7
1	B	3149	TYR	2.7
1	B	3865	ALA	2.7
1	A	3582	GLU	2.7
1	B	3766	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1365	PHE	2.7
1	B	2985	ASN	2.6
1	B	2257	PHE	2.6
1	A	3476	ARG	2.6
1	B	3605	GLU	2.6
1	B	2346	PHE	2.6
1	B	2903	ILE	2.6
1	B	2831	MET	2.6
1	B	3949	GLY	2.6
1	A	3980	ILE	2.6
1	B	2384	GLU	2.6
1	B	3979	ASN	2.6
1	B	1365	PHE	2.6
1	A	3299	LEU	2.5
1	B	3584	MET	2.5
1	A	2141	ILE	2.5
1	A	3467	SER	2.5
1	B	1468	PHE	2.5
1	A	2944	ILE	2.5
1	A	3469	GLU	2.5
1	A	3377	MET	2.5
1	A	3605	GLU	2.5
1	B	1884	GLU	2.5
1	A	3180	GLY	2.5
1	A	2701	SER	2.5
1	B	3555	TYR	2.5
1	B	2907	ALA	2.5
1	A	2370	SER	2.5
1	A	2905	SER	2.5
1	A	3135	GLU	2.4
1	B	2706	GLU	2.4
1	B	2819	GLU	2.4
1	B	3173	ALA	2.4
1	B	3162	SER	2.4
1	B	3488	VAL	2.4
1	B	2374	GLU	2.4
1	A	3924	TRP	2.4
1	B	2730	VAL	2.4
1	A	2349	ASP	2.4
1	A	2459	HIS	2.4
1	A	1424	PHE	2.4
1	B	3150	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	3293	ILE	2.4
1	A	2380	LEU	2.4
1	B	2380	LEU	2.4
1	B	2381	GLU	2.4
1	A	3521	ASN	2.4
1	B	2989	PRO	2.4
1	B	2697	SER	2.4
1	A	2825	THR	2.4
1	A	2922	THR	2.4
1	A	2379	SER	2.3
1	A	3179	ASN	2.3
1	B	2144	THR	2.3
1	A	2942	ASP	2.3
1	B	2752	VAL	2.3
1	B	2760	GLY	2.3
1	B	2836	ALA	2.3
1	A	3309	THR	2.3
1	A	3982	TRP	2.3
1	B	2480	LYS	2.3
1	B	2030	ASN	2.3
1	B	2147	ASN	2.3
1	A	2906	PRO	2.3
1	A	3949	GLY	2.3
1	B	2846	GLY	2.3
1	B	2984	VAL	2.3
1	A	3547	ASP	2.3
1	A	2941	THR	2.2
1	B	2897	ASN	2.2
1	A	2140	ASP	2.2
1	A	2616	LEU	2.2
1	A	3945	LEU	2.2
1	B	2171	ASP	2.2
1	B	3179	ASN	2.2
1	A	2940	PHE	2.2
1	B	3143	LYS	2.2
1	B	3287	SER	2.2
1	A	2694	LEU	2.2
1	A	2728	LEU	2.2
1	A	2945	VAL	2.2
1	B	1987	PHE	2.2
1	A	3148	TYR	2.2
1	B	3261	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	3486	VAL	2.2
1	A	2144	THR	2.2
1	A	3472	HIS	2.2
1	B	2826	ALA	2.2
1	B	2987	ARG	2.2
1	A	3737	THR	2.2
1	B	2823	LEU	2.2
1	A	3162	SER	2.1
1	B	3469	GLU	2.1
1	B	3473	ALA	2.1
1	B	3160	SER	2.1
1	A	3149	TYR	2.1
1	B	2476	LYS	2.1
1	A	1740	THR	2.1
1	A	2699	LEU	2.1
1	A	3557	LEU	2.1
1	A	2836	ALA	2.1
1	B	3487	ASP	2.1
1	B	2387	ARG	2.1
1	B	3468	ARG	2.1
1	B	3741	ASN	2.1
1	A	2954	PHE	2.1
1	A	1600	ASP	2.1
1	A	3474	GLY	2.1
1	A	3764	LYS	2.1
1	B	2898	LYS	2.1
1	B	2988	SER	2.1
1	A	3479	VAL	2.1
1	B	2448	ASP	2.1
1	A	2182	GLU	2.1
1	A	2761	ALA	2.1
1	A	3161	PRO	2.0
1	A	2893	ASP	2.0
1	A	4033	LEU	2.0
1	B	2364	ASP	2.0
1	B	3579	GLU	2.0
1	A	3320	LEU	2.0
1	B	1923	SER	2.0
1	B	4018	SER	2.0
1	A	2752	VAL	2.0
1	A	2157	ASP	2.0
1	A	3915	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	3492	PHE	2.0
1	B	2563	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

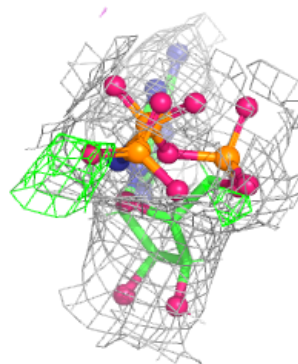
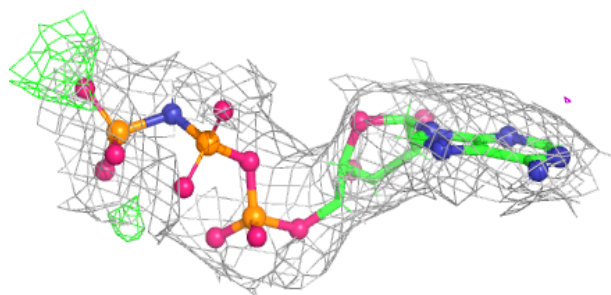
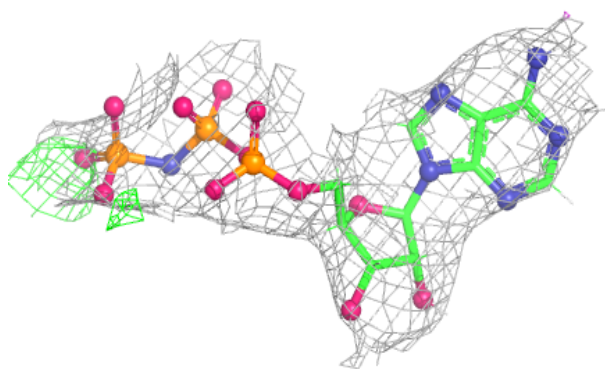
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ANP	A	5004	31/31	0.89	0.16	49,72,160,227	0
2	ANP	B	5003	31/31	0.89	0.18	43,75,101,161	0
2	ANP	B	5001	31/31	0.91	0.16	31,57,180,372	0
2	ANP	A	5003	31/31	0.91	0.16	21,52,121,134	0
2	ANP	B	5004	31/31	0.91	0.14	47,78,162,183	0
3	MG	B	5005	1/1	0.91	0.21	54,54,54,54	0
3	MG	A	5005	1/1	0.92	0.27	50,50,50,50	0
2	ANP	A	5001	31/31	0.93	0.14	23,51,183,503	0
2	ANP	A	5002	31/31	0.95	0.13	36,66,98,149	0
2	ANP	B	5002	31/31	0.95	0.14	28,67,122,162	0

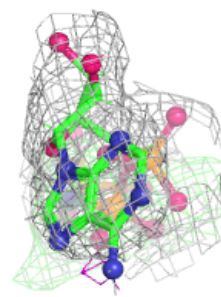
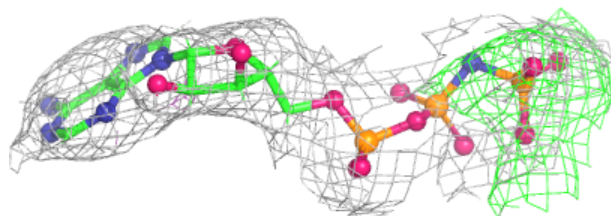
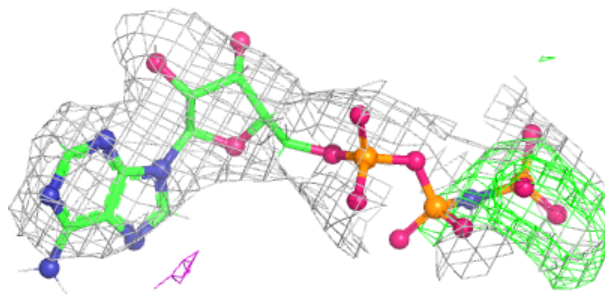
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

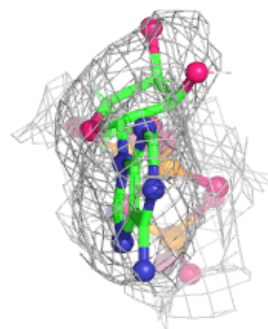
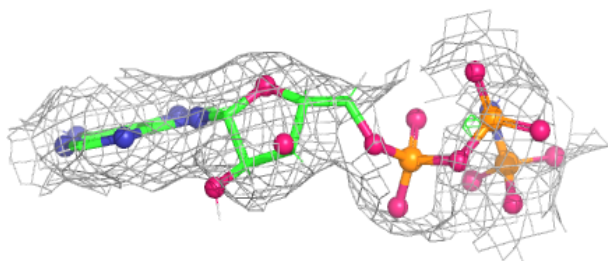
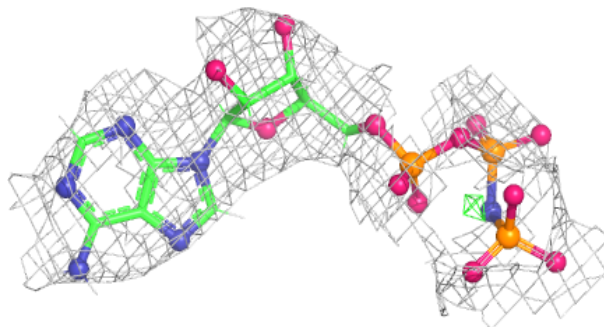
**Electron density around ANP B 5003:**

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

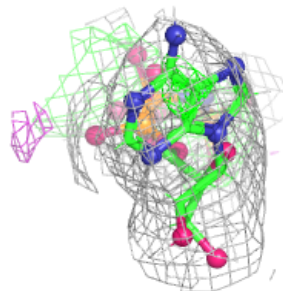
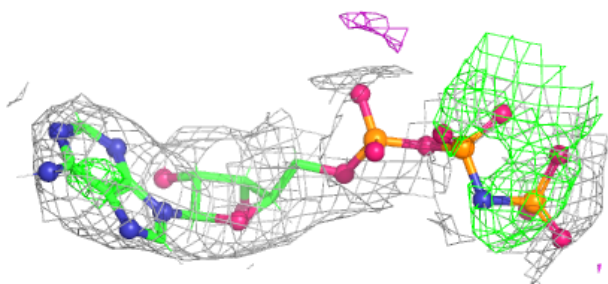
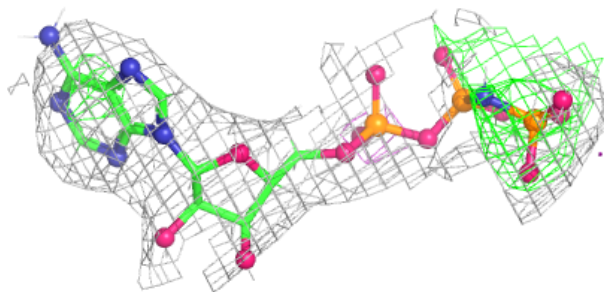


Electron density around ANP B 5001:

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

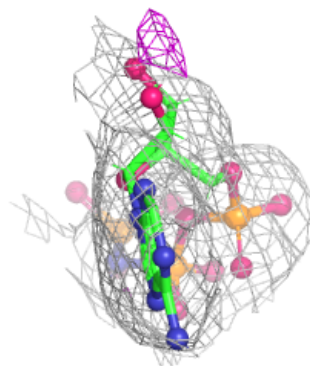
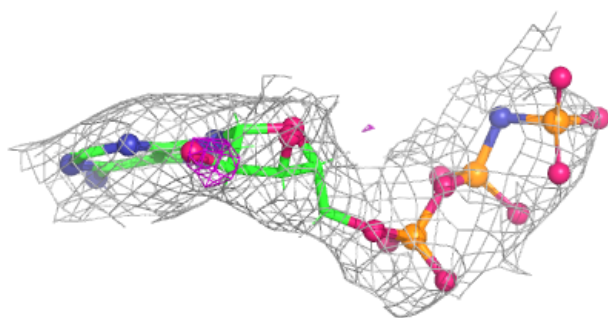
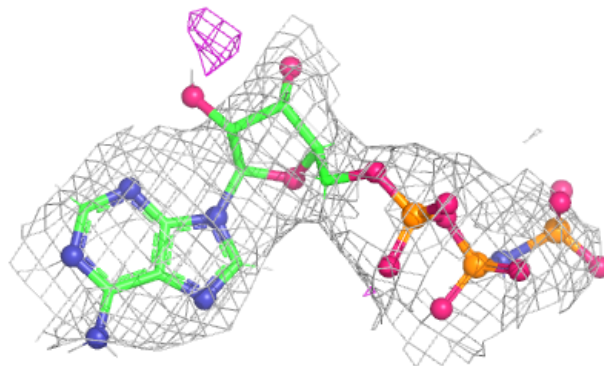
**Electron density around ANP A 5003:**

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

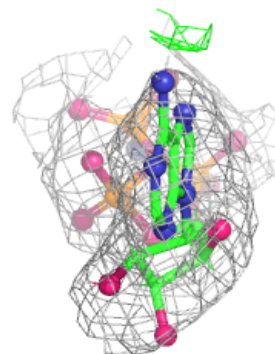
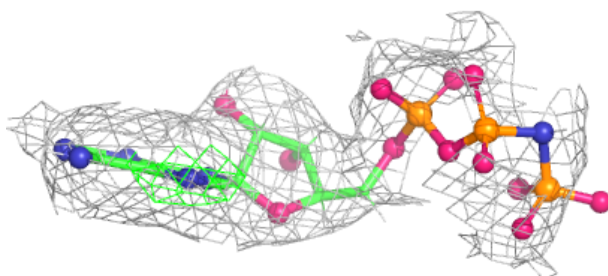
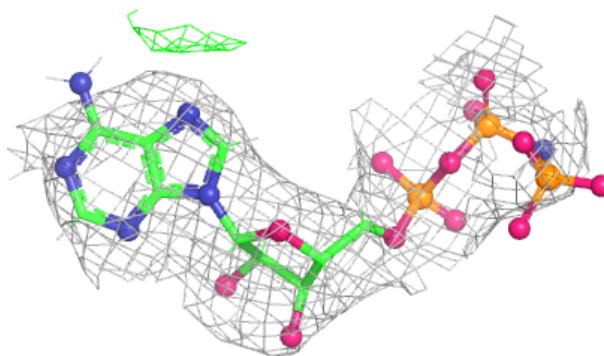


Electron density around ANP B 5004:

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

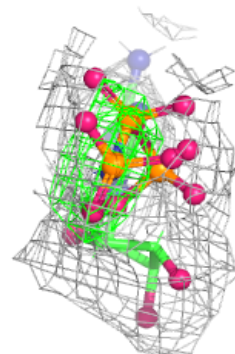
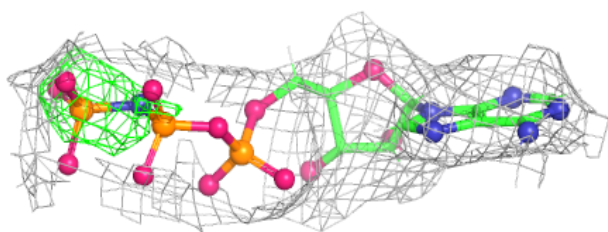
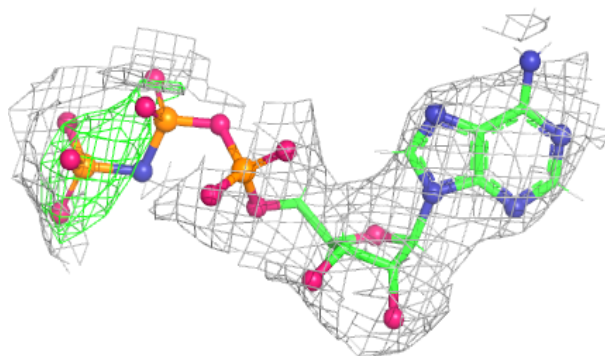
**Electron density around ANP A 5001:**

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

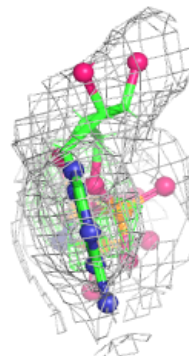
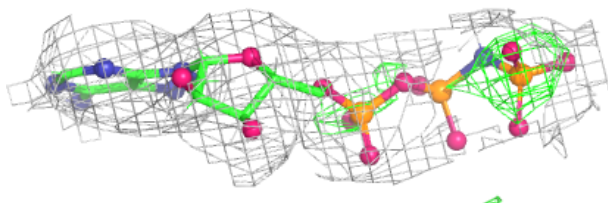
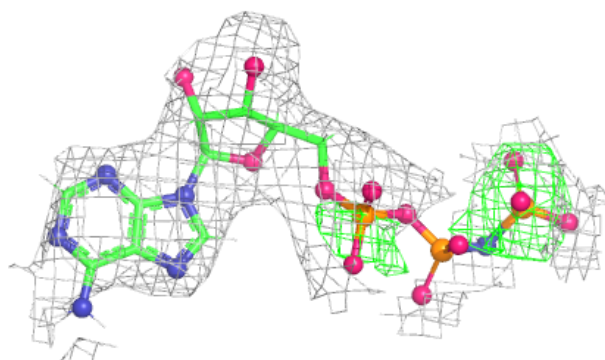


Electron density around ANP A 5002:

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

**Electron density around ANP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.