



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:22 AM UTC

PDB ID : 4LNI / pdb_00004lni
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of the transition state complex
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.
Deposited on : 2013-07-11
Resolution : 2.58 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

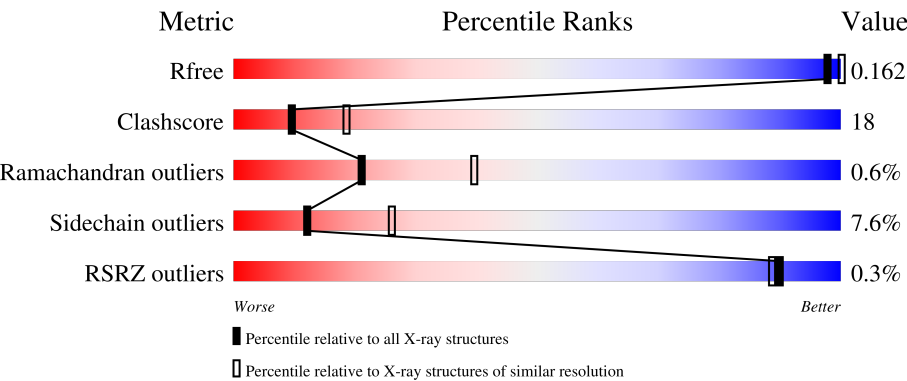
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	443	64%30%6%
1	B	443	63%31%6%
1	C	443	67%28%. .
1	D	443	62%33%5%

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Mol	Chain	Length	Quality of chain
1	E	443	
1	F	443	
1	G	443	
1	H	443	
1	I	443	
1	J	443	
1	K	443	
1	L	443	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P3S	D	501	-	-	X	-
2	P3S	G	601	-	-	X	-
2	P3S	H	601	-	-	X	-

2 Entry composition

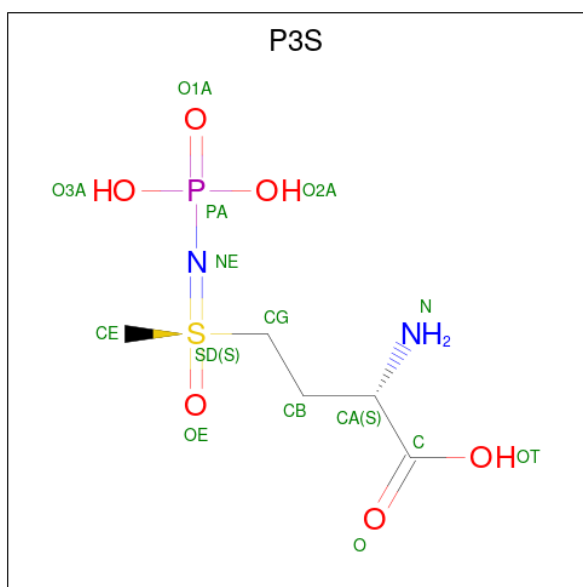
There are 5 unique types of molecules in this entry. The entry contains 86960 atoms, of which 41847 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase.

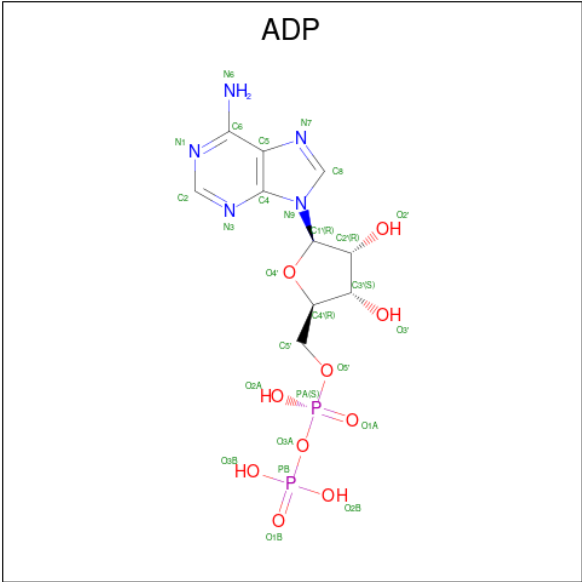
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	B	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	C	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	D	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	E	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	F	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	G	443	Total	C	H	N	O	S	0	0	0
			7009	2259	3474	590	670	16			
1	H	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	I	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	J	441	Total	C	H	N	O	S	0	0	0
			6980	2250	3459	587	668	16			
1	K	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	L	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			

- Molecule 2 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (CCD ID: P3S) (formula: $C_5H_{13}N_2O_6PS$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	G	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	H	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	I	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	J	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	K	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	L	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		

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



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total 3 Mg 3	0	0
4	B	3	Total 3 Mg 3	0	0
4	C	3	Total 3 Mg 3	0	0
4	D	3	Total 3 Mg 3	0	0
4	E	3	Total 3 Mg 3	0	0
4	F	3	Total 3 Mg 3	0	0
4	G	3	Total 3 Mg 3	0	0
4	H	3	Total 3 Mg 3	0	0
4	I	3	Total 3 Mg 3	0	0
4	J	3	Total 3 Mg 3	0	0
4	K	3	Total 3 Mg 3	0	0
4	L	3	Total 3 Mg 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	177	Total 177 O 177	0	0
5	B	178	Total 178 O 178	0	0
5	C	183	Total 183 O 183	0	0
5	D	200	Total 200 O 200	0	0
5	E	168	Total 168 O 168	0	0
5	F	166	Total 166 O 166	0	0
5	G	184	Total 184 O 184	0	0
5	H	174	Total 174 O 174	0	0

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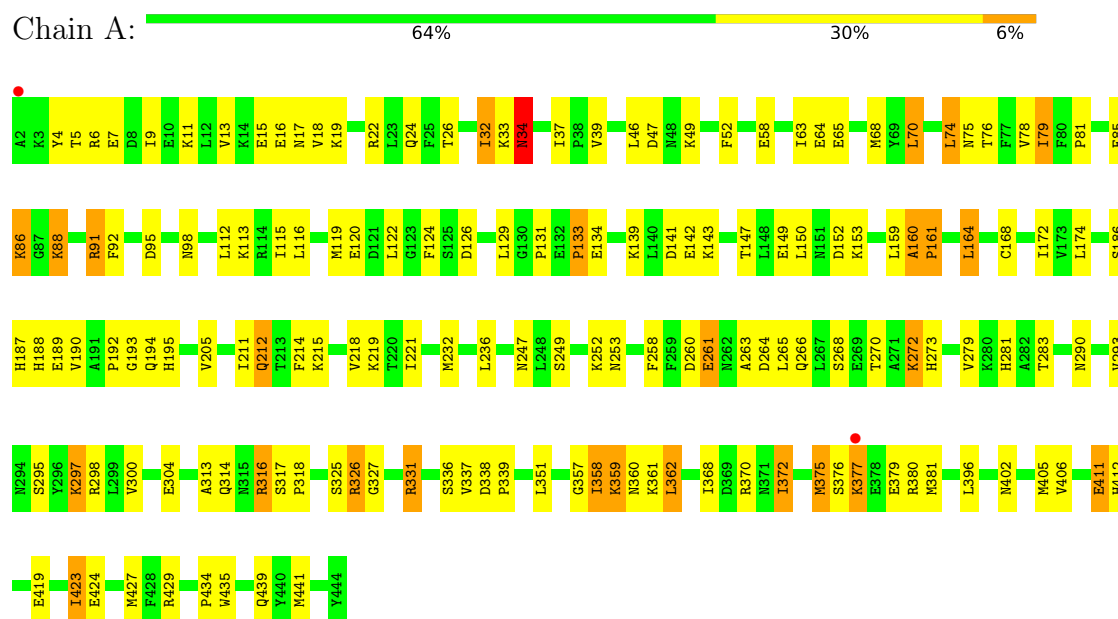
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	189	Total 189	O 189	0	0
5	J	194	Total 194	O 194	0	0
5	K	191	Total 191	O 191	0	0
5	L	163	Total 163	O 163	0	0

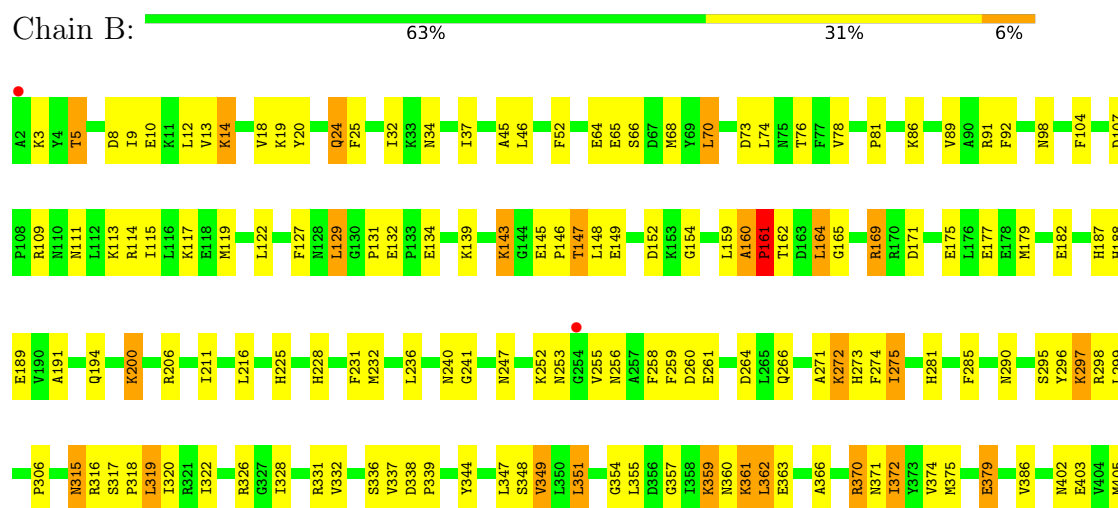
3 Residue-property plots

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

• Molecule 1: Glutamine synthetase



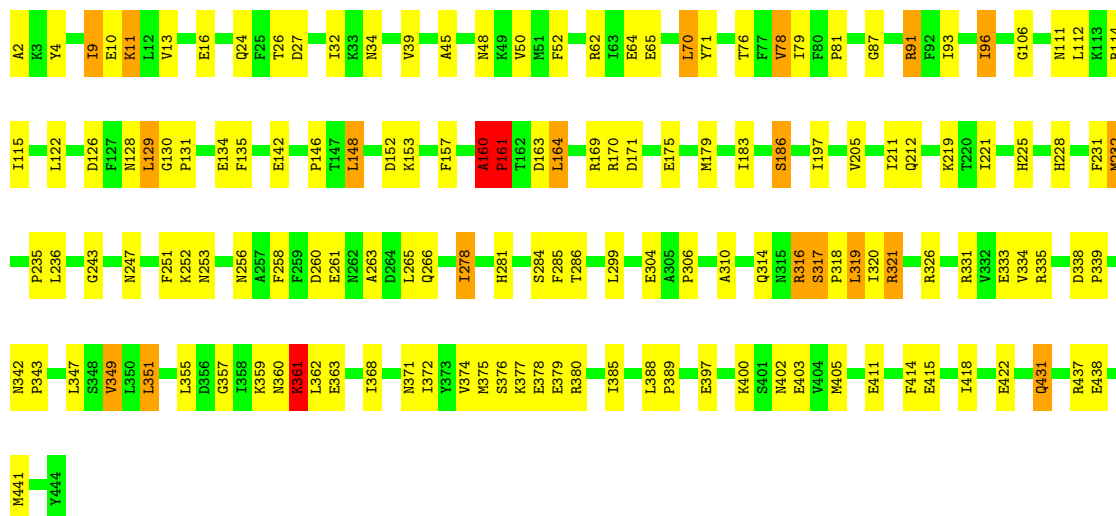
• Molecule 1: Glutamine synthetase





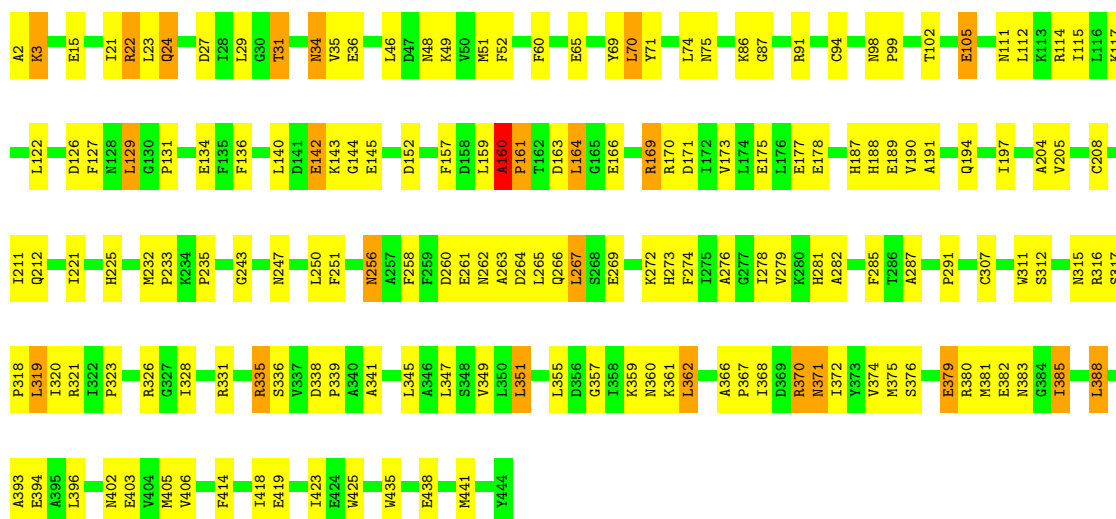
• Molecule 1: Glutamine synthetase

Chain C: 67% 28% . .



• Molecule 1: Glutamine synthetase

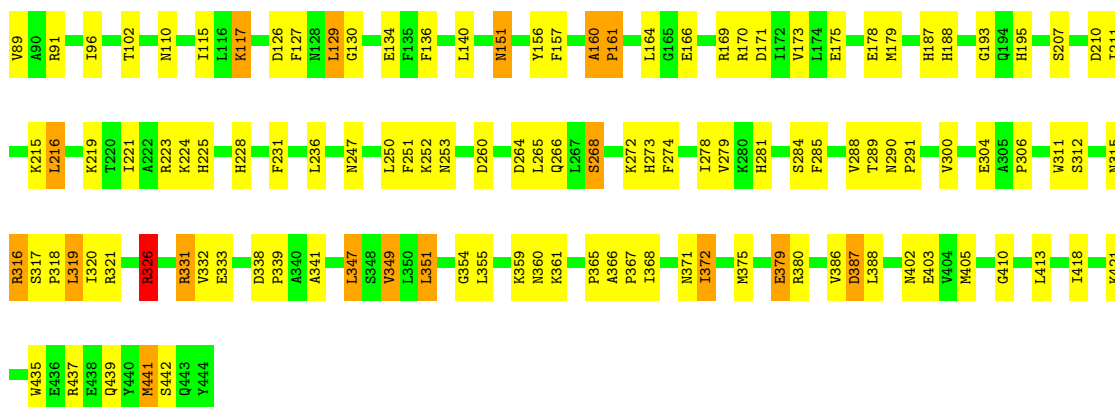
Chain D: 62% 33% 5%



• Molecule 1: Glutamine synthetase

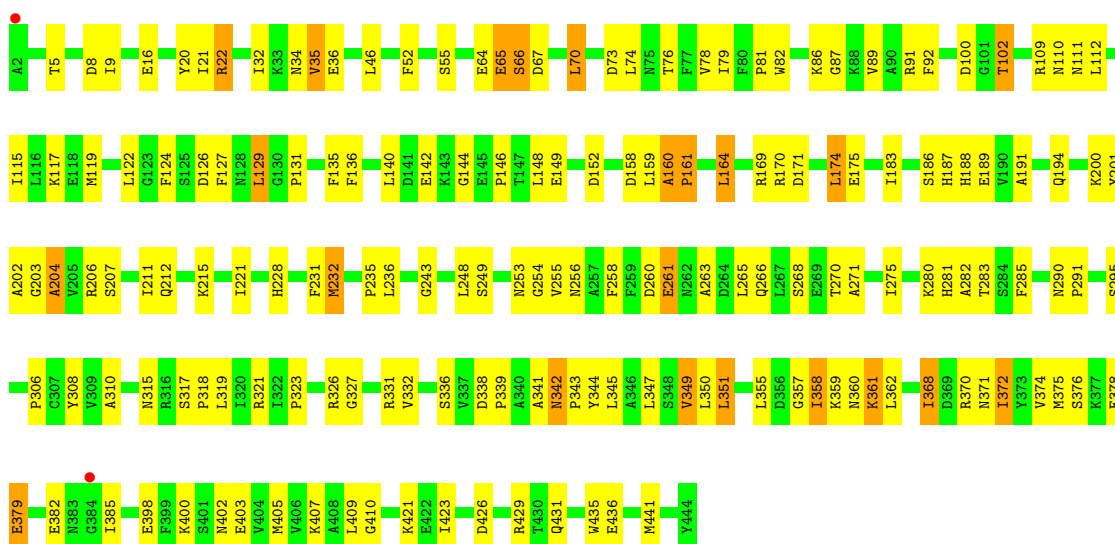
Chain E: 65% 30% 5%





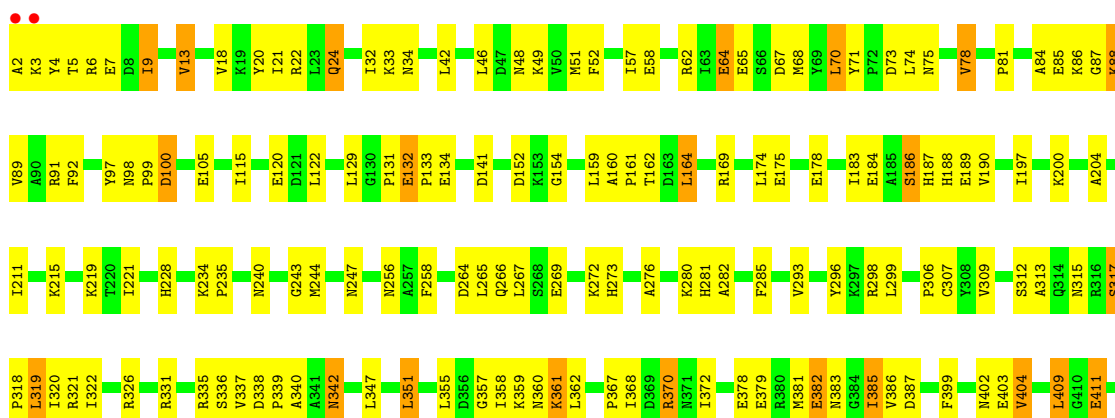
• Molecule 1: Glutamine synthetase

Chain F: 61% 34% 5%



• Molecule 1: Glutamine synthetase

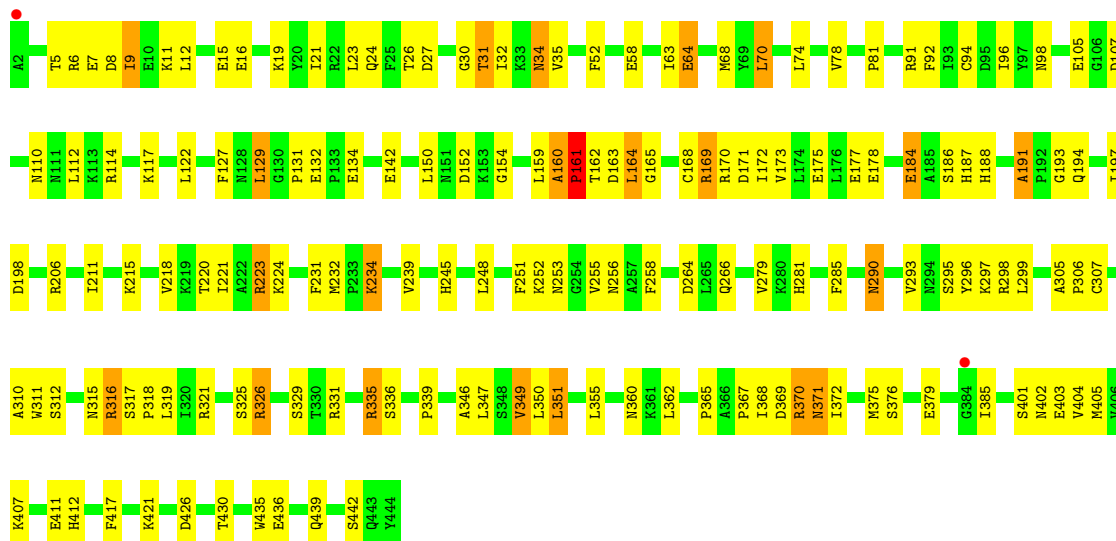
Chain G: 63% 31% 5%





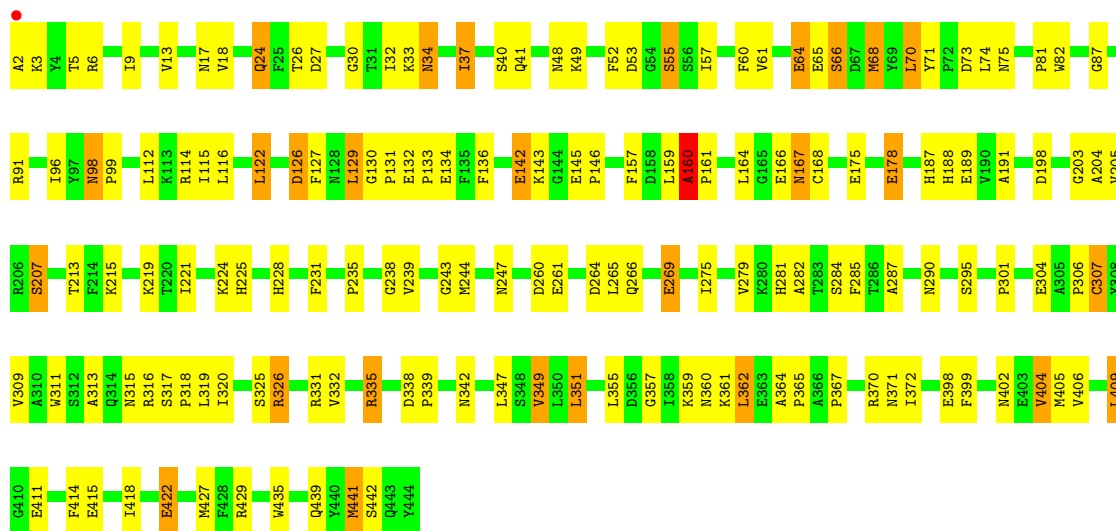
• Molecule 1: Glutamine synthetase

Chain H: 64% 31% 5%



• Molecule 1: Glutamine synthetase

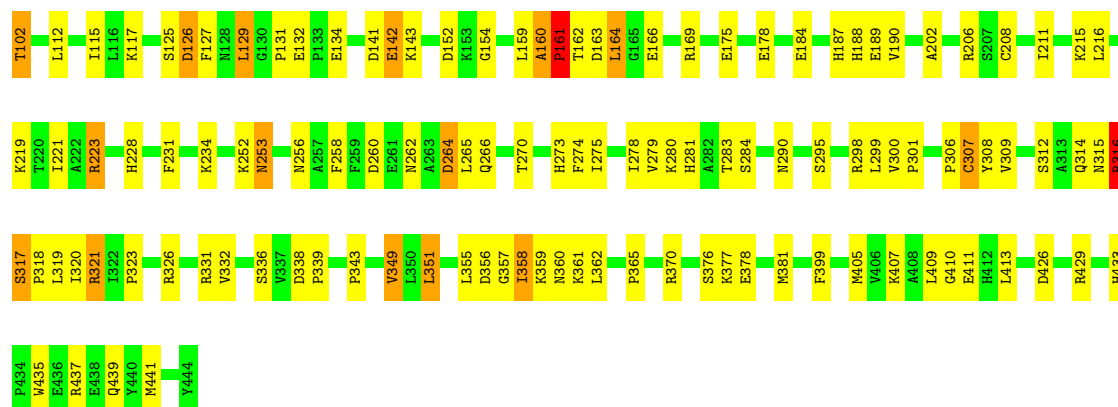
Chain I: 63% 30% 6%



• Molecule 1: Glutamine synthetase

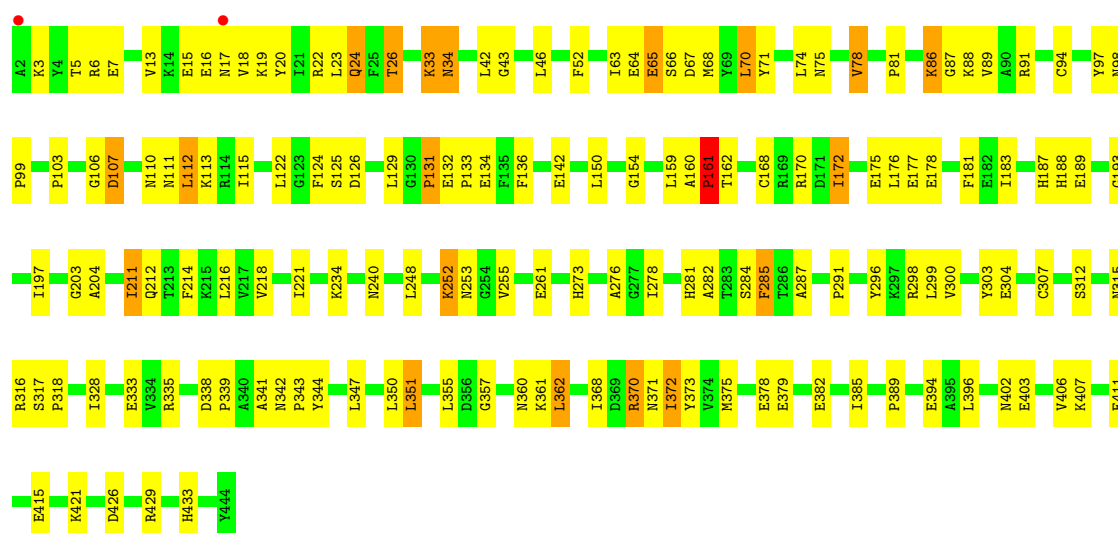
Chain J: 65% 29% 5%





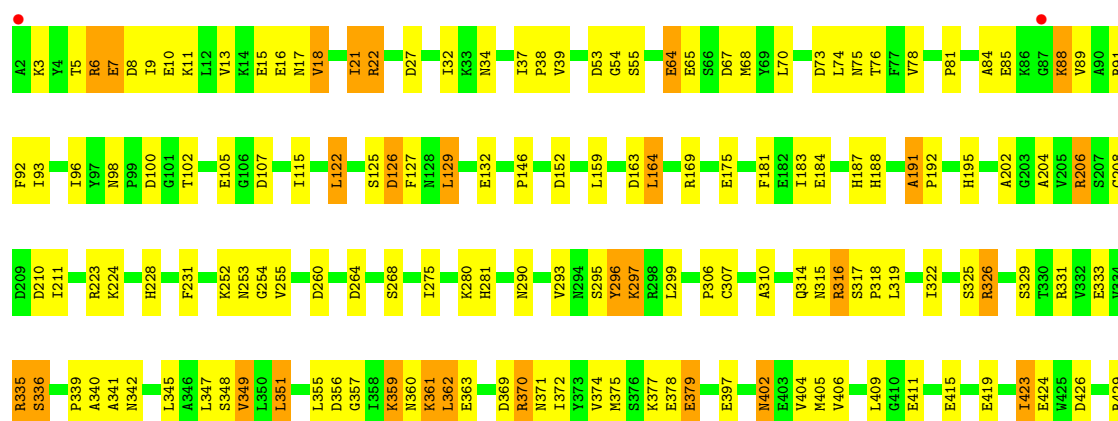
• Molecule 1: Glutamine synthetase

Chain K: 65% 31% •



• Molecule 1: Glutamine synthetase

Chain L: 64% 29% 7%



T430	P434
Q431	W435
	E436
	R437
	E438
	Q439
	Y440
	M441
	S442
	Q443
	Y444

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.20Å 141.60Å 142.10Å 60.29° 67.38° 76.20°	Depositor
Resolution (Å)	117.10 – 2.58 117.10 – 2.58	Depositor EDS
% Data completeness (in resolution range)	90.8 (117.10-2.58) 90.8 (117.10-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.6.4_486, CNS 1.2	Depositor
R, R_{free}	0.165 , 0.223 0.159 , 0.162	Depositor DCC
R_{free} test set	21985 reflections (11.18%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	1.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	86960	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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: P3S, MG, 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	1.15	6/3618 (0.2%)	1.26	14/4895 (0.3%)
1	B	1.18	4/3618 (0.1%)	1.28	23/4895 (0.5%)
1	C	1.18	4/3618 (0.1%)	1.35	9/4895 (0.2%)
1	D	1.17	5/3618 (0.1%)	1.28	14/4895 (0.3%)
1	E	1.19	6/3618 (0.2%)	1.40	19/4895 (0.4%)
1	F	1.14	2/3618 (0.1%)	1.23	13/4895 (0.3%)
1	G	1.14	3/3618 (0.1%)	1.21	15/4895 (0.3%)
1	H	1.16	6/3618 (0.2%)	1.52	21/4895 (0.4%)
1	I	1.15	1/3618 (0.0%)	1.41	23/4895 (0.5%)
1	J	1.17	3/3604 (0.1%)	1.53	18/4877 (0.4%)
1	K	1.20	3/3618 (0.1%)	1.48	15/4895 (0.3%)
1	L	1.15	4/3618 (0.1%)	1.23	20/4895 (0.4%)
All	All	1.17	47/43402 (0.1%)	1.35	204/58722 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	H	0	1
1	I	0	1
All	All	0	9

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	190	VAL	CA-CB	8.61	1.64	1.54
1	E	161	PRO	N-CD	7.98	1.58	1.47
1	H	279	VAL	CA-CB	7.26	1.62	1.54
1	B	366	ALA	CA-CB	-7.08	1.42	1.53
1	E	161	PRO	CA-C	6.71	1.61	1.52
1	H	346	ALA	CA-CB	-6.68	1.42	1.53
1	C	334	VAL	CA-CB	6.53	1.61	1.53
1	F	204	ALA	CA-CB	-6.42	1.43	1.53
1	A	279	VAL	CA-CB	6.27	1.61	1.54
1	L	264	ASP	CA-C	6.23	1.60	1.52
1	D	197	ILE	C-O	-6.22	1.17	1.24
1	G	367	PRO	C-O	-6.08	1.16	1.23
1	K	197	ILE	C-O	-6.03	1.17	1.24
1	A	26	THR	C-O	-6.00	1.17	1.24
1	J	65	GLU	CA-C	-5.99	1.46	1.53
1	L	211	ILE	CA-CB	-5.99	1.47	1.54
1	J	202	ALA	CA-CB	-5.88	1.43	1.53
1	J	18	VAL	CA-CB	-5.87	1.47	1.54
1	L	18	VAL	CA-CB	-5.86	1.47	1.54
1	H	197	ILE	C-O	-5.86	1.18	1.24
1	L	191	ALA	CA-CB	5.84	1.62	1.53
1	H	160	ALA	CA-C	-5.82	1.46	1.53
1	C	317	SER	CA-C	5.77	1.60	1.52
1	C	183	ILE	CA-CB	5.75	1.60	1.54
1	C	106	GLY	C-O	-5.61	1.20	1.24
1	K	106	GLY	C-O	-5.61	1.18	1.24
1	E	278	ILE	CA-CB	-5.53	1.47	1.54
1	D	279	VAL	CA-C	5.50	1.59	1.52
1	A	423	ILE	CA-C	5.49	1.59	1.52
1	D	250	LEU	C-O	-5.48	1.17	1.24
1	F	35	VAL	CA-CB	5.43	1.62	1.54
1	H	442	SER	CA-C	-5.42	1.45	1.52
1	H	305	ALA	CA-CB	-5.41	1.46	1.53
1	B	315	ASN	CA-C	5.41	1.59	1.52
1	B	45	ALA	CA-CB	-5.37	1.44	1.53
1	E	173	VAL	CA-CB	5.35	1.61	1.54
1	A	313	ALA	CA-C	5.34	1.59	1.52
1	A	26	THR	CA-C	-5.29	1.46	1.52
1	G	403	GLU	C-O	-5.26	1.17	1.24
1	E	53	ASP	CA-C	5.24	1.59	1.52
1	I	239	VAL	N-CA	5.22	1.52	1.46
1	E	223	ARG	C-O	-5.21	1.18	1.24
1	K	278	ILE	CA-CB	-5.16	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	VAL	N-CA	-5.15	1.40	1.46
1	D	190	VAL	CA-CB	5.11	1.60	1.54
1	B	332	VAL	CA-CB	-5.10	1.48	1.54
1	D	169	ARG	CB-CG	-5.08	1.37	1.52

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	160	ALA	CA-C-N	44.53	175.50	119.84
1	H	160	ALA	C-N-CA	44.53	175.50	119.84
1	J	160	ALA	CA-C-N	44.39	175.33	119.84
1	J	160	ALA	C-N-CA	44.39	175.33	119.84
1	K	160	ALA	CA-C-N	40.21	170.10	119.84
1	K	160	ALA	C-N-CA	40.21	170.10	119.84
1	I	160	ALA	CA-C-N	33.51	161.73	119.84
1	I	160	ALA	C-N-CA	33.51	161.73	119.84
1	C	160	ALA	CA-C-N	29.72	156.99	119.84
1	C	160	ALA	C-N-CA	29.72	156.99	119.84
1	E	160	ALA	CA-C-N	29.49	156.71	119.84
1	E	160	ALA	C-N-CA	29.49	156.71	119.84
1	D	160	ALA	CA-C-N	21.91	147.23	119.84
1	D	160	ALA	C-N-CA	21.91	147.23	119.84
1	B	160	ALA	CA-C-N	18.31	142.73	119.84
1	B	160	ALA	C-N-CA	18.31	142.73	119.84
1	A	160	ALA	CA-C-N	17.68	141.94	119.84
1	A	160	ALA	C-N-CA	17.68	141.94	119.84
1	E	160	ALA	C-N-CD	-15.51	61.42	125.00
1	K	160	ALA	C-N-CD	-13.80	68.41	125.00
1	F	160	ALA	CA-C-N	13.51	136.72	119.84
1	F	160	ALA	C-N-CA	13.51	136.72	119.84
1	C	160	ALA	C-N-CD	-13.12	71.20	125.00
1	H	160	ALA	C-N-CD	-13.04	71.56	125.00
1	J	160	ALA	C-N-CD	-12.98	71.76	125.00
1	E	160	ALA	O-C-N	12.65	132.56	121.30
1	I	160	ALA	C-N-CD	-11.42	78.18	125.00
1	F	160	ALA	C-N-CD	-10.43	82.25	125.00
1	D	160	ALA	C-N-CD	-10.31	82.73	125.00
1	G	160	ALA	C-N-CD	-9.45	99.81	120.60
1	L	132	GLU	CA-C-N	-9.38	108.11	119.84
1	L	132	GLU	C-N-CA	-9.38	108.11	119.84
1	B	160	ALA	C-N-CD	-9.34	86.70	125.00
1	E	161	PRO	CA-N-CD	-9.09	99.27	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	410	GLY	CA-C-O	-8.54	116.34	122.23
1	L	191	ALA	CA-C-N	-8.42	111.31	119.90
1	L	191	ALA	C-N-CA	-8.42	111.31	119.90
1	C	161	PRO	CA-N-CD	-8.11	100.64	112.00
1	G	293	VAL	N-CA-C	-8.01	102.63	110.72
1	A	37	ILE	CA-C-N	-7.98	112.13	120.03
1	A	37	ILE	C-N-CA	-7.98	112.13	120.03
1	L	54	GLY	N-CA-C	-7.85	106.03	114.67
1	E	288	VAL	N-CA-C	7.84	118.64	110.72
1	L	37	ILE	CA-C-N	-7.77	112.34	120.03
1	L	37	ILE	C-N-CA	-7.77	112.34	120.03
1	E	161	PRO	N-CA-C	-7.69	96.63	112.47
1	A	160	ALA	C-N-CD	-7.68	93.49	125.00
1	K	132	GLU	CA-C-N	-7.65	110.28	119.84
1	K	132	GLU	C-N-CA	-7.65	110.28	119.84
1	E	338	ASP	CA-C-N	-7.62	112.17	121.00
1	E	338	ASP	C-N-CA	-7.62	112.17	121.00
1	E	161	PRO	N-CA-CB	7.60	111.23	103.25
1	G	160	ALA	CA-C-N	7.58	145.19	127.00
1	G	160	ALA	C-N-CA	7.58	145.19	127.00
1	B	132	GLU	CA-C-N	-7.34	110.66	119.84
1	B	132	GLU	C-N-CA	-7.34	110.66	119.84
1	E	366	ALA	CA-C-N	7.27	127.31	119.90
1	E	366	ALA	C-N-CA	7.27	127.31	119.90
1	B	232	MET	CA-C-N	7.26	126.52	118.97
1	B	232	MET	C-N-CA	7.26	126.52	118.97
1	K	211	ILE	CB-CA-C	-7.23	102.38	112.14
1	H	293	VAL	N-CA-C	-7.20	103.28	110.62
1	L	293	VAL	N-CA-C	-7.18	103.29	110.62
1	E	300	VAL	CA-C-N	-7.17	112.54	120.14
1	E	300	VAL	C-N-CA	-7.17	112.54	120.14
1	L	342	ASN	CA-C-N	-7.17	111.78	119.24
1	L	342	ASN	C-N-CA	-7.17	111.78	119.24
1	J	234	LYS	CA-C-N	-7.10	111.66	119.19
1	J	234	LYS	C-N-CA	-7.10	111.66	119.19
1	F	358	ILE	CB-CA-C	-7.04	103.01	111.81
1	G	317	SER	CA-C-N	-7.00	111.10	119.84
1	G	317	SER	C-N-CA	-7.00	111.10	119.84
1	G	190	VAL	N-CA-C	6.99	117.70	110.36
1	J	37	ILE	CA-C-N	-6.94	113.16	120.03
1	J	37	ILE	C-N-CA	-6.94	113.16	120.03
1	H	232	MET	CA-C-N	6.90	126.42	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	232	MET	C-N-CA	6.90	126.42	119.24
1	K	161	PRO	CA-N-CD	-6.85	102.41	112.00
1	J	433	HIS	CA-C-N	-6.82	111.77	119.28
1	J	433	HIS	C-N-CA	-6.82	111.77	119.28
1	H	168	CYS	N-CA-C	-6.65	103.73	110.97
1	B	410	GLY	CA-C-O	-6.55	117.71	122.23
1	I	238	GLY	N-CA-C	6.54	124.22	115.59
1	E	326	ARG	CG-CD-NE	-6.50	97.70	112.00
1	C	160	ALA	O-C-N	6.47	128.67	121.43
1	L	307	CYS	N-CA-C	-6.38	106.71	114.75
1	A	120	GLU	N-CA-C	-6.35	104.44	111.36
1	E	316	ARG	N-CA-C	-6.32	105.15	112.92
1	L	322	ILE	CA-C-N	-6.32	113.78	120.03
1	L	322	ILE	C-N-CA	-6.32	113.78	120.03
1	B	89	VAL	N-CA-C	6.29	117.36	108.36
1	D	366	ALA	CA-C-N	6.29	126.30	119.89
1	D	366	ALA	C-N-CA	6.29	126.30	119.89
1	L	411	GLU	N-CA-C	6.26	117.77	111.07
1	L	341	ALA	N-CA-C	6.26	118.37	110.24
1	I	37	ILE	CA-C-N	-6.25	113.84	120.03
1	I	37	ILE	C-N-CA	-6.25	113.84	120.03
1	B	297	LYS	N-CA-C	-6.14	105.79	113.28
1	F	410	GLY	CA-C-O	-6.13	118.00	122.23
1	J	316	ARG	N-CA-C	-6.09	105.77	112.72
1	J	275	ILE	CB-CA-C	-6.08	103.93	112.14
1	D	385	ILE	CB-CA-C	-6.07	104.68	111.23
1	K	160	ALA	O-C-N	6.04	127.52	121.30
1	K	131	PRO	CA-C-O	-6.03	114.50	121.86
1	C	225	HIS	N-CA-C	-5.99	105.90	112.72
1	K	161	PRO	N-CA-C	-5.99	100.14	112.47
1	J	161	PRO	CA-N-CD	-5.97	103.64	112.00
1	H	307	CYS	N-CA-C	-5.90	107.31	114.75
1	B	206	ARG	N-CA-C	-5.89	104.94	111.71
1	H	430	THR	N-CA-C	-5.85	106.19	113.38
1	B	169	ARG	N-CA-C	-5.82	105.01	111.36
1	I	130	GLY	CA-C-N	5.82	125.58	119.76
1	I	130	GLY	C-N-CA	5.82	125.58	119.76
1	C	321	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	A	358	ILE	CB-CA-C	-5.79	104.23	112.22
1	B	37	ILE	CA-C-N	-5.75	113.77	119.92
1	B	37	ILE	C-N-CA	-5.75	113.77	119.92
1	I	287	ALA	N-CA-C	-5.72	105.18	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	89	VAL	N-CA-C	5.71	116.10	108.11
1	A	300	VAL	CA-C-N	-5.70	114.09	119.85
1	A	300	VAL	C-N-CA	-5.70	114.09	119.85
1	A	34	ASN	N-CA-C	5.69	117.18	108.42
1	D	98	ASN	CA-C-N	-5.69	112.73	119.84
1	D	98	ASN	C-N-CA	-5.69	112.73	119.84
1	A	293	VAL	N-CA-C	-5.65	105.00	110.42
1	I	98	ASN	CA-C-N	-5.64	113.86	119.56
1	I	98	ASN	C-N-CA	-5.64	113.86	119.56
1	J	321	ARG	CA-C-N	-5.62	118.78	122.60
1	J	321	ARG	C-N-CA	-5.62	118.78	122.60
1	H	132	GLU	CA-C-N	-5.61	112.83	119.84
1	H	132	GLU	C-N-CA	-5.61	112.83	119.84
1	B	66	SER	N-CA-C	5.57	117.03	111.07
1	A	359	LYS	N-CA-C	-5.57	105.22	112.23
1	G	120	GLU	N-CA-C	-5.56	105.38	111.82
1	H	191	ALA	CA-C-N	-5.55	114.04	119.76
1	H	191	ALA	C-N-CA	-5.55	114.04	119.76
1	G	184	GLU	N-CA-C	-5.55	106.18	113.12
1	D	60	PHE	CA-C-O	5.53	121.15	117.94
1	B	275	ILE	CB-CA-C	-5.52	104.81	112.04
1	I	342	ASN	CA-C-N	-5.50	112.95	119.05
1	I	342	ASN	C-N-CA	-5.50	112.95	119.05
1	L	336	SER	N-CA-C	-5.44	105.77	112.90
1	G	340	ALA	N-CA-C	-5.43	106.66	113.28
1	H	290	ASN	CA-C-N	-5.40	114.36	120.89
1	H	290	ASN	C-N-CA	-5.40	114.36	120.89
1	G	132	GLU	CA-C-N	-5.39	113.10	119.84
1	G	132	GLU	C-N-CA	-5.39	113.10	119.84
1	H	30	GLY	N-CA-C	-5.37	107.27	115.00
1	K	433	HIS	N-CA-C	5.37	117.70	110.29
1	I	178	GLU	N-CA-C	5.36	118.04	111.82
1	K	168	CYS	N-CA-C	-5.34	105.37	111.14
1	I	364	ALA	CA-C-N	5.34	125.32	120.03
1	I	364	ALA	C-N-CA	5.34	125.32	120.03
1	E	410	GLY	CA-C-O	-5.34	118.30	122.52
1	B	66	SER	CB-CA-C	-5.33	102.52	110.88
1	D	212	GLN	N-CA-C	-5.32	105.15	111.69
1	L	296	TYR	CA-CB-CG	-5.31	104.34	113.90
1	F	66	SER	N-CA-C	5.30	117.47	111.11
1	G	322	ILE	CB-CA-C	-5.30	105.09	111.18
1	B	177	GLU	N-CA-C	-5.29	105.60	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	THR	CA-C-N	5.26	125.20	119.78
1	D	102	THR	C-N-CA	5.26	125.20	119.78
1	J	132	GLU	CA-C-N	-5.25	113.28	119.84
1	J	132	GLU	C-N-CA	-5.25	113.28	119.84
1	G	13	VAL	CB-CA-C	-5.25	105.16	111.88
1	D	388	LEU	CA-C-N	5.24	125.16	119.76
1	D	388	LEU	C-N-CA	5.24	125.16	119.76
1	I	191	ALA	CA-C-N	-5.24	114.37	119.76
1	I	191	ALA	C-N-CA	-5.24	114.37	119.76
1	J	358	ILE	CB-CA-C	-5.23	105.12	111.87
1	E	102	THR	N-CA-C	5.23	116.41	109.93
1	I	132	GLU	CA-C-N	-5.22	113.31	119.84
1	I	132	GLU	C-N-CA	-5.22	113.31	119.84
1	B	322	ILE	CA-C-N	-5.21	114.87	120.03
1	B	322	ILE	C-N-CA	-5.21	114.87	120.03
1	K	113	LYS	N-CA-C	5.20	116.95	111.28
1	F	65	GLU	CA-C-N	5.20	127.56	120.54
1	F	65	GLU	C-N-CA	5.20	127.56	120.54
1	B	107	ASP	CA-C-N	5.20	124.38	118.97
1	B	107	ASP	C-N-CA	5.20	124.38	118.97
1	C	278	ILE	N-CA-C	-5.17	105.46	110.42
1	I	213	THR	N-CA-C	-5.15	105.85	111.82
1	I	145	GLU	CA-C-N	-5.14	114.62	119.76
1	I	145	GLU	C-N-CA	-5.14	114.62	119.76
1	A	212	GLN	N-CA-C	-5.13	105.87	111.82
1	L	325	SER	CA-C-N	-5.12	115.40	122.16
1	L	325	SER	C-N-CA	-5.12	115.40	122.16
1	F	232	MET	CA-C-N	-5.12	113.27	118.85
1	F	232	MET	C-N-CA	-5.12	113.27	118.85
1	B	241	GLY	N-CA-C	-5.09	104.78	112.41
1	K	212	GLN	N-CA-C	-5.08	105.93	111.82
1	F	55	SER	N-CA-C	-5.07	107.09	113.28
1	F	174	LEU	N-CA-C	5.07	116.50	111.07
1	L	340	ALA	N-CA-C	-5.07	105.94	111.82
1	E	89	VAL	CB-CA-C	-5.07	103.58	110.42
1	H	107	ASP	CA-C-N	5.05	124.49	119.24
1	H	107	ASP	C-N-CA	5.05	124.49	119.24
1	H	165	GLY	N-CA-C	-5.05	106.98	115.62
1	G	385	ILE	N-CA-C	5.04	115.59	107.73
1	H	234	LYS	CA-C-N	-5.03	114.48	119.56
1	H	234	LYS	C-N-CA	-5.03	114.48	119.56
1	A	424	GLU	N-CA-C	-5.02	105.89	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	ILE	CG1-CB-CG2	-5.01	95.67	110.70
1	F	331	ARG	N-CA-C	5.00	116.12	108.42

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ALA	Peptide
1	B	160	ALA	Peptide
1	C	160	ALA	Mainchain,Peptide
1	D	160	ALA	Peptide
1	E	160	ALA	Peptide
1	F	160	ALA	Peptide
1	H	160	ALA	Peptide
1	I	160	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3535	3477	3466	127	0
1	B	3535	3477	3466	117	0
1	C	3535	3477	3466	124	0
1	D	3535	3477	3466	135	0
1	E	3535	3477	3466	124	0
1	F	3535	3477	3466	149	0
1	G	3535	3474	3466	146	0
1	H	3535	3477	3466	133	0
1	I	3535	3477	3466	142	0
1	J	3521	3459	3448	127	0
1	K	3535	3477	3466	124	0
1	L	3535	3477	3466	133	0
2	A	15	12	10	5	0
2	B	15	12	10	2	0
2	C	15	12	10	5	0
2	D	15	12	10	7	0
2	E	15	12	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	15	12	10	5	0
2	G	15	12	10	7	0
2	H	15	12	10	6	0
2	I	15	12	10	3	0
2	J	15	12	10	3	0
2	K	15	12	10	4	0
2	L	15	12	10	1	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	1	0
3	F	27	0	12	1	0
3	G	27	0	12	0	0
3	H	27	0	12	0	0
3	I	27	0	12	0	0
3	J	27	0	12	0	0
3	K	27	0	12	0	0
3	L	27	0	12	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
4	I	3	0	0	0	0
4	J	3	0	0	0	0
4	K	3	0	0	0	0
4	L	3	0	0	0	0
5	A	177	0	0	11	0
5	B	178	0	0	14	0
5	C	183	0	0	14	0
5	D	200	0	0	14	0
5	E	168	0	0	12	0
5	F	166	0	0	15	0
5	G	184	0	0	20	0
5	H	174	0	0	17	0
5	I	189	0	0	17	0
5	J	194	0	0	20	0
5	K	191	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	163	0	0	11	0
All	All	45113	41847	41838	1510	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1510) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:601:P3S:SD	2:H:601:P3S:CE	2.01	1.48
2:G:601:P3S:SD	2:G:601:P3S:CE	2.01	1.46
2:F:601:P3S:SD	2:F:601:P3S:CE	2.02	1.45
2:D:501:P3S:CE	2:D:501:P3S:SD	2.03	1.43
1:I:357:GLY:HA2	1:I:362:LEU:CD1	1.64	1.27
1:I:357:GLY:HA2	1:I:362:LEU:HD13	1.16	1.15
2:G:601:P3S:CE	2:G:601:P3S:CG	2.24	1.14
1:K:211:ILE:HG13	5:K:635:HOH:O	1.49	1.13
2:F:601:P3S:CE	2:F:601:P3S:CG	2.34	1.05
1:F:100:ASP:OD1	1:F:102:THR:CG2	2.06	1.03
1:B:147:THR:HG22	1:B:149:GLU:H	1.24	1.01
1:I:2:ALA:HB2	5:I:766:HOH:O	1.63	0.97
1:C:321:ARG:NH1	5:C:602:HOH:O	1.98	0.97
1:L:22:ARG:HH11	1:L:89:VAL:HG11	1.30	0.97
1:G:3:LYS:NZ	1:G:4:TYR:CE2	2.33	0.96
1:F:100:ASP:OD1	1:F:102:THR:HG22	1.63	0.96
1:A:232:MET:HE2	1:G:441:MET:HA	1.48	0.95
2:D:501:P3S:CE	2:D:501:P3S:CG	2.44	0.94
1:D:266:GLN:HB2	1:D:326:ARG:HD2	1.48	0.94
1:G:3:LYS:NZ	1:G:4:TYR:CD2	2.34	0.94
1:D:326:ARG:CZ	5:D:712:HOH:O	2.18	0.92
1:G:269:GLU:HG2	5:G:745:HOH:O	1.71	0.90
2:H:601:P3S:CE	2:H:601:P3S:CG	2.50	0.89
1:L:224:LYS:HE2	5:L:642:HOH:O	1.71	0.89
1:H:8:ASP:O	1:H:11:LYS:HG2	1.72	0.88
1:L:223:ARG:HG3	5:L:700:HOH:O	1.74	0.88
1:F:206:ARG:NH1	5:F:748:HOH:O	2.07	0.88
1:J:252:LYS:HE3	5:J:749:HOH:O	1.75	0.86
1:H:31:THR:HG21	5:H:811:HOH:O	1.75	0.86
1:G:3:LYS:NZ	1:G:4:TYR:CZ	2.44	0.85
1:K:429:ARG:HD3	5:K:697:HOH:O	1.75	0.85
1:J:16:GLU:O	1:J:88:LYS:HE3	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:411:GLU:HG2	5:G:824:HOH:O	1.78	0.84
2:G:601:P3S:CG	2:G:601:P3S:HEC3	2.06	0.84
1:L:11:LYS:HE2	1:L:15:GLU:OE2	1.79	0.83
1:C:411:GLU:O	1:C:415:GLU:HG2	1.77	0.83
1:G:3:LYS:NZ	1:G:4:TYR:CG	2.46	0.83
1:I:357:GLY:CA	1:I:362:LEU:HD13	2.06	0.83
1:J:264:ASP:OD1	5:J:763:HOH:O	1.96	0.83
1:L:423:ILE:HD12	1:L:423:ILE:C	2.03	0.83
1:J:68:MET:HE2	1:J:98:ASN:HA	1.60	0.82
1:I:357:GLY:CA	1:I:362:LEU:CD1	2.54	0.82
1:D:122:LEU:HD21	1:D:359:LYS:HG2	1.62	0.82
1:I:81:PRO:HG2	1:I:175:GLU:OE2	1.80	0.81
1:L:254:GLY:O	1:L:255:VAL:HG23	1.80	0.81
1:D:142:GLU:H	1:D:142:GLU:CD	1.88	0.81
1:G:13:VAL:HG13	1:G:18:VAL:HB	1.63	0.81
1:H:266:GLN:HB2	1:H:326:ARG:HD2	1.62	0.81
1:C:349:VAL:HG22	1:C:405:MET:SD	2.21	0.81
1:F:131:PRO:CB	1:F:211:ILE:HD11	2.12	0.80
1:H:81:PRO:HG2	1:H:175:GLU:OE1	1.81	0.80
1:B:357:GLY:HA2	1:B:362:LEU:HD22	1.64	0.80
1:A:232:MET:HE2	1:G:441:MET:CA	2.12	0.80
1:L:65:GLU:OE1	1:L:65:GLU:HA	1.80	0.80
1:D:326:ARG:NH2	5:D:712:HOH:O	2.15	0.79
1:I:362:LEU:HD12	1:I:362:LEU:H	1.47	0.79
1:J:83:THR:HB	1:K:170:ARG:HH22	1.48	0.78
1:C:380:ARG:HB2	1:C:385:ILE:HB	1.65	0.78
1:J:83:THR:HB	1:K:170:ARG:NH2	1.98	0.78
1:K:429:ARG:CD	5:K:697:HOH:O	2.30	0.78
1:K:370:ARG:HD2	5:K:700:HOH:O	1.83	0.77
1:L:357:GLY:HA2	1:L:362:LEU:HD22	1.66	0.77
1:F:9:ILE:HG13	1:F:74:LEU:HD12	1.64	0.77
1:E:13:VAL:HG13	1:E:18:VAL:HB	1.65	0.77
1:A:52:PHE:CE1	1:A:70:LEU:HD13	2.20	0.77
1:H:223:ARG:HH11	1:H:223:ARG:HG2	1.50	0.76
1:A:150:LEU:HD23	1:A:193:GLY:HA3	1.65	0.76
2:G:601:P3S:HEC3	2:G:601:P3S:HGC2	1.67	0.76
1:L:22:ARG:NH1	1:L:89:VAL:HG11	1.98	0.76
1:G:3:LYS:NZ	1:G:4:TYR:CD1	2.54	0.76
1:B:351:LEU:HD22	1:B:355:LEU:HG	1.68	0.76
5:A:693:HOH:O	1:B:143:LYS:HD3	1.84	0.75
1:K:131:PRO:CG	1:K:211:ILE:HD11	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:GLU:OE2	1:F:407:LYS:HE2	1.86	0.75
1:L:13:VAL:HG13	1:L:18:VAL:HB	1.69	0.75
1:G:399:PHE:HZ	1:G:409:LEU:HD22	1.52	0.75
1:G:368:ILE:CD1	1:G:385:ILE:HD11	2.16	0.74
1:B:9:ILE:O	1:B:13:VAL:HG23	1.86	0.74
2:F:601:P3S:CG	2:F:601:P3S:HEC3	2.17	0.74
1:G:3:LYS:NZ	1:G:4:TYR:CE1	2.54	0.74
1:D:256:ASN:HD22	1:D:258:PHE:H	1.35	0.74
1:I:357:GLY:HA2	1:I:362:LEU:HD11	1.66	0.74
1:E:372:ILE:HA	1:E:375:MET:HE2	1.68	0.73
1:H:105:GLU:OE1	5:H:866:HOH:O	2.04	0.73
1:I:189:GLU:OE2	2:I:501:P3S:HEC3	1.88	0.73
1:F:16:GLU:HG2	1:F:79:ILE:CD1	2.18	0.73
1:K:122:LEU:CD2	1:K:124:PHE:HE1	2.02	0.73
1:I:9:ILE:HG13	1:I:74:LEU:HD12	1.69	0.73
1:F:271:ALA:O	1:F:275:ILE:HG12	1.89	0.73
1:J:211:ILE:HG22	1:J:215:LYS:HE2	1.71	0.73
1:F:131:PRO:HB2	1:F:211:ILE:HD11	1.72	0.72
1:K:122:LEU:CD2	1:K:124:PHE:CE1	2.72	0.72
1:G:5:THR:HB	5:G:850:HOH:O	1.89	0.71
1:I:351:LEU:HD22	1:I:355:LEU:HG	1.71	0.71
1:C:316:ARG:HD3	2:C:501:P3S:OE	1.90	0.71
1:H:152:ASP:HB3	1:H:164:LEU:HB2	1.70	0.71
1:J:265:LEU:O	1:J:326:ARG:NH1	2.24	0.71
1:J:407:LYS:HG2	5:J:671:HOH:O	1.89	0.71
1:G:51:MET:HE1	1:H:325:SER:OG	1.91	0.71
1:C:321:ARG:CZ	5:C:602:HOH:O	2.32	0.71
1:C:368:ILE:HG12	1:C:385:ILE:HD11	1.71	0.71
1:D:319:LEU:CD2	1:D:336:SER:HB2	2.21	0.70
1:I:24:GLN:NE2	1:I:91:ARG:HH11	1.89	0.70
1:J:300:VAL:HG13	1:J:301:PRO:HD2	1.73	0.70
1:H:368:ILE:HD12	1:H:385:ILE:HD11	1.72	0.70
1:A:52:PHE:CD1	1:A:70:LEU:HD13	2.26	0.70
1:J:266:GLN:HB2	1:J:326:ARG:HD2	1.74	0.70
1:K:131:PRO:HG3	1:K:211:ILE:HD11	1.73	0.70
1:J:357:GLY:HA2	1:J:362:LEU:HD12	1.74	0.70
1:F:5:THR:HG23	1:F:8:ASP:H	1.57	0.70
1:F:372:ILE:HD11	1:F:385:ILE:HG21	1.73	0.70
1:L:5:THR:HG22	1:L:8:ASP:CG	2.16	0.70
1:G:265:LEU:O	1:G:326:ARG:NH1	2.25	0.70
1:H:285:PHE:HB2	1:H:349:VAL:HG11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:MET:HE2	1:F:235:PRO:HA	1.72	0.69
1:G:3:LYS:CE	1:G:4:TYR:CE2	2.75	0.69
1:I:335:ARG:HD3	5:I:647:HOH:O	1.92	0.69
1:J:24:GLN:HE21	1:J:91:ARG:HD3	1.57	0.69
1:D:115:ILE:HG22	1:D:351:LEU:HD13	1.73	0.69
1:K:115:ILE:HG22	1:K:351:LEU:HD13	1.73	0.69
1:L:351:LEU:HD22	1:L:355:LEU:HG	1.74	0.69
1:D:262:ASN:ND2	5:D:764:HOH:O	2.17	0.69
1:K:281:HIS:HD2	1:K:402:ASN:HD21	1.40	0.69
1:F:5:THR:HG22	1:F:8:ASP:OD2	1.91	0.69
1:B:379:GLU:HG3	5:B:673:HOH:O	1.90	0.69
1:H:187:HIS:HD2	1:H:188:HIS:O	1.76	0.69
1:I:96:ILE:N	1:I:96:ILE:HD12	2.07	0.69
1:K:99:PRO:HG2	1:L:314:GLN:HE22	1.56	0.69
1:C:65:GLU:OE2	5:C:750:HOH:O	2.11	0.69
1:B:370:ARG:NE	5:B:686:HOH:O	2.26	0.69
1:C:142:GLU:CD	1:C:142:GLU:H	2.00	0.69
1:L:152:ASP:HB3	1:L:164:LEU:HB2	1.75	0.69
1:G:351:LEU:HD22	1:G:355:LEU:HG	1.75	0.69
1:F:345:LEU:HD22	1:F:409:LEU:HD22	1.75	0.68
1:L:402:ASN:C	1:L:402:ASN:HD22	2.01	0.68
1:G:68:MET:HE2	1:G:98:ASN:HA	1.76	0.68
1:C:24:GLN:HE21	1:C:34:ASN:HD22	1.40	0.68
1:A:150:LEU:CD2	1:A:192:PRO:O	2.42	0.68
1:D:126:ASP:HB2	1:D:251:PHE:HB2	1.76	0.68
1:E:9:ILE:O	1:E:13:VAL:HG23	1.94	0.68
1:E:81:PRO:HD2	1:E:179:MET:HE2	1.75	0.68
1:D:2:ALA:HB3	1:D:75:ASN:HD21	1.59	0.68
1:F:169:ARG:CD	1:F:186:SER:OG	2.42	0.68
1:C:351:LEU:HD22	1:C:355:LEU:HG	1.76	0.67
1:C:377:LYS:HG3	1:C:378:GLU:N	2.09	0.67
1:E:175:GLU:HG3	1:E:221:ILE:HD11	1.75	0.67
1:J:24:GLN:NE2	1:J:91:ARG:HH11	1.92	0.67
1:J:161:PRO:O	1:J:164:LEU:HD13	1.94	0.67
1:A:265:LEU:O	1:A:326:ARG:NH1	2.28	0.67
1:D:131:PRO:HB3	1:D:211:ILE:HD11	1.76	0.67
1:J:252:LYS:CE	5:J:749:HOH:O	2.39	0.67
1:L:423:ILE:HD12	1:L:423:ILE:O	1.94	0.67
1:F:115:ILE:HG22	1:F:351:LEU:HD13	1.75	0.67
1:G:152:ASP:HB3	1:G:164:LEU:HB2	1.76	0.67
1:B:139:LYS:O	1:B:147:THR:HB	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:HIS:HD2	1:F:402:ASN:HD21	1.42	0.67
1:I:269:GLU:CD	1:I:269:GLU:H	2.03	0.67
1:F:429:ARG:HD2	5:F:799:HOH:O	1.94	0.67
1:A:427:MET:HE1	5:G:869:HOH:O	1.93	0.66
1:B:315:ASN:O	1:B:318:PRO:HD2	1.95	0.66
1:A:16:GLU:HG2	1:A:79:ILE:HD13	1.76	0.66
1:L:163:ASP:OD2	1:L:169:ARG:NH2	2.28	0.66
1:G:399:PHE:CZ	1:G:409:LEU:HD22	2.30	0.66
1:C:131:PRO:HB3	1:C:211:ILE:HD11	1.77	0.66
1:E:3:LYS:HB3	1:E:75:ASN:ND2	2.11	0.66
1:J:274:PHE:CE2	1:J:278:ILE:HD11	2.30	0.66
1:B:187:HIS:HD2	1:B:188:HIS:O	1.78	0.66
1:D:27:ASP:OD1	1:D:31:THR:HG23	1.95	0.66
1:F:285:PHE:HB2	1:F:349:VAL:HG11	1.78	0.66
1:F:359:LYS:CE	5:F:737:HOH:O	2.43	0.66
1:H:360:ASN:HB2	1:H:362:LEU:CD1	2.25	0.66
1:H:376:SER:OG	1:H:379:GLU:HB2	1.96	0.66
1:A:187:HIS:HD2	1:A:188:HIS:O	1.78	0.66
1:B:161:PRO:HG2	1:C:219:LYS:HB3	1.77	0.66
1:H:91:ARG:C	1:H:91:ARG:HD2	2.21	0.66
1:G:6:ARG:HD2	1:G:46:LEU:HD13	1.78	0.65
1:J:62:ARG:NH1	5:J:790:HOH:O	2.29	0.65
1:G:68:MET:HE3	1:G:99:PRO:HD3	1.78	0.65
1:L:81:PRO:HG2	1:L:175:GLU:OE2	1.95	0.65
1:F:285:PHE:HB2	1:F:349:VAL:CG1	2.26	0.65
1:F:261:GLU:CD	1:F:261:GLU:H	2.04	0.65
1:H:52:PHE:CE1	1:H:70:LEU:HD13	2.32	0.65
1:F:100:ASP:OD1	1:F:102:THR:HG23	1.92	0.65
1:D:24:GLN:HE21	1:D:91:ARG:HD3	1.61	0.65
1:D:204:ALA:HB1	1:D:347:LEU:HD13	1.78	0.65
1:J:34:ASN:CG	1:K:159:LEU:CD2	2.70	0.65
1:A:172:ILE:HD12	1:A:218:VAL:HA	1.78	0.65
1:B:281:HIS:HD2	1:B:402:ASN:HD21	1.45	0.65
1:H:19:LYS:HD3	5:H:863:HOH:O	1.96	0.65
1:K:110:ASN:ND2	5:K:745:HOH:O	2.30	0.65
1:K:170:ARG:HB3	5:K:636:HOH:O	1.96	0.65
1:G:169:ARG:HG3	1:G:197:ILE:HD11	1.78	0.65
1:H:206:ARG:NH1	5:H:731:HOH:O	2.30	0.65
1:C:377:LYS:HG3	1:C:378:GLU:H	1.62	0.64
1:D:351:LEU:HD22	1:D:355:LEU:HG	1.80	0.64
1:D:189:GLU:OE2	2:D:501:P3S:HEC3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:LYS:HZ1	1:G:4:TYR:CE2	1.54	0.64
1:K:338:ASP:HB2	1:K:339:PRO:HD2	1.78	0.64
1:K:378:GLU:O	1:K:382:GLU:HG2	1.98	0.64
1:B:285:PHE:HB2	1:B:349:VAL:CG1	2.27	0.64
1:G:7:GLU:HA	1:G:7:GLU:OE1	1.97	0.64
1:G:20:TYR:HB2	1:G:89:VAL:HG22	1.80	0.64
1:J:407:LYS:CG	5:J:671:HOH:O	2.45	0.64
1:K:261:GLU:HG2	5:K:680:HOH:O	1.96	0.64
1:H:142:GLU:OE1	1:H:142:GLU:HA	1.97	0.64
1:H:150:LEU:HD22	1:H:193:GLY:HA3	1.79	0.64
1:J:351:LEU:HD22	1:J:355:LEU:HG	1.80	0.64
1:F:357:GLY:HA2	1:F:362:LEU:HD22	1.79	0.64
1:I:142:GLU:OE1	1:I:143:LYS:HG3	1.98	0.64
1:I:167:ASN:ND2	1:I:168:CYS:H	1.96	0.64
1:J:429:ARG:HD3	5:J:750:HOH:O	1.97	0.64
1:J:98:ASN:HD22	1:J:102:THR:HG22	1.63	0.64
1:B:290:ASN:HB3	1:B:295:SER:HB3	1.79	0.64
1:F:306:PRO:HB3	1:F:319:LEU:HA	1.80	0.64
1:J:189:GLU:OE2	2:J:501:P3S:HEC3	1.98	0.64
1:L:306:PRO:HB3	1:L:319:LEU:HA	1.78	0.64
1:D:357:GLY:HA2	1:D:362:LEU:HD22	1.79	0.64
1:G:68:MET:CE	1:G:98:ASN:HA	2.28	0.64
1:G:342:ASN:C	1:G:342:ASN:HD22	2.06	0.64
1:I:68:MET:CE	1:I:98:ASN:HA	2.28	0.64
1:I:167:ASN:HA	5:I:617:HOH:O	1.97	0.64
1:J:52:PHE:CE1	1:J:70:LEU:HD13	2.33	0.64
1:A:142:GLU:N	1:A:142:GLU:CD	2.56	0.63
1:E:359:LYS:HE2	5:E:626:HOH:O	1.98	0.63
1:J:32:ILE:HG23	1:K:159:LEU:HG	1.79	0.63
1:B:231:PHE:O	1:B:339:PRO:HG2	1.98	0.63
1:G:32:ILE:HG23	1:H:159:LEU:HD13	1.79	0.63
1:L:91:ARG:HD2	1:L:91:ARG:C	2.22	0.63
1:A:131:PRO:HB3	1:A:211:ILE:HD11	1.79	0.63
1:A:338:ASP:HB2	1:A:339:PRO:HD2	1.80	0.63
1:G:21:ILE:HD13	1:G:42:LEU:HD13	1.80	0.63
1:K:17:ASN:HA	5:K:703:HOH:O	1.98	0.63
1:A:281:HIS:HD2	1:A:402:ASN:HD21	1.47	0.63
1:F:148:LEU:HD21	1:L:437:ARG:HD3	1.79	0.63
1:E:285:PHE:HB2	1:E:349:VAL:HG11	1.80	0.63
1:F:189:GLU:OE2	2:F:601:P3S:HEC3	1.99	0.63
1:K:357:GLY:HA2	1:K:362:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ARG:HD2	1:D:34:ASN:OD1	1.99	0.63
1:D:136:PHE:CD1	1:D:235:PRO:HG2	2.33	0.63
1:G:368:ILE:HG21	1:G:372:ILE:HD12	1.81	0.63
1:L:419:GLU:O	1:L:423:ILE:HG23	1.99	0.63
1:A:134:GLU:OE1	2:A:501:P3S:N	2.32	0.62
1:E:351:LEU:HD22	1:E:355:LEU:HG	1.80	0.62
1:A:172:ILE:HD13	1:A:221:ILE:HB	1.81	0.62
1:A:316:ARG:NH1	2:A:501:P3S:O2A	2.31	0.62
1:H:351:LEU:HD22	1:H:355:LEU:HG	1.81	0.62
1:J:206:ARG:NH2	5:J:672:HOH:O	2.32	0.62
1:B:111:ASN:OD1	1:B:114:ARG:NH1	2.31	0.62
1:E:349:VAL:HG22	1:E:405:MET:SD	2.39	0.62
1:L:231:PHE:HB3	1:L:339:PRO:HB2	1.82	0.62
1:B:425:TRP:O	1:B:429:ARG:HG2	1.98	0.62
1:F:400:LYS:HE3	5:F:776:HOH:O	1.98	0.62
1:G:24:GLN:NE2	1:G:91:ARG:HH11	1.96	0.62
1:L:281:HIS:HE1	1:L:356:ASP:OD2	1.83	0.62
1:L:378:GLU:HG3	1:L:379:GLU:N	2.14	0.62
1:L:84:ALA:HA	1:L:88:LYS:HB3	1.81	0.62
1:L:96:ILE:N	1:L:96:ILE:HD12	2.14	0.62
1:J:115:ILE:HG22	1:J:351:LEU:HD13	1.82	0.62
1:L:377:LYS:HG3	5:L:726:HOH:O	1.99	0.62
1:A:419:GLU:O	1:A:423:ILE:HG12	2.00	0.62
1:C:65:GLU:O	1:C:65:GLU:HG3	1.99	0.62
1:D:24:GLN:NE2	1:D:91:ARG:HH11	1.98	0.62
1:D:178:GLU:HG3	5:D:798:HOH:O	2.00	0.62
2:D:501:P3S:CG	2:D:501:P3S:HEC3	2.29	0.62
1:H:318:PRO:HB3	1:H:372:ILE:HD11	1.80	0.62
1:H:360:ASN:HB2	1:H:362:LEU:HD11	1.82	0.62
1:G:187:HIS:HD2	1:G:188:HIS:O	1.83	0.62
1:J:273:HIS:HB3	1:J:358:ILE:HA	1.82	0.62
1:B:91:ARG:HD2	1:B:91:ARG:C	2.25	0.62
1:D:311:TRP:CZ2	1:D:367:PRO:HG3	2.35	0.62
1:E:110:ASN:ND2	5:E:640:HOH:O	2.31	0.62
1:I:65:GLU:HG3	1:I:65:GLU:O	2.00	0.62
1:K:26:THR:HG21	1:K:344:TYR:HE1	1.65	0.62
1:E:9:ILE:HG13	1:E:74:LEU:HD22	1.81	0.61
1:H:32:ILE:HG23	1:I:159:LEU:HG	1.82	0.61
1:K:86:LYS:HG3	5:K:714:HOH:O	2.00	0.61
1:B:273:HIS:CE1	1:B:361:LYS:HB3	2.36	0.61
1:J:290:ASN:HB3	1:J:295:SER:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:313:ALA:HB1	5:G:735:HOH:O	1.99	0.61
1:J:231:PHE:HB3	1:J:339:PRO:HB2	1.83	0.61
1:C:129:LEU:HD22	1:C:130:GLY:N	2.15	0.61
1:C:148:LEU:HD12	1:I:441:MET:HE1	1.81	0.61
1:D:394:GLU:HB2	5:D:660:HOH:O	2.00	0.61
1:G:115:ILE:HG22	1:G:351:LEU:HD13	1.82	0.61
1:J:24:GLN:HB3	1:J:34:ASN:HB3	1.83	0.61
1:A:357:GLY:HA2	1:A:362:LEU:HD22	1.83	0.61
1:B:143:LYS:HE2	1:B:145:GLU:HG3	1.81	0.61
1:E:211:ILE:HG22	1:E:215:LYS:HE2	1.83	0.61
1:E:311:TRP:CZ2	1:E:367:PRO:HG3	2.36	0.61
1:G:273:HIS:O	1:G:276:ALA:HB3	2.00	0.61
1:F:270:THR:HG23	1:F:358:ILE:HD12	1.82	0.61
1:H:285:PHE:HB2	1:H:349:VAL:CG1	2.31	0.61
1:I:357:GLY:O	1:I:362:LEU:HD12	1.99	0.61
1:D:256:ASN:HD21	1:D:258:PHE:HB2	1.66	0.61
1:L:317:SER:N	1:L:318:PRO:CD	2.64	0.61
1:I:167:ASN:HB3	5:I:617:HOH:O	2.00	0.60
1:D:111:ASN:OD1	1:D:114:ARG:NH1	2.34	0.60
1:H:375:MET:HE3	1:H:379:GLU:HG2	1.82	0.60
1:A:5:THR:O	1:A:6:ARG:C	2.45	0.60
1:D:105:GLU:CD	1:D:105:GLU:H	2.08	0.60
1:E:117:LYS:HD2	5:E:630:HOH:O	2.02	0.60
2:F:601:P3S:HEC3	2:F:601:P3S:HGC2	1.82	0.60
1:G:4:TYR:H	1:G:75:ASN:ND2	1.99	0.60
1:K:411:GLU:O	1:K:415:GLU:HG2	2.02	0.60
1:C:236:LEU:HD12	5:C:710:HOH:O	2.02	0.60
1:J:377:LYS:NZ	1:J:381:MET:HE3	2.16	0.60
1:L:426:ASP:HB2	5:L:671:HOH:O	2.02	0.60
1:D:208:CYS:SG	1:D:347:LEU:HD12	2.41	0.60
1:J:219:LYS:HB3	1:K:161:PRO:HG2	1.82	0.60
1:D:318:PRO:HB3	1:D:372:ILE:HD11	1.84	0.60
1:E:170:ARG:NH1	1:F:86:LYS:HD3	2.17	0.60
1:C:52:PHE:CE1	1:C:70:LEU:HD13	2.37	0.60
1:E:20:TYR:C	1:E:21:ILE:HD12	2.27	0.60
1:F:261:GLU:CD	1:F:261:GLU:N	2.60	0.60
1:H:335:ARG:HD3	5:H:766:HOH:O	2.02	0.60
1:I:142:GLU:H	1:I:142:GLU:CD	2.10	0.60
1:I:315:ASN:OD1	1:I:318:PRO:HD3	2.01	0.60
1:B:298:ARG:NH2	1:B:336:SER:O	2.35	0.59
1:G:247:ASN:HB3	1:G:331:ARG:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:205:VAL:HB	5:I:625:HOH:O	2.00	0.59
1:I:349:VAL:HG22	1:I:405:MET:SD	2.42	0.59
1:D:70:LEU:HD23	1:D:94:CYS:SG	2.42	0.59
1:F:342:ASN:C	1:F:342:ASN:HD22	2.10	0.59
1:K:317:SER:OG	1:K:372:ILE:HG12	2.01	0.59
1:C:357:GLY:HA2	1:C:362:LEU:HD12	1.82	0.59
1:F:175:GLU:HG3	1:F:221:ILE:HD11	1.84	0.59
1:G:211:ILE:HG22	1:G:215:LYS:HE2	1.85	0.59
1:C:170:ARG:HG2	5:C:713:HOH:O	2.02	0.59
1:D:27:ASP:OD2	1:D:27:ASP:C	2.44	0.59
1:G:122:LEU:HD11	1:G:359:LYS:HG3	1.84	0.59
1:L:204:ALA:HB1	1:L:347:LEU:HD13	1.84	0.59
1:A:189:GLU:OE2	2:A:501:P3S:HEC3	2.03	0.59
1:D:2:ALA:HB1	5:D:791:HOH:O	2.02	0.59
1:F:129:LEU:HG	1:F:347:LEU:HD11	1.83	0.59
1:H:223:ARG:HH11	1:H:223:ARG:CG	2.15	0.59
1:I:187:HIS:HD2	1:I:188:HIS:O	1.85	0.59
1:K:333:GLU:OE2	1:K:335:ARG:HD2	2.01	0.59
1:B:68:MET:HE1	1:B:98:ASN:OD1	2.03	0.59
1:D:2:ALA:O	1:D:3:LYS:C	2.45	0.59
1:E:170:ARG:CZ	1:F:86:LYS:HD3	2.33	0.59
1:H:317:SER:N	1:H:318:PRO:CD	2.66	0.59
1:F:117:LYS:HG3	5:F:818:HOH:O	2.02	0.59
1:I:53:ASP:OD2	1:I:55:SER:HB3	2.02	0.59
1:K:252:LYS:O	1:K:253:ASN:HB2	2.03	0.59
1:H:170:ARG:NH1	1:H:171:ASP:OD2	2.36	0.59
1:B:189:GLU:OE2	2:B:501:P3S:HEC3	2.03	0.58
1:C:131:PRO:CB	1:C:211:ILE:HD11	2.33	0.58
1:C:333:GLU:CD	5:C:602:HOH:O	2.46	0.58
1:L:402:ASN:ND2	1:L:405:MET:H	2.00	0.58
1:A:150:LEU:HD23	1:A:192:PRO:O	2.02	0.58
1:G:189:GLU:OE2	2:G:601:P3S:HEC3	2.03	0.58
1:B:306:PRO:HB3	1:B:319:LEU:HA	1.84	0.58
1:C:316:ARG:NH1	2:C:501:P3S:O3A	2.36	0.58
1:L:349:VAL:HG22	1:L:405:MET:SD	2.44	0.58
1:B:127:PHE:CD2	1:B:351:LEU:HG	2.38	0.58
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.86	0.58
1:D:317:SER:N	1:D:318:PRO:CD	2.66	0.58
1:F:169:ARG:HD3	1:F:186:SER:OG	2.03	0.58
1:H:316:ARG:HD3	2:H:601:P3S:OE	2.04	0.58
1:B:154:GLY:HA2	1:B:162:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ILE:HG22	1:E:64:GLU:OE2	2.03	0.58
1:I:261:GLU:HB2	1:I:266:GLN:HE21	1.69	0.58
1:L:169:ARG:HD3	1:L:195:HIS:HB3	1.84	0.58
1:A:112:LEU:HD12	1:A:205:VAL:HG22	1.85	0.58
1:E:96:ILE:N	1:E:96:ILE:HD12	2.18	0.58
1:H:127:PHE:CD2	1:H:351:LEU:HG	2.39	0.58
1:H:27:ASP:OD2	1:H:31:THR:HG23	2.04	0.58
1:H:281:HIS:NE2	1:H:404:VAL:HG11	2.19	0.58
1:A:316:ARG:HD2	2:A:501:P3S:OE	2.03	0.58
1:A:368:ILE:HG21	1:A:372:ILE:HD12	1.86	0.58
1:I:429:ARG:NH2	5:I:687:HOH:O	2.37	0.58
1:J:9:ILE:O	1:J:13:VAL:HG23	2.04	0.58
1:B:129:LEU:HG	1:B:347:LEU:HD11	1.86	0.57
1:D:23:LEU:HB3	1:D:70:LEU:CD2	2.35	0.57
1:F:152:ASP:HB3	1:F:164:LEU:HB2	1.86	0.57
1:A:290:ASN:HB3	1:A:295:SER:HB3	1.85	0.57
1:C:175:GLU:HG3	1:C:221:ILE:HD11	1.86	0.57
1:E:317:SER:N	1:E:318:PRO:CD	2.67	0.57
1:J:154:GLY:HA2	1:J:162:THR:HG22	1.85	0.57
1:J:279:VAL:HG11	1:J:365:PRO:HG2	1.86	0.57
1:A:52:PHE:CE1	1:A:70:LEU:CD1	2.88	0.57
1:B:25:PHE:CD2	1:B:70:LEU:HD11	2.39	0.57
1:F:5:THR:HG22	1:F:8:ASP:CG	2.28	0.57
1:J:34:ASN:ND2	1:K:159:LEU:HD22	2.19	0.57
1:J:134:GLU:OE2	2:J:501:P3S:N	2.38	0.57
1:L:402:ASN:O	1:L:406:VAL:HG23	2.04	0.57
1:I:261:GLU:HA	1:I:266:GLN:HG2	1.87	0.57
1:J:161:PRO:O	1:J:164:LEU:CD1	2.53	0.57
1:K:131:PRO:CB	1:K:211:ILE:HD11	2.34	0.57
1:F:370:ARG:HD3	1:F:375:MET:HE3	1.86	0.57
1:K:122:LEU:O	1:K:122:LEU:HD23	2.05	0.57
1:B:285:PHE:HB2	1:B:349:VAL:HG11	1.85	0.57
1:B:115:ILE:HD12	1:B:348:SER:HB3	1.86	0.57
1:C:338:ASP:HB2	1:C:339:PRO:HD2	1.86	0.57
1:C:418:ILE:O	1:C:422:GLU:HG3	2.05	0.57
1:D:91:ARG:HD2	1:D:91:ARG:C	2.30	0.57
1:D:170:ARG:NH1	1:D:171:ASP:OD2	2.38	0.57
1:G:368:ILE:HD11	1:G:385:ILE:HD11	1.85	0.57
1:I:68:MET:HE3	1:I:98:ASN:HA	1.86	0.57
1:A:139:LYS:HD2	1:A:149:GLU:HG2	1.86	0.57
1:D:159:LEU:HD22	1:E:32:ILE:CG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:ILE:O	1:F:81:PRO:HD3	2.05	0.57
1:F:253:ASN:ND2	5:F:766:HOH:O	2.38	0.57
1:G:86:LYS:HG2	1:H:170:ARG:CZ	2.35	0.57
1:I:99:PRO:HG2	1:J:314:GLN:NE2	2.19	0.57
1:K:187:HIS:HD2	1:K:188:HIS:O	1.87	0.57
1:B:386:VAL:HG12	5:B:618:HOH:O	2.05	0.56
1:D:117:LYS:NZ	5:D:689:HOH:O	2.38	0.56
1:H:7:GLU:HG3	5:H:860:HOH:O	2.05	0.56
1:C:122:LEU:HD11	1:C:359:LYS:HB3	1.87	0.56
1:E:285:PHE:HB2	1:E:349:VAL:CG1	2.34	0.56
1:H:329:SER:O	1:H:331:ARG:HD3	2.05	0.56
1:L:415:GLU:HB2	5:L:669:HOH:O	2.04	0.56
1:C:16:GLU:HG2	1:C:79:ILE:CD1	2.35	0.56
1:D:160:ALA:HB2	1:D:166:GLU:OE2	2.06	0.56
1:E:368:ILE:CG2	1:E:375:MET:HE1	2.36	0.56
1:F:349:VAL:HG22	1:F:405:MET:SD	2.45	0.56
1:G:281:HIS:HD2	1:G:402:ASN:HD21	1.53	0.56
1:H:173:VAL:O	1:H:177:GLU:HG3	2.05	0.56
1:J:5:THR:HG22	1:J:8:ASP:OD1	2.05	0.56
1:J:34:ASN:CG	1:K:159:LEU:HD21	2.31	0.56
1:K:24:GLN:NE2	1:K:91:ARG:HH11	2.03	0.56
1:L:252:LYS:O	1:L:253:ASN:HB2	2.05	0.56
1:E:170:ARG:HG2	5:E:753:HOH:O	2.04	0.56
1:L:360:ASN:HB2	1:L:362:LEU:HD13	1.88	0.56
1:C:317:SER:N	1:C:318:PRO:CD	2.68	0.56
1:F:202:ALA:HB1	1:F:206:ARG:NE	2.21	0.56
1:D:419:GLU:O	1:D:423:ILE:HD13	2.06	0.56
1:F:211:ILE:HG22	1:F:215:LYS:HE2	1.87	0.56
1:K:403:GLU:OE1	1:K:403:GLU:HA	2.04	0.56
1:L:125:SER:HB3	1:L:126:ASP:OD1	2.05	0.56
1:D:264:ASP:OD2	1:D:265:LEU:N	2.39	0.56
1:D:269:GLU:HG2	5:D:703:HOH:O	2.06	0.56
1:J:52:PHE:CD1	1:J:70:LEU:HD13	2.41	0.56
1:B:117:LYS:HE2	5:B:681:HOH:O	2.05	0.56
1:H:368:ILE:CD1	1:H:385:ILE:HD11	2.36	0.56
1:I:37:ILE:HD12	1:I:41:GLN:HB2	1.88	0.56
1:L:317:SER:H	1:L:318:PRO:CD	2.18	0.56
1:G:2:ALA:HA	5:G:796:HOH:O	2.06	0.56
2:G:601:P3S:CE	2:G:601:P3S:HGC1	2.31	0.56
1:H:426:ASP:HB2	5:H:794:HOH:O	2.04	0.56
1:K:211:ILE:CG1	5:K:635:HOH:O	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ASN:HB3	1:C:71:TYR:CD1	2.41	0.56
1:J:126:ASP:HB3	5:J:718:HOH:O	2.06	0.56
1:F:265:LEU:O	1:F:326:ARG:NH1	2.39	0.55
1:G:306:PRO:HB3	1:G:319:LEU:HA	1.88	0.55
1:G:338:ASP:HB2	1:G:339:PRO:HD2	1.88	0.55
1:B:122:LEU:HD11	1:B:359:LYS:HG3	1.88	0.55
1:E:306:PRO:HB3	1:E:319:LEU:HA	1.87	0.55
1:I:167:ASN:CA	5:I:617:HOH:O	2.53	0.55
1:J:45:ALA:HA	5:J:663:HOH:O	2.04	0.55
1:B:317:SER:N	1:B:318:PRO:CD	2.69	0.55
1:L:9:ILE:HG13	1:L:74:LEU:HD12	1.87	0.55
1:A:115:ILE:HG22	1:A:351:LEU:HD23	1.87	0.55
1:B:319:LEU:HD13	1:B:320:ILE:HG13	1.88	0.55
1:D:161:PRO:O	1:D:164:LEU:HD13	2.06	0.55
1:I:112:LEU:HD12	1:I:205:VAL:HG22	1.88	0.55
1:G:3:LYS:HE2	1:G:4:TYR:CE2	2.40	0.55
1:G:159:LEU:HD13	1:L:32:ILE:HG23	1.88	0.55
1:I:265:LEU:O	1:I:326:ARG:NH1	2.40	0.55
1:E:134:GLU:OE1	2:E:501:P3S:N	2.40	0.55
1:E:311:TRP:CH2	1:E:367:PRO:HG3	2.41	0.55
1:G:105:GLU:HG2	1:G:105:GLU:O	2.05	0.55
1:B:113:LYS:HG2	5:B:750:HOH:O	2.05	0.55
1:B:159:LEU:HD11	1:C:34:ASN:CG	2.32	0.55
1:L:316:ARG:HD3	2:L:501:P3S:OE	2.07	0.55
1:C:112:LEU:HD12	1:C:205:VAL:HG22	1.89	0.55
1:F:360:ASN:O	1:F:361:LYS:C	2.48	0.55
1:J:429:ARG:CD	5:J:750:HOH:O	2.51	0.55
1:A:32:ILE:HD13	1:A:33:LYS:N	2.22	0.54
1:A:336:SER:O	1:A:337:VAL:C	2.46	0.54
1:E:272:LYS:NZ	1:E:311:TRP:CH2	2.76	0.54
1:H:8:ASP:C	1:H:11:LYS:HG2	2.33	0.54
1:A:261:GLU:CD	1:A:261:GLU:H	2.14	0.54
1:G:7:GLU:OE1	1:G:7:GLU:CA	2.54	0.54
1:D:441:MET:O	1:J:228:HIS:HE1	1.89	0.54
1:E:3:LYS:HB3	1:E:75:ASN:HD21	1.71	0.54
1:G:3:LYS:CE	1:G:4:TYR:CD2	2.90	0.54
1:L:443:GLN:NE2	5:L:734:HOH:O	2.39	0.54
1:C:231:PHE:HB3	1:C:339:PRO:HB2	1.90	0.54
1:D:311:TRP:CH2	1:D:367:PRO:HG3	2.42	0.54
1:E:319:LEU:HD13	1:E:320:ILE:HG13	1.88	0.54
1:G:58:GLU:HB2	5:G:705:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:GLY:HA2	1:G:162:THR:HG22	1.88	0.54
1:H:231:PHE:HB3	1:H:339:PRO:HB2	1.88	0.54
1:J:377:LYS:HZ3	1:J:381:MET:HE3	1.70	0.54
1:A:32:ILE:HG23	1:F:159:LEU:HD13	1.88	0.54
1:C:2:ALA:HB3	5:C:783:HOH:O	2.07	0.54
1:C:129:LEU:HG	1:C:347:LEU:HD11	1.88	0.54
1:E:169:ARG:HE	1:E:195:HIS:HD2	1.54	0.54
1:F:16:GLU:HG2	1:F:79:ILE:HD13	1.90	0.54
1:G:321:ARG:NH2	1:L:67:ASP:OD2	2.41	0.54
1:H:24:GLN:HE21	1:H:91:ARG:HD3	1.70	0.54
1:H:68:MET:HE1	1:H:98:ASN:OD1	2.08	0.54
1:K:175:GLU:HG3	1:K:221:ILE:HD11	1.89	0.54
1:G:9:ILE:HD13	1:G:74:LEU:HG	1.90	0.54
1:G:281:HIS:NE2	1:G:404:VAL:HG11	2.22	0.54
1:J:24:GLN:NE2	1:J:91:ARG:HD3	2.20	0.54
1:L:370:ARG:HD2	1:L:375:MET:SD	2.46	0.54
1:A:372:ILE:HG23	1:A:375:MET:HE3	1.89	0.54
1:A:435:TRP:CD1	1:G:431:GLN:HG2	2.42	0.54
1:G:6:ARG:N	5:G:850:HOH:O	2.41	0.54
1:H:163:ASP:CG	1:H:169:ARG:HH22	2.15	0.54
1:J:407:LYS:HD3	5:J:678:HOH:O	2.07	0.54
1:C:306:PRO:HB3	1:C:319:LEU:HA	1.90	0.54
1:E:24:GLN:NE2	1:E:91:ARG:HD3	2.23	0.54
1:E:236:LEU:HD12	5:E:708:HOH:O	2.07	0.54
1:L:85:GLU:O	1:L:85:GLU:HG2	2.07	0.54
1:C:62:ARG:HH11	1:C:62:ARG:HG2	1.73	0.54
1:C:256:ASN:OD1	1:C:258:PHE:HB2	2.08	0.54
1:F:140:LEU:HD21	1:F:228:HIS:HB2	1.89	0.54
1:L:76:THR:HG21	1:L:93:ILE:HB	1.88	0.54
1:C:9:ILE:O	1:C:13:VAL:HG13	2.09	0.54
1:D:393:ALA:HB2	1:D:425:TRP:CE2	2.43	0.54
1:E:127:PHE:CD2	1:E:351:LEU:HG	2.43	0.54
1:E:386:VAL:HG22	5:E:604:HOH:O	2.07	0.54
1:G:86:LYS:HD3	5:H:716:HOH:O	2.07	0.54
1:J:152:ASP:HB3	1:J:164:LEU:HB2	1.90	0.54
1:A:247:ASN:OD1	1:A:331:ARG:HD2	2.07	0.53
1:E:187:HIS:HD2	1:E:188:HIS:O	1.90	0.53
1:L:3:LYS:HB3	1:L:75:ASN:OD1	2.08	0.53
1:L:74:LEU:N	1:L:74:LEU:HD22	2.22	0.53
1:D:282:ALA:HA	1:D:285:PHE:CZ	2.44	0.53
1:E:164:LEU:HA	5:E:764:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:ASN:OD1	1:F:318:PRO:HD3	2.07	0.53
1:G:141:ASP:OD2	1:G:141:ASP:C	2.51	0.53
1:I:34:ASN:CG	1:J:159:LEU:HD11	2.34	0.53
1:I:65:GLU:O	1:I:65:GLU:CG	2.57	0.53
1:I:167:ASN:CB	5:I:617:HOH:O	2.55	0.53
1:K:170:ARG:CB	5:K:636:HOH:O	2.55	0.53
1:L:78:VAL:HG12	1:L:91:ARG:HG3	1.90	0.53
1:L:208:CYS:SG	1:L:347:LEU:HD12	2.48	0.53
1:F:131:PRO:O	5:F:731:HOH:O	2.19	0.53
1:H:191:ALA:H	1:H:194:GLN:HE21	1.55	0.53
1:H:369:ASP:O	1:H:370:ARG:HG3	2.07	0.53
1:F:148:LEU:HD21	1:L:437:ARG:CD	2.38	0.53
1:A:16:GLU:HG2	1:A:79:ILE:CD1	2.38	0.53
1:B:5:THR:HG23	1:B:8:ASP:OD2	2.09	0.53
1:C:403:GLU:HG3	5:C:674:HOH:O	2.08	0.53
1:I:219:LYS:HB3	1:J:161:PRO:HG2	1.90	0.53
1:I:311:TRP:CZ2	1:I:367:PRO:HD3	2.44	0.53
1:B:147:THR:HG22	1:B:149:GLU:N	2.08	0.53
1:G:78:VAL:HG12	1:G:91:ARG:HG3	1.91	0.53
1:E:268:SER:O	1:E:272:LYS:HG2	2.09	0.53
1:G:378:GLU:HA	1:G:378:GLU:OE1	2.09	0.53
1:I:282:ALA:HA	1:I:285:PHE:CZ	2.44	0.53
1:J:306:PRO:HB3	1:J:319:LEU:HA	1.91	0.53
1:A:6:ARG:NH2	1:A:47:ASP:OD1	2.41	0.53
1:D:159:LEU:HD22	1:E:32:ILE:HG21	1.90	0.53
1:F:202:ALA:HB1	1:F:206:ARG:CZ	2.39	0.53
1:F:249:SER:HA	1:F:258:PHE:CE1	2.44	0.53
1:H:24:GLN:NE2	1:H:91:ARG:HH11	2.06	0.53
1:H:256:ASN:OD1	1:H:258:PHE:HB2	2.09	0.53
1:L:129:LEU:HG	1:L:347:LEU:HD21	1.89	0.53
1:B:427:MET:O	1:B:431:GLN:HG2	2.09	0.53
1:C:252:LYS:O	1:C:253:ASN:HB2	2.09	0.53
1:E:76:THR:O	1:E:78:VAL:HG23	2.09	0.53
1:G:22:ARG:HG3	1:G:89:VAL:CG1	2.38	0.53
1:D:281:HIS:HD2	1:D:402:ASN:HD21	1.58	0.52
1:E:22:ARG:HD2	1:E:34:ASN:ND2	2.25	0.52
1:E:372:ILE:O	1:E:375:MET:HB3	2.09	0.52
1:K:65:GLU:CD	5:K:653:HOH:O	2.52	0.52
1:B:76:THR:O	1:B:78:VAL:HG23	2.09	0.52
1:D:131:PRO:CB	1:D:211:ILE:HD11	2.39	0.52
1:E:252:LYS:O	1:E:253:ASN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:PRO:HG2	5:G:726:HOH:O	2.09	0.52
1:I:231:PHE:HB3	1:I:339:PRO:HB2	1.91	0.52
5:D:668:HOH:O	1:E:51:MET:HE3	2.09	0.52
1:G:2:ALA:CA	5:G:796:HOH:O	2.58	0.52
1:G:183:ILE:HB	1:L:38:PRO:HG2	1.90	0.52
1:I:30:GLY:HA3	5:I:691:HOH:O	2.09	0.52
1:E:216:LEU:C	1:E:216:LEU:CD2	2.83	0.52
1:G:312:SER:HB2	1:G:368:ILE:O	2.09	0.52
1:K:154:GLY:HA2	1:K:162:THR:HG22	1.91	0.52
1:A:298:ARG:NH2	1:A:336:SER:O	2.42	0.52
1:B:317:SER:H	1:B:318:PRO:CD	2.23	0.52
1:C:260:ASP:OD1	1:C:263:ALA:HB2	2.10	0.52
1:E:317:SER:N	1:E:318:PRO:HD2	2.24	0.52
1:F:52:PHE:CE1	1:F:70:LEU:HD13	2.44	0.52
1:F:308:TYR:HB2	1:F:372:ILE:HD13	1.90	0.52
1:H:129:LEU:HG	1:H:347:LEU:HD11	1.90	0.52
1:B:104:PHE:HA	5:B:668:HOH:O	2.08	0.52
1:D:383:ASN:HB2	1:D:385:ILE:HG12	1.91	0.52
1:F:376:SER:OG	1:F:379:GLU:HB2	2.09	0.52
1:H:311:TRP:CZ2	1:H:367:PRO:HD3	2.44	0.52
1:J:298:ARG:NH2	1:J:336:SER:O	2.42	0.52
1:B:371:ASN:C	1:B:371:ASN:HD22	2.18	0.52
1:C:232:MET:HE3	1:C:235:PRO:HB3	1.91	0.52
1:C:304:GLU:OE1	2:C:501:P3S:HEC1	2.09	0.52
1:D:112:LEU:HD12	1:D:205:VAL:HG22	1.91	0.52
1:I:160:ALA:HB2	1:I:166:GLU:CD	2.35	0.52
1:C:48:ASN:HB3	1:C:71:TYR:CE1	2.45	0.52
1:H:9:ILE:HG12	1:H:92:PHE:HZ	1.74	0.52
1:J:187:HIS:HD2	1:J:188:HIS:O	1.92	0.52
1:L:53:ASP:OD2	1:L:55:SER:HB3	2.10	0.52
1:L:360:ASN:O	1:L:361:LYS:C	2.51	0.52
1:A:76:THR:O	1:A:91:ARG:NH1	2.43	0.52
2:H:601:P3S:CG	2:H:601:P3S:HEC3	2.37	0.52
1:K:91:ARG:HD2	1:K:91:ARG:C	2.35	0.52
1:B:13:VAL:HG13	1:B:18:VAL:HB	1.92	0.52
1:J:142:GLU:OE1	1:J:143:LYS:HD2	2.10	0.52
1:J:413:LEU:HD23	5:J:735:HOH:O	2.10	0.52
1:A:427:MET:CE	5:G:823:HOH:O	2.58	0.51
1:D:281:HIS:CG	1:D:405:MET:HE3	2.44	0.51
1:E:52:PHE:CE1	1:E:70:LEU:HD13	2.45	0.51
1:E:321:ARG:NH2	1:F:67:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:280:LYS:HE2	1:L:281:HIS:CE1	2.45	0.51
1:A:304:GLU:OE1	1:A:316:ARG:HG2	2.10	0.51
1:B:252:LYS:O	1:B:253:ASN:HB2	2.08	0.51
1:B:370:ARG:HA	1:C:64:GLU:HG2	1.92	0.51
1:G:73:ASP:OD1	1:G:73:ASP:C	2.54	0.51
1:G:370:ARG:HA	1:L:64:GLU:HG2	1.92	0.51
1:J:91:ARG:HD2	1:J:91:ARG:C	2.35	0.51
1:K:122:LEU:HD22	1:K:124:PHE:CE1	2.44	0.51
1:E:170:ARG:NH1	1:E:171:ASP:OD2	2.44	0.51
1:E:311:TRP:CB	1:E:320:ILE:HB	2.40	0.51
1:F:243:GLY:C	1:F:339:PRO:HD3	2.35	0.51
1:G:169:ARG:HG3	1:G:197:ILE:CD1	2.41	0.51
1:I:27:ASP:OD2	1:I:27:ASP:C	2.52	0.51
1:J:57:ILE:HD12	1:J:57:ILE:N	2.26	0.51
1:K:64:GLU:HG2	1:L:370:ARG:HA	1.91	0.51
1:L:100:ASP:OD1	1:L:102:THR:HG23	2.10	0.51
1:L:202:ALA:HB1	1:L:206:ARG:HG2	1.92	0.51
1:C:81:PRO:HB2	1:C:175:GLU:OE1	2.10	0.51
1:D:152:ASP:HB3	1:D:164:LEU:HB2	1.92	0.51
1:H:63:ILE:HD11	1:I:304:GLU:HG2	1.93	0.51
1:H:281:HIS:CG	1:H:405:MET:HE3	2.45	0.51
1:B:349:VAL:HG22	1:B:405:MET:SD	2.51	0.51
1:C:400:LYS:HE2	1:C:418:ILE:HD13	1.92	0.51
1:D:319:LEU:HD13	1:D:320:ILE:HG13	1.92	0.51
1:I:362:LEU:HD12	1:I:362:LEU:N	2.19	0.51
1:J:437:ARG:O	1:J:441:MET:HB3	2.10	0.51
1:B:191:ALA:H	1:B:194:GLN:HE21	1.58	0.51
1:I:347:LEU:N	1:I:347:LEU:HD22	2.24	0.51
1:J:223:ARG:HG2	5:J:638:HOH:O	2.10	0.51
1:K:216:LEU:HD13	1:L:159:LEU:HD23	1.92	0.51
1:L:317:SER:N	1:L:318:PRO:HD2	2.26	0.51
1:C:285:PHE:HB2	1:C:349:VAL:CG1	2.40	0.51
1:E:157:PHE:CE2	1:F:35:VAL:HB	2.46	0.51
1:H:34:ASN:ND2	1:I:159:LEU:HD22	2.25	0.51
1:H:220:THR:HG22	1:H:224:LYS:NZ	2.26	0.51
1:J:24:GLN:HE22	1:J:91:ARG:HH11	1.56	0.51
1:K:396:LEU:HD11	1:K:421:LYS:HB2	1.92	0.51
1:A:325:SER:HB3	5:B:766:HOH:O	2.09	0.51
1:D:51:MET:HG2	1:D:69:TYR:CE2	2.46	0.51
1:F:368:ILE:HG12	1:F:385:ILE:HD11	1.93	0.51
1:G:319:LEU:HD13	1:G:320:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:285:PHE:HB2	1:I:349:VAL:HG11	1.92	0.51
1:K:317:SER:N	1:K:318:PRO:CD	2.73	0.51
1:B:317:SER:N	1:B:318:PRO:HD2	2.26	0.51
1:B:431:GLN:NE2	5:B:685:HOH:O	2.43	0.51
1:E:115:ILE:HG22	1:E:351:LEU:HD13	1.93	0.51
1:F:16:GLU:O	1:F:16:GLU:HG3	2.09	0.51
1:I:338:ASP:HB2	1:I:339:PRO:HD2	1.92	0.51
1:J:316:ARG:HD2	2:J:501:P3S:OE	2.11	0.51
1:K:172:ILE:HD13	1:K:221:ILE:HB	1.91	0.51
1:K:426:ASP:HB2	5:K:652:HOH:O	2.11	0.51
1:A:24:GLN:HB3	1:A:32:ILE:HD11	1.93	0.51
1:A:377:LYS:HD3	1:A:380:ARG:HH22	1.76	0.51
1:D:86:LYS:NZ	5:D:674:HOH:O	2.43	0.51
1:H:402:ASN:OD1	1:H:404:VAL:HG12	2.11	0.51
1:K:52:PHE:CE1	1:K:70:LEU:HD13	2.45	0.51
1:K:285:PHE:CD1	1:K:285:PHE:C	2.89	0.51
1:A:152:ASP:HB3	1:A:164:LEU:HB2	1.94	0.50
1:D:48:ASN:HB3	1:D:71:TYR:CE1	2.46	0.50
1:E:368:ILE:HG21	1:E:375:MET:HE1	1.94	0.50
1:F:22:ARG:HG3	1:F:89:VAL:HG11	1.92	0.50
1:G:91:ARG:HD2	1:G:91:ARG:C	2.36	0.50
1:G:419:GLU:HA	5:G:793:HOH:O	2.11	0.50
1:L:125:SER:C	1:L:126:ASP:OD1	2.54	0.50
1:B:171:ASP:OD2	1:B:225:HIS:NE2	2.44	0.50
1:C:186:SER:HB2	1:C:197:ILE:HG12	1.92	0.50
1:D:256:ASN:ND2	1:D:258:PHE:HB2	2.26	0.50
1:E:272:LYS:HE3	1:E:272:LYS:HA	1.92	0.50
1:I:306:PRO:HB3	1:I:319:LEU:HA	1.93	0.50
1:L:74:LEU:CD2	1:L:74:LEU:H	2.24	0.50
1:L:91:ARG:HD2	1:L:92:PHE:N	2.26	0.50
1:B:5:THR:CG2	1:B:8:ASP:OD2	2.59	0.50
1:C:10:GLU:O	1:C:13:VAL:HG22	2.12	0.50
1:C:16:GLU:HG2	1:C:79:ILE:HD13	1.92	0.50
1:D:374:VAL:O	1:D:374:VAL:HG12	2.12	0.50
1:G:64:GLU:O	1:G:65:GLU:HG2	2.10	0.50
1:G:86:LYS:HG2	1:H:170:ARG:NH1	2.26	0.50
1:H:403:GLU:O	1:H:407:LYS:HG2	2.11	0.50
1:F:187:HIS:HD2	1:F:188:HIS:O	1.95	0.50
1:G:175:GLU:HG3	1:G:221:ILE:HD11	1.92	0.50
1:K:296:TYR:CD1	1:K:296:TYR:N	2.77	0.50
1:C:314:GLN:NE2	1:D:99:PRO:HG3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:GLN:HE22	1:E:91:ARG:HH11	1.59	0.50
1:E:437:ARG:O	1:E:441:MET:HB3	2.12	0.50
1:F:203:GLY:H	1:F:206:ARG:NH2	2.09	0.50
1:J:317:SER:H	1:J:318:PRO:HD2	1.77	0.50
1:L:5:THR:HG22	1:L:8:ASP:OD2	2.11	0.50
1:C:310:ALA:HA	5:C:695:HOH:O	2.10	0.50
1:E:272:LYS:NZ	1:E:311:TRP:CZ2	2.80	0.50
1:H:281:HIS:HD2	1:H:402:ASN:HD21	1.58	0.50
1:D:403:GLU:OE1	1:D:403:GLU:HA	2.12	0.50
1:G:234:LYS:HD3	1:G:298:ARG:HA	1.93	0.50
1:I:129:LEU:HD13	1:I:131:PRO:HG3	1.92	0.50
1:K:284:SER:CB	1:K:402:ASN:HD22	2.24	0.50
1:B:256:ASN:OD1	1:B:258:PHE:HB2	2.11	0.50
1:C:128:ASN:ND2	5:C:775:HOH:O	2.44	0.50
1:H:154:GLY:HA2	1:H:162:THR:HG22	1.93	0.50
1:L:127:PHE:CE2	1:L:351:LEU:HG	2.47	0.50
1:L:315:ASN:OD1	1:L:318:PRO:HD3	2.12	0.50
1:D:360:ASN:O	1:D:361:LYS:C	2.55	0.50
1:F:441:MET:O	1:L:228:HIS:HE1	1.94	0.50
1:G:215:LYS:O	1:G:219:LYS:HD3	2.12	0.50
1:G:282:ALA:HA	1:G:285:PHE:CZ	2.47	0.50
1:K:81:PRO:HG2	1:K:175:GLU:OE2	2.12	0.50
1:K:351:LEU:HD22	1:K:355:LEU:HG	1.94	0.50
1:K:402:ASN:O	1:K:406:VAL:HG23	2.12	0.50
1:L:310:ALA:HA	5:L:741:HOH:O	2.11	0.50
1:L:369:ASP:O	1:L:370:ARG:HB3	2.11	0.50
1:A:161:PRO:O	1:A:164:LEU:HD13	2.12	0.49
1:F:109:ARG:HG3	1:F:344:TYR:CE2	2.47	0.49
1:F:169:ARG:HD2	1:F:186:SER:OG	2.11	0.49
1:H:127:PHE:CE2	1:H:351:LEU:HG	2.46	0.49
1:B:274:PHE:CE1	1:B:354:GLY:HA3	2.47	0.49
1:I:96:ILE:N	1:I:96:ILE:CD1	2.75	0.49
1:I:281:HIS:O	1:I:284:SER:HB2	2.11	0.49
1:I:290:ASN:HB3	1:I:295:SER:HB3	1.93	0.49
1:I:317:SER:N	1:I:318:PRO:CD	2.76	0.49
1:C:228:HIS:HE1	1:I:441:MET:O	1.95	0.49
1:H:35:VAL:HB	1:I:157:PHE:CE2	2.47	0.49
1:H:223:ARG:CG	1:H:223:ARG:NH1	2.74	0.49
1:I:133:PRO:HB3	1:I:244:MET:HG3	1.94	0.49
1:J:260:ASP:C	1:J:260:ASP:OD1	2.55	0.49
1:A:372:ILE:HA	1:A:375:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:PHE:HB2	1:B:349:VAL:HG13	1.94	0.49
1:D:129:LEU:HG	1:D:347:LEU:HD21	1.94	0.49
1:H:175:GLU:HG3	1:H:221:ILE:HD11	1.94	0.49
1:A:68:MET:HE1	1:A:98:ASN:OD1	2.12	0.49
1:B:264:ASP:OD2	1:B:272:LYS:HE3	2.12	0.49
1:C:314:GLN:HE22	1:D:99:PRO:HG3	1.76	0.49
1:F:343:PRO:O	1:F:347:LEU:HD23	2.12	0.49
1:G:357:GLY:HA2	1:G:362:LEU:HD12	1.94	0.49
1:H:122:LEU:HD12	1:H:355:LEU:HD22	1.93	0.49
1:G:62:ARG:HD2	5:G:866:HOH:O	2.12	0.49
1:B:131:PRO:CB	1:B:211:ILE:HD11	2.42	0.49
1:B:247:ASN:HB3	1:B:331:ARG:HD2	1.93	0.49
1:D:319:LEU:HD23	1:D:336:SER:HB2	1.94	0.49
1:H:23:LEU:HD22	1:H:94:CYS:SG	2.53	0.49
1:D:371:ASN:C	1:D:371:ASN:HD22	2.19	0.49
1:F:202:ALA:HA	1:F:206:ARG:HH21	1.78	0.49
1:G:131:PRO:HB3	1:G:211:ILE:HD11	1.95	0.49
1:H:63:ILE:HG23	1:H:64:GLU:N	2.28	0.49
1:L:439:GLN:HE21	1:L:439:GLN:HA	1.77	0.49
1:D:380:ARG:O	1:D:383:ASN:O	2.30	0.49
1:E:20:TYR:O	1:E:21:ILE:HD12	2.13	0.49
5:F:849:HOH:O	1:L:297:LYS:HD2	2.12	0.49
1:G:351:LEU:HD22	1:G:355:LEU:CG	2.42	0.49
1:L:187:HIS:HD2	1:L:188:HIS:O	1.95	0.49
1:H:252:LYS:O	1:H:253:ASN:HB2	2.13	0.49
1:I:317:SER:N	1:I:318:PRO:HD2	2.27	0.49
1:A:314:GLN:NE2	5:A:705:HOH:O	2.46	0.48
5:A:727:HOH:O	1:B:86:LYS:HE3	2.12	0.48
1:D:326:ARG:NE	5:D:712:HOH:O	2.37	0.48
1:E:62:ARG:NH1	1:E:64:GLU:OE1	2.43	0.48
1:F:260:ASP:HB2	1:F:268:SER:HA	1.95	0.48
1:G:256:ASN:OD1	1:G:258:PHE:HB2	2.13	0.48
1:H:206:ARG:NH2	5:H:738:HOH:O	2.46	0.48
1:J:317:SER:N	1:J:318:PRO:HD2	2.27	0.48
1:K:133:PRO:HG2	1:K:214:PHE:CE2	2.48	0.48
1:B:431:GLN:HG3	1:H:435:TRP:CD1	2.48	0.48
1:C:414:PHE:CZ	1:C:418:ILE:HD12	2.48	0.48
1:E:231:PHE:HB3	1:E:339:PRO:HB2	1.94	0.48
1:I:360:ASN:O	1:I:361:LYS:C	2.57	0.48
1:B:81:PRO:HG2	1:B:175:GLU:OE2	2.14	0.48
1:D:335:ARG:NH1	2:D:501:P3S:O1A	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:LYS:NZ	5:E:637:HOH:O	2.44	0.48
1:G:386:VAL:HG22	5:G:714:HOH:O	2.12	0.48
1:K:67:ASP:CG	1:L:314:GLN:HB2	2.39	0.48
1:C:126:ASP:HB2	1:C:251:PHE:HB2	1.95	0.48
1:F:136:PHE:CD1	1:F:235:PRO:HG2	2.49	0.48
1:L:349:VAL:HB	5:L:628:HOH:O	2.12	0.48
1:B:372:ILE:O	1:B:375:MET:HB2	2.14	0.48
1:B:437:ARG:O	1:B:441:MET:HB3	2.13	0.48
1:C:285:PHE:HB2	1:C:349:VAL:HG11	1.95	0.48
1:D:161:PRO:HG2	1:E:219:LYS:HB3	1.96	0.48
1:H:34:ASN:CG	1:I:159:LEU:HD22	2.38	0.48
1:J:320:ILE:CG2	1:J:332:VAL:HG13	2.43	0.48
1:D:316:ARG:HH11	1:E:66:SER:HB2	1.78	0.48
1:F:282:ALA:HA	1:F:285:PHE:CE2	2.48	0.48
1:F:426:ASP:CG	5:F:855:HOH:O	2.56	0.48
1:H:215:LYS:HG2	1:H:231:PHE:CE2	2.48	0.48
1:I:32:ILE:O	1:I:33:LYS:HD2	2.13	0.48
1:I:402:ASN:OD1	1:I:404:VAL:HG13	2.14	0.48
1:J:34:ASN:CG	1:K:159:LEU:HD22	2.35	0.48
1:L:127:PHE:CD2	1:L:351:LEU:HG	2.49	0.48
1:D:414:PHE:CZ	1:D:418:ILE:HD12	2.49	0.48
2:D:501:P3S:HEC3	2:D:501:P3S:HGC2	1.94	0.48
5:D:724:HOH:O	1:J:219:LYS:HE2	2.12	0.48
1:E:63:ILE:O	1:E:66:SER:OG	2.32	0.48
1:E:360:ASN:O	1:E:361:LYS:C	2.57	0.48
1:I:9:ILE:HG13	1:I:74:LEU:CD1	2.42	0.48
1:J:34:ASN:ND2	1:K:159:LEU:CD2	2.76	0.48
1:K:103:PRO:HG2	5:K:667:HOH:O	2.14	0.48
1:K:189:GLU:OE2	2:K:501:P3S:HEC3	2.13	0.48
1:B:24:GLN:HB3	1:B:34:ASN:HB3	1.95	0.48
1:B:134:GLU:OE1	2:B:501:P3S:N	2.47	0.48
1:C:281:HIS:HD2	1:C:402:ASN:HD21	1.62	0.48
1:H:105:GLU:N	5:H:780:HOH:O	2.45	0.48
1:H:245:HIS:CD2	1:H:335:ARG:HB3	2.48	0.48
1:J:281:HIS:HE1	1:J:356:ASP:OD1	1.96	0.48
1:B:147:THR:CG2	1:B:148:LEU:N	2.77	0.48
1:C:78:VAL:HG12	1:C:91:ARG:CG	2.43	0.48
1:I:74:LEU:N	1:I:74:LEU:HD22	2.29	0.48
1:K:6:ARG:HG3	1:K:46:LEU:HD13	1.96	0.48
1:L:5:THR:HG21	1:L:7:GLU:OE2	2.14	0.48
1:A:297:LYS:HD3	1:A:297:LYS:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:PRO:O	1:C:164:LEU:HD13	2.14	0.48
1:D:52:PHE:CE1	1:D:70:LEU:HD12	2.49	0.48
1:D:265:LEU:O	1:D:326:ARG:NH1	2.46	0.48
1:G:115:ILE:HG22	1:G:351:LEU:CD1	2.43	0.48
1:I:399:PHE:HZ	1:I:409:LEU:HD22	1.78	0.48
1:L:146:PRO:HG3	1:L:228:HIS:CD2	2.49	0.48
1:A:252:LYS:O	1:A:253:ASN:HB2	2.13	0.47
1:A:429:ARG:HD2	5:A:647:HOH:O	2.13	0.47
1:E:127:PHE:CE2	1:E:351:LEU:HG	2.49	0.47
1:J:9:ILE:HG13	1:J:74:LEU:HD22	1.95	0.47
1:L:74:LEU:N	1:L:74:LEU:CD2	2.77	0.47
1:A:150:LEU:HD11	1:A:236:LEU:HD11	1.95	0.47
1:A:232:MET:HE2	1:G:441:MET:CB	2.45	0.47
1:C:360:ASN:O	1:C:361:LYS:C	2.57	0.47
1:C:431:GLN:HG2	1:I:435:TRP:CD1	2.49	0.47
1:F:436:GLU:OE2	1:L:297:LYS:HE3	2.14	0.47
1:I:247:ASN:HB3	1:I:331:ARG:HD2	1.95	0.47
1:K:316:ARG:HD3	2:K:501:P3S:OE	2.15	0.47
1:G:64:GLU:HG2	1:H:371:ASN:N	2.29	0.47
1:H:296:TYR:N	1:H:296:TYR:CD1	2.81	0.47
1:A:11:LYS:HE3	1:A:15:GLU:OE1	2.14	0.47
1:B:5:THR:CG2	1:B:8:ASP:CG	2.87	0.47
1:B:191:ALA:H	1:B:194:GLN:NE2	2.12	0.47
1:I:48:ASN:HB3	1:I:71:TYR:CE1	2.49	0.47
1:I:52:PHE:CE1	1:I:70:LEU:HD13	2.49	0.47
1:J:216:LEU:HD13	1:K:159:LEU:HD12	1.96	0.47
1:L:125:SER:CB	1:L:126:ASP:OD1	2.61	0.47
1:C:134:GLU:OE1	2:C:501:P3S:N	2.47	0.47
1:D:287:ALA:HB1	1:D:396:LEU:HD23	1.97	0.47
1:D:376:SER:O	1:D:379:GLU:HB2	2.14	0.47
1:E:311:TRP:HB3	1:E:320:ILE:HB	1.95	0.47
1:J:256:ASN:OD1	1:J:258:PHE:HB2	2.14	0.47
1:L:441:MET:O	1:L:441:MET:HG3	2.14	0.47
1:A:150:LEU:HD12	1:A:150:LEU:H	1.79	0.47
1:D:338:ASP:HB2	1:D:339:PRO:HD2	1.95	0.47
1:D:362:LEU:HA	5:D:756:HOH:O	2.14	0.47
1:E:272:LYS:HE3	1:E:272:LYS:CA	2.43	0.47
1:F:127:PHE:CZ	1:F:248:LEU:HD22	2.49	0.47
1:F:319:LEU:CD1	1:F:336:SER:HB2	2.45	0.47
1:H:34:ASN:OD1	1:I:159:LEU:HD13	2.14	0.47
1:H:376:SER:OG	1:H:379:GLU:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:407:LYS:NZ	5:J:787:HOH:O	2.42	0.47
1:K:429:ARG:NH2	5:K:664:HOH:O	2.47	0.47
1:A:4:TYR:H	1:A:75:ASN:ND2	2.13	0.47
1:A:283:THR:HG23	5:A:612:HOH:O	2.15	0.47
1:B:131:PRO:HB3	1:B:211:ILE:HD11	1.97	0.47
1:B:360:ASN:O	1:B:361:LYS:C	2.58	0.47
1:D:247:ASN:HB3	1:D:331:ARG:HD2	1.96	0.47
1:D:266:GLN:CB	1:D:326:ARG:HD2	2.32	0.47
1:H:312:SER:HB2	1:H:368:ILE:O	2.15	0.47
1:J:317:SER:H	1:J:318:PRO:CD	2.27	0.47
1:J:349:VAL:HG22	1:J:405:MET:SD	2.55	0.47
1:J:399:PHE:HZ	1:J:409:LEU:HD22	1.80	0.47
1:B:19:LYS:HB3	1:B:20:TYR:CE2	2.50	0.47
1:B:260:ASP:O	1:B:266:GLN:HA	2.14	0.47
1:E:24:GLN:NE2	1:E:91:ARG:HH11	2.13	0.47
1:F:91:ARG:HD2	1:F:92:PHE:N	2.30	0.47
1:F:359:LYS:HE2	5:F:737:HOH:O	2.11	0.47
1:G:67:ASP:OD2	1:H:321:ARG:NH2	2.48	0.47
1:G:68:MET:CE	1:G:99:PRO:HD3	2.44	0.47
1:G:317:SER:N	1:G:318:PRO:CD	2.78	0.47
1:H:318:PRO:HA	1:H:372:ILE:HD12	1.97	0.47
1:H:435:TRP:O	1:H:439:GLN:HG2	2.15	0.47
1:I:285:PHE:HB2	1:I:349:VAL:CG1	2.45	0.47
1:J:65:GLU:OE1	1:J:65:GLU:HA	2.14	0.47
1:J:312:SER:HB3	1:J:315:ASN:HB3	1.96	0.47
1:F:161:PRO:O	1:F:164:LEU:HD13	2.14	0.47
1:G:161:PRO:O	1:G:164:LEU:HD13	2.15	0.47
1:H:184:GLU:HB3	1:H:198:ASP:HB2	1.97	0.47
1:I:142:GLU:CD	1:I:142:GLU:N	2.73	0.47
1:J:317:SER:N	1:J:318:PRO:CD	2.78	0.47
1:A:270:THR:HG23	1:A:358:ILE:HD12	1.97	0.46
1:J:100:ASP:OD2	1:J:102:THR:HB	2.15	0.46
1:K:312:SER:HB3	1:K:315:ASN:HB3	1.97	0.46
1:L:107:ASP:OD1	1:L:107:ASP:C	2.56	0.46
1:A:376:SER:OG	1:A:379:GLU:HB2	2.15	0.46
1:F:435:TRP:CD1	1:L:431:GLN:HG2	2.49	0.46
1:H:234:LYS:HD3	1:H:298:ARG:HA	1.97	0.46
1:B:296:TYR:CD1	1:B:296:TYR:N	2.83	0.46
1:B:338:ASP:HB2	1:B:339:PRO:HD2	1.97	0.46
1:D:142:GLU:CD	1:D:142:GLU:N	2.64	0.46
1:F:371:ASN:O	1:F:374:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:ALA:HB1	1:G:347:LEU:CD2	2.46	0.46
1:H:172:ILE:HD13	1:H:218:VAL:HG22	1.96	0.46
1:I:275:ILE:O	1:I:279:VAL:HG23	2.15	0.46
1:K:65:GLU:OE2	5:K:653:HOH:O	2.20	0.46
1:K:125:SER:C	1:K:126:ASP:OD2	2.57	0.46
1:L:434:PRO:HD2	5:L:719:HOH:O	2.16	0.46
1:A:434:PRO:HG2	1:G:434:PRO:HG2	1.96	0.46
1:H:169:ARG:HD2	1:H:186:SER:OG	2.16	0.46
1:K:375:MET:CE	1:K:379:GLU:HG2	2.46	0.46
1:E:435:TRP:O	1:E:439:GLN:HG2	2.15	0.46
1:F:117:LYS:HE3	5:F:818:HOH:O	2.15	0.46
1:F:403:GLU:OE2	1:F:407:LYS:CE	2.61	0.46
1:G:186:SER:HB2	1:G:197:ILE:HD13	1.96	0.46
1:I:115:ILE:HG22	1:I:351:LEU:HD13	1.96	0.46
1:I:313:ALA:HB1	5:I:634:HOH:O	2.15	0.46
1:J:306:PRO:HG2	1:J:336:SER:N	2.30	0.46
1:J:361:LYS:HE2	5:J:677:HOH:O	2.16	0.46
1:A:159:LEU:HD13	1:B:32:ILE:HG23	1.98	0.46
1:A:172:ILE:CD1	1:A:221:ILE:HB	2.45	0.46
1:B:414:PHE:O	1:B:418:ILE:HG12	2.15	0.46
1:B:423:ILE:HG13	5:B:737:HOH:O	2.15	0.46
1:C:342:ASN:O	1:C:343:PRO:C	2.58	0.46
1:C:355:LEU:O	1:C:359:LYS:HG2	2.15	0.46
1:H:117:LYS:NZ	5:H:740:HOH:O	2.43	0.46
1:H:131:PRO:HB3	1:H:211:ILE:HD11	1.96	0.46
1:I:136:PHE:CD1	1:I:235:PRO:HG2	2.50	0.46
1:I:175:GLU:HG3	1:I:221:ILE:HD11	1.97	0.46
1:J:376:SER:O	1:J:377:LYS:C	2.59	0.46
1:L:296:TYR:CD1	1:L:296:TYR:N	2.83	0.46
1:L:306:PRO:HG2	1:L:336:SER:HA	1.98	0.46
1:A:168:CYS:O	1:A:172:ILE:HG12	2.16	0.46
1:E:140:LEU:HD21	1:E:228:HIS:HB2	1.96	0.46
1:H:8:ASP:O	1:H:11:LYS:CG	2.55	0.46
1:H:306:PRO:HG2	1:H:336:SER:CA	2.45	0.46
1:J:129:LEU:O	1:J:131:PRO:HD3	2.15	0.46
1:B:165:GLY:O	1:B:169:ARG:HB2	2.16	0.46
1:D:187:HIS:HD2	1:D:188:HIS:O	1.99	0.46
1:D:260:ASP:O	1:D:266:GLN:HA	2.15	0.46
1:D:291:PRO:HG3	1:D:341:ALA:HA	1.98	0.46
1:G:134:GLU:OE2	2:G:601:P3S:N	2.49	0.46
1:G:204:ALA:HB1	1:G:347:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:371:ASN:HD22	1:H:371:ASN:C	2.23	0.46
1:I:5:THR:O	1:I:6:ARG:C	2.59	0.46
1:J:264:ASP:OD1	1:J:264:ASP:O	2.34	0.46
1:D:347:LEU:HD23	1:D:347:LEU:HA	1.88	0.46
1:F:378:GLU:O	1:F:382:GLU:HG2	2.16	0.46
1:G:264:ASP:C	1:G:266:GLN:N	2.73	0.46
1:G:267:LEU:HG	1:G:326:ARG:HH12	1.81	0.46
1:H:191:ALA:H	1:H:194:GLN:NE2	2.13	0.46
1:K:16:GLU:HB2	1:K:18:VAL:HG23	1.97	0.46
1:K:107:ASP:C	1:K:107:ASP:OD1	2.58	0.46
1:A:133:PRO:HG2	1:A:214:PHE:CE2	2.51	0.46
1:E:58:GLU:HB2	5:E:609:HOH:O	2.16	0.46
1:E:225:HIS:HD2	5:E:663:HOH:O	1.99	0.46
1:G:48:ASN:OD1	1:G:71:TYR:HA	2.16	0.46
1:H:248:LEU:HD11	1:H:350:LEU:HD13	1.98	0.46
1:K:150:LEU:HD22	1:K:193:GLY:HA3	1.97	0.46
1:L:202:ALA:CB	1:L:206:ARG:HG2	2.45	0.46
1:A:64:GLU:OE2	1:F:371:ASN:HB2	2.16	0.45
1:A:427:MET:HE3	5:G:823:HOH:O	2.15	0.45
1:A:435:TRP:CH2	1:A:439:GLN:HG3	2.52	0.45
1:C:372:ILE:H	1:C:372:ILE:HG13	1.48	0.45
1:C:377:LYS:CG	1:C:378:GLU:N	2.76	0.45
1:E:136:PHE:HA	1:E:193:GLY:O	2.16	0.45
1:G:336:SER:O	1:G:337:VAL:C	2.58	0.45
1:H:198:ASP:HA	5:H:842:HOH:O	2.15	0.45
1:I:435:TRP:O	1:I:439:GLN:HG2	2.16	0.45
1:L:423:ILE:HG13	1:L:424:GLU:N	2.31	0.45
1:D:171:ASP:OD1	1:D:225:HIS:HE1	1.98	0.45
1:H:11:LYS:HG3	1:H:12:LEU:N	2.31	0.45
1:H:105:GLU:HG3	1:H:412:HIS:CB	2.47	0.45
1:I:13:VAL:HG13	1:I:18:VAL:HB	1.98	0.45
1:I:99:PRO:HG2	1:J:314:GLN:HE22	1.81	0.45
1:L:6:ARG:HD2	1:L:10:GLU:OE2	2.16	0.45
1:L:68:MET:HE1	1:L:98:ASN:OD1	2.15	0.45
1:L:409:LEU:HD23	1:L:409:LEU:HA	1.73	0.45
1:B:73:ASP:OD2	1:B:73:ASP:C	2.57	0.45
1:C:2:ALA:CB	5:C:783:HOH:O	2.65	0.45
1:E:273:HIS:CE1	1:E:361:LYS:HB3	2.51	0.45
1:G:132:GLU:O	1:G:244:MET:HA	2.16	0.45
1:G:368:ILE:CG2	1:G:372:ILE:HD12	2.45	0.45
1:G:402:ASN:OD1	1:G:402:ASN:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:THR:CG2	5:H:811:HOH:O	2.46	0.45
1:I:64:GLU:HG2	1:J:370:ARG:C	2.41	0.45
1:I:73:ASP:C	1:I:73:ASP:OD1	2.59	0.45
1:I:301:PRO:HD3	1:I:307:CYS:SG	2.57	0.45
1:A:249:SER:HA	1:A:258:PHE:CE1	2.51	0.45
1:A:270:THR:CG2	1:A:358:ILE:HD12	2.47	0.45
1:A:317:SER:N	1:A:318:PRO:CD	2.79	0.45
1:B:297:LYS:NZ	1:H:436:GLU:OE1	2.46	0.45
1:C:232:MET:HE2	1:I:441:MET:HA	1.99	0.45
5:C:751:HOH:O	1:I:427:MET:HE3	2.16	0.45
1:D:24:GLN:HE21	1:D:91:ARG:HH11	1.63	0.45
1:D:321:ARG:NH2	1:E:67:ASP:OD2	2.50	0.45
1:D:328:ILE:HG12	1:D:328:ILE:O	2.16	0.45
1:E:247:ASN:OD1	1:E:331:ARG:HD2	2.17	0.45
1:F:200:LYS:HG3	1:F:201:TYR:N	2.30	0.45
1:G:379:GLU:HA	1:G:382:GLU:HG2	1.98	0.45
1:H:24:GLN:HE22	1:H:91:ARG:HH11	1.64	0.45
1:J:315:ASN:OD1	1:J:318:PRO:HD3	2.16	0.45
1:A:6:ARG:HG3	1:A:46:LEU:HD13	1.98	0.45
1:A:13:VAL:HG13	1:A:18:VAL:HB	1.97	0.45
1:C:129:LEU:HD22	1:C:129:LEU:C	2.42	0.45
1:C:160:ALA:HA	1:C:163:ASP:O	2.17	0.45
1:I:244:MET:HE1	5:I:622:HOH:O	2.17	0.45
1:A:86:LYS:HG2	1:F:170:ARG:CZ	2.47	0.45
1:A:88:LYS:HE2	5:A:666:HOH:O	2.16	0.45
1:D:375:MET:HE2	1:D:379:GLU:HB3	1.99	0.45
1:K:183:ILE:HD12	1:K:183:ILE:N	2.31	0.45
1:K:328:ILE:HG12	1:K:328:ILE:O	2.15	0.45
1:L:281:HIS:CE1	1:L:356:ASP:OD2	2.67	0.45
1:A:159:LEU:HG	1:B:34:ASN:ND2	2.31	0.45
1:A:261:GLU:CD	1:A:261:GLU:N	2.74	0.45
1:A:360:ASN:O	1:A:361:LYS:C	2.60	0.45
1:C:148:LEU:CD1	1:I:441:MET:HE1	2.46	0.45
1:C:372:ILE:HA	1:C:375:MET:HG2	1.98	0.45
1:D:173:VAL:O	1:D:177:GLU:HG3	2.16	0.45
1:G:99:PRO:O	1:G:100:ASP:O	2.34	0.45
1:I:26:THR:HG22	1:I:27:ASP:O	2.16	0.45
1:A:317:SER:N	1:A:318:PRO:HD2	2.31	0.45
1:C:39:VAL:HG22	1:C:39:VAL:O	2.17	0.45
1:C:438:GLU:HG3	5:C:703:HOH:O	2.16	0.45
1:D:159:LEU:HD23	1:E:216:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:TRP:HA	1:D:438:GLU:OE2	2.16	0.45
1:E:86:LYS:NZ	5:E:627:HOH:O	2.50	0.45
1:L:329:SER:O	1:L:331:ARG:HD3	2.17	0.45
1:C:278:ILE:CG2	1:C:320:ILE:HD11	2.46	0.45
1:E:129:LEU:HG	1:E:347:LEU:HD21	1.99	0.45
1:I:134:GLU:OE1	2:I:501:P3S:N	2.50	0.45
1:I:398:GLU:HG2	5:I:755:HOH:O	2.16	0.45
1:K:389:PRO:HA	1:K:394:GLU:OE1	2.17	0.45
1:A:412:HIS:HA	5:A:634:HOH:O	2.16	0.45
1:E:6:ARG:HD3	1:E:46:LEU:HD13	1.98	0.45
1:E:291:PRO:HG3	1:E:341:ALA:HA	1.98	0.45
1:F:131:PRO:CG	1:F:211:ILE:HD11	2.47	0.45
1:F:260:ASP:CG	1:F:263:ALA:HB2	2.42	0.45
1:G:62:ARG:CG	5:G:866:HOH:O	2.64	0.45
1:H:134:GLU:OE1	2:H:601:P3S:N	2.50	0.45
1:J:5:THR:HG22	1:J:8:ASP:CG	2.42	0.45
1:J:208:CYS:SG	1:J:343:PRO:HB2	2.56	0.45
1:L:423:ILE:C	1:L:423:ILE:CD1	2.71	0.45
1:A:372:ILE:HA	1:A:375:MET:HE2	1.98	0.44
1:D:243:GLY:C	1:D:339:PRO:HD3	2.42	0.44
1:D:273:HIS:O	1:D:276:ALA:HB3	2.17	0.44
1:D:282:ALA:HA	1:D:285:PHE:CE2	2.52	0.44
1:E:47:ASP:O	1:E:49:LYS:HD2	2.18	0.44
1:E:264:ASP:O	1:E:265:LEU:HB2	2.17	0.44
1:G:306:PRO:HG2	1:G:336:SER:N	2.32	0.44
1:L:122:LEU:HD11	1:L:359:LYS:HD3	1.99	0.44
1:A:143:LYS:HE3	1:F:149:GLU:OE1	2.18	0.44
1:C:78:VAL:HG12	1:C:91:ARG:HG2	1.99	0.44
1:E:260:ASP:OD2	1:E:260:ASP:C	2.57	0.44
1:E:304:GLU:OE2	2:E:501:P3S:HEC1	2.18	0.44
1:E:375:MET:HG3	1:E:379:GLU:HB3	2.00	0.44
1:G:64:GLU:C	1:G:65:GLU:HG2	2.42	0.44
1:I:61:VAL:HB	1:I:65:GLU:OE1	2.17	0.44
1:I:122:LEU:HD21	1:I:359:LYS:HG3	1.98	0.44
1:J:321:ARG:O	1:J:323:PRO:HD3	2.17	0.44
1:K:282:ALA:HA	1:K:285:PHE:CZ	2.52	0.44
1:B:328:ILE:HG12	1:B:328:ILE:O	2.17	0.44
1:D:345:LEU:O	1:D:349:VAL:HG22	2.17	0.44
1:E:55:SER:HA	1:E:61:VAL:O	2.18	0.44
1:F:202:ALA:HB3	1:F:207:SER:HB2	1.99	0.44
1:F:283:THR:O	1:F:398:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:THR:O	1:H:6:ARG:C	2.59	0.44
1:H:131:PRO:CB	1:H:211:ILE:HD11	2.47	0.44
1:H:290:ASN:HB3	1:H:295:SER:HB3	1.99	0.44
1:J:399:PHE:CZ	1:J:409:LEU:HD22	2.52	0.44
1:A:63:ILE:HG22	1:A:64:GLU:OE2	2.17	0.44
1:C:388:LEU:HB3	1:C:389:PRO:HD2	1.99	0.44
1:F:317:SER:N	1:F:318:PRO:CD	2.81	0.44
1:H:52:PHE:CD1	1:H:70:LEU:HD13	2.53	0.44
1:L:100:ASP:OD1	1:L:100:ASP:C	2.60	0.44
1:C:152:ASP:HB3	1:C:164:LEU:HB2	1.99	0.44
1:C:243:GLY:C	1:C:339:PRO:HD3	2.43	0.44
1:E:315:ASN:O	1:E:321:ARG:HB2	2.18	0.44
1:J:117:LYS:HD2	5:J:675:HOH:O	2.17	0.44
1:K:291:PRO:HG3	1:K:341:ALA:HA	1.99	0.44
1:B:9:ILE:HG21	1:B:92:PHE:HZ	1.82	0.44
1:B:306:PRO:CB	1:B:319:LEU:HA	2.48	0.44
1:C:45:ALA:HA	1:C:50:VAL:HG23	1.98	0.44
1:C:170:ARG:HG3	5:D:648:HOH:O	2.17	0.44
1:C:247:ASN:HB3	1:C:331:ARG:HD2	1.99	0.44
1:C:317:SER:N	1:C:318:PRO:HD2	2.33	0.44
1:C:368:ILE:HD12	1:C:368:ILE:N	2.33	0.44
1:F:321:ARG:NH1	3:F:602:ADP:O1B	2.51	0.44
1:H:74:LEU:HD22	1:H:74:LEU:N	2.33	0.44
1:K:176:LEU:O	1:K:181:PHE:HB2	2.17	0.44
1:K:285:PHE:C	1:K:285:PHE:HD1	2.26	0.44
1:L:223:ARG:HG3	1:L:223:ARG:HH11	1.83	0.44
1:A:5:THR:C	1:A:7:GLU:N	2.76	0.44
1:A:427:MET:CE	5:G:869:HOH:O	2.59	0.44
1:A:441:MET:O	1:G:228:HIS:HE1	2.00	0.44
1:B:236:LEU:HD12	5:B:773:HOH:O	2.18	0.44
1:D:163:ASP:CG	1:D:169:ARG:HH22	2.25	0.44
1:D:307:CYS:HA	1:D:388:LEU:HD12	2.00	0.44
1:E:24:GLN:HE21	1:E:91:ARG:HD3	1.83	0.44
1:F:82:TRP:HE3	1:F:175:GLU:OE1	2.01	0.44
1:F:140:LEU:HD23	1:F:146:PRO:HA	2.00	0.44
1:H:8:ASP:CA	1:H:11:LYS:HE2	2.48	0.44
1:I:221:ILE:O	1:I:225:HIS:HD2	1.99	0.44
1:J:5:THR:HG23	1:J:8:ASP:H	1.83	0.44
1:K:360:ASN:O	1:K:361:LYS:C	2.59	0.44
1:D:127:PHE:CD2	1:D:351:LEU:HG	2.53	0.44
1:F:32:ILE:HD13	1:F:212:GLN:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:THR:HG23	1:F:358:ILE:CD1	2.47	0.44
1:G:296:TYR:CD1	1:G:296:TYR:N	2.86	0.44
1:I:282:ALA:HA	1:I:285:PHE:CE2	2.53	0.44
1:J:68:MET:CE	1:J:99:PRO:HD3	2.46	0.44
1:K:3:LYS:HB3	1:K:75:ASN:OD1	2.17	0.44
1:K:5:THR:O	1:K:6:ARG:C	2.61	0.44
1:L:181:PHE:CE2	1:L:210:ASP:HB3	2.53	0.44
1:A:150:LEU:HD12	1:A:150:LEU:N	2.33	0.44
1:A:153:LYS:HA	1:A:192:PRO:HB3	2.00	0.44
1:E:375:MET:HG2	1:E:380:ARG:HG3	1.99	0.44
1:F:171:ASP:HA	1:F:174:LEU:HD12	2.00	0.44
1:G:81:PRO:HG2	1:G:175:GLU:OE2	2.18	0.44
1:H:317:SER:H	1:H:318:PRO:CD	2.30	0.44
1:I:34:ASN:C	1:I:34:ASN:HD22	2.26	0.44
1:I:55:SER:HB3	1:I:66:SER:HB3	1.99	0.44
1:J:281:HIS:O	1:J:284:SER:HB2	2.17	0.44
1:K:68:MET:HE1	1:K:98:ASN:OD1	2.18	0.44
1:K:248:LEU:HD11	1:K:350:LEU:HD13	2.00	0.44
1:L:73:ASP:OD2	1:L:73:ASP:C	2.60	0.44
1:L:378:GLU:HG3	1:L:379:GLU:H	1.81	0.44
1:A:19:LYS:C	1:A:39:VAL:HG13	2.43	0.43
1:A:273:HIS:HB2	1:A:358:ILE:HD13	1.99	0.43
1:D:134:GLU:OE1	2:D:501:P3S:N	2.50	0.43
1:D:143:LYS:O	1:D:145:GLU:HG2	2.17	0.43
1:D:161:PRO:O	1:D:164:LEU:CD1	2.66	0.43
1:D:351:LEU:O	1:D:355:LEU:HG	2.17	0.43
1:E:126:ASP:HB2	1:E:251:PHE:HB2	1.99	0.43
1:F:76:THR:O	1:F:78:VAL:HG23	2.17	0.43
1:F:290:ASN:HB3	1:F:295:SER:HB3	2.00	0.43
1:G:306:PRO:HG3	1:G:335:ARG:HB2	2.00	0.43
1:I:9:ILE:CG1	1:I:74:LEU:HD12	2.44	0.43
1:I:24:GLN:NE2	1:I:91:ARG:HD3	2.32	0.43
1:J:279:VAL:HG13	1:J:309:VAL:HG12	2.00	0.43
1:J:307:CYS:HB3	1:J:308:TYR:CD1	2.53	0.43
1:K:287:ALA:HB1	1:K:396:LEU:HD23	2.00	0.43
1:L:68:MET:HE3	1:L:98:ASN:HA	2.00	0.43
1:A:147:THR:HB	5:A:641:HOH:O	2.18	0.43
1:A:317:SER:H	1:A:318:PRO:CD	2.31	0.43
1:D:52:PHE:CD1	1:D:70:LEU:HD12	2.53	0.43
1:D:256:ASN:HD22	1:D:256:ASN:C	2.25	0.43
1:E:169:ARG:HE	1:E:195:HIS:CD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:LEU:HD12	1:F:355:LEU:HD22	1.99	0.43
1:F:275:ILE:HD11	1:F:332:VAL:HG22	2.00	0.43
1:G:9:ILE:HG21	1:G:92:PHE:HZ	1.83	0.43
1:H:26:THR:HG22	1:H:27:ASP:O	2.18	0.43
1:I:269:GLU:CD	1:I:269:GLU:N	2.75	0.43
1:I:441:MET:O	1:I:441:MET:HG3	2.18	0.43
1:B:402:ASN:OD1	1:B:402:ASN:C	2.60	0.43
1:F:256:ASN:OD1	1:F:258:PHE:HB2	2.19	0.43
1:F:260:ASP:HB3	1:F:263:ALA:HB3	2.00	0.43
1:F:315:ASN:O	1:F:318:PRO:HD2	2.17	0.43
1:G:273:HIS:HB3	1:G:358:ILE:HA	2.00	0.43
1:K:122:LEU:HD22	1:K:124:PHE:CD1	2.53	0.43
1:A:194:GLN:C	1:A:195:HIS:CD2	2.97	0.43
1:A:260:ASP:O	1:A:266:GLN:HA	2.18	0.43
1:D:402:ASN:O	1:D:406:VAL:HG23	2.18	0.43
1:F:310:ALA:HB1	1:F:368:ILE:HD13	2.01	0.43
1:H:68:MET:HE3	1:H:98:ASN:HA	1.99	0.43
1:H:96:ILE:HD12	1:H:96:ILE:N	2.33	0.43
1:H:110:ASN:OD1	5:H:723:HOH:O	2.21	0.43
1:A:370:ARG:NH1	1:A:379:GLU:OE2	2.50	0.43
1:B:5:THR:HG22	1:B:8:ASP:CG	2.43	0.43
1:C:62:ARG:HH12	1:C:65:GLU:CD	2.26	0.43
1:C:96:ILE:HD12	1:C:96:ILE:N	2.33	0.43
1:D:370:ARG:HH11	1:D:370:ARG:HB3	1.81	0.43
1:E:281:HIS:CD2	1:E:405:MET:HE3	2.53	0.43
1:E:387:ASP:OD1	1:E:387:ASP:N	2.51	0.43
1:G:219:LYS:HB3	1:H:161:PRO:HG2	2.00	0.43
1:G:264:ASP:C	1:G:266:GLN:H	2.25	0.43
1:K:26:THR:HG21	1:K:344:TYR:CE1	2.51	0.43
1:A:375:MET:HE2	1:A:375:MET:HB2	1.78	0.43
1:C:135:PHE:HB3	1:C:231:PHE:CE1	2.54	0.43
1:C:212:GLN:HA	1:C:212:GLN:OE1	2.18	0.43
1:D:157:PHE:CZ	1:E:35:VAL:HB	2.53	0.43
1:G:351:LEU:HD22	1:G:355:LEU:CD1	2.48	0.43
1:G:387:ASP:OD2	1:G:387:ASP:N	2.51	0.43
1:H:142:GLU:OE1	1:H:142:GLU:CA	2.67	0.43
1:L:351:LEU:HD22	1:L:355:LEU:CG	2.45	0.43
1:A:219:LYS:NZ	5:A:654:HOH:O	2.50	0.43
1:F:110:ASN:O	1:F:111:ASN:C	2.61	0.43
1:F:291:PRO:HG3	1:F:341:ALA:HA	2.00	0.43
1:I:279:VAL:HG13	1:I:309:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:7:GLU:CD	1:K:7:GLU:H	2.27	0.43
1:K:19:LYS:C	1:K:20:TYR:CD1	2.97	0.43
1:K:421:LYS:HA	1:K:421:LYS:HD3	1.94	0.43
1:F:321:ARG:O	1:F:323:PRO:HD3	2.18	0.43
1:H:317:SER:N	1:H:318:PRO:HD2	2.33	0.43
1:I:40:SER:HB3	5:I:736:HOH:O	2.18	0.43
1:J:252:LYS:O	1:J:253:ASN:CG	2.62	0.43
1:K:129:LEU:HD22	1:K:347:LEU:HD11	2.01	0.43
1:K:281:HIS:CD2	1:K:402:ASN:HD21	2.27	0.43
1:K:342:ASN:O	1:K:343:PRO:C	2.60	0.43
1:L:402:ASN:ND2	1:L:404:VAL:N	2.67	0.43
1:B:10:GLU:O	1:B:14:LYS:HE2	2.19	0.43
1:D:191:ALA:H	1:D:194:GLN:HE21	1.65	0.43
1:E:289:THR:OG1	1:E:290:ASN:ND2	2.51	0.43
1:F:285:PHE:HB2	1:F:349:VAL:HG13	1.98	0.43
2:H:601:P3S:HEC3	2:H:601:P3S:HGC2	2.00	0.43
1:I:55:SER:CB	1:I:66:SER:HB3	2.48	0.43
1:I:112:LEU:C	1:I:112:LEU:HD13	2.44	0.43
1:I:415:GLU:HB2	5:I:681:HOH:O	2.17	0.43
1:J:175:GLU:HG3	1:J:221:ILE:HD11	2.00	0.43
1:K:42:LEU:O	1:K:43:GLY:C	2.61	0.43
1:K:315:ASN:OD1	1:K:317:SER:HB3	2.19	0.43
1:A:74:LEU:HA	1:A:92:PHE:HE2	1.84	0.43
1:A:79:ILE:O	1:A:81:PRO:HD3	2.19	0.43
1:C:380:ARG:HB2	1:C:385:ILE:CB	2.44	0.43
1:D:22:ARG:NH1	1:D:36:GLU:OE1	2.52	0.43
1:D:159:LEU:HD22	1:E:32:ILE:HG23	2.01	0.43
1:D:414:PHE:CZ	1:D:418:ILE:CD1	3.02	0.43
1:F:282:ALA:HA	1:F:285:PHE:CZ	2.54	0.43
1:H:63:ILE:CD1	1:I:304:GLU:HG2	2.47	0.43
1:I:129:LEU:HD12	1:I:207:SER:HB3	2.00	0.43
1:I:146:PRO:HB3	1:I:228:HIS:CG	2.54	0.43
1:I:243:GLY:C	1:I:339:PRO:HD3	2.44	0.43
1:L:439:GLN:HA	1:L:439:GLN:NE2	2.34	0.43
1:A:316:ARG:CD	2:A:501:P3S:OE	2.67	0.42
1:B:336:SER:O	1:B:337:VAL:C	2.62	0.42
1:C:24:GLN:HE21	1:C:34:ASN:ND2	2.11	0.42
1:C:175:GLU:O	1:C:179:MET:HG3	2.18	0.42
1:C:321:ARG:NE	5:C:602:HOH:O	2.45	0.42
1:F:202:ALA:HB1	1:F:206:ARG:NH2	2.34	0.42
1:F:254:GLY:O	1:F:255:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:ILE:N	1:G:115:ILE:HD12	2.33	0.42
1:H:27:ASP:OD1	1:H:58:GLU:HB2	2.19	0.42
1:H:315:ASN:OD1	1:H:318:PRO:HD3	2.19	0.42
1:I:127:PHE:CE2	1:I:347:LEU:HD12	2.53	0.42
1:I:320:ILE:CG2	1:I:332:VAL:HG13	2.49	0.42
1:J:129:LEU:HD13	1:J:131:PRO:HG3	2.00	0.42
1:L:316:ARG:HG2	1:L:335:ARG:CZ	2.49	0.42
1:L:326:ARG:HD3	1:L:326:ARG:HA	1.96	0.42
1:B:52:PHE:CD1	1:B:52:PHE:N	2.86	0.42
1:E:279:VAL:HG11	1:E:365:PRO:HG2	2.00	0.42
1:E:316:ARG:HB2	1:F:66:SER:OG	2.19	0.42
1:F:260:ASP:HB2	1:F:268:SER:CA	2.49	0.42
1:I:82:TRP:HB2	1:I:224:LYS:NZ	2.33	0.42
1:J:81:PRO:HB2	5:J:720:HOH:O	2.19	0.42
1:K:46:LEU:HD23	1:K:46:LEU:HA	1.78	0.42
1:L:115:ILE:HG13	1:L:348:SER:HB2	2.00	0.42
1:L:316:ARG:HG2	1:L:335:ARG:NH2	2.34	0.42
1:L:371:ASN:O	1:L:374:VAL:HG22	2.19	0.42
1:A:33:LYS:HE2	1:F:158:ASP:OD2	2.19	0.42
1:B:152:ASP:HB3	1:B:164:LEU:HB2	2.01	0.42
1:F:421:LYS:HA	1:F:421:LYS:HD3	1.85	0.42
1:H:8:ASP:CB	1:H:11:LYS:HE2	2.49	0.42
1:H:306:PRO:HG2	1:H:336:SER:HA	1.99	0.42
1:I:52:PHE:CD1	1:I:70:LEU:HD13	2.54	0.42
1:I:347:LEU:HD13	1:I:347:LEU:HA	1.84	0.42
1:J:35:VAL:HG22	1:J:36:GLU:N	2.33	0.42
1:K:234:LYS:HD3	1:K:298:ARG:HA	2.01	0.42
1:K:368:ILE:HD11	1:K:385:ILE:HD11	2.01	0.42
1:L:27:ASP:OD2	1:L:27:ASP:C	2.62	0.42
1:A:32:ILE:HD12	1:F:159:LEU:CD2	2.49	0.42
1:B:360:ASN:HB2	1:B:362:LEU:HD13	2.01	0.42
1:C:335:ARG:HH21	1:C:335:ARG:HD3	1.70	0.42
1:D:263:ALA:CB	1:D:267:LEU:O	2.68	0.42
1:E:317:SER:H	1:E:318:PRO:CD	2.30	0.42
1:F:319:LEU:HD12	1:F:336:SER:HB2	2.01	0.42
1:G:71:TYR:CE1	1:G:97:TYR:HB2	2.53	0.42
1:G:368:ILE:CG2	1:G:372:ILE:CD1	2.97	0.42
1:H:365:PRO:HB2	5:H:807:HOH:O	2.18	0.42
1:I:3:LYS:HB3	1:I:75:ASN:OD1	2.19	0.42
1:I:429:ARG:HD3	5:I:773:HOH:O	2.19	0.42
1:J:295:SER:OG	1:J:338:ASP:OD1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:178:GLU:HA	1:K:178:GLU:OE1	2.20	0.42
1:A:33:LYS:O	1:A:34:ASN:HB3	2.18	0.42
1:A:368:ILE:CG2	1:A:372:ILE:HD12	2.49	0.42
1:B:146:PRO:HG3	1:B:228:HIS:CD2	2.54	0.42
1:B:255:VAL:HG12	1:B:256:ASN:N	2.34	0.42
1:C:157:PHE:CE2	1:D:35:VAL:HB	2.54	0.42
1:D:317:SER:N	1:D:318:PRO:HD2	2.34	0.42
1:G:5:THR:O	1:G:6:ARG:C	2.61	0.42
1:H:164:LEU:HA	1:H:164:LEU:HD12	1.77	0.42
1:A:112:LEU:HD13	1:A:116:LEU:CD1	2.50	0.42
1:B:119:MET:SD	1:B:127:PHE:HB2	2.60	0.42
1:B:317:SER:H	1:B:318:PRO:HD2	1.82	0.42
1:E:316:ARG:HH21	1:F:66:SER:HB3	1.84	0.42
1:F:20:TYR:HB2	1:F:89:VAL:HG22	2.01	0.42
1:K:33:LYS:O	1:K:34:ASN:HB3	2.19	0.42
1:A:65:GLU:HB2	5:A:667:HOH:O	2.19	0.42
1:C:377:LYS:CG	1:C:378:GLU:H	2.28	0.42
1:E:284:SER:CB	1:E:402:ASN:HD22	2.33	0.42
1:E:320:ILE:CG2	1:E:332:VAL:HG13	2.50	0.42
1:G:115:ILE:HD12	1:G:115:ILE:H	1.85	0.42
1:H:215:LYS:HG2	1:H:231:PHE:CZ	2.54	0.42
1:H:371:ASN:C	1:H:371:ASN:ND2	2.76	0.42
1:I:48:ASN:HB3	1:I:71:TYR:CD1	2.54	0.42
1:J:283:THR:HG23	5:J:659:HOH:O	2.20	0.42
1:K:13:VAL:HG13	1:K:18:VAL:HB	2.00	0.42
1:A:16:GLU:O	1:A:17:ASN:HB2	2.20	0.42
1:C:76:THR:HG21	1:C:93:ILE:HB	2.00	0.42
1:C:146:PRO:HG3	1:C:228:HIS:CD2	2.55	0.42
1:C:347:LEU:O	1:C:351:LEU:HB2	2.19	0.42
1:C:375:MET:HE3	1:C:379:GLU:HG2	2.02	0.42
1:E:91:ARG:HD2	1:E:91:ARG:C	2.45	0.42
1:E:129:LEU:HD13	1:E:207:SER:OG	2.20	0.42
1:E:130:GLY:HA3	3:E:502:ADP:H1'	2.02	0.42
1:F:22:ARG:NH1	1:F:36:GLU:OE2	2.53	0.42
1:F:100:ASP:OD1	1:F:100:ASP:C	2.62	0.42
1:H:9:ILE:HD13	1:H:74:LEU:HD12	2.02	0.42
1:H:402:ASN:OD1	1:H:402:ASN:C	2.63	0.42
1:J:23:LEU:HD23	1:J:23:LEU:HA	1.85	0.42
1:K:136:PHE:CZ	5:K:766:HOH:O	2.69	0.42
1:K:371:ASN:HD21	1:K:373:TYR:HB2	1.85	0.42
1:A:317:SER:H	1:A:318:PRO:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:PHE:CE2	1:B:351:LEU:HG	2.55	0.42
1:C:170:ARG:HH11	1:C:171:ASP:CG	2.27	0.42
1:C:371:ASN:O	1:C:374:VAL:HG22	2.20	0.42
1:D:175:GLU:HG3	1:D:221:ILE:HD11	2.02	0.42
1:D:232:MET:HA	1:D:233:PRO:HD3	1.91	0.42
1:E:171:ASP:OD1	1:E:225:HIS:CE1	2.73	0.42
1:G:9:ILE:O	1:G:13:VAL:HG23	2.20	0.42
1:K:304:GLU:OE2	2:K:501:P3S:HEC1	2.20	0.42
1:L:306:PRO:HG2	1:L:335:ARG:C	2.44	0.42
1:A:9:ILE:HD13	1:A:92:PHE:CZ	2.55	0.42
1:C:319:LEU:O	1:C:319:LEU:HD22	2.20	0.42
1:E:166:GLU:HB3	5:E:764:HOH:O	2.20	0.42
1:E:266:GLN:HB2	1:E:326:ARG:HD2	2.02	0.42
1:J:141:ASP:OD2	1:J:141:ASP:C	2.63	0.42
1:K:240:ASN:HD22	1:K:303:TYR:HD2	1.67	0.42
1:A:49:LYS:HA	1:A:49:LYS:HD3	1.80	0.41
1:A:405:MET:O	1:A:406:VAL:C	2.63	0.41
1:B:175:GLU:O	1:B:179:MET:HG3	2.20	0.41
1:B:426:ASP:HB2	5:B:687:HOH:O	2.20	0.41
1:C:115:ILE:HG22	1:C:351:LEU:HD13	2.02	0.41
1:C:299:LEU:HD22	1:C:306:PRO:O	2.19	0.41
1:C:351:LEU:O	1:C:355:LEU:HG	2.20	0.41
1:D:48:ASN:HB3	1:D:71:TYR:CD1	2.55	0.41
1:D:272:LYS:HZ3	1:D:311:TRP:HH2	1.62	0.41
1:D:368:ILE:HG13	1:D:385:ILE:HD11	2.01	0.41
1:E:216:LEU:O	1:E:216:LEU:HD23	2.20	0.41
1:E:421:LYS:HA	1:E:421:LYS:HD3	1.88	0.41
1:I:279:VAL:HG11	1:I:365:PRO:HG2	2.02	0.41
1:I:371:ASN:C	1:I:371:ASN:HD22	2.26	0.41
1:K:134:GLU:OE1	2:K:501:P3S:N	2.53	0.41
1:L:105:GLU:O	1:L:105:GLU:CG	2.68	0.41
1:B:259:PHE:CE1	1:B:326:ARG:HG3	2.55	0.41
1:C:11:LYS:HB3	1:C:11:LYS:HE3	1.83	0.41
1:C:111:ASN:OD1	1:C:114:ARG:NH1	2.53	0.41
1:C:232:MET:HE1	1:I:441:MET:HB2	2.01	0.41
1:E:274:PHE:CE1	1:E:354:GLY:HA3	2.55	0.41
1:E:312:SER:HB3	1:E:315:ASN:HB3	2.02	0.41
1:E:371:ASN:C	1:E:371:ASN:HD22	2.28	0.41
1:F:281:HIS:CD2	1:F:402:ASN:HD21	2.30	0.41
1:H:285:PHE:CD1	1:H:285:PHE:C	2.98	0.41
1:I:112:LEU:HD13	1:I:116:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:203:GLY:O	1:I:204:ALA:C	2.63	0.41
1:I:260:ASP:O	1:I:266:GLN:HA	2.20	0.41
1:K:122:LEU:HD23	1:K:124:PHE:CE1	2.55	0.41
1:K:177:GLU:HG3	1:K:183:ILE:HD13	2.00	0.41
1:K:273:HIS:O	1:K:276:ALA:HB3	2.19	0.41
1:L:345:LEU:HD22	1:L:409:LEU:HD22	2.02	0.41
1:L:402:ASN:HD22	1:L:404:VAL:N	2.17	0.41
1:A:427:MET:HE2	5:G:823:HOH:O	2.18	0.41
1:C:4:TYR:HB3	1:C:9:ILE:HD13	2.02	0.41
1:C:286:THR:HG21	1:C:389:PRO:HG2	2.02	0.41
1:D:22:ARG:O	1:D:91:ARG:HA	2.20	0.41
1:F:310:ALA:O	1:F:318:PRO:HB2	2.20	0.41
1:G:360:ASN:O	1:G:361:LYS:C	2.63	0.41
1:J:67:ASP:O	1:J:68:MET:HE3	2.21	0.41
1:J:262:ASN:HA	5:J:706:HOH:O	2.19	0.41
1:J:360:ASN:O	1:J:361:LYS:C	2.62	0.41
1:K:78:VAL:HG12	1:K:91:ARG:HG3	2.02	0.41
1:K:172:ILE:CD1	1:K:218:VAL:HA	2.49	0.41
1:L:191:ALA:O	1:L:192:PRO:C	2.59	0.41
1:L:402:ASN:ND2	1:L:404:VAL:H	2.18	0.41
1:B:371:ASN:N	1:C:64:GLU:HG2	2.35	0.41
1:D:152:ASP:OD2	1:D:152:ASP:C	2.64	0.41
1:F:429:ARG:CD	5:F:799:HOH:O	2.62	0.41
1:G:6:ARG:CD	1:G:46:LEU:HD13	2.49	0.41
1:G:22:ARG:HG3	1:G:89:VAL:HG11	2.02	0.41
1:J:91:ARG:HD2	1:J:92:PHE:N	2.35	0.41
1:J:435:TRP:O	1:J:439:GLN:HG2	2.20	0.41
1:J:437:ARG:O	1:J:441:MET:CB	2.68	0.41
1:K:211:ILE:CD1	5:K:635:HOH:O	2.61	0.41
1:K:317:SER:N	1:K:318:PRO:HD2	2.35	0.41
1:A:411:GLU:OE1	1:A:411:GLU:HA	2.20	0.41
1:B:109:ARG:HG3	1:B:344:TYR:CE2	2.56	0.41
1:G:243:GLY:C	1:G:339:PRO:HD3	2.46	0.41
1:G:309:VAL:CG2	1:G:386:VAL:HG23	2.50	0.41
1:H:417:PHE:O	1:H:421:LYS:HG2	2.20	0.41
1:I:126:ASP:HB3	5:I:671:HOH:O	2.20	0.41
1:I:418:ILE:O	1:I:422:GLU:HB2	2.19	0.41
1:K:23:LEU:HD22	1:K:94:CYS:SG	2.61	0.41
1:L:333:GLU:OE2	1:L:335:ARG:HD2	2.21	0.41
1:A:11:LYS:HE3	1:A:15:GLU:CD	2.46	0.41
1:D:321:ARG:O	1:D:323:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:ARG:HG3	1:F:89:VAL:CG1	2.51	0.41
1:F:135:PHE:HB3	1:F:231:PHE:CE1	2.56	0.41
1:F:260:ASP:O	1:F:266:GLN:HA	2.21	0.41
1:G:273:HIS:ND1	1:G:362:LEU:O	2.52	0.41
1:H:52:PHE:CE1	1:H:70:LEU:CD1	3.04	0.41
1:H:187:HIS:HE1	5:H:840:HOH:O	2.02	0.41
1:K:300:VAL:O	1:K:300:VAL:HG23	2.19	0.41
1:L:370:ARG:HD3	5:L:702:HOH:O	2.19	0.41
1:B:371:ASN:C	1:B:371:ASN:ND2	2.78	0.41
1:B:403:GLU:HG2	5:B:615:HOH:O	2.20	0.41
1:D:171:ASP:OD1	1:D:225:HIS:CE1	2.74	0.41
1:D:312:SER:HB3	1:D:315:ASN:HB3	2.03	0.41
1:E:210:ASP:O	1:E:211:ILE:C	2.62	0.41
1:F:119:MET:HG2	1:F:124:PHE:HB2	2.03	0.41
1:F:338:ASP:HB2	1:F:339:PRO:HD2	2.01	0.41
1:G:78:VAL:HG12	1:G:91:ARG:CG	2.51	0.41
1:I:167:ASN:HD22	1:I:168:CYS:H	1.67	0.41
1:I:221:ILE:HA	1:I:221:ILE:HD13	1.81	0.41
1:I:402:ASN:O	1:I:406:VAL:HG23	2.21	0.41
1:A:212:GLN:OE1	1:A:215:LYS:NZ	2.53	0.41
1:B:52:PHE:CE1	1:B:70:LEU:HD13	2.56	0.41
1:E:156:TYR:CZ	1:E:157:PHE:CE1	3.08	0.41
1:F:142:GLU:C	1:F:144:GLY:H	2.28	0.41
1:G:52:PHE:CE1	1:G:70:LEU:HD13	2.55	0.41
1:G:62:ARG:HE	1:G:62:ARG:HB3	1.73	0.41
1:G:381:MET:O	1:G:383:ASN:O	2.39	0.41
1:G:429:ARG:HD3	5:G:862:HOH:O	2.20	0.41
1:H:251:PHE:HA	1:H:255:VAL:O	2.21	0.41
1:J:160:ALA:HB2	1:J:166:GLU:CD	2.45	0.41
1:A:95:ASP:OD2	1:A:113:LYS:NZ	2.53	0.41
1:A:190:VAL:HA	5:A:602:HOH:O	2.20	0.41
1:A:263:ALA:O	1:A:264:ASP:C	2.64	0.41
1:A:268:SER:O	1:A:272:LYS:HG2	2.20	0.41
1:B:8:ASP:O	1:B:12:LEU:HB2	2.20	0.41
1:B:46:LEU:HD22	1:B:74:LEU:HD21	2.01	0.41
1:B:319:LEU:CD1	1:B:320:ILE:HG13	2.50	0.41
1:B:419:GLU:HG3	5:B:737:HOH:O	2.21	0.41
1:C:62:ARG:NH1	1:C:65:GLU:CD	2.78	0.41
1:C:278:ILE:HG21	1:C:320:ILE:HD11	2.02	0.41
1:C:351:LEU:HD22	1:C:355:LEU:CG	2.46	0.41
1:D:122:LEU:HD11	1:D:359:LYS:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:PHE:CE2	1:D:278:ILE:HD11	2.56	0.41
1:D:371:ASN:C	1:D:371:ASN:ND2	2.79	0.41
1:E:52:PHE:CD1	1:E:70:LEU:HD13	2.56	0.41
1:E:388:LEU:HD23	1:E:388:LEU:HA	1.79	0.41
1:E:413:LEU:HD23	1:E:413:LEU:HA	1.91	0.41
1:F:73:ASP:HA	5:F:800:HOH:O	2.20	0.41
1:F:129:LEU:HD13	1:F:131:PRO:HD3	2.01	0.41
1:F:248:LEU:HD11	1:F:350:LEU:HD13	2.02	0.41
1:F:326:ARG:O	1:F:327:GLY:C	2.61	0.41
1:F:351:LEU:HD22	1:F:355:LEU:HG	2.03	0.41
1:F:431:GLN:HG2	1:L:435:TRP:CD1	2.56	0.41
1:G:49:LYS:HA	1:G:49:LYS:HD3	1.86	0.41
1:H:234:LYS:HE3	1:H:239:VAL:O	2.21	0.41
1:I:52:PHE:CE1	1:I:68:MET:HB3	2.56	0.41
1:I:316:ARG:HD3	2:I:501:P3S:OE	2.20	0.41
1:J:142:GLU:CD	1:J:143:LYS:HD2	2.46	0.41
1:J:280:LYS:HG3	1:J:281:HIS:N	2.36	0.41
1:K:22:ARG:HD3	1:K:34:ASN:OD1	2.21	0.41
1:K:111:ASN:O	1:K:112:LEU:C	2.64	0.41
1:K:142:GLU:CD	1:K:142:GLU:H	2.28	0.41
1:L:426:ASP:HA	1:L:429:ARG:HG2	2.03	0.41
1:B:182:GLU:HB2	1:B:200:LYS:HB2	2.02	0.41
1:C:266:GLN:HB2	1:C:326:ARG:HD2	2.02	0.41
1:F:203:GLY:O	1:F:204:ALA:C	2.64	0.41
1:F:359:LYS:NZ	5:F:737:HOH:O	2.26	0.41
1:G:312:SER:HB3	1:G:315:ASN:HB3	2.03	0.41
1:G:315:ASN:O	1:G:318:PRO:HD2	2.21	0.41
1:G:368:ILE:HG22	1:G:372:ILE:CD1	2.51	0.41
1:J:376:SER:C	1:J:378:GLU:N	2.79	0.41
1:L:347:LEU:HD23	1:L:347:LEU:HA	1.79	0.41
1:L:397:GLU:OE1	1:L:397:GLU:HA	2.21	0.41
1:A:5:THR:O	1:A:7:GLU:N	2.54	0.40
1:A:326:ARG:HB3	1:A:327:GLY:H	1.71	0.40
1:C:26:THR:HG22	1:C:27:ASP:O	2.21	0.40
1:D:140:LEU:HD22	1:D:144:GLY:O	2.21	0.40
1:E:151:ASN:OD1	1:E:195:HIS:HE1	2.03	0.40
1:F:191:ALA:H	1:F:194:GLN:HE21	1.68	0.40
1:I:409:LEU:HD23	1:I:414:PHE:HA	2.03	0.40
1:K:282:ALA:HA	1:K:285:PHE:CE2	2.57	0.40
1:L:275:ILE:HD13	1:L:275:ILE:HG21	1.87	0.40
1:L:439:GLN:HE21	1:L:439:GLN:CA	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:OD2	1:A:141:ASP:C	2.64	0.40
1:A:402:ASN:OD1	1:A:402:ASN:C	2.63	0.40
1:B:115:ILE:HD12	1:B:348:SER:CB	2.48	0.40
1:C:65:GLU:O	1:C:65:GLU:CG	2.65	0.40
1:C:335:ARG:NH1	2:C:501:P3S:OE	2.55	0.40
1:E:250:LEU:HD23	1:E:250:LEU:HA	1.81	0.40
1:F:46:LEU:HA	1:F:46:LEU:HD23	1.78	0.40
1:F:74:LEU:H	1:F:74:LEU:HD22	1.85	0.40
1:F:266:GLN:HB2	1:F:326:ARG:HH11	1.86	0.40
1:G:84:ALA:CB	1:G:88:LYS:HG3	2.52	0.40
1:H:310:ALA:HA	5:H:823:HOH:O	2.21	0.40
1:J:18:VAL:HA	1:J:88:LYS:HG2	2.03	0.40
1:J:435:TRP:CH2	1:J:439:GLN:HG3	2.56	0.40
1:L:290:ASN:HB3	1:L:295:SER:HB3	2.03	0.40
1:L:306:PRO:HG2	1:L:336:SER:CA	2.50	0.40
1:B:371:ASN:O	1:B:374:VAL:HG22	2.20	0.40
1:D:46:LEU:HD22	1:D:74:LEU:HD21	2.03	0.40
1:E:170:ARG:NH2	1:F:86:LYS:HD3	2.35	0.40
1:F:280:LYS:NZ	5:F:836:HOH:O	2.45	0.40
1:G:57:ILE:HD12	1:G:57:ILE:N	2.37	0.40
1:I:74:LEU:N	1:I:74:LEU:CD2	2.84	0.40
1:J:9:ILE:HG21	1:J:92:PHE:HZ	1.86	0.40
1:K:71:TYR:CE1	1:K:97:TYR:HB2	2.57	0.40
1:K:403:GLU:OE2	1:K:407:LYS:HE2	2.21	0.40
1:K:429:ARG:NH2	5:K:732:HOH:O	2.54	0.40
1:A:370:ARG:HG3	1:A:375:MET:HE1	2.03	0.40
1:B:271:ALA:O	1:B:275:ILE:HG13	2.20	0.40
1:D:27:ASP:OD2	1:D:29:LEU:N	2.54	0.40
1:I:198:ASP:HA	5:I:601:HOH:O	2.21	0.40
1:J:315:ASN:O	1:J:318:PRO:HD2	2.20	0.40
1:K:203:GLY:O	1:K:204:ALA:C	2.65	0.40
1:L:21:ILE:HD11	1:L:39:VAL:HG23	2.03	0.40
1:L:402:ASN:HB2	5:L:720:HOH:O	2.20	0.40
1:A:119:MET:HG2	1:A:124:PHE:HB2	2.04	0.40
1:B:143:LYS:O	1:B:143:LYS:CG	2.69	0.40
1:B:331:ARG:N	5:B:666:HOH:O	2.50	0.40
1:D:129:LEU:HD12	1:D:347:LEU:HD11	2.03	0.40
1:G:68:MET:HE1	5:G:742:HOH:O	2.21	0.40
1:G:309:VAL:HG21	1:G:386:VAL:HG23	2.04	0.40
1:I:68:MET:HE3	1:I:68:MET:HA	2.02	0.40
1:J:127:PHE:CD2	1:J:351:LEU:HG	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:163:ASP:CG	1:J:169:ARG:HH22	2.29	0.40
1:L:260:ASP:HB2	1:L:268:SER:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/443 (100%)	407 (92%)	32 (7%)	2 (0%)	24	44
1	B	441/443 (100%)	417 (95%)	22 (5%)	2 (0%)	24	44
1	C	441/443 (100%)	414 (94%)	22 (5%)	5 (1%)	11	24
1	D	441/443 (100%)	407 (92%)	31 (7%)	3 (1%)	18	36
1	E	441/443 (100%)	417 (95%)	21 (5%)	3 (1%)	18	36
1	F	441/443 (100%)	410 (93%)	28 (6%)	3 (1%)	18	36
1	G	441/443 (100%)	403 (91%)	34 (8%)	4 (1%)	14	29
1	H	441/443 (100%)	420 (95%)	20 (4%)	1 (0%)	43	63
1	I	441/443 (100%)	414 (94%)	24 (5%)	3 (1%)	18	36
1	J	439/443 (99%)	413 (94%)	23 (5%)	3 (1%)	18	36
1	K	441/443 (100%)	416 (94%)	23 (5%)	2 (0%)	24	44
1	L	441/443 (100%)	416 (94%)	24 (5%)	1 (0%)	43	63
All	All	5290/5316 (100%)	4954 (94%)	304 (6%)	32 (1%)	21	39

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO
1	B	161	PRO

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Mol	Chain	Res	Type
1	C	161	PRO
1	C	361	LYS
1	D	161	PRO
1	E	161	PRO
1	F	161	PRO
1	G	100	ASP
1	H	161	PRO
1	I	161	PRO
1	J	161	PRO
1	K	161	PRO
1	C	261	GLU
1	D	3	LYS
1	L	361	LYS
1	F	361	LYS
1	B	361	LYS
1	C	265	LEU
1	E	268	SER
1	G	361	LYS
1	I	60	PHE
1	D	87	GLY
1	E	87	GLY
1	G	133	PRO
1	A	133	PRO
1	J	87	GLY
1	K	87	GLY
1	C	87	GLY
1	F	87	GLY
1	I	87	GLY
1	J	317	SER
1	G	87	GLY

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	382/382 (100%)	350 (92%)	32 (8%)	10 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	382/382 (100%)	353 (92%)	29 (8%)	12	26
1	C	382/382 (100%)	357 (94%)	25 (6%)	15	33
1	D	382/382 (100%)	357 (94%)	25 (6%)	15	33
1	E	382/382 (100%)	354 (93%)	28 (7%)	13	27
1	F	382/382 (100%)	361 (94%)	21 (6%)	19	39
1	G	382/382 (100%)	352 (92%)	30 (8%)	11	24
1	H	382/382 (100%)	351 (92%)	31 (8%)	11	23
1	I	382/382 (100%)	345 (90%)	37 (10%)	8	16
1	J	381/382 (100%)	350 (92%)	31 (8%)	11	23
1	K	382/382 (100%)	356 (93%)	26 (7%)	14	31
1	L	382/382 (100%)	349 (91%)	33 (9%)	10	21
All	All	4583/4584 (100%)	4235 (92%)	348 (8%)	12	26

All (348) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	32	ILE
1	A	34	ASN
1	A	58	GLU
1	A	70	LEU
1	A	74	LEU
1	A	78	VAL
1	A	79	ILE
1	A	85	GLU
1	A	86	LYS
1	A	88	LYS
1	A	91	ARG
1	A	122	LEU
1	A	126	ASP
1	A	129	LEU
1	A	164	LEU
1	A	174	LEU
1	A	186	SER
1	A	261	GLU
1	A	272	LYS
1	A	297	LYS
1	A	316	ARG

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Mol	Chain	Res	Type
1	A	326	ARG
1	A	331	ARG
1	A	359	LYS
1	A	362	LEU
1	A	372	ILE
1	A	375	MET
1	A	377	LYS
1	A	381	MET
1	A	396	LEU
1	A	411	GLU
1	B	3	LYS
1	B	5	THR
1	B	14	LYS
1	B	24	GLN
1	B	64	GLU
1	B	65	GLU
1	B	70	LEU
1	B	129	LEU
1	B	143	LYS
1	B	147	THR
1	B	161	PRO
1	B	164	LEU
1	B	200	LYS
1	B	216	LEU
1	B	240	ASN
1	B	261	GLU
1	B	272	LYS
1	B	299	LEU
1	B	316	ARG
1	B	319	LEU
1	B	349	VAL
1	B	351	LEU
1	B	359	LYS
1	B	362	LEU
1	B	363	GLU
1	B	370	ARG
1	B	372	ILE
1	B	379	GLU
1	B	441	MET
1	C	9	ILE
1	C	11	LYS
1	C	32	ILE

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Mol	Chain	Res	Type
1	C	70	LEU
1	C	78	VAL
1	C	91	ARG
1	C	129	LEU
1	C	148	LEU
1	C	153	LYS
1	C	164	LEU
1	C	169	ARG
1	C	186	SER
1	C	232	MET
1	C	284	SER
1	C	316	ARG
1	C	319	LEU
1	C	349	VAL
1	C	351	LEU
1	C	361	LYS
1	C	363	GLU
1	C	376	SER
1	C	397	GLU
1	C	431	GLN
1	C	437	ARG
1	C	441	MET
1	D	15	GLU
1	D	21	ILE
1	D	22	ARG
1	D	24	GLN
1	D	31	THR
1	D	34	ASN
1	D	49	LYS
1	D	65	GLU
1	D	70	LEU
1	D	105	GLU
1	D	129	LEU
1	D	142	GLU
1	D	164	LEU
1	D	256	ASN
1	D	261	GLU
1	D	267	LEU
1	D	319	LEU
1	D	335	ARG
1	D	351	LEU
1	D	362	LEU

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Mol	Chain	Res	Type
1	D	370	ARG
1	D	371	ASN
1	D	379	GLU
1	D	381	MET
1	D	382	GLU
1	E	3	LYS
1	E	14	LYS
1	E	28	ILE
1	E	49	LYS
1	E	56	SER
1	E	58	GLU
1	E	63	ILE
1	E	70	LEU
1	E	117	LYS
1	E	129	LEU
1	E	151	ASN
1	E	178	GLU
1	E	216	LEU
1	E	224	LYS
1	E	319	LEU
1	E	326	ARG
1	E	331	ARG
1	E	333	GLU
1	E	347	LEU
1	E	349	VAL
1	E	351	LEU
1	E	372	ILE
1	E	379	GLU
1	E	387	ASP
1	E	403	GLU
1	E	418	ILE
1	E	441	MET
1	E	442	SER
1	F	21	ILE
1	F	22	ARG
1	F	34	ASN
1	F	64	GLU
1	F	65	GLU
1	F	70	LEU
1	F	102	THR
1	F	112	LEU
1	F	126	ASP

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Mol	Chain	Res	Type
1	F	129	LEU
1	F	164	LEU
1	F	183	ILE
1	F	236	LEU
1	F	261	GLU
1	F	342	ASN
1	F	349	VAL
1	F	351	LEU
1	F	368	ILE
1	F	372	ILE
1	F	379	GLU
1	F	423	ILE
1	G	9	ILE
1	G	24	GLN
1	G	33	LYS
1	G	34	ASN
1	G	64	GLU
1	G	70	LEU
1	G	78	VAL
1	G	85	GLU
1	G	88	LYS
1	G	129	LEU
1	G	164	LEU
1	G	174	LEU
1	G	178	GLU
1	G	186	SER
1	G	200	LYS
1	G	240	ASN
1	G	272	LYS
1	G	280	LYS
1	G	299	LEU
1	G	307	CYS
1	G	319	LEU
1	G	342	ASN
1	G	351	LEU
1	G	370	ARG
1	G	382	GLU
1	G	404	VAL
1	G	409	LEU
1	G	411	GLU
1	G	422	GLU
1	G	441	MET

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Mol	Chain	Res	Type
1	H	9	ILE
1	H	15	GLU
1	H	16	GLU
1	H	21	ILE
1	H	31	THR
1	H	34	ASN
1	H	64	GLU
1	H	70	LEU
1	H	78	VAL
1	H	112	LEU
1	H	114	ARG
1	H	129	LEU
1	H	161	PRO
1	H	164	LEU
1	H	169	ARG
1	H	178	GLU
1	H	184	GLU
1	H	223	ARG
1	H	264	ASP
1	H	297	LYS
1	H	299	LEU
1	H	316	ARG
1	H	319	LEU
1	H	326	ARG
1	H	335	ARG
1	H	349	VAL
1	H	351	LEU
1	H	370	ARG
1	H	371	ASN
1	H	401	SER
1	H	411	GLU
1	I	17	ASN
1	I	24	GLN
1	I	34	ASN
1	I	49	LYS
1	I	55	SER
1	I	57	ILE
1	I	64	GLU
1	I	66	SER
1	I	68	MET
1	I	70	LEU
1	I	114	ARG

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Mol	Chain	Res	Type
1	I	122	LEU
1	I	126	ASP
1	I	129	LEU
1	I	142	GLU
1	I	164	LEU
1	I	167	ASN
1	I	178	GLU
1	I	207	SER
1	I	215	LYS
1	I	264	ASP
1	I	269	GLU
1	I	307	CYS
1	I	325	SER
1	I	326	ARG
1	I	335	ARG
1	I	349	VAL
1	I	351	LEU
1	I	362	LEU
1	I	370	ARG
1	I	372	ILE
1	I	404	VAL
1	I	409	LEU
1	I	411	GLU
1	I	422	GLU
1	I	441	MET
1	I	442	SER
1	J	24	GLN
1	J	49	LYS
1	J	64	GLU
1	J	68	MET
1	J	70	LEU
1	J	85	GLU
1	J	100	ASP
1	J	102	THR
1	J	112	LEU
1	J	125	SER
1	J	126	ASP
1	J	129	LEU
1	J	142	GLU
1	J	161	PRO
1	J	164	LEU
1	J	178	GLU

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Mol	Chain	Res	Type
1	J	184	GLU
1	J	190	VAL
1	J	223	ARG
1	J	253	ASN
1	J	264	ASP
1	J	270	THR
1	J	299	LEU
1	J	307	CYS
1	J	316	ARG
1	J	331	ARG
1	J	349	VAL
1	J	351	LEU
1	J	359	LYS
1	J	411	GLU
1	J	426	ASP
1	K	15	GLU
1	K	24	GLN
1	K	26	THR
1	K	33	LYS
1	K	34	ASN
1	K	63	ILE
1	K	65	GLU
1	K	66	SER
1	K	70	LEU
1	K	74	LEU
1	K	78	VAL
1	K	86	LYS
1	K	88	LYS
1	K	107	ASP
1	K	112	LEU
1	K	161	PRO
1	K	172	ILE
1	K	252	LYS
1	K	255	VAL
1	K	285	PHE
1	K	299	LEU
1	K	307	CYS
1	K	351	LEU
1	K	362	LEU
1	K	370	ARG
1	K	372	ILE
1	L	6	ARG

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Mol	Chain	Res	Type
1	L	7	GLU
1	L	16	GLU
1	L	17	ASN
1	L	21	ILE
1	L	22	ARG
1	L	34	ASN
1	L	64	GLU
1	L	70	LEU
1	L	88	LYS
1	L	122	LEU
1	L	126	ASP
1	L	129	LEU
1	L	164	LEU
1	L	183	ILE
1	L	184	GLU
1	L	206	ARG
1	L	297	LYS
1	L	299	LEU
1	L	316	ARG
1	L	326	ARG
1	L	335	ARG
1	L	349	VAL
1	L	351	LEU
1	L	359	LYS
1	L	362	LEU
1	L	363	GLU
1	L	370	ARG
1	L	372	ILE
1	L	379	GLU
1	L	402	ASN
1	L	423	ILE
1	L	441	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (158) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	75	ASN
1	A	167	ASN
1	A	187	HIS
1	A	240	ASN
1	A	266	GLN

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Mol	Chain	Res	Type
1	A	281	HIS
1	A	314	GLN
1	A	416	HIS
1	A	443	GLN
1	B	24	GLN
1	B	34	ASN
1	B	167	ASN
1	B	187	HIS
1	B	194	GLN
1	B	228	HIS
1	B	253	ASN
1	B	281	HIS
1	B	290	ASN
1	B	371	ASN
1	B	412	HIS
1	B	416	HIS
1	B	431	GLN
1	C	34	ASN
1	C	128	ASN
1	C	167	ASN
1	C	187	HIS
1	C	194	GLN
1	C	228	HIS
1	C	240	ASN
1	C	281	HIS
1	C	290	ASN
1	C	314	GLN
1	C	360	ASN
1	C	412	HIS
1	C	431	GLN
1	D	24	GLN
1	D	75	ASN
1	D	110	ASN
1	D	167	ASN
1	D	187	HIS
1	D	194	GLN
1	D	225	HIS
1	D	228	HIS
1	D	240	ASN
1	D	245	HIS
1	D	253	ASN
1	D	256	ASN

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Mol	Chain	Res	Type
1	D	290	ASN
1	D	314	GLN
1	D	402	ASN
1	E	24	GLN
1	E	34	ASN
1	E	75	ASN
1	E	110	ASN
1	E	187	HIS
1	E	195	HIS
1	E	225	HIS
1	E	228	HIS
1	E	281	HIS
1	E	290	ASN
1	E	314	GLN
1	E	371	ASN
1	F	98	ASN
1	F	110	ASN
1	F	128	ASN
1	F	167	ASN
1	F	187	HIS
1	F	194	GLN
1	F	228	HIS
1	F	240	ASN
1	F	247	ASN
1	F	253	ASN
1	F	281	HIS
1	F	314	GLN
1	F	342	ASN
1	F	431	GLN
1	G	24	GLN
1	G	34	ASN
1	G	41	GLN
1	G	167	ASN
1	G	187	HIS
1	G	194	GLN
1	G	228	HIS
1	G	240	ASN
1	G	281	HIS
1	G	314	GLN
1	G	342	ASN
1	G	360	ASN
1	G	431	GLN

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Mol	Chain	Res	Type
1	H	17	ASN
1	H	24	GLN
1	H	128	ASN
1	H	167	ASN
1	H	187	HIS
1	H	194	GLN
1	H	212	GLN
1	H	228	HIS
1	H	240	ASN
1	H	281	HIS
1	H	290	ASN
1	H	314	GLN
1	H	360	ASN
1	H	371	ASN
1	I	24	GLN
1	I	34	ASN
1	I	110	ASN
1	I	128	ASN
1	I	167	ASN
1	I	187	HIS
1	I	225	HIS
1	I	240	ASN
1	I	266	GLN
1	I	290	ASN
1	I	371	ASN
1	I	431	GLN
1	J	24	GLN
1	J	34	ASN
1	J	41	GLN
1	J	128	ASN
1	J	167	ASN
1	J	187	HIS
1	J	194	GLN
1	J	228	HIS
1	J	240	ASN
1	J	281	HIS
1	J	290	ASN
1	J	314	GLN
1	J	412	HIS
1	J	431	GLN
1	J	443	GLN
1	K	24	GLN

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Mol	Chain	Res	Type
1	K	110	ASN
1	K	167	ASN
1	K	187	HIS
1	K	212	GLN
1	K	240	ASN
1	K	262	ASN
1	K	281	HIS
1	K	290	ASN
1	K	314	GLN
1	K	371	ASN
1	K	412	HIS
1	K	416	HIS
1	L	110	ASN
1	L	128	ASN
1	L	167	ASN
1	L	187	HIS
1	L	194	GLN
1	L	228	HIS
1	L	240	ASN
1	L	281	HIS
1	L	290	ASN
1	L	314	GLN
1	L	402	ASN
1	L	431	GLN
1	L	439	GLN
1	L	443	GLN

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

Of 60 ligands modelled in this entry, 36 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	F	602	4	28,29,29	1.37	4 (14%)	43,45,45	2.31	18 (41%)
3	ADP	G	602	4	28,29,29	1.55	5 (17%)	43,45,45	2.07	13 (30%)
2	P3S	D	501	4	11,14,14	2.72	5 (45%)	9,21,21	4.93	4 (44%)
2	P3S	G	601	4	11,14,14	2.67	4 (36%)	9,21,21	5.71	5 (55%)
2	P3S	F	601	4	11,14,14	2.59	5 (45%)	9,21,21	4.83	4 (44%)
3	ADP	K	502	4	28,29,29	1.41	4 (14%)	43,45,45	2.24	14 (32%)
3	ADP	L	502	4	28,29,29	1.49	4 (14%)	43,45,45	2.12	14 (32%)
3	ADP	B	502	4	28,29,29	1.36	6 (21%)	43,45,45	2.33	15 (34%)
2	P3S	H	601	4	11,14,14	2.86	6 (54%)	9,21,21	4.92	3 (33%)
2	P3S	K	501	4	11,14,14	2.53	4 (36%)	9,21,21	4.66	3 (33%)
2	P3S	B	501	4	11,14,14	2.61	4 (36%)	9,21,21	5.96	7 (77%)
3	ADP	I	502	4	28,29,29	1.53	6 (21%)	43,45,45	2.16	16 (37%)
3	ADP	D	502	4	28,29,29	1.32	4 (14%)	43,45,45	1.98	14 (32%)
2	P3S	L	501	4	11,14,14	2.63	4 (36%)	9,21,21	4.72	3 (33%)
2	P3S	C	501	4	11,14,14	2.49	4 (36%)	9,21,21	5.10	5 (55%)
2	P3S	A	501	4	11,14,14	2.81	5 (45%)	9,21,21	6.15	3 (33%)
2	P3S	J	501	4	11,14,14	2.41	4 (36%)	9,21,21	5.61	3 (33%)
3	ADP	E	502	4	28,29,29	1.35	6 (21%)	43,45,45	2.41	13 (30%)
3	ADP	A	502	4	28,29,29	1.27	3 (10%)	43,45,45	2.07	11 (25%)
3	ADP	J	502	4	28,29,29	1.52	5 (17%)	43,45,45	2.04	16 (37%)
2	P3S	E	501	4	11,14,14	2.47	4 (36%)	9,21,21	6.44	6 (66%)
3	ADP	C	502	4	28,29,29	1.38	3 (10%)	43,45,45	2.32	16 (37%)
3	ADP	H	602	4	28,29,29	1.48	5 (17%)	43,45,45	2.08	13 (30%)
2	P3S	I	501	4	11,14,14	2.56	4 (36%)	9,21,21	5.34	6 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	F	602	4	-	8/16/32/32	0/3/3/3
3	ADP	G	602	4	-	3/16/32/32	0/3/3/3
2	P3S	D	501	4	-	4/9/16/16	-
2	P3S	G	601	4	-	4/9/16/16	-
2	P3S	F	601	4	-	4/9/16/16	-
3	ADP	K	502	4	-	4/16/32/32	0/3/3/3
3	ADP	L	502	4	-	7/16/32/32	0/3/3/3
3	ADP	B	502	4	-	5/16/32/32	0/3/3/3
2	P3S	H	601	4	-	4/9/16/16	-
2	P3S	K	501	4	-	4/9/16/16	-
2	P3S	B	501	4	-	4/9/16/16	-
3	ADP	I	502	4	-	4/16/32/32	0/3/3/3
3	ADP	D	502	4	-	5/16/32/32	0/3/3/3
2	P3S	L	501	4	-	4/9/16/16	-
2	P3S	C	501	4	-	4/9/16/16	-
2	P3S	A	501	4	-	4/9/16/16	-
2	P3S	J	501	4	-	4/9/16/16	-
3	ADP	E	502	4	-	4/16/32/32	0/3/3/3
3	ADP	A	502	4	-	3/16/32/32	0/3/3/3
3	ADP	J	502	4	-	6/16/32/32	0/3/3/3
2	P3S	E	501	4	-	4/9/16/16	-
3	ADP	C	502	4	-	3/16/32/32	0/3/3/3
3	ADP	H	602	4	-	7/16/32/32	0/3/3/3
2	P3S	I	501	4	-	4/9/16/16	-

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	P3S	CE-SD	6.01	2.03	1.75
2	F	601	P3S	CE-SD	5.76	2.02	1.75
2	H	601	P3S	CE-SD	5.61	2.01	1.75
2	G	601	P3S	CE-SD	5.60	2.01	1.75
2	J	501	P3S	CE-SD	5.51	2.01	1.75
2	L	501	P3S	CE-SD	5.50	2.01	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	P3S	CE-SD	5.33	2.00	1.75
2	K	501	P3S	CE-SD	5.26	2.00	1.75
2	A	501	P3S	CE-SD	5.19	1.99	1.75
2	I	501	P3S	OE-SD	5.19	1.71	1.45
3	L	502	ADP	C5-C4	5.06	1.48	1.39
2	E	501	P3S	CE-SD	5.05	1.99	1.75
2	C	501	P3S	CE-SD	5.02	1.99	1.75
3	G	602	ADP	C5-C4	4.85	1.47	1.39
2	I	501	P3S	CE-SD	4.83	1.98	1.75
2	G	601	P3S	OE-SD	4.73	1.69	1.45
2	B	501	P3S	OE-SD	4.71	1.69	1.45
2	A	501	P3S	CB-CG	-4.69	1.48	1.52
2	K	501	P3S	OE-SD	4.60	1.68	1.45
2	L	501	P3S	OE-SD	4.53	1.68	1.45
2	H	601	P3S	OE-SD	4.51	1.68	1.45
2	E	501	P3S	OE-SD	4.47	1.68	1.45
2	A	501	P3S	OE-SD	4.47	1.68	1.45
3	I	502	ADP	C5-C4	4.44	1.47	1.39
2	D	501	P3S	OE-SD	4.40	1.67	1.45
2	C	501	P3S	OE-SD	4.30	1.67	1.45
2	J	501	P3S	OE-SD	4.25	1.67	1.45
3	K	502	ADP	C5-C4	4.25	1.46	1.39
2	F	601	P3S	OE-SD	4.16	1.66	1.45
3	J	502	ADP	C5-C4	4.10	1.46	1.39
3	J	502	ADP	PA-O3A	4.05	1.63	1.59
3	H	602	ADP	C5-C4	4.05	1.46	1.39
3	B	502	ADP	C5-C4	3.94	1.46	1.39
3	A	502	ADP	C5-C4	3.91	1.46	1.39
3	C	502	ADP	C5-C4	3.86	1.46	1.39
3	E	502	ADP	C5-C4	3.51	1.45	1.39
3	F	602	ADP	C4-N9	-3.44	1.30	1.37
3	G	602	ADP	PA-O3A	3.37	1.63	1.59
3	D	502	ADP	C5-C4	3.18	1.44	1.39
3	C	502	ADP	C4-N9	-3.16	1.31	1.37
3	D	502	ADP	C4-N9	-3.07	1.31	1.37
3	I	502	ADP	C5-C6	3.06	1.49	1.41
3	H	602	ADP	C5-N7	-3.04	1.33	1.39
3	F	602	ADP	PB-O2B	-2.98	1.43	1.54
2	D	501	P3S	PA-NE	2.98	1.69	1.58
3	F	602	ADP	C5-C4	2.93	1.44	1.39
2	K	501	P3S	O-C	2.92	1.30	1.22
2	H	601	P3S	O-C	2.91	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	ADP	C5-N7	-2.91	1.33	1.39
2	L	501	P3S	O-C	2.91	1.30	1.22
2	L	501	P3S	PA-NE	2.87	1.69	1.58
2	C	501	P3S	O-C	2.87	1.30	1.22
2	E	501	P3S	O-C	2.87	1.30	1.22
3	H	602	ADP	C8-N7	2.86	1.37	1.31
2	H	601	P3S	PA-NE	2.85	1.68	1.58
3	F	602	ADP	C5-C6	2.84	1.48	1.41
3	G	602	ADP	C8-N7	2.84	1.37	1.31
2	G	601	P3S	PA-O1A	2.83	1.51	1.46
2	G	601	P3S	O-C	2.81	1.30	1.22
2	I	501	P3S	O-C	2.74	1.30	1.22
3	G	602	ADP	C5-N7	-2.74	1.34	1.39
3	D	502	ADP	C5-N7	-2.71	1.34	1.39
2	F	601	P3S	PA-NE	2.69	1.68	1.58
2	D	501	P3S	CB-CG	-2.68	1.50	1.52
2	B	501	P3S	O-C	2.67	1.30	1.22
2	C	501	P3S	PA-NE	2.62	1.68	1.58
2	J	501	P3S	O-C	2.60	1.29	1.22
3	E	502	ADP	PA-O3A	2.55	1.62	1.59
2	F	601	P3S	CB-CG	-2.53	1.50	1.52
2	D	501	P3S	O-C	2.53	1.29	1.22
2	I	501	P3S	PA-O2A	-2.52	1.49	1.54
2	E	501	P3S	CB-CG	2.52	1.55	1.52
3	A	502	ADP	C5-N7	-2.51	1.34	1.39
3	J	502	ADP	C5-C6	2.49	1.47	1.41
3	L	502	ADP	C8-N7	2.48	1.36	1.31
3	B	502	ADP	C5-N7	-2.48	1.34	1.39
3	D	502	ADP	PB-O2B	-2.48	1.45	1.54
2	A	501	P3S	O-C	2.48	1.29	1.22
2	H	601	P3S	CB-CG	-2.41	1.50	1.52
3	K	502	ADP	C4-N9	-2.40	1.32	1.37
2	K	501	P3S	PA-NE	2.40	1.67	1.58
3	K	502	ADP	C5-C6	2.37	1.47	1.41
2	B	501	P3S	PA-NE	2.36	1.67	1.58
3	J	502	ADP	C8-N7	2.36	1.36	1.31
3	E	502	ADP	C8-N7	2.34	1.36	1.31
3	K	502	ADP	C8-N7	2.34	1.36	1.31
3	L	502	ADP	C5-C6	2.33	1.47	1.41
2	H	601	P3S	PA-O1A	2.32	1.50	1.46
2	F	601	P3S	O-C	2.31	1.28	1.22
3	L	502	ADP	PB-O2B	-2.30	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	502	ADP	C8-N7	2.27	1.36	1.31
2	A	501	P3S	PA-NE	2.26	1.66	1.58
3	E	502	ADP	C4-N9	-2.23	1.33	1.37
3	B	502	ADP	C5-C6	2.21	1.47	1.41
3	I	502	ADP	C4-N9	-2.20	1.33	1.37
3	B	502	ADP	C8-N9	-2.20	1.33	1.37
2	J	501	P3S	PA-NE	2.15	1.66	1.58
3	I	502	ADP	C5-N7	-2.13	1.35	1.39
3	G	602	ADP	C5-C6	2.10	1.46	1.41
3	E	502	ADP	PB-O2B	-2.10	1.47	1.54
3	J	502	ADP	C5-N7	-2.09	1.35	1.39
3	E	502	ADP	C5-N7	-2.06	1.35	1.39
3	H	602	ADP	C5-C6	2.06	1.46	1.41
3	H	602	ADP	O4'-C4'	-2.04	1.40	1.45
3	I	502	ADP	PB-O2B	-2.04	1.47	1.54
3	A	502	ADP	C8-N7	2.02	1.35	1.31
3	B	502	ADP	C4-N9	-2.02	1.33	1.37
3	B	502	ADP	C8-N7	2.01	1.35	1.31

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	P3S	OE-SD-CE	15.66	134.05	109.21
2	E	501	P3S	OE-SD-CE	15.08	133.12	109.21
2	B	501	P3S	OE-SD-CE	14.17	131.68	109.21
2	J	501	P3S	OE-SD-CE	13.34	130.37	109.21
2	G	601	P3S	OE-SD-CE	12.25	128.63	109.21
2	H	601	P3S	OE-SD-CE	11.78	127.89	109.21
2	I	501	P3S	OE-SD-CE	11.66	127.71	109.21
2	D	501	P3S	OE-SD-CE	10.93	126.54	109.21
2	K	501	P3S	OE-SD-CE	10.88	126.47	109.21
2	C	501	P3S	CE-SD-CG	-10.53	68.35	105.17
2	G	601	P3S	CE-SD-CG	-10.46	68.60	105.17
2	F	601	P3S	OE-SD-CE	9.84	124.81	109.21
2	E	501	P3S	CE-SD-CG	-9.47	72.08	105.17
2	F	601	P3S	CE-SD-CG	-9.35	72.47	105.17
2	J	501	P3S	CE-SD-CG	-9.19	73.05	105.17
2	L	501	P3S	CE-SD-CG	-9.16	73.16	105.17
2	L	501	P3S	OE-SD-CE	9.15	123.73	109.21
2	C	501	P3S	OE-SD-CE	9.03	123.53	109.21
2	B	501	P3S	CE-SD-CG	-8.97	73.80	105.17
2	I	501	P3S	CE-SD-CG	-8.67	74.86	105.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	P3S	CE-SD-CG	-8.49	75.51	105.17
2	D	501	P3S	CE-SD-CG	-8.43	75.70	105.17
2	K	501	P3S	CE-SD-CG	-7.92	77.50	105.17
2	H	601	P3S	CE-SD-CG	-7.73	78.16	105.17
3	E	502	ADP	N3-C2-N1	-7.40	117.38	128.58
3	C	502	ADP	N3-C2-N1	-6.21	119.18	128.58
3	K	502	ADP	N3-C2-N1	-6.18	119.23	128.58
3	G	602	ADP	O4'-C1'-N9	5.74	119.12	108.09
3	F	602	ADP	N3-C2-N1	-5.60	120.10	128.58
3	L	502	ADP	O4'-C1'-N9	5.50	118.64	108.09
3	E	502	ADP	O4'-C1'-N9	5.29	118.26	108.09
3	H	602	ADP	N3-C2-N1	-5.24	120.65	128.58
3	G	602	ADP	C5-C4-N3	-5.15	119.62	126.72
3	D	502	ADP	N3-C2-N1	-5.12	120.83	128.58
3	K	502	ADP	O4'-C1'-N9	5.11	117.91	108.09
3	A	502	ADP	C5-C4-N3	-5.08	119.72	126.72
3	E	502	ADP	C2-N3-C4	5.00	124.04	111.83
3	J	502	ADP	C5-C4-N3	-4.98	119.86	126.72
3	B	502	ADP	N3-C2-N1	-4.92	121.13	128.58
3	L	502	ADP	C5-C4-N3	-4.90	119.97	126.72
3	I	502	ADP	C5-C4-N3	-4.84	120.05	126.72
3	A	502	ADP	N3-C2-N1	-4.82	121.28	128.58
3	B	502	ADP	C5-C4-N3	-4.81	120.10	126.72
3	B	502	ADP	C4-N9-C8	4.77	110.74	105.74
3	I	502	ADP	C4-C5-N7	-4.76	105.14	110.58
3	B	502	ADP	O4'-C1'-N9	4.73	117.18	108.09
3	H	602	ADP	C5-C4-N3	-4.70	120.25	126.72
3	A	502	ADP	O4'-C1'-N9	4.67	117.06	108.09
3	K	502	ADP	C2-N1-C6	4.60	126.28	118.73
3	B	502	ADP	N3-C4-N9	4.41	134.67	127.17
2	L	501	P3S	CB-CA-C	4.40	122.09	110.45
3	J	502	ADP	N3-C2-N1	-4.39	121.94	128.58
3	E	502	ADP	C5-C4-N3	-4.36	120.72	126.72
3	A	502	ADP	N3-C4-N9	4.32	134.52	127.17
3	J	502	ADP	C2-N3-C4	4.32	122.37	111.83
2	C	501	P3S	CB-CA-C	4.28	121.78	110.45
2	J	501	P3S	CB-CA-C	4.25	121.70	110.45
2	E	501	P3S	OT-C-O	-4.23	114.49	124.08
3	H	602	ADP	C2-N3-C4	4.22	122.15	111.83
3	G	602	ADP	N3-C4-N9	4.18	134.28	127.17
3	I	502	ADP	N3-C2-N1	-4.16	122.29	128.58
3	L	502	ADP	N3-C4-N9	4.16	134.24	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	602	ADP	N3-C4-N9	4.13	134.19	127.17
3	C	502	ADP	C2-N3-C4	4.12	121.90	111.83
3	F	602	ADP	O4'-C1'-N9	4.12	116.00	108.09
3	C	502	ADP	C5-C4-N3	-4.09	121.09	126.72
3	E	502	ADP	N3-C4-N9	4.07	134.09	127.17
3	A	502	ADP	C2-N3-C4	4.05	121.73	111.83
3	F	602	ADP	O2B-PB-O3A	4.03	118.16	104.64
2	B	501	P3S	CB-CA-C	3.98	120.99	110.45
3	K	502	ADP	C2-N3-C4	3.97	121.53	111.83
3	B	502	ADP	C2-N3-C4	3.96	121.50	111.83
3	C	502	ADP	O3A-PB-O1B	-3.94	90.32	111.04
3	J	502	ADP	N3-C4-N9	3.94	133.86	127.17
3	C	502	ADP	O4'-C1'-N9	3.91	115.59	108.09
2	F	601	P3S	CB-CA-C	3.87	120.70	110.45
2	E	501	P3S	CB-CA-C	3.85	120.64	110.45
3	K	502	ADP	C6-C5-N7	3.84	139.49	132.09
3	F	602	ADP	C2-N3-C4	3.83	121.18	111.83
3	E	502	ADP	C2-N1-C6	3.82	125.01	118.73
3	C	502	ADP	C2-N1-C6	3.81	124.98	118.73
3	C	502	ADP	N3-C4-N9	3.78	133.59	127.17
3	B	502	ADP	C4-C5-N7	-3.77	106.27	110.58
2	H	601	P3S	CB-CA-C	3.75	120.38	110.45
3	L	502	ADP	N3-C2-N1	-3.75	122.91	128.58
3	C	502	ADP	O2A-PA-O1A	3.72	129.77	112.44
2	I	501	P3S	CB-CA-C	3.71	120.27	110.45
3	K	502	ADP	O3B-PB-O2B	3.70	121.67	107.80
3	F	602	ADP	C4-N9-C1'	-3.68	118.02	126.63
3	E	502	ADP	C4-N9-C8	3.68	109.60	105.74
3	B	502	ADP	N9-C8-N7	-3.67	108.73	113.94
3	I	502	ADP	C2-N3-C4	3.67	120.79	111.83
3	C	502	ADP	O3B-PB-O1B	3.66	125.08	110.83
3	F	602	ADP	C4-N9-C8	3.65	109.57	105.74
3	D	502	ADP	C4-N9-C8	3.63	109.55	105.74
3	F	602	ADP	O2A-PA-O1A	3.60	129.21	112.44
2	D	501	P3S	CB-CA-C	3.57	119.89	110.45
3	B	502	ADP	C5-N7-C8	3.52	108.99	103.45
3	F	602	ADP	C6-C5-C4	-3.50	112.40	117.18
3	D	502	ADP	C2-N1-C6	3.48	124.45	118.73
3	I	502	ADP	C5-N7-C8	3.47	108.90	103.45
3	F	602	ADP	C6-C5-N7	3.46	138.75	132.09
2	E	501	P3S	O3A-PA-O1A	-3.45	106.56	113.77
3	I	502	ADP	N3-C4-N9	3.45	133.03	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	ADP	C2-N3-C4	3.44	120.22	111.83
2	C	501	P3S	CE-SD-NE	3.43	119.46	107.48
2	I	501	P3S	OT-C-O	-3.40	116.36	124.08
2	A	501	P3S	CB-CA-C	3.39	119.43	110.45
3	C	502	ADP	C4-N9-C8	3.39	109.30	105.74
3	L	502	ADP	C4-C5-N7	-3.39	106.71	110.58
3	L	502	ADP	C2-N3-C4	3.37	120.07	111.83
3	I	502	ADP	C4-N9-C8	3.36	109.27	105.74
3	K	502	ADP	C5-C4-N3	-3.36	122.09	126.72
3	J	502	ADP	C6-C5-N7	3.36	138.57	132.09
3	F	602	ADP	O3A-PB-O1B	-3.36	93.38	111.04
3	F	602	ADP	O3B-PB-O2B	3.36	120.38	107.80
3	B	502	ADP	O3B-PB-O2B	3.31	120.21	107.80
3	I	502	ADP	C6-C5-N7	3.31	138.46	132.09
3	D	502	ADP	C5-C4-N3	-3.28	122.20	126.72
3	G	602	ADP	C2-N3-C4	3.19	119.63	111.83
2	G	601	P3S	CE-SD-NE	3.18	118.61	107.48
3	E	502	ADP	C6-C5-N7	3.18	138.22	132.09
2	G	601	P3S	CB-CA-C	3.17	118.86	110.45
3	H	602	ADP	C4-N9-C8	3.16	109.06	105.74
3	L	502	ADP	C4-N9-C8	3.16	109.06	105.74
2	D	501	P3S	O2A-PA-O1A	-3.11	107.27	113.77
2	G	601	P3S	OT-C-O	-3.05	117.17	124.08
3	I	502	ADP	O4'-C1'-N9	3.04	113.93	108.09
3	I	502	ADP	O3B-PB-O1B	3.02	122.60	110.83
3	J	502	ADP	C4-N9-C1'	-2.99	119.65	126.63
2	I	501	P3S	O2A-PA-O1A	-2.98	107.54	113.77
3	K	502	ADP	C6-C5-C4	-2.98	113.11	117.18
3	D	502	ADP	O4'-C1'-N9	2.97	113.80	108.09
3	D	502	ADP	N3-C4-N9	2.96	132.20	127.17
3	I	502	ADP	N9-C8-N7	-2.96	109.74	113.94
3	G	602	ADP	C4-C5-N7	-2.96	107.20	110.58
3	J	502	ADP	C4-C5-N7	-2.95	107.21	110.58
3	E	502	ADP	C6-C5-C4	-2.94	113.16	117.18
3	H	602	ADP	O3B-PB-O3A	-2.88	94.99	104.64
3	K	502	ADP	C4-N9-C1'	-2.85	119.96	126.63
2	I	501	P3S	CE-SD-NE	2.85	117.43	107.48
3	B	502	ADP	C6-C5-N7	2.84	137.56	132.09
3	F	602	ADP	C2-N1-C6	2.84	123.39	118.73
3	B	502	ADP	C2-N1-C6	2.83	123.37	118.73
3	A	502	ADP	O2A-PA-O1A	2.81	125.53	112.44
2	E	501	P3S	O2A-PA-O1A	2.80	119.61	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	602	ADP	O2B-PB-O1B	-2.80	99.92	110.83
3	L	502	ADP	C5-N7-C8	2.80	107.85	103.45
3	K	502	ADP	C4-C5-N7	-2.79	107.39	110.58
3	G	602	ADP	N3-C2-N1	-2.78	124.37	128.58
3	L	502	ADP	C6-C5-N7	2.76	137.41	132.09
3	G	602	ADP	O3B-PB-O1B	2.75	121.54	110.83
3	D	502	ADP	N9-C8-N7	-2.74	110.05	113.94
3	D	502	ADP	O2A-PA-O3A	2.72	114.63	107.27
3	B	502	ADP	O3'-C3'-C2'	-2.67	103.25	111.82
3	H	602	ADP	C6-C5-N7	2.66	137.22	132.09
3	D	502	ADP	C4-N9-C1'	-2.66	120.42	126.63
3	D	502	ADP	O3B-PB-O2B	2.66	117.76	107.80
2	B	501	P3S	O3A-PA-O1A	-2.63	108.27	113.77
3	J	502	ADP	C4-N9-C8	2.63	108.50	105.74
3	C	502	ADP	O2B-PB-O3A	2.62	113.43	104.64
3	I	502	ADP	C2-N1-C6	2.55	122.92	118.73
3	C	502	ADP	C6-C5-N7	2.54	137.00	132.09
3	B	502	ADP	O5'-PA-O1A	-2.52	98.94	108.94
3	K	502	ADP	C1'-N9-C8	2.51	132.67	127.09
3	I	502	ADP	O2A-PA-O1A	2.50	124.08	112.44
3	F	602	ADP	C5-C4-N3	-2.49	123.28	126.72
3	E	502	ADP	O4'-C4'-C3'	2.46	110.04	105.15
3	K	502	ADP	O2A-PA-O1A	2.45	123.86	112.44
2	K	501	P3S	CB-CA-C	2.45	116.94	110.45
3	A	502	ADP	C6-C5-N7	2.45	136.81	132.09
3	G	602	ADP	C4-N9-C8	2.45	108.31	105.74
3	H	602	ADP	C2-N1-C6	2.44	122.74	118.73
3	H	602	ADP	C4-N9-C1'	-2.44	120.93	126.63
3	G	602	ADP	O2A-PA-O1A	2.43	123.75	112.44
3	H	602	ADP	N9-C8-N7	-2.43	110.49	113.94
3	F	602	ADP	N3-C4-N9	2.42	131.29	127.17
3	A	502	ADP	O3B-PB-O2B	2.41	116.85	107.80
3	E	502	ADP	N9-C8-N7	-2.40	110.52	113.94
3	G	602	ADP	C5-N7-C8	2.40	107.23	103.45
3	J	502	ADP	C5-N7-C8	2.40	107.23	103.45
3	F	602	ADP	C1'-N9-C8	2.39	132.40	127.09
3	L	502	ADP	C2-N1-C6	2.39	122.65	118.73
3	F	602	ADP	O3B-PB-O1B	2.38	120.11	110.83
3	L	502	ADP	N9-C8-N7	-2.36	110.59	113.94
3	L	502	ADP	O2B-PB-O3A	2.36	112.55	104.64
3	D	502	ADP	C6-C5-N7	2.35	136.62	132.09
3	I	502	ADP	C4-N9-C1'	-2.30	121.24	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	602	ADP	O3B-PB-O2B	2.30	116.42	107.80
3	K	502	ADP	O3B-PB-O1B	2.29	119.77	110.83
3	C	502	ADP	C4-N9-C1'	-2.29	121.27	126.63
3	H	602	ADP	O2A-PA-O1A	2.28	123.06	112.44
3	J	502	ADP	C2'-C1'-N9	2.28	118.96	113.30
3	J	502	ADP	O2A-PA-O1A	2.26	122.97	112.44
3	E	502	ADP	O2A-PA-O1A	2.25	122.92	112.44
3	J	502	ADP	O4'-C1'-C2'	-2.25	101.80	106.62
3	A	502	ADP	O2A-PA-O3A	-2.23	101.23	107.27
3	I	502	ADP	O2B-PB-O3A	2.22	112.09	104.64
3	J	502	ADP	N9-C8-N7	-2.22	110.79	113.94
3	H	602	ADP	C4-C5-N7	-2.21	108.06	110.58
3	G	602	ADP	O4'-C4'-C3'	2.18	109.49	105.15
3	E	502	ADP	C4-N9-C1'	-2.17	121.55	126.63
3	J	502	ADP	C6-C5-C4	-2.17	114.22	117.18
2	C	501	P3S	OT-C-O	-2.17	119.17	124.08
3	L	502	ADP	O2A-PA-O1A	2.16	122.47	112.44
3	H	602	ADP	C5-N7-C8	2.15	106.83	103.45
3	J	502	ADP	C1'-N9-C8	2.14	131.84	127.09
3	K	502	ADP	N3-C4-N9	2.13	130.79	127.17
3	J	502	ADP	O4'-C1'-N9	2.13	112.18	108.09
3	A	502	ADP	C4-N9-C1'	-2.12	121.67	126.63
2	F	601	P3S	CB-CA-N	-2.12	104.60	110.12
3	C	502	ADP	O3B-PB-O2B	2.11	115.72	107.80
3	I	502	ADP	C3'-C2'-C1'	-2.10	97.48	101.46
2	B	501	P3S	CE-SD-NE	2.10	114.83	107.48
3	A	502	ADP	C4-C5-N7	-2.08	108.20	110.58
3	F	602	ADP	O3'-C3'-C4'	-2.07	105.13	111.08
3	G	602	ADP	O3A-PB-O1B	-2.07	100.16	111.04
3	C	502	ADP	N9-C8-N7	-2.07	111.00	113.94
2	B	501	P3S	O3A-PA-O2A	2.06	114.66	106.57
3	B	502	ADP	O2A-PA-O1A	2.04	121.95	112.44
3	C	502	ADP	C4-C5-N7	-2.03	108.26	110.58
3	D	502	ADP	O2A-PA-O1A	2.03	121.89	112.44
2	B	501	P3S	OT-C-O	-2.02	119.49	124.08
3	L	502	ADP	C4-N9-C1'	-2.02	121.91	126.63
3	D	502	ADP	C4-C5-N7	-2.00	108.29	110.58

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	P3S	O-C-CA-N
3	B	502	ADP	PA-O3A-PB-O2B
3	D	502	ADP	PA-O3A-PB-O2B
3	E	502	ADP	PA-O3A-PB-O2B
3	H	602	ADP	PA-O3A-PB-O2B
3	I	502	ADP	PA-O3A-PB-O2B
3	J	502	ADP	PA-O3A-PB-O2B
3	K	502	ADP	PA-O3A-PB-O2B
3	L	502	ADP	PA-O3A-PB-O2B
2	F	601	P3S	OT-C-CA-CB
2	E	501	P3S	OT-C-CA-N
2	G	601	P3S	OT-C-CA-N
2	I	501	P3S	OT-C-CA-N
2	L	501	P3S	OT-C-CA-N
2	A	501	P3S	OT-C-CA-N
2	B	501	P3S	OT-C-CA-N
2	C	501	P3S	OT-C-CA-N
2	D	501	P3S	OT-C-CA-N
2	F	601	P3S	OT-C-CA-N
2	J	501	P3S	OT-C-CA-N
2	K	501	P3S	OT-C-CA-N
2	H	601	P3S	OT-C-CA-N
2	D	501	P3S	OT-C-CA-CB
2	H	601	P3S	OT-C-CA-CB
2	F	601	P3S	O-C-CA-CB
2	B	501	P3S	OT-C-CA-CB
2	D	501	P3S	O-C-CA-CB
2	H	601	P3S	O-C-CA-CB
2	K	501	P3S	OT-C-CA-CB
2	L	501	P3S	OT-C-CA-CB
3	F	602	ADP	O4'-C4'-C5'-O5'
3	L	502	ADP	O4'-C4'-C5'-O5'
3	L	502	ADP	C3'-C4'-C5'-O5'
3	A	502	ADP	PA-O3A-PB-O1B
3	C	502	ADP	PA-O3A-PB-O1B
2	J	501	P3S	OT-C-CA-CB
2	K	501	P3S	O-C-CA-CB
3	B	502	ADP	C2'-C1'-N9-C8
2	A	501	P3S	O-C-CA-CB
2	B	501	P3S	O-C-CA-CB
2	C	501	P3S	OT-C-CA-CB
2	C	501	P3S	O-C-CA-CB
2	E	501	P3S	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	I	501	P3S	O-C-CA-CB
2	J	501	P3S	O-C-CA-CB
2	L	501	P3S	O-C-CA-CB
2	B	501	P3S	O-C-CA-N
2	C	501	P3S	O-C-CA-N
2	D	501	P3S	O-C-CA-N
2	E	501	P3S	O-C-CA-N
2	F	601	P3S	O-C-CA-N
2	G	601	P3S	O-C-CA-N
2	H	601	P3S	O-C-CA-N
2	I	501	P3S	O-C-CA-N
2	J	501	P3S	O-C-CA-N
2	K	501	P3S	O-C-CA-N
2	L	501	P3S	O-C-CA-N
2	A	501	P3S	OT-C-CA-CB
2	E	501	P3S	OT-C-CA-CB
2	G	601	P3S	O-C-CA-CB
2	I	501	P3S	OT-C-CA-CB
3	A	502	ADP	C2'-C1'-N9-C8
2	G	601	P3S	OT-C-CA-CB
3	C	502	ADP	C2'-C1'-N9-C8
3	D	502	ADP	C2'-C1'-N9-C8
3	E	502	ADP	C2'-C1'-N9-C8
3	F	602	ADP	C2'-C1'-N9-C8
3	G	602	ADP	C2'-C1'-N9-C8
3	H	602	ADP	C2'-C1'-N9-C8
3	I	502	ADP	C2'-C1'-N9-C8
3	J	502	ADP	C2'-C1'-N9-C8
3	K	502	ADP	C2'-C1'-N9-C8
3	L	502	ADP	C2'-C1'-N9-C8
3	F	602	ADP	C5'-O5'-PA-O1A
3	F	602	ADP	C5'-O5'-PA-O2A
3	F	602	ADP	C5'-O5'-PA-O3A
3	H	602	ADP	C5'-O5'-PA-O3A
3	G	602	ADP	PA-O3A-PB-O1B
3	H	602	ADP	PA-O3A-PB-O1B
3	J	502	ADP	O4'-C4'-C5'-O5'
3	K	502	ADP	O4'-C1'-N9-C8
3	D	502	ADP	O4'-C1'-N9-C8
3	I	502	ADP	O4'-C1'-N9-C8
3	B	502	ADP	PA-O3A-PB-O1B
3	E	502	ADP	PA-O3A-PB-O1B

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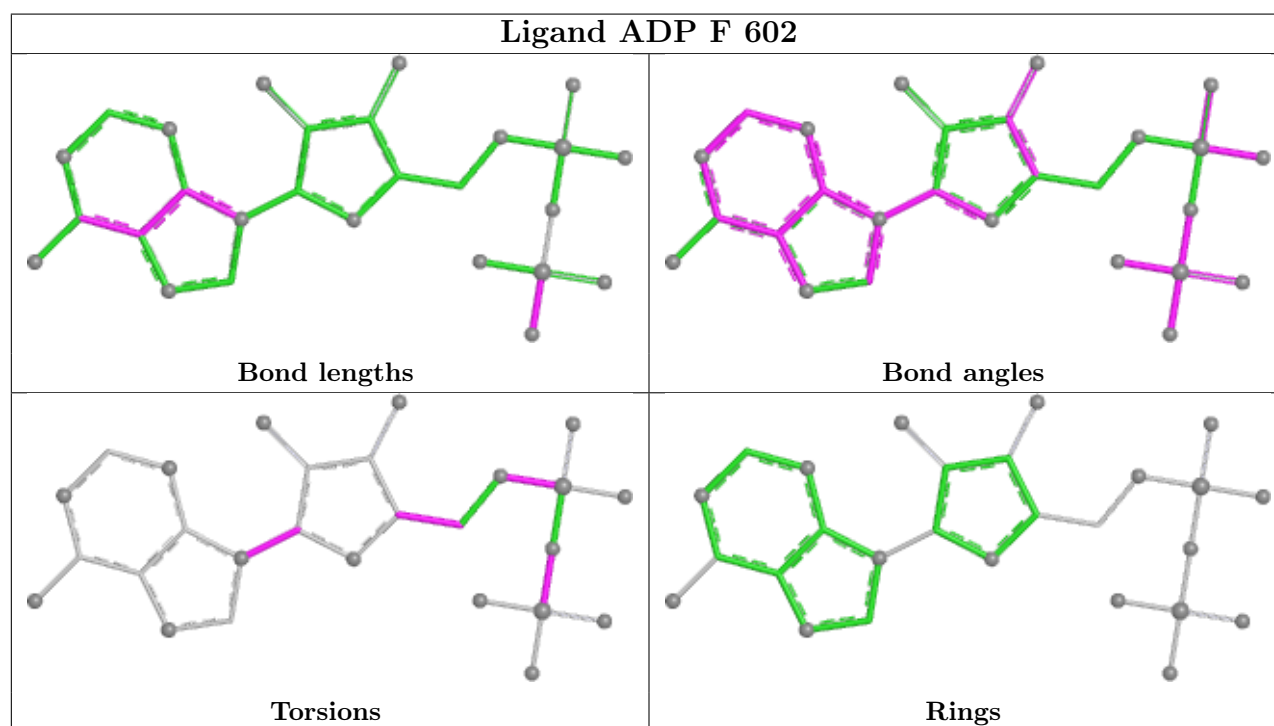
Mol	Chain	Res	Type	Atoms
3	F	602	ADP	PA-O3A-PB-O1B
3	K	502	ADP	PA-O3A-PB-O1B
3	D	502	ADP	PA-O3A-PB-O3B
3	H	602	ADP	PA-O3A-PB-O3B
3	J	502	ADP	PA-O3A-PB-O3B
3	L	502	ADP	PA-O3A-PB-O3B
3	A	502	ADP	O4'-C1'-N9-C8
3	E	502	ADP	O4'-C1'-N9-C8
3	F	602	ADP	O4'-C1'-N9-C8
3	H	602	ADP	O4'-C1'-N9-C8
3	J	502	ADP	O4'-C1'-N9-C8
3	L	502	ADP	O4'-C1'-N9-C8
3	D	502	ADP	O4'-C4'-C5'-O5'
3	H	602	ADP	O4'-C4'-C5'-O5'
3	C	502	ADP	O4'-C1'-N9-C8
3	G	602	ADP	O4'-C1'-N9-C8
3	B	502	ADP	C2'-C1'-N9-C4
3	F	602	ADP	C2'-C1'-N9-C4
3	J	502	ADP	C2'-C1'-N9-C4
3	L	502	ADP	PA-O3A-PB-O1B
3	B	502	ADP	O4'-C1'-N9-C8
3	I	502	ADP	O4'-C4'-C5'-O5'

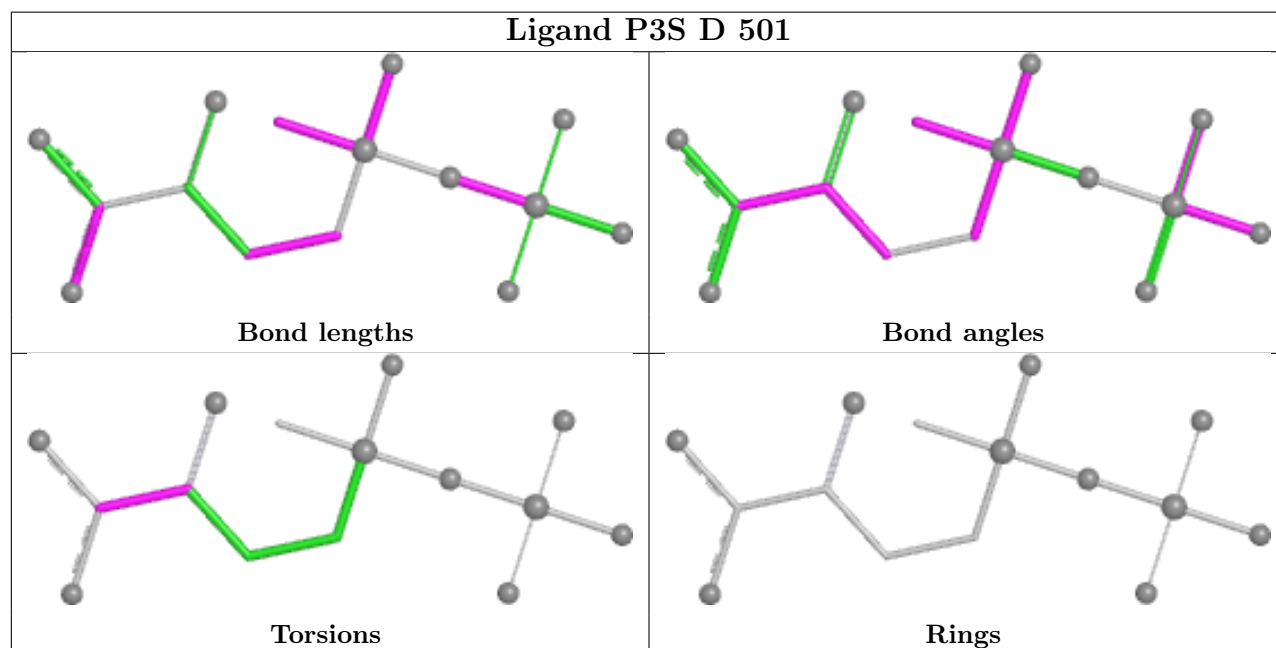
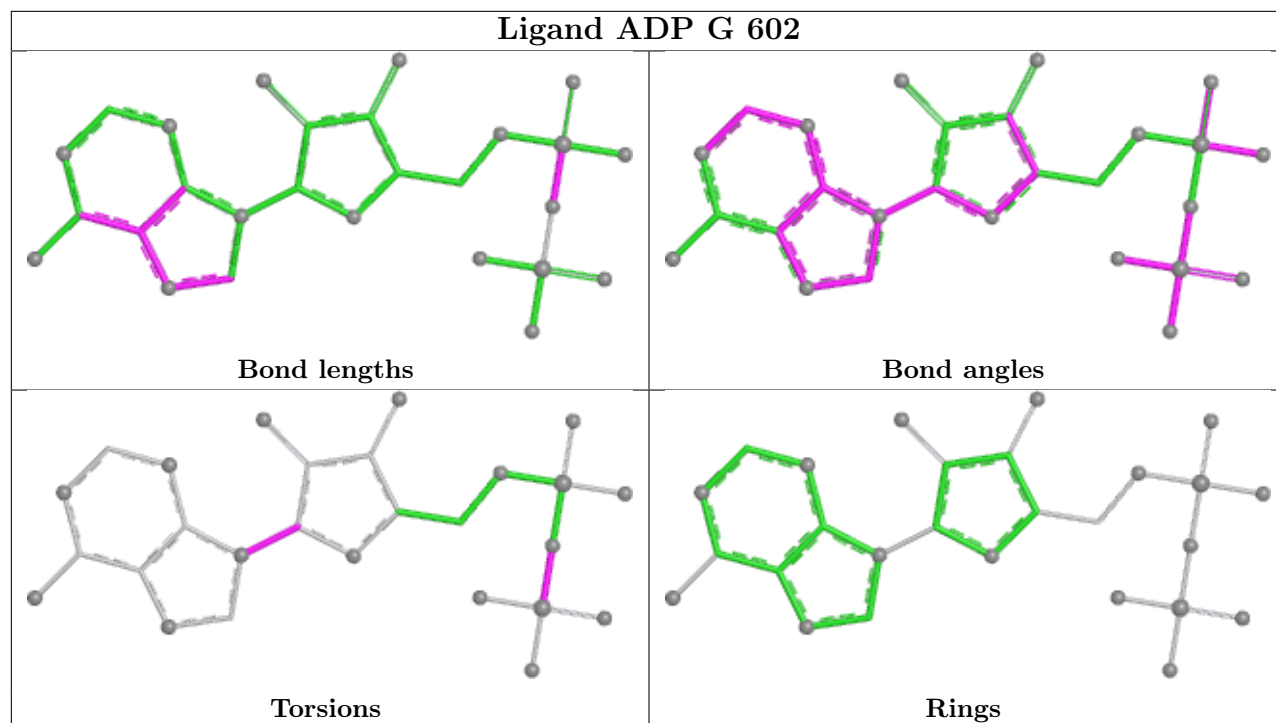
There are no ring outliers.

14 monomers are involved in 52 short contacts:

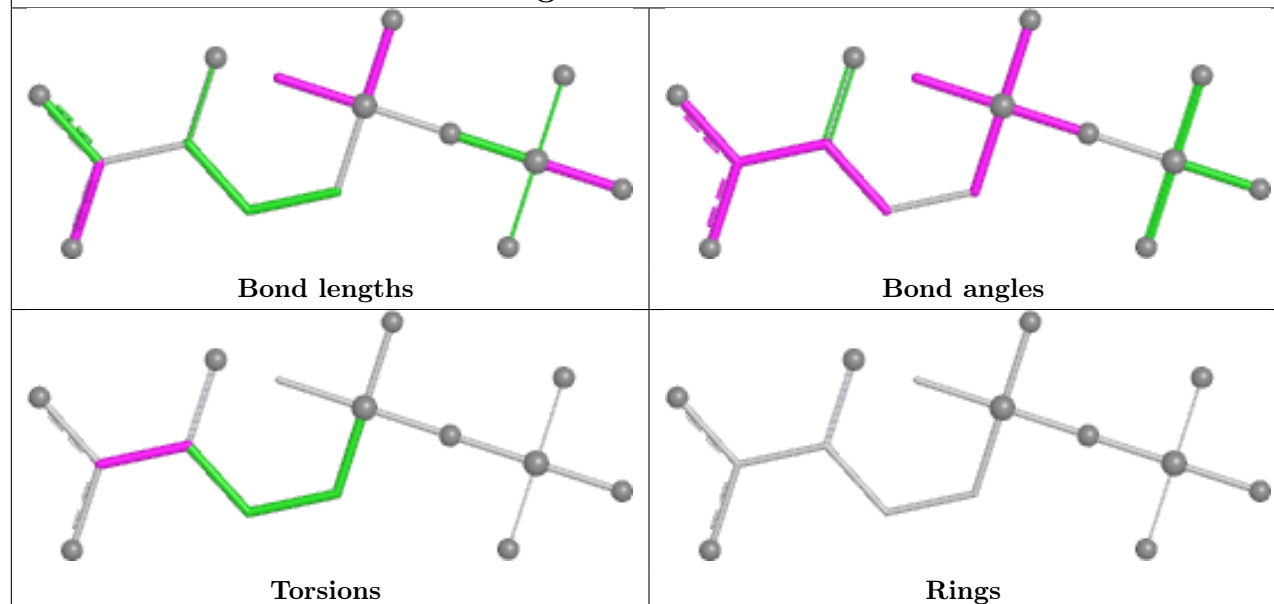
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	602	ADP	1	0
2	D	501	P3S	7	0
2	G	601	P3S	7	0
2	F	601	P3S	5	0
2	H	601	P3S	6	0
2	K	501	P3S	4	0
2	B	501	P3S	2	0
2	L	501	P3S	1	0
2	C	501	P3S	5	0
2	A	501	P3S	5	0
2	J	501	P3S	3	0
3	E	502	ADP	1	0
2	E	501	P3S	2	0
2	I	501	P3S	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

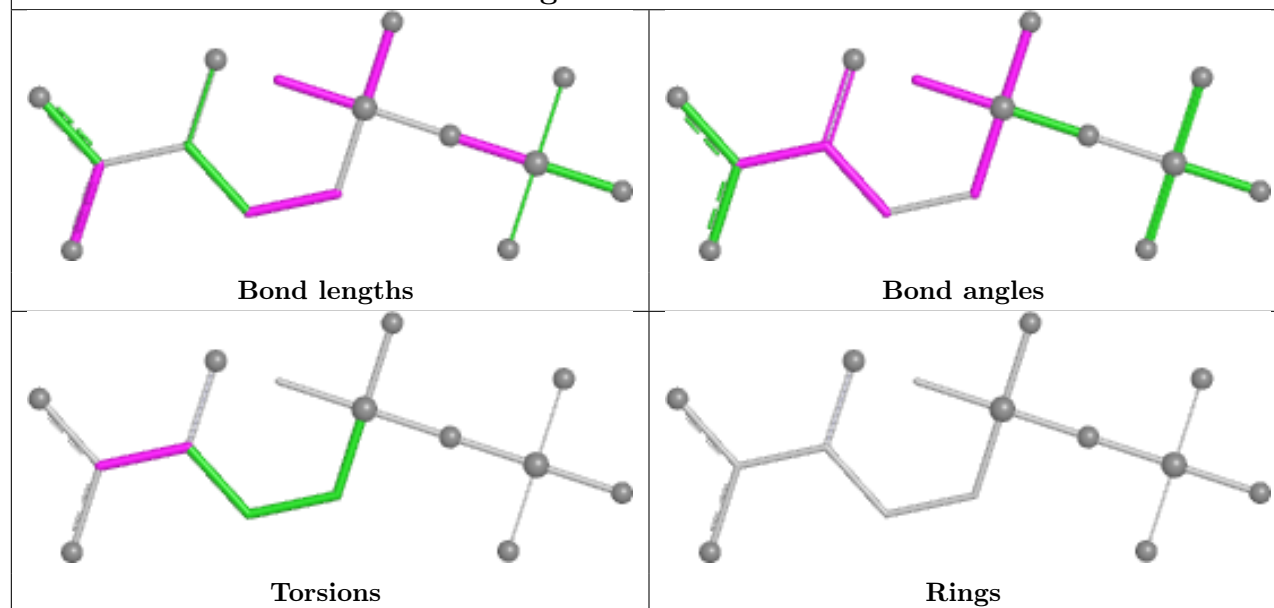


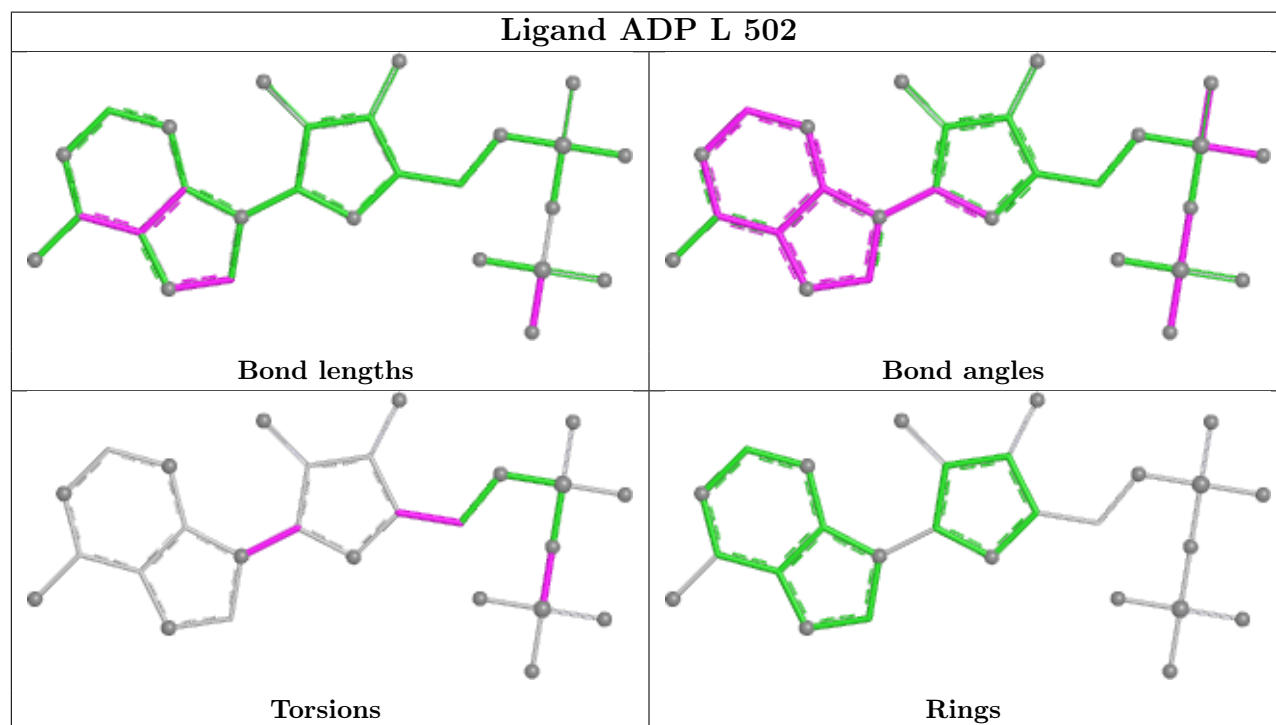
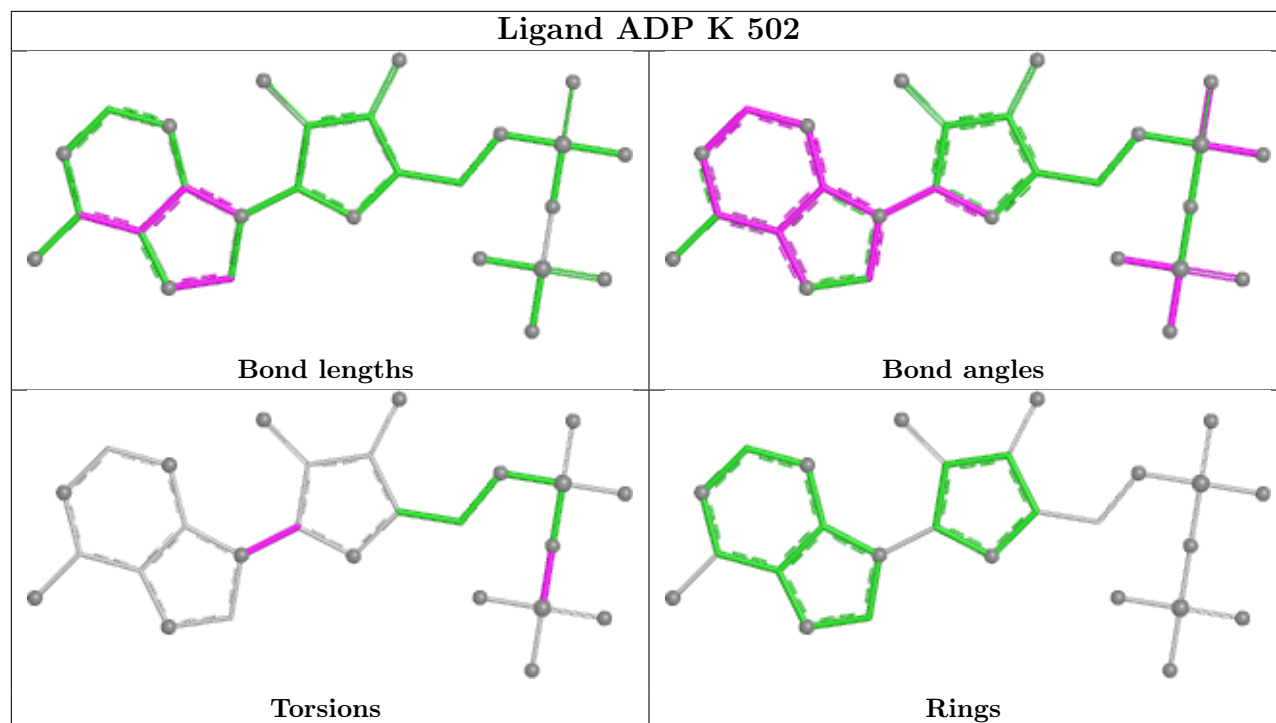


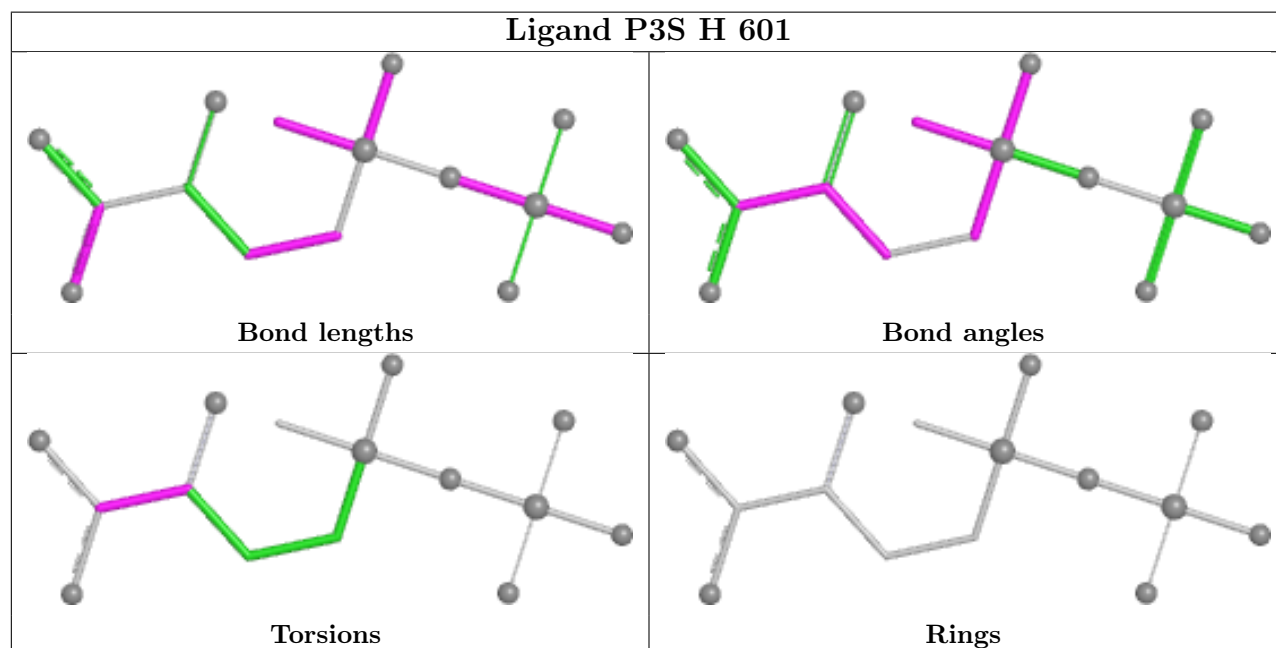
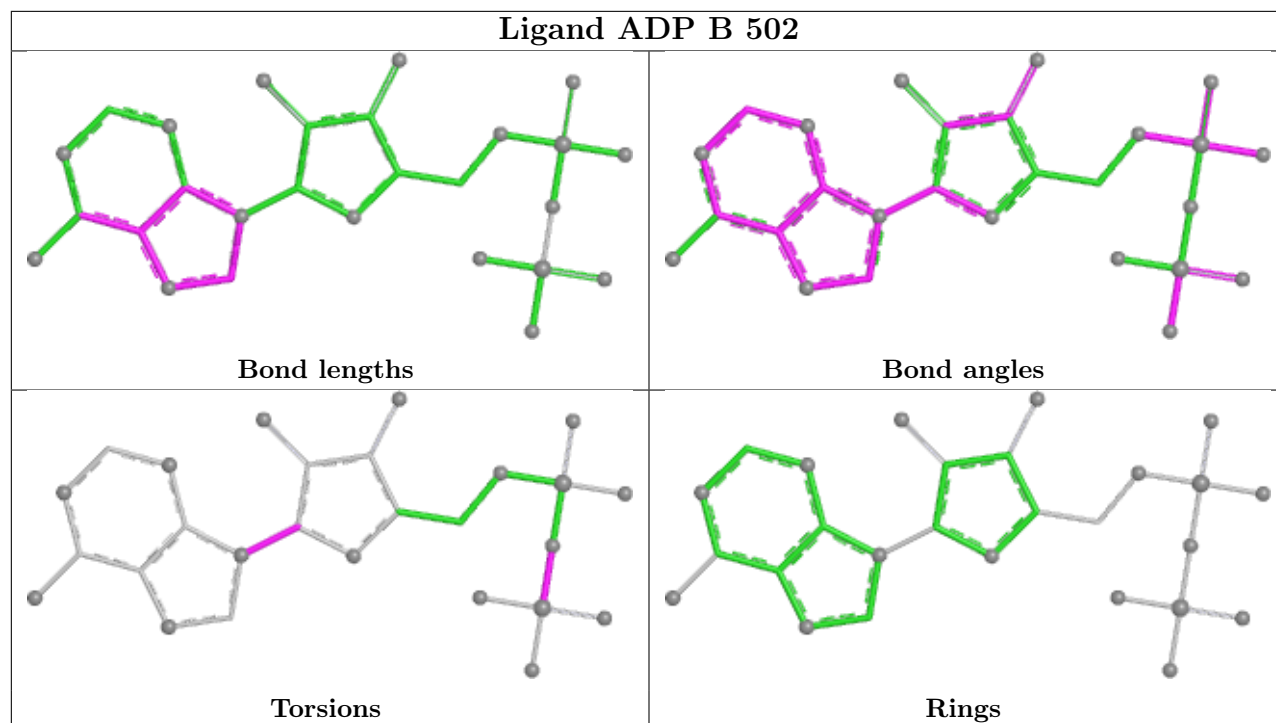
Ligand P3S G 601



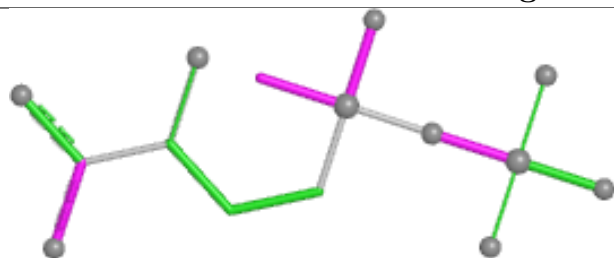
Ligand P3S F 601



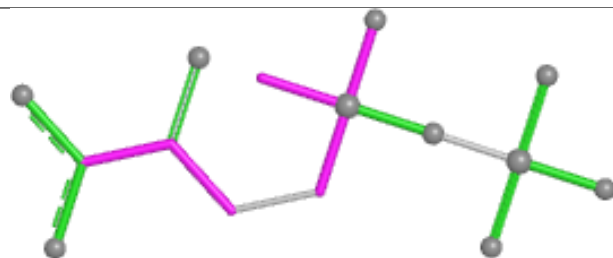




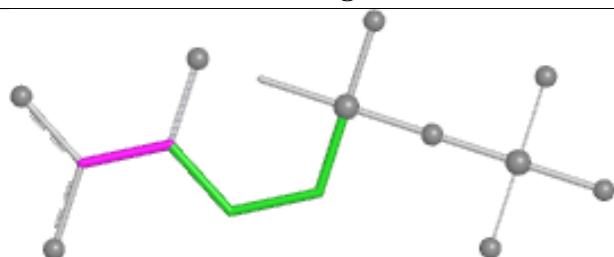
Ligand P3S K 501



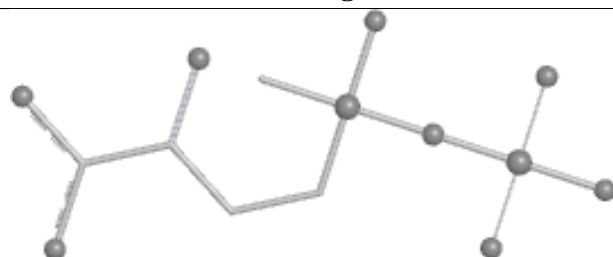
Bond lengths



Bond angles

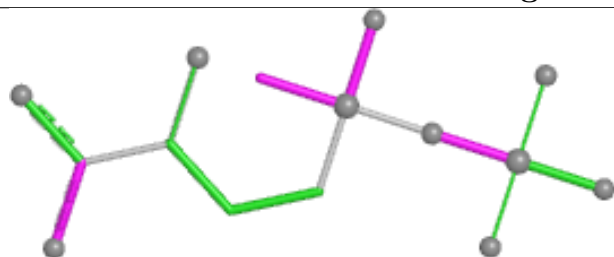


Torsions

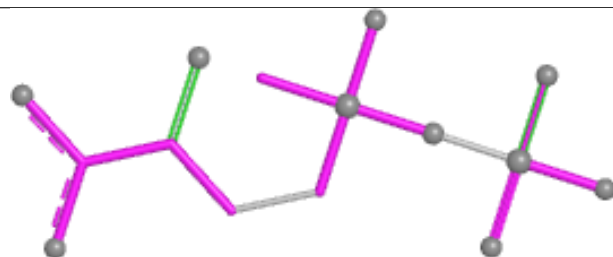


Rings

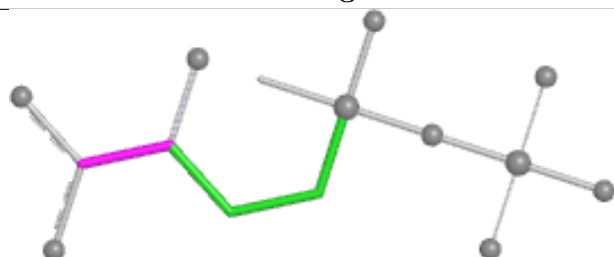
Ligand P3S B 501



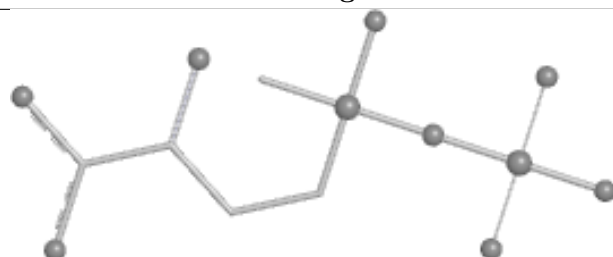
Bond lengths



Bond angles

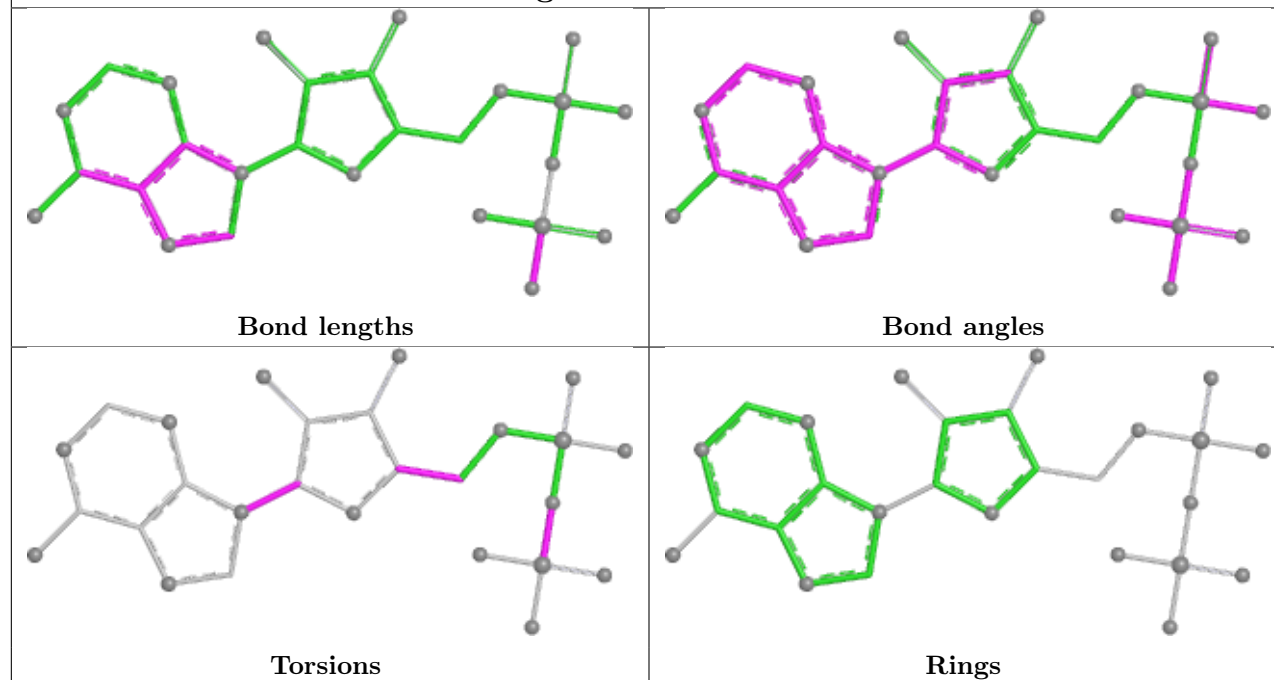


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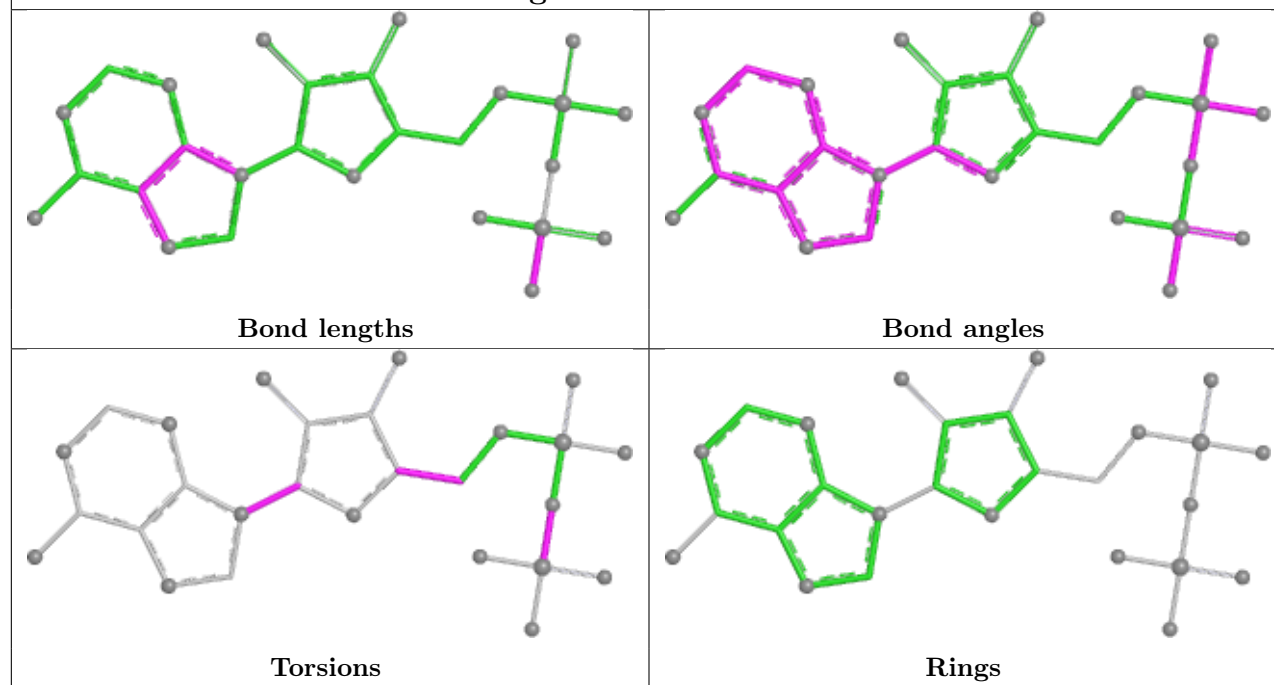


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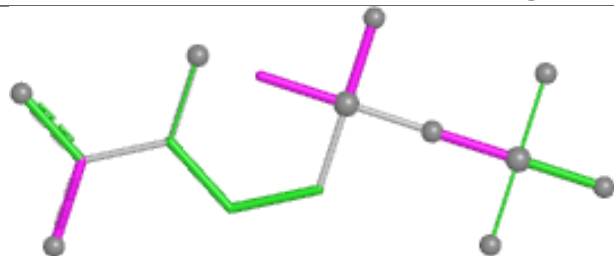
Ligand ADP I 502



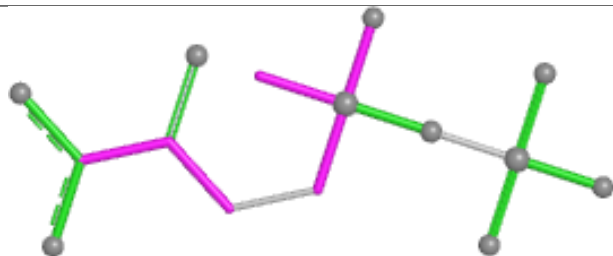
Ligand ADP D 502



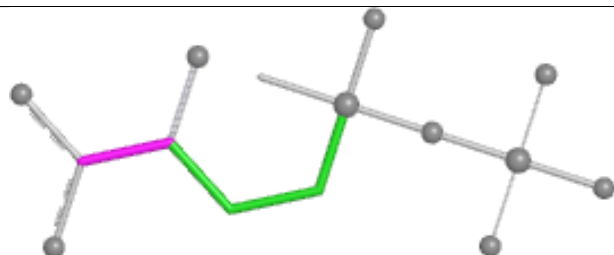
Ligand P3S L 501



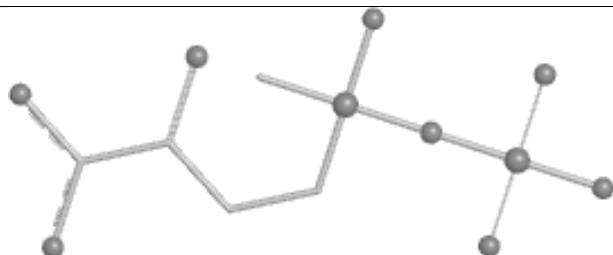
Bond lengths



Bond angles

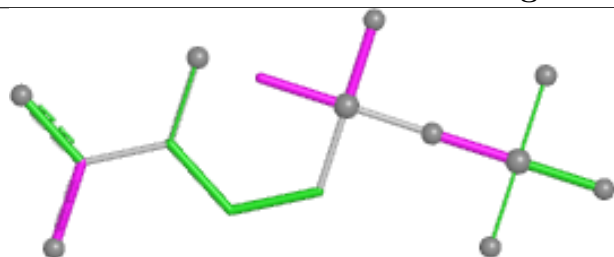


Torsions

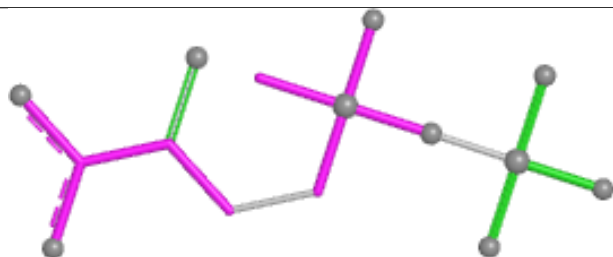


Rings

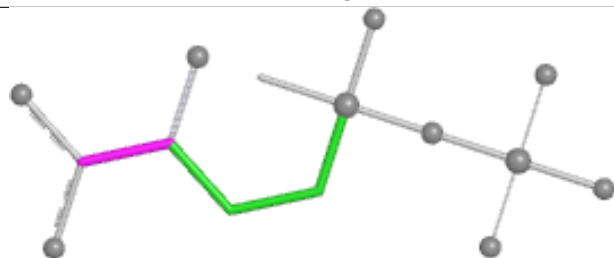
Ligand P3S C 501



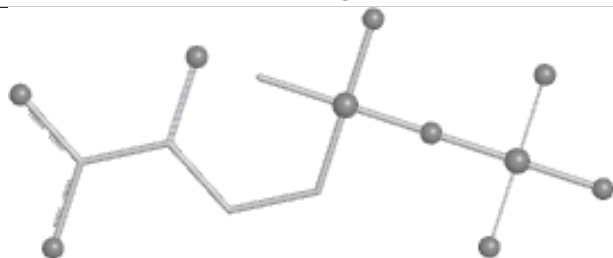
Bond lengths



Bond angles

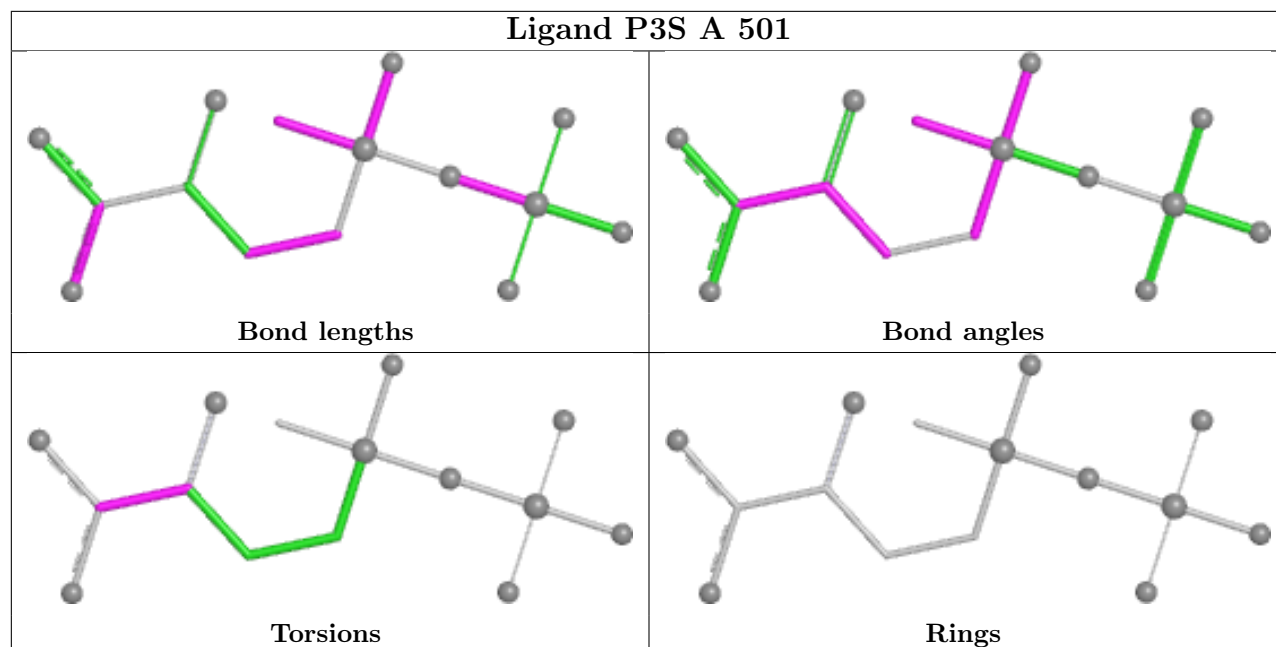


Torsions

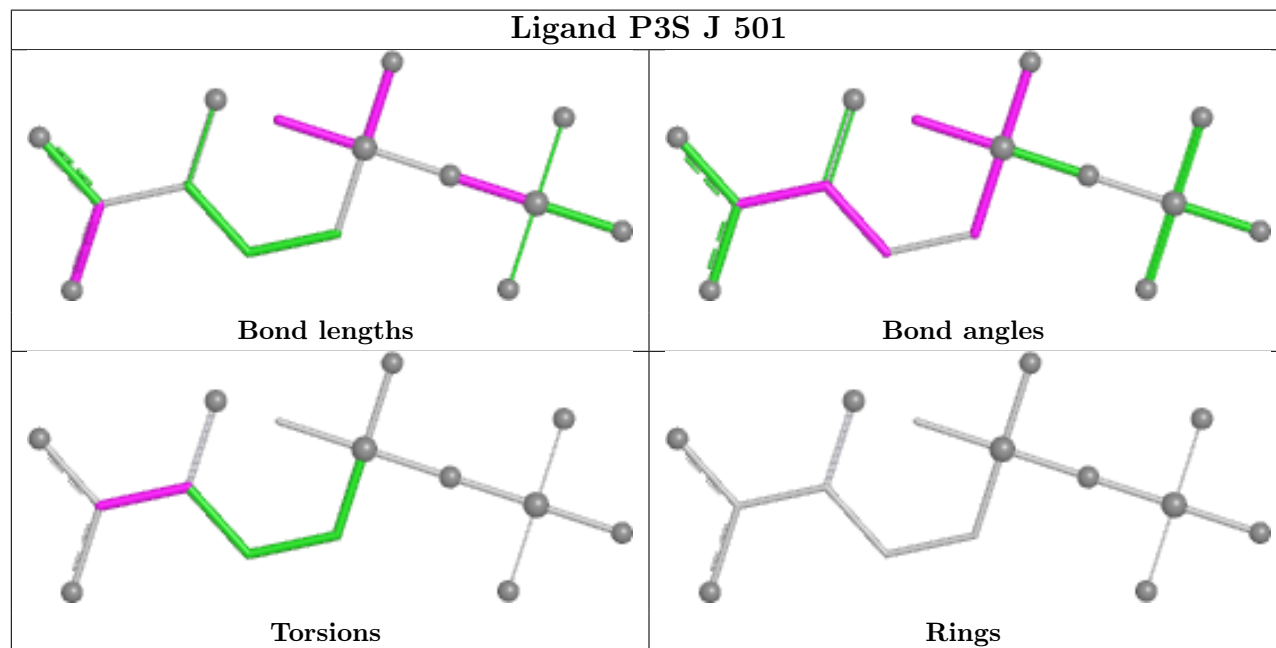


Rings

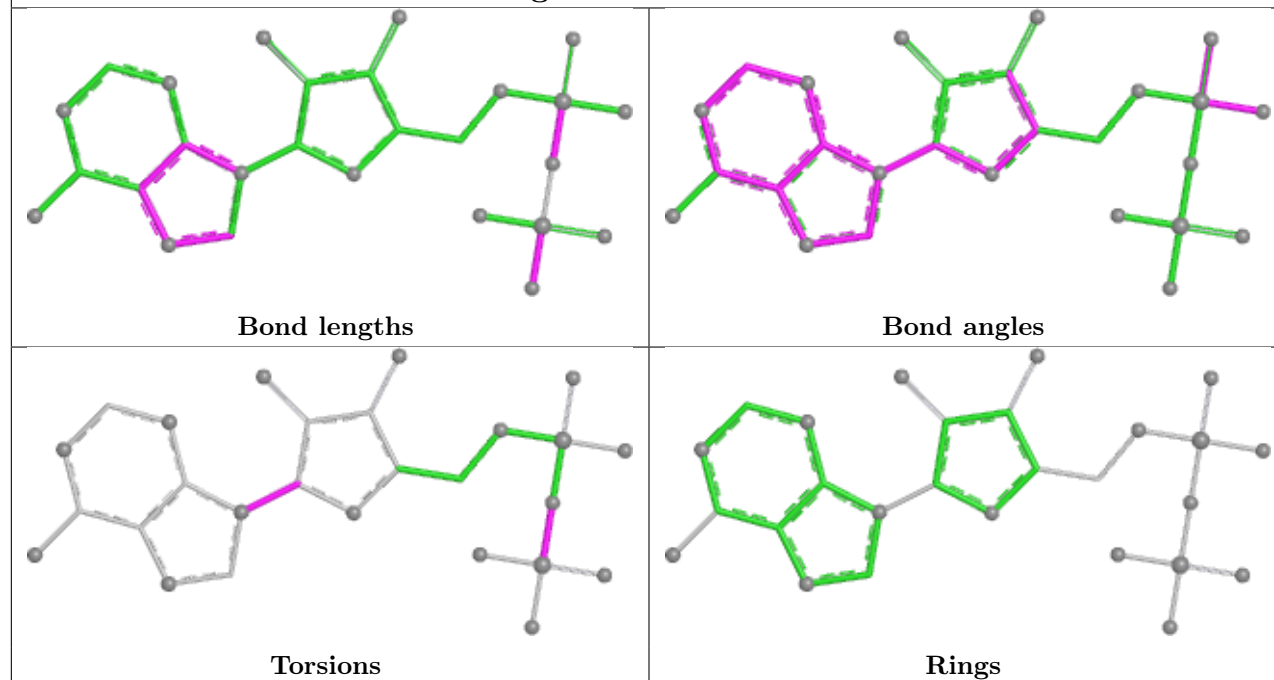
Ligand P3S A 501



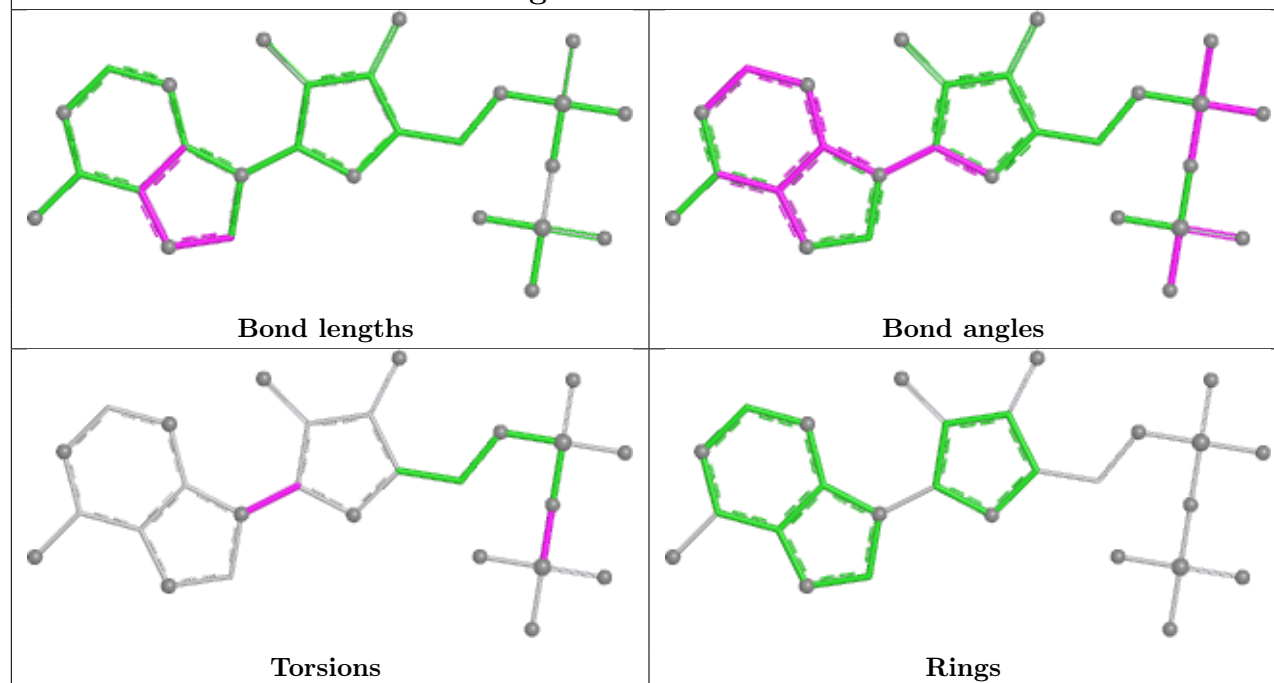
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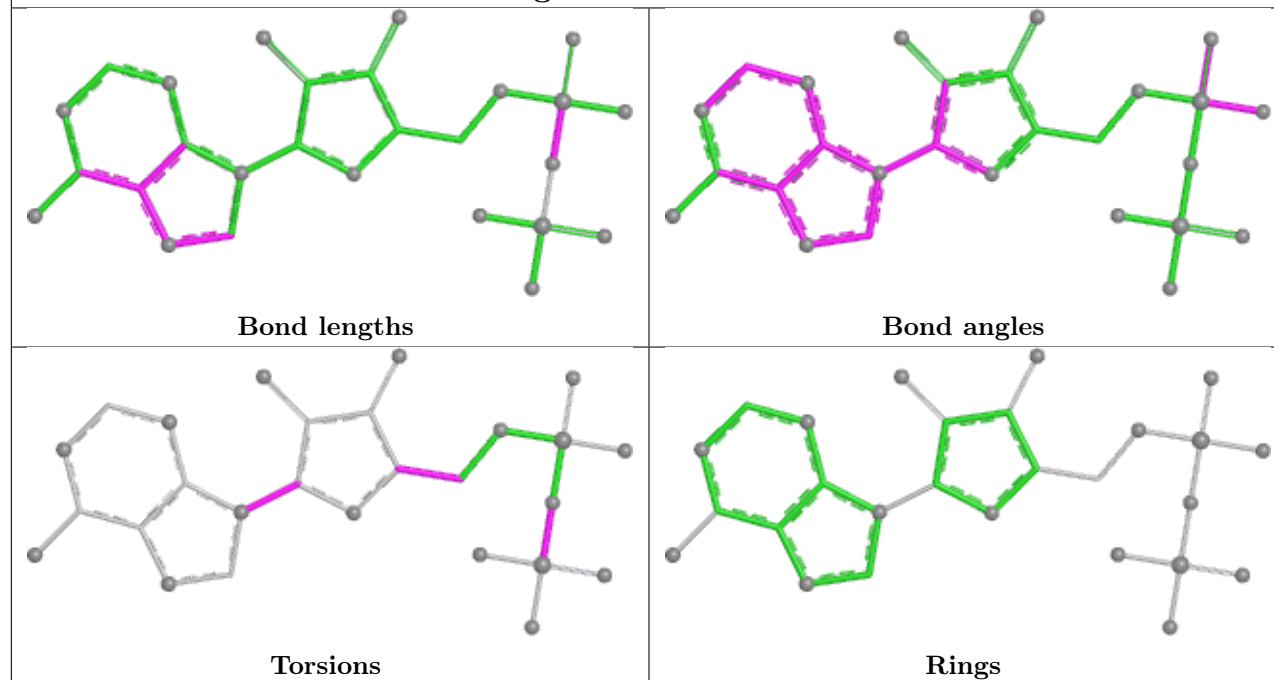
Ligand ADP E 502



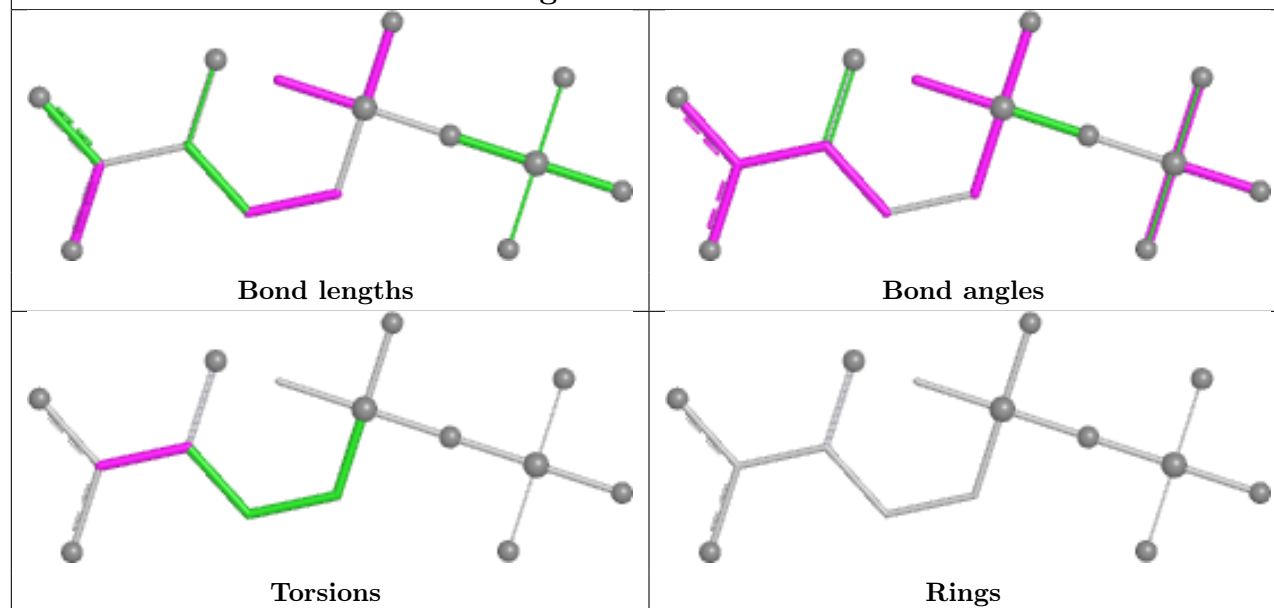
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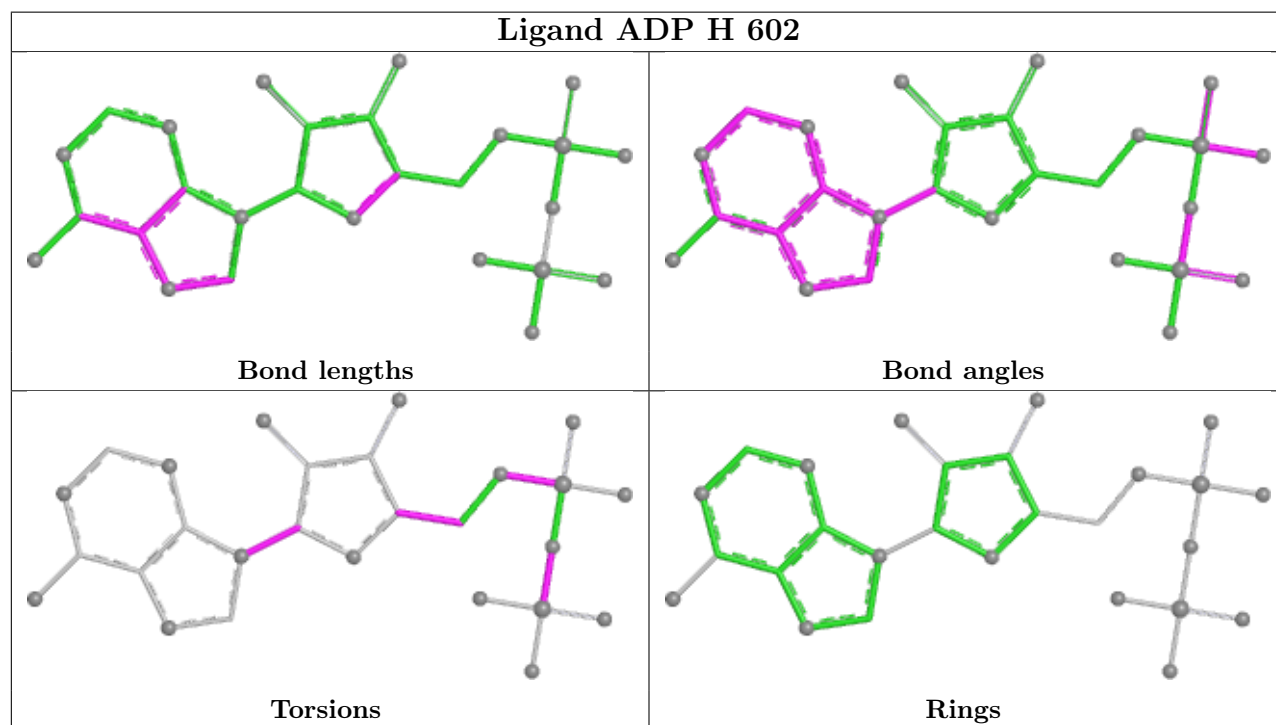
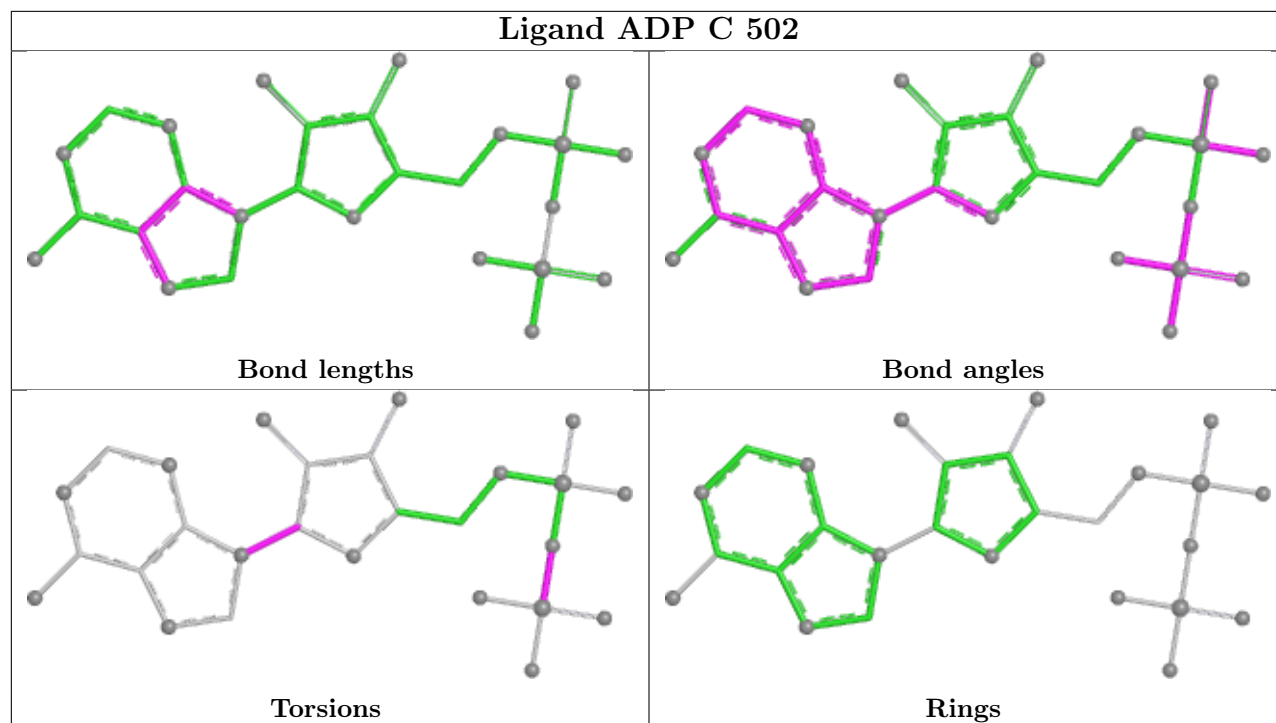


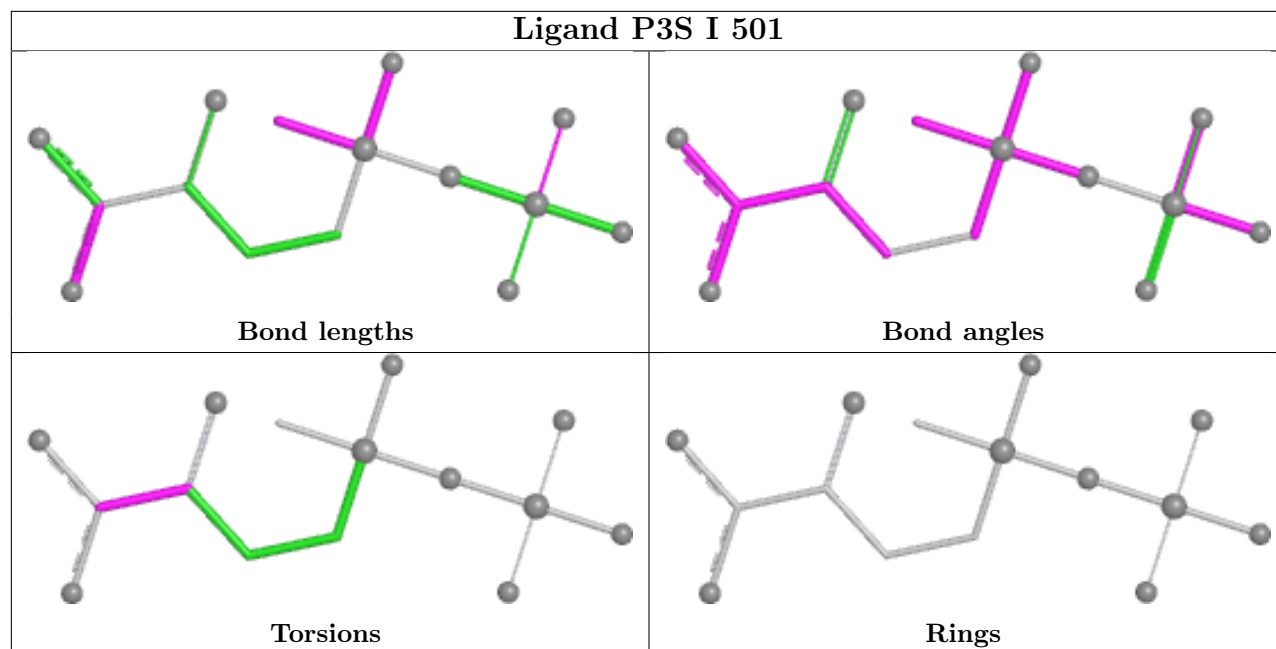
Ligand ADP J 502



Ligand P3S E 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/443 (100%)	-0.55	2 (0%) 87 86	8, 20, 46, 82	0
1	B	443/443 (100%)	-0.56	2 (0%) 87 86	9, 20, 49, 83	0
1	C	443/443 (100%)	-0.55	0 100 100	8, 20, 48, 73	0
1	D	443/443 (100%)	-0.55	0 100 100	8, 20, 45, 73	0
1	E	443/443 (100%)	-0.59	1 (0%) 91 90	6, 20, 45, 74	0
1	F	443/443 (100%)	-0.52	2 (0%) 87 86	8, 21, 48, 83	0
1	G	443/443 (100%)	-0.53	2 (0%) 87 86	8, 21, 49, 75	0
1	H	443/443 (100%)	-0.55	2 (0%) 87 86	7, 21, 46, 78	0
1	I	443/443 (100%)	-0.56	1 (0%) 91 90	7, 20, 46, 77	0
1	J	441/443 (99%)	-0.59	0 100 100	7, 20, 43, 67	0
1	K	443/443 (100%)	-0.54	2 (0%) 87 86	8, 21, 47, 74	0
1	L	443/443 (100%)	-0.49	2 (0%) 87 86	9, 22, 49, 83	0
All	All	5314/5316 (99%)	-0.55	16 (0%) 90 89	6, 20, 48, 83	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	ALA	5.5
1	K	17	ASN	3.9
1	L	2	ALA	3.8
1	A	2	ALA	3.8
1	K	2	ALA	3.5
1	B	2	ALA	3.2
1	E	2	ALA	2.8
1	H	2	ALA	2.8
1	G	2	ALA	2.5
1	F	384	GLY	2.5
1	H	384	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	87	GLY	2.3
1	G	3	LYS	2.2
1	I	2	ALA	2.1
1	B	254	GLY	2.1
1	A	377	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	P3S	A	501	15/15	0.97	0.08	8,16,28,34	0
2	P3S	E	501	15/15	0.97	0.08	7,15,26,33	0
2	P3S	K	501	15/15	0.97	0.07	10,15,21,23	0
2	P3S	L	501	15/15	0.97	0.07	13,18,26,32	0
4	MG	B	504	1/1	0.97	0.10	4,4,4,4	0
4	MG	F	605	1/1	0.97	0.08	5,5,5,5	0
2	P3S	G	601	15/15	0.98	0.07	13,24,38,39	0
2	P3S	H	601	15/15	0.98	0.07	9,13,21,26	0
2	P3S	I	501	15/15	0.98	0.07	9,13,27,28	0
2	P3S	J	501	15/15	0.98	0.07	8,16,22,24	0
2	P3S	C	501	15/15	0.98	0.06	4,13,27,40	0
2	P3S	D	501	15/15	0.98	0.07	8,18,34,41	0
3	ADP	A	502	27/27	0.98	0.06	14,18,24,25	0
3	ADP	B	502	27/27	0.98	0.06	11,19,23,28	0
3	ADP	D	502	27/27	0.98	0.06	11,19,28,32	0
4	MG	A	504	1/1	0.98	0.07	4,4,4,4	0
4	MG	A	505	1/1	0.98	0.11	6,6,6,6	0
2	P3S	B	501	15/15	0.98	0.07	7,15,22,31	0

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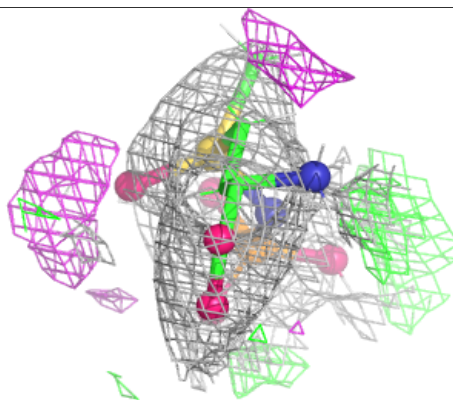
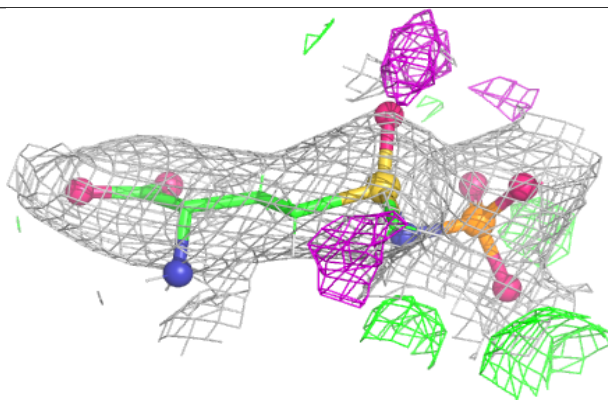
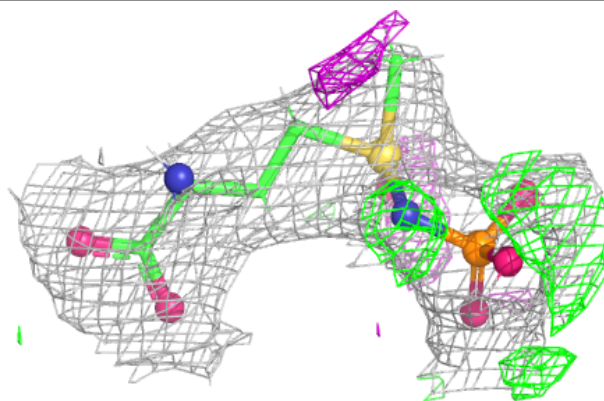
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	B	505	1/1	0.98	0.09	7,7,7,7	0
4	MG	D	505	1/1	0.98	0.11	1,1,1,1	0
4	MG	E	504	1/1	0.98	0.10	3,3,3,3	0
4	MG	E	505	1/1	0.98	0.09	4,4,4,4	0
2	P3S	F	601	15/15	0.98	0.07	12,21,32,45	0
4	MG	G	603	1/1	0.98	0.07	4,4,4,4	0
4	MG	J	503	1/1	0.98	0.14	5,5,5,5	0
3	ADP	C	502	27/27	0.99	0.05	11,18,21,23	0
3	ADP	E	502	27/27	0.99	0.05	8,15,23,31	0
4	MG	B	503	1/1	0.99	0.14	0,0,0,0	0
3	ADP	F	602	27/27	0.99	0.05	10,20,27,30	0
3	ADP	G	602	27/27	0.99	0.05	16,22,31,32	0
4	MG	C	503	1/1	0.99	0.13	0,0,0,0	0
4	MG	C	505	1/1	0.99	0.09	5,5,5,5	0
4	MG	D	503	1/1	0.99	0.12	5,5,5,5	0
4	MG	D	504	1/1	0.99	0.03	2,2,2,2	0
3	ADP	H	602	27/27	0.99	0.05	11,18,23,25	0
4	MG	E	503	1/1	0.99	0.12	1,1,1,1	0
3	ADP	I	502	27/27	0.99	0.05	13,18,25,26	0
3	ADP	J	502	27/27	0.99	0.05	13,18,24,33	0
3	ADP	K	502	27/27	0.99	0.05	8,15,22,25	0
3	ADP	L	502	27/27	0.99	0.06	16,24,35,37	0
4	MG	G	604	1/1	0.99	0.07	10,10,10,10	0
4	MG	G	605	1/1	0.99	0.09	7,7,7,7	0
4	MG	H	604	1/1	0.99	0.07	5,5,5,5	0
4	MG	I	503	1/1	0.99	0.10	0,0,0,0	0
4	MG	I	505	1/1	0.99	0.08	6,6,6,6	0
4	MG	A	503	1/1	0.99	0.11	4,4,4,4	0
4	MG	J	505	1/1	0.99	0.10	0,0,0,0	0
4	MG	K	504	1/1	0.99	0.06	5,5,5,5	0
4	MG	K	505	1/1	0.99	0.10	1,1,1,1	0
4	MG	L	503	1/1	0.99	0.08	2,2,2,2	0
4	MG	L	504	1/1	0.99	0.06	7,7,7,7	0
4	MG	L	505	1/1	0.99	0.05	0,0,0,0	0
4	MG	J	504	1/1	1.00	0.06	4,4,4,4	0
4	MG	F	603	1/1	1.00	0.07	5,5,5,5	0
4	MG	K	503	1/1	1.00	0.09	0,0,0,0	0
4	MG	H	605	1/1	1.00	0.10	1,1,1,1	0
4	MG	F	604	1/1	1.00	0.08	6,6,6,6	0
4	MG	I	504	1/1	1.00	0.07	5,5,5,5	0
4	MG	C	504	1/1	1.00	0.04	6,6,6,6	0
4	MG	H	603	1/1	1.00	0.10	1,1,1,1	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.

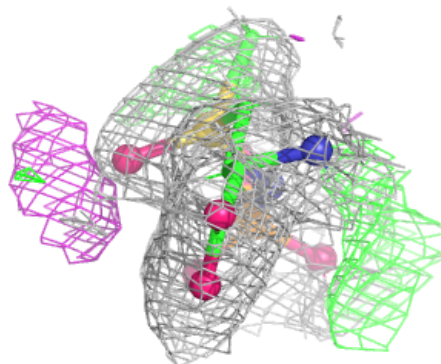
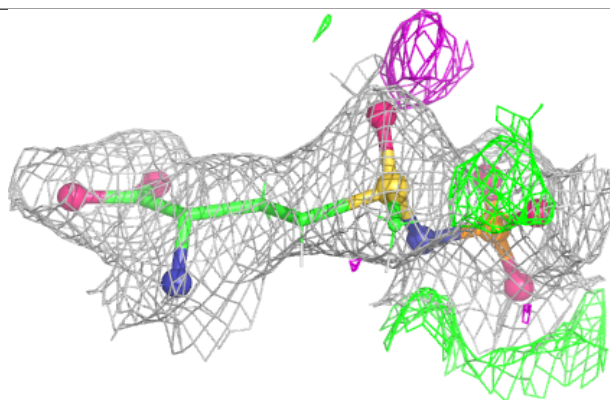
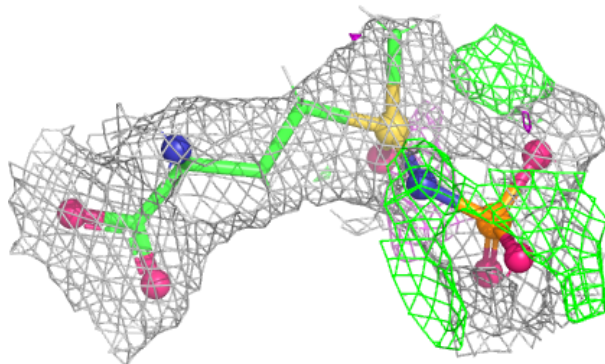
Electron density around P3S A 501:

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

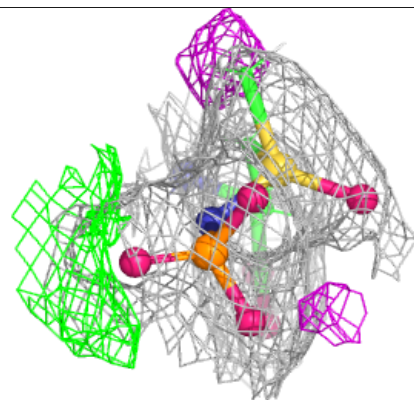
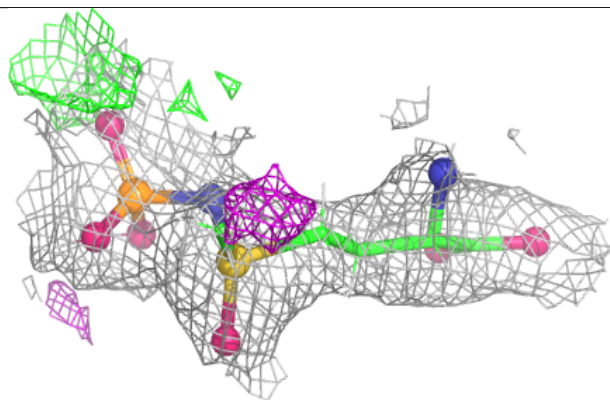
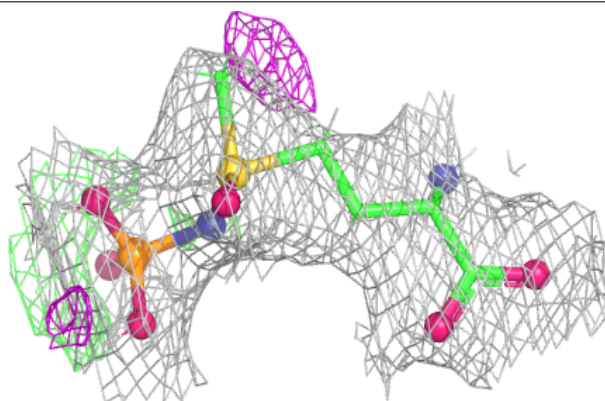


Electron density around P3S E 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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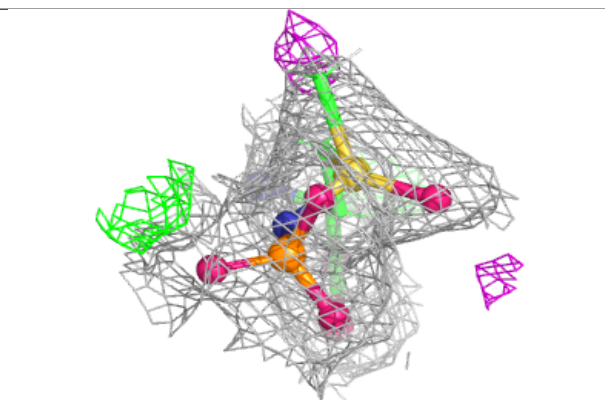
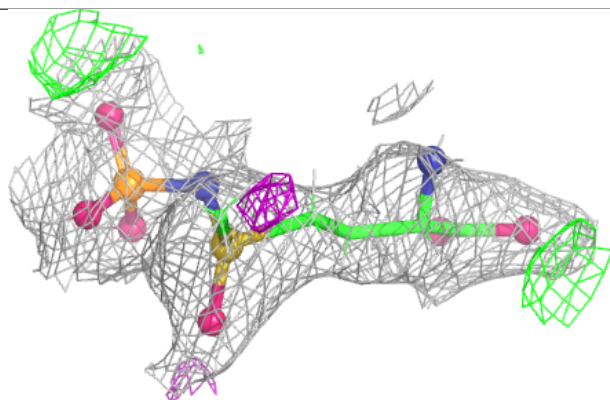
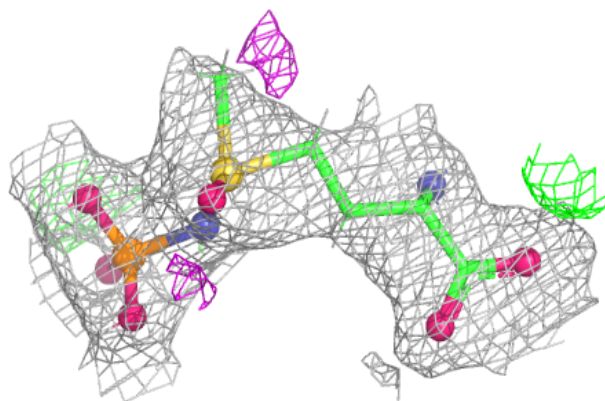
**Electron density around P3S K 501:**

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and green (positive)

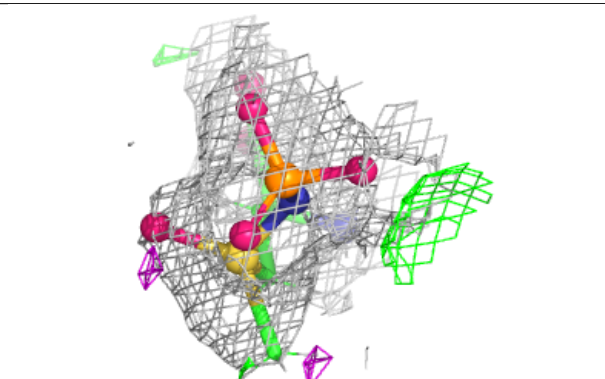
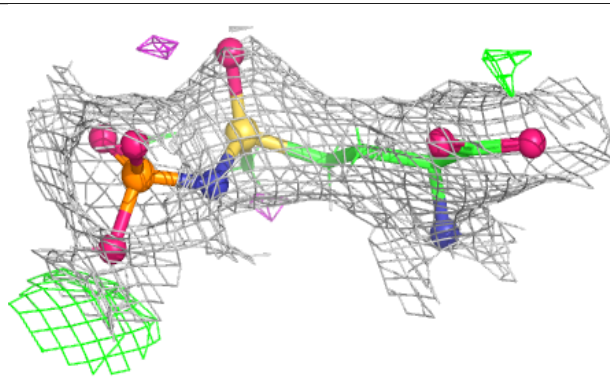
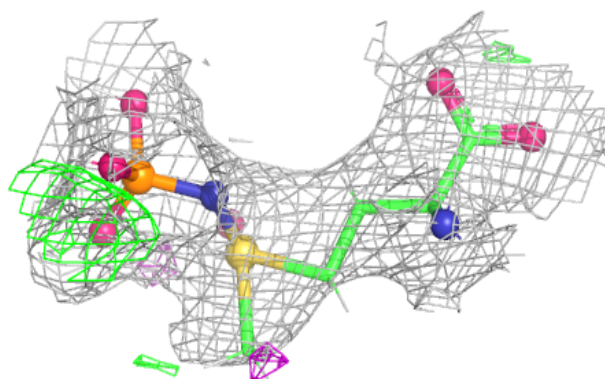


Electron density around P3S L 501:

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and green (positive)

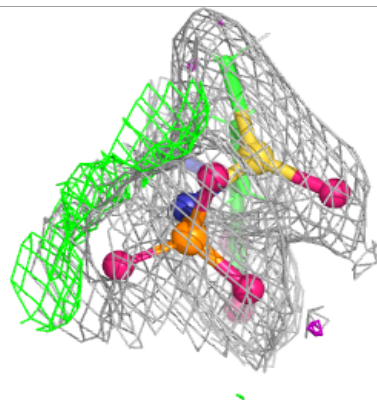
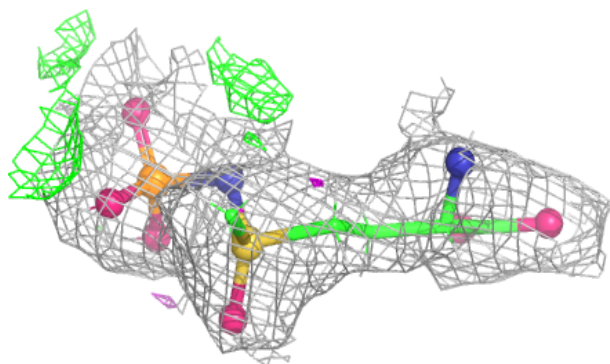
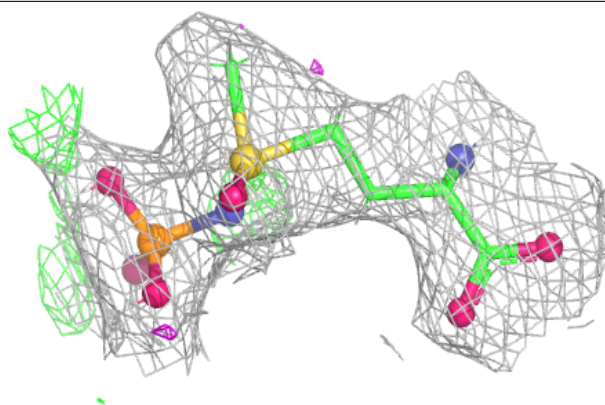
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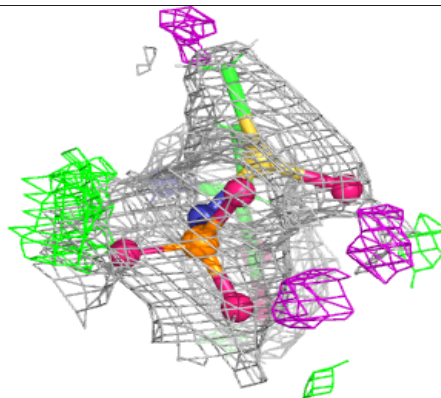
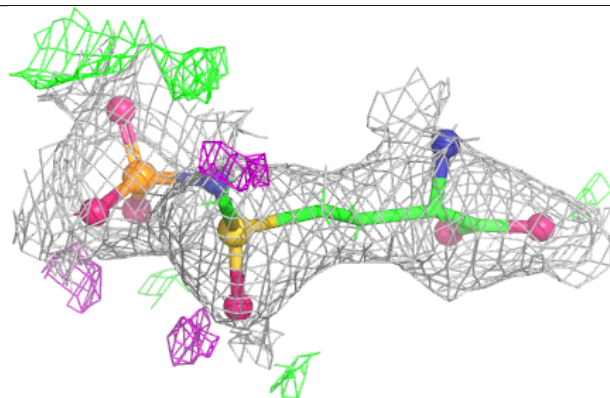
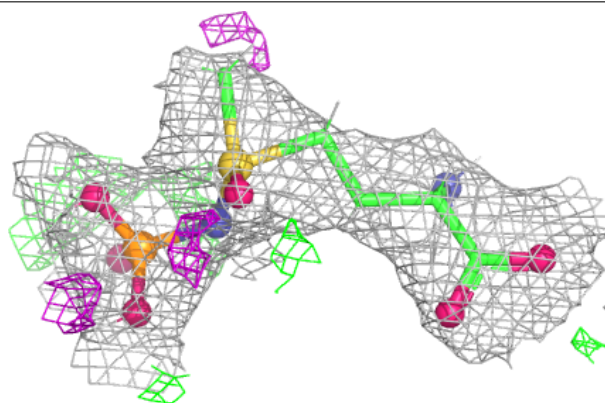


Electron density around P3S H 601:

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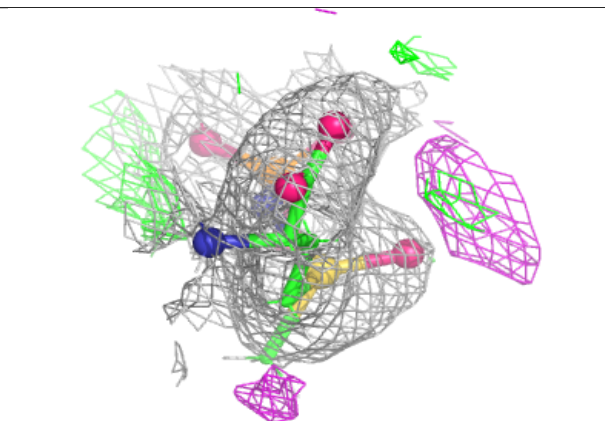
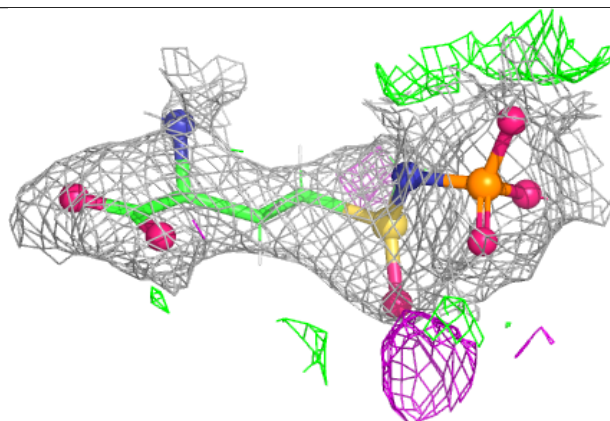
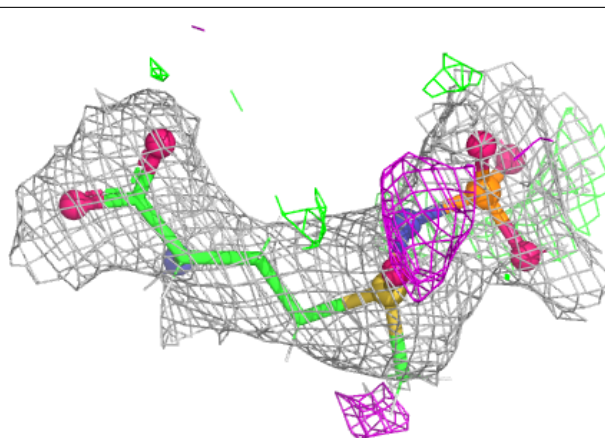
**Electron density around P3S I 501:**

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and green (positive)

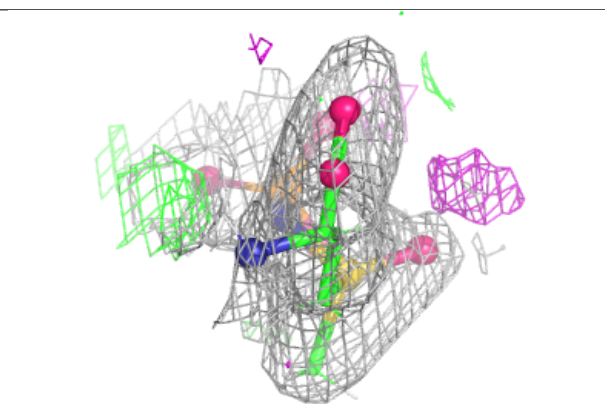
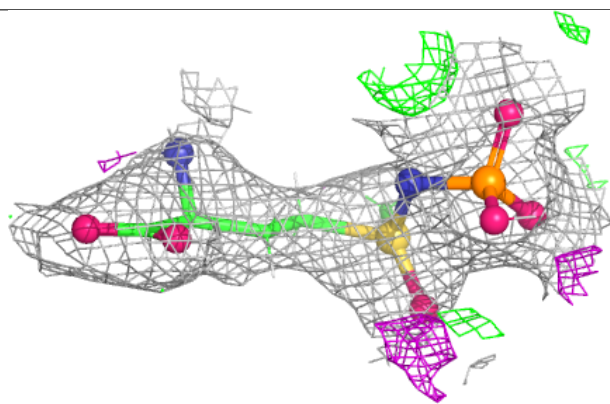
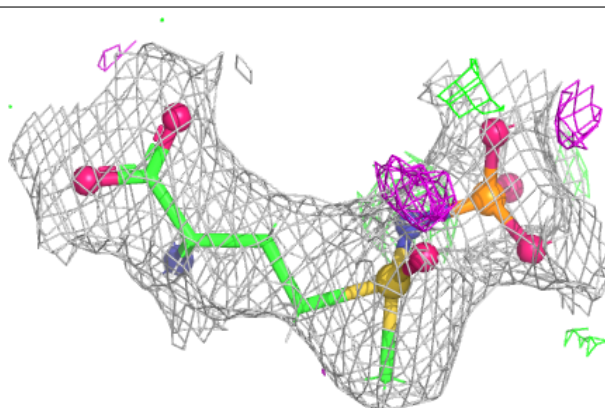


Electron density around P3S J 501:

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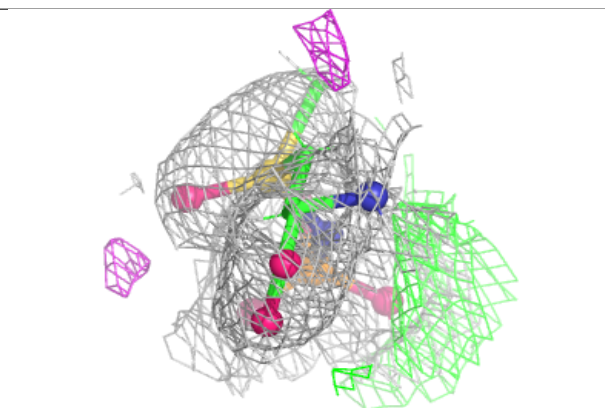
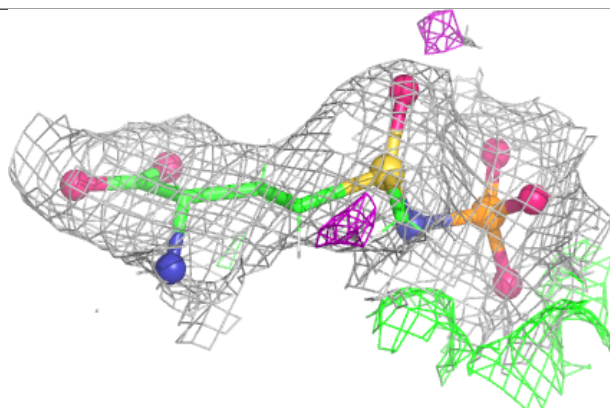
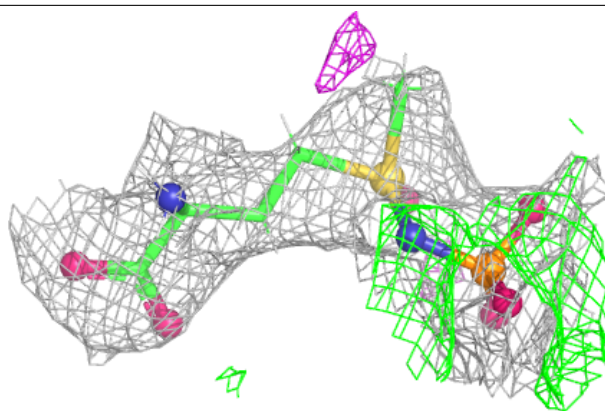
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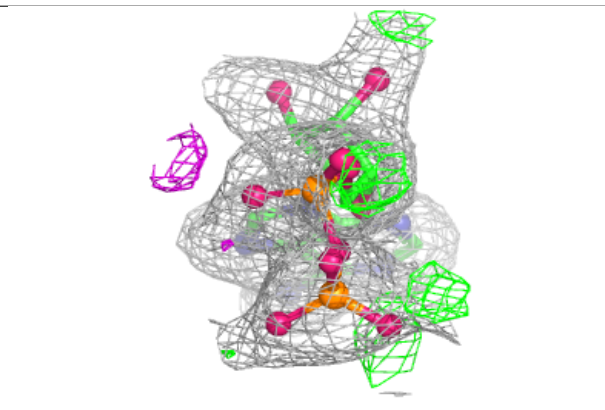
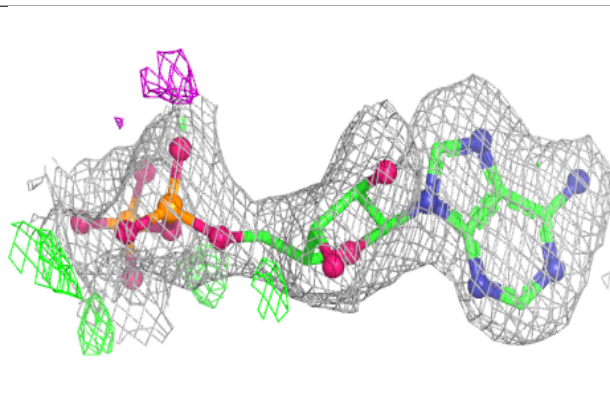
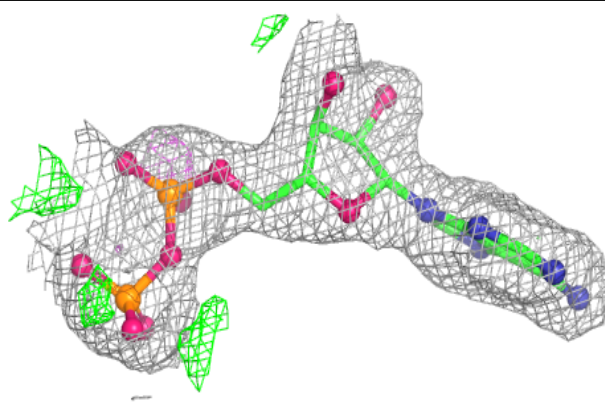


Electron density around P3S D 501:

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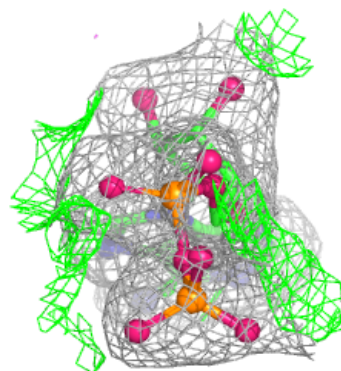
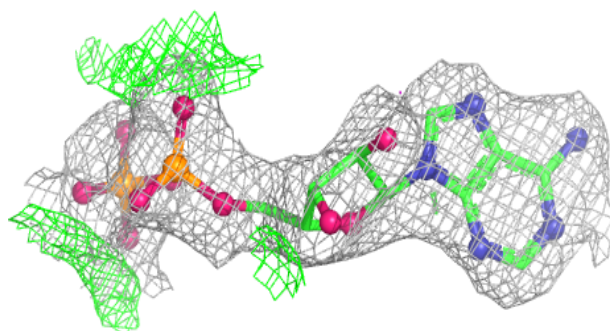
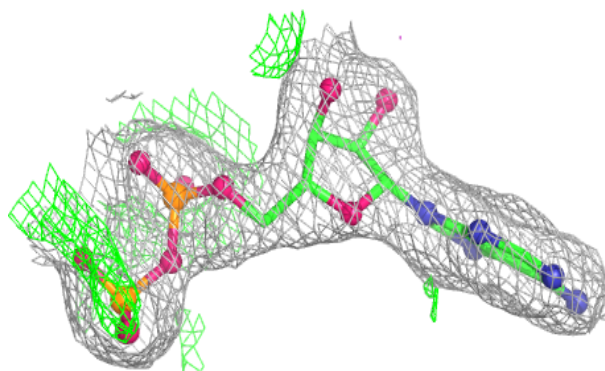
**Electron density around ADP A 502:**

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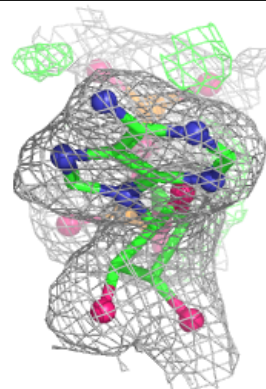
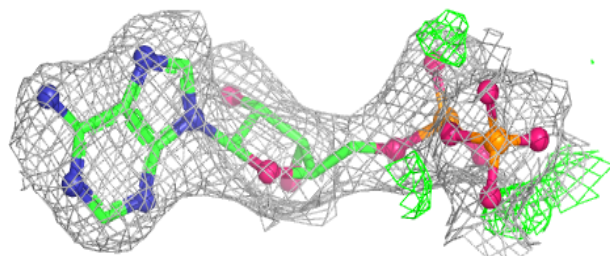
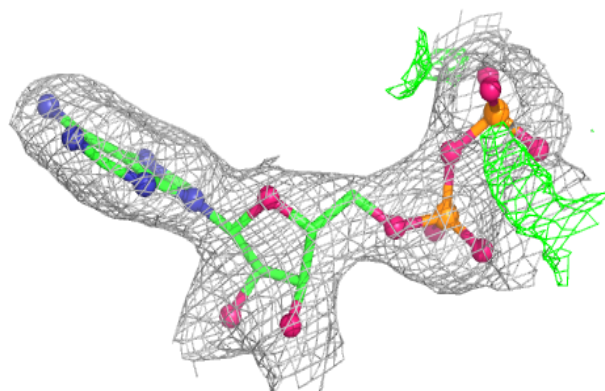


Electron density around ADP B 502:

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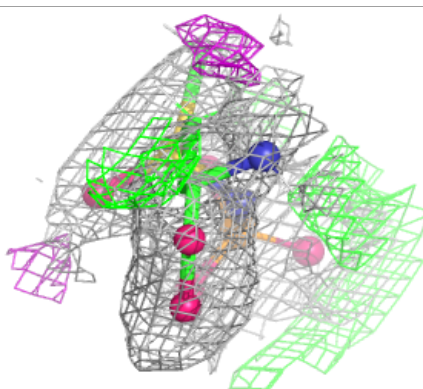
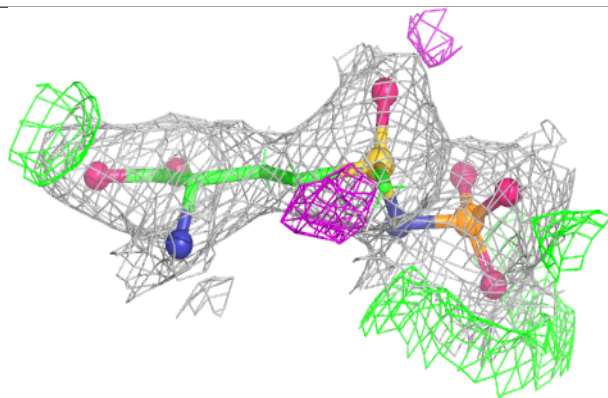
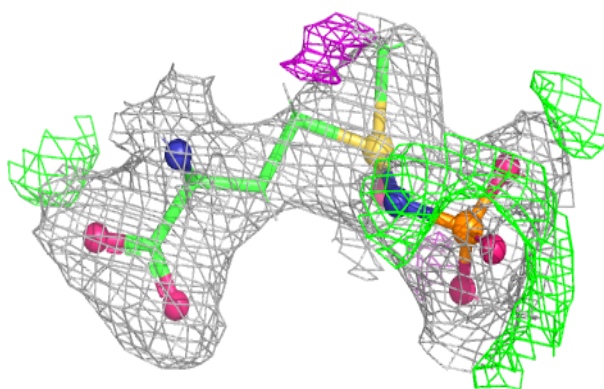
**Electron density around ADP D 502:**

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

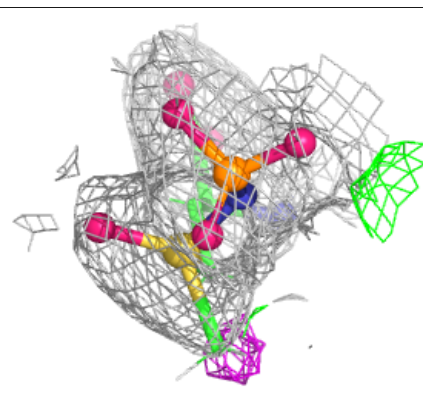
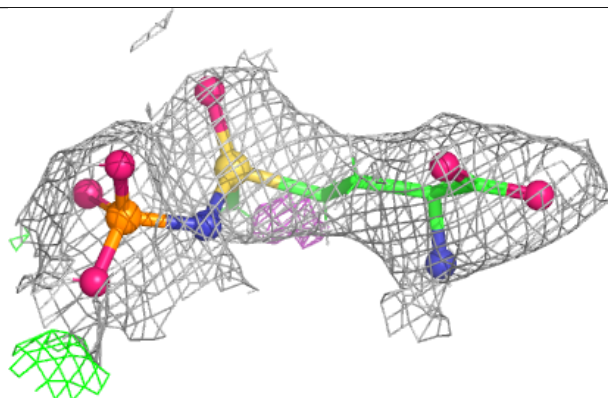
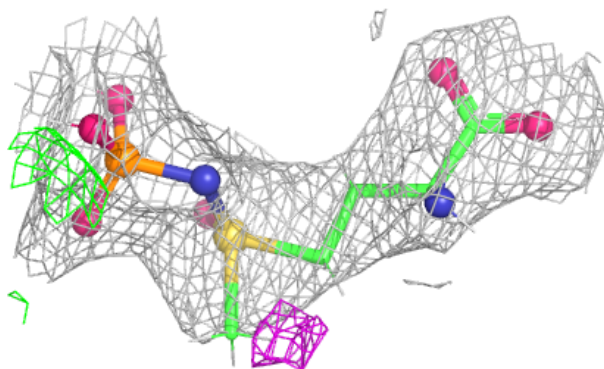


Electron density around P3S B 501:

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

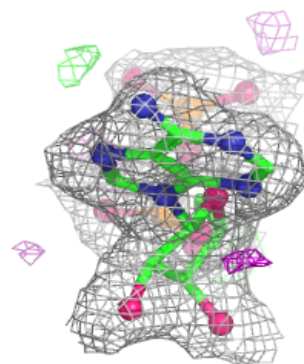
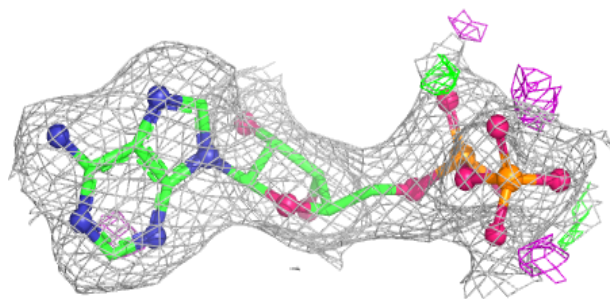
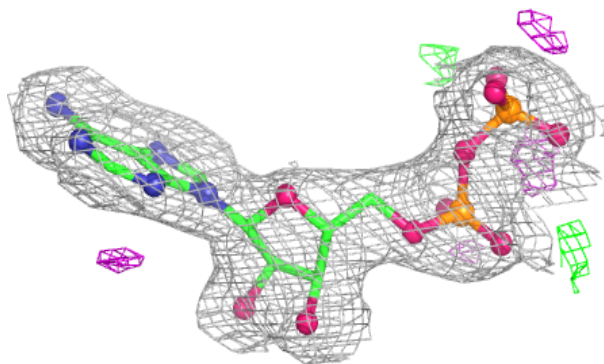
**Electron density around P3S F 601:**

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

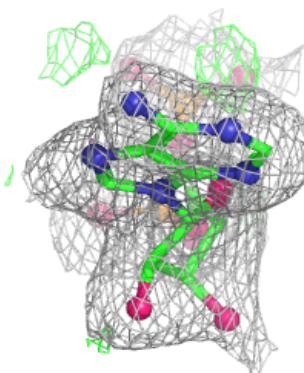
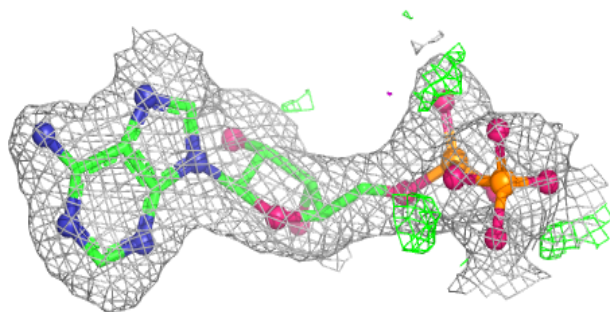
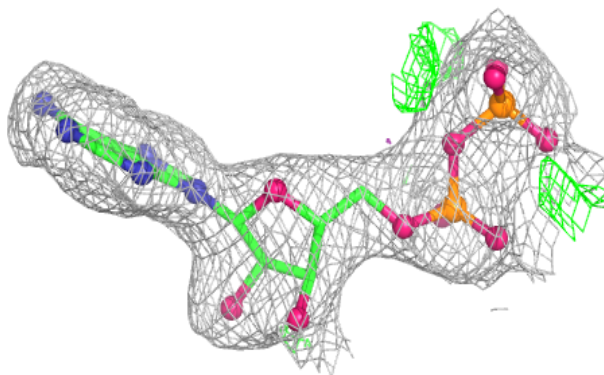


Electron density around ADP C 502:

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

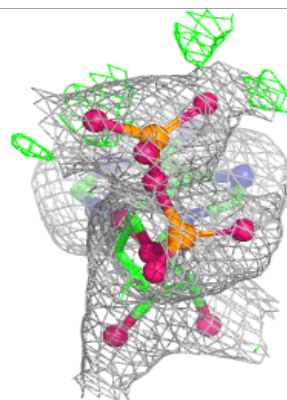
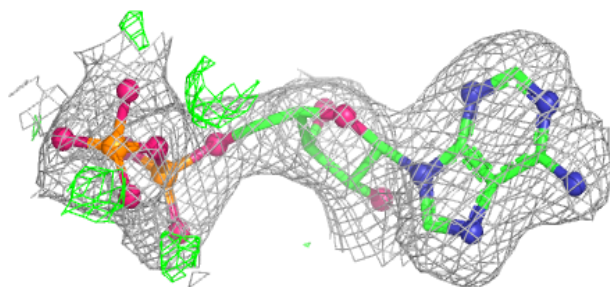
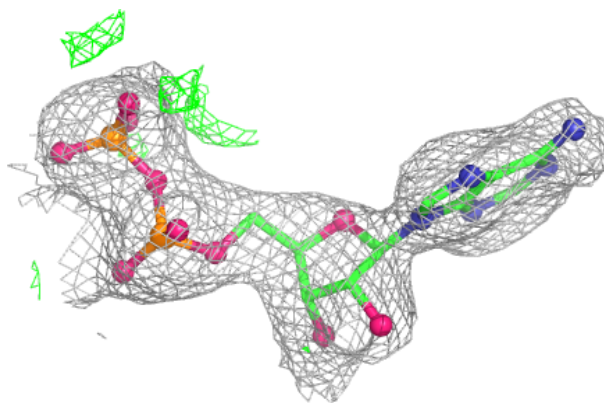
**Electron density around ADP E 502:**

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

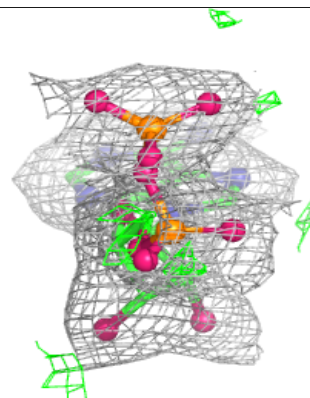
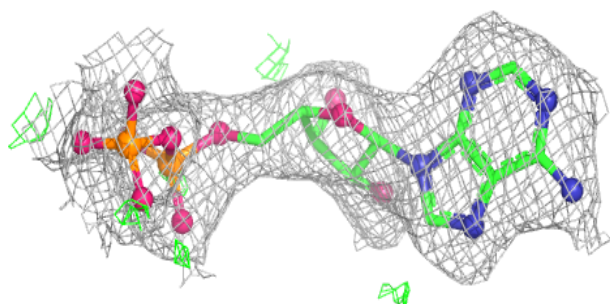
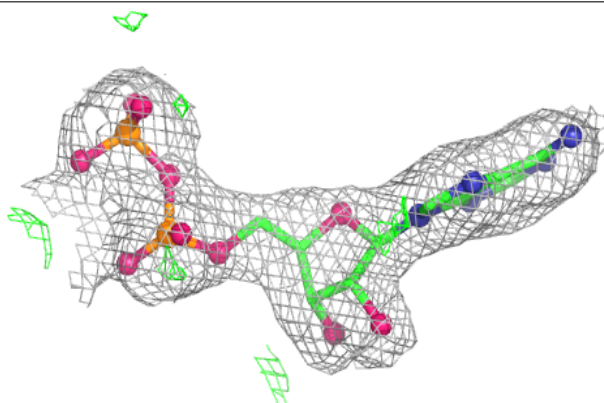


Electron density around ADP F 602:

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

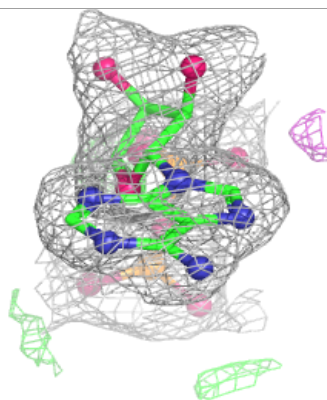
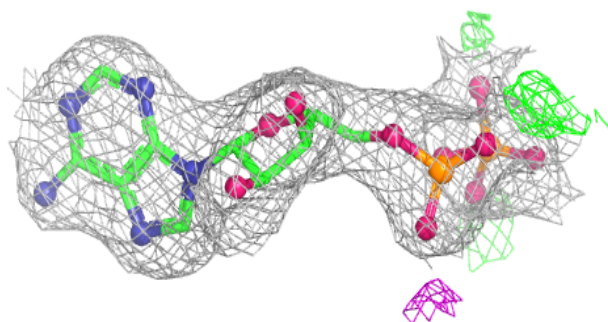
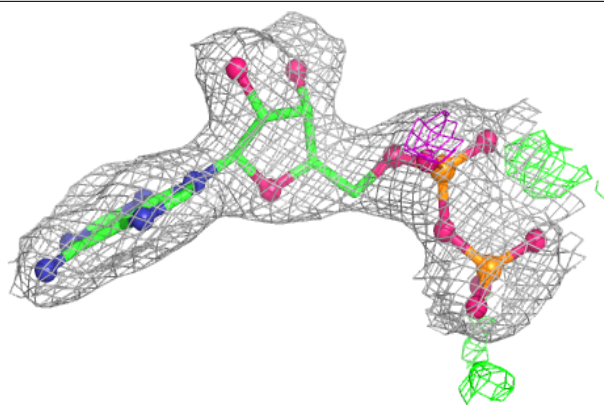
**Electron density around ADP G 602:**

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

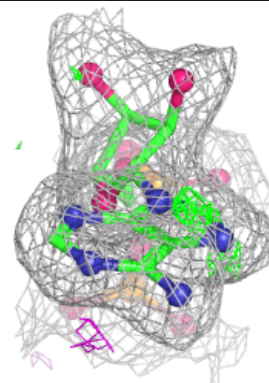
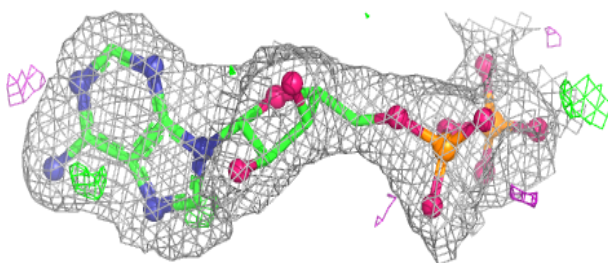
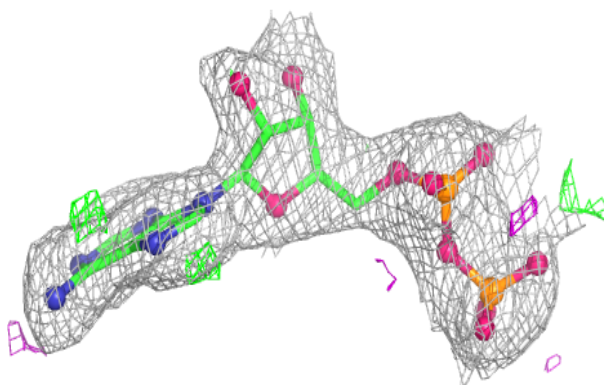


Electron density around ADP H 602:

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

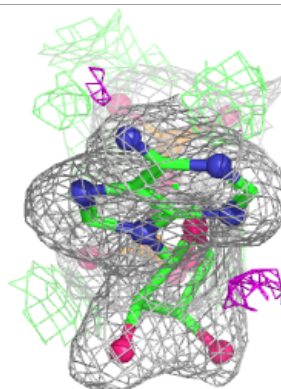
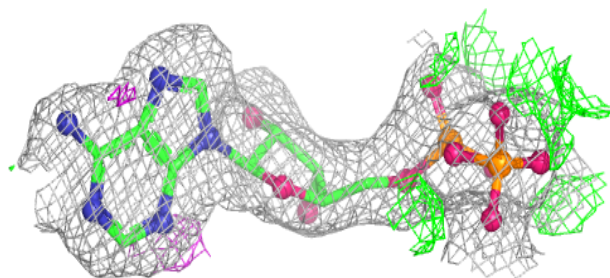
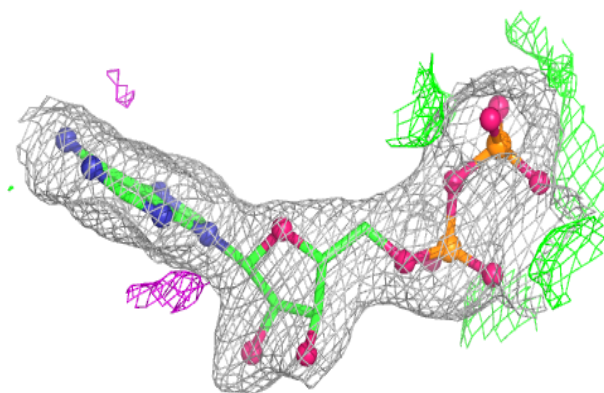
**Electron density around ADP I 502:**

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

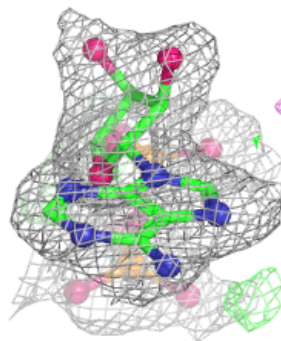
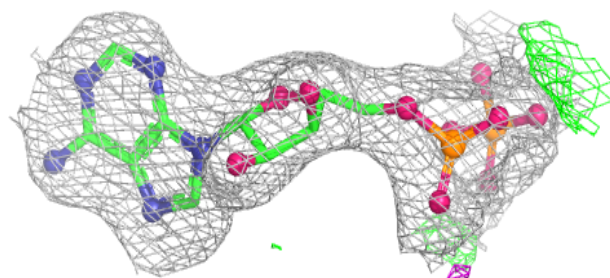
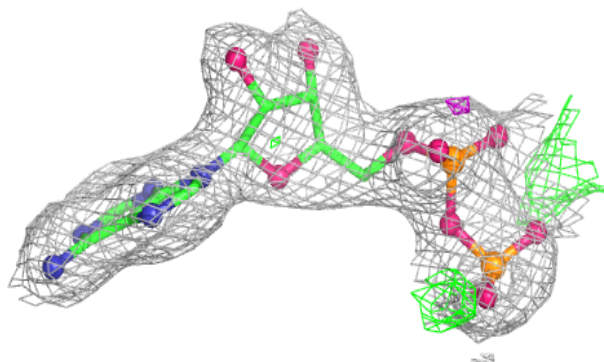


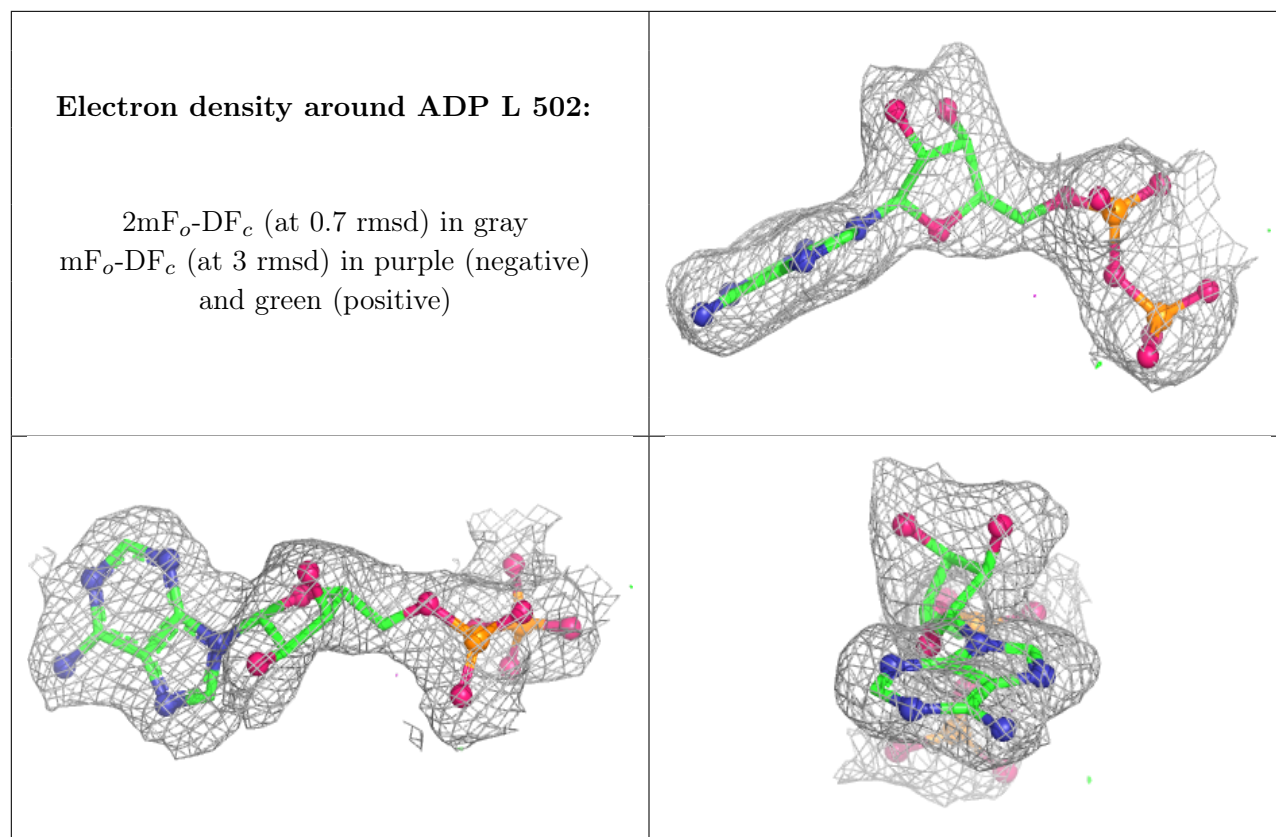
Electron density around ADP J 502:

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

**Electron density around ADP K 502:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.