



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2022 – 02:08 PM EDT

PDB ID : 7TEN
Title : Crystal structure of the *Listeria monocytogenes* GS-Met-Sox-P- ADP complex to 3.5 Angstrom
Authors : Schumacher, M.A.
Deposited on : 2022-01-05
Resolution : 3.50 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

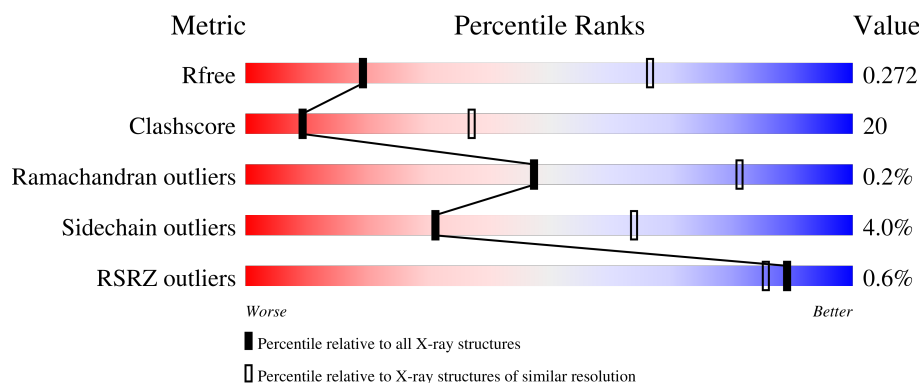
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	447	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 58% 38% .. </div> </div>
1	B	447	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 54% 44% .. </div> </div>
1	D	447	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 57% 39% .. </div> </div>
1	E	447	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 53% 43% .. </div> </div>
1	H	447	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 58% 39% .. </div> </div>

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Mol	Chain	Length	Quality of chain
1	J	447	<div><div><div>%</div><div><div></div><div>51%</div><div>45%</div><div></div></div><div>..</div></div></div>
1	M	447	<div><div><div>%</div><div><div></div><div>56%</div><div>40%</div><div></div></div><div>..</div></div></div>
1	O	447	<div><div><div></div><div><div></div><div>59%</div><div>38%</div><div></div></div><div>..</div></div></div>
1	Q	447	<div><div><div></div><div><div></div><div>55%</div><div>42%</div><div></div></div><div>..</div></div></div>
1	S	447	<div><div><div>2%</div><div><div></div><div>61%</div><div>35%</div><div></div></div><div>..</div></div></div>
1	U	447	<div><div><div>%</div><div><div></div><div>59%</div><div>38%</div><div></div></div><div>..</div></div></div>
1	W	447	<div><div><div>%</div><div><div></div><div>60%</div><div>37%</div><div></div></div><div>..</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 42583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3512	2248	586	660	18			
1	E	442	Total	C	N	O	S	0	0	0
			3496	2243	585	650	18			
1	B	442	Total	C	N	O	S	0	0	0
			3505	2246	580	661	18			
1	D	442	Total	C	N	O	S	0	0	0
			3509	2248	587	656	18			
1	H	442	Total	C	N	O	S	0	0	0
			3525	2257	584	666	18			
1	J	442	Total	C	N	O	S	0	0	0
			3496	2241	587	650	18			
1	M	442	Total	C	N	O	S	0	0	0
			3501	2241	583	659	18			
1	O	442	Total	C	N	O	S	0	0	0
			3508	2247	588	655	18			
1	Q	442	Total	C	N	O	S	0	0	0
			3503	2243	581	661	18			
1	S	442	Total	C	N	O	S	0	0	0
			3497	2242	588	649	18			
1	U	442	Total	C	N	O	S	0	0	0
			3515	2250	586	661	18			
1	W	442	Total	C	N	O	S	0	0	0
			3512	2249	587	658	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A5D5GA79
A	-1	SER	-	expression tag	UNP A0A5D5GA79
A	0	HIS	-	expression tag	UNP A0A5D5GA79
A	402	ASN	ASP	conflict	UNP A0A5D5GA79
E	-2	GLY	-	expression tag	UNP A0A5D5GA79

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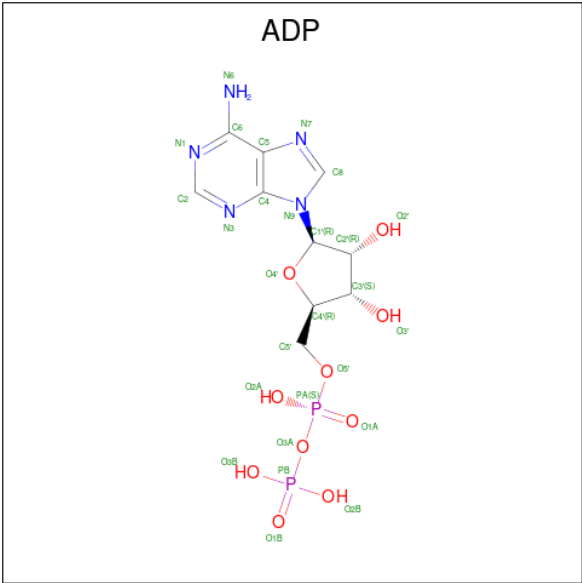
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP A0A5D5GA79
E	0	HIS	-	expression tag	UNP A0A5D5GA79
E	402	ASN	ASP	conflict	UNP A0A5D5GA79
B	-2	GLY	-	expression tag	UNP A0A5D5GA79
B	-1	SER	-	expression tag	UNP A0A5D5GA79
B	0	HIS	-	expression tag	UNP A0A5D5GA79
B	402	ASN	ASP	conflict	UNP A0A5D5GA79
D	-2	GLY	-	expression tag	UNP A0A5D5GA79
D	-1	SER	-	expression tag	UNP A0A5D5GA79
D	0	HIS	-	expression tag	UNP A0A5D5GA79
D	402	ASN	ASP	conflict	UNP A0A5D5GA79
H	-2	GLY	-	expression tag	UNP A0A5D5GA79
H	-1	SER	-	expression tag	UNP A0A5D5GA79
H	0	HIS	-	expression tag	UNP A0A5D5GA79
H	402	ASN	ASP	conflict	UNP A0A5D5GA79
J	-2	GLY	-	expression tag	UNP A0A5D5GA79
J	-1	SER	-	expression tag	UNP A0A5D5GA79
J	0	HIS	-	expression tag	UNP A0A5D5GA79
J	402	ASN	ASP	conflict	UNP A0A5D5GA79
M	-2	GLY	-	expression tag	UNP A0A5D5GA79
M	-1	SER	-	expression tag	UNP A0A5D5GA79
M	0	HIS	-	expression tag	UNP A0A5D5GA79
M	402	ASN	ASP	conflict	UNP A0A5D5GA79
O	-2	GLY	-	expression tag	UNP A0A5D5GA79
O	-1	SER	-	expression tag	UNP A0A5D5GA79
O	0	HIS	-	expression tag	UNP A0A5D5GA79
O	402	ASN	ASP	conflict	UNP A0A5D5GA79
Q	-2	GLY	-	expression tag	UNP A0A5D5GA79
Q	-1	SER	-	expression tag	UNP A0A5D5GA79
Q	0	HIS	-	expression tag	UNP A0A5D5GA79
Q	402	ASN	ASP	conflict	UNP A0A5D5GA79
S	-2	GLY	-	expression tag	UNP A0A5D5GA79
S	-1	SER	-	expression tag	UNP A0A5D5GA79
S	0	HIS	-	expression tag	UNP A0A5D5GA79
S	402	ASN	ASP	conflict	UNP A0A5D5GA79
U	-2	GLY	-	expression tag	UNP A0A5D5GA79
U	-1	SER	-	expression tag	UNP A0A5D5GA79
U	0	HIS	-	expression tag	UNP A0A5D5GA79
U	402	ASN	ASP	conflict	UNP A0A5D5GA79
W	-2	GLY	-	expression tag	UNP A0A5D5GA79
W	-1	SER	-	expression tag	UNP A0A5D5GA79
W	0	HIS	-	expression tag	UNP A0A5D5GA79

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Chain	Residue	Modelled	Actual	Comment	Reference
W	402	ASN	ASP	conflict	UNP A0A5D5GA79

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



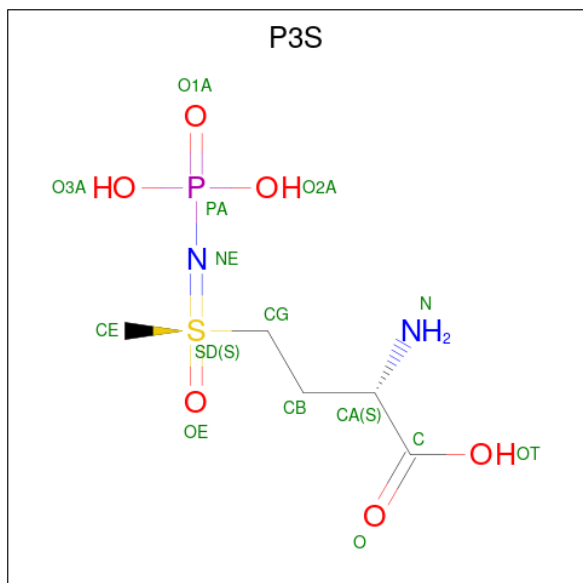
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	Q	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	S	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

- Molecule 3 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (three-letter code: P3S) (formula: $C_5H_{13}N_2O_6PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	E	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	B	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	D	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	H	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	J	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	M	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	O	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	Q	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		

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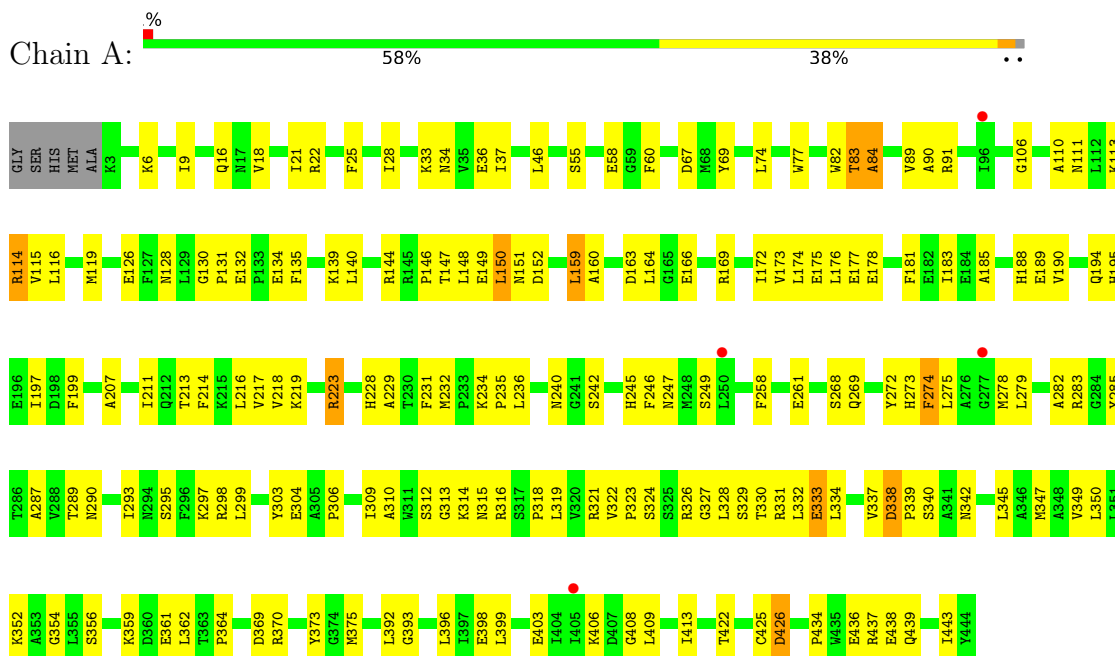
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	S	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	U	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	W	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		

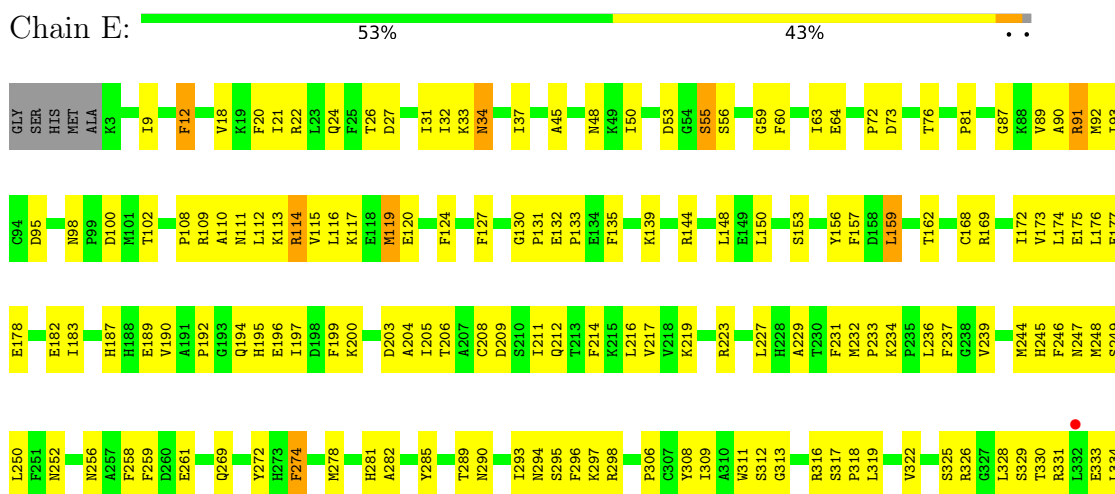
3 Residue-property plots

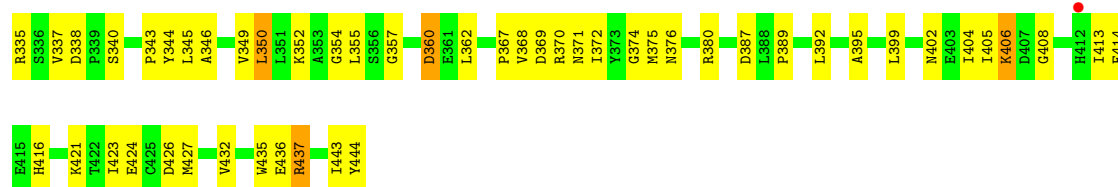
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glutamine synthetase



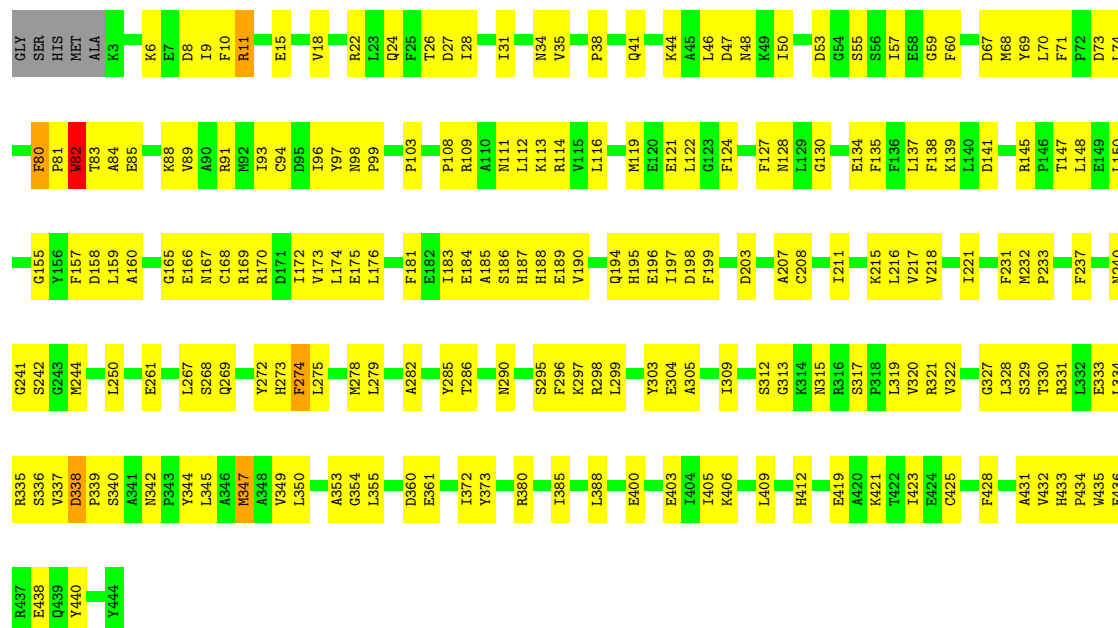
• Molecule 1: Glutamine synthetase





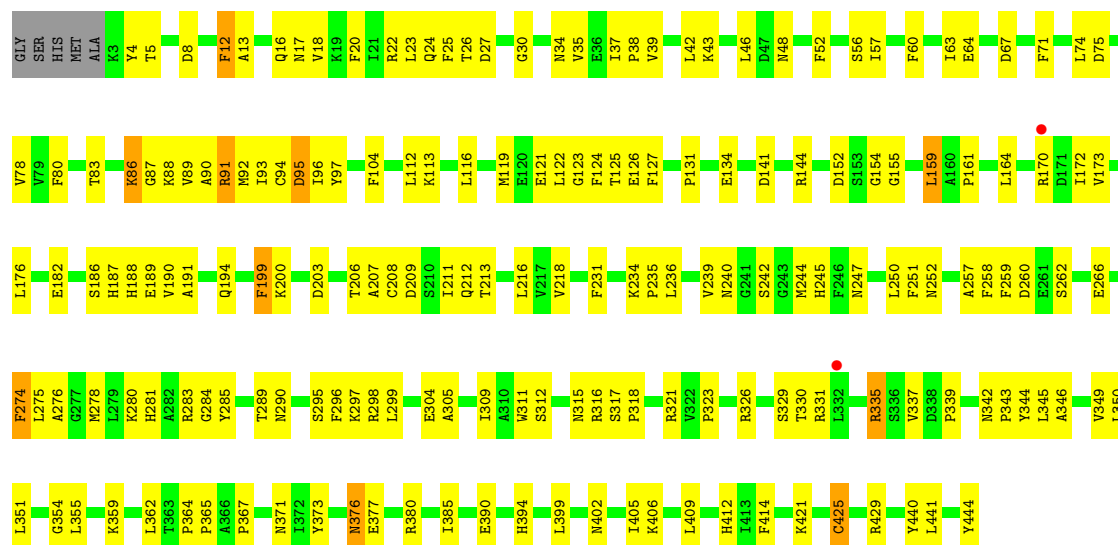
● Molecule 1: Glutamine synthetase

Chain B: 54% 44% ..



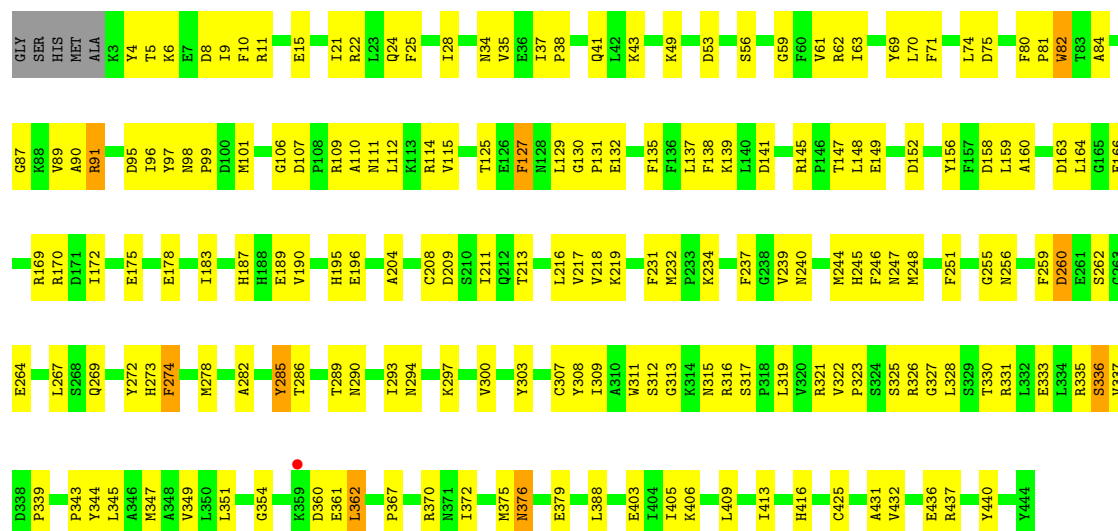
● Molecule 1: Glutamine synthetase

Chain D: 57% 39% ..



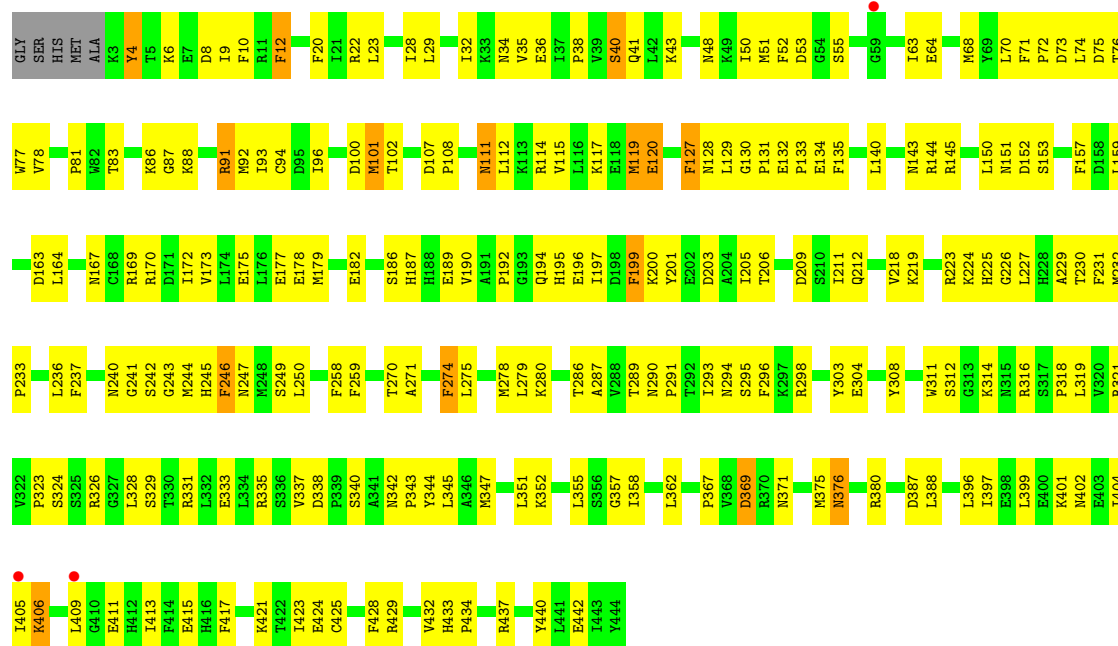
- Molecule 1: Glutamine synthetase

Chain H:  58% 39% ..



- Molecule 1: Glutamine synthetase

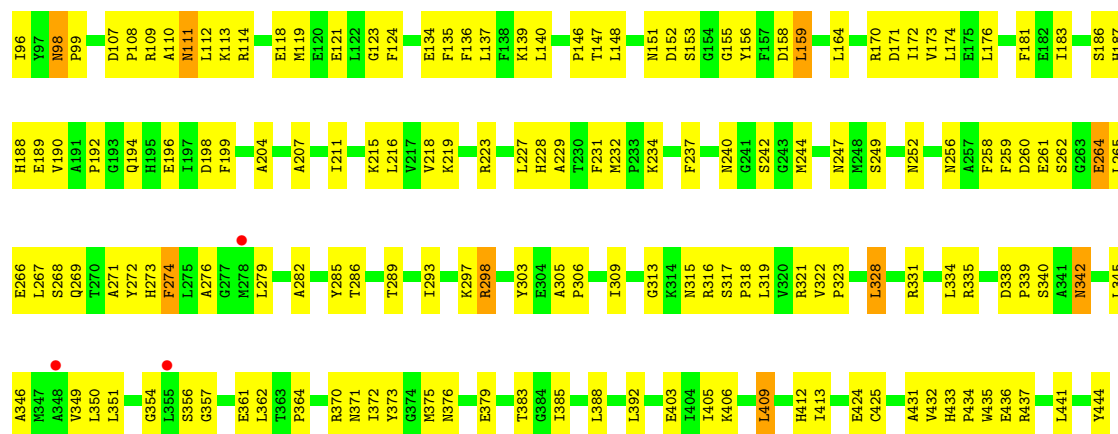
Chain J:  51% 45% ..

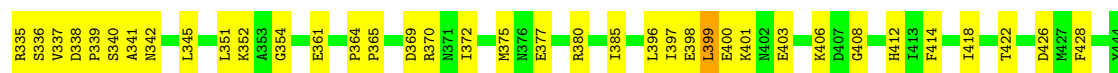


- Molecule 1: Glutamine synthetase

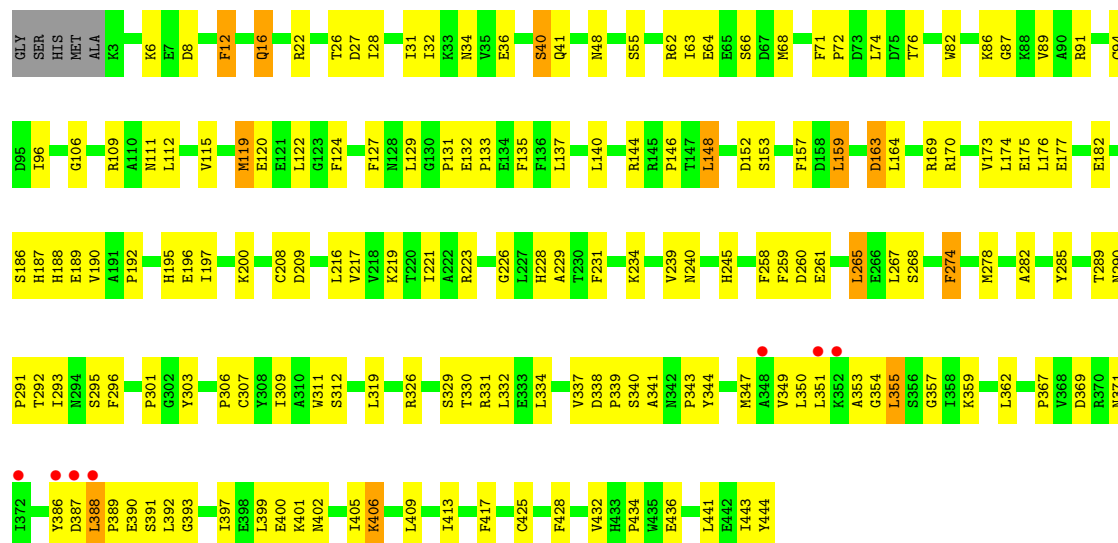
Chain M:  56% 40% ..



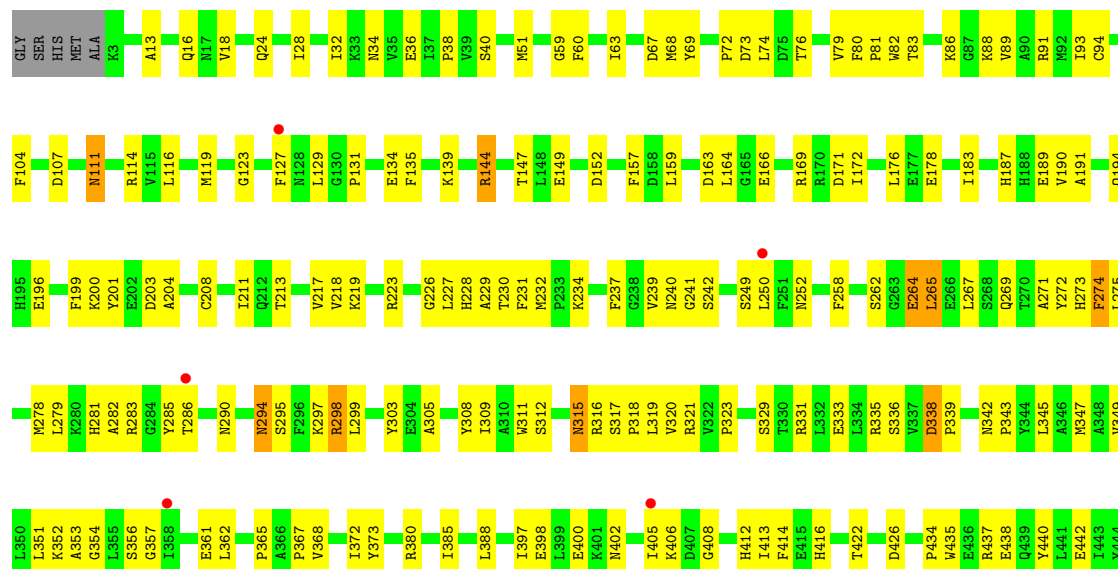




• Molecule 1: Glutamine synthetase

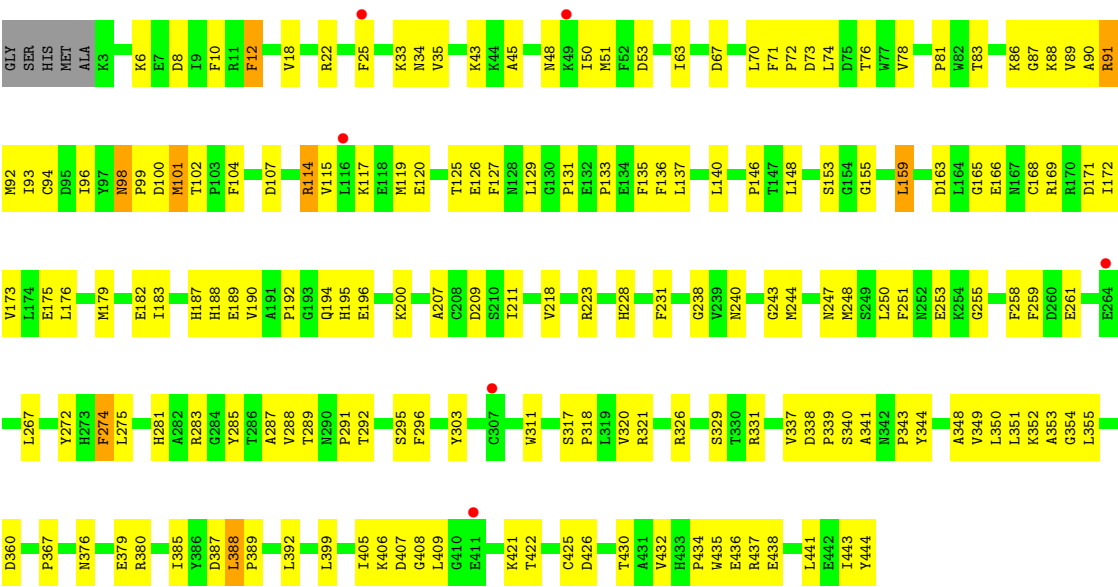


• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	112.61Å 137.61Å 138.02Å 60.75° 87.16° 68.40°	Depositor
Resolution (Å)	63.88 – 3.50 63.88 – 3.50	Depositor EDS
% Data completeness (in resolution range)	74.3 (63.88-3.50) 74.3 (63.88-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.201 , 0.273 0.200 , 0.272	Depositor DCC
R_{free} test set	1988 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	98.8	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	42583	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/3597	0.53	0/4867
1	B	0.31	0/3590	0.57	0/4859
1	D	0.31	0/3595	0.54	0/4864
1	E	0.33	0/3583	0.59	3/4851 (0.1%)
1	H	0.33	0/3610	0.57	0/4883
1	J	0.30	0/3582	0.56	1/4848 (0.0%)
1	M	0.31	0/3585	0.55	0/4852
1	O	0.31	0/3594	0.53	0/4863
1	Q	0.30	0/3587	0.55	0/4854
1	S	0.32	0/3583	0.56	3/4849 (0.1%)
1	U	0.31	0/3600	0.52	0/4870
1	W	0.31	0/3598	0.54	1/4868 (0.0%)
All	All	0.31	0/43104	0.55	8/58328 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	355	LEU	CA-CB-CG	6.48	130.21	115.30
1	S	388	LEU	CA-CB-CG	6.39	130.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	355	LEU	CA-CB-CG	5.64	128.27	115.30
1	W	388	LEU	CA-CB-CG	5.43	127.79	115.30
1	E	298	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	E	350	LEU	CA-CB-CG	5.22	127.31	115.30
1	S	355	LEU	CA-CB-CG	5.16	127.17	115.30
1	S	265	LEU	CB-CG-CD1	5.11	119.68	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	THR	Peptide
1	E	34	ASN	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	3512	0	3421	142	0
1	B	3505	0	3399	170	0
1	D	3509	0	3417	151	0
1	E	3496	0	3395	167	0
1	H	3525	0	3433	147	0
1	J	3496	0	3404	180	0
1	M	3501	0	3399	161	0
1	O	3508	0	3418	149	0
1	Q	3503	0	3402	142	0
1	S	3497	0	3407	127	0
1	U	3515	0	3420	151	0
1	W	3512	0	3419	134	0
2	A	27	0	12	5	0
2	B	27	0	12	5	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	H	27	0	12	3	0
2	J	27	0	12	5	0
2	M	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	27	0	12	4	0
2	Q	27	0	12	1	0
2	S	27	0	12	2	0
2	U	27	0	12	2	0
2	W	27	0	12	0	0
3	A	15	0	10	1	0
3	B	15	0	10	3	0
3	D	15	0	10	2	0
3	E	15	0	8	0	0
3	H	15	0	10	2	0
3	J	15	0	10	1	0
3	M	15	0	10	3	0
3	O	15	0	10	2	0
3	Q	15	0	10	0	0
3	S	15	0	10	0	0
3	U	15	0	10	2	0
3	W	15	0	10	0	0
All	All	42583	0	41196	1649	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 20.

All (1649) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:51:MET:HE3	1:U:69:TYR:CZ	1.92	1.03
1:M:170:ARG:NH1	1:O:36:GLU:OE2	1.97	0.98
1:U:51:MET:CE	1:U:69:TYR:CZ	2.49	0.96
1:U:51:MET:CE	1:U:69:TYR:CE1	2.50	0.95
1:D:119:MET:HG2	1:D:351:LEU:HD21	1.49	0.95
1:D:329:SER:HA	2:D:501:ADP:HN61	1.36	0.89
1:U:51:MET:HE3	1:U:69:TYR:CE2	2.08	0.89
1:O:151:ASN:ND2	1:O:152:ASP:OD2	2.05	0.88
1:B:68:MET:HA	1:B:99:PRO:HD3	1.56	0.87
1:Q:80:PHE:HB2	1:Q:89:VAL:HG23	1.54	0.87
1:M:189:GLU:HG3	1:M:190:VAL:H	1.39	0.87
1:H:267:LEU:HD21	1:H:326:ARG:HE	1.39	0.86
1:J:289:THR:HB	1:J:337:VAL:HG22	1.57	0.86
1:U:51:MET:HE1	1:U:69:TYR:CE1	2.10	0.86
1:D:83:THR:HA	1:D:86:LYS:HE3	1.58	0.85
1:U:18:VAL:HA	1:U:88:LYS:HB3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:144:ARG:NH2	1:S:223:ARG:O	2.09	0.85
1:J:237:PHE:HE2	1:M:431:ALA:HA	1.42	0.85
1:O:100:ASP:HB2	1:O:102:THR:HG22	1.58	0.85
1:H:28:ILE:HG13	1:H:59:GLY:HA3	1.57	0.84
1:J:402:ASN:HB3	1:J:405:ILE:HD11	1.60	0.84
1:M:183:ILE:HD12	1:M:199:PHE:HB3	1.60	0.83
1:B:183:ILE:HG23	1:D:38:PRO:HG2	1.61	0.83
1:E:313:GLY:HA2	1:E:322:VAL:HB	1.61	0.82
1:O:290:ASN:ND2	1:O:338:ASP:OD2	2.12	0.82
1:Q:20:PHE:HB2	1:Q:89:VAL:HG12	1.62	0.82
1:U:234:LYS:NZ	1:U:239:VAL:O	2.12	0.82
1:J:345:LEU:HD21	1:J:413:ILE:HD13	1.61	0.82
1:U:139:LYS:NZ	1:U:149:GLU:OE1	2.12	0.82
1:M:159:LEU:HD13	1:O:216:LEU:CD1	2.09	0.82
1:H:321:ARG:NH2	2:H:501:ADP:O3B	2.14	0.81
1:A:183:ILE:HD12	1:A:199:PHE:HB3	1.62	0.80
1:U:189:GLU:HB3	1:U:194:GLN:HB3	1.64	0.80
1:H:209:ASP:OD1	1:H:344:TYR:OH	2.00	0.80
1:H:290:ASN:ND2	1:H:336:SER:O	2.13	0.80
1:M:159:LEU:HG	1:O:34:ASN:HB2	1.62	0.80
1:E:189:GLU:HG3	1:E:190:VAL:H	1.44	0.80
1:E:18:VAL:HG11	1:E:90:ALA:HB2	1.62	0.80
1:M:170:ARG:HH22	1:O:22:ARG:HH12	1.29	0.80
1:J:209:ASP:OD1	1:J:344:TYR:OH	1.99	0.79
1:B:216:LEU:HD13	1:W:159:LEU:HD13	1.61	0.79
1:J:189:GLU:HG3	1:J:190:VAL:H	1.48	0.78
1:M:342:ASN:HB3	1:M:345:LEU:HB2	1.64	0.78
1:U:219:LYS:HA	1:U:229:ALA:HB3	1.64	0.78
1:J:167:ASN:O	1:U:86:LYS:NZ	2.18	0.77
1:A:22:ARG:HH21	1:O:170:ARG:HH22	1.31	0.77
1:U:60:PHE:O	1:U:412:HIS:NE2	2.18	0.77
1:B:189:GLU:HG3	1:B:190:VAL:H	1.50	0.76
1:H:234:LYS:NZ	1:H:239:VAL:O	2.14	0.76
1:J:100:ASP:HB2	1:J:102:THR:HG22	1.68	0.76
1:E:285:TYR:CE1	1:E:350:LEU:HD12	2.21	0.75
1:E:329:SER:HA	2:E:501:ADP:HN61	1.51	0.75
1:O:189:GLU:HG3	1:O:190:VAL:H	1.48	0.75
1:A:194:GLN:HE21	1:A:242:SER:HB3	1.49	0.75
1:Q:189:GLU:HB3	1:Q:194:GLN:HB3	1.66	0.75
1:M:159:LEU:HD21	1:O:34:ASN:HD22	1.51	0.75
1:H:96:ILE:HG12	1:H:107:ASP:OD2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:309:ILE:HG23	1:Q:319:LEU:HD22	1.69	0.74
1:M:187:HIS:ND1	1:M:188:HIS:O	2.21	0.74
1:M:98:ASN:OD1	1:M:99:PRO:HD2	1.88	0.74
1:O:69:TYR:HE1	1:O:99:PRO:HB3	1.52	0.74
1:W:153:SER:HA	1:W:192:PRO:HB3	1.70	0.73
1:E:352:LYS:HG2	1:E:408:GLY:HA3	1.71	0.73
1:O:370:ARG:HH21	1:O:375:MET:HG2	1.53	0.73
1:Q:314:LYS:HG2	1:Q:324:SER:HB3	1.70	0.73
1:J:433:HIS:CD2	1:M:433:HIS:CD2	2.77	0.73
1:Q:163:ASP:OD2	1:Q:169:ARG:NH1	2.21	0.73
1:J:32:ILE:HG12	1:J:212:GLN:HB3	1.71	0.73
1:W:155:GLY:O	1:W:188:HIS:ND1	2.21	0.73
1:A:352:LYS:HD3	1:A:408:GLY:HA2	1.69	0.73
1:B:97:TYR:HD2	1:B:103:PRO:HA	1.54	0.73
1:J:230:THR:OG1	1:M:441:LEU:O	2.07	0.73
1:W:189:GLU:HG3	1:W:190:VAL:H	1.54	0.72
1:J:91:ARG:HH21	1:J:93:ILE:HD11	1.54	0.72
1:J:143:ASN:HB3	1:J:145:ARG:HD3	1.71	0.72
1:A:290:ASN:ND2	1:A:338:ASP:OD2	2.23	0.72
1:E:91:ARG:HH21	1:E:93:ILE:HD11	1.54	0.72
1:J:240:ASN:HA	1:J:303:TYR:HB3	1.72	0.72
1:J:290:ASN:ND2	1:J:338:ASP:OD2	2.22	0.72
1:U:38:PRO:HB2	1:U:40:SER:H	1.53	0.72
1:E:100:ASP:HB2	1:E:102:THR:HG22	1.71	0.72
1:W:338:ASP:OD1	1:W:340:SER:OG	2.08	0.71
1:E:174:LEU:HA	1:E:177:GLU:HB3	1.73	0.71
1:B:22:ARG:NH2	1:W:166:GLU:OE2	2.22	0.71
1:J:323:PRO:O	1:J:326:ARG:NH1	2.23	0.71
1:D:208:CYS:HB3	1:D:343:PRO:HB2	1.71	0.71
1:M:247:ASN:HB3	1:M:331:ARG:HD2	1.72	0.71
1:W:247:ASN:OD1	1:W:331:ARG:NH1	2.24	0.71
1:Q:338:ASP:OD1	1:Q:340:SER:OG	2.09	0.71
1:S:234:LYS:NZ	1:S:239:VAL:O	2.22	0.71
1:U:290:ASN:ND2	1:U:338:ASP:OD2	2.23	0.71
1:E:114:ARG:HD3	1:E:115:VAL:HG13	1.73	0.71
1:E:130:GLY:O	1:E:247:ASN:ND2	2.23	0.71
1:U:166:GLU:OE2	1:W:22:ARG:NH2	2.24	0.71
1:A:189:GLU:HG3	1:A:190:VAL:H	1.56	0.70
1:U:315:ASN:ND2	1:W:63:ILE:O	2.24	0.70
1:B:9:ILE:HD11	1:B:74:LEU:HB3	1.73	0.70
1:B:183:ILE:HD12	1:B:199:PHE:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:402:ASN:HB3	1:S:405:ILE:HD11	1.73	0.70
1:H:131:PRO:HG3	1:H:211:ILE:HD11	1.73	0.70
1:J:404:ILE:HD12	1:J:404:ILE:H	1.56	0.70
1:W:78:VAL:HG22	1:W:91:ARG:HD2	1.72	0.70
1:D:182:GLU:HG2	1:D:200:LYS:HD2	1.74	0.70
1:W:96:ILE:N	1:W:107:ASP:OD2	2.25	0.70
1:H:147:THR:HG23	1:H:149:GLU:H	1.56	0.70
1:O:338:ASP:OD1	1:O:340:SER:OG	2.07	0.70
1:J:232:MET:HG2	1:J:233:PRO:HD2	1.71	0.70
1:B:85:GLU:N	1:B:85:GLU:OE1	2.24	0.69
1:S:189:GLU:HG3	1:S:190:VAL:H	1.58	0.69
1:U:434:PRO:HA	1:U:437:ARG:HG3	1.74	0.69
1:W:22:ARG:HD2	1:W:89:VAL:HG11	1.74	0.69
1:O:247:ASN:OD1	1:O:331:ARG:NH1	2.23	0.69
1:U:189:GLU:HG3	1:U:190:VAL:H	1.58	0.69
1:W:376:ASN:HB2	1:W:379:GLU:HB2	1.75	0.69
1:A:28:ILE:O	1:A:342:ASN:ND2	2.26	0.69
1:H:159:LEU:HG	1:J:34:ASN:HB2	1.75	0.69
1:H:437:ARG:NH1	1:O:235:PRO:O	2.26	0.69
1:J:96:ILE:HG22	1:J:107:ASP:OD2	1.93	0.69
1:Q:300:VAL:HG11	1:W:430:THR:HG22	1.75	0.69
1:S:388:LEU:HD23	1:S:389:PRO:HD2	1.74	0.68
1:E:285:TYR:HE1	1:E:350:LEU:HD12	1.59	0.68
1:D:191:ALA:HB2	1:D:240:ASN:HB2	1.75	0.68
1:W:296:PHE:HE2	1:W:392:LEU:HA	1.58	0.68
1:E:150:LEU:HD21	1:E:236:LEU:HD11	1.76	0.68
1:B:24:GLN:HG2	1:B:34:ASN:HB2	1.74	0.68
1:S:338:ASP:OD1	1:S:340:SER:OG	2.12	0.68
1:A:159:LEU:HG	1:E:34:ASN:HB2	1.75	0.68
1:A:274:PHE:CE2	1:A:354:GLY:HA3	2.29	0.68
1:J:357:GLY:HA2	1:J:362:LEU:HD12	1.76	0.68
1:J:440:TYR:OH	1:M:424:GLU:OE2	2.11	0.68
1:Q:274:PHE:CE2	1:Q:354:GLY:HA3	2.28	0.68
1:U:191:ALA:HB2	1:U:240:ASN:HB2	1.75	0.68
1:B:282:ALA:HB3	1:B:309:ILE:HD13	1.75	0.68
1:H:115:VAL:HG12	1:H:351:LEU:HD23	1.76	0.67
1:H:169:ARG:HA	1:H:172:ILE:HD12	1.76	0.67
1:A:356:SER:HA	1:A:359:LYS:HE2	1.76	0.67
1:S:291:PRO:HG3	1:S:341:ALA:HA	1.76	0.67
1:H:163:ASP:OD2	1:H:169:ARG:NH1	2.27	0.67
1:H:260:ASP:OD1	1:H:262:SER:OG	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:289:THR:HB	1:Q:337:VAL:HG12	1.75	0.67
1:W:18:VAL:HG11	1:W:90:ALA:HB2	1.74	0.67
1:A:321:ARG:NH2	2:A:501:ADP:O3B	2.26	0.67
1:B:321:ARG:NH2	2:B:501:ADP:O3B	2.26	0.67
1:J:170:ARG:HD2	1:U:86:LYS:HE2	1.77	0.67
1:J:371:ASN:HD22	1:U:63:ILE:HG21	1.58	0.67
1:E:153:SER:HA	1:E:192:PRO:HB3	1.76	0.67
1:U:51:MET:HE1	1:U:69:TYR:CZ	2.25	0.67
1:B:60:PHE:O	1:B:412:HIS:NE2	2.27	0.67
1:D:321:ARG:NH2	2:D:501:ADP:O3B	2.25	0.67
1:D:91:ARG:HH21	1:D:93:ILE:HD11	1.59	0.67
1:U:51:MET:HE3	1:U:69:TYR:CE1	2.22	0.67
1:M:28:ILE:HG12	1:M:59:GLY:HA3	1.76	0.67
1:Q:111:ASN:OD1	1:Q:114:ARG:NH2	2.24	0.67
1:Q:189:GLU:HG3	1:Q:190:VAL:H	1.60	0.67
1:W:119:MET:HG2	1:W:351:LEU:HD21	1.75	0.67
1:A:111:ASN:OD1	1:A:114:ARG:NH2	2.28	0.67
1:A:219:LYS:HA	1:A:229:ALA:HB3	1.75	0.67
1:O:331:ARG:HD3	2:O:501:ADP:C4	2.29	0.67
1:B:183:ILE:HD11	1:B:197:ILE:HG22	1.76	0.66
1:H:273:HIS:CB	1:H:361:GLU:HG2	2.26	0.66
1:D:121:GLU:HG3	1:D:122:LEU:HD23	1.77	0.66
1:Q:159:LEU:HG	1:S:34:ASN:HB2	1.76	0.66
1:H:300:VAL:HG11	1:O:430:THR:HG22	1.76	0.66
1:Q:232:MET:HE2	1:W:437:ARG:HA	1.78	0.66
1:Q:308:TYR:OH	1:Q:380:ARG:NH1	2.28	0.66
1:E:73:ASP:OD2	1:E:113:LYS:NZ	2.26	0.66
1:S:289:THR:HB	1:S:337:VAL:HG22	1.78	0.66
1:O:273:HIS:ND1	1:O:362:LEU:O	2.28	0.66
1:E:432:VAL:HG22	1:B:237:PHE:HB2	1.77	0.66
1:B:267:LEU:HB2	1:B:272:TYR:HE1	1.60	0.66
1:M:216:LEU:HD13	1:S:159:LEU:HD13	1.78	0.66
1:U:281:HIS:ND1	1:U:402:ASN:OD1	2.27	0.66
1:A:22:ARG:HH21	1:O:170:ARG:NH2	1.93	0.65
1:H:267:LEU:HB2	1:H:272:TYR:HE1	1.61	0.65
1:M:317:SER:HB2	1:M:372:ILE:HG22	1.79	0.65
1:D:83:THR:HG21	1:D:89:VAL:H	1.61	0.65
1:Q:403:GLU:HA	1:Q:406:LYS:HD3	1.78	0.65
1:S:231:PHE:HB3	1:S:339:PRO:HG2	1.79	0.65
1:A:216:LEU:HD13	1:O:159:LEU:HD13	1.76	0.65
1:E:157:PHE:HB3	1:Q:33:LYS:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ALA:HA	1:B:88:LYS:HA	1.77	0.65
1:S:87:GLY:O	1:S:89:VAL:HG23	1.97	0.65
1:H:327:GLY:N	1:H:330:THR:OG1	2.30	0.65
1:J:134:GLU:OE2	1:J:243:GLY:N	2.26	0.65
1:O:331:ARG:HD3	2:O:501:ADP:C5	2.31	0.65
1:O:176:LEU:HG	1:O:217:VAL:HG11	1.78	0.65
1:W:114:ARG:NH2	1:W:407:ASP:O	2.25	0.65
1:O:20:PHE:HB2	1:O:89:VAL:HG22	1.78	0.65
1:O:79:VAL:HA	1:O:90:ALA:HA	1.79	0.65
1:A:326:ARG:HG2	1:A:330:THR:HG23	1.79	0.65
1:B:286:THR:HG21	1:B:388:LEU:HD22	1.79	0.65
1:E:159:LEU:HD13	1:Q:216:LEU:HD13	1.78	0.65
1:A:6:LYS:HG2	1:A:74:LEU:HD21	1.77	0.64
1:D:18:VAL:HA	1:D:88:LYS:HB3	1.79	0.64
1:O:409:LEU:O	1:O:413:ILE:HB	1.97	0.64
1:J:314:LYS:HB2	1:U:67:ASP:HB2	1.79	0.64
1:U:13:ALA:HA	1:U:18:VAL:HG22	1.79	0.64
1:E:285:TYR:HB3	1:E:405:ILE:HG21	1.79	0.64
1:E:402:ASN:HB3	1:E:405:ILE:HD11	1.77	0.64
1:J:311:TRP:HA	1:J:318:PRO:HB2	1.79	0.64
1:O:127:PHE:HB3	1:O:204:ALA:HB2	1.79	0.64
1:Q:237:PHE:HB2	1:W:432:VAL:HG22	1.80	0.64
1:D:91:ARG:NH2	1:D:213:THR:OG1	2.30	0.64
1:U:28:ILE:O	1:U:342:ASN:ND2	2.30	0.64
1:A:33:LYS:HB3	1:O:157:PHE:HB3	1.80	0.64
1:M:282:ALA:HB3	1:M:309:ILE:HD13	1.79	0.64
1:J:170:ARG:HB3	1:U:86:LYS:HZ1	1.63	0.64
1:B:34:ASN:HD22	1:W:159:LEU:HG	1.62	0.64
1:E:203:ASP:HB3	1:E:206:THR:HG22	1.80	0.64
1:D:159:LEU:HG	1:H:34:ASN:ND2	2.12	0.64
1:E:274:PHE:CE2	1:E:354:GLY:HA3	2.33	0.63
1:S:86:LYS:HG3	1:S:87:GLY:H	1.62	0.63
1:U:282:ALA:HA	1:U:285:TYR:CZ	2.33	0.63
1:E:176:LEU:HG	1:E:217:VAL:HG11	1.79	0.63
1:A:338:ASP:OD1	1:A:340:SER:OG	2.16	0.63
1:J:413:ILE:O	1:J:417:PHE:N	2.30	0.63
1:H:432:VAL:HA	1:H:436:GLU:OE2	1.98	0.63
1:B:97:TYR:CD2	1:B:103:PRO:HA	2.34	0.63
1:D:274:PHE:CE2	1:D:354:GLY:HA3	2.33	0.63
1:M:159:LEU:HD13	1:O:216:LEU:HD12	1.79	0.63
1:Q:328:LEU:O	2:Q:501:ADP:N6	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:278:MET:O	1:S:282:ALA:N	2.31	0.63
1:U:152:ASP:HB3	1:U:164:LEU:H	1.64	0.63
1:U:315:ASN:HD22	1:U:316:ARG:H	1.47	0.63
1:W:48:ASN:HB3	1:W:71:PHE:CD1	2.33	0.63
1:A:34:ASN:ND2	1:O:159:LEU:HG	2.13	0.63
1:W:275:LEU:HD21	1:W:320:VAL:HG11	1.81	0.63
1:A:247:ASN:ND2	1:A:333:GLU:OE1	2.31	0.62
1:H:209:ASP:O	1:H:213:THR:OG1	2.10	0.62
1:J:28:ILE:HD11	1:J:417:PHE:HB2	1.81	0.62
1:S:293:ILE:HD11	1:S:425:CYS:HA	1.80	0.62
1:W:240:ASN:HA	1:W:303:TYR:HB3	1.80	0.62
1:A:437:ARG:NH1	1:D:235:PRO:O	2.32	0.62
1:E:48:ASN:OD1	1:E:72:PRO:HD2	1.99	0.62
1:D:189:GLU:HG3	1:D:190:VAL:H	1.62	0.62
1:W:209:ASP:OD1	1:W:344:TYR:OH	2.10	0.62
1:E:290:ASN:HB3	1:E:295:SER:HB3	1.80	0.62
1:D:298:ARG:HG2	1:D:299:LEU:HD23	1.81	0.62
1:H:240:ASN:HA	1:H:303:TYR:HB3	1.81	0.62
1:M:321:ARG:NH2	2:M:501:ADP:O3B	2.25	0.62
1:W:86:LYS:HG3	1:W:87:GLY:H	1.64	0.62
1:U:349:VAL:HG13	1:U:405:ILE:HD12	1.82	0.62
1:B:18:VAL:HA	1:B:88:LYS:HB3	1.80	0.62
1:H:189:GLU:HG3	1:H:190:VAL:H	1.65	0.62
1:E:9:ILE:HA	1:E:12:PHE:HB2	1.82	0.62
1:B:84:ALA:HB1	1:B:88:LYS:HG3	1.82	0.62
1:Q:297:LYS:NZ	1:W:436:GLU:OE1	2.27	0.62
1:S:405:ILE:HD12	1:S:406:LYS:N	2.15	0.62
1:E:316:ARG:O	1:E:335:ARG:NH2	2.33	0.61
1:M:234:LYS:HD2	1:M:298:ARG:HA	1.82	0.61
1:M:293:ILE:HD11	1:M:425:CYS:HA	1.80	0.61
1:M:331:ARG:HD3	2:M:501:ADP:C5	2.35	0.61
1:M:112:LEU:HD21	1:M:204:ALA:HB1	1.82	0.61
1:M:286:THR:HG21	1:M:388:LEU:HD22	1.80	0.61
1:J:433:HIS:CG	1:M:433:HIS:HD2	2.19	0.61
1:S:351:LEU:O	1:S:355:LEU:HG	2.00	0.61
1:E:144:ARG:NH2	1:E:223:ARG:O	2.33	0.61
1:S:146:PRO:HG3	1:U:442:GLU:HG2	1.81	0.61
1:A:306:PRO:HB3	1:A:319:LEU:HA	1.81	0.61
1:E:294:ASN:ND2	1:B:436:GLU:OE1	2.33	0.61
1:B:274:PHE:CE2	1:B:354:GLY:HA3	2.34	0.61
1:S:290:ASN:HB2	1:S:296:PHE:HE1	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASP:CG	1:O:321:ARG:HH11	2.03	0.61
1:D:30:GLY:O	1:D:212:GLN:NE2	2.32	0.61
1:D:289:THR:HB	1:D:337:VAL:HG22	1.81	0.61
1:M:328:LEU:HD23	1:M:328:LEU:H	1.65	0.61
1:W:189:GLU:HG3	1:W:190:VAL:N	2.14	0.61
1:A:329:SER:HA	2:A:501:ADP:HN61	1.64	0.61
1:E:237:PHE:CE2	1:B:431:ALA:HA	2.36	0.61
1:H:74:LEU:HD12	1:H:74:LEU:H	1.65	0.61
1:J:405:ILE:HD12	1:J:406:LYS:N	2.15	0.61
1:M:152:ASP:HB3	1:M:164:LEU:HG	1.83	0.61
1:M:267:LEU:HB2	1:M:272:TYR:CE1	2.35	0.61
1:A:232:MET:HE1	1:D:441:LEU:HB2	1.83	0.61
1:B:172:ILE:HG21	1:B:218:VAL:HG12	1.83	0.61
1:M:219:LYS:HA	1:M:229:ALA:HB3	1.83	0.61
1:H:152:ASP:HB3	1:H:164:LEU:H	1.66	0.61
1:J:129:LEU:HD11	1:J:246:PHE:CD1	2.36	0.61
1:M:38:PRO:HB2	1:M:40:SER:H	1.66	0.61
1:W:380:ARG:HB2	1:W:385:ILE:HG13	1.82	0.61
1:H:326:ARG:HG2	1:H:330:THR:HG23	1.82	0.61
1:M:60:PHE:O	1:M:412:HIS:NE2	2.31	0.61
1:O:28:ILE:HG23	1:O:29:LEU:HG	1.82	0.61
1:O:141:ASP:OD1	1:O:145:ARG:N	2.26	0.61
1:B:127:PHE:HE2	1:B:347:MET:HG3	1.65	0.60
1:Q:110:ALA:HA	1:Q:113:LYS:HD2	1.84	0.60
1:U:28:ILE:HG13	1:U:59:GLY:HA3	1.83	0.60
1:A:312:SER:OG	1:A:315:ASN:HB3	2.01	0.60
1:D:285:TYR:HB2	1:D:349:VAL:HG11	1.82	0.60
1:U:274:PHE:CE2	1:U:354:GLY:HA3	2.36	0.60
1:D:123:GLY:O	1:D:252:ASN:ND2	2.35	0.60
1:D:342:ASN:HB3	1:D:345:LEU:HB2	1.84	0.60
1:O:169:ARG:HD3	1:O:195:HIS:HB3	1.84	0.60
1:B:111:ASN:OD1	1:B:114:ARG:NH2	2.34	0.60
1:J:114:ARG:HD2	1:J:115:VAL:HG13	1.82	0.60
1:E:21:ILE:HG13	1:E:90:ALA:HB3	1.83	0.60
1:E:326:ARG:O	1:E:330:THR:N	2.35	0.60
1:M:370:ARG:NH2	1:M:375:MET:SD	2.74	0.60
1:S:112:LEU:HA	1:S:115:VAL:HG22	1.84	0.60
1:A:304:GLU:OE2	1:E:56:SER:OG	2.19	0.60
1:H:246:PHE:HB3	1:H:248:MET:HE1	1.84	0.60
1:J:270:THR:O	1:J:274:PHE:N	2.32	0.60
1:M:338:ASP:OD1	1:M:340:SER:OG	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:319:LEU:HD23	1:U:320:VAL:HG23	1.84	0.60
1:A:34:ASN:HD21	1:O:159:LEU:HG	1.67	0.60
1:D:236:LEU:HD12	1:D:239:VAL:HG21	1.82	0.60
1:H:274:PHE:CE2	1:H:354:GLY:HA3	2.36	0.60
1:S:27:ASP:OD1	1:S:31:ILE:N	2.33	0.60
1:B:349:VAL:HG13	1:B:405:ILE:HG23	1.83	0.60
1:Q:60:PHE:O	1:Q:412:HIS:NE2	2.34	0.60
1:U:279:LEU:HD22	1:U:309:ILE:HG22	1.84	0.60
1:B:155:GLY:O	1:B:188:HIS:ND1	2.35	0.60
1:B:313:GLY:HA2	1:B:322:VAL:HB	1.83	0.60
1:D:18:VAL:HG11	1:D:90:ALA:HB2	1.84	0.60
1:D:305:ALA:O	1:D:373:TYR:OH	2.16	0.60
1:H:106:GLY:O	1:H:413:ILE:HD11	2.01	0.60
1:M:95:ASP:OD2	1:M:109:ARG:HD3	2.02	0.60
1:M:403:GLU:HA	1:M:406:LYS:HB2	1.84	0.60
1:Q:48:ASN:HB3	1:Q:71:PHE:CE1	2.36	0.60
1:U:127:PHE:HB3	1:U:204:ALA:HB2	1.84	0.60
1:J:40:SER:OG	1:J:41:GLN:NE2	2.34	0.59
1:W:349:VAL:HG12	1:W:350:LEU:HD12	1.84	0.59
1:Q:282:ALA:HB3	1:Q:309:ILE:HD13	1.85	0.59
1:S:55:SER:HB2	1:S:63:ILE:HA	1.84	0.59
1:A:83:THR:O	1:A:84:ALA:O	2.20	0.59
1:H:370:ARG:NH2	1:H:375:MET:SD	2.74	0.59
1:M:258:PHE:HA	1:M:271:ALA:HB2	1.82	0.59
1:B:329:SER:HA	2:B:501:ADP:HN61	1.67	0.59
1:J:169:ARG:HD3	1:J:195:HIS:HB3	1.84	0.59
1:U:240:ASN:HA	1:U:303:TYR:HB3	1.85	0.59
1:W:81:PRO:HG2	1:W:175:GLU:HG3	1.84	0.59
1:B:165:GLY:HA2	1:B:168:CYS:HB3	1.84	0.59
1:H:208:CYS:SG	1:H:343:PRO:HB2	2.43	0.59
1:M:11:ARG:O	1:M:15:GLU:HB2	2.02	0.59
1:M:72:PRO:HA	1:M:94:CYS:HA	1.85	0.59
1:M:134:GLU:HG2	1:M:196:GLU:HB2	1.85	0.59
1:E:117:LYS:HA	1:E:120:GLU:HB2	1.83	0.59
1:S:48:ASN:HB3	1:S:71:PHE:CE1	2.38	0.59
1:M:171:ASP:HA	1:M:174:LEU:HD12	1.85	0.58
1:U:147:THR:HG23	1:U:149:GLU:H	1.68	0.58
1:B:338:ASP:OD1	1:B:340:SER:OG	2.21	0.58
1:D:25:PHE:HB2	1:D:96:ILE:HD11	1.86	0.58
1:D:159:LEU:HD13	1:H:216:LEU:HD13	1.85	0.58
1:U:187:HIS:HB3	1:W:35:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:258:PHE:HA	1:U:271:ALA:HB2	1.85	0.58
1:B:48:ASN:HB3	1:B:71:PHE:CG	2.38	0.58
1:B:73:ASP:HB2	1:B:94:CYS:SG	2.43	0.58
1:B:261:GLU:OE1	1:B:261:GLU:N	2.33	0.58
1:A:247:ASN:HB3	1:A:331:ARG:HD2	1.85	0.58
1:H:84:ALA:HB1	1:H:87:GLY:C	2.24	0.58
1:H:111:ASN:OD1	1:H:114:ARG:NH2	2.24	0.58
1:H:286:THR:HG21	1:H:388:LEU:HD22	1.84	0.58
1:B:41:GLN:OE1	1:B:44:LYS:NZ	2.25	0.58
1:B:403:GLU:HG2	1:B:406:LYS:HD3	1.86	0.58
1:M:264:GLU:HB2	1:M:272:TYR:OH	2.02	0.58
1:S:357:GLY:HA2	1:S:362:LEU:HD12	1.85	0.58
1:A:67:ASP:HB2	1:O:314:LYS:HB2	1.85	0.58
1:D:125:THR:HG22	1:D:126:GLU:HG3	1.85	0.58
1:J:405:ILE:HD12	1:J:406:LYS:H	1.69	0.58
1:U:241:GLY:HA3	1:U:298:ARG:HG3	1.85	0.58
1:A:279:LEU:HD22	1:A:309:ILE:HG22	1.86	0.58
1:A:436:GLU:OE2	1:D:297:LYS:NZ	2.37	0.58
1:J:433:HIS:CG	1:M:433:HIS:CD2	2.92	0.58
1:E:435:TRP:CH2	1:B:428:PHE:HB2	2.39	0.58
1:B:240:ASN:HA	1:B:303:TYR:HB3	1.86	0.58
1:B:244:MET:H	1:B:338:ASP:HA	1.68	0.58
1:J:237:PHE:CE2	1:M:431:ALA:HA	2.32	0.58
1:M:334:LEU:HD23	1:M:350:LEU:HD21	1.86	0.58
1:S:122:LEU:HD11	1:S:359:LYS:HD3	1.85	0.58
1:S:436:GLU:OE1	1:U:297:LYS:NZ	2.36	0.58
1:B:189:GLU:HB3	1:B:194:GLN:HB3	1.86	0.58
1:D:71:PHE:O	1:D:95:ASP:N	2.34	0.58
1:O:18:VAL:HG11	1:O:90:ALA:HB2	1.85	0.58
1:O:342:ASN:HB3	1:O:345:LEU:HB2	1.86	0.58
1:S:109:ARG:NH1	1:S:209:ASP:OD2	2.25	0.58
1:U:72:PRO:HA	1:U:94:CYS:HA	1.86	0.58
1:W:187:HIS:NE2	1:W:196:GLU:HB3	2.19	0.58
1:E:189:GLU:HG3	1:E:190:VAL:HG23	1.85	0.57
1:D:60:PHE:HE2	1:D:96:ILE:HG12	1.69	0.57
1:O:323:PRO:O	1:O:326:ARG:NH1	2.36	0.57
1:W:165:GLY:O	1:W:169:ARG:N	2.21	0.57
1:E:206:THR:HA	1:E:209:ASP:HB2	1.85	0.57
1:D:80:PHE:O	1:D:83:THR:HG22	2.04	0.57
1:U:159:LEU:HD21	1:W:34:ASN:HD22	1.69	0.57
1:A:289:THR:HB	1:A:337:VAL:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:208:CYS:HB3	1:S:343:PRO:HB2	1.86	0.57
1:A:370:ARG:NH2	1:A:375:MET:SD	2.77	0.57
1:D:83:THR:OG1	1:D:87:GLY:O	2.23	0.57
1:Q:9:ILE:HD12	1:Q:74:LEU:HB3	1.87	0.57
1:S:8:ASP:O	1:S:12:PHE:HB2	2.05	0.57
1:E:437:ARG:HG3	1:B:232:MET:HE1	1.87	0.57
1:W:182:GLU:OE1	1:W:200:LYS:HD2	2.04	0.57
1:A:268:SER:OG	1:A:269:GLN:N	2.38	0.57
1:B:353:ALA:HB2	1:B:405:ILE:HD11	1.86	0.57
1:Q:319:LEU:HD23	1:Q:320:VAL:HG23	1.86	0.57
1:U:139:LYS:O	1:U:147:THR:HG22	2.05	0.57
1:A:6:LYS:NZ	1:A:46:LEU:O	2.24	0.57
1:J:397:ILE:O	1:J:401:LYS:HG2	2.05	0.57
1:A:282:ALA:HA	1:A:285:TYR:CE2	2.40	0.57
1:E:370:ARG:HE	1:E:375:MET:HG2	1.70	0.57
1:H:5:THR:N	1:H:8:ASP:OD2	2.37	0.57
1:J:231:PHE:HB2	1:M:444:TYR:OXT	2.05	0.57
1:J:290:ASN:HB3	1:J:295:SER:HB3	1.85	0.57
1:M:159:LEU:HD13	1:O:216:LEU:HD11	1.85	0.57
1:U:76:THR:HG21	1:U:93:ILE:HB	1.86	0.57
1:D:52:PHE:HE2	1:D:57:ILE:HD12	1.70	0.57
1:H:125:THR:N	1:H:251:PHE:O	2.33	0.57
1:M:434:PRO:O	1:M:437:ARG:N	2.37	0.57
1:O:295:SER:O	1:O:298:ARG:HG2	2.05	0.57
1:W:91:ARG:HH21	1:W:93:ILE:HD11	1.70	0.57
1:H:112:LEU:HD21	1:H:204:ALA:HB1	1.87	0.56
1:H:328:LEU:O	2:H:501:ADP:N6	2.38	0.56
1:J:152:ASP:OD2	1:J:164:LEU:N	2.27	0.56
1:M:437:ARG:O	1:M:441:LEU:HB2	2.05	0.56
1:S:432:VAL:HG22	1:U:237:PHE:HB2	1.87	0.56
1:W:244:MET:N	1:W:337:VAL:O	2.38	0.56
1:A:314:LYS:HG2	1:A:324:SER:HB3	1.87	0.56
1:M:357:GLY:O	1:M:361:GLU:HA	2.05	0.56
1:E:132:GLU:HB2	1:E:245:HIS:HB2	1.87	0.56
1:E:427:MET:HE2	1:B:435:TRP:HZ2	1.69	0.56
1:B:69:TYR:CD1	1:B:99:PRO:HA	2.41	0.56
1:B:273:HIS:CB	1:B:361:GLU:HG2	2.35	0.56
1:O:245:HIS:ND1	1:O:333:GLU:OE2	2.38	0.56
1:S:26:THR:HG1	1:S:344:TYR:HE2	1.52	0.56
1:S:434:PRO:HG3	1:U:434:PRO:HD2	1.88	0.56
1:U:249:SER:HA	1:U:258:PHE:CE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:LYS:HA	1:E:229:ALA:HB3	1.86	0.56
1:A:183:ILE:HD11	1:A:197:ILE:HG22	1.86	0.56
1:E:309:ILE:HA	1:E:319:LEU:HD12	1.88	0.56
1:E:311:TRP:HA	1:E:318:PRO:HB2	1.88	0.56
1:B:321:ARG:NH1	1:B:333:GLU:OE1	2.39	0.56
1:E:197:ILE:HB	1:E:214:PHE:HZ	1.71	0.56
1:J:318:PRO:O	1:J:335:ARG:HD2	2.06	0.56
1:M:34:ASN:ND2	1:S:159:LEU:HG	2.21	0.56
1:Q:326:ARG:HG2	1:Q:330:THR:HG23	1.86	0.56
1:U:59:GLY:HA2	1:U:416:HIS:HD2	1.69	0.56
1:W:100:ASP:HB2	1:W:102:THR:HG22	1.87	0.56
1:A:261:GLU:OE1	1:A:261:GLU:N	2.36	0.56
1:E:234:LYS:NZ	1:E:239:VAL:O	2.35	0.56
1:D:95:ASP:HB3	1:D:97:TYR:HE1	1.69	0.56
1:M:111:ASN:ND2	1:M:413:ILE:HD12	2.20	0.56
1:W:352:LYS:HG2	1:W:408:GLY:HA3	1.87	0.56
1:E:32:ILE:HG12	1:E:212:GLN:HB3	1.87	0.56
1:B:98:ASN:OD1	1:B:99:PRO:HD2	2.05	0.56
1:J:237:PHE:HD2	1:M:432:VAL:HG23	1.70	0.56
1:O:106:GLY:HA2	1:O:413:ILE:HG13	1.88	0.56
1:Q:69:TYR:CE1	1:Q:99:PRO:HA	2.41	0.56
1:B:24:GLN:HB2	1:B:93:ILE:HG13	1.88	0.56
1:B:57:ILE:HG21	1:B:60:PHE:CE2	2.41	0.56
1:S:405:ILE:HD12	1:S:406:LYS:H	1.71	0.56
1:W:289:THR:HB	1:W:337:VAL:HG22	1.88	0.56
1:J:6:LYS:HA	1:J:74:LEU:HD23	1.88	0.56
1:A:323:PRO:HG2	1:A:331:ARG:NE	2.21	0.55
1:O:311:TRP:CZ2	1:O:367:PRO:HB3	2.41	0.55
1:A:282:ALA:HB3	1:A:309:ILE:HD13	1.87	0.55
1:E:182:GLU:OE1	1:E:200:LYS:HD2	2.07	0.55
1:B:69:TYR:HD1	1:B:99:PRO:HA	1.71	0.55
1:H:231:PHE:HB3	1:H:339:PRO:HB2	1.89	0.55
1:J:52:PHE:HZ	1:J:96:ILE:HD12	1.70	0.55
1:W:104:PHE:HB3	1:W:107:ASP:HB2	1.88	0.55
1:A:134:GLU:O	1:A:242:SER:HB2	2.05	0.55
1:B:166:GLU:OE2	1:D:22:ARG:NH2	2.38	0.55
1:H:82:TRP:O	1:H:84:ALA:N	2.38	0.55
1:W:274:PHE:HE2	1:W:354:GLY:HA3	1.71	0.55
1:W:281:HIS:HD2	1:W:353:ALA:HB1	1.71	0.55
1:A:132:GLU:HB2	1:A:245:HIS:HB2	1.87	0.55
1:E:389:PRO:HB2	1:E:395:ALA:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ASN:OD1	1:B:317:SER:OG	2.19	0.55
1:D:323:PRO:O	1:D:326:ARG:NH1	2.40	0.55
1:H:96:ILE:HB	1:H:107:ASP:HB2	1.88	0.55
1:Q:48:ASN:HB3	1:Q:71:PHE:CD1	2.41	0.55
1:Q:117:LYS:HA	1:Q:120:GLU:HG3	1.87	0.55
1:D:245:HIS:HE1	3:D:502:P3S:NE	2.04	0.55
1:H:135:PHE:HB3	1:H:231:PHE:CE2	2.42	0.55
1:D:161:PRO:HD2	1:H:219:LYS:HE3	1.89	0.55
1:D:209:ASP:OD1	1:D:344:TYR:OH	2.23	0.55
1:M:139:LYS:O	1:M:147:THR:HG22	2.05	0.55
1:M:256:ASN:HD22	1:M:328:LEU:HA	1.72	0.55
1:O:351:LEU:O	1:O:355:LEU:HG	2.07	0.55
1:Q:244:MET:HE2	1:Q:339:PRO:HA	1.88	0.55
1:S:274:PHE:HE2	1:S:354:GLY:HA3	1.72	0.55
1:U:305:ALA:N	1:U:373:TYR:OH	2.39	0.55
1:J:10:PHE:CE1	1:J:43:LYS:HG3	2.42	0.55
1:U:73:ASP:OD1	1:U:74:LEU:N	2.40	0.55
1:B:159:LEU:HD11	1:D:34:ASN:HD22	1.72	0.55
1:J:153:SER:HA	1:J:192:PRO:HB3	1.89	0.55
1:S:6:LYS:HG3	1:S:74:LEU:HD21	1.88	0.55
1:J:219:LYS:HA	1:J:229:ALA:HB3	1.89	0.55
1:M:51:MET:HB3	1:M:69:TYR:HA	1.89	0.55
1:M:305:ALA:N	1:M:373:TYR:OH	2.40	0.55
1:O:376:ASN:O	1:O:380:ARG:HG3	2.06	0.55
1:Q:147:THR:OG1	1:Q:148:LEU:N	2.39	0.55
1:E:237:PHE:HE2	1:B:431:ALA:HA	1.71	0.54
1:B:167:ASN:HA	1:B:170:ARG:HB3	1.89	0.54
1:D:390:GLU:HG3	1:D:394:HIS:ND1	2.23	0.54
1:U:400:GLU:HA	1:U:406:LYS:HD2	1.89	0.54
1:O:91:ARG:HH21	1:O:93:ILE:HD11	1.72	0.54
1:Q:257:ALA:O	1:Q:270:THR:OG1	2.24	0.54
1:A:327:GLY:N	1:A:330:THR:OG1	2.40	0.54
1:A:403:GLU:HA	1:A:406:LYS:HD3	1.89	0.54
1:E:209:ASP:OD1	1:E:344:TYR:OH	2.19	0.54
1:M:215:LYS:HG2	1:M:231:PHE:CE1	2.43	0.54
1:O:21:ILE:HD13	1:O:42:LEU:HD13	1.88	0.54
1:O:285:TYR:HB2	1:O:349:VAL:HG11	1.88	0.54
1:S:22:ARG:HD2	1:S:89:VAL:HG11	1.89	0.54
1:E:108:PRO:HB3	1:E:345:LEU:HD13	1.90	0.54
1:E:249:SER:HA	1:E:258:PHE:CE2	2.42	0.54
1:E:346:ALA:O	1:E:350:LEU:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ILE:HG23	1:B:70:LEU:HB2	1.90	0.54
1:H:323:PRO:HG2	1:H:331:ARG:NE	2.23	0.54
1:M:137:LEU:HD13	1:M:227:LEU:HD13	1.90	0.54
1:S:292:THR:HB	1:U:440:TYR:CE2	2.43	0.54
1:B:305:ALA:O	1:B:373:TYR:OH	2.20	0.54
1:J:135:PHE:HB3	1:J:231:PHE:CE1	2.43	0.54
1:Q:167:ASN:HA	1:Q:170:ARG:HB3	1.88	0.54
1:U:16:GLN:HB2	1:U:18:VAL:HG13	1.89	0.54
1:B:109:ARG:HG3	1:B:344:TYR:CE1	2.42	0.54
1:D:13:ALA:O	1:D:17:ASN:N	2.37	0.54
1:H:360:ASP:O	1:H:361:GLU:HB3	2.06	0.54
1:U:311:TRP:NE1	1:U:365:PRO:O	2.31	0.54
1:W:311:TRP:CH2	1:W:367:PRO:HB3	2.42	0.54
1:E:187:HIS:HB3	1:Q:35:VAL:HG23	1.88	0.54
1:B:38:PRO:HG2	1:W:183:ILE:HB	1.90	0.54
1:H:232:MET:HE1	1:O:441:LEU:HB2	1.89	0.54
1:H:278:MET:O	1:H:282:ALA:N	2.40	0.54
1:O:63:ILE:O	1:O:66:SER:OG	2.26	0.54
1:O:329:SER:HA	2:O:501:ADP:HN61	1.73	0.54
1:Q:231:PHE:HB3	1:Q:339:PRO:HB2	1.88	0.54
1:E:124:PHE:CD1	1:E:250:LEU:HB3	2.42	0.54
1:J:100:ASP:O	1:J:101:MET:HB2	2.07	0.54
1:J:111:ASN:O	1:J:115:VAL:HG22	2.07	0.54
1:M:173:VAL:HG13	1:M:183:ILE:HG21	1.89	0.54
1:J:132:GLU:HB2	1:J:245:HIS:HB2	1.88	0.54
1:S:63:ILE:O	1:S:66:SER:OG	2.26	0.54
1:W:292:THR:OG1	1:W:295:SER:N	2.39	0.54
1:M:261:GLU:HA	1:M:266:GLU:HA	1.90	0.54
1:U:159:LEU:HD11	1:W:34:ASN:HD22	1.73	0.54
1:E:261:GLU:OE1	1:E:261:GLU:N	2.37	0.53
1:H:80:PHE:HB2	1:H:89:VAL:HB	1.89	0.53
1:U:82:TRP:CD1	1:U:83:THR:HG23	2.42	0.53
1:W:351:LEU:HG	1:W:355:LEU:HD23	1.90	0.53
1:E:135:PHE:CE1	1:E:195:HIS:HB2	2.43	0.53
1:E:189:GLU:HB3	1:E:194:GLN:HG2	1.90	0.53
1:H:38:PRO:HD2	1:H:41:GLN:HG2	1.89	0.53
1:J:304:GLU:HB3	3:J:502:P3S:HGC1	1.90	0.53
1:O:69:TYR:CE1	1:O:99:PRO:HB3	2.39	0.53
1:Q:308:TYR:CE2	1:Q:380:ARG:HD3	2.43	0.53
1:A:166:GLU:OE2	1:E:22:ARG:NH2	2.42	0.53
1:D:52:PHE:CE2	1:D:57:ILE:HD12	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:ASP:HA	1:H:11:ARG:NH1	2.23	0.53
1:O:309:ILE:HG12	1:O:386:TYR:O	2.09	0.53
1:S:274:PHE:CE2	1:S:354:GLY:HA3	2.42	0.53
1:U:176:LEU:HG	1:U:217:VAL:HG11	1.91	0.53
1:E:346:ALA:HA	1:E:349:VAL:HG12	1.89	0.53
1:M:306:PRO:HG3	1:M:335:ARG:HB2	1.90	0.53
1:Q:215:LYS:HA	1:Q:218:VAL:HG22	1.91	0.53
1:E:352:LYS:HG2	1:E:408:GLY:CA	2.37	0.53
1:B:400:GLU:HA	1:B:406:LYS:HD2	1.89	0.53
1:M:256:ASN:ND2	1:M:328:LEU:O	2.42	0.53
1:S:76:THR:HB	1:S:91:ARG:HH12	1.73	0.53
1:U:333:GLU:OE2	1:U:335:ARG:NH2	2.42	0.53
1:W:281:HIS:CD2	1:W:353:ALA:HB1	2.42	0.53
1:A:163:ASP:OD2	1:A:169:ARG:NH1	2.41	0.53
1:E:357:GLY:HA2	1:E:362:LEU:HD13	1.91	0.53
1:B:80:PHE:HB2	1:B:89:VAL:HB	1.89	0.53
1:J:150:LEU:HD13	1:J:192:PRO:HB2	1.91	0.53
1:M:21:ILE:HD13	1:M:42:LEU:HD13	1.90	0.53
1:O:288:VAL:HG23	1:O:399:LEU:HD11	1.90	0.53
1:E:306:PRO:HB3	1:E:319:LEU:HA	1.91	0.53
1:H:309:ILE:HA	1:H:319:LEU:HD12	1.91	0.53
1:H:335:ARG:NH1	3:H:502:P3S:OE	2.41	0.53
1:J:246:PHE:CD2	1:J:337:VAL:HG21	2.44	0.53
1:S:62:ARG:NH1	1:S:64:GLU:OE1	2.42	0.53
1:A:147:THR:OG1	1:A:148:LEU:N	2.41	0.53
1:A:152:ASP:OD2	1:A:188:HIS:NE2	2.31	0.53
1:E:76:THR:O	1:E:92:MET:HA	2.09	0.53
1:J:130:GLY:HA3	2:J:501:ADP:O2'	2.08	0.53
1:M:110:ALA:HA	1:M:113:LYS:HB2	1.91	0.53
1:M:316:ARG:HH11	3:M:502:P3S:HEC2	1.74	0.53
1:O:22:ARG:HD2	1:O:89:VAL:HG11	1.91	0.53
1:O:148:LEU:HD23	1:O:148:LEU:H	1.73	0.53
1:W:388:LEU:HD23	1:W:389:PRO:HD2	1.90	0.53
1:B:321:ARG:NH2	1:D:67:ASP:OD2	2.39	0.53
1:D:74:LEU:HA	1:D:92:MET:SD	2.49	0.53
1:D:112:LEU:O	1:D:116:LEU:HB2	2.09	0.53
1:D:376:ASN:O	1:D:380:ARG:HG2	2.09	0.53
1:H:213:THR:O	1:H:217:VAL:HG23	2.09	0.53
1:M:189:GLU:HG3	1:M:190:VAL:HG23	1.91	0.53
1:M:146:PRO:HB3	1:M:228:HIS:CG	2.44	0.53
1:Q:152:ASP:HB3	1:Q:164:LEU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:169:ARG:HD3	1:Q:195:HIS:HB3	1.90	0.53
1:B:169:ARG:HD3	1:B:195:HIS:ND1	2.24	0.52
1:M:33:LYS:HB3	1:S:157:PHE:HB3	1.91	0.52
1:Q:170:ARG:NH1	1:S:36:GLU:OE2	2.42	0.52
1:A:174:LEU:HD21	1:E:20:PHE:HE2	1.74	0.52
1:H:11:ARG:O	1:H:15:GLU:HB2	2.08	0.52
1:M:119:MET:HB2	1:M:124:PHE:HB2	1.91	0.52
1:S:261:GLU:OE1	1:S:261:GLU:N	2.41	0.52
1:U:271:ALA:O	1:U:275:LEU:HD12	2.08	0.52
1:W:72:PRO:HA	1:W:94:CYS:HA	1.90	0.52
1:D:122:LEU:HD21	1:D:359:LYS:HE2	1.91	0.52
1:M:282:ALA:HA	1:M:285:TYR:CE2	2.43	0.52
1:Q:232:MET:HE3	1:W:441:LEU:HD13	1.90	0.52
1:S:170:ARG:HA	1:S:173:VAL:HG22	1.91	0.52
1:A:315:ASN:ND2	1:E:64:GLU:HA	2.24	0.52
1:B:67:ASP:CG	1:W:321:ARG:HH11	2.12	0.52
1:J:409:LEU:O	1:J:413:ILE:HB	2.10	0.52
1:M:159:LEU:HD21	1:O:34:ASN:ND2	2.21	0.52
1:O:304:GLU:O	1:O:335:ARG:NH2	2.43	0.52
1:Q:315:ASN:ND2	1:S:64:GLU:HA	2.23	0.52
1:W:287:ALA:HB3	1:W:399:LEU:HD12	1.91	0.52
1:E:316:ARG:CZ	1:Q:66:SER:HB3	2.39	0.52
1:D:421:LYS:O	1:D:425:CYS:HB2	2.10	0.52
1:J:91:ARG:HE	1:J:93:ILE:HG13	1.73	0.52
1:J:432:VAL:HG22	1:M:237:PHE:HB2	1.92	0.52
1:O:326:ARG:HB3	1:O:330:THR:HG23	1.92	0.52
1:Q:273:HIS:CB	1:Q:361:GLU:HG2	2.39	0.52
1:U:213:THR:O	1:U:217:VAL:HG23	2.09	0.52
1:U:231:PHE:HB3	1:U:339:PRO:HB2	1.90	0.52
1:D:127:PHE:CE1	1:D:351:LEU:HB2	2.45	0.52
1:D:275:LEU:O	1:D:278:MET:N	2.38	0.52
1:O:402:ASN:O	1:O:406:LYS:HB2	2.10	0.52
1:A:313:GLY:HA2	1:A:322:VAL:CG2	2.40	0.52
1:H:169:ARG:HD3	1:H:195:HIS:ND1	2.25	0.52
1:J:182:GLU:HG2	1:J:200:LYS:HD2	1.92	0.52
1:J:286:THR:HG21	1:J:388:LEU:HD22	1.92	0.52
1:O:314:LYS:HD3	1:O:324:SER:HB3	1.92	0.52
1:Q:52:PHE:CD1	1:Q:70:LEU:HG	2.45	0.52
1:W:127:PHE:HE2	1:W:248:MET:HB3	1.74	0.52
1:B:267:LEU:HB2	1:B:272:TYR:CE1	2.43	0.52
1:D:34:ASN:OD1	1:D:35:VAL:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:PHE:CE2	1:H:351:LEU:HD13	2.45	0.52
1:J:293:ILE:HD11	1:J:425:CYS:HA	1.92	0.52
1:O:48:ASN:HB3	1:O:71:PHE:CE1	2.45	0.52
1:U:311:TRP:CH2	1:U:367:PRO:HB3	2.45	0.52
1:W:115:VAL:HG21	1:W:348:ALA:HA	1.90	0.52
1:A:231:PHE:HB3	1:A:339:PRO:HG2	1.91	0.52
1:E:443:ILE:HG23	1:E:444:TYR:CD2	2.45	0.52
1:J:144:ARG:NH2	1:J:223:ARG:O	2.42	0.52
1:U:123:GLY:O	1:U:252:ASN:ND2	2.43	0.52
1:E:436:GLU:OE1	1:B:297:LYS:NZ	2.43	0.52
1:B:331:ARG:HD3	2:B:501:ADP:C5	2.45	0.52
1:M:12:PHE:O	1:M:16:GLN:HG2	2.10	0.52
1:D:172:ILE:HD13	1:D:218:VAL:HA	1.91	0.51
1:O:91:ARG:HE	1:O:93:ILE:HG13	1.75	0.51
1:D:231:PHE:HB3	1:D:339:PRO:HB2	1.91	0.51
1:O:203:ASP:HB3	1:O:206:THR:HG22	1.91	0.51
1:Q:290:ASN:ND2	1:Q:338:ASP:OD2	2.32	0.51
1:E:53:ASP:OD1	1:E:55:SER:HB3	2.09	0.51
1:D:234:LYS:HD3	1:D:298:ARG:HA	1.91	0.51
1:Q:159:LEU:HD13	1:S:216:LEU:HD12	1.93	0.51
1:Q:342:ASN:HB3	1:Q:345:LEU:HB2	1.93	0.51
1:W:338:ASP:O	1:W:340:SER:N	2.37	0.51
1:A:135:PHE:HB3	1:A:231:PHE:CE2	2.46	0.51
1:E:256:ASN:ND2	1:E:328:LEU:O	2.43	0.51
1:B:203:ASP:OD1	1:B:203:ASP:N	2.41	0.51
1:J:127:PHE:CE1	1:J:351:LEU:HD13	2.46	0.51
1:J:249:SER:HA	1:J:258:PHE:CE2	2.46	0.51
1:J:345:LEU:HD21	1:J:413:ILE:HG21	1.92	0.51
1:M:244:MET:HB2	1:M:339:PRO:HD3	1.91	0.51
1:Q:152:ASP:OD2	1:Q:163:ASP:HA	2.10	0.51
1:U:172:ILE:HD13	1:U:218:VAL:HG12	1.91	0.51
1:U:203:ASP:OD1	1:U:203:ASP:N	2.37	0.51
1:U:315:ASN:HD22	1:U:316:ARG:N	2.08	0.51
1:U:352:LYS:HD3	1:U:408:GLY:HA2	1.92	0.51
1:A:151:ASN:HB2	1:A:164:LEU:HD12	1.92	0.51
1:B:315:ASN:ND2	1:D:63:ILE:O	2.42	0.51
1:D:24:GLN:HG3	1:D:93:ILE:HG12	1.92	0.51
1:D:187:HIS:HE1	1:D:189:GLU:OE2	1.93	0.51
1:Q:328:LEU:HD23	1:Q:328:LEU:H	1.76	0.51
1:U:305:ALA:O	1:U:373:TYR:OH	2.18	0.51
1:W:125:THR:HG22	1:W:126:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:LEU:O	1:E:162:THR:N	2.43	0.51
1:H:98:ASN:HB3	1:H:99:PRO:HD2	1.93	0.51
1:H:403:GLU:HA	1:H:406:LYS:HD3	1.91	0.51
1:U:312:SER:HB2	1:U:368:VAL:O	2.10	0.51
1:W:189:GLU:HB3	1:W:194:GLN:HG2	1.93	0.51
1:W:351:LEU:O	1:W:355:LEU:HG	2.11	0.51
1:J:294:ASN:HD22	1:M:436:GLU:HB3	1.74	0.51
1:W:285:TYR:HB2	1:W:349:VAL:HG11	1.92	0.51
1:A:159:LEU:HD13	1:E:216:LEU:HD12	1.92	0.51
1:E:81:PRO:HB3	1:E:178:GLU:HG2	1.93	0.51
1:B:208:CYS:HA	1:B:211:ILE:HD12	1.93	0.51
1:Q:267:LEU:HB2	1:Q:272:TYR:HE1	1.76	0.51
1:U:397:ILE:HA	1:U:400:GLU:HG2	1.93	0.51
1:A:403:GLU:HG2	1:A:406:LYS:HD3	1.93	0.51
1:H:6:LYS:HG2	1:H:74:LEU:HD21	1.93	0.51
1:M:80:PHE:HB2	1:M:89:VAL:HB	1.91	0.51
1:Q:28:ILE:HG23	1:Q:29:LEU:HG	1.93	0.51
1:W:259:PHE:CE2	1:W:261:GLU:HG3	2.46	0.51
1:B:217:VAL:O	1:B:221:ILE:HB	2.11	0.51
1:D:250:LEU:HB2	1:D:257:ALA:HB3	1.93	0.51
1:H:345:LEU:HG	1:H:409:LEU:HD23	1.92	0.51
1:J:6:LYS:HG3	1:J:74:LEU:HD21	1.93	0.51
1:J:429:ARG:O	1:M:297:LYS:HD2	2.11	0.51
1:S:76:THR:HB	1:S:91:ARG:NH1	2.26	0.51
1:B:111:ASN:CG	1:B:114:ARG:HH21	2.14	0.50
1:D:155:GLY:O	1:D:188:HIS:ND1	2.44	0.50
1:J:28:ILE:HG23	1:J:29:LEU:HG	1.93	0.50
1:J:338:ASP:OD1	1:J:340:SER:OG	2.25	0.50
1:J:376:ASN:O	1:J:380:ARG:HG3	2.11	0.50
1:A:298:ARG:NH1	3:A:502:P3S:OT	2.40	0.50
1:B:127:PHE:CE2	1:B:347:MET:HG3	2.46	0.50
1:J:76:THR:O	1:J:92:MET:HA	2.11	0.50
1:O:184:GLU:H	1:O:199:PHE:HA	1.76	0.50
1:A:21:ILE:HA	1:A:90:ALA:O	2.12	0.50
1:D:95:ASP:OD2	1:D:113:LYS:NZ	2.44	0.50
1:O:188:HIS:HD2	1:O:195:HIS:CD2	2.29	0.50
1:A:67:ASP:OD2	1:O:321:ARG:NH1	2.42	0.50
1:E:278:MET:O	1:E:282:ALA:N	2.45	0.50
1:B:148:LEU:HD23	1:B:148:LEU:O	2.12	0.50
1:D:25:PHE:CB	1:D:96:ILE:HD11	2.41	0.50
1:H:139:LYS:O	1:H:147:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:PHE:CE2	1:H:327:GLY:HA2	2.47	0.50
1:M:321:ARG:HH22	2:M:501:ADP:PB	2.32	0.50
1:O:246:PHE:CD2	1:O:337:VAL:HG21	2.47	0.50
1:Q:9:ILE:CD1	1:Q:74:LEU:HB3	2.42	0.50
1:Q:130:GLY:O	1:Q:247:ASN:HB2	2.11	0.50
1:A:172:ILE:HG21	1:A:218:VAL:HG12	1.93	0.50
1:E:117:LYS:HD2	1:E:120:GLU:HG3	1.92	0.50
1:M:189:GLU:HG3	1:M:190:VAL:N	2.17	0.50
1:O:141:ASP:OD1	1:O:141:ASP:N	2.42	0.50
1:S:119:MET:HB2	1:S:124:PHE:HB2	1.93	0.50
1:U:234:LYS:HD2	1:U:297:LYS:O	2.11	0.50
1:D:125:THR:N	1:D:251:PHE:O	2.37	0.50
1:J:223:ARG:HA	1:J:227:LEU:O	2.12	0.50
1:J:319:LEU:HD12	1:J:388:LEU:HD11	1.94	0.50
1:M:135:PHE:HB3	1:M:231:PHE:CE2	2.46	0.50
1:O:247:ASN:HB3	1:O:331:ARG:HD2	1.93	0.50
1:U:321:ARG:NH1	1:W:67:ASP:OD1	2.45	0.50
1:E:289:THR:HB	1:E:337:VAL:HG22	1.94	0.50
1:E:316:ARG:NH2	1:Q:66:SER:HB3	2.26	0.50
1:H:282:ALA:HA	1:H:285:TYR:CE2	2.46	0.50
1:M:153:SER:HA	1:M:192:PRO:HB3	1.94	0.50
1:A:146:PRO:HB3	1:A:228:HIS:HB2	1.92	0.50
1:J:328:LEU:HD12	1:J:329:SER:N	2.27	0.50
1:A:310:ALA:O	1:A:318:PRO:HB2	2.12	0.49
1:B:139:LYS:O	1:B:147:THR:HG22	2.12	0.49
1:M:140:LEU:HD11	1:M:223:ARG:HG3	1.94	0.49
1:O:250:LEU:HD12	1:O:258:PHE:HE1	1.77	0.49
1:U:24:GLN:HE22	1:U:80:PHE:HZ	1.60	0.49
1:U:51:MET:HE3	1:U:69:TYR:CD2	2.47	0.49
1:W:267:LEU:HB3	1:W:272:TYR:CE2	2.47	0.49
1:A:272:TYR:O	1:A:364:PRO:HG3	2.11	0.49
1:A:304:GLU:H	1:A:373:TYR:HE2	1.59	0.49
1:B:121:GLU:HG3	1:B:122:LEU:HD12	1.93	0.49
1:J:8:ASP:O	1:J:12:PHE:HB2	2.12	0.49
1:O:203:ASP:O	1:O:207:ALA:N	2.42	0.49
1:Q:187:HIS:NE2	1:Q:196:GLU:HB3	2.28	0.49
1:S:296:PHE:HB3	1:S:390:GLU:O	2.13	0.49
1:U:434:PRO:O	1:U:438:GLU:HG3	2.13	0.49
1:A:316:ARG:HG2	1:A:321:ARG:HD3	1.94	0.49
1:E:325:SER:HB2	1:Q:51:MET:SD	2.53	0.49
1:H:10:PHE:CZ	1:H:43:LYS:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:311:TRP:CH2	1:H:367:PRO:HB3	2.48	0.49
1:O:278:MET:O	1:O:282:ALA:N	2.45	0.49
1:S:174:LEU:HA	1:S:177:GLU:HB3	1.95	0.49
1:U:329:SER:HA	2:U:501:ADP:HN61	1.77	0.49
1:E:308:TYR:OH	1:E:380:ARG:NH2	2.46	0.49
1:E:331:ARG:HD3	2:E:501:ADP:C4	2.47	0.49
1:B:8:ASP:OD1	1:B:8:ASP:N	2.41	0.49
1:B:176:LEU:HG	1:B:217:VAL:HG11	1.94	0.49
1:H:132:GLU:O	1:H:244:MET:HA	2.13	0.49
1:B:304:GLU:OE2	1:D:56:SER:OG	2.30	0.49
1:D:141:ASP:O	1:D:144:ARG:N	2.30	0.49
1:M:4:TYR:CD2	1:M:75:ASP:HA	2.47	0.49
1:Q:51:MET:HE2	1:Q:67:ASP:HB3	1.95	0.49
1:S:153:SER:HA	1:S:192:PRO:HB3	1.94	0.49
1:U:315:ASN:O	1:U:321:ARG:HB2	2.12	0.49
1:H:107:ASP:OD1	1:H:110:ALA:N	2.46	0.49
1:H:313:GLY:HA2	1:H:322:VAL:HG22	1.94	0.49
1:J:247:ASN:OD1	1:J:331:ARG:NH1	2.39	0.49
1:O:156:TYR:HB2	1:O:190:VAL:HA	1.94	0.49
1:O:189:GLU:HG3	1:O:190:VAL:N	2.22	0.49
1:Q:214:PHE:O	1:Q:218:VAL:HG13	2.11	0.49
1:Q:278:MET:O	1:Q:282:ALA:N	2.43	0.49
1:S:137:LEU:HD12	1:S:195:HIS:CD2	2.47	0.49
1:U:163:ASP:OD2	1:U:169:ARG:NH1	2.46	0.49
1:A:331:ARG:HD3	2:A:501:ADP:C8	2.47	0.49
1:E:189:GLU:HG3	1:E:190:VAL:N	2.19	0.49
1:Q:308:TYR:CZ	1:Q:380:ARG:HD3	2.48	0.49
1:S:133:PRO:HD2	1:S:197:ILE:O	2.13	0.49
1:S:387:ASP:OD1	1:S:387:ASP:N	2.44	0.49
1:U:79:VAL:HG13	1:U:89:VAL:O	2.12	0.49
1:W:137:LEU:HD12	1:W:195:HIS:NE2	2.28	0.49
1:A:116:LEU:O	1:A:119:MET:HG2	2.13	0.49
1:H:376:ASN:H	1:H:379:GLU:HB2	1.78	0.49
1:M:152:ASP:HB3	1:M:164:LEU:H	1.78	0.49
1:S:311:TRP:CH2	1:S:367:PRO:HB3	2.48	0.49
1:U:342:ASN:HB3	1:U:345:LEU:HB2	1.94	0.49
1:W:135:PHE:HD1	1:W:136:PHE:O	1.96	0.49
1:E:131:PRO:HG3	1:E:211:ILE:HD11	1.95	0.49
1:E:135:PHE:O	1:E:194:GLN:HA	2.12	0.49
1:E:169:ARG:HB3	1:E:197:ILE:HD11	1.95	0.49
1:B:159:LEU:HD21	1:D:34:ASN:HD22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:ARG:HG3	1:H:344:TYR:CE1	2.47	0.49
1:H:316:ARG:HB2	1:J:63:ILE:HD11	1.94	0.49
1:J:246:PHE:HD2	1:J:337:VAL:HG21	1.77	0.49
1:M:305:ALA:O	1:M:373:TYR:OH	2.22	0.49
1:O:169:ARG:HA	1:O:172:ILE:HD12	1.94	0.49
1:U:111:ASN:OD1	1:U:114:ARG:NH2	2.30	0.49
1:W:288:VAL:HG11	1:W:349:VAL:HG21	1.95	0.49
1:D:405:ILE:O	1:D:409:LEU:HB2	2.13	0.48
1:H:4:TYR:HD2	1:H:75:ASP:HA	1.78	0.48
1:M:219:LYS:NZ	1:M:229:ALA:O	2.46	0.48
1:S:68:MET:HE2	1:S:96:ILE:HG22	1.93	0.48
1:S:135:PHE:HB3	1:S:231:PHE:CE1	2.48	0.48
1:S:152:ASP:OD2	1:S:164:LEU:N	2.43	0.48
1:U:157:PHE:O	1:W:34:ASN:N	2.44	0.48
1:W:231:PHE:HB3	1:W:339:PRO:HG2	1.93	0.48
1:A:207:ALA:O	1:A:211:ILE:N	2.45	0.48
1:H:24:GLN:HG2	1:H:34:ASN:HB3	1.95	0.48
1:M:108:PRO:HA	1:M:111:ASN:HB2	1.95	0.48
1:M:433:HIS:HB2	1:M:434:PRO:HD2	1.94	0.48
1:Q:28:ILE:O	1:Q:342:ASN:ND2	2.43	0.48
1:S:163:ASP:OD2	1:S:188:HIS:HD2	1.95	0.48
1:A:115:VAL:HG13	1:A:352:LYS:HG3	1.94	0.48
1:A:232:MET:CE	1:D:441:LEU:HB2	2.42	0.48
1:B:215:LYS:HG2	1:B:231:PHE:CE1	2.48	0.48
1:J:169:ARG:HB3	1:J:197:ILE:HD11	1.95	0.48
1:M:259:PHE:CE1	1:M:261:GLU:HB3	2.48	0.48
1:A:240:ASN:HA	1:A:303:TYR:HB3	1.95	0.48
1:E:111:ASN:O	1:E:115:VAL:HG22	2.14	0.48
1:E:169:ARG:HD3	1:E:195:HIS:ND1	2.29	0.48
1:E:281:HIS:CD2	1:E:404:ILE:HD13	2.48	0.48
1:H:246:PHE:CG	1:H:337:VAL:HG21	2.49	0.48
1:U:199:PHE:O	2:U:501:ADP:O3'	2.25	0.48
1:A:83:THR:O	1:A:83:THR:HG23	2.13	0.48
1:E:135:PHE:HB3	1:E:231:PHE:CE1	2.48	0.48
1:D:83:THR:HG21	1:D:89:VAL:N	2.26	0.48
1:D:134:GLU:HB2	1:D:242:SER:HB2	1.96	0.48
1:D:207:ALA:O	1:D:211:ILE:HG13	2.13	0.48
1:D:440:TYR:HD2	1:D:444:TYR:CE2	2.32	0.48
1:H:237:PHE:HB2	1:O:432:VAL:HG22	1.96	0.48
1:M:207:ALA:O	1:M:211:ILE:N	2.46	0.48
1:M:273:HIS:CB	1:M:361:GLU:HG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:276:ALA:HB2	1:M:364:PRO:HA	1.95	0.48
1:Q:323:PRO:HG2	1:Q:331:ARG:NE	2.29	0.48
1:S:72:PRO:HA	1:S:94:CYS:HA	1.94	0.48
1:W:10:PHE:CZ	1:W:43:LYS:HE3	2.48	0.48
1:W:114:ARG:HD3	1:W:115:VAL:HG13	1.96	0.48
1:A:16:GLN:HB2	1:A:18:VAL:HG13	1.95	0.48
1:A:249:SER:HA	1:A:258:PHE:CE2	2.49	0.48
1:B:403:GLU:HA	1:B:406:LYS:HD3	1.94	0.48
1:B:434:PRO:O	1:B:438:GLU:HG3	2.14	0.48
1:D:208:CYS:HB2	1:D:344:TYR:CE1	2.48	0.48
1:O:138:PHE:HB3	1:O:147:THR:O	2.14	0.48
1:Q:95:ASP:OD2	1:Q:109:ARG:HB3	2.14	0.48
1:A:173:VAL:HG13	1:A:183:ILE:HG21	1.94	0.48
1:E:133:PRO:HA	1:E:244:MET:HA	1.96	0.48
1:E:187:HIS:NE2	1:E:196:GLU:HB3	2.29	0.48
1:E:318:PRO:HB3	1:E:372:ILE:HD11	1.95	0.48
1:D:43:LYS:HA	1:D:46:LEU:HB2	1.94	0.48
1:J:371:ASN:ND2	1:U:63:ILE:HG21	2.27	0.48
1:M:176:LEU:O	1:M:181:PHE:HB2	2.13	0.48
1:A:176:LEU:O	1:A:181:PHE:HB2	2.12	0.48
1:D:124:PHE:CZ	1:D:250:LEU:HD13	2.48	0.48
1:W:250:LEU:HD11	1:W:274:PHE:CD1	2.49	0.48
1:E:334:LEU:HD13	1:E:350:LEU:HD11	1.95	0.48
1:B:67:ASP:O	1:B:99:PRO:HG3	2.14	0.48
1:D:289:THR:OG1	1:D:290:ASN:ND2	2.47	0.48
1:H:172:ILE:HG21	1:H:218:VAL:HG12	1.95	0.48
1:J:402:ASN:O	1:J:406:LYS:HB2	2.14	0.48
1:O:37:ILE:HD12	1:O:38:PRO:O	2.13	0.48
1:Q:112:LEU:O	1:Q:116:LEU:HG	2.14	0.48
1:Q:400:GLU:HA	1:Q:406:LYS:HD2	1.96	0.48
1:D:194:GLN:HE21	1:D:242:SER:HB3	1.79	0.48
1:O:316:ARG:NH1	3:O:502:P3S:O3A	2.47	0.48
1:W:98:ASN:OD1	1:W:99:PRO:HD2	2.14	0.48
1:A:173:VAL:O	1:A:177:GLU:N	2.42	0.47
1:E:308:TYR:HD2	1:E:372:ILE:HG22	1.78	0.47
1:E:344:TYR:O	1:E:345:LEU:HD12	2.14	0.47
1:D:26:THR:HG22	1:D:27:ASP:O	2.14	0.47
1:J:321:ARG:NH2	2:J:501:ADP:O3B	2.46	0.47
1:O:131:PRO:HG3	1:O:211:ILE:HD11	1.96	0.47
1:Q:225:HIS:HB3	1:Q:227:LEU:HD12	1.95	0.47
1:S:312:SER:OG	1:S:369:ASP:OD1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLY:HA2	1:A:396:LEU:HD12	1.95	0.47
1:H:130:GLY:N	1:H:247:ASN:O	2.38	0.47
1:J:352:LYS:HG3	1:J:404:ILE:HG22	1.96	0.47
1:O:9:ILE:HA	1:O:12:PHE:HB2	1.94	0.47
1:Q:286:THR:HA	1:Q:289:THR:OG1	2.14	0.47
1:S:175:GLU:HG3	1:S:221:ILE:HD11	1.95	0.47
1:U:317:SER:HB2	1:U:372:ILE:HG22	1.95	0.47
1:E:156:TYR:HD1	1:E:190:VAL:HG22	1.79	0.47
1:B:108:PRO:HB3	1:B:345:LEU:HD13	1.96	0.47
1:D:91:ARG:HE	1:D:93:ILE:HG13	1.78	0.47
1:M:111:ASN:HD21	1:M:409:LEU:C	2.17	0.47
1:O:34:ASN:OD1	1:O:35:VAL:N	2.47	0.47
1:O:402:ASN:HB3	1:O:405:ILE:HD11	1.95	0.47
1:Q:191:ALA:O	1:Q:194:GLN:HB2	2.14	0.47
1:S:329:SER:HA	2:S:501:ADP:HN61	1.79	0.47
1:S:353:ALA:HB2	1:S:405:ILE:HG23	1.96	0.47
1:W:8:ASP:O	1:W:12:PHE:HB2	2.14	0.47
1:E:133:PRO:HG3	1:E:244:MET:HG3	1.95	0.47
1:D:27:ASP:HA	1:D:60:PHE:HE1	1.79	0.47
1:H:251:PHE:HA	1:H:255:GLY:O	2.13	0.47
1:J:232:MET:O	1:J:242:SER:OG	2.26	0.47
1:A:234:LYS:HD2	1:A:297:LYS:O	2.15	0.47
1:E:81:PRO:HG2	1:E:175:GLU:OE1	2.15	0.47
1:D:203:ASP:O	1:D:207:ALA:N	2.48	0.47
1:D:346:ALA:O	1:D:350:LEU:HG	2.15	0.47
1:J:140:LEU:HB2	1:J:226:GLY:O	2.13	0.47
1:W:6:LYS:HG3	1:W:74:LEU:HD21	1.96	0.47
1:U:345:LEU:HD11	1:U:413:ILE:HD13	1.96	0.47
1:A:106:GLY:HA2	1:A:413:ILE:HG13	1.97	0.47
1:B:53:ASP:OD1	1:B:55:SER:N	2.47	0.47
1:B:184:GLU:N	1:B:198:ASP:O	2.42	0.47
1:B:290:ASN:ND2	1:B:336:SER:O	2.44	0.47
1:B:319:LEU:HD23	1:B:320:VAL:HG23	1.96	0.47
1:D:4:TYR:N	1:D:75:ASP:OD1	2.46	0.47
1:D:280:LYS:O	1:D:283:ARG:NE	2.48	0.47
1:H:9:ILE:HD11	1:H:74:LEU:HB3	1.97	0.47
1:H:141:ASP:OD1	1:H:145:ARG:N	2.29	0.47
1:J:119:MET:HG3	1:J:120:GLU:N	2.30	0.47
1:J:173:VAL:O	1:J:177:GLU:N	2.38	0.47
1:J:189:GLU:HG3	1:J:190:VAL:N	2.25	0.47
1:M:123:GLY:O	1:M:252:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:249:SER:HA	1:M:258:PHE:CE2	2.49	0.47
1:O:152:ASP:HB3	1:O:164:LEU:HG	1.96	0.47
1:O:165:GLY:HA3	1:O:195:HIS:HE1	1.79	0.47
1:Q:414:PHE:O	1:Q:418:ILE:HG22	2.14	0.47
1:S:187:HIS:NE2	1:S:196:GLU:HB3	2.30	0.47
1:E:405:ILE:HD12	1:E:406:LYS:N	2.30	0.47
1:B:34:ASN:HD22	1:W:159:LEU:CG	2.25	0.47
1:J:83:THR:HB	1:J:87:GLY:O	2.14	0.47
1:J:201:TYR:HB3	2:J:501:ADP:N3	2.30	0.47
1:J:245:HIS:ND1	1:J:333:GLU:OE2	2.48	0.47
1:J:270:THR:HB	1:J:358:ILE:HD13	1.97	0.47
1:M:268:SER:OG	1:M:269:GLN:N	2.47	0.47
1:O:189:GLU:HG2	1:O:194:GLN:NE2	2.30	0.47
1:Q:95:ASP:OD1	1:Q:109:ARG:NH2	2.45	0.47
1:S:132:GLU:OE1	1:S:245:HIS:ND1	2.48	0.47
1:U:208:CYS:HB3	1:U:343:PRO:HB2	1.97	0.47
1:D:274:PHE:CE2	1:D:278:MET:HE3	2.50	0.47
1:H:267:LEU:HB2	1:H:272:TYR:CE1	2.44	0.47
1:M:33:LYS:HB3	1:S:157:PHE:CB	2.45	0.47
1:M:349:VAL:HG22	1:M:405:ILE:HD12	1.97	0.47
1:O:85:GLU:C	1:O:86:LYS:HD2	2.36	0.47
1:O:323:PRO:HD2	1:O:331:ARG:O	2.15	0.47
1:U:131:PRO:HD2	1:U:199:PHE:HE2	1.79	0.47
1:B:141:ASP:OD1	1:B:145:ARG:N	2.43	0.47
1:B:296:PHE:HA	1:B:299:LEU:HD12	1.98	0.47
1:J:314:LYS:HB3	1:J:324:SER:HB3	1.97	0.47
1:M:376:ASN:HB3	1:M:379:GLU:HG3	1.97	0.47
1:U:290:ASN:ND2	1:U:336:SER:O	2.30	0.47
1:E:168:CYS:O	1:E:172:ILE:HG13	2.15	0.46
1:H:187:HIS:NE2	1:H:196:GLU:HB3	2.30	0.46
1:J:81:PRO:HG2	1:J:175:GLU:OE1	2.15	0.46
1:M:188:HIS:ND1	1:M:189:GLU:O	2.43	0.46
1:M:279:LEU:HD22	1:M:309:ILE:HG22	1.97	0.46
1:Q:168:CYS:O	1:Q:172:ILE:HG13	2.15	0.46
1:S:231:PHE:HB3	1:S:339:PRO:CG	2.46	0.46
1:U:51:MET:CE	1:U:69:TYR:CD1	2.98	0.46
1:U:226:GLY:C	1:U:227:LEU:HD23	2.35	0.46
1:W:87:GLY:O	1:W:89:VAL:HG23	2.15	0.46
1:A:139:LYS:NZ	1:A:149:GLU:HB3	2.30	0.46
1:B:60:PHE:HE2	1:B:96:ILE:HD13	1.80	0.46
1:B:173:VAL:HG13	1:B:183:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:THR:HG23	1:D:88:LYS:HA	1.96	0.46
1:D:161:PRO:HD3	1:H:219:LYS:HB3	1.97	0.46
1:M:313:GLY:HA2	1:M:322:VAL:CG2	2.45	0.46
1:Q:97:TYR:HA	1:Q:103:PRO:HA	1.98	0.46
1:Q:377:GLU:HG3	1:Q:380:ARG:HE	1.81	0.46
1:E:183:ILE:HD13	1:E:199:PHE:HB3	1.96	0.46
1:E:357:GLY:HA2	1:E:362:LEU:CD1	2.46	0.46
1:H:160:ALA:HB2	1:H:166:GLU:OE2	2.16	0.46
1:O:153:SER:HA	1:O:192:PRO:HB3	1.98	0.46
1:S:152:ASP:CG	1:S:164:LEU:H	2.19	0.46
1:U:274:PHE:CD2	1:U:354:GLY:HA3	2.50	0.46
1:W:114:ARG:HH12	1:W:408:GLY:HA2	1.80	0.46
1:D:48:ASN:HB3	1:D:71:PHE:CE1	2.51	0.46
1:J:4:TYR:HB2	1:J:75:ASP:OD1	2.13	0.46
1:J:129:LEU:HD22	1:J:347:MET:SD	2.55	0.46
1:M:96:ILE:HG12	1:M:107:ASP:OD2	2.14	0.46
1:S:290:ASN:HB2	1:S:296:PHE:CE1	2.49	0.46
1:W:405:ILE:O	1:W:409:LEU:HB2	2.15	0.46
1:A:140:LEU:HD13	1:A:144:ARG:HD2	1.98	0.46
1:B:157:PHE:CE2	1:D:52:PHE:HB2	2.50	0.46
1:M:66:SER:O	1:M:68:MET:HG3	2.15	0.46
1:M:172:ILE:CG2	1:M:218:VAL:HG12	2.46	0.46
1:O:78:VAL:O	1:O:91:ARG:N	2.49	0.46
1:Q:283:ARG:HB3	1:Q:398:GLU:OE1	2.15	0.46
1:A:126:GLU:HB3	1:A:128:ASN:OD1	2.16	0.46
1:E:87:GLY:O	1:E:89:VAL:HG23	2.15	0.46
1:E:316:ARG:NH2	1:Q:53:ASP:OD1	2.49	0.46
1:D:188:HIS:ND1	1:D:189:GLU:O	2.43	0.46
1:H:24:GLN:OE1	1:H:91:ARG:HD3	2.16	0.46
1:H:232:MET:HE1	1:O:437:ARG:HA	1.97	0.46
1:H:315:ASN:ND2	1:J:64:GLU:HA	2.31	0.46
1:O:172:ILE:HG21	1:O:218:VAL:HG22	1.98	0.46
1:W:48:ASN:HB3	1:W:71:PHE:CE1	2.50	0.46
1:J:187:HIS:NE2	1:J:196:GLU:HB3	2.30	0.46
1:J:250:LEU:HD11	1:J:274:PHE:CE1	2.51	0.46
1:J:287:ALA:HB3	1:J:399:LEU:HD13	1.96	0.46
1:M:111:ASN:OD1	1:M:114:ARG:NH2	2.49	0.46
1:H:95:ASP:OD2	1:H:109:ARG:HD3	2.16	0.46
1:M:151:ASN:O	1:M:164:LEU:HD12	2.15	0.46
1:M:189:GLU:HB3	1:M:194:GLN:HB3	1.98	0.46
1:O:273:HIS:HB3	1:O:357:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:316:ARG:HB2	1:W:63:ILE:HD11	1.98	0.46
1:W:422:THR:O	1:W:426:ASP:N	2.48	0.46
1:E:173:VAL:HG12	1:E:197:ILE:HG21	1.98	0.46
1:M:23:LEU:HD22	1:M:94:CYS:SG	2.56	0.46
1:M:63:ILE:HG21	1:S:371:ASN:HD22	1.81	0.46
1:O:170:ARG:HA	1:O:173:VAL:HG22	1.98	0.46
1:O:260:ASP:OD1	1:O:263:GLY:N	2.48	0.46
1:Q:69:TYR:HE1	1:Q:99:PRO:HA	1.81	0.46
1:W:83:THR:O	1:W:88:LYS:HA	2.15	0.46
1:E:423:ILE:HD12	1:E:426:ASP:HB3	1.98	0.46
1:B:167:ASN:HB3	1:B:170:ARG:HE	1.79	0.46
1:B:216:LEU:CD1	1:W:159:LEU:HD13	2.41	0.46
1:B:421:LYS:O	1:B:425:CYS:HB2	2.15	0.46
1:D:296:PHE:HB3	1:D:390:GLU:O	2.16	0.46
1:J:131:PRO:HD2	1:J:199:PHE:HE2	1.81	0.46
1:J:331:ARG:HD3	2:J:501:ADP:C8	2.51	0.46
1:S:312:SER:OG	1:S:369:ASP:HA	2.16	0.46
1:U:129:LEU:HD22	1:U:347:MET:SD	2.56	0.46
1:U:135:PHE:HB3	1:U:231:PHE:CE2	2.51	0.46
1:U:144:ARG:HD2	1:U:223:ARG:NH2	2.31	0.46
1:U:194:GLN:HE21	1:U:242:SER:HB3	1.81	0.46
1:U:264:GLU:O	1:U:265:LEU:HG	2.16	0.46
1:U:422:THR:O	1:U:426:ASP:HB2	2.16	0.46
1:W:101:MET:O	1:W:101:MET:HG3	2.15	0.46
1:E:360:ASP:HB3	1:E:362:LEU:HD11	1.98	0.45
1:B:34:ASN:ND2	1:W:159:LEU:CD2	2.78	0.45
1:B:315:ASN:ND2	1:D:64:GLU:HA	2.31	0.45
1:D:304:GLU:OE2	3:D:502:P3S:HEC3	2.16	0.45
1:J:131:PRO:HA	1:J:245:HIS:O	2.16	0.45
1:J:150:LEU:HD11	1:J:236:LEU:HD11	1.98	0.45
1:J:280:LYS:HE3	1:J:280:LYS:HB2	1.57	0.45
1:O:48:ASN:OD1	1:O:72:PRO:HD2	2.16	0.45
1:U:127:PHE:CZ	1:U:351:LEU:HD13	2.51	0.45
1:U:406:LYS:HG2	1:U:414:PHE:CE1	2.51	0.45
1:E:435:TRP:HE3	1:E:436:GLU:HG2	1.81	0.45
1:D:95:ASP:HB3	1:D:97:TYR:CE1	2.49	0.45
1:H:244:MET:O	1:H:337:VAL:HG23	2.16	0.45
1:M:240:ASN:HA	1:M:303:TYR:HB3	1.98	0.45
1:Q:292:THR:O	1:Q:295:SER:OG	2.31	0.45
1:S:406:LYS:HB3	1:S:406:LYS:HE3	1.72	0.45
1:B:24:GLN:HA	1:B:34:ASN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:THR:HG22	1:B:27:ASP:O	2.17	0.45
1:D:23:LEU:HB3	1:D:94:CYS:SG	2.57	0.45
1:H:138:PHE:CE1	1:O:441:LEU:HD11	2.51	0.45
1:J:296:PHE:N	1:J:296:PHE:CD1	2.84	0.45
1:M:274:PHE:CE2	1:M:354:GLY:HA3	2.50	0.45
1:S:106:GLY:HA2	1:S:413:ILE:HG12	1.98	0.45
1:S:131:PRO:O	1:S:133:PRO:HD3	2.16	0.45
1:S:260:ASP:CB	1:S:268:SER:HA	2.46	0.45
1:S:290:ASN:HB3	1:S:295:SER:HB3	1.97	0.45
1:U:273:HIS:CB	1:U:361:GLU:HG2	2.45	0.45
1:W:78:VAL:HG21	1:W:179:MET:HE3	1.99	0.45
1:W:127:PHE:CE2	1:W:248:MET:HB3	2.50	0.45
1:E:371:ASN:OD1	1:E:374:GLY:N	2.48	0.45
1:B:60:PHE:CE2	1:B:96:ILE:HD13	2.51	0.45
1:B:112:LEU:HD12	1:B:112:LEU:HA	1.77	0.45
1:B:233:PRO:HG2	1:B:295:SER:HB3	1.98	0.45
1:D:152:ASP:HB3	1:D:164:LEU:HB2	1.97	0.45
1:D:316:ARG:HB3	1:D:335:ARG:NH2	2.31	0.45
1:D:350:LEU:O	1:D:354:GLY:N	2.38	0.45
1:H:362:LEU:HD23	1:H:362:LEU:O	2.15	0.45
1:J:434:PRO:HG2	1:M:434:PRO:HG3	1.98	0.45
1:Q:141:ASP:OD1	1:Q:145:ARG:N	2.49	0.45
1:Q:380:ARG:HA	1:Q:385:ILE:HD11	1.97	0.45
1:S:140:LEU:HD12	1:S:146:PRO:HA	1.98	0.45
1:U:157:PHE:HB3	1:W:33:LYS:HB3	1.98	0.45
1:W:243:GLY:HA2	1:W:338:ASP:HA	1.98	0.45
1:D:244:MET:N	1:D:337:VAL:O	2.48	0.45
1:D:326:ARG:O	1:D:330:THR:N	2.50	0.45
1:H:286:THR:HA	1:H:289:THR:OG1	2.16	0.45
1:J:291:PRO:HB2	1:J:421:LYS:HE3	1.99	0.45
1:M:187:HIS:HE1	1:M:189:GLU:OE2	1.99	0.45
1:Q:106:GLY:HA3	1:Q:412:HIS:CD2	2.51	0.45
1:Q:295:SER:O	1:Q:299:LEU:HG	2.16	0.45
1:S:173:VAL:HG11	1:S:186:SER:HB3	1.99	0.45
1:U:183:ILE:HD12	1:U:199:PHE:HB3	1.99	0.45
1:U:241:GLY:O	3:U:502:P3S:N	2.49	0.45
1:E:150:LEU:CD2	1:E:236:LEU:HD11	2.45	0.45
1:B:135:PHE:HB3	1:B:231:PHE:CE2	2.52	0.45
1:D:315:ASN:O	1:D:321:ARG:HB2	2.17	0.45
1:Q:21:ILE:HG12	1:Q:42:LEU:HD13	1.98	0.45
1:U:316:ARG:NE	1:W:53:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:HA	1:A:409:LEU:HD12	1.98	0.45
1:E:326:ARG:O	1:E:329:SER:N	2.49	0.45
1:B:312:SER:HB3	1:B:315:ASN:HB3	1.99	0.45
1:H:409:LEU:O	1:H:413:ILE:HB	2.16	0.45
1:J:78:VAL:HG22	1:J:91:ARG:HD2	1.99	0.45
1:W:296:PHE:CE2	1:W:392:LEU:HA	2.46	0.45
1:W:341:ALA:O	1:W:343:PRO:HD3	2.17	0.45
1:A:282:ALA:HA	1:A:285:TYR:CZ	2.51	0.45
1:B:406:LYS:HA	1:B:409:LEU:HD12	1.99	0.45
1:H:25:PHE:CE1	1:H:70:LEU:HD21	2.51	0.45
1:H:325:SER:HB2	1:J:51:MET:SD	2.57	0.45
1:J:72:PRO:HA	1:J:94:CYS:HA	1.97	0.45
1:O:83:THR:OG1	1:O:89:VAL:HB	2.17	0.45
1:O:144:ARG:NH2	1:O:223:ARG:O	2.50	0.45
1:O:188:HIS:CD2	1:O:195:HIS:CD2	3.03	0.45
1:Q:290:ASN:ND2	1:Q:336:SER:O	2.36	0.45
1:S:326:ARG:HB3	1:S:330:THR:HG23	1.99	0.45
1:U:250:LEU:HG	1:U:274:PHE:HE1	1.81	0.45
1:U:267:LEU:HB2	1:U:272:TYR:HE1	1.82	0.45
1:W:258:PHE:HZ	1:W:274:PHE:CD1	2.35	0.45
1:A:392:LEU:O	1:A:396:LEU:HG	2.16	0.45
1:E:26:THR:HG22	1:E:27:ASP:O	2.17	0.45
1:E:172:ILE:O	1:E:175:GLU:HB2	2.17	0.45
1:E:232:MET:HG2	1:E:233:PRO:HD2	1.98	0.45
1:E:368:VAL:HG22	1:E:370:ARG:HG2	1.98	0.45
1:E:444:TYR:CE1	1:B:31:ILE:HD11	2.52	0.45
1:B:135:PHE:HE2	1:B:137:LEU:HD21	1.82	0.45
1:J:128:ASN:HB2	1:J:249:SER:O	2.16	0.45
1:J:170:ARG:HB3	1:U:86:LYS:NZ	2.32	0.45
1:J:316:ARG:O	1:J:335:ARG:NH2	2.50	0.45
1:S:293:ILE:HG21	1:S:428:PHE:CD1	2.52	0.45
1:W:434:PRO:O	1:W:438:GLU:HG3	2.17	0.45
1:W:443:ILE:HG13	1:W:444:TYR:H	1.81	0.45
1:E:45:ALA:HA	1:E:50:ILE:HG12	1.99	0.45
1:E:59:GLY:C	1:E:60:PHE:HD1	2.21	0.45
1:B:328:LEU:HD23	1:B:328:LEU:H	1.82	0.45
1:D:281:HIS:HB3	1:D:402:ASN:HD21	1.81	0.45
1:H:316:ARG:NH1	3:H:502:P3S:O2A	2.48	0.45
1:J:108:PRO:HB3	1:J:345:LEU:HD13	1.99	0.45
1:J:321:ARG:NH2	1:J:333:GLU:OE2	2.50	0.45
1:J:421:LYS:HA	1:J:424:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:184:GLU:OE2	2:O:501:ADP:H2'	2.17	0.45
1:U:286:THR:HG21	1:U:388:LEU:HD22	1.98	0.45
1:W:25:PHE:CE1	1:W:70:LEU:HD11	2.52	0.45
1:W:129:LEU:HA	1:W:247:ASN:O	2.17	0.45
1:B:207:ALA:O	1:B:211:ILE:N	2.50	0.44
1:D:250:LEU:HD12	1:D:258:PHE:CE1	2.52	0.44
1:M:286:THR:HA	1:M:289:THR:OG1	2.17	0.44
1:O:87:GLY:O	1:O:89:VAL:HG23	2.18	0.44
1:Q:215:LYS:HE3	1:Q:215:LYS:HB2	1.76	0.44
1:Q:315:ASN:HD22	1:Q:316:ARG:H	1.66	0.44
1:Q:321:ARG:O	1:Q:333:GLU:HB3	2.17	0.44
1:A:83:THR:HG21	1:A:89:VAL:H	1.82	0.44
1:A:110:ALA:HA	1:A:113:LYS:HD2	1.99	0.44
1:A:297:LYS:HD2	1:D:429:ARG:O	2.16	0.44
1:B:68:MET:HE2	1:B:68:MET:HB3	1.51	0.44
1:B:172:ILE:HG23	1:B:217:VAL:HG12	1.98	0.44
1:B:331:ARG:HD3	2:B:501:ADP:N7	2.31	0.44
1:D:351:LEU:O	1:D:355:LEU:HG	2.16	0.44
1:J:23:LEU:HB3	1:J:94:CYS:SG	2.57	0.44
1:J:129:LEU:HD12	1:J:247:ASN:O	2.18	0.44
1:J:131:PRO:O	1:J:133:PRO:HD3	2.17	0.44
1:O:135:PHE:HB3	1:O:231:PHE:CE1	2.52	0.44
3:O:502:P3S:HN1	3:O:502:P3S:HGC2	1.46	0.44
1:Q:261:GLU:OE1	1:Q:261:GLU:N	2.27	0.44
1:S:301:PRO:HD3	1:S:307:CYS:SG	2.56	0.44
1:U:286:THR:HG21	1:U:388:LEU:CD2	2.48	0.44
1:U:353:ALA:HB2	1:U:405:ILE:HD11	1.98	0.44
1:W:91:ARG:NH2	1:W:93:ILE:HD11	2.33	0.44
1:E:95:ASP:OD1	1:E:109:ARG:HB3	2.17	0.44
1:E:159:LEU:HD23	1:E:159:LEU:HA	1.79	0.44
1:B:134:GLU:O	1:B:242:SER:HB2	2.17	0.44
1:H:21:ILE:HA	1:H:90:ALA:O	2.17	0.44
1:O:194:GLN:C	1:O:195:HIS:HD2	2.21	0.44
1:O:291:PRO:HB2	1:O:421:LYS:HE3	2.00	0.44
1:Q:98:ASN:HB3	1:Q:99:PRO:HD2	1.99	0.44
1:Q:132:GLU:O	1:Q:244:MET:HA	2.17	0.44
1:Q:327:GLY:N	1:Q:330:THR:OG1	2.50	0.44
1:S:176:LEU:HG	1:S:217:VAL:HG11	1.99	0.44
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.89	0.44
1:E:110:ALA:O	1:E:114:ARG:N	2.50	0.44
1:E:246:PHE:CE2	1:E:337:VAL:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ALA:HA	1:D:37:ILE:HG22	1.99	0.44
1:D:309:ILE:HG13	1:D:309:ILE:O	2.17	0.44
1:H:232:MET:SD	1:O:440:TYR:HB2	2.58	0.44
1:J:194:GLN:NE2	1:J:241:GLY:O	2.36	0.44
1:Q:370:ARG:NE	1:Q:375:MET:SD	2.88	0.44
1:W:168:CYS:O	1:W:172:ILE:HG13	2.17	0.44
1:W:173:VAL:HA	1:W:176:LEU:HD12	1.98	0.44
1:A:185:ALA:HA	1:E:37:ILE:HG22	1.99	0.44
1:A:342:ASN:HB3	1:A:345:LEU:HB2	1.99	0.44
1:E:296:PHE:CZ	1:E:392:LEU:HD12	2.53	0.44
1:J:20:PHE:HA	1:J:38:PRO:HA	1.99	0.44
1:J:311:TRP:CZ2	1:J:367:PRO:HB3	2.53	0.44
1:O:284:GLY:HA2	1:O:398:GLU:O	2.17	0.44
1:S:82:TRP:HH2	1:S:216:LEU:HD21	1.82	0.44
1:A:163:ASP:OD1	1:A:188:HIS:HD2	2.01	0.44
1:A:287:ALA:HB3	1:A:399:LEU:HD12	1.98	0.44
1:E:98:ASN:HB2	1:E:102:THR:HG23	1.99	0.44
1:B:113:LYS:HA	1:B:116:LEU:HD12	1.99	0.44
1:B:278:MET:HB3	1:B:285:TYR:OH	2.17	0.44
1:D:16:GLN:HB3	1:D:88:LYS:NZ	2.33	0.44
1:D:96:ILE:HD12	1:D:96:ILE:H	1.82	0.44
1:H:159:LEU:HD11	1:J:34:ASN:HD22	1.83	0.44
1:J:201:TYR:N	2:J:501:ADP:O2'	2.50	0.44
1:M:172:ILE:HG21	1:M:218:VAL:HG12	2.00	0.44
1:O:150:LEU:HD21	1:O:236:LEU:HD11	1.99	0.44
1:Q:81:PRO:HG2	1:Q:175:GLU:OE1	2.18	0.44
1:Q:319:LEU:O	1:Q:334:LEU:HD12	2.18	0.44
1:S:169:ARG:O	1:S:173:VAL:HG13	2.17	0.44
1:A:144:ARG:HB3	1:A:223:ARG:NH2	2.33	0.44
1:E:274:PHE:HD2	1:E:274:PHE:O	2.01	0.44
1:B:215:LYS:HG2	1:B:231:PHE:CZ	2.52	0.44
1:B:282:ALA:HA	1:B:285:TYR:CZ	2.52	0.44
1:H:129:LEU:HD22	1:H:347:MET:SD	2.57	0.44
1:H:232:MET:HE2	1:O:441:LEU:HD13	2.00	0.44
1:J:172:ILE:HD13	1:J:218:VAL:HG22	2.00	0.44
1:M:313:GLY:HA2	1:M:322:VAL:HG23	1.99	0.44
1:O:85:GLU:O	1:O:85:GLU:HG2	2.17	0.44
1:O:159:LEU:O	1:O:162:THR:N	2.48	0.44
1:Q:140:LEU:HD23	1:Q:146:PRO:HA	2.00	0.44
1:Q:160:ALA:HA	1:Q:161:PRO:HA	1.73	0.44
1:E:113:LYS:HG3	1:E:205:ILE:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:MET:HE3	1:E:127:PHE:HB2	2.00	0.44
1:B:176:LEU:O	1:B:181:PHE:HB2	2.18	0.44
1:B:419:GLU:O	1:B:423:ILE:HG13	2.17	0.44
1:D:247:ASN:OD1	1:D:331:ARG:NH1	2.48	0.44
1:Q:137:LEU:HD23	1:Q:229:ALA:HA	2.00	0.44
1:W:172:ILE:HG21	1:W:218:VAL:HG22	2.00	0.44
1:A:232:MET:HE3	1:A:235:PRO:HB3	1.99	0.44
1:A:331:ARG:HD3	2:A:501:ADP:C5	2.52	0.44
1:E:293:ILE:HD12	1:B:440:TYR:OH	2.18	0.44
1:B:112:LEU:O	1:B:116:LEU:HG	2.18	0.44
1:B:327:GLY:N	1:B:330:THR:OG1	2.51	0.44
1:B:334:LEU:HD22	1:B:350:LEU:HD21	2.00	0.44
1:J:428:PHE:HD1	1:M:435:TRP:CZ3	2.36	0.44
1:M:69:TYR:CE1	1:M:99:PRO:HA	2.53	0.44
1:Q:16:GLN:H	1:Q:16:GLN:HG2	1.61	0.44
1:W:140:LEU:HD11	1:W:228:HIS:HB2	2.00	0.44
1:A:146:PRO:HB3	1:A:228:HIS:CB	2.48	0.43
1:B:189:GLU:HG3	1:B:190:VAL:N	2.26	0.43
1:D:266:GLU:HB2	1:D:326:ARG:HE	1.83	0.43
1:H:431:ALA:HA	1:O:237:PHE:CD2	2.53	0.43
1:M:334:LEU:CD2	1:M:350:LEU:HD21	2.48	0.43
1:Q:267:LEU:HB2	1:Q:272:TYR:CE1	2.52	0.43
1:S:182:GLU:CB	1:S:200:LYS:HB2	2.48	0.43
1:S:296:PHE:HE2	1:S:392:LEU:HA	1.82	0.43
1:A:219:LYS:NZ	1:D:444:TYR:OXT	2.34	0.43
1:A:331:ARG:HD3	2:A:501:ADP:N7	2.33	0.43
1:E:311:TRP:CH2	1:E:367:PRO:HB3	2.54	0.43
1:D:173:VAL:HA	1:D:176:LEU:HD12	2.00	0.43
1:D:260:ASP:O	1:D:262:SER:N	2.51	0.43
1:H:112:LEU:HD12	1:H:112:LEU:HA	1.82	0.43
1:H:282:ALA:HB3	1:H:309:ILE:HD13	1.99	0.43
1:H:294:ASN:ND2	1:O:436:GLU:OE2	2.51	0.43
1:Q:112:LEU:HD23	1:Q:205:ILE:HG22	2.00	0.43
1:Q:260:ASP:O	1:Q:262:SER:N	2.45	0.43
1:W:45:ALA:HA	1:W:50:ILE:HG12	2.00	0.43
1:W:258:PHE:HZ	1:W:274:PHE:HD1	1.65	0.43
1:A:290:ASN:HD22	1:A:295:SER:HB2	1.84	0.43
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.84	0.43
1:B:333:GLU:OE2	1:B:335:ARG:NH2	2.52	0.43
1:H:376:ASN:HB2	1:H:379:GLU:OE2	2.18	0.43
1:J:143:ASN:HB3	1:J:145:ARG:CD	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:82:TRP:CD1	1:O:83:THR:HG23	2.53	0.43
1:O:342:ASN:ND2	1:O:345:LEU:HD13	2.33	0.43
1:W:76:THR:O	1:W:92:MET:HA	2.17	0.43
1:W:133:PRO:HB3	1:W:244:MET:HG3	1.99	0.43
1:W:238:GLY:HA2	1:W:303:TYR:OH	2.18	0.43
1:A:82:TRP:HE3	1:A:175:GLU:OE1	2.01	0.43
1:B:28:ILE:O	1:B:342:ASN:ND2	2.52	0.43
1:B:166:GLU:CD	1:D:22:ARG:HH22	2.22	0.43
1:D:377:GLU:O	1:D:380:ARG:HG3	2.19	0.43
1:H:156:TYR:CZ	1:J:53:ASP:HB3	2.53	0.43
1:M:321:ARG:HB2	1:M:335:ARG:HD2	2.00	0.43
1:Q:131:PRO:HA	1:Q:245:HIS:O	2.17	0.43
1:S:40:SER:OG	1:S:41:GLN:OE1	2.37	0.43
1:S:127:PHE:CD1	1:S:351:LEU:HD13	2.53	0.43
1:S:146:PRO:CG	1:U:442:GLU:HG2	2.48	0.43
1:A:22:ARG:HD3	1:A:36:GLU:HB2	2.01	0.43
1:E:245:HIS:CE1	1:E:335:ARG:NH1	2.87	0.43
1:B:317:SER:HB2	1:B:372:ILE:HG22	2.01	0.43
1:D:5:THR:OG1	1:D:8:ASP:HB3	2.17	0.43
1:J:22:ARG:NH1	1:J:36:GLU:OE2	2.52	0.43
1:M:52:PHE:CD1	1:M:70:LEU:HG	2.54	0.43
1:O:84:ALA:O	1:O:85:GLU:HB3	2.18	0.43
1:O:287:ALA:HB3	1:O:399:LEU:HD12	2.00	0.43
1:O:293:ILE:HG21	1:O:428:PHE:CD1	2.54	0.43
1:Q:8:ASP:O	1:Q:12:PHE:N	2.49	0.43
1:Q:316:ARG:HE	1:S:66:SER:HB3	1.83	0.43
1:S:285:TYR:HB2	1:S:349:VAL:HG11	2.00	0.43
1:W:283:ARG:HB3	1:W:283:ARG:CZ	2.48	0.43
1:W:326:ARG:O	1:W:329:SER:N	2.52	0.43
1:A:150:LEU:HD11	1:A:236:LEU:HD21	2.00	0.43
1:A:285:TYR:HB2	1:A:349:VAL:HG11	2.01	0.43
1:E:345:LEU:HD21	1:E:413:ILE:HG21	2.00	0.43
1:B:6:LYS:NZ	1:B:46:LEU:O	2.33	0.43
1:H:322:VAL:HG23	1:H:322:VAL:O	2.19	0.43
1:J:50:ILE:HD13	1:J:50:ILE:HA	1.94	0.43
1:J:131:PRO:HG3	1:J:211:ILE:HD11	2.00	0.43
1:Q:44:LYS:O	1:Q:44:LYS:HG3	2.18	0.43
1:S:428:PHE:HD1	1:U:435:TRP:CZ3	2.36	0.43
1:U:218:VAL:HG23	1:U:219:LYS:HG3	2.01	0.43
1:W:387:ASP:OD1	1:W:387:ASP:N	2.50	0.43
1:A:160:ALA:N	1:A:166:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PHE:HB3	1:A:339:PRO:CG	2.48	0.43
1:E:246:PHE:O	1:E:333:GLU:HA	2.18	0.43
1:E:296:PHE:HD1	1:E:296:PHE:N	2.17	0.43
1:B:241:GLY:O	3:B:502:P3S:N	2.52	0.43
1:B:360:ASP:O	1:B:361:GLU:HB3	2.19	0.43
1:D:39:VAL:O	1:D:42:LEU:HB2	2.18	0.43
1:H:37:ILE:HD12	1:H:41:GLN:HB2	2.00	0.43
1:H:183:ILE:HG23	1:J:38:PRO:CG	2.48	0.43
1:J:135:PHE:HB3	1:J:231:PHE:CD1	2.54	0.43
1:J:423:ILE:HD12	1:J:423:ILE:HA	1.92	0.43
1:J:442:GLU:HA	1:M:228:HIS:CE1	2.53	0.43
1:O:51:MET:HG2	1:O:69:TYR:CE2	2.54	0.43
1:Q:247:ASN:OD1	1:Q:333:GLU:HB2	2.19	0.43
1:W:131:PRO:O	1:W:133:PRO:HD3	2.19	0.43
1:W:146:PRO:HB3	1:W:228:HIS:CD2	2.54	0.43
1:A:283:ARG:HD3	1:A:398:GLU:OE1	2.19	0.43
1:D:96:ILE:HD12	1:D:96:ILE:N	2.33	0.43
1:D:154:GLY:HA3	1:D:188:HIS:NE2	2.33	0.43
1:J:296:PHE:N	1:J:296:PHE:HD1	2.16	0.43
1:M:48:ASN:HB3	1:M:71:PHE:CE1	2.54	0.43
1:O:205:ILE:HG13	1:O:206:THR:N	2.33	0.43
1:O:342:ASN:HD22	1:O:345:LEU:HD13	1.84	0.43
1:Q:275:LEU:HD12	1:Q:332:LEU:HD13	2.01	0.43
1:Q:284:GLY:O	1:Q:399:LEU:HD12	2.19	0.43
1:Q:352:LYS:HD3	1:Q:408:GLY:HA2	2.01	0.43
1:W:117:LYS:HA	1:W:120:GLU:HB2	2.00	0.43
1:E:112:LEU:O	1:E:116:LEU:HB2	2.19	0.43
1:B:130:GLY:HA3	2:B:501:ADP:H1'	2.00	0.43
1:J:237:PHE:CD2	1:M:432:VAL:HG23	2.52	0.43
1:M:47:ASP:HB3	1:M:49:LYS:HD2	2.00	0.43
1:M:216:LEU:HD22	1:S:159:LEU:HD11	2.01	0.43
1:Q:21:ILE:CD1	1:Q:39:VAL:HA	2.49	0.43
1:Q:61:VAL:HG22	1:Q:62:ARG:H	1.84	0.43
1:S:441:LEU:HB2	1:U:232:MET:HE2	2.00	0.43
1:U:308:TYR:CE2	1:U:380:ARG:HD3	2.53	0.43
1:A:28:ILE:HG22	1:A:58:GLU:O	2.19	0.43
1:B:160:ALA:HB2	1:B:166:GLU:OE1	2.18	0.43
1:B:268:SER:OG	1:B:269:GLN:N	2.52	0.43
1:D:104:PHE:CZ	1:D:412:HIS:HE1	2.37	0.43
1:D:316:ARG:HB2	1:H:63:ILE:HD11	2.00	0.43
1:J:186:SER:OG	1:U:36:GLU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:233:PRO:HG2	1:J:294:ASN:OD1	2.19	0.43
1:M:51:MET:HB3	1:M:51:MET:HE3	1.93	0.43
1:M:383:THR:HG21	1:M:385:ILE:HG23	2.01	0.43
1:U:131:PRO:HG2	1:U:211:ILE:HD11	2.00	0.43
1:U:164:LEU:HD23	1:U:164:LEU:HA	1.85	0.43
1:A:246:PHE:CD2	1:A:337:VAL:HG21	2.54	0.42
1:E:236:LEU:HD12	1:E:239:VAL:HG21	2.01	0.42
1:D:276:ALA:HB1	1:D:362:LEU:HB3	2.01	0.42
1:H:137:LEU:HD23	1:H:137:LEU:HA	1.87	0.42
1:H:148:LEU:O	1:H:148:LEU:HD23	2.19	0.42
1:H:246:PHE:HB3	1:H:248:MET:CE	2.48	0.42
1:J:9:ILE:HA	1:J:12:PHE:HB2	2.01	0.42
1:M:156:TYR:CZ	1:O:53:ASP:HB3	2.54	0.42
1:M:159:LEU:HA	1:M:159:LEU:HD23	1.81	0.42
1:M:351:LEU:HD12	1:M:351:LEU:HA	1.83	0.42
1:M:403:GLU:HA	1:M:406:LYS:HD3	1.99	0.42
1:M:432:VAL:HG12	1:M:433:HIS:H	1.84	0.42
1:O:334:LEU:CD2	1:O:337:VAL:HG23	2.49	0.42
1:Q:277:GLY:O	1:Q:281:HIS:HB2	2.19	0.42
1:Q:316:ARG:HB3	1:Q:335:ARG:NH1	2.34	0.42
1:Q:397:ILE:O	1:Q:401:LYS:HG3	2.19	0.42
1:Q:428:PHE:HB2	1:W:435:TRP:CZ3	2.54	0.42
1:S:392:LEU:HA	1:S:392:LEU:HD12	1.93	0.42
1:U:282:ALA:HA	1:U:285:TYR:CE2	2.54	0.42
1:U:294:ASN:ND2	1:U:294:ASN:O	2.52	0.42
1:E:399:LEU:HD22	1:E:414:PHE:HE1	1.83	0.42
1:B:119:MET:O	1:B:124:PHE:N	2.51	0.42
1:D:203:ASP:HB3	1:D:206:THR:HG22	2.01	0.42
1:J:440:TYR:HB3	1:M:232:MET:HG3	2.00	0.42
1:Q:86:LYS:HG3	1:Q:87:GLY:H	1.83	0.42
1:Q:104:PHE:HB3	1:Q:107:ASP:HB2	2.01	0.42
1:Q:317:SER:HB2	1:Q:372:ILE:HG22	2.01	0.42
1:W:25:PHE:HE1	1:W:70:LEU:HD11	1.83	0.42
1:A:37:ILE:HG22	1:O:185:ALA:HA	2.00	0.42
1:E:293:ILE:HD11	1:E:424:GLU:HG2	2.00	0.42
1:E:405:ILE:H	1:E:405:ILE:HG13	1.62	0.42
1:D:317:SER:N	1:D:318:PRO:HD2	2.34	0.42
1:J:246:PHE:CE2	1:J:337:VAL:HG11	2.54	0.42
1:M:146:PRO:HB3	1:M:228:HIS:CB	2.50	0.42
1:M:282:ALA:HA	1:M:285:TYR:CZ	2.54	0.42
1:M:316:ARG:HD3	3:M:502:P3S:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:423:ILE:HD12	1:O:423:ILE:HA	1.87	0.42
1:Q:203:ASP:OD1	1:Q:206:THR:HB	2.19	0.42
1:Q:364:PRO:HA	1:Q:365:PRO:HD3	1.91	0.42
1:Q:422:THR:O	1:Q:426:ASP:HB2	2.19	0.42
1:U:189:GLU:OE1	3:U:502:P3S:HGC2	2.20	0.42
1:U:380:ARG:HG2	1:U:385:ILE:HD11	2.00	0.42
1:W:70:LEU:HD23	1:W:70:LEU:HA	1.86	0.42
1:A:293:ILE:HD11	1:A:425:CYS:HA	2.00	0.42
1:E:211:ILE:O	1:E:214:PHE:N	2.52	0.42
1:D:170:ARG:NH2	1:H:22:ARG:HH21	2.18	0.42
1:D:295:SER:O	1:D:299:LEU:HG	2.20	0.42
1:H:49:LYS:HA	1:H:69:TYR:CE2	2.55	0.42
1:J:157:PHE:HE1	1:J:187:HIS:ND1	2.16	0.42
1:J:244:MET:H	1:J:338:ASP:HA	1.84	0.42
1:M:91:ARG:HD2	1:M:92:MET:N	2.34	0.42
1:O:326:ARG:O	1:O:330:THR:N	2.52	0.42
1:S:331:ARG:HD3	2:S:501:ADP:C5	2.54	0.42
1:W:251:PHE:HA	1:W:255:GLY:O	2.20	0.42
1:A:150:LEU:HD12	1:A:150:LEU:H	1.84	0.42
1:E:296:PHE:N	1:E:296:PHE:CD1	2.87	0.42
1:B:345:LEU:O	1:B:349:VAL:HB	2.19	0.42
1:J:91:ARG:HH21	1:J:93:ILE:CD1	2.27	0.42
1:J:112:LEU:HD13	1:J:344:TYR:O	2.20	0.42
1:J:278:MET:H	1:J:278:MET:HG2	1.66	0.42
1:M:95:ASP:OD1	1:M:109:ARG:NH2	2.53	0.42
1:M:316:ARG:NH1	3:M:502:P3S:O3A	2.52	0.42
1:O:421:LYS:HA	1:O:421:LYS:HD3	1.77	0.42
1:E:247:ASN:OD1	1:E:333:GLU:HG3	2.20	0.42
1:E:297:LYS:HE2	1:B:431:ALA:O	2.20	0.42
1:B:244:MET:O	1:B:337:VAL:HG23	2.19	0.42
1:B:275:LEU:O	1:B:279:LEU:HD23	2.19	0.42
1:H:436:GLU:O	1:H:440:TYR:HD1	2.02	0.42
1:J:34:ASN:OD1	1:J:35:VAL:N	2.52	0.42
1:J:53:ASP:OD1	1:J:55:SER:HB3	2.20	0.42
1:J:258:PHE:CD1	1:J:271:ALA:HB2	2.54	0.42
1:O:62:ARG:H	1:O:62:ARG:HG3	1.71	0.42
1:O:98:ASN:OD1	1:O:99:PRO:HD2	2.19	0.42
1:O:290:ASN:HB3	1:O:295:SER:HB2	2.01	0.42
1:Q:282:ALA:HA	1:Q:285:TYR:CE2	2.55	0.42
1:U:159:LEU:HD21	1:W:34:ASN:ND2	2.34	0.42
1:U:228:HIS:NE2	1:U:230:THR:HB	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:PHE:HB3	1:B:339:PRO:HB2	2.01	0.42
1:B:250:LEU:HD11	1:B:274:PHE:HE1	1.85	0.42
1:B:305:ALA:N	1:B:373:TYR:OH	2.52	0.42
1:D:364:PRO:HA	1:D:365:PRO:HD3	1.88	0.42
1:H:132:GLU:CD	1:H:245:HIS:HB2	2.40	0.42
1:J:70:LEU:HD23	1:J:70:LEU:HA	1.85	0.42
1:J:308:TYR:HD1	1:J:387:ASP:HA	1.83	0.42
1:O:293:ILE:HG21	1:O:428:PHE:CE1	2.55	0.42
1:Q:11:ARG:HA	1:Q:11:ARG:HD2	1.90	0.42
1:Q:128:ASN:O	1:Q:248:MET:HA	2.19	0.42
1:Q:296:PHE:CD1	1:Q:299:LEU:HD12	2.55	0.42
1:Q:315:ASN:HD22	1:Q:316:ARG:N	2.18	0.42
1:S:129:LEU:HD22	1:S:347:MET:SD	2.59	0.42
1:S:240:ASN:HA	1:S:303:TYR:HB3	2.01	0.42
1:U:295:SER:O	1:U:299:LEU:HG	2.20	0.42
1:A:131:PRO:HG2	1:A:199:PHE:CZ	2.55	0.42
1:E:131:PRO:O	1:E:133:PRO:HD3	2.19	0.42
1:E:139:LYS:HA	1:E:227:LEU:HD23	2.01	0.42
1:B:321:ARG:HH21	1:D:67:ASP:CG	2.20	0.42
1:H:71:PHE:HB2	1:H:97:TYR:CE1	2.54	0.42
1:H:132:GLU:OE2	1:H:245:HIS:HB2	2.19	0.42
1:J:411:GLU:O	1:J:415:GLU:HB2	2.19	0.42
1:M:264:GLU:O	1:M:265:LEU:HG	2.20	0.42
1:O:208:CYS:SG	1:O:347:MET:HG3	2.60	0.42
1:Q:43:LYS:HD3	1:Q:46:LEU:HD12	2.02	0.42
1:S:401:LYS:O	1:S:401:LYS:HG3	2.19	0.42
1:A:9:ILE:HD12	1:A:74:LEU:HD23	2.01	0.42
1:A:144:ARG:HB3	1:A:223:ARG:HH22	1.85	0.42
1:E:197:ILE:HB	1:E:214:PHE:CZ	2.52	0.42
1:E:362:LEU:HD12	1:E:362:LEU:H	1.84	0.42
1:D:131:PRO:HG2	1:D:199:PHE:CE2	2.55	0.42
1:D:312:SER:HB3	1:D:318:PRO:HG3	2.01	0.42
1:H:61:VAL:HG22	1:H:62:ARG:H	1.85	0.42
1:J:52:PHE:CZ	1:J:96:ILE:HD12	2.52	0.42
1:J:342:ASN:HA	1:J:343:PRO:HD3	1.94	0.42
1:O:309:ILE:HG13	1:O:309:ILE:O	2.19	0.42
1:Q:234:LYS:NZ	1:Q:239:VAL:O	2.28	0.42
1:Q:291:PRO:HD3	1:Q:341:ALA:HB2	2.02	0.42
1:S:68:MET:HE2	1:S:96:ILE:CG2	2.50	0.42
1:S:219:LYS:HB3	1:S:229:ALA:HB3	2.01	0.42
1:S:228:HIS:CE1	1:U:442:GLU:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:306:PRO:HB3	1:S:319:LEU:HA	2.01	0.42
1:U:79:VAL:O	1:U:81:PRO:HD3	2.20	0.42
1:A:316:ARG:HG2	1:A:321:ARG:CD	2.50	0.42
1:E:406:LYS:HE3	1:E:406:LYS:HB3	1.96	0.42
1:B:159:LEU:HG	1:D:34:ASN:HB2	2.02	0.42
1:H:101:MET:N	1:H:101:MET:SD	2.93	0.42
1:J:205:ILE:O	1:J:209:ASP:OD2	2.37	0.42
1:M:317:SER:N	1:M:318:PRO:HD2	2.35	0.42
1:Q:218:VAL:HG21	1:Q:231:PHE:CZ	2.55	0.42
1:S:170:ARG:O	1:S:174:LEU:HG	2.19	0.42
1:A:275:LEU:HD11	1:A:332:LEU:HD22	2.01	0.41
1:A:434:PRO:O	1:A:438:GLU:HG3	2.20	0.41
1:E:119:MET:HE1	1:E:124:PHE:HB3	2.02	0.41
1:B:82:TRP:O	1:B:83:THR:C	2.58	0.41
1:D:323:PRO:HG2	1:D:331:ARG:CZ	2.50	0.41
1:D:371:ASN:HD22	1:H:63:ILE:HG21	1.84	0.41
1:H:170:ARG:HD2	1:J:86:LYS:HE2	2.02	0.41
1:M:346:ALA:O	1:M:349:VAL:HG12	2.19	0.41
1:S:393:GLY:O	1:S:397:ILE:HG13	2.19	0.41
1:U:104:PHE:O	1:U:107:ASP:HB3	2.20	0.41
1:U:234:LYS:HD2	1:U:298:ARG:HA	2.02	0.41
1:A:278:MET:O	1:A:282:ALA:N	2.53	0.41
1:E:24:GLN:HB2	1:E:33:LYS:O	2.20	0.41
1:E:31:ILE:O	1:E:33:LYS:HD3	2.20	0.41
1:E:309:ILE:HG13	1:E:309:ILE:O	2.20	0.41
1:B:174:LEU:HD21	1:D:20:PHE:HE2	1.85	0.41
1:H:323:PRO:HG2	1:H:331:ARG:HE	1.85	0.41
1:J:159:LEU:HG	1:U:34:ASN:ND2	2.35	0.41
1:M:170:ARG:CZ	1:M:170:ARG:HB2	2.49	0.41
1:O:59:GLY:C	1:O:60:PHE:HD1	2.24	0.41
1:O:278:MET:HB2	1:O:285:TYR:OH	2.20	0.41
1:O:406:LYS:HB3	1:O:406:LYS:HE3	1.71	0.41
1:S:140:LEU:HB2	1:S:226:GLY:O	2.20	0.41
1:S:148:LEU:HD23	1:S:148:LEU:H	1.86	0.41
1:W:392:LEU:HD23	1:W:425:CYS:HB2	2.01	0.41
1:A:213:THR:O	1:A:217:VAL:HG23	2.19	0.41
1:E:127:PHE:HB3	1:E:204:ALA:HB2	2.01	0.41
1:E:237:PHE:HD2	1:B:432:VAL:HG23	1.86	0.41
1:B:11:ARG:O	1:B:15:GLU:HB2	2.21	0.41
1:H:349:VAL:HG13	1:H:405:ILE:HG23	2.02	0.41
1:J:159:LEU:HD12	1:U:32:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:159:LEU:HD13	1:S:216:LEU:CD1	2.49	0.41
1:Q:252:ASN:N	1:Q:255:GLY:O	2.40	0.41
1:S:32:ILE:HD12	1:S:32:ILE:H	1.85	0.41
1:S:443:ILE:HG13	1:S:444:TYR:CD2	2.55	0.41
1:W:274:PHE:CE2	1:W:354:GLY:HA3	2.53	0.41
1:W:317:SER:N	1:W:318:PRO:HD2	2.35	0.41
1:A:214:PHE:O	1:A:218:VAL:HG13	2.20	0.41
1:E:387:ASP:OD1	1:E:387:ASP:N	2.48	0.41
1:D:371:ASN:ND2	1:H:63:ILE:HG21	2.36	0.41
1:M:155:GLY:N	1:M:158:ASP:OD2	2.31	0.41
1:S:334:LEU:HD22	1:S:350:LEU:HD21	2.02	0.41
1:U:282:ALA:O	1:U:286:THR:HG23	2.21	0.41
1:W:127:PHE:CD1	1:W:351:LEU:HD13	2.55	0.41
1:W:291:PRO:HB2	1:W:421:LYS:HE3	2.02	0.41
1:W:406:LYS:HE3	1:W:406:LYS:HB3	1.90	0.41
1:A:313:GLY:HA2	1:A:322:VAL:HG22	2.02	0.41
1:E:33:LYS:HD2	1:E:33:LYS:HA	1.81	0.41
1:E:380:ARG:H	1:E:380:ARG:HG3	1.67	0.41
1:B:319:LEU:HD12	1:B:388:LEU:HD11	2.02	0.41
1:D:8:ASP:O	1:D:12:PHE:HB2	2.21	0.41
1:H:247:ASN:HB3	1:H:331:ARG:HD2	2.02	0.41
1:H:274:PHE:CD2	1:H:354:GLY:HA3	2.55	0.41
1:H:311:TRP:CZ2	1:H:367:PRO:HB3	2.56	0.41
1:J:312:SER:OG	1:J:369:ASP:OD1	2.38	0.41
1:J:375:MET:HE2	1:J:380:ARG:HB3	2.03	0.41
1:J:396:LEU:HD11	1:J:421:LYS:HB2	2.02	0.41
1:M:69:TYR:CD1	1:M:99:PRO:HA	2.55	0.41
1:O:256:ASN:ND2	1:O:330:THR:HB	2.36	0.41
1:S:265:LEU:CD1	1:S:267:LEU:HB2	2.51	0.41
1:U:267:LEU:HB2	1:U:272:TYR:CE1	2.55	0.41
1:A:130:GLY:HA2	1:A:131:PRO:HD3	1.86	0.41
1:A:273:HIS:CB	1:A:361:GLU:HG2	2.49	0.41
1:A:295:SER:O	1:A:299:LEU:HG	2.21	0.41
1:E:402:ASN:O	1:E:406:LYS:HB2	2.21	0.41
1:B:380:ARG:HA	1:B:385:ILE:HD11	2.01	0.41
1:D:350:LEU:HD23	1:D:350:LEU:HA	1.87	0.41
1:D:380:ARG:HB2	1:D:385:ILE:HG13	2.03	0.41
1:H:22:ARG:HA	1:H:35:VAL:O	2.21	0.41
1:J:442:GLU:HA	1:M:228:HIS:NE2	2.35	0.41
1:M:315:ASN:OD1	1:M:318:PRO:HD3	2.20	0.41
1:Q:168:CYS:HA	1:Q:225:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:131:PRO:HD2	1:U:199:PHE:CE2	2.54	0.41
1:U:323:PRO:HG2	1:U:331:ARG:NE	2.36	0.41
1:W:117:LYS:HA	1:W:117:LYS:HD3	1.87	0.41
1:W:207:ALA:O	1:W:211:ILE:HG13	2.21	0.41
1:A:312:SER:HB2	1:A:369:ASP:HA	2.02	0.41
1:B:108:PRO:HB3	1:B:345:LEU:CD1	2.50	0.41
1:B:187:HIS:NE2	1:B:196:GLU:HB3	2.35	0.41
1:J:48:ASN:HB3	1:J:71:PHE:CE1	2.56	0.41
1:O:151:ASN:O	1:O:164:LEU:HD12	2.21	0.41
1:U:318:PRO:HG2	1:U:320:VAL:O	2.21	0.41
1:E:338:ASP:O	1:E:340:SER:N	2.46	0.41
1:B:134:GLU:OE2	3:B:502:P3S:HBC1	2.21	0.41
1:D:83:THR:HA	1:D:86:LYS:CE	2.41	0.41
1:D:405:ILE:H	1:D:405:ILE:HG13	1.71	0.41
1:J:78:VAL:HG21	1:J:179:MET:HE3	2.03	0.41
1:M:260:ASP:O	1:M:262:SER:N	2.42	0.41
1:U:68:MET:HB3	1:U:68:MET:HE2	1.85	0.41
1:U:282:ALA:HB3	1:U:309:ILE:HD13	2.02	0.41
1:A:152:ASP:HB3	1:A:164:LEU:H	1.85	0.41
1:A:334:LEU:HD22	1:A:350:LEU:HD11	2.03	0.41
1:A:422:THR:O	1:A:426:ASP:HB2	2.20	0.41
1:E:208:CYS:HB3	1:E:343:PRO:HB2	2.03	0.41
1:E:421:LYS:HA	1:E:424:GLU:HB3	2.02	0.41
1:B:81:PRO:HG2	1:B:175:GLU:OE1	2.21	0.41
1:B:138:PHE:CE2	1:B:150:LEU:HG	2.56	0.41
1:B:298:ARG:NH1	3:B:502:P3S:OT	2.53	0.41
1:D:311:TRP:CZ2	1:D:367:PRO:HB3	2.56	0.41
1:H:111:ASN:HD21	1:H:409:LEU:C	2.24	0.41
1:H:312:SER:OG	1:H:313:GLY:N	2.53	0.41
1:J:117:LYS:HD3	1:J:117:LYS:HA	1.61	0.41
1:M:21:ILE:CD1	1:M:42:LEU:HD13	2.51	0.41
1:M:317:SER:N	1:M:318:PRO:CD	2.84	0.41
1:M:323:PRO:HG2	1:M:331:ARG:CZ	2.50	0.41
1:M:392:LEU:HB3	1:M:425:CYS:SG	2.60	0.41
1:O:80:PHE:HD1	1:O:80:PHE:HA	1.75	0.41
1:O:412:HIS:O	1:O:416:HIS:HB2	2.21	0.41
1:Q:131:PRO:HD2	1:Q:199:PHE:CE2	2.56	0.41
1:Q:221:ILE:HD13	1:Q:221:ILE:HA	1.88	0.41
1:S:16:GLN:HE21	1:S:16:GLN:HB2	1.74	0.41
1:S:119:MET:H	1:S:119:MET:HG3	1.68	0.41
1:S:152:ASP:HB3	1:S:164:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:134:GLU:HG2	1:U:196:GLU:HB2	2.03	0.41
1:E:269:GLN:HA	1:E:272:TYR:HB2	2.02	0.41
1:O:25:PHE:CE2	1:O:57:ILE:HD13	2.56	0.41
1:Q:249:SER:HA	1:Q:258:PHE:CE2	2.56	0.41
1:S:309:ILE:HG12	1:S:386:TYR:O	2.21	0.41
1:A:22:ARG:HD2	1:A:34:ASN:OD1	2.21	0.40
1:D:127:PHE:CD1	1:D:351:LEU:HD22	2.57	0.40
1:D:349:VAL:HG13	1:D:405:ILE:CG2	2.51	0.40
1:H:321:ARG:O	1:H:333:GLU:HB3	2.20	0.40
1:J:81:PRO:HB3	1:J:178:GLU:HG2	2.03	0.40
1:M:136:PHE:CE2	1:M:242:SER:HB3	2.56	0.40
1:S:28:ILE:HD11	1:S:417:PHE:HB2	2.03	0.40
1:U:283:ARG:HB3	1:U:398:GLU:OE1	2.21	0.40
1:A:315:ASN:ND2	1:E:63:ILE:HG23	2.36	0.40
1:A:439:GLN:O	1:A:443:ILE:HG13	2.21	0.40
1:B:35:VAL:HG23	1:W:187:HIS:HB3	2.03	0.40
1:B:403:GLU:HG2	1:B:406:LYS:NZ	2.36	0.40
1:H:53:ASP:OD2	1:H:56:SER:OG	2.39	0.40
1:H:297:LYS:NZ	1:O:431:ALA:O	2.49	0.40
1:O:401:LYS:HA	1:O:401:LYS:HD2	1.80	0.40
1:S:265:LEU:H	1:S:265:LEU:HG	1.34	0.40
1:U:127:PHE:CE2	1:U:351:LEU:HD13	2.56	0.40
1:U:218:VAL:HG21	1:U:231:PHE:CE1	2.56	0.40
1:W:91:ARG:HH21	1:W:93:ILE:CD1	2.33	0.40
1:W:148:LEU:HD23	1:W:148:LEU:H	1.87	0.40
1:A:9:ILE:HG23	1:A:77:TRP:CZ3	2.57	0.40
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.91	0.40
1:A:315:ASN:HA	1:E:63:ILE:O	2.21	0.40
1:B:28:ILE:HG12	1:B:59:GLY:HA3	2.02	0.40
1:D:399:LEU:HD22	1:D:414:PHE:HE1	1.87	0.40
1:H:69:TYR:HB3	1:H:71:PHE:HE1	1.86	0.40
1:H:89:VAL:HG12	1:H:90:ALA:H	1.84	0.40
1:H:109:ARG:HG3	1:H:344:TYR:HE1	1.86	0.40
1:H:109:ARG:HA	1:H:344:TYR:CD1	2.57	0.40
1:H:130:GLY:HA3	2:H:501:ADP:H1'	2.03	0.40
1:J:68:MET:SD	1:J:96:ILE:HD11	2.61	0.40
1:J:275:LEU:O	1:J:279:LEU:HB2	2.21	0.40
1:M:71:PHE:HA	1:M:72:PRO:HD3	1.92	0.40
1:M:118:GLU:HA	1:M:121:GLU:HG2	2.02	0.40
1:M:370:ARG:HG2	1:M:371:ASN:H	1.86	0.40
1:O:48:ASN:HB3	1:O:71:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:351:LEU:HD12	1:Q:351:LEU:HA	1.93	0.40
1:Q:352:LYS:HD3	1:Q:408:GLY:CA	2.50	0.40
1:S:219:LYS:H	1:S:219:LYS:HG2	1.70	0.40
1:U:116:LEU:O	1:U:119:MET:HG2	2.21	0.40
1:U:357:GLY:O	1:U:361:GLU:HA	2.21	0.40
1:W:100:ASP:O	1:W:101:MET:HB3	2.21	0.40
1:A:139:LYS:O	1:A:147:THR:HG22	2.22	0.40
1:E:312:SER:OG	1:E:369:ASP:OD1	2.40	0.40
1:B:34:ASN:ND2	1:W:159:LEU:HD23	2.37	0.40
1:B:159:LEU:HD13	1:D:216:LEU:CD1	2.50	0.40
1:H:293:ILE:HD11	1:H:425:CYS:HA	2.03	0.40
1:H:317:SER:OG	1:H:372:ILE:HG22	2.21	0.40
1:H:436:GLU:OE1	1:O:294:ASN:ND2	2.43	0.40
1:J:112:LEU:HD12	1:J:112:LEU:HA	1.92	0.40
1:O:16:GLN:O	1:O:88:LYS:HD2	2.22	0.40
1:O:45:ALA:HA	1:O:50:ILE:HG12	2.04	0.40
1:O:397:ILE:O	1:O:401:LYS:HG2	2.22	0.40
1:Q:159:LEU:HD11	1:S:34:ASN:HD22	1.86	0.40
1:Q:287:ALA:HB1	1:Q:396:LEU:HD23	2.03	0.40
1:S:86:LYS:HG3	1:S:87:GLY:N	2.34	0.40
1:S:402:ASN:O	1:S:406:LYS:HB2	2.22	0.40
1:U:200:LYS:HG2	1:U:201:TYR:H	1.86	0.40
1:W:73:ASP:N	1:W:93:ILE:O	2.44	0.40
1:A:135:PHE:CE2	1:A:195:HIS:HB2	2.56	0.40
1:B:119:MET:HB3	1:B:355:LEU:HD11	2.04	0.40
1:D:78:VAL:HG22	1:D:91:ARG:HD2	2.04	0.40
1:D:284:GLY:O	1:D:399:LEU:HA	2.21	0.40
1:H:81:PRO:HG2	1:H:175:GLU:OE1	2.21	0.40
1:J:9:ILE:HD12	1:J:77:TRP:CE3	2.57	0.40
1:J:203:ASP:HB3	1:J:206:THR:HG22	2.03	0.40
1:J:224:LYS:HE2	1:J:224:LYS:HB2	1.91	0.40
1:J:295:SER:O	1:J:298:ARG:HG2	2.20	0.40
1:S:258:PHE:CE2	1:S:332:LEU:HD23	2.57	0.40
1:S:409:LEU:HD12	1:S:409:LEU:HA	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/447 (98%)	389 (88%)	49 (11%)	2 (0%)	29	68
1	B	440/447 (98%)	393 (89%)	46 (10%)	1 (0%)	47	81
1	D	440/447 (98%)	397 (90%)	43 (10%)	0	100	100
1	E	440/447 (98%)	396 (90%)	44 (10%)	0	100	100
1	H	440/447 (98%)	393 (89%)	45 (10%)	2 (0%)	29	68
1	J	440/447 (98%)	393 (89%)	47 (11%)	0	100	100
1	M	440/447 (98%)	390 (89%)	48 (11%)	2 (0%)	29	68
1	O	440/447 (98%)	404 (92%)	36 (8%)	0	100	100
1	Q	440/447 (98%)	390 (89%)	50 (11%)	0	100	100
1	S	440/447 (98%)	398 (90%)	42 (10%)	0	100	100
1	U	440/447 (98%)	388 (88%)	50 (11%)	2 (0%)	29	68
1	W	440/447 (98%)	412 (94%)	28 (6%)	0	100	100
All	All	5280/5364 (98%)	4743 (90%)	528 (10%)	9 (0%)	47	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	A	362	LEU
1	H	362	LEU
1	M	362	LEU
1	U	362	LEU
1	B	82	TRP
1	H	264	GLU
1	M	264	GLU
1	U	264	GLU

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	375/386 (97%)	360 (96%)	15 (4%)	31	64
1	B	373/386 (97%)	360 (96%)	13 (4%)	36	67
1	D	374/386 (97%)	361 (96%)	13 (4%)	36	67
1	E	370/386 (96%)	353 (95%)	17 (5%)	27	61
1	H	378/386 (98%)	363 (96%)	15 (4%)	31	64
1	J	371/386 (96%)	349 (94%)	22 (6%)	19	53
1	M	372/386 (96%)	355 (95%)	17 (5%)	27	61
1	O	374/386 (97%)	361 (96%)	13 (4%)	36	67
1	Q	373/386 (97%)	360 (96%)	13 (4%)	36	67
1	S	371/386 (96%)	356 (96%)	15 (4%)	31	64
1	U	375/386 (97%)	360 (96%)	15 (4%)	31	64
1	W	375/386 (97%)	362 (96%)	13 (4%)	36	67
All	All	4481/4632 (97%)	4300 (96%)	181 (4%)	31	64

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PHE
1	A	55	SER
1	A	60	PHE
1	A	69	TYR
1	A	91	ARG
1	A	114	ARG
1	A	150	LEU
1	A	159	LEU
1	A	178	GLU
1	A	223	ARG
1	A	274	PHE
1	A	333	GLU
1	A	338	ASP
1	A	347	MET

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Mol	Chain	Res	Type
1	A	426	ASP
1	E	12	PHE
1	E	55	SER
1	E	91	ARG
1	E	114	ARG
1	E	119	MET
1	E	148	LEU
1	E	159	LEU
1	E	248	MET
1	E	252	ASN
1	E	259	PHE
1	E	274	PHE
1	E	317	SER
1	E	360	ASP
1	E	376	ASN
1	E	406	LYS
1	E	416	HIS
1	E	437	ARG
1	B	10	PHE
1	B	11	ARG
1	B	47	ASP
1	B	80	PHE
1	B	82	TRP
1	B	91	ARG
1	B	128	ASN
1	B	158	ASP
1	B	186	SER
1	B	274	PHE
1	B	338	ASP
1	B	347	MET
1	B	433	HIS
1	D	12	PHE
1	D	86	LYS
1	D	91	ARG
1	D	95	ASP
1	D	159	LEU
1	D	186	SER
1	D	199	PHE
1	D	259	PHE
1	D	274	PHE
1	D	335	ARG
1	D	376	ASN

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Mol	Chain	Res	Type
1	D	406	LYS
1	D	425	CYS
1	H	82	TRP
1	H	91	ARG
1	H	127	PHE
1	H	158	ASP
1	H	178	GLU
1	H	256	ASN
1	H	260	ASP
1	H	269	GLN
1	H	274	PHE
1	H	285	TYR
1	H	307	CYS
1	H	308	TYR
1	H	336	SER
1	H	376	ASN
1	H	416	HIS
1	J	4	TYR
1	J	12	PHE
1	J	40	SER
1	J	73	ASP
1	J	88	LYS
1	J	91	ARG
1	J	101	MET
1	J	111	ASN
1	J	119	MET
1	J	120	GLU
1	J	127	PHE
1	J	151	ASN
1	J	163	ASP
1	J	199	PHE
1	J	225	HIS
1	J	246	PHE
1	J	259	PHE
1	J	274	PHE
1	J	369	ASP
1	J	376	ASN
1	J	406	LYS
1	J	437	ARG
1	M	47	ASP
1	M	51	MET
1	M	60	PHE

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Mol	Chain	Res	Type
1	M	91	ARG
1	M	98	ASN
1	M	111	ASN
1	M	148	LEU
1	M	159	LEU
1	M	186	SER
1	M	198	ASP
1	M	274	PHE
1	M	298	ARG
1	M	319	LEU
1	M	328	LEU
1	M	342	ASN
1	M	356	SER
1	M	409	LEU
1	O	12	PHE
1	O	14	ASP
1	O	27	ASP
1	O	75	ASP
1	O	91	ARG
1	O	119	MET
1	O	120	GLU
1	O	159	LEU
1	O	259	PHE
1	O	274	PHE
1	O	355	LEU
1	O	380	ARG
1	O	406	LYS
1	Q	12	PHE
1	Q	17	ASN
1	Q	62	ARG
1	Q	91	ARG
1	Q	141	ASP
1	Q	144	ARG
1	Q	178	GLU
1	Q	223	ARG
1	Q	274	PHE
1	Q	319	LEU
1	Q	328	LEU
1	Q	369	ASP
1	Q	399	LEU
1	S	12	PHE
1	S	16	GLN

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Mol	Chain	Res	Type
1	S	40	SER
1	S	111	ASN
1	S	119	MET
1	S	120	GLU
1	S	148	LEU
1	S	159	LEU
1	S	163	ASP
1	S	259	PHE
1	S	274	PHE
1	S	391	SER
1	S	399	LEU
1	S	400	GLU
1	S	406	LYS
1	U	91	ARG
1	U	111	ASN
1	U	144	ARG
1	U	171	ASP
1	U	178	GLU
1	U	262	SER
1	U	265	LEU
1	U	269	GLN
1	U	274	PHE
1	U	278	MET
1	U	294	ASN
1	U	298	ARG
1	U	315	ASN
1	U	338	ASP
1	U	356	SER
1	W	12	PHE
1	W	51	MET
1	W	91	ARG
1	W	98	ASN
1	W	101	MET
1	W	114	ARG
1	W	159	LEU
1	W	163	ASP
1	W	171	ASP
1	W	223	ARG
1	W	253	GLU
1	W	274	PHE
1	W	360	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	HIS
1	B	34	ASN
1	B	128	ASN
1	D	245	HIS
1	H	34	ASN
1	H	315	ASN
1	H	412	HIS
1	J	41	GLN
1	J	290	ASN
1	J	371	ASN
1	M	256	ASN
1	M	315	ASN
1	M	342	ASN
1	M	433	HIS
1	O	195	HIS
1	O	290	ASN
1	O	342	ASN
1	Q	34	ASN
1	Q	212	GLN
1	S	16	GLN
1	U	34	ASN
1	U	269	GLN
1	U	294	ASN
1	U	315	ASN
1	U	416	HIS
1	W	24	GLN
1	W	281	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	P3S	H	502	-	11,14,14	1.77	2 (18%)	12,21,21	12.29	6 (50%)
3	P3S	U	502	-	11,14,14	1.84	3 (27%)	12,21,21	12.87	5 (41%)
2	ADP	B	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.42	4 (13%)
2	ADP	H	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.48	4 (13%)
3	P3S	A	502	-	11,14,14	1.96	3 (27%)	12,21,21	13.22	4 (33%)
3	P3S	E	502	-	11,14,14	1.94	3 (27%)	12,21,21	13.63	5 (41%)
2	ADP	U	501	-	24,29,29	1.02	1 (4%)	29,45,45	1.39	4 (13%)
3	P3S	B	502	-	11,14,14	1.83	2 (18%)	12,21,21	12.09	6 (50%)
2	ADP	A	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.47	4 (13%)
3	P3S	O	502	-	11,14,14	1.75	3 (27%)	12,21,21	12.36	4 (33%)
3	P3S	W	502	-	11,14,14	1.88	3 (27%)	12,21,21	12.54	3 (25%)
2	ADP	W	501	-	24,29,29	0.99	1 (4%)	29,45,45	1.35	4 (13%)
2	ADP	J	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.43	5 (17%)
2	ADP	M	501	-	24,29,29	0.99	1 (4%)	29,45,45	1.45	4 (13%)
3	P3S	J	502	-	11,14,14	1.86	3 (27%)	12,21,21	13.11	5 (41%)
2	ADP	E	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.44	3 (10%)
3	P3S	M	502	-	11,14,14	1.75	3 (27%)	12,21,21	13.34	6 (50%)
2	ADP	O	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.44	3 (10%)
2	ADP	S	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.37	3 (10%)
2	ADP	D	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.48	4 (13%)
3	P3S	Q	502	-	11,14,14	1.86	4 (36%)	12,21,21	12.71	4 (33%)
3	P3S	S	502	-	11,14,14	1.97	3 (27%)	12,21,21	13.09	4 (33%)
2	ADP	Q	501	-	24,29,29	0.99	2 (8%)	29,45,45	1.33	4 (13%)
3	P3S	D	502	-	11,14,14	1.90	3 (27%)	12,21,21	12.18	4 (33%)

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	P3S	H	502	-	-	8/9/16/16	-
3	P3S	U	502	-	-	6/9/16/16	-
2	ADP	B	501	-	-	4/12/32/32	0/3/3/3
2	ADP	H	501	-	-	3/12/32/32	0/3/3/3
3	P3S	A	502	-	-	6/9/16/16	-
3	P3S	E	502	-	-	7/9/16/16	-
2	ADP	U	501	-	-	7/12/32/32	0/3/3/3
3	P3S	B	502	-	-	6/9/16/16	-
2	ADP	A	501	-	-	6/12/32/32	0/3/3/3
3	P3S	O	502	-	-	7/9/16/16	-
3	P3S	W	502	-	-	4/9/16/16	-
2	ADP	W	501	-	-	5/12/32/32	0/3/3/3
2	ADP	J	501	-	-	2/12/32/32	0/3/3/3
2	ADP	M	501	-	-	6/12/32/32	0/3/3/3
3	P3S	J	502	-	-	7/9/16/16	-
2	ADP	E	501	-	-	1/12/32/32	0/3/3/3
3	P3S	M	502	-	-	7/9/16/16	-
2	ADP	O	501	-	-	2/12/32/32	0/3/3/3
2	ADP	S	501	-	-	4/12/32/32	0/3/3/3
2	ADP	D	501	-	-	2/12/32/32	0/3/3/3
3	P3S	Q	502	-	-	8/9/16/16	-
3	P3S	S	502	-	-	8/9/16/16	-
2	ADP	Q	501	-	-	3/12/32/32	0/3/3/3
3	P3S	D	502	-	-	7/9/16/16	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	P3S	PA-NE	3.57	1.72	1.59
3	M	502	P3S	PA-NE	3.53	1.72	1.59
3	A	502	P3S	PA-NE	3.50	1.72	1.59
3	S	502	P3S	PA-NE	3.50	1.72	1.59
3	D	502	P3S	PA-NE	3.49	1.72	1.59
3	U	502	P3S	PA-NE	3.39	1.71	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	P3S	PA-NE	3.38	1.71	1.59
3	A	502	P3S	PA-O1A	3.37	1.52	1.46
3	Q	502	P3S	PA-NE	3.37	1.71	1.59
3	E	502	P3S	PA-O1A	3.29	1.51	1.46
3	O	502	P3S	PA-NE	3.28	1.71	1.59
3	W	502	P3S	PA-O1A	3.26	1.51	1.46
3	S	502	P3S	PA-O1A	3.24	1.51	1.46
3	H	502	P3S	PA-NE	3.21	1.71	1.59
3	J	502	P3S	PA-NE	3.19	1.71	1.59
3	H	502	P3S	PA-O1A	3.15	1.51	1.46
3	W	502	P3S	PA-NE	3.10	1.70	1.59
3	U	502	P3S	PA-O1A	3.09	1.51	1.46
3	J	502	P3S	PA-O1A	3.07	1.51	1.46
3	B	502	P3S	PA-O1A	2.96	1.51	1.46
3	E	502	P3S	CB-CG	2.93	1.55	1.52
3	D	502	P3S	PA-O1A	2.86	1.51	1.46
3	Q	502	P3S	PA-O1A	2.82	1.51	1.46
3	D	502	P3S	CB-CG	2.69	1.55	1.52
3	S	502	P3S	CB-CG	2.69	1.55	1.52
2	U	501	ADP	C5-C4	2.59	1.47	1.40
2	W	501	ADP	C5-C4	2.57	1.47	1.40
2	Q	501	ADP	C5-C4	2.52	1.47	1.40
3	J	502	P3S	CB-CG	2.52	1.55	1.52
2	B	501	ADP	C5-C4	2.51	1.47	1.40
3	Q	502	P3S	CB-CG	2.51	1.55	1.52
2	M	501	ADP	C5-C4	2.49	1.47	1.40
2	S	501	ADP	C5-C4	2.48	1.47	1.40
2	A	501	ADP	C5-C4	2.47	1.47	1.40
2	J	501	ADP	C5-C4	2.46	1.47	1.40
3	W	502	P3S	CB-CG	2.46	1.55	1.52
2	O	501	ADP	C5-C4	2.44	1.47	1.40
3	O	502	P3S	PA-O1A	2.43	1.50	1.46
2	H	501	ADP	C5-C4	2.42	1.47	1.40
3	M	502	P3S	PA-O1A	2.39	1.50	1.46
3	A	502	P3S	CB-CG	2.37	1.55	1.52
2	E	501	ADP	C5-C4	2.35	1.47	1.40
3	M	502	P3S	CB-CG	2.33	1.55	1.52
2	D	501	ADP	C5-C4	2.30	1.47	1.40
3	O	502	P3S	CB-CG	2.29	1.55	1.52
3	U	502	P3S	CB-CG	2.05	1.54	1.52
2	Q	501	ADP	O4'-C1'	2.02	1.43	1.41
3	Q	502	P3S	PA-O2A	-2.00	1.50	1.54

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	502	P3S	OE-SD-CG	42.47	141.61	108.37
3	S	502	P3S	OE-SD-CG	40.86	140.35	108.37
3	M	502	P3S	OE-SD-CG	39.23	139.07	108.37
3	J	502	P3S	OE-SD-CG	38.99	138.89	108.37
3	Q	502	P3S	OE-SD-CG	38.92	138.83	108.37
3	W	502	P3S	OE-SD-CG	38.72	138.67	108.37
3	A	502	P3S	OE-SD-CG	38.38	138.41	108.37
3	D	502	P3S	OE-SD-CG	38.31	138.36	108.37
3	U	502	P3S	OE-SD-CG	37.67	137.85	108.37
3	O	502	P3S	OE-SD-CG	37.49	137.71	108.37
3	H	502	P3S	OE-SD-CG	36.68	137.08	108.37
3	B	502	P3S	OE-SD-CG	36.09	136.62	108.37
3	A	502	P3S	OE-SD-CE	-22.39	73.59	109.24
3	M	502	P3S	OE-SD-CE	-22.10	74.06	109.24
3	U	502	P3S	OE-SD-CE	-21.35	75.25	109.24
3	J	502	P3S	OE-SD-CE	-20.68	76.32	109.24
3	H	502	P3S	OE-SD-CE	-19.14	78.77	109.24
3	B	502	P3S	OE-SD-CE	-18.51	79.77	109.24
3	E	502	P3S	OE-SD-CE	-18.40	79.94	109.24
3	Q	502	P3S	OE-SD-CE	-18.24	80.21	109.24
3	O	502	P3S	OE-SD-CE	-18.23	80.21	109.24
3	S	502	P3S	OE-SD-CE	-17.36	81.60	109.24
3	W	502	P3S	OE-SD-CE	-17.06	82.08	109.24
3	D	502	P3S	OE-SD-CE	-15.37	84.77	109.24
3	A	502	P3S	CE-SD-NE	10.39	143.79	107.48
3	J	502	P3S	CE-SD-NE	9.74	141.53	107.48
3	U	502	P3S	CE-SD-NE	9.69	141.34	107.48
3	M	502	P3S	CE-SD-NE	9.42	140.41	107.48
3	B	502	P3S	CE-SD-NE	9.15	139.45	107.48
3	W	502	P3S	CE-SD-NE	9.14	139.41	107.48
3	O	502	P3S	CE-SD-NE	8.92	138.66	107.48
3	H	502	P3S	CE-SD-NE	8.88	138.50	107.48
3	Q	502	P3S	CE-SD-NE	8.55	137.37	107.48
3	E	502	P3S	CE-SD-NE	8.44	136.96	107.48
3	S	502	P3S	CE-SD-NE	8.25	136.33	107.48
3	D	502	P3S	CE-SD-NE	7.46	133.54	107.48
2	H	501	ADP	PA-O3A-PB	-3.81	119.76	132.83
2	A	501	ADP	PA-O3A-PB	-3.66	120.25	132.83
2	D	501	ADP	PA-O3A-PB	-3.56	120.61	132.83
2	D	501	ADP	N3-C2-N1	-3.50	123.21	128.68
2	S	501	ADP	N3-C2-N1	-3.46	123.26	128.68
2	O	501	ADP	N3-C2-N1	-3.41	123.36	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	ADP	N3-C2-N1	-3.36	123.42	128.68
2	J	501	ADP	N3-C2-N1	-3.35	123.45	128.68
2	D	501	ADP	C4-C5-N7	-3.35	105.91	109.40
2	J	501	ADP	PA-O3A-PB	-3.32	121.44	132.83
2	U	501	ADP	PA-O3A-PB	-3.31	121.47	132.83
2	A	501	ADP	N3-C2-N1	-3.30	123.52	128.68
2	O	501	ADP	C4-C5-N7	-3.28	105.98	109.40
2	M	501	ADP	PA-O3A-PB	-3.22	121.76	132.83
2	B	501	ADP	N3-C2-N1	-3.19	123.70	128.68
2	M	501	ADP	N3-C2-N1	-3.17	123.72	128.68
2	Q	501	ADP	N3-C2-N1	-3.14	123.76	128.68
2	S	501	ADP	C4-C5-N7	-3.13	106.14	109.40
2	H	501	ADP	N3-C2-N1	-3.12	123.81	128.68
2	W	501	ADP	N3-C2-N1	-3.09	123.85	128.68
3	D	502	P3S	O3A-PA-O1A	-3.04	106.94	113.45
2	U	501	ADP	N3-C2-N1	-3.02	123.96	128.68
2	E	501	ADP	C4-C5-N7	-3.00	106.27	109.40
3	B	502	P3S	O2A-PA-O1A	-2.99	107.03	113.45
2	B	501	ADP	PA-O3A-PB	-2.97	122.62	132.83
2	O	501	ADP	PA-O3A-PB	-2.93	122.76	132.83
2	Q	501	ADP	C3'-C2'-C1'	2.92	105.38	100.98
2	B	501	ADP	C3'-C2'-C1'	2.90	105.35	100.98
2	W	501	ADP	C4-C5-N7	-2.86	106.41	109.40
2	E	501	ADP	PA-O3A-PB	-2.81	123.19	132.83
2	U	501	ADP	C3'-C2'-C1'	2.77	105.15	100.98
3	Q	502	P3S	O3A-PA-O1A	-2.75	107.55	113.45
2	M	501	ADP	C3'-C2'-C1'	2.73	105.08	100.98
2	H	501	ADP	C4-C5-N7	-2.72	106.56	109.40
3	O	502	P3S	O3A-PA-O1A	-2.71	107.64	113.45
2	B	501	ADP	C4-C5-N7	-2.67	106.61	109.40
2	M	501	ADP	C4-C5-N7	-2.62	106.67	109.40
2	A	501	ADP	C4-C5-N7	-2.61	106.68	109.40
2	W	501	ADP	C3'-C2'-C1'	2.59	104.88	100.98
2	Q	501	ADP	PA-O3A-PB	-2.58	123.97	132.83
2	J	501	ADP	C4-C5-N7	-2.55	106.74	109.40
2	Q	501	ADP	C4-C5-N7	-2.52	106.77	109.40
2	A	501	ADP	C3'-C2'-C1'	2.50	104.74	100.98
3	U	502	P3S	O2A-PA-O1A	-2.49	108.11	113.45
2	S	501	ADP	PA-O3A-PB	-2.47	124.34	132.83
3	E	502	P3S	OT-C-CA	2.45	121.73	113.38
2	U	501	ADP	C4-C5-N7	-2.44	106.86	109.40
2	H	501	ADP	C3'-C2'-C1'	2.39	104.58	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	ADP	C3'-C2'-C1'	2.37	104.55	100.98
3	A	502	P3S	O2A-PA-O1A	-2.36	108.38	113.45
3	H	502	P3S	O3A-PA-O1A	-2.30	108.51	113.45
3	U	502	P3S	O3A-PA-O1A	-2.26	108.61	113.45
3	B	502	P3S	O3A-PA-O1A	-2.24	108.65	113.45
3	H	502	P3S	O2A-PA-O1A	-2.24	108.66	113.45
3	M	502	P3S	O3A-PA-O1A	-2.18	108.77	113.45
3	B	502	P3S	OT-C-CA	2.17	120.78	113.38
3	S	502	P3S	OT-C-CA	2.16	120.75	113.38
2	D	501	ADP	C3'-C2'-C1'	2.15	104.22	100.98
3	J	502	P3S	O3A-PA-O1A	-2.14	108.86	113.45
3	H	502	P3S	OT-C-CA	2.13	120.64	113.38
3	M	502	P3S	OT-C-CA	2.11	120.58	113.38
2	J	501	ADP	O3B-PB-O2B	2.11	115.69	107.64
2	W	501	ADP	PA-O3A-PB	-2.06	125.75	132.83
3	E	502	P3S	OT-C-O	-2.05	119.43	124.09
3	M	502	P3S	O2A-PA-O1A	-2.02	109.12	113.45
3	J	502	P3S	OT-C-O	-2.02	119.51	124.09

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ADP	C5'-O5'-PA-O1A
2	A	501	ADP	C3'-C4'-C5'-O5'
2	B	501	ADP	C5'-O5'-PA-O1A
2	B	501	ADP	C5'-O5'-PA-O2A
2	D	501	ADP	O4'-C4'-C5'-O5'
2	H	501	ADP	C5'-O5'-PA-O1A
2	H	501	ADP	C5'-O5'-PA-O2A
2	M	501	ADP	C5'-O5'-PA-O2A
2	M	501	ADP	C3'-C4'-C5'-O5'
2	Q	501	ADP	C3'-C4'-C5'-O5'
2	S	501	ADP	C5'-O5'-PA-O3A
2	U	501	ADP	C5'-O5'-PA-O1A
2	W	501	ADP	C5'-O5'-PA-O1A
3	A	502	P3S	CB-CG-SD-CE
3	A	502	P3S	CA-CB-CG-SD
3	E	502	P3S	O-C-CA-N
3	B	502	P3S	CB-CG-SD-CE
3	B	502	P3S	O-C-CA-N
3	D	502	P3S	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
3	D	502	P3S	N-CA-CB-CG
3	H	502	P3S	CB-CG-SD-OE
3	H	502	P3S	CB-CG-SD-CE
3	H	502	P3S	O-C-CA-N
3	J	502	P3S	CB-CG-SD-OE
3	M	502	P3S	CB-CG-SD-OE
3	M	502	P3S	CB-CG-SD-CE
3	M	502	P3S	O-C-CA-N
3	O	502	P3S	N-CA-CB-CG
3	Q	502	P3S	CB-CG-SD-OE
3	Q	502	P3S	CB-CG-SD-CE
3	Q	502	P3S	N-CA-CB-CG
3	Q	502	P3S	O-C-CA-N
3	S	502	P3S	CB-CG-SD-CE
3	S	502	P3S	N-CA-CB-CG
3	S	502	P3S	O-C-CA-N
3	U	502	P3S	CB-CG-SD-OE
2	J	501	ADP	O4'-C4'-C5'-O5'
2	J	501	ADP	C3'-C4'-C5'-O5'
2	Q	501	ADP	O4'-C4'-C5'-O5'
3	E	502	P3S	OT-C-CA-N
3	B	502	P3S	OT-C-CA-N
3	D	502	P3S	OT-C-CA-N
3	M	502	P3S	OT-C-CA-N
3	O	502	P3S	OT-C-CA-N
3	Q	502	P3S	OT-C-CA-N
2	D	501	ADP	C3'-C4'-C5'-O5'
3	O	502	P3S	OT-C-CA-CB
3	U	502	P3S	OT-C-CA-CB
3	E	502	P3S	CA-CB-CG-SD
3	H	502	P3S	OT-C-CA-N
3	O	502	P3S	O-C-CA-CB
3	U	502	P3S	O-C-CA-CB
3	S	502	P3S	OT-C-CA-N
2	U	501	ADP	C3'-C4'-C5'-O5'
3	D	502	P3S	OT-C-CA-CB
3	D	502	P3S	O-C-CA-CB
2	A	501	ADP	O4'-C4'-C5'-O5'
2	M	501	ADP	O4'-C4'-C5'-O5'
3	D	502	P3S	C-CA-CB-CG
3	Q	502	P3S	C-CA-CB-CG
3	S	502	P3S	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	U	502	P3S	OT-C-CA-N
2	W	501	ADP	PA-O3A-PB-O1B
2	O	501	ADP	O4'-C4'-C5'-O5'
3	J	502	P3S	OT-C-CA-N
3	A	502	P3S	O-C-CA-N
3	D	502	P3S	O-C-CA-N
3	J	502	P3S	O-C-CA-N
3	O	502	P3S	O-C-CA-N
3	U	502	P3S	O-C-CA-N
3	W	502	P3S	O-C-CA-N
3	U	502	P3S	CA-CB-CG-SD
2	W	501	ADP	PA-O3A-PB-O2B
2	A	501	ADP	C5'-O5'-PA-O3A
2	M	501	ADP	C5'-O5'-PA-O3A
2	W	501	ADP	C5'-O5'-PA-O3A
3	B	502	P3S	CA-CB-CG-SD
2	U	501	ADP	PB-O3A-PA-O2A
3	S	502	P3S	CB-CG-SD-OE
3	H	502	P3S	OT-C-CA-CB
3	S	502	P3S	OT-C-CA-CB
3	S	502	P3S	O-C-CA-CB
2	A	501	ADP	C5'-O5'-PA-O2A
2	M	501	ADP	C5'-O5'-PA-O1A
2	U	501	ADP	C5'-O5'-PA-O2A
3	E	502	P3S	CB-CG-SD-CE
3	J	502	P3S	CB-CG-SD-CE
3	O	502	P3S	CB-CG-SD-CE
3	H	502	P3S	O-C-CA-CB
3	M	502	P3S	OT-C-CA-CB
3	M	502	P3S	O-C-CA-CB
2	S	501	ADP	PA-O3A-PB-O1B
3	E	502	P3S	OT-C-CA-CB
3	E	502	P3S	O-C-CA-CB
3	B	502	P3S	OT-C-CA-CB
3	B	502	P3S	O-C-CA-CB
2	Q	501	ADP	PB-O3A-PA-O2A
2	E	501	ADP	O4'-C4'-C5'-O5'
3	H	502	P3S	CA-CB-CG-SD
3	Q	502	P3S	O-C-CA-CB
3	J	502	P3S	CA-CB-CG-SD
3	O	502	P3S	C-CA-CB-CG
3	A	502	P3S	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	J	502	P3S	O-C-CA-CB
3	Q	502	P3S	OT-C-CA-CB
3	A	502	P3S	OT-C-CA-N
2	A	501	ADP	PB-O3A-PA-O2A
2	M	501	ADP	PB-O3A-PA-O1A
2	U	501	ADP	PB-O3A-PA-O1A
2	B	501	ADP	C3'-C4'-C5'-O5'
2	O	501	ADP	C3'-C4'-C5'-O5'
3	W	502	P3S	OT-C-CA-N
3	W	502	P3S	O-C-CA-CB
3	W	502	P3S	OT-C-CA-CB
2	U	501	ADP	O4'-C4'-C5'-O5'
3	A	502	P3S	OT-C-CA-CB
3	J	502	P3S	OT-C-CA-CB
2	B	501	ADP	C5'-O5'-PA-O3A
2	H	501	ADP	C5'-O5'-PA-O3A
2	U	501	ADP	C5'-O5'-PA-O3A
3	E	502	P3S	N-CA-CB-CG
3	H	502	P3S	N-CA-CB-CG
3	M	502	P3S	N-CA-CB-CG
2	W	501	ADP	O4'-C4'-C5'-O5'
2	S	501	ADP	C5'-O5'-PA-O1A
2	S	501	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

19 monomers are involved in 50 short contacts:

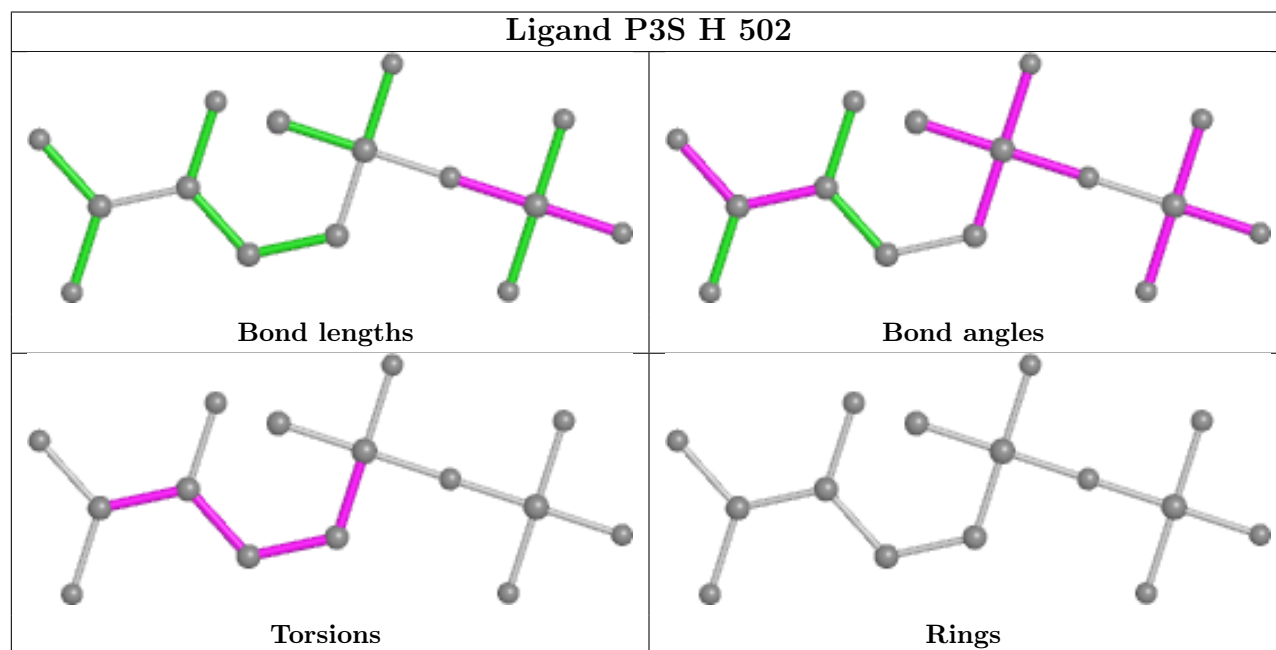
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	502	P3S	2	0
3	U	502	P3S	2	0
2	B	501	ADP	5	0
2	H	501	ADP	3	0
3	A	502	P3S	1	0
2	U	501	ADP	2	0
3	B	502	P3S	3	0
2	A	501	ADP	5	0
3	O	502	P3S	2	0
2	J	501	ADP	5	0
2	M	501	ADP	3	0
3	J	502	P3S	1	0
2	E	501	ADP	2	0
3	M	502	P3S	3	0

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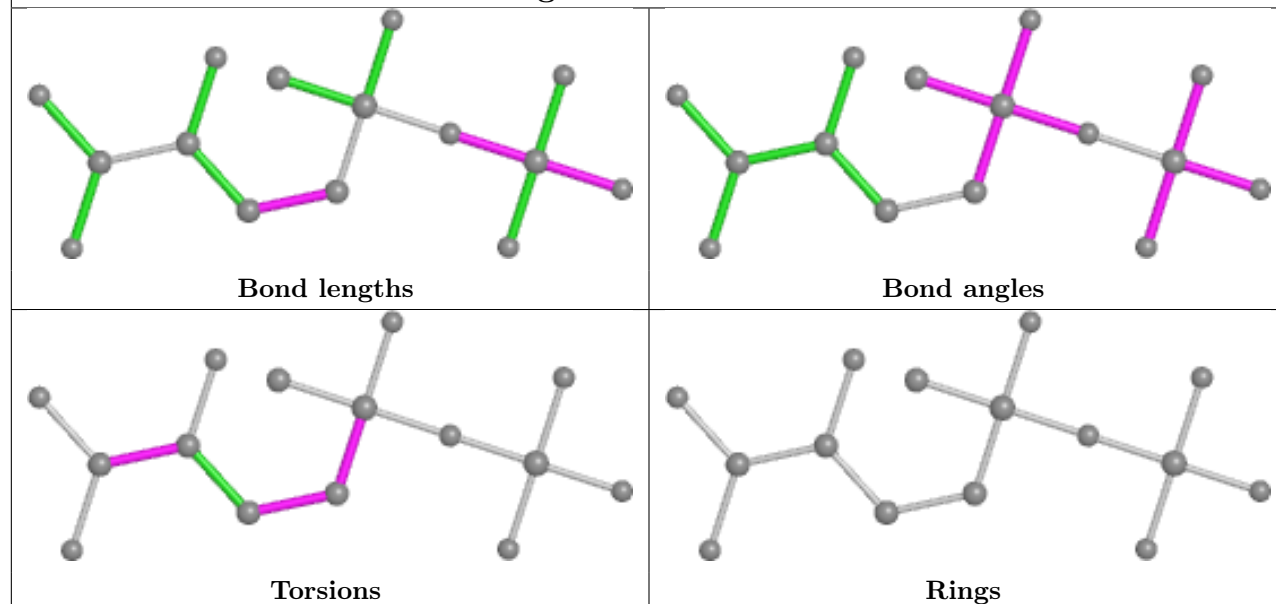
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	501	ADP	4	0
2	S	501	ADP	2	0
2	D	501	ADP	2	0
2	Q	501	ADP	1	0
3	D	502	P3S	2	0

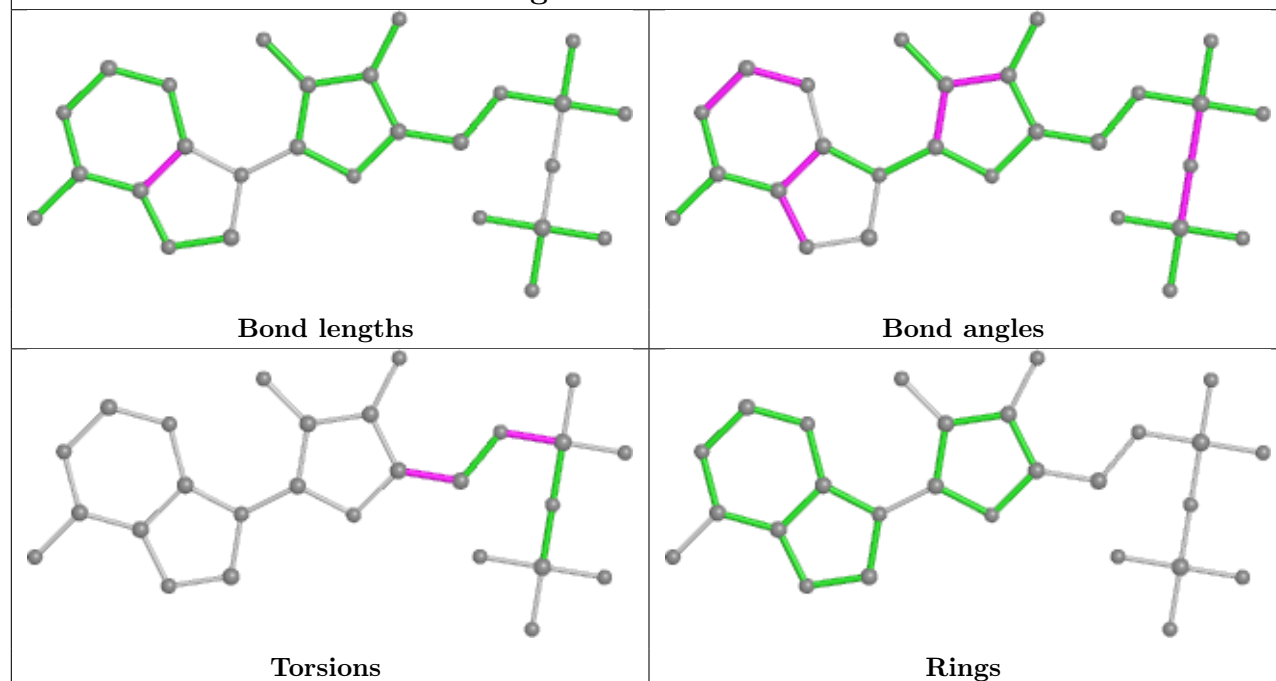
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

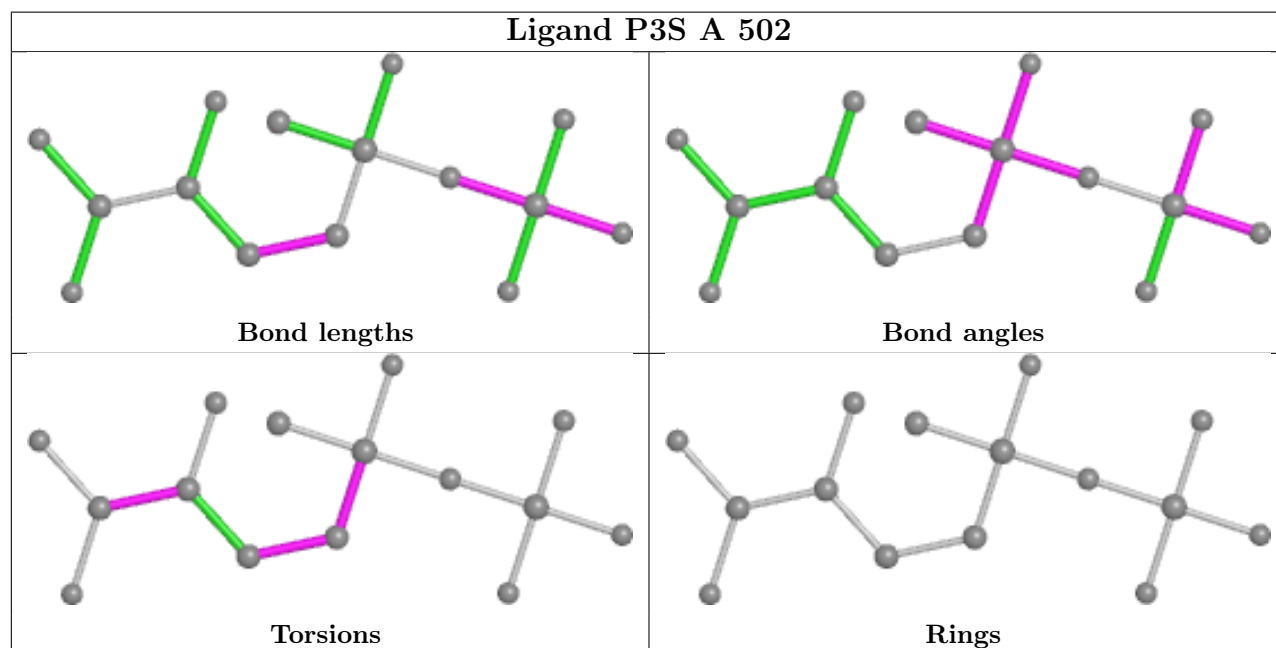
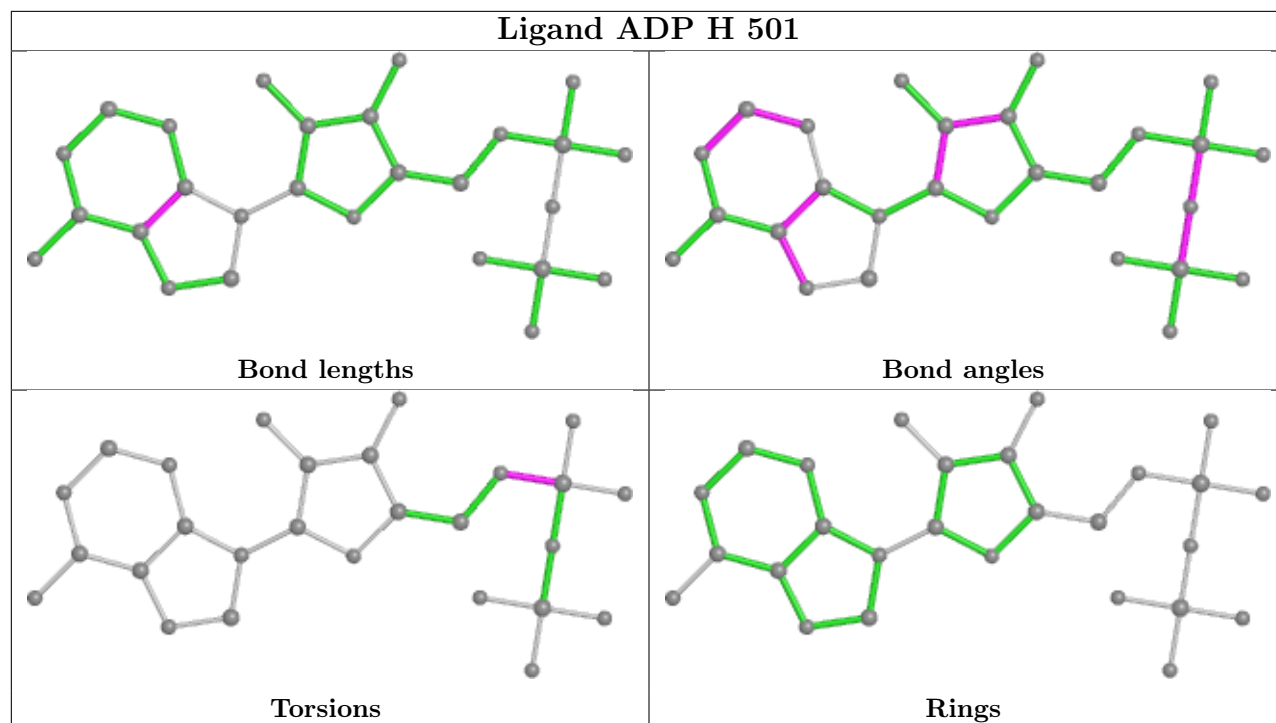


Ligand P3S U 502

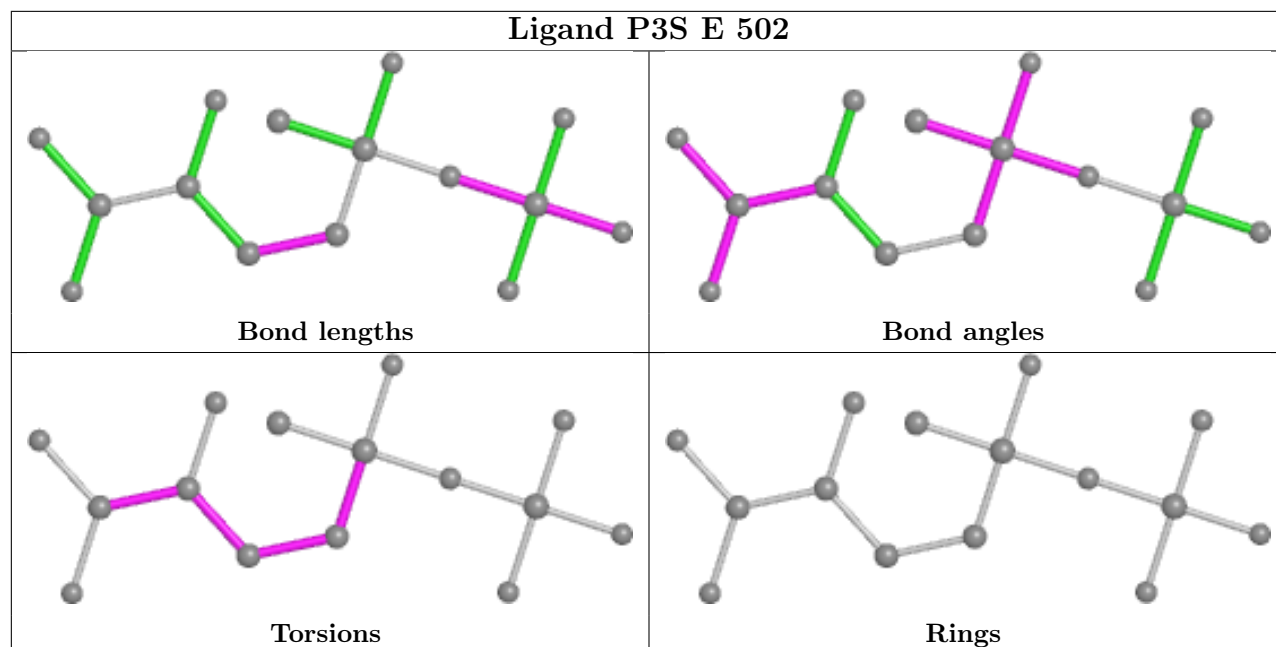


Ligand ADP B 501

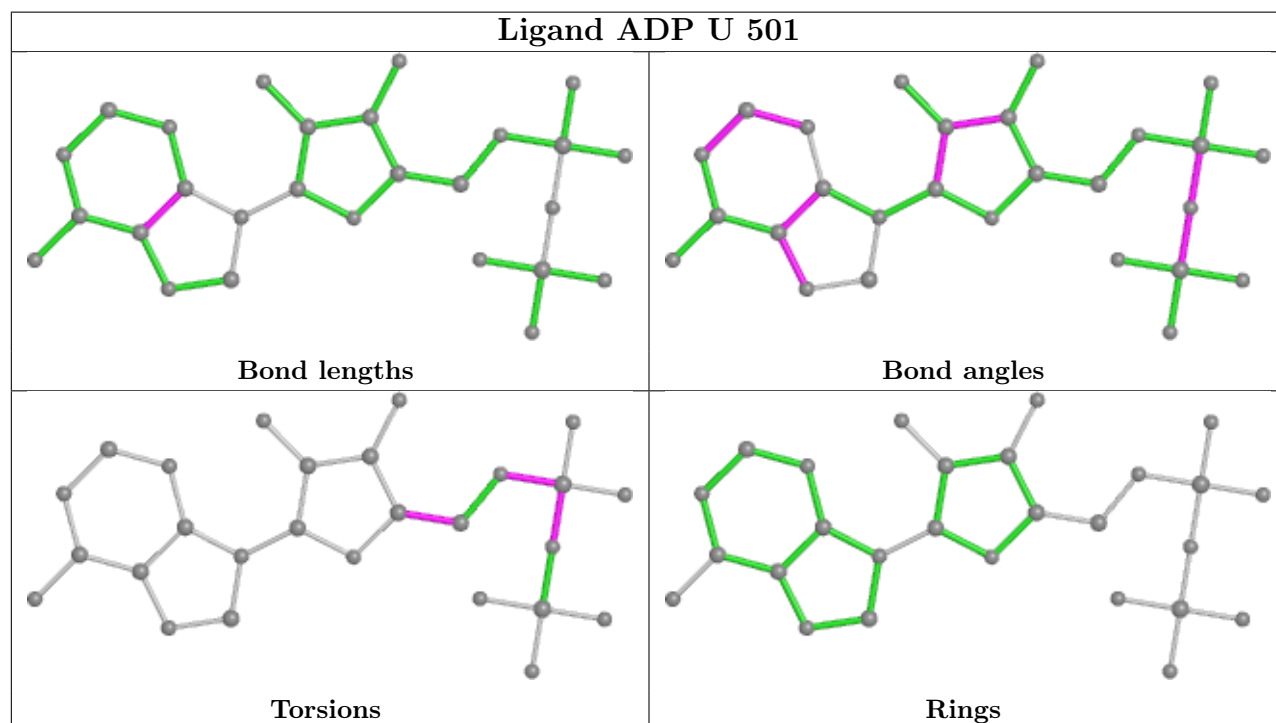




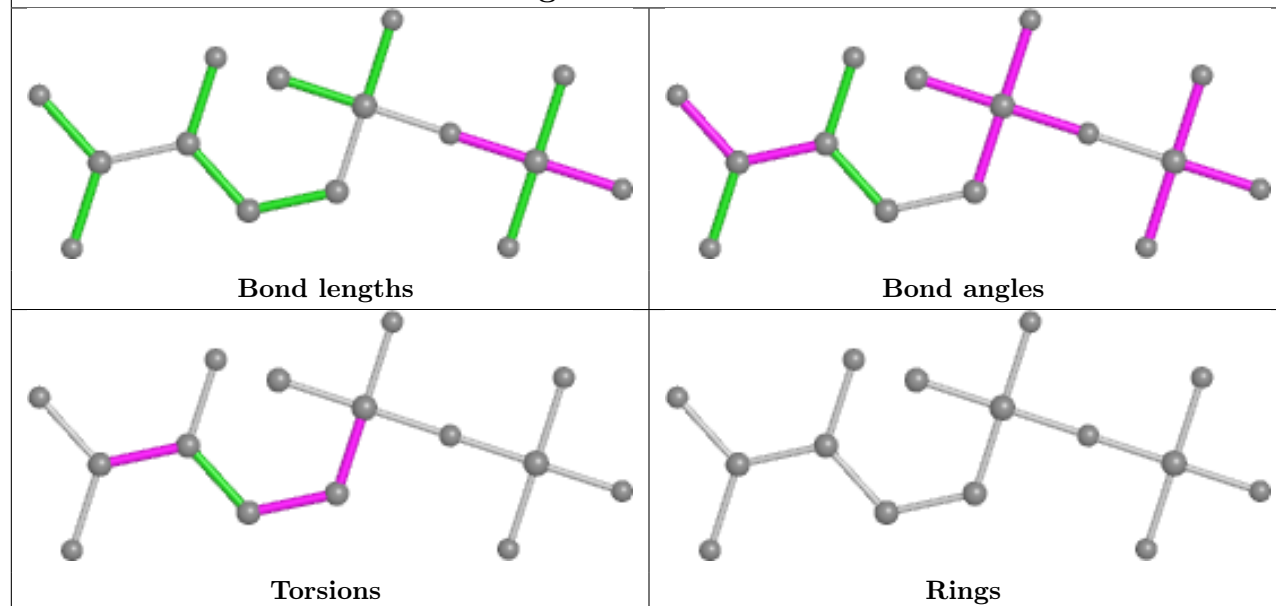
Ligand P3S E 502



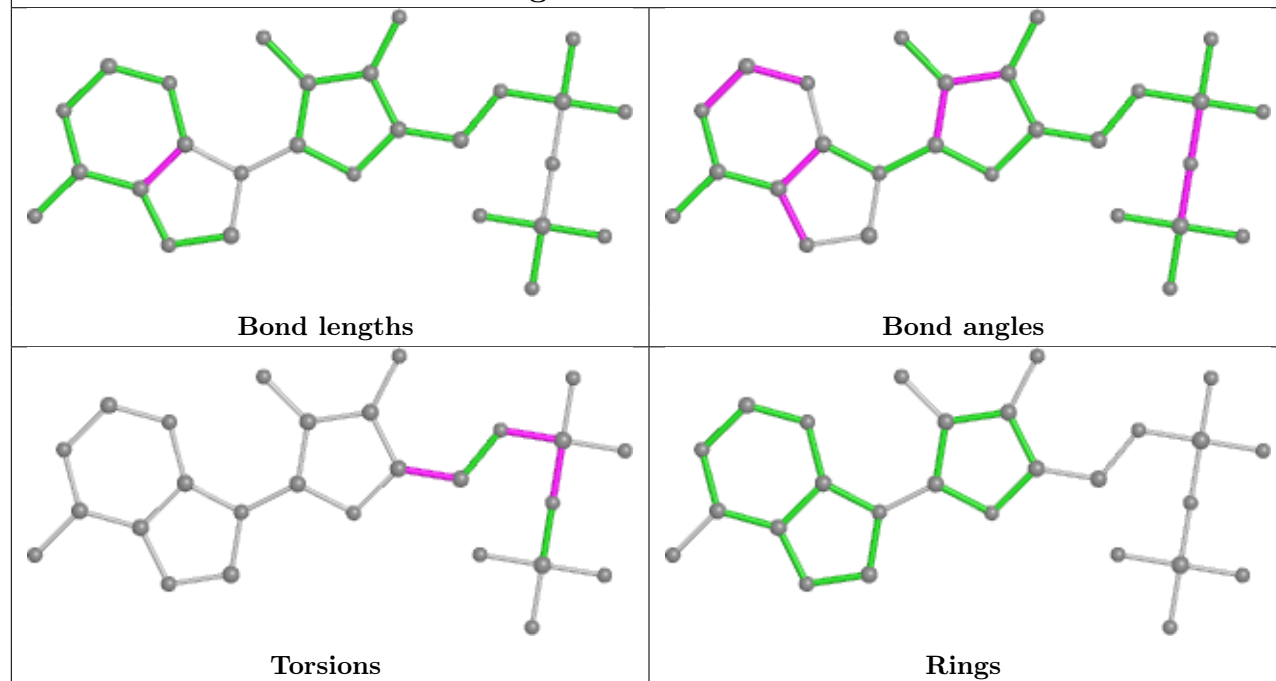
Ligand ADP U 501



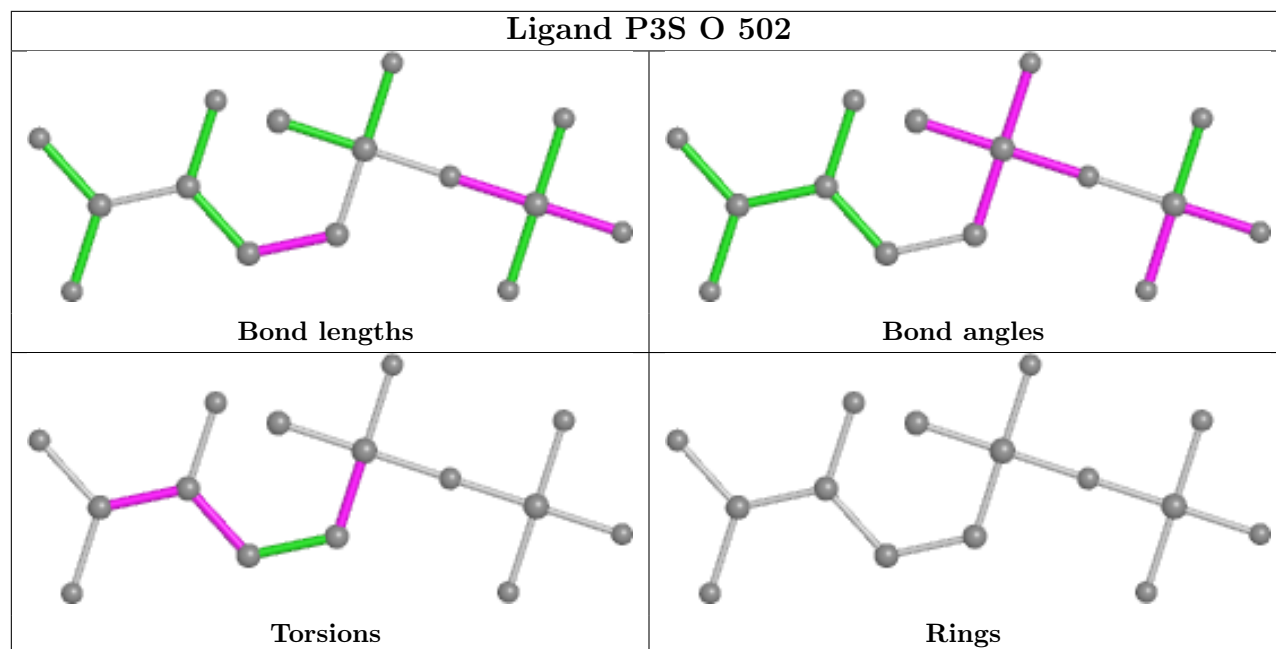
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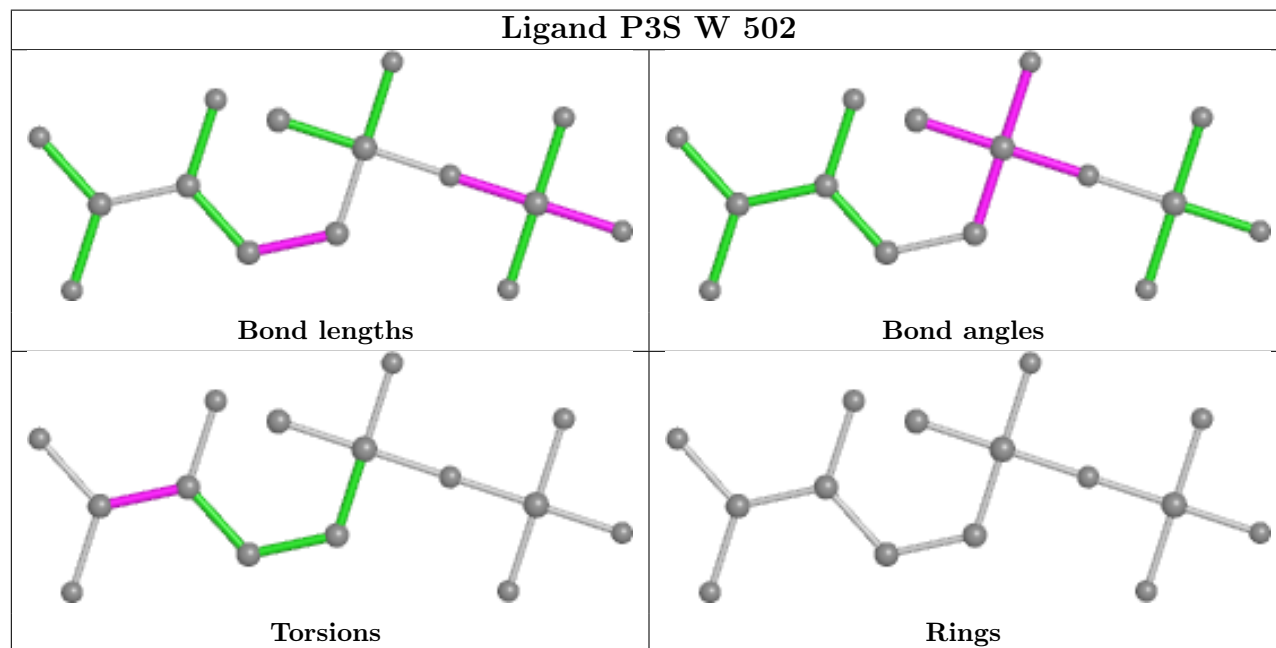
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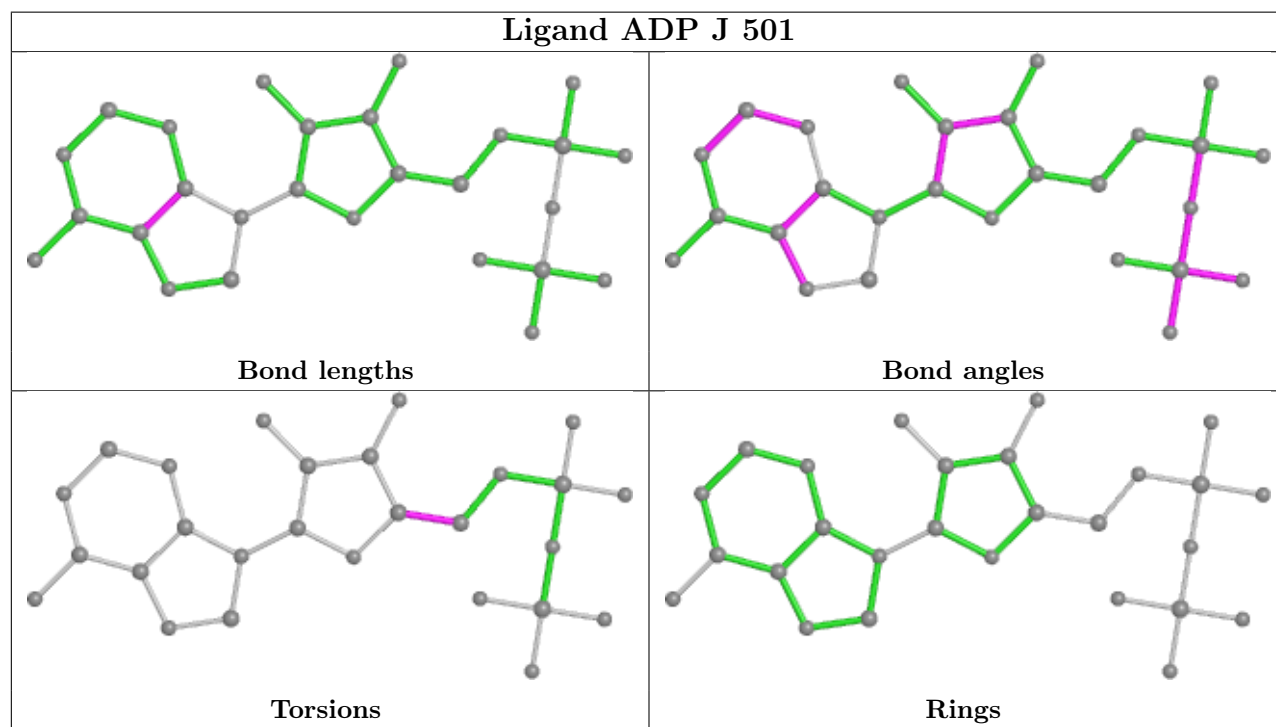
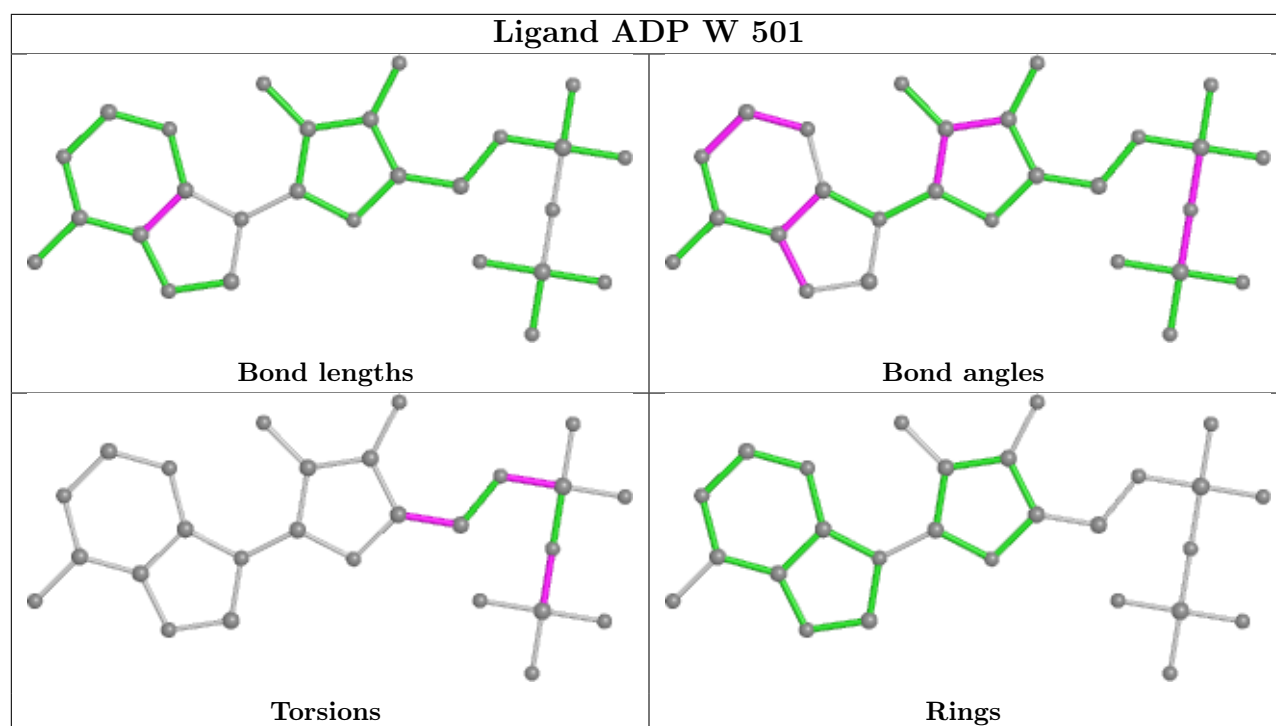


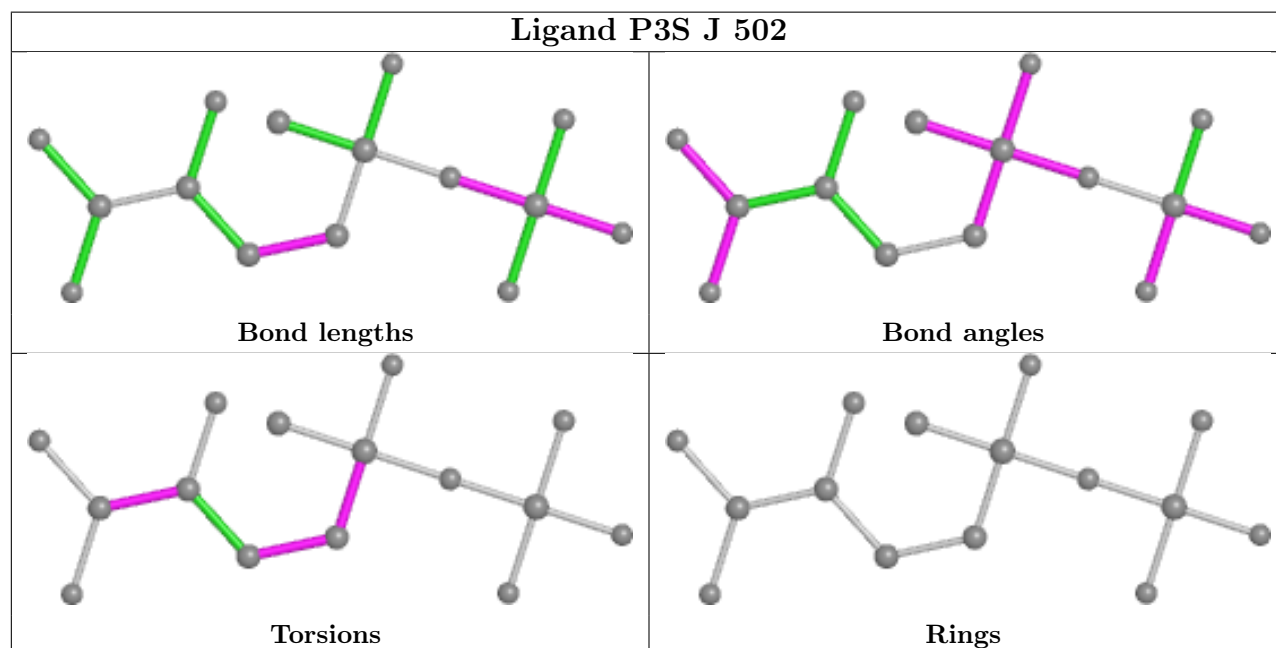
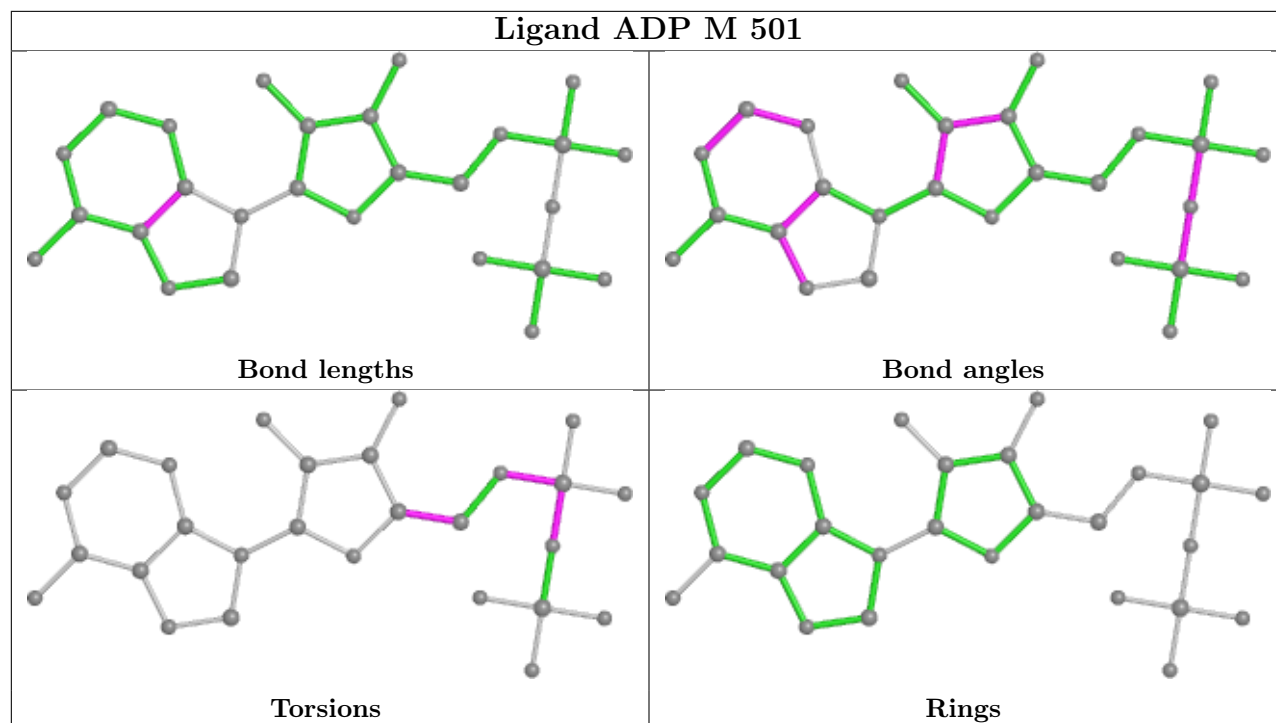
Ligand P3S O 502



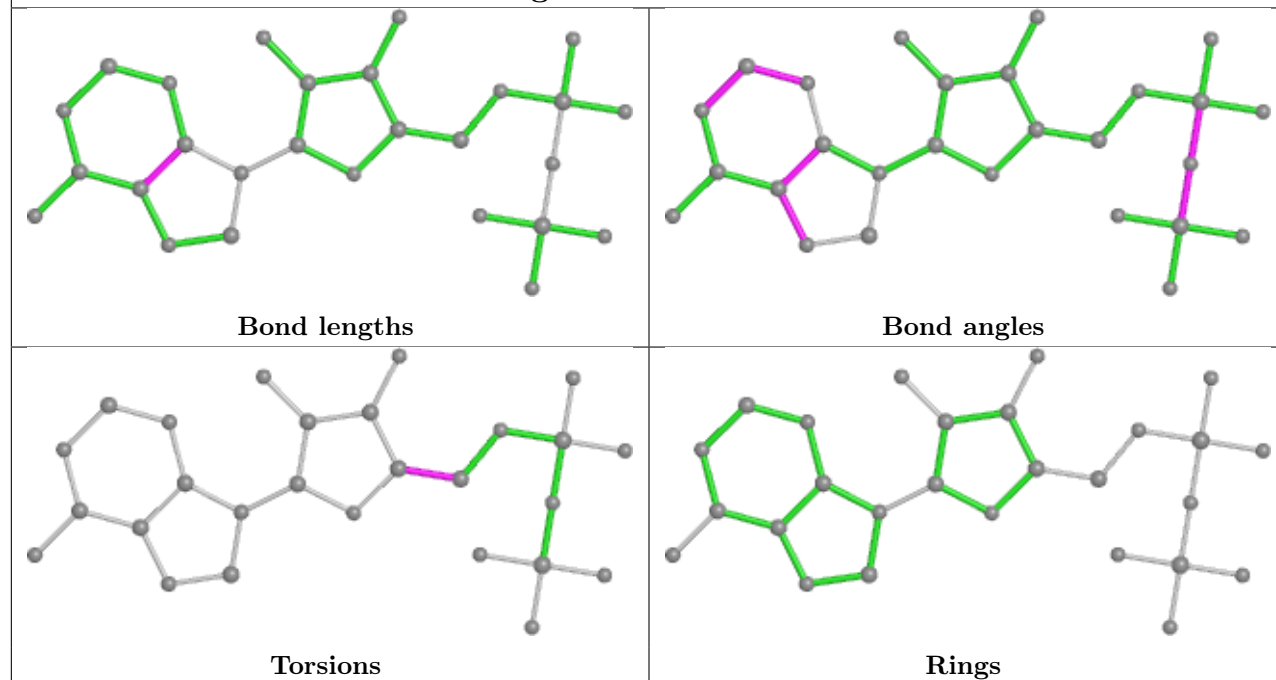
Ligand P3S W 502



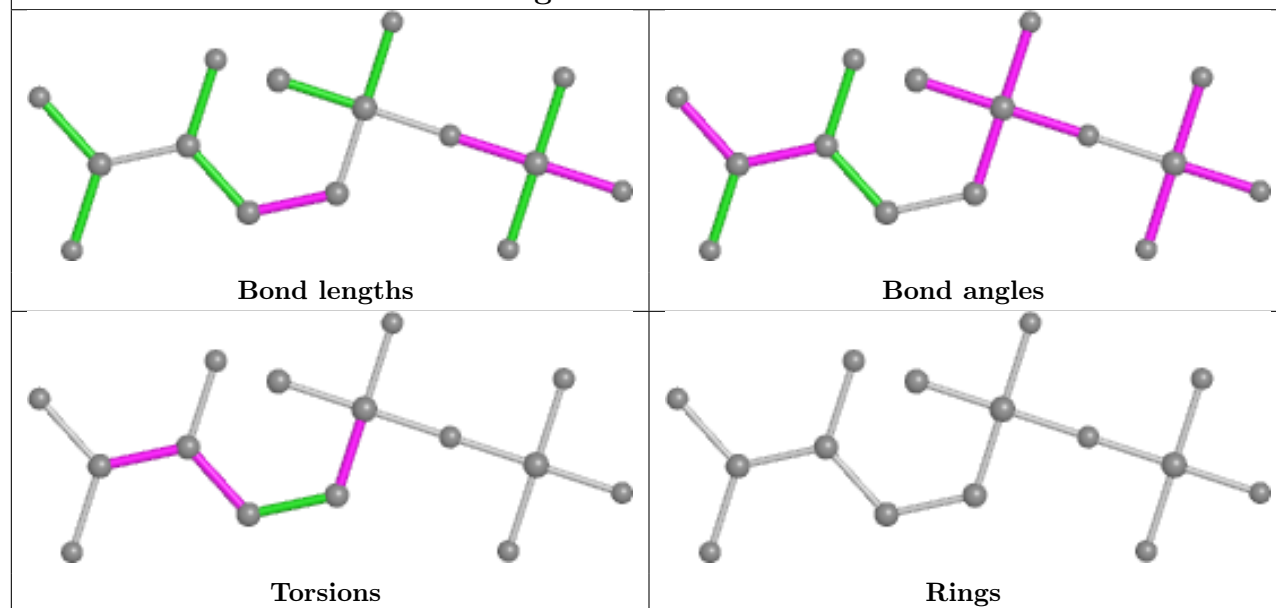


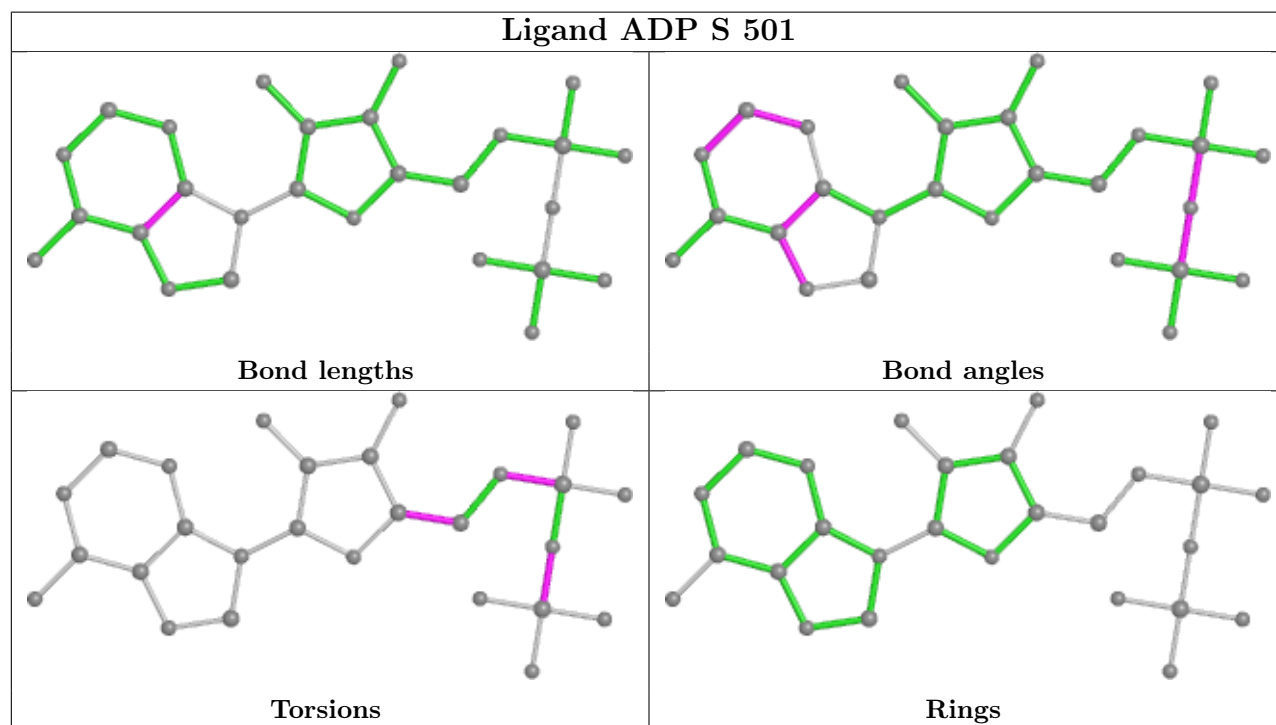
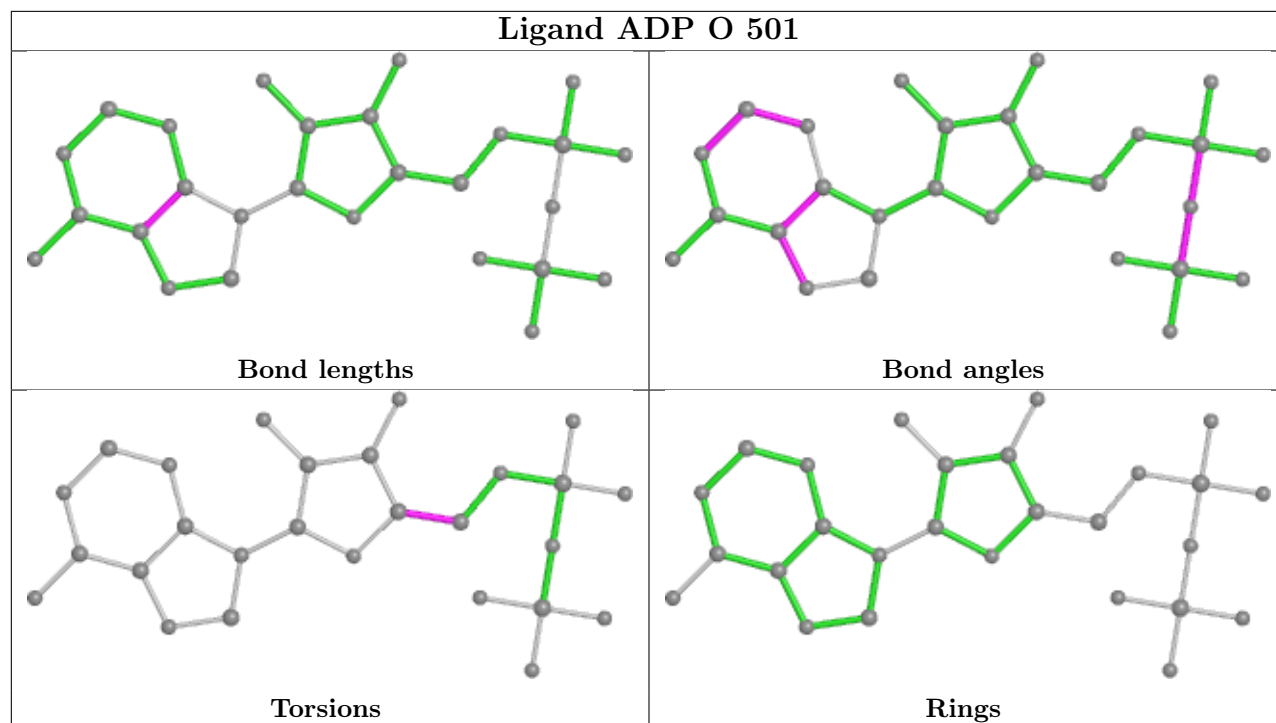


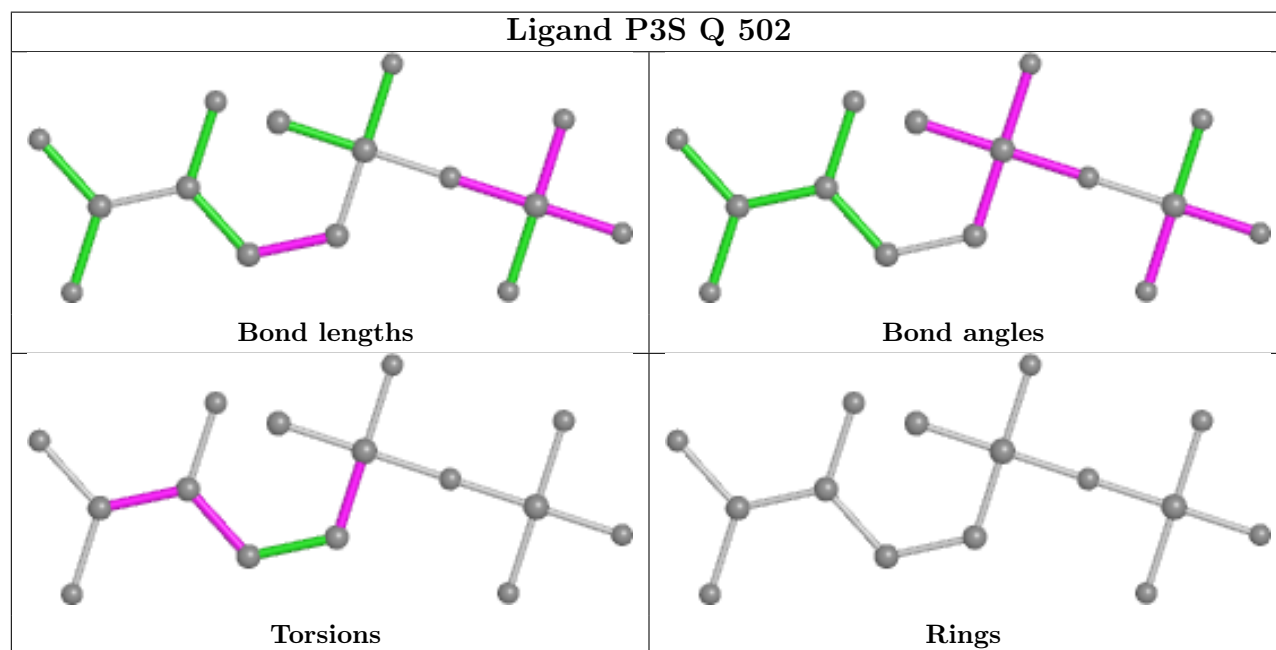
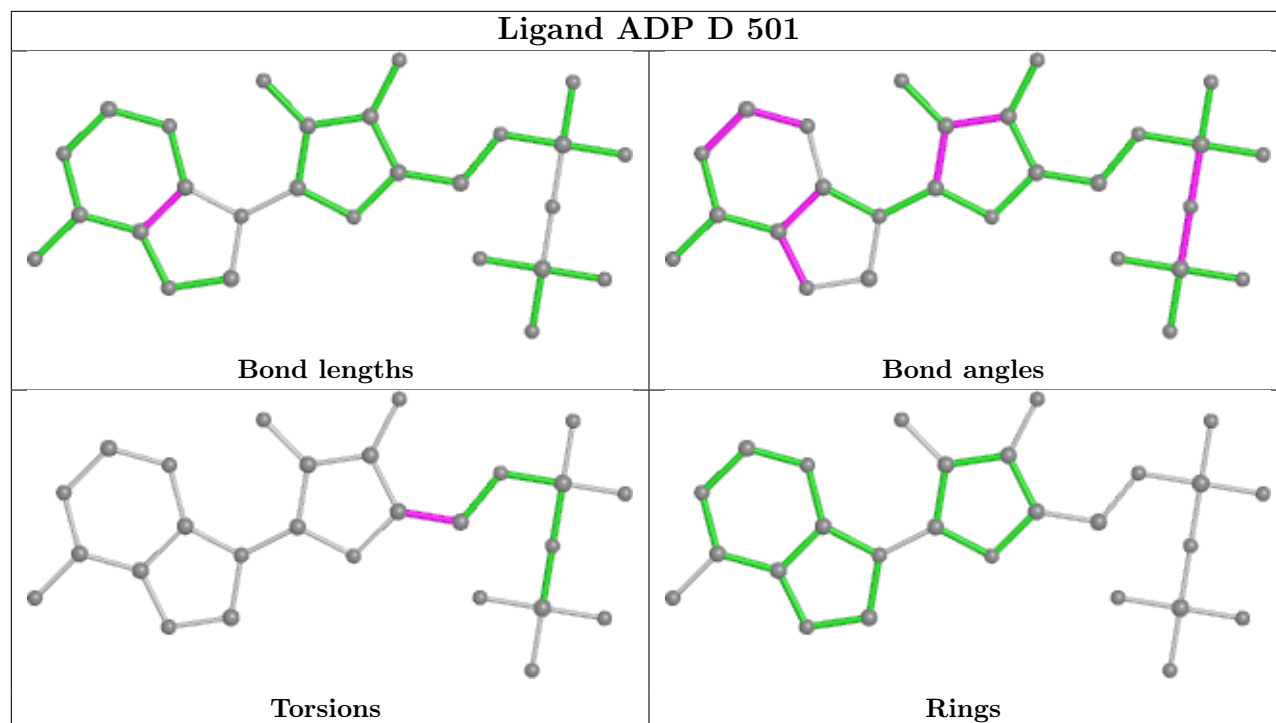
Ligand ADP E 501



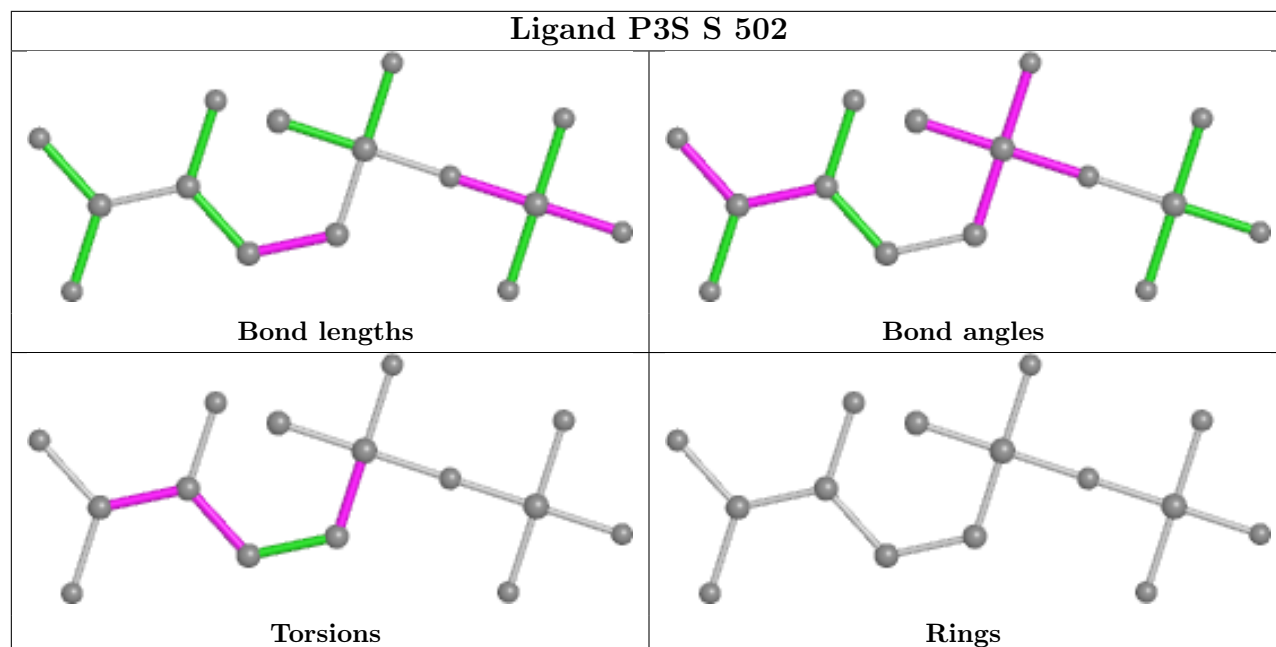
Ligand P3S M 502



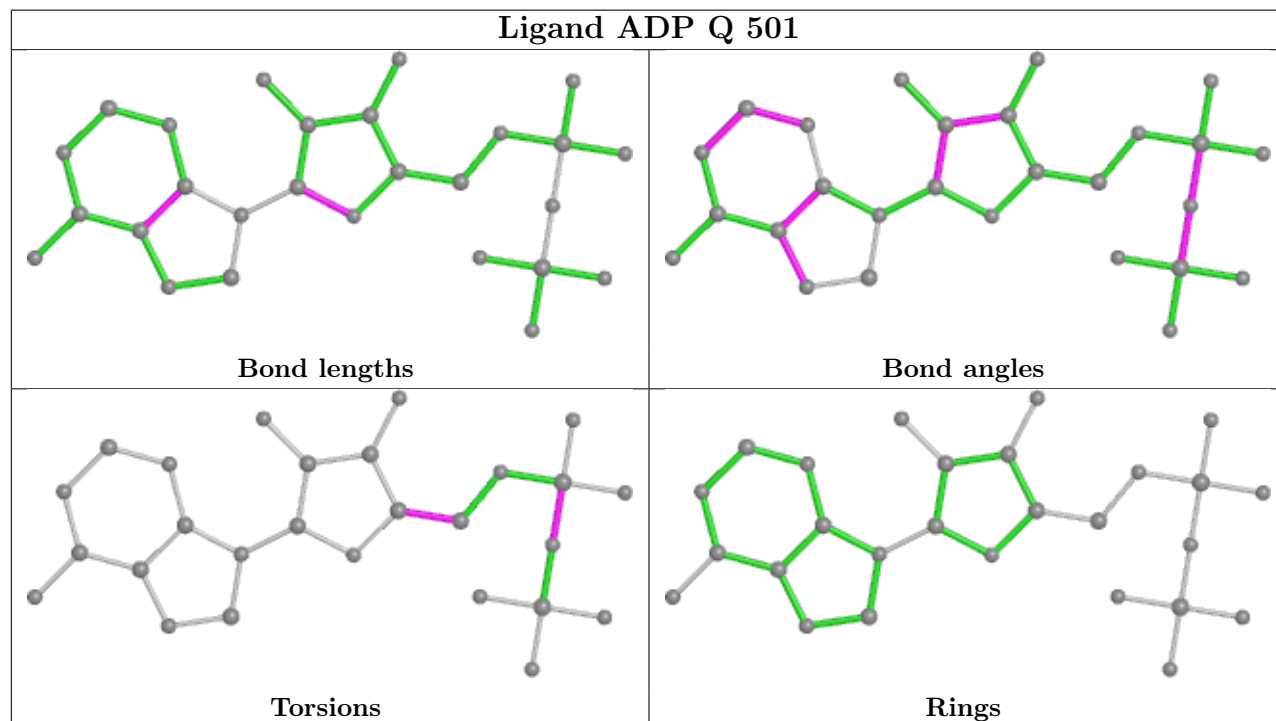


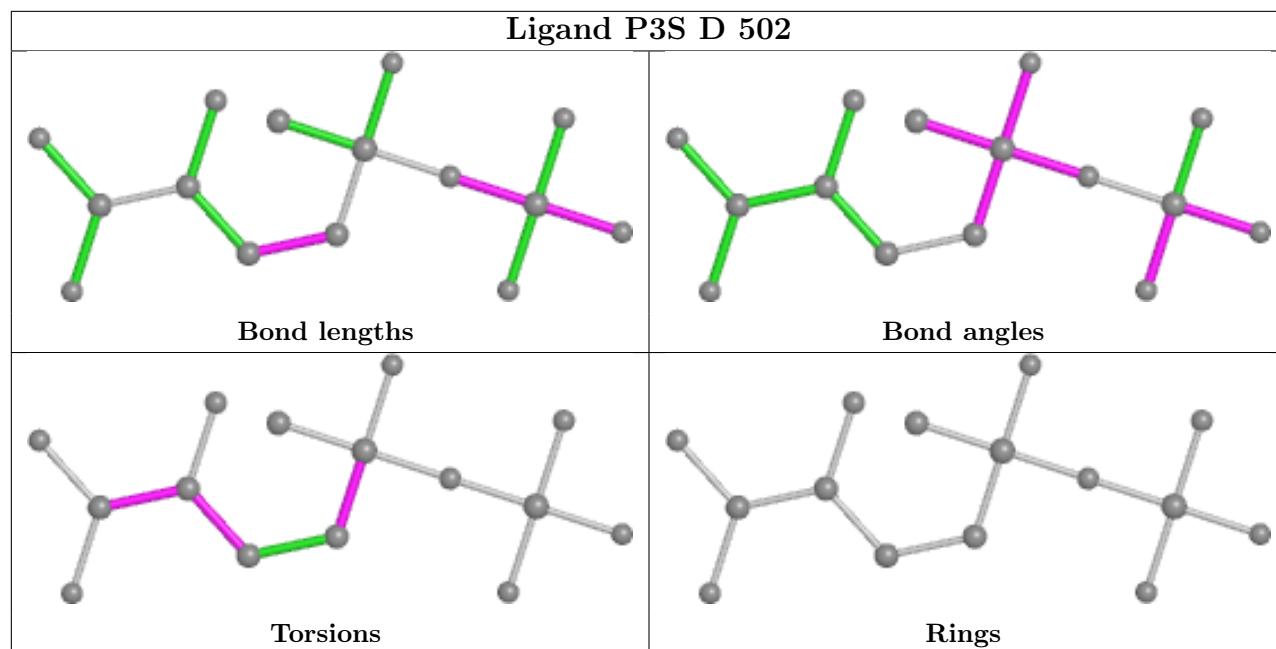


Ligand P3S S 502



Ligand ADP Q 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	442/447 (98%)	-0.35	4 (0%) 84 79	55, 100, 152, 201	0
1	B	442/447 (98%)	-0.39	0 100 100	56, 112, 163, 242	0
1	D	442/447 (98%)	-0.36	2 (0%) 91 88	50, 102, 150, 228	0
1	E	442/447 (98%)	-0.38	2 (0%) 91 88	56, 102, 152, 202	0
1	H	442/447 (98%)	-0.34	1 (0%) 95 93	60, 104, 157, 234	0
1	J	442/447 (98%)	-0.34	3 (0%) 87 83	64, 113, 172, 230	0
1	M	442/447 (98%)	-0.29	3 (0%) 87 83	60, 116, 172, 207	0
1	O	442/447 (98%)	-0.30	1 (0%) 95 93	46, 106, 163, 223	0
1	Q	442/447 (98%)	-0.33	0 100 100	56, 112, 162, 220	0
1	S	442/447 (98%)	-0.24	7 (1%) 72 66	66, 115, 170, 216	0
1	U	442/447 (98%)	-0.26	5 (1%) 80 75	72, 121, 165, 257	0
1	W	442/447 (98%)	-0.18	6 (1%) 75 69	70, 123, 181, 270	0
All	All	5304/5364 (98%)	-0.31	34 (0%) 89 86	46, 111, 166, 270	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	387	ASP	4.1
1	U	405	ILE	3.1
1	J	59	GLY	3.1
1	W	116	LEU	3.0
1	S	348	ALA	3.0
1	E	332	LEU	3.0
1	W	307	CYS	2.6
1	D	332	LEU	2.6
1	U	358	ILE	2.5
1	H	359	LYS	2.5
1	E	412	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	U	127	PHE	2.5
1	J	409	LEU	2.5
1	U	286	THR	2.5
1	S	372	ILE	2.4
1	W	411	GLU	2.4
1	A	405	ILE	2.4
1	M	278	MET	2.4
1	W	25	PHE	2.3
1	W	49	LYS	2.3
1	O	353	ALA	2.3
1	S	388	LEU	2.3
1	A	96	ILE	2.2
1	S	352	LYS	2.2
1	D	170	ARG	2.1
1	M	348	ALA	2.1
1	A	250	LEU	2.1
1	J	405	ILE	2.1
1	S	351	LEU	2.1
1	S	386	TYR	2.1
1	U	250	LEU	2.1
1	W	264	GLU	2.1
1	A	277	GLY	2.0
1	M	355	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.

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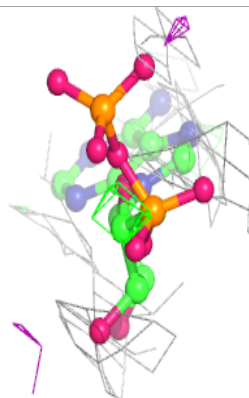
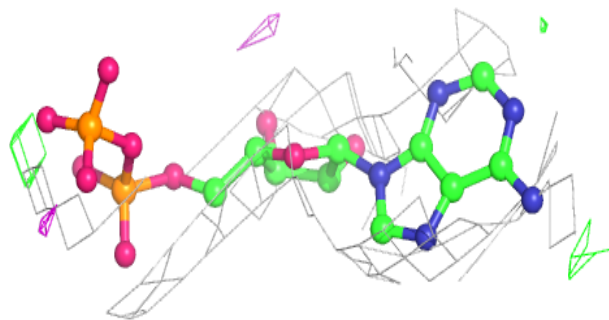
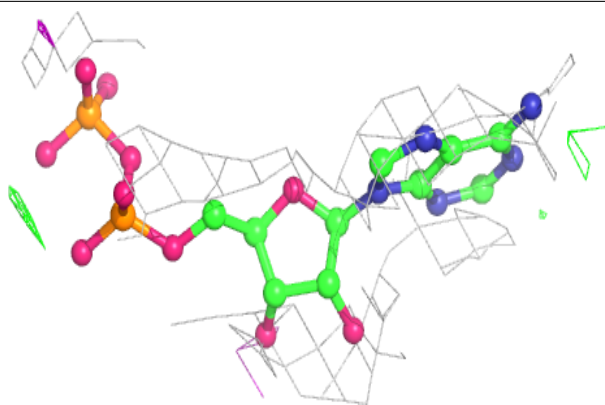
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	E	501	27/27	0.84	0.20	89,117,140,146	0
2	ADP	M	501	27/27	0.85	0.24	101,119,131,136	0
2	ADP	J	501	27/27	0.86	0.24	109,128,144,148	0
2	ADP	U	501	27/27	0.87	0.23	102,122,141,154	0
2	ADP	W	501	27/27	0.87	0.27	115,135,143,148	0
2	ADP	A	501	27/27	0.89	0.23	86,105,127,129	0
2	ADP	D	501	27/27	0.89	0.23	80,97,112,117	0
2	ADP	B	501	27/27	0.90	0.20	83,97,112,119	0
2	ADP	H	501	27/27	0.90	0.22	92,107,122,127	0
2	ADP	S	501	27/27	0.91	0.22	95,114,124,140	0
2	ADP	O	501	27/27	0.92	0.19	84,91,114,118	0
2	ADP	Q	501	27/27	0.93	0.22	94,111,116,121	0
3	P3S	H	502	15/15	0.93	0.23	90,100,114,117	0
3	P3S	M	502	15/15	0.93	0.23	82,88,95,96	0
3	P3S	S	502	15/15	0.93	0.25	98,114,120,123	0
3	P3S	D	502	15/15	0.94	0.27	72,80,107,118	0
3	P3S	E	502	15/15	0.95	0.21	91,96,118,118	0
3	P3S	B	502	15/15	0.95	0.24	83,97,112,116	0
3	P3S	O	502	15/15	0.95	0.22	73,82,109,109	0
3	P3S	Q	502	15/15	0.95	0.23	86,93,116,125	0
3	P3S	A	502	15/15	0.95	0.23	82,88,100,104	0
3	P3S	U	502	15/15	0.95	0.22	101,110,122,125	0
3	P3S	W	502	15/15	0.95	0.21	95,101,121,122	0
3	P3S	J	502	15/15	0.96	0.22	86,91,108,109	0

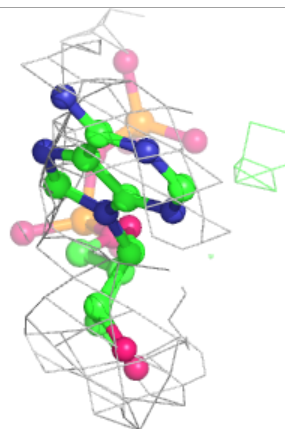
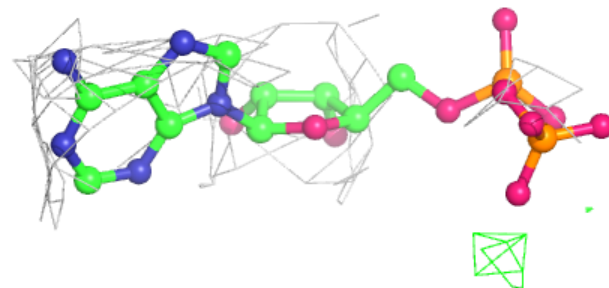
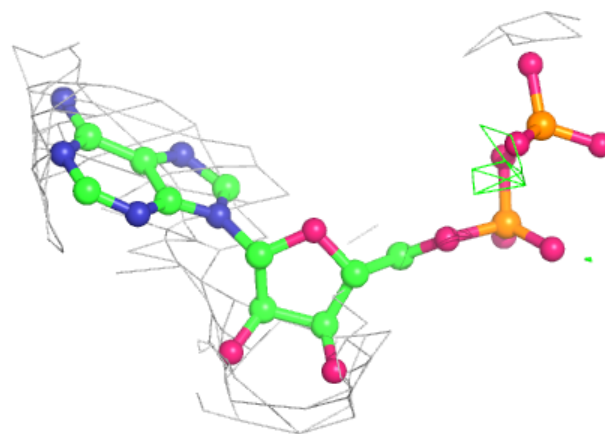
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP E 501:

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

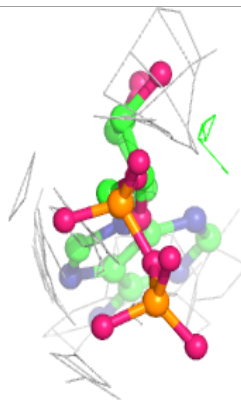
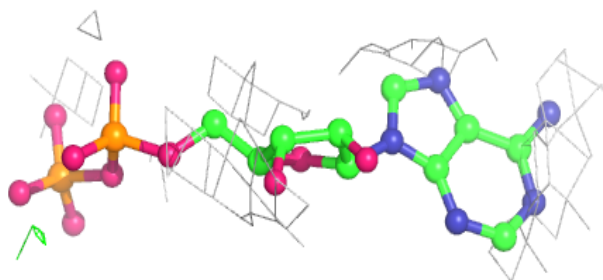
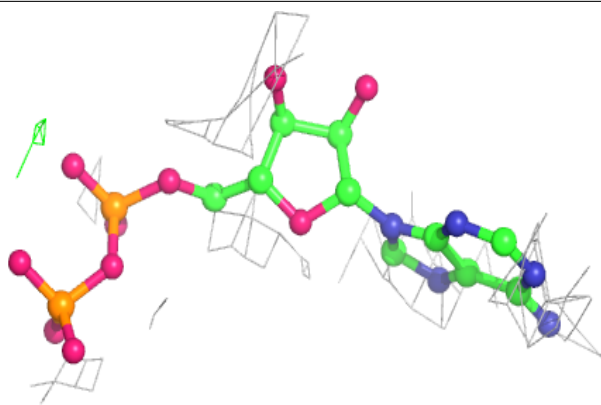
**Electron density around ADP M 501:**

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

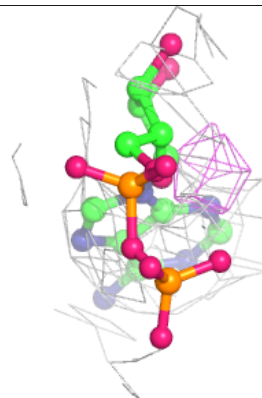
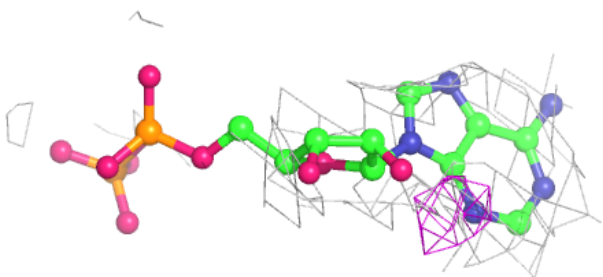
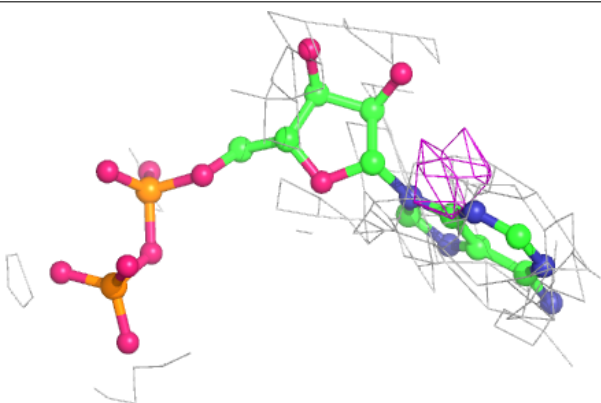


Electron density around ADP J 501:

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

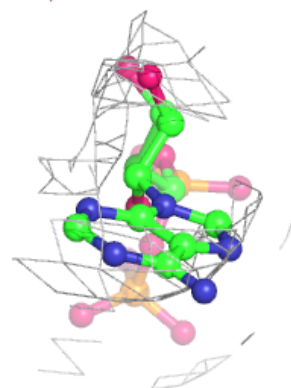
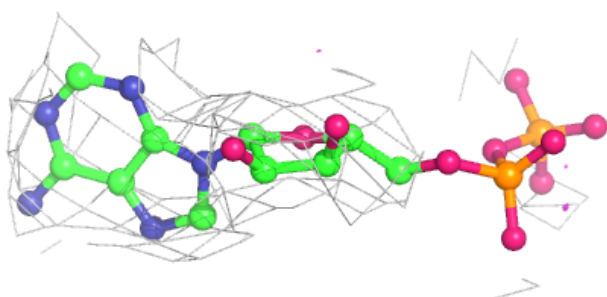
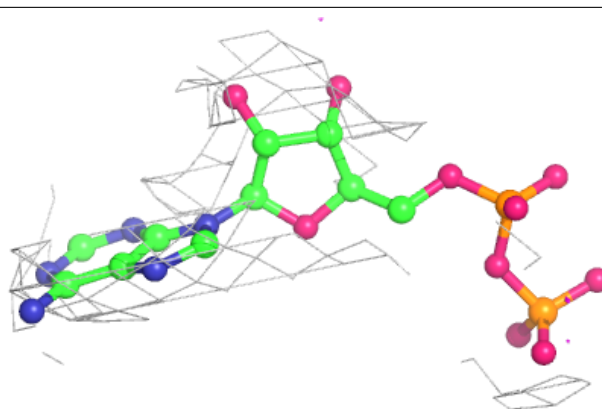
**Electron density around ADP U 501:**

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

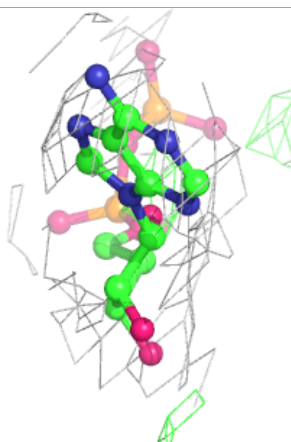
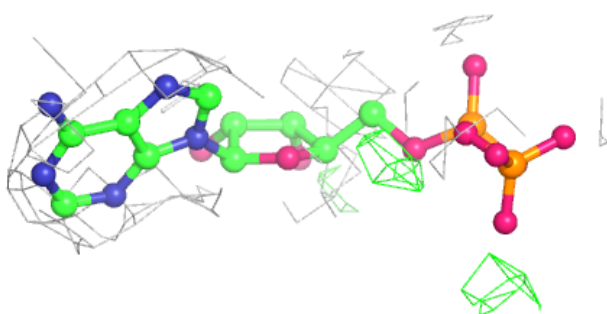
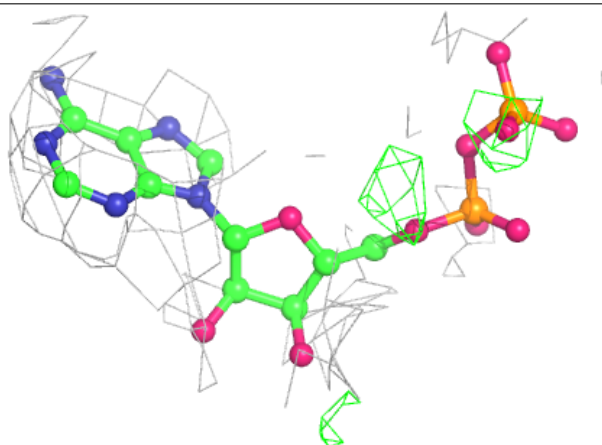


Electron density around ADP W 501:

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

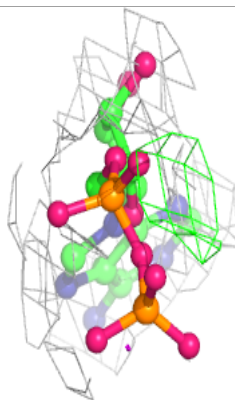
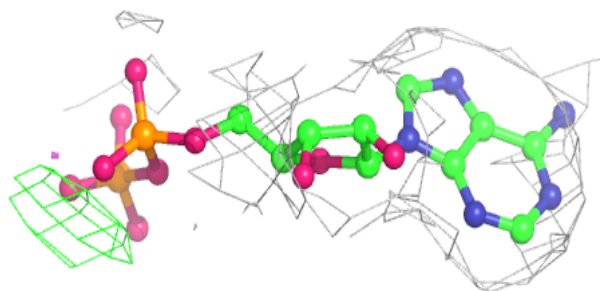
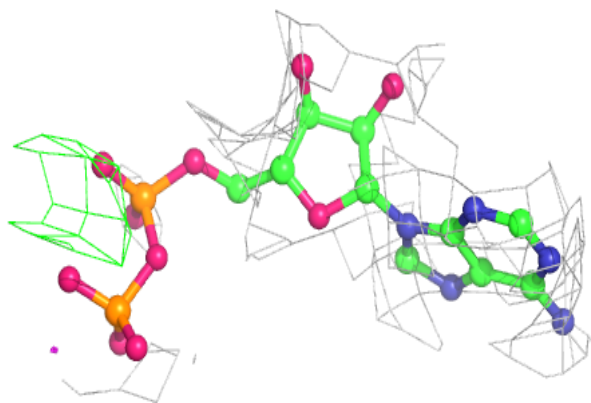
**Electron density around ADP A 501:**

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

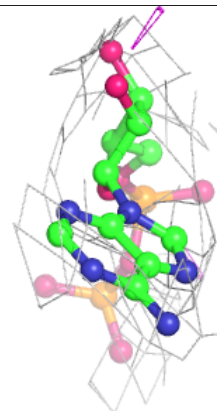
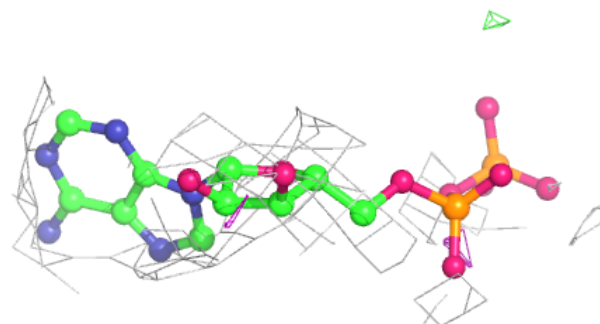
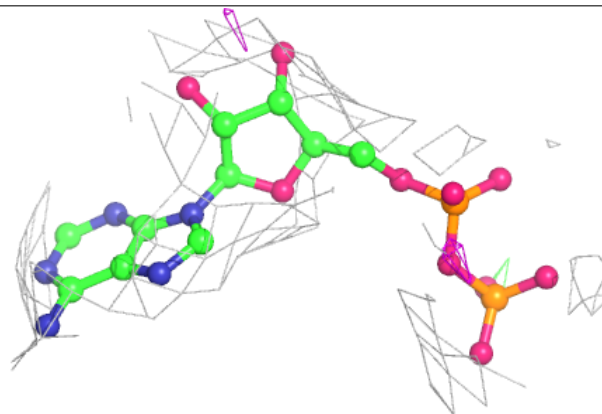


Electron density around ADP D 501:

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

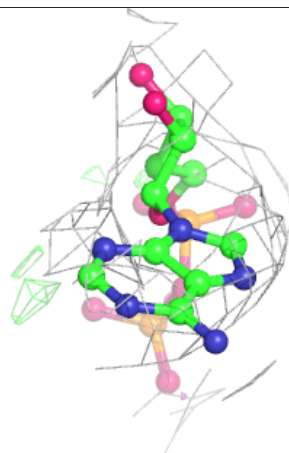
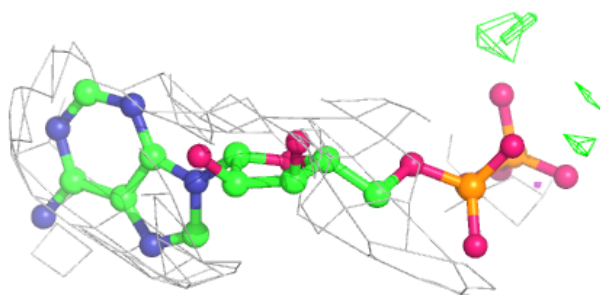
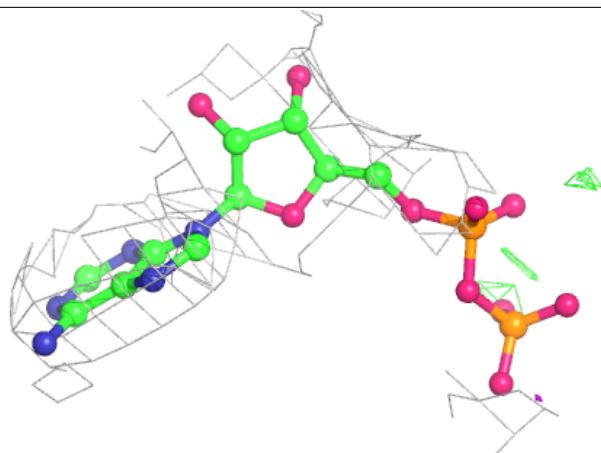
**Electron density around ADP B 501:**

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

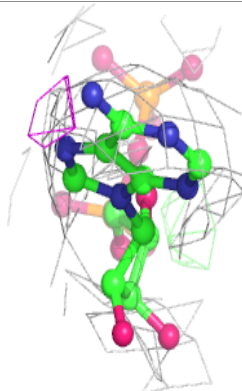
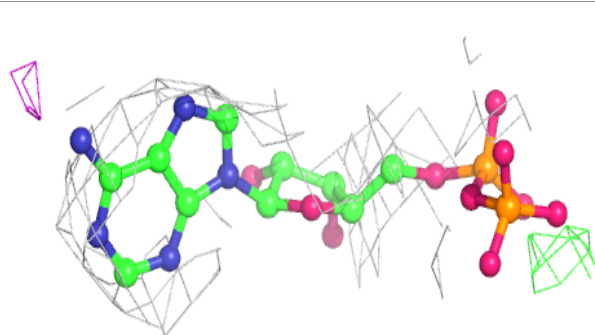
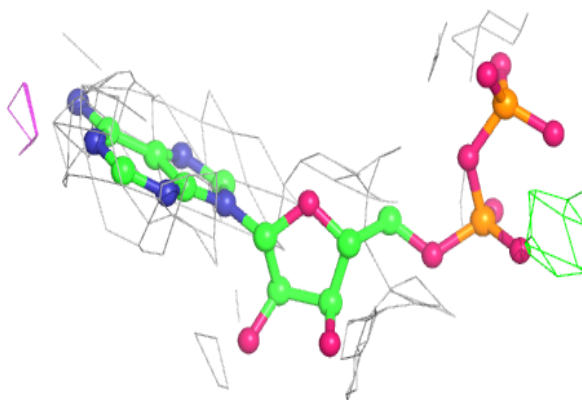


Electron density around ADP H 501:

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

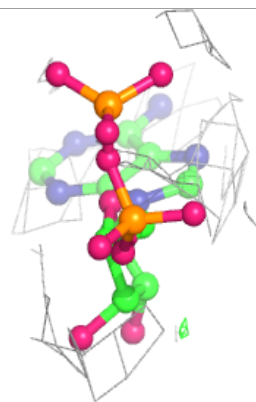
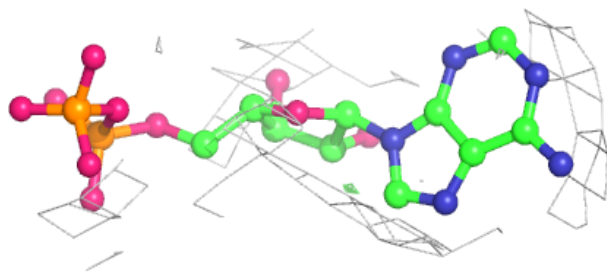
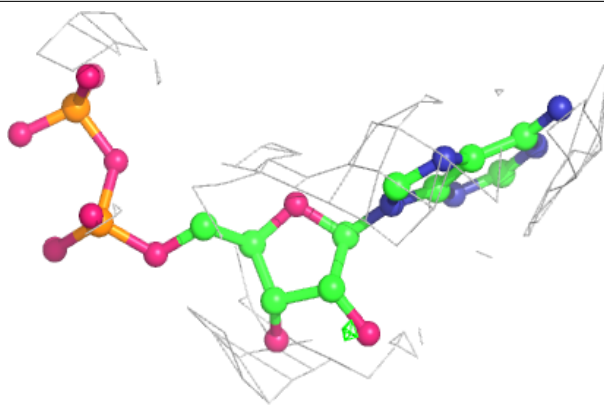
**Electron density around ADP S 501:**

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

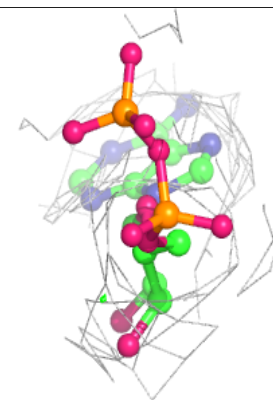
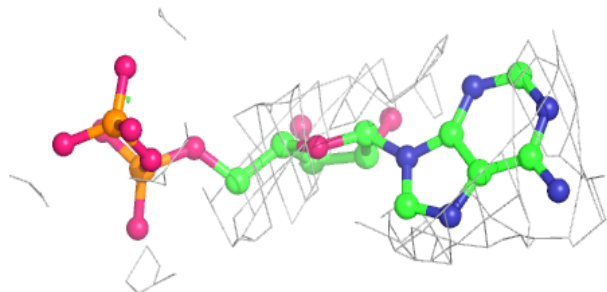
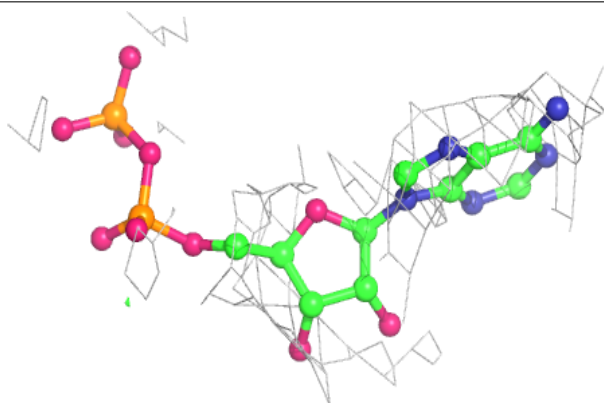


Electron density around ADP O 501:

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

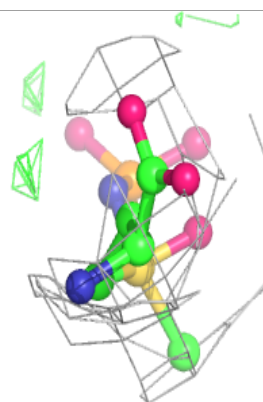
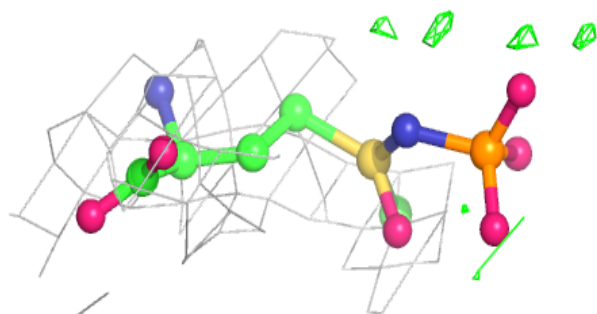
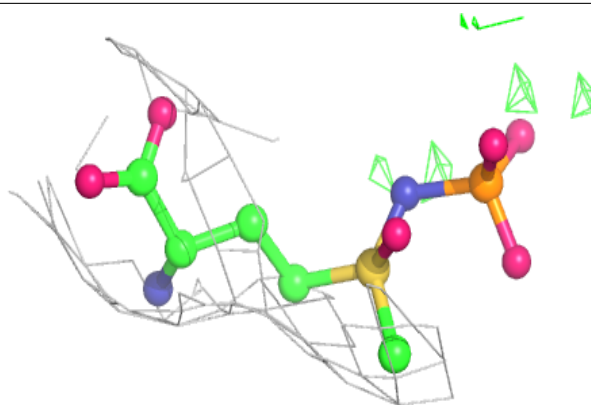
**Electron density around ADP Q 501:**

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

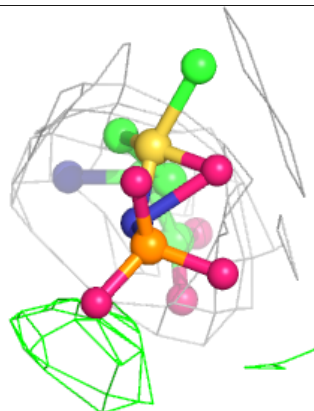
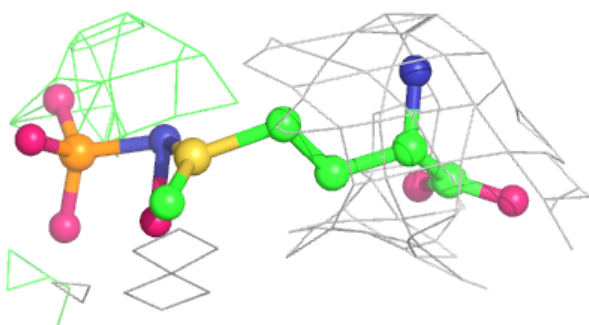
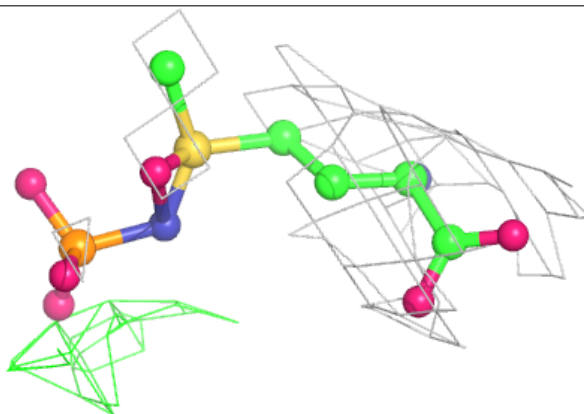


Electron density around P3S H 502:

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

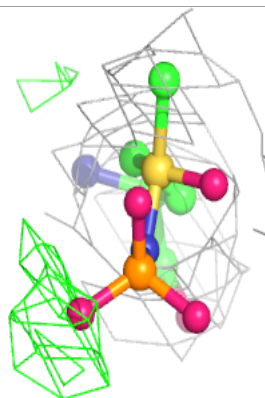
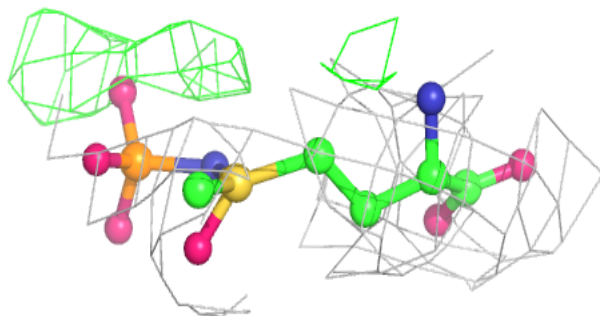
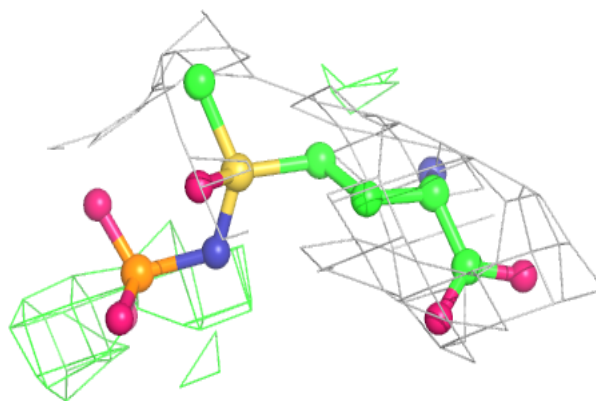
**Electron density around P3S M 502:**

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

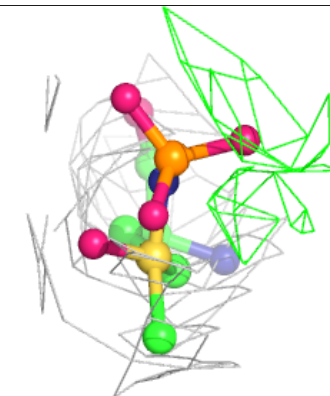
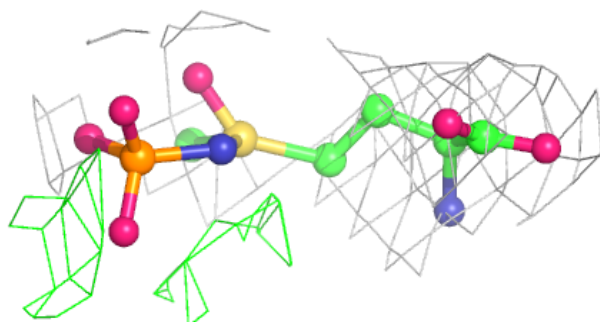
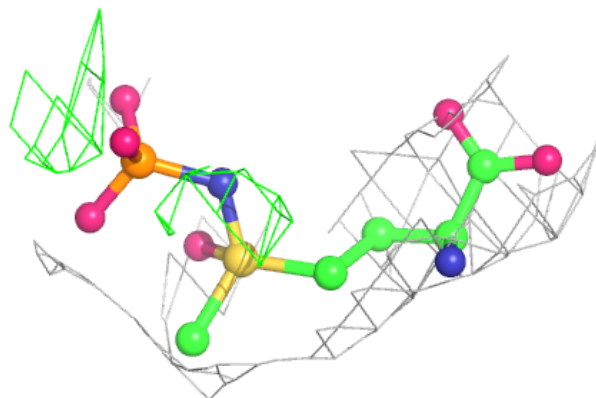


Electron density around P3S S 502:

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

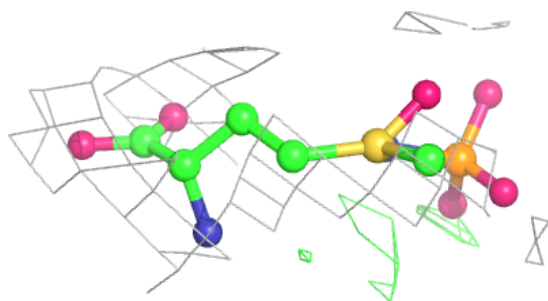
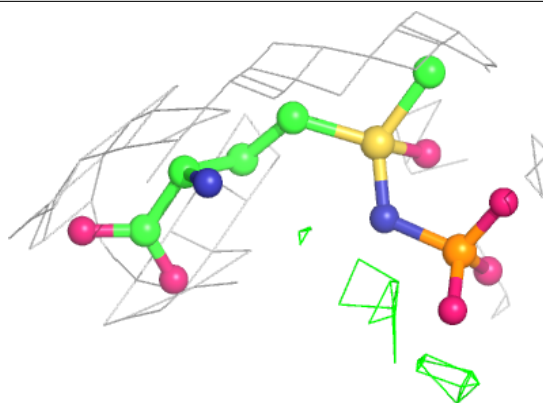
**Electron density around P3S D 502:**

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

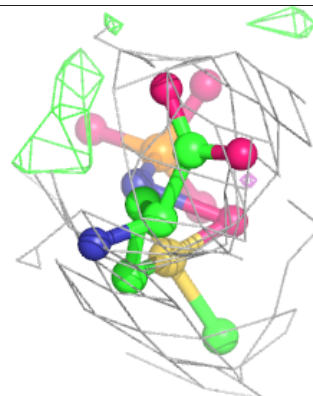
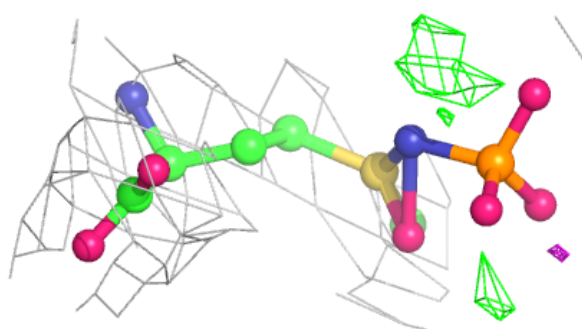
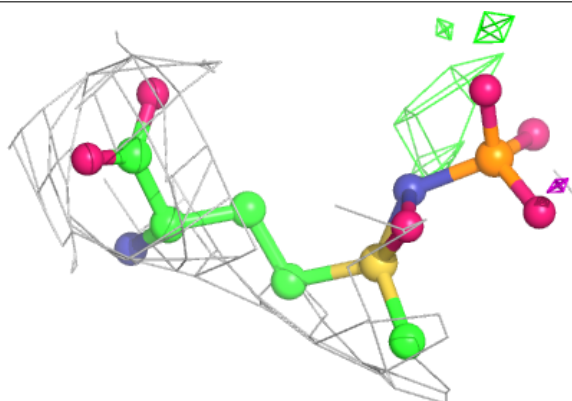


Electron density around P3S E 502:

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

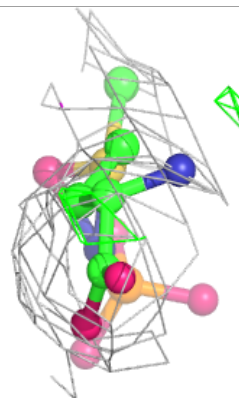
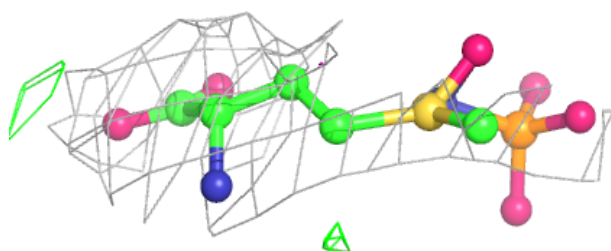
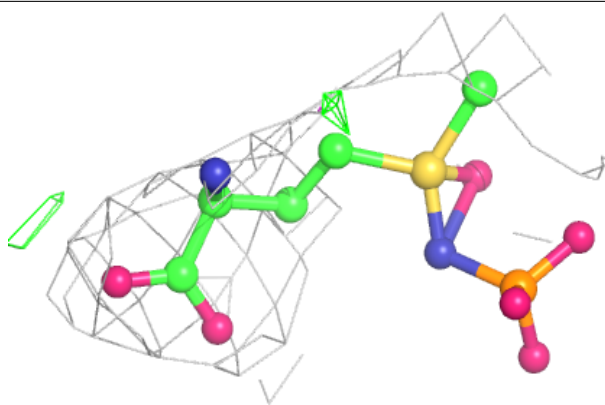
**Electron density around P3S B 502:**

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

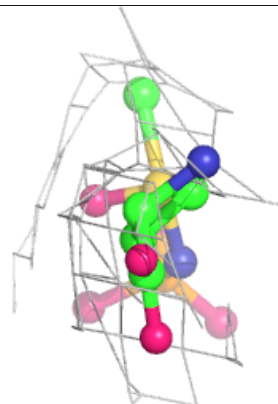
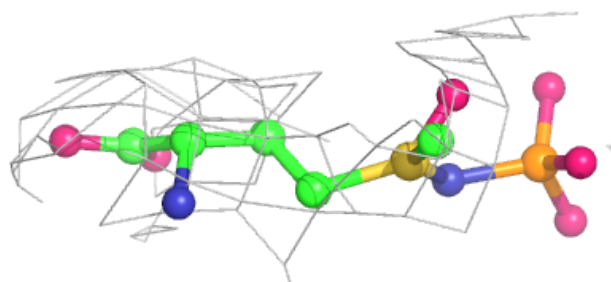
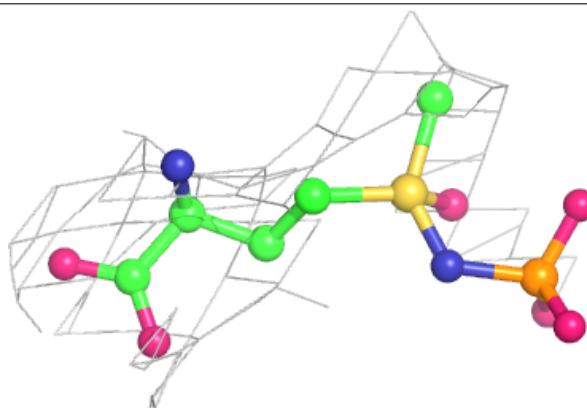


Electron density around P3S O 502:

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

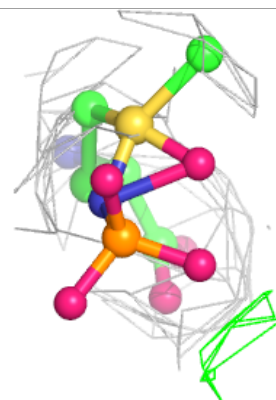
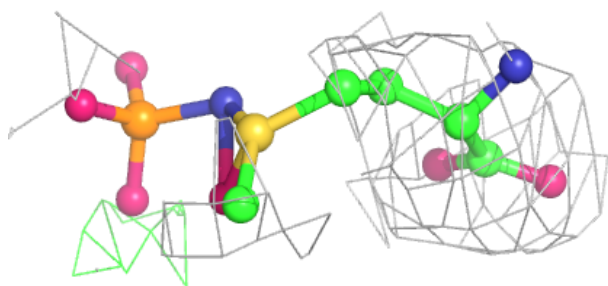
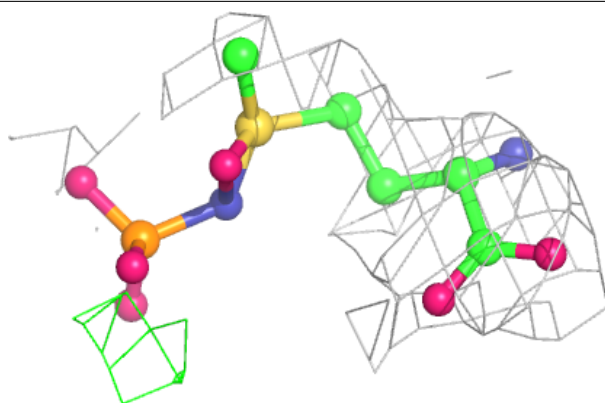
**Electron density around P3S Q 502:**

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

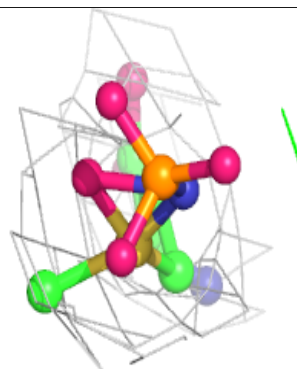
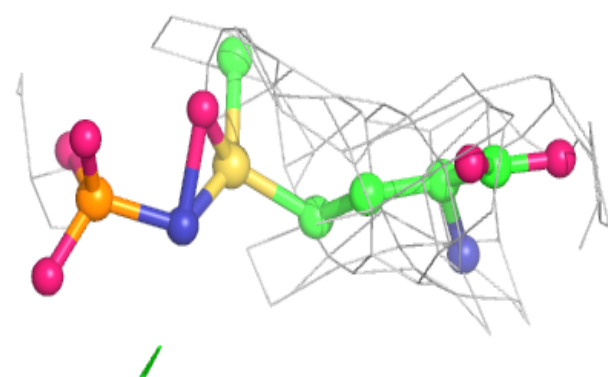
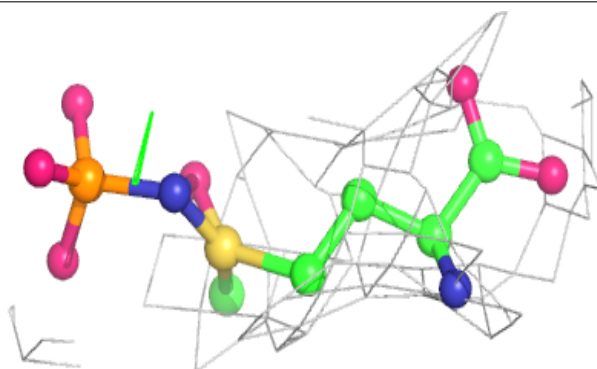


Electron density around P3S A 502:

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

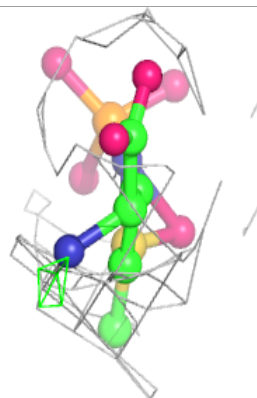
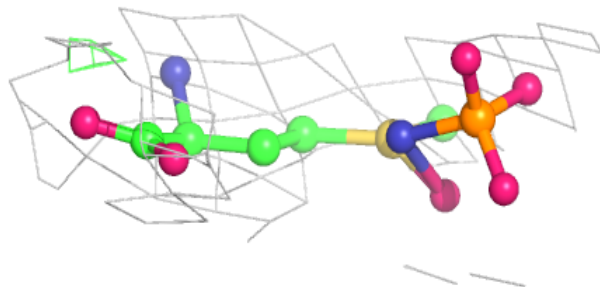
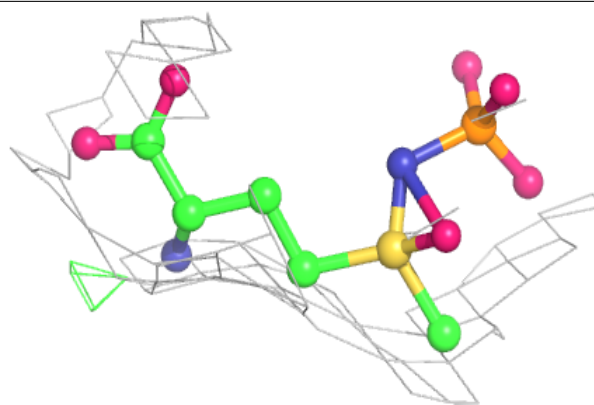
**Electron density around P3S U 502:**

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

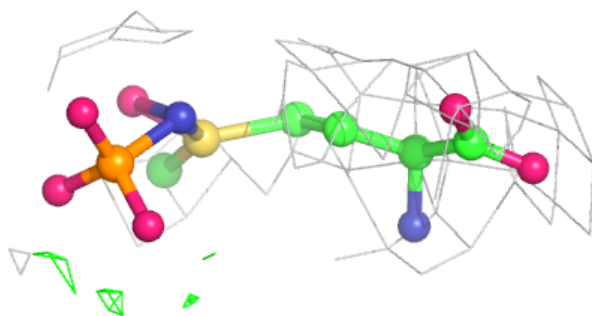
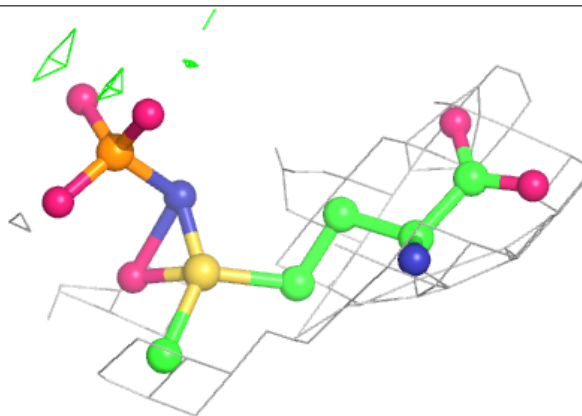


Electron density around P3S W 502:

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

**Electron density around P3S 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.