



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 01:07 AM EDT

PDB ID : 3ISS
Title : Crystal structure of enolpyruvyl-UDP-GlcNAc synthase (MurA):UDP-N-acetyl-muramic acid:phosphite from Escherichia coli
Authors : Jackson, S.G.; Zhang, F.; Chindemi, P.; Junop, M.S.; Berti, P.J.
Deposited on : 2009-08-27
Resolution : 2.50 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 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 : 2.23.2
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) : 2.23.2

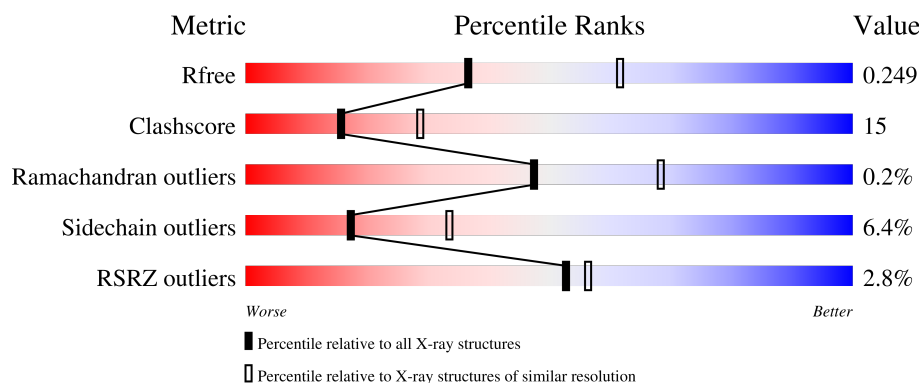
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	418	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>.</div> </div> </div>
1	B	418	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>.</div> </div> </div>
1	C	418	<div> <div></div> <div> <div></div> <div>77%</div> <div>21%</div> <div>.</div> </div> </div>
1	D	418	<div> <div></div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
1	E	418	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	418	<div><div><div>2%</div><div>74%</div><div>23%</div><div></div></div></div>
1	G	418	<div><div><div>2%</div><div>73%</div><div>25%</div><div></div></div></div>
1	H	418	<div><div><div>%</div><div>78%</div><div>20%</div><div></div></div></div>
1	I	418	<div><div><div>8%</div><div>72%</div><div>24%</div><div></div></div></div>
1	J	418	<div><div><div>2%</div><div>74%</div><div>24%</div><div></div></div></div>
1	K	418	<div><div><div>%</div><div>77%</div><div>21%</div><div></div></div></div>
1	L	418	<div><div><div>11%</div><div>70%</div><div>28%</div><div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39025 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	B	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	C	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	D	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	E	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	F	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	G	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	H	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	I	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	J	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	K	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	L	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			

There are 12 discrepancies between the modelled and reference sequences:

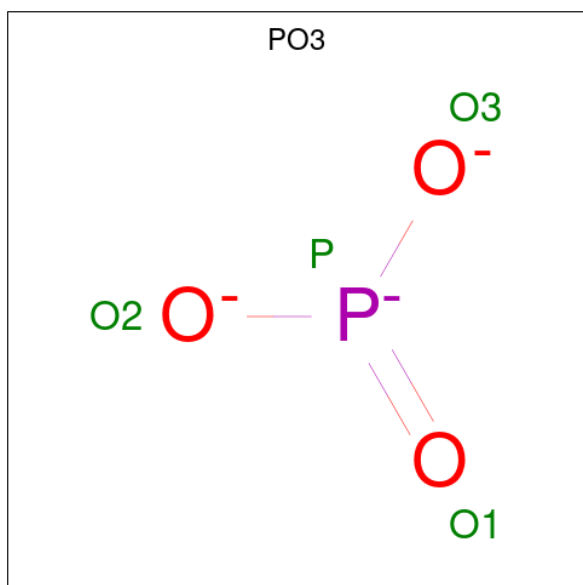
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASP	ASN	engineered mutation	UNP P0A749
B	67	ASP	ASN	engineered mutation	UNP P0A749
C	67	ASP	ASN	engineered mutation	UNP P0A749
D	67	ASP	ASN	engineered mutation	UNP P0A749
E	67	ASP	ASN	engineered mutation	UNP P0A749

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Chain	Residue	Modelled	Actual	Comment	Reference
F	67	ASP	ASN	engineered mutation	UNP P0A749
G	67	ASP	ASN	engineered mutation	UNP P0A749
H	67	ASP	ASN	engineered mutation	UNP P0A749
I	67	ASP	ASN	engineered mutation	UNP P0A749
J	67	ASP	ASN	engineered mutation	UNP P0A749
K	67	ASP	ASN	engineered mutation	UNP P0A749
L	67	ASP	ASN	engineered mutation	UNP P0A749

- Molecule 2 is PHOSPHITE ION (three-letter code: PO3) (formula: O₃P).



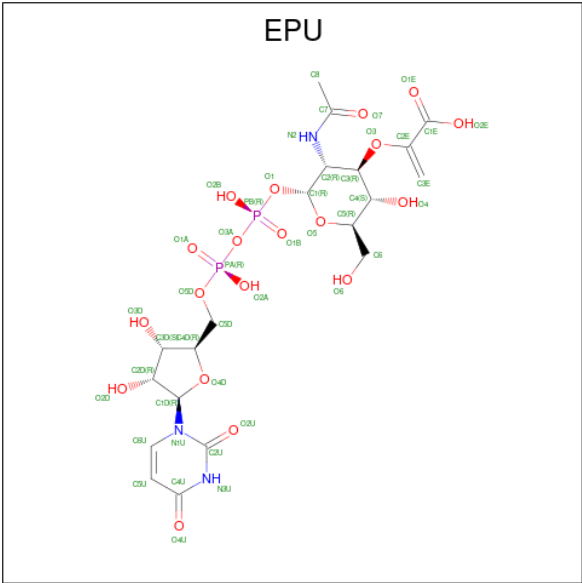
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 4 3 1	0	0
2	B	1	Total O P 4 3 1	0	0
2	C	1	Total O P 4 3 1	0	0
2	D	1	Total O P 4 3 1	0	0
2	E	1	Total O P 4 3 1	0	0
2	F	1	Total O P 4 3 1	0	0
2	G	1	Total O P 4 3 1	0	0
2	H	1	Total O P 4 3 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	O	P	0	0
			4	3	1		
2	J	1	Total	O	P	0	0
			4	3	1		
2	K	1	Total	O	P	0	0
			4	3	1		
2	L	1	Total	O	P	0	0
			4	3	1		

- Molecule 3 is URIDINE-DIPHOSPHATE-2(N-ACETYLGLUCOSAMINYL) BUTYRIC ACID (three-letter code: EPU) (formula: C₂₀H₂₉N₃O₁₉P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	C	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	D	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	E	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	F	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	G	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	I	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	J	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	K	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	L	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

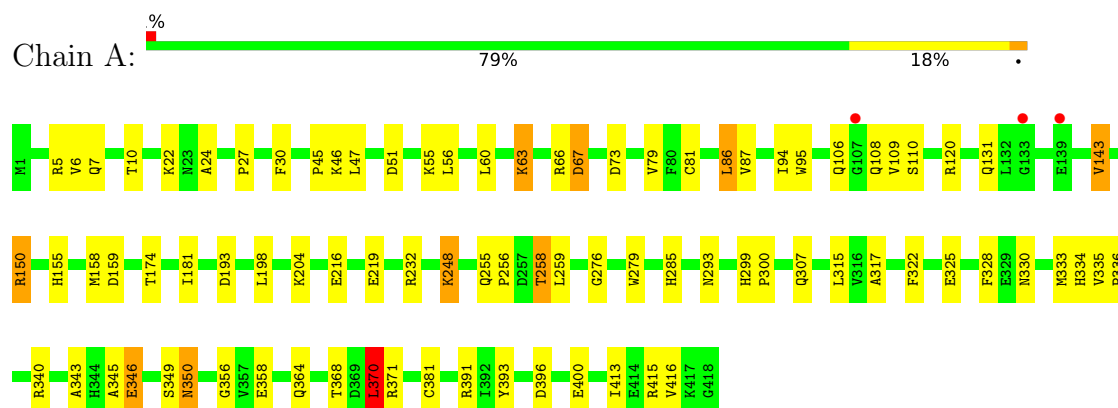
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	63	Total	O	0	0
			63	63		
4	C	112	Total	O	0	0
			112	112		
4	D	106	Total	O	0	0
			106	106		
4	E	83	Total	O	0	0
			83	83		
4	F	69	Total	O	0	0
			69	69		
4	G	54	Total	O	0	0
			54	54		
4	H	84	Total	O	0	0
			84	84		
4	I	43	Total	O	0	0
			43	43		
4	J	55	Total	O	0	0
			55	55		
4	K	69	Total	O	0	0
			69	69		
4	L	36	Total	O	0	0
			36	36		

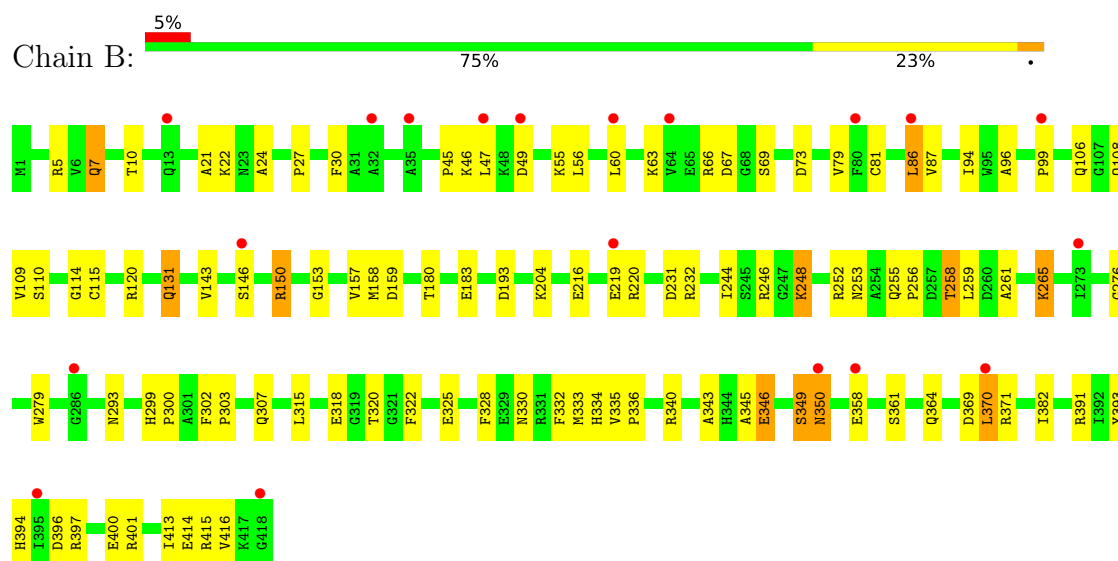
3 Residue-property plots

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.

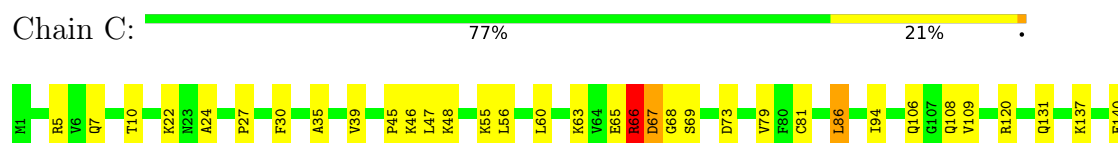
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

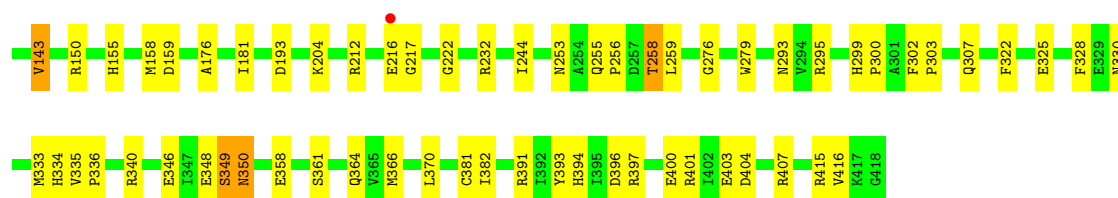


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



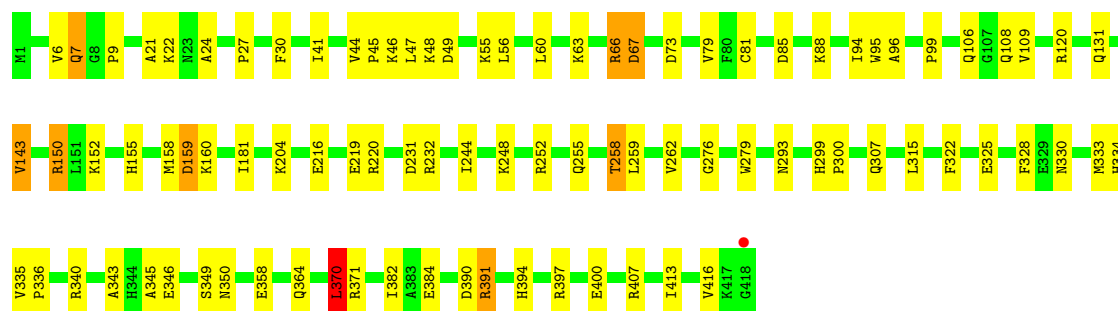
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





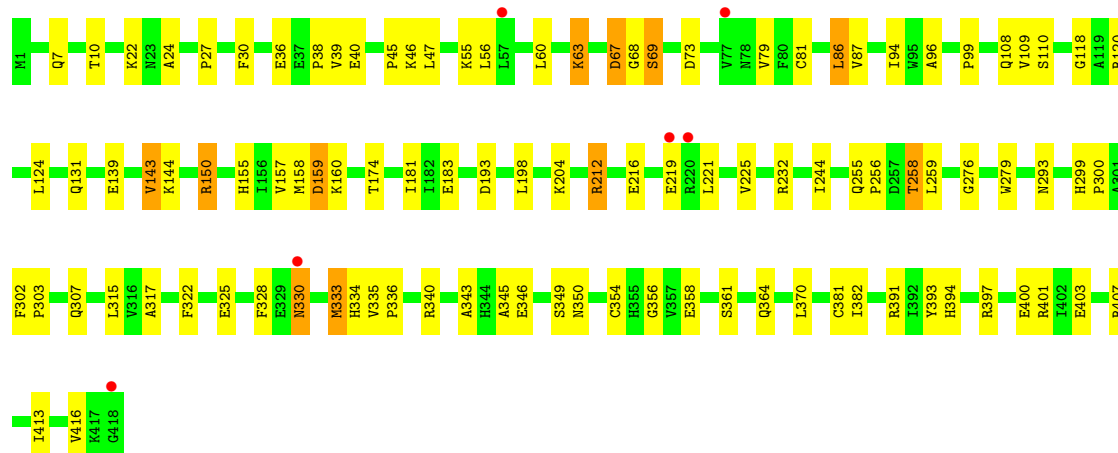
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain D: 78% 20%



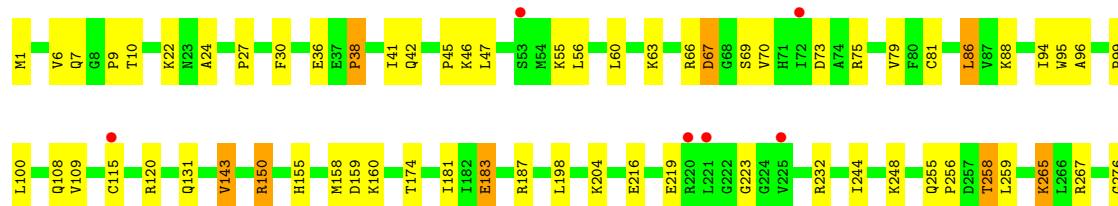
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

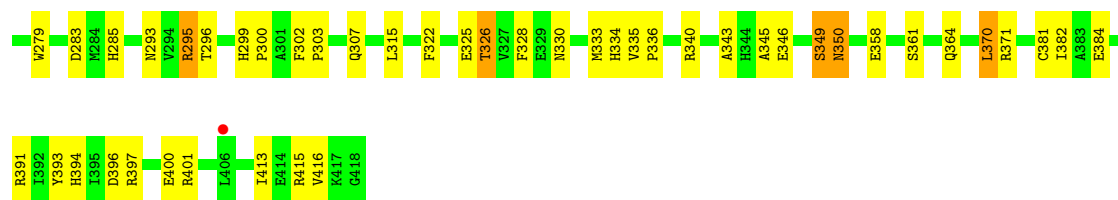
Chain E: 75% 22%



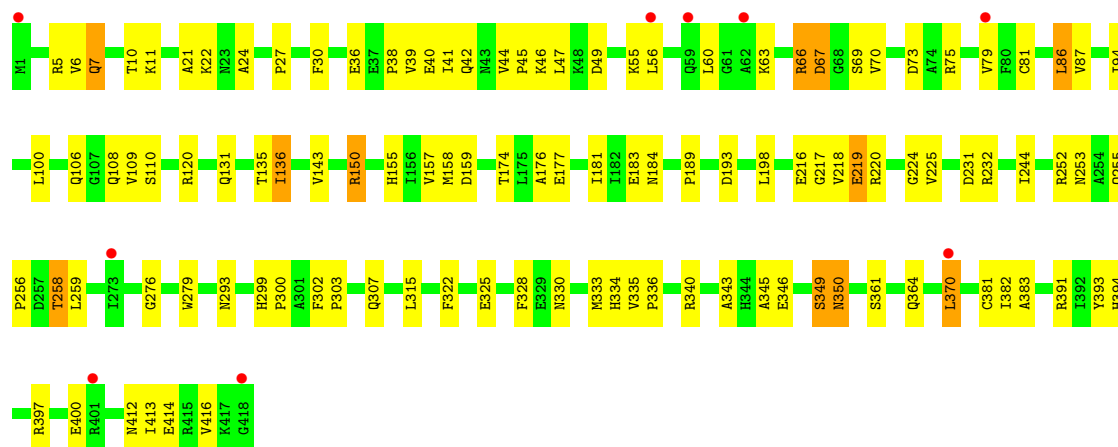
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain F: 74% 23%

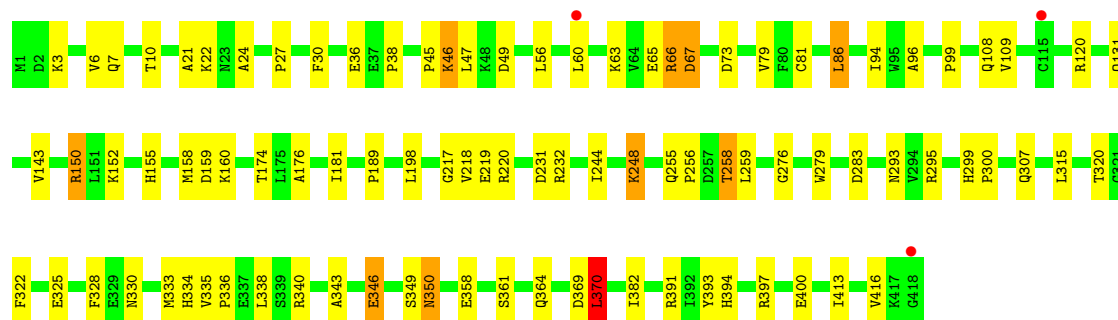
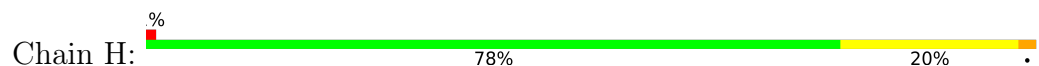




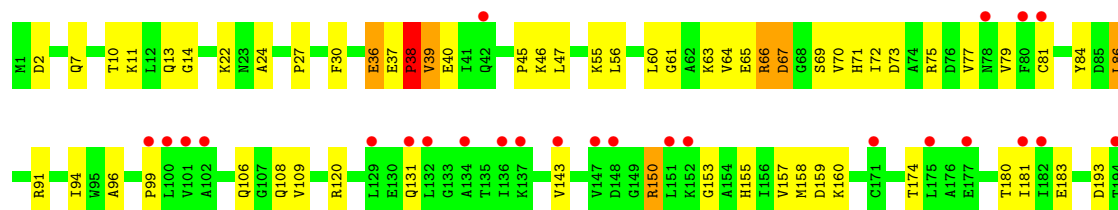
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

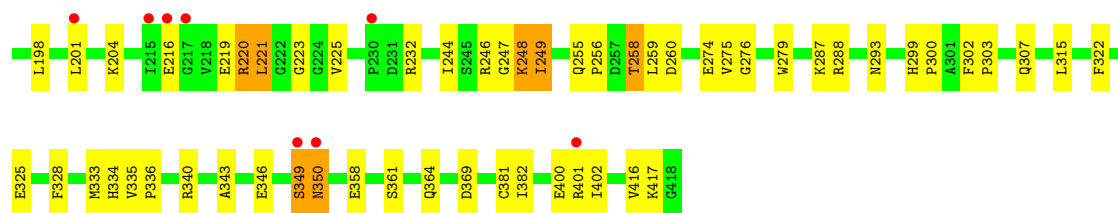


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

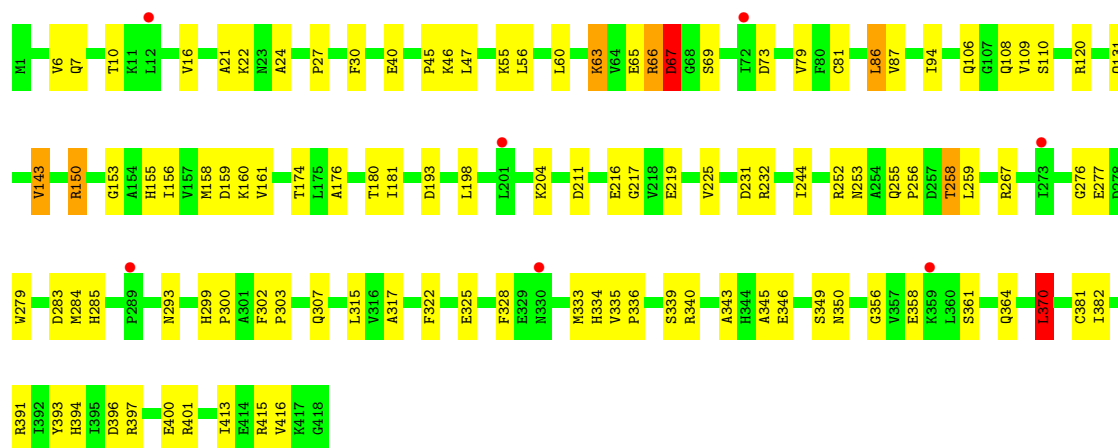
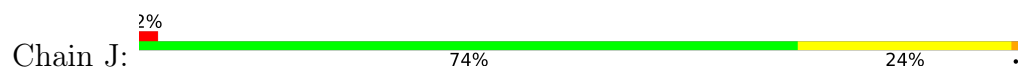


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

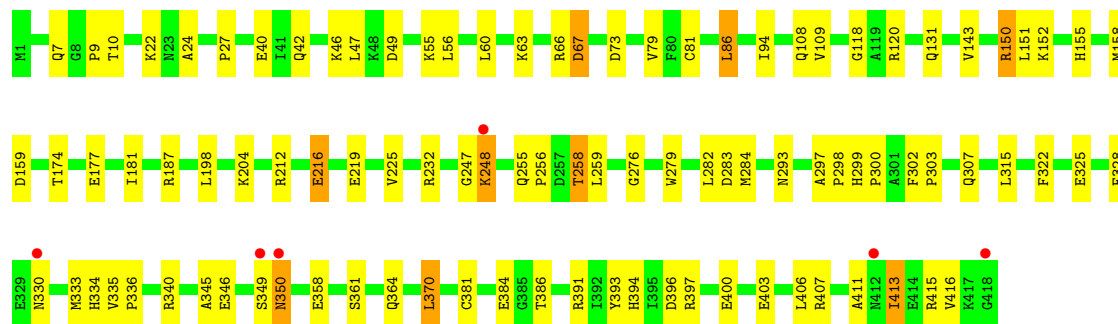
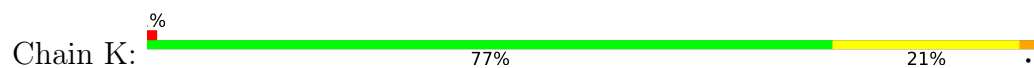




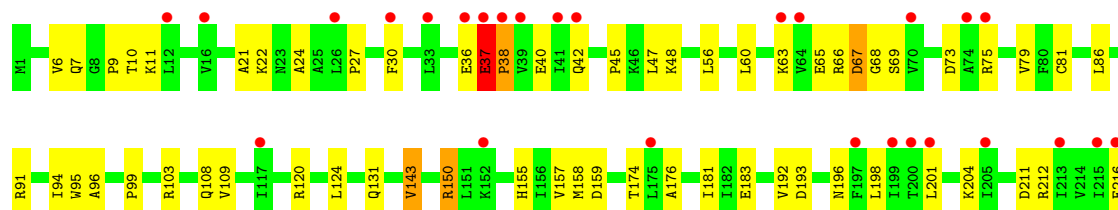
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

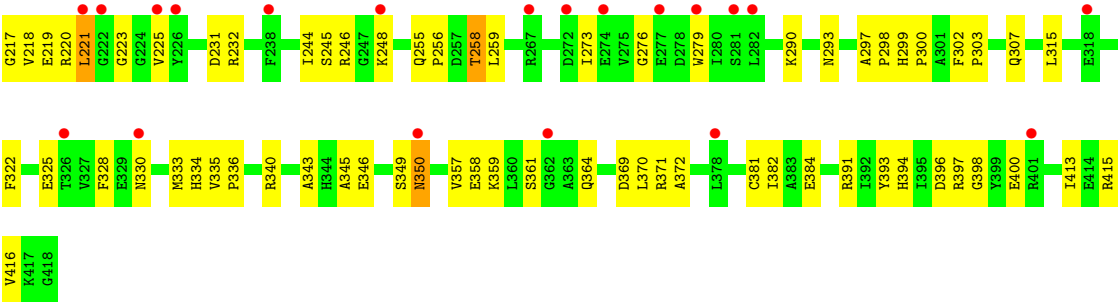


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.51Å 120.91Å 139.73Å 111.52° 104.44° 90.19°	Depositor
Resolution (Å)	47.48 – 2.50 47.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.48-2.50) 97.6 (47.48-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.222 , 0.254 0.217 , 0.249	Depositor DCC
R_{free} test set	8367 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	39025	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.08% 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: EPU, PO3

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	0.49	0/3176	0.61	1/4298 (0.0%)
1	B	0.51	1/3176 (0.0%)	0.60	3/4298 (0.1%)
1	C	0.54	0/3176	0.63	3/4298 (0.1%)
1	D	0.53	0/3176	0.62	2/4298 (0.0%)
1	E	0.51	0/3176	0.65	1/4298 (0.0%)
1	F	0.56	1/3176 (0.0%)	0.60	1/4298 (0.0%)
1	G	0.50	0/3176	0.62	2/4298 (0.0%)
1	H	0.53	0/3176	0.59	3/4298 (0.1%)
1	I	0.52	0/3176	0.59	1/4298 (0.0%)
1	J	0.48	0/3176	0.58	2/4298 (0.0%)
1	K	0.51	0/3176	0.59	2/4298 (0.0%)
1	L	0.52	0/3176	0.61	1/4298 (0.0%)
All	All	0.52	2/38112 (0.0%)	0.61	22/51576 (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	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	115	CYS	CB-SG	-5.21	1.73	1.81
1	B	115	CYS	C-N	-5.09	1.22	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	ASP	CB-CG-OD1	18.46	134.91	118.30
1	A	67	ASP	CB-CG-OD1	17.43	133.98	118.30
1	G	67	ASP	CB-CG-OD1	14.32	131.18	118.30
1	D	67	ASP	N-CA-CB	-14.03	85.34	110.60
1	C	67	ASP	N-CA-CB	-10.81	91.13	110.60
1	J	67	ASP	CB-CA-C	-7.38	95.64	110.40
1	C	67	ASP	CB-CA-C	-6.38	97.63	110.40
1	K	67	ASP	CB-CA-C	-5.97	98.47	110.40
1	L	37	GLU	C-N-CD	-5.92	107.58	120.60
1	I	369	ASP	CB-CA-C	5.82	122.04	110.40
1	C	68	GLY	N-CA-C	-5.80	98.61	113.10
1	H	370	LEU	CB-CA-C	-5.72	99.34	110.20
1	H	67	ASP	CB-CG-OD1	5.62	123.36	118.30
1	K	370	LEU	CB-CA-C	-5.45	99.84	110.20
1	H	67	ASP	CB-CA-C	-5.43	99.54	110.40
1	B	114	GLY	O-C-N	-5.39	114.07	122.70
1	B	115	CYS	O-C-N	-5.21	114.36	122.70
1	B	370	LEU	CB-CA-C	-5.10	100.50	110.20
1	D	370	LEU	CB-CA-C	-5.10	100.52	110.20
1	J	370	LEU	CB-CA-C	-5.08	100.54	110.20
1	F	370	LEU	CB-CA-C	-5.04	100.63	110.20
1	G	370	LEU	CB-CA-C	-5.03	100.64	110.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	66	ARG	Peptide
1	D	66	ARG	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	3133	0	3210	68	0
1	B	3133	0	3208	93	0
1	C	3133	0	3210	81	0
1	D	3133	0	3210	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3133	0	3210	90	0
1	F	3133	0	3210	103	0
1	G	3133	0	3210	106	0
1	H	3133	0	3210	88	0
1	I	3133	0	3210	107	0
1	J	3133	0	3210	92	0
1	K	3133	0	3210	123	0
1	L	3133	0	3210	122	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	1	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	1	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	2	0
3	D	44	0	26	0	0
3	E	44	0	26	2	0
3	F	44	0	26	3	0
3	G	44	0	26	0	0
3	H	44	0	26	3	0
3	I	44	0	26	1	0
3	J	44	0	26	1	0
3	K	44	0	26	0	0
3	L	44	0	26	2	0
4	A	79	0	0	7	0
4	B	63	0	0	14	0
4	C	112	0	0	11	0
4	D	106	0	0	5	0
4	E	83	0	0	2	0
4	F	69	0	0	7	0
4	G	54	0	0	15	0
4	H	84	0	0	9	0
4	I	43	0	0	10	0
4	J	55	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	69	0	0	12	0
4	L	36	0	0	8	0
All	All	39025	0	38830	1129	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 15.

All (1129) 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:K:248:LYS:CD	1:K:283:ASP:HA	1.32	1.55
1:K:248:LYS:HD2	1:K:283:ASP:CA	1.49	1.39
1:E:370:LEU:CD1	1:E:397:ARG:HB2	1.60	1.32
1:B:370:LEU:CD1	1:B:397:ARG:HB2	1.59	1.30
1:C:370:LEU:CD1	1:C:397:ARG:HB2	1.64	1.27
1:L:67:ASP:HB3	1:L:69:SER:O	1.33	1.27
1:D:370:LEU:CD1	1:D:397:ARG:HB2	1.64	1.26
1:J:370:LEU:CD1	1:J:397:ARG:HB2	1.66	1.25
1:K:370:LEU:CD1	1:K:397:ARG:HB2	1.65	1.24
1:G:370:LEU:CD1	1:G:397:ARG:HB2	1.66	1.24
1:F:370:LEU:CD1	1:F:397:ARG:HB2	1.69	1.22
1:H:370:LEU:CD1	1:H:397:ARG:HB2	1.70	1.21
1:L:370:LEU:CD1	1:L:397:ARG:HB2	1.73	1.18
1:I:37:GLU:CG	1:I:38:PRO:HD2	1.75	1.17
1:K:248:LYS:HE3	1:K:248:LYS:HA	1.18	1.13
1:K:248:LYS:HA	1:K:248:LYS:CE	1.61	1.12
1:I:37:GLU:HG3	1:I:38:PRO:HD2	1.20	1.10
1:E:403:GLU:HG3	4:E:756:HOH:O	1.50	1.09
1:I:248:LYS:O	1:I:249:ILE:HG22	1.54	1.08
1:I:37:GLU:HG3	1:I:38:PRO:CD	1.85	1.07
1:L:290:LYS:HB3	4:L:743:HOH:O	1.52	1.06
1:K:330:ASN:HB3	4:K:714:HOH:O	1.55	1.05
1:E:370:LEU:HD11	1:E:397:ARG:CB	1.87	1.04
1:G:370:LEU:HD11	1:G:397:ARG:CB	1.87	1.04
1:K:248:LYS:HE3	1:K:248:LYS:CA	1.89	1.03
1:E:370:LEU:HD11	1:E:397:ARG:HB2	1.37	1.01
1:K:370:LEU:HD11	1:K:397:ARG:HB2	1.41	1.01
1:C:370:LEU:HD11	1:C:397:ARG:HB2	1.42	1.00
1:B:370:LEU:HD11	1:B:397:ARG:CB	1.90	1.00
1:F:370:LEU:HD11	1:F:397:ARG:CB	1.92	1.00
1:B:370:LEU:CD1	1:B:397:ARG:CB	2.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:VAL:HG12	1:G:219:GLU:N	1.76	0.99
1:F:370:LEU:HD11	1:F:397:ARG:HB2	1.44	0.99
1:B:370:LEU:HD13	1:B:397:ARG:HB2	1.45	0.99
1:E:370:LEU:CD1	1:E:397:ARG:CB	2.41	0.98
1:C:370:LEU:HD11	1:C:397:ARG:CB	1.94	0.98
1:L:273:ILE:HB	4:L:704:HOH:O	1.63	0.98
1:K:152:LYS:HE2	1:K:177:GLU:OE1	1.63	0.97
1:J:370:LEU:HD11	1:J:397:ARG:CB	1.93	0.97
1:B:370:LEU:HD11	1:B:397:ARG:HB2	1.41	0.97
1:K:370:LEU:HD11	1:K:397:ARG:CB	1.95	0.97
1:D:370:LEU:HD11	1:D:397:ARG:CB	1.95	0.96
1:J:370:LEU:CD1	1:J:397:ARG:CB	2.44	0.96
1:H:370:LEU:HD11	1:H:397:ARG:CB	1.95	0.96
1:L:192:VAL:HG12	4:L:433:HOH:O	1.64	0.95
1:H:370:LEU:CD1	1:H:397:ARG:CB	2.43	0.95
1:G:370:LEU:CD1	1:G:397:ARG:CB	2.42	0.95
1:D:370:LEU:CD1	1:D:397:ARG:CB	2.45	0.94
1:L:48:LYS:HE2	4:L:761:HOH:O	1.68	0.93
1:G:370:LEU:HD11	1:G:397:ARG:HB2	1.44	0.93
1:F:391:ARG:NH1	1:F:393:TYR:HE2	1.66	0.93
1:C:370:LEU:HD13	1:C:397:ARG:HB2	1.48	0.93
1:L:370:LEU:HD11	1:L:397:ARG:CB	1.98	0.93
1:D:370:LEU:HD11	1:D:397:ARG:HB2	1.45	0.93
1:C:370:LEU:CD1	1:C:397:ARG:CB	2.45	0.93
1:E:370:LEU:HD13	1:E:397:ARG:HB2	1.49	0.92
1:D:370:LEU:HD13	1:D:397:ARG:HB2	1.47	0.92
1:K:370:LEU:CD1	1:K:397:ARG:CB	2.48	0.92
1:L:67:ASP:CB	1:L:69:SER:H	1.83	0.91
1:A:22:LYS:HE3	1:A:370:LEU:HD21	1.51	0.91
1:K:248:LYS:HD3	1:K:282:LEU:O	1.71	0.91
3:C:603:EPU:O4	3:C:603:EPU:HE31	1.69	0.91
1:L:370:LEU:CD1	1:L:397:ARG:CB	2.48	0.91
1:J:370:LEU:HD11	1:J:397:ARG:HB2	1.48	0.90
1:B:391:ARG:HD3	4:B:607:HOH:O	1.71	0.89
1:K:46:LYS:C	1:K:47:LEU:HD23	1.92	0.89
1:F:370:LEU:CD1	1:F:397:ARG:CB	2.47	0.89
1:J:370:LEU:HD13	1:J:397:ARG:HB2	1.52	0.89
1:I:37:GLU:CG	1:I:38:PRO:CD	2.47	0.88
1:B:246:ARG:HD2	4:B:786:HOH:O	1.73	0.88
1:K:370:LEU:HD13	1:K:397:ARG:HB2	1.54	0.87
1:B:131:GLN:HG2	4:B:720:HOH:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:391:ARG:NH1	1:F:393:TYR:CE2	2.42	0.87
1:G:5:ARG:HD2	1:G:414:GLU:OE2	1.73	0.87
1:E:330:ASN:HB3	1:H:330:ASN:CG	1.94	0.87
1:G:218:VAL:CG1	1:G:219:GLU:N	2.38	0.87
1:K:248:LYS:NZ	1:K:284:MET:HG2	1.89	0.87
1:H:370:LEU:HD13	1:H:397:ARG:HB2	1.55	0.87
1:H:370:LEU:HD11	1:H:397:ARG:HB2	1.55	0.86
1:E:330:ASN:N	1:E:330:ASN:HD22	1.72	0.86
1:K:247:GLY:O	1:K:248:LYS:CE	2.23	0.86
1:F:1:MET:HE1	1:F:391:ARG:NH1	1.90	0.86
1:J:293:ASN:CB	4:J:760:HOH:O	2.22	0.86
1:K:248:LYS:HE2	1:K:282:LEU:O	1.75	0.85
1:F:391:ARG:HH11	1:F:393:TYR:HE2	1.16	0.85
1:F:370:LEU:HD13	1:F:397:ARG:HB2	1.59	0.85
1:L:370:LEU:HD11	1:L:397:ARG:HB2	1.55	0.85
1:L:370:LEU:HD13	1:L:397:ARG:HB2	1.59	0.84
1:G:66:ARG:HG3	1:G:67:ASP:O	1.77	0.84
1:G:370:LEU:HD13	1:G:397:ARG:HB2	1.57	0.84
1:I:220:ARG:HG3	1:I:221:LEU:N	1.93	0.83
1:C:150:ARG:HB2	4:C:462:HOH:O	1.80	0.82
3:H:608:EPU:O4	3:H:608:EPU:HE31	1.79	0.82
1:K:150:ARG:HH12	1:K:219:GLU:HA	1.44	0.82
1:L:204:LYS:HD3	1:L:216:GLU:HB3	1.62	0.82
1:L:245:SER:O	1:L:246:ARG:HB2	1.80	0.82
1:J:66:ARG:HG3	1:J:67:ASP:O	1.81	0.81
1:E:400:GLU:O	1:E:401:ARG:HB2	1.79	0.81
1:L:232:ARG:HB3	1:L:258:THR:CG2	2.10	0.81
1:K:248:LYS:HD3	1:K:283:ASP:HA	1.60	0.81
1:L:204:LYS:HD3	1:L:216:GLU:CB	2.11	0.81
1:L:67:ASP:CG	1:L:69:SER:N	2.29	0.80
1:G:11:LYS:CE	4:G:796:HOH:O	2.29	0.80
1:G:11:LYS:HE3	4:G:796:HOH:O	1.80	0.80
1:I:232:ARG:HB3	1:I:258:THR:CG2	2.12	0.80
1:F:1:MET:HE1	1:F:391:ARG:HH12	1.43	0.79
1:I:293:ASN:ND2	1:I:322:PHE:H	1.79	0.79
1:E:330:ASN:N	1:E:330:ASN:ND2	2.30	0.79
1:G:232:ARG:HB3	1:G:258:THR:CG2	2.11	0.79
1:I:248:LYS:O	1:I:249:ILE:CG2	2.30	0.79
1:F:293:ASN:ND2	1:F:322:PHE:H	1.80	0.79
1:I:84:TYR:CE2	4:I:824:HOH:O	2.34	0.79
1:L:48:LYS:CE	4:L:761:HOH:O	2.26	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:GLU:HG2	1:I:38:PRO:HD2	1.61	0.79
1:D:232:ARG:HB3	1:D:258:THR:CG2	2.13	0.79
1:J:232:ARG:HB3	1:J:258:THR:CG2	2.13	0.79
1:C:293:ASN:ND2	1:C:322:PHE:H	1.80	0.78
1:H:232:ARG:HB3	1:H:258:THR:CG2	2.13	0.78
1:F:60:LEU:HA	1:F:79:VAL:HG13	1.66	0.78
1:G:218:VAL:CG1	1:G:219:GLU:H	1.95	0.78
1:L:36:GLU:O	1:L:37:GLU:HB3	1.81	0.78
1:B:232:ARG:HB3	1:B:258:THR:CG2	2.13	0.78
1:F:400:GLU:HG2	1:F:401:ARG:HG2	1.63	0.78
3:C:603:EPU:O4	3:C:603:EPU:C3E	2.32	0.78
1:J:66:ARG:C	1:J:67:ASP:O	2.14	0.78
1:H:293:ASN:ND2	1:H:322:PHE:H	1.81	0.77
1:L:36:GLU:O	1:L:37:GLU:CB	2.32	0.77
1:C:232:ARG:HB3	1:C:258:THR:CG2	2.15	0.77
1:A:120:ARG:HD2	4:A:780:HOH:O	1.84	0.77
1:A:232:ARG:HB3	1:A:258:THR:CG2	2.14	0.77
1:B:293:ASN:ND2	1:B:322:PHE:H	1.82	0.77
1:L:218:VAL:HG23	1:L:219:GLU:N	1.99	0.77
1:D:22:LYS:HE3	1:D:370:LEU:HD21	1.66	0.76
1:K:247:GLY:O	1:K:248:LYS:NZ	2.19	0.75
1:L:60:LEU:HA	1:L:79:VAL:HG13	1.68	0.75
1:G:293:ASN:ND2	1:G:322:PHE:H	1.84	0.75
1:H:3:LYS:HD2	4:H:498:HOH:O	1.86	0.75
1:J:66:ARG:O	1:J:67:ASP:O	2.03	0.75
1:L:357:VAL:HG12	1:L:358:GLU:N	2.02	0.75
1:A:232:ARG:HB3	1:A:258:THR:HG21	1.70	0.74
1:G:60:LEU:HA	1:G:79:VAL:HG13	1.69	0.74
1:B:22:LYS:HE3	1:B:370:LEU:HD21	1.68	0.74
1:K:248:LYS:CE	1:K:283:ASP:HA	2.17	0.74
1:A:293:ASN:ND2	1:A:322:PHE:H	1.86	0.74
1:K:248:LYS:CD	1:K:282:LEU:O	2.36	0.74
1:K:212:ARG:NH1	4:K:735:HOH:O	2.20	0.74
1:B:60:LEU:HA	1:B:79:VAL:HG13	1.69	0.74
1:C:60:LEU:HA	1:C:79:VAL:HG13	1.70	0.73
1:D:60:LEU:HA	1:D:79:VAL:HG13	1.70	0.73
1:F:232:ARG:HB3	1:F:258:THR:CG2	2.18	0.73
1:E:60:LEU:HA	1:E:79:VAL:HG13	1.70	0.73
1:E:183:GLU:OE2	1:E:212:ARG:CZ	2.36	0.73
1:K:232:ARG:HB3	1:K:258:THR:CG2	2.18	0.73
1:E:232:ARG:HB3	1:E:258:THR:CG2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ASN:ND2	1:D:322:PHE:H	1.85	0.73
1:A:60:LEU:HA	1:A:79:VAL:HG13	1.70	0.73
1:K:60:LEU:HA	1:K:79:VAL:HG13	1.70	0.73
1:A:368:THR:HB	4:A:556:HOH:O	1.89	0.73
1:L:232:ARG:HB3	1:L:258:THR:HG21	1.70	0.73
1:L:255:GLN:O	1:L:258:THR:HB	1.89	0.73
1:E:293:ASN:ND2	1:E:322:PHE:H	1.87	0.72
1:D:67:ASP:CG	1:D:67:ASP:O	2.24	0.72
1:F:255:GLN:O	1:F:258:THR:HB	1.89	0.72
1:H:232:ARG:HB3	1:H:258:THR:HG21	1.70	0.72
1:L:357:VAL:CG1	1:L:358:GLU:N	2.53	0.72
1:I:60:LEU:HA	1:I:79:VAL:HG13	1.70	0.72
1:K:248:LYS:CD	1:K:283:ASP:CA	2.28	0.72
1:I:84:TYR:HE2	4:I:824:HOH:O	1.68	0.72
1:J:293:ASN:ND2	1:J:322:PHE:H	1.88	0.72
1:F:296:THR:O	1:F:326:THR:HB	1.89	0.72
1:C:391:ARG:HG3	1:C:393:TYR:HE2	1.53	0.72
1:I:232:ARG:HB3	1:I:258:THR:HG21	1.70	0.71
1:D:232:ARG:HB3	1:D:258:THR:HG21	1.72	0.71
1:L:293:ASN:ND2	1:L:322:PHE:H	1.87	0.71
1:I:39:VAL:HG12	1:I:72:ILE:O	1.91	0.71
1:H:60:LEU:HA	1:H:79:VAL:HG13	1.71	0.71
1:L:67:ASP:CG	1:L:67:ASP:OXT	2.29	0.71
1:B:232:ARG:HB3	1:B:258:THR:HG21	1.72	0.71
1:J:24:ALA:O	1:J:27:PRO:HD2	1.90	0.71
1:J:255:GLN:O	1:J:258:THR:HB	1.91	0.71
1:F:326:THR:CG2	1:F:326:THR:O	2.39	0.71
1:J:66:ARG:HG3	1:J:67:ASP:N	2.06	0.71
1:B:5:ARG:HD2	1:B:414:GLU:OE2	1.90	0.71
1:B:255:GLN:O	1:B:258:THR:HB	1.90	0.71
1:I:248:LYS:C	1:I:249:ILE:CG2	2.59	0.71
1:A:5:ARG:HD3	4:A:420:HOH:O	1.90	0.70
1:C:232:ARG:HB3	1:C:258:THR:HG21	1.70	0.70
1:I:255:GLN:O	1:I:258:THR:HB	1.91	0.70
1:D:255:GLN:O	1:D:258:THR:HB	1.91	0.70
1:G:370:LEU:HD11	1:G:397:ARG:HB3	1.73	0.70
1:G:24:ALA:O	1:G:27:PRO:HD2	1.91	0.70
1:L:24:ALA:O	1:L:27:PRO:HD2	1.90	0.70
1:K:255:GLN:O	1:K:258:THR:HB	1.91	0.70
1:C:255:GLN:O	1:C:258:THR:HB	1.91	0.70
1:E:325:GLU:HG2	1:E:328:PHE:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLN:O	1:A:258:THR:HB	1.90	0.70
1:E:183:GLU:OE2	1:E:212:ARG:NH2	2.25	0.70
1:I:247:GLY:HA2	1:I:248:LYS:HE2	1.74	0.70
1:F:155:HIS:NE2	1:F:183:GLU:OE1	2.25	0.69
1:J:60:LEU:HA	1:J:79:VAL:HG13	1.73	0.69
1:K:248:LYS:HE3	1:K:248:LYS:N	2.06	0.69
1:G:232:ARG:HB3	1:G:258:THR:HG21	1.72	0.69
1:L:67:ASP:CB	1:L:69:SER:N	2.55	0.69
1:F:232:ARG:HB3	1:F:258:THR:HG21	1.73	0.69
1:I:220:ARG:CG	1:I:221:LEU:N	2.56	0.69
1:J:211:ASP:HB3	4:K:452:HOH:O	1.92	0.69
1:K:247:GLY:C	1:K:248:LYS:HE3	2.12	0.69
1:K:248:LYS:CE	1:K:282:LEU:O	2.40	0.69
1:K:340:ARG:NH1	1:K:364:GLN:O	2.25	0.69
1:H:293:ASN:HD22	1:H:322:PHE:H	1.39	0.69
1:E:232:ARG:HB3	1:E:258:THR:HG21	1.74	0.68
1:I:401:ARG:HA	4:I:436:HOH:O	1.92	0.68
1:F:88:LYS:NZ	4:F:637:HOH:O	2.20	0.68
1:K:232:ARG:HB3	1:K:258:THR:HG21	1.75	0.68
1:I:276:GLY:HA3	1:I:279:TRP:NE1	2.07	0.68
1:D:371:ARG:NH2	4:D:459:HOH:O	2.27	0.68
1:K:22:LYS:HE3	1:K:370:LEU:HD21	1.75	0.68
1:K:248:LYS:NZ	1:K:282:LEU:HD23	2.09	0.68
1:L:67:ASP:CG	1:L:69:SER:H	1.92	0.68
1:L:299:HIS:CG	1:L:300:PRO:HA	2.29	0.68
1:C:22:LYS:HE3	1:C:370:LEU:HD21	1.76	0.68
1:F:1:MET:CE	1:F:391:ARG:NH1	2.57	0.68
1:A:371:ARG:NH2	4:A:426:HOH:O	2.26	0.67
1:K:248:LYS:NZ	1:K:284:MET:N	2.42	0.67
1:A:46:LYS:NZ	1:A:67:ASP:OXT	2.25	0.67
1:K:293:ASN:ND2	1:K:322:PHE:H	1.92	0.67
1:H:22:LYS:HE3	1:H:370:LEU:HD21	1.77	0.67
1:J:232:ARG:HB3	1:J:258:THR:HG21	1.75	0.67
1:I:303:PRO:HA	4:I:419:HOH:O	1.94	0.67
1:G:255:GLN:O	1:G:258:THR:HB	1.94	0.67
1:J:22:LYS:HE3	1:J:370:LEU:HD21	1.77	0.67
1:C:401:ARG:HD2	1:C:404:ASP:OD2	1.95	0.67
1:J:293:ASN:HB2	4:J:760:HOH:O	1.88	0.66
1:G:325:GLU:HG2	1:G:328:PHE:O	1.95	0.66
1:H:255:GLN:O	1:H:258:THR:HB	1.95	0.66
1:B:246:ARG:CD	4:B:786:HOH:O	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:THR:O	1:F:326:THR:HG23	1.94	0.66
1:K:66:ARG:HG3	1:K:67:ASP:O	1.96	0.66
1:K:152:LYS:CE	1:K:177:GLU:OE1	2.40	0.66
1:F:293:ASN:HD22	1:F:322:PHE:H	1.43	0.66
1:H:325:GLU:HG2	1:H:328:PHE:O	1.96	0.66
1:A:24:ALA:O	1:A:27:PRO:HD2	1.96	0.66
1:K:247:GLY:O	1:K:248:LYS:HE3	1.94	0.66
1:B:370:LEU:HD11	1:B:397:ARG:C	2.17	0.66
1:I:401:ARG:CA	4:I:436:HOH:O	2.44	0.66
1:E:118:GLY:HA2	1:E:330:ASN:OD1	1.96	0.65
1:I:46:LYS:HG2	1:I:66:ARG:NH2	2.10	0.65
1:L:22:LYS:HE3	1:L:370:LEU:HD21	1.78	0.65
1:C:35:ALA:HB1	1:C:222:GLY:O	1.96	0.65
1:D:370:LEU:HD11	1:D:397:ARG:C	2.16	0.65
1:E:333:MET:O	1:E:336:PRO:HD2	1.97	0.65
1:K:248:LYS:HZ1	1:K:284:MET:HG2	1.61	0.65
1:F:299:HIS:CG	1:F:300:PRO:HA	2.31	0.65
1:G:333:MET:O	1:G:336:PRO:HD2	1.97	0.65
1:I:66:ARG:NH2	1:I:67:ASP:OD1	2.30	0.65
1:L:67:ASP:OD1	1:L:69:SER:N	2.30	0.65
1:C:403:GLU:HG3	4:C:463:HOH:O	1.98	0.64
1:C:108:GLN:NE2	4:C:444:HOH:O	2.30	0.64
1:E:255:GLN:O	1:E:258:THR:HB	1.97	0.64
1:E:330:ASN:ND2	1:E:330:ASN:H	1.94	0.64
1:K:63:LYS:HB2	1:K:73:ASP:HB3	1.79	0.64
1:J:299:HIS:CG	1:J:300:PRO:HA	2.33	0.64
1:C:330:ASN:ND2	1:C:330:ASN:O	2.30	0.64
1:F:88:LYS:CE	4:F:637:HOH:O	2.46	0.64
1:B:24:ALA:O	1:B:27:PRO:HD2	1.97	0.64
1:G:218:VAL:HG12	1:G:219:GLU:H	1.53	0.63
1:I:120:ARG:HD2	4:I:438:HOH:O	1.98	0.63
1:I:201:LEU:HB2	1:I:221:LEU:HD22	1.80	0.63
1:A:22:LYS:HE3	1:A:370:LEU:CD2	2.28	0.63
1:G:6:VAL:HG22	1:G:413:ILE:HG13	1.80	0.63
1:G:177:GLU:HG3	4:G:433:HOH:O	1.97	0.63
1:L:63:LYS:HB2	1:L:73:ASP:HB3	1.80	0.63
1:H:218:VAL:HG23	1:H:219:GLU:N	2.12	0.63
1:L:325:GLU:HG2	1:L:328:PHE:O	1.98	0.63
1:K:330:ASN:CB	4:K:714:HOH:O	2.26	0.63
1:K:276:GLY:HA3	1:K:279:TRP:NE1	2.14	0.63
1:D:63:LYS:HB2	1:D:73:ASP:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:248:LYS:HD2	1:K:283:ASP:CB	2.28	0.63
1:H:63:LYS:HB2	1:H:73:ASP:HB3	1.81	0.63
1:H:370:LEU:HD11	1:H:397:ARG:HB3	1.78	0.63
1:I:299:HIS:CG	1:I:300:PRO:HA	2.33	0.63
1:K:248:LYS:HE2	1:K:282:LEU:HD23	1.81	0.63
1:L:67:ASP:OD1	1:L:68:GLY:C	2.35	0.63
1:B:322:PHE:CE1	1:H:346:GLU:HG3	2.34	0.63
1:K:204:LYS:HD2	1:K:216:GLU:HG2	1.81	0.63
1:K:394:HIS:CE1	4:K:811:HOH:O	2.52	0.63
1:L:42:GLN:HA	1:L:69:SER:OG	1.99	0.63
1:G:299:HIS:CG	1:G:300:PRO:HA	2.33	0.62
1:C:340:ARG:NH1	1:C:364:GLN:O	2.32	0.62
1:B:46:LYS:NZ	4:B:434:HOH:O	2.29	0.62
1:J:267:ARG:NH1	4:J:697:HOH:O	2.29	0.62
1:K:325:GLU:HG2	1:K:328:PHE:O	1.99	0.62
1:E:330:ASN:HB3	1:H:330:ASN:ND2	2.14	0.62
1:K:299:HIS:CG	1:K:300:PRO:HA	2.34	0.62
1:B:276:GLY:HA3	1:B:279:TRP:NE1	2.15	0.62
1:B:299:HIS:CG	1:B:300:PRO:HA	2.35	0.62
1:G:63:LYS:HB2	1:G:73:ASP:HB3	1.80	0.62
1:K:248:LYS:HD2	1:K:283:ASP:HA	0.63	0.62
1:C:370:LEU:HD11	1:C:397:ARG:C	2.20	0.62
1:D:293:ASN:HD22	1:D:322:PHE:H	1.48	0.62
1:E:22:LYS:HE3	1:E:370:LEU:HD21	1.82	0.62
1:B:401:ARG:HG3	4:B:444:HOH:O	1.99	0.62
1:J:325:GLU:HG2	1:J:328:PHE:O	1.99	0.62
1:B:370:LEU:HD12	1:B:394:HIS:O	1.99	0.61
1:A:299:HIS:CG	1:A:300:PRO:HA	2.36	0.61
1:C:333:MET:O	1:C:336:PRO:HD2	2.00	0.61
1:J:120:ARG:HD2	4:J:673:HOH:O	1.99	0.61
1:B:333:MET:O	1:B:336:PRO:HD2	2.00	0.61
1:D:299:HIS:CG	1:D:300:PRO:HA	2.36	0.61
1:K:248:LYS:HZ3	1:K:284:MET:N	1.98	0.61
1:B:370:LEU:HD13	1:B:397:ARG:CB	2.21	0.61
1:E:299:HIS:CG	1:E:300:PRO:HA	2.35	0.61
1:L:150:ARG:NH2	1:L:218:VAL:O	2.31	0.61
1:A:120:ARG:HD3	1:A:328:PHE:CE1	2.36	0.61
1:E:24:ALA:O	1:E:27:PRO:HD2	2.00	0.61
1:F:63:LYS:HB2	1:F:73:ASP:HB3	1.83	0.61
1:B:346:GLU:HG3	1:H:322:PHE:CE1	2.36	0.60
1:F:248:LYS:HD3	1:F:283:ASP:CG	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:LYS:CD	4:G:796:HOH:O	2.48	0.60
1:D:160:LYS:HD2	1:F:295:ARG:HH21	1.65	0.60
1:K:403:GLU:HB2	1:K:413:ILE:HD13	1.82	0.60
1:J:63:LYS:HB2	1:J:73:ASP:HB3	1.83	0.60
1:J:276:GLY:HA3	1:J:279:TRP:NE1	2.17	0.60
1:J:161:VAL:HA	4:J:437:HOH:O	2.00	0.60
1:B:60:LEU:HA	1:B:79:VAL:CG1	2.31	0.60
1:C:330:ASN:CG	1:D:330:ASN:ND2	2.55	0.60
1:D:67:ASP:O	1:D:67:ASP:OD1	2.19	0.60
1:F:1:MET:HE3	1:F:391:ARG:NH2	2.17	0.60
1:G:42:GLN:NE2	4:G:420:HOH:O	2.33	0.60
1:C:325:GLU:HG2	1:C:328:PHE:O	2.01	0.60
1:E:47:LEU:HD21	1:E:400:GLU:N	2.17	0.60
1:G:44:VAL:O	1:G:66:ARG:NH2	2.31	0.60
1:G:340:ARG:NH1	1:G:364:GLN:O	2.35	0.60
1:J:333:MET:O	1:J:336:PRO:HD2	2.01	0.60
1:K:46:LYS:O	1:K:47:LEU:HD23	2.00	0.60
1:K:24:ALA:O	1:K:27:PRO:HD2	2.02	0.60
1:K:333:MET:O	1:K:336:PRO:HD2	2.02	0.60
1:F:276:GLY:HA3	1:F:279:TRP:NE1	2.17	0.60
1:G:7:GLN:HB2	1:G:412:ASN:CG	2.22	0.60
1:G:177:GLU:N	4:G:433:HOH:O	2.34	0.60
1:G:299:HIS:ND1	1:G:300:PRO:HA	2.17	0.60
1:I:333:MET:O	1:I:336:PRO:HD2	2.02	0.60
1:J:283:ASP:OD2	1:J:285:HIS:CE1	2.55	0.60
1:G:252:ARG:O	1:G:253:ASN:HB2	2.00	0.59
1:H:160:LYS:HE3	3:H:608:EPU:O2U	2.02	0.59
1:J:284:MET:O	1:J:285:HIS:C	2.40	0.59
1:J:370:LEU:HD11	1:J:397:ARG:HB3	1.82	0.59
1:C:258:THR:HG22	1:C:259:LEU:HG	1.84	0.59
1:J:370:LEU:HD11	1:J:397:ARG:C	2.22	0.59
1:L:36:GLU:O	1:L:37:GLU:CG	2.51	0.59
1:D:47:LEU:HD21	1:D:400:GLU:N	2.17	0.59
1:D:120:ARG:HD3	1:D:328:PHE:CE1	2.37	0.59
1:E:370:LEU:HD12	1:E:394:HIS:O	2.03	0.59
1:C:63:LYS:HB2	1:C:73:ASP:HB3	1.85	0.59
1:J:370:LEU:HD12	1:J:394:HIS:O	2.02	0.59
1:L:276:GLY:HA3	1:L:279:TRP:NE1	2.17	0.59
1:C:212:ARG:NH1	4:C:437:HOH:O	2.34	0.59
1:G:22:LYS:HE3	1:G:370:LEU:HD21	1.84	0.59
1:I:24:ALA:O	1:I:27:PRO:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:276:GLY:HA3	1:H:279:TRP:NE1	2.18	0.59
1:B:332:PHE:N	4:B:427:HOH:O	2.35	0.59
1:E:67:ASP:OD1	1:E:69:SER:N	2.36	0.59
1:E:370:LEU:HD11	1:E:397:ARG:C	2.23	0.59
1:I:61:GLY:O	1:I:77:VAL:HA	2.03	0.59
1:C:299:HIS:CG	1:C:300:PRO:HA	2.38	0.58
1:D:333:MET:O	1:D:336:PRO:HD2	2.03	0.58
1:F:60:LEU:HA	1:F:79:VAL:CG1	2.33	0.58
1:F:370:LEU:HD11	1:F:397:ARG:HB3	1.81	0.58
1:B:350:ASN:ND2	4:B:437:HOH:O	2.35	0.58
1:C:370:LEU:HD13	1:C:397:ARG:CB	2.27	0.58
1:K:391:ARG:HG3	1:K:393:TYR:HE2	1.68	0.58
1:A:63:LYS:HB2	1:A:73:ASP:HB3	1.85	0.58
1:F:47:LEU:HD21	1:F:400:GLU:N	2.18	0.58
1:G:383:ALA:HB3	4:G:511:HOH:O	2.02	0.58
1:J:391:ARG:HG3	1:J:393:TYR:CE2	2.38	0.58
1:D:370:LEU:HD12	1:D:394:HIS:O	2.03	0.58
1:J:391:ARG:HG3	1:J:393:TYR:HE2	1.68	0.58
1:B:63:LYS:HB2	1:B:73:ASP:HB3	1.85	0.58
1:C:295:ARG:NE	4:C:430:HOH:O	2.34	0.58
1:C:370:LEU:HD12	1:C:394:HIS:O	2.04	0.58
1:H:66:ARG:NE	1:H:67:ASP:O	2.36	0.58
1:I:293:ASN:HD22	1:I:322:PHE:H	1.51	0.58
1:K:42:GLN:NE2	4:K:434:HOH:O	2.36	0.58
1:B:322:PHE:HE1	1:H:346:GLU:HG3	1.68	0.58
1:C:293:ASN:HD22	1:C:322:PHE:H	1.49	0.58
1:C:60:LEU:HA	1:C:79:VAL:CG1	2.34	0.58
1:F:371:ARG:NH2	4:F:427:HOH:O	2.36	0.58
1:G:276:GLY:HA3	1:G:279:TRP:NE1	2.19	0.58
1:I:64:VAL:HA	1:I:71:HIS:O	2.03	0.58
1:K:248:LYS:CE	1:K:282:LEU:HD23	2.33	0.58
1:E:67:ASP:OD1	1:E:68:GLY:C	2.37	0.58
3:F:606:EPU:HE31	3:F:606:EPU:O4	2.03	0.58
1:H:333:MET:O	1:H:336:PRO:HD2	2.04	0.58
1:H:370:LEU:HD11	1:H:397:ARG:C	2.24	0.58
1:K:47:LEU:HD23	1:K:47:LEU:N	2.16	0.58
1:C:276:GLY:HA3	1:C:279:TRP:NE1	2.18	0.58
1:A:333:MET:O	1:A:336:PRO:HD2	2.03	0.57
1:L:36:GLU:O	1:L:37:GLU:HG2	2.04	0.57
1:A:66:ARG:NH2	1:A:67:ASP:OD1	2.30	0.57
1:L:370:LEU:HD11	1:L:397:ARG:C	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:NE	4:B:786:HOH:O	2.37	0.57
1:C:391:ARG:HG3	1:C:393:TYR:CE2	2.37	0.57
1:G:60:LEU:HA	1:G:79:VAL:CG1	2.34	0.57
1:B:22:LYS:HE3	1:B:370:LEU:CD2	2.34	0.57
1:J:66:ARG:CG	1:J:67:ASP:O	2.50	0.57
1:L:370:LEU:HD11	1:L:397:ARG:HB3	1.84	0.57
1:H:299:HIS:CG	1:H:300:PRO:HA	2.39	0.57
1:L:258:THR:HG22	1:L:259:LEU:HG	1.86	0.57
1:E:370:LEU:HD11	1:E:397:ARG:HB3	1.83	0.57
1:F:340:ARG:NH1	1:F:364:GLN:O	2.37	0.57
1:A:325:GLU:HG2	1:A:328:PHE:O	2.05	0.57
1:A:391:ARG:HG3	1:A:393:TYR:CE2	2.39	0.57
1:C:24:ALA:O	1:C:27:PRO:HD2	2.04	0.57
1:G:46:LYS:HA	1:G:66:ARG:HH12	1.70	0.57
1:H:94:ILE:HA	1:H:109:VAL:HG11	1.87	0.57
1:D:22:LYS:HE3	1:D:370:LEU:CD2	2.34	0.57
1:I:258:THR:HG22	1:I:259:LEU:HG	1.87	0.57
1:L:120:ARG:HD3	1:L:328:PHE:CE1	2.40	0.57
1:L:219:GLU:O	1:L:220:ARG:HG3	2.05	0.56
1:B:391:ARG:HG3	1:B:393:TYR:CE2	2.40	0.56
1:I:60:LEU:HA	1:I:79:VAL:CG1	2.36	0.56
1:A:391:ARG:HG3	1:A:393:TYR:HE2	1.69	0.56
1:E:63:LYS:HB2	1:E:73:ASP:HB3	1.88	0.56
1:I:246:ARG:HG2	1:I:287:LYS:O	2.05	0.56
1:J:47:LEU:HD21	1:J:400:GLU:N	2.20	0.56
1:K:391:ARG:HG3	1:K:393:TYR:CE2	2.40	0.56
1:L:60:LEU:HA	1:L:79:VAL:CG1	2.35	0.56
1:G:293:ASN:HD22	1:G:322:PHE:H	1.51	0.56
1:A:60:LEU:HA	1:A:79:VAL:CG1	2.36	0.56
1:A:293:ASN:HD22	1:A:322:PHE:H	1.54	0.56
1:F:333:MET:O	1:F:336:PRO:HD2	2.05	0.56
1:H:120:ARG:HD3	1:H:328:PHE:HE1	1.71	0.56
1:G:391:ARG:HG3	1:G:393:TYR:HE2	1.71	0.55
1:H:60:LEU:HA	1:H:79:VAL:CG1	2.36	0.55
1:I:36:GLU:HG3	1:I:221:LEU:O	2.06	0.55
1:L:47:LEU:HD21	1:L:400:GLU:N	2.21	0.55
1:B:325:GLU:HG2	1:B:328:PHE:O	2.06	0.55
1:K:120:ARG:HD3	1:K:328:PHE:CE1	2.41	0.55
1:K:370:LEU:HD11	1:K:397:ARG:C	2.27	0.55
1:F:330:ASN:HB3	1:G:330:ASN:ND2	2.22	0.55
1:J:299:HIS:ND1	1:J:300:PRO:HA	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ALA:O	1:D:27:PRO:HD2	2.06	0.55
1:K:248:LYS:HG3	1:K:283:ASP:OD1	2.06	0.55
1:A:47:LEU:HD21	1:A:400:GLU:N	2.22	0.55
1:I:11:LYS:HE2	1:I:248:LYS:HE3	1.87	0.55
1:C:46:LYS:O	1:C:47:LEU:HD23	2.06	0.55
1:E:293:ASN:HD22	1:E:322:PHE:H	1.52	0.55
1:G:370:LEU:HD12	1:G:394:HIS:O	2.07	0.55
1:A:46:LYS:CE	1:A:67:ASP:OXT	2.55	0.55
1:F:1:MET:HE3	1:F:391:ARG:CZ	2.37	0.55
1:H:299:HIS:ND1	1:H:300:PRO:HA	2.21	0.55
1:L:38:PRO:O	1:L:223:GLY:HA3	2.07	0.55
1:D:60:LEU:HA	1:D:79:VAL:CG1	2.36	0.55
1:F:94:ILE:HA	1:F:109:VAL:HG11	1.89	0.55
1:K:60:LEU:HA	1:K:79:VAL:CG1	2.36	0.55
1:C:45:PRO:HB2	1:C:47:LEU:HG	1.89	0.55
1:D:45:PRO:HB2	1:D:47:LEU:HG	1.89	0.55
1:D:407:ARG:HG3	4:D:423:HOH:O	2.06	0.55
1:K:247:GLY:O	1:K:248:LYS:HG2	2.06	0.55
1:K:248:LYS:NZ	1:K:284:MET:H	2.03	0.55
1:L:211:ASP:OD1	1:L:211:ASP:N	2.33	0.55
1:B:299:HIS:ND1	1:B:300:PRO:HA	2.22	0.55
1:I:325:GLU:HG2	1:I:328:PHE:O	2.07	0.55
1:K:370:LEU:HD12	1:K:394:HIS:O	2.07	0.55
1:G:39:VAL:HG23	1:G:224:GLY:O	2.08	0.54
1:A:258:THR:HG22	1:A:259:LEU:HG	1.89	0.54
1:L:45:PRO:HB2	1:L:47:LEU:HG	1.89	0.54
1:L:75:ARG:HA	1:L:103:ARG:HH22	1.71	0.54
1:B:369:ASP:OD1	1:B:369:ASP:C	2.45	0.54
1:D:22:LYS:CE	1:D:370:LEU:HD21	2.37	0.54
1:J:60:LEU:HA	1:J:79:VAL:CG1	2.37	0.54
1:H:47:LEU:HD21	1:H:400:GLU:N	2.22	0.54
1:A:276:GLY:HA3	1:A:279:TRP:NE1	2.23	0.54
1:F:120:ARG:HD3	1:F:328:PHE:HE1	1.71	0.54
1:F:258:THR:HG22	1:F:259:LEU:HG	1.89	0.54
1:K:94:ILE:HA	1:K:109:VAL:HG11	1.90	0.54
1:B:391:ARG:HG3	1:B:393:TYR:HE2	1.70	0.54
1:G:370:LEU:HD11	1:G:397:ARG:C	2.28	0.54
1:C:120:ARG:HD3	1:C:328:PHE:CE1	2.43	0.54
1:D:325:GLU:HG2	1:D:328:PHE:O	2.07	0.54
1:E:60:LEU:HA	1:E:79:VAL:CG1	2.36	0.54
3:H:608:EPU:O4	3:H:608:EPU:C3E	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:HA	1:B:109:VAL:HG11	1.90	0.54
1:D:94:ILE:HA	1:D:109:VAL:HG11	1.89	0.54
1:E:94:ILE:HA	1:E:109:VAL:HG11	1.89	0.54
1:G:24:ALA:C	1:G:27:PRO:HD2	2.28	0.54
1:J:66:ARG:HG3	1:J:67:ASP:C	2.28	0.54
1:L:11:LYS:HD2	1:L:246:ARG:O	2.07	0.54
1:B:46:LYS:O	1:B:47:LEU:HD23	2.08	0.54
1:F:150:ARG:HH22	1:F:219:GLU:HA	1.73	0.54
1:G:94:ILE:HA	1:G:109:VAL:HG11	1.89	0.54
1:I:299:HIS:ND1	1:I:300:PRO:HA	2.22	0.54
1:D:220:ARG:HD2	4:D:733:HOH:O	2.08	0.53
1:I:13:GLN:HA	1:I:249:ILE:HG22	1.89	0.53
1:I:47:LEU:HD21	1:I:400:GLU:N	2.23	0.53
1:J:258:THR:HG22	1:J:259:LEU:HG	1.89	0.53
1:L:218:VAL:HG23	1:L:219:GLU:H	1.74	0.53
1:A:120:ARG:HD3	1:A:328:PHE:HE1	1.73	0.53
1:B:47:LEU:HD21	1:B:400:GLU:N	2.23	0.53
1:B:370:LEU:HD11	1:B:397:ARG:HB3	1.87	0.53
1:L:150:ARG:HH12	1:L:219:GLU:HA	1.74	0.53
1:G:120:ARG:HD3	1:G:328:PHE:CE1	2.43	0.53
1:G:36:GLU:OE1	1:G:220:ARG:CZ	2.56	0.53
1:I:276:GLY:HA3	1:I:279:TRP:CD1	2.43	0.53
1:L:244:ILE:HD12	1:L:382:ILE:HD13	1.89	0.53
1:D:120:ARG:HD3	1:D:328:PHE:HE1	1.73	0.53
1:D:258:THR:HG22	1:D:259:LEU:HG	1.90	0.53
1:G:150:ARG:NH2	4:G:752:HOH:O	2.41	0.53
1:I:335:VAL:HB	1:I:336:PRO:HD3	1.90	0.53
1:A:94:ILE:HA	1:A:109:VAL:HG11	1.91	0.53
1:B:146:SER:HB2	4:B:452:HOH:O	2.09	0.53
1:F:325:GLU:HG2	1:F:328:PHE:O	2.07	0.53
1:B:150:ARG:HH12	1:B:219:GLU:HA	1.73	0.53
1:C:244:ILE:HD12	1:C:382:ILE:HD13	1.90	0.53
1:D:276:GLY:HA3	1:D:279:TRP:NE1	2.24	0.53
1:F:285:HIS:CE1	1:H:152:LYS:HZ3	2.26	0.53
1:G:218:VAL:HG12	1:G:220:ARG:H	1.73	0.53
1:H:24:ALA:O	1:H:27:PRO:HD2	2.08	0.53
1:H:370:LEU:HD13	1:H:397:ARG:CB	2.26	0.53
1:H:391:ARG:HG3	1:H:393:TYR:CE2	2.44	0.53
1:L:67:ASP:HB2	1:L:69:SER:H	1.67	0.53
1:B:22:LYS:CE	1:B:370:LEU:HD21	2.38	0.53
1:H:3:LYS:CE	4:H:498:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:LEU:HD22	1:G:343:ALA:HB1	1.91	0.52
1:H:45:PRO:HB2	1:H:47:LEU:HG	1.91	0.52
1:K:212:ARG:NH2	4:K:738:HOH:O	2.40	0.52
1:K:299:HIS:ND1	1:K:300:PRO:HA	2.23	0.52
1:K:152:LYS:HD3	1:K:177:GLU:HB2	1.92	0.52
1:A:120:ARG:CD	4:A:780:HOH:O	2.51	0.52
1:E:299:HIS:ND1	1:E:300:PRO:HA	2.23	0.52
1:F:22:LYS:HE3	1:F:370:LEU:HD21	1.92	0.52
1:K:258:THR:HG22	1:K:259:LEU:HG	1.90	0.52
1:L:24:ALA:C	1:L:27:PRO:HD2	2.30	0.52
1:B:293:ASN:HD22	1:B:322:PHE:H	1.55	0.52
1:F:66:ARG:HB3	1:F:70:VAL:HG22	1.91	0.52
1:F:370:LEU:HD11	1:F:397:ARG:C	2.30	0.52
1:G:391:ARG:HG3	1:G:393:TYR:CE2	2.44	0.52
1:H:120:ARG:HD3	1:H:328:PHE:CE1	2.44	0.52
1:J:24:ALA:C	1:J:27:PRO:HD2	2.29	0.52
1:B:120:ARG:HD3	1:B:328:PHE:CE1	2.45	0.52
1:L:192:VAL:C	4:L:433:HOH:O	2.48	0.52
1:C:330:ASN:O	1:C:330:ASN:CG	2.48	0.52
1:E:391:ARG:HG3	1:E:393:TYR:CE2	2.44	0.52
1:F:38:PRO:O	1:F:223:GLY:HA3	2.09	0.52
1:G:47:LEU:HD21	1:G:400:GLU:N	2.24	0.52
1:H:258:THR:HG22	1:H:259:LEU:HG	1.92	0.52
1:J:46:LYS:HZ3	1:J:67:ASP:HB2	1.75	0.52
1:K:276:GLY:HA3	1:K:279:TRP:CE2	2.45	0.52
1:L:299:HIS:ND1	1:L:300:PRO:HA	2.24	0.52
1:B:244:ILE:HD12	1:B:382:ILE:HD13	1.92	0.52
1:C:334:HIS:H	1:C:334:HIS:CD2	2.28	0.52
1:J:370:LEU:HD13	1:J:397:ARG:CB	2.27	0.52
1:G:120:ARG:HD3	1:G:328:PHE:HE1	1.75	0.52
1:L:219:GLU:O	1:L:220:ARG:CG	2.58	0.52
1:A:46:LYS:O	1:A:47:LEU:HD23	2.10	0.52
1:F:299:HIS:ND1	1:F:300:PRO:HA	2.24	0.52
1:G:176:ALA:C	4:G:433:HOH:O	2.49	0.51
1:J:16:VAL:HB	4:J:425:HOH:O	2.09	0.51
1:K:120:ARG:HD3	1:K:328:PHE:HE1	1.74	0.51
1:L:196:ASN:ND2	4:L:433:HOH:O	2.43	0.51
1:L:333:MET:O	1:L:336:PRO:HD2	2.10	0.51
1:A:346:GLU:HG3	1:E:322:PHE:HE1	1.76	0.51
1:C:10:THR:HG21	4:C:476:HOH:O	2.10	0.51
1:H:369:ASP:HB2	4:H:449:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:GLY:HA3	1:I:279:TRP:CE2	2.46	0.51
1:J:46:LYS:NZ	1:J:67:ASP:OXT	2.43	0.51
1:H:340:ARG:NH1	1:H:364:GLN:O	2.43	0.51
1:L:201:LEU:CB	1:L:221:LEU:HD23	2.41	0.51
1:L:335:VAL:HB	1:L:336:PRO:HD3	1.91	0.51
1:C:66:ARG:HE	1:C:67:ASP:HB3	1.75	0.51
1:E:330:ASN:HB3	1:H:330:ASN:OD1	2.10	0.51
1:F:36:GLU:O	1:F:75:ARG:HG2	2.11	0.51
1:I:120:ARG:HD3	1:I:328:PHE:CE1	2.45	0.51
1:E:276:GLY:HA3	1:E:279:TRP:NE1	2.26	0.51
1:F:88:LYS:HE2	4:F:637:HOH:O	2.10	0.51
1:G:150:ARG:HH22	1:G:219:GLU:HA	1.76	0.51
1:H:370:LEU:HD12	1:H:394:HIS:O	2.11	0.51
1:I:94:ILE:HA	1:I:109:VAL:HG11	1.92	0.51
1:I:204:LYS:HB2	1:I:216:GLU:HB3	1.92	0.51
1:K:22:LYS:HE3	1:K:370:LEU:CD2	2.41	0.51
1:C:47:LEU:HD21	1:C:400:GLU:N	2.25	0.51
1:D:150:ARG:HH22	1:D:219:GLU:HA	1.75	0.51
1:E:325:GLU:CG	1:E:328:PHE:O	2.58	0.51
1:I:350:ASN:HD22	1:I:350:ASN:H	1.58	0.51
1:L:193:ASP:HA	4:L:433:HOH:O	2.10	0.51
1:L:391:ARG:HG3	1:L:393:TYR:CE2	2.45	0.51
1:A:340:ARG:NH1	1:A:364:GLN:O	2.44	0.51
1:B:258:THR:HG22	1:B:259:LEU:HG	1.92	0.51
1:F:120:ARG:HD3	1:F:328:PHE:CE1	2.46	0.51
1:G:177:GLU:CA	4:G:433:HOH:O	2.57	0.51
1:E:258:THR:HG22	1:E:259:LEU:HG	1.92	0.51
1:F:335:VAL:HB	1:F:336:PRO:HD3	1.93	0.51
1:I:66:ARG:HD2	1:I:70:VAL:HG22	1.92	0.51
1:L:94:ILE:HA	1:L:109:VAL:HG11	1.93	0.51
1:L:204:LYS:HD3	1:L:216:GLU:CG	2.40	0.51
1:E:391:ARG:HG3	1:E:393:TYR:HE2	1.76	0.51
1:H:150:ARG:HH22	1:H:219:GLU:HA	1.75	0.51
1:B:276:GLY:HA3	1:B:279:TRP:CE2	2.46	0.50
1:E:120:ARG:HD3	1:E:328:PHE:HE1	1.76	0.50
1:K:22:LYS:CE	1:K:370:LEU:HD21	2.41	0.50
1:B:66:ARG:O	1:B:67:ASP:OXT	2.30	0.50
1:I:340:ARG:NH1	1:I:364:GLN:O	2.44	0.50
1:J:340:ARG:NH1	1:J:364:GLN:O	2.45	0.50
1:L:334:HIS:CD2	1:L:334:HIS:H	2.29	0.50
1:K:248:LYS:HZ2	1:K:284:MET:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:THR:HG22	1:G:381:CYS:O	2.11	0.50
1:G:66:ARG:O	1:G:67:ASP:O	2.30	0.50
1:J:293:ASN:HB3	4:J:760:HOH:O	2.02	0.50
1:A:334:HIS:H	1:A:334:HIS:CD2	2.29	0.50
1:I:220:ARG:HG3	1:I:221:LEU:H	1.74	0.50
1:I:334:HIS:CD2	1:I:334:HIS:H	2.28	0.50
1:L:37:GLU:O	1:L:37:GLU:HG3	2.10	0.50
1:D:252:ARG:NH2	4:D:428:HOH:O	2.43	0.50
1:F:325:GLU:CG	1:F:328:PHE:O	2.59	0.50
1:G:66:ARG:HB2	1:G:70:VAL:HG22	1.94	0.50
1:H:3:LYS:NZ	4:H:498:HOH:O	2.25	0.50
1:H:276:GLY:HA3	1:H:279:TRP:CE2	2.46	0.50
1:H:391:ARG:HG3	1:H:393:TYR:HE2	1.77	0.50
1:J:276:GLY:HA3	1:J:279:TRP:CE2	2.47	0.50
1:C:120:ARG:HD2	4:C:797:HOH:O	2.11	0.50
1:C:391:ARG:CG	1:C:393:TYR:CE2	2.95	0.50
1:D:155:HIS:HD2	1:D:181:ILE:HB	1.77	0.50
1:D:262:VAL:HG23	4:D:422:HOH:O	2.11	0.50
1:F:1:MET:CE	1:F:391:ARG:CZ	2.89	0.50
1:F:24:ALA:O	1:F:27:PRO:HD2	2.12	0.50
1:H:150:ARG:HH12	1:H:219:GLU:HA	1.77	0.50
1:I:10:THR:HG22	1:I:381:CYS:O	2.12	0.50
1:J:94:ILE:HA	1:J:109:VAL:HG11	1.93	0.50
1:L:42:GLN:HG2	1:L:69:SER:OG	2.12	0.50
1:F:45:PRO:HB2	1:F:47:LEU:HG	1.92	0.50
1:I:66:ARG:O	1:I:67:ASP:OXT	2.29	0.50
1:D:244:ILE:HD12	1:D:382:ILE:HD13	1.93	0.50
1:E:22:LYS:HE3	1:E:370:LEU:CD2	2.42	0.50
1:F:66:ARG:O	1:F:67:ASP:O	2.30	0.50
1:C:94:ILE:HA	1:C:109:VAL:HG11	1.93	0.49
1:F:276:GLY:HA3	1:F:279:TRP:CE2	2.47	0.49
1:G:218:VAL:HG13	1:G:219:GLU:H	1.74	0.49
1:H:46:LYS:O	1:H:47:LEU:HD23	2.12	0.49
1:H:176:ALA:O	1:H:217:GLY:HA3	2.12	0.49
1:I:66:ARG:O	1:I:67:ASP:C	2.50	0.49
1:K:56:LEU:HB2	1:K:86:LEU:CD2	2.42	0.49
1:K:293:ASN:HD22	1:K:322:PHE:H	1.58	0.49
1:L:276:GLY:HA3	1:L:279:TRP:CE2	2.47	0.49
1:G:276:GLY:HA3	1:G:279:TRP:CE2	2.47	0.49
1:I:37:GLU:HB3	1:I:223:GLY:HA3	1.94	0.49
1:I:275:VAL:HG23	1:I:275:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:370:LEU:HD12	1:L:394:HIS:O	2.12	0.49
1:A:56:LEU:HB2	1:A:86:LEU:CD2	2.43	0.49
1:B:346:GLU:HG3	1:H:322:PHE:HE1	1.76	0.49
1:C:370:LEU:HD11	1:C:397:ARG:HB3	1.90	0.49
1:G:184:ASN:ND2	4:G:421:HOH:O	2.45	0.49
1:L:370:LEU:HD13	1:L:397:ARG:CB	2.32	0.49
1:E:120:ARG:HD3	1:E:328:PHE:CE1	2.47	0.49
1:F:350:ASN:H	1:F:350:ASN:ND2	2.11	0.49
1:E:370:LEU:HD13	1:E:397:ARG:CB	2.26	0.49
1:A:87:VAL:HG21	1:A:110:SER:HB3	1.94	0.49
1:K:10:THR:HG22	1:K:381:CYS:O	2.13	0.49
1:K:174:THR:HG21	1:K:198:LEU:HD13	1.94	0.49
1:K:248:LYS:HG3	1:K:283:ASP:CG	2.33	0.49
1:K:364:GLN:HB3	4:K:451:HOH:O	2.12	0.49
1:J:335:VAL:HB	1:J:336:PRO:HD3	1.94	0.49
1:D:334:HIS:H	1:D:334:HIS:CD2	2.31	0.49
1:E:45:PRO:HB2	1:E:47:LEU:HG	1.95	0.49
1:I:2:ASP:OD1	1:I:417:LYS:CD	2.61	0.49
1:B:334:HIS:CD2	1:B:334:HIS:H	2.29	0.49
1:C:276:GLY:HA3	1:C:279:TRP:CE2	2.48	0.49
1:D:299:HIS:ND1	1:D:300:PRO:HA	2.28	0.49
1:F:96:ALA:O	1:F:99:PRO:HD2	2.13	0.49
1:G:334:HIS:CD2	1:G:334:HIS:H	2.29	0.49
1:J:22:LYS:CE	1:J:370:LEU:HD21	2.43	0.49
1:L:256:PRO:C	1:L:258:THR:H	2.16	0.49
1:H:67:ASP:C	1:H:67:ASP:OD1	2.51	0.49
1:K:152:LYS:CD	1:K:177:GLU:OE1	2.61	0.49
1:K:187:ARG:NH2	4:K:452:HOH:O	2.34	0.49
1:B:24:ALA:C	1:B:27:PRO:HD2	2.32	0.48
1:E:36:GLU:HG3	1:E:221:LEU:O	2.13	0.48
1:E:10:THR:HG22	1:E:381:CYS:O	2.13	0.48
1:E:340:ARG:NH1	1:E:364:GLN:O	2.46	0.48
1:G:46:LYS:HA	1:G:66:ARG:NH1	2.27	0.48
1:H:66:ARG:HG3	1:H:67:ASP:O	2.13	0.48
1:A:299:HIS:ND1	1:A:300:PRO:HA	2.28	0.48
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.94	0.48
1:J:150:ARG:HH12	1:J:219:GLU:HA	1.77	0.48
1:L:174:THR:HG21	1:L:198:LEU:HD13	1.95	0.48
1:K:24:ALA:C	1:K:27:PRO:HD2	2.33	0.48
1:A:24:ALA:C	1:A:27:PRO:HD2	2.34	0.48
1:D:109:VAL:O	1:D:143:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:LEU:HB2	1:G:86:LEU:CD2	2.43	0.48
1:L:22:LYS:HE3	1:L:370:LEU:CD2	2.43	0.48
1:L:96:ALA:O	1:L:99:PRO:HD2	2.13	0.48
1:A:45:PRO:HB2	1:A:47:LEU:HG	1.96	0.48
1:C:348:GLU:HG3	1:F:322:PHE:CE2	2.49	0.48
1:D:370:LEU:HD13	1:D:397:ARG:CB	2.26	0.48
1:J:315:LEU:HD22	1:J:343:ALA:HB1	1.96	0.48
1:H:56:LEU:HB2	1:H:86:LEU:CD2	2.43	0.48
1:I:66:ARG:CB	1:I:70:VAL:HG22	2.43	0.48
1:I:81:CYS:HA	1:I:108:GLN:O	2.14	0.48
1:K:204:LYS:CD	1:K:216:GLU:HG2	2.44	0.48
1:K:248:LYS:HE2	1:K:282:LEU:C	2.34	0.48
1:H:3:LYS:CD	4:H:498:HOH:O	2.53	0.48
1:I:63:LYS:HB2	1:I:73:ASP:HB3	1.95	0.48
1:L:109:VAL:O	1:L:143:VAL:HG13	2.14	0.48
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.96	0.48
1:F:370:LEU:HD12	1:F:394:HIS:O	2.13	0.48
1:I:350:ASN:H	1:I:350:ASN:ND2	2.12	0.48
1:J:160:LYS:HE3	3:J:610:EPU:O2U	2.12	0.48
1:L:30:PHE:HE1	1:L:56:LEU:HD23	1.78	0.48
1:L:340:ARG:NH1	1:L:364:GLN:O	2.47	0.48
1:A:150:ARG:HH22	1:A:219:GLU:HA	1.79	0.48
1:A:315:LEU:HD22	1:A:343:ALA:HB1	1.96	0.48
1:C:22:LYS:HE3	1:C:370:LEU:CD2	2.41	0.48
1:B:400:GLU:HG3	4:B:444:HOH:O	2.13	0.47
1:D:46:LYS:NZ	1:D:67:ASP:O	2.33	0.47
1:F:350:ASN:H	1:F:350:ASN:HD22	1.59	0.47
1:E:124:LEU:HB2	3:E:605:EPU:O4U	2.14	0.47
1:E:150:ARG:HH22	1:E:219:GLU:HA	1.78	0.47
1:F:160:LYS:HE3	3:F:606:EPU:O2U	2.14	0.47
1:G:335:VAL:HB	1:G:336:PRO:HD3	1.96	0.47
1:G:370:LEU:HD13	1:G:397:ARG:CB	2.29	0.47
1:I:201:LEU:CB	1:I:221:LEU:HD22	2.43	0.47
1:B:315:LEU:HD22	1:B:343:ALA:HB1	1.96	0.47
1:D:150:ARG:HH12	1:D:219:GLU:HA	1.78	0.47
1:I:36:GLU:O	1:I:75:ARG:HG2	2.14	0.47
1:L:22:LYS:CE	1:L:370:LEU:HD21	2.44	0.47
1:L:396:ASP:OD2	1:L:415:ARG:NH2	2.46	0.47
1:E:30:PHE:HE1	1:E:56:LEU:HD23	1.80	0.47
1:F:155:HIS:HD2	1:F:181:ILE:HB	1.80	0.47
1:F:302:PHE:HA	1:F:303:PRO:HD3	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:22:LYS:HE3	1:J:370:LEU:CD2	2.43	0.47
1:K:22:LYS:HE2	1:K:49:ASP:OD2	2.15	0.47
1:K:334:HIS:H	1:K:334:HIS:CD2	2.31	0.47
1:L:155:HIS:HD2	1:L:181:ILE:HB	1.79	0.47
1:E:24:ALA:C	1:E:27:PRO:HD2	2.34	0.47
1:J:401:ARG:NH2	4:J:438:HOH:O	2.47	0.47
1:L:6:VAL:HG22	1:L:413:ILE:HG13	1.95	0.47
1:B:340:ARG:NH1	1:B:364:GLN:O	2.47	0.47
1:E:22:LYS:CE	1:E:370:LEU:HD21	2.45	0.47
1:E:46:LYS:O	1:E:47:LEU:HD23	2.15	0.47
1:J:334:HIS:H	1:J:334:HIS:CD2	2.32	0.47
1:K:248:LYS:HD2	1:K:283:ASP:C	2.26	0.47
1:L:315:LEU:HD21	1:L:345:ALA:HB2	1.95	0.47
1:L:315:LEU:HD22	1:L:343:ALA:HB1	1.97	0.47
1:B:45:PRO:HB2	1:B:47:LEU:HG	1.97	0.47
1:C:299:HIS:ND1	1:C:300:PRO:HA	2.30	0.47
1:C:350:ASN:HD22	1:C:350:ASN:H	1.63	0.47
1:E:150:ARG:HH12	1:E:219:GLU:HA	1.79	0.47
1:E:334:HIS:CD2	1:E:334:HIS:H	2.31	0.47
1:F:244:ILE:HD12	1:F:382:ILE:HD13	1.96	0.47
1:H:232:ARG:HD3	1:H:258:THR:HG23	1.96	0.47
1:L:302:PHE:HA	1:L:303:PRO:HD3	1.75	0.47
1:C:253:ASN:OD1	4:C:484:HOH:O	2.20	0.47
1:C:256:PRO:C	1:C:258:THR:H	2.18	0.47
1:C:330:ASN:ND2	1:D:330:ASN:ND2	2.63	0.47
1:D:335:VAL:HB	1:D:336:PRO:HD3	1.96	0.47
1:E:204:LYS:HB2	1:E:216:GLU:HB3	1.97	0.47
1:G:41:ILE:O	1:G:69:SER:HB3	2.15	0.47
1:I:248:LYS:C	1:I:249:ILE:HG23	2.35	0.47
1:K:403:GLU:CB	1:K:413:ILE:HD13	2.45	0.47
1:A:256:PRO:C	1:A:258:THR:H	2.17	0.47
1:B:87:VAL:HG21	1:B:110:SER:HB3	1.95	0.47
1:D:159:ASP:OD1	1:F:265:LYS:NZ	2.47	0.47
1:F:81:CYS:HA	1:F:108:GLN:O	2.15	0.47
1:H:65:GLU:OE2	4:H:446:HOH:O	2.20	0.47
1:E:335:VAL:HB	1:E:336:PRO:HD3	1.96	0.47
1:K:232:ARG:HD3	1:K:258:THR:HG23	1.97	0.47
1:G:21:ALA:HA	1:G:231:ASP:HB2	1.97	0.46
1:G:174:THR:HG21	1:G:198:LEU:HD13	1.98	0.46
1:L:21:ALA:HA	1:L:231:ASP:HB2	1.95	0.46
1:B:261:ALA:HA	1:E:157:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:GLN:HG3	1:E:144:LYS:HG2	1.97	0.46
1:E:174:THR:HG21	1:E:198:LEU:HD13	1.98	0.46
1:H:22:LYS:HE2	1:H:49:ASP:OD2	2.15	0.46
1:K:407:ARG:NH1	1:K:413:ILE:O	2.48	0.46
1:L:357:VAL:HG12	1:L:359:LYS:N	2.29	0.46
1:C:204:LYS:HB2	1:C:216:GLU:HB3	1.98	0.46
1:E:315:LEU:HD22	1:E:343:ALA:HB1	1.97	0.46
1:F:56:LEU:HB2	1:F:86:LEU:CD2	2.46	0.46
1:G:258:THR:HG22	1:G:259:LEU:HG	1.97	0.46
1:H:22:LYS:HE3	1:H:370:LEU:CD2	2.45	0.46
1:H:340:ARG:NH2	4:H:453:HOH:O	2.25	0.46
1:I:303:PRO:HA	4:I:643:HOH:O	2.15	0.46
1:B:150:ARG:HH22	1:B:219:GLU:HA	1.79	0.46
1:F:187:ARG:NH1	4:F:454:HOH:O	2.32	0.46
1:J:120:ARG:HD3	1:J:328:PHE:CE1	2.51	0.46
1:B:30:PHE:HE1	1:B:56:LEU:HD23	1.80	0.46
1:D:66:ARG:O	1:D:66:ARG:HG3	2.15	0.46
1:C:56:LEU:HB2	1:C:86:LEU:CD2	2.46	0.46
1:E:56:LEU:HB2	1:E:86:LEU:CD2	2.45	0.46
1:J:106:GLN:HE21	1:J:108:GLN:HE22	1.63	0.46
1:K:386:THR:HB	4:K:436:HOH:O	2.16	0.46
1:B:56:LEU:HB2	1:B:86:LEU:CD2	2.44	0.46
1:C:10:THR:HG22	1:C:381:CYS:O	2.16	0.46
1:C:120:ARG:HD3	1:C:328:PHE:HE1	1.79	0.46
1:G:45:PRO:HB2	1:G:47:LEU:HG	1.97	0.46
1:H:155:HIS:HD2	1:H:181:ILE:HB	1.81	0.46
1:I:201:LEU:O	1:I:221:LEU:HD23	2.16	0.46
1:K:248:LYS:CG	1:K:283:ASP:OD1	2.63	0.46
1:A:10:THR:HG22	1:A:381:CYS:O	2.15	0.46
1:E:315:LEU:HD21	1:E:345:ALA:HB2	1.98	0.46
1:F:174:THR:HG21	1:F:198:LEU:HD13	1.98	0.46
1:H:299:HIS:O	4:H:447:HOH:O	2.21	0.46
1:H:315:LEU:HD22	1:H:343:ALA:HB1	1.97	0.46
1:E:139:GLU:CG	1:E:144:LYS:HD2	2.46	0.46
1:I:402:ILE:N	4:I:436:HOH:O	2.38	0.46
1:A:396:ASP:OD2	1:A:415:ARG:NH2	2.47	0.45
1:G:22:LYS:HE3	1:G:370:LEU:CD2	2.47	0.45
1:K:335:VAL:HB	1:K:336:PRO:HD3	1.98	0.45
1:B:265:LYS:NZ	1:E:159:ASP:OD1	2.50	0.45
1:C:106:GLN:HE21	1:C:108:GLN:HE22	1.64	0.45
1:C:155:HIS:HD2	1:C:181:ILE:HB	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:LYS:HB2	1:F:216:GLU:HB3	1.99	0.45
1:F:370:LEU:HD13	1:F:397:ARG:CB	2.35	0.45
1:G:75:ARG:NH1	4:G:813:HOH:O	2.23	0.45
1:J:285:HIS:N	4:J:444:HOH:O	2.48	0.45
1:B:302:PHE:HA	1:B:303:PRO:HD3	1.75	0.45
1:E:118:GLY:CA	1:E:330:ASN:OD1	2.64	0.45
1:F:150:ARG:HH12	1:F:219:GLU:HA	1.81	0.45
1:G:7:GLN:HB2	1:G:412:ASN:ND2	2.30	0.45
1:H:350:ASN:HD22	1:H:350:ASN:H	1.64	0.45
1:I:45:PRO:HB2	1:I:47:LEU:HG	1.97	0.45
1:J:256:PRO:C	1:J:258:THR:H	2.19	0.45
1:J:302:PHE:HA	1:J:303:PRO:HD3	1.77	0.45
1:L:120:ARG:HD3	1:L:328:PHE:HE1	1.80	0.45
1:A:315:LEU:HD21	1:A:345:ALA:HB2	1.98	0.45
1:C:24:ALA:C	1:C:27:PRO:HD2	2.36	0.45
1:E:276:GLY:HA3	1:E:279:TRP:CE2	2.51	0.45
1:F:10:THR:HG22	1:F:381:CYS:O	2.16	0.45
1:F:24:ALA:C	1:F:27:PRO:HD2	2.37	0.45
1:F:248:LYS:HD3	1:F:283:ASP:OD2	2.17	0.45
1:H:334:HIS:H	1:H:334:HIS:CD2	2.35	0.45
1:I:37:GLU:HG2	1:I:38:PRO:CD	2.35	0.45
1:B:396:ASP:OD2	1:B:415:ARG:NH2	2.50	0.45
1:E:109:VAL:O	1:E:143:VAL:HG13	2.15	0.45
1:F:66:ARG:CB	1:F:70:VAL:HG22	2.45	0.45
1:G:67:ASP:OXT	1:G:67:ASP:OD1	2.34	0.45
1:I:2:ASP:OD1	1:I:417:LYS:HD3	2.17	0.45
1:I:150:ARG:HH12	1:I:219:GLU:HA	1.81	0.45
1:B:320:THR:HG21	1:H:320:THR:HG21	1.98	0.45
1:G:155:HIS:HD2	1:G:181:ILE:HB	1.81	0.45
1:H:325:GLU:CG	1:H:328:PHE:O	2.65	0.45
1:K:66:ARG:NE	1:K:67:ASP:O	2.50	0.45
1:A:330:ASN:HB3	1:B:330:ASN:ND2	2.31	0.45
1:D:21:ALA:HA	1:D:231:ASP:HB2	1.98	0.45
1:D:204:LYS:HB2	1:D:216:GLU:HB3	1.99	0.45
1:F:330:ASN:ND2	1:G:330:ASN:HB3	2.32	0.45
1:L:37:GLU:HA	1:L:38:PRO:HA	1.69	0.45
1:B:220:ARG:HA	4:B:487:HOH:O	2.15	0.45
1:B:232:ARG:HD3	1:B:258:THR:HG23	1.99	0.45
1:B:369:ASP:OD1	1:B:371:ARG:N	2.43	0.45
1:D:390:ASP:O	1:D:391:ARG:CB	2.63	0.45
1:J:252:ARG:O	1:J:253:ASN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:PRO:O	1:L:223:GLY:CA	2.65	0.45
1:E:160:LYS:HE3	3:E:605:EPU:O2U	2.17	0.45
1:H:295:ARG:NE	4:H:451:HOH:O	2.50	0.45
1:I:56:LEU:HB2	1:I:86:LEU:CD2	2.47	0.45
1:I:260:ASP:HB2	4:I:820:HOH:O	2.17	0.45
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.99	0.45
1:H:350:ASN:H	1:H:350:ASN:ND2	2.15	0.45
1:I:219:GLU:O	1:I:219:GLU:CG	2.65	0.45
1:I:275:VAL:O	1:I:275:VAL:CG2	2.65	0.45
1:L:81:CYS:HA	1:L:108:GLN:O	2.17	0.45
1:E:67:ASP:CG	1:E:69:SER:N	2.70	0.44
1:A:150:ARG:HH12	1:A:219:GLU:HA	1.83	0.44
1:J:81:CYS:HA	1:J:108:GLN:O	2.17	0.44
1:J:204:LYS:HB2	1:J:216:GLU:HB3	1.98	0.44
1:J:244:ILE:HD12	1:J:382:ILE:HD13	1.99	0.44
1:K:118:GLY:HA3	4:K:446:HOH:O	2.17	0.44
1:D:276:GLY:HA3	1:D:279:TRP:CE2	2.52	0.44
1:B:248:LYS:HB2	1:B:248:LYS:HE3	1.46	0.44
1:E:256:PRO:C	1:E:258:THR:H	2.21	0.44
1:G:177:GLU:HA	4:G:433:HOH:O	2.17	0.44
1:L:10:THR:HG22	1:L:381:CYS:O	2.18	0.44
1:A:6:VAL:HG22	1:A:413:ILE:HG13	1.98	0.44
1:C:22:LYS:CE	1:C:370:LEU:HD21	2.45	0.44
1:G:349:SER:HB3	1:G:350:ASN:H	1.61	0.44
1:H:6:VAL:HG22	1:H:413:ILE:HG13	1.99	0.44
1:I:24:ALA:C	1:I:27:PRO:HD2	2.37	0.44
1:B:204:LYS:HB2	1:B:216:GLU:HB3	1.99	0.44
1:B:256:PRO:C	1:B:258:THR:H	2.20	0.44
1:C:5:ARG:NH1	4:C:428:HOH:O	2.50	0.44
1:I:256:PRO:C	1:I:258:THR:H	2.20	0.44
1:J:87:VAL:HG21	1:J:110:SER:HB3	2.00	0.44
1:J:150:ARG:HH22	1:J:219:GLU:HA	1.82	0.44
1:K:151:LEU:C	1:K:152:LYS:HG2	2.38	0.44
1:K:155:HIS:HD2	1:K:181:ILE:HB	1.82	0.44
1:L:219:GLU:C	1:L:220:ARG:HG3	2.38	0.44
1:L:391:ARG:HG3	1:L:393:TYR:HE2	1.83	0.44
1:B:22:LYS:HE2	1:B:49:ASP:OD2	2.17	0.44
1:F:46:LYS:O	1:F:47:LEU:HD23	2.18	0.44
1:F:256:PRO:C	1:F:258:THR:H	2.21	0.44
1:I:155:HIS:HD2	1:I:181:ILE:HB	1.82	0.44
1:K:47:LEU:HD21	1:K:400:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ALA:C	1:D:27:PRO:HD2	2.38	0.44
1:L:27:PRO:HG3	1:L:95:TRP:CH2	2.53	0.44
1:A:285:HIS:HB3	1:D:152:LYS:CD	2.47	0.44
1:B:81:CYS:HA	1:B:108:GLN:O	2.18	0.44
1:C:396:ASP:OD2	1:C:415:ARG:NH2	2.49	0.44
1:D:96:ALA:O	1:D:99:PRO:HD2	2.18	0.44
1:E:302:PHE:HA	1:E:303:PRO:HD3	1.73	0.44
1:H:81:CYS:HA	1:H:108:GLN:O	2.18	0.44
1:L:176:ALA:O	1:L:217:GLY:HA3	2.18	0.44
1:L:357:VAL:CG1	1:L:358:GLU:H	2.27	0.44
1:A:155:HIS:HD2	1:A:181:ILE:HB	1.82	0.43
1:A:219:GLU:O	1:A:219:GLU:HG2	2.17	0.43
1:D:85:ASP:HA	1:D:88:LYS:HE2	1.99	0.43
1:G:256:PRO:C	1:G:258:THR:H	2.21	0.43
1:K:256:PRO:C	1:K:258:THR:H	2.20	0.43
1:L:350:ASN:H	1:L:350:ASN:HD22	1.66	0.43
1:B:96:ALA:O	1:B:99:PRO:HD2	2.18	0.43
1:G:66:ARG:C	1:G:67:ASP:O	2.55	0.43
1:H:24:ALA:C	1:H:27:PRO:HD2	2.37	0.43
1:J:10:THR:HG22	1:J:381:CYS:O	2.18	0.43
1:K:302:PHE:HA	1:K:303:PRO:HD3	1.78	0.43
1:L:183:GLU:OE2	1:L:212:ARG:CZ	2.65	0.43
1:L:350:ASN:H	1:L:350:ASN:ND2	2.16	0.43
1:C:350:ASN:H	1:C:350:ASN:ND2	2.15	0.43
1:D:340:ARG:NH1	1:D:364:GLN:O	2.51	0.43
1:F:396:ASP:OD2	1:F:415:ARG:NH2	2.49	0.43
1:I:46:LYS:O	1:I:47:LEU:HD23	2.17	0.43
1:L:371:ARG:NH1	1:L:398:GLY:O	2.51	0.43
1:A:109:VAL:O	1:A:143:VAL:HG13	2.19	0.43
1:A:317:ALA:O	1:A:356:GLY:HA3	2.18	0.43
1:F:334:HIS:CD2	1:F:334:HIS:H	2.36	0.43
1:G:244:ILE:HD12	1:G:382:ILE:HD13	2.00	0.43
1:I:40:GLU:HB3	1:I:225:VAL:HG22	1.99	0.43
1:J:315:LEU:HD21	1:J:345:ALA:HB2	1.99	0.43
1:L:219:GLU:HG2	1:L:220:ARG:HG3	2.00	0.43
1:L:293:ASN:HD22	1:L:322:PHE:H	1.63	0.43
1:A:22:LYS:HB2	1:A:47:LEU:HD12	2.00	0.43
1:D:6:VAL:HG22	1:D:413:ILE:HG13	1.99	0.43
1:E:87:VAL:HG21	1:E:110:SER:HB3	2.00	0.43
1:G:46:LYS:HE2	1:G:67:ASP:OD1	2.18	0.43
1:I:11:LYS:HE2	1:I:248:LYS:CE	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:GLY:O	1:I:249:ILE:HB	2.19	0.43
1:I:91:ARG:HG2	2:I:509:PO3:O1	2.19	0.43
1:I:276:GLY:CA	1:I:279:TRP:CE2	3.01	0.43
1:J:45:PRO:HB2	1:J:47:LEU:HG	2.00	0.43
1:D:9:PRO:HD3	1:D:384:GLU:HA	2.00	0.43
1:D:81:CYS:HA	1:D:108:GLN:O	2.17	0.43
1:G:41:ILE:HG22	1:G:44:VAL:CG2	2.49	0.43
1:H:30:PHE:HE1	1:H:56:LEU:HD23	1.83	0.43
1:H:36:GLU:OE1	1:H:220:ARG:NH2	2.51	0.43
1:I:30:PHE:HE1	1:I:56:LEU:HD23	1.82	0.43
1:H:256:PRO:C	1:H:258:THR:H	2.21	0.43
1:J:174:THR:HG21	1:J:198:LEU:HD13	2.00	0.43
1:J:176:ALA:O	1:J:217:GLY:HA3	2.19	0.43
1:J:396:ASP:OD2	1:J:415:ARG:NH2	2.51	0.43
1:L:232:ARG:HD3	1:L:258:THR:HG23	2.00	0.43
1:C:407:ARG:NH1	4:C:463:HOH:O	2.38	0.43
1:F:6:VAL:HG22	1:F:413:ILE:HG13	2.01	0.43
1:F:27:PRO:HG3	1:F:95:TRP:CH2	2.54	0.43
1:H:335:VAL:HB	1:H:336:PRO:HD3	2.00	0.43
1:J:283:ASP:OD1	1:J:284:MET:N	2.52	0.43
1:K:248:LYS:HZ3	1:K:282:LEU:HD23	1.80	0.43
1:B:350:ASN:ND2	1:B:350:ASN:H	2.16	0.43
1:F:42:GLN:HG2	1:F:69:SER:OG	2.19	0.43
1:G:22:LYS:HE2	1:G:49:ASP:OD2	2.19	0.43
1:G:40:GLU:HB3	1:G:225:VAL:HG22	2.01	0.43
1:G:81:CYS:HA	1:G:108:GLN:O	2.18	0.43
1:K:67:ASP:OD1	1:K:67:ASP:C	2.57	0.43
1:L:124:LEU:HB2	3:L:612:EPU:O4U	2.19	0.43
1:A:30:PHE:HE1	1:A:56:LEU:HD23	1.84	0.43
1:A:276:GLY:HA3	1:A:279:TRP:CE2	2.53	0.43
1:D:315:LEU:HD22	1:D:343:ALA:HB1	2.00	0.43
1:I:120:ARG:HD3	1:I:328:PHE:HE1	1.84	0.43
1:F:315:LEU:HD22	1:F:343:ALA:HB1	1.99	0.42
1:F:391:ARG:NH1	1:F:393:TYR:OH	2.52	0.42
1:J:56:LEU:HB2	1:J:86:LEU:CD2	2.48	0.42
1:K:297:ALA:HB1	1:K:298:PRO:CD	2.49	0.42
1:F:333:MET:HG3	4:F:442:HOH:O	2.18	0.42
1:G:5:ARG:HB3	1:G:414:GLU:HG3	2.00	0.42
1:G:30:PHE:HE1	1:G:56:LEU:HD23	1.84	0.42
1:H:21:ALA:HA	1:H:231:ASP:HB2	2.01	0.42
1:H:232:ARG:CB	1:H:258:THR:CG2	2.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:244:ILE:HD12	1:H:382:ILE:HD13	2.01	0.42
1:I:66:ARG:HB2	1:I:70:VAL:HG22	2.00	0.42
1:K:258:THR:HG21	4:K:442:HOH:O	2.19	0.42
1:K:350:ASN:H	1:K:350:ASN:ND2	2.17	0.42
1:E:81:CYS:HA	1:E:108:GLN:O	2.18	0.42
1:E:244:ILE:HD12	1:E:382:ILE:HD13	2.00	0.42
1:F:232:ARG:CB	1:F:258:THR:CG2	2.93	0.42
1:I:37:GLU:CG	1:I:38:PRO:N	2.82	0.42
1:I:96:ALA:O	1:I:99:PRO:HD2	2.19	0.42
1:I:302:PHE:HA	1:I:303:PRO:HD3	1.80	0.42
1:J:6:VAL:HG22	1:J:413:ILE:HG13	2.01	0.42
1:L:91:ARG:HD2	2:L:512:PO3:O1	2.18	0.42
1:A:232:ARG:CB	1:A:258:THR:CG2	2.94	0.42
1:F:41:ILE:O	1:F:69:SER:HA	2.19	0.42
1:G:87:VAL:HG21	1:G:110:SER:HB3	2.00	0.42
1:G:315:LEU:HD21	1:G:345:ALA:HB2	2.01	0.42
1:K:81:CYS:HA	1:K:108:GLN:O	2.19	0.42
1:D:315:LEU:HD21	1:D:345:ALA:HB2	2.00	0.42
1:K:396:ASP:OD2	1:K:415:ARG:NH2	2.52	0.42
1:B:315:LEU:HD21	1:B:345:ALA:HB2	2.02	0.42
1:B:370:LEU:HD11	1:B:397:ARG:CA	2.45	0.42
1:G:157:VAL:HA	1:G:183:GLU:HB2	2.01	0.42
1:H:338:LEU:HD23	1:H:338:LEU:HA	1.88	0.42
1:J:153:GLY:HA2	1:J:180:THR:OG1	2.19	0.42
1:K:406:LEU:C	1:K:411:ALA:HB3	2.40	0.42
1:A:27:PRO:HG3	1:A:95:TRP:CH2	2.54	0.42
1:A:350:ASN:HD22	1:A:350:ASN:H	1.68	0.42
1:C:366:MET:O	4:C:436:HOH:O	2.22	0.42
1:E:370:LEU:HD11	1:E:397:ARG:CA	2.48	0.42
1:G:106:GLN:HE21	1:G:108:GLN:HE22	1.67	0.42
1:G:176:ALA:O	1:G:217:GLY:HA3	2.18	0.42
1:I:219:GLU:O	1:I:219:GLU:HG2	2.20	0.42
1:I:244:ILE:HD12	1:I:382:ILE:HD13	2.02	0.42
1:I:247:GLY:CA	1:I:248:LYS:HE2	2.46	0.42
1:J:40:GLU:HB3	1:J:225:VAL:HG22	2.01	0.42
1:K:370:LEU:HD11	1:K:397:ARG:HB3	1.91	0.42
1:L:204:LYS:HD3	1:L:216:GLU:HG2	2.00	0.42
1:C:391:ARG:CG	1:C:393:TYR:HE2	2.24	0.42
1:G:11:LYS:HD3	4:G:796:HOH:O	2.16	0.42
1:C:81:CYS:HA	1:C:108:GLN:O	2.20	0.42
1:D:7:GLN:HA	1:D:7:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:PHE:HA	1:G:303:PRO:HD3	1.82	0.42
1:I:153:GLY:HA2	1:I:180:THR:OG1	2.20	0.42
1:I:246:ARG:HH21	1:I:288:ARG:HD2	1.83	0.42
1:K:350:ASN:H	1:K:350:ASN:HD22	1.68	0.42
1:A:174:THR:HG21	1:A:198:LEU:HD13	2.02	0.42
1:C:67:ASP:HB2	1:C:69:SER:O	2.20	0.42
3:F:606:EPU:O4	3:F:606:EPU:C3E	2.67	0.42
1:G:46:LYS:CE	1:G:67:ASP:OD1	2.67	0.42
1:G:135:THR:C	1:G:136:ILE:HG12	2.40	0.42
1:H:248:LYS:HE3	1:H:283:ASP:OD2	2.20	0.42
1:I:315:LEU:HD22	1:I:343:ALA:HB1	2.02	0.42
1:B:350:ASN:H	1:B:350:ASN:HD22	1.68	0.41
1:C:348:GLU:CG	1:F:322:PHE:CE2	3.03	0.41
1:F:267:ARG:NH1	4:F:432:HOH:O	2.51	0.41
1:G:189:PRO:HD3	1:G:299:HIS:CD2	2.54	0.41
1:J:317:ALA:O	1:J:356:GLY:HA3	2.20	0.41
1:K:247:GLY:O	1:K:248:LYS:CG	2.68	0.41
1:D:94:ILE:HD12	1:D:109:VAL:HG11	2.01	0.41
1:I:22:LYS:HB2	1:I:47:LEU:HD12	2.02	0.41
1:I:160:LYS:HE3	3:I:609:EPU:O2U	2.20	0.41
1:K:9:PRO:HD3	1:K:384:GLU:HA	2.03	0.41
1:K:330:ASN:HB3	1:L:330:ASN:ND2	2.35	0.41
1:A:46:LYS:HE2	4:A:436:HOH:O	2.20	0.41
1:E:354:CYS:O	4:E:425:HOH:O	2.22	0.41
1:F:391:ARG:NH1	1:F:393:TYR:CZ	2.87	0.41
1:J:156:ILE:HA	4:J:534:HOH:O	2.20	0.41
1:A:81:CYS:HA	1:A:108:GLN:O	2.19	0.41
1:A:346:GLU:HG3	1:E:322:PHE:CE1	2.53	0.41
1:E:155:HIS:HD2	1:E:181:ILE:HB	1.84	0.41
1:I:106:GLN:HE21	1:I:108:GLN:HE22	1.68	0.41
1:B:318:GLU:OE2	4:B:814:HOH:O	2.21	0.41
1:C:109:VAL:O	1:C:143:VAL:HG13	2.21	0.41
1:D:66:ARG:O	1:D:67:ASP:OXT	2.39	0.41
1:F:109:VAL:O	1:F:143:VAL:HG13	2.20	0.41
1:F:349:SER:HB3	1:F:350:ASN:H	1.71	0.41
1:K:40:GLU:HB3	1:K:225:VAL:HG22	2.02	0.41
1:C:349:SER:HB3	1:C:350:ASN:H	1.66	0.41
1:F:30:PHE:HE1	1:F:56:LEU:HD23	1.86	0.41
1:I:350:ASN:HD22	1:I:350:ASN:N	2.18	0.41
1:J:21:ALA:HA	1:J:231:ASP:HB2	2.02	0.41
1:L:94:ILE:HD12	1:L:109:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:297:ALA:HB1	1:L:298:PRO:CD	2.51	0.41
1:L:369:ASP:HB3	1:L:372:ALA:HB3	2.03	0.41
1:D:232:ARG:HD3	1:D:258:THR:HG23	2.02	0.41
1:E:317:ALA:O	1:E:356:GLY:HA3	2.20	0.41
1:I:349:SER:HB3	1:I:350:ASN:H	1.65	0.41
1:J:109:VAL:O	1:J:143:VAL:HG13	2.20	0.41
1:L:40:GLU:HB3	1:L:225:VAL:HG22	2.03	0.41
1:B:157:VAL:HA	1:B:183:GLU:HB2	2.03	0.41
1:B:370:LEU:HD23	3:B:602:EPU:O2E	2.21	0.41
1:C:176:ALA:O	1:C:217:GLY:HA3	2.21	0.41
1:C:330:ASN:CG	1:D:330:ASN:HD22	2.24	0.41
1:G:100:LEU:HD23	1:G:100:LEU:HA	1.89	0.41
1:G:232:ARG:HD3	1:G:258:THR:HG23	2.03	0.41
1:H:22:LYS:CE	1:H:370:LEU:HD21	2.47	0.41
1:I:401:ARG:N	4:I:436:HOH:O	2.52	0.41
1:J:336:PRO:O	1:J:339:SER:HB2	2.20	0.41
1:A:106:GLN:HE21	1:A:108:GLN:HE22	1.69	0.41
1:A:204:LYS:HB2	1:A:216:GLU:HB3	2.03	0.41
1:B:153:GLY:HA2	1:B:180:THR:OG1	2.21	0.41
1:C:30:PHE:HE1	1:C:56:LEU:HD23	1.85	0.41
1:E:139:GLU:HG2	1:E:144:LYS:HD2	2.03	0.41
1:F:330:ASN:CG	1:G:330:ASN:CG	2.79	0.41
1:G:412:ASN:HA	4:G:426:HOH:O	2.21	0.41
1:H:96:ALA:O	1:H:99:PRO:HD2	2.21	0.41
1:H:370:LEU:CD1	1:H:397:ARG:HB3	2.39	0.41
1:I:150:ARG:HH22	1:I:219:GLU:HA	1.85	0.41
1:J:293:ASN:HD22	1:J:322:PHE:H	1.62	0.41
1:L:201:LEU:HB2	1:L:221:LEU:HD23	2.03	0.41
1:L:357:VAL:HG12	1:L:359:LYS:H	1.85	0.41
1:A:248:LYS:HB2	1:A:248:LYS:HE2	1.78	0.41
1:B:7:GLN:NE2	4:B:449:HOH:O	2.54	0.41
1:D:248:LYS:HE3	1:D:248:LYS:HB2	1.90	0.41
1:D:370:LEU:HD11	1:D:397:ARG:CA	2.49	0.41
1:F:315:LEU:HD21	1:F:345:ALA:HB2	2.03	0.41
1:H:189:PRO:HD3	1:H:299:HIS:CD2	2.56	0.41
1:I:157:VAL:HA	1:I:183:GLU:HB2	2.03	0.41
1:J:155:HIS:HD2	1:J:181:ILE:HB	1.85	0.41
1:J:325:GLU:CG	1:J:328:PHE:O	2.67	0.41
1:K:297:ALA:HB1	1:K:298:PRO:HD2	2.03	0.41
1:K:330:ASN:ND2	1:L:330:ASN:HB3	2.36	0.41
1:L:9:PRO:HD3	1:L:384:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:612:EPU:O2A	3:L:612:EPU:O1B	2.37	0.41
1:J:30:PHE:HE1	1:J:56:LEU:HD23	1.86	0.40
1:D:27:PRO:HG3	1:D:95:TRP:CH2	2.56	0.40
1:D:30:PHE:HE1	1:D:56:LEU:HD23	1.86	0.40
1:D:106:GLN:HE21	1:D:108:GLN:HE22	1.69	0.40
1:E:96:ALA:O	1:E:99:PRO:HD2	2.20	0.40
1:H:174:THR:HG21	1:H:198:LEU:HD13	2.04	0.40
1:K:247:GLY:O	1:K:248:LYS:CD	2.69	0.40
1:K:315:LEU:HD21	1:K:345:ALA:HB2	2.03	0.40
1:L:30:PHE:CE1	1:L:56:LEU:HD23	2.56	0.40
1:A:51:ASP:OD1	4:A:434:HOH:O	2.22	0.40
1:B:21:ALA:HA	1:B:231:ASP:HB2	2.02	0.40
1:B:252:ARG:O	1:B:253:ASN:HB2	2.21	0.40
1:E:40:GLU:HB3	1:E:225:VAL:HG22	2.03	0.40
1:E:403:GLU:OE2	1:J:277:GLU:OE2	2.39	0.40
1:F:100:LEU:HD23	1:F:100:LEU:HA	1.93	0.40
1:I:174:THR:HG21	1:I:198:LEU:HD13	2.03	0.40
1:L:157:VAL:HA	1:L:183:GLU:HB2	2.04	0.40
1:B:106:GLN:HE21	1:B:108:GLN:HE22	1.69	0.40
1:B:349:SER:HB3	1:B:350:ASN:H	1.70	0.40
1:D:22:LYS:HE2	1:D:49:ASP:OD2	2.22	0.40
1:F:9:PRO:HD3	1:F:384:GLU:HA	2.02	0.40
1:J:46:LYS:HZ1	1:J:67:ASP:HB3	1.87	0.40
1:J:277:GLU:CG	4:J:783:HOH:O	2.70	0.40
1:J:391:ARG:CG	1:J:393:TYR:CE2	3.04	0.40
1:B:120:ARG:HD3	1:B:328:PHE:HE1	1.83	0.40
1:C:302:PHE:HA	1:C:303:PRO:HD3	1.73	0.40
1:C:350:ASN:HD22	1:C:350:ASN:N	2.19	0.40
1:D:41:ILE:HG22	1:D:44:VAL:CG2	2.51	0.40
1:E:47:LEU:HD23	1:E:47:LEU:HA	1.81	0.40
1:E:407:ARG:NH1	1:E:413:ILE:O	2.54	0.40
1:K:248:LYS:HD2	1:K:284:MET:N	2.35	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	414/418 (99%)	403 (97%)	10 (2%)	1 (0%)	47	68
1	B	414/418 (99%)	404 (98%)	10 (2%)	0	100	100
1	C	414/418 (99%)	401 (97%)	13 (3%)	0	100	100
1	D	414/418 (99%)	404 (98%)	9 (2%)	1 (0%)	47	68
1	E	414/418 (99%)	403 (97%)	11 (3%)	0	100	100
1	F	414/418 (99%)	404 (98%)	10 (2%)	0	100	100
1	G	414/418 (99%)	402 (97%)	12 (3%)	0	100	100
1	H	414/418 (99%)	403 (97%)	10 (2%)	1 (0%)	47	68
1	I	414/418 (99%)	399 (96%)	13 (3%)	2 (0%)	29	48
1	J	414/418 (99%)	404 (98%)	9 (2%)	1 (0%)	47	68
1	K	414/418 (99%)	403 (97%)	11 (3%)	0	100	100
1	L	414/418 (99%)	400 (97%)	12 (3%)	2 (0%)	29	48
All	All	4968/5016 (99%)	4830 (97%)	130 (3%)	8 (0%)	47	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	37	GLU
1	L	38	PRO
1	A	370	LEU
1	H	370	LEU
1	I	38	PRO
1	J	370	LEU
1	D	370	LEU
1	I	39	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	312 (94%)	19 (6%)	20	39
1	B	331/331 (100%)	309 (93%)	22 (7%)	16	32
1	C	331/331 (100%)	309 (93%)	22 (7%)	16	32
1	D	331/331 (100%)	315 (95%)	16 (5%)	25	48
1	E	331/331 (100%)	307 (93%)	24 (7%)	14	27
1	F	331/331 (100%)	309 (93%)	22 (7%)	16	32
1	G	331/331 (100%)	310 (94%)	21 (6%)	18	34
1	H	331/331 (100%)	311 (94%)	20 (6%)	19	37
1	I	331/331 (100%)	303 (92%)	28 (8%)	10	21
1	J	331/331 (100%)	309 (93%)	22 (7%)	16	32
1	K	331/331 (100%)	312 (94%)	19 (6%)	20	39
1	L	331/331 (100%)	311 (94%)	20 (6%)	19	37
All	All	3972/3972 (100%)	3717 (94%)	255 (6%)	17	33

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	55	LYS
1	A	63	LYS
1	A	86	LEU
1	A	131	GLN
1	A	143	VAL
1	A	150	ARG
1	A	158	MET
1	A	159	ASP
1	A	193	ASP
1	A	248	LYS
1	A	258	THR
1	A	307	GLN
1	A	346	GLU
1	A	349	SER
1	A	350	ASN
1	A	358	GLU
1	A	370	LEU
1	A	416	VAL
1	B	7	GLN
1	B	10	THR
1	B	55	LYS

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Mol	Chain	Res	Type
1	B	69	SER
1	B	86	LEU
1	B	131	GLN
1	B	143	VAL
1	B	150	ARG
1	B	158	MET
1	B	159	ASP
1	B	193	ASP
1	B	248	LYS
1	B	258	THR
1	B	265	LYS
1	B	307	GLN
1	B	346	GLU
1	B	349	SER
1	B	350	ASN
1	B	358	GLU
1	B	361	SER
1	B	413	ILE
1	B	416	VAL
1	C	7	GLN
1	C	39	VAL
1	C	48	LYS
1	C	55	LYS
1	C	65	GLU
1	C	66	ARG
1	C	86	LEU
1	C	131	GLN
1	C	137	LYS
1	C	140	GLU
1	C	143	VAL
1	C	158	MET
1	C	159	ASP
1	C	193	ASP
1	C	258	THR
1	C	307	GLN
1	C	346	GLU
1	C	349	SER
1	C	350	ASN
1	C	358	GLU
1	C	361	SER
1	C	416	VAL
1	D	7	GLN

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Mol	Chain	Res	Type
1	D	48	LYS
1	D	55	LYS
1	D	131	GLN
1	D	143	VAL
1	D	150	ARG
1	D	158	MET
1	D	159	ASP
1	D	258	THR
1	D	307	GLN
1	D	346	GLU
1	D	349	SER
1	D	350	ASN
1	D	358	GLU
1	D	391	ARG
1	D	416	VAL
1	E	7	GLN
1	E	38	PRO
1	E	39	VAL
1	E	55	LYS
1	E	63	LYS
1	E	69	SER
1	E	86	LEU
1	E	131	GLN
1	E	143	VAL
1	E	150	ARG
1	E	158	MET
1	E	159	ASP
1	E	193	ASP
1	E	212	ARG
1	E	258	THR
1	E	307	GLN
1	E	330	ASN
1	E	333	MET
1	E	346	GLU
1	E	349	SER
1	E	350	ASN
1	E	358	GLU
1	E	361	SER
1	E	416	VAL
1	F	7	GLN
1	F	38	PRO
1	F	55	LYS

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Mol	Chain	Res	Type
1	F	67	ASP
1	F	86	LEU
1	F	131	GLN
1	F	143	VAL
1	F	150	ARG
1	F	158	MET
1	F	159	ASP
1	F	183	GLU
1	F	258	THR
1	F	265	LYS
1	F	295	ARG
1	F	307	GLN
1	F	326	THR
1	F	346	GLU
1	F	349	SER
1	F	350	ASN
1	F	358	GLU
1	F	361	SER
1	F	416	VAL
1	G	7	GLN
1	G	38	PRO
1	G	55	LYS
1	G	66	ARG
1	G	86	LEU
1	G	131	GLN
1	G	136	ILE
1	G	143	VAL
1	G	150	ARG
1	G	158	MET
1	G	159	ASP
1	G	193	ASP
1	G	216	GLU
1	G	219	GLU
1	G	258	THR
1	G	307	GLN
1	G	346	GLU
1	G	349	SER
1	G	350	ASN
1	G	361	SER
1	G	416	VAL
1	H	7	GLN
1	H	10	THR

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Mol	Chain	Res	Type
1	H	38	PRO
1	H	46	LYS
1	H	66	ARG
1	H	86	LEU
1	H	131	GLN
1	H	143	VAL
1	H	150	ARG
1	H	158	MET
1	H	159	ASP
1	H	248	LYS
1	H	258	THR
1	H	307	GLN
1	H	346	GLU
1	H	349	SER
1	H	350	ASN
1	H	358	GLU
1	H	361	SER
1	H	416	VAL
1	I	7	GLN
1	I	36	GLU
1	I	38	PRO
1	I	55	LYS
1	I	65	GLU
1	I	66	ARG
1	I	67	ASP
1	I	69	SER
1	I	86	LEU
1	I	131	GLN
1	I	143	VAL
1	I	150	ARG
1	I	158	MET
1	I	159	ASP
1	I	193	ASP
1	I	220	ARG
1	I	221	LEU
1	I	248	LYS
1	I	249	ILE
1	I	258	THR
1	I	274	GLU
1	I	307	GLN
1	I	346	GLU
1	I	349	SER

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Mol	Chain	Res	Type
1	I	350	ASN
1	I	358	GLU
1	I	361	SER
1	I	416	VAL
1	J	7	GLN
1	J	55	LYS
1	J	63	LYS
1	J	65	GLU
1	J	66	ARG
1	J	67	ASP
1	J	69	SER
1	J	86	LEU
1	J	131	GLN
1	J	143	VAL
1	J	150	ARG
1	J	158	MET
1	J	159	ASP
1	J	193	ASP
1	J	258	THR
1	J	307	GLN
1	J	346	GLU
1	J	349	SER
1	J	350	ASN
1	J	358	GLU
1	J	361	SER
1	J	416	VAL
1	K	7	GLN
1	K	55	LYS
1	K	86	LEU
1	K	131	GLN
1	K	143	VAL
1	K	150	ARG
1	K	158	MET
1	K	159	ASP
1	K	216	GLU
1	K	248	LYS
1	K	258	THR
1	K	307	GLN
1	K	346	GLU
1	K	349	SER
1	K	350	ASN
1	K	358	GLU

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Mol	Chain	Res	Type
1	K	361	SER
1	K	413	ILE
1	K	416	VAL
1	L	7	GLN
1	L	37	GLU
1	L	65	GLU
1	L	66	ARG
1	L	67	ASP
1	L	86	LEU
1	L	131	GLN
1	L	143	VAL
1	L	150	ARG
1	L	158	MET
1	L	159	ASP
1	L	221	LEU
1	L	248	LYS
1	L	258	THR
1	L	307	GLN
1	L	346	GLU
1	L	349	SER
1	L	350	ASN
1	L	361	SER
1	L	416	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	42	GLN
1	A	59	GLN
1	A	106	GLN
1	A	155	HIS
1	A	184	ASN
1	A	293	ASN
1	A	334	HIS
1	A	344	HIS
1	A	350	ASN
1	B	7	GLN
1	B	42	GLN
1	B	59	GLN
1	B	106	GLN
1	B	184	ASN

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Mol	Chain	Res	Type
1	B	293	ASN
1	B	334	HIS
1	B	344	HIS
1	B	350	ASN
1	C	7	GLN
1	C	42	GLN
1	C	59	GLN
1	C	106	GLN
1	C	155	HIS
1	C	184	ASN
1	C	293	ASN
1	C	330	ASN
1	C	334	HIS
1	C	344	HIS
1	C	350	ASN
1	D	7	GLN
1	D	42	GLN
1	D	59	GLN
1	D	71	HIS
1	D	106	GLN
1	D	155	HIS
1	D	184	ASN
1	D	293	ASN
1	D	330	ASN
1	D	334	HIS
1	D	350	ASN
1	E	42	GLN
1	E	59	GLN
1	E	106	GLN
1	E	184	ASN
1	E	293	ASN
1	E	330	ASN
1	E	334	HIS
1	E	344	HIS
1	E	350	ASN
1	F	7	GLN
1	F	42	GLN
1	F	59	GLN
1	F	71	HIS
1	F	106	GLN
1	F	184	ASN
1	F	293	ASN

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Mol	Chain	Res	Type
1	F	334	HIS
1	F	344	HIS
1	F	350	ASN
1	G	7	GLN
1	G	42	GLN
1	G	59	GLN
1	G	106	GLN
1	G	155	HIS
1	G	184	ASN
1	G	293	ASN
1	G	334	HIS
1	G	344	HIS
1	G	350	ASN
1	H	7	GLN
1	H	59	GLN
1	H	106	GLN
1	H	155	HIS
1	H	184	ASN
1	H	293	ASN
1	H	334	HIS
1	H	350	ASN
1	I	7	GLN
1	I	42	GLN
1	I	59	GLN
1	I	106	GLN
1	I	155	HIS
1	I	184	ASN
1	I	293	ASN
1	I	334	HIS
1	I	344	HIS
1	I	350	ASN
1	J	7	GLN
1	J	42	GLN
1	J	59	GLN
1	J	106	GLN
1	J	184	ASN
1	J	293	ASN
1	J	334	HIS
1	J	344	HIS
1	J	350	ASN
1	K	7	GLN
1	K	42	GLN

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Mol	Chain	Res	Type
1	K	59	GLN
1	K	106	GLN
1	K	184	ASN
1	K	293	ASN
1	K	334	HIS
1	K	344	HIS
1	K	350	ASN
1	K	364	GLN
1	L	7	GLN
1	L	42	GLN
1	L	59	GLN
1	L	106	GLN
1	L	155	HIS
1	L	184	ASN
1	L	293	ASN
1	L	334	HIS
1	L	350	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	EPU	A	601	-	36,46,46	2.35	11 (30%)	45,69,69	1.87	8 (17%)
3	EPU	G	607	-	36,46,46	2.16	7 (19%)	45,69,69	1.95	9 (20%)
2	PO3	C	502	-	0,3,3	-	-	0,3,3	-	-
3	EPU	F	606	-	36,46,46	2.29	13 (36%)	45,69,69	1.76	8 (17%)
3	EPU	E	605	-	36,46,46	2.30	8 (22%)	45,69,69	1.79	12 (26%)
3	EPU	B	602	-	36,46,46	2.22	6 (16%)	45,69,69	1.85	9 (20%)
2	PO3	J	510	-	0,3,3	-	-	0,3,3	-	-
2	PO3	D	503	-	0,3,3	-	-	0,3,3	-	-
2	PO3	F	506	-	0,3,3	-	-	0,3,3	-	-
2	PO3	B	502	-	0,3,3	-	-	0,3,3	-	-
3	EPU	L	612	-	36,46,46	2.24	9 (25%)	45,69,69	2.02	9 (20%)
2	PO3	H	508	-	0,3,3	-	-	0,3,3	-	-
3	EPU	J	610	-	36,46,46	2.33	9 (25%)	45,69,69	2.15	12 (26%)
3	EPU	K	611	-	36,46,46	2.27	7 (19%)	45,69,69	1.81	9 (20%)
3	EPU	C	603	-	36,46,46	2.31	11 (30%)	45,69,69	1.96	8 (17%)
3	EPU	I	609	-	36,46,46	2.40	11 (30%)	45,69,69	1.98	8 (17%)
3	EPU	H	608	-	36,46,46	2.12	9 (25%)	45,69,69	1.92	7 (15%)
2	PO3	E	504	-	0,3,3	-	-	0,3,3	-	-
3	EPU	D	604	-	36,46,46	2.22	10 (27%)	45,69,69	2.26	11 (24%)
2	PO3	A	501	-	0,3,3	-	-	0,3,3	-	-
2	PO3	I	509	-	0,3,3	-	-	0,3,3	-	-
2	PO3	G	507	-	0,3,3	-	-	0,3,3	-	-
2	PO3	K	511	-	0,3,3	-	-	0,3,3	-	-
2	PO3	L	512	-	0,3,3	-	-	0,3,3	-	-

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	EPU	A	601	-	-	6/26/71/71	0/3/3/3
3	EPU	E	605	-	-	7/26/71/71	0/3/3/3
3	EPU	G	607	-	-	6/26/71/71	0/3/3/3
3	EPU	K	611	-	-	5/26/71/71	0/3/3/3
3	EPU	C	603	-	-	5/26/71/71	0/3/3/3
3	EPU	I	609	-	-	7/26/71/71	0/3/3/3
3	EPU	B	602	-	-	5/26/71/71	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPU	H	608	-	-	6/26/71/71	0/3/3/3
3	EPU	D	604	-	-	6/26/71/71	0/3/3/3
3	EPU	L	612	-	-	10/26/71/71	0/3/3/3
3	EPU	F	606	-	-	7/26/71/71	0/3/3/3
3	EPU	J	610	-	-	8/26/71/71	0/3/3/3

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	611	EPU	C3E-C2E	9.77	1.52	1.33
3	E	605	EPU	C3E-C2E	9.77	1.52	1.33
3	J	610	EPU	C3E-C2E	9.65	1.51	1.33
3	B	602	EPU	C3E-C2E	9.59	1.51	1.33
3	I	609	EPU	C3E-C2E	9.54	1.51	1.33
3	A	601	EPU	C3E-C2E	9.53	1.51	1.33
3	L	612	EPU	C3E-C2E	9.50	1.51	1.33
3	G	607	EPU	C3E-C2E	9.31	1.51	1.33
3	D	604	EPU	C3E-C2E	9.24	1.51	1.33
3	C	603	EPU	C3E-C2E	8.77	1.50	1.33
3	H	608	EPU	C3E-C2E	8.76	1.50	1.33
3	F	606	EPU	C3E-C2E	8.52	1.49	1.33
3	C	603	EPU	O3-C3	-4.42	1.38	1.44
3	F	606	EPU	O3-C3	-4.26	1.38	1.44
3	B	602	EPU	O3-C3	-4.22	1.38	1.44
3	A	601	EPU	C6U-N1U	-4.09	1.30	1.35
3	I	609	EPU	C6U-N1U	-4.00	1.30	1.35
3	B	602	EPU	C6U-N1U	-3.99	1.30	1.35
3	K	611	EPU	C6U-N1U	-3.98	1.30	1.35
3	J	610	EPU	C6U-N1U	-3.82	1.31	1.35
3	I	609	EPU	O3-C3	-3.67	1.39	1.44
3	C	603	EPU	C6U-N1U	-3.63	1.31	1.35
3	F	606	EPU	C6U-N1U	-3.60	1.31	1.35
3	H	608	EPU	C6U-N1U	-3.53	1.31	1.35
3	E	605	EPU	O3-C3	-3.51	1.39	1.44
3	L	612	EPU	C6U-N1U	-3.49	1.31	1.35
3	I	609	EPU	PB-O1	-3.45	1.51	1.60
3	E	605	EPU	C6U-N1U	-3.40	1.31	1.35
3	D	604	EPU	O3-C3	-3.25	1.39	1.44
3	A	601	EPU	O3-C3	-3.24	1.39	1.44
3	L	612	EPU	C3-C2	-3.23	1.47	1.53
3	G	607	EPU	C6U-N1U	-3.23	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	610	EPU	O3-C3	-3.22	1.40	1.44
3	H	608	EPU	C2U-N3U	-3.21	1.31	1.38
3	F	606	EPU	C2D-C1D	-3.12	1.49	1.53
3	L	612	EPU	O3-C3	-3.09	1.40	1.44
3	D	604	EPU	C6U-N1U	-3.04	1.32	1.35
3	K	611	EPU	O3-C3	-3.02	1.40	1.44
3	A	601	EPU	PB-O1	-2.99	1.52	1.60
3	D	604	EPU	C2U-N3U	-2.95	1.32	1.38
3	E	605	EPU	C2U-N3U	-2.93	1.32	1.38
3	I	609	EPU	C2U-N3U	-2.89	1.32	1.38
3	J	610	EPU	C3-C2	-2.88	1.48	1.53
3	F	606	EPU	PB-O2B	-2.84	1.42	1.55
3	C	603	EPU	C2U-N3U	-2.84	1.32	1.38
3	J	610	EPU	C2U-N3U	-2.73	1.32	1.38
3	A	601	EPU	C2U-N3U	-2.73	1.32	1.38
3	G	607	EPU	C2U-N3U	-2.72	1.32	1.38
3	J	610	EPU	C2D-C1D	-2.71	1.49	1.53
3	I	609	EPU	PA-O2A	-2.61	1.43	1.55
3	D	604	EPU	PB-O2B	-2.59	1.43	1.55
3	L	612	EPU	C2U-N3U	-2.59	1.33	1.38
3	H	608	EPU	O3-C3	-2.57	1.40	1.44
3	F	606	EPU	C2U-N3U	-2.54	1.33	1.38
3	H	608	EPU	C2D-C1D	-2.51	1.50	1.53
3	D	604	EPU	O5-C5	-2.51	1.38	1.44
3	K	611	EPU	C3-C2	-2.49	1.48	1.53
3	H	608	EPU	PB-O2B	-2.47	1.43	1.55
3	F	606	EPU	O4D-C4D	-2.47	1.39	1.45
3	D	604	EPU	PA-O2A	-2.44	1.43	1.55
3	C	603	EPU	PB-O2B	-2.44	1.43	1.55
3	F	606	EPU	C1-C2	-2.42	1.49	1.53
3	F	606	EPU	PB-O1	-2.39	1.54	1.60
3	A	601	EPU	PA-O2A	-2.37	1.44	1.55
3	E	605	EPU	C2D-C1D	-2.36	1.50	1.53
3	L	612	EPU	C2D-C1D	-2.34	1.50	1.53
3	A	601	EPU	PB-O2B	-2.34	1.44	1.55
3	H	608	EPU	PB-O1	-2.29	1.54	1.60
3	I	609	EPU	PB-O2B	-2.29	1.44	1.55
3	G	607	EPU	PB-O2B	-2.29	1.44	1.55
3	A	601	EPU	C2D-C1D	-2.28	1.50	1.53
3	E	605	EPU	PA-O2A	-2.28	1.44	1.55
3	F	606	EPU	PA-O2A	-2.28	1.44	1.55
3	C	603	EPU	PA-O2A	-2.28	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	EPU	C3-C2	-2.27	1.49	1.53
3	I	609	EPU	C2D-C1D	-2.27	1.50	1.53
3	C	603	EPU	C2D-C1D	-2.26	1.50	1.53
3	E	605	EPU	C3D-C2D	-2.26	1.47	1.53
3	D	604	EPU	PA-O1A	-2.26	1.42	1.50
3	J	610	EPU	C1-C2	-2.24	1.49	1.53
3	F	606	EPU	PB-O1B	-2.22	1.43	1.50
3	C	603	EPU	O7-C7	-2.22	1.18	1.23
3	A	601	EPU	PA-O1A	-2.21	1.43	1.50
3	K	611	EPU	PA-O2A	-2.20	1.45	1.55
3	I	609	EPU	C3-C2	-2.20	1.49	1.53
3	I	609	EPU	O4D-C4D	-2.19	1.40	1.45
3	L	612	EPU	C3D-C2D	-2.18	1.47	1.53
3	G	607	EPU	C2D-C1D	-2.17	1.50	1.53
3	K	611	EPU	PB-O2B	-2.16	1.45	1.55
3	D	604	EPU	O7-C7	-2.15	1.18	1.23
3	J	610	EPU	C2-N2	-2.14	1.42	1.45
3	B	602	EPU	C2D-C1D	-2.14	1.50	1.53
3	F	606	EPU	C4-C5	-2.14	1.48	1.53
3	F	606	EPU	O7-C7	-2.13	1.18	1.23
3	D	604	EPU	C2D-C1D	-2.13	1.50	1.53
3	C	603	EPU	C4-C5	-2.13	1.48	1.53
3	E	605	EPU	C1-C2	-2.11	1.49	1.53
3	A	601	EPU	O4D-C4D	-2.09	1.40	1.45
3	L	612	EPU	PA-O2A	-2.08	1.45	1.55
3	J	610	EPU	O5-C5	-2.08	1.39	1.44
3	H	608	EPU	PB-O1B	-2.08	1.43	1.50
3	H	608	EPU	PA-O2A	-2.07	1.45	1.55
3	I	609	EPU	O7-C7	-2.06	1.18	1.23
3	K	611	EPU	PB-O1B	-2.06	1.43	1.50
3	L	612	EPU	O4D-C4D	-2.05	1.40	1.45
3	B	602	EPU	PA-O2A	-2.05	1.45	1.55
3	G	607	EPU	PA-O2A	-2.04	1.45	1.55
3	G	607	EPU	PB-O1	-2.04	1.55	1.60
3	C	603	EPU	PB-O1	-2.02	1.55	1.60
3	A	601	EPU	O7-C7	-2.01	1.18	1.23
3	B	602	EPU	PB-O2B	-2.01	1.45	1.55

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	608	EPU	C1E-C2E-C3E	-8.98	104.31	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	607	EPU	C1E-C2E-C3E	-8.63	104.96	121.07
3	D	604	EPU	C1E-C2E-C3E	-8.13	105.90	121.07
3	B	602	EPU	C1E-C2E-C3E	-7.74	106.63	121.07
3	L	612	EPU	C1E-C2E-C3E	-7.31	107.42	121.07
3	J	610	EPU	C1E-C2E-C3E	-7.18	107.67	121.07
3	C	603	EPU	C3-C2-N2	-6.68	99.82	110.91
3	D	604	EPU	O5-C1-O1	-6.45	102.94	111.36
3	K	611	EPU	C1E-C2E-C3E	-6.37	109.18	121.07
3	I	609	EPU	O5-C1-O1	-6.31	103.12	111.36
3	F	606	EPU	C1E-C2E-C3E	-6.29	109.34	121.07
3	E	605	EPU	C1E-C2E-C3E	-6.19	109.52	121.07
3	C	603	EPU	C1E-C2E-C3E	-5.68	110.47	121.07
3	J	610	EPU	O5-C1-O1	-5.52	104.15	111.36
3	A	601	EPU	C3-C2-N2	-5.50	101.78	110.91
3	I	609	EPU	C3-C2-N2	-5.38	101.98	110.91
3	A	601	EPU	C1E-C2E-C3E	-5.32	111.13	121.07
3	J	610	EPU	C3-C2-N2	-5.24	102.21	110.91
3	I	609	EPU	C1E-C2E-C3E	-5.16	111.44	121.07
3	A	601	EPU	O5-C1-O1	-4.95	104.90	111.36
3	K	611	EPU	O5-C1-O1	-4.82	105.07	111.36
3	L	612	EPU	C3-C2-N2	-4.69	103.13	110.91
3	L	612	EPU	PB-O3A-PA	-4.43	117.61	132.83
3	F	606	EPU	C3-C2-N2	-4.30	103.77	110.91
3	G	607	EPU	C3-C2-N2	-4.25	103.85	110.91
3	K	611	EPU	C3-C2-N2	-4.22	103.90	110.91
3	D	604	EPU	C1-O5-C5	-4.05	105.74	113.69
3	L	612	EPU	O5-C1-O1	-4.02	106.11	111.36
3	D	604	EPU	O5-C1-C2	-3.97	102.82	110.58
3	E	605	EPU	C3-C2-N2	-3.71	104.75	110.91
3	D	604	EPU	C3-C2-N2	-3.58	104.96	110.91
3	B	602	EPU	C3D-C2D-C1D	3.52	106.27	100.98
3	L	612	EPU	O3D-C3D-C2D	-3.43	100.74	111.82
3	D	604	EPU	C3-C4-C5	-3.35	102.53	109.66
3	I	609	EPU	C6-C5-C4	-3.28	105.33	113.00
3	D	604	EPU	C1-C2-N2	3.24	116.58	111.00
3	F	606	EPU	O5-C1-C2	-3.22	104.28	110.58
3	A	601	EPU	C6-C5-C4	-3.19	105.53	113.00
3	J	610	EPU	O4D-C1D-C2D	-3.18	102.28	106.93
3	E	605	EPU	O5-C1-C2	-3.15	104.43	110.58
3	J	610	EPU	O3D-C3D-C4D	-3.03	102.29	111.05
3	H	608	EPU	C3-C2-N2	-3.03	105.88	110.91
3	G	607	EPU	C3D-C2D-C1D	3.00	105.49	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	609	EPU	O6-C6-C5	-2.98	101.07	111.29
3	C	603	EPU	C3D-C2D-C1D	2.96	105.43	100.98
3	H	608	EPU	O3-C3-C2	2.91	113.36	107.91
3	C	603	EPU	C8-C7-N2	2.91	121.02	116.10
3	K	611	EPU	C3D-C2D-C1D	2.88	105.32	100.98
3	C	603	EPU	C2-N2-C7	-2.82	116.33	123.18
3	J	610	EPU	PB-O3A-PA	-2.81	123.19	132.83
3	H	608	EPU	C3D-C2D-C1D	2.77	105.15	100.98
3	C	603	EPU	O5-C1-C2	-2.74	105.23	110.58
3	J	610	EPU	C6-C5-C4	-2.73	106.60	113.00
3	K	611	EPU	O5-C1-C2	-2.71	105.28	110.58
3	E	605	EPU	O3D-C3D-C2D	-2.71	103.06	111.82
3	G	607	EPU	O5-C1-O1	-2.71	107.83	111.36
3	J	610	EPU	O6-C6-C5	-2.70	102.03	111.29
3	F	606	EPU	O5-C1-O1	-2.67	107.88	111.36
3	B	602	EPU	C3-C2-N2	-2.63	106.54	110.91
3	L	612	EPU	C6-C5-C4	-2.63	106.85	113.00
3	J	610	EPU	C2-N2-C7	-2.57	116.94	123.18
3	L	612	EPU	C1-C2-N2	-2.54	106.63	111.00
3	K	611	EPU	O2A-PA-O1A	2.54	124.79	112.24
3	H	608	EPU	C1-C2-N2	-2.53	106.65	111.00
3	C	603	EPU	O4-C4-C3	-2.52	103.26	109.94
3	E	605	EPU	O2B-PB-O1B	2.48	124.48	112.24
3	G	607	EPU	O3-C3-C2	2.47	112.53	107.91
3	A	601	EPU	O6-C6-C5	-2.47	102.82	111.29
3	F	606	EPU	C3D-C2D-C1D	2.45	104.67	100.98
3	F	606	EPU	C1-C2-C3	-2.43	105.42	109.88
3	D	604	EPU	C3D-C2D-C1D	2.42	104.62	100.98
3	E	605	EPU	O2D-C2D-C3D	-2.42	104.01	111.82
3	A	601	EPU	C3D-C2D-C1D	2.40	104.59	100.98
3	L	612	EPU	O3A-PB-O1	2.36	107.24	102.48
3	E	605	EPU	C2-N2-C7	-2.32	117.53	123.18
3	E	605	EPU	O2A-PA-O1A	2.31	123.64	112.24
3	B	602	EPU	C2-N2-C7	-2.29	117.61	123.18
3	F	606	EPU	O3D-C3D-C2D	-2.29	104.42	111.82
3	K	611	EPU	C5U-C4U-N3U	-2.27	118.32	123.31
3	F	606	EPU	C2D-C3D-C4D	2.26	107.04	102.64
3	G	607	EPU	C1-C2-N2	-2.23	107.16	111.00
3	G	607	EPU	O3A-PB-O1	-2.23	97.98	102.48
3	J	610	EPU	O5D-PA-O1A	-2.23	100.34	109.07
3	D	604	EPU	O2D-C2D-C3D	-2.21	104.68	111.82
3	H	608	EPU	O5-C1-C2	-2.20	106.29	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	611	EPU	C2-N2-C7	-2.19	117.85	123.18
3	B	602	EPU	PB-O3A-PA	-2.18	125.34	132.83
3	I	609	EPU	O3D-C3D-C2D	-2.18	104.77	111.82
3	B	602	EPU	O2A-PA-O1A	2.17	122.98	112.24
3	G	607	EPU	O2B-PB-O1B	2.16	122.92	112.24
3	E	605	EPU	O3A-PB-O1	-2.16	98.13	102.48
3	I	609	EPU	C2-N2-C7	-2.15	117.95	123.18
3	B	602	EPU	O3D-C3D-C2D	-2.15	104.87	111.82
3	B	602	EPU	O5-C1-O1	-2.14	108.57	111.36
3	D	604	EPU	O6-C6-C5	-2.13	103.97	111.29
3	A	601	EPU	C2-N2-C7	-2.13	117.99	123.18
3	J	610	EPU	O2A-PA-O1A	2.13	122.78	112.24
3	B	602	EPU	O4D-C1D-C2D	-2.13	103.81	106.93
3	E	605	EPU	PB-O3A-PA	-2.13	125.53	132.83
3	L	612	EPU	O6-C6-C5	-2.13	104.00	111.29
3	K	611	EPU	O4-C4-C5	2.12	114.57	109.30
3	C	603	EPU	O5-C1-O1	-2.08	108.65	111.36
3	I	609	EPU	O4D-C4D-C5D	-2.07	102.57	109.37
3	J	610	EPU	O3A-PB-O1	-2.07	98.32	102.48
3	H	608	EPU	O2A-PA-O1A	2.06	122.41	112.24
3	E	605	EPU	O4D-C1D-C2D	-2.05	103.93	106.93
3	E	605	EPU	O1-C1-C2	2.04	112.09	108.40
3	G	607	EPU	O2D-C2D-C3D	-2.03	105.25	111.82
3	A	601	EPU	O4-C4-C3	-2.03	104.57	109.94
3	D	604	EPU	O3D-C3D-C2D	-2.00	105.35	111.82

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	EPU	C2D-C1D-N1U-C6U
3	A	601	EPU	O4D-C1D-N1U-C6U
3	B	602	EPU	C2D-C1D-N1U-C6U
3	B	602	EPU	C5D-O5D-PA-O1A
3	B	602	EPU	C5D-O5D-PA-O2A
3	C	603	EPU	C5D-O5D-PA-O1A
3	D	604	EPU	C5D-O5D-PA-O1A
3	E	605	EPU	C2D-C1D-N1U-C6U
3	E	605	EPU	O4D-C1D-N1U-C6U
3	E	605	EPU	C5D-O5D-PA-O2A
3	F	606	EPU	C2D-C1D-N1U-C6U
3	F	606	EPU	O4D-C1D-N1U-C6U

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Mol	Chain	Res	Type	Atoms
3	F	606	EPU	C5D-O5D-PA-O2A
3	F	606	EPU	C5D-O5D-PA-O3A
3	G	607	EPU	C5D-O5D-PA-O1A
3	G	607	EPU	C5D-O5D-PA-O2A
3	H	608	EPU	C2D-C1D-N1U-C6U
3	H	608	EPU	O4D-C1D-N1U-C6U
3	H	608	EPU	C5D-O5D-PA-O1A
3	H	608	EPU	C5D-O5D-PA-O2A
3	I	609	EPU	C2D-C1D-N1U-C6U
3	I	609	EPU	O4D-C1D-N1U-C6U
3	J	610	EPU	C2D-C1D-N1U-C6U
3	J	610	EPU	C5D-O5D-PA-O1A
3	K	611	EPU	C5D-O5D-PA-O1A
3	L	612	EPU	C2D-C1D-N1U-C6U
3	L	612	EPU	O4D-C1D-N1U-C6U
3	L	612	EPU	O4D-C4D-C5D-O5D
3	L	612	EPU	C5D-O5D-PA-O2A
3	L	612	EPU	C5D-O5D-PA-O3A
3	L	612	EPU	C4-C5-C6-O6
3	A	601	EPU	O4D-C4D-C5D-O5D
3	F	606	EPU	C3D-C4D-C5D-O5D
3	I	609	EPU	O4D-C4D-C5D-O5D
3	L	612	EPU	O5-C5-C6-O6
3	J	610	EPU	C4-C5-C6-O6
3	L	612	EPU	C3D-C4D-C5D-O5D
3	A	601	EPU	C3D-C4D-C5D-O5D
3	F	606	EPU	O4D-C4D-C5D-O5D
3	E	605	EPU	O4D-C4D-C5D-O5D
3	D	604	EPU	C1-O1-PB-O3A
3	E	605	EPU	C3D-C4D-C5D-O5D
3	I	609	EPU	C3D-C4D-C5D-O5D
3	J	610	EPU	PB-O3A-PA-O1A
3	K	611	EPU	PB-O3A-PA-O1A
3	I	609	EPU	C4-C5-C6-O6
3	G	607	EPU	C1-O1-PB-O3A
3	A	601	EPU	C4-C5-C6-O6
3	C	603	EPU	C5D-O5D-PA-O3A
3	D	604	EPU	C5D-O5D-PA-O3A
3	E	605	EPU	C5D-O5D-PA-O3A
3	J	610	EPU	C5D-O5D-PA-O3A
3	B	602	EPU	PB-O3A-PA-O2A
3	J	610	EPU	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	L	612	EPU	PB-O3A-PA-O2A
3	D	604	EPU	O5-C5-C6-O6
3	C	603	EPU	C5D-O5D-PA-O2A
3	D	604	EPU	C5D-O5D-PA-O2A
3	J	610	EPU	C5D-O5D-PA-O2A
3	K	611	EPU	C5D-O5D-PA-O2A
3	J	610	EPU	O5-C5-C6-O6
3	C	603	EPU	PB-O3A-PA-O2A
3	F	606	EPU	PB-O3A-PA-O2A
3	I	609	EPU	PB-O3A-PA-O2A
3	K	611	EPU	PB-O3A-PA-O2A
3	D	604	EPU	PA-O3A-PB-O1B
3	B	602	EPU	C5D-O5D-PA-O3A
3	G	607	EPU	C5D-O5D-PA-O3A
3	H	608	EPU	C5D-O5D-PA-O3A
3	K	611	EPU	C5D-O5D-PA-O3A
3	C	603	EPU	PB-O3A-PA-O1A
3	E	605	EPU	PB-O3A-PA-O2A
3	G	607	EPU	PB-O3A-PA-O1A
3	G	607	EPU	PA-O3A-PB-O2B
3	H	608	EPU	PB-O3A-PA-O1A
3	I	609	EPU	PB-O3A-PA-O1A
3	L	612	EPU	PB-O3A-PA-O1A
3	A	601	EPU	C5D-O5D-PA-O1A

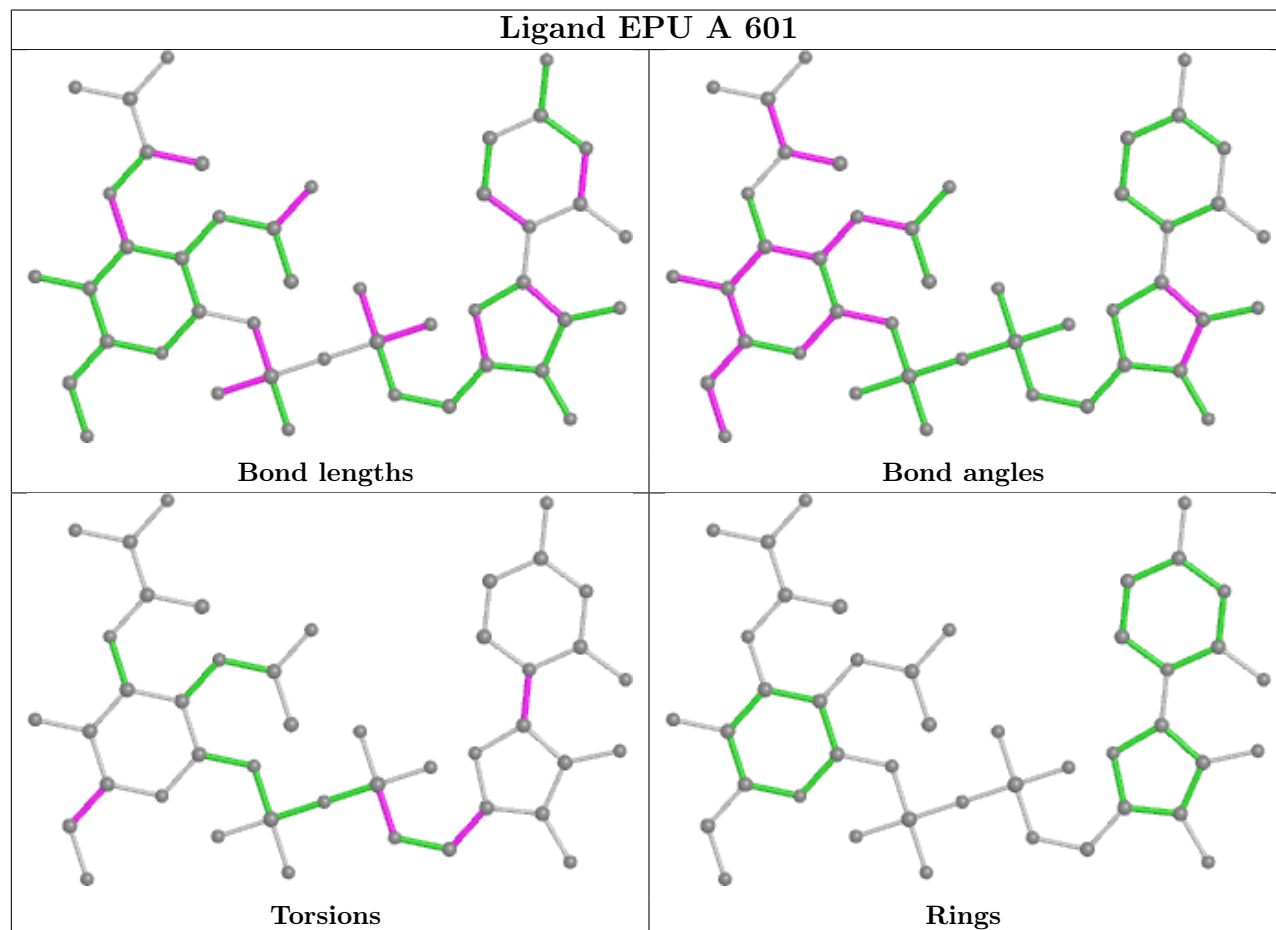
There are no ring outliers.

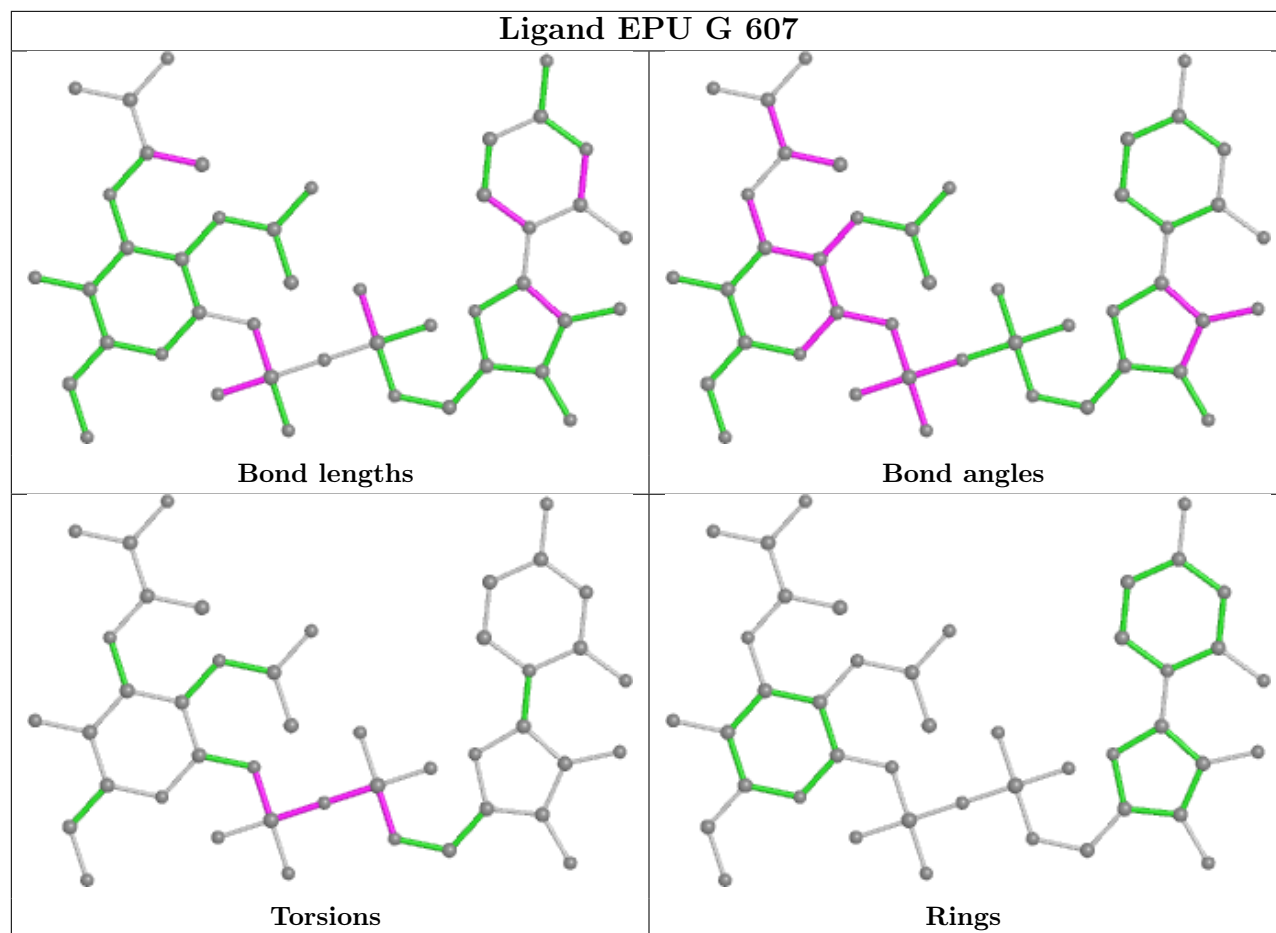
10 monomers are involved in 17 short contacts:

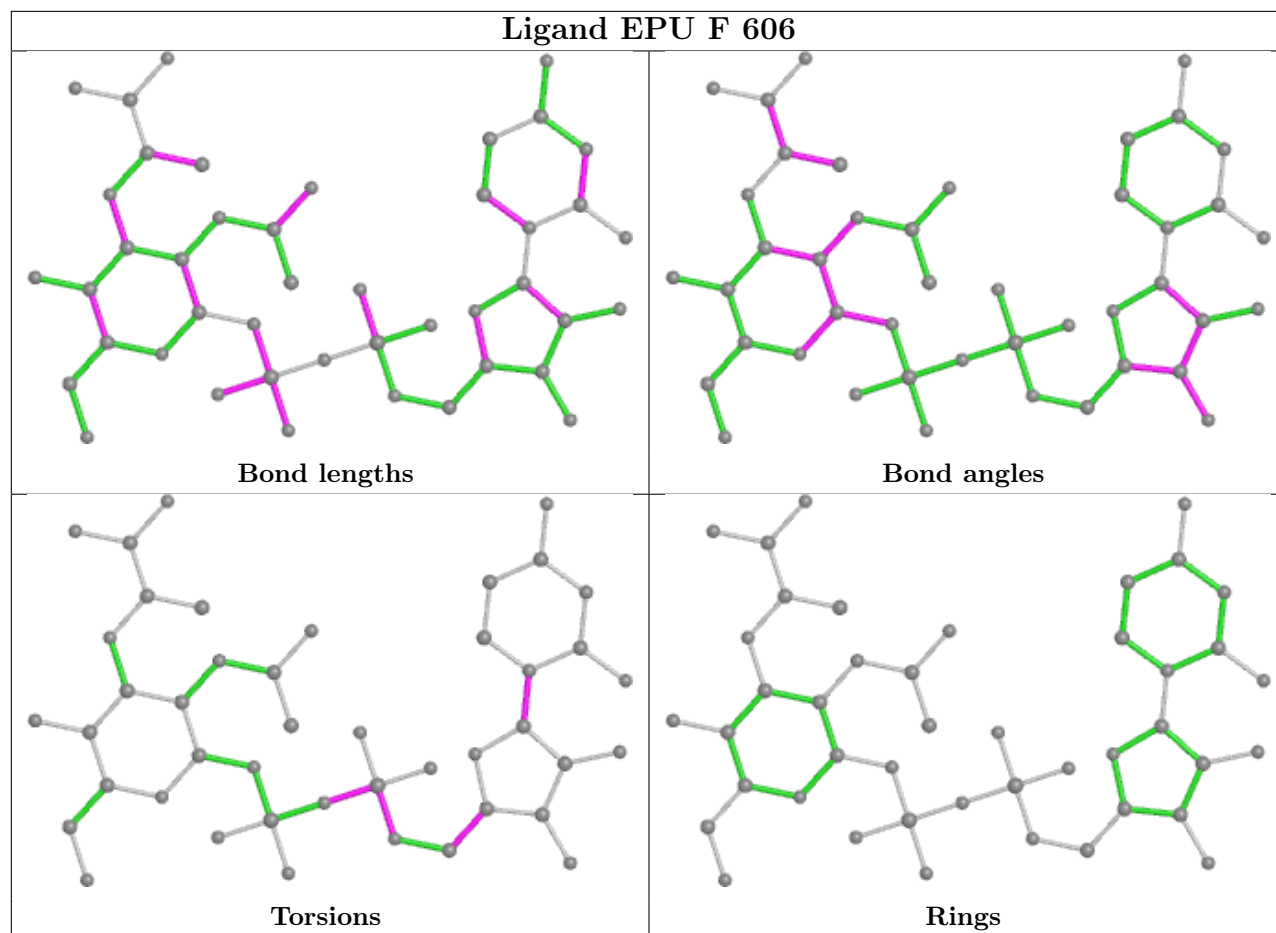
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	606	EPU	3	0
3	E	605	EPU	2	0
3	B	602	EPU	1	0
3	L	612	EPU	2	0
3	J	610	EPU	1	0
3	C	603	EPU	2	0
3	I	609	EPU	1	0
3	H	608	EPU	3	0
2	I	509	PO3	1	0
2	L	512	PO3	1	0

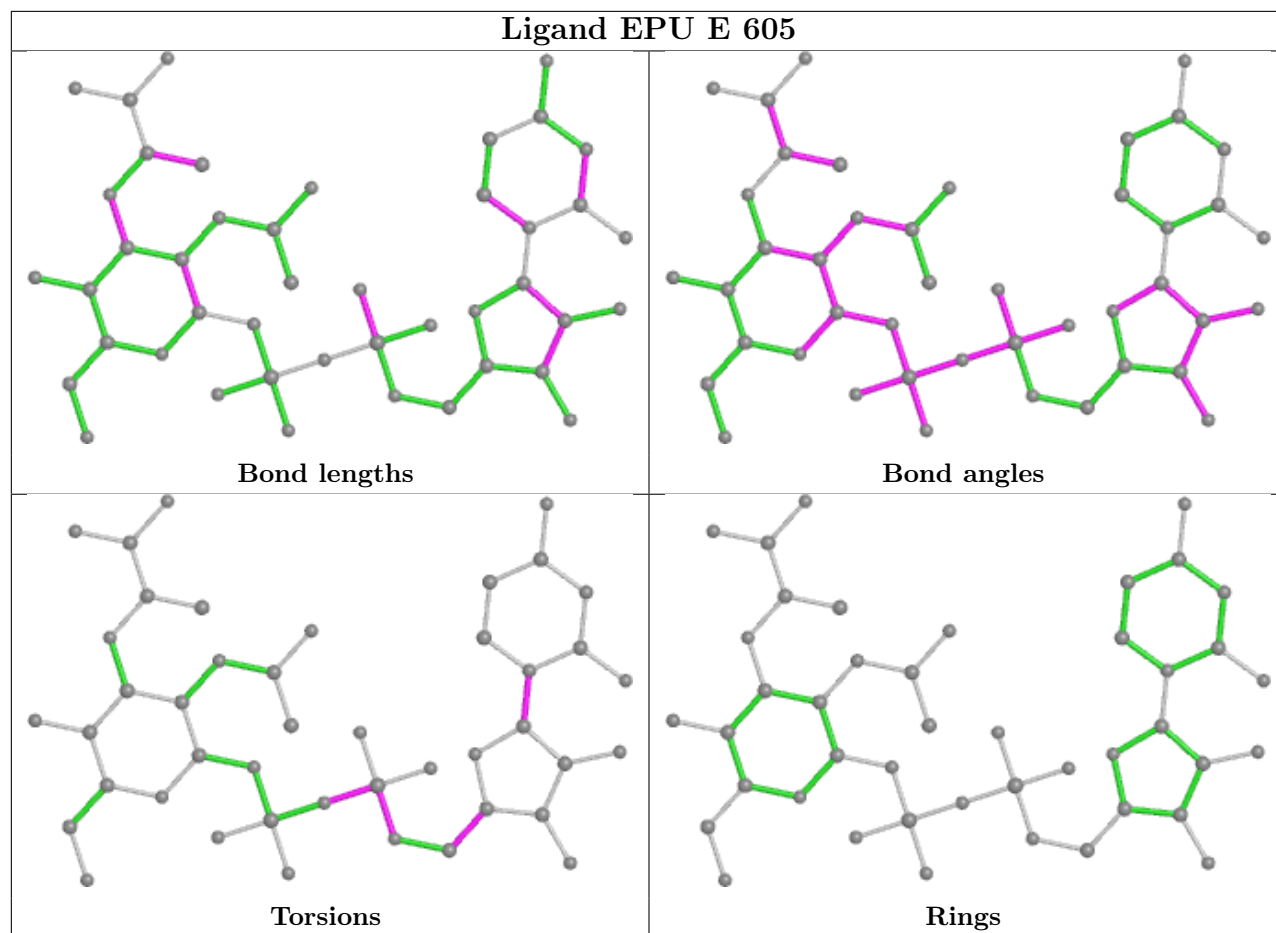
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

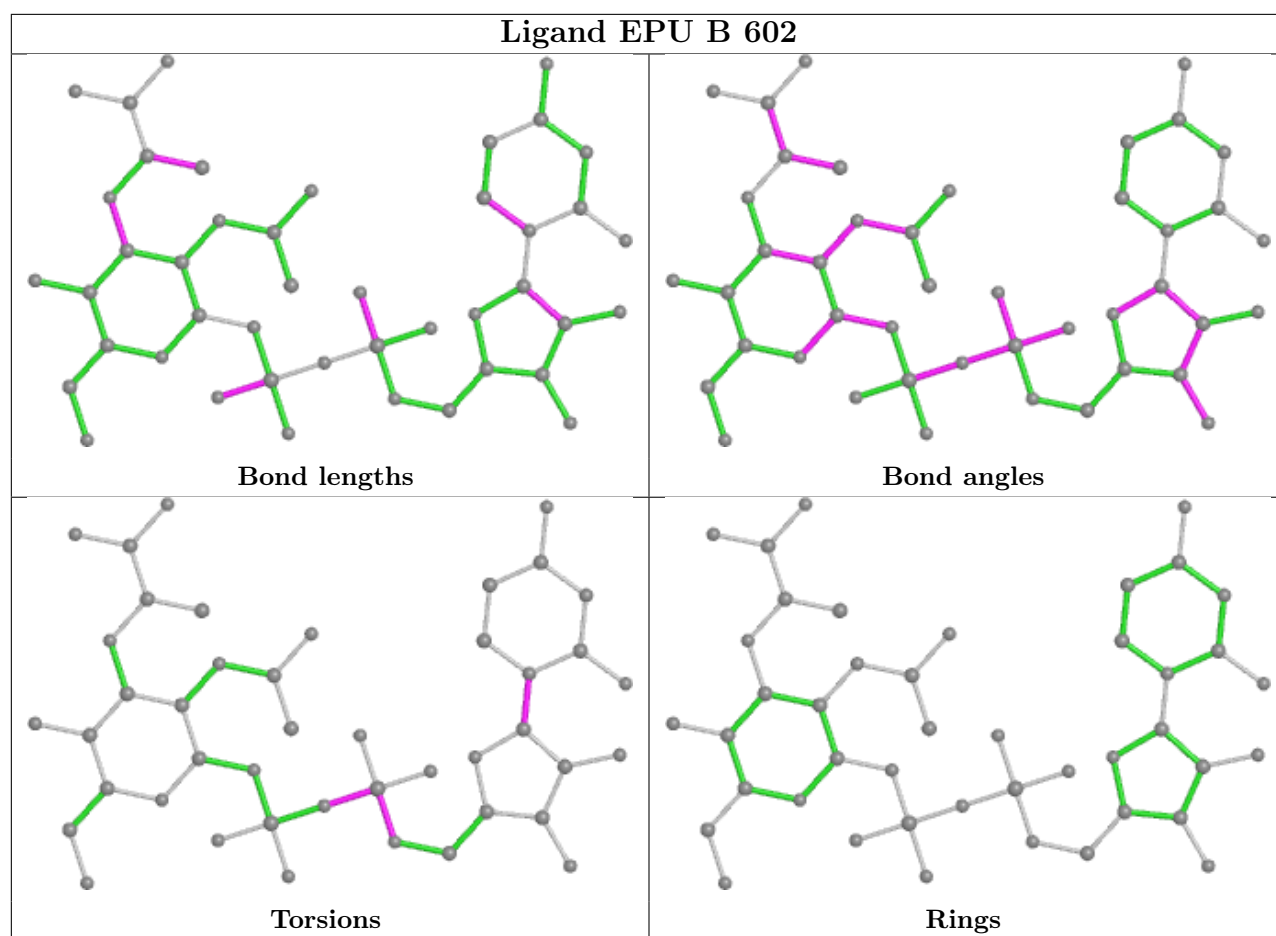
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

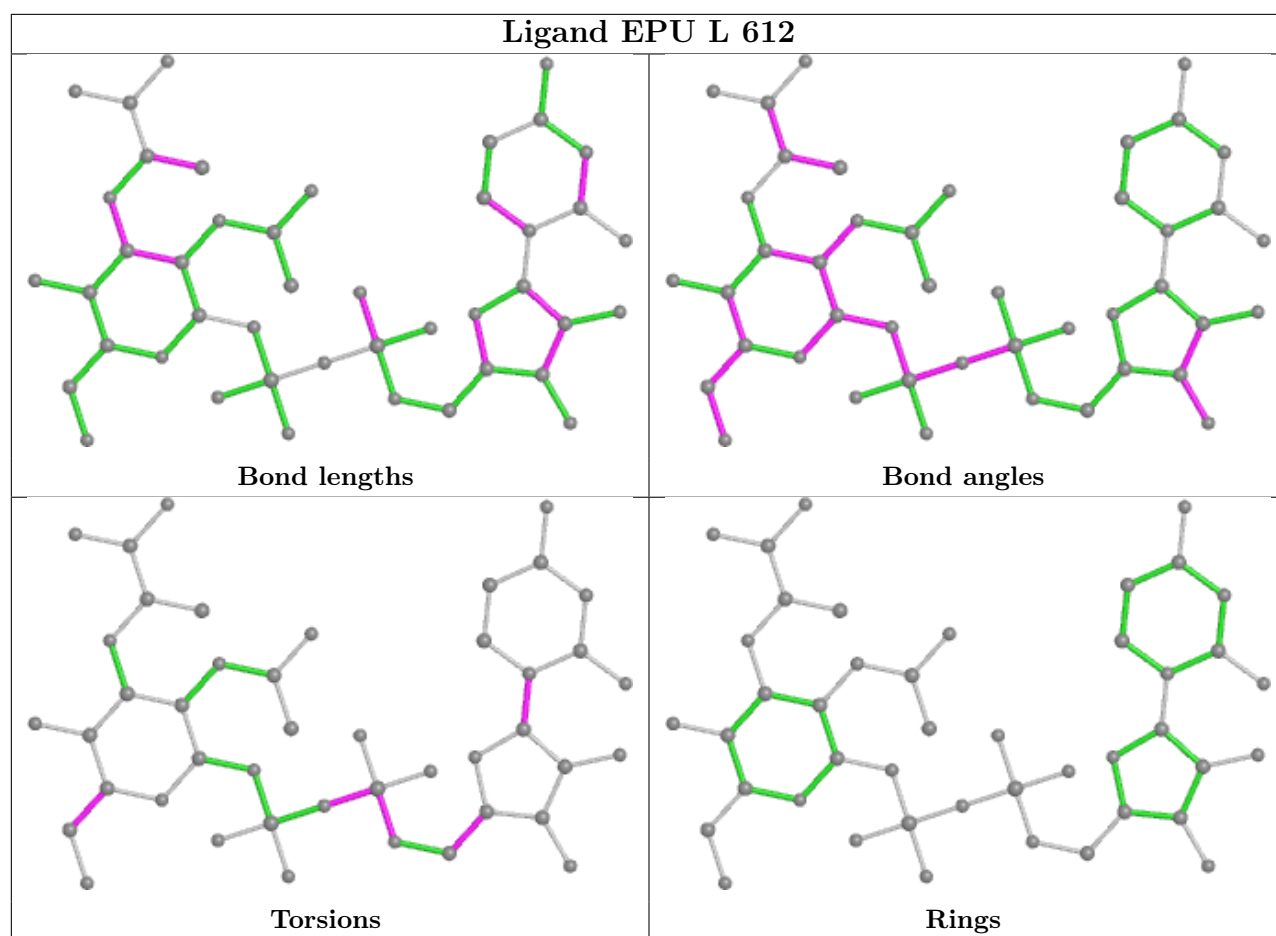


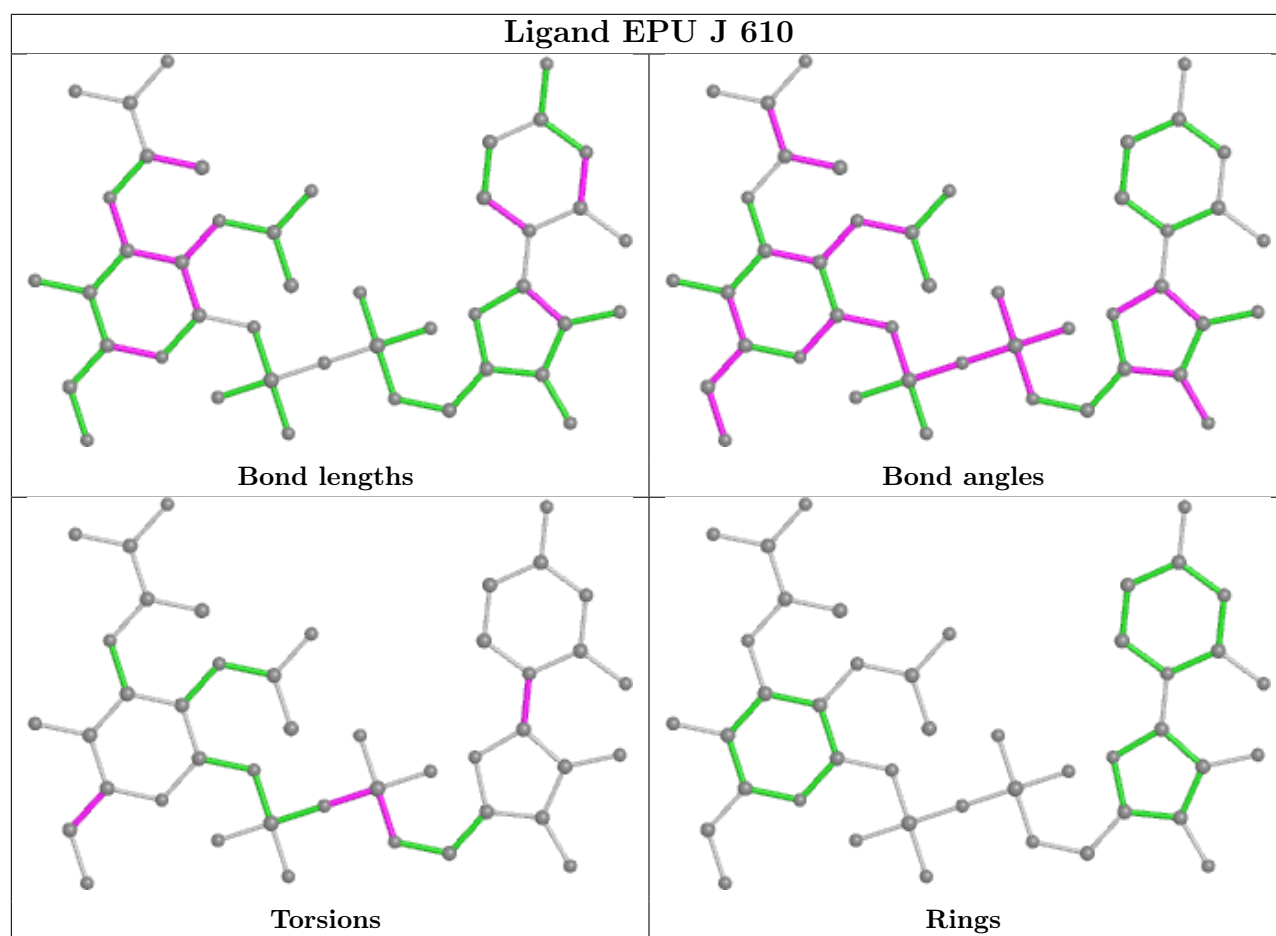


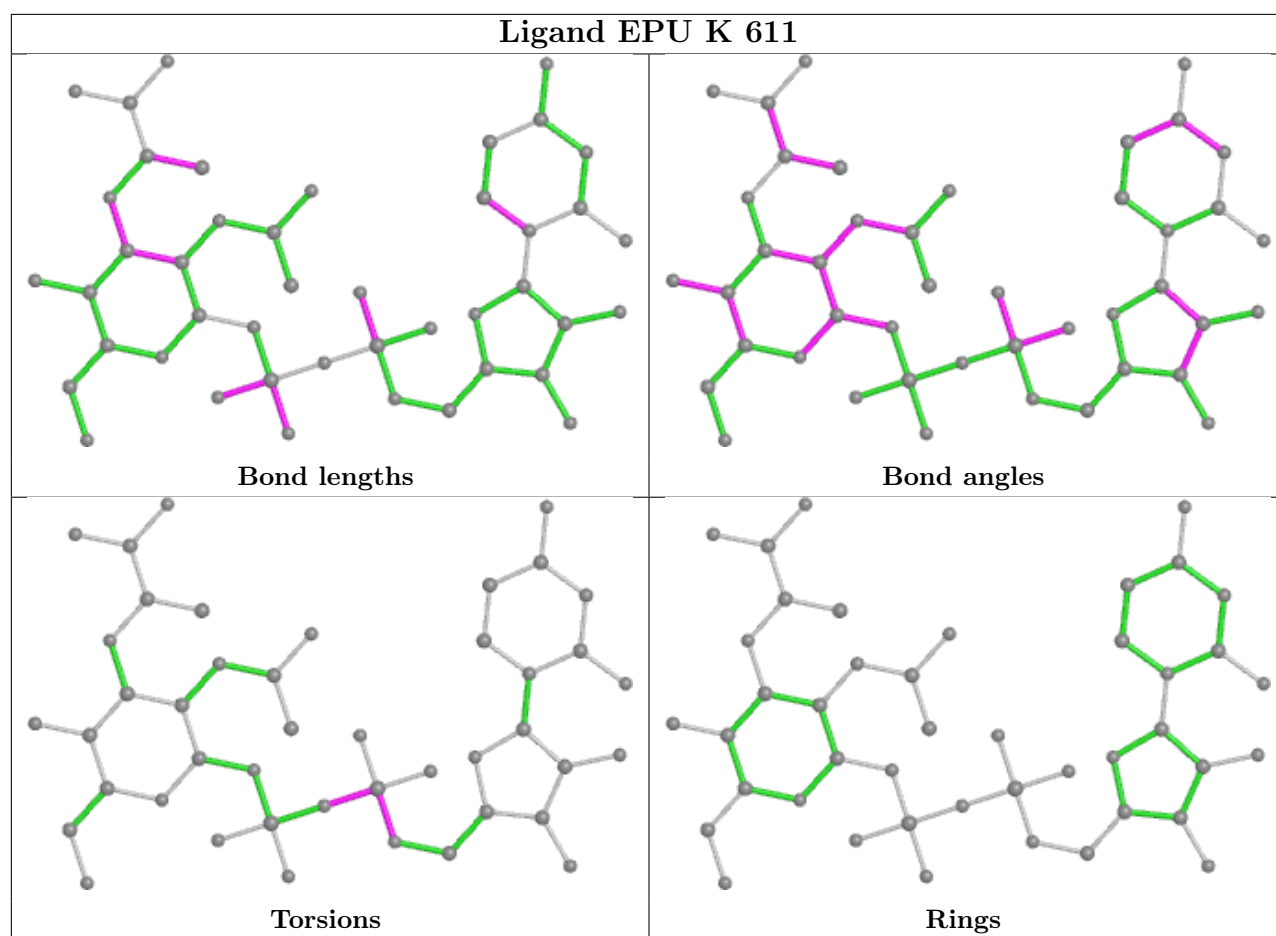


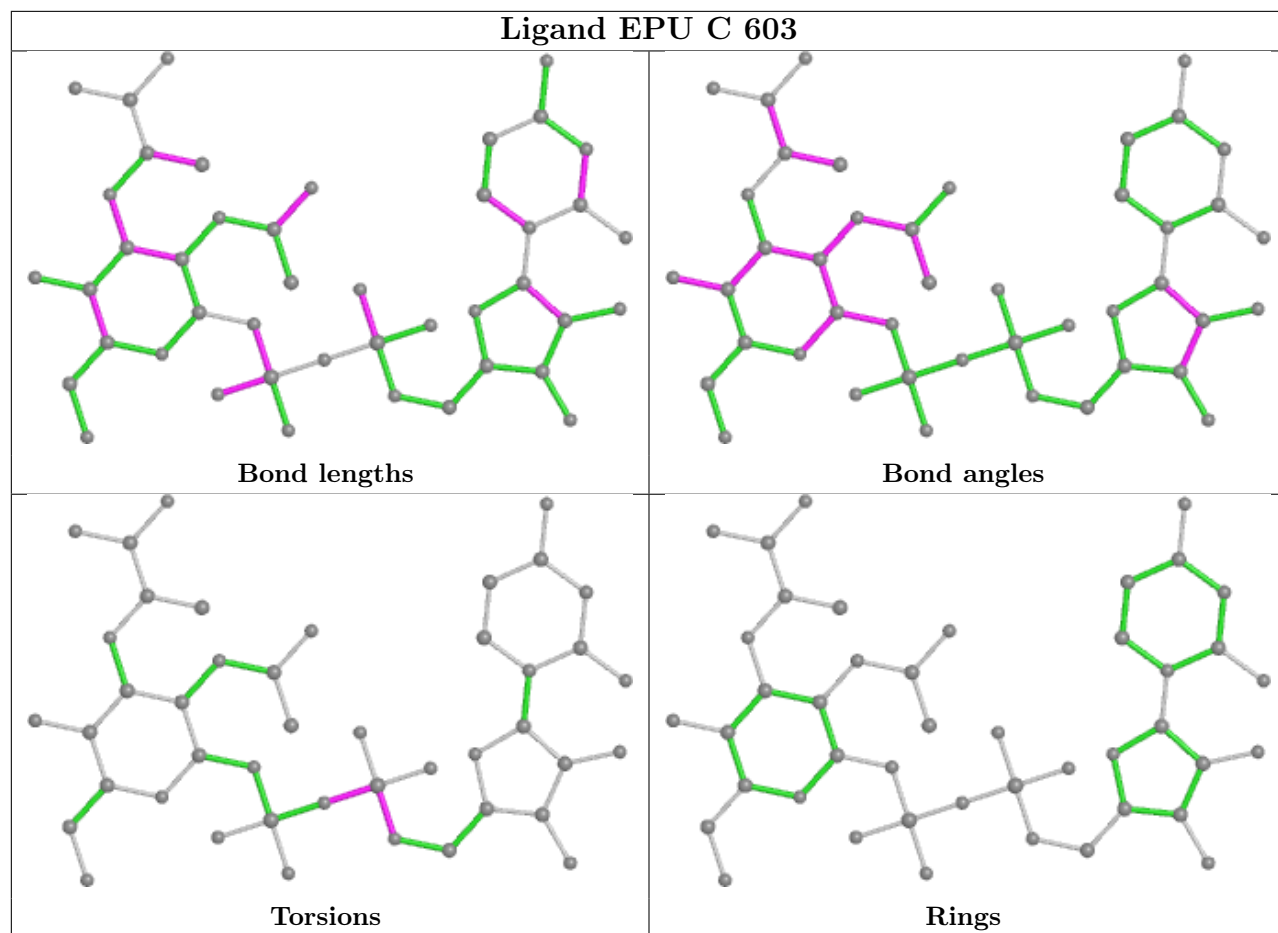


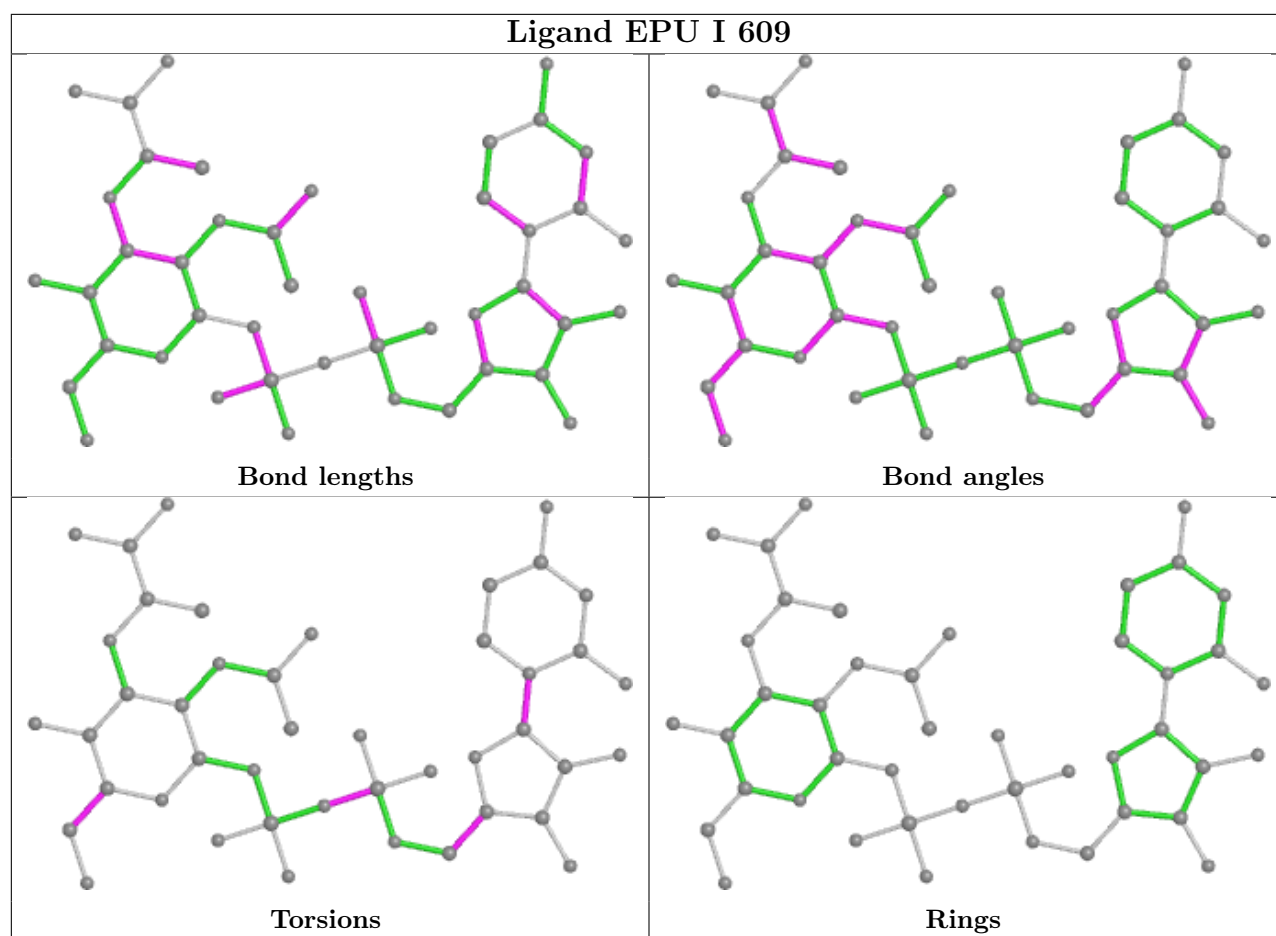


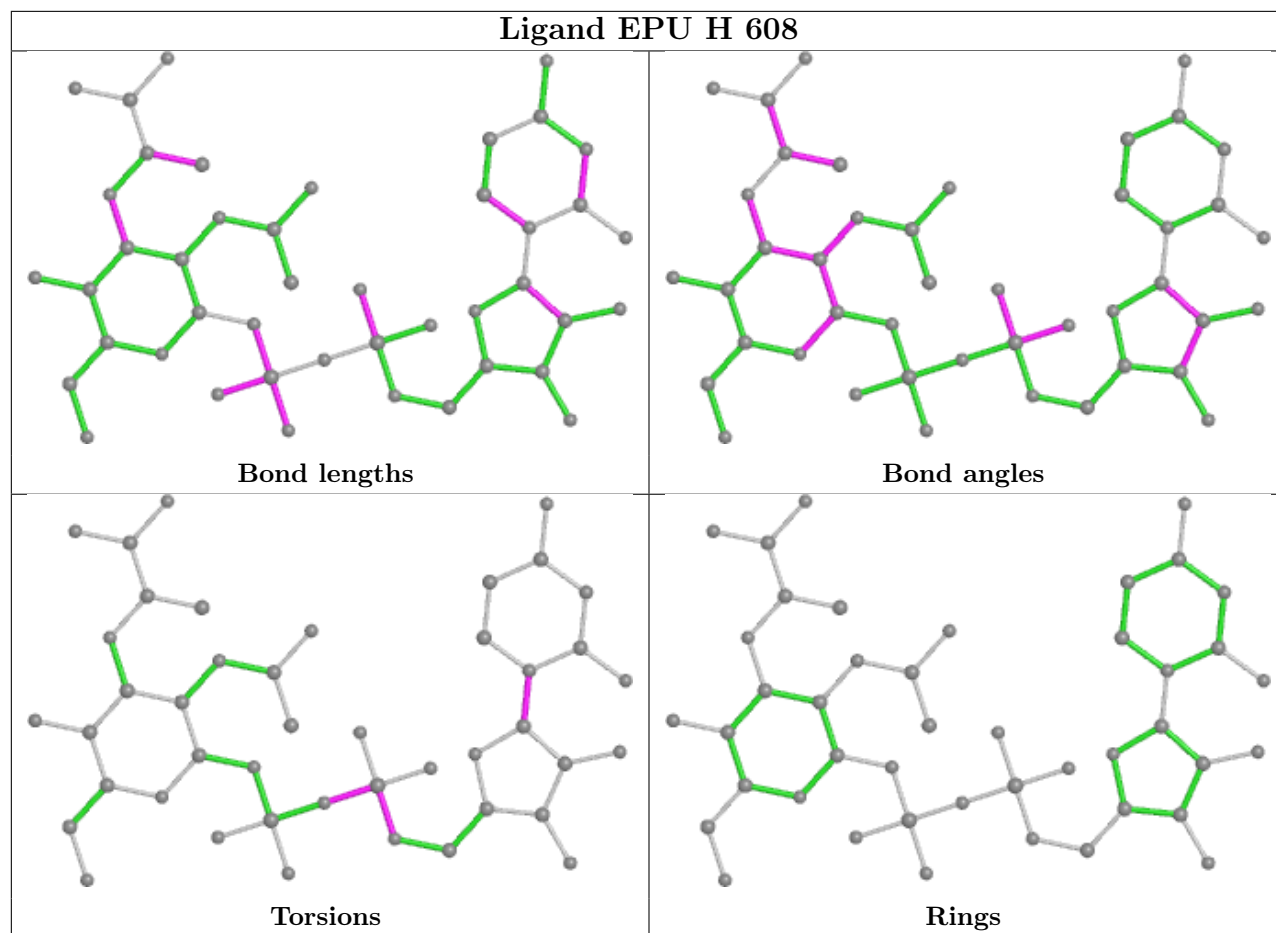


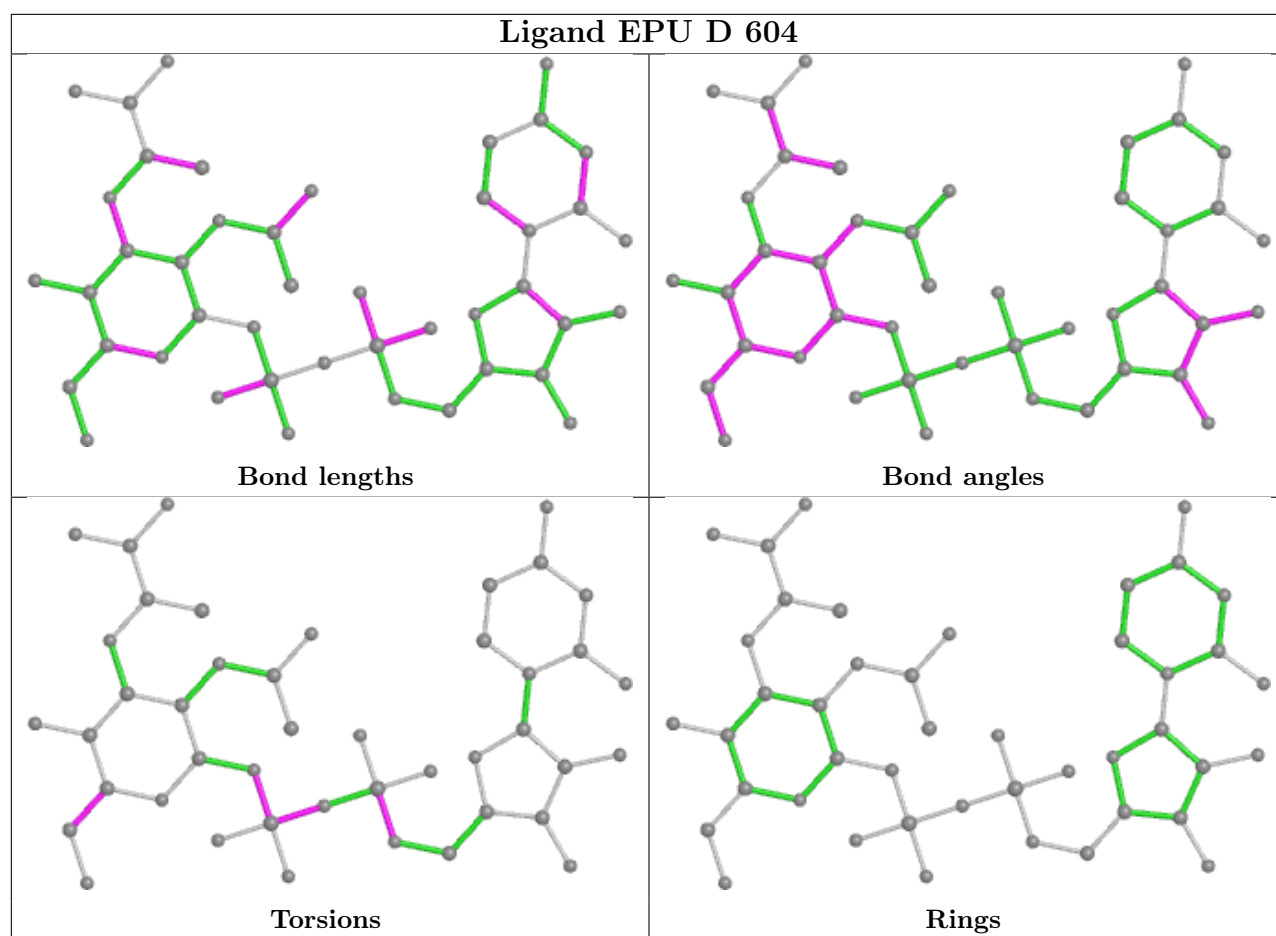












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1
1	B	1
1	J	1
1	F	1
1	A	1
1	E	1
1	C	1
1	H	1
1	K	1
1	G	1

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Mol	Chain	Number of breaks
1	D	1
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	67:ASP	C	68:GLY	N	4.56
1	B	67:ASP	C	68:GLY	N	4.44
1	J	67:ASP	C	68:GLY	N	4.32
1	F	67:ASP	C	68:GLY	N	4.14
1	A	67:ASP	C	68:GLY	N	4.12
1	E	67:ASP	C	68:GLY	N	4.04
1	C	67:ASP	C	68:GLY	N	3.98
1	H	67:ASP	C	68:GLY	N	3.89
1	K	67:ASP	C	68:GLY	N	3.87
1	G	67:ASP	C	68:GLY	N	3.85
1	D	67:ASP	C	68:GLY	N	3.83
1	L	67:ASP	C	68:GLY	N	3.29

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	418/418 (100%)	-0.14	3 (0%) 87 89	36, 55, 83, 120	0
1	B	418/418 (100%)	0.25	19 (4%) 33 36	37, 67, 100, 186	0
1	C	418/418 (100%)	-0.25	1 (0%) 95 95	26, 48, 71, 116	0
1	D	418/418 (100%)	-0.31	1 (0%) 95 95	30, 48, 72, 118	0
1	E	418/418 (100%)	-0.12	6 (1%) 75 77	32, 52, 77, 143	0
1	F	418/418 (100%)	-0.05	7 (1%) 70 72	33, 55, 85, 127	0
1	G	418/418 (100%)	0.06	9 (2%) 62 65	34, 61, 98, 147	0
1	H	418/418 (100%)	-0.21	3 (0%) 87 89	32, 51, 69, 132	0
1	I	418/418 (100%)	0.34	33 (7%) 12 12	38, 71, 118, 170	0
1	J	418/418 (100%)	0.03	7 (1%) 70 72	34, 64, 97, 128	0
1	K	418/418 (100%)	-0.10	6 (1%) 75 77	29, 53, 79, 169	0
1	L	418/418 (100%)	0.59	47 (11%) 5 4	42, 81, 129, 203	0
All	All	5016/5016 (100%)	0.01	142 (2%) 53 56	26, 57, 99, 203	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	418	GLY	8.6
1	L	222	GLY	7.0
1	L	221	LEU	6.6
1	L	215	ILE	6.0
1	I	215	ILE	5.9
1	I	81	CYS	5.8
1	E	418	GLY	5.4
1	I	216	GLU	5.1
1	I	177	GLU	4.9
1	I	136	ILE	4.9
1	L	39	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	418	GLY	4.7
1	D	418	GLY	4.7
1	K	418	GLY	4.6
1	I	152	LYS	4.4
1	G	418	GLY	4.3
1	I	99	PRO	4.2
1	I	134	ALA	4.2
1	J	201	LEU	4.1
1	F	225	VAL	3.9
1	I	181	ILE	3.8
1	L	63	LYS	3.8
1	L	41	ILE	3.8
1	L	12	LEU	3.7
1	L	199	ILE	3.6
1	G	401	ARG	3.5
1	I	148	ASP	3.5
1	E	57	LEU	3.4
1	L	75	ARG	3.4
1	L	216	GLU	3.4
1	J	359	LYS	3.4
1	B	395	ILE	3.4
1	L	225	VAL	3.4
1	B	47	LEU	3.3
1	L	197	PHE	3.3
1	B	273	ILE	3.3
1	I	132	LEU	3.3
1	L	37	GLU	3.2
1	G	59	GLN	3.2
1	L	401	ARG	3.2
1	G	1	MET	3.2
1	I	147	VAL	3.1
1	E	77	VAL	3.1
1	B	146	SER	3.1
1	L	279	TRP	3.1
1	L	277	GLU	3.1
1	K	248	LYS	3.1
1	J	72	ILE	3.0
1	G	56	LEU	3.0
1	L	213	ILE	3.0
1	B	370	LEU	3.0
1	L	175	LEU	3.0
1	K	349	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	282	LEU	2.9
1	J	273	ILE	2.9
1	I	217	GLY	2.9
1	F	72	ILE	2.9
1	K	330	ASN	2.8
1	L	30	PHE	2.8
1	J	12	LEU	2.8
1	I	349	SER	2.8
1	L	205	ILE	2.8
1	H	60	LEU	2.8
1	L	201	LEU	2.8
1	K	412	ASN	2.7
1	L	200	THR	2.7
1	E	220	ARG	2.7
1	B	286	GLY	2.7
1	G	273	ILE	2.7
1	I	194	THR	2.6
1	I	350	ASN	2.6
1	A	133	GLY	2.6
1	B	60	LEU	2.6
1	B	219	GLU	2.6
1	I	102	ALA	2.6
1	L	64	VAL	2.6
1	L	26	LEU	2.6
1	I	143	VAL	2.6
1	E	330	ASN	2.6
1	L	267	ARG	2.6
1	B	80	PHE	2.6
1	I	401	ARG	2.5
1	B	35	ALA	2.5
1	G	79	VAL	2.5
1	B	358	GLU	2.5
1	I	137	LYS	2.5
1	F	53	SER	2.5
1	I	131	GLN	2.5
1	K	350	ASN	2.5
1	J	289	PRO	2.5
1	L	226	TYR	2.5
1	B	49	ASP	2.5
1	I	230	PRO	2.5
1	F	115	CYS	2.4
1	I	201	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	99	PRO	2.4
1	F	221	LEU	2.4
1	A	139	GLU	2.4
1	H	115	CYS	2.4
1	L	238	PHE	2.4
1	I	171	CYS	2.4
1	I	175	LEU	2.4
1	L	272	ASP	2.3
1	A	107	GLY	2.3
1	I	129	LEU	2.3
1	B	64	VAL	2.3
1	L	16	VAL	2.3
1	B	32	ALA	2.3
1	L	281	SER	2.3
1	I	42	GLN	2.3
1	I	78	ASN	2.3
1	L	326	THR	2.3
1	B	13	GLN	2.3
1	F	406	LEU	2.3
1	L	274	GLU	2.3
1	I	151	LEU	2.3
1	L	152	LYS	2.3
1	I	80	PHE	2.3
1	L	248	LYS	2.2
1	G	62	ALA	2.2
1	L	33	LEU	2.2
1	L	42	GLN	2.2
1	I	182	ILE	2.2
1	L	117	ILE	2.2
1	L	362	GLY	2.2
1	L	330	ASN	2.2
1	L	350	ASN	2.2
1	C	216	GLU	2.2
1	E	219	GLU	2.2
1	L	36	GLU	2.1
1	L	38	PRO	2.1
1	L	74	ALA	2.1
1	J	330	ASN	2.1
1	I	101	VAL	2.1
1	F	220	ARG	2.1
1	I	100	LEU	2.1
1	L	378	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	318	GLU	2.1
1	G	370	LEU	2.0
1	B	350	ASN	2.0
1	L	70	VAL	2.0
1	B	86	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO3	B	502	4/4	0.89	0.15	61,70,74,81	0
2	PO3	A	501	4/4	0.92	0.27	65,66,69,73	0
2	PO3	D	503	4/4	0.92	0.22	52,56,65,67	0
3	EPU	I	609	44/44	0.92	0.17	55,65,70,74	0
2	PO3	K	511	4/4	0.94	0.32	56,69,71,79	0
2	PO3	L	512	4/4	0.94	0.23	68,73,83,85	0
2	PO3	H	508	4/4	0.94	0.25	54,56,57,63	0
3	EPU	D	604	44/44	0.95	0.12	32,43,53,59	0
3	EPU	F	606	44/44	0.95	0.14	33,41,52,67	0
3	EPU	G	607	44/44	0.95	0.17	39,50,58,65	0
3	EPU	B	602	44/44	0.95	0.14	43,51,59,68	0
3	EPU	A	601	44/44	0.96	0.15	38,51,59,63	0
3	EPU	H	608	44/44	0.96	0.14	37,50,61,63	0
2	PO3	E	504	4/4	0.96	0.23	58,64,65,68	0
3	EPU	J	610	44/44	0.96	0.13	42,48,54,61	0
3	EPU	K	611	44/44	0.96	0.13	33,44,52,69	0
3	EPU	L	612	44/44	0.96	0.15	56,64,70,77	0
2	PO3	C	502	4/4	0.97	0.27	59,66,66,70	0

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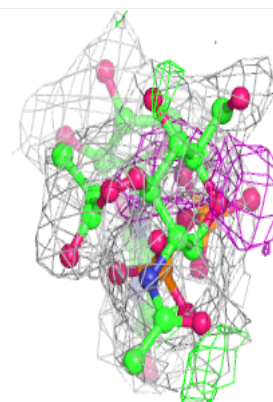
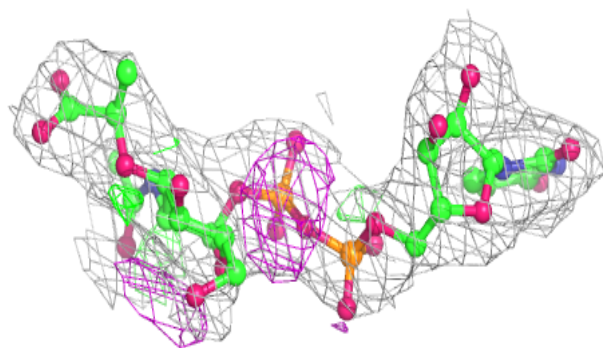
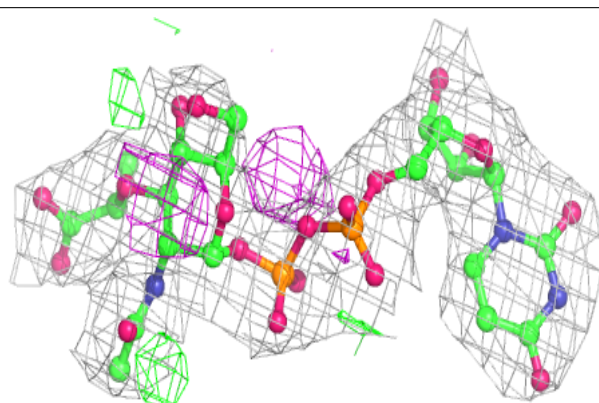
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO3	I	509	4/4	0.97	0.24	49,72,72,87	0
3	EPU	C	603	44/44	0.97	0.13	33,41,49,61	0
2	PO3	F	506	4/4	0.97	0.23	71,73,76,77	0
3	EPU	E	605	44/44	0.97	0.13	34,42,56,62	0
2	PO3	G	507	4/4	0.97	0.20	50,53,55,58	0
2	PO3	J	510	4/4	0.98	0.23	53,65,65,68	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.

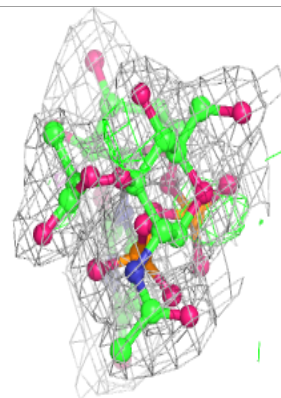
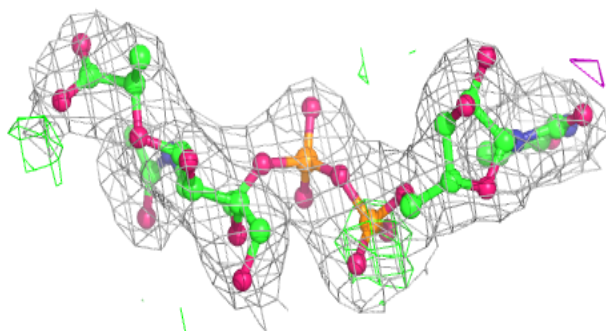
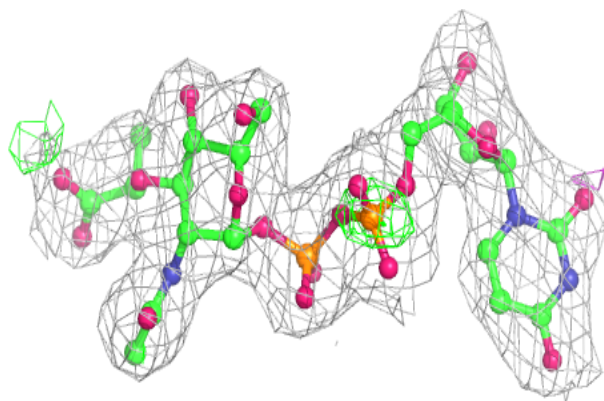
Electron density around EPU I 609:

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

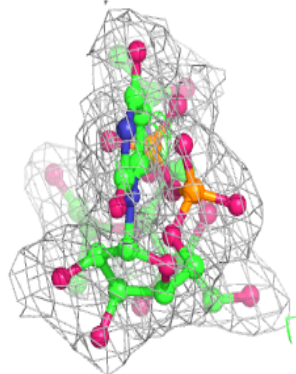
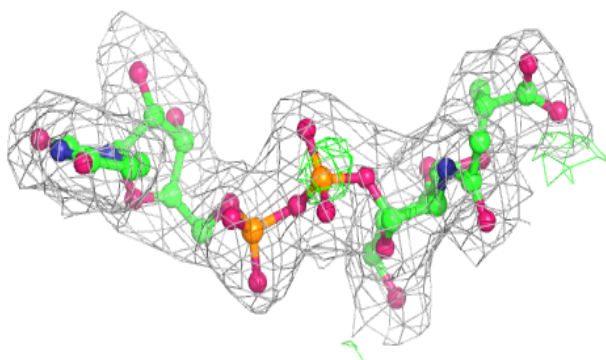
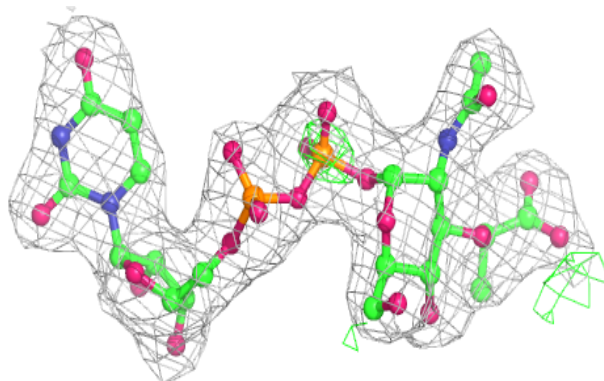


Electron density around EPU D 604:

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

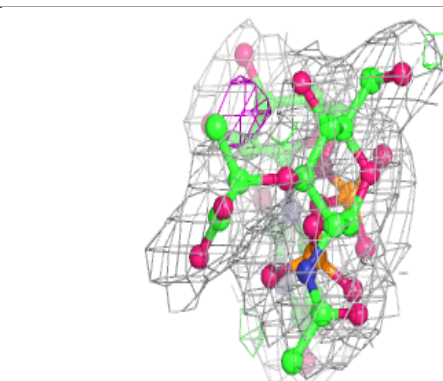
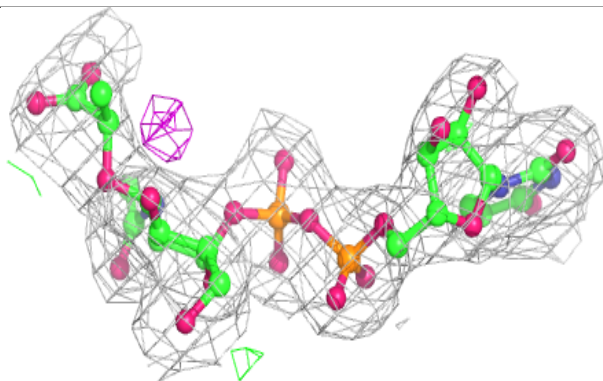
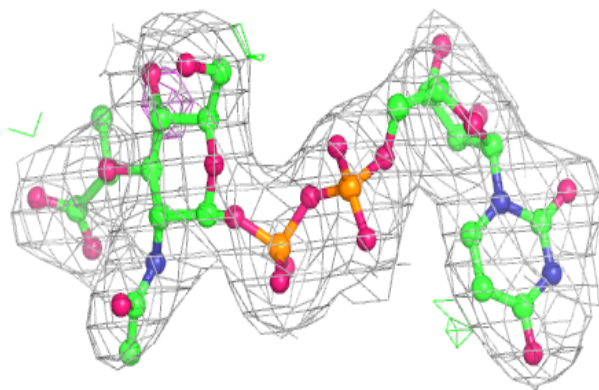
**Electron density around EPU F 606:**

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

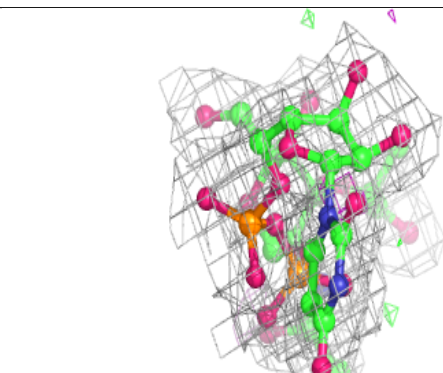
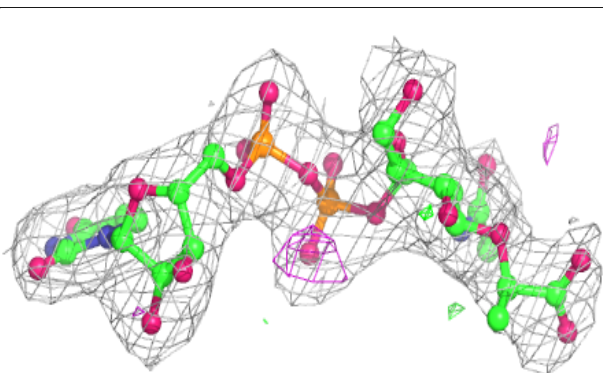
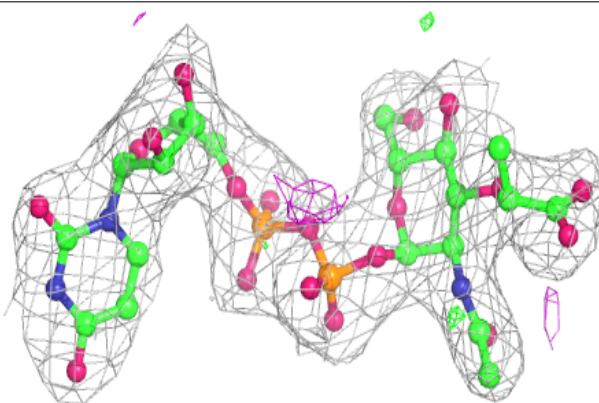


Electron density around EPU G 607:

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

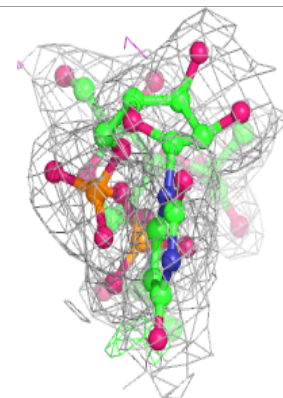
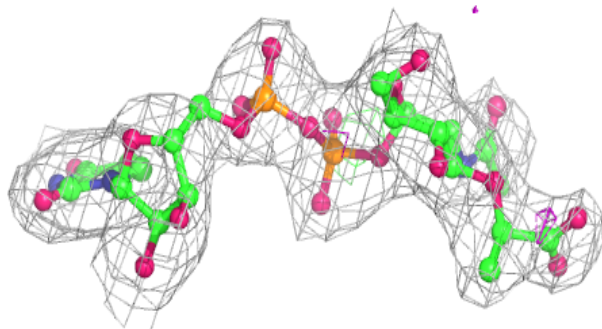
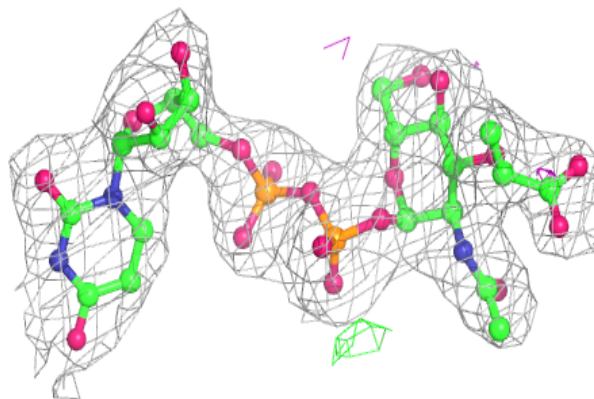
**Electron density around EPU B 602:**

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

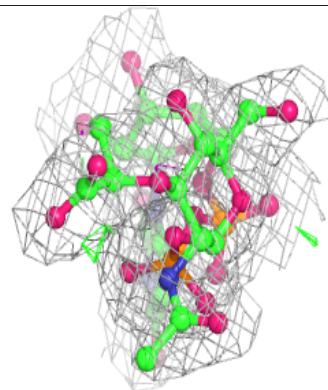
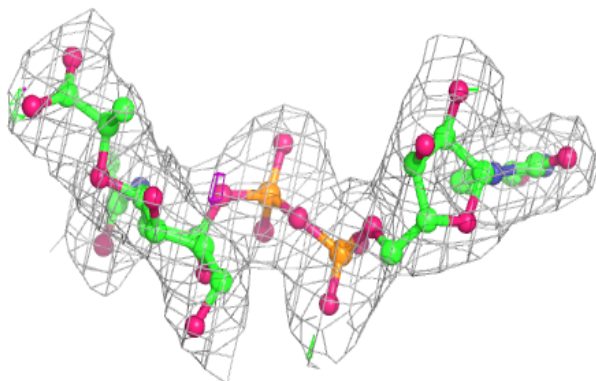
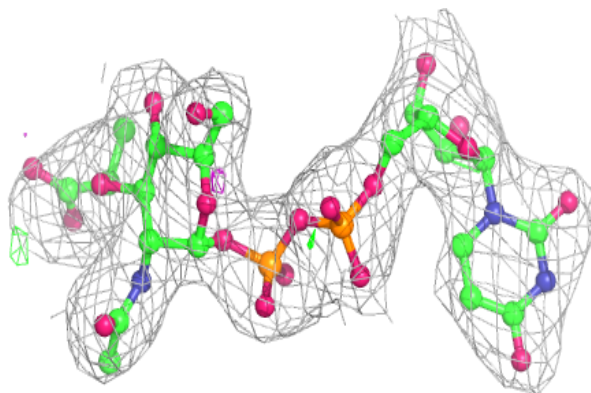


Electron density around EPU A 601:

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

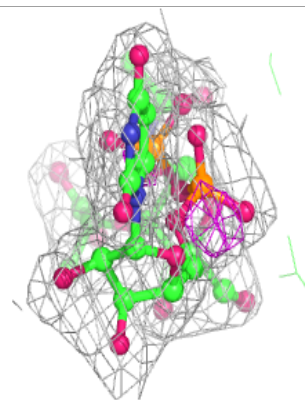
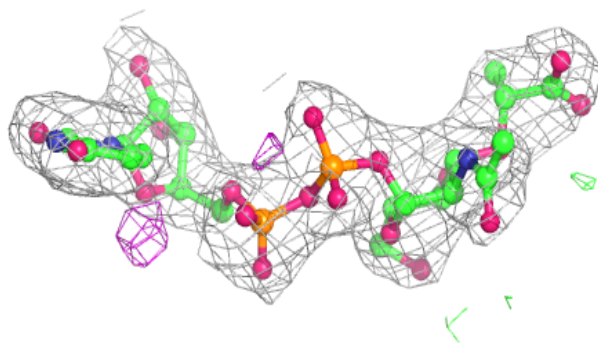
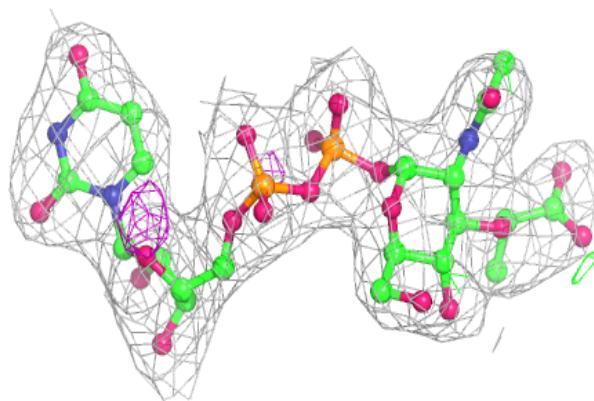
**Electron density around EPU H 608:**

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

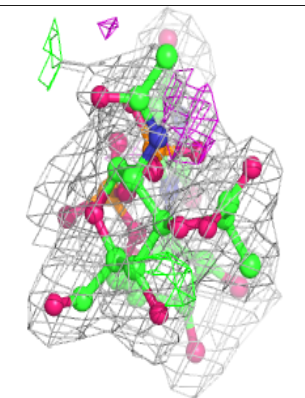
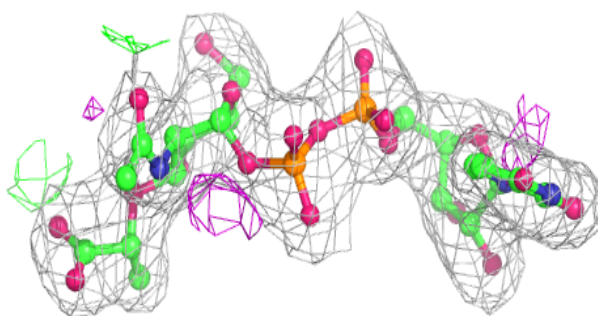
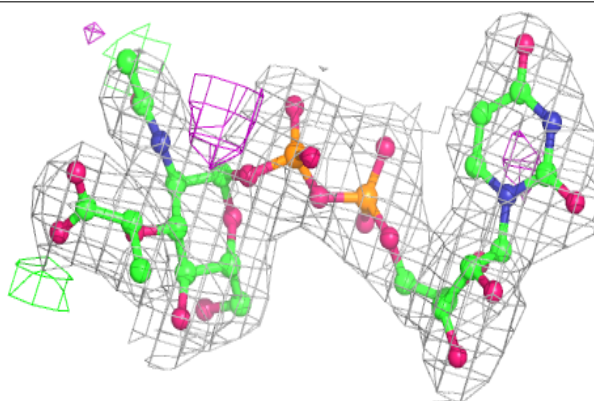


Electron density around EPU J 610:

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

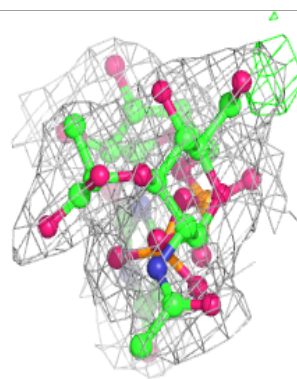
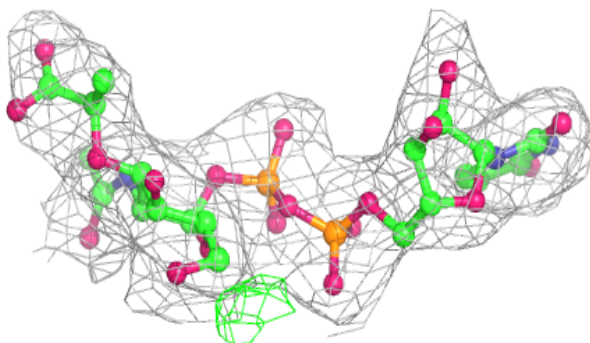
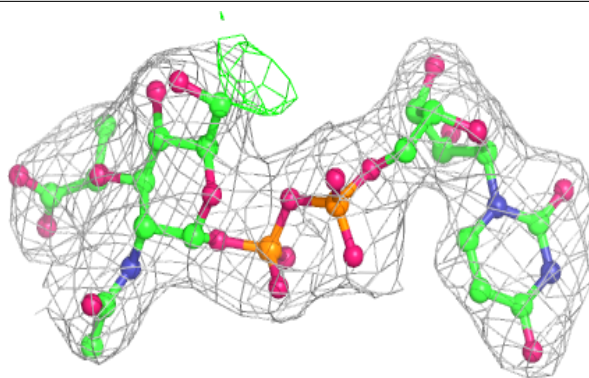
**Electron density around EPU K 611:**

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

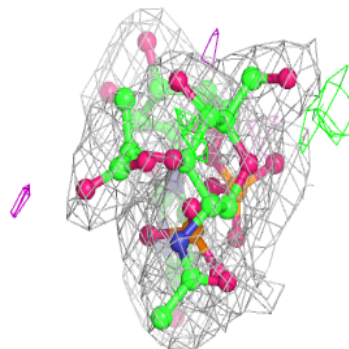
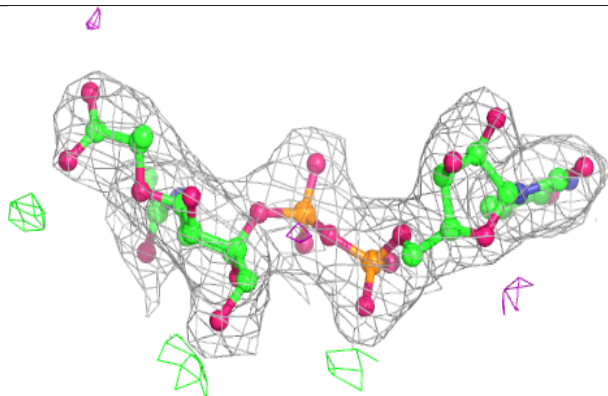
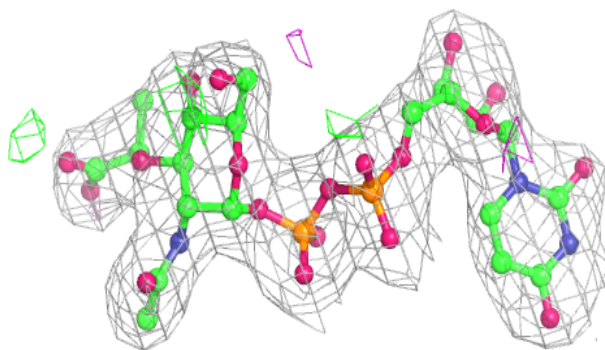


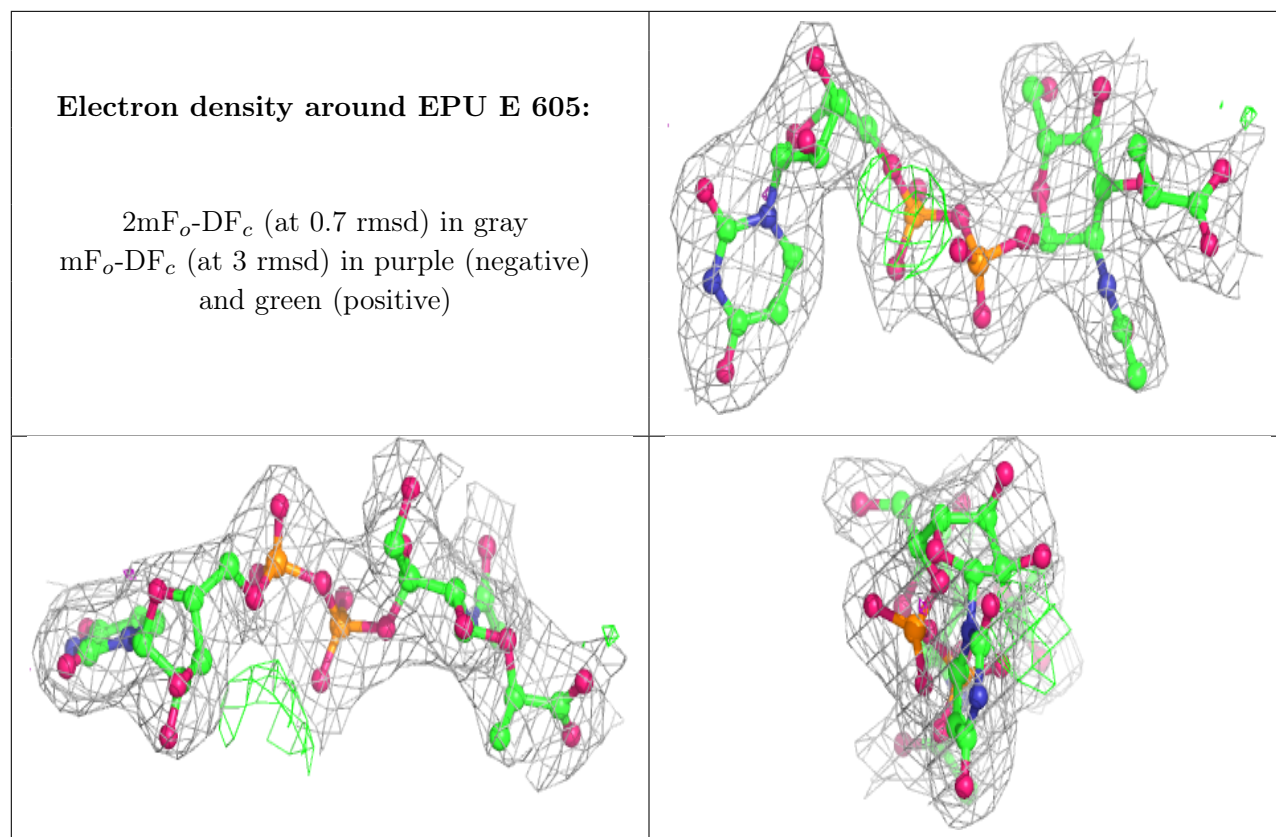
Electron density around EPU L 612:

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

**Electron density around EPU C 603:**

$2mF_o-DF_c$ (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.