



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:34 AM UTC

PDB ID : 3CF0 / pdb_00003cf0
Title : Structure of D2 subdomain of P97/VCP in complex with ADP
Authors : Davies, J.M.; Brunger, A.T.; Weis, W.I.
Deposited on : 2008-03-01
Resolution : 3.00 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

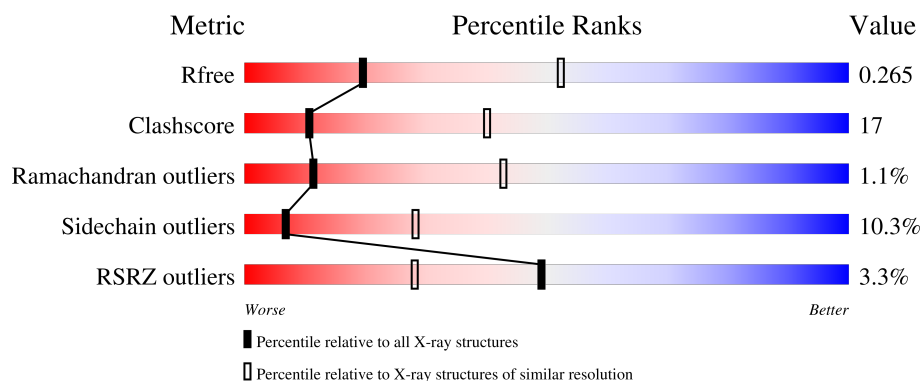
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



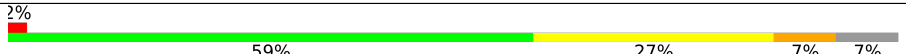
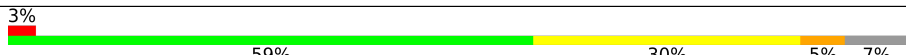
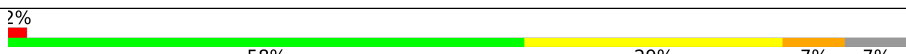
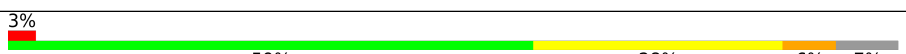
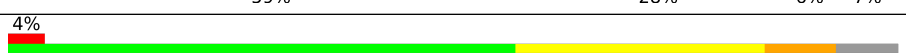
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	301	
1	B	301	
1	C	301	
1	D	301	
1	E	301	

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Mol	Chain	Length	Quality of chain
1	F	301	
1	G	301	
1	H	301	
1	I	301	
1	J	301	
1	K	301	
1	L	301	
1	M	301	
1	N	301	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31164 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	B	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	C	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	D	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	E	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	F	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	G	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	H	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	I	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	J	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	K	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	L	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	M	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			
1	N	281	Total	C	N	O	S	0	0	0
			2199	1391	382	414	12			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

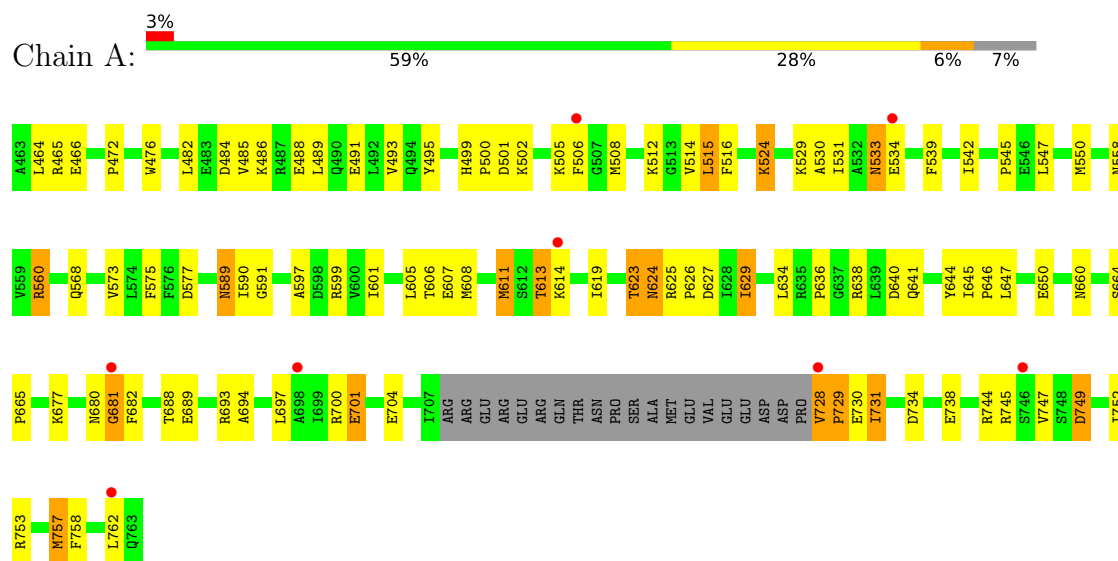


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

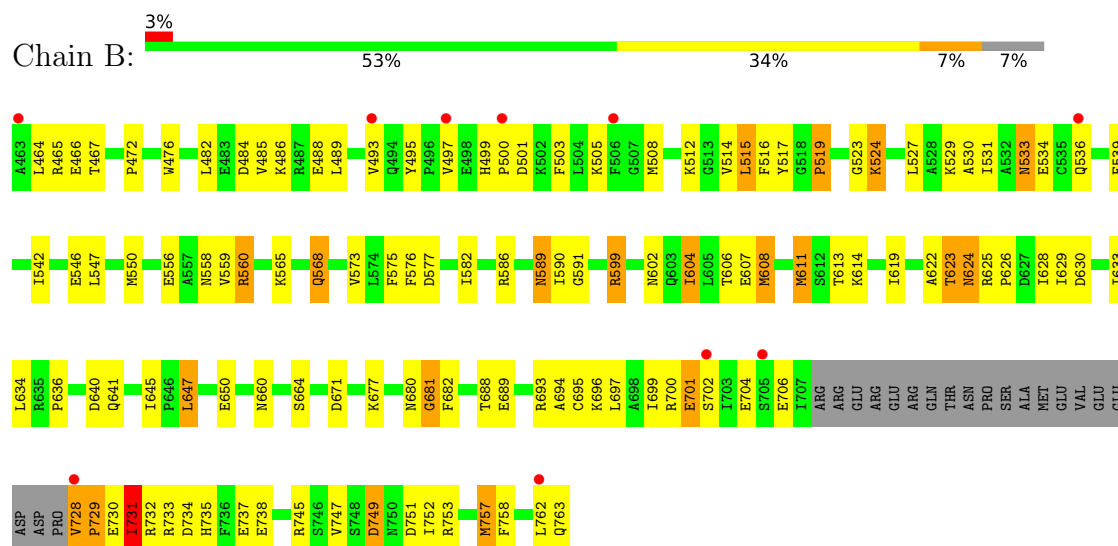
3 Residue-property plots [i](#)

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.

- Molecule 1: Transitional endoplasmic reticulum ATPase

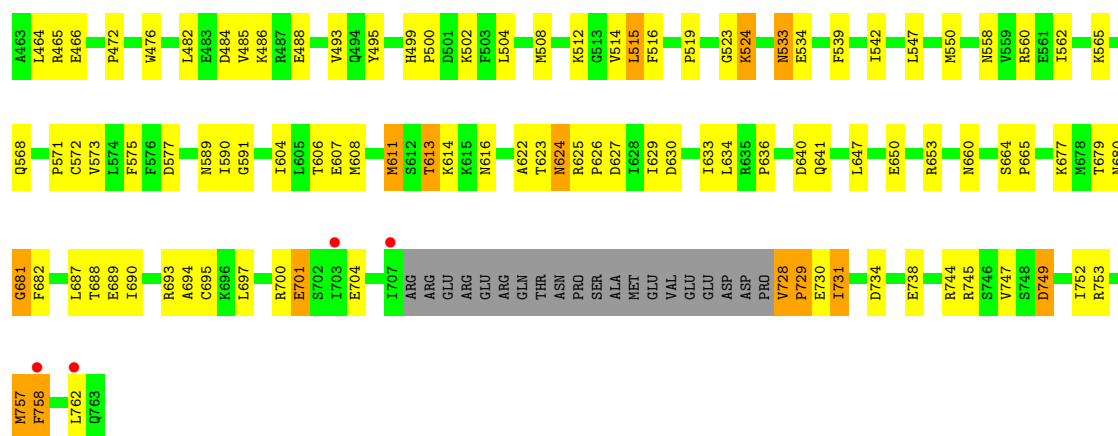


- Molecule 1: Transitional endoplasmic reticulum ATPase

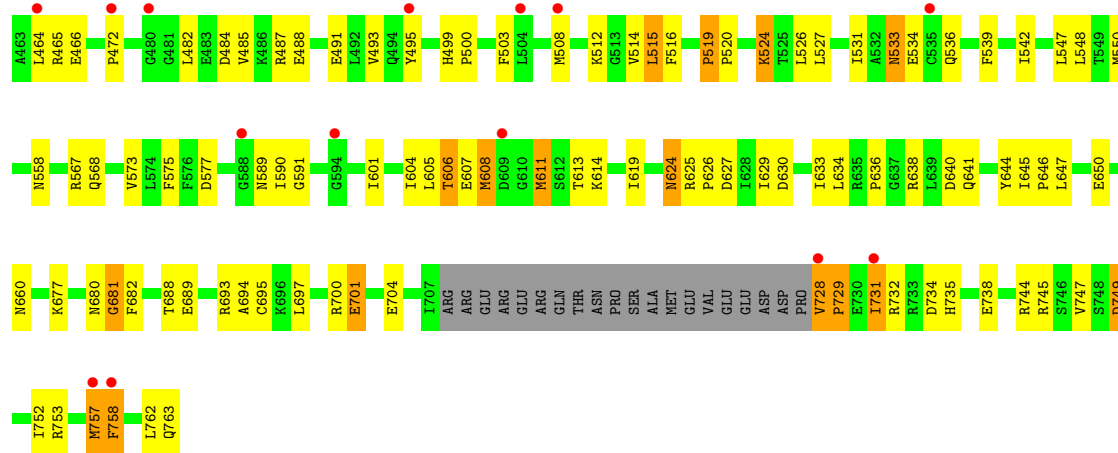


- Molecule 1: Transitional endoplasmic reticulum ATPase

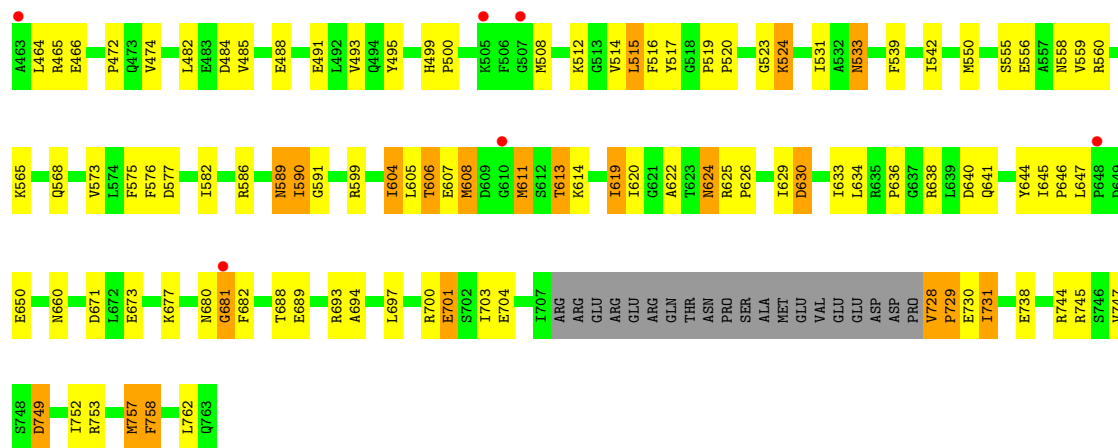




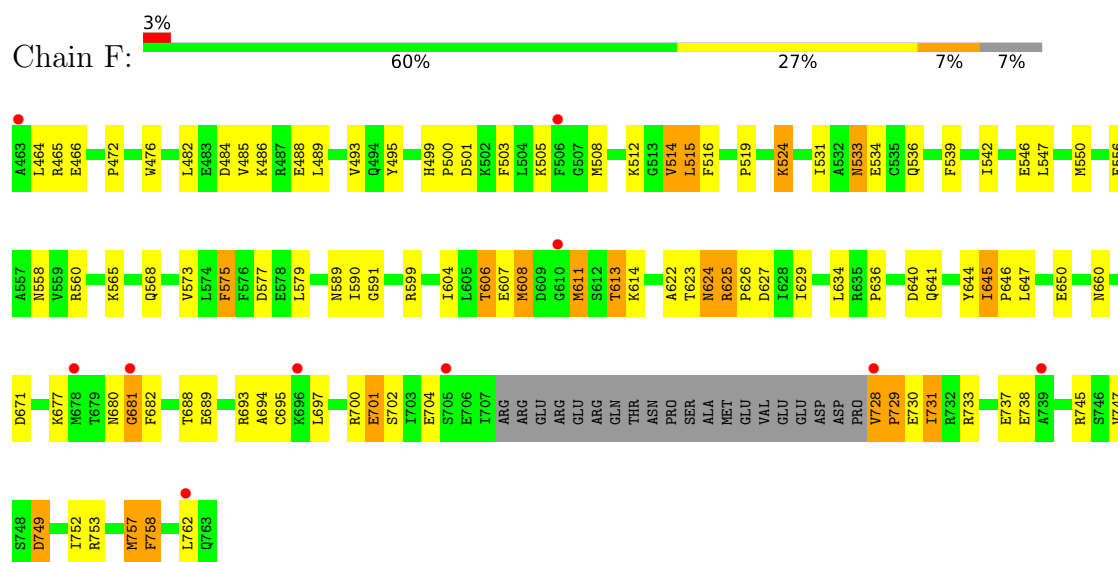
• Molecule 1: Transitional endoplasmic reticulum ATPase



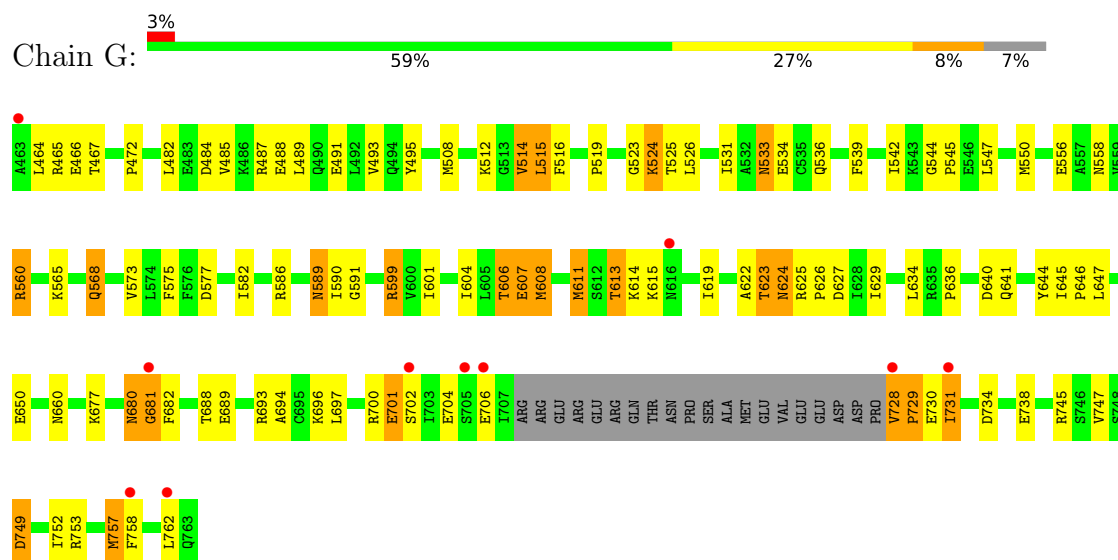
• Molecule 1: Transitional endoplasmic reticulum ATPase



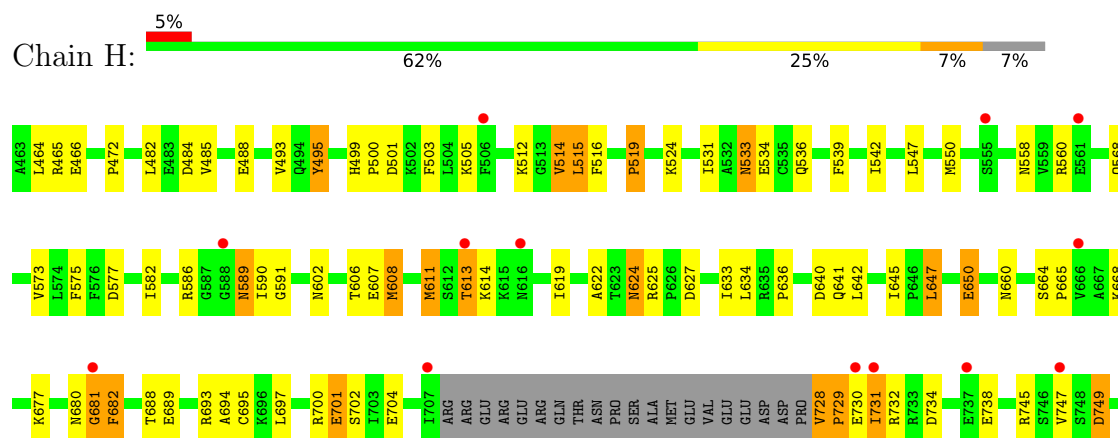
• Molecule 1: Transitional endoplasmic reticulum ATPase

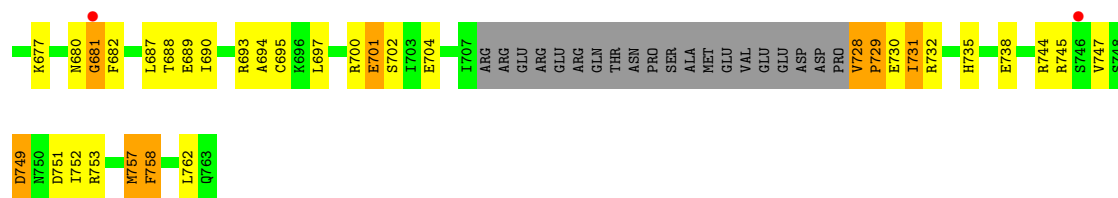


• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase

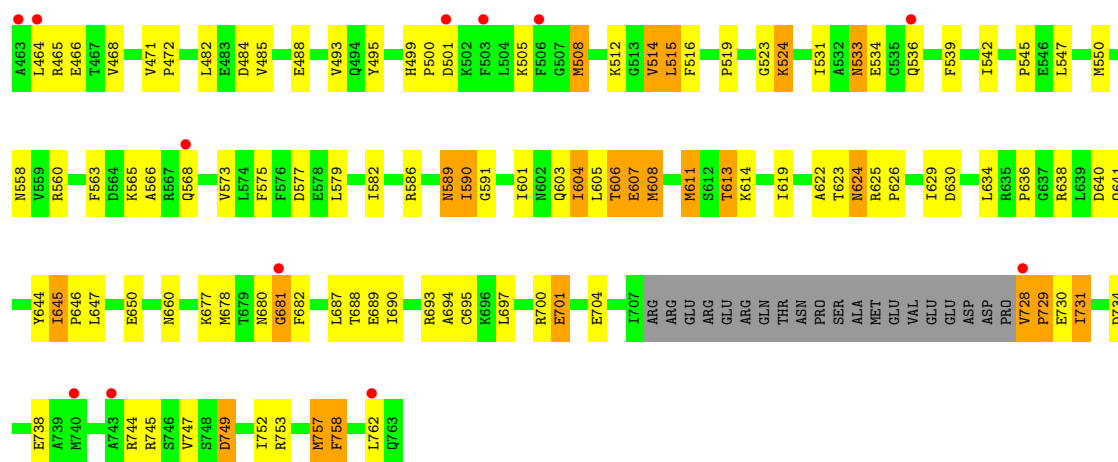




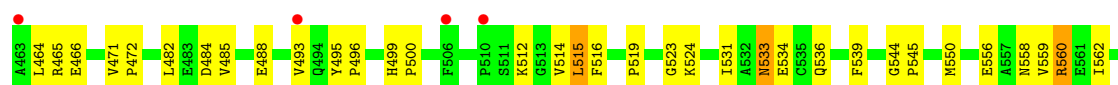
• Molecule 1: Transitional endoplasmic reticulum ATPase

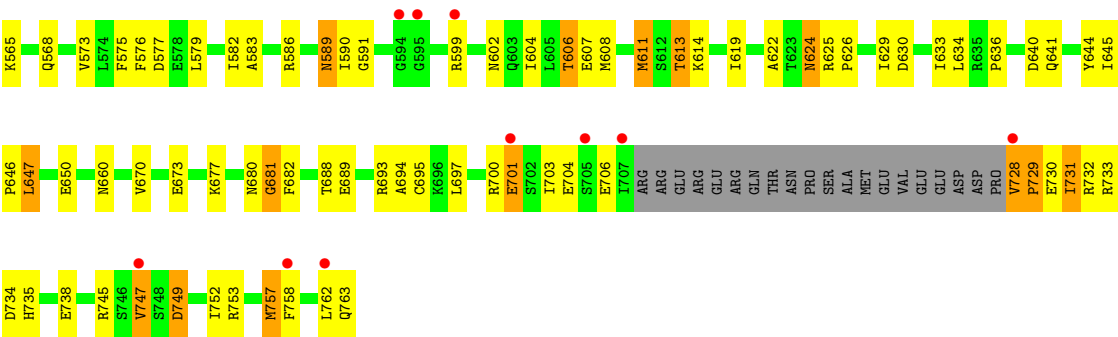


• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.32Å 167.22Å 209.47Å 90.00° 112.29° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-3.00) 96.3 (30.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.243 , 0.262 0.237 , 0.265	Depositor DCC
R_{free} test set	9759 reflections (8.84%)	wwPDB-VP
Wilson B-factor (Å ²)	84.5	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 96.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-1/2*h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31164	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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	1.01	2/2236 (0.1%)	1.15	3/3015 (0.1%)
1	B	1.14	4/2236 (0.2%)	1.21	7/3015 (0.2%)
1	C	1.16	2/2236 (0.1%)	1.23	9/3015 (0.3%)
1	D	1.05	0/2236	1.16	6/3015 (0.2%)
1	E	1.24	3/2236 (0.1%)	1.24	10/3015 (0.3%)
1	F	1.07	1/2236 (0.0%)	1.17	8/3015 (0.3%)
1	G	1.16	1/2236 (0.0%)	1.25	8/3015 (0.3%)
1	H	1.08	1/2236 (0.0%)	1.18	6/3015 (0.2%)
1	I	1.23	0/2236	1.27	12/3015 (0.4%)
1	J	1.09	0/2236	1.18	5/3015 (0.2%)
1	K	1.05	1/2236 (0.0%)	1.16	7/3015 (0.2%)
1	L	1.15	3/2236 (0.1%)	1.20	7/3015 (0.2%)
1	M	1.17	5/2236 (0.2%)	1.25	11/3015 (0.4%)
1	N	1.08	2/2236 (0.1%)	1.19	6/3015 (0.2%)
All	All	1.12	25/31304 (0.1%)	1.20	105/42210 (0.2%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	625	ARG	N-CA	-6.39	1.40	1.46
1	E	619	ILE	CA-CB	-6.38	1.46	1.54
1	E	620	ILE	CA-CB	-6.17	1.46	1.54
1	L	685	ALA	CA-CB	-6.07	1.44	1.53
1	M	468	VAL	CA-CB	5.88	1.60	1.53
1	A	597	ALA	CA-CB	-5.86	1.44	1.53
1	M	519	PRO	C-O	5.77	1.30	1.24
1	K	620	ILE	CA-CB	-5.65	1.47	1.54
1	B	497	VAL	CA-CB	5.58	1.62	1.54
1	E	519	PRO	C-O	5.42	1.30	1.24
1	L	577	ASP	CA-C	5.38	1.60	1.53
1	B	628	ILE	C-O	-5.34	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	682	PHE	CA-C	-5.31	1.46	1.52
1	N	619	ILE	CA-CB	-5.31	1.47	1.54
1	C	519	PRO	C-O	5.24	1.30	1.24
1	L	469	VAL	CA-CB	-5.24	1.48	1.54
1	A	629	ILE	CA-CB	5.23	1.59	1.54
1	C	607	GLU	C-O	-5.17	1.17	1.24
1	B	602	ASN	N-CA	-5.15	1.40	1.46
1	B	731	ILE	CA-CB	5.10	1.59	1.53
1	M	590	ILE	CA-CB	5.10	1.60	1.54
1	G	601	ILE	C-O	5.07	1.30	1.24
1	M	566	ALA	CA-CB	-5.07	1.45	1.53
1	M	619	ILE	CA-CB	-5.05	1.48	1.54
1	N	576	PHE	CA-C	-5.00	1.46	1.52

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	519	PRO	CA-C-N	9.29	129.05	119.76
1	N	519	PRO	C-N-CA	9.29	129.05	119.76
1	J	519	PRO	CA-C-N	8.08	127.84	119.76
1	J	519	PRO	C-N-CA	8.08	127.84	119.76
1	I	645	ILE	CA-C-N	7.89	128.34	120.52
1	I	645	ILE	C-N-CA	7.89	128.34	120.52
1	B	519	PRO	CA-C-N	7.67	127.43	119.76
1	B	519	PRO	C-N-CA	7.67	127.43	119.76
1	C	519	PRO	CA-C-N	7.67	127.95	119.90
1	C	519	PRO	C-N-CA	7.67	127.95	119.90
1	M	519	PRO	CA-C-N	7.55	128.66	120.13
1	M	519	PRO	C-N-CA	7.55	128.66	120.13
1	D	519	PRO	CA-C-N	7.46	127.22	119.76
1	D	519	PRO	C-N-CA	7.46	127.22	119.76
1	H	519	PRO	CA-C-N	7.44	127.20	119.76
1	H	519	PRO	C-N-CA	7.44	127.20	119.76
1	K	519	PRO	CA-C-N	7.43	127.70	119.90
1	K	519	PRO	C-N-CA	7.43	127.70	119.90
1	F	519	PRO	CA-C-N	7.08	127.34	119.90
1	F	519	PRO	C-N-CA	7.08	127.34	119.90
1	G	608	MET	N-CA-C	-6.72	105.64	114.31
1	L	519	PRO	CA-C-N	6.62	126.85	119.90
1	L	519	PRO	C-N-CA	6.62	126.85	119.90
1	M	608	MET	N-CA-C	-6.44	106.00	114.31
1	A	601	ILE	N-CA-C	-6.27	104.22	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	608	MET	N-CA-C	-6.22	106.28	114.31
1	G	645	ILE	CA-C-N	6.20	126.65	120.52
1	G	645	ILE	C-N-CA	6.20	126.65	120.52
1	G	519	PRO	CA-C-N	6.08	125.84	119.76
1	G	519	PRO	C-N-CA	6.08	125.84	119.76
1	L	608	MET	N-CA-C	-6.03	106.26	113.97
1	E	519	PRO	CA-C-N	6.02	126.22	119.90
1	E	519	PRO	C-N-CA	6.02	126.22	119.90
1	I	519	PRO	CA-C-N	5.98	126.18	119.90
1	I	519	PRO	C-N-CA	5.98	126.18	119.90
1	M	758	PHE	N-CA-C	-5.94	103.98	111.11
1	I	470	GLU	CA-C-N	-5.92	117.59	123.04
1	I	470	GLU	C-N-CA	-5.92	117.59	123.04
1	F	608	MET	N-CA-C	-5.82	106.83	114.04
1	K	645	ILE	CA-C-N	5.77	126.23	120.52
1	K	645	ILE	C-N-CA	5.77	126.23	120.52
1	J	645	ILE	CA-C-N	5.76	126.22	120.52
1	J	645	ILE	C-N-CA	5.76	126.22	120.52
1	A	645	ILE	CA-C-N	5.73	127.04	120.85
1	A	645	ILE	C-N-CA	5.73	127.04	120.85
1	N	645	ILE	CA-C-N	5.71	126.18	120.52
1	N	645	ILE	C-N-CA	5.71	126.18	120.52
1	E	474	VAL	N-CA-C	5.70	117.20	108.71
1	C	758	PHE	N-CA-C	-5.69	104.98	111.07
1	K	758	PHE	N-CA-C	-5.69	104.29	111.11
1	I	758	PHE	N-CA-C	-5.61	105.07	111.07
1	M	630	ASP	CA-C-N	5.59	125.70	119.32
1	M	630	ASP	C-N-CA	5.59	125.70	119.32
1	F	645	ILE	CA-C-N	5.59	126.05	120.52
1	F	645	ILE	C-N-CA	5.59	126.05	120.52
1	H	695	CYS	CB-CA-C	-5.56	102.08	110.92
1	I	590	ILE	N-CA-C	5.55	115.79	110.74
1	D	548	LEU	N-CA-C	5.53	117.31	111.28
1	H	608	MET	N-CA-C	-5.53	107.17	114.31
1	L	645	ILE	CA-C-N	5.49	125.96	120.52
1	L	645	ILE	C-N-CA	5.49	125.96	120.52
1	E	608	MET	N-CA-C	-5.47	107.15	113.88
1	C	572	CYS	CA-C-N	-5.46	115.92	122.90
1	C	572	CYS	C-N-CA	-5.46	115.92	122.90
1	K	695	CYS	CB-CA-C	-5.43	102.28	110.92
1	N	583	ALA	N-CA-C	-5.43	105.05	110.97
1	I	695	CYS	CB-CA-C	-5.42	102.14	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	695	CYS	CB-CA-C	-5.41	102.32	110.92
1	M	645	ILE	CA-C-N	5.39	125.85	120.52
1	M	645	ILE	C-N-CA	5.39	125.85	120.52
1	K	608	MET	N-CA-C	-5.35	107.41	114.04
1	F	575	PHE	N-CA-C	5.34	117.36	108.02
1	D	608	MET	N-CA-C	-5.33	107.44	114.31
1	B	608	MET	N-CA-C	-5.31	107.18	113.97
1	B	664	SER	N-CA-C	5.30	117.78	108.82
1	E	758	PHE	N-CA-C	-5.29	104.76	111.11
1	I	600	VAL	N-CA-C	5.28	115.49	110.53
1	L	590	ILE	N-CA-C	5.27	115.54	110.74
1	C	695	CYS	CB-CA-C	-5.27	102.54	110.92
1	H	758	PHE	N-CA-C	-5.27	105.43	111.07
1	G	615	LYS	CA-C-N	-5.27	114.35	123.25
1	G	615	LYS	C-N-CA	-5.27	114.35	123.25
1	D	758	PHE	N-CA-C	-5.25	105.45	111.07
1	M	601	ILE	N-CA-C	-5.25	104.53	111.09
1	F	758	PHE	N-CA-C	-5.23	104.83	111.11
1	L	664	SER	N-CA-C	5.22	117.64	108.82
1	C	493	VAL	N-CA-C	5.20	116.49	112.12
1	B	630	ASP	CA-C-N	5.19	125.49	119.47
1	B	630	ASP	C-N-CA	5.19	125.49	119.47
1	M	695	CYS	CB-CA-C	-5.19	102.67	110.92
1	D	695	CYS	CB-CA-C	-5.17	102.70	110.92
1	F	695	CYS	CB-CA-C	-5.17	102.71	110.92
1	G	680	ASN	N-CA-C	5.16	121.79	110.80
1	N	695	CYS	CB-CA-C	-5.14	102.74	110.92
1	H	732	ARG	N-CA-C	5.13	117.67	109.81
1	I	608	MET	N-CA-C	-5.13	107.57	113.88
1	E	630	ASP	CA-C-N	5.12	125.16	119.32
1	E	630	ASP	C-N-CA	5.12	125.16	119.32
1	I	633	ILE	CG1-CB-CG2	-5.10	95.39	110.70
1	E	559	VAL	N-CA-C	-5.10	105.42	110.62
1	M	590	ILE	N-CA-C	5.07	115.35	110.74
1	E	520	PRO	CB-CA-C	-5.05	105.34	111.46
1	E	590	ILE	N-CA-C	5.02	115.31	110.74
1	C	630	ASP	CA-C-N	5.01	125.03	119.32
1	C	630	ASP	C-N-CA	5.01	125.03	119.32

There are no chirality outliers.

There are no planarity outliers.

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	2199	0	2220	78	1
1	B	2199	0	2220	85	1
1	C	2199	0	2220	67	0
1	D	2199	0	2220	76	0
1	E	2199	0	2220	81	2
1	F	2199	0	2220	74	1
1	G	2199	0	2220	84	0
1	H	2199	0	2220	74	2
1	I	2199	0	2220	69	1
1	J	2199	0	2220	81	0
1	K	2199	0	2220	84	0
1	L	2199	0	2220	71	0
1	M	2199	0	2220	78	2
1	N	2199	0	2220	74	1
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	2	0
2	D	27	0	12	1	0
2	E	27	0	12	2	0
2	F	27	0	12	1	0
2	G	27	0	12	3	0
2	H	27	0	12	1	0
2	I	27	0	12	2	0
2	J	27	0	12	1	0
2	K	27	0	12	2	0
2	L	27	0	12	3	0
2	M	27	0	12	2	0
2	N	27	0	12	3	0
All	All	31164	0	31248	1042	6

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 17.

All (1042) 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:G:568:GLN:O	1:J:466:GLU:CD	1.93	1.12
1:E:680:ASN:C	1:E:682:PHE:H	1.61	1.07
1:F:680:ASN:C	1:F:682:PHE:H	1.65	0.99
1:G:680:ASN:C	1:G:682:PHE:H	1.70	0.98
1:D:680:ASN:C	1:D:682:PHE:H	1.69	0.98
1:G:568:GLN:O	1:J:466:GLU:CG	2.11	0.97
1:M:680:ASN:C	1:M:682:PHE:H	1.69	0.97
1:C:680:ASN:C	1:C:682:PHE:H	1.71	0.97
1:A:680:ASN:C	1:A:682:PHE:H	1.71	0.96
1:J:680:ASN:C	1:J:682:PHE:H	1.69	0.96
1:I:680:ASN:C	1:I:682:PHE:H	1.68	0.96
1:B:680:ASN:C	1:B:682:PHE:H	1.70	0.95
1:A:744:ARG:HD3	1:N:763:GLN:C	1.91	0.94
1:H:680:ASN:C	1:H:682:PHE:H	1.71	0.93
1:G:568:GLN:HG2	1:J:466:GLU:CG	1.99	0.92
1:K:680:ASN:C	1:K:682:PHE:H	1.71	0.92
1:N:680:ASN:C	1:N:682:PHE:H	1.73	0.91
1:E:680:ASN:O	1:E:682:PHE:N	2.04	0.91
1:L:680:ASN:C	1:L:682:PHE:H	1.72	0.89
1:M:728:VAL:N	1:M:729:PRO:HD3	1.91	0.85
1:E:749:ASP:HA	1:E:752:ILE:HD12	1.59	0.84
1:C:728:VAL:N	1:C:729:PRO:HD3	1.92	0.84
1:B:728:VAL:N	1:B:729:PRO:HD3	1.92	0.84
1:E:680:ASN:C	1:E:682:PHE:N	2.34	0.84
1:H:464:LEU:HD22	1:H:558:ASN:HB3	1.60	0.84
1:H:728:VAL:N	1:H:729:PRO:HD3	1.93	0.83
1:A:728:VAL:N	1:A:729:PRO:HD3	1.94	0.83
1:G:728:VAL:N	1:G:729:PRO:HD3	1.94	0.83
1:L:728:VAL:N	1:L:729:PRO:HD3	1.93	0.83
1:F:728:VAL:N	1:F:729:PRO:HD3	1.95	0.82
1:I:728:VAL:N	1:I:729:PRO:HD3	1.93	0.82
1:C:636:PRO:HA	1:C:640:ASP:OD2	1.79	0.82
1:D:464:LEU:HD22	1:D:558:ASN:HB3	1.62	0.82
1:K:728:VAL:N	1:K:729:PRO:HD3	1.95	0.82
1:E:728:VAL:N	1:E:729:PRO:HD3	1.94	0.82
1:F:680:ASN:C	1:F:682:PHE:N	2.37	0.82
1:D:487:ARG:HD2	1:E:700:ARG:HH21	1.45	0.81
1:F:680:ASN:O	1:F:682:PHE:N	2.13	0.81
1:J:728:VAL:N	1:J:729:PRO:HD3	1.96	0.81
1:G:636:PRO:HA	1:G:640:ASP:OD2	1.82	0.80
1:C:749:ASP:HA	1:C:752:ILE:HD12	1.63	0.80
1:I:680:ASN:O	1:I:682:PHE:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:728:VAL:N	1:N:729:PRO:HD3	1.96	0.80
1:H:749:ASP:HA	1:H:752:ILE:HD12	1.62	0.80
1:B:680:ASN:O	1:B:682:PHE:N	2.15	0.80
1:G:568:GLN:O	1:J:466:GLU:HG2	1.81	0.80
1:A:636:PRO:HA	1:A:640:ASP:OD2	1.80	0.79
1:K:464:LEU:HD22	1:K:558:ASN:HB3	1.65	0.79
1:D:728:VAL:N	1:D:729:PRO:HD3	1.97	0.78
1:G:568:GLN:HG2	1:J:466:GLU:HG3	1.66	0.78
1:D:749:ASP:HA	1:D:752:ILE:HD12	1.65	0.78
1:F:636:PRO:HA	1:F:640:ASP:OD2	1.83	0.78
1:M:680:ASN:C	1:M:682:PHE:N	2.42	0.78
1:A:680:ASN:C	1:A:682:PHE:N	2.42	0.77
1:B:680:ASN:C	1:B:682:PHE:N	2.41	0.77
1:K:680:ASN:C	1:K:682:PHE:N	2.40	0.77
1:J:680:ASN:C	1:J:682:PHE:N	2.42	0.77
1:M:636:PRO:HA	1:M:640:ASP:OD2	1.83	0.77
1:E:464:LEU:HD22	1:E:558:ASN:HB3	1.65	0.76
1:M:464:LEU:HD22	1:M:558:ASN:HB3	1.65	0.76
1:J:636:PRO:HA	1:J:640:ASP:OD2	1.84	0.76
1:C:680:ASN:C	1:C:682:PHE:N	2.42	0.76
1:H:680:ASN:C	1:H:682:PHE:N	2.43	0.76
1:G:680:ASN:O	1:G:682:PHE:N	2.19	0.76
1:K:749:ASP:HA	1:K:752:ILE:HD12	1.68	0.75
1:L:749:ASP:HA	1:L:752:ILE:HD12	1.68	0.75
1:D:487:ARG:NE	1:E:700:ARG:NH2	2.34	0.75
1:D:487:ARG:CD	1:E:700:ARG:HH21	2.00	0.75
1:H:636:PRO:HA	1:H:640:ASP:OD2	1.87	0.75
1:N:749:ASP:HA	1:N:752:ILE:HD12	1.68	0.75
1:C:680:ASN:O	1:C:682:PHE:N	2.19	0.75
1:K:680:ASN:O	1:K:682:PHE:N	2.20	0.75
1:M:680:ASN:O	1:M:682:PHE:N	2.20	0.75
1:K:636:PRO:HA	1:K:640:ASP:OD2	1.86	0.74
1:F:749:ASP:HA	1:F:752:ILE:HD12	1.70	0.74
1:L:636:PRO:HA	1:L:640:ASP:OD2	1.87	0.74
1:E:636:PRO:HA	1:E:640:ASP:OD2	1.86	0.74
1:L:680:ASN:C	1:L:682:PHE:N	2.43	0.74
1:N:636:PRO:HA	1:N:640:ASP:OD2	1.88	0.73
1:N:464:LEU:HD22	1:N:558:ASN:HB3	1.71	0.73
1:M:749:ASP:HA	1:M:752:ILE:HD12	1.68	0.73
1:H:680:ASN:O	1:H:682:PHE:N	2.21	0.73
1:M:681:GLY:HA3	1:M:745:ARG:HH21	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:763:GLN:C	1:C:744:ARG:HD3	2.14	0.73
1:I:636:PRO:HA	1:I:640:ASP:OD2	1.89	0.72
1:F:514:VAL:HG22	1:F:641:GLN:HB2	1.71	0.72
1:D:680:ASN:O	1:D:682:PHE:N	2.23	0.72
1:J:680:ASN:O	1:J:682:PHE:N	2.23	0.72
1:G:568:GLN:HG2	1:J:466:GLU:HG2	1.71	0.71
1:K:681:GLY:HA3	1:K:745:ARG:HH21	1.55	0.71
1:L:680:ASN:O	1:L:682:PHE:N	2.23	0.71
1:N:680:ASN:C	1:N:682:PHE:N	2.44	0.71
1:E:681:GLY:HA3	1:E:745:ARG:HH21	1.55	0.71
1:G:749:ASP:HA	1:G:752:ILE:HD12	1.71	0.71
1:J:464:LEU:HD22	1:J:558:ASN:HB3	1.72	0.71
1:A:464:LEU:HD22	1:A:558:ASN:HB3	1.71	0.71
1:A:680:ASN:O	1:A:682:PHE:N	2.23	0.71
1:B:749:ASP:HA	1:B:752:ILE:HD12	1.71	0.71
1:D:487:ARG:HD2	1:E:700:ARG:NH2	2.06	0.71
1:A:681:GLY:HA3	1:A:745:ARG:HH21	1.54	0.70
1:M:697:LEU:O	1:M:701:GLU:HB2	1.91	0.70
1:D:636:PRO:HA	1:D:640:ASP:OD2	1.91	0.70
1:D:681:GLY:HA3	1:D:745:ARG:HH21	1.56	0.70
1:D:487:ARG:HE	1:E:700:ARG:NH2	1.88	0.70
1:G:681:GLY:HA3	1:G:745:ARG:HH21	1.56	0.70
1:A:749:ASP:HA	1:A:752:ILE:HD12	1.72	0.70
1:F:464:LEU:HD22	1:F:558:ASN:HB3	1.73	0.70
1:L:681:GLY:HA3	1:L:745:ARG:HH21	1.57	0.69
1:G:680:ASN:C	1:G:682:PHE:N	2.43	0.69
1:B:636:PRO:HA	1:B:640:ASP:OD2	1.93	0.69
1:D:697:LEU:O	1:D:701:GLU:HB2	1.93	0.69
1:I:464:LEU:HD22	1:I:558:ASN:HB3	1.75	0.69
1:L:464:LEU:HD22	1:L:558:ASN:HB3	1.75	0.69
1:H:681:GLY:HA3	1:H:745:ARG:HH21	1.57	0.68
1:G:697:LEU:O	1:G:701:GLU:HB2	1.93	0.68
1:C:697:LEU:O	1:C:701:GLU:HB2	1.94	0.68
1:I:749:ASP:HA	1:I:752:ILE:HD12	1.76	0.68
1:N:680:ASN:O	1:N:682:PHE:N	2.27	0.67
1:J:749:ASP:HA	1:J:752:ILE:HD12	1.76	0.67
1:J:763:GLN:C	1:K:744:ARG:HD3	2.19	0.67
1:N:514:VAL:HG22	1:N:641:GLN:HB2	1.75	0.67
1:D:514:VAL:HG22	1:D:641:GLN:HB2	1.76	0.67
1:F:681:GLY:HA3	1:F:745:ARG:HH21	1.59	0.66
1:C:758:PHE:HB3	1:C:762:LEU:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:493:VAL:CG2	1:G:531:ILE:HD11	2.26	0.66
1:H:514:VAL:HG22	1:H:641:GLN:HB2	1.77	0.66
1:M:606:THR:C	1:M:608:MET:H	2.04	0.66
1:B:650:GLU:HB3	1:B:677:LYS:NZ	2.10	0.66
1:J:697:LEU:O	1:J:701:GLU:HB2	1.96	0.66
1:A:694:ALA:HB1	1:A:731:ILE:HD11	1.76	0.66
1:A:697:LEU:O	1:A:701:GLU:HB2	1.95	0.65
1:C:464:LEU:HD22	1:C:558:ASN:HB3	1.77	0.65
1:K:575:PHE:CE2	1:K:577:ASP:HB2	2.32	0.65
1:G:464:LEU:HD22	1:G:558:ASN:HB3	1.77	0.65
1:H:493:VAL:CG2	1:H:531:ILE:HD11	2.27	0.65
1:H:694:ALA:HB1	1:H:731:ILE:HD11	1.79	0.65
1:B:681:GLY:HA3	1:B:745:ARG:HH21	1.62	0.65
1:K:753:ARG:O	1:K:757:MET:HG2	1.98	0.64
1:C:681:GLY:HA3	1:C:745:ARG:HH21	1.62	0.64
1:F:606:THR:C	1:F:608:MET:H	2.05	0.64
1:M:472:PRO:HG3	1:M:539:PHE:HB2	1.79	0.64
1:H:533:ASN:C	1:H:533:ASN:ND2	2.55	0.64
1:I:533:ASN:C	1:I:533:ASN:ND2	2.56	0.64
1:I:650:GLU:HB3	1:I:677:LYS:NZ	2.12	0.64
1:D:487:ARG:CD	1:E:700:ARG:NH2	2.59	0.64
1:M:728:VAL:N	1:M:729:PRO:CD	2.61	0.64
1:M:514:VAL:HG22	1:M:641:GLN:HB2	1.80	0.63
1:L:697:LEU:O	1:L:701:GLU:HB2	1.98	0.63
1:A:758:PHE:HB3	1:A:762:LEU:HD12	1.81	0.63
1:D:763:GLN:C	1:E:744:ARG:HD3	2.24	0.63
1:E:493:VAL:CG2	1:E:531:ILE:HD11	2.28	0.63
1:C:472:PRO:HG3	1:C:539:PHE:HB2	1.81	0.63
1:J:624:ASN:C	1:J:624:ASN:HD22	2.07	0.63
1:E:575:PHE:CE2	1:E:577:ASP:HB2	2.33	0.62
1:B:464:LEU:HD22	1:B:558:ASN:HB3	1.79	0.62
1:I:493:VAL:CG2	1:I:531:ILE:HD11	2.29	0.62
1:M:694:ALA:HB1	1:M:731:ILE:HD11	1.80	0.62
1:L:493:VAL:CG2	1:L:531:ILE:HD11	2.30	0.62
1:N:697:LEU:O	1:N:701:GLU:HB2	1.99	0.62
1:L:728:VAL:N	1:L:729:PRO:CD	2.62	0.62
1:K:697:LEU:O	1:K:701:GLU:HB2	1.99	0.62
1:L:650:GLU:HB3	1:L:677:LYS:NZ	2.15	0.62
1:M:650:GLU:HB3	1:M:677:LYS:NZ	2.15	0.62
1:C:650:GLU:HB3	1:C:677:LYS:NZ	2.15	0.62
1:D:487:ARG:NE	1:E:700:ARG:HH21	1.95	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:728:VAL:N	1:C:729:PRO:CD	2.62	0.62
1:E:688:THR:OG1	2:E:900:ADP:H1'	2.00	0.62
1:B:728:VAL:N	1:B:729:PRO:CD	2.61	0.62
1:A:728:VAL:N	1:A:729:PRO:CD	2.63	0.62
1:I:514:VAL:HG22	1:I:641:GLN:HB2	1.81	0.61
1:K:688:THR:OG1	2:K:900:ADP:H1'	2.00	0.61
1:E:697:LEU:O	1:E:701:GLU:HB2	2.01	0.61
1:J:681:GLY:HA3	1:J:745:ARG:HH21	1.63	0.61
1:E:514:VAL:HG22	1:E:641:GLN:HB2	1.83	0.61
1:F:650:GLU:HB3	1:F:677:LYS:NZ	2.16	0.61
1:H:728:VAL:N	1:H:729:PRO:CD	2.63	0.61
1:B:688:THR:OG1	2:B:900:ADP:H1'	2.01	0.61
1:M:758:PHE:HB3	1:M:762:LEU:HD12	1.83	0.61
1:A:650:GLU:HB3	1:A:677:LYS:NZ	2.16	0.61
1:G:568:GLN:C	1:J:466:GLU:HG2	2.24	0.61
1:L:514:VAL:HG22	1:L:641:GLN:HB2	1.82	0.61
1:M:606:THR:O	1:M:608:MET:N	2.33	0.61
1:B:758:PHE:HB3	1:B:762:LEU:HD12	1.82	0.60
1:N:575:PHE:CE2	1:N:577:ASP:HB2	2.36	0.60
1:B:624:ASN:HD22	1:B:625:ARG:HG2	1.65	0.60
1:C:694:ALA:HB1	1:C:731:ILE:HD11	1.83	0.60
1:H:697:LEU:O	1:H:701:GLU:HB2	2.01	0.60
1:L:694:ALA:HB1	1:L:731:ILE:HD11	1.82	0.60
1:C:514:VAL:HG22	1:C:641:GLN:HB2	1.83	0.60
1:F:728:VAL:N	1:F:729:PRO:CD	2.65	0.60
1:A:688:THR:OG1	2:A:900:ADP:H1'	2.02	0.60
1:J:514:VAL:HG22	1:J:641:GLN:HB2	1.84	0.60
1:A:515:LEU:HD12	1:A:634:LEU:HD21	1.84	0.60
1:G:728:VAL:N	1:G:729:PRO:CD	2.65	0.60
1:G:624:ASN:HD22	1:G:625:ARG:HG2	1.67	0.60
1:K:728:VAL:N	1:K:729:PRO:CD	2.64	0.60
1:K:650:GLU:HB3	1:K:677:LYS:NZ	2.16	0.60
1:J:465:ARG:HG2	1:J:466:GLU:N	2.17	0.60
1:A:508:MET:SD	1:B:696:LYS:HG3	2.42	0.59
1:E:728:VAL:N	1:E:729:PRO:CD	2.64	0.59
1:H:515:LEU:HD12	1:H:634:LEU:HD21	1.83	0.59
1:G:514:VAL:HG22	1:G:641:GLN:HB2	1.84	0.59
1:D:464:LEU:HD22	1:D:558:ASN:CB	2.31	0.59
1:G:523:GLY:HA2	2:G:900:ADP:O1A	2.02	0.59
1:G:758:PHE:HB3	1:G:762:LEU:HD12	1.85	0.59
1:H:758:PHE:HB3	1:H:762:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:GLU:O	1:A:693:ARG:HG3	2.03	0.59
1:I:680:ASN:C	1:I:682:PHE:N	2.40	0.59
1:I:697:LEU:O	1:I:701:GLU:HB2	2.01	0.59
1:M:493:VAL:CG2	1:M:531:ILE:HD11	2.33	0.59
1:E:689:GLU:O	1:E:693:ARG:HG3	2.03	0.59
1:J:758:PHE:HB3	1:J:762:LEU:HD12	1.84	0.59
1:E:694:ALA:HB1	1:E:731:ILE:HD11	1.85	0.58
1:F:645:ILE:N	1:F:645:ILE:HD12	2.18	0.58
1:K:694:ALA:HB1	1:K:731:ILE:HD11	1.85	0.58
1:N:650:GLU:HB3	1:N:677:LYS:NZ	2.17	0.58
1:E:758:PHE:HB3	1:E:762:LEU:HD12	1.86	0.58
1:H:624:ASN:HD22	1:H:625:ARG:HG2	1.68	0.58
1:L:556:GLU:OE2	1:L:599:ARG:NH1	2.36	0.58
1:A:575:PHE:CE2	1:A:577:ASP:HB2	2.39	0.58
1:G:575:PHE:CE2	1:G:577:ASP:HB2	2.38	0.58
1:K:465:ARG:HG2	1:K:466:GLU:N	2.19	0.58
1:N:606:THR:C	1:N:608:MET:H	2.12	0.58
1:N:681:GLY:HA3	1:N:745:ARG:HH21	1.67	0.58
1:F:533:ASN:C	1:F:533:ASN:ND2	2.60	0.58
1:E:650:GLU:HB3	1:E:677:LYS:NZ	2.19	0.58
1:G:568:GLN:O	1:J:466:GLU:OE1	2.21	0.58
1:N:728:VAL:N	1:N:729:PRO:CD	2.65	0.58
1:N:758:PHE:HB3	1:N:762:LEU:HD12	1.85	0.58
1:A:514:VAL:HG22	1:A:641:GLN:HB2	1.86	0.58
1:A:547:LEU:HA	1:A:550:MET:HE3	1.86	0.58
1:D:694:ALA:HB1	1:D:731:ILE:HD11	1.84	0.58
1:E:472:PRO:HG3	1:E:539:PHE:HB2	1.86	0.58
1:I:728:VAL:N	1:I:729:PRO:CD	2.63	0.58
1:I:758:PHE:HB3	1:I:762:LEU:HD12	1.86	0.58
1:J:689:GLU:O	1:J:693:ARG:HG3	2.03	0.58
1:K:533:ASN:C	1:K:533:ASN:ND2	2.61	0.58
1:I:516:PHE:O	1:I:622:ALA:HA	2.03	0.58
1:C:512:LYS:NZ	1:C:611:MET:O	2.34	0.58
1:L:582:ILE:O	1:L:586:ARG:HG2	2.03	0.57
1:D:758:PHE:HB3	1:D:762:LEU:HD12	1.86	0.57
1:H:689:GLU:O	1:H:693:ARG:HG3	2.04	0.57
1:I:681:GLY:HA3	1:I:745:ARG:HH21	1.68	0.57
1:K:514:VAL:HG22	1:K:641:GLN:HB2	1.85	0.57
1:C:547:LEU:HA	1:C:550:MET:HE3	1.87	0.57
1:I:582:ILE:O	1:I:586:ARG:HG2	2.04	0.57
1:K:689:GLU:O	1:K:693:ARG:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:523:GLY:HA2	2:L:900:ADP:O1A	2.04	0.57
1:C:660:ASN:ND2	1:C:688:THR:HA	2.20	0.57
1:D:624:ASN:HD22	1:D:625:ARG:HG2	1.69	0.57
1:D:728:VAL:N	1:D:729:PRO:CD	2.67	0.57
1:G:650:GLU:HB3	1:G:677:LYS:NZ	2.20	0.57
1:J:515:LEU:HD12	1:J:634:LEU:HD21	1.86	0.57
1:B:493:VAL:CG2	1:B:531:ILE:HD11	2.35	0.57
1:B:514:VAL:HG22	1:B:641:GLN:HB2	1.85	0.57
1:E:515:LEU:HD12	1:E:634:LEU:HD21	1.86	0.57
1:H:606:THR:C	1:H:608:MET:H	2.13	0.57
1:J:650:GLU:HB3	1:J:677:LYS:NZ	2.20	0.57
1:M:688:THR:OG1	2:M:900:ADP:H1'	2.05	0.57
1:E:582:ILE:O	1:E:586:ARG:HG2	2.04	0.57
1:G:694:ALA:HB1	1:G:731:ILE:HD11	1.86	0.57
1:H:547:LEU:HA	1:H:550:MET:HE3	1.86	0.57
1:F:694:ALA:HB1	1:F:731:ILE:HD11	1.85	0.57
1:I:694:ALA:HB1	1:I:731:ILE:HD11	1.86	0.57
1:K:758:PHE:HB3	1:K:762:LEU:HD12	1.85	0.57
1:L:575:PHE:CE2	1:L:577:ASP:HB2	2.39	0.57
1:M:533:ASN:C	1:M:533:ASN:ND2	2.63	0.57
1:A:660:ASN:ND2	1:A:688:THR:HA	2.19	0.57
1:B:694:ALA:HB1	1:B:731:ILE:HD11	1.86	0.57
1:D:625:ARG:HB3	1:D:625:ARG:NH1	2.20	0.57
1:J:472:PRO:HG3	1:J:539:PHE:HB2	1.86	0.57
1:J:728:VAL:N	1:J:729:PRO:CD	2.65	0.57
1:L:515:LEU:HD12	1:L:634:LEU:HD21	1.85	0.57
1:L:753:ARG:O	1:L:757:MET:HG2	2.05	0.57
1:F:688:THR:OG1	2:F:900:ADP:H1'	2.04	0.57
1:F:465:ARG:HG2	1:F:466:GLU:N	2.20	0.56
1:B:753:ARG:O	1:B:757:MET:HG2	2.05	0.56
1:G:512:LYS:NZ	1:G:611:MET:O	2.38	0.56
1:C:465:ARG:HG2	1:C:466:GLU:N	2.21	0.56
1:C:624:ASN:HD22	1:C:625:ARG:HG2	1.70	0.56
1:G:472:PRO:HG3	1:G:539:PHE:HB2	1.87	0.56
1:I:482:LEU:HB3	1:I:485:VAL:HG22	1.87	0.56
1:I:575:PHE:CE2	1:I:577:ASP:HB2	2.39	0.56
1:K:606:THR:C	1:K:608:MET:H	2.14	0.56
1:L:758:PHE:HB3	1:L:762:LEU:HD12	1.86	0.56
1:M:606:THR:C	1:M:608:MET:N	2.61	0.56
1:F:758:PHE:HB3	1:F:762:LEU:HD12	1.86	0.56
1:G:689:GLU:O	1:G:693:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:547:LEU:HA	1:F:550:MET:HE3	1.87	0.56
1:A:472:PRO:HG3	1:A:539:PHE:HB2	1.87	0.56
1:C:575:PHE:CE2	1:C:577:ASP:HB2	2.40	0.56
1:J:533:ASN:C	1:J:533:ASN:ND2	2.64	0.56
1:D:689:GLU:O	1:D:693:ARG:HG3	2.05	0.55
1:M:464:LEU:HD22	1:M:558:ASN:CB	2.35	0.55
1:K:472:PRO:HG3	1:K:539:PHE:HB2	1.89	0.55
1:N:630:ASP:O	1:N:633:ILE:HD12	2.06	0.55
1:F:482:LEU:HB3	1:F:485:VAL:HG22	1.87	0.55
1:E:533:ASN:C	1:E:533:ASN:ND2	2.65	0.55
1:G:582:ILE:O	1:G:586:ARG:HG2	2.06	0.55
1:J:660:ASN:ND2	1:J:688:THR:HA	2.22	0.55
1:A:700:ARG:O	1:A:704:GLU:HB2	2.07	0.55
1:E:700:ARG:O	1:E:704:GLU:HB2	2.07	0.55
1:L:630:ASP:O	1:L:633:ILE:HD12	2.07	0.55
1:M:547:LEU:HA	1:M:550:MET:HE3	1.89	0.55
1:A:465:ARG:HG2	1:A:466:GLU:N	2.21	0.55
1:F:533:ASN:HD22	1:F:534:GLU:N	2.05	0.55
1:L:700:ARG:O	1:L:704:GLU:HB2	2.07	0.55
1:E:465:ARG:HG2	1:E:466:GLU:N	2.22	0.55
1:N:688:THR:OG1	2:N:900:ADP:H1'	2.07	0.55
1:F:515:LEU:HD12	1:F:634:LEU:HD21	1.88	0.54
1:H:650:GLU:HB3	1:H:677:LYS:NZ	2.23	0.54
1:I:472:PRO:HB2	1:I:533:ASN:HB2	1.89	0.54
1:B:575:PHE:CE2	1:B:577:ASP:HB2	2.43	0.54
1:C:533:ASN:C	1:C:533:ASN:ND2	2.65	0.54
1:D:700:ARG:O	1:D:704:GLU:HB2	2.07	0.54
1:F:472:PRO:HG3	1:F:539:PHE:HB2	1.89	0.54
1:F:624:ASN:HD22	1:F:625:ARG:HG2	1.71	0.54
1:M:613:THR:HG23	1:M:614:LYS:HG3	1.88	0.54
1:A:624:ASN:HD22	1:A:625:ARG:HG2	1.73	0.54
1:K:516:PHE:HB3	1:K:524:LYS:HG2	1.90	0.54
1:H:688:THR:OG1	2:H:900:ADP:H1'	2.08	0.54
1:I:533:ASN:HD22	1:I:534:GLU:N	2.05	0.54
1:N:694:ALA:HB1	1:N:731:ILE:HD11	1.89	0.54
1:A:606:THR:C	1:A:608:MET:H	2.15	0.54
1:E:624:ASN:HD22	1:E:625:ARG:HG2	1.72	0.54
1:E:660:ASN:ND2	1:E:688:THR:HA	2.23	0.54
1:F:606:THR:O	1:F:608:MET:N	2.41	0.54
1:J:625:ARG:NH1	1:J:625:ARG:HB3	2.23	0.54
1:C:689:GLU:O	1:C:693:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:472:PRO:HB2	1:N:533:ASN:HB2	1.89	0.54
1:I:689:GLU:O	1:I:693:ARG:HG3	2.07	0.54
1:J:624:ASN:HD22	1:J:625:ARG:HG2	1.73	0.54
1:M:575:PHE:CE2	1:M:577:ASP:HB2	2.43	0.54
1:A:533:ASN:C	1:A:533:ASN:ND2	2.65	0.54
1:D:465:ARG:HG2	1:D:466:GLU:N	2.23	0.54
1:D:575:PHE:CE2	1:D:577:ASP:HB2	2.43	0.54
1:N:753:ARG:O	1:N:757:MET:HG2	2.08	0.54
1:D:633:ILE:O	1:D:633:ILE:HG22	2.08	0.54
1:J:515:LEU:HD21	1:J:623:THR:HG22	1.89	0.54
1:C:700:ARG:O	1:C:704:GLU:HB2	2.07	0.54
1:M:624:ASN:C	1:M:624:ASN:HD22	2.15	0.54
1:F:689:GLU:O	1:F:693:ARG:HG3	2.08	0.53
1:M:689:GLU:O	1:M:693:ARG:HG3	2.09	0.53
1:A:624:ASN:HD22	1:A:624:ASN:C	2.16	0.53
1:D:606:THR:C	1:D:608:MET:H	2.17	0.53
1:E:645:ILE:HD12	1:E:645:ILE:N	2.23	0.53
1:G:516:PHE:HB3	1:G:524:LYS:HG2	1.90	0.53
1:K:576:PHE:CE2	1:K:604:ILE:HD13	2.44	0.53
1:E:495:TYR:N	1:E:495:TYR:CD2	2.75	0.53
1:G:533:ASN:C	1:G:533:ASN:ND2	2.66	0.53
1:M:515:LEU:HD21	1:M:623:THR:HG22	1.91	0.53
1:N:689:GLU:O	1:N:693:ARG:HG3	2.09	0.53
1:A:613:THR:HG23	1:A:614:LYS:HG3	1.91	0.53
1:D:464:LEU:HD13	1:D:550:MET:HG3	1.89	0.53
1:H:660:ASN:ND2	1:H:688:THR:HA	2.24	0.53
1:G:688:THR:OG1	2:G:900:ADP:H1'	2.09	0.53
1:H:575:PHE:CE2	1:H:577:ASP:HB2	2.44	0.53
1:M:625:ARG:HB3	1:M:625:ARG:NH1	2.24	0.53
1:N:465:ARG:HG2	1:N:466:GLU:N	2.24	0.53
1:D:472:PRO:HG3	1:D:539:PHE:HB2	1.90	0.53
1:F:660:ASN:ND2	1:F:688:THR:HA	2.24	0.53
1:F:753:ARG:O	1:F:757:MET:HG2	2.09	0.53
1:M:605:LEU:HD22	1:M:638:ARG:HD3	1.91	0.53
1:M:660:ASN:ND2	1:M:688:THR:HA	2.24	0.53
1:C:464:LEU:HD22	1:C:558:ASN:CB	2.39	0.53
1:C:508:MET:SD	1:G:696:LYS:HG3	2.49	0.53
1:C:606:THR:C	1:C:608:MET:H	2.16	0.53
1:J:694:ALA:HB1	1:J:731:ILE:HD11	1.91	0.53
1:C:482:LEU:HB3	1:C:485:VAL:HG22	1.91	0.52
1:D:567:ARG:HH21	1:D:611:MET:CG	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:512:LYS:NZ	1:J:611:MET:O	2.42	0.52
1:J:560:ARG:HG3	1:J:560:ARG:HH11	1.73	0.52
1:L:606:THR:C	1:L:608:MET:H	2.18	0.52
1:H:464:LEU:HD13	1:H:550:MET:HG3	1.90	0.52
1:H:753:ARG:O	1:H:757:MET:HG2	2.09	0.52
1:K:464:LEU:HD22	1:K:558:ASN:CB	2.37	0.52
1:B:606:THR:C	1:B:608:MET:H	2.17	0.52
1:G:753:ARG:O	1:G:757:MET:HG2	2.10	0.52
1:I:465:ARG:HG2	1:I:466:GLU:N	2.23	0.52
1:L:624:ASN:HD22	1:L:625:ARG:HG2	1.73	0.52
1:F:730:GLU:N	1:F:730:GLU:CD	2.67	0.52
1:J:560:ARG:HG3	1:J:560:ARG:NH1	2.24	0.52
1:K:700:ARG:O	1:K:704:GLU:HB2	2.09	0.52
1:B:689:GLU:O	1:B:693:ARG:HG3	2.10	0.52
1:E:560:ARG:HG3	1:E:560:ARG:HH11	1.74	0.52
1:F:606:THR:C	1:F:608:MET:N	2.64	0.52
1:J:533:ASN:HD22	1:J:534:GLU:N	2.07	0.52
1:K:533:ASN:HD22	1:K:534:GLU:N	2.07	0.52
1:L:472:PRO:HG3	1:L:539:PHE:HB2	1.91	0.52
1:L:660:ASN:ND2	1:L:688:THR:HA	2.24	0.52
1:B:516:PHE:HB3	1:B:524:LYS:HG2	1.90	0.52
1:K:624:ASN:HD22	1:K:624:ASN:C	2.17	0.52
1:B:533:ASN:C	1:B:533:ASN:ND2	2.67	0.52
1:D:650:GLU:HB3	1:D:677:LYS:NZ	2.24	0.52
1:F:697:LEU:O	1:F:701:GLU:HB2	2.09	0.52
1:G:465:ARG:HG2	1:G:466:GLU:N	2.23	0.52
1:H:700:ARG:O	1:H:704:GLU:HB2	2.10	0.52
1:I:700:ARG:O	1:I:704:GLU:HB2	2.10	0.52
1:D:516:PHE:HB3	1:D:524:LYS:HG2	1.91	0.52
1:G:606:THR:C	1:G:608:MET:H	2.17	0.52
1:K:660:ASN:ND2	1:K:688:THR:HA	2.25	0.52
1:A:605:LEU:HD22	1:A:638:ARG:HD3	1.91	0.52
1:G:590:ILE:HG13	1:G:591:GLY:H	1.75	0.52
1:M:465:ARG:HG2	1:M:466:GLU:N	2.25	0.52
1:N:650:GLU:HB3	1:N:677:LYS:HZ1	1.75	0.52
1:H:624:ASN:HD22	1:H:624:ASN:C	2.17	0.51
1:J:613:THR:HG23	1:J:614:LYS:HG3	1.92	0.51
1:L:689:GLU:O	1:L:693:ARG:HG3	2.10	0.51
1:N:606:THR:C	1:N:608:MET:N	2.68	0.51
1:N:730:GLU:N	1:N:730:GLU:CD	2.68	0.51
1:E:613:THR:HG23	1:E:614:LYS:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:688:THR:OG1	2:L:900:ADP:H1'	2.09	0.51
1:A:472:PRO:HB2	1:A:533:ASN:HB2	1.92	0.51
1:C:502:LYS:HE2	1:G:706:GLU:OE2	2.10	0.51
1:M:512:LYS:NZ	1:M:611:MET:O	2.43	0.51
1:I:660:ASN:ND2	1:I:688:THR:HA	2.25	0.51
1:J:688:THR:OG1	2:J:900:ADP:H1'	2.09	0.51
1:B:472:PRO:HB2	1:B:533:ASN:HB2	1.93	0.51
1:H:625:ARG:NH1	1:H:627:ASP:OD1	2.44	0.51
1:M:624:ASN:HD22	1:M:625:ARG:HG2	1.75	0.51
1:D:515:LEU:HD12	1:D:634:LEU:HD21	1.91	0.51
1:G:515:LEU:HD12	1:G:634:LEU:HD21	1.92	0.51
1:H:533:ASN:HD22	1:H:534:GLU:N	2.08	0.51
1:M:700:ARG:O	1:M:704:GLU:HB2	2.11	0.51
1:L:624:ASN:HD22	1:L:624:ASN:C	2.19	0.51
1:L:681:GLY:HA3	1:L:745:ARG:NH2	2.25	0.51
1:L:730:GLU:N	1:L:730:GLU:CD	2.69	0.51
1:M:495:TYR:N	1:M:495:TYR:CD2	2.78	0.51
1:N:660:ASN:ND2	1:N:688:THR:HA	2.26	0.51
1:A:533:ASN:HD22	1:A:534:GLU:N	2.09	0.51
1:E:499:HIS:N	1:E:500:PRO:HD3	2.25	0.51
1:F:472:PRO:HB2	1:F:533:ASN:HB2	1.92	0.51
1:J:606:THR:C	1:J:608:MET:H	2.17	0.51
1:K:464:LEU:HD13	1:K:550:MET:HG3	1.92	0.51
1:E:644:TYR:C	1:E:645:ILE:HD12	2.36	0.51
1:G:624:ASN:HD22	1:G:624:ASN:C	2.19	0.51
1:I:472:PRO:HG3	1:I:539:PHE:HB2	1.92	0.51
1:B:464:LEU:HD13	1:B:550:MET:HG3	1.93	0.50
1:B:516:PHE:O	1:B:622:ALA:HA	2.11	0.50
1:J:700:ARG:O	1:J:704:GLU:HB2	2.11	0.50
1:I:606:THR:C	1:I:608:MET:H	2.19	0.50
1:C:495:TYR:N	1:C:495:TYR:CD2	2.78	0.50
1:E:495:TYR:N	1:E:495:TYR:HD2	2.08	0.50
1:H:465:ARG:HG2	1:H:466:GLU:N	2.27	0.50
1:B:633:ILE:O	1:B:633:ILE:HG22	2.11	0.50
1:C:495:TYR:N	1:C:495:TYR:HD2	2.10	0.50
1:G:560:ARG:NH1	1:G:560:ARG:HG3	2.26	0.50
1:L:512:LYS:NZ	1:L:611:MET:O	2.44	0.50
1:M:515:LEU:HD12	1:M:634:LEU:HD21	1.92	0.50
1:N:515:LEU:HD12	1:N:634:LEU:HD21	1.94	0.50
1:A:495:TYR:N	1:A:495:TYR:CD2	2.79	0.50
1:I:495:TYR:N	1:I:495:TYR:CD2	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:482:LEU:HB3	1:K:485:VAL:HG22	1.92	0.50
1:M:495:TYR:N	1:M:495:TYR:HD2	2.10	0.50
1:C:681:GLY:HA3	1:C:745:ARG:HE	1.77	0.50
1:C:753:ARG:O	1:C:757:MET:HG2	2.11	0.50
1:D:493:VAL:CG2	1:D:531:ILE:HD11	2.42	0.50
1:D:660:ASN:ND2	1:D:688:THR:HA	2.26	0.50
1:E:464:LEU:HD13	1:E:550:MET:HG3	1.93	0.50
1:G:482:LEU:HB3	1:G:485:VAL:HG22	1.93	0.50
1:C:688:THR:OG1	2:C:900:ADP:H1'	2.12	0.50
1:D:688:THR:OG1	2:D:900:ADP:H1'	2.11	0.50
1:E:516:PHE:HB3	1:E:524:LYS:HG2	1.94	0.50
1:G:730:GLU:N	1:G:730:GLU:CD	2.70	0.50
1:H:464:LEU:HD22	1:H:558:ASN:CB	2.36	0.50
1:H:590:ILE:HG13	1:H:591:GLY:H	1.77	0.50
1:G:533:ASN:HD22	1:G:534:GLU:N	2.10	0.49
1:J:493:VAL:CG2	1:J:531:ILE:HD11	2.41	0.49
1:L:645:ILE:HD12	1:L:645:ILE:N	2.27	0.49
1:A:482:LEU:HB3	1:A:485:VAL:HG22	1.93	0.49
1:K:512:LYS:NZ	1:K:611:MET:O	2.44	0.49
1:B:697:LEU:O	1:B:701:GLU:HB2	2.12	0.49
1:E:560:ARG:HG3	1:E:560:ARG:NH1	2.26	0.49
1:G:625:ARG:HH12	1:G:627:ASP:CG	2.21	0.49
1:H:495:TYR:N	1:H:495:TYR:CD2	2.79	0.49
1:J:582:ILE:O	1:J:586:ARG:HG2	2.11	0.49
1:L:681:GLY:HA3	1:L:745:ARG:HE	1.77	0.49
1:N:512:LYS:NZ	1:N:611:MET:O	2.43	0.49
1:E:512:LYS:NZ	1:E:611:MET:O	2.44	0.49
1:E:550:MET:HG2	1:E:555:SER:O	2.12	0.49
1:G:525:THR:O	1:G:526:LEU:C	2.56	0.49
1:J:590:ILE:HG13	1:J:591:GLY:H	1.77	0.49
1:L:495:TYR:N	1:L:495:TYR:CD2	2.80	0.49
1:A:512:LYS:NZ	1:A:611:MET:O	2.43	0.49
1:I:523:GLY:HA2	2:I:900:ADP:O1A	2.13	0.49
1:I:730:GLU:N	1:I:730:GLU:CD	2.70	0.49
1:L:465:ARG:HG2	1:L:466:GLU:N	2.27	0.49
1:G:700:ARG:O	1:G:704:GLU:HB2	2.12	0.49
1:H:495:TYR:N	1:H:495:TYR:HD2	2.10	0.49
1:H:606:THR:C	1:H:608:MET:N	2.68	0.49
1:L:464:LEU:HD13	1:L:550:MET:HG3	1.94	0.49
1:H:512:LYS:NZ	1:H:611:MET:O	2.45	0.49
1:G:472:PRO:HB2	1:G:533:ASN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:613:THR:HG23	1:K:614:LYS:HG3	1.93	0.49
1:M:508:MET:HG3	1:M:508:MET:O	2.10	0.49
1:B:524:LYS:HD2	1:B:622:ALA:HB1	1.95	0.49
1:D:499:HIS:CD2	1:E:703:ILE:HD13	2.48	0.49
1:K:605:LEU:HD22	1:K:638:ARG:HD3	1.95	0.49
1:N:472:PRO:HG3	1:N:539:PHE:HB2	1.94	0.49
1:N:533:ASN:C	1:N:533:ASN:ND2	2.71	0.49
1:B:700:ARG:O	1:B:704:GLU:HB2	2.13	0.49
1:E:464:LEU:HD22	1:E:558:ASN:CB	2.38	0.49
1:F:493:VAL:CG2	1:F:531:ILE:HD11	2.43	0.49
1:I:544:GLY:N	1:I:545:PRO:CD	2.75	0.49
1:K:493:VAL:CG2	1:K:531:ILE:HD11	2.42	0.49
1:K:495:TYR:N	1:K:495:TYR:CD2	2.81	0.49
1:D:608:MET:HG3	1:D:619:ILE:CD1	2.43	0.48
1:G:606:THR:O	1:G:608:MET:N	2.46	0.48
1:I:624:ASN:HD22	1:I:625:ARG:HG2	1.77	0.48
1:J:508:MET:O	1:J:508:MET:HG3	2.13	0.48
1:N:700:ARG:O	1:N:704:GLU:HB2	2.13	0.48
1:I:512:LYS:NZ	1:I:611:MET:O	2.45	0.48
1:N:626:PRO:HA	1:N:629:ILE:HG12	1.94	0.48
1:A:545:PRO:HA	1:N:602:ASN:OD1	2.13	0.48
1:A:626:PRO:HA	1:A:629:ILE:HG12	1.95	0.48
1:A:688:THR:HG1	2:A:900:ADP:H1'	1.77	0.48
1:C:533:ASN:HD22	1:C:534:GLU:N	2.10	0.48
1:N:493:VAL:CG2	1:N:531:ILE:HD11	2.43	0.48
1:H:472:PRO:HG3	1:H:539:PHE:HB2	1.94	0.48
1:J:516:PHE:O	1:J:622:ALA:HA	2.13	0.48
1:A:625:ARG:NH1	1:A:627:ASP:OD1	2.47	0.48
1:F:556:GLU:OE2	1:F:599:ARG:NH1	2.46	0.48
1:A:495:TYR:N	1:A:495:TYR:HD2	2.12	0.48
1:B:556:GLU:OE2	1:B:599:ARG:NH1	2.47	0.48
1:C:660:ASN:HD22	1:C:688:THR:HA	1.79	0.48
1:H:472:PRO:HB2	1:H:533:ASN:HB2	1.95	0.48
1:H:606:THR:O	1:H:608:MET:N	2.46	0.48
1:H:660:ASN:HD22	1:H:688:THR:HA	1.79	0.48
1:K:644:TYR:CE2	1:K:646:PRO:HB3	2.49	0.48
1:N:589:ASN:OD1	1:N:589:ASN:N	2.37	0.48
1:A:608:MET:HG3	1:A:619:ILE:CD1	2.43	0.48
1:B:660:ASN:ND2	1:B:688:THR:HA	2.28	0.48
1:C:606:THR:C	1:C:608:MET:N	2.70	0.48
1:C:758:PHE:HB3	1:C:762:LEU:CD1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:575:PHE:CE2	1:F:577:ASP:HB2	2.48	0.48
1:G:495:TYR:CD2	1:G:495:TYR:N	2.81	0.48
1:L:508:MET:O	1:L:508:MET:HG3	2.12	0.48
1:B:495:TYR:N	1:B:495:TYR:CD2	2.82	0.48
1:B:523:GLY:HA2	2:B:900:ADP:O1A	2.14	0.48
1:C:515:LEU:HD21	1:C:623:THR:HG22	1.94	0.48
1:E:624:ASN:HD22	1:E:624:ASN:C	2.22	0.48
1:F:606:THR:HG22	1:I:465:ARG:HD2	1.96	0.48
1:J:482:LEU:HB3	1:J:485:VAL:HG22	1.96	0.48
1:B:590:ILE:HG13	1:B:591:GLY:H	1.78	0.48
1:C:523:GLY:HA2	2:C:900:ADP:O1A	2.13	0.48
1:D:482:LEU:HB3	1:D:485:VAL:HG22	1.96	0.48
1:K:499:HIS:N	1:K:500:PRO:HD3	2.28	0.48
1:M:626:PRO:HA	1:M:629:ILE:HG12	1.95	0.48
1:H:493:VAL:HG21	1:H:531:ILE:CG1	2.44	0.47
1:H:512:LYS:HE2	1:H:512:LYS:HB3	1.76	0.47
1:B:606:THR:C	1:B:608:MET:N	2.72	0.47
1:B:730:GLU:N	1:B:730:GLU:CD	2.72	0.47
1:E:590:ILE:HG13	1:E:591:GLY:H	1.79	0.47
1:I:493:VAL:HG21	1:I:531:ILE:CG1	2.44	0.47
1:I:524:LYS:HD2	1:I:622:ALA:HB1	1.97	0.47
1:M:495:TYR:CD1	1:N:703:ILE:HD12	2.49	0.47
1:M:681:GLY:HA3	1:M:745:ARG:NH2	2.26	0.47
1:E:516:PHE:O	1:E:622:ALA:HA	2.14	0.47
1:G:560:ARG:HG3	1:G:560:ARG:HH11	1.77	0.47
1:C:650:GLU:HB3	1:C:677:LYS:HZ1	1.80	0.47
1:G:660:ASN:ND2	1:G:688:THR:HA	2.29	0.47
1:H:482:LEU:HB3	1:H:485:VAL:HG22	1.95	0.47
1:K:560:ARG:HG3	1:K:560:ARG:NH1	2.30	0.47
1:B:560:ARG:NH1	1:B:560:ARG:HG3	2.29	0.47
1:D:495:TYR:CD2	1:D:495:TYR:N	2.83	0.47
1:E:493:VAL:HG21	1:E:531:ILE:CG1	2.45	0.47
1:E:650:GLU:H	1:E:650:GLU:CD	2.22	0.47
1:I:644:TYR:C	1:I:645:ILE:HD12	2.39	0.47
1:J:556:GLU:OE2	1:J:599:ARG:NH1	2.47	0.47
1:J:660:ASN:HD22	1:J:688:THR:HA	1.78	0.47
1:L:533:ASN:C	1:L:533:ASN:ND2	2.71	0.47
1:M:499:HIS:N	1:M:500:PRO:HD3	2.30	0.47
1:D:624:ASN:HD22	1:D:624:ASN:C	2.23	0.47
1:F:613:THR:HG23	1:F:614:LYS:HG3	1.96	0.47
1:G:625:ARG:NH1	1:G:627:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ARG:O	1:A:757:MET:HG2	2.14	0.47
1:B:560:ARG:HG3	1:B:560:ARG:HH11	1.79	0.47
1:E:472:PRO:HB2	1:E:533:ASN:HB2	1.96	0.47
1:E:605:LEU:HD22	1:E:638:ARG:HD3	1.97	0.47
1:E:625:ARG:NH1	1:E:625:ARG:HB3	2.30	0.47
1:H:611:MET:HE3	1:H:611:MET:HB3	1.77	0.47
1:K:576:PHE:CZ	1:K:604:ILE:HD13	2.49	0.47
1:K:624:ASN:HD22	1:K:625:ARG:HG2	1.78	0.47
1:K:625:ARG:HH12	1:K:627:ASP:CG	2.21	0.47
1:L:515:LEU:HD21	1:L:623:THR:HG22	1.95	0.47
1:L:560:ARG:NH1	1:L:560:ARG:HG3	2.30	0.47
1:N:482:LEU:HB3	1:N:485:VAL:HG22	1.97	0.47
1:B:650:GLU:HB3	1:B:677:LYS:HZ1	1.79	0.47
1:G:606:THR:C	1:G:608:MET:N	2.71	0.47
1:H:582:ILE:O	1:H:586:ARG:HG2	2.14	0.47
1:B:582:ILE:O	1:B:586:ARG:HG2	2.15	0.47
1:G:493:VAL:HG21	1:G:531:ILE:HD11	1.96	0.47
1:H:681:GLY:HA3	1:H:745:ARG:NH2	2.28	0.47
1:J:575:PHE:CE2	1:J:577:ASP:HB2	2.50	0.47
1:J:650:GLU:H	1:J:650:GLU:CD	2.23	0.47
1:J:681:GLY:HA3	1:J:745:ARG:HE	1.79	0.47
1:K:732:ARG:O	1:K:735:HIS:HB2	2.14	0.47
1:M:645:ILE:N	1:M:645:ILE:HD12	2.30	0.47
1:A:650:GLU:HB3	1:A:677:LYS:HZ1	1.79	0.47
1:B:495:TYR:HB3	1:B:503:PHE:HE2	1.80	0.47
1:G:556:GLU:OE2	1:G:599:ARG:NH1	2.48	0.47
1:J:464:LEU:HD13	1:J:550:MET:HG3	1.96	0.47
1:B:515:LEU:HD12	1:B:634:LEU:HD21	1.96	0.46
1:F:512:LYS:NZ	1:F:611:MET:O	2.45	0.46
1:F:590:ILE:HG13	1:F:591:GLY:H	1.79	0.46
1:F:650:GLU:HB3	1:F:677:LYS:HZ1	1.79	0.46
1:G:613:THR:HG23	1:G:614:LYS:HG3	1.96	0.46
1:A:508:MET:O	1:A:508:MET:HG3	2.15	0.46
1:A:516:PHE:HB3	1:A:524:LYS:HG2	1.97	0.46
1:D:499:HIS:N	1:D:500:PRO:HD3	2.30	0.46
1:D:606:THR:C	1:D:608:MET:N	2.72	0.46
1:I:495:TYR:N	1:I:495:TYR:HD2	2.13	0.46
1:I:640:ASP:HB2	1:I:641:GLN:HE21	1.80	0.46
1:L:495:TYR:N	1:L:495:TYR:HD2	2.14	0.46
1:B:465:ARG:HG2	1:B:466:GLU:N	2.31	0.46
1:E:644:TYR:CE2	1:E:646:PRO:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:499:HIS:N	1:L:500:PRO:HD3	2.30	0.46
1:L:613:THR:HG23	1:L:614:LYS:HG3	1.98	0.46
1:M:730:GLU:N	1:M:730:GLU:CD	2.73	0.46
1:N:523:GLY:HA2	2:N:900:ADP:O1A	2.15	0.46
1:A:590:ILE:HG13	1:A:591:GLY:H	1.80	0.46
1:B:467:THR:HB	1:B:565:LYS:HD2	1.97	0.46
1:D:590:ILE:HG13	1:D:591:GLY:H	1.81	0.46
1:D:613:THR:HG23	1:D:614:LYS:HG3	1.97	0.46
1:E:630:ASP:O	1:E:633:ILE:HD12	2.15	0.46
1:H:625:ARG:HH12	1:H:627:ASP:CG	2.24	0.46
1:K:501:ASP:HB2	1:K:505:LYS:HE3	1.98	0.46
1:B:493:VAL:HG21	1:B:531:ILE:CG1	2.46	0.46
1:C:624:ASN:HD22	1:C:624:ASN:C	2.24	0.46
1:C:660:ASN:HD21	1:C:688:THR:CB	2.29	0.46
1:F:624:ASN:HD22	1:F:624:ASN:C	2.23	0.46
1:I:688:THR:OG1	2:I:900:ADP:H1'	2.15	0.46
1:B:472:PRO:HG3	1:B:539:PHE:HB2	1.97	0.46
1:E:482:LEU:HB3	1:E:485:VAL:HG22	1.98	0.46
1:K:625:ARG:HB3	1:K:625:ARG:NH1	2.31	0.46
1:L:606:THR:C	1:L:608:MET:N	2.73	0.46
1:C:524:LYS:HD2	1:C:622:ALA:HB1	1.98	0.46
1:C:613:THR:HG23	1:C:614:LYS:HG3	1.97	0.46
1:K:611:MET:HE3	1:K:611:MET:HB3	1.79	0.46
1:N:729:PRO:C	1:N:730:GLU:CD	2.83	0.46
1:B:495:TYR:N	1:B:495:TYR:HD2	2.14	0.46
1:D:508:MET:O	1:D:508:MET:HG3	2.16	0.46
1:E:575:PHE:CZ	1:E:577:ASP:HB2	2.50	0.46
1:F:533:ASN:ND2	1:F:534:GLU:N	2.64	0.46
1:G:547:LEU:HA	1:G:550:MET:HE3	1.97	0.46
1:G:608:MET:HG3	1:G:619:ILE:CD1	2.46	0.46
1:K:508:MET:O	1:K:508:MET:HG3	2.16	0.46
1:B:501:ASP:HB2	1:B:505:LYS:HE3	1.98	0.46
1:C:476:TRP:CE3	1:C:486:LYS:HG2	2.51	0.46
1:E:508:MET:O	1:E:508:MET:HG3	2.15	0.46
1:F:644:TYR:C	1:F:645:ILE:HD12	2.41	0.46
1:K:625:ARG:NH1	1:K:627:ASP:OD1	2.48	0.46
1:N:495:TYR:N	1:N:495:TYR:CD2	2.83	0.46
1:N:647:LEU:HD21	1:N:747:VAL:HG21	1.97	0.46
1:C:515:LEU:HD12	1:C:634:LEU:HD21	1.97	0.46
1:C:625:ARG:NH1	1:C:627:ASP:OD1	2.49	0.46
1:H:645:ILE:N	1:H:645:ILE:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:582:ILE:O	1:N:586:ARG:HG2	2.16	0.46
1:F:524:LYS:HD2	1:F:622:ALA:HB1	1.98	0.45
1:G:495:TYR:N	1:G:495:TYR:HD2	2.14	0.45
1:J:499:HIS:N	1:J:500:PRO:HD3	2.31	0.45
1:N:464:LEU:HD13	1:N:550:MET:HG3	1.98	0.45
1:N:650:GLU:CD	1:N:650:GLU:H	2.24	0.45
1:A:660:ASN:HD22	1:A:688:THR:HA	1.81	0.45
1:G:464:LEU:HD13	1:G:550:MET:HG3	1.97	0.45
1:I:645:ILE:HD12	1:I:645:ILE:N	2.30	0.45
1:N:624:ASN:C	1:N:624:ASN:HD22	2.24	0.45
1:B:681:GLY:HA3	1:B:745:ARG:HE	1.81	0.45
1:D:495:TYR:N	1:D:495:TYR:HD2	2.15	0.45
1:I:731:ILE:HD13	1:I:731:ILE:C	2.42	0.45
1:I:753:ARG:O	1:I:757:MET:HG2	2.17	0.45
1:K:495:TYR:N	1:K:495:TYR:HD2	2.14	0.45
1:K:626:PRO:HA	1:K:629:ILE:HG12	1.97	0.45
1:A:499:HIS:N	1:A:500:PRO:HD3	2.31	0.45
1:B:613:THR:HG23	1:B:614:LYS:HG3	1.99	0.45
1:D:567:ARG:HH21	1:D:611:MET:HG3	1.81	0.45
1:I:508:MET:O	1:I:508:MET:HG3	2.17	0.45
1:I:626:PRO:HA	1:I:629:ILE:HG12	1.98	0.45
1:J:605:LEU:HD22	1:J:638:ARG:HD3	1.98	0.45
1:K:542:ILE:HD11	1:K:562:ILE:HG23	1.97	0.45
1:M:493:VAL:HG21	1:M:531:ILE:CG1	2.46	0.45
1:M:644:TYR:CE2	1:M:646:PRO:HB3	2.51	0.45
1:N:732:ARG:O	1:N:735:HIS:HB2	2.16	0.45
1:B:476:TRP:CE3	1:B:486:LYS:HG2	2.52	0.45
1:B:681:GLY:HA3	1:B:745:ARG:NH2	2.31	0.45
1:C:464:LEU:HD13	1:C:550:MET:HG3	1.98	0.45
1:D:753:ARG:O	1:D:757:MET:HG2	2.17	0.45
1:F:660:ASN:HD22	1:F:688:THR:HA	1.82	0.45
1:G:493:VAL:HG21	1:G:531:ILE:CG1	2.46	0.45
1:M:589:ASN:OD1	1:M:625:ARG:NH2	2.50	0.45
1:A:611:MET:HE3	1:A:611:MET:HB3	1.86	0.45
1:D:547:LEU:HA	1:D:550:MET:HE3	1.98	0.45
1:D:644:TYR:CE2	1:D:646:PRO:HB3	2.51	0.45
1:F:508:MET:O	1:F:508:MET:HG3	2.15	0.45
1:G:681:GLY:HA3	1:G:745:ARG:NH2	2.28	0.45
1:I:547:LEU:HA	1:I:550:MET:HE3	1.97	0.45
1:J:625:ARG:NH1	1:J:627:ASP:OD1	2.49	0.45
1:J:626:PRO:HA	1:J:629:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:533:ASN:HD22	1:M:534:GLU:N	2.14	0.45
1:C:633:ILE:O	1:C:633:ILE:HG22	2.16	0.45
1:D:680:ASN:C	1:D:682:PHE:N	2.41	0.45
1:G:467:THR:HB	1:G:565:LYS:HD2	1.98	0.45
1:I:611:MET:HE3	1:I:611:MET:HB3	1.78	0.45
1:K:515:LEU:HD12	1:K:634:LEU:HD21	1.98	0.45
1:K:660:ASN:HD22	1:K:688:THR:HA	1.82	0.45
1:N:611:MET:HE3	1:N:611:MET:HB3	1.83	0.45
1:E:681:GLY:HA3	1:E:745:ARG:NH2	2.27	0.45
1:H:501:ASP:HB2	1:H:505:LYS:HE3	1.99	0.45
1:I:464:LEU:HD13	1:I:550:MET:HG3	1.99	0.45
1:N:575:PHE:CZ	1:N:577:ASP:HB2	2.51	0.45
1:K:582:ILE:O	1:K:586:ARG:HG2	2.17	0.45
1:N:464:LEU:HD22	1:N:558:ASN:CB	2.43	0.45
1:N:681:GLY:HA3	1:N:745:ARG:HE	1.81	0.45
1:A:464:LEU:HD22	1:A:558:ASN:CB	2.44	0.45
1:J:606:THR:C	1:J:608:MET:N	2.75	0.45
1:K:547:LEU:HA	1:K:550:MET:HE3	1.98	0.45
1:L:590:ILE:HG13	1:L:591:GLY:H	1.81	0.45
1:M:516:PHE:O	1:M:622:ALA:HA	2.16	0.45
1:A:502:LYS:HE2	1:B:706:GLU:OE2	2.17	0.44
1:B:482:LEU:HB3	1:B:485:VAL:HG22	1.99	0.44
1:B:645:ILE:HD12	1:B:645:ILE:N	2.33	0.44
1:C:512:LYS:HE2	1:C:512:LYS:HB3	1.79	0.44
1:K:687:LEU:HA	1:K:690:ILE:HD12	1.99	0.44
1:M:501:ASP:O	1:M:505:LYS:HG3	2.17	0.44
1:N:606:THR:O	1:N:608:MET:N	2.50	0.44
1:N:624:ASN:HD22	1:N:625:ARG:HG2	1.82	0.44
1:B:611:MET:HE3	1:B:611:MET:HB3	1.83	0.44
1:D:681:GLY:HA3	1:D:745:ARG:NH2	2.28	0.44
1:K:730:GLU:N	1:K:730:GLU:CD	2.75	0.44
1:L:611:MET:HB3	1:L:611:MET:HE3	1.73	0.44
1:M:582:ILE:O	1:M:586:ARG:HG2	2.18	0.44
1:G:512:LYS:HE2	1:G:512:LYS:HB3	1.86	0.44
1:H:634:LEU:HD22	1:H:642:LEU:HD21	2.00	0.44
1:J:495:TYR:N	1:J:495:TYR:CD2	2.86	0.44
1:K:465:ARG:HG2	1:K:466:GLU:H	1.82	0.44
1:L:626:PRO:HA	1:L:629:ILE:HG12	1.99	0.44
1:A:501:ASP:O	1:A:505:LYS:HG3	2.18	0.44
1:B:527:LEU:O	1:B:531:ILE:HG22	2.17	0.44
1:B:626:PRO:HA	1:B:629:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:PRO:HA	1:C:616:ASN:HB3	1.99	0.44
1:H:499:HIS:N	1:H:500:PRO:HD3	2.32	0.44
1:I:482:LEU:HB3	1:I:485:VAL:CG2	2.47	0.44
1:K:751:ASP:O	1:K:752:ILE:C	2.60	0.44
1:M:590:ILE:HG13	1:M:591:GLY:H	1.82	0.44
1:M:464:LEU:HD13	1:M:550:MET:HG3	1.99	0.44
1:M:660:ASN:HD22	1:M:688:THR:HA	1.82	0.44
1:N:499:HIS:N	1:N:500:PRO:HD3	2.33	0.44
1:A:730:GLU:N	1:A:730:GLU:CD	2.75	0.44
1:F:476:TRP:CE3	1:F:486:LYS:HG2	2.53	0.44
1:F:644:TYR:CE2	1:F:646:PRO:HB3	2.53	0.44
1:G:516:PHE:O	1:G:622:ALA:HA	2.18	0.44
1:H:763:GLN:C	1:M:744:ARG:HD3	2.42	0.44
1:L:560:ARG:HG3	1:L:560:ARG:HH11	1.82	0.44
1:A:681:GLY:HA3	1:A:745:ARG:NH2	2.28	0.44
1:E:523:GLY:HA2	2:E:900:ADP:O1A	2.16	0.44
1:E:611:MET:HB3	1:E:611:MET:HE3	1.71	0.44
1:H:613:THR:HG23	1:H:614:LYS:HG3	1.99	0.44
1:I:625:ARG:NH1	1:I:627:ASP:OD1	2.51	0.44
1:J:753:ARG:O	1:J:757:MET:HG2	2.18	0.44
1:M:512:LYS:HE2	1:M:512:LYS:HB3	1.79	0.44
1:D:630:ASP:O	1:D:633:ILE:HD12	2.18	0.44
1:F:515:LEU:HD21	1:F:623:THR:HG22	1.99	0.44
1:G:508:MET:O	1:G:508:MET:HG3	2.17	0.44
1:H:501:ASP:O	1:H:505:LYS:HG3	2.18	0.44
1:J:660:ASN:HD21	1:J:688:THR:CB	2.29	0.44
1:K:472:PRO:HB2	1:K:533:ASN:HB2	1.99	0.44
1:M:650:GLU:HB3	1:M:677:LYS:HZ1	1.82	0.44
1:M:681:GLY:HA3	1:M:745:ARG:HE	1.83	0.44
1:A:644:TYR:CE2	1:A:646:PRO:HB3	2.53	0.44
1:B:519:PRO:HG3	1:B:647:LEU:HD12	2.00	0.44
1:F:729:PRO:C	1:F:730:GLU:CD	2.86	0.44
1:K:560:ARG:HG3	1:K:560:ARG:HH11	1.83	0.44
1:N:495:TYR:N	1:N:495:TYR:HD2	2.15	0.44
1:N:644:TYR:CE2	1:N:646:PRO:HB3	2.53	0.44
1:C:730:GLU:CD	1:C:730:GLU:N	2.76	0.43
1:H:519:PRO:HG3	1:H:647:LEU:HD12	2.00	0.43
1:H:730:GLU:CD	1:H:730:GLU:N	2.76	0.43
1:J:730:GLU:CD	1:J:730:GLU:N	2.76	0.43
1:K:542:ILE:HD11	1:K:562:ILE:CG2	2.47	0.43
1:K:645:ILE:N	1:K:645:ILE:HD12	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:613:THR:HG23	1:N:614:LYS:HG3	2.00	0.43
1:A:493:VAL:CG2	1:A:531:ILE:HD11	2.49	0.43
1:D:533:ASN:ND2	1:D:533:ASN:C	2.76	0.43
1:E:512:LYS:HB3	1:E:512:LYS:HE2	1.69	0.43
1:E:608:MET:HG3	1:E:619:ILE:CD1	2.48	0.43
1:F:626:PRO:HA	1:F:629:ILE:HG12	1.99	0.43
1:L:522:CYS:HB3	1:L:645:ILE:HG22	1.99	0.43
1:A:606:THR:C	1:A:608:MET:N	2.71	0.43
1:B:589:ASN:OD1	1:B:589:ASN:N	2.35	0.43
1:E:465:ARG:HG2	1:E:466:GLU:H	1.82	0.43
1:E:606:THR:C	1:E:608:MET:H	2.26	0.43
1:J:465:ARG:HG2	1:J:466:GLU:H	1.79	0.43
1:M:625:ARG:HB3	1:M:625:ARG:HH11	1.82	0.43
1:N:559:VAL:HA	1:N:562:ILE:HD12	2.01	0.43
1:B:650:GLU:CD	1:B:650:GLU:H	2.26	0.43
1:C:664:SER:HA	1:C:665:PRO:HD3	1.87	0.43
1:F:495:TYR:N	1:F:495:TYR:CD2	2.85	0.43
1:G:487:ARG:HE	1:H:700:ARG:NH2	2.16	0.43
1:G:523:GLY:CA	2:G:900:ADP:O1A	2.66	0.43
1:G:544:GLY:N	1:G:545:PRO:CD	2.81	0.43
1:H:650:GLU:CD	1:H:650:GLU:H	2.26	0.43
1:I:660:ASN:HD21	1:I:688:THR:CB	2.32	0.43
1:A:501:ASP:HB2	1:A:505:LYS:HE3	1.99	0.43
1:B:624:ASN:HD22	1:B:624:ASN:C	2.26	0.43
1:F:700:ARG:O	1:F:704:GLU:HB2	2.18	0.43
1:F:731:ILE:HD13	1:F:731:ILE:C	2.44	0.43
1:K:515:LEU:HD21	1:K:623:THR:HG22	1.99	0.43
1:L:523:GLY:CA	2:L:900:ADP:O1A	2.66	0.43
1:K:606:THR:C	1:K:608:MET:N	2.71	0.43
1:L:482:LEU:HB3	1:L:485:VAL:HG22	2.00	0.43
1:E:730:GLU:CD	1:E:730:GLU:N	2.77	0.43
1:L:604:ILE:O	1:L:608:MET:HB2	2.19	0.43
1:M:753:ARG:O	1:M:757:MET:HG2	2.18	0.43
1:A:476:TRP:CE3	1:A:486:LYS:HG2	2.54	0.43
1:B:508:MET:O	1:B:508:MET:HG3	2.17	0.43
1:B:547:LEU:HA	1:B:550:MET:HE3	2.00	0.43
1:C:653:ARG:HD2	1:C:679:THR:OG1	2.19	0.43
1:H:589:ASN:OD1	1:H:625:ARG:NH2	2.52	0.43
1:I:608:MET:HG3	1:I:619:ILE:CD1	2.48	0.43
1:J:534:GLU:C	1:J:536:GLN:H	2.27	0.43
1:N:579:LEU:HD23	1:N:579:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:LEU:HA	1:B:489:LEU:HD23	1.83	0.43
1:C:516:PHE:HB3	1:C:524:LYS:HG2	2.01	0.43
1:D:625:ARG:NH1	1:D:627:ASP:OD1	2.51	0.43
1:G:640:ASP:HB2	1:G:641:GLN:HE21	1.84	0.43
1:K:519:PRO:HA	1:K:520:PRO:HD3	1.81	0.43
1:M:523:GLY:HA2	2:M:900:ADP:O1A	2.18	0.43
1:D:526:LEU:N	1:D:526:LEU:HD23	2.34	0.43
1:E:589:ASN:OD1	1:E:625:ARG:NH2	2.52	0.43
1:L:464:LEU:HD22	1:L:558:ASN:CB	2.45	0.43
1:A:625:ARG:NH1	1:A:625:ARG:HB3	2.33	0.42
1:B:527:LEU:HD23	1:B:527:LEU:HA	1.91	0.42
1:C:590:ILE:HG13	1:C:591:GLY:H	1.84	0.42
1:F:599:ARG:NH2	1:I:552:PHE:HB3	2.34	0.42
1:G:589:ASN:OD1	1:G:625:ARG:NH2	2.52	0.42
1:J:527:LEU:HD23	1:J:527:LEU:HA	1.92	0.42
1:N:556:GLU:OE2	1:N:599:ARG:NH1	2.52	0.42
1:A:560:ARG:HG3	1:A:560:ARG:NH1	2.34	0.42
1:A:607:GLU:O	1:A:611:MET:HB2	2.19	0.42
1:A:757:MET:HG2	1:A:757:MET:H	1.71	0.42
1:A:758:PHE:HB3	1:A:762:LEU:CD1	2.47	0.42
1:B:733:ARG:O	1:B:737:GLU:HG3	2.20	0.42
1:F:516:PHE:HB3	1:F:524:LYS:HG2	2.02	0.42
1:I:476:TRP:CE3	1:I:486:LYS:HG2	2.54	0.42
1:D:625:ARG:HB3	1:D:625:ARG:HH11	1.83	0.42
1:D:645:ILE:N	1:D:645:ILE:HD12	2.33	0.42
1:F:489:LEU:HD23	1:F:489:LEU:HA	1.86	0.42
1:F:495:TYR:N	1:F:495:TYR:HD2	2.17	0.42
1:F:516:PHE:O	1:F:622:ALA:HA	2.18	0.42
1:F:650:GLU:CD	1:F:650:GLU:H	2.27	0.42
1:M:482:LEU:HB3	1:M:485:VAL:HG22	2.01	0.42
1:A:575:PHE:CZ	1:A:577:ASP:HB2	2.54	0.42
1:C:687:LEU:HA	1:C:690:ILE:HD12	2.00	0.42
1:E:493:VAL:HG21	1:E:531:ILE:HD11	2.00	0.42
1:L:471:VAL:HA	1:L:472:PRO:HD3	1.84	0.42
1:L:731:ILE:C	1:L:731:ILE:HD13	2.45	0.42
1:L:732:ARG:O	1:L:735:HIS:HB2	2.18	0.42
1:B:499:HIS:N	1:B:500:PRO:HD3	2.34	0.42
1:C:626:PRO:HA	1:C:629:ILE:HG12	2.02	0.42
1:D:519:PRO:HA	1:D:520:PRO:HD3	1.86	0.42
1:D:534:GLU:C	1:D:536:GLN:H	2.27	0.42
1:E:731:ILE:C	1:E:731:ILE:HD13	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:589:ASN:OD1	1:J:625:ARG:NH2	2.52	0.42
1:K:482:LEU:HB3	1:K:485:VAL:CG2	2.50	0.42
1:K:516:PHE:O	1:K:622:ALA:HA	2.20	0.42
1:A:464:LEU:HD13	1:A:550:MET:HG3	2.02	0.42
1:A:482:LEU:HB3	1:A:485:VAL:CG2	2.50	0.42
1:C:625:ARG:HH12	1:C:627:ASP:CG	2.26	0.42
1:D:512:LYS:HB3	1:D:512:LYS:HE2	1.77	0.42
1:I:515:LEU:HD12	1:I:634:LEU:HD21	2.00	0.42
1:J:601:ILE:HG21	1:J:633:ILE:HD11	2.02	0.42
1:K:575:PHE:CZ	1:K:577:ASP:HB2	2.54	0.42
1:A:529:LYS:O	1:A:530:ALA:C	2.63	0.42
1:D:626:PRO:HA	1:D:629:ILE:HG12	2.01	0.42
1:F:625:ARG:NH1	1:F:627:ASP:OD1	2.52	0.42
1:I:642:LEU:N	1:I:642:LEU:HD22	2.35	0.42
1:M:471:VAL:HA	1:M:472:PRO:HD3	1.86	0.42
1:N:670:VAL:HG22	1:N:733:ARG:HA	2.01	0.42
1:A:515:LEU:HD21	1:A:623:THR:HG22	2.01	0.42
1:B:464:LEU:HD11	1:B:546:GLU:HG3	2.01	0.42
1:F:681:GLY:HA3	1:F:745:ARG:NH2	2.31	0.42
1:H:495:TYR:HB3	1:H:503:PHE:HE2	1.83	0.42
1:I:556:GLU:OE2	1:I:599:ARG:NH1	2.52	0.42
1:K:501:ASP:O	1:K:505:LYS:HG3	2.19	0.42
1:M:758:PHE:HB3	1:M:762:LEU:CD1	2.49	0.42
1:N:590:ILE:HG13	1:N:591:GLY:H	1.83	0.42
1:A:650:GLU:CD	1:A:650:GLU:H	2.27	0.42
1:G:575:PHE:CZ	1:G:577:ASP:HB2	2.54	0.42
1:G:644:TYR:CE2	1:G:646:PRO:HB3	2.55	0.42
1:I:542:ILE:HD11	1:I:562:ILE:CG2	2.50	0.42
1:J:517:TYR:CZ	1:J:644:TYR:HB2	2.55	0.42
1:K:523:GLY:HA2	2:K:900:ADP:O1A	2.20	0.42
1:L:729:PRO:C	1:L:730:GLU:CD	2.88	0.42
1:B:512:LYS:NZ	1:B:611:MET:O	2.47	0.42
1:C:472:PRO:HB2	1:C:533:ASN:HB2	2.02	0.42
1:C:681:GLY:HA3	1:C:745:ARG:NH2	2.31	0.42
1:D:495:TYR:HB3	1:D:503:PHE:HE2	1.85	0.42
1:D:732:ARG:O	1:D:735:HIS:HB2	2.20	0.42
1:H:602:ASN:OD1	1:M:545:PRO:HA	2.20	0.42
1:H:681:GLY:HA3	1:H:745:ARG:HE	1.85	0.42
1:K:749:ASP:OD1	1:K:749:ASP:N	2.53	0.42
1:L:493:VAL:HG21	1:L:531:ILE:CG1	2.50	0.42
1:L:501:ASP:HB2	1:L:505:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:650:GLU:H	1:M:650:GLU:CD	2.28	0.42
1:H:664:SER:HA	1:H:665:PRO:HD3	1.89	0.41
1:K:681:GLY:HA3	1:K:745:ARG:NH2	2.29	0.41
1:K:731:ILE:HD13	1:K:731:ILE:C	2.45	0.41
1:M:493:VAL:HG21	1:M:531:ILE:HD11	2.02	0.41
1:M:603:GLN:O	1:M:604:ILE:C	2.63	0.41
1:B:556:GLU:O	1:B:559:VAL:HG23	2.19	0.41
1:D:512:LYS:NZ	1:D:611:MET:O	2.48	0.41
1:J:464:LEU:HD22	1:J:558:ASN:CB	2.45	0.41
1:L:472:PRO:HB2	1:L:533:ASN:HB2	2.02	0.41
1:L:607:GLU:O	1:L:611:MET:HB2	2.20	0.41
1:M:482:LEU:HB3	1:M:485:VAL:CG2	2.50	0.41
1:M:536:GLN:OE1	1:M:536:GLN:HA	2.20	0.41
1:M:563:PHE:CD2	1:M:607:GLU:HB3	2.55	0.41
1:N:495:TYR:N	1:N:496:PRO:HD2	2.35	0.41
1:N:516:PHE:O	1:N:622:ALA:HA	2.21	0.41
1:B:608:MET:HG3	1:B:619:ILE:CD1	2.50	0.41
1:C:499:HIS:N	1:C:500:PRO:HD3	2.36	0.41
1:D:625:ARG:HH12	1:D:627:ASP:CG	2.27	0.41
1:H:519:PRO:HG3	1:H:647:LEU:CD1	2.50	0.41
1:H:534:GLU:C	1:H:536:GLN:H	2.29	0.41
1:I:630:ASP:O	1:I:633:ILE:HD12	2.20	0.41
1:K:650:GLU:CD	1:K:650:GLU:H	2.28	0.41
1:M:516:PHE:HB3	1:M:524:LYS:HG2	2.02	0.41
1:F:733:ARG:O	1:F:737:GLU:HG3	2.20	0.41
1:F:757:MET:HG2	1:F:757:MET:H	1.71	0.41
1:G:729:PRO:C	1:G:730:GLU:CD	2.89	0.41
1:H:493:VAL:HG21	1:H:531:ILE:HD11	1.98	0.41
1:H:515:LEU:C	1:H:515:LEU:CD2	2.93	0.41
1:I:650:GLU:HB3	1:I:677:LYS:HZ3	1.85	0.41
1:M:611:MET:HE3	1:M:611:MET:HB3	1.84	0.41
1:E:491:GLU:HG2	1:E:495:TYR:CE1	2.56	0.41
1:E:606:THR:C	1:E:608:MET:N	2.78	0.41
1:F:499:HIS:N	1:F:500:PRO:HD3	2.35	0.41
1:G:626:PRO:HA	1:G:629:ILE:HG12	2.02	0.41
1:I:471:VAL:HA	1:I:472:PRO:HD3	1.88	0.41
1:I:495:TYR:HB3	1:I:503:PHE:HE2	1.86	0.41
1:I:624:ASN:HD22	1:I:624:ASN:C	2.28	0.41
1:L:495:TYR:HB3	1:L:503:PHE:HE2	1.85	0.41
1:N:660:ASN:HD22	1:N:688:THR:HA	1.85	0.41
1:A:589:ASN:OD1	1:A:625:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:482:LEU:HB3	1:F:485:VAL:CG2	2.50	0.41
1:F:645:ILE:N	1:F:645:ILE:CD1	2.83	0.41
1:F:671:ASP:OD1	1:F:671:ASP:C	2.64	0.41
1:H:633:ILE:O	1:H:633:ILE:HG22	2.20	0.41
1:M:678:MET:HE2	1:M:678:MET:HA	2.01	0.41
1:D:605:LEU:HD22	1:D:638:ARG:HD3	2.03	0.41
1:G:534:GLU:C	1:G:536:GLN:H	2.28	0.41
1:H:533:ASN:ND2	1:H:534:GLU:N	2.68	0.41
1:I:534:GLU:C	1:I:536:GLN:H	2.28	0.41
1:I:660:ASN:HD22	1:I:688:THR:HA	1.84	0.41
1:J:547:LEU:HA	1:J:550:MET:HE3	2.02	0.41
1:N:534:GLU:C	1:N:536:GLN:H	2.28	0.41
1:N:544:GLY:N	1:N:545:PRO:CD	2.84	0.41
1:N:706:GLU:H	1:N:706:GLU:HG3	1.71	0.41
1:B:534:GLU:C	1:B:536:GLN:H	2.28	0.41
1:B:671:ASP:OD1	1:B:671:ASP:C	2.63	0.41
1:B:732:ARG:O	1:B:735:HIS:HB2	2.20	0.41
1:D:491:GLU:HG2	1:D:495:TYR:CE1	2.56	0.41
1:E:517:TYR:CZ	1:E:644:TYR:HB2	2.56	0.41
1:E:671:ASP:OD1	1:E:671:ASP:C	2.63	0.41
1:E:753:ARG:O	1:E:757:MET:HG2	2.21	0.41
1:G:491:GLU:HG2	1:G:495:TYR:CE1	2.55	0.41
1:H:660:ASN:HD21	1:H:688:THR:CB	2.34	0.41
1:H:731:ILE:C	1:H:731:ILE:HD13	2.46	0.41
1:I:527:LEU:HD23	1:I:527:LEU:HA	1.87	0.41
1:K:512:LYS:HE2	1:K:512:LYS:HB3	1.74	0.41
1:N:731:ILE:HD13	1:N:731:ILE:C	2.45	0.41
1:A:491:GLU:HG2	1:A:495:TYR:CE1	2.56	0.41
1:B:512:LYS:HE2	1:B:512:LYS:HB3	1.77	0.41
1:C:508:MET:O	1:C:508:MET:HG3	2.21	0.41
1:D:575:PHE:CZ	1:D:577:ASP:HB2	2.56	0.41
1:E:626:PRO:HA	1:E:629:ILE:HG12	2.03	0.41
1:F:495:TYR:HB3	1:F:503:PHE:HE2	1.86	0.41
1:F:625:ARG:HH12	1:F:627:ASP:CG	2.29	0.41
1:G:465:ARG:HG2	1:G:466:GLU:H	1.85	0.41
1:H:516:PHE:O	1:H:622:ALA:HA	2.21	0.41
1:J:471:VAL:HA	1:J:472:PRO:HD3	1.88	0.41
1:J:472:PRO:HB2	1:J:533:ASN:HB2	2.01	0.41
1:J:624:ASN:C	1:J:624:ASN:ND2	2.77	0.41
1:L:497:VAL:HG13	1:L:498:GLU:HG3	2.03	0.41
1:M:687:LEU:HA	1:M:690:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:560:ARG:NH1	1:N:560:ARG:HG3	2.36	0.41
1:B:529:LYS:O	1:B:530:ALA:C	2.62	0.41
1:D:611:MET:HE3	1:D:611:MET:HB3	1.82	0.41
1:F:464:LEU:HD11	1:F:546:GLU:HG3	2.02	0.41
1:G:758:PHE:HB3	1:G:762:LEU:CD1	2.51	0.41
1:I:613:THR:HG23	1:I:614:LYS:HG3	2.03	0.41
1:N:625:ARG:HB3	1:N:625:ARG:NH1	2.36	0.41
1:E:499:HIS:O	1:E:500:PRO:C	2.63	0.40
1:E:576:PHE:CE2	1:E:604:ILE:HD13	2.56	0.40
1:F:493:VAL:HG21	1:F:531:ILE:CG1	2.51	0.40
1:G:607:GLU:O	1:G:611:MET:HB2	2.21	0.40
1:H:608:MET:HG3	1:H:619:ILE:CD1	2.52	0.40
1:J:491:GLU:HG2	1:J:495:TYR:CE1	2.55	0.40
1:J:660:ASN:ND2	1:J:688:THR:OG1	2.50	0.40
1:N:471:VAL:HA	1:N:472:PRO:HD3	1.86	0.40
1:B:536:GLN:OE1	1:B:536:GLN:HA	2.21	0.40
1:D:601:ILE:HG21	1:D:633:ILE:HD11	2.03	0.40
1:K:493:VAL:HG21	1:K:531:ILE:CG1	2.51	0.40
1:L:754:LYS:HA	1:L:757:MET:HG3	2.03	0.40
1:N:512:LYS:HE2	1:N:512:LYS:HB3	1.78	0.40
1:B:501:ASP:O	1:B:505:LYS:HG3	2.22	0.40
1:B:751:ASP:O	1:B:752:ILE:C	2.62	0.40
1:C:542:ILE:HG12	1:C:562:ILE:HD13	2.02	0.40
1:D:527:LEU:HD23	1:D:527:LEU:HA	1.96	0.40
1:J:481:GLY:O	1:J:482:LEU:HB2	2.21	0.40
1:J:495:TYR:HB3	1:J:503:PHE:HE2	1.86	0.40
1:K:508:MET:SD	1:L:696:LYS:HG3	2.61	0.40
1:L:575:PHE:HA	1:L:620:ILE:O	2.22	0.40
1:A:512:LYS:HE2	1:A:512:LYS:HB3	1.70	0.40
1:A:560:ARG:HG3	1:A:560:ARG:HH11	1.85	0.40
1:A:664:SER:HA	1:A:665:PRO:HD3	1.92	0.40
1:C:500:PRO:O	1:C:504:LEU:HD13	2.22	0.40
1:D:744:ARG:HD3	1:L:763:GLN:C	2.46	0.40
1:E:556:GLU:OE2	1:E:599:ARG:NH1	2.55	0.40
1:F:501:ASP:HB2	1:F:505:LYS:HE3	2.02	0.40
1:G:515:LEU:HD21	1:G:623:THR:HG22	2.03	0.40
1:J:493:VAL:HG21	1:J:531:ILE:CG1	2.51	0.40
1:J:495:TYR:N	1:J:495:TYR:HD2	2.19	0.40
1:J:583:ALA:O	1:J:584:LYS:C	2.61	0.40
1:K:489:LEU:HD23	1:K:489:LEU:HA	1.91	0.40
1:K:579:LEU:HD23	1:K:579:LEU:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:660:ASN:HD21	1:K:688:THR:CB	2.35	0.40
1:L:501:ASP:O	1:L:505:LYS:HG3	2.22	0.40
1:L:547:LEU:HA	1:L:550:MET:HE3	2.02	0.40
1:M:501:ASP:HB2	1:M:505:LYS:HE3	2.04	0.40
1:M:660:ASN:HD21	1:M:688:THR:CB	2.34	0.40
1:N:688:THR:HG1	2:N:900:ADP:H1'	1.86	0.40
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.91	0.40
1:A:506:PHE:CD2	1:B:699:ILE:HG12	2.56	0.40
1:B:517:TYR:HA	1:B:623:THR:O	2.22	0.40
1:B:576:PHE:CZ	1:B:604:ILE:HD13	2.56	0.40
1:F:534:GLU:C	1:F:536:GLN:H	2.29	0.40
1:G:489:LEU:HD23	1:G:489:LEU:HA	1.94	0.40
1:I:512:LYS:HB3	1:I:512:LYS:HE2	1.85	0.40
1:J:489:LEU:HD23	1:J:489:LEU:HA	1.93	0.40
1:K:590:ILE:HG13	1:K:591:GLY:H	1.86	0.40
1:K:650:GLU:HB3	1:K:677:LYS:HZ1	1.85	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:668:LYS:NZ	1:N:673:GLU:OE1[4_455]	1.57	0.63
1:A:614:LYS:CE	1:M:536:GLN:O[4_455]	1.88	0.32
1:E:673:GLU:OE1	1:H:668:LYS:NZ[4_454]	1.90	0.30
1:B:568:GLN:OE1	1:M:505:LYS:NZ[4_455]	2.10	0.10
1:E:671:ASP:OD1	1:H:668:LYS:NZ[4_454]	2.10	0.10
1:F:749:ASP:OD1	1:F:749:ASP:OD1[2_454]	2.16	0.04

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	277/301 (92%)	255 (92%)	20 (7%)	2 (1%)	18	53
1	B	277/301 (92%)	254 (92%)	20 (7%)	3 (1%)	11	43
1	C	277/301 (92%)	252 (91%)	23 (8%)	2 (1%)	18	53
1	D	277/301 (92%)	252 (91%)	22 (8%)	3 (1%)	11	43
1	E	277/301 (92%)	254 (92%)	20 (7%)	3 (1%)	11	43
1	F	277/301 (92%)	250 (90%)	23 (8%)	4 (1%)	9	36
1	G	277/301 (92%)	252 (91%)	22 (8%)	3 (1%)	11	43
1	H	277/301 (92%)	251 (91%)	22 (8%)	4 (1%)	9	36
1	I	277/301 (92%)	253 (91%)	22 (8%)	2 (1%)	18	53
1	J	277/301 (92%)	253 (91%)	21 (8%)	3 (1%)	11	43
1	K	277/301 (92%)	253 (91%)	20 (7%)	4 (1%)	9	36
1	L	277/301 (92%)	254 (92%)	20 (7%)	3 (1%)	11	43
1	M	277/301 (92%)	250 (90%)	23 (8%)	4 (1%)	9	36
1	N	277/301 (92%)	247 (89%)	27 (10%)	3 (1%)	11	43
All	All	3878/4214 (92%)	3530 (91%)	305 (8%)	43 (1%)	11	43

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	681	GLY
1	B	681	GLY
1	C	681	GLY
1	D	681	GLY
1	E	607	GLU
1	E	681	GLY
1	F	607	GLU
1	F	681	GLY
1	G	681	GLY
1	H	681	GLY
1	I	681	GLY
1	J	681	GLY
1	K	681	GLY
1	L	579	LEU
1	L	681	GLY
1	M	681	GLY
1	N	681	GLY
1	D	607	GLU
1	F	579	LEU

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Mol	Chain	Res	Type
1	G	607	GLU
1	H	607	GLU
1	M	607	GLU
1	B	607	GLU
1	H	650	GLU
1	K	607	GLU
1	M	579	LEU
1	J	607	GLU
1	K	579	LEU
1	A	729	PRO
1	C	729	PRO
1	D	729	PRO
1	E	729	PRO
1	F	729	PRO
1	G	729	PRO
1	H	729	PRO
1	I	729	PRO
1	J	729	PRO
1	M	729	PRO
1	N	607	GLU
1	K	729	PRO
1	N	729	PRO
1	B	729	PRO
1	L	729	PRO

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	236/255 (92%)	212 (90%)	24 (10%)	7	29
1	B	236/255 (92%)	211 (89%)	25 (11%)	6	27
1	C	236/255 (92%)	213 (90%)	23 (10%)	8	30
1	D	236/255 (92%)	214 (91%)	22 (9%)	8	32
1	E	236/255 (92%)	213 (90%)	23 (10%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	236/255 (92%)	210 (89%)	26 (11%)	6	25
1	G	236/255 (92%)	208 (88%)	28 (12%)	5	22
1	H	236/255 (92%)	211 (89%)	25 (11%)	6	27
1	I	236/255 (92%)	211 (89%)	25 (11%)	6	27
1	J	236/255 (92%)	214 (91%)	22 (9%)	8	32
1	K	236/255 (92%)	212 (90%)	24 (10%)	7	29
1	L	236/255 (92%)	213 (90%)	23 (10%)	8	30
1	M	236/255 (92%)	209 (89%)	27 (11%)	5	24
1	N	236/255 (92%)	212 (90%)	24 (10%)	7	29
All	All	3304/3570 (92%)	2963 (90%)	341 (10%)	7	28

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	ASP
1	A	488	GLU
1	A	515	LEU
1	A	524	LYS
1	A	533	ASN
1	A	542	ILE
1	A	560	ARG
1	A	568	GLN
1	A	573	VAL
1	A	589	ASN
1	A	599	ARG
1	A	611	MET
1	A	613	THR
1	A	623	THR
1	A	624	ASN
1	A	647	LEU
1	A	701	GLU
1	A	728	VAL
1	A	731	ILE
1	A	734	ASP
1	A	738	GLU
1	A	747	VAL
1	A	749	ASP
1	A	757	MET
1	B	484	ASP

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Mol	Chain	Res	Type
1	B	488	GLU
1	B	515	LEU
1	B	524	LYS
1	B	533	ASN
1	B	542	ILE
1	B	560	ARG
1	B	568	GLN
1	B	573	VAL
1	B	589	ASN
1	B	599	ARG
1	B	604	ILE
1	B	611	MET
1	B	623	THR
1	B	624	ASN
1	B	647	LEU
1	B	701	GLU
1	B	702	SER
1	B	728	VAL
1	B	731	ILE
1	B	734	ASP
1	B	738	GLU
1	B	747	VAL
1	B	749	ASP
1	B	757	MET
1	C	484	ASP
1	C	488	GLU
1	C	515	LEU
1	C	524	LYS
1	C	533	ASN
1	C	560	ARG
1	C	565	LYS
1	C	568	GLN
1	C	573	VAL
1	C	589	ASN
1	C	604	ILE
1	C	611	MET
1	C	613	THR
1	C	624	ASN
1	C	647	LEU
1	C	701	GLU
1	C	728	VAL
1	C	731	ILE

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Mol	Chain	Res	Type
1	C	734	ASP
1	C	738	GLU
1	C	747	VAL
1	C	749	ASP
1	C	757	MET
1	D	484	ASP
1	D	488	GLU
1	D	515	LEU
1	D	524	LYS
1	D	533	ASN
1	D	542	ILE
1	D	568	GLN
1	D	573	VAL
1	D	589	ASN
1	D	604	ILE
1	D	606	THR
1	D	611	MET
1	D	624	ASN
1	D	647	LEU
1	D	701	GLU
1	D	728	VAL
1	D	731	ILE
1	D	734	ASP
1	D	738	GLU
1	D	747	VAL
1	D	749	ASP
1	D	757	MET
1	E	484	ASP
1	E	488	GLU
1	E	515	LEU
1	E	524	LYS
1	E	533	ASN
1	E	542	ILE
1	E	565	LYS
1	E	568	GLN
1	E	573	VAL
1	E	589	ASN
1	E	604	ILE
1	E	606	THR
1	E	611	MET
1	E	613	THR
1	E	624	ASN

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Mol	Chain	Res	Type
1	E	647	LEU
1	E	701	GLU
1	E	728	VAL
1	E	731	ILE
1	E	738	GLU
1	E	747	VAL
1	E	749	ASP
1	E	757	MET
1	F	484	ASP
1	F	488	GLU
1	F	514	VAL
1	F	515	LEU
1	F	524	LYS
1	F	533	ASN
1	F	542	ILE
1	F	560	ARG
1	F	565	LYS
1	F	568	GLN
1	F	573	VAL
1	F	589	ASN
1	F	604	ILE
1	F	606	THR
1	F	611	MET
1	F	613	THR
1	F	624	ASN
1	F	647	LEU
1	F	701	GLU
1	F	702	SER
1	F	728	VAL
1	F	731	ILE
1	F	738	GLU
1	F	747	VAL
1	F	749	ASP
1	F	757	MET
1	G	484	ASP
1	G	488	GLU
1	G	514	VAL
1	G	515	LEU
1	G	524	LYS
1	G	533	ASN
1	G	542	ILE
1	G	560	ARG

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Mol	Chain	Res	Type
1	G	568	GLN
1	G	573	VAL
1	G	589	ASN
1	G	599	ARG
1	G	604	ILE
1	G	606	THR
1	G	611	MET
1	G	613	THR
1	G	623	THR
1	G	624	ASN
1	G	647	LEU
1	G	701	GLU
1	G	702	SER
1	G	728	VAL
1	G	731	ILE
1	G	734	ASP
1	G	738	GLU
1	G	747	VAL
1	G	749	ASP
1	G	757	MET
1	H	484	ASP
1	H	488	GLU
1	H	495	TYR
1	H	514	VAL
1	H	515	LEU
1	H	524	LYS
1	H	533	ASN
1	H	542	ILE
1	H	560	ARG
1	H	568	GLN
1	H	573	VAL
1	H	589	ASN
1	H	611	MET
1	H	613	THR
1	H	624	ASN
1	H	647	LEU
1	H	701	GLU
1	H	702	SER
1	H	728	VAL
1	H	731	ILE
1	H	734	ASP
1	H	738	GLU

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Mol	Chain	Res	Type
1	H	747	VAL
1	H	749	ASP
1	H	757	MET
1	I	484	ASP
1	I	488	GLU
1	I	504	LEU
1	I	514	VAL
1	I	515	LEU
1	I	524	LYS
1	I	533	ASN
1	I	542	ILE
1	I	560	ARG
1	I	568	GLN
1	I	573	VAL
1	I	589	ASN
1	I	606	THR
1	I	611	MET
1	I	624	ASN
1	I	629	ILE
1	I	647	LEU
1	I	701	GLU
1	I	728	VAL
1	I	731	ILE
1	I	734	ASP
1	I	738	GLU
1	I	747	VAL
1	I	749	ASP
1	I	757	MET
1	J	484	ASP
1	J	488	GLU
1	J	515	LEU
1	J	524	LYS
1	J	533	ASN
1	J	542	ILE
1	J	568	GLN
1	J	573	VAL
1	J	589	ASN
1	J	599	ARG
1	J	604	ILE
1	J	611	MET
1	J	624	ASN
1	J	647	LEU

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Mol	Chain	Res	Type
1	J	701	GLU
1	J	728	VAL
1	J	731	ILE
1	J	734	ASP
1	J	738	GLU
1	J	747	VAL
1	J	749	ASP
1	J	757	MET
1	K	471	VAL
1	K	484	ASP
1	K	488	GLU
1	K	515	LEU
1	K	524	LYS
1	K	533	ASN
1	K	542	ILE
1	K	568	GLN
1	K	573	VAL
1	K	589	ASN
1	K	599	ARG
1	K	604	ILE
1	K	606	THR
1	K	611	MET
1	K	624	ASN
1	K	647	LEU
1	K	701	GLU
1	K	702	SER
1	K	728	VAL
1	K	731	ILE
1	K	738	GLU
1	K	747	VAL
1	K	749	ASP
1	K	757	MET
1	L	484	ASP
1	L	488	GLU
1	L	515	LEU
1	L	524	LYS
1	L	533	ASN
1	L	542	ILE
1	L	565	LYS
1	L	568	GLN
1	L	573	VAL
1	L	589	ASN

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Mol	Chain	Res	Type
1	L	604	ILE
1	L	606	THR
1	L	611	MET
1	L	613	THR
1	L	624	ASN
1	L	647	LEU
1	L	701	GLU
1	L	728	VAL
1	L	731	ILE
1	L	738	GLU
1	L	747	VAL
1	L	749	ASP
1	L	757	MET
1	M	484	ASP
1	M	488	GLU
1	M	508	MET
1	M	514	VAL
1	M	515	LEU
1	M	524	LYS
1	M	533	ASN
1	M	542	ILE
1	M	560	ARG
1	M	565	LYS
1	M	568	GLN
1	M	573	VAL
1	M	589	ASN
1	M	604	ILE
1	M	606	THR
1	M	611	MET
1	M	613	THR
1	M	624	ASN
1	M	647	LEU
1	M	701	GLU
1	M	728	VAL
1	M	731	ILE
1	M	734	ASP
1	M	738	GLU
1	M	747	VAL
1	M	749	ASP
1	M	757	MET
1	N	484	ASP
1	N	488	GLU

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Mol	Chain	Res	Type
1	N	515	LEU
1	N	524	LYS
1	N	533	ASN
1	N	560	ARG
1	N	565	LYS
1	N	568	GLN
1	N	573	VAL
1	N	589	ASN
1	N	604	ILE
1	N	606	THR
1	N	611	MET
1	N	613	THR
1	N	624	ASN
1	N	647	LEU
1	N	701	GLU
1	N	728	VAL
1	N	731	ILE
1	N	734	ASP
1	N	738	GLU
1	N	747	VAL
1	N	749	ASP
1	N	757	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	490	GLN
1	A	533	ASN
1	A	558	ASN
1	A	624	ASN
1	A	641	GLN
1	A	660	ASN
1	B	490	GLN
1	B	533	ASN
1	B	558	ASN
1	B	568	GLN
1	B	624	ASN
1	B	641	GLN
1	B	660	ASN
1	C	490	GLN
1	C	533	ASN
1	C	558	ASN

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Mol	Chain	Res	Type
1	C	603	GLN
1	C	624	ASN
1	C	641	GLN
1	C	660	ASN
1	C	763	GLN
1	D	490	GLN
1	D	499	HIS
1	D	533	ASN
1	D	603	GLN
1	D	624	ASN
1	D	660	ASN
1	E	490	GLN
1	E	499	HIS
1	E	533	ASN
1	E	558	ASN
1	E	603	GLN
1	E	624	ASN
1	E	641	GLN
1	E	660	ASN
1	F	490	GLN
1	F	533	ASN
1	F	558	ASN
1	F	624	ASN
1	F	641	GLN
1	F	660	ASN
1	G	490	GLN
1	G	533	ASN
1	G	558	ASN
1	G	624	ASN
1	G	641	GLN
1	G	660	ASN
1	H	490	GLN
1	H	494	GLN
1	H	533	ASN
1	H	603	GLN
1	H	624	ASN
1	H	641	GLN
1	H	660	ASN
1	I	490	GLN
1	I	494	GLN
1	I	533	ASN
1	I	558	ASN

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Mol	Chain	Res	Type
1	I	603	GLN
1	I	624	ASN
1	I	641	GLN
1	I	660	ASN
1	J	490	GLN
1	J	533	ASN
1	J	558	ASN
1	J	603	GLN
1	J	624	ASN
1	J	641	GLN
1	J	660	ASN
1	J	763	GLN
1	K	490	GLN
1	K	533	ASN
1	K	558	ASN
1	K	624	ASN
1	K	660	ASN
1	K	763	GLN
1	L	490	GLN
1	L	533	ASN
1	L	558	ASN
1	L	603	GLN
1	L	624	ASN
1	L	641	GLN
1	L	660	ASN
1	L	763	GLN
1	M	490	GLN
1	M	533	ASN
1	M	558	ASN
1	M	603	GLN
1	M	624	ASN
1	M	641	GLN
1	M	660	ASN
1	M	763	GLN
1	N	490	GLN
1	N	533	ASN
1	N	558	ASN
1	N	603	GLN
1	N	624	ASN
1	N	641	GLN
1	N	660	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 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$
2	ADP	G	900	-	28,29,29	2.13	5 (17%)	43,45,45	4.05	11 (25%)
2	ADP	J	900	-	28,29,29	1.98	5 (17%)	43,45,45	4.06	10 (23%)
2	ADP	K	900	-	28,29,29	2.01	4 (14%)	43,45,45	3.94	11 (25%)
2	ADP	M	900	-	28,29,29	2.02	5 (17%)	43,45,45	4.24	10 (23%)
2	ADP	N	900	-	28,29,29	1.89	4 (14%)	43,45,45	4.12	14 (32%)
2	ADP	C	900	-	28,29,29	2.13	5 (17%)	43,45,45	4.40	12 (27%)
2	ADP	H	900	-	28,29,29	1.83	3 (10%)	43,45,45	3.95	11 (25%)
2	ADP	B	900	-	28,29,29	2.05	5 (17%)	43,45,45	3.95	11 (25%)
2	ADP	A	900	-	28,29,29	1.83	4 (14%)	43,45,45	4.01	11 (25%)
2	ADP	F	900	-	28,29,29	1.76	3 (10%)	43,45,45	4.24	12 (27%)
2	ADP	I	900	-	28,29,29	1.93	4 (14%)	43,45,45	4.03	9 (20%)
2	ADP	L	900	-	28,29,29	2.09	5 (17%)	43,45,45	4.02	11 (25%)
2	ADP	E	900	-	28,29,29	1.98	4 (14%)	43,45,45	3.89	12 (27%)
2	ADP	D	900	-	28,29,29	1.99	5 (17%)	43,45,45	4.52	11 (25%)

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	ADP	G	900	-	-	0/16/32/32	0/3/3/3
2	ADP	J	900	-	-	0/16/32/32	0/3/3/3
2	ADP	K	900	-	-	0/16/32/32	0/3/3/3
2	ADP	M	900	-	-	2/16/32/32	0/3/3/3
2	ADP	N	900	-	-	0/16/32/32	0/3/3/3
2	ADP	C	900	-	-	1/16/32/32	0/3/3/3
2	ADP	H	900	-	-	1/16/32/32	0/3/3/3
2	ADP	B	900	-	-	0/16/32/32	0/3/3/3
2	ADP	A	900	-	-	0/16/32/32	0/3/3/3
2	ADP	F	900	-	-	0/16/32/32	0/3/3/3
2	ADP	I	900	-	-	1/16/32/32	0/3/3/3
2	ADP	L	900	-	-	1/16/32/32	0/3/3/3
2	ADP	E	900	-	-	0/16/32/32	0/3/3/3
2	ADP	D	900	-	-	0/16/32/32	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	900	ADP	C8-N9	-8.69	1.22	1.37
2	L	900	ADP	C8-N9	-8.42	1.23	1.37
2	E	900	ADP	C8-N9	-8.29	1.23	1.37
2	C	900	ADP	C8-N9	-8.12	1.23	1.37
2	H	900	ADP	C8-N9	-8.09	1.23	1.37
2	D	900	ADP	C8-N9	-8.05	1.23	1.37
2	B	900	ADP	C8-N9	-7.87	1.24	1.37
2	K	900	ADP	C8-N9	-7.83	1.24	1.37
2	M	900	ADP	C8-N9	-7.68	1.24	1.37
2	J	900	ADP	C8-N9	-7.55	1.24	1.37
2	N	900	ADP	C8-N9	-7.55	1.24	1.37
2	A	900	ADP	C8-N9	-7.27	1.25	1.37
2	F	900	ADP	C8-N9	-7.22	1.25	1.37
2	I	900	ADP	C8-N9	-6.91	1.25	1.37
2	G	900	ADP	C8-N7	-4.36	1.23	1.31
2	I	900	ADP	C5-C4	4.32	1.46	1.39
2	A	900	ADP	C5-C4	4.07	1.46	1.39
2	E	900	ADP	C8-N7	-3.90	1.24	1.31
2	I	900	ADP	C8-N7	-3.89	1.24	1.31
2	C	900	ADP	C5-C4	3.88	1.46	1.39
2	K	900	ADP	C5-C4	3.82	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	900	ADP	C8-N7	-3.82	1.24	1.31
2	M	900	ADP	C5-C4	3.75	1.45	1.39
2	B	900	ADP	C8-N7	-3.71	1.24	1.31
2	B	900	ADP	PA-O3A	3.68	1.63	1.59
2	N	900	ADP	C8-N7	-3.66	1.24	1.31
2	N	900	ADP	C5-C4	3.65	1.45	1.39
2	C	900	ADP	C8-N7	-3.62	1.24	1.31
2	M	900	ADP	C8-N7	-3.58	1.24	1.31
2	L	900	ADP	PA-O3A	3.58	1.63	1.59
2	J	900	ADP	C8-N7	-3.54	1.24	1.31
2	J	900	ADP	C5-C4	3.49	1.45	1.39
2	D	900	ADP	C8-N7	-3.49	1.25	1.31
2	C	900	ADP	C4-N9	-3.41	1.30	1.37
2	F	900	ADP	C8-N7	-3.35	1.25	1.31
2	K	900	ADP	C8-N7	-3.29	1.25	1.31
2	K	900	ADP	PA-O3A	3.27	1.63	1.59
2	M	900	ADP	PA-O3A	3.27	1.63	1.59
2	D	900	ADP	C5-C4	3.20	1.44	1.39
2	E	900	ADP	C5-C4	3.20	1.44	1.39
2	C	900	ADP	PA-O3A	3.18	1.62	1.59
2	B	900	ADP	C5-C4	3.14	1.44	1.39
2	A	900	ADP	C8-N7	-3.10	1.25	1.31
2	L	900	ADP	C5-C4	3.09	1.44	1.39
2	J	900	ADP	PA-O3A	3.01	1.62	1.59
2	F	900	ADP	C5-C4	2.99	1.44	1.39
2	H	900	ADP	C5-C4	2.97	1.44	1.39
2	I	900	ADP	C4-N9	-2.96	1.31	1.37
2	D	900	ADP	C4-N9	-2.96	1.31	1.37
2	J	900	ADP	C4-N9	-2.85	1.31	1.37
2	G	900	ADP	C4-N9	-2.75	1.32	1.37
2	B	900	ADP	C4-N9	-2.54	1.32	1.37
2	H	900	ADP	C8-N7	-2.49	1.26	1.31
2	G	900	ADP	PA-O3A	2.46	1.62	1.59
2	D	900	ADP	PA-O3A	2.42	1.62	1.59
2	G	900	ADP	C5-C4	2.42	1.43	1.39
2	M	900	ADP	C4-N9	-2.41	1.32	1.37
2	L	900	ADP	C4-N9	-2.19	1.33	1.37
2	E	900	ADP	C4-N9	-2.17	1.33	1.37
2	A	900	ADP	C4-N9	-2.09	1.33	1.37
2	N	900	ADP	C4-N9	-2.05	1.33	1.37

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	ADP	N9-C8-N7	20.87	143.55	113.94
2	C	900	ADP	N9-C8-N7	20.59	143.15	113.94
2	M	900	ADP	N9-C8-N7	19.92	142.19	113.94
2	F	900	ADP	N9-C8-N7	19.55	141.67	113.94
2	G	900	ADP	N9-C8-N7	19.17	141.13	113.94
2	N	900	ADP	N9-C8-N7	19.15	141.11	113.94
2	I	900	ADP	N9-C8-N7	19.12	141.07	113.94
2	L	900	ADP	N9-C8-N7	18.93	140.79	113.94
2	A	900	ADP	N9-C8-N7	18.90	140.75	113.94
2	J	900	ADP	N9-C8-N7	18.86	140.70	113.94
2	K	900	ADP	N9-C8-N7	18.73	140.51	113.94
2	B	900	ADP	N9-C8-N7	18.65	140.40	113.94
2	E	900	ADP	N9-C8-N7	18.34	139.95	113.94
2	H	900	ADP	N9-C8-N7	17.92	139.37	113.94
2	D	900	ADP	C4-N9-C8	-12.97	92.12	105.74
2	F	900	ADP	C4-N9-C8	-12.41	92.71	105.74
2	C	900	ADP	C4-N9-C8	-12.06	93.07	105.74
2	M	900	ADP	C4-N9-C8	-12.04	93.09	105.74
2	D	900	ADP	C5-N7-C8	-11.73	85.02	103.45
2	C	900	ADP	C5-N7-C8	-11.47	85.42	103.45
2	H	900	ADP	C4-N9-C8	-11.45	93.71	105.74
2	K	900	ADP	C4-N9-C8	-11.44	93.73	105.74
2	N	900	ADP	C4-N9-C8	-11.38	93.79	105.74
2	A	900	ADP	C4-N9-C8	-11.28	93.89	105.74
2	J	900	ADP	C4-N9-C8	-11.27	93.90	105.74
2	I	900	ADP	C5-N7-C8	-11.11	85.98	103.45
2	L	900	ADP	C4-N9-C8	-11.04	94.14	105.74
2	B	900	ADP	C4-N9-C8	-10.85	94.34	105.74
2	G	900	ADP	C4-N9-C8	-10.82	94.38	105.74
2	F	900	ADP	C5-N7-C8	-10.80	86.48	103.45
2	M	900	ADP	C5-N7-C8	-10.79	86.49	103.45
2	G	900	ADP	C5-N7-C8	-10.47	87.00	103.45
2	J	900	ADP	C5-N7-C8	-10.38	87.13	103.45
2	N	900	ADP	C5-N7-C8	-10.38	87.14	103.45
2	E	900	ADP	C4-N9-C8	-10.31	94.91	105.74
2	B	900	ADP	C5-N7-C8	-10.26	87.32	103.45
2	A	900	ADP	C5-N7-C8	-10.23	87.37	103.45
2	L	900	ADP	C5-N7-C8	-10.23	87.38	103.45
2	I	900	ADP	C4-N9-C8	-9.96	95.28	105.74
2	E	900	ADP	C5-N7-C8	-9.84	87.99	103.45
2	K	900	ADP	C5-N7-C8	-9.81	88.03	103.45
2	H	900	ADP	C5-N7-C8	-9.49	88.53	103.45
2	D	900	ADP	N3-C2-N1	-5.58	120.13	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	900	ADP	C4-N9-C1'	5.56	139.64	126.63
2	D	900	ADP	C4-N9-C1'	5.38	139.21	126.63
2	F	900	ADP	C4-N9-C1'	5.31	139.05	126.63
2	M	900	ADP	C4-N9-C1'	5.26	138.94	126.63
2	C	900	ADP	C4-N9-C1'	4.95	138.21	126.63
2	G	900	ADP	C4-N9-C1'	4.86	138.01	126.63
2	H	900	ADP	C4-N9-C1'	4.79	137.84	126.63
2	F	900	ADP	N3-C2-N1	-4.78	121.34	128.58
2	E	900	ADP	C4-N9-C1'	4.74	137.72	126.63
2	I	900	ADP	C4-N9-C1'	4.64	137.48	126.63
2	A	900	ADP	C4-N9-C1'	4.60	137.40	126.63
2	E	900	ADP	N3-C2-N1	-4.59	121.64	128.58
2	L	900	ADP	C4-N9-C1'	4.50	137.16	126.63
2	C	900	ADP	N3-C2-N1	-4.42	121.89	128.58
2	N	900	ADP	N3-C2-N1	-4.39	121.94	128.58
2	H	900	ADP	N3-C2-N1	-4.37	121.96	128.58
2	K	900	ADP	C4-N9-C1'	4.33	136.76	126.63
2	B	900	ADP	C4-N9-C1'	4.32	136.74	126.63
2	J	900	ADP	N3-C2-N1	-4.29	122.09	128.58
2	N	900	ADP	C4-N9-C1'	4.29	136.66	126.63
2	M	900	ADP	N3-C2-N1	-4.19	122.24	128.58
2	H	900	ADP	C5-C4-N3	-4.13	121.03	126.72
2	A	900	ADP	N3-C2-N1	-4.01	122.51	128.58
2	H	900	ADP	O3B-PB-O2B	4.01	122.84	107.80
2	G	900	ADP	N3-C2-N1	-3.97	122.57	128.58
2	I	900	ADP	N3-C2-N1	-3.89	122.69	128.58
2	L	900	ADP	N3-C2-N1	-3.85	122.76	128.58
2	H	900	ADP	C2'-C1'-N9	-3.84	103.77	113.30
2	B	900	ADP	C2'-C1'-N9	-3.62	104.32	113.30
2	I	900	ADP	O3B-PB-O2B	3.61	121.32	107.80
2	J	900	ADP	C5-C4-N3	-3.55	121.83	126.72
2	G	900	ADP	C5-C4-N3	-3.51	121.89	126.72
2	L	900	ADP	C2'-C1'-N9	-3.50	104.61	113.30
2	C	900	ADP	C2'-C1'-N9	-3.49	104.64	113.30
2	L	900	ADP	C5-C4-N3	-3.45	121.96	126.72
2	K	900	ADP	N3-C2-N1	-3.44	123.37	128.58
2	D	900	ADP	C2'-C1'-N9	-3.36	104.96	113.30
2	M	900	ADP	C5-C4-N3	-3.35	122.10	126.72
2	M	900	ADP	C2'-C1'-N9	-3.35	104.99	113.30
2	K	900	ADP	C5-C4-N3	-3.30	122.17	126.72
2	C	900	ADP	O4'-C1'-N9	3.27	114.37	108.09
2	E	900	ADP	C2'-C1'-N9	-3.26	105.20	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	900	ADP	C5-C4-N3	-3.26	122.23	126.72
2	G	900	ADP	C2'-C1'-N9	-3.25	105.23	113.30
2	E	900	ADP	C5-C4-N3	-3.25	122.25	126.72
2	D	900	ADP	C2-N1-C6	3.25	124.06	118.73
2	F	900	ADP	C2'-C1'-N9	-3.22	105.30	113.30
2	J	900	ADP	O3B-PB-O2B	3.20	119.80	107.80
2	F	900	ADP	C5-C4-N3	-3.20	122.31	126.72
2	A	900	ADP	C2'-C1'-N9	-3.15	105.48	113.30
2	G	900	ADP	C2-N3-C4	3.12	119.44	111.83
2	E	900	ADP	C2-N3-C4	3.09	119.39	111.83
2	A	900	ADP	C5-C4-N3	-3.07	122.48	126.72
2	D	900	ADP	C2-N3-C4	3.07	119.33	111.83
2	B	900	ADP	N3-C2-N1	-3.05	123.96	128.58
2	I	900	ADP	C2'-C1'-N9	-3.05	105.72	113.30
2	J	900	ADP	C2-N3-C4	3.05	119.29	111.83
2	H	900	ADP	C2-N3-C4	2.99	119.14	111.83
2	N	900	ADP	O3B-PB-O2B	2.98	118.96	107.80
2	N	900	ADP	C2'-C1'-N9	-2.95	105.98	113.30
2	B	900	ADP	C5-C4-N3	-2.95	122.66	126.72
2	I	900	ADP	C2-N1-C6	2.94	123.56	118.73
2	L	900	ADP	C2-N3-C4	2.92	118.96	111.83
2	C	900	ADP	C2-N3-C4	2.87	118.83	111.83
2	C	900	ADP	C5-C4-N3	-2.86	122.77	126.72
2	G	900	ADP	O3B-PB-O2B	2.85	118.50	107.80
2	F	900	ADP	C2-N3-C4	2.85	118.79	111.83
2	N	900	ADP	C2-N3-C4	2.83	118.75	111.83
2	D	900	ADP	O3B-PB-O2B	2.83	118.41	107.80
2	K	900	ADP	C2-N3-C4	2.77	118.60	111.83
2	M	900	ADP	C2-N3-C4	2.75	118.54	111.83
2	L	900	ADP	N3-C4-N9	2.72	131.79	127.17
2	D	900	ADP	O4'-C1'-N9	2.70	113.28	108.09
2	J	900	ADP	C2'-C1'-N9	-2.68	106.65	113.30
2	K	900	ADP	C2'-C1'-N9	-2.67	106.66	113.30
2	D	900	ADP	C5-C4-N3	-2.67	123.04	126.72
2	C	900	ADP	O3B-PB-O2B	2.67	117.82	107.80
2	A	900	ADP	O3B-PB-O2B	2.59	117.51	107.80
2	B	900	ADP	O3'-C3'-C4'	-2.55	103.76	111.08
2	A	900	ADP	C2-N3-C4	2.54	118.05	111.83
2	E	900	ADP	N3-C4-N9	2.54	131.49	127.17
2	M	900	ADP	O3B-PB-O2B	2.54	117.33	107.80
2	N	900	ADP	C6-C5-C4	-2.52	113.73	117.18
2	N	900	ADP	N3-C4-N9	2.49	131.40	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	900	ADP	O3'-C3'-C4'	-2.46	104.01	111.08
2	A	900	ADP	C2-N1-C6	2.46	122.77	118.73
2	N	900	ADP	C2-N1-C6	2.42	122.70	118.73
2	C	900	ADP	C2-N1-C6	2.41	122.68	118.73
2	K	900	ADP	O2B-PB-O3A	-2.40	96.59	104.64
2	G	900	ADP	O3B-PB-O3A	-2.40	96.59	104.64
2	K	900	ADP	O3B-PB-O2B	2.40	116.80	107.80
2	G	900	ADP	N3-C4-N9	2.40	131.24	127.17
2	H	900	ADP	N3-C4-N9	2.40	131.24	127.17
2	N	900	ADP	O3A-PA-O1A	2.34	117.75	110.70
2	B	900	ADP	C2-N3-C4	2.32	117.50	111.83
2	F	900	ADP	O3B-PB-O2B	2.32	116.50	107.80
2	E	900	ADP	O3B-PB-O2B	2.31	116.48	107.80
2	J	900	ADP	N3-C4-N9	2.31	131.09	127.17
2	F	900	ADP	C2-N1-C6	2.30	122.50	118.73
2	E	900	ADP	O3B-PB-O3A	-2.25	97.09	104.64
2	A	900	ADP	O3'-C3'-C4'	-2.19	104.78	111.08
2	M	900	ADP	N3-C4-N9	2.18	130.88	127.17
2	F	900	ADP	O4'-C1'-N9	2.16	112.23	108.09
2	B	900	ADP	O3B-PB-O1B	2.08	118.93	110.83
2	H	900	ADP	C2-N1-C6	2.07	122.13	118.73
2	K	900	ADP	N3-C4-N9	2.07	130.69	127.17
2	I	900	ADP	O2'-C2'-C1'	-2.07	102.99	110.10
2	B	900	ADP	N3-C4-N9	2.05	130.66	127.17
2	C	900	ADP	C2'-C3'-C4'	2.05	106.58	102.61
2	L	900	ADP	O3B-PB-O2B	2.04	115.44	107.80
2	L	900	ADP	O3A-PA-O1A	2.03	116.82	110.70
2	E	900	ADP	O2A-PA-O1A	2.01	121.81	112.44
2	F	900	ADP	O2'-C2'-C1'	-2.01	103.17	110.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

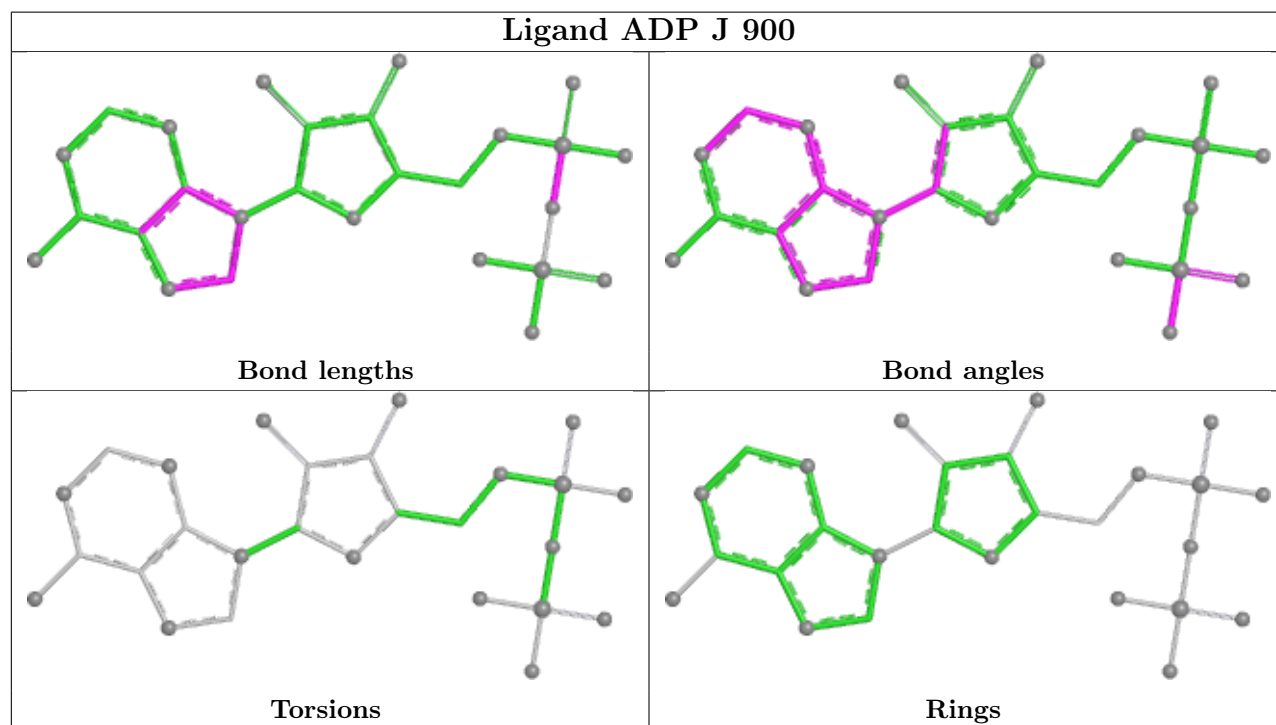
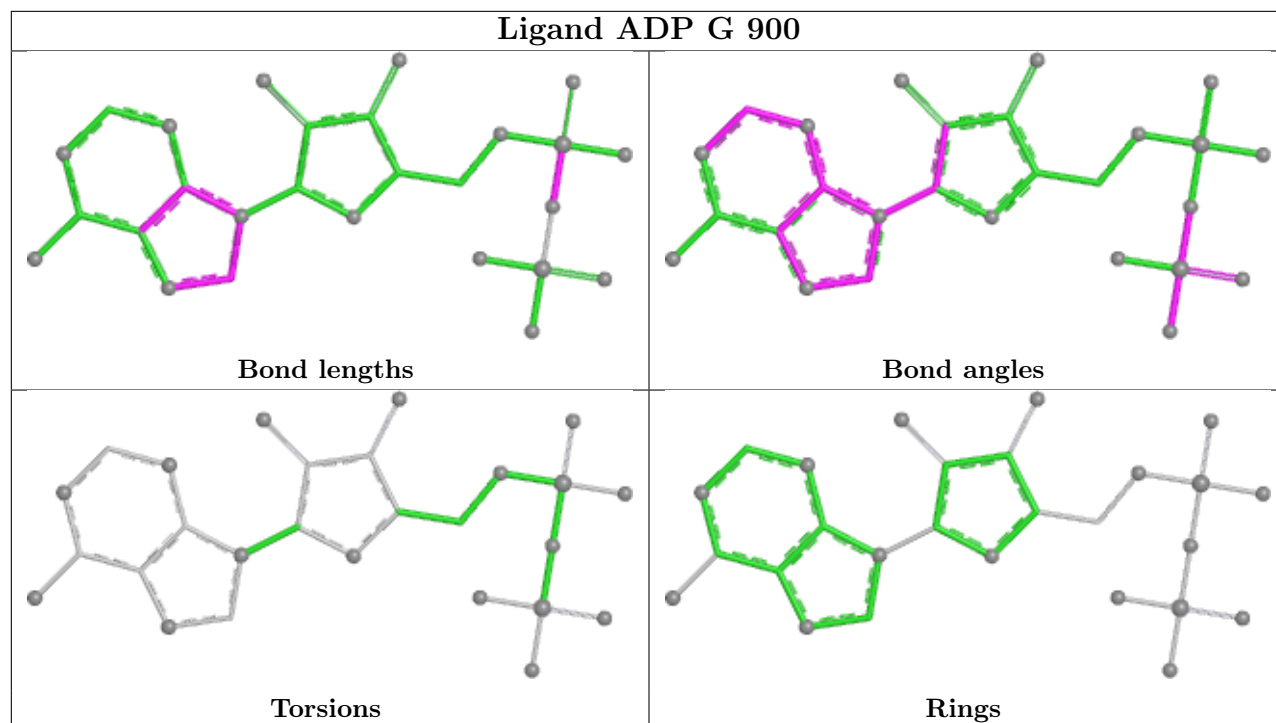
Mol	Chain	Res	Type	Atoms
2	M	900	ADP	O4'-C4'-C5'-O5'
2	M	900	ADP	C3'-C4'-C5'-O5'
2	C	900	ADP	C3'-C4'-C5'-O5'
2	L	900	ADP	C3'-C4'-C5'-O5'
2	H	900	ADP	C3'-C4'-C5'-O5'
2	I	900	ADP	C3'-C4'-C5'-O5'

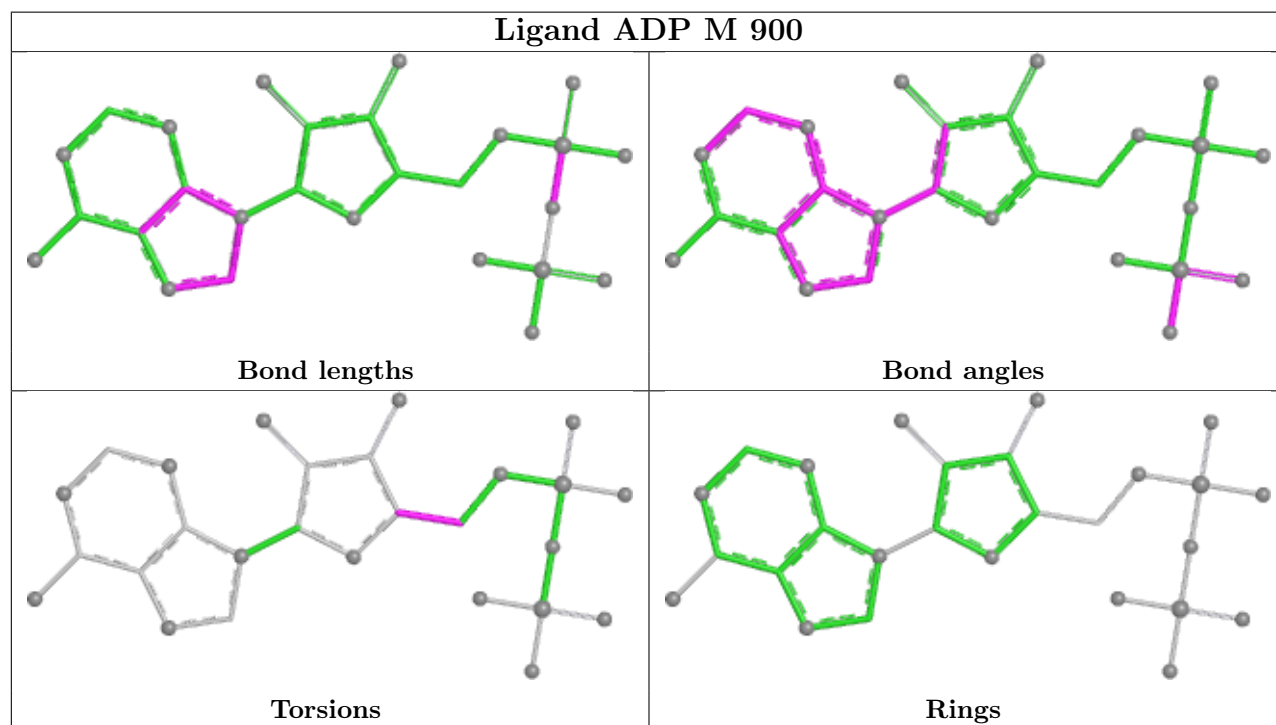
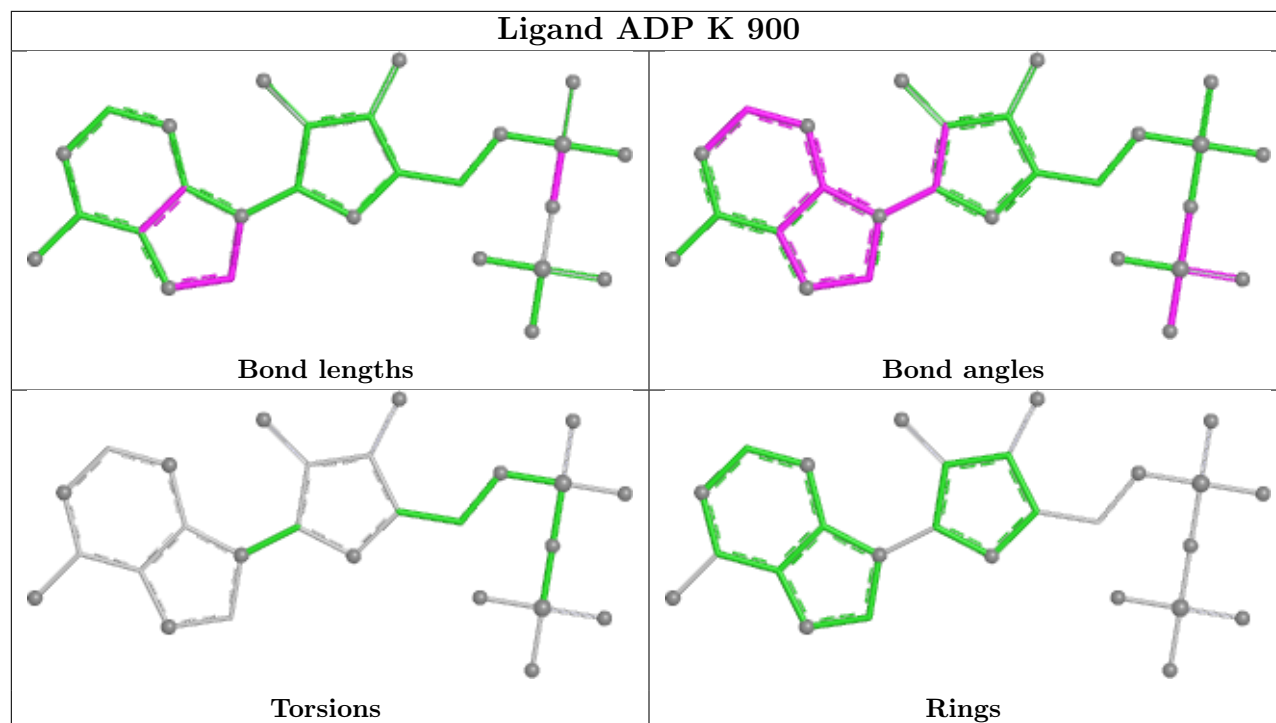
There are no ring outliers.

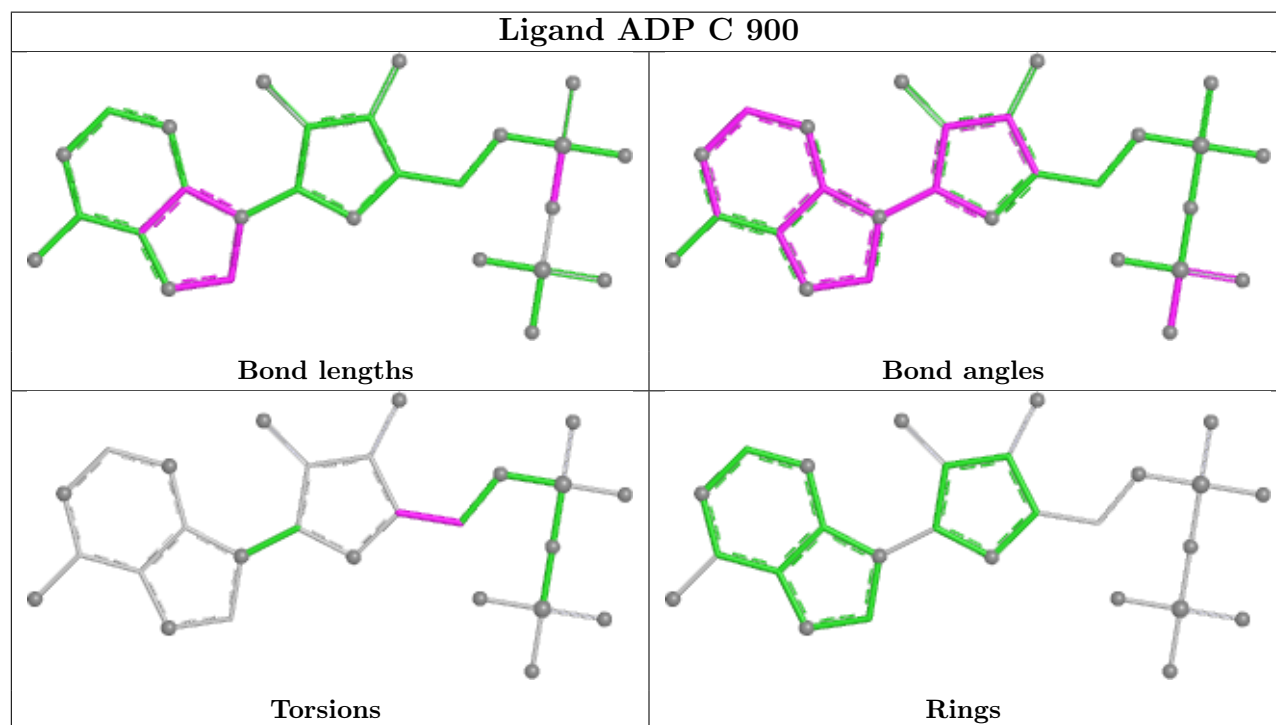
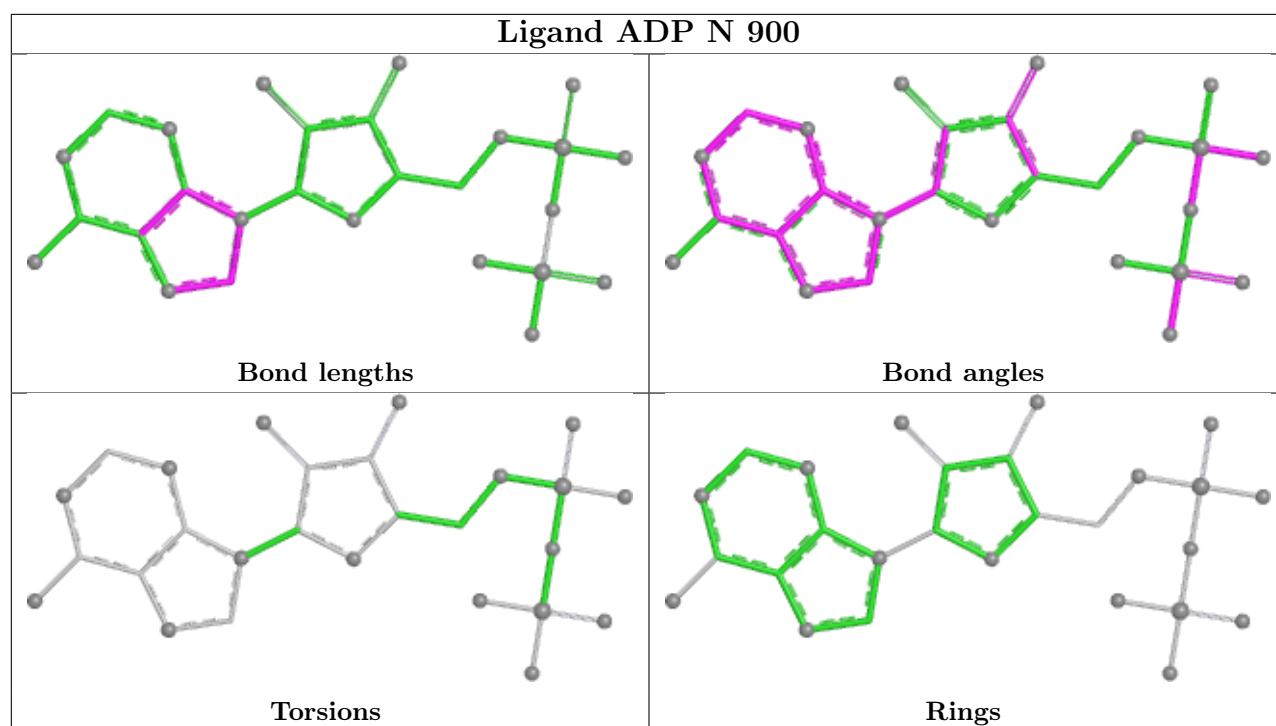
14 monomers are involved in 27 short contacts:

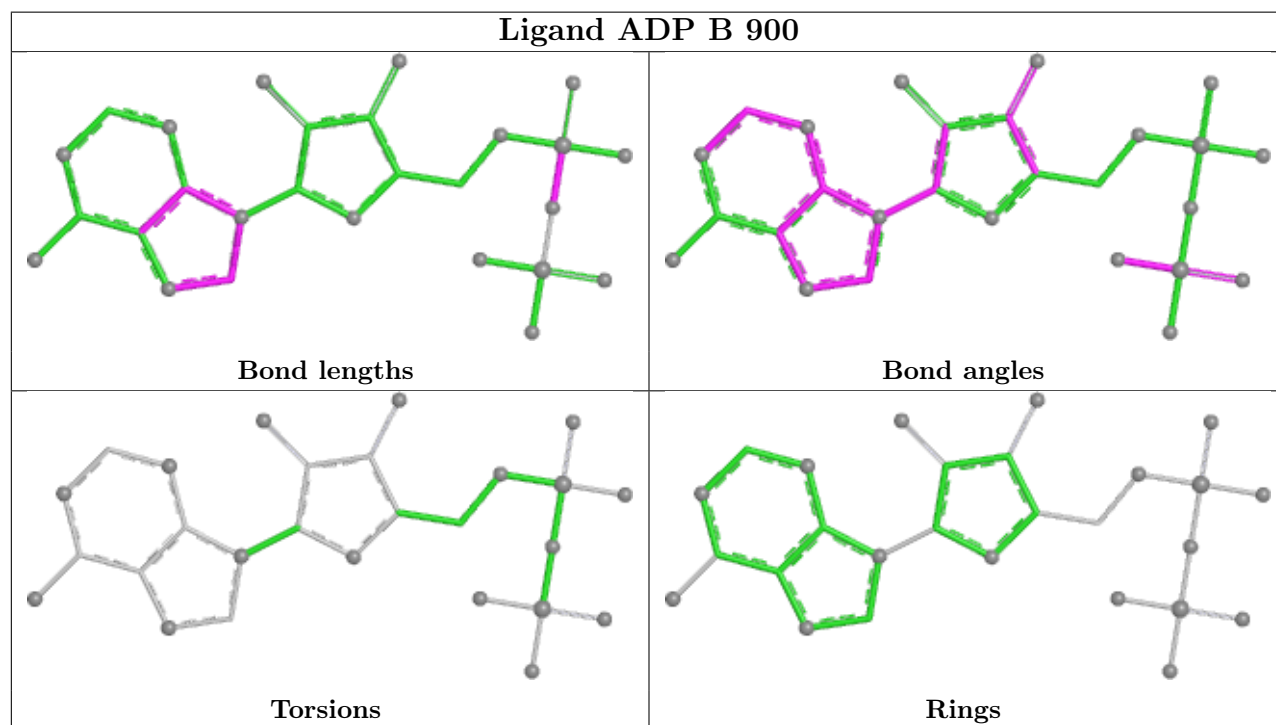
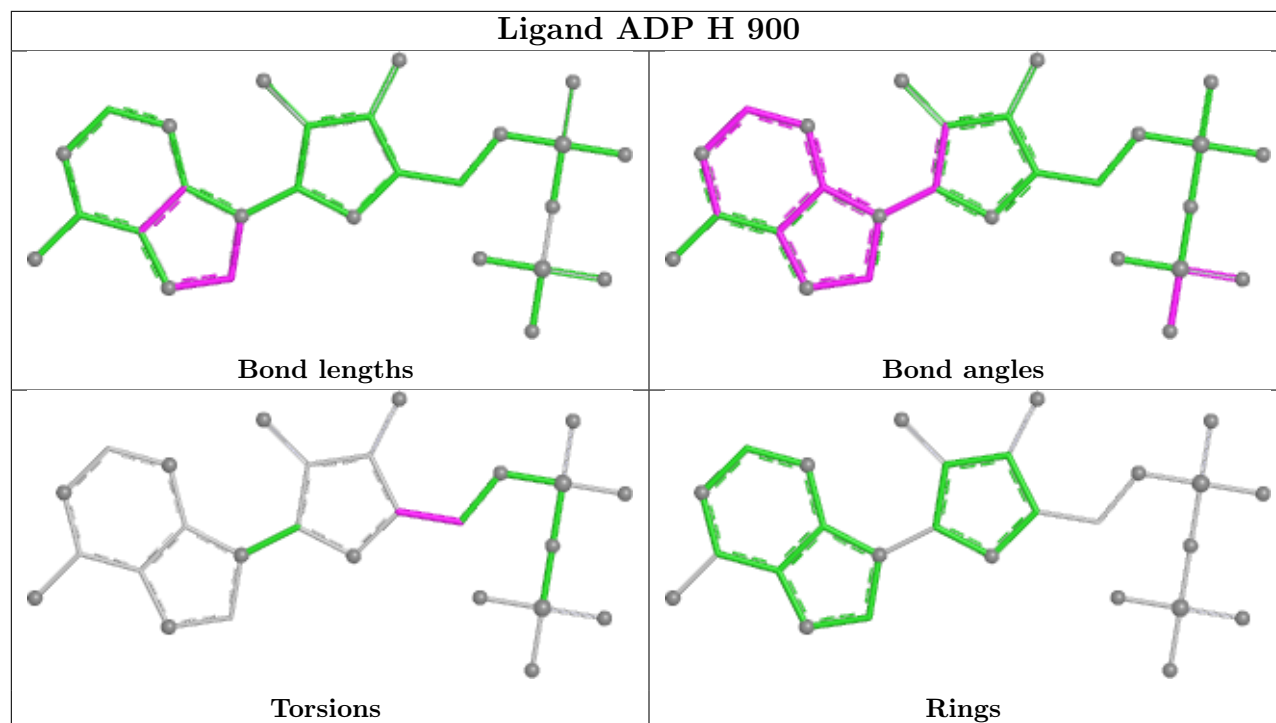
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	900	ADP	3	0
2	J	900	ADP	1	0
2	K	900	ADP	2	0
2	M	900	ADP	2	0
2	N	900	ADP	3	0
2	C	900	ADP	2	0
2	H	900	ADP	1	0
2	B	900	ADP	2	0
2	A	900	ADP	2	0
2	F	900	ADP	1	0
2	I	900	ADP	2	0
2	L	900	ADP	3	0
2	E	900	ADP	2	0
2	D	900	ADP	1	0

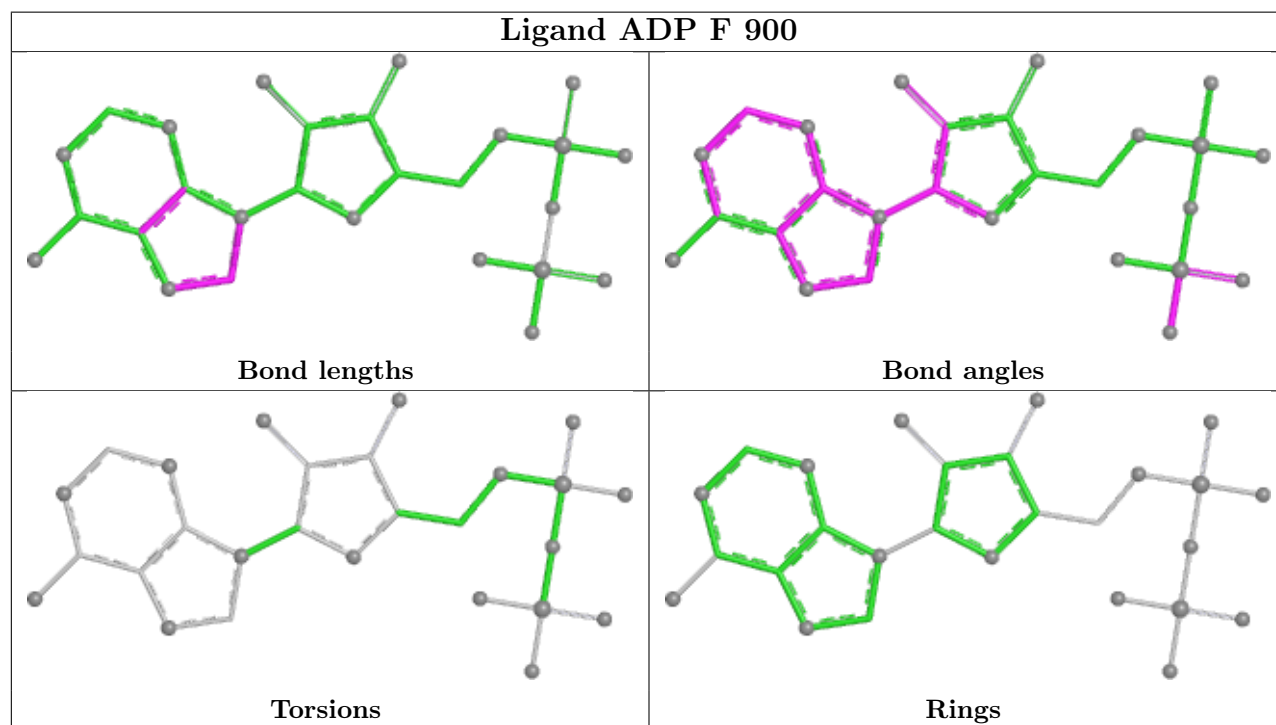
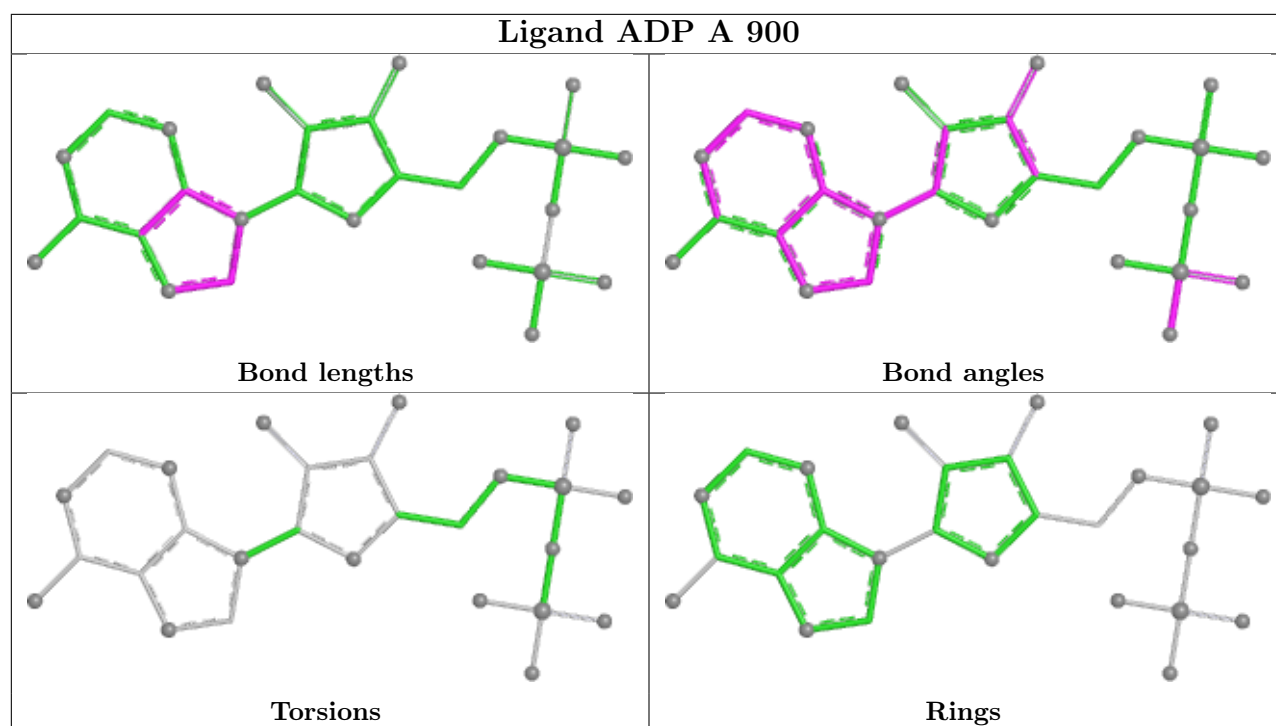
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



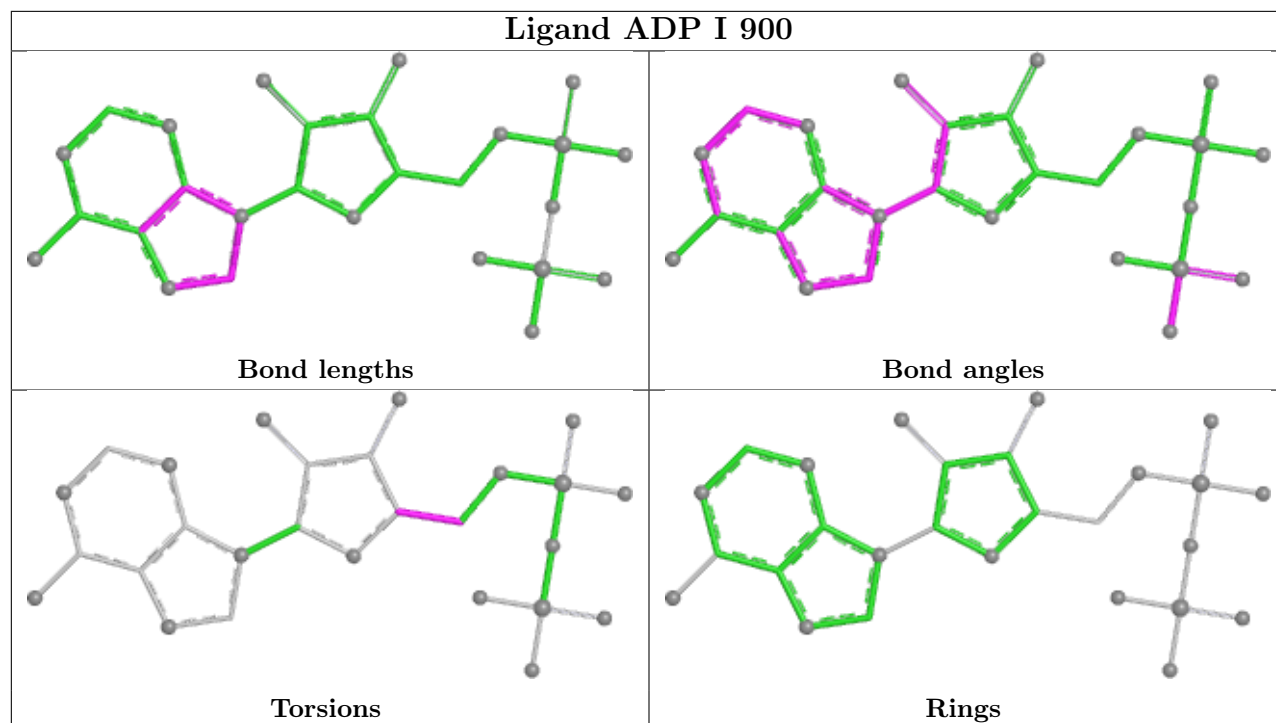




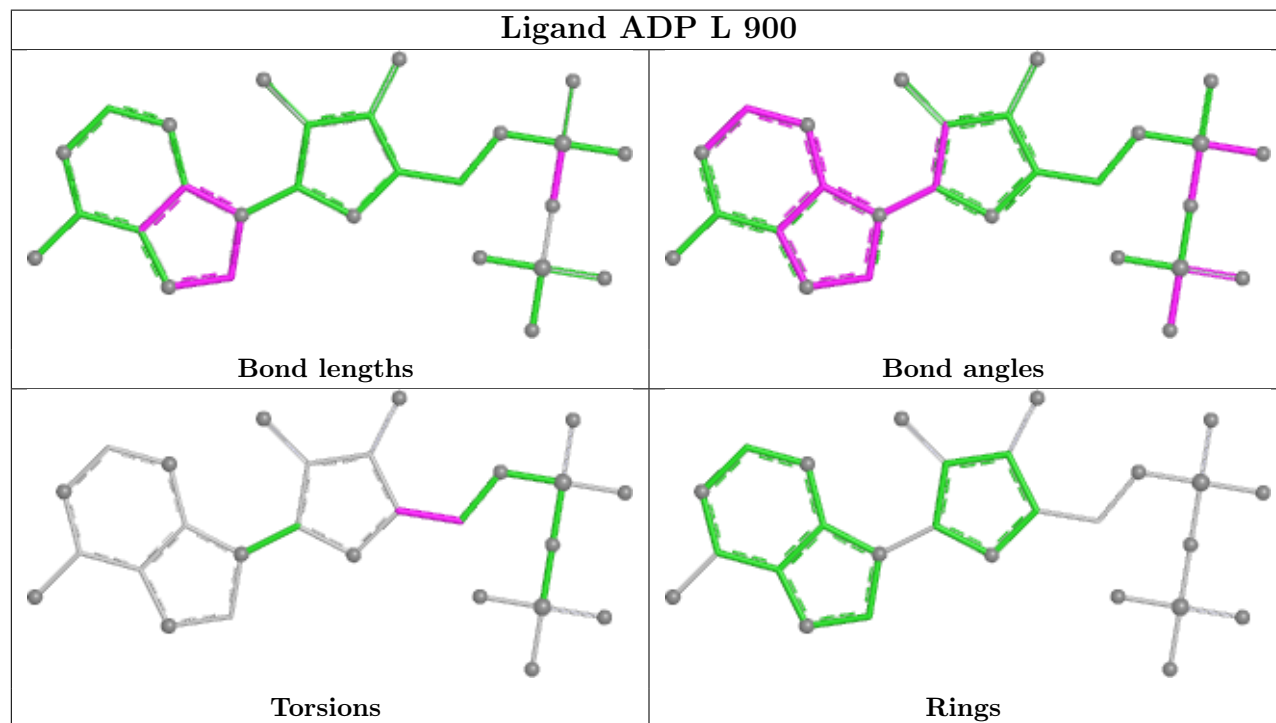


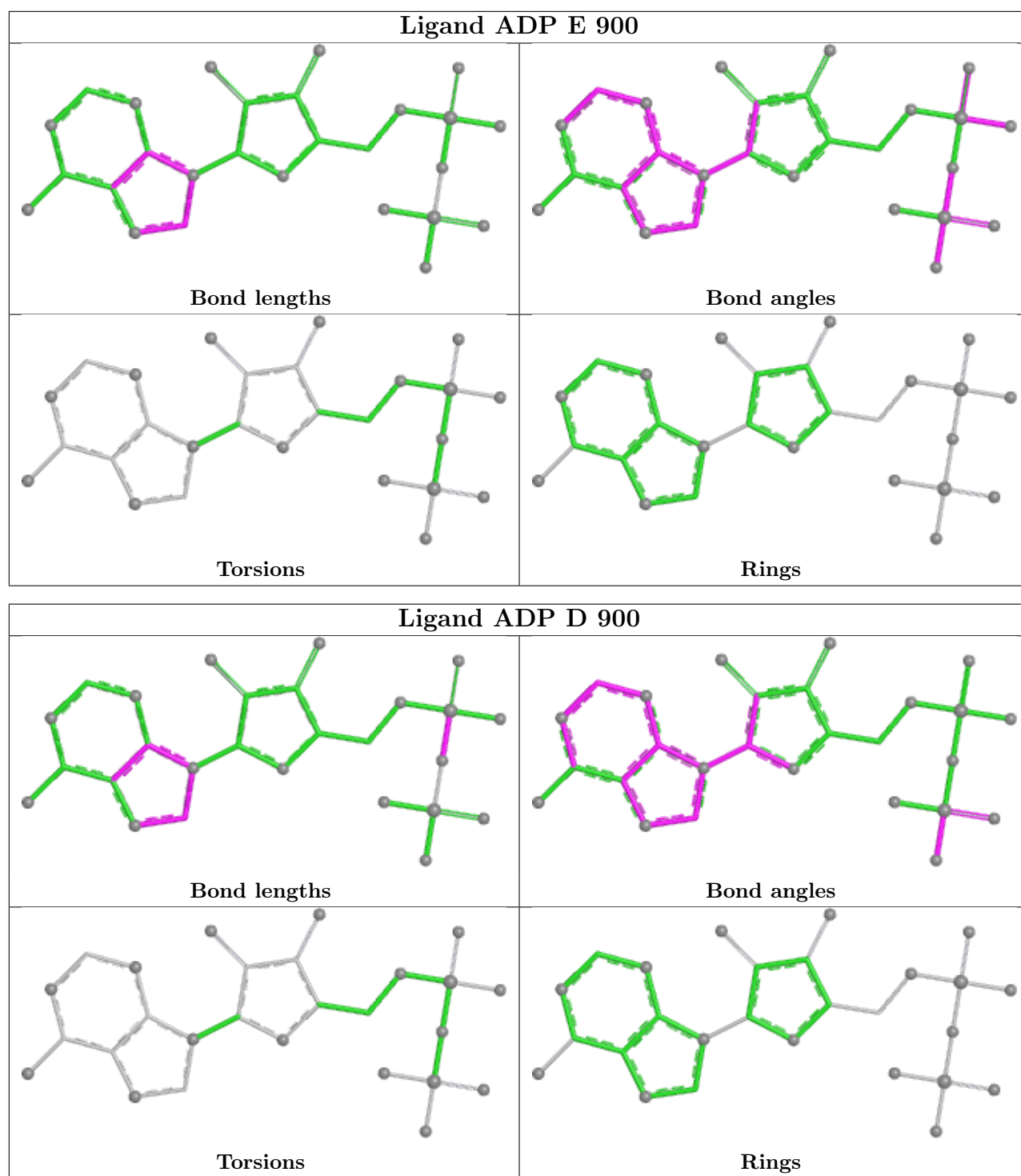


Ligand ADP I 900



Ligand ADP L 900





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	281/301 (93%)	0.34	8 (2%) 55 32	42, 85, 134, 163	0
1	B	281/301 (93%)	0.24	10 (3%) 46 26	42, 85, 134, 163	0
1	C	281/301 (93%)	0.21	4 (1%) 73 51	42, 85, 134, 163	0
1	D	281/301 (93%)	0.57	14 (4%) 34 18	42, 85, 134, 163	0
1	E	281/301 (93%)	0.15	6 (2%) 63 40	42, 85, 134, 163	0
1	F	281/301 (93%)	0.44	10 (3%) 46 26	42, 85, 134, 163	0
1	G	281/301 (93%)	0.32	10 (3%) 46 26	42, 85, 134, 163	0
1	H	281/301 (93%)	0.45	15 (5%) 32 16	42, 85, 134, 163	0
1	I	281/301 (93%)	0.12	5 (1%) 67 44	42, 85, 134, 163	0
1	J	281/301 (93%)	0.30	8 (2%) 55 32	42, 85, 134, 163	0
1	K	281/301 (93%)	0.23	6 (2%) 63 40	42, 85, 134, 163	0
1	L	281/301 (93%)	0.19	9 (3%) 50 29	42, 85, 134, 163	0
1	M	281/301 (93%)	0.29	12 (4%) 40 21	42, 85, 134, 163	0
1	N	281/301 (93%)	0.44	14 (4%) 34 18	42, 85, 134, 163	0
All	All	3934/4214 (93%)	0.31	131 (3%) 49 28	42, 85, 135, 163	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	681	GLY	6.1
1	D	495	TYR	4.1
1	M	536	GLN	3.8
1	H	506	PHE	3.8
1	B	463	ALA	3.7
1	J	681	GLY	3.7
1	F	739	ALA	3.7
1	I	762	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	588	GLY	3.5
1	C	762	LEU	3.4
1	N	728	VAL	3.4
1	G	702	SER	3.4
1	A	762	LEU	3.3
1	H	762	LEU	3.3
1	J	762	LEU	3.2
1	M	501	ASP	3.2
1	F	705	SER	3.2
1	L	507	GLY	3.2
1	N	705	SER	3.1
1	G	728	VAL	3.1
1	G	762	LEU	3.1
1	H	681	GLY	3.1
1	A	698	ALA	3.1
1	B	705	SER	3.1
1	M	743	ALA	3.1
1	A	746	SER	3.0
1	H	588	GLY	3.0
1	K	681	GLY	3.0
1	C	707	ILE	3.0
1	B	728	VAL	2.9
1	E	610	GLY	2.9
1	N	510	PRO	2.9
1	L	705	SER	2.9
1	M	762	LEU	2.9
1	D	480	GLY	2.8
1	I	681	GLY	2.8
1	F	506	PHE	2.8
1	D	535	CYS	2.8
1	G	463	ALA	2.8
1	L	568	GLN	2.8
1	G	706	GLU	2.8
1	F	681	GLY	2.7
1	N	463	ALA	2.7
1	B	762	LEU	2.7
1	K	463	ALA	2.7
1	L	463	ALA	2.7
1	M	503	PHE	2.7
1	G	616	ASN	2.7
1	N	758	PHE	2.6
1	F	762	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	508	MET	2.6
1	N	599	ARG	2.6
1	L	508	MET	2.5
1	N	506	PHE	2.5
1	N	701	GLU	2.5
1	H	737	GLU	2.5
1	D	731	ILE	2.5
1	B	506	PHE	2.5
1	D	594	GLY	2.5
1	K	746	SER	2.5
1	J	535	CYS	2.5
1	D	728	VAL	2.5
1	H	555	SER	2.4
1	M	506	PHE	2.4
1	D	609	ASP	2.4
1	E	505	LYS	2.4
1	B	493	VAL	2.4
1	F	678	MET	2.4
1	J	746	SER	2.4
1	M	728	VAL	2.4
1	N	493	VAL	2.4
1	H	707	ILE	2.4
1	M	463	ALA	2.4
1	D	472	PRO	2.4
1	N	595	GLY	2.4
1	G	758	PHE	2.4
1	L	728	VAL	2.4
1	N	594	GLY	2.3
1	C	758	PHE	2.3
1	E	681	GLY	2.3
1	H	731	ILE	2.3
1	I	588	GLY	2.3
1	A	728	VAL	2.3
1	E	507	GLY	2.3
1	D	504	LEU	2.3
1	J	758	PHE	2.3
1	B	500	PRO	2.3
1	C	703	ILE	2.3
1	I	636	PRO	2.3
1	F	463	ALA	2.3
1	H	613	THR	2.3
1	B	702	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	613	THR	2.2
1	L	536	GLN	2.2
1	H	616	ASN	2.2
1	A	681	GLY	2.2
1	A	614	LYS	2.2
1	D	758	PHE	2.2
1	N	707	ILE	2.2
1	J	558	ASN	2.2
1	E	463	ALA	2.2
1	F	728	VAL	2.1
1	H	761	THR	2.1
1	F	696	LYS	2.1
1	E	648	PRO	2.1
1	J	728	VAL	2.1
1	N	747	VAL	2.1
1	M	464	LEU	2.1
1	D	757	MET	2.1
1	H	730	GLU	2.1
1	J	463	ALA	2.1
1	A	534	GLU	2.1
1	F	610	GLY	2.1
1	H	561	GLU	2.1
1	G	731	ILE	2.1
1	K	609	ASP	2.1
1	L	707	ILE	2.1
1	M	740	MET	2.1
1	B	536	GLN	2.1
1	G	681	GLY	2.1
1	I	510	PRO	2.1
1	H	666	VAL	2.1
1	D	464	LEU	2.1
1	M	568	GLN	2.1
1	A	506	PHE	2.0
1	K	507	GLY	2.0
1	L	729	PRO	2.0
1	B	497	VAL	2.0
1	N	762	LEU	2.0
1	G	705	SER	2.0
1	H	747	VAL	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 ⓘ

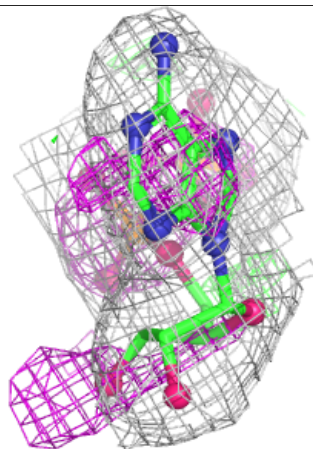
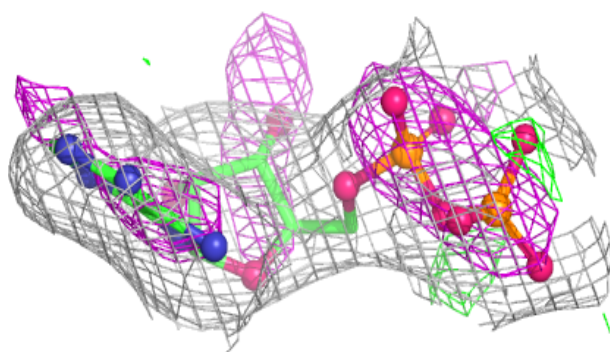
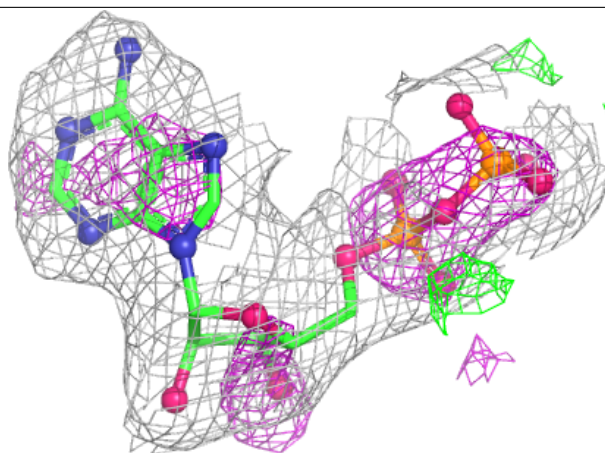
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	900	27/27	0.86	0.12	64,66,69,72	0
2	ADP	K	900	27/27	0.88	0.11	64,66,69,72	0
2	ADP	D	900	27/27	0.89	0.11	64,66,69,72	0
2	ADP	H	900	27/27	0.90	0.10	64,66,69,72	0
2	ADP	C	900	27/27	0.91	0.11	64,66,69,72	0
2	ADP	F	900	27/27	0.91	0.10	64,66,69,72	0
2	ADP	L	900	27/27	0.91	0.11	64,66,69,72	0
2	ADP	N	900	27/27	0.91	0.10	64,66,69,72	0
2	ADP	J	900	27/27	0.92	0.10	64,66,69,72	0
2	ADP	B	900	27/27	0.92	0.10	64,66,69,72	0
2	ADP	G	900	27/27	0.92	0.11	64,66,69,72	0
2	ADP	E	900	27/27	0.92	0.09	64,66,69,72	0
2	ADP	M	900	27/27	0.93	0.10	64,66,69,72	0
2	ADP	I	900	27/27	0.95	0.09	64,66,69,72	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.

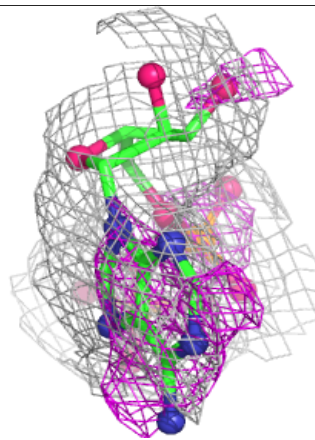
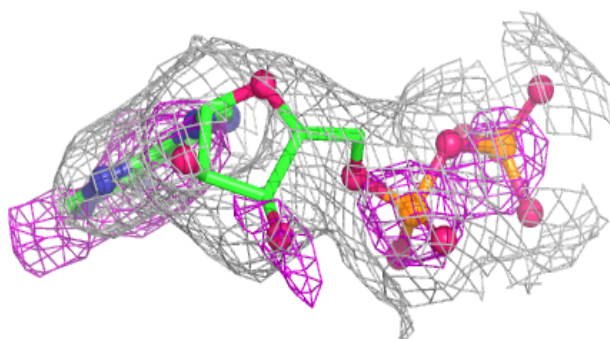
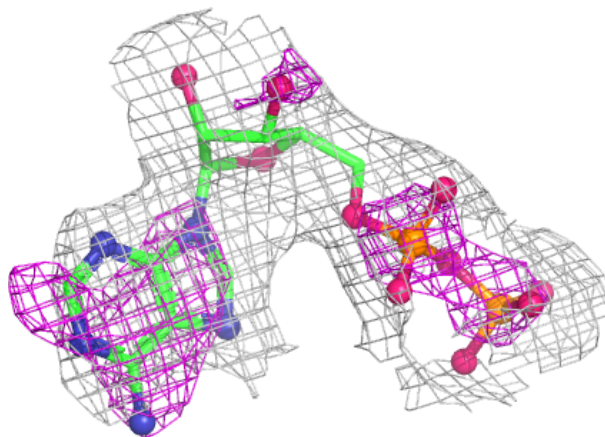
Electron density around ADP A 900:

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



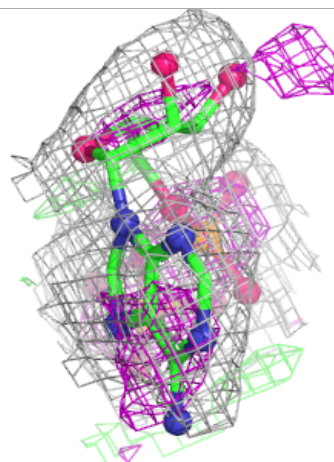
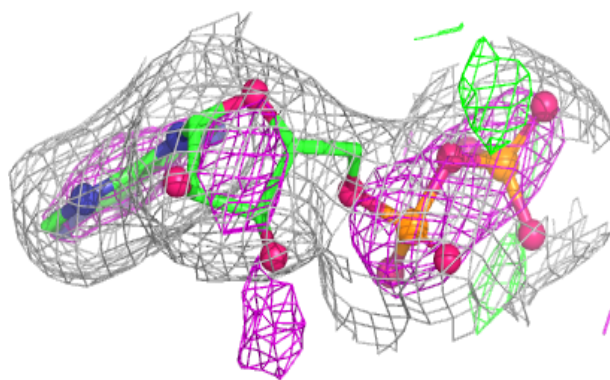
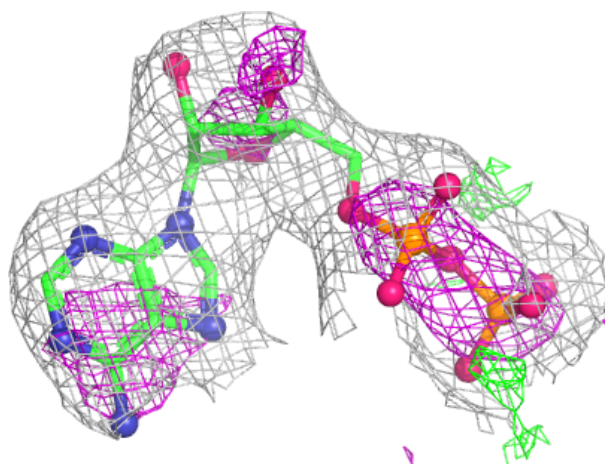
Electron density around ADP K 900:

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



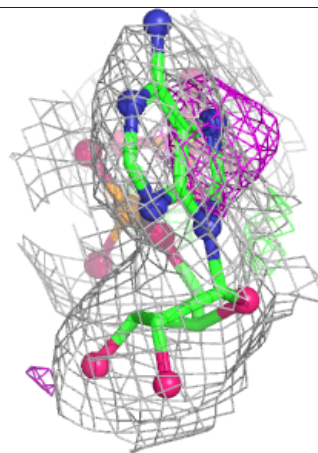
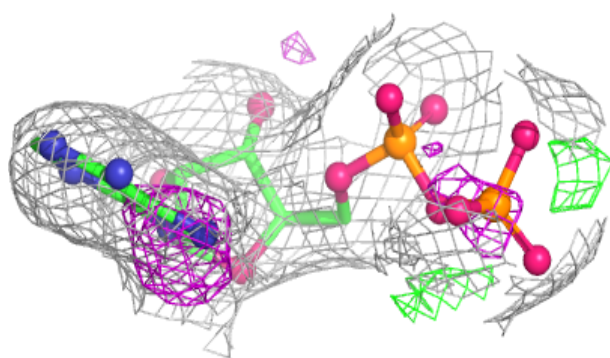
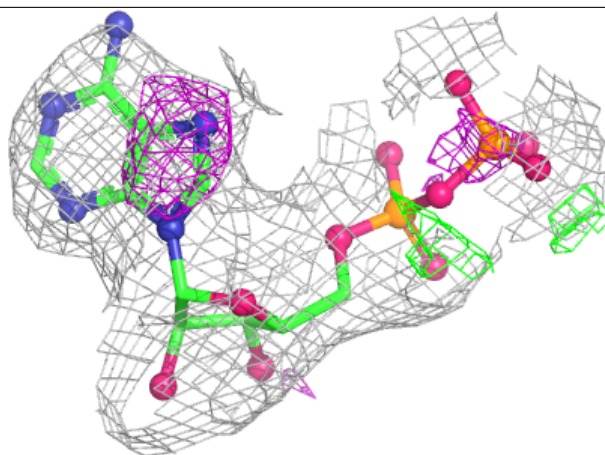
Electron density around ADP D 900:

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



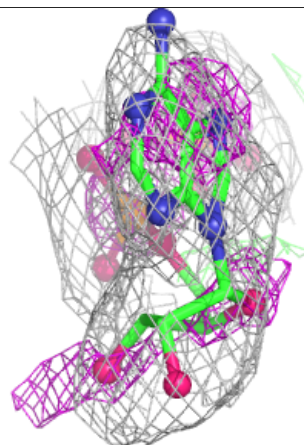
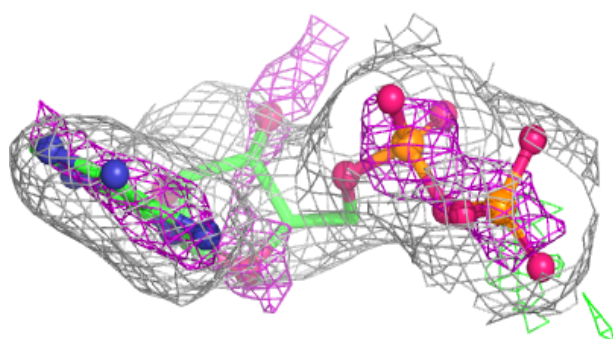
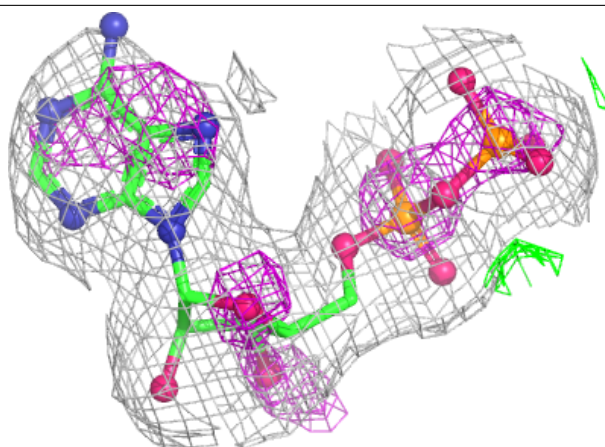
Electron density around ADP H 900:

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



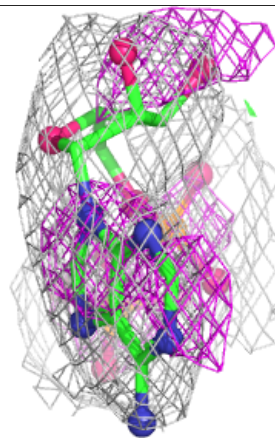
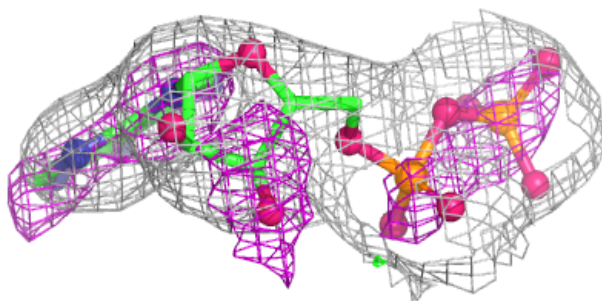
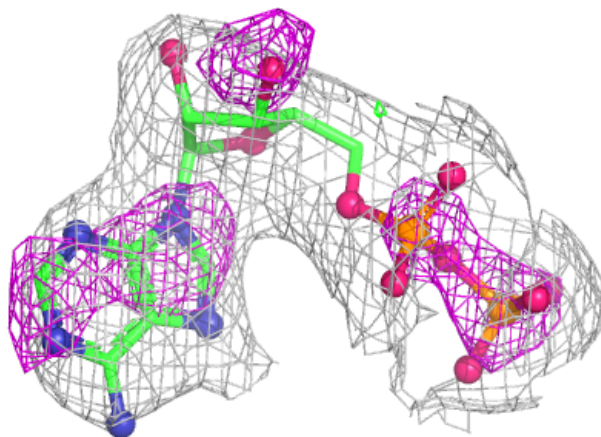
Electron density around ADP C 900:

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



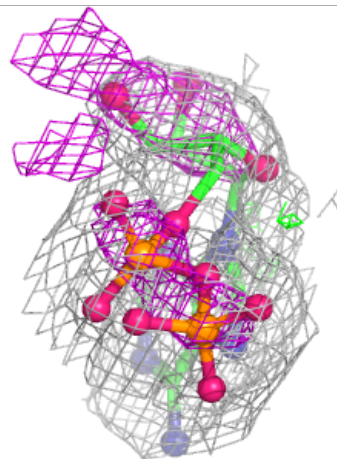
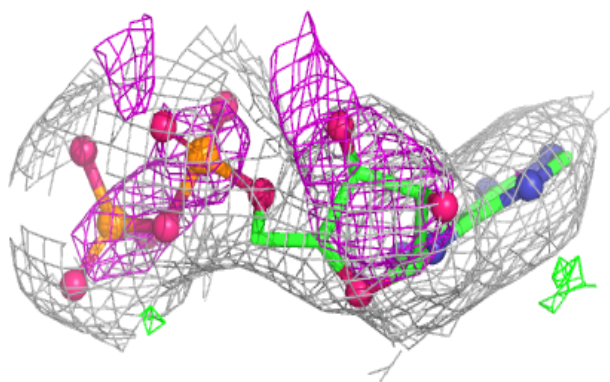
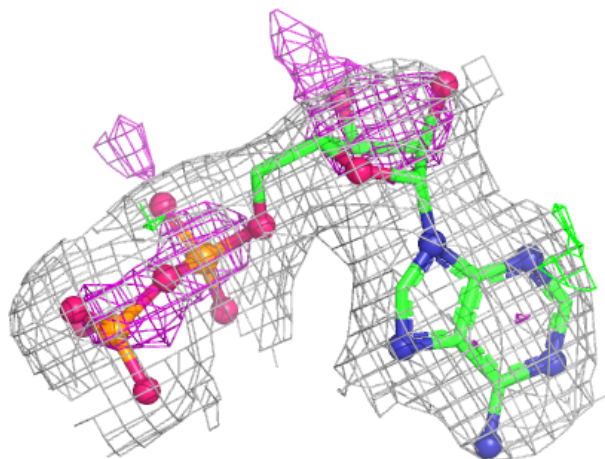
Electron density around ADP F 900:

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



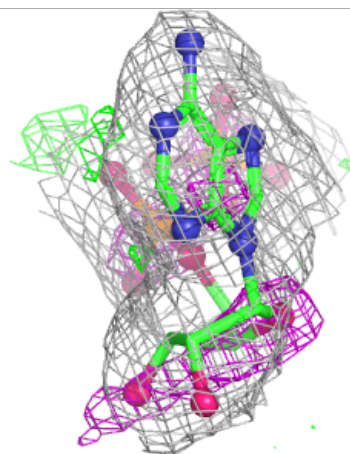
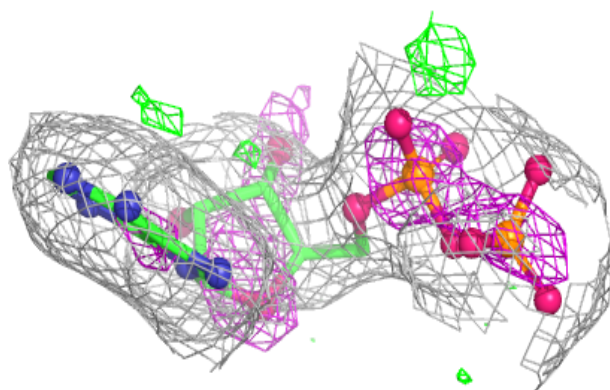
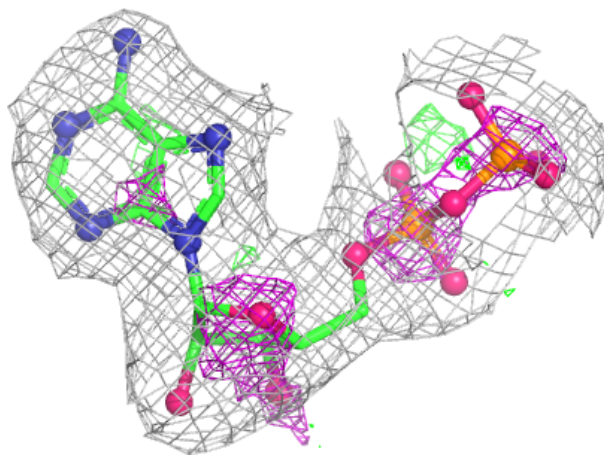
Electron density around ADP L 900:

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



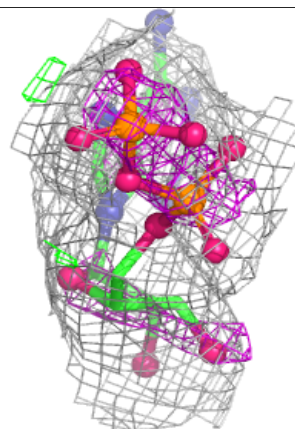
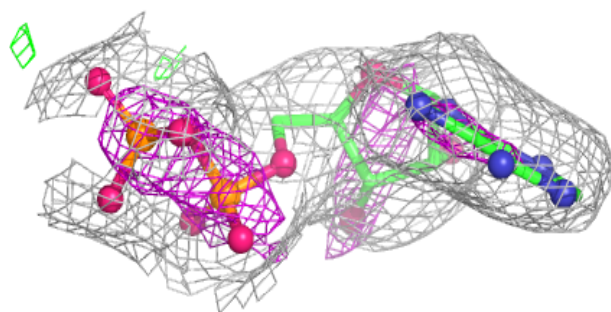
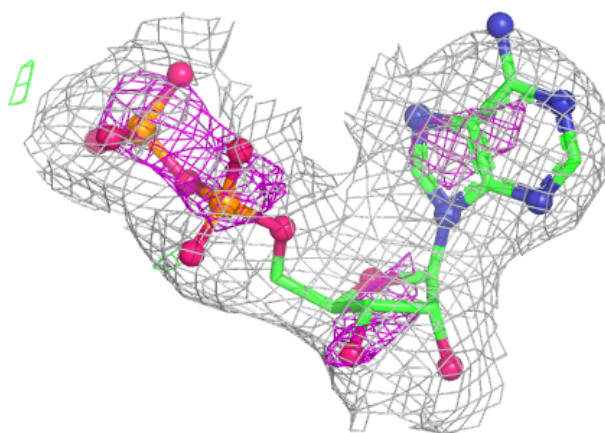
Electron density around ADP N 900:

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



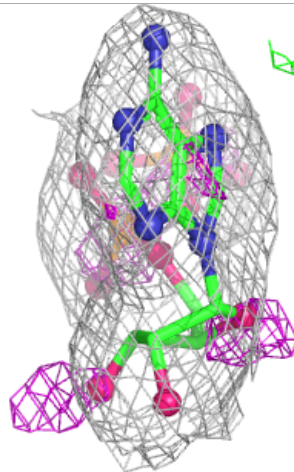
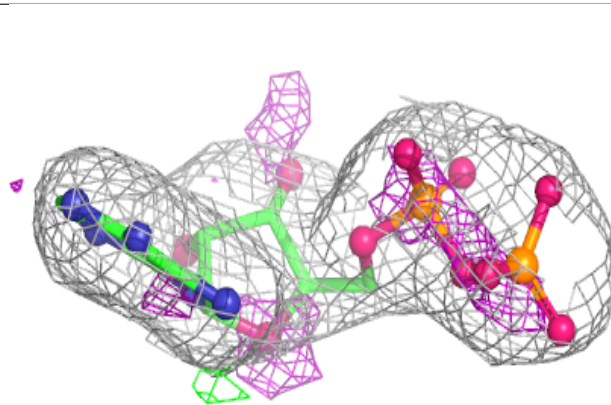
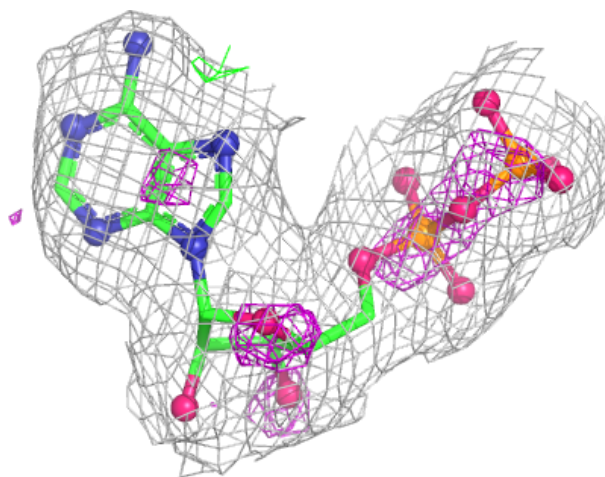
Electron density around ADP J 900:

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



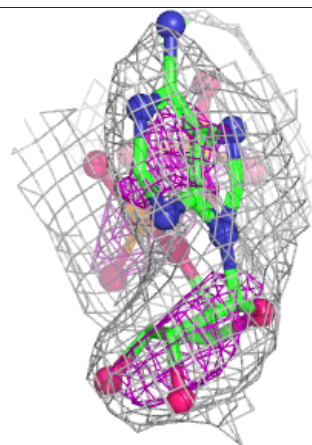
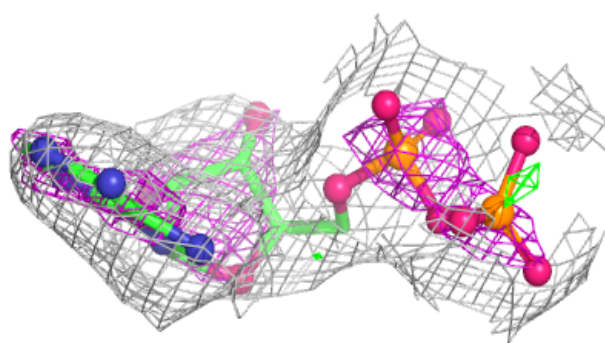
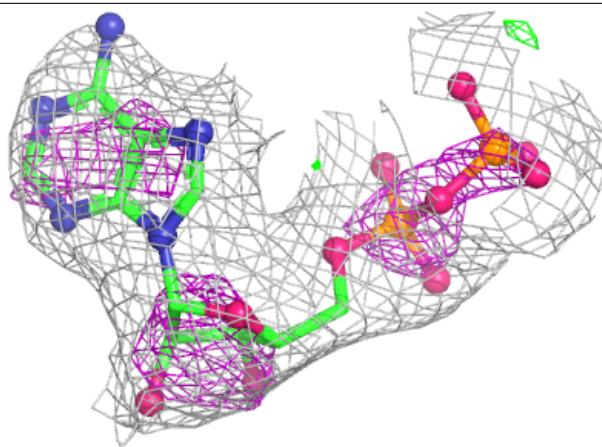
Electron density around ADP B 900:

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



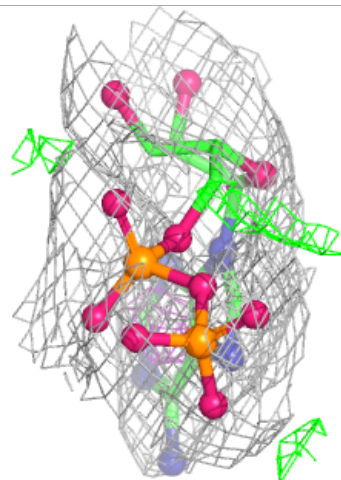
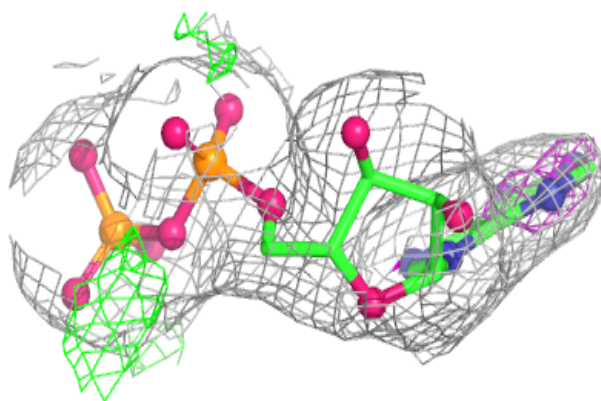
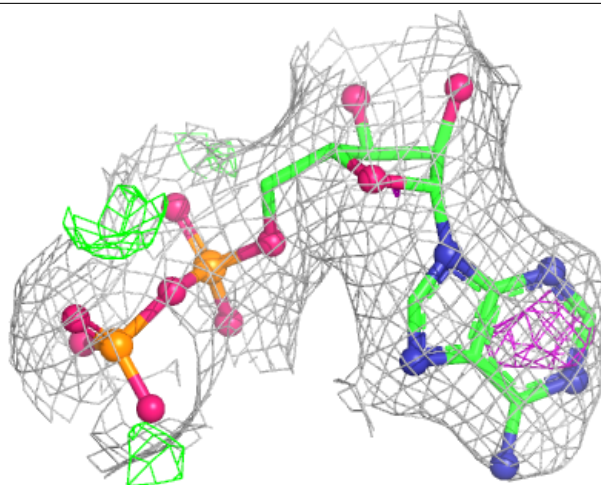
Electron density around ADP G 900:

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



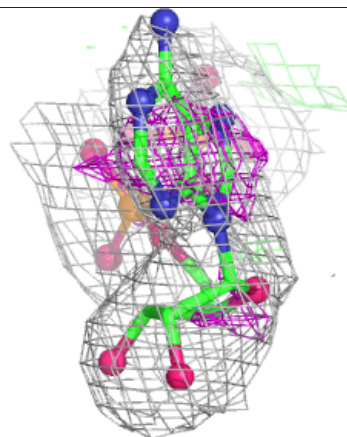
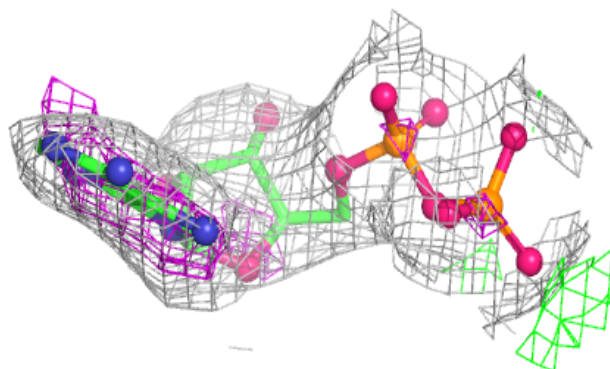
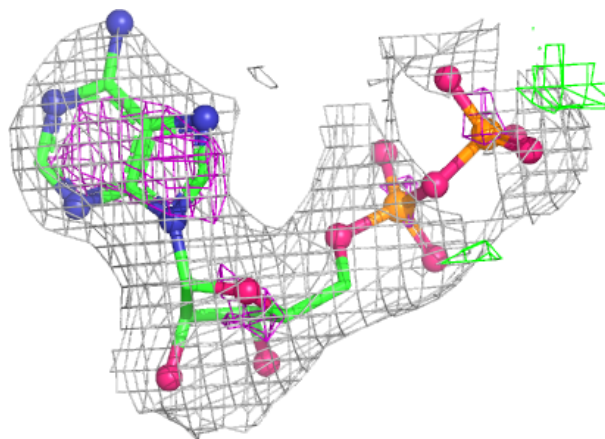
Electron density around ADP E 900:

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



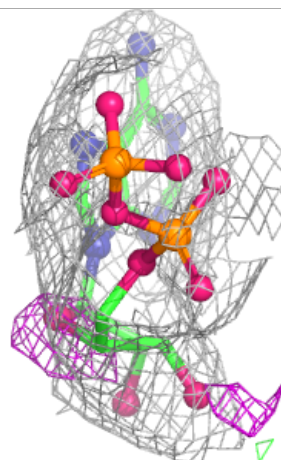
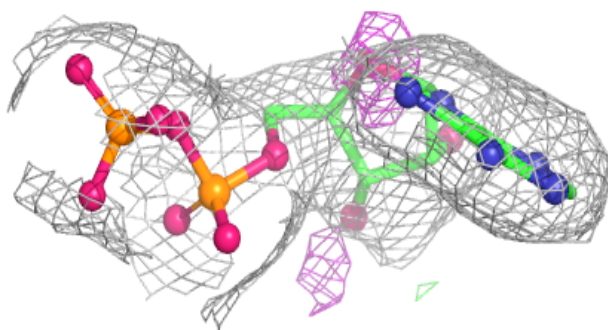
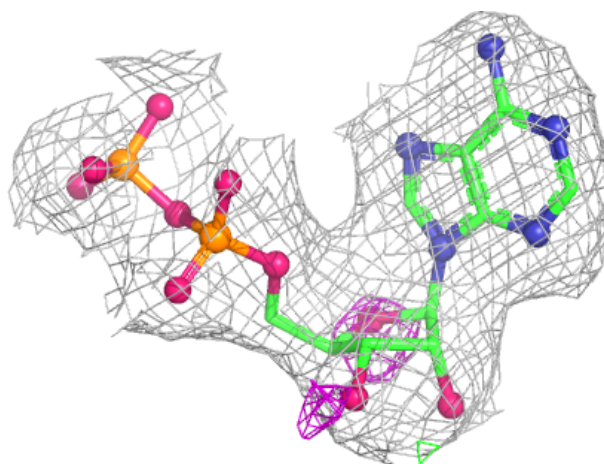
Electron density around ADP M 900:

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



Electron density around ADP I 900:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.