



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:35 PM UTC

PDB ID : 2C39 / pdb_00002c39
Title : RNase PH core of the archaeal exosome in complex with ADP
Authors : Lorentzen, E.; Conti, E.
Deposited on : 2005-10-05
Resolution : 3.30 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

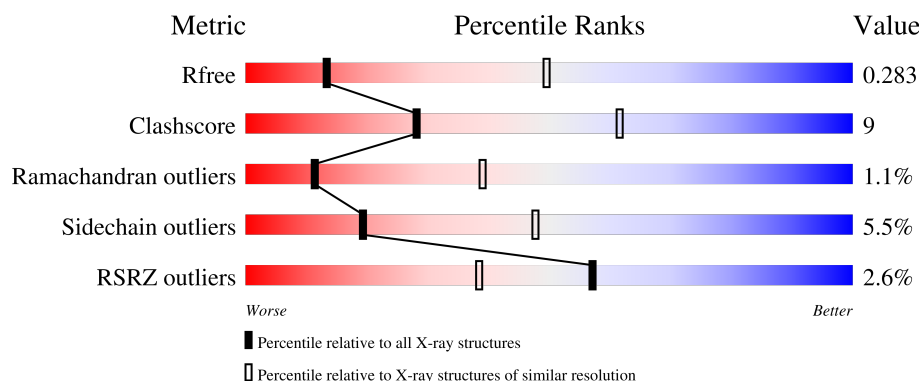
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	275	2% 81% 12% • 5%
1	C	275	% 74% 19% • 5%
1	E	275	75% 18% • 5%
1	G	275	3% 78% 15% • 5%
1	I	275	% 77% 16% • 5%

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Mol	Chain	Length	Quality of chain
1	K	275	
1	M	275	
1	O	275	
1	Q	275	
1	S	275	
1	U	275	
1	W	275	
2	B	248	
2	D	248	
2	F	248	
2	H	248	
2	J	248	
2	L	248	
2	N	248	
2	P	248	
2	R	248	
2	T	248	
2	V	248	
2	X	248	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 45814 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROBABLE EXOSOME COMPLEX EXONUCLEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1944	1239	320	380	5			
1	C	260	Total	C	N	O	S	0	0	0
			1947	1243	321	378	5			
1	E	260	Total	C	N	O	S	0	0	0
			1968	1253	325	385	5			
1	G	260	Total	C	N	O	S	0	0	0
			1961	1250	323	383	5			
1	I	260	Total	C	N	O	S	0	0	0
			1954	1247	323	379	5			
1	K	260	Total	C	N	O	S	0	0	0
			1958	1249	323	381	5			
1	M	260	Total	C	N	O	S	0	0	0
			1960	1249	324	382	5			
1	O	260	Total	C	N	O	S	0	0	0
			1951	1246	323	377	5			
1	Q	260	Total	C	N	O	S	0	0	0
			1953	1245	322	381	5			
1	S	259	Total	C	N	O	S	0	0	0
			1955	1245	323	382	5			
1	U	255	Total	C	N	O	S	0	0	0
			1908	1219	317	367	5			
1	W	259	Total	C	N	O	S	0	0	0
			1950	1245	322	378	5			

- Molecule 2 is a protein called PROBABLE EXOSOME COMPLEX EXONUCLEASE 1.

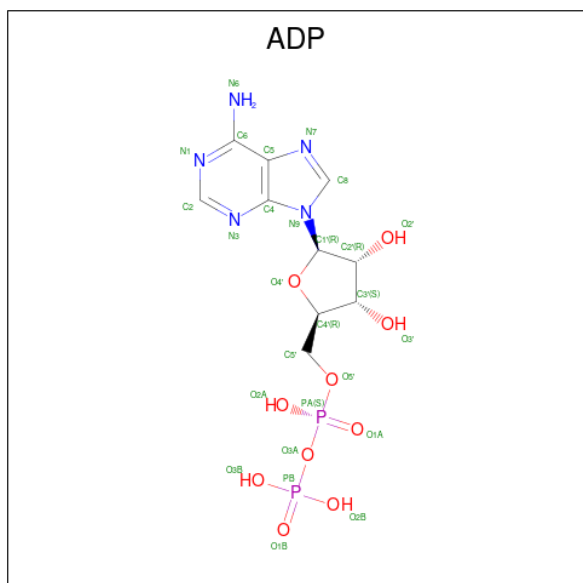
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1812	1145	317	340	10			
2	D	248	Total	C	N	O	S	0	0	0
			1900	1198	330	360	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	241	Total	C	N	O	S	0	0	0
			1838	1161	317	350	10			
2	H	230	Total	C	N	O	S	0	0	0
			1732	1094	302	327	9			
2	J	241	Total	C	N	O	S	0	0	0
			1844	1165	321	348	10			
2	L	247	Total	C	N	O	S	0	0	0
			1890	1194	328	357	11			
2	N	239	Total	C	N	O	S	0	0	0
			1809	1144	313	342	10			
2	P	248	Total	C	N	O	S	0	0	0
			1904	1202	332	358	12			
2	R	248	Total	C	N	O	S	0	0	0
			1880	1188	332	348	12			
2	T	248	Total	C	N	O	S	0	0	0
			1884	1193	328	351	12			
2	V	239	Total	C	N	O	S	0	0	0
			1815	1148	318	339	10			
2	X	239	Total	C	N	O	S	0	0	0
			1821	1148	315	348	10			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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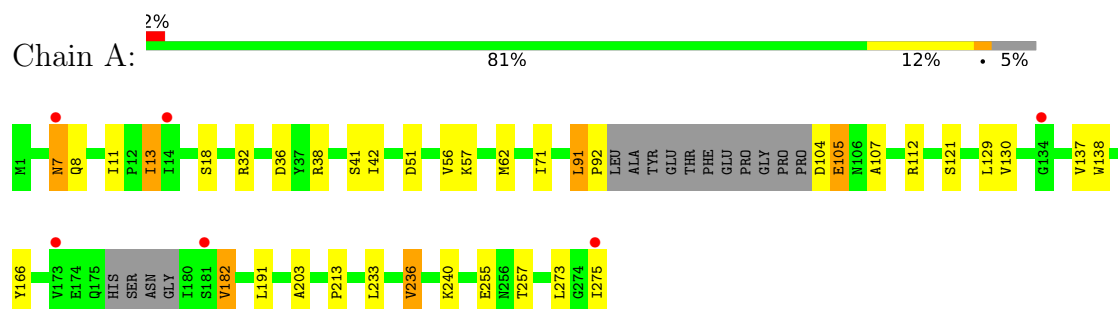
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	O	P		0	0
			17	5	10	2			
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	O	P			0	0
			9	7	2				
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	R	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	T	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	V	1	Total	C	O	P		0	0
			17	5	10	2			
3	X	1	Total	C	O	P		0	0
			17	5	10	2			

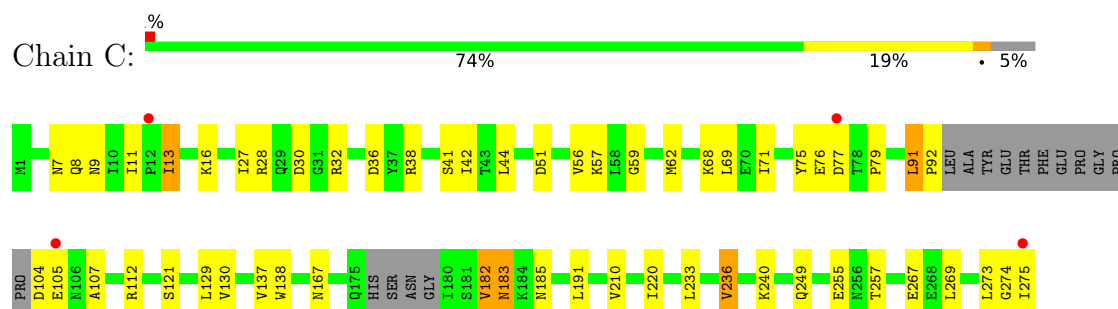
3 Residue-property plots [i](#)

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.

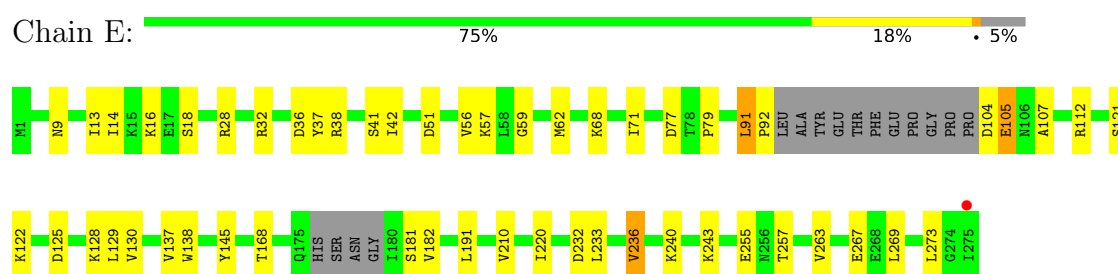
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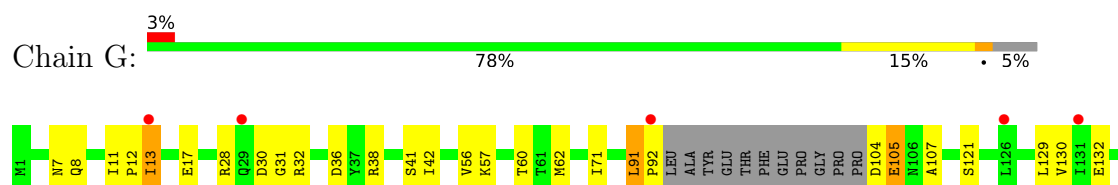
• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



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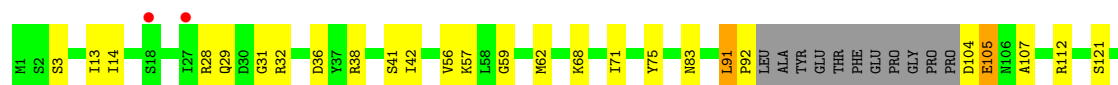
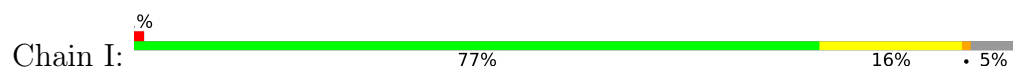


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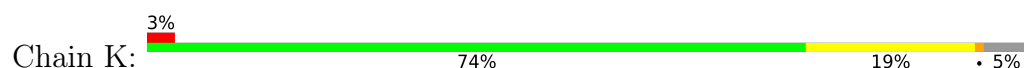




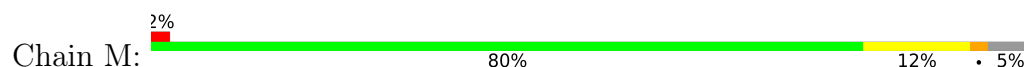
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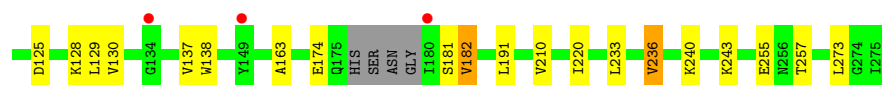
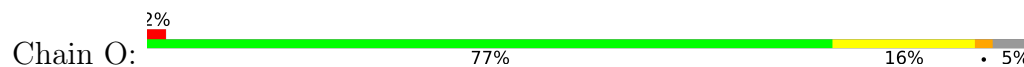
• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



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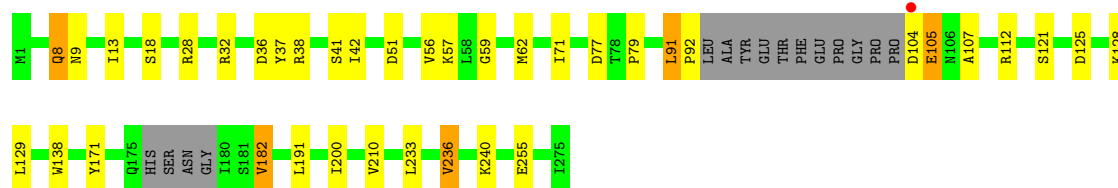


• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



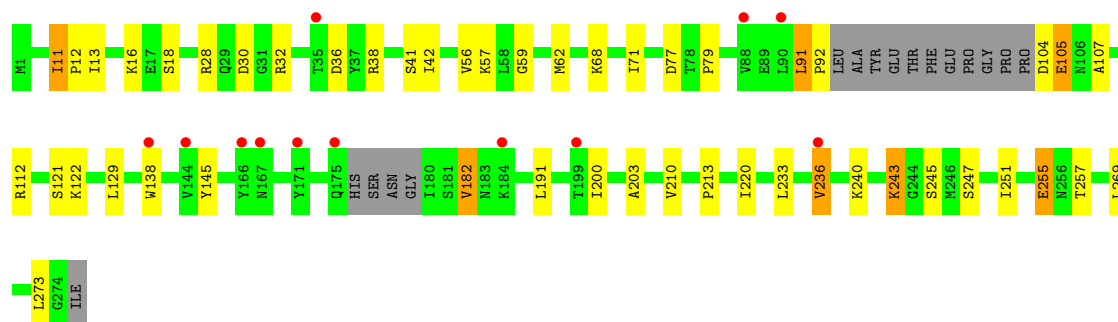
- Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

Chain Q: 



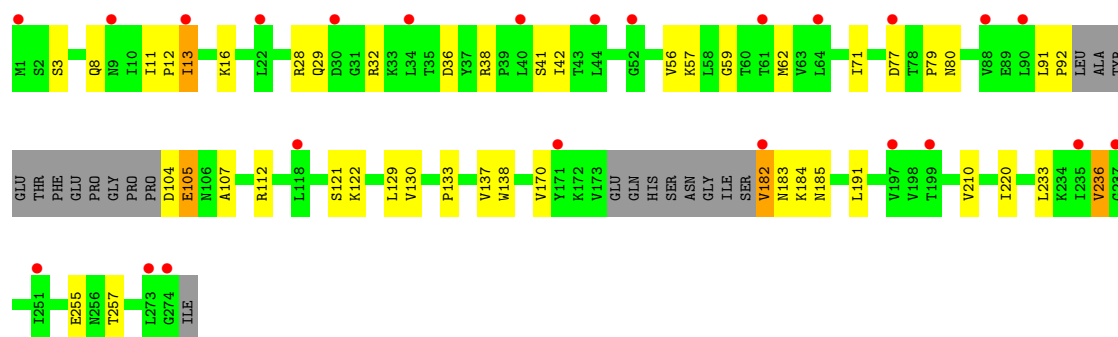
- Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

Chain S: 



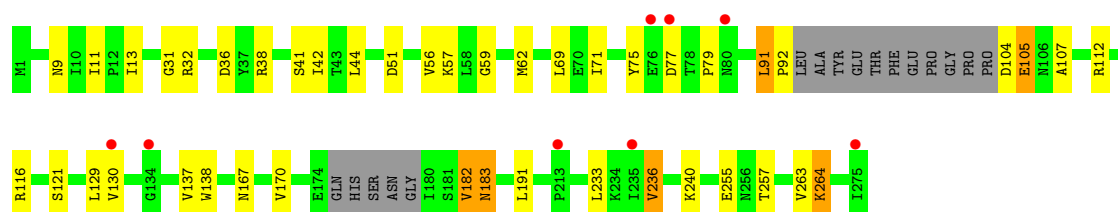
- Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

Chain U: 



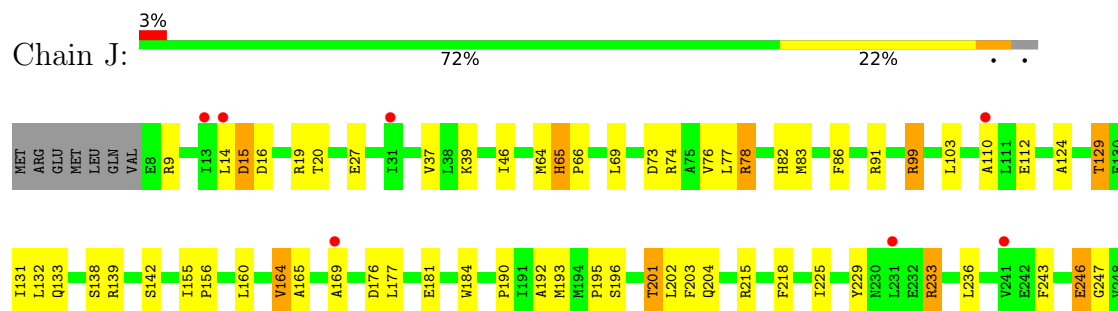
- Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

Chain W: 

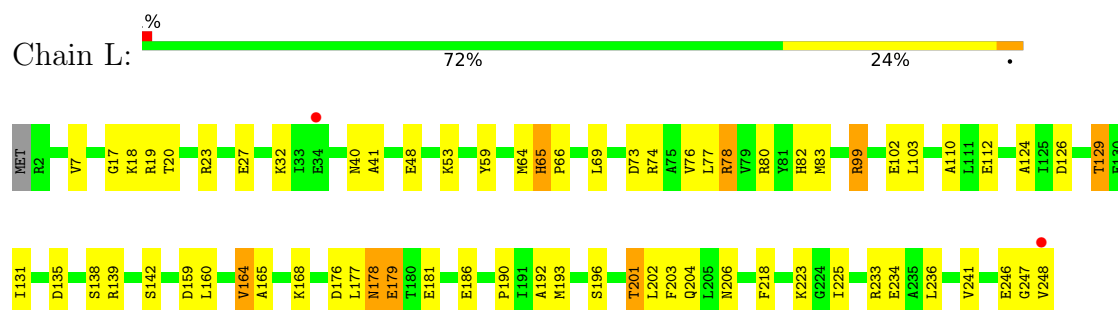


- Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

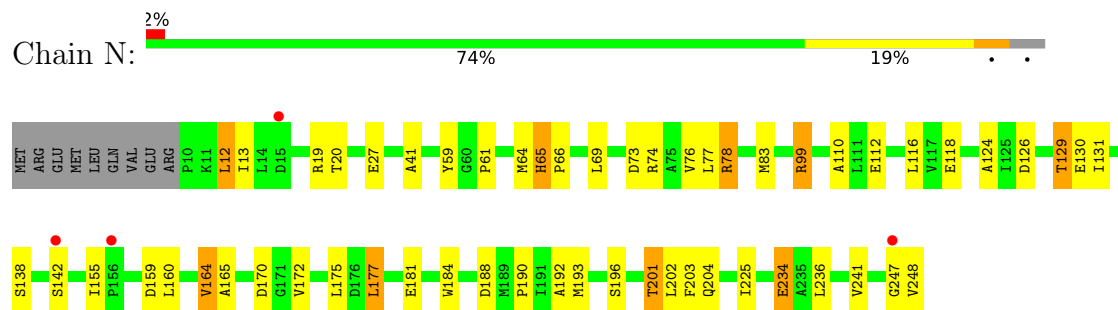
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1



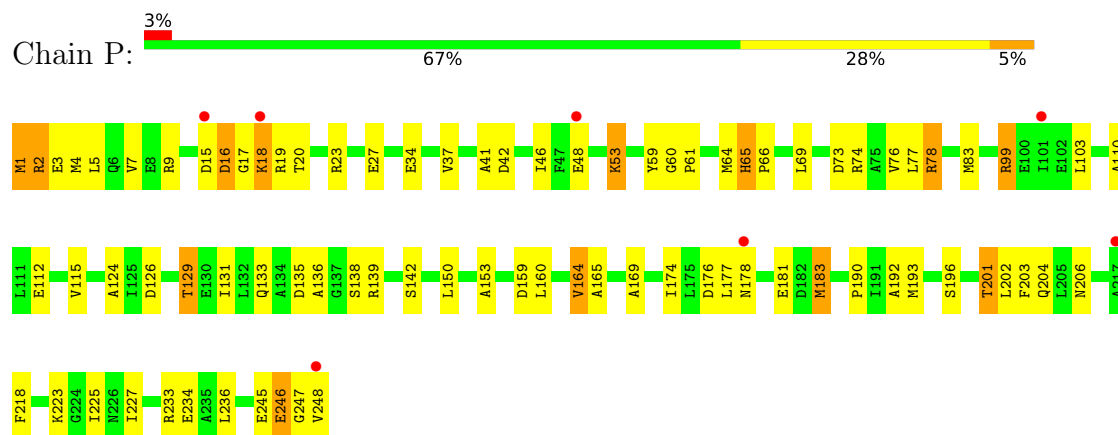
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1



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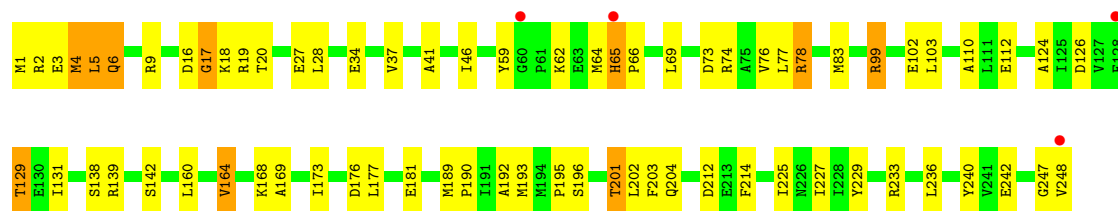


• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

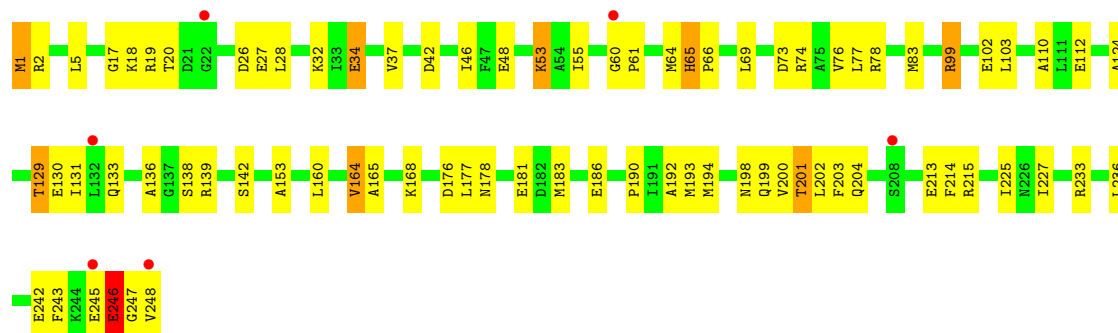


• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

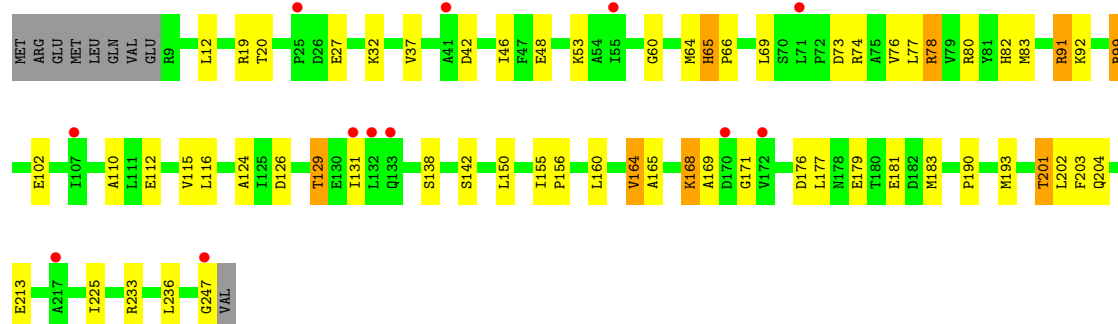




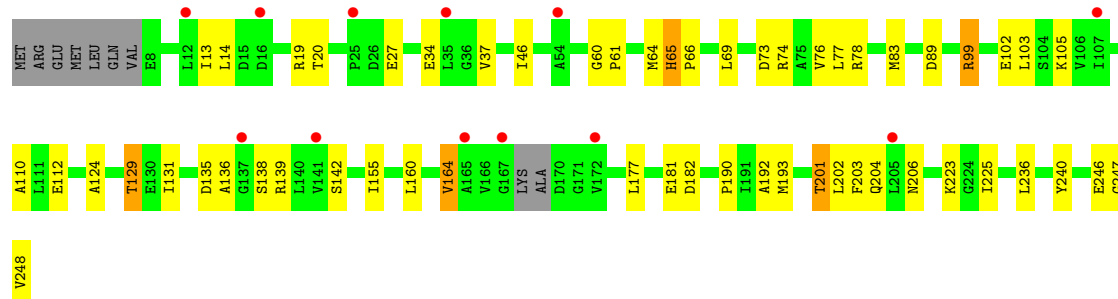
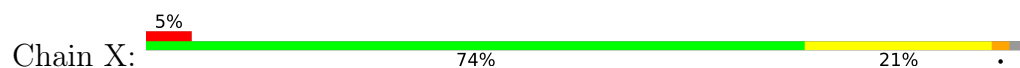
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1



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• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	206.20Å 214.00Å 432.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.25 – 3.30 93.25 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (93.25-3.30) 93.5 (93.25-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.274 , 0.295 0.265 , 0.283	Depositor DCC
R_{free} test set	4015 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.048 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	45814	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/1969	0.86	2/2678 (0.1%)
1	C	0.66	0/1972	0.87	2/2680 (0.1%)
1	E	0.59	0/1993	0.87	2/2706 (0.1%)
1	G	0.60	0/1986	0.86	2/2697 (0.1%)
1	I	0.57	0/1979	0.85	1/2688 (0.0%)
1	K	0.66	0/1983	0.87	0/2693
1	M	0.59	0/1985	0.84	3/2696 (0.1%)
1	O	0.67	0/1976	0.88	2/2684 (0.1%)
1	Q	0.61	0/1978	0.84	0/2688
1	S	0.60	0/1980	0.84	2/2690 (0.1%)
1	U	0.60	0/1933	0.86	0/2628
1	W	0.59	0/1975	0.85	2/2682 (0.1%)
2	B	0.57	0/1840	0.88	0/2494
2	D	0.64	0/1928	0.94	2/2606 (0.1%)
2	F	0.60	0/1866	0.89	0/2524
2	H	0.59	0/1757	0.88	0/2377
2	J	0.57	0/1872	0.85	0/2530
2	L	0.64	0/1918	0.94	2/2592 (0.1%)
2	N	0.59	0/1837	0.89	0/2487
2	P	0.64	0/1932	0.93	2/2609 (0.1%)
2	R	0.64	0/1908	0.94	5/2578 (0.2%)
2	T	0.62	0/1912	0.90	5/2584 (0.2%)
2	V	0.64	0/1843	0.88	0/2494
2	X	0.60	0/1848	0.89	0/2501
All	All	0.61	0/46170	0.88	34/62586 (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
2	D	0	2
2	L	0	1
2	P	0	1
2	R	0	2
2	T	0	1
All	All	0	7

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	9	ARG	CA-C-N	9.14	129.19	119.78
2	R	9	ARG	C-N-CA	9.14	129.19	119.78
2	D	18	LYS	N-CA-C	8.12	121.01	110.53
2	L	246	GLU	N-CA-C	7.08	117.94	108.38
2	D	246	GLU	N-CA-C	6.85	117.54	107.88
2	L	18	LYS	N-CA-C	6.81	120.59	110.52
2	R	6	GLN	N-CA-C	6.48	120.40	110.36
1	G	132	GLU	CA-C-N	6.35	127.78	119.84
1	G	132	GLU	C-N-CA	6.35	127.78	119.84
2	T	18	LYS	N-CA-C	5.99	118.63	110.55
2	R	4	MET	N-CA-C	-5.75	94.91	111.00
1	M	11	ILE	CA-C-N	5.73	125.73	119.89
1	M	11	ILE	C-N-CA	5.73	125.73	119.89
2	R	18	LYS	N-CA-C	5.71	118.87	110.59
1	E	181	SER	N-CA-C	5.54	115.43	108.45
1	O	11	ILE	CA-C-N	5.52	125.52	119.89
1	O	11	ILE	C-N-CA	5.52	125.52	119.89
2	P	246	GLU	N-CA-C	5.46	116.44	108.14
1	C	11	ILE	CA-C-N	5.44	125.44	119.89
1	C	11	ILE	C-N-CA	5.44	125.44	119.89
2	P	18	LYS	N-CA-C	5.39	117.83	110.55
1	A	11	ILE	CA-C-N	5.37	125.37	119.89
1	A	11	ILE	C-N-CA	5.37	125.37	119.89
1	E	9	ASN	N-CA-C	5.33	117.43	108.96
2	T	178	ASN	N-CA-C	-5.28	103.06	110.35
1	I	29	GLN	N-CA-C	5.10	116.65	111.14
2	T	194	MET	CA-C-N	5.09	124.70	119.05
2	T	194	MET	C-N-CA	5.09	124.70	119.05
1	W	11	ILE	CA-C-N	5.08	125.07	119.89
1	W	11	ILE	C-N-CA	5.08	125.07	119.89
1	M	181	SER	N-CA-C	5.06	117.57	110.14
2	T	246	GLU	N-CA-C	5.04	116.85	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	11	ILE	CA-C-N	5.03	125.02	119.89
1	S	11	ILE	C-N-CA	5.03	125.02	119.89

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	1	MET	Peptide
2	D	17	GLY	Peptide
2	L	17	GLY	Peptide
2	P	17	GLY	Peptide
2	R	17	GLY	Peptide
2	R	5	LEU	Peptide
2	T	17	GLY	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	1944	0	1969	21	0
1	C	1947	0	1982	30	0
1	E	1968	0	2013	35	0
1	G	1961	0	2003	34	0
1	I	1954	0	1997	33	0
1	K	1958	0	2001	37	0
1	M	1960	0	2003	20	0
1	O	1951	0	1995	26	0
1	Q	1953	0	1988	23	0
1	S	1955	0	1996	30	0
1	U	1908	0	1950	26	0
1	W	1950	0	1997	26	0
2	B	1812	0	1810	43	0
2	D	1900	0	1920	52	0
2	F	1838	0	1852	49	0
2	H	1732	0	1740	51	0
2	J	1844	0	1870	49	0
2	L	1890	0	1915	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1809	0	1817	43	0
2	P	1904	0	1938	51	0
2	R	1880	0	1904	44	0
2	T	1884	0	1913	52	0
2	V	1815	0	1836	42	0
2	X	1821	0	1820	36	0
3	B	27	0	12	4	0
3	D	27	0	12	4	0
3	F	17	0	7	1	0
3	H	27	0	12	2	0
3	J	9	0	0	1	0
3	L	27	0	12	3	0
3	N	27	0	12	3	0
3	P	27	0	12	3	0
3	R	27	0	12	1	0
3	T	27	0	12	3	0
3	V	17	0	7	2	0
3	X	17	0	7	1	0
All	All	45814	0	46346	823	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 (823) 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)
2:R:99:ARG:NH1	3:R:404:ADP:O2A	1.85	1.09
2:T:1:MET:H2	2:T:2:ARG:HA	1.24	1.00
2:T:1:MET:N	2:T:2:ARG:HA	1.75	1.00
1:E:243:LYS:HG2	2:F:112:GLU:OE1	1.61	0.98
2:D:99:ARG:NH1	3:D:404:ADP:O2A	2.03	0.91
1:G:249:GLN:H	1:G:249:GLN:HE21	1.18	0.90
2:P:99:ARG:NH1	3:P:404:ADP:O2A	2.07	0.87
2:L:78:ARG:HD3	2:L:126:ASP:OD1	1.75	0.86
2:H:227:ILE:HD12	2:H:248:VAL:HG13	1.59	0.83
2:V:99:ARG:NH1	3:V:404:ADP:O2A	2.12	0.81
2:T:99:ARG:NH1	3:T:404:ADP:O2A	2.13	0.81
1:G:249:GLN:HE21	1:G:249:GLN:N	1.77	0.81
2:J:64:MET:HE2	2:J:124:ALA:HB2	1.66	0.78
2:F:99:ARG:NH1	3:F:404:ADP:O2A	2.16	0.77
2:L:64:MET:HE2	2:L:124:ALA:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:53:LYS:HG3	2:T:133:GLN:HB2	1.67	0.76
2:D:64:MET:HE2	2:D:124:ALA:HB2	1.67	0.76
2:H:48:GLU:HG2	2:H:53:LYS:HG2	1.67	0.75
2:L:99:ARG:NH1	3:L:404:ADP:O2A	2.19	0.75
2:N:77:LEU:HD12	2:N:112:GLU:HG3	1.69	0.74
2:N:99:ARG:HH12	3:N:404:ADP:PA	2.09	0.74
2:R:78:ARG:HD3	2:R:126:ASP:OD1	1.88	0.74
2:X:64:MET:HE2	2:X:124:ALA:HB2	1.70	0.73
2:R:64:MET:HE2	2:R:124:ALA:HB2	1.70	0.73
2:V:64:MET:HE2	2:V:124:ALA:HB2	1.71	0.73
2:H:64:MET:HE2	2:H:124:ALA:HB2	1.70	0.72
2:P:53:LYS:HG3	2:P:133:GLN:HB2	1.69	0.72
2:B:64:MET:HE2	2:B:124:ALA:HB2	1.70	0.72
2:T:243:PHE:HZ	2:T:246:GLU:HG2	1.54	0.72
2:F:64:MET:HE2	2:F:124:ALA:HB2	1.72	0.72
2:L:77:LEU:HD12	2:L:112:GLU:HG3	1.72	0.72
2:H:99:ARG:NH1	3:H:404:ADP:O2A	2.22	0.72
2:J:99:ARG:HH12	3:J:404:ADP:PB	2.11	0.72
2:T:64:MET:HE2	2:T:124:ALA:HB2	1.72	0.72
2:P:64:MET:HE2	2:P:124:ALA:HB2	1.71	0.71
2:B:175:LEU:HD22	2:B:248:VAL:HG21	1.72	0.71
1:W:51:ASP:OD2	1:W:69:LEU:HB2	1.92	0.70
2:F:77:LEU:HD12	2:F:112:GLU:HG3	1.73	0.70
2:X:223:LYS:HB3	2:X:248:VAL:HG11	1.72	0.70
2:F:129:THR:HG21	2:F:142:SER:OG	1.90	0.70
2:R:77:LEU:HD12	2:R:112:GLU:HG3	1.73	0.70
2:H:78:ARG:HD3	2:H:126:ASP:OD1	1.92	0.70
2:L:48:GLU:HG2	2:L:53:LYS:HG2	1.72	0.70
2:T:66:PRO:HG2	2:T:69:LEU:HD12	1.74	0.69
2:N:99:ARG:NH1	3:N:404:ADP:O2A	2.25	0.69
2:F:48:GLU:OE1	2:F:53:LYS:HE2	1.92	0.69
2:D:77:LEU:HD12	2:D:112:GLU:HG3	1.73	0.69
2:T:77:LEU:HD12	2:T:112:GLU:HG3	1.74	0.69
1:G:243:LYS:HG2	2:H:112:GLU:OE1	1.92	0.69
2:B:66:PRO:HG2	2:B:69:LEU:HD12	1.75	0.69
2:D:65:HIS:CB	2:D:66:PRO:HD3	2.22	0.68
2:X:129:THR:HG21	2:X:142:SER:OG	1.93	0.68
2:J:77:LEU:HD12	2:J:112:GLU:HG3	1.75	0.68
2:B:34:GLU:HB3	2:B:240:TYR:HD1	1.59	0.68
2:T:1:MET:N	2:T:2:ARG:CA	2.56	0.68
1:K:42:ILE:HG12	1:K:56:VAL:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:64:MET:HE2	2:N:124:ALA:HB2	1.74	0.68
2:B:77:LEU:HD12	2:B:112:GLU:HG3	1.77	0.67
2:N:12:LEU:HD21	2:N:184:TRP:HB2	1.75	0.67
2:J:243:PHE:HZ	2:J:246:GLU:HG2	1.60	0.67
2:V:77:LEU:HD12	2:V:112:GLU:HG3	1.75	0.67
2:X:66:PRO:HG2	2:X:69:LEU:HD12	1.77	0.67
2:L:65:HIS:CB	2:L:66:PRO:HD3	2.23	0.67
1:I:112:ARG:NH2	2:J:99:ARG:HB2	2.10	0.67
2:V:65:HIS:CB	2:V:66:PRO:HD3	2.24	0.67
2:N:66:PRO:HG2	2:N:69:LEU:HD12	1.77	0.67
2:H:34:GLU:HB3	2:H:240:TYR:HD1	1.58	0.66
1:M:42:ILE:HG12	1:M:56:VAL:HG22	1.76	0.66
2:N:129:THR:HG21	2:N:142:SER:OG	1.95	0.66
1:G:42:ILE:HG12	1:G:56:VAL:HG22	1.78	0.66
2:P:65:HIS:CB	2:P:66:PRO:HD3	2.25	0.66
1:U:41:SER:HB2	1:U:57:LYS:HB2	1.78	0.66
2:B:136:ALA:HA	3:B:404:ADP:O3'	1.95	0.66
1:E:243:LYS:CE	2:F:108:ARG:HH21	2.08	0.66
2:L:66:PRO:HG2	2:L:69:LEU:HD12	1.76	0.66
2:F:65:HIS:CB	2:F:66:PRO:HD3	2.25	0.66
2:H:227:ILE:HD13	2:H:248:VAL:HG22	1.78	0.66
2:V:168:LYS:HD2	2:V:213:GLU:OE1	1.96	0.66
1:K:112:ARG:NH2	2:L:99:ARG:HB2	2.10	0.65
2:P:77:LEU:HD12	2:P:112:GLU:HG3	1.78	0.65
2:B:99:ARG:HH12	3:B:404:ADP:PA	2.20	0.65
2:R:66:PRO:HG2	2:R:69:LEU:HD12	1.79	0.65
2:X:77:LEU:HD12	2:X:112:GLU:HG3	1.79	0.65
2:B:78:ARG:HD3	2:B:126:ASP:OD1	1.96	0.65
2:H:66:PRO:HG2	2:H:69:LEU:HD12	1.79	0.65
2:N:65:HIS:CB	2:N:66:PRO:HD3	2.27	0.65
2:J:65:HIS:CB	2:J:66:PRO:HD3	2.26	0.65
1:Q:42:ILE:HG12	1:Q:56:VAL:HG22	1.79	0.65
1:Q:51:ASP:OD1	1:Q:171:TYR:HE1	1.79	0.65
2:H:65:HIS:CB	2:H:66:PRO:HD3	2.26	0.65
2:H:129:THR:HG21	2:H:142:SER:OG	1.97	0.64
2:B:65:HIS:CB	2:B:66:PRO:HD3	2.26	0.64
2:X:65:HIS:CB	2:X:66:PRO:HD3	2.27	0.64
2:J:66:PRO:HG2	2:J:69:LEU:HD12	1.79	0.64
2:H:77:LEU:HD12	2:H:112:GLU:HG3	1.78	0.64
2:B:164:VAL:HG22	2:B:225:ILE:HG13	1.80	0.64
2:L:19:ARG:HD2	2:L:181:GLU:OE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:164:VAL:HG22	2:R:225:ILE:HG13	1.80	0.64
2:T:65:HIS:CB	2:T:66:PRO:HD3	2.28	0.64
2:P:66:PRO:HG2	2:P:69:LEU:HD12	1.79	0.63
2:V:78:ARG:HD3	2:V:126:ASP:OD1	1.99	0.63
2:V:129:THR:HG21	2:V:142:SER:OG	1.97	0.63
2:F:164:VAL:HG22	2:F:225:ILE:HG13	1.80	0.63
2:V:66:PRO:HG2	2:V:69:LEU:HD12	1.79	0.63
3:P:404:ADP:O2A	3:P:404:ADP:O2B	2.16	0.63
2:T:1:MET:HG3	2:T:1:MET:O	1.98	0.63
2:F:66:PRO:HG2	2:F:69:LEU:HD12	1.81	0.63
1:S:240:LYS:HB2	2:T:203:PHE:HB3	1.81	0.63
2:D:66:PRO:HG2	2:D:69:LEU:HD12	1.81	0.63
2:H:164:VAL:HG22	2:H:225:ILE:HG13	1.80	0.62
1:G:91:LEU:HD22	2:L:80:ARG:HH12	1.65	0.62
2:R:65:HIS:CB	2:R:66:PRO:HD3	2.29	0.62
2:B:129:THR:HG21	2:B:142:SER:OG	2.00	0.62
1:W:42:ILE:HG12	1:W:56:VAL:HG22	1.82	0.62
2:R:227:ILE:HD12	2:R:248:VAL:HG13	1.82	0.62
2:F:48:GLU:HG2	2:F:53:LYS:HG2	1.81	0.61
2:N:175:LEU:CD2	2:N:248:VAL:HG21	2.30	0.61
1:S:41:SER:HB2	1:S:57:LYS:HB2	1.81	0.61
2:J:164:VAL:HG22	2:J:225:ILE:HG13	1.82	0.61
2:L:129:THR:HG21	2:L:142:SER:OG	2.00	0.61
2:T:129:THR:HG21	2:T:142:SER:OG	2.01	0.61
2:T:164:VAL:HG22	2:T:225:ILE:HG13	1.82	0.61
2:X:34:GLU:HB3	2:X:240:TYR:HD1	1.65	0.61
2:X:73:ASP:OD2	2:X:74:ARG:HG3	2.00	0.61
1:O:41:SER:HB2	1:O:57:LYS:HB2	1.83	0.61
1:K:41:SER:HB2	1:K:57:LYS:HB2	1.83	0.61
1:M:41:SER:HB2	1:M:57:LYS:HB2	1.82	0.61
2:J:129:THR:HG21	2:J:142:SER:OG	2.01	0.61
2:B:9:ARG:NH2	2:B:184:TRP:O	2.34	0.60
2:B:138:SER:OG	3:B:404:ADP:O2B	2.18	0.60
1:S:42:ILE:HG12	1:S:56:VAL:HG22	1.82	0.60
2:V:179:GLU:O	2:V:183:MET:HB2	2.01	0.60
2:D:83:MET:HE2	2:D:99:ARG:HH21	1.66	0.60
1:A:42:ILE:HG12	1:A:56:VAL:HG22	1.83	0.60
1:C:41:SER:HB2	1:C:57:LYS:HB2	1.83	0.60
2:P:1:MET:HG3	2:P:3:GLU:H	1.67	0.60
1:W:116:ARG:HD3	2:X:206:ASN:HB3	1.83	0.60
1:Q:71:ILE:HD12	1:Q:182:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ILE:HD12	1:E:182:VAL:HG22	1.83	0.60
1:K:6:SER:C	1:K:8:GLN:H	2.10	0.60
2:P:164:VAL:HG22	2:P:225:ILE:HG13	1.84	0.60
1:K:51:ASP:OD2	1:K:69:LEU:HB2	2.02	0.60
1:U:42:ILE:HG12	1:U:56:VAL:HG22	1.84	0.60
2:N:177:LEU:HD12	2:N:188:ASP:OD1	2.01	0.60
2:T:55:ILE:HG22	2:T:130:GLU:HB2	1.82	0.60
2:H:83:MET:HE2	2:H:99:ARG:HH21	1.67	0.59
2:L:83:MET:HE2	2:L:99:ARG:HH21	1.66	0.59
1:Q:41:SER:HB2	1:Q:57:LYS:HB2	1.82	0.59
1:G:148:ASP:OD1	2:L:40:ASN:HB2	2.02	0.59
1:U:112:ARG:NH2	2:V:99:ARG:HB2	2.17	0.59
1:I:42:ILE:HG12	1:I:56:VAL:HG22	1.84	0.59
2:V:164:VAL:HG22	2:V:225:ILE:HG13	1.84	0.59
1:M:71:ILE:HD12	1:M:182:VAL:HG22	1.85	0.59
1:W:41:SER:HB2	1:W:57:LYS:HB2	1.84	0.59
2:X:164:VAL:HG22	2:X:225:ILE:HG13	1.83	0.59
2:J:82:HIS:HE1	1:K:145:TYR:OH	1.86	0.59
1:O:42:ILE:HG12	1:O:56:VAL:HG22	1.85	0.59
1:C:42:ILE:HG12	1:C:56:VAL:HG22	1.85	0.59
1:I:14:ILE:HG22	2:V:116:LEU:HD22	1.85	0.59
2:L:164:VAL:HG22	2:L:225:ILE:HG13	1.85	0.59
2:N:130:GLU:HG3	1:Q:91:LEU:HD13	1.84	0.59
1:S:71:ILE:HD12	1:S:182:VAL:HG22	1.84	0.59
1:I:248:LEU:HD23	2:J:218:PHE:CZ	2.38	0.58
1:E:41:SER:HB2	1:E:57:LYS:HB2	1.86	0.58
2:N:164:VAL:HG22	2:N:225:ILE:HG13	1.83	0.58
1:G:41:SER:HB2	1:G:57:LYS:HB2	1.84	0.58
2:L:73:ASP:OD2	2:L:74:ARG:HG3	2.04	0.58
2:N:110:ALA:HB1	2:N:201:THR:CG2	2.34	0.58
2:L:234:GLU:HG3	2:L:241:VAL:CG2	2.33	0.58
2:B:180:THR:HA	2:B:183:MET:HE2	1.86	0.58
1:C:71:ILE:HD12	1:C:182:VAL:HG22	1.86	0.57
2:D:129:THR:HG21	2:D:142:SER:OG	2.03	0.57
2:H:48:GLU:HG2	2:H:53:LYS:CG	2.35	0.57
2:P:110:ALA:HB1	2:P:201:THR:CG2	2.34	0.57
2:R:129:THR:HG21	2:R:142:SER:OG	2.04	0.57
2:T:26:ASP:O	2:T:248:VAL:HB	2.03	0.57
2:F:73:ASP:OD2	2:F:74:ARG:HG3	2.05	0.57
1:G:71:ILE:HD12	1:G:182:VAL:HG22	1.87	0.57
2:D:110:ALA:HB1	2:D:201:THR:CG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ILE:HG21	2:N:118:GLU:OE1	2.04	0.57
2:F:83:MET:HE2	2:F:99:ARG:HH21	1.69	0.57
2:N:129:THR:HG21	2:N:142:SER:HG	1.67	0.57
2:N:78:ARG:HD3	2:N:126:ASP:OD1	2.04	0.57
2:V:19:ARG:HD2	2:V:181:GLU:OE2	2.04	0.57
2:L:110:ALA:HB1	2:L:201:THR:CG2	2.34	0.57
2:H:89:ASP:OD2	2:H:89:ASP:N	2.27	0.56
2:T:19:ARG:HD2	2:T:181:GLU:OE2	2.04	0.56
1:A:71:ILE:HD12	1:A:182:VAL:HG22	1.87	0.56
1:E:42:ILE:HG12	1:E:56:VAL:HG22	1.86	0.56
2:R:73:ASP:OD2	2:R:74:ARG:HG3	2.06	0.56
2:R:110:ALA:HB1	2:R:201:THR:CG2	2.35	0.56
2:T:110:ALA:HB1	2:T:201:THR:CG2	2.35	0.56
1:W:71:ILE:HD12	1:W:182:VAL:HG22	1.88	0.56
2:X:110:ALA:HB1	2:X:201:THR:CG2	2.36	0.56
2:P:19:ARG:HD2	2:P:181:GLU:OE2	2.05	0.56
1:A:32:ARG:HB2	1:A:36:ASP:HB2	1.87	0.56
1:I:31:GLY:HA2	2:V:233:ARG:NH1	2.20	0.56
2:P:83:MET:HE2	2:P:99:ARG:HH21	1.70	0.56
2:T:83:MET:HE2	2:T:99:ARG:HH21	1.69	0.56
2:D:164:VAL:HG22	2:D:225:ILE:HG13	1.87	0.56
1:K:57:LYS:HG2	1:K:62:MET:HG2	1.88	0.56
2:L:32:LYS:HB3	2:L:48:GLU:HB2	1.88	0.56
2:P:129:THR:HG21	2:P:142:SER:OG	2.06	0.56
1:S:255:GLU:OE2	2:T:215:ARG:NH2	2.39	0.56
2:F:110:ALA:HB1	2:F:201:THR:CG2	2.36	0.56
1:G:249:GLN:H	1:G:249:GLN:NE2	1.96	0.56
1:K:32:ARG:HB2	1:K:36:ASP:HB2	1.88	0.56
2:L:168:LYS:HE2	2:L:186:GLU:HB2	1.88	0.56
2:P:203:PHE:HE1	2:P:218:PHE:CE1	2.24	0.56
2:X:83:MET:HE2	2:X:99:ARG:HH21	1.71	0.56
1:O:57:LYS:HG2	1:O:62:MET:HG2	1.87	0.55
2:D:19:ARG:HD2	2:D:181:GLU:OE2	2.06	0.55
2:F:233:ARG:CZ	1:W:31:GLY:HA2	2.35	0.55
2:T:55:ILE:CG2	2:T:130:GLU:HB2	2.35	0.55
1:C:32:ARG:HB2	1:C:36:ASP:HB2	1.87	0.55
2:F:243:PHE:CZ	2:F:246:GLU:HG2	2.42	0.55
2:J:133:GLN:NE2	1:K:48:LYS:HB2	2.22	0.55
1:I:41:SER:HB2	1:I:57:LYS:HB2	1.88	0.55
2:N:83:MET:HE2	2:N:99:ARG:HH21	1.70	0.55
2:H:73:ASP:OD2	2:H:74:ARG:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:227:ILE:CD1	2:H:248:VAL:HG13	2.35	0.55
1:I:71:ILE:HD12	1:I:182:VAL:HG22	1.89	0.55
2:R:83:MET:HE2	2:R:99:ARG:HH21	1.71	0.55
2:T:28:LEU:HG	2:T:248:VAL:HG21	1.89	0.55
2:H:135:ASP:O	2:H:136:ALA:HB3	2.07	0.55
2:V:83:MET:HE2	2:V:99:ARG:HH21	1.72	0.55
2:P:73:ASP:OD2	2:P:74:ARG:HG3	2.07	0.55
2:F:129:THR:HG21	2:F:142:SER:HG	1.70	0.54
2:H:88:THR:HG21	3:H:404:ADP:C2	2.43	0.54
2:J:86:PHE:HA	1:K:68:LYS:HD3	1.87	0.54
1:I:32:ARG:HB2	1:I:36:ASP:HB2	1.89	0.54
1:O:71:ILE:HD12	1:O:182:VAL:HG22	1.90	0.54
2:T:73:ASP:OD2	2:T:74:ARG:HG3	2.08	0.54
1:E:243:LYS:CE	2:F:108:ARG:NH2	2.70	0.54
1:K:71:ILE:HD12	1:K:182:VAL:HG22	1.89	0.54
1:U:32:ARG:HB2	1:U:36:ASP:HB2	1.89	0.54
1:C:183:ASN:C	1:C:183:ASN:ND2	2.65	0.54
1:E:51:ASP:O	1:E:168:THR:HA	2.07	0.54
2:H:110:ALA:HB1	2:H:201:THR:CG2	2.37	0.54
1:E:121:SER:O	1:E:122:LYS:HB3	2.07	0.54
2:N:19:ARG:HD2	2:N:181:GLU:OE2	2.07	0.54
1:O:240:LYS:HB2	2:P:203:PHE:HB3	1.90	0.54
1:C:240:LYS:HB2	2:D:203:PHE:HB3	1.89	0.53
2:H:80:ARG:NH1	2:H:130:GLU:OE2	2.42	0.53
1:U:71:ILE:HD12	1:U:182:VAL:HG22	1.90	0.53
2:V:73:ASP:OD2	2:V:74:ARG:HG3	2.08	0.53
2:J:83:MET:HE2	2:J:99:ARG:HH21	1.74	0.53
2:T:243:PHE:CZ	2:T:246:GLU:HG2	2.41	0.53
2:H:227:ILE:CD1	2:H:248:VAL:HG22	2.38	0.53
1:O:32:ARG:HB2	1:O:36:ASP:HB2	1.91	0.53
2:T:34:GLU:HG3	2:T:46:ILE:HB	1.90	0.53
1:U:57:LYS:HG2	1:U:62:MET:HG2	1.91	0.53
2:P:48:GLU:HG2	2:P:53:LYS:HB3	1.91	0.53
2:B:110:ALA:HB1	2:B:201:THR:CG2	2.39	0.53
2:D:223:LYS:HB3	2:D:248:VAL:CG1	2.39	0.53
1:G:32:ARG:HB2	1:G:36:ASP:HB2	1.91	0.53
1:I:57:LYS:HG2	1:I:62:MET:HG2	1.91	0.53
1:E:32:ARG:HB2	1:E:36:ASP:HB2	1.90	0.53
2:P:159:ASP:OD2	2:P:196:SER:HB2	2.08	0.53
2:B:51:ASN:HB2	2:B:135:ASP:OD2	2.09	0.53
2:D:99:ARG:HH12	3:D:404:ADP:PA	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:ARG:NH1	2:D:233:ARG:HG3	2.24	0.53
2:R:212:ASP:OD1	2:R:212:ASP:N	2.39	0.53
2:X:223:LYS:HB3	2:X:248:VAL:CG1	2.38	0.53
1:E:243:LYS:HE3	2:F:108:ARG:HH21	1.73	0.52
1:M:32:ARG:HB2	1:M:36:ASP:HB2	1.90	0.52
1:G:91:LEU:H	1:G:92:PRO:CD	2.23	0.52
1:Q:57:LYS:HG2	1:Q:62:MET:HG2	1.90	0.52
2:T:42:ASP:O	2:T:153:ALA:HA	2.09	0.52
2:J:91:ARG:HB2	1:K:68:LYS:HG2	1.91	0.52
2:X:223:LYS:CB	2:X:248:VAL:HG11	2.38	0.52
1:E:125:ASP:HB3	1:E:128:LYS:HD2	1.91	0.52
2:H:131:ILE:HG12	2:H:138:SER:HB2	1.91	0.52
2:P:193:MET:HG3	2:P:225:ILE:HD13	1.92	0.52
2:F:78:ARG:HD3	2:F:126:ASP:OD1	2.10	0.52
2:H:192:ALA:HB3	2:H:202:LEU:HB3	1.92	0.52
1:W:32:ARG:HB2	1:W:36:ASP:HB2	1.91	0.52
2:H:129:THR:HG21	2:H:142:SER:HG	1.73	0.52
2:L:23:ARG:HH21	2:L:178:ASN:HD21	1.56	0.52
1:S:269:LEU:O	1:S:273:LEU:HG	2.10	0.52
1:C:112:ARG:NH1	2:D:102:GLU:OE1	2.42	0.52
2:D:73:ASP:OD2	2:D:74:ARG:HG3	2.10	0.52
2:L:193:MET:HG3	2:L:225:ILE:HD13	1.92	0.52
2:H:82:HIS:HE1	1:I:145:TYR:OH	1.92	0.52
1:E:112:ARG:NH2	2:F:99:ARG:HB2	2.25	0.52
2:L:131:ILE:HD11	2:L:142:SER:HB2	1.92	0.52
1:S:57:LYS:HG2	1:S:62:MET:HG2	1.92	0.51
1:W:183:ASN:C	1:W:183:ASN:ND2	2.66	0.51
2:B:193:MET:HG3	2:B:225:ILE:HD13	1.92	0.51
1:Q:32:ARG:HB2	1:Q:36:ASP:HB2	1.91	0.51
1:C:51:ASP:OD2	1:C:69:LEU:HB2	2.10	0.51
1:G:91:LEU:H	1:G:92:PRO:HD3	1.75	0.51
2:R:19:ARG:HD2	2:R:181:GLU:OE2	2.09	0.51
2:R:34:GLU:HB3	2:R:240:TYR:HD1	1.75	0.51
1:W:91:LEU:H	1:W:92:PRO:CD	2.23	0.51
1:A:57:LYS:HG2	1:A:62:MET:HG2	1.93	0.51
2:L:83:MET:HE2	2:L:99:ARG:NH2	2.25	0.51
1:S:32:ARG:HB2	1:S:36:ASP:HB2	1.91	0.51
2:X:131:ILE:HG12	2:X:138:SER:HB2	1.93	0.51
2:J:133:GLN:OE1	1:K:48:LYS:HG2	2.10	0.51
1:S:91:LEU:H	1:S:92:PRO:CD	2.24	0.51
2:D:28:LEU:O	2:D:245:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:MET:HE1	2:H:76:VAL:HB	1.92	0.51
1:E:263:VAL:O	1:E:267:GLU:HG3	2.11	0.51
2:P:42:ASP:O	2:P:153:ALA:HA	2.11	0.51
2:P:190:PRO:HG2	2:P:204:GLN:HB2	1.92	0.51
1:S:145:TYR:OH	2:V:82:HIS:HE1	1.92	0.51
2:X:135:ASP:O	2:X:136:ALA:HB3	2.11	0.51
2:B:19:ARG:HD2	2:B:181:GLU:OE2	2.11	0.51
1:E:91:LEU:H	1:E:92:PRO:CD	2.23	0.51
2:F:131:ILE:HG12	2:F:138:SER:HB2	1.94	0.50
2:T:136:ALA:N	3:T:404:ADP:O3'	2.36	0.50
1:Q:240:LYS:HB2	2:R:203:PHE:HB3	1.93	0.50
2:B:73:ASP:OD2	2:B:74:ARG:HG3	2.10	0.50
1:G:30:ASP:OD1	1:G:31:GLY:N	2.44	0.50
2:J:64:MET:HE1	2:J:76:VAL:HB	1.94	0.50
2:L:135:ASP:OD1	2:L:179:GLU:HB2	2.11	0.50
2:P:16:ASP:C	2:P:18:LYS:H	2.19	0.50
1:A:91:LEU:H	1:A:92:PRO:HD3	1.76	0.50
2:F:19:ARG:HD2	2:F:181:GLU:OE2	2.11	0.50
1:K:91:LEU:H	1:K:92:PRO:CD	2.25	0.50
2:R:168:LYS:HG3	2:R:173:ILE:HG13	1.92	0.50
1:C:91:LEU:H	1:C:92:PRO:HD3	1.76	0.50
2:T:27:GLU:HG2	2:T:247:GLY:HA2	1.94	0.50
2:T:227:ILE:HD12	2:T:248:VAL:HG13	1.94	0.50
1:C:91:LEU:H	1:C:92:PRO:CD	2.24	0.50
2:D:83:MET:HE2	2:D:99:ARG:NH2	2.26	0.50
2:J:110:ALA:HB1	2:J:201:THR:CG2	2.42	0.50
2:L:131:ILE:HG12	2:L:138:SER:HB2	1.92	0.50
2:P:131:ILE:HG12	2:P:138:SER:HB2	1.92	0.50
1:E:91:LEU:H	1:E:92:PRO:HD3	1.76	0.50
2:V:110:ALA:HB1	2:V:201:THR:CG2	2.41	0.50
2:V:131:ILE:HD11	2:V:142:SER:HB2	1.93	0.50
2:X:129:THR:HG21	2:X:142:SER:HG	1.76	0.50
1:A:41:SER:HB2	1:A:57:LYS:HB2	1.92	0.49
2:R:2:ARG:HG2	2:R:3:GLU:H	1.77	0.49
1:C:57:LYS:HG2	1:C:62:MET:HG2	1.93	0.49
1:E:243:LYS:HE2	2:F:108:ARG:HH21	1.74	0.49
2:T:213:GLU:O	2:T:214:PHE:C	2.54	0.49
1:E:57:LYS:HG2	1:E:62:MET:HG2	1.94	0.49
2:H:19:ARG:HD2	2:H:181:GLU:OE2	2.12	0.49
2:J:73:ASP:OD2	2:J:74:ARG:HG3	2.12	0.49
1:O:91:LEU:H	1:O:92:PRO:CD	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ARG:NH2	2:D:99:ARG:HB2	2.27	0.49
1:E:28:ARG:CZ	1:E:210:VAL:HG13	2.43	0.49
1:E:243:LYS:HE3	2:F:108:ARG:NH2	2.27	0.49
1:G:91:LEU:HD22	2:L:80:ARG:NH1	2.27	0.49
2:L:223:LYS:HB3	2:L:248:VAL:CG1	2.43	0.49
1:Q:91:LEU:H	1:Q:92:PRO:HD3	1.76	0.49
1:E:91:LEU:N	1:E:92:PRO:CD	2.76	0.49
2:P:192:ALA:HB3	2:P:202:LEU:HB3	1.95	0.49
2:J:27:GLU:HG2	2:J:247:GLY:HA2	1.95	0.49
2:P:1:MET:HG2	2:P:4:MET:HG3	1.95	0.49
1:C:68:LYS:HG2	2:F:91:ARG:HB2	1.94	0.49
2:D:131:ILE:HD11	2:D:142:SER:HB2	1.94	0.49
2:T:131:ILE:HG12	2:T:138:SER:HB2	1.94	0.49
2:V:27:GLU:HG2	2:V:247:GLY:HA2	1.95	0.49
1:A:91:LEU:H	1:A:92:PRO:CD	2.26	0.49
1:M:91:LEU:H	1:M:92:PRO:CD	2.25	0.49
2:P:15:ASP:C	2:P:16:ASP:O	2.55	0.49
1:Q:129:LEU:HB3	1:Q:138:TRP:HB2	1.95	0.49
1:A:104:ASP:HB3	1:A:107:ALA:HB3	1.95	0.49
2:D:131:ILE:HG12	2:D:138:SER:HB2	1.95	0.49
1:W:91:LEU:H	1:W:92:PRO:HD3	1.77	0.49
2:B:131:ILE:HG12	2:B:138:SER:HB2	1.95	0.49
1:E:38:ARG:HD2	1:E:59:GLY:HA3	1.95	0.49
1:E:104:ASP:CG	1:E:105:GLU:N	2.71	0.49
1:I:240:LYS:HB2	2:J:203:PHE:HB3	1.95	0.49
1:O:121:SER:HB3	1:O:236:VAL:HG11	1.94	0.49
2:P:183:MET:HE3	2:P:183:MET:HA	1.95	0.49
2:B:169:ALA:O	2:B:171:GLY:N	2.42	0.48
2:F:168:LYS:HE2	2:F:186:GLU:HB2	1.93	0.48
1:M:91:LEU:H	1:M:92:PRO:HD3	1.78	0.48
1:U:104:ASP:CG	1:U:105:GLU:N	2.71	0.48
1:W:57:LYS:HG2	1:W:62:MET:HG2	1.94	0.48
1:C:27:ILE:HD11	2:T:233:ARG:HH12	1.78	0.48
2:D:233:ARG:NH2	1:G:31:GLY:HA2	2.28	0.48
2:N:118:GLU:CD	2:N:118:GLU:H	2.20	0.48
1:G:91:LEU:N	1:G:92:PRO:CD	2.76	0.48
2:H:27:GLU:HG2	2:H:247:GLY:HA2	1.96	0.48
1:K:112:ARG:NH1	2:L:102:GLU:OE1	2.46	0.48
2:N:190:PRO:HG2	2:N:204:GLN:HB2	1.94	0.48
1:S:121:SER:HB3	1:S:236:VAL:HG11	1.95	0.48
2:D:159:ASP:OD2	2:D:196:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:234:GLU:HG3	2:N:241:VAL:HG21	1.94	0.48
1:O:91:LEU:H	1:O:92:PRO:HD3	1.78	0.48
2:V:131:ILE:HG12	2:V:138:SER:HB2	1.96	0.48
1:W:91:LEU:N	1:W:92:PRO:CD	2.76	0.48
2:X:192:ALA:HB3	2:X:202:LEU:HB3	1.96	0.48
2:D:193:MET:HG3	2:D:225:ILE:HD13	1.94	0.48
2:N:131:ILE:HG12	2:N:138:SER:HB2	1.94	0.48
1:A:7:ASN:H	1:A:7:ASN:ND2	2.11	0.48
2:B:175:LEU:HD22	2:B:248:VAL:CG2	2.43	0.48
1:O:163:ALA:HA	1:O:273:LEU:HD21	1.95	0.48
1:Q:104:ASP:CG	1:Q:105:GLU:N	2.71	0.48
2:T:190:PRO:HG2	2:T:204:GLN:HB2	1.96	0.48
2:X:103:LEU:HD21	2:X:139:ARG:CZ	2.43	0.48
2:J:193:MET:HG3	2:J:225:ILE:HD13	1.95	0.48
2:R:27:GLU:HG2	2:R:247:GLY:HA2	1.95	0.48
2:T:192:ALA:HB3	2:T:202:LEU:HB3	1.96	0.48
2:F:131:ILE:HD11	2:F:142:SER:HB2	1.96	0.48
1:M:91:LEU:N	1:M:92:PRO:CD	2.77	0.48
2:N:64:MET:HE1	2:N:76:VAL:HB	1.95	0.48
2:N:73:ASP:OD2	2:N:74:ARG:HG3	2.14	0.48
1:Q:125:ASP:CG	1:Q:128:LYS:HG3	2.39	0.48
1:S:68:LYS:HG2	2:V:91:ARG:HB2	1.94	0.48
1:U:91:LEU:H	1:U:92:PRO:HD3	1.78	0.48
1:A:166:TYR:HB3	1:A:273:LEU:HD22	1.96	0.48
2:D:233:ARG:HG3	2:D:233:ARG:HH11	1.79	0.48
2:N:12:LEU:HD22	2:N:181:GLU:HA	1.95	0.48
1:Q:91:LEU:H	1:Q:92:PRO:CD	2.26	0.48
2:B:83:MET:HE2	2:B:99:ARG:HH21	1.79	0.47
2:N:202:LEU:HD23	2:N:203:PHE:N	2.29	0.47
1:Q:112:ARG:NH2	2:R:99:ARG:HB2	2.29	0.47
1:S:251:ILE:HD12	2:T:200:VAL:HG21	1.96	0.47
2:V:37:VAL:HG11	2:V:46:ILE:HG13	1.96	0.47
2:J:14:LEU:O	2:J:16:ASP:N	2.44	0.47
2:N:234:GLU:HG3	2:N:241:VAL:CG2	2.44	0.47
1:W:121:SER:HB3	1:W:236:VAL:HG11	1.96	0.47
1:I:104:ASP:HB3	1:I:107:ALA:HB3	1.96	0.47
2:R:2:ARG:HG2	2:R:3:GLU:N	2.29	0.47
1:U:104:ASP:HB3	1:U:107:ALA:HB3	1.97	0.47
1:U:121:SER:O	1:U:122:LYS:HB2	2.14	0.47
2:B:27:GLU:HG2	2:B:247:GLY:HA2	1.97	0.47
1:E:129:LEU:HB3	1:E:138:TRP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:64:MET:HE1	2:F:76:VAL:HB	1.96	0.47
2:N:131:ILE:HD11	2:N:142:SER:HB2	1.95	0.47
2:P:135:ASP:O	2:P:136:ALA:HB3	2.14	0.47
1:S:129:LEU:HB3	1:S:138:TRP:HB2	1.96	0.47
2:T:28:LEU:O	2:T:245:GLU:HB3	2.15	0.47
2:T:83:MET:HE2	2:T:99:ARG:NH2	2.30	0.47
2:V:83:MET:HB2	2:V:92:LYS:HD3	1.97	0.47
2:V:99:ARG:HH12	3:V:404:ADP:PA	2.37	0.47
2:H:83:MET:HE2	2:H:99:ARG:NH2	2.29	0.47
1:I:104:ASP:CG	1:I:105:GLU:N	2.71	0.47
1:A:121:SER:HB3	1:A:236:VAL:HG11	1.95	0.47
2:D:13:ILE:HD13	2:D:19:ARG:HG2	1.95	0.47
2:H:86:PHE:HA	1:I:68:LYS:HD3	1.97	0.47
1:A:91:LEU:N	1:A:92:PRO:CD	2.77	0.47
1:C:38:ARG:HD2	1:C:59:GLY:HA3	1.97	0.47
2:F:27:GLU:HG2	2:F:247:GLY:HA2	1.95	0.47
1:I:38:ARG:HD2	1:I:59:GLY:HA3	1.97	0.47
2:J:190:PRO:HG2	2:J:204:GLN:HB2	1.96	0.47
2:P:1:MET:HE2	2:P:2:ARG:HG3	1.95	0.47
1:S:91:LEU:H	1:S:92:PRO:HD3	1.79	0.47
2:V:32:LYS:HB3	2:V:48:GLU:HB2	1.97	0.47
2:F:26:ASP:HB2	2:F:248:VAL:HG12	1.95	0.47
2:H:131:ILE:HD11	2:H:142:SER:HB2	1.97	0.47
2:H:193:MET:HG3	2:H:225:ILE:HD13	1.97	0.47
1:I:121:SER:HB3	1:I:236:VAL:HG11	1.96	0.47
1:M:104:ASP:HB3	1:M:107:ALA:HB3	1.97	0.47
1:I:28:ARG:CZ	1:I:210:VAL:HG13	2.45	0.47
2:T:64:MET:HE1	2:T:76:VAL:HB	1.97	0.47
2:F:83:MET:HE2	2:F:99:ARG:NH2	2.30	0.46
2:L:179:GLU:HG3	3:L:404:ADP:O2'	2.15	0.46
2:P:41:ALA:HA	2:P:59:TYR:CE2	2.50	0.46
2:J:83:MET:HE2	2:J:99:ARG:NH2	2.30	0.46
2:N:27:GLU:HG2	2:N:247:GLY:HA2	1.98	0.46
1:O:77:ASP:O	1:O:79:PRO:HD3	2.15	0.46
1:Q:91:LEU:N	1:Q:92:PRO:CD	2.78	0.46
1:U:91:LEU:H	1:U:92:PRO:CD	2.28	0.46
2:B:34:GLU:HB3	2:B:240:TYR:CD1	2.46	0.46
1:G:104:ASP:CG	1:G:105:GLU:N	2.73	0.46
2:J:19:ARG:HD2	2:J:181:GLU:OE2	2.15	0.46
2:N:83:MET:HE2	2:N:99:ARG:NH2	2.31	0.46
1:S:91:LEU:N	1:S:92:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:91:LEU:N	1:K:92:PRO:CD	2.79	0.46
2:L:234:GLU:HG3	2:L:241:VAL:HG21	1.98	0.46
2:P:227:ILE:HD12	2:P:248:VAL:HG22	1.97	0.46
1:Q:38:ARG:HD2	1:Q:59:GLY:HA3	1.97	0.46
1:C:91:LEU:N	1:C:92:PRO:CD	2.78	0.46
1:G:91:LEU:CD2	2:L:80:ARG:HH12	2.28	0.46
2:J:192:ALA:HB3	2:J:202:LEU:HB3	1.96	0.46
2:J:196:SER:HB3	1:O:27:ILE:HG21	1.96	0.46
2:P:23:ARG:HH21	2:P:178:ASN:ND2	2.14	0.46
2:V:193:MET:HG3	2:V:225:ILE:HD13	1.97	0.46
1:W:129:LEU:HB3	1:W:138:TRP:HB2	1.97	0.46
1:M:104:ASP:CG	1:M:105:GLU:N	2.73	0.46
2:X:193:MET:HG3	2:X:225:ILE:HD13	1.98	0.46
2:P:27:GLU:HG2	2:P:247:GLY:HA2	1.98	0.46
2:R:131:ILE:HD11	2:R:142:SER:HB2	1.98	0.46
1:U:38:ARG:HD2	1:U:59:GLY:HA3	1.98	0.46
2:D:202:LEU:HD23	2:D:203:PHE:N	2.31	0.46
1:E:104:ASP:HB3	1:E:107:ALA:HB3	1.98	0.46
2:H:28:LEU:HG	2:H:248:VAL:HG21	1.98	0.46
1:K:91:LEU:H	1:K:92:PRO:HD3	1.80	0.46
2:R:64:MET:HE1	2:R:76:VAL:HB	1.98	0.46
2:R:192:ALA:HB3	2:R:202:LEU:HB3	1.97	0.46
1:E:32:ARG:CZ	1:E:38:ARG:HG3	2.46	0.46
2:H:202:LEU:HD23	2:H:203:PHE:N	2.31	0.46
2:J:160:LEU:HD11	2:J:236:LEU:HD22	1.98	0.46
2:L:64:MET:HE1	2:L:76:VAL:HB	1.98	0.46
2:R:190:PRO:HG2	2:R:204:GLN:HB2	1.97	0.46
1:C:28:ARG:CZ	1:C:210:VAL:HG13	2.46	0.46
2:F:192:ALA:HB3	2:F:202:LEU:HB3	1.98	0.45
1:G:57:LYS:HG2	1:G:62:MET:HG2	1.98	0.45
1:M:57:LYS:HG2	1:M:62:MET:HG2	1.97	0.45
2:D:65:HIS:CB	2:D:66:PRO:CD	2.94	0.45
1:O:91:LEU:N	1:O:92:PRO:CD	2.79	0.45
2:P:60:GLY:O	2:P:61:PRO:C	2.60	0.45
2:X:27:GLU:HG2	2:X:247:GLY:HA2	1.97	0.45
1:W:240:LYS:HB2	2:X:203:PHE:HB3	1.98	0.45
2:P:37:VAL:HG11	2:P:46:ILE:HG13	1.98	0.45
1:W:77:ASP:O	1:W:79:PRO:HD3	2.16	0.45
1:C:269:LEU:O	1:C:273:LEU:HG	2.17	0.45
1:I:125:ASP:OD2	1:I:128:LYS:HE3	2.16	0.45
1:K:243:LYS:HD3	2:L:74:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:83:MET:HE2	2:R:99:ARG:NH2	2.31	0.45
2:V:42:ASP:CG	2:V:60:GLY:H	2.24	0.45
2:V:168:LYS:HE3	2:V:171:GLY:HA2	1.97	0.45
2:D:1:MET:C	2:D:3:GLU:N	2.73	0.45
2:J:233:ARG:NH1	1:O:31:GLY:HA2	2.31	0.45
1:K:3:SER:HB3	2:L:78:ARG:HG3	1.97	0.45
1:Q:8:GLN:O	1:Q:8:GLN:HG2	2.16	0.45
2:V:48:GLU:OE1	2:V:53:LYS:HE2	2.17	0.45
2:V:160:LEU:HD11	2:V:236:LEU:HD22	1.99	0.45
1:W:38:ARG:HD2	1:W:59:GLY:HA3	1.99	0.45
1:A:129:LEU:HB3	1:A:138:TRP:HB2	1.99	0.45
1:C:75:TYR:N	1:C:75:TYR:CD1	2.85	0.45
2:D:183:MET:HE3	2:D:184:TRP:CZ2	2.51	0.45
1:I:91:LEU:H	1:I:92:PRO:HD3	1.82	0.45
2:L:23:ARG:HH12	2:L:176:ASP:HB3	1.82	0.45
1:Q:121:SER:HB3	1:Q:236:VAL:HG11	1.97	0.45
2:B:192:ALA:HB3	2:B:202:LEU:HB3	1.99	0.45
1:I:75:TYR:CE2	1:I:83:ASN:OD1	2.70	0.45
2:J:131:ILE:HG12	2:J:138:SER:HB2	1.97	0.45
1:K:77:ASP:O	1:K:79:PRO:HD3	2.16	0.45
1:A:32:ARG:CZ	1:A:38:ARG:HG3	2.47	0.45
2:D:192:ALA:HB3	2:D:202:LEU:HB3	1.99	0.45
3:D:404:ADP:H5'2	3:D:404:ADP:O3B	2.16	0.45
2:F:210:THR:HG23	2:F:213:GLU:OE1	2.16	0.45
1:I:91:LEU:H	1:I:92:PRO:CD	2.30	0.45
2:P:83:MET:HE2	2:P:99:ARG:NH2	2.31	0.45
2:R:131:ILE:HG12	2:R:138:SER:HB2	1.99	0.45
2:R:195:PRO:HG2	2:R:229:TYR:CD1	2.52	0.45
2:X:61:PRO:HD3	2:X:155:ILE:HD11	1.99	0.45
2:B:131:ILE:HD11	2:B:142:SER:HB2	1.99	0.45
1:E:14:ILE:HG22	2:N:116:LEU:HD22	1.99	0.45
2:J:131:ILE:HD11	2:J:142:SER:HB2	1.99	0.45
2:X:19:ARG:HD2	2:X:181:GLU:OE2	2.16	0.45
1:C:129:LEU:HB3	1:C:138:TRP:HB2	1.99	0.44
2:J:37:VAL:HG11	2:J:46:ILE:HG13	1.99	0.44
2:R:212:ASP:C	2:R:214:PHE:N	2.75	0.44
2:T:32:LYS:HB3	2:T:48:GLU:HB2	1.98	0.44
1:G:104:ASP:HB3	1:G:107:ALA:HB3	1.99	0.44
2:H:91:ARG:HB2	1:I:68:LYS:HG2	1.99	0.44
1:I:130:VAL:HA	1:I:137:VAL:HG12	1.98	0.44
1:O:6:SER:C	1:O:8:GLN:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:190:PRO:HG2	2:V:204:GLN:HB2	1.99	0.44
2:B:91:ARG:HB2	1:E:68:LYS:HG2	2.00	0.44
1:E:121:SER:HB3	1:E:236:VAL:HG11	1.98	0.44
2:J:86:PHE:HB2	1:K:50:ALA:HB2	1.98	0.44
1:K:130:VAL:HA	1:K:137:VAL:HG12	1.99	0.44
2:L:27:GLU:HG2	2:L:247:GLY:HA2	2.00	0.44
1:O:130:VAL:HA	1:O:137:VAL:HG12	1.99	0.44
2:T:37:VAL:HG11	2:T:46:ILE:HG13	1.99	0.44
1:U:91:LEU:N	1:U:92:PRO:CD	2.79	0.44
1:W:104:ASP:HB3	1:W:107:ALA:HB3	1.99	0.44
2:B:99:ARG:NH1	3:B:404:ADP:O2A	2.50	0.44
2:L:41:ALA:HA	2:L:59:TYR:CE2	2.53	0.44
1:M:130:VAL:HA	1:M:137:VAL:HG12	1.99	0.44
2:R:62:LYS:NZ	2:R:126:ASP:OD2	2.48	0.44
1:S:16:LYS:HG3	1:S:220:ILE:HB	2.00	0.44
2:B:190:PRO:HG2	2:B:204:GLN:HB2	1.99	0.44
2:H:48:GLU:CG	2:H:53:LYS:HG2	2.41	0.44
2:J:39:LYS:HA	2:J:39:LYS:HD2	1.85	0.44
1:O:32:ARG:CZ	1:O:38:ARG:HG3	2.47	0.44
1:S:28:ARG:CZ	1:S:210:VAL:HG13	2.48	0.44
1:W:32:ARG:CZ	1:W:38:ARG:HG3	2.48	0.44
1:W:264:LYS:H	1:W:264:LYS:HG3	1.66	0.44
2:X:182:ASP:CG	3:X:404:ADP:H5'1	2.43	0.44
2:F:159:ASP:OD2	2:F:196:SER:HB2	2.17	0.44
2:L:192:ALA:HB3	2:L:202:LEU:HB3	1.99	0.44
1:S:104:ASP:CG	1:S:105:GLU:N	2.75	0.44
2:X:131:ILE:HD11	2:X:142:SER:HB2	2.00	0.44
2:D:160:LEU:HD11	2:D:236:LEU:HD22	2.00	0.44
1:K:28:ARG:CZ	1:K:210:VAL:HG13	2.48	0.44
1:O:112:ARG:NH2	2:P:99:ARG:HB2	2.33	0.44
2:P:1:MET:HG3	2:P:3:GLU:N	2.30	0.44
1:G:232:ASP:OD1	1:G:232:ASP:C	2.60	0.44
1:G:240:LYS:HB2	2:H:203:PHE:HB3	2.00	0.44
1:S:38:ARG:HD2	1:S:59:GLY:HA3	1.99	0.44
1:U:129:LEU:HB3	1:U:138:TRP:HB2	2.00	0.44
1:A:240:LYS:HB2	2:B:203:PHE:HB3	2.00	0.44
2:H:227:ILE:HD12	2:H:248:VAL:CG1	2.41	0.44
2:P:169:ALA:HB2	2:P:174:ILE:HD13	2.00	0.44
1:E:130:VAL:HA	1:E:137:VAL:HG12	2.00	0.43
2:F:135:ASP:O	2:F:136:ALA:HB3	2.18	0.43
2:X:83:MET:HE2	2:X:99:ARG:NH2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3:SER:HB3	2:J:78:ARG:CG	2.47	0.43
1:K:27:ILE:HG21	2:R:196:SER:HB3	2.00	0.43
2:L:165:ALA:HA	2:L:190:PRO:HA	1.99	0.43
2:N:13:ILE:CD1	2:N:172:VAL:HB	2.48	0.43
2:T:165:ALA:HA	2:T:190:PRO:HA	2.00	0.43
2:V:64:MET:HE1	2:V:76:VAL:HB	2.00	0.43
2:B:41:ALA:HA	2:B:59:TYR:CE2	2.54	0.43
2:B:64:MET:HE1	2:B:76:VAL:HB	2.01	0.43
1:C:121:SER:HB3	1:C:236:VAL:HG11	2.00	0.43
2:D:214:PHE:O	2:D:218:PHE:HB2	2.18	0.43
1:G:203:ALA:HB2	1:G:213:PRO:HG3	1.99	0.43
1:M:121:SER:HB3	1:M:236:VAL:HG11	2.01	0.43
2:P:160:LEU:HD11	2:P:236:LEU:HD22	2.00	0.43
1:U:13:ILE:H	1:U:13:ILE:HG13	1.61	0.43
2:V:12:LEU:HD22	2:V:181:GLU:HG3	2.00	0.43
1:A:112:ARG:NH1	2:B:102:GLU:OE1	2.51	0.43
2:F:41:ALA:HA	2:F:59:TYR:CE2	2.54	0.43
1:I:91:LEU:N	1:I:92:PRO:CD	2.81	0.43
2:J:103:LEU:HD21	2:J:139:ARG:CZ	2.48	0.43
1:O:38:ARG:HD2	1:O:59:GLY:HA3	2.00	0.43
1:S:112:ARG:NH1	2:T:102:GLU:OE1	2.52	0.43
1:U:80:ASN:OD1	1:U:133:PRO:HB3	2.18	0.43
1:A:104:ASP:CG	1:A:105:GLU:N	2.76	0.43
1:K:38:ARG:HD2	1:K:59:GLY:HA3	2.00	0.43
2:L:190:PRO:HG2	2:L:204:GLN:HB2	2.00	0.43
1:Q:77:ASP:O	1:Q:79:PRO:HD3	2.18	0.43
1:Q:104:ASP:HB3	1:Q:107:ALA:HB3	2.00	0.43
1:S:11:ILE:HA	1:S:12:PRO:HD3	1.93	0.43
2:X:190:PRO:HG2	2:X:204:GLN:HB2	1.99	0.43
1:A:130:VAL:HA	1:A:137:VAL:HG12	2.00	0.43
2:B:202:LEU:HD23	2:B:203:PHE:N	2.33	0.43
2:D:190:PRO:HG2	2:D:204:GLN:HB2	1.99	0.43
1:G:121:SER:HB3	1:G:236:VAL:HG11	1.99	0.43
2:N:61:PRO:HD3	2:N:155:ILE:HD11	2.01	0.43
1:O:104:ASP:CG	1:O:105:GLU:N	2.77	0.43
1:U:77:ASP:O	1:U:79:PRO:HD3	2.18	0.43
2:D:27:GLU:HG2	2:D:247:GLY:HA2	2.01	0.43
1:G:145:TYR:OH	2:L:82:HIS:HE1	2.01	0.43
2:T:131:ILE:HD11	2:T:142:SER:HB2	2.01	0.43
2:T:160:LEU:HD11	2:T:236:LEU:HD22	2.00	0.43
2:N:12:LEU:HD12	2:N:170:ASP:OD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:165:ALA:HA	2:P:190:PRO:HA	2.00	0.43
1:S:32:ARG:CZ	1:S:38:ARG:HG3	2.49	0.43
1:S:91:LEU:HD22	2:V:80:ARG:HH12	1.83	0.43
1:W:105:GLU:OE1	2:X:105:LYS:HG3	2.19	0.43
1:E:240:LYS:HB2	2:F:203:PHE:HB3	2.00	0.43
2:F:65:HIS:CB	2:F:66:PRO:CD	2.97	0.43
1:G:130:VAL:HA	1:G:137:VAL:HG12	2.00	0.43
2:H:61:PRO:HD3	2:H:155:ILE:HD11	2.01	0.43
2:J:155:ILE:HA	2:J:156:PRO:HD3	1.88	0.43
2:L:23:ARG:HH21	2:L:178:ASN:ND2	2.15	0.43
1:M:32:ARG:CZ	1:M:38:ARG:HG3	2.48	0.43
1:C:104:ASP:HB3	1:C:107:ALA:HB3	2.01	0.43
2:N:193:MET:HG3	2:N:225:ILE:HD13	2.00	0.43
2:P:223:LYS:HB3	2:P:248:VAL:CG1	2.48	0.43
2:V:155:ILE:HA	2:V:156:PRO:HD3	1.88	0.43
1:C:130:VAL:HA	1:C:137:VAL:HG12	2.01	0.42
1:S:104:ASP:HB3	1:S:107:ALA:HB3	2.01	0.42
1:U:112:ARG:NH1	2:V:102:GLU:OE1	2.49	0.42
2:V:165:ALA:HA	2:V:190:PRO:HA	2.01	0.42
2:D:1:MET:C	2:D:3:GLU:H	2.26	0.42
2:H:160:LEU:HD11	2:H:236:LEU:HD22	2.00	0.42
1:I:32:ARG:CZ	1:I:38:ARG:HG3	2.48	0.42
2:L:65:HIS:CB	2:L:66:PRO:CD	2.95	0.42
1:S:77:ASP:O	1:S:79:PRO:HD3	2.19	0.42
1:U:11:ILE:HA	1:U:12:PRO:HD3	1.94	0.42
2:B:82:HIS:HB3	2:B:130:GLU:OE2	2.19	0.42
2:B:129:THR:HG21	2:B:142:SER:HG	1.83	0.42
2:D:135:ASP:O	2:D:136:ALA:HB3	2.20	0.42
1:U:32:ARG:CZ	1:U:38:ARG:HG3	2.49	0.42
1:U:121:SER:HB3	1:U:236:VAL:HG11	2.00	0.42
2:X:34:GLU:HB3	2:X:240:TYR:CD1	2.50	0.42
1:A:13:ILE:H	1:A:13:ILE:HG13	1.69	0.42
2:B:159:ASP:OD2	2:B:196:SER:HB2	2.19	0.42
2:H:165:ALA:HA	2:H:190:PRO:HA	2.02	0.42
1:M:28:ARG:CZ	1:M:210:VAL:HG13	2.49	0.42
2:R:41:ALA:HA	2:R:59:TYR:CE2	2.54	0.42
2:V:115:VAL:CG2	2:V:150:LEU:HD13	2.49	0.42
2:X:160:LEU:HD11	2:X:236:LEU:HD22	2.02	0.42
1:E:16:LYS:HG3	1:E:220:ILE:HB	2.01	0.42
1:G:60:THR:HB	2:L:40:ASN:ND2	2.35	0.42
1:M:11:ILE:HA	1:M:12:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:159:ASP:OD2	2:N:196:SER:HB2	2.19	0.42
2:P:131:ILE:HD11	2:P:142:SER:HB2	2.01	0.42
2:V:202:LEU:HD23	2:V:203:PHE:N	2.34	0.42
1:C:77:ASP:O	1:C:79:PRO:HD3	2.19	0.42
2:D:136:ALA:HA	3:D:404:ADP:H5'2	2.02	0.42
2:F:19:ARG:HD3	2:F:174:ILE:HG21	2.01	0.42
2:H:224:GLY:HA2	2:H:248:VAL:HG11	2.01	0.42
1:K:13:ILE:H	1:K:13:ILE:HG13	1.67	0.42
2:N:192:ALA:HB3	2:N:202:LEU:HB3	2.01	0.42
1:O:174:GLU:O	1:O:181:SER:N	2.47	0.42
2:V:83:MET:HE2	2:V:99:ARG:NH2	2.34	0.42
2:B:82:HIS:HE1	1:E:145:TYR:OH	2.02	0.42
2:F:190:PRO:HG2	2:F:204:GLN:HB2	2.02	0.42
1:G:13:ILE:O	1:G:17:GLU:HG3	2.20	0.42
1:G:60:THR:HB	2:L:40:ASN:HD21	1.83	0.42
2:L:159:ASP:OD1	2:L:160:LEU:N	2.53	0.42
1:M:112:ARG:NH2	2:N:99:ARG:HB2	2.34	0.42
2:N:41:ALA:HA	2:N:59:TYR:CE2	2.55	0.42
3:N:404:ADP:O3B	3:N:404:ADP:O3'	2.30	0.42
2:P:23:ARG:HH12	2:P:176:ASP:HB3	1.85	0.42
1:U:130:VAL:HA	1:U:137:VAL:HG12	2.00	0.42
1:W:104:ASP:CG	1:W:105:GLU:N	2.78	0.42
2:D:233:ARG:HH11	2:D:233:ARG:CG	2.33	0.42
2:F:160:LEU:HD11	2:F:236:LEU:HD22	2.01	0.42
1:G:32:ARG:CZ	1:G:38:ARG:HG3	2.50	0.42
2:L:99:ARG:HH12	3:L:404:ADP:PA	2.40	0.42
1:Q:112:ARG:NH1	2:R:102:GLU:OE1	2.53	0.42
2:R:193:MET:HG3	2:R:225:ILE:HD13	2.00	0.42
1:U:28:ARG:CZ	1:U:210:VAL:HG13	2.50	0.42
2:B:227:ILE:HD12	2:B:248:VAL:HG13	2.01	0.42
2:D:9:ARG:HG3	2:D:184:TRP:HB3	2.01	0.42
2:D:227:ILE:HD12	2:D:248:VAL:HG22	2.01	0.42
1:E:77:ASP:O	1:E:79:PRO:HD3	2.20	0.42
1:G:30:ASP:OD1	1:G:32:ARG:HG2	2.20	0.42
2:J:129:THR:HG21	2:J:142:SER:HG	1.85	0.42
1:K:88:VAL:HG12	1:K:89:GLU:N	2.35	0.42
2:N:165:ALA:HA	2:N:190:PRO:HA	2.01	0.42
1:Q:28:ARG:CZ	1:Q:210:VAL:HG13	2.50	0.42
2:R:2:ARG:CD	2:R:4:MET:HG2	2.50	0.42
1:S:247:SER:HA	2:T:198:ASN:O	2.20	0.42
2:D:29:ARG:C	2:D:245:GLU:HB3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:165:ALA:HA	2:F:190:PRO:HA	2.02	0.42
2:P:78:ARG:HD3	2:P:126:ASP:OD1	2.20	0.42
1:U:3:SER:HB3	2:V:78:ARG:CG	2.50	0.42
2:X:64:MET:HE1	2:X:76:VAL:HB	2.02	0.42
1:A:166:TYR:HB2	1:A:273:LEU:HD21	2.01	0.41
1:C:75:TYR:N	1:C:75:TYR:HD1	2.17	0.41
1:I:129:LEU:HB3	1:I:138:TRP:HB2	2.02	0.41
2:J:132:LEU:HD22	1:K:64:LEU:CD2	2.50	0.41
1:K:104:ASP:CG	1:K:105:GLU:N	2.78	0.41
2:L:159:ASP:OD2	2:L:196:SER:HB2	2.19	0.41
1:M:38:ARG:HD2	1:M:59:GLY:HA3	2.02	0.41
1:O:125:ASP:CG	1:O:128:LYS:HG3	2.44	0.41
2:P:64:MET:HE1	2:P:76:VAL:HB	2.02	0.41
2:R:3:GLU:CB	2:R:5:LEU:N	2.83	0.41
2:R:103:LEU:HD21	2:R:139:ARG:CZ	2.50	0.41
2:R:129:THR:O	2:R:129:THR:HG22	2.20	0.41
1:W:130:VAL:HA	1:W:137:VAL:HG12	2.02	0.41
1:C:13:ILE:H	1:C:13:ILE:HG13	1.69	0.41
2:D:37:VAL:HG11	2:D:46:ILE:HG13	2.02	0.41
2:D:42:ASP:O	2:D:153:ALA:HA	2.19	0.41
2:D:129:THR:O	2:D:129:THR:HG22	2.20	0.41
2:J:243:PHE:CZ	2:J:246:GLU:HG2	2.47	0.41
1:O:11:ILE:HA	1:O:12:PRO:HD3	1.92	0.41
1:O:16:LYS:HG3	1:O:220:ILE:HB	2.02	0.41
2:R:16:ASP:HB3	2:R:17:GLY:H	1.76	0.41
2:T:193:MET:HG3	2:T:225:ILE:HD13	2.01	0.41
2:B:37:VAL:HG11	2:B:46:ILE:HG13	2.02	0.41
2:F:48:GLU:CG	2:F:53:LYS:HG2	2.48	0.41
1:O:28:ARG:CZ	1:O:210:VAL:HG13	2.50	0.41
2:P:99:ARG:NH2	3:P:404:ADP:O2B	2.53	0.41
2:R:37:VAL:HG11	2:R:46:ILE:HG13	2.02	0.41
2:R:160:LEU:HD11	2:R:236:LEU:HD22	2.03	0.41
2:T:60:GLY:O	2:T:61:PRO:C	2.61	0.41
2:D:183:MET:HE3	2:D:184:TRP:CE2	2.55	0.41
2:H:59:TYR:CE1	1:I:92:PRO:HA	2.55	0.41
1:I:203:ALA:HB2	1:I:213:PRO:HG3	2.03	0.41
2:L:202:LEU:HD23	2:L:203:PHE:N	2.35	0.41
1:U:16:LYS:HG3	1:U:220:ILE:HB	2.03	0.41
2:X:37:VAL:HG11	2:X:46:ILE:HG13	2.02	0.41
2:D:60:GLY:O	2:D:61:PRO:C	2.63	0.41
2:F:37:VAL:HG11	2:F:46:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:TYR:CZ	1:I:92:PRO:HA	2.55	0.41
2:J:65:HIS:CB	2:J:66:PRO:CD	2.97	0.41
1:K:11:ILE:HA	1:K:12:PRO:HD3	1.94	0.41
1:O:129:LEU:HB3	1:O:138:TRP:HB2	2.02	0.41
2:P:103:LEU:HD21	2:P:139:ARG:CZ	2.51	0.41
2:B:165:ALA:HA	2:B:190:PRO:HA	2.03	0.41
1:C:16:LYS:HG3	1:C:220:ILE:HB	2.03	0.41
2:D:155:ILE:HA	2:D:156:PRO:HD3	1.88	0.41
2:F:155:ILE:HA	2:F:156:PRO:HD3	1.89	0.41
2:X:60:GLY:O	2:X:61:PRO:C	2.64	0.41
1:G:11:ILE:HA	1:G:12:PRO:HD3	1.93	0.41
2:H:195:PRO:HG2	2:H:229:TYR:CD1	2.55	0.41
1:I:252:ASP:OD1	2:J:215:ARG:NH1	2.54	0.41
2:J:195:PRO:HG2	2:J:229:TYR:CD1	2.56	0.41
1:K:104:ASP:HB3	1:K:107:ALA:HB3	2.03	0.41
1:M:77:ASP:O	1:M:79:PRO:HD3	2.21	0.41
2:R:28:LEU:HG	2:R:248:VAL:HG21	2.03	0.41
1:S:245:SER:HB2	2:T:199:GLN:HB3	2.02	0.41
2:T:32:LYS:HE2	2:T:34:GLU:OE2	2.20	0.41
1:C:183:ASN:ND2	1:C:185:ASN:OD1	2.38	0.41
1:M:240:LYS:HB2	2:N:203:PHE:HB3	2.03	0.41
2:N:159:ASP:OD1	2:N:160:LEU:N	2.54	0.41
2:P:169:ALA:HB2	2:P:174:ILE:CD1	2.51	0.41
2:B:26:ASP:O	2:B:248:VAL:HG23	2.21	0.41
2:H:190:PRO:HG2	2:H:204:GLN:HB2	2.02	0.41
1:I:248:LEU:CD2	2:J:218:PHE:CZ	3.04	0.41
2:J:9:ARG:HG2	2:J:184:TRP:CE3	2.56	0.41
1:M:16:LYS:HG3	1:M:220:ILE:HB	2.03	0.41
1:Q:32:ARG:CZ	1:Q:38:ARG:HG3	2.50	0.41
1:S:203:ALA:HB2	1:S:213:PRO:HG3	2.02	0.41
2:X:65:HIS:CB	2:X:66:PRO:CD	2.98	0.41
1:C:274:GLY:O	1:C:275:ILE:HB	2.21	0.41
2:D:30:SER:N	2:D:245:GLU:HB3	2.36	0.41
2:D:165:ALA:HA	2:D:190:PRO:HA	2.03	0.41
1:E:269:LEU:O	1:E:273:LEU:HG	2.20	0.41
2:F:13:ILE:HD11	2:F:169:ALA:HB3	2.03	0.41
2:H:116:LEU:HD12	2:H:156:PRO:HB2	2.03	0.41
2:J:202:LEU:HD23	2:J:203:PHE:N	2.36	0.41
1:K:129:LEU:HB3	1:K:138:TRP:HB2	2.03	0.41
1:K:240:LYS:HB2	2:L:203:PHE:HB3	2.02	0.41
2:L:160:LEU:HD11	2:L:236:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:16:ASP:C	2:P:18:LYS:N	2.79	0.40
2:T:103:LEU:HD21	2:T:139:ARG:CZ	2.51	0.40
2:T:138:SER:OG	3:T:404:ADP:O3B	2.29	0.40
1:W:75:TYR:HD2	1:W:75:TYR:N	2.20	0.40
1:A:203:ALA:HB2	1:A:213:PRO:HG3	2.04	0.40
2:D:41:ALA:HA	2:D:59:TYR:CE2	2.56	0.40
2:J:165:ALA:HA	2:J:190:PRO:HA	2.03	0.40
2:L:103:LEU:HD21	2:L:139:ARG:CZ	2.51	0.40
2:P:245:GLU:O	2:P:246:GLU:HB3	2.22	0.40
2:R:2:ARG:HD2	2:R:4:MET:HG2	2.02	0.40
1:S:243:LYS:HG2	2:T:112:GLU:OE1	2.21	0.40
1:K:32:ARG:CZ	1:K:38:ARG:HG3	2.51	0.40
2:N:160:LEU:HD11	2:N:236:LEU:HD22	2.04	0.40
2:P:115:VAL:CG2	2:P:150:LEU:HD13	2.51	0.40
1:U:183:ASN:O	1:U:185:ASN:N	2.52	0.40
1:C:44:LEU:HD22	1:C:167:ASN:HB2	2.03	0.40
2:D:16:ASP:C	2:D:18:LYS:H	2.29	0.40
2:F:193:MET:HG3	2:F:225:ILE:HD13	2.03	0.40
1:G:28:ARG:CZ	1:G:210:VAL:HG13	2.51	0.40
1:G:129:LEU:HB3	1:G:138:TRP:HB2	2.02	0.40
2:H:39:LYS:HG2	1:I:148:ASP:OD2	2.22	0.40
2:J:91:ARG:HD2	1:K:141:TRP:CG	2.57	0.40
1:K:6:SER:C	1:K:8:GLN:N	2.76	0.40
1:K:247:SER:O	1:K:250:ASP:HB2	2.21	0.40
2:R:189:MET:HE1	2:R:214:PHE:HD1	1.87	0.40
1:W:112:ARG:NH1	2:X:102:GLU:OE1	2.53	0.40
2:F:202:LEU:HD23	2:F:203:PHE:N	2.37	0.40
2:H:135:ASP:O	2:H:136:ALA:CB	2.70	0.40
1:W:44:LEU:HD22	1:W:167:ASN:HB2	2.03	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	254/275 (92%)	241 (95%)	10 (4%)	3 (1%)	10	37
1	C	254/275 (92%)	240 (94%)	8 (3%)	6 (2%)	4	24
1	E	254/275 (92%)	241 (95%)	11 (4%)	2 (1%)	16	45
1	G	254/275 (92%)	239 (94%)	11 (4%)	4 (2%)	7	31
1	I	254/275 (92%)	242 (95%)	10 (4%)	2 (1%)	16	45
1	K	254/275 (92%)	240 (94%)	11 (4%)	3 (1%)	10	37
1	M	254/275 (92%)	240 (94%)	11 (4%)	3 (1%)	10	37
1	O	254/275 (92%)	245 (96%)	7 (3%)	2 (1%)	16	45
1	Q	254/275 (92%)	238 (94%)	13 (5%)	3 (1%)	10	37
1	S	253/275 (92%)	242 (96%)	9 (4%)	2 (1%)	16	45
1	U	249/275 (90%)	236 (95%)	11 (4%)	2 (1%)	16	45
1	W	253/275 (92%)	241 (95%)	9 (4%)	3 (1%)	10	37
2	B	239/248 (96%)	221 (92%)	15 (6%)	3 (1%)	9	35
2	D	246/248 (99%)	231 (94%)	10 (4%)	5 (2%)	6	27
2	F	239/248 (96%)	226 (95%)	10 (4%)	3 (1%)	9	35
2	H	226/248 (91%)	216 (96%)	8 (4%)	2 (1%)	14	43
2	J	239/248 (96%)	225 (94%)	10 (4%)	4 (2%)	7	30
2	L	245/248 (99%)	231 (94%)	13 (5%)	1 (0%)	30	60
2	N	237/248 (96%)	224 (94%)	12 (5%)	1 (0%)	30	60
2	P	246/248 (99%)	230 (94%)	13 (5%)	3 (1%)	10	37
2	R	246/248 (99%)	230 (94%)	13 (5%)	3 (1%)	10	37
2	T	246/248 (99%)	233 (95%)	11 (4%)	2 (1%)	16	45
2	V	237/248 (96%)	218 (92%)	15 (6%)	4 (2%)	7	30
2	X	235/248 (95%)	223 (95%)	11 (5%)	1 (0%)	30	60
All	All	5922/6276 (94%)	5593 (94%)	262 (4%)	67 (1%)	11	39

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	8	GLN
2	J	15	ASP
2	P	16	ASP
1	Q	8	GLN
2	V	91	ARG
2	V	169	ALA

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Mol	Chain	Res	Type
1	A	8	GLN
1	A	105	GLU
1	C	8	GLN
1	C	9	ASN
1	C	105	GLU
2	D	7	VAL
1	E	105	GLU
1	G	7	ASN
1	G	105	GLU
1	I	105	GLU
1	K	105	GLU
1	M	105	GLU
1	O	105	GLU
1	Q	105	GLU
2	R	169	ALA
1	S	105	GLU
1	U	105	GLU
1	U	184	LYS
1	W	105	GLU
1	C	7	ASN
1	C	76	GLU
2	F	169	ALA
1	W	9	ASN
2	B	170	ASP
2	D	176	ASP
2	H	176	ASP
2	V	176	ASP
2	B	176	ASP
2	D	2	ARG
2	D	16	ASP
2	F	176	ASP
2	J	65	HIS
2	J	169	ALA
1	K	76	GLU
2	P	7	VAL
2	R	176	ASP
2	T	176	ASP
2	V	65	HIS
2	B	65	HIS
2	D	65	HIS
2	F	65	HIS
2	H	65	HIS

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Mol	Chain	Res	Type
2	J	176	ASP
2	L	65	HIS
1	M	8	GLN
2	N	65	HIS
2	P	65	HIS
2	R	65	HIS
2	X	65	HIS
2	T	65	HIS
1	C	91	LEU
1	K	91	LEU
1	O	91	LEU
1	S	91	LEU
1	W	91	LEU
1	E	91	LEU
1	G	91	LEU
1	Q	91	LEU
1	A	91	LEU
1	I	91	LEU
1	M	91	LEU

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	212/242 (88%)	201 (95%)	11 (5%)	21	49
1	C	212/242 (88%)	201 (95%)	11 (5%)	21	49
1	E	218/242 (90%)	209 (96%)	9 (4%)	27	55
1	G	216/242 (89%)	207 (96%)	9 (4%)	26	55
1	I	214/242 (88%)	206 (96%)	8 (4%)	30	58
1	K	215/242 (89%)	203 (94%)	12 (6%)	19	47
1	M	216/242 (89%)	205 (95%)	11 (5%)	21	50
1	O	213/242 (88%)	204 (96%)	9 (4%)	26	55
1	Q	214/242 (88%)	204 (95%)	10 (5%)	23	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	216/242 (89%)	204 (94%)	12 (6%)	19	47
1	U	208/242 (86%)	198 (95%)	10 (5%)	23	52
1	W	214/242 (88%)	203 (95%)	11 (5%)	21	50
2	B	186/208 (89%)	175 (94%)	11 (6%)	18	46
2	D	200/208 (96%)	185 (92%)	15 (8%)	12	38
2	F	193/208 (93%)	182 (94%)	11 (6%)	18	47
2	H	179/208 (86%)	168 (94%)	11 (6%)	17	45
2	J	194/208 (93%)	184 (95%)	10 (5%)	21	49
2	L	199/208 (96%)	186 (94%)	13 (6%)	15	43
2	N	188/208 (90%)	179 (95%)	9 (5%)	23	52
2	P	201/208 (97%)	184 (92%)	17 (8%)	10	33
2	R	194/208 (93%)	183 (94%)	11 (6%)	18	47
2	T	196/208 (94%)	180 (92%)	16 (8%)	10	35
2	V	189/208 (91%)	181 (96%)	8 (4%)	26	55
2	X	191/208 (92%)	180 (94%)	11 (6%)	18	47
All	All	4878/5400 (90%)	4612 (94%)	266 (6%)	19	48

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	13	ILE
1	A	18	SER
1	A	51	ASP
1	A	182	VAL
1	A	191	LEU
1	A	233	LEU
1	A	236	VAL
1	A	255	GLU
1	A	257	THR
1	A	275	ILE
2	B	12	LEU
2	B	13	ILE
2	B	20	THR
2	B	26	ASP
2	B	78	ARG
2	B	89	ASP

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Mol	Chain	Res	Type
2	B	99	ARG
2	B	129	THR
2	B	164	VAL
2	B	177	LEU
2	B	201	THR
1	C	13	ILE
1	C	30	ASP
1	C	182	VAL
1	C	183	ASN
1	C	191	LEU
1	C	233	LEU
1	C	236	VAL
1	C	249	GLN
1	C	255	GLU
1	C	257	THR
1	C	267	GLU
2	D	1	MET
2	D	2	ARG
2	D	7	VAL
2	D	8	GLU
2	D	20	THR
2	D	34	GLU
2	D	78	ARG
2	D	99	ARG
2	D	129	THR
2	D	164	VAL
2	D	177	LEU
2	D	201	THR
2	D	212	ASP
2	D	233	ARG
2	D	245	GLU
1	E	13	ILE
1	E	18	SER
1	E	37	TYR
1	E	191	LEU
1	E	232	ASP
1	E	233	LEU
1	E	236	VAL
1	E	255	GLU
1	E	257	THR
2	F	15	ASP
2	F	18	LYS

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Mol	Chain	Res	Type
2	F	20	THR
2	F	34	GLU
2	F	39	LYS
2	F	78	ARG
2	F	99	ARG
2	F	129	THR
2	F	164	VAL
2	F	177	LEU
2	F	201	THR
1	G	13	ILE
1	G	182	VAL
1	G	191	LEU
1	G	206	ASP
1	G	233	LEU
1	G	236	VAL
1	G	249	GLN
1	G	255	GLU
1	G	257	THR
2	H	20	THR
2	H	39	LYS
2	H	78	ARG
2	H	89	ASP
2	H	99	ARG
2	H	129	THR
2	H	164	VAL
2	H	177	LEU
2	H	178	ASN
2	H	201	THR
2	H	212	ASP
1	I	13	ILE
1	I	182	VAL
1	I	191	LEU
1	I	232	ASP
1	I	233	LEU
1	I	236	VAL
1	I	255	GLU
1	I	257	THR
2	J	15	ASP
2	J	20	THR
2	J	78	ARG
2	J	99	ARG
2	J	129	THR

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Mol	Chain	Res	Type
2	J	164	VAL
2	J	177	LEU
2	J	201	THR
2	J	233	ARG
2	J	246	GLU
1	K	13	ILE
1	K	24	GLU
1	K	30	ASP
1	K	182	VAL
1	K	191	LEU
1	K	232	ASP
1	K	233	LEU
1	K	236	VAL
1	K	249	GLN
1	K	255	GLU
1	K	257	THR
1	K	275	ILE
2	L	7	VAL
2	L	20	THR
2	L	78	ARG
2	L	99	ARG
2	L	129	THR
2	L	164	VAL
2	L	177	LEU
2	L	178	ASN
2	L	179	GLU
2	L	201	THR
2	L	206	ASN
2	L	218	PHE
2	L	233	ARG
1	M	8	GLN
1	M	13	ILE
1	M	29	GLN
1	M	170	VAL
1	M	182	VAL
1	M	191	LEU
1	M	233	LEU
1	M	236	VAL
1	M	255	GLU
1	M	257	THR
1	M	275	ILE
2	N	12	LEU

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Mol	Chain	Res	Type
2	N	20	THR
2	N	78	ARG
2	N	99	ARG
2	N	129	THR
2	N	164	VAL
2	N	177	LEU
2	N	201	THR
2	N	234	GLU
1	O	13	ILE
1	O	18	SER
1	O	182	VAL
1	O	191	LEU
1	O	233	LEU
1	O	236	VAL
1	O	243	LYS
1	O	255	GLU
1	O	257	THR
2	P	1	MET
2	P	2	ARG
2	P	5	LEU
2	P	9	ARG
2	P	20	THR
2	P	34	GLU
2	P	53	LYS
2	P	78	ARG
2	P	99	ARG
2	P	129	THR
2	P	164	VAL
2	P	177	LEU
2	P	183	MET
2	P	201	THR
2	P	206	ASN
2	P	233	ARG
2	P	234	GLU
1	Q	9	ASN
1	Q	13	ILE
1	Q	18	SER
1	Q	37	TYR
1	Q	182	VAL
1	Q	191	LEU
1	Q	200	ILE
1	Q	233	LEU

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Mol	Chain	Res	Type
1	Q	236	VAL
1	Q	255	GLU
2	R	1	MET
2	R	6	GLN
2	R	20	THR
2	R	78	ARG
2	R	99	ARG
2	R	129	THR
2	R	164	VAL
2	R	177	LEU
2	R	201	THR
2	R	233	ARG
2	R	242	GLU
1	S	13	ILE
1	S	18	SER
1	S	30	ASP
1	S	122	LYS
1	S	182	VAL
1	S	191	LEU
1	S	200	ILE
1	S	233	LEU
1	S	236	VAL
1	S	243	LYS
1	S	255	GLU
1	S	257	THR
2	T	1	MET
2	T	5	LEU
2	T	20	THR
2	T	34	GLU
2	T	53	LYS
2	T	78	ARG
2	T	99	ARG
2	T	129	THR
2	T	164	VAL
2	T	168	LYS
2	T	177	LEU
2	T	183	MET
2	T	186	GLU
2	T	201	THR
2	T	242	GLU
2	T	246	GLU
1	U	8	GLN

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Mol	Chain	Res	Type
1	U	13	ILE
1	U	29	GLN
1	U	170	VAL
1	U	182	VAL
1	U	191	LEU
1	U	233	LEU
1	U	236	VAL
1	U	255	GLU
1	U	257	THR
2	V	20	THR
2	V	78	ARG
2	V	99	ARG
2	V	129	THR
2	V	164	VAL
2	V	168	LYS
2	V	177	LEU
2	V	201	THR
1	W	13	ILE
1	W	170	VAL
1	W	182	VAL
1	W	183	ASN
1	W	191	LEU
1	W	233	LEU
1	W	236	VAL
1	W	255	GLU
1	W	257	THR
1	W	263	VAL
1	W	264	LYS
2	X	13	ILE
2	X	14	LEU
2	X	20	THR
2	X	78	ARG
2	X	89	ASP
2	X	99	ARG
2	X	129	THR
2	X	164	VAL
2	X	177	LEU
2	X	201	THR
2	X	246	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
2	B	178	ASN
2	B	216	GLN
1	C	83	ASN
2	D	133	GLN
2	D	178	ASN
2	D	216	GLN
1	E	83	ASN
2	F	82	HIS
2	F	216	GLN
1	G	83	ASN
1	G	249	GLN
2	H	178	ASN
2	H	216	GLN
1	I	183	ASN
1	I	256	ASN
2	J	82	HIS
2	J	178	ASN
2	J	216	GLN
1	K	9	ASN
1	K	83	ASN
1	K	183	ASN
1	K	185	ASN
2	L	40	ASN
2	L	82	HIS
2	L	178	ASN
2	L	216	GLN
1	M	83	ASN
1	M	183	ASN
2	N	178	ASN
2	N	216	GLN
1	O	8	GLN
1	O	183	ASN
2	P	178	ASN
2	P	216	GLN
1	Q	83	ASN
2	R	6	GLN
2	R	82	HIS
2	R	216	GLN
1	S	9	ASN
1	S	29	GLN
1	S	83	ASN
1	S	256	ASN

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Mol	Chain	Res	Type
2	T	40	ASN
2	T	82	HIS
2	T	216	GLN
1	U	83	ASN
1	U	183	ASN
2	V	82	HIS
2	V	216	GLN
2	X	133	GLN
2	X	216	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](#)

12 ligands are modelled in this entry.

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	$\# Z > 2$
3	ADP	T	404	-	28,29,29	1.43	6 (21%)	43,45,45	1.85	10 (23%)
3	ADP	V	404	-	16,17,29	1.22	2 (12%)	22,26,45	1.11	1 (4%)
3	ADP	F	404	-	16,17,29	1.86	3 (18%)	22,26,45	1.07	1 (4%)
3	ADP	X	404	-	16,17,29	2.09	3 (18%)	22,26,45	1.32	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	404	-	28,29,29	1.62	5 (17%)	43,45,45	1.81	7 (16%)
3	ADP	L	404	-	28,29,29	1.51	3 (10%)	43,45,45	1.93	11 (25%)
3	ADP	H	404	-	28,29,29	1.47	4 (14%)	43,45,45	1.95	10 (23%)
3	ADP	N	404	-	28,29,29	1.57	5 (17%)	43,45,45	1.80	8 (18%)
3	ADP	D	404	-	28,29,29	1.51	4 (14%)	43,45,45	2.00	12 (27%)
3	ADP	R	404	-	28,29,29	1.63	5 (17%)	43,45,45	1.81	10 (23%)
3	ADP	P	404	-	28,29,29	1.49	5 (17%)	43,45,45	2.09	13 (30%)
3	ADP	J	404	-	6,8,29	0.94	0	12,13,45	1.05	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	T	404	-	-	3/16/32/32	0/3/3/3
3	ADP	V	404	-	-	0/12/25/32	0/1/1/3
3	ADP	F	404	-	-	2/12/25/32	0/1/1/3
3	ADP	X	404	-	-	6/12/25/32	0/1/1/3
3	ADP	B	404	-	-	6/16/32/32	0/3/3/3
3	ADP	L	404	-	-	3/16/32/32	0/3/3/3
3	ADP	H	404	-	-	3/16/32/32	0/3/3/3
3	ADP	N	404	-	-	5/16/32/32	0/3/3/3
3	ADP	D	404	-	-	1/16/32/32	0/3/3/3
3	ADP	R	404	-	-	3/16/32/32	0/3/3/3
3	ADP	P	404	-	-	5/16/32/32	0/3/3/3
3	ADP	J	404	-	-	0/6/6/32	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	404	ADP	O4'-C1'	6.32	1.57	1.43
3	F	404	ADP	O4'-C1'	5.47	1.55	1.43
3	B	404	ADP	C5-C4	5.29	1.48	1.39
3	R	404	ADP	C5-C4	5.23	1.48	1.39
3	N	404	ADP	C5-C4	5.12	1.48	1.39
3	L	404	ADP	C5-C4	5.10	1.48	1.39
3	H	404	ADP	C5-C4	4.95	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	ADP	C5-C4	4.75	1.47	1.39
3	P	404	ADP	C5-C4	4.57	1.47	1.39
3	T	404	ADP	C5-C4	4.26	1.46	1.39
3	B	404	ADP	PA-O3A	3.62	1.63	1.59
3	F	404	ADP	PA-O3A	3.61	1.63	1.59
3	L	404	ADP	C5-C6	3.59	1.51	1.41
3	V	404	ADP	PA-O3A	3.41	1.63	1.59
3	X	404	ADP	PA-O3A	3.39	1.63	1.59
3	R	404	ADP	PA-O3A	3.19	1.62	1.59
3	X	404	ADP	C1'-C2'	3.18	1.57	1.51
3	R	404	ADP	C5-C6	3.09	1.49	1.41
3	B	404	ADP	C5-C6	2.97	1.49	1.41
3	H	404	ADP	C5-C6	2.96	1.49	1.41
3	N	404	ADP	PA-O3A	2.93	1.62	1.59
3	P	404	ADP	C5-C6	2.89	1.49	1.41
3	N	404	ADP	C5-C6	2.83	1.48	1.41
3	D	404	ADP	C5-N7	-2.77	1.34	1.39
3	D	404	ADP	C5-C6	2.71	1.48	1.41
3	T	404	ADP	C5-N7	-2.71	1.34	1.39
3	D	404	ADP	C8-N7	2.55	1.36	1.31
3	R	404	ADP	C8-N7	2.46	1.36	1.31
3	H	404	ADP	C8-N7	2.40	1.36	1.31
3	F	404	ADP	C1'-C2'	2.39	1.56	1.51
3	N	404	ADP	C8-N7	2.36	1.36	1.31
3	T	404	ADP	C4-N9	-2.35	1.32	1.37
3	T	404	ADP	PA-O3A	2.28	1.62	1.59
3	P	404	ADP	PA-O3A	2.25	1.61	1.59
3	P	404	ADP	C5-N7	-2.23	1.35	1.39
3	T	404	ADP	C8-N7	2.23	1.36	1.31
3	T	404	ADP	C5-C6	2.22	1.47	1.41
3	B	404	ADP	C5-N7	-2.20	1.35	1.39
3	V	404	ADP	O4'-C1'	2.17	1.48	1.43
3	P	404	ADP	C8-N7	2.14	1.35	1.31
3	R	404	ADP	C5-N7	-2.12	1.35	1.39
3	L	404	ADP	C8-N7	2.12	1.35	1.31
3	H	404	ADP	PA-O3A	2.10	1.61	1.59
3	B	404	ADP	C8-N7	2.09	1.35	1.31
3	N	404	ADP	C5-N7	-2.04	1.35	1.39

All (86) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	ADP	C5-C4-N3	-6.15	118.25	126.72
3	H	404	ADP	C5-C4-N3	-6.02	118.42	126.72
3	N	404	ADP	C5-C4-N3	-5.98	118.49	126.72
3	L	404	ADP	C5-C4-N3	-5.77	118.77	126.72
3	R	404	ADP	C5-C4-N3	-5.68	118.89	126.72
3	P	404	ADP	C5-C4-N3	-5.68	118.90	126.72
3	D	404	ADP	C5-C4-N3	-5.52	119.12	126.72
3	T	404	ADP	C5-C4-N3	-5.21	119.54	126.72
3	P	404	ADP	N3-C4-N9	4.92	135.53	127.17
3	N	404	ADP	N3-C4-N9	4.91	135.51	127.17
3	B	404	ADP	N3-C4-N9	4.86	135.43	127.17
3	H	404	ADP	N3-C4-N9	4.83	135.37	127.17
3	T	404	ADP	N3-C4-N9	4.70	135.16	127.17
3	L	404	ADP	C4-C5-N7	-4.38	105.58	110.58
3	R	404	ADP	N3-C4-N9	4.29	134.46	127.17
3	D	404	ADP	N3-C4-N9	4.16	134.25	127.17
3	P	404	ADP	N3-C2-N1	-4.13	122.33	128.58
3	L	404	ADP	N3-C4-N9	4.11	134.16	127.17
3	H	404	ADP	C2-N3-C4	4.04	121.69	111.83
3	N	404	ADP	C2-N3-C4	4.02	121.65	111.83
3	P	404	ADP	C2-N3-C4	3.99	121.58	111.83
3	B	404	ADP	C2-N3-C4	3.86	121.26	111.83
3	D	404	ADP	N3-C2-N1	-3.82	122.80	128.58
3	D	404	ADP	C2-N3-C4	3.78	121.06	111.83
3	L	404	ADP	C2-N3-C4	3.72	120.92	111.83
3	X	404	ADP	C1'-C2'-C3'	3.71	107.55	101.63
3	N	404	ADP	N3-C2-N1	-3.66	123.05	128.58
3	P	404	ADP	C4-N9-C8	3.64	109.56	105.74
3	T	404	ADP	C2'-C1'-N9	-3.63	104.29	113.30
3	D	404	ADP	C4-C5-N7	-3.61	106.45	110.58
3	T	404	ADP	C4-N9-C8	3.61	109.53	105.74
3	R	404	ADP	C2-N3-C4	3.60	120.63	111.83
3	D	404	ADP	O4'-C1'-N9	3.59	114.98	108.09
3	H	404	ADP	N3-C2-N1	-3.57	123.17	128.58
3	P	404	ADP	C4-C5-N7	-3.55	106.53	110.58
3	B	404	ADP	N3-C2-N1	-3.48	123.31	128.58
3	P	404	ADP	C2'-C1'-N9	-3.48	104.66	113.30
3	V	404	ADP	C1'-C2'-C3'	3.44	107.13	101.63
3	T	404	ADP	C2-N3-C4	3.42	120.17	111.83
3	H	404	ADP	C2'-C1'-N9	-3.39	104.89	113.30
3	B	404	ADP	C4-C5-N7	-3.35	106.75	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	404	ADP	C4-C5-N7	-3.33	106.78	110.58
3	T	404	ADP	N3-C2-N1	-3.28	123.62	128.58
3	L	404	ADP	N3-C2-N1	-3.10	123.90	128.58
3	F	404	ADP	C1'-C2'-C3'	3.03	106.47	101.63
3	L	404	ADP	O4'-C1'-N9	3.03	113.91	108.09
3	R	404	ADP	N3-C2-N1	-3.00	124.04	128.58
3	H	404	ADP	C4-C5-N7	-2.99	107.16	110.58
3	H	404	ADP	O4'-C1'-N9	2.96	113.77	108.09
3	P	404	ADP	C5-N7-C8	2.95	108.08	103.45
3	X	404	ADP	O4'-C1'-C2'	-2.91	100.75	105.76
3	L	404	ADP	C6-C5-N7	2.82	137.54	132.09
3	D	404	ADP	O3A-PA-O1A	-2.81	102.26	110.70
3	N	404	ADP	C4-C5-N7	-2.79	107.39	110.58
3	L	404	ADP	C5-N7-C8	2.76	107.78	103.45
3	D	404	ADP	C5-N7-C8	2.69	107.67	103.45
3	P	404	ADP	N9-C8-N7	-2.60	110.25	113.94
3	R	404	ADP	O4'-C1'-N9	2.58	113.04	108.09
3	T	404	ADP	C4-C5-N7	-2.54	107.68	110.58
3	L	404	ADP	O3B-PB-O2B	2.50	117.19	107.80
3	D	404	ADP	C2'-C1'-N9	-2.45	107.21	113.30
3	D	404	ADP	C6-C5-N7	2.42	136.76	132.09
3	P	404	ADP	C6-C5-N7	2.42	136.75	132.09
3	B	404	ADP	C5-N7-C8	2.39	107.21	103.45
3	T	404	ADP	N9-C8-N7	-2.36	110.58	113.94
3	R	404	ADP	C6-C5-N7	2.36	136.64	132.09
3	D	404	ADP	C4-N9-C8	2.25	108.10	105.74
3	H	404	ADP	C6-C5-N7	2.24	136.41	132.09
3	T	404	ADP	C5-N7-C8	2.20	106.91	103.45
3	H	404	ADP	C5-N7-C8	2.20	106.91	103.45
3	L	404	ADP	C2'-C1'-N9	-2.18	107.89	113.30
3	R	404	ADP	C5-N7-C8	2.17	106.86	103.45
3	L	404	ADP	C4-N9-C8	2.17	108.02	105.74
3	R	404	ADP	O3B-PB-O2B	2.15	115.84	107.80
3	N	404	ADP	C6-C5-N7	2.14	136.21	132.09
3	P	404	ADP	O3B-PB-O2B	2.09	115.65	107.80
3	B	404	ADP	C2-N1-C6	2.08	122.15	118.73
3	N	404	ADP	O4'-C1'-N9	2.08	112.08	108.09
3	P	404	ADP	C2-N1-C6	2.07	122.14	118.73
3	N	404	ADP	C5-N7-C8	2.07	106.70	103.45
3	D	404	ADP	O3A-PB-O1B	-2.06	100.20	111.04
3	R	404	ADP	O3A-PA-O1A	-2.06	104.52	110.70
3	J	404	ADP	O3B-PB-O1B	2.01	118.67	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	404	ADP	N6-C6-N1	2.01	122.85	118.38
3	P	404	ADP	O3A-PA-O1A	-2.00	104.68	110.70
3	H	404	ADP	C4-N9-C8	2.00	107.84	105.74

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	ADP	C5'-O5'-PA-O2A
3	B	404	ADP	C5'-O5'-PA-O3A
3	H	404	ADP	C5'-O5'-PA-O3A
3	L	404	ADP	PB-O3A-PA-O5'
3	N	404	ADP	C5'-O5'-PA-O1A
3	N	404	ADP	C5'-O5'-PA-O3A
3	P	404	ADP	C5'-O5'-PA-O1A
3	R	404	ADP	C5'-O5'-PA-O1A
3	T	404	ADP	C5'-O5'-PA-O1A
3	T	404	ADP	C5'-O5'-PA-O3A
3	X	404	ADP	C5'-O5'-PA-O1A
3	B	404	ADP	O4'-C4'-C5'-O5'
3	L	404	ADP	O4'-C4'-C5'-O5'
3	L	404	ADP	C3'-C4'-C5'-O5'
3	X	404	ADP	O4'-C4'-C5'-O5'
3	B	404	ADP	C3'-C4'-C5'-O5'
3	N	404	ADP	O4'-C4'-C5'-O5'
3	X	404	ADP	C3'-C4'-C5'-O5'
3	F	404	ADP	C3'-C4'-C5'-O5'
3	N	404	ADP	C3'-C4'-C5'-O5'
3	B	404	ADP	PB-O3A-PA-O5'
3	D	404	ADP	PB-O3A-PA-O5'
3	P	404	ADP	PA-O3A-PB-O1B
3	H	404	ADP	C5'-O5'-PA-O1A
3	N	404	ADP	C5'-O5'-PA-O2A
3	P	404	ADP	C5'-O5'-PA-O2A
3	P	404	ADP	C5'-O5'-PA-O3A
3	T	404	ADP	C5'-O5'-PA-O2A
3	X	404	ADP	C5'-O5'-PA-O2A
3	X	404	ADP	C5'-O5'-PA-O3A
3	F	404	ADP	O4'-C4'-C5'-O5'
3	R	404	ADP	PB-O3A-PA-O5'
3	B	404	ADP	PA-O3A-PB-O1B
3	P	404	ADP	PA-O3A-PB-O2B

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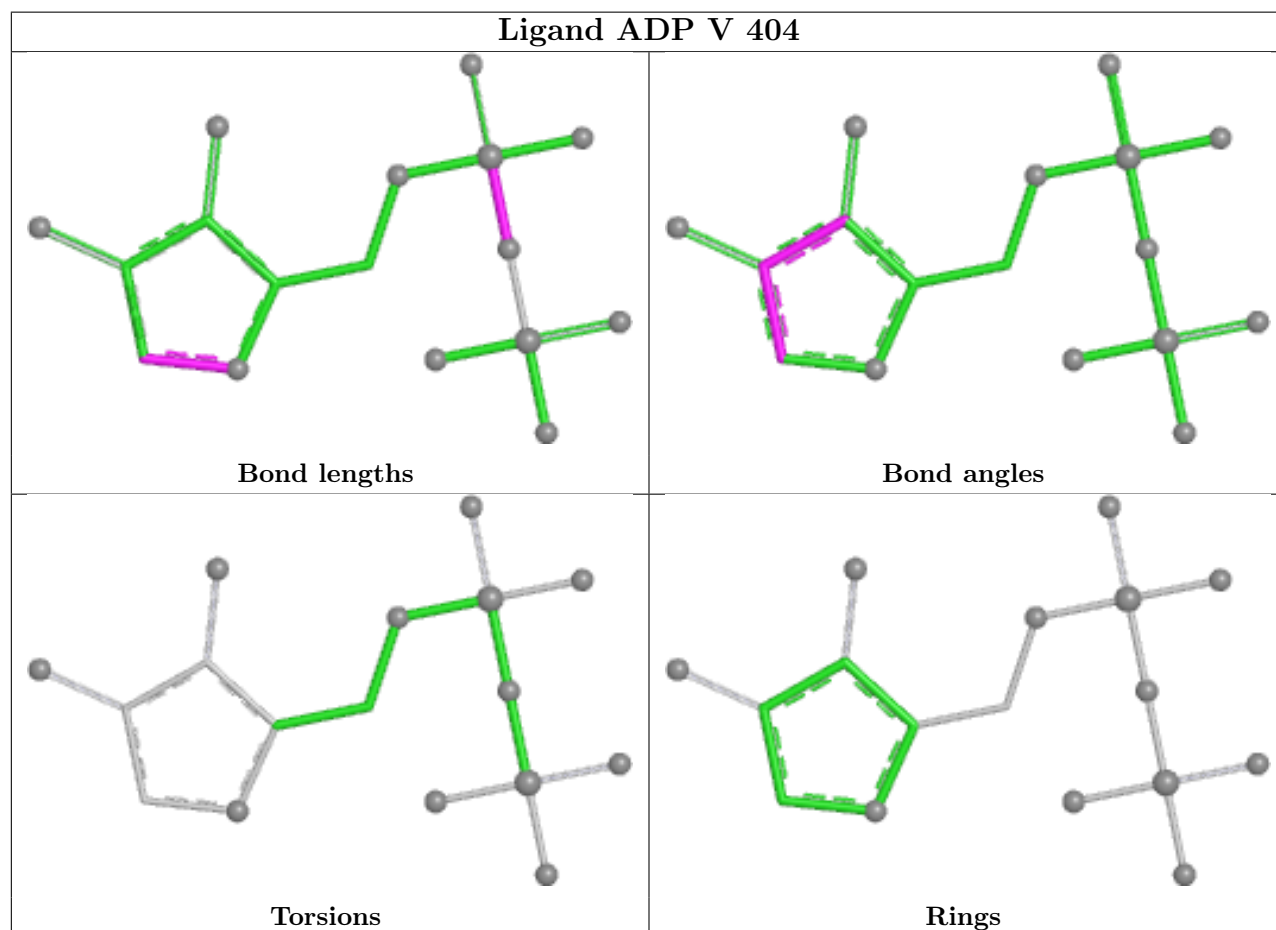
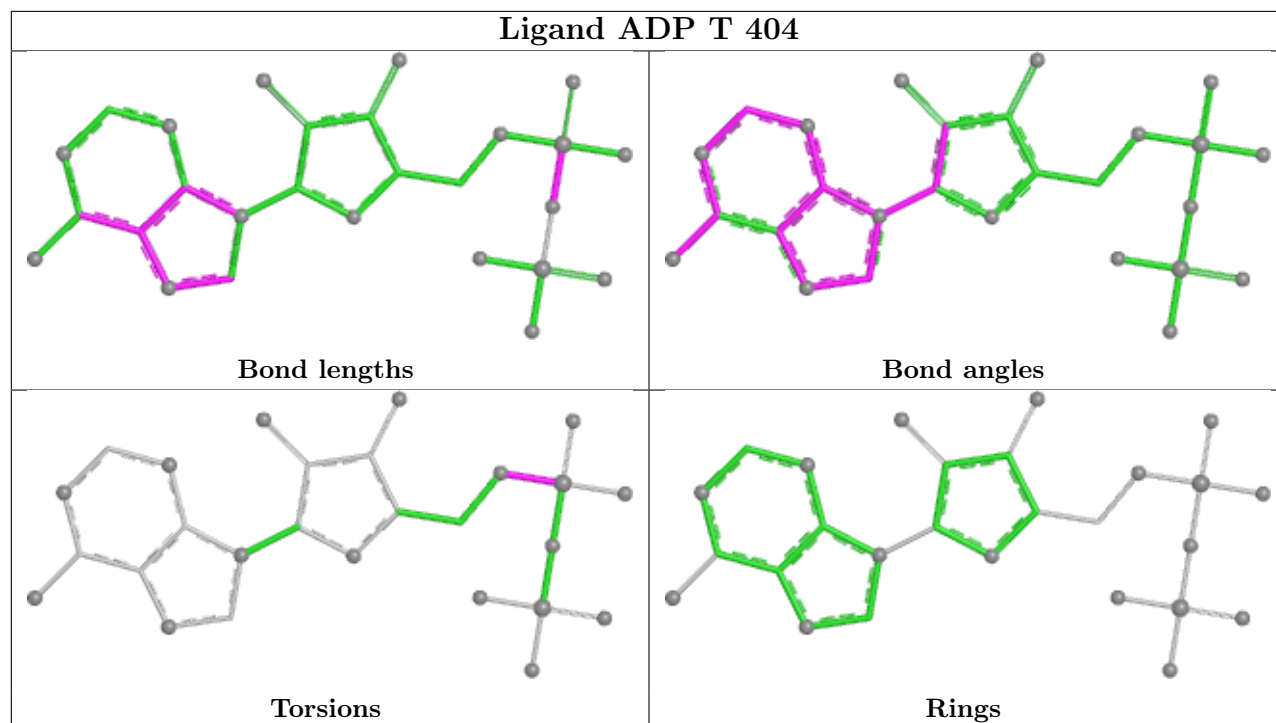
Mol	Chain	Res	Type	Atoms
3	H	404	ADP	O4'-C4'-C5'-O5'
3	X	404	ADP	PA-O3A-PB-O1B
3	R	404	ADP	O4'-C4'-C5'-O5'

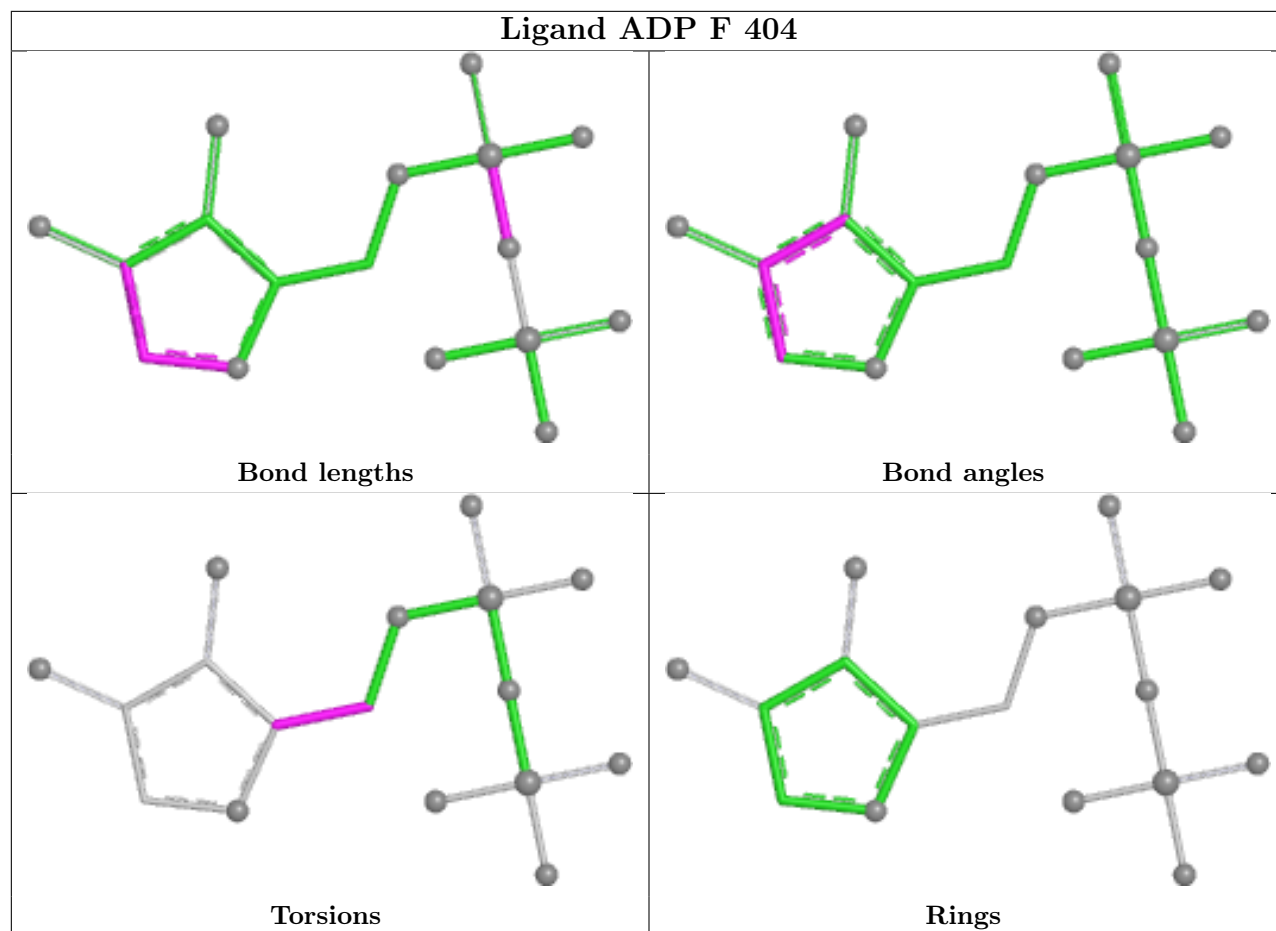
There are no ring outliers.

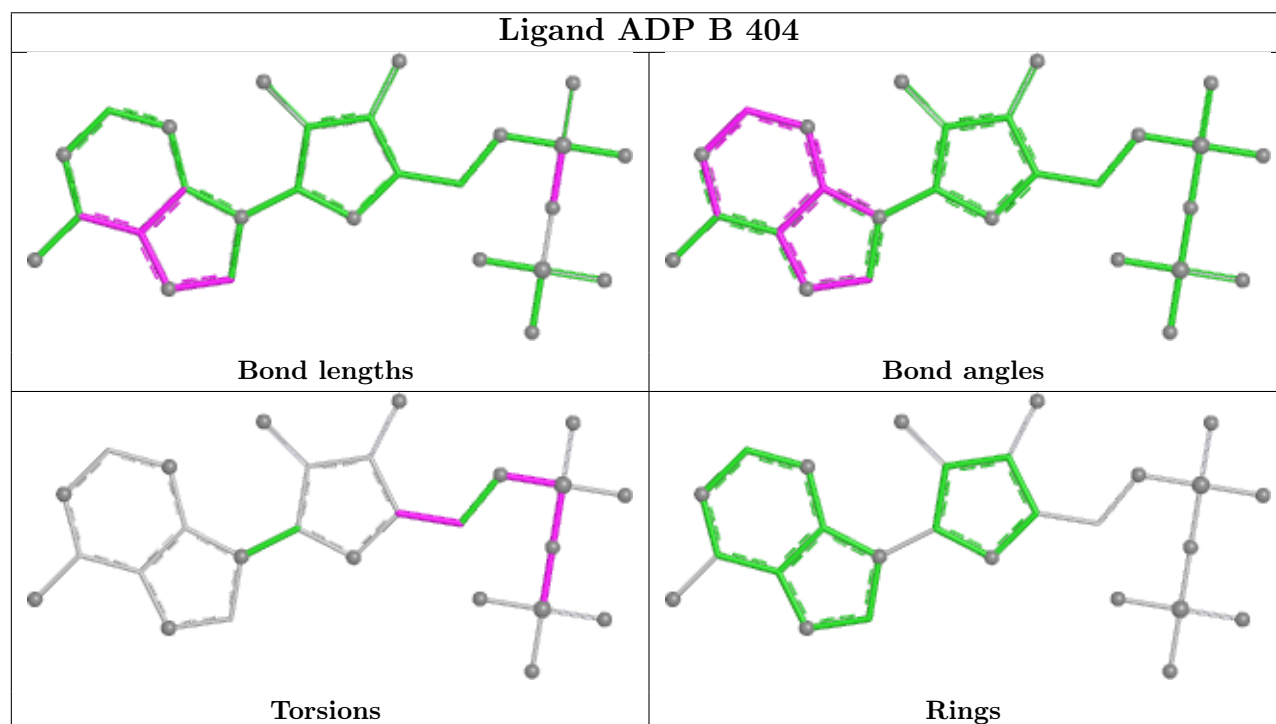
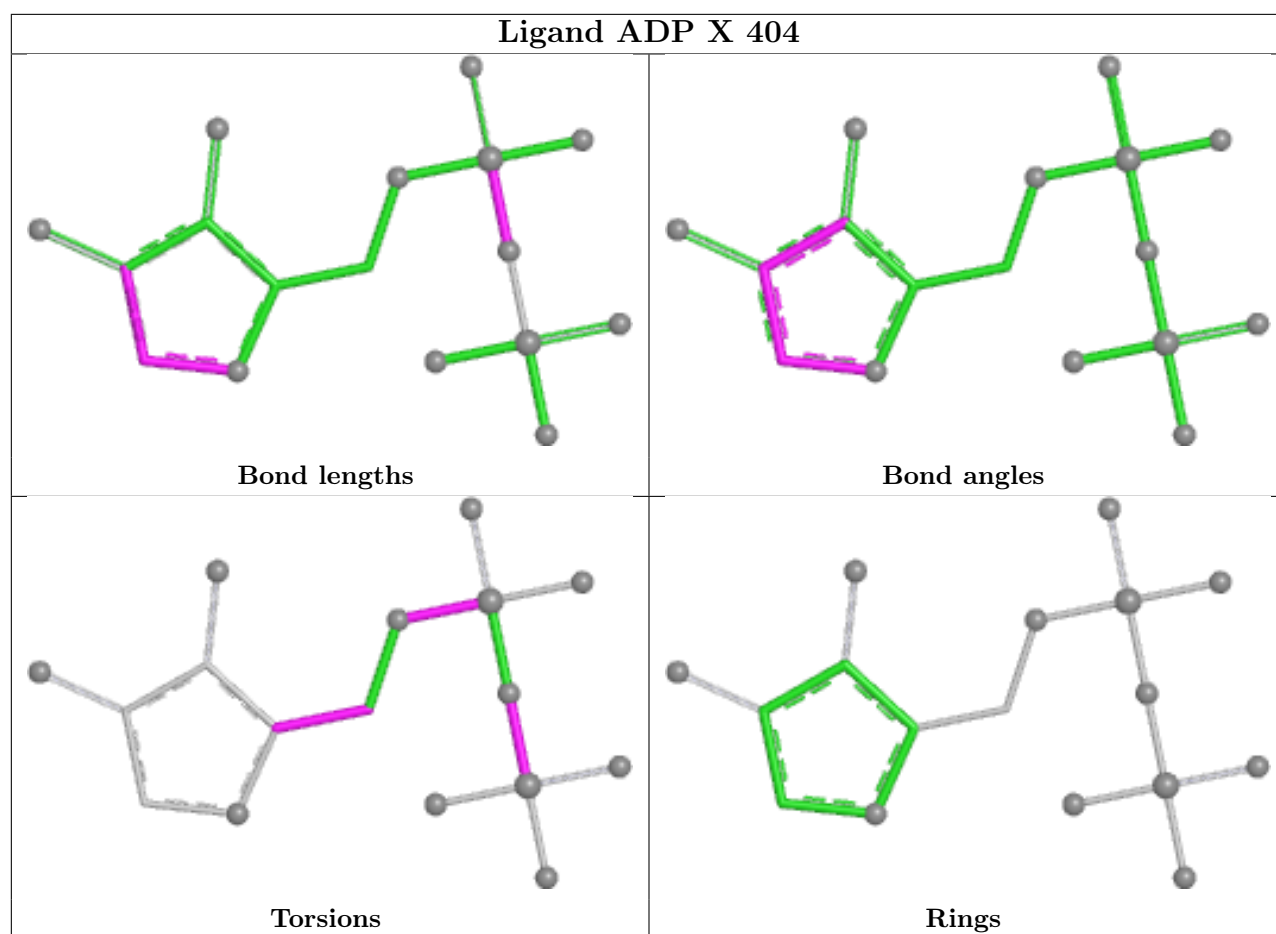
12 monomers are involved in 28 short contacts:

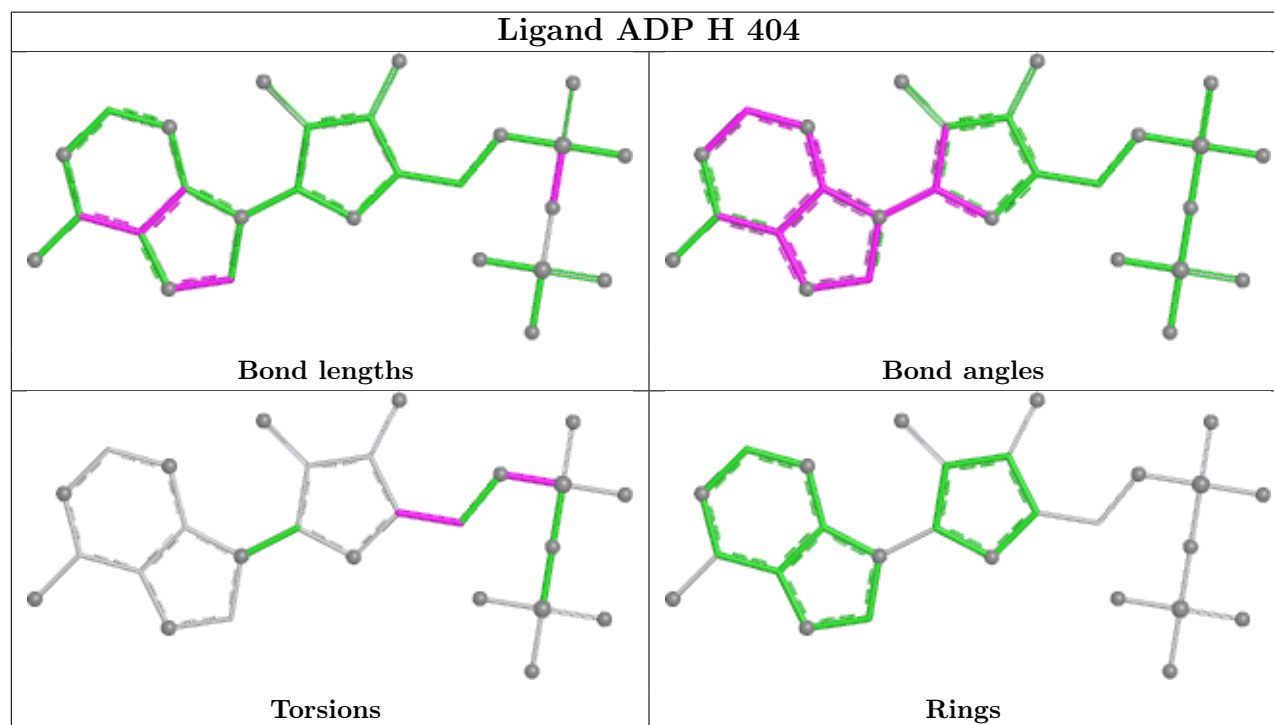
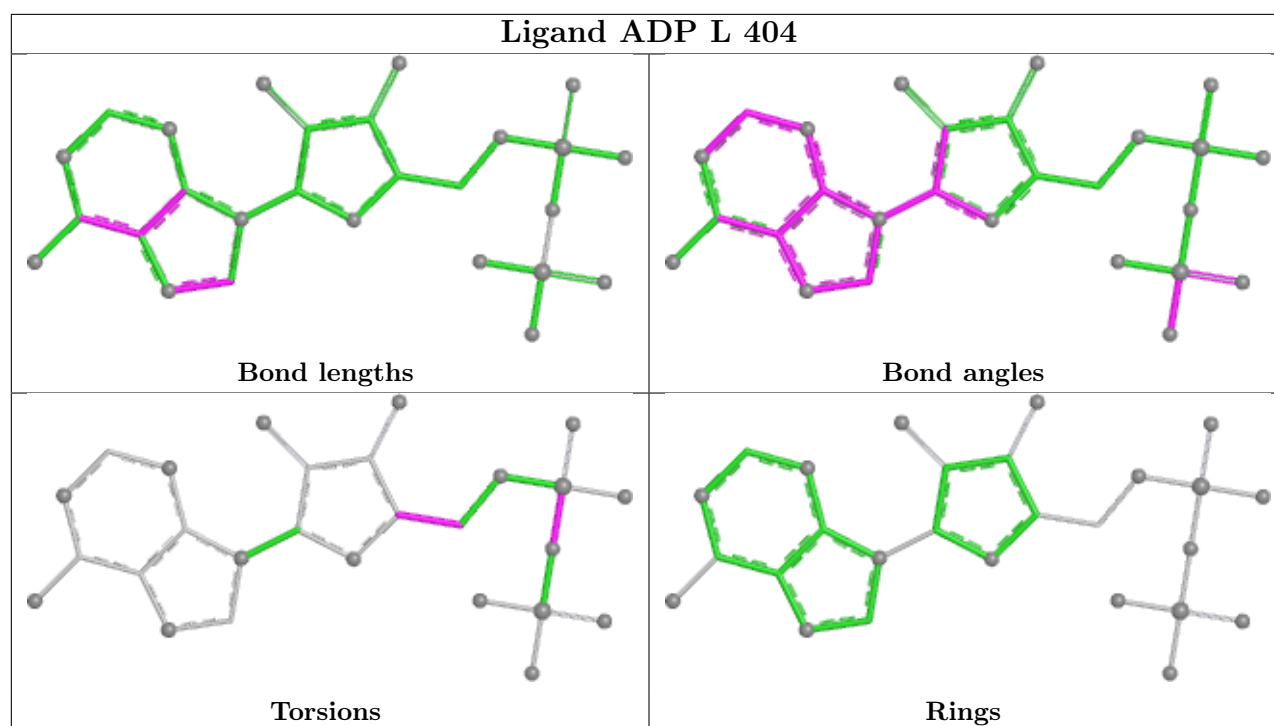
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	404	ADP	3	0
3	V	404	ADP	2	0
3	F	404	ADP	1	0
3	X	404	ADP	1	0
3	B	404	ADP	4	0
3	L	404	ADP	3	0
3	H	404	ADP	2	0
3	N	404	ADP	3	0
3	D	404	ADP	4	0
3	R	404	ADP	1	0
3	P	404	ADP	3	0
3	J	404	ADP	1	0

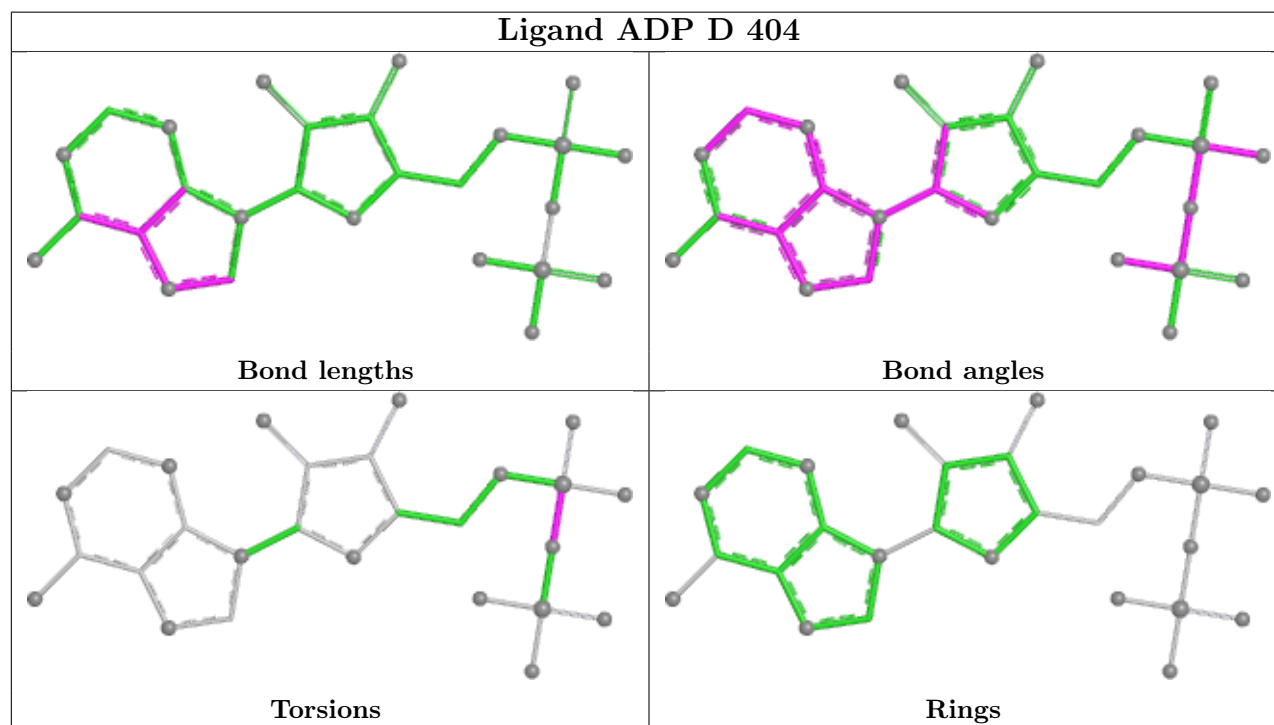
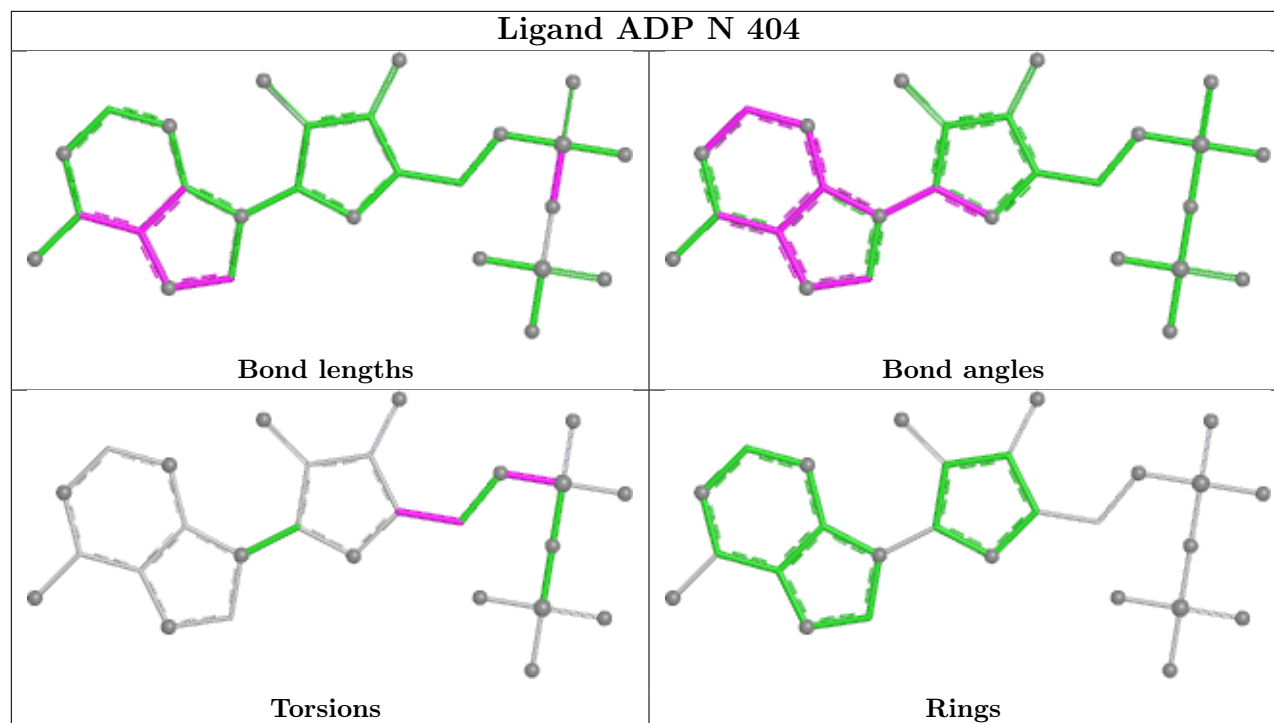
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

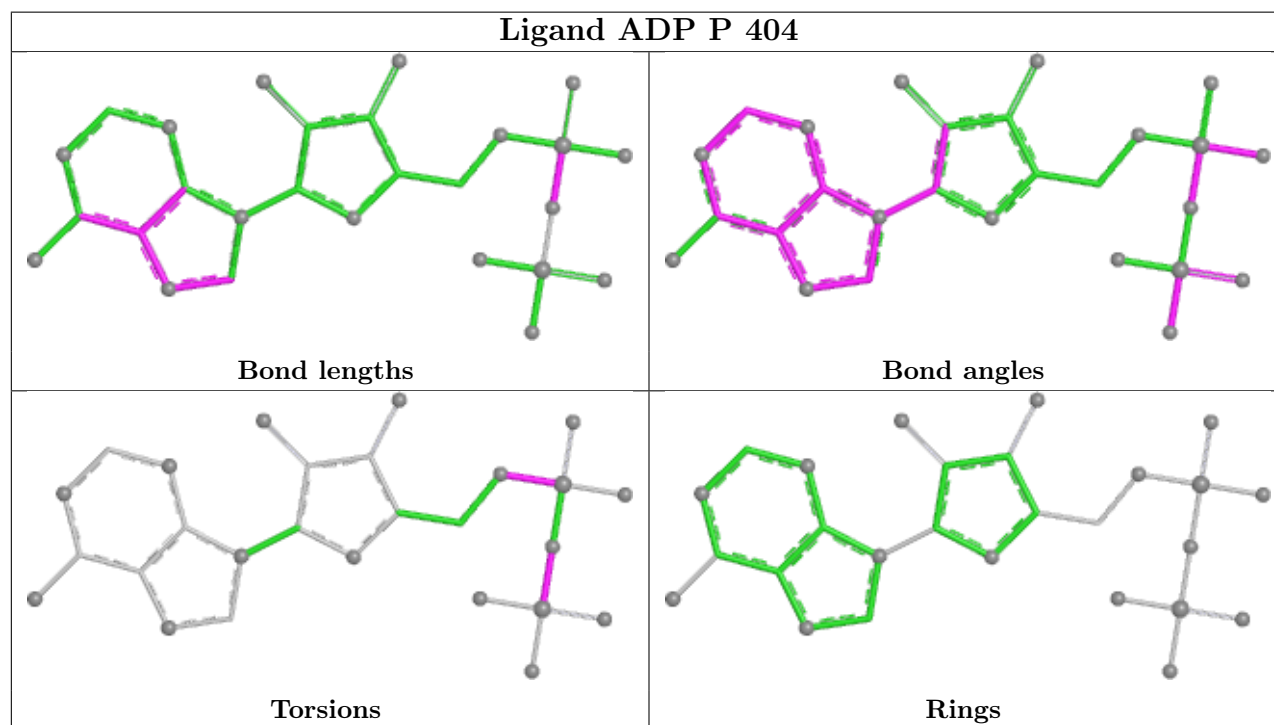
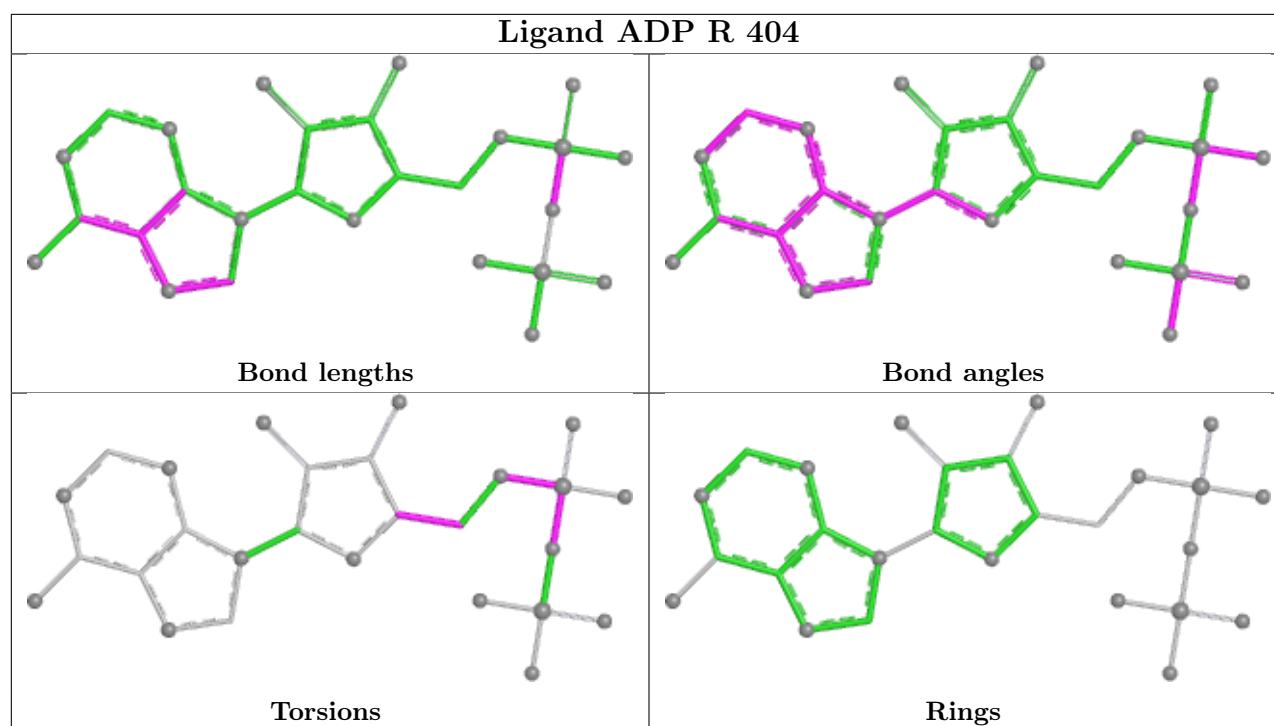


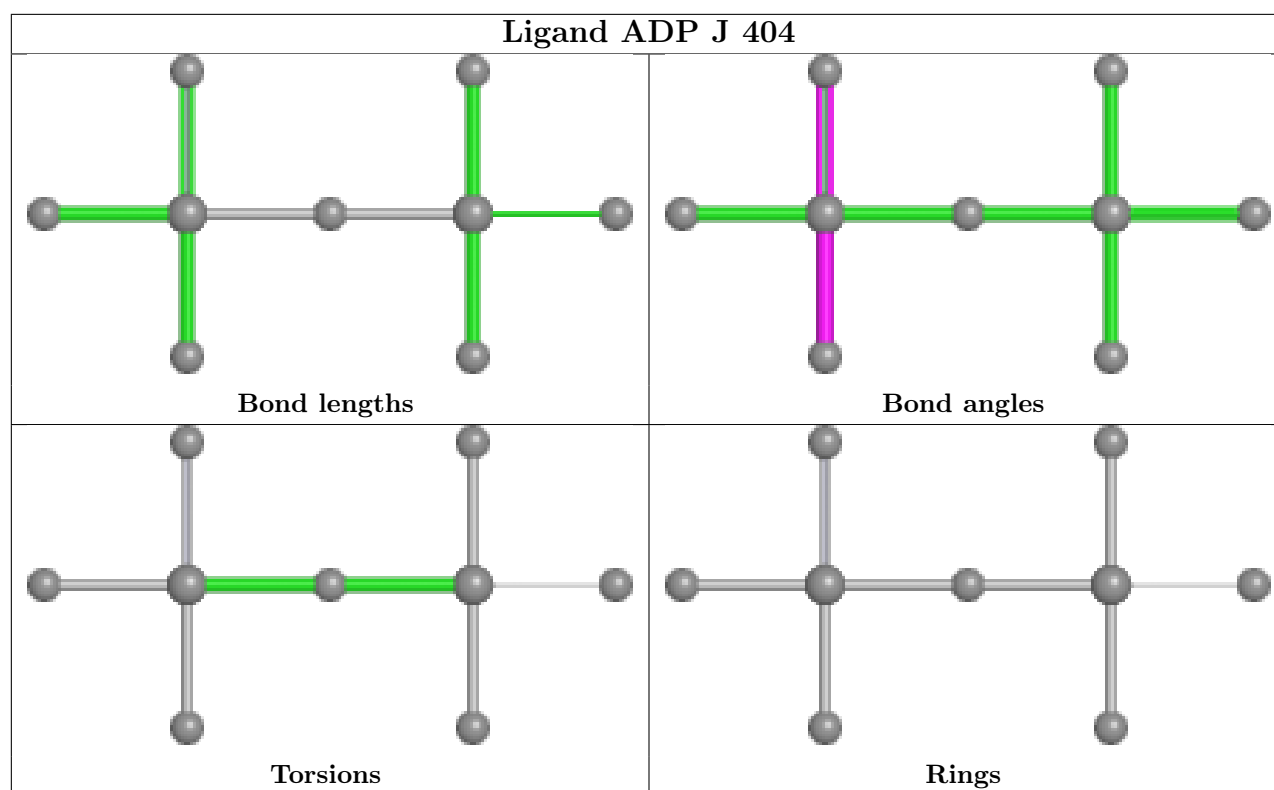












5.7 Other polymers [i](#)

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	260/275 (94%)	0.31	6 (2%) 61 42	46, 53, 67, 74	0
1	C	260/275 (94%)	0.30	4 (1%) 72 53	46, 53, 67, 75	0
1	E	260/275 (94%)	0.17	1 (0%) 88 79	46, 53, 67, 74	0
1	G	260/275 (94%)	0.45	7 (2%) 56 37	46, 53, 67, 74	0
1	I	260/275 (94%)	0.36	4 (1%) 72 53	46, 53, 67, 73	0
1	K	260/275 (94%)	0.42	8 (3%) 51 35	46, 53, 67, 75	0
1	M	260/275 (94%)	0.32	5 (1%) 66 48	46, 53, 67, 75	0
1	O	260/275 (94%)	0.48	6 (2%) 61 42	46, 53, 67, 75	0
1	Q	260/275 (94%)	0.21	1 (0%) 88 79	46, 53, 67, 74	0
1	S	259/275 (94%)	0.48	12 (4%) 37 25	46, 53, 67, 73	0
1	U	255/275 (92%)	0.80	24 (9%) 14 11	46, 53, 66, 73	0
1	W	259/275 (94%)	0.48	8 (3%) 51 35	46, 53, 67, 75	0
2	B	241/248 (97%)	0.20	1 (0%) 88 79	46, 52, 68, 80	0
2	D	248/248 (100%)	0.34	4 (1%) 70 52	45, 52, 68, 80	0
2	F	241/248 (97%)	0.19	4 (1%) 69 50	46, 52, 68, 80	0
2	H	230/248 (92%)	0.52	8 (3%) 47 31	46, 52, 69, 80	0
2	J	241/248 (97%)	0.40	7 (2%) 53 35	46, 52, 68, 80	0
2	L	247/248 (99%)	0.36	2 (0%) 82 68	45, 52, 68, 80	0
2	N	239/248 (96%)	0.26	4 (1%) 69 50	46, 52, 69, 79	0
2	P	248/248 (100%)	0.40	7 (2%) 55 36	45, 52, 68, 80	0
2	R	248/248 (100%)	0.30	4 (1%) 70 52	45, 52, 69, 80	0
2	T	248/248 (100%)	0.36	6 (2%) 59 40	45, 52, 69, 79	0
2	V	239/248 (96%)	0.69	12 (5%) 34 23	46, 52, 68, 79	0
2	X	239/248 (96%)	0.61	12 (5%) 34 23	46, 52, 69, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	6022/6276 (95%)	0.39	157 (2%) 57 38	45, 52, 68, 80	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	166	TYR	4.1
2	L	248	VAL	3.7
1	O	134	GLY	3.7
1	C	12	PRO	3.7
2	X	172	VAL	3.7
1	S	171	TYR	3.5
2	T	248	VAL	3.3
1	K	275	ILE	3.3
2	R	60	GLY	3.3
1	S	138	TRP	3.3
1	A	134	GLY	3.2
1	M	275	ILE	3.2
2	B	15	ASP	3.1
2	N	247	GLY	3.1
2	N	15	ASP	3.1
2	V	170	ASP	3.1
1	U	52	GLY	3.1
1	E	275	ILE	3.0
1	K	149	TYR	3.0
1	U	273	LEU	3.0
2	J	169	ALA	3.0
2	H	171	GLY	3.0
2	F	165	ALA	2.9
2	V	132	LEU	2.9
2	X	54	ALA	2.9
2	H	131	ILE	2.9
1	U	44	LEU	2.9
1	S	175	GLN	2.9
1	A	181	SER	2.8
2	X	12	LEU	2.8
2	F	247	GLY	2.8
1	I	275	ILE	2.8
1	U	171	TYR	2.7
2	V	217	ALA	2.7
1	S	167	ASN	2.7
1	W	213	PRO	2.7
1	O	180	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	W	134	GLY	2.6
2	V	247	GLY	2.6
1	O	104	ASP	2.6
1	Q	104	ASP	2.6
1	G	126	LEU	2.6
1	U	64	LEU	2.6
2	T	60	GLY	2.6
1	W	275	ILE	2.6
1	O	36	ASP	2.6
1	U	88	VAL	2.6
1	M	6	SER	2.5
1	M	77	ASP	2.5
1	U	30	ASP	2.5
2	V	41	ALA	2.5
1	C	275	ILE	2.5
1	S	144	VAL	2.5
2	R	248	VAL	2.5
2	X	165	ALA	2.5
1	A	275	ILE	2.5
1	C	77	ASP	2.5
2	V	55	ILE	2.5
1	U	61	THR	2.5
1	S	88	VAL	2.5
1	S	199	THR	2.4
1	K	37	TYR	2.4
2	H	246	GLU	2.4
1	U	9	ASN	2.4
2	P	178	ASN	2.4
1	K	120	ASP	2.4
2	V	131	ILE	2.4
1	U	40	LEU	2.4
1	G	155	ASP	2.4
1	M	134	GLY	2.4
2	D	60	GLY	2.4
2	X	137	GLY	2.4
1	I	27	ILE	2.4
2	D	161	ILE	2.4
1	U	1	MET	2.4
1	U	197	VAL	2.4
2	P	248	VAL	2.4
2	V	25	PRO	2.4
1	I	248	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	13	ILE	2.3
2	P	101	ILE	2.3
1	K	171	TYR	2.3
1	S	184	LYS	2.3
1	W	130	VAL	2.3
2	X	141	VAL	2.3
1	K	13	ILE	2.3
1	O	80	ASN	2.3
2	P	15	ASP	2.3
2	P	48	GLU	2.3
2	V	71	LEU	2.3
2	V	133	GLN	2.3
1	C	105	GLU	2.2
2	F	60	GLY	2.2
2	H	60	GLY	2.2
1	O	149	TYR	2.2
1	G	29	GLN	2.2
1	W	80	ASN	2.2
2	D	73	ASP	2.2
1	A	14	ILE	2.2
1	G	237	GLY	2.2
2	P	217	ALA	2.2
1	U	182	VAL	2.2
2	J	231	LEU	2.2
2	H	228	ILE	2.2
2	J	13	ILE	2.2
2	H	140	LEU	2.2
2	X	35	LEU	2.2
2	X	205	LEU	2.2
2	R	65	HIS	2.2
2	F	248	VAL	2.1
1	U	90	LEU	2.1
1	U	118	LEU	2.1
2	H	205	LEU	2.1
1	U	274	GLY	2.1
2	T	22	GLY	2.1
1	A	7	ASN	2.1
1	S	236	VAL	2.1
1	U	251	ILE	2.1
2	J	31	ILE	2.1
1	U	22	LEU	2.1
2	T	132	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	18	SER	2.1
2	N	142	SER	2.1
1	K	104	ASP	2.1
2	V	172	VAL	2.1
1	G	131	ILE	2.1
2	P	18	LYS	2.1
2	X	25	PRO	2.1
2	X	167	GLY	2.1
2	H	147	SER	2.1
1	K	251	ILE	2.1
1	M	180	ILE	2.1
1	U	34	LEU	2.1
1	U	235	ILE	2.1
1	W	235	ILE	2.1
2	V	107	ILE	2.1
1	U	13	ILE	2.1
2	X	16	ASP	2.1
2	N	156	PRO	2.1
1	A	173	VAL	2.0
2	T	208	SER	2.0
2	X	107	ILE	2.0
2	J	110	ALA	2.0
1	G	92	PRO	2.0
2	R	128	PHE	2.0
1	W	76	GLU	2.0
2	T	245	GLU	2.0
2	J	241	VAL	2.0
2	D	160	LEU	2.0
2	J	14	LEU	2.0
1	S	35	THR	2.0
1	U	199	THR	2.0
1	U	77	ASP	2.0
1	W	77	ASP	2.0
1	U	237	GLY	2.0
2	L	34	GLU	2.0
1	S	90	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

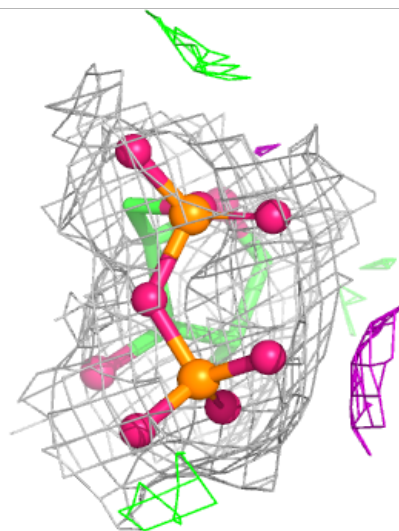
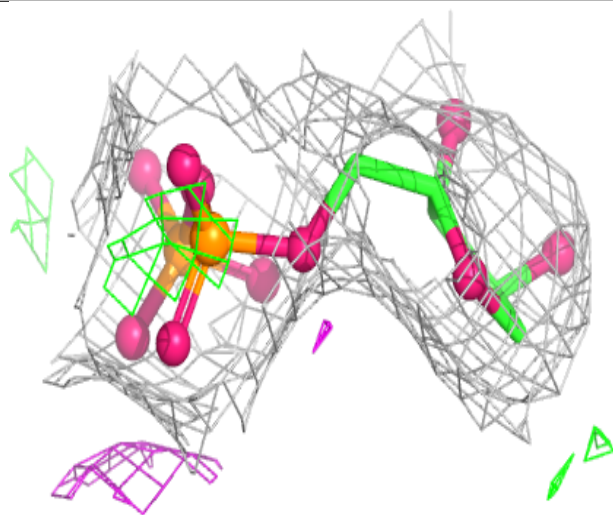
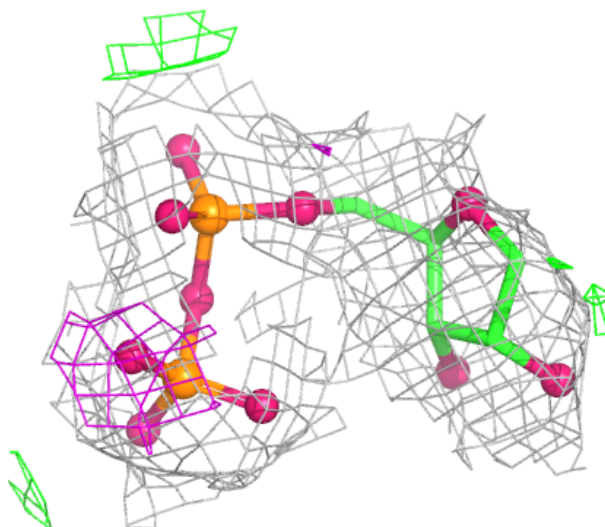
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	V	404	17/27	0.78	0.14	90,93,95,95	0
3	ADP	X	404	17/27	0.81	0.14	86,87,89,89	0
3	ADP	F	404	17/27	0.84	0.12	91,94,95,95	0
3	ADP	H	404	27/27	0.84	0.14	116,117,119,119	0
3	ADP	J	404	9/27	0.89	0.07	100,100,101,101	0
3	ADP	B	404	27/27	0.92	0.08	79,90,95,95	0
3	ADP	N	404	27/27	0.92	0.09	59,62,64,64	0
3	ADP	L	404	27/27	0.94	0.08	52,54,56,58	0
3	ADP	D	404	27/27	0.94	0.08	48,50,51,51	0
3	ADP	R	404	27/27	0.95	0.08	47,55,58,58	0
3	ADP	P	404	27/27	0.96	0.07	33,39,41,42	0
3	ADP	T	404	27/27	0.96	0.07	55,60,63,63	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.

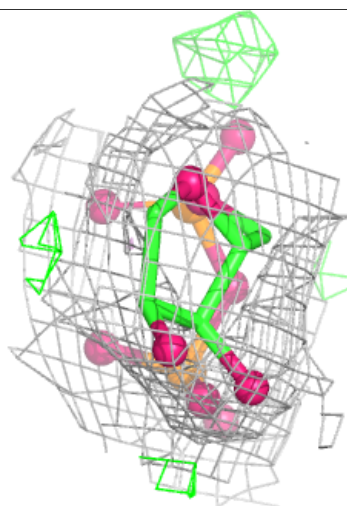
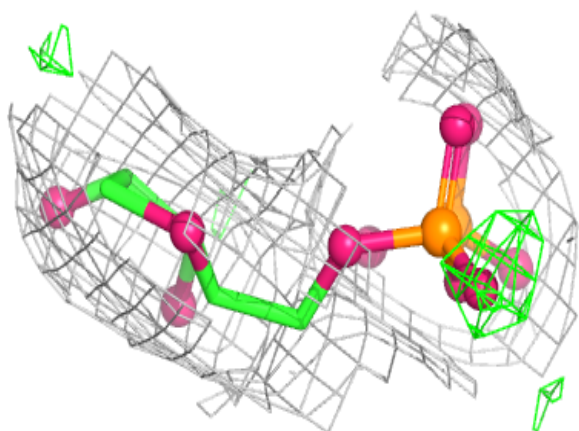
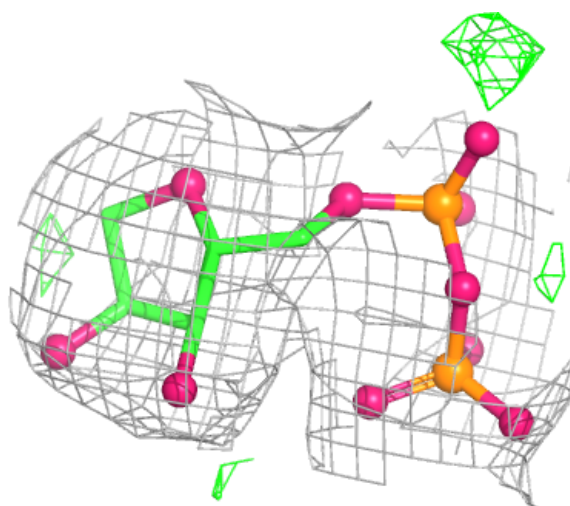
Electron density around ADP V 404:

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



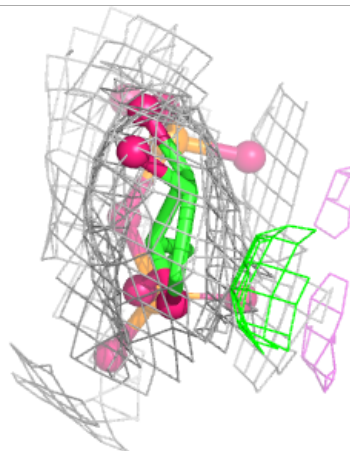
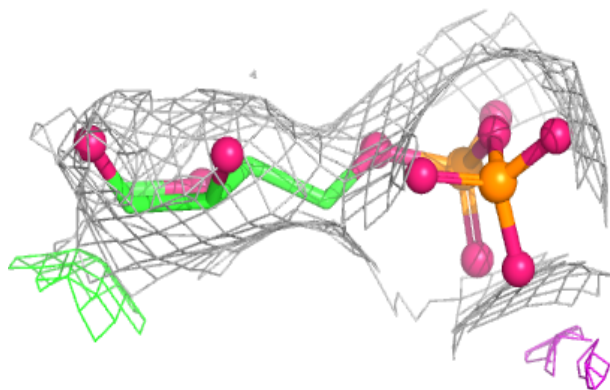
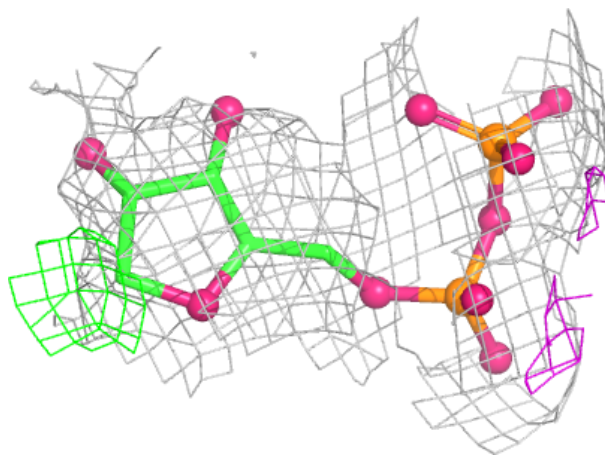
Electron density around ADP X 404:

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and green (positive)



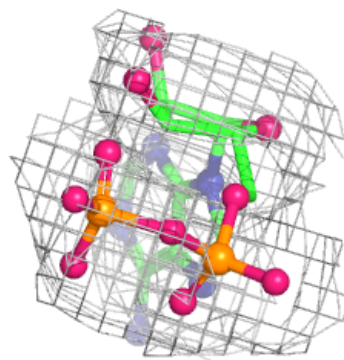
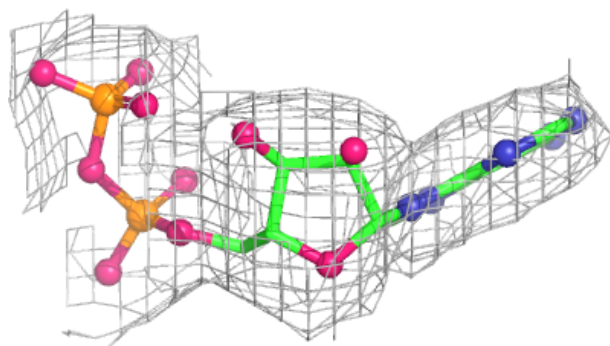
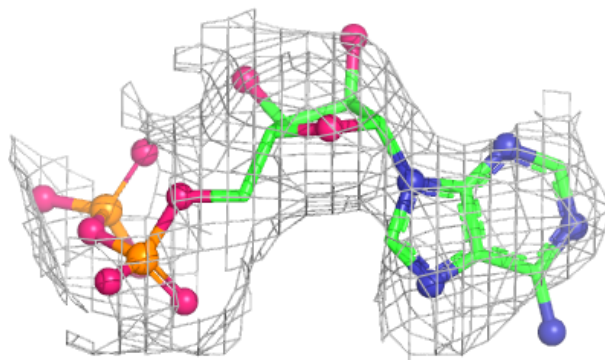
Electron density around ADP F 404:

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and green (positive)



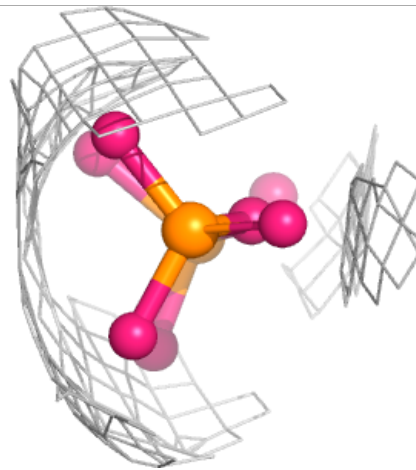
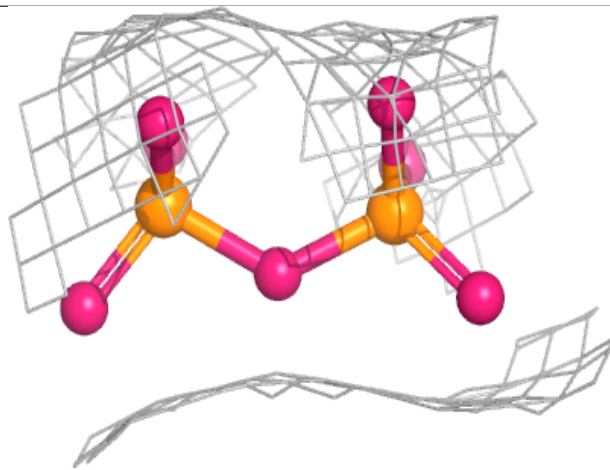
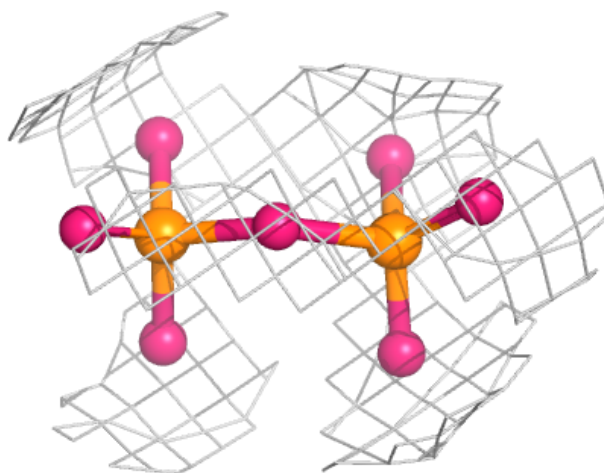
Electron density around ADP H 404:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



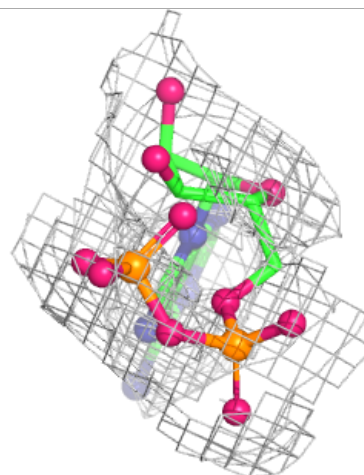
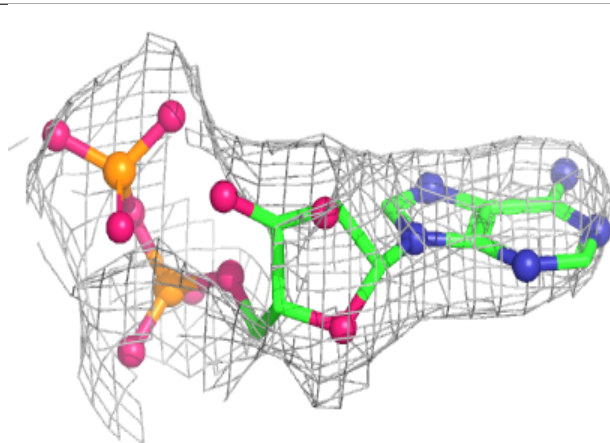
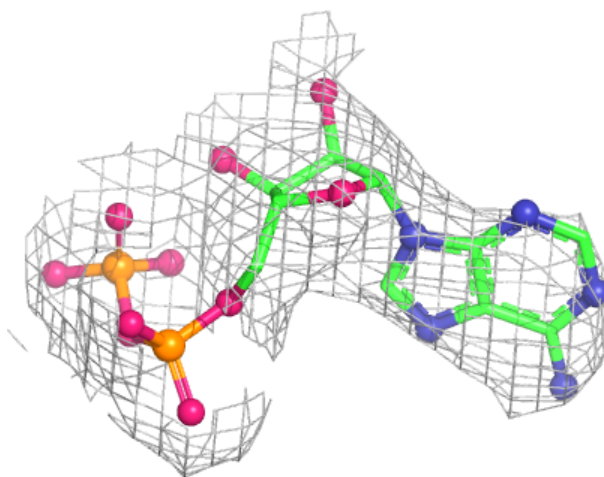
Electron density around ADP J 404:

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and green (positive)



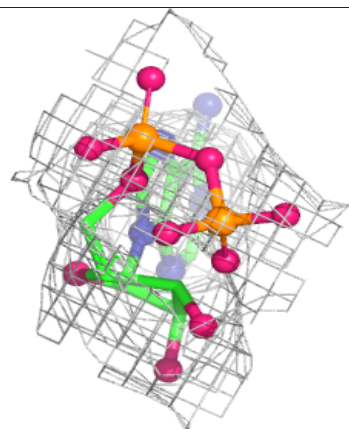
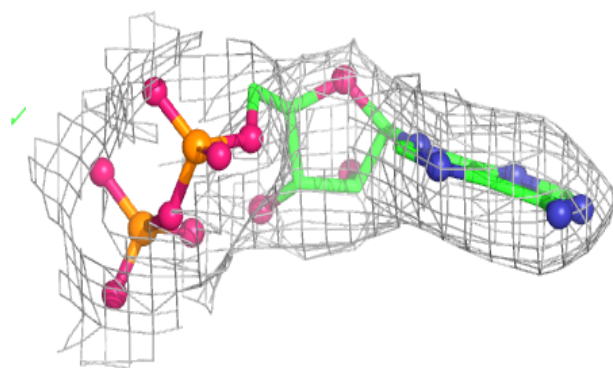
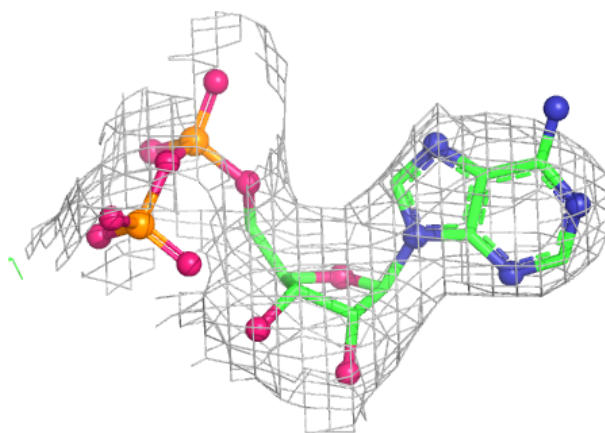
Electron density around ADP B 404:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

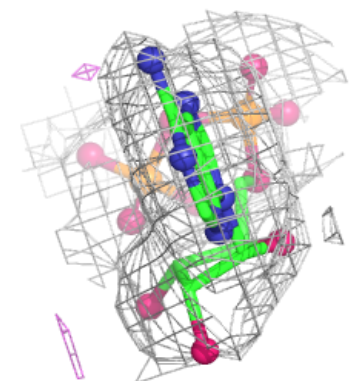
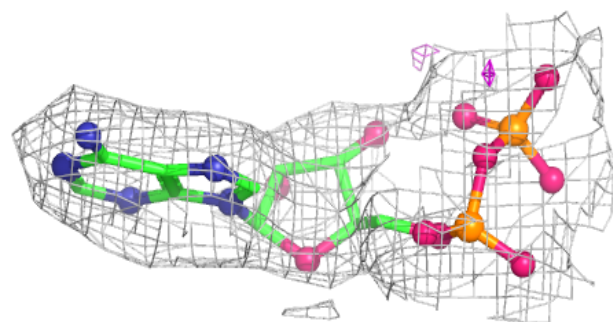
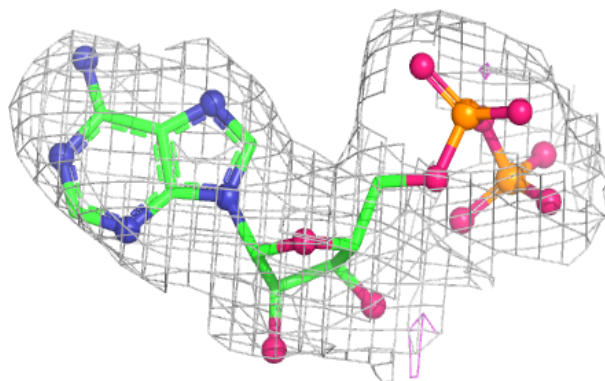


Electron density around ADP N 404:

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

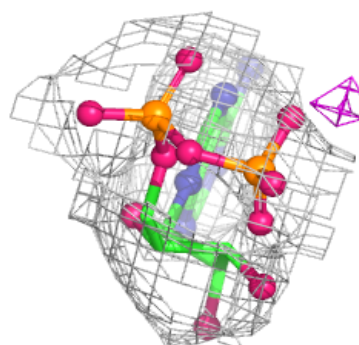
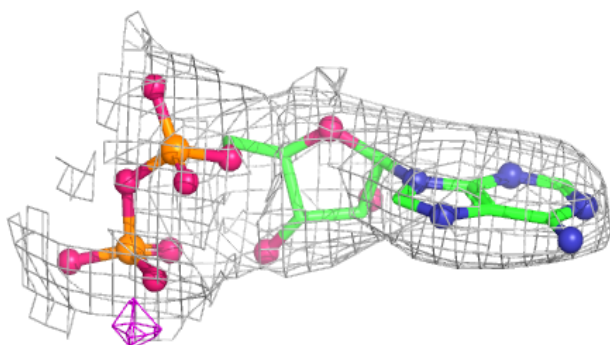
**Electron density around ADP L 404:**

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

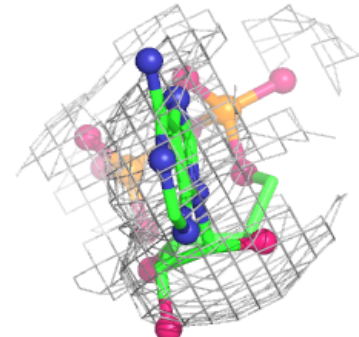
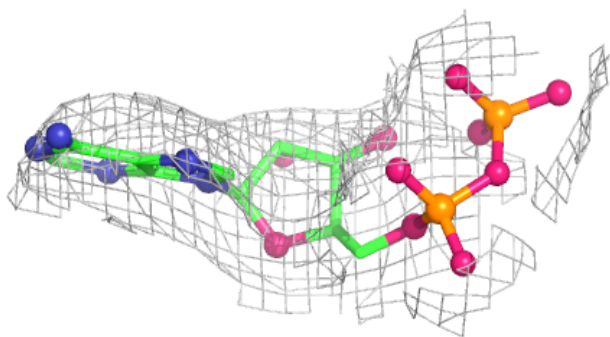
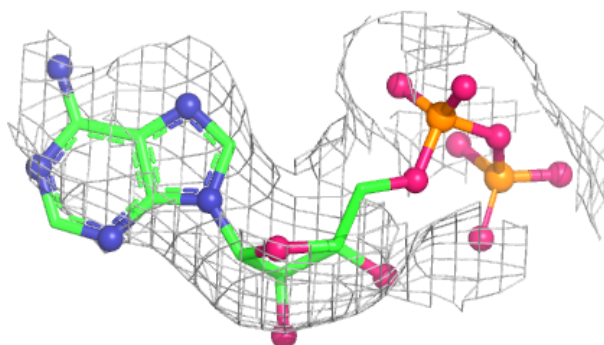


Electron density around ADP D 404:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

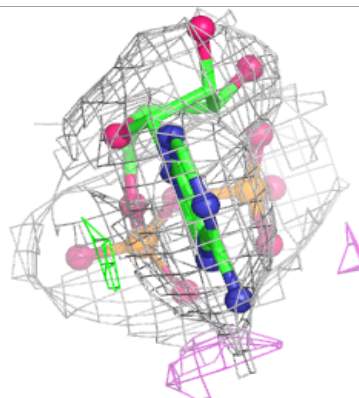
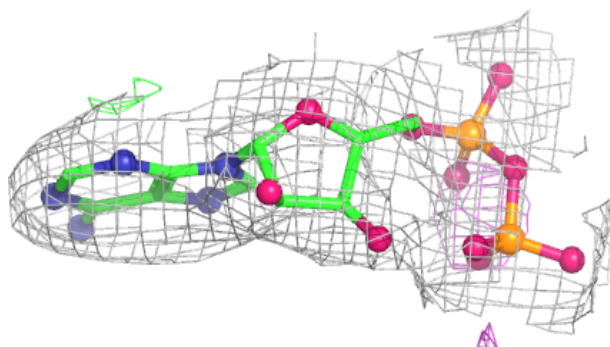
**Electron density around ADP R 404:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

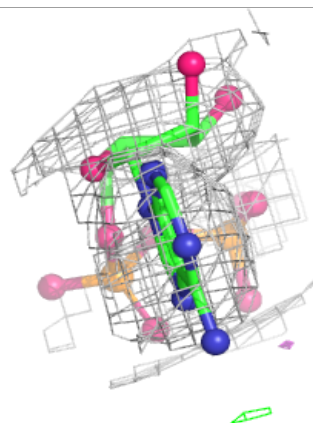
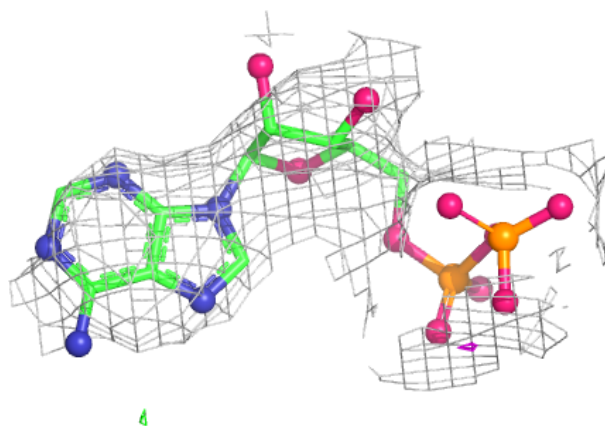


Electron density around ADP P 404:

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

**Electron density around ADP T 404:**

$2mF_o-DF_c$ (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.