



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:26 am BST

PDB ID : 3SWD  
Title : E. coli MurA in complex with UDP-N-acetylmuramic acid and covalent adduct of PEP with Cys115  
Authors : Zhu, J.-Y.; Schonbrunn, E.  
Deposited on : 2011-07-13  
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](mailto: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.

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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 : 2.11  
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) : 2.11

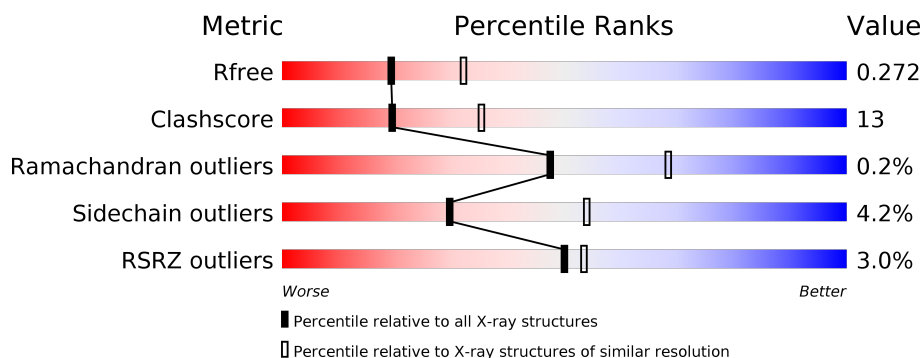
# 1 Overall quality at a glance

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>80%</div> <div>19%</div> <div>.</div> </div> </div>
1	B	418	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
1	C	418	<div> <div></div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
1	D	418	<div> <div></div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
1	E	418	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
1	F	418	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	418	
1	H	418	
1	I	418	
1	J	418	
1	K	418	
1	L	418	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	IAS	I	67	-	-	X	-
1	IAS	K	67	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39035 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	P	S	0	0	0
			3143	1970	556	600	1	16			
1	B	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			
1	C	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			
1	D	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			
1	E	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			
1	F	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			
1	G	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			
1	H	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			
1	I	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			
1	J	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			
1	K	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			
1	L	418	Total	C	N	O	P	S	0	0	0
			3143	1970	556	600	1	16			

There are 12 discrepancies between the modelled and reference sequences:

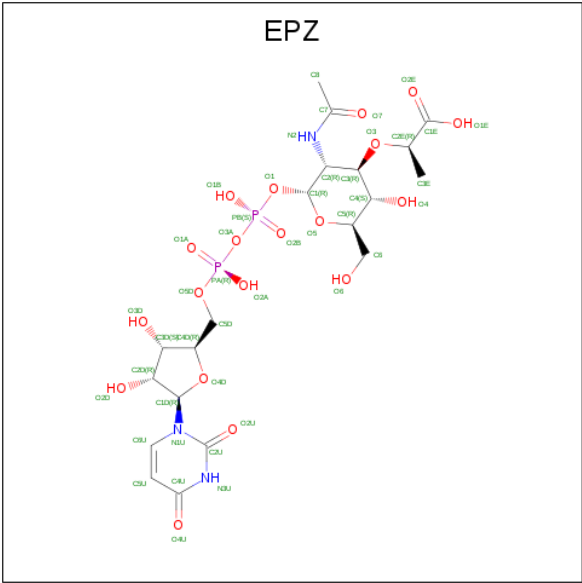
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749
B	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749
C	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749
D	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749
E	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749

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Chain	Residue	Modelled	Actual	Comment	Reference
F	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749
G	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749
H	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749
I	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749
J	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749
K	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749
L	67	IAS	ASN	ENGINEERED MUTATION	UNP P0A749

- Molecule 2 is (2R)-2-{{[(2R,3R,4R,5S,6R)-3-(acetylamino)-2-{{[(S)-{{[(R)-{{[(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]oxy}-5-hydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-4-yl]oxy}propanoic acid (three-letter code: EPZ) (formula: C<sub>20</sub>H<sub>31</sub>N<sub>3</sub>O<sub>19</sub>P<sub>2</sub>).



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

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

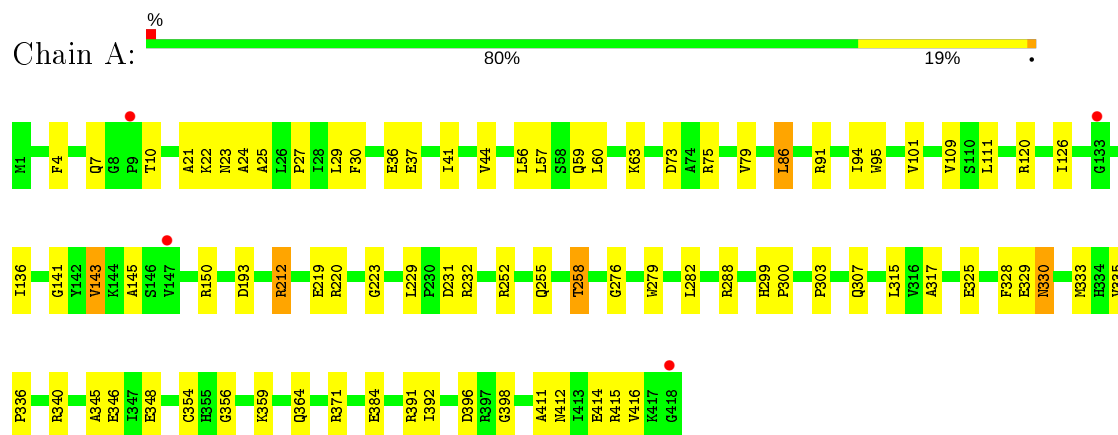
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	B	58	Total	O	0	0
			58	58		
3	C	105	Total	O	0	0
			105	105		
3	D	104	Total	O	0	0
			104	104		
3	E	86	Total	O	0	0
			86	86		
3	F	63	Total	O	0	0
			63	63		
3	G	47	Total	O	0	0
			47	47		
3	H	73	Total	O	0	0
			73	73		
3	I	42	Total	O	0	0
			42	42		
3	J	45	Total	O	0	0
			45	45		
3	K	60	Total	O	0	0
			60	60		
3	L	32	Total	O	0	0
			32	32		

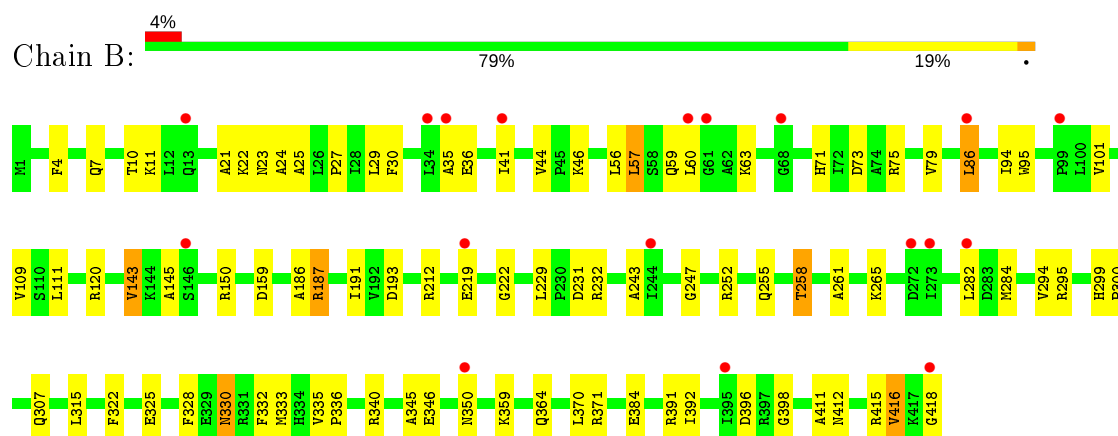
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

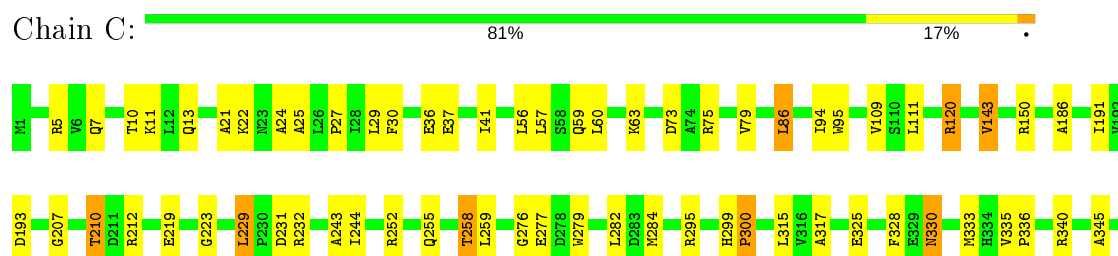
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

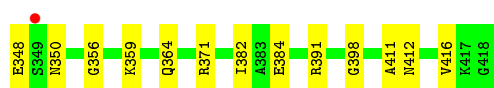


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



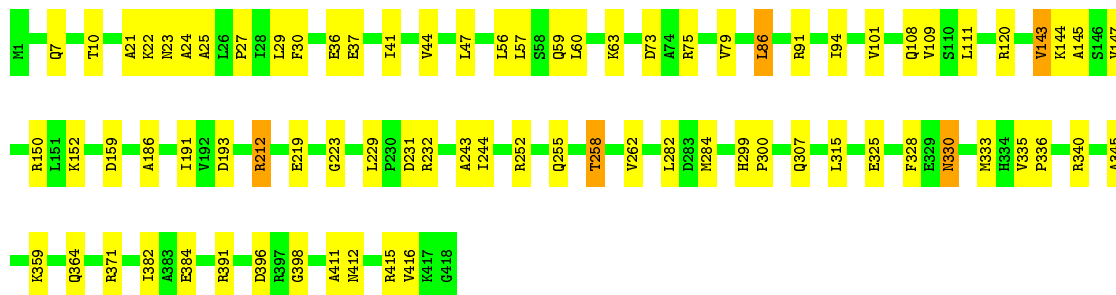
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





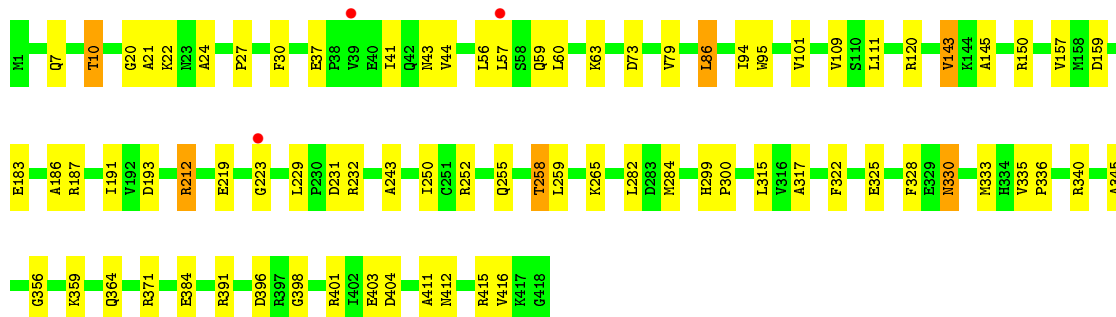
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain D: 81% 18%



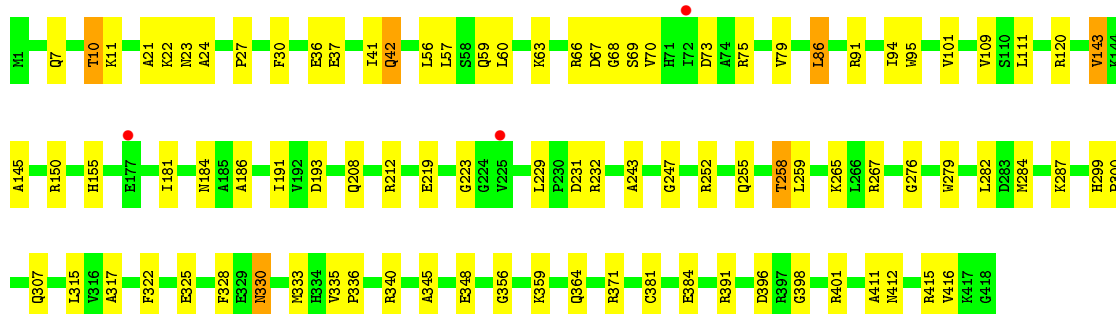
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain E: 81% 17%



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

Chain F: 78% 21%

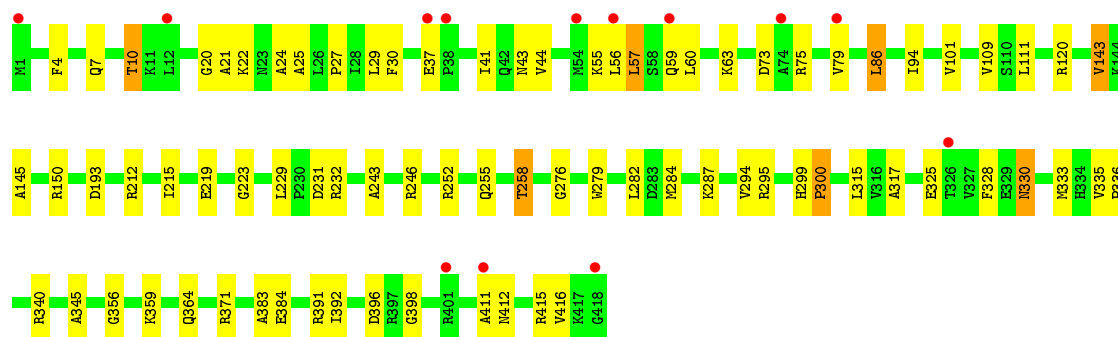


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

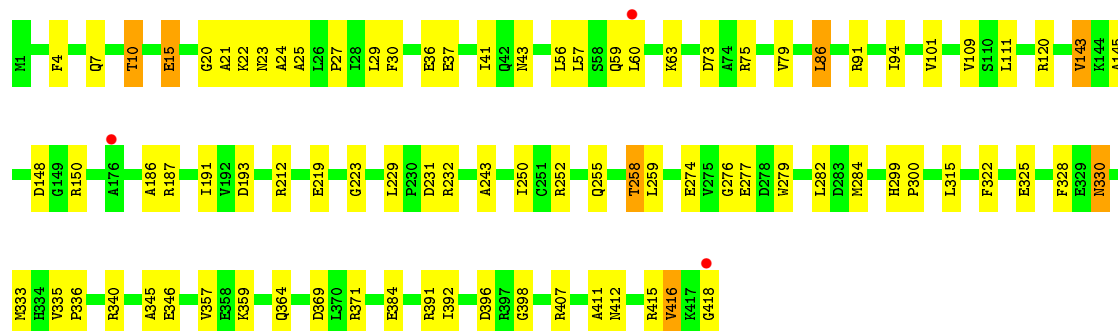
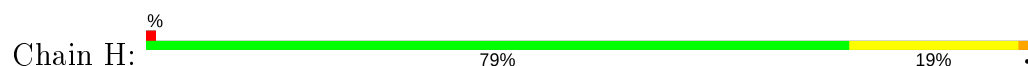
Chain G: 81% 17%



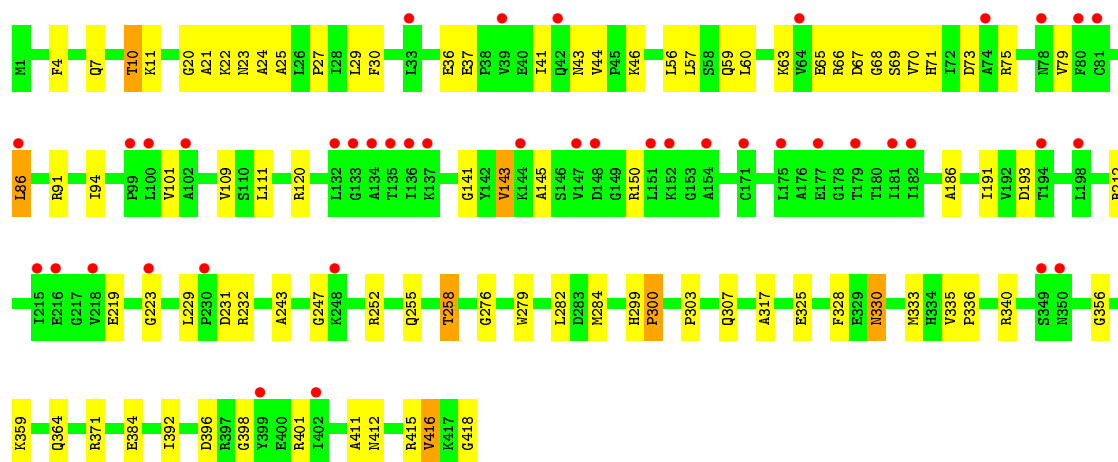
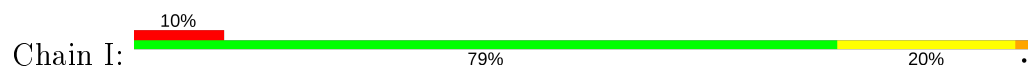




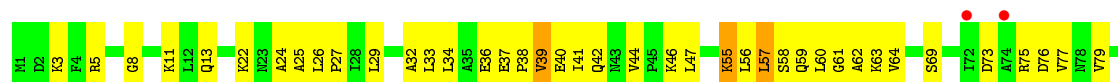
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

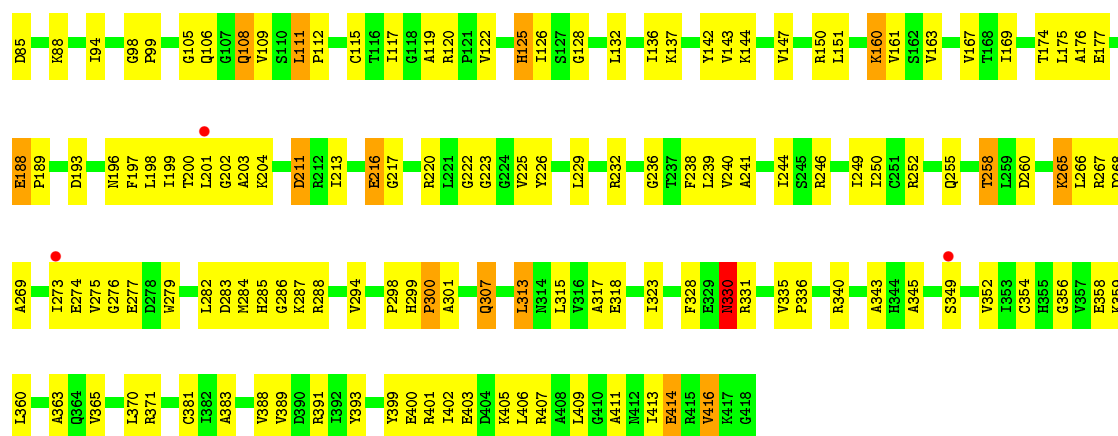


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

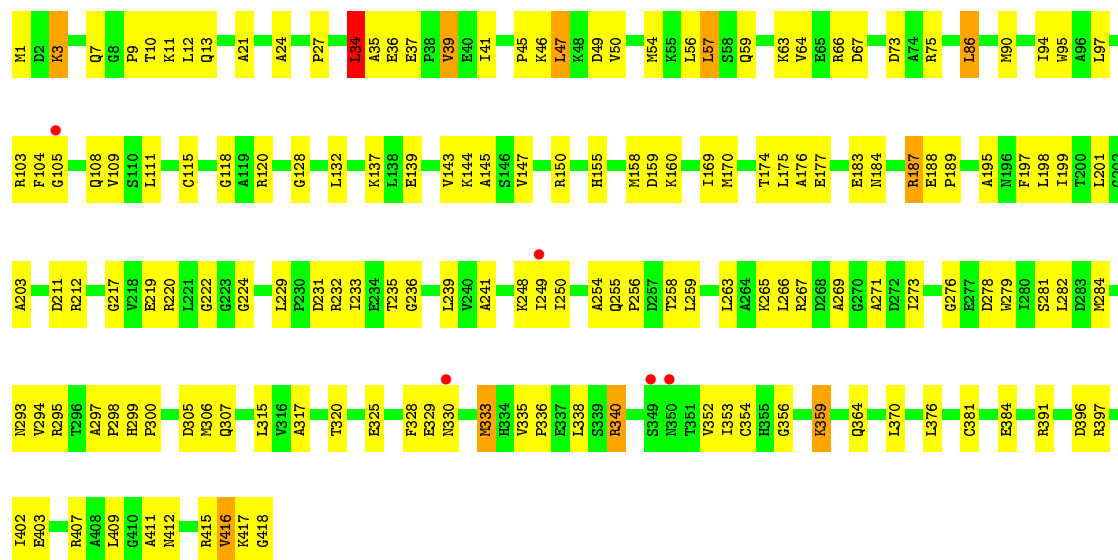


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

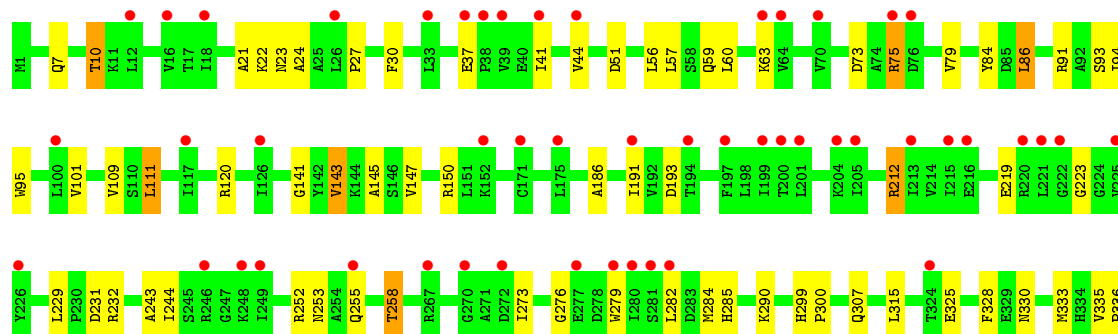
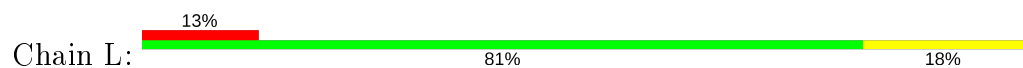


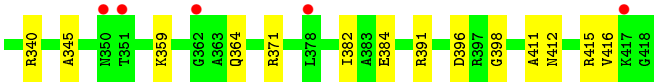


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



• 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, $\alpha$ , $\beta$ , $\gamma$	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)	97.5 (47.48-2.50) 97.6 (47.48-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.51Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.226 , 0.280 0.219 , 0.272	Depositor DCC
$R_{free}$ test set	8367 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	39035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: QPA, EPZ, IAS

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	0.56	0/3161	0.97	3/4278 (0.1%)
1	B	0.55	0/3161	0.90	2/4278 (0.0%)
1	C	0.61	1/3161 (0.0%)	0.92	4/4278 (0.1%)
1	D	0.62	0/3161	1.09	6/4278 (0.1%)
1	E	0.58	0/3161	0.91	2/4278 (0.0%)
1	F	0.59	3/3161 (0.1%)	0.92	2/4278 (0.0%)
1	G	0.56	0/3161	0.90	2/4278 (0.0%)
1	H	0.59	0/3161	0.92	2/4278 (0.0%)
1	I	0.55	0/3161	0.91	2/4278 (0.0%)
1	J	0.70	2/3161 (0.1%)	1.01	0/4278
1	K	0.72	0/3161	1.00	2/4278 (0.0%)
1	L	0.52	0/3161	1.07	7/4278 (0.2%)
All	All	0.60	6/37932 (0.0%)	0.96	34/51336 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	381	CYS	CB-SG	-5.45	1.73	1.81
1	J	330	ASN	CG-OD1	5.32	1.35	1.24
1	C	350	ASN	CG-OD1	5.14	1.35	1.24
1	F	381	CYS	CB-SG	-5.10	1.73	1.81
1	F	184	ASN	CG-OD1	5.04	1.35	1.24
1	F	42	GLN	CD-OE1	5.01	1.34	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	75	ARG	NE-CZ-NH1	-20.39	110.11	120.30
1	D	120	ARG	NE-CZ-NH1	-20.14	110.23	120.30
1	D	212	ARG	NE-CZ-NH1	-19.88	110.36	120.30
1	L	75	ARG	NE-CZ-NH2	19.34	129.97	120.30
1	L	212	ARG	NE-CZ-NH1	-19.15	110.73	120.30
1	L	212	ARG	NE-CZ-NH2	18.74	129.67	120.30
1	A	212	ARG	NE-CZ-NH1	-18.43	111.09	120.30
1	D	212	ARG	NE-CZ-NH2	18.29	129.44	120.30
1	D	120	ARG	NE-CZ-NH2	18.07	129.33	120.30
1	A	212	ARG	NE-CZ-NH2	17.89	129.25	120.30
1	L	212	ARG	CD-NE-CZ	9.63	137.08	123.60
1	C	212	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	I	212	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	H	212	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	A	212	ARG	CD-NE-CZ	9.38	136.73	123.60
1	D	212	ARG	CD-NE-CZ	9.23	136.53	123.60
1	F	212	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	B	212	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	I	212	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	E	212	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	B	212	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	F	212	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	G	212	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	H	212	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	E	212	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	L	75	ARG	CD-NE-CZ	7.91	134.67	123.60
1	D	120	ARG	CD-NE-CZ	7.61	134.26	123.60
1	C	212	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	G	212	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	K	34	LEU	CA-CB-CG	6.96	131.30	115.30
1	C	120	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	L	75	ARG	CG-CD-NE	5.28	122.89	111.80
1	K	417	LYS	N-CA-C	5.24	125.14	111.00
1	C	120	ARG	NE-CZ-NH2	-5.16	117.72	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	187	ARG	Sidechain
1	K	340	ARG	Sidechain

## 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	3143	0	3210	66	1
1	B	3143	0	3211	77	0
1	C	3143	0	3210	64	0
1	D	3143	0	3210	60	0
1	E	3143	0	3211	76	0
1	F	3143	0	3211	82	0
1	G	3143	0	3211	66	0
1	H	3143	0	3210	73	0
1	I	3143	0	3211	74	1
1	J	3143	0	3211	171	0
1	K	3143	0	3211	152	0
1	L	3143	0	3210	65	0
2	A	44	0	28	0	0
2	B	44	0	28	2	0
2	C	44	0	28	1	0
2	D	44	0	28	0	0
2	E	44	0	28	0	0
2	F	44	0	28	0	0
2	G	44	0	28	1	0
2	H	44	0	28	0	0
2	I	44	0	28	2	0
2	J	44	0	28	2	0
2	K	44	0	28	3	0
2	L	44	0	28	1	0
3	A	76	0	0	4	0
3	B	58	0	0	7	0
3	C	105	0	0	4	0
3	D	104	0	0	7	0
3	E	86	0	0	5	0
3	F	63	0	0	4	0
3	G	47	0	0	5	0
3	H	73	0	0	5	0
3	I	42	0	0	4	0
3	J	45	0	0	10	0
3	K	60	0	0	5	0
3	L	32	0	0	5	0
All	All	39035	0	38863	984	1

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 13.

All (984) 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:C:11:LYS:NZ	1:C:13:GLN:OE1	1.75	1.18
1:J:405:LYS:O	1:J:409:LEU:HD12	1.46	1.13
1:E:403:GLU:HG3	3:E:660:HOH:O	1.46	1.13
1:K:66:ARG:HG3	1:K:67:IAS:OXT	1.51	1.09
1:K:370:LEU:HD11	1:K:397:ARG:HB2	1.39	1.04
1:K:233:ILE:HA	1:K:306:MET:HE2	1.40	1.04
1:K:45:PRO:HG2	1:K:47:LEU:HD11	1.51	0.92
1:I:60:LEU:HA	1:I:79:VAL:HG13	1.52	0.91
1:D:60:LEU:HA	1:D:79:VAL:HG13	1.53	0.91
1:F:60:LEU:HA	1:F:79:VAL:HG13	1.50	0.91
1:K:174:THR:HG21	1:K:198:LEU:HD13	1.53	0.90
1:L:60:LEU:HA	1:L:79:VAL:HG13	1.51	0.90
1:B:150:ARG:HH12	1:B:219:GLU:HA	1.35	0.90
1:C:150:ARG:HH12	1:C:219:GLU:HA	1.36	0.90
1:C:60:LEU:HA	1:C:79:VAL:HG13	1.53	0.90
1:G:60:LEU:HA	1:G:79:VAL:HG13	1.53	0.90
1:H:60:LEU:HA	1:H:79:VAL:HG13	1.53	0.90
1:E:60:LEU:HA	1:E:79:VAL:HG13	1.52	0.90
1:B:60:LEU:HA	1:B:79:VAL:HG13	1.52	0.89
1:J:294:VAL:HB	1:J:323:ILE:HD13	1.52	0.89
1:J:60:LEU:HA	1:J:79:VAL:CG1	2.03	0.89
1:L:150:ARG:HH12	1:L:219:GLU:HA	1.36	0.89
1:E:150:ARG:HH12	1:E:219:GLU:HA	1.37	0.88
1:I:150:ARG:HH12	1:I:219:GLU:HA	1.38	0.88
1:A:150:ARG:HH12	1:A:219:GLU:HA	1.39	0.88
1:A:60:LEU:HA	1:A:79:VAL:HG13	1.54	0.88
1:F:150:ARG:HH12	1:F:219:GLU:HA	1.38	0.87
1:D:150:ARG:HH12	1:D:219:GLU:HA	1.39	0.87
1:H:150:ARG:HH12	1:H:219:GLU:HA	1.41	0.86
1:J:405:LYS:O	1:J:409:LEU:CD1	2.22	0.86
1:H:219:GLU:HG2	3:H:663:HOH:O	1.74	0.86
1:K:3:LYS:NZ	1:K:418:GLY:C	2.30	0.85
1:G:150:ARG:HH12	1:G:219:GLU:HA	1.43	0.83
1:K:183:GLU:OE1	1:K:212:ARG:HB2	1.79	0.83
1:K:255:GLN:O	1:K:258:THR:HG22	1.79	0.82
1:J:41:ILE:O	1:J:69:SER:HB2	1.79	0.82
1:K:46:LYS:HG2	1:K:66:ARG:NH2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:47:LEU:HD21	1:J:400:GLU:N	1.96	0.81
1:L:273:ILE:HB	3:L:622:HOH:O	1.79	0.80
1:H:15:GLU:OE2	1:H:252:ARG:NH1	2.15	0.80
1:J:59:GLN:O	1:J:79:VAL:HG11	1.80	0.79
1:A:303:PRO:HA	3:A:625:HOH:O	1.82	0.79
1:K:407:ARG:HA	1:K:411:ALA:HB3	1.65	0.78
1:E:404:ASP:OD1	1:J:277:GLU:HB3	1.84	0.78
1:H:274:GLU:HG2	3:H:665:HOH:O	1.84	0.77
1:K:295:ARG:HG3	1:K:295:ARG:HH11	1.50	0.77
1:K:108:GLN:HG2	1:K:144:LYS:NZ	2.00	0.77
1:C:207:GLY:O	1:C:210:THR:HG23	1.85	0.76
1:D:232:ARG:HB3	1:D:258:THR:CG2	2.15	0.76
1:F:66:ARG:HB3	1:F:70:VAL:HG22	1.65	0.76
1:I:232:ARG:HB3	1:I:258:THR:HG21	1.67	0.76
1:J:11:LYS:HE3	1:J:13:GLN:OE1	1.85	0.76
1:J:315:LEU:HD22	1:J:343:ALA:HB1	1.68	0.75
1:L:232:ARG:HB3	1:L:258:THR:HG21	1.68	0.75
1:H:232:ARG:HB3	1:H:258:THR:CG2	2.16	0.75
1:D:232:ARG:HB3	1:D:258:THR:HG21	1.69	0.75
1:I:120:ARG:HD2	3:I:621:HOH:O	1.85	0.75
1:K:36:GLU:HB2	1:K:220:ARG:NH2	2.02	0.75
1:I:232:ARG:HB3	1:I:258:THR:CG2	2.16	0.75
1:K:39:VAL:HG23	1:K:224:GLY:H	1.51	0.75
1:K:56:LEU:HD12	1:K:86:LEU:HD23	1.68	0.75
1:K:109:VAL:O	1:K:143:VAL:HG12	1.85	0.75
1:K:233:ILE:HA	1:K:306:MET:CE	2.16	0.74
1:A:232:ARG:HB3	1:A:258:THR:CG2	2.18	0.74
1:J:24:ALA:O	1:J:27:PRO:HD2	1.87	0.74
1:L:232:ARG:HB3	1:L:258:THR:CG2	2.17	0.74
1:G:232:ARG:HB3	1:G:258:THR:CG2	2.18	0.74
1:E:401:ARG:HG2	1:J:277:GLU:CD	2.06	0.74
1:J:8:GLY:HA3	1:J:383:ALA:O	1.87	0.74
1:C:232:ARG:HB3	1:C:258:THR:HG21	1.70	0.74
1:A:232:ARG:HB3	1:A:258:THR:HG21	1.68	0.73
1:B:232:ARG:HB3	1:B:258:THR:CG2	2.19	0.73
1:G:232:ARG:HB3	1:G:258:THR:HG21	1.71	0.73
1:J:22:LYS:HD3	1:J:371:ARG:HH21	1.54	0.73
1:J:199:ILE:O	1:J:202:GLY:N	2.22	0.73
1:F:330:ASN:HB3	1:G:330:ASN:ND2	2.04	0.73
1:F:66:ARG:HB3	1:F:70:VAL:CG2	2.19	0.72
1:K:187:ARG:NH1	1:K:300:PRO:HD3	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:VAL:HG23	1:K:224:GLY:N	2.05	0.72
1:J:335:VAL:HB	1:J:336:PRO:HD3	1.69	0.72
2:L:501:EPZ:H5DA	2:L:501:EPZ:H6U	1.69	0.72
1:H:232:ARG:HB3	1:H:258:THR:HG21	1.70	0.72
1:F:401:ARG:HG2	3:F:649:HOH:O	1.89	0.72
1:D:159:ASP:OD1	1:F:265:LYS:HE2	1.88	0.72
1:C:232:ARG:HB3	1:C:258:THR:CG2	2.20	0.71
1:D:252:ARG:HD2	3:D:640:HOH:O	1.90	0.71
1:B:232:ARG:HB3	1:B:258:THR:HG21	1.71	0.71
1:F:232:ARG:HB3	1:F:258:THR:HG21	1.71	0.71
1:J:117:ILE:HG22	1:J:331:ARG:HG3	1.72	0.71
1:F:232:ARG:HB3	1:F:258:THR:CG2	2.20	0.71
1:B:333:MET:O	1:B:336:PRO:HD2	1.90	0.71
1:G:333:MET:O	1:G:336:PRO:HD2	1.90	0.71
1:J:34:LEU:HD22	1:J:175:LEU:HD12	1.72	0.70
1:K:330:ASN:HB3	3:L:632:HOH:O	1.90	0.70
1:J:60:LEU:HD23	1:J:79:VAL:HG13	1.71	0.70
1:C:11:LYS:HE2	3:C:676:HOH:O	1.91	0.70
1:I:67:IAS:OD1	1:I:69:SER:N	2.24	0.70
1:J:109:VAL:O	1:J:143:VAL:HG13	1.91	0.70
1:K:115:QPA:H9	1:K:115:QPA:O13	1.91	0.69
1:K:57:LEU:HB3	1:K:64:VAL:HG21	1.73	0.69
1:J:161:VAL:HA	3:J:621:HOH:O	1.92	0.69
1:B:322:PHE:CE1	1:H:346:GLU:HG3	2.27	0.69
1:J:174:THR:HG21	1:J:198:LEU:HD13	1.74	0.69
1:J:238:PHE:O	1:J:241:ALA:HB3	1.92	0.69
1:H:369:ASP:HB2	3:H:629:HOH:O	1.93	0.68
1:C:333:MET:O	1:C:336:PRO:HD2	1.93	0.68
1:E:232:ARG:HB3	1:E:258:THR:CG2	2.23	0.68
1:B:265:LYS:HE2	1:E:159:ASP:OD1	1.94	0.68
1:E:232:ARG:HB3	1:E:258:THR:HG21	1.73	0.68
1:G:24:ALA:O	1:G:27:PRO:HD2	1.94	0.68
1:A:24:ALA:O	1:A:27:PRO:HD2	1.94	0.68
1:D:59:GLN:O	1:D:79:VAL:HG11	1.94	0.67
1:I:333:MET:O	1:I:336:PRO:HD2	1.93	0.67
1:A:120:ARG:HD2	3:A:662:HOH:O	1.95	0.67
1:K:10:THR:HG22	1:K:381:CYS:O	1.93	0.67
1:K:66:ARG:CG	1:K:67:IAS:OXT	2.36	0.67
1:B:59:GLN:O	1:B:79:VAL:HG11	1.95	0.67
1:H:120:ARG:HD3	1:H:328:PHE:CE1	2.29	0.67
1:J:299:HIS:ND1	1:J:300:PRO:HA	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ARG:NH1	1:C:364:GLN:O	2.28	0.66
1:K:67:IAS:OD1	1:K:67:IAS:C	2.40	0.66
1:L:24:ALA:O	1:L:27:PRO:HD2	1.96	0.66
1:J:22:LYS:HB3	1:J:371:ARG:NH2	2.10	0.66
1:D:333:MET:O	1:D:336:PRO:HD2	1.96	0.66
1:E:59:GLN:O	1:E:79:VAL:HG11	1.96	0.66
1:H:15:GLU:HG3	1:H:250:ILE:HB	1.78	0.66
1:F:67:IAS:OD1	1:F:69:SER:N	2.29	0.66
1:G:59:GLN:O	1:G:79:VAL:HG11	1.96	0.66
1:H:59:GLN:O	1:H:79:VAL:HG11	1.96	0.65
1:J:38:PRO:HD3	1:J:75:ARG:HH21	1.60	0.65
1:C:59:GLN:O	1:C:79:VAL:HG11	1.96	0.65
1:K:50:VAL:O	1:K:54:MET:HG3	1.95	0.65
1:F:59:GLN:O	1:F:79:VAL:HG11	1.96	0.65
1:K:250:ILE:HD13	1:K:281:SER:HB2	1.79	0.65
1:G:340:ARG:NH1	1:G:364:GLN:O	2.30	0.65
1:A:120:ARG:HD3	1:A:328:PHE:CE1	2.31	0.65
1:L:59:GLN:O	1:L:79:VAL:HG11	1.96	0.64
1:B:187:ARG:HD3	3:B:619:HOH:O	1.97	0.64
1:B:120:ARG:HD3	1:B:328:PHE:CE1	2.32	0.64
1:F:255:GLN:O	1:F:258:THR:HB	1.98	0.64
1:G:120:ARG:HD3	1:G:328:PHE:CE1	2.33	0.64
1:J:111:LEU:HD23	1:J:112:PRO:HD2	1.77	0.64
1:K:139:GLU:HG3	1:K:144:LYS:HD2	1.78	0.64
1:L:333:MET:O	1:L:336:PRO:HD2	1.98	0.64
1:D:47:LEU:HA	3:D:671:HOH:O	1.96	0.64
1:K:250:ILE:HD13	1:K:281:SER:CB	2.28	0.64
1:L:255:GLN:O	1:L:258:THR:HB	1.98	0.64
1:J:117:ILE:CG2	1:J:331:ARG:HG3	2.27	0.64
1:K:340:ARG:NH1	1:L:84:TYR:CE1	2.65	0.64
1:D:24:ALA:O	1:D:27:PRO:HD2	1.98	0.64
1:J:402:ILE:O	1:J:406:LEU:HB2	1.98	0.64
1:K:128:GLY:HA3	1:K:169:ILE:HD11	1.79	0.64
1:K:299:HIS:CG	1:K:300:PRO:HA	2.32	0.64
1:E:330:ASN:ND2	1:H:330:ASN:HB3	2.12	0.64
1:K:3:LYS:HZ3	1:K:418:GLY:C	2.00	0.64
1:L:120:ARG:HD3	1:L:328:PHE:CE1	2.33	0.64
1:L:335:VAL:HB	1:L:336:PRO:HD3	1.80	0.64
1:B:24:ALA:O	1:B:27:PRO:HD2	1.98	0.64
1:E:330:ASN:HB3	1:H:330:ASN:ND2	2.13	0.64
1:J:120:ARG:HD2	3:J:637:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:GLN:O	1:C:258:THR:HB	1.98	0.64
1:E:120:ARG:HD3	1:E:328:PHE:CE1	2.32	0.63
1:H:333:MET:O	1:H:336:PRO:HD2	1.98	0.63
1:K:97:LEU:HB2	1:K:109:VAL:HG21	1.80	0.63
1:E:401:ARG:HG2	1:J:277:GLU:OE2	1.98	0.63
1:J:287:LYS:HA	1:J:287:LYS:HE2	1.79	0.63
1:K:150:ARG:NH2	1:K:177:GLU:HG2	2.13	0.63
1:I:59:GLN:O	1:I:79:VAL:HG11	1.98	0.63
1:K:3:LYS:HB2	1:K:416:VAL:HG22	1.79	0.63
1:A:255:GLN:O	1:A:258:THR:HB	1.99	0.63
1:D:262:VAL:HG23	3:D:610:HOH:O	1.97	0.63
1:J:232:ARG:HB3	1:J:258:THR:HG23	1.79	0.63
1:F:333:MET:O	1:F:336:PRO:HD2	1.99	0.63
1:B:346:GLU:HG3	1:H:322:PHE:CE1	2.35	0.62
1:E:250:ILE:HG12	3:E:620:HOH:O	2.00	0.62
1:J:60:LEU:HA	1:J:79:VAL:HG13	1.81	0.62
1:D:152:LYS:HD2	3:D:650:HOH:O	1.98	0.62
1:D:255:GLN:O	1:D:258:THR:HB	1.98	0.62
1:K:12:LEU:HD12	1:K:241:ALA:HB1	1.80	0.62
1:J:211:ASP:OD2	1:K:187:ARG:NH1	2.31	0.62
1:D:335:VAL:HB	1:D:336:PRO:HD3	1.81	0.62
1:D:10:THR:HG21	1:D:411:ALA:HA	1.81	0.62
1:F:267:ARG:NH1	3:F:617:HOH:O	2.31	0.62
1:J:288:ARG:NH1	1:J:318:GLU:HB2	2.15	0.62
1:A:59:GLN:O	1:A:79:VAL:HG11	1.99	0.62
1:J:25:ALA:O	1:J:29:LEU:HD13	2.00	0.62
1:K:232:ARG:HB2	1:K:259:LEU:HD21	1.81	0.62
1:K:233:ILE:CA	1:K:306:MET:HE2	2.25	0.62
1:J:41:ILE:HD12	1:J:41:ILE:N	2.15	0.62
1:J:47:LEU:HD21	1:J:399:TYR:C	2.20	0.62
1:J:42:GLN:HA	1:J:69:SER:HB3	1.82	0.62
1:C:120:ARG:HD3	1:C:328:PHE:CE1	2.35	0.62
1:B:159:ASP:OD1	1:E:265:LYS:HE2	1.99	0.62
1:I:303:PRO:HB3	3:I:636:HOH:O	2.00	0.62
1:J:150:ARG:NH2	1:J:177:GLU:HB3	2.15	0.62
1:A:333:MET:O	1:A:336:PRO:HD2	1.99	0.61
2:B:501:EPZ:H5DA	2:B:501:EPZ:H6U	1.81	0.61
1:F:66:ARG:HB2	1:F:70:VAL:HG23	1.81	0.61
1:J:323:ILE:HB	1:J:352:VAL:CG1	2.29	0.61
1:K:118:GLY:HA3	3:K:629:HOH:O	2.00	0.61
1:A:330:ASN:HB3	1:B:330:ASN:ND2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:ALA:O	1:E:27:PRO:HD2	2.00	0.61
1:B:255:GLN:O	1:B:258:THR:HB	2.00	0.61
1:C:359:LYS:HE2	1:C:384:GLU:HB2	1.82	0.61
1:F:340:ARG:NH1	1:F:364:GLN:O	2.33	0.61
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.83	0.61
1:G:359:LYS:HE2	1:G:384:GLU:HB2	1.83	0.61
1:K:137:LYS:HE2	1:K:139:GLU:OE1	2.01	0.61
1:D:359:LYS:HE2	1:D:384:GLU:HB2	1.83	0.61
1:F:330:ASN:ND2	1:G:330:ASN:HB3	2.16	0.61
1:K:12:LEU:CD1	1:K:241:ALA:HB1	2.30	0.61
1:A:10:THR:HG21	1:A:411:ALA:HA	1.82	0.61
1:C:120:ARG:HD2	3:C:694:HOH:O	2.00	0.61
1:K:105:GLY:HA2	1:K:147:VAL:HG12	1.83	0.61
1:E:359:LYS:HE2	1:E:384:GLU:HB2	1.82	0.61
1:G:150:ARG:NH2	3:G:635:HOH:O	2.34	0.61
1:F:42:GLN:HG2	1:F:69:SER:OG	2.01	0.60
1:A:56:LEU:HB2	1:A:86:LEU:HD22	1.83	0.60
1:F:120:ARG:HD3	1:F:328:PHE:CE1	2.35	0.60
2:K:501:EPZ:H6U	2:K:501:EPZ:H5DA	1.82	0.60
1:E:404:ASP:OD2	1:J:277:GLU:HG2	2.02	0.60
1:B:46:LYS:NZ	3:B:615:HOH:O	2.34	0.60
1:E:333:MET:O	1:E:336:PRO:HD2	2.01	0.60
1:H:255:GLN:O	1:H:258:THR:HB	2.02	0.60
1:C:10:THR:HG21	1:C:411:ALA:HA	1.82	0.60
1:H:340:ARG:NH1	1:H:364:GLN:O	2.34	0.60
1:J:204:LYS:CB	1:J:216:GLU:HB3	2.32	0.60
1:J:276:GLY:HA3	1:J:279:TRP:NE1	2.17	0.60
1:K:258:THR:HG21	3:K:625:HOH:O	2.02	0.60
1:J:126:ILE:HG23	1:J:136:ILE:HD12	1.83	0.60
1:J:3:LYS:HD3	1:J:388:VAL:CG1	2.32	0.60
1:B:359:LYS:HE2	1:B:384:GLU:HB2	1.83	0.60
1:I:120:ARG:HD3	1:I:328:PHE:CE1	2.37	0.60
1:B:10:THR:HG21	1:B:411:ALA:HA	1.84	0.59
1:G:255:GLN:O	1:G:258:THR:HB	2.02	0.59
1:K:370:LEU:CD1	1:K:397:ARG:HB2	2.24	0.59
1:B:322:PHE:HE1	1:H:346:GLU:HG3	1.67	0.59
1:I:335:VAL:HB	1:I:336:PRO:HD3	1.85	0.59
1:J:406:LEU:O	1:J:411:ALA:HB3	2.01	0.59
1:I:359:LYS:HE2	1:I:384:GLU:HB2	1.85	0.59
1:C:60:LEU:HA	1:C:79:VAL:CG1	2.31	0.59
1:F:24:ALA:O	1:F:27:PRO:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:255:GLN:O	1:I:258:THR:HB	2.02	0.59
1:K:220:ARG:HG3	1:K:220:ARG:HH11	1.66	0.59
2:I:501:EPZ:H6U	2:I:501:EPZ:H5DA	1.85	0.59
1:F:335:VAL:HB	1:F:336:PRO:HD3	1.85	0.59
1:F:66:ARG:CB	1:F:70:VAL:CG2	2.80	0.59
1:K:402:ILE:HG23	1:K:403:GLU:N	2.18	0.59
1:J:236:GLY:O	1:J:240:VAL:HG23	2.03	0.58
1:L:10:THR:HG21	1:L:411:ALA:HA	1.83	0.58
1:L:37:GLU:HB2	1:L:223:GLY:N	2.17	0.58
1:I:340:ARG:NH1	1:I:364:GLN:O	2.36	0.58
1:J:255:GLN:O	1:J:258:THR:HB	2.03	0.58
2:J:501:EPZ:H5DA	2:J:501:EPZ:H6U	1.85	0.58
1:K:94:ILE:HA	1:K:109:VAL:HG11	1.84	0.58
1:G:56:LEU:HB2	1:G:86:LEU:HD22	1.86	0.58
1:H:24:ALA:O	1:H:27:PRO:HD2	2.03	0.58
1:D:109:VAL:O	1:D:143:VAL:HG13	2.02	0.58
1:G:383:ALA:HB3	3:G:623:HOH:O	2.02	0.58
1:K:340:ARG:HH21	1:L:141:GLY:HA3	1.68	0.58
1:F:10:THR:HG21	1:F:411:ALA:HA	1.85	0.58
1:A:109:VAL:O	1:A:143:VAL:HG13	2.04	0.58
1:C:11:LYS:NZ	1:C:13:GLN:CD	2.56	0.58
1:K:333:MET:O	1:K:336:PRO:HD2	2.04	0.58
1:J:22:LYS:HB3	1:J:371:ARG:HH21	1.67	0.58
1:L:73:ASP:OD1	1:L:75:ARG:HD3	2.03	0.58
1:E:255:GLN:O	1:E:258:THR:HB	2.04	0.57
1:H:120:ARG:HD3	1:H:328:PHE:HE1	1.69	0.57
1:J:267:ARG:NH1	3:J:639:HOH:O	2.36	0.57
1:K:340:ARG:HG2	1:L:111:LEU:HB3	1.85	0.57
1:L:359:LYS:HE2	1:L:384:GLU:HB2	1.85	0.57
1:A:359:LYS:HE2	1:A:384:GLU:HB2	1.86	0.57
1:F:359:LYS:HE2	1:F:384:GLU:HB2	1.85	0.57
1:F:66:ARG:CB	1:F:70:VAL:HG23	2.34	0.57
1:I:24:ALA:O	1:I:27:PRO:HD2	2.05	0.57
1:I:66:ARG:O	1:I:67:IAS:C	2.52	0.57
1:H:359:LYS:HE2	1:H:384:GLU:HB2	1.85	0.57
1:C:325:GLU:HG2	1:C:328:PHE:O	2.03	0.57
1:J:204:LYS:HB2	1:J:216:GLU:HB3	1.84	0.57
1:L:109:VAL:O	1:L:143:VAL:HG13	2.05	0.57
1:E:109:VAL:O	1:E:143:VAL:HG13	2.04	0.57
1:H:325:GLU:HG2	1:H:328:PHE:O	2.04	0.57
1:J:232:ARG:HB3	1:J:258:THR:CG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:252:ARG:HH11	1:J:252:ARG:HG3	1.69	0.57
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.85	0.56
1:B:71:HIS:HD2	3:B:644:HOH:O	1.86	0.56
1:J:22:LYS:HD3	1:J:371:ARG:NH2	2.19	0.56
1:K:266:LEU:O	1:K:269:ALA:N	2.38	0.56
1:K:340:ARG:NH1	1:K:364:GLN:O	2.38	0.56
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.87	0.56
1:J:266:LEU:O	1:J:269:ALA:HB3	2.05	0.56
1:B:71:HIS:CD2	3:B:644:HOH:O	2.58	0.56
1:G:325:GLU:HG2	1:G:328:PHE:O	2.04	0.56
1:J:240:VAL:O	1:J:244:ILE:HG12	2.06	0.56
1:J:391:ARG:HD2	1:J:393:TYR:HE2	1.69	0.56
1:B:56:LEU:HB2	1:B:86:LEU:HD22	1.87	0.56
1:G:10:THR:HG21	1:G:411:ALA:HA	1.86	0.56
1:G:55:LYS:NZ	3:G:614:HOH:O	2.33	0.56
1:J:267:ARG:HD2	3:J:639:HOH:O	2.05	0.56
1:J:55:LYS:NZ	3:J:625:HOH:O	2.30	0.56
1:K:276:GLY:HA3	1:K:279:TRP:CE2	2.41	0.56
1:L:325:GLU:HG2	1:L:328:PHE:O	2.06	0.56
1:F:359:LYS:NZ	1:F:384:GLU:OE1	2.36	0.56
1:H:10:THR:HG21	1:H:411:ALA:HA	1.87	0.56
1:K:143:VAL:HG13	1:K:143:VAL:O	2.06	0.56
1:J:406:LEU:O	1:J:411:ALA:CB	2.53	0.55
1:K:254:ALA:O	1:K:278:ASP:HA	2.06	0.55
1:K:47:LEU:CD1	1:K:50:VAL:HG23	2.36	0.55
1:I:109:VAL:O	1:I:143:VAL:HG13	2.06	0.55
1:J:246:ARG:NH2	1:J:288:ARG:HD2	2.20	0.55
1:L:290:LYS:HB3	3:L:626:HOH:O	2.05	0.55
1:C:24:ALA:O	1:C:27:PRO:HD2	2.05	0.55
1:H:109:VAL:O	1:H:143:VAL:HG13	2.07	0.55
1:K:325:GLU:HG2	1:K:328:PHE:O	2.07	0.55
1:E:56:LEU:HB2	1:E:86:LEU:HD22	1.88	0.55
1:J:85:ASP:HA	1:J:88:LYS:HE2	1.88	0.55
1:J:3:LYS:HD3	1:J:388:VAL:HG12	1.89	0.55
1:K:340:ARG:NH2	1:L:141:GLY:HA3	2.22	0.55
1:K:407:ARG:CA	1:K:411:ALA:HB3	2.36	0.55
1:I:330:ASN:HB3	1:J:330:ASN:OD1	2.07	0.55
1:L:340:ARG:NH1	1:L:364:GLN:O	2.40	0.55
1:D:56:LEU:HB2	1:D:86:LEU:HD22	1.88	0.55
1:E:335:VAL:HB	1:E:336:PRO:HD3	1.88	0.55
1:E:10:THR:HG21	1:E:411:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10:THR:HG21	1:I:411:ALA:HA	1.89	0.55
1:L:299:HIS:CG	1:L:300:PRO:HA	2.42	0.55
1:A:325:GLU:HG2	1:A:328:PHE:O	2.08	0.54
1:D:37:GLU:HB2	1:D:223:GLY:N	2.22	0.54
1:B:340:ARG:NH1	1:B:364:GLN:O	2.40	0.54
1:G:299:HIS:ND1	1:G:300:PRO:HA	2.23	0.54
1:K:3:LYS:HZ1	1:K:418:GLY:C	2.10	0.54
1:G:109:VAL:O	1:G:143:VAL:HG13	2.07	0.54
1:J:5:ARG:HD2	1:J:414:GLU:OE1	2.08	0.54
1:K:11:LYS:HD2	1:K:13:GLN:OE1	2.07	0.54
1:B:299:HIS:CG	1:B:300:PRO:HA	2.43	0.54
1:E:37:GLU:HB2	1:E:223:GLY:N	2.23	0.54
1:E:150:ARG:NH1	1:E:219:GLU:HA	2.17	0.54
1:E:330:ASN:OD1	1:H:330:ASN:OD1	2.26	0.54
1:A:252:ARG:HH11	1:A:252:ARG:HG3	1.73	0.54
1:H:335:VAL:HB	1:H:336:PRO:HD3	1.89	0.54
1:J:299:HIS:CG	1:J:300:PRO:HA	2.43	0.54
1:C:150:ARG:NH1	1:C:219:GLU:HA	2.16	0.54
1:F:299:HIS:CG	1:F:300:PRO:HA	2.43	0.54
1:J:128:GLY:HA3	1:J:169:ILE:CD1	2.38	0.54
1:K:27:PRO:HG3	1:K:95:TRP:CZ3	2.42	0.54
1:L:252:ARG:HG3	1:L:252:ARG:HH11	1.73	0.54
1:L:56:LEU:HB2	1:L:86:LEU:HD22	1.90	0.54
1:C:37:GLU:HB2	1:C:223:GLY:N	2.23	0.53
1:G:120:ARG:HD3	1:G:328:PHE:HE1	1.72	0.53
1:G:335:VAL:HB	1:G:336:PRO:HD3	1.89	0.53
1:A:37:GLU:HB2	1:A:223:GLY:N	2.24	0.53
1:K:235:THR:O	1:K:239:LEU:HG	2.07	0.53
1:D:325:GLU:HG2	1:D:328:PHE:O	2.07	0.53
1:K:36:GLU:O	1:K:37:GLU:HG2	2.08	0.53
1:I:65:GLU:HG3	1:I:71:HIS:HB2	1.90	0.53
1:B:60:LEU:HA	1:B:79:VAL:CG1	2.32	0.53
1:G:37:GLU:HB2	1:G:223:GLY:N	2.23	0.53
2:G:501:EPZ:H5DA	2:G:501:EPZ:H6U	1.89	0.53
1:G:60:LEU:HA	1:G:79:VAL:CG1	2.35	0.53
1:E:252:ARG:HH11	1:E:252:ARG:HG3	1.72	0.53
1:I:67:IAS:CG	1:I:69:SER:N	2.72	0.53
1:J:282:LEU:HD23	1:J:283:ASP:N	2.23	0.53
1:A:371:ARG:NH2	3:A:608:HOH:O	2.40	0.53
1:A:56:LEU:HB2	1:A:86:LEU:CD2	2.39	0.53
1:B:261:ALA:HB3	3:B:604:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:ARG:NH1	1:L:219:GLU:HA	2.16	0.53
1:D:299:HIS:CG	1:D:300:PRO:HA	2.44	0.53
1:I:37:GLU:HB2	1:I:223:GLY:N	2.23	0.53
1:K:183:GLU:OE2	1:K:212:ARG:HD2	2.08	0.53
1:B:299:HIS:ND1	1:B:300:PRO:HA	2.24	0.53
1:E:219:GLU:HG2	3:E:661:HOH:O	2.08	0.53
1:E:359:LYS:NZ	1:E:384:GLU:OE1	2.33	0.53
1:K:120:ARG:HD3	1:K:328:PHE:CE1	2.44	0.53
1:L:371:ARG:NH1	1:L:398:GLY:O	2.42	0.53
2:C:501:EPZ:H5DA	2:C:501:EPZ:H6U	1.91	0.52
1:D:63:LYS:HB2	1:D:73:ASP:HB3	1.91	0.52
1:E:325:GLU:HG2	1:E:328:PHE:O	2.09	0.52
1:J:46:LYS:HB2	1:J:400:GLU:HG3	1.90	0.52
1:C:109:VAL:O	1:C:143:VAL:HG13	2.09	0.52
1:F:252:ARG:HH11	1:F:252:ARG:HG3	1.74	0.52
1:K:150:ARG:HH21	1:K:177:GLU:HG2	1.72	0.52
1:K:24:ALA:O	1:K:27:PRO:HD2	2.10	0.52
1:E:340:ARG:NH1	1:E:364:GLN:O	2.42	0.52
1:F:330:ASN:CG	1:G:330:ASN:CG	2.68	0.52
1:H:252:ARG:HH11	1:H:252:ARG:HG3	1.75	0.52
1:A:340:ARG:NH1	1:A:364:GLN:O	2.42	0.52
1:B:265:LYS:CE	1:E:159:ASP:OD1	2.58	0.52
1:I:46:LYS:HG2	1:I:66:ARG:NH2	2.25	0.52
1:J:176:ALA:O	1:J:217:GLY:HA3	2.10	0.52
1:J:196:ASN:HB2	1:J:226:TYR:OH	2.10	0.52
1:C:5:ARG:NH1	3:C:614:HOH:O	2.29	0.52
1:J:42:GLN:OE1	1:J:225:VAL:HG11	2.09	0.52
1:K:187:ARG:NH1	1:K:300:PRO:CD	2.72	0.52
1:J:128:GLY:HA3	1:J:169:ILE:HD11	1.91	0.52
1:E:120:ARG:HD3	1:E:328:PHE:HE1	1.71	0.52
1:E:299:HIS:ND1	1:E:300:PRO:HA	2.24	0.52
1:K:108:GLN:HG2	1:K:144:LYS:CE	2.40	0.52
1:A:330:ASN:ND2	1:B:330:ASN:HB3	2.24	0.52
1:H:56:LEU:HB2	1:H:86:LEU:HD22	1.91	0.52
1:I:325:GLU:HG2	1:I:328:PHE:O	2.10	0.52
1:H:282:LEU:C	1:H:282:LEU:HD23	2.30	0.52
1:J:73:ASP:CG	1:J:75:ARG:HG2	2.31	0.52
1:F:60:LEU:HA	1:F:79:VAL:CG1	2.32	0.51
1:H:37:GLU:HB2	1:H:223:GLY:N	2.26	0.51
1:K:183:GLU:O	1:K:184:ASN:CB	2.58	0.51
1:K:1:MET:CE	1:K:391:ARG:HB3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:LEU:HA	1:E:79:VAL:CG1	2.34	0.51
1:J:163:VAL:O	1:J:167:VAL:HG23	2.09	0.51
1:J:315:LEU:HD21	1:J:345:ALA:HB2	1.92	0.51
1:K:338:LEU:HD21	1:K:376:LEU:HD23	1.92	0.51
1:E:21:ALA:HA	1:E:231:ASP:HB2	1.92	0.51
1:I:359:LYS:NZ	1:I:384:GLU:OE1	2.41	0.51
1:I:60:LEU:HA	1:I:79:VAL:CG1	2.33	0.51
1:J:401:ARG:O	1:J:405:LYS:HG3	2.11	0.51
1:K:254:ALA:O	1:K:256:PRO:HD3	2.11	0.51
1:K:353:ILE:N	1:K:353:ILE:HD12	2.25	0.51
1:A:22:LYS:NZ	1:A:23:ASN:OD1	2.44	0.51
1:B:150:ARG:NH1	1:B:219:GLU:HA	2.16	0.51
1:C:56:LEU:HB2	1:C:86:LEU:HD22	1.91	0.51
1:J:122:VAL:O	1:J:122:VAL:HG23	2.10	0.51
1:L:120:ARG:HD3	1:L:328:PHE:HE1	1.74	0.51
1:F:150:ARG:NH1	1:F:219:GLU:HA	2.18	0.51
1:K:407:ARG:HG3	1:K:411:ALA:O	2.10	0.51
1:B:120:ARG:HD3	1:B:328:PHE:HE1	1.74	0.51
1:G:359:LYS:NZ	1:G:384:GLU:OE1	2.40	0.51
1:J:136:ILE:HG22	1:J:137:LYS:N	2.25	0.51
1:J:213:ILE:HD11	3:J:618:HOH:O	2.09	0.51
1:A:396:ASP:OD2	1:A:415:ARG:NH2	2.44	0.51
1:B:21:ALA:HA	1:B:231:ASP:HB2	1.91	0.51
1:H:359:LYS:NZ	1:H:384:GLU:OE1	2.37	0.51
1:J:391:ARG:HD2	1:J:393:TYR:CE2	2.46	0.51
1:C:252:ARG:HH11	1:C:252:ARG:HG3	1.76	0.51
1:A:346:GLU:HG3	1:E:322:PHE:HE1	1.76	0.51
1:A:288:ARG:HB2	3:D:690:HOH:O	2.11	0.51
1:B:36:GLU:O	1:B:75:ARG:HG2	2.11	0.51
1:J:22:LYS:HE3	1:J:370:LEU:HD12	1.92	0.51
1:L:285:HIS:CD2	3:L:623:HOH:O	2.62	0.51
1:I:41:ILE:HD12	1:I:41:ILE:N	2.26	0.51
1:J:197:PHE:O	1:J:200:THR:HB	2.10	0.51
1:J:299:HIS:CE1	1:J:300:PRO:HA	2.46	0.51
1:K:195:ALA:O	1:K:199:ILE:HG13	2.10	0.51
1:C:299:HIS:CG	1:C:300:PRO:HA	2.46	0.50
1:D:21:ALA:HA	1:D:231:ASP:HB2	1.93	0.50
1:F:109:VAL:O	1:F:143:VAL:HG13	2.11	0.50
1:G:63:LYS:HB2	1:G:73:ASP:HB3	1.93	0.50
1:A:282:LEU:HD23	1:A:282:LEU:C	2.32	0.50
1:E:299:HIS:CG	1:E:300:PRO:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ALA:HA	1:F:231:ASP:HB2	1.93	0.50
1:H:299:HIS:CG	1:H:300:PRO:HA	2.46	0.50
1:J:94:ILE:HA	1:J:109:VAL:HG11	1.92	0.50
1:K:295:ARG:NH1	1:K:295:ARG:HG3	2.24	0.50
1:L:150:ARG:HH12	1:L:219:GLU:CA	2.17	0.50
1:A:120:ARG:HD3	1:A:328:PHE:HE1	1.73	0.50
1:A:41:ILE:N	1:A:41:ILE:HD12	2.25	0.50
1:B:30:PHE:HE1	1:B:56:LEU:HD23	1.77	0.50
1:C:282:LEU:C	1:C:282:LEU:HD23	2.32	0.50
1:I:67:IAS:OD1	1:I:69:SER:O	2.29	0.50
1:K:103:ARG:HD3	1:K:104:PHE:CZ	2.46	0.50
1:K:297:ALA:HB1	1:K:298:PRO:HD2	1.94	0.50
1:K:66:ARG:HG3	1:K:67:IAS:N	2.25	0.50
1:F:56:LEU:HB2	1:F:86:LEU:HD22	1.92	0.50
1:G:21:ALA:HA	1:G:231:ASP:HB2	1.92	0.50
1:J:119:ALA:O	1:J:120:ARG:HG2	2.11	0.50
1:J:98:GLY:O	1:J:99:PRO:C	2.49	0.50
1:K:75:ARG:HG2	3:K:603:HOH:O	2.11	0.50
1:C:295:ARG:NH2	1:F:348:GLU:OE1	2.41	0.50
1:F:330:ASN:OD1	1:G:330:ASN:OD1	2.29	0.50
1:G:56:LEU:HB2	1:G:86:LEU:CD2	2.41	0.50
1:J:60:LEU:HD22	1:J:79:VAL:O	2.11	0.50
1:G:396:ASP:OD2	1:G:415:ARG:NH2	2.45	0.50
1:K:340:ARG:NH1	1:L:84:TYR:HE1	2.08	0.50
1:E:56:LEU:HB2	1:E:86:LEU:CD2	2.42	0.50
1:F:67:IAS:OD1	1:F:69:SER:O	2.30	0.50
1:I:56:LEU:HB2	1:I:86:LEU:HD22	1.92	0.50
1:K:271:ALA:HB1	1:K:282:LEU:HG	1.94	0.50
1:A:63:LYS:HB2	1:A:73:ASP:HB3	1.93	0.50
1:H:41:ILE:N	1:H:41:ILE:HD12	2.26	0.50
1:I:401:ARG:HA	3:I:619:HOH:O	2.11	0.50
1:J:111:LEU:HD23	1:J:112:PRO:CD	2.41	0.50
1:L:299:HIS:ND1	1:L:300:PRO:HA	2.27	0.50
1:F:37:GLU:HB2	1:F:223:GLY:N	2.27	0.50
1:F:325:GLU:HG2	1:F:328:PHE:O	2.11	0.50
1:I:299:HIS:CG	1:I:300:PRO:HA	2.46	0.50
1:J:5:ARG:NH1	1:J:416:VAL:HG11	2.27	0.50
1:K:233:ILE:HD12	1:K:305:ASP:HB2	1.93	0.50
1:G:252:ARG:HH11	1:G:252:ARG:HG3	1.76	0.49
1:G:299:HIS:CG	1:G:300:PRO:HA	2.47	0.49
1:J:37:GLU:HB2	1:J:222:GLY:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:HIS:ND1	1:F:300:PRO:HA	2.26	0.49
1:F:371:ARG:NH1	1:F:398:GLY:O	2.45	0.49
1:I:282:LEU:C	1:I:282:LEU:HD23	2.33	0.49
1:J:5:ARG:NH1	1:J:5:ARG:HB2	2.27	0.49
1:C:120:ARG:HD3	1:C:328:PHE:HE1	1.76	0.49
1:C:348:GLU:HG3	1:F:322:PHE:CE2	2.47	0.49
1:G:7:GLN:HB2	1:G:412:ASN:HB3	1.94	0.49
1:I:66:ARG:C	1:I:67:IAS:OXT	2.45	0.49
1:E:404:ASP:OD2	1:J:277:GLU:CG	2.60	0.49
1:K:297:ALA:HB1	1:K:298:PRO:CD	2.42	0.49
1:K:66:ARG:NE	1:K:67:IAS:OXT	2.44	0.49
1:A:22:LYS:HD2	1:A:398:GLY:HA2	1.95	0.49
1:C:330:ASN:ND2	1:D:330:ASN:HB3	2.27	0.49
1:E:404:ASP:OD2	1:J:277:GLU:OE1	2.31	0.49
1:J:407:ARG:HA	1:J:411:ALA:HB3	1.94	0.49
1:K:27:PRO:HG3	1:K:95:TRP:CH2	2.48	0.49
1:K:97:LEU:HB2	1:K:109:VAL:CG2	2.42	0.49
1:B:94:ILE:HA	1:B:109:VAL:HG11	1.94	0.49
1:C:7:GLN:HB2	1:C:412:ASN:HB3	1.93	0.49
1:J:307:GLN:HG2	1:J:323:ILE:HG21	1.95	0.49
1:J:5:ARG:HH12	1:J:416:VAL:HG11	1.77	0.49
1:D:56:LEU:HB2	1:D:86:LEU:CD2	2.43	0.49
1:I:67:IAS:OD1	1:I:68:GLY:C	2.51	0.49
1:I:66:ARG:O	1:I:67:IAS:OXT	2.30	0.49
1:J:108:GLN:HG2	1:J:144:LYS:HE2	1.95	0.49
1:K:24:ALA:C	1:K:27:PRO:HD2	2.33	0.49
1:A:359:LYS:NZ	1:A:384:GLU:OE1	2.39	0.49
1:K:21:ALA:HA	1:K:231:ASP:HB2	1.93	0.49
1:B:325:GLU:HG2	1:B:328:PHE:O	2.11	0.49
1:D:94:ILE:HA	1:D:109:VAL:HG11	1.95	0.49
1:H:63:LYS:HB2	1:H:73:ASP:HB3	1.95	0.49
1:L:51:ASP:HB3	3:L:628:HOH:O	2.13	0.49
1:G:22:LYS:HD2	1:G:398:GLY:HA2	1.95	0.49
1:H:299:HIS:ND1	1:H:300:PRO:HA	2.28	0.49
1:I:63:LYS:HB2	1:I:73:ASP:HB3	1.95	0.49
1:B:350:ASN:OD1	3:B:618:HOH:O	2.20	0.48
1:D:299:HIS:ND1	1:D:300:PRO:HA	2.28	0.48
1:C:330:ASN:HB3	1:D:330:ASN:ND2	2.27	0.48
1:F:120:ARG:HD3	1:F:328:PHE:HE1	1.78	0.48
1:J:29:LEU:O	1:J:32:ALA:HB3	2.12	0.48
1:L:63:LYS:HB2	1:L:73:ASP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:ASP:OD2	1:D:415:ARG:NH2	2.45	0.48
1:F:186:ALA:HB3	1:F:191:ILE:CD1	2.44	0.48
1:F:396:ASP:OD2	1:F:415:ARG:NH2	2.44	0.48
1:I:299:HIS:ND1	1:I:300:PRO:HA	2.28	0.48
1:J:201:LEU:HD22	1:J:223:GLY:HA2	1.96	0.48
1:L:21:ALA:HA	1:L:231:ASP:HB2	1.95	0.48
1:L:396:ASP:OD2	1:L:415:ARG:NH2	2.44	0.48
1:C:56:LEU:HB2	1:C:86:LEU:CD2	2.43	0.48
1:E:94:ILE:HA	1:E:109:VAL:HG11	1.96	0.48
1:H:56:LEU:HB2	1:H:86:LEU:CD2	2.44	0.48
1:B:35:ALA:HB1	1:B:222:GLY:O	2.13	0.48
1:D:150:ARG:NH1	1:D:219:GLU:HA	2.19	0.48
1:E:330:ASN:CG	1:H:330:ASN:CG	2.72	0.48
1:I:252:ARG:HH11	1:I:252:ARG:HG3	1.78	0.48
1:J:150:ARG:CZ	1:J:177:GLU:HB3	2.43	0.48
1:J:340:ARG:HH12	1:J:363:ALA:HB1	1.79	0.48
1:K:158:MET:O	1:K:159:ASP:C	2.52	0.48
1:A:299:HIS:CG	1:A:300:PRO:HA	2.49	0.48
1:B:109:VAL:O	1:B:143:VAL:HG13	2.13	0.48
1:K:155:HIS:CE1	3:K:653:HOH:O	2.67	0.48
1:A:94:ILE:HA	1:A:109:VAL:HG11	1.94	0.48
1:D:232:ARG:CB	1:D:258:THR:CG2	2.91	0.48
1:E:7:GLN:HB2	1:E:412:ASN:HB3	1.96	0.48
1:H:21:ALA:HA	1:H:231:ASP:HB2	1.94	0.48
1:K:233:ILE:O	1:K:306:MET:HE1	2.14	0.48
1:B:396:ASP:OD2	1:B:415:ARG:NH2	2.46	0.48
1:D:340:ARG:NH1	1:D:364:GLN:O	2.46	0.48
1:F:94:ILE:HA	1:F:109:VAL:HG11	1.95	0.48
1:F:36:GLU:O	1:F:75:ARG:HG2	2.14	0.48
1:F:7:GLN:HB2	1:F:412:ASN:HB3	1.96	0.48
1:H:94:ILE:HA	1:H:109:VAL:HG11	1.94	0.48
1:H:232:ARG:CB	1:H:258:THR:CG2	2.90	0.48
1:L:30:PHE:HE1	1:L:56:LEU:HD23	1.79	0.48
1:L:56:LEU:HB2	1:L:86:LEU:CD2	2.42	0.48
1:L:22:LYS:HD2	1:L:398:GLY:HA2	1.96	0.48
1:E:30:PHE:HE1	1:E:56:LEU:HD23	1.78	0.47
1:G:287:LYS:HE2	3:G:646:HOH:O	2.13	0.47
1:K:36:GLU:C	1:K:37:GLU:HG2	2.34	0.47
1:L:60:LEU:HA	1:L:79:VAL:CG1	2.33	0.47
1:A:150:ARG:NH1	1:A:219:GLU:HA	2.19	0.47
1:A:346:GLU:HG3	1:E:322:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:ILE:HA	1:G:109:VAL:HG11	1.94	0.47
1:J:62:ALA:O	1:J:64:VAL:HG23	2.13	0.47
1:L:315:LEU:HD21	1:L:345:ALA:HB2	1.97	0.47
1:A:330:ASN:CG	1:B:330:ASN:CG	2.72	0.47
1:B:63:LYS:HB2	1:B:73:ASP:HB3	1.95	0.47
1:D:371:ARG:NH1	1:D:398:GLY:O	2.46	0.47
1:J:143:VAL:HG22	1:J:143:VAL:O	2.13	0.47
1:J:403:GLU:CB	1:J:413:ILE:HD13	2.44	0.47
1:C:348:GLU:CD	1:F:322:PHE:CE2	2.88	0.47
1:I:150:ARG:NH1	1:I:219:GLU:HA	2.18	0.47
1:J:198:LEU:O	1:J:203:ALA:CB	2.62	0.47
1:J:33:LEU:HD21	1:J:57:LEU:HD12	1.97	0.47
1:K:35:ALA:HB1	1:K:222:GLY:O	2.15	0.47
1:B:282:LEU:HD23	1:B:282:LEU:C	2.35	0.47
1:B:56:LEU:HB2	1:B:86:LEU:CD2	2.45	0.47
1:J:265:LYS:HE2	1:J:268:ASP:OD2	2.15	0.47
1:J:365:VAL:CG2	1:J:389:VAL:HG22	2.44	0.47
1:K:402:ILE:CG2	1:K:403:GLU:N	2.78	0.47
1:C:63:LYS:HB2	1:C:73:ASP:HB3	1.95	0.47
1:E:22:LYS:HD2	1:E:398:GLY:HA2	1.96	0.47
1:G:41:ILE:HD12	1:G:41:ILE:N	2.30	0.47
1:J:142:TYR:CB	1:J:144:LYS:HE3	2.45	0.47
1:K:315:LEU:HD23	1:K:354:CYS:HB3	1.97	0.47
1:J:136:ILE:CG2	1:J:137:LYS:N	2.78	0.47
1:K:47:LEU:HD12	1:K:50:VAL:HG23	1.97	0.47
1:E:63:LYS:HB2	1:E:73:ASP:HB3	1.97	0.47
3:E:681:HOH:O	1:J:277:GLU:HB2	2.15	0.47
1:G:150:ARG:NH1	1:G:219:GLU:HA	2.22	0.47
1:G:371:ARG:NH1	1:G:398:GLY:O	2.48	0.47
1:J:60:LEU:CD2	1:J:79:VAL:HG13	2.44	0.47
1:D:186:ALA:HB3	1:D:191:ILE:CD1	2.45	0.47
1:H:36:GLU:O	1:H:75:ARG:HG2	2.15	0.47
1:I:396:ASP:OD2	1:I:415:ARG:NH2	2.48	0.47
1:K:236:GLY:HA3	1:K:306:MET:HE1	1.96	0.47
1:L:282:LEU:HD23	1:L:282:LEU:C	2.35	0.47
1:E:317:ALA:O	1:E:356:GLY:HA3	2.15	0.46
1:K:108:GLN:HG2	1:K:144:LYS:HZ2	1.80	0.46
1:L:94:ILE:HA	1:L:109:VAL:HG11	1.97	0.46
1:F:63:LYS:HB2	1:F:73:ASP:HB3	1.96	0.46
1:I:22:LYS:HD2	1:I:398:GLY:HA2	1.97	0.46
1:D:282:LEU:C	1:D:282:LEU:HD23	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:56:LEU:HB2	1:I:86:LEU:CD2	2.45	0.46
1:K:139:GLU:HG3	1:K:144:LYS:CD	2.44	0.46
1:A:36:GLU:O	1:A:75:ARG:HG2	2.16	0.46
1:B:22:LYS:HD2	1:B:398:GLY:HA2	1.97	0.46
1:C:232:ARG:CB	1:C:258:THR:CG2	2.92	0.46
1:F:56:LEU:HB2	1:F:86:LEU:CD2	2.45	0.46
1:J:147:VAL:HG13	1:J:147:VAL:O	2.15	0.46
1:C:94:ILE:HA	1:C:109:VAL:HG11	1.98	0.46
1:C:371:ARG:NH1	1:C:398:GLY:O	2.48	0.46
1:G:232:ARG:CB	1:G:258:THR:CG2	2.93	0.46
1:G:243:ALA:HA	1:G:284:MET:HG3	1.98	0.46
1:H:60:LEU:HA	1:H:79:VAL:CG1	2.35	0.46
1:J:147:VAL:HG21	1:J:151:LEU:HD23	1.97	0.46
1:J:22:LYS:O	1:J:26:LEU:HD13	2.15	0.46
1:J:313:LEU:C	1:J:313:LEU:HD23	2.36	0.46
1:K:105:GLY:HA2	1:K:147:VAL:CG1	2.45	0.46
1:L:143:VAL:O	1:L:143:VAL:HG22	2.14	0.46
1:L:232:ARG:CB	1:L:258:THR:CG2	2.91	0.46
1:H:371:ARG:NH1	1:H:398:GLY:O	2.48	0.46
1:I:22:LYS:NZ	1:I:23:ASN:OD1	2.48	0.46
1:K:56:LEU:HB2	1:K:86:LEU:HD23	1.97	0.46
1:A:60:LEU:HA	1:A:79:VAL:CG1	2.36	0.46
1:D:143:VAL:O	1:D:143:VAL:HG22	2.16	0.46
1:E:371:ARG:NH1	1:E:398:GLY:O	2.48	0.46
1:F:22:LYS:HD2	1:F:398:GLY:HA2	1.97	0.46
1:H:4:PHE:CD2	1:H:392:ILE:HG21	2.51	0.46
1:C:36:GLU:O	1:C:75:ARG:HG2	2.16	0.46
1:E:41:ILE:HD12	1:E:41:ILE:N	2.31	0.46
1:K:197:PHE:CZ	1:K:201:LEU:HD11	2.51	0.46
1:K:276:GLY:HA3	1:K:279:TRP:NE1	2.31	0.46
1:A:371:ARG:NH1	1:A:398:GLY:O	2.48	0.46
1:D:359:LYS:NZ	1:D:384:GLU:OE1	2.46	0.46
1:J:204:LYS:HB3	1:J:216:GLU:HB3	1.97	0.46
1:B:370:LEU:HD21	2:B:501:EPZ:O2E	2.15	0.46
1:E:359:LYS:CE	1:E:384:GLU:HB2	2.46	0.46
1:G:282:LEU:C	1:G:282:LEU:HD23	2.36	0.46
1:H:416:VAL:HG23	1:H:418:GLY:H	1.81	0.46
1:J:120:ARG:HD3	1:J:328:PHE:CE1	2.51	0.46
1:J:406:LEU:C	1:J:411:ALA:HB3	2.36	0.46
1:B:186:ALA:HB3	1:B:191:ILE:CD1	2.46	0.45
1:G:41:ILE:HG22	1:G:44:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:IAS:OD1	1:F:68:GLY:C	2.54	0.45
1:I:143:VAL:O	1:I:143:VAL:HG22	2.16	0.45
1:I:371:ARG:NH1	1:I:398:GLY:O	2.49	0.45
1:J:125:HIS:HE1	3:J:626:HOH:O	1.98	0.45
1:J:358:GLU:OE1	1:J:359:LYS:HG2	2.15	0.45
1:A:317:ALA:O	1:A:356:GLY:HA3	2.16	0.45
1:B:41:ILE:HD12	1:B:41:ILE:N	2.31	0.45
1:C:244:ILE:HD12	1:C:382:ILE:HD13	1.99	0.45
1:I:94:ILE:HA	1:I:109:VAL:HG11	1.97	0.45
1:J:188:GLU:OE1	3:J:619:HOH:O	2.21	0.45
1:J:283:ASP:OD2	1:J:285:HIS:CE1	2.69	0.45
1:D:22:LYS:NZ	1:D:23:ASN:OD1	2.47	0.45
1:F:282:LEU:C	1:F:282:LEU:HD23	2.36	0.45
1:I:67:IAS:CG	1:I:69:SER:H	2.29	0.45
1:J:199:ILE:HA	1:J:203:ALA:H	1.82	0.45
1:J:56:LEU:O	1:J:60:LEU:HG	2.17	0.45
1:B:232:ARG:CB	1:B:258:THR:CG2	2.92	0.45
1:H:232:ARG:HD3	1:H:258:THR:HG23	1.99	0.45
1:K:317:ALA:O	1:K:356:GLY:HA3	2.16	0.45
1:K:407:ARG:C	1:K:409:LEU:H	2.20	0.45
1:D:315:LEU:HD21	1:D:345:ALA:HB2	1.97	0.45
1:F:41:ILE:N	1:F:41:ILE:HD12	2.32	0.45
1:K:359:LYS:HD3	1:K:384:GLU:HB2	1.99	0.45
1:A:30:PHE:HE1	1:A:56:LEU:HD23	1.81	0.45
1:C:276:GLY:HA3	1:C:279:TRP:NE1	2.31	0.45
1:F:22:LYS:NZ	1:F:23:ASN:OD1	2.50	0.45
1:H:143:VAL:HG22	1:H:143:VAL:O	2.16	0.45
1:I:232:ARG:CB	1:I:258:THR:CG2	2.90	0.45
1:I:141:GLY:HA3	1:J:340:ARG:NH2	2.32	0.45
1:D:371:ARG:NH2	3:D:644:HOH:O	2.50	0.45
1:J:201:LEU:CD2	1:J:223:GLY:HA2	2.47	0.45
1:J:249:ILE:HG12	1:J:250:ILE:N	2.32	0.45
1:A:276:GLY:HA3	1:A:279:TRP:NE1	2.32	0.45
1:D:7:GLN:HB2	1:D:412:ASN:HB3	1.99	0.45
1:K:1:MET:O	1:K:3:LYS:HE3	2.16	0.45
1:K:220:ARG:NH1	1:K:220:ARG:HG3	2.31	0.45
1:C:348:GLU:CG	1:F:322:PHE:CE2	3.00	0.45
1:G:359:LYS:CE	1:G:384:GLU:HB2	2.47	0.45
1:K:335:VAL:HB	1:K:336:PRO:HD3	1.99	0.45
1:A:21:ALA:HA	1:A:231:ASP:HB2	1.98	0.44
1:B:243:ALA:HA	1:B:284:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ARG:NH1	1:B:398:GLY:O	2.49	0.44
1:D:244:ILE:HD12	1:D:382:ILE:HD13	1.99	0.44
1:H:396:ASP:OD2	1:H:415:ARG:NH2	2.48	0.44
1:J:36:GLU:OE2	1:J:220:ARG:NE	2.50	0.44
1:K:396:ASP:OD2	1:K:415:ARG:NH2	2.48	0.44
1:L:41:ILE:N	1:L:41:ILE:HD12	2.32	0.44
1:D:41:ILE:HG22	1:D:44:VAL:CG2	2.47	0.44
1:E:315:LEU:HD21	1:E:345:ALA:HB2	1.99	0.44
1:K:271:ALA:HB2	1:K:284:MET:SD	2.56	0.44
1:K:90:MET:HB2	1:K:397:ARG:NH2	2.32	0.44
1:F:276:GLY:HA3	1:F:279:TRP:NE1	2.31	0.44
1:K:370:LEU:HA	1:K:370:LEU:HD12	1.51	0.44
1:D:22:LYS:HD2	1:D:398:GLY:HA2	1.99	0.44
1:K:63:LYS:HB2	1:K:73:ASP:HB3	2.00	0.44
1:B:7:GLN:HB2	1:B:412:ASN:HB3	1.99	0.44
1:E:150:ARG:HH12	1:E:219:GLU:CA	2.20	0.44
1:F:243:ALA:HA	1:F:284:MET:HG3	1.98	0.44
1:I:186:ALA:HB3	1:I:191:ILE:CD1	2.48	0.44
1:L:24:ALA:C	1:L:27:PRO:HD2	2.37	0.44
1:A:7:GLN:HB2	1:A:412:ASN:HB3	2.00	0.44
1:B:252:ARG:HH11	1:B:252:ARG:HG3	1.81	0.44
1:A:330:ASN:OD1	1:B:330:ASN:OD1	2.35	0.44
1:C:299:HIS:ND1	1:C:300:PRO:HA	2.33	0.44
1:C:59:GLN:O	1:C:79:VAL:CG1	2.66	0.44
1:G:24:ALA:C	1:G:27:PRO:HD2	2.38	0.44
1:H:30:PHE:HE1	1:H:56:LEU:HD23	1.83	0.44
1:I:25:ALA:O	1:I:29:LEU:HD13	2.17	0.44
1:C:27:PRO:HG3	1:C:95:TRP:CH2	2.52	0.44
1:E:282:LEU:C	1:E:282:LEU:HD23	2.37	0.44
1:B:332:PHE:N	3:B:609:HOH:O	2.51	0.44
1:D:159:ASP:OD1	1:F:265:LYS:CE	2.63	0.44
1:D:243:ALA:HA	1:D:284:MET:HG3	1.98	0.44
1:J:61:GLY:HA3	1:J:77:VAL:HA	2.00	0.44
1:L:276:GLY:HA3	1:L:279:TRP:NE1	2.33	0.44
1:L:27:PRO:HG3	1:L:95:TRP:CH2	2.52	0.44
1:A:354:CYS:HB2	3:A:626:HOH:O	2.18	0.44
1:C:21:ALA:HA	1:C:231:ASP:HB2	1.98	0.44
1:C:243:ALA:HA	1:C:284:MET:HG3	2.00	0.44
1:D:252:ARG:HH11	1:D:252:ARG:HG3	1.82	0.44
1:D:41:ILE:N	1:D:41:ILE:HD12	2.33	0.44
1:G:30:PHE:HE1	1:G:56:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:GLY:HA3	1:I:279:TRP:NE1	2.33	0.44
1:J:24:ALA:C	1:J:27:PRO:HD2	2.37	0.44
1:K:108:GLN:HG2	1:K:144:LYS:HZ1	1.79	0.44
1:K:49:ASP:OD2	1:K:370:LEU:HD21	2.17	0.44
1:A:25:ALA:O	1:A:29:LEU:HD13	2.18	0.43
1:D:59:GLN:O	1:D:79:VAL:CG1	2.63	0.43
1:I:36:GLU:O	1:I:75:ARG:HG2	2.18	0.43
1:J:317:ALA:O	1:J:356:GLY:HA3	2.18	0.43
1:K:7:GLN:HB2	1:K:412:ASN:CG	2.38	0.43
1:A:299:HIS:ND1	1:A:300:PRO:HA	2.33	0.43
1:B:24:ALA:C	1:B:27:PRO:HD2	2.38	0.43
1:H:186:ALA:HB3	1:H:191:ILE:CD1	2.47	0.43
1:I:101:VAL:HG21	1:I:145:ALA:HB3	2.00	0.43
1:J:115:QPA:O13	1:J:115:QPA:H9	2.18	0.43
1:J:244:ILE:CG2	1:J:313:LEU:HA	2.47	0.43
1:K:265:LYS:HE2	1:K:293:ASN:O	2.18	0.43
1:L:359:LYS:NZ	1:L:384:GLU:OE1	2.42	0.43
1:A:4:PHE:CD2	1:A:392:ILE:HG21	2.53	0.43
1:D:108:GLN:HG3	1:D:144:LYS:HG2	2.00	0.43
1:E:396:ASP:OD2	1:E:415:ARG:NH2	2.51	0.43
1:E:59:GLN:O	1:E:79:VAL:CG1	2.65	0.43
1:H:20:GLY:HA3	1:H:43:ASN:O	2.18	0.43
1:I:30:PHE:HE1	1:I:56:LEU:HD23	1.82	0.43
1:J:58:SER:C	1:J:60:LEU:N	2.71	0.43
1:J:60:LEU:O	1:J:79:VAL:HG12	2.19	0.43
1:K:267:ARG:HG3	1:K:273:ILE:HD12	2.00	0.43
1:K:370:LEU:HD23	2:K:501:EPZ:O2E	2.18	0.43
1:A:315:LEU:HD21	1:A:345:ALA:HB2	2.00	0.43
1:D:60:LEU:HA	1:D:79:VAL:CG1	2.35	0.43
1:K:187:ARG:HH12	1:K:300:PRO:CD	2.30	0.43
1:L:60:LEU:CA	1:L:79:VAL:HG13	2.37	0.43
1:L:7:GLN:HB2	1:L:412:ASN:HB3	2.00	0.43
1:C:22:LYS:HD2	1:C:398:GLY:HA2	1.99	0.43
1:J:41:ILE:HG22	1:J:44:VAL:CG2	2.49	0.43
1:B:22:LYS:NZ	1:B:23:ASN:OD1	2.48	0.43
1:C:41:ILE:HD12	1:C:41:ILE:N	2.34	0.43
1:E:186:ALA:HB3	1:E:191:ILE:CD1	2.48	0.43
1:F:232:ARG:CB	1:F:258:THR:CG2	2.93	0.43
1:I:41:ILE:O	1:I:69:SER:HA	2.17	0.43
1:J:142:TYR:HB2	1:J:144:LYS:HE3	1.99	0.43
1:J:5:ARG:CB	1:J:5:ARG:HH11	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:CB	1:A:258:THR:CG2	2.92	0.43
1:G:4:PHE:CD2	1:G:392:ILE:HG21	2.53	0.43
1:H:22:LYS:NZ	1:H:23:ASN:OD1	2.51	0.43
1:J:276:GLY:HA3	1:J:279:TRP:CE2	2.54	0.43
1:J:41:ILE:HD12	1:J:41:ILE:H	1.83	0.43
1:J:57:LEU:HB3	1:J:64:VAL:HG21	2.01	0.43
1:K:198:LEU:O	1:K:203:ALA:HB3	2.18	0.43
1:D:30:PHE:HE1	1:D:56:LEU:HD23	1.84	0.43
1:E:232:ARG:CB	1:E:258:THR:CG2	2.96	0.43
1:F:27:PRO:HG3	1:F:95:TRP:CH2	2.54	0.43
1:G:101:VAL:HG21	1:G:145:ALA:CB	2.49	0.43
1:H:357:VAL:HG13	3:H:602:HOH:O	2.17	0.43
1:K:183:GLU:O	1:K:184:ASN:HB3	2.19	0.43
1:A:143:VAL:O	1:A:143:VAL:HG22	2.19	0.43
1:G:412:ASN:HA	3:G:608:HOH:O	2.18	0.43
1:I:21:ALA:HA	1:I:231:ASP:HB2	2.01	0.43
1:I:7:GLN:HB2	1:I:412:ASN:HB3	2.01	0.43
1:J:46:LYS:N	1:J:400:GLU:OE1	2.34	0.43
1:B:4:PHE:CD2	1:B:392:ILE:HG21	2.54	0.43
1:F:359:LYS:CE	1:F:384:GLU:HB2	2.49	0.43
1:H:7:GLN:HB2	1:H:412:ASN:HB3	2.00	0.43
1:K:94:ILE:HD12	1:K:109:VAL:HG11	2.01	0.43
1:K:34:LEU:HD22	1:K:175:LEU:HD12	2.00	0.43
1:L:59:GLN:O	1:L:79:VAL:CG1	2.65	0.43
1:B:232:ARG:HD3	1:B:258:THR:HG23	2.01	0.42
1:F:317:ALA:O	1:F:356:GLY:HA3	2.19	0.42
1:H:150:ARG:HH12	1:H:219:GLU:CA	2.22	0.42
1:D:232:ARG:HD3	1:D:258:THR:HG23	2.00	0.42
1:G:20:GLY:HA3	1:G:43:ASN:O	2.19	0.42
1:G:276:GLY:HA3	1:G:279:TRP:NE1	2.34	0.42
1:J:120:ARG:CD	3:J:637:HOH:O	2.60	0.42
1:I:330:ASN:OD1	1:J:330:ASN:CB	2.67	0.42
1:J:41:ILE:HG22	1:J:44:VAL:HG23	2.01	0.42
2:J:501:EPZ:C6U	2:J:501:EPZ:H5DA	2.48	0.42
1:K:169:ILE:O	1:K:170:MET:C	2.57	0.42
1:D:36:GLU:O	1:D:75:ARG:HG2	2.19	0.42
1:G:294:VAL:HG12	1:G:295:ARG:N	2.34	0.42
1:I:59:GLN:O	1:I:79:VAL:CG1	2.66	0.42
1:J:3:LYS:HB2	1:J:389:VAL:O	2.19	0.42
2:K:501:EPZ:C6U	2:K:501:EPZ:H5DA	2.48	0.42
1:L:101:VAL:HG21	1:L:145:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:VAL:HG21	1:B:145:ALA:CB	2.50	0.42
1:C:186:ALA:HB3	1:C:191:ILE:CD1	2.49	0.42
1:C:258:THR:HG22	1:C:259:LEU:HG	2.00	0.42
1:D:147:VAL:O	1:D:147:VAL:HG13	2.18	0.42
1:F:24:ALA:C	1:F:27:PRO:HD2	2.40	0.42
1:F:70:VAL:O	1:F:70:VAL:HG12	2.18	0.42
1:G:25:ALA:O	1:G:29:LEU:HD13	2.19	0.42
1:I:20:GLY:HA3	1:I:43:ASN:O	2.19	0.42
1:K:188:GLU:HA	1:K:189:PRO:HD3	1.88	0.42
1:L:186:ALA:HB3	1:L:191:ILE:CD1	2.49	0.42
1:A:141:GLY:HA3	1:B:340:ARG:NH2	2.34	0.42
1:F:59:GLN:O	1:F:79:VAL:CG1	2.64	0.42
1:G:59:GLN:O	1:G:79:VAL:CG1	2.65	0.42
2:I:501:EPZ:C6U	2:I:501:EPZ:H5DA	2.50	0.42
1:J:220:ARG:HG3	1:J:220:ARG:HH11	1.83	0.42
1:K:315:LEU:HA	1:K:315:LEU:HD23	1.86	0.42
1:A:101:VAL:HG21	1:A:145:ALA:HB3	2.01	0.42
1:B:359:LYS:NZ	1:B:384:GLU:OE1	2.45	0.42
1:E:20:GLY:HA3	1:E:43:ASN:O	2.19	0.42
1:F:11:LYS:HE2	1:F:247:GLY:HA2	2.02	0.42
1:F:258:THR:HG22	1:F:259:LEU:HG	2.01	0.42
1:G:246:ARG:HG2	1:G:287:LYS:O	2.20	0.42
1:G:57:LEU:HA	1:G:57:LEU:HD12	1.88	0.42
1:H:59:GLN:O	1:H:79:VAL:CG1	2.65	0.42
1:J:198:LEU:HA	1:J:198:LEU:HD23	1.84	0.42
1:K:1:MET:HE1	1:K:391:ARG:HB3	2.00	0.42
1:K:352:VAL:O	1:K:352:VAL:HG13	2.19	0.42
1:E:183:GLU:OE2	1:E:212:ARG:NH1	2.53	0.42
1:F:150:ARG:HH12	1:F:219:GLU:CA	2.21	0.42
1:I:416:VAL:HG23	1:I:418:GLY:H	1.84	0.42
1:J:58:SER:C	1:J:60:LEU:H	2.23	0.42
1:J:5:ARG:CB	1:J:5:ARG:NH1	2.83	0.42
1:C:150:ARG:HH12	1:C:219:GLU:CA	2.20	0.42
1:C:330:ASN:CG	1:D:330:ASN:CG	2.78	0.42
1:B:261:ALA:HA	1:E:157:VAL:HG11	2.02	0.42
1:F:208:GLN:OE1	1:F:208:GLN:N	2.47	0.42
1:G:317:ALA:O	1:G:356:GLY:HA3	2.20	0.42
1:H:243:ALA:HA	1:H:284:MET:HG3	2.02	0.42
1:K:137:LYS:HE2	1:K:139:GLU:CD	2.40	0.42
1:L:22:LYS:NZ	1:L:23:ASN:OD1	2.47	0.42
1:A:220:ARG:HG3	1:A:220:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ALA:C	1:A:27:PRO:HD2	2.39	0.42
1:B:359:LYS:CE	1:B:384:GLU:HB2	2.50	0.42
1:C:315:LEU:HD21	1:C:345:ALA:HB2	2.02	0.42
1:H:101:VAL:HG21	1:H:145:ALA:HB3	2.02	0.42
1:H:150:ARG:NH1	1:H:219:GLU:HA	2.21	0.42
1:H:24:ALA:C	1:H:27:PRO:HD2	2.39	0.42
1:J:189:PRO:HD3	1:J:299:HIS:CD2	2.55	0.42
1:L:243:ALA:HA	1:L:284:MET:HG3	2.01	0.42
1:C:24:ALA:C	1:C:27:PRO:HD2	2.40	0.42
1:D:25:ALA:O	1:D:29:LEU:HD13	2.20	0.42
1:D:24:ALA:C	1:D:27:PRO:HD2	2.41	0.42
1:I:11:LYS:HE2	1:I:247:GLY:HA2	2.02	0.42
1:J:105:GLY:HA2	1:J:147:VAL:CG1	2.49	0.42
1:J:273:ILE:HG22	1:J:274:GLU:N	2.35	0.42
1:K:259:LEU:HD23	3:K:606:HOH:O	2.20	0.42
1:B:41:ILE:HG22	1:B:44:VAL:CG2	2.50	0.41
1:F:101:VAL:HG21	1:F:145:ALA:CB	2.50	0.41
1:J:160:LYS:HD3	1:K:295:ARG:HE	1.84	0.41
1:H:232:ARG:CD	1:H:258:THR:HG23	2.50	0.41
1:H:315:LEU:HD21	1:H:345:ALA:HB2	2.02	0.41
1:I:243:ALA:HA	1:I:284:MET:HG3	2.02	0.41
1:J:108:GLN:CG	1:J:144:LYS:HE2	2.51	0.41
1:J:402:ILE:HG12	1:J:406:LEU:CD1	2.51	0.41
1:J:39:VAL:CG2	1:J:40:GLU:N	2.83	0.41
1:B:101:VAL:HG21	1:B:145:ALA:HB3	2.02	0.41
1:F:287:LYS:HA	1:H:148:ASP:OD2	2.20	0.41
1:F:150:ARG:HB2	3:F:632:HOH:O	2.20	0.41
1:H:276:GLY:HA3	1:H:279:TRP:NE1	2.35	0.41
1:H:407:ARG:HG3	3:H:643:HOH:O	2.19	0.41
1:I:317:ALA:O	1:I:356:GLY:HA3	2.20	0.41
1:C:25:ALA:O	1:C:29:LEU:HD13	2.21	0.41
1:C:317:ALA:O	1:C:356:GLY:HA3	2.20	0.41
1:G:101:VAL:HG21	1:G:145:ALA:HB3	2.02	0.41
1:I:41:ILE:HG22	1:I:44:VAL:CG2	2.51	0.41
1:L:93:SER:C	1:L:95:TRP:N	2.74	0.41
1:C:30:PHE:HE1	1:C:56:LEU:HD23	1.85	0.41
1:C:359:LYS:NZ	1:C:384:GLU:OE1	2.43	0.41
1:F:371:ARG:NH2	3:F:612:HOH:O	2.54	0.41
1:G:315:LEU:HD21	1:G:345:ALA:HB2	2.01	0.41
1:I:4:PHE:CD2	1:I:392:ILE:HG21	2.55	0.41
1:J:239:LEU:HB3	1:J:282:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:265:LYS:HE2	1:K:294:VAL:HG22	2.01	0.41
1:L:101:VAL:HG21	1:L:145:ALA:CB	2.50	0.41
1:L:147:VAL:HG13	1:L:147:VAL:O	2.19	0.41
1:L:232:ARG:HD3	1:L:258:THR:HG23	2.03	0.41
1:C:229:LEU:HA	3:C:666:HOH:O	2.20	0.41
1:E:24:ALA:C	1:E:27:PRO:HD2	2.41	0.41
1:I:120:ARG:HD3	1:I:328:PHE:HE1	1.81	0.41
1:I:44:VAL:HG12	1:I:66:ARG:HH12	1.86	0.41
1:J:60:LEU:HA	1:J:79:VAL:HG12	1.95	0.41
1:K:233:ILE:CD1	1:K:305:ASP:HB2	2.49	0.41
1:A:232:ARG:HD3	1:A:258:THR:HG23	2.03	0.41
1:B:11:LYS:HE2	1:B:247:GLY:HA2	2.02	0.41
1:D:252:ARG:NH2	3:D:616:HOH:O	2.52	0.41
1:E:258:THR:HG22	1:E:259:LEU:HG	2.02	0.41
1:F:30:PHE:HE1	1:F:56:LEU:HD23	1.84	0.41
1:G:215:ILE:HD12	1:G:215:ILE:N	2.36	0.41
1:H:101:VAL:HG21	1:H:145:ALA:CB	2.51	0.41
1:I:330:ASN:OD1	1:J:330:ASN:HB3	2.20	0.41
1:J:22:LYS:N	3:J:607:HOH:O	2.53	0.41
1:J:402:ILE:HG12	1:J:406:LEU:HD12	2.01	0.41
1:B:143:VAL:HG22	1:B:143:VAL:O	2.20	0.41
1:B:294:VAL:HG12	1:B:295:ARG:N	2.36	0.41
1:K:34:LEU:HD22	1:K:175:LEU:CD1	2.50	0.41
1:K:232:ARG:HB2	1:K:259:LEU:CD2	2.49	0.41
1:K:295:ARG:NH1	1:K:295:ARG:CG	2.84	0.41
1:K:41:ILE:N	1:K:41:ILE:HD12	2.36	0.41
1:L:244:ILE:HD12	1:L:382:ILE:HD13	2.02	0.41
1:L:41:ILE:HG22	1:L:44:VAL:CG2	2.50	0.41
1:A:101:VAL:HG21	1:A:145:ALA:CB	2.51	0.41
1:B:416:VAL:HG23	1:B:418:GLY:H	1.85	0.41
1:C:243:ALA:HA	1:C:284:MET:CG	2.51	0.41
1:E:243:ALA:HA	1:E:284:MET:CG	2.51	0.41
1:F:66:ARG:CB	1:F:70:VAL:HG22	2.43	0.41
1:H:22:LYS:HD2	1:H:398:GLY:HA2	2.02	0.41
1:J:132:LEU:HA	1:J:132:LEU:HD23	1.88	0.41
1:K:320:THR:HG23	1:K:354:CYS:O	2.21	0.41
1:B:315:LEU:HD21	1:B:345:ALA:HB2	2.03	0.41
1:E:150:ARG:HB2	3:E:676:HOH:O	2.20	0.41
1:E:232:ARG:HD3	1:E:258:THR:HG23	2.03	0.41
1:I:66:ARG:HD2	1:I:70:VAL:HG22	2.03	0.41
1:J:188:GLU:OE2	1:J:299:HIS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:ALA:O	1:K:217:GLY:HA3	2.21	0.41
1:A:348:GLU:HG3	1:E:322:PHE:CE2	2.56	0.40
1:A:41:ILE:HG22	1:A:44:VAL:CG2	2.51	0.40
1:E:101:VAL:HG21	1:E:145:ALA:HB3	2.03	0.40
1:F:315:LEU:HD21	1:F:345:ALA:HB2	2.02	0.40
1:G:294:VAL:CG1	1:G:295:ARG:N	2.84	0.40
1:H:258:THR:HG22	1:H:259:LEU:HG	2.03	0.40
1:E:330:ASN:CG	1:H:330:ASN:HB3	2.41	0.40
1:H:359:LYS:CE	1:H:384:GLU:HB2	2.49	0.40
1:I:101:VAL:HG21	1:I:145:ALA:CB	2.50	0.40
1:B:25:ALA:O	1:B:29:LEU:HD13	2.21	0.40
1:B:27:PRO:HG3	1:B:95:TRP:CH2	2.57	0.40
1:E:41:ILE:HG22	1:E:44:VAL:CG2	2.50	0.40
1:F:143:VAL:HG22	1:F:143:VAL:O	2.21	0.40
1:F:101:VAL:HG21	1:F:145:ALA:HB3	2.02	0.40
1:H:25:ALA:O	1:H:29:LEU:HD13	2.21	0.40
1:J:284:MET:C	1:J:286:GLY:H	2.25	0.40
1:K:132:LEU:HD11	1:K:169:ILE:HG23	2.02	0.40
1:K:9:PRO:HD3	1:K:384:GLU:HA	2.02	0.40
1:A:359:LYS:CE	1:A:384:GLU:HB2	2.51	0.40
1:A:27:PRO:HG3	1:A:95:TRP:CH2	2.56	0.40
1:B:57:LEU:HD12	1:B:57:LEU:HA	1.88	0.40
1:C:277:GLU:HG2	1:C:277:GLU:O	2.22	0.40
1:E:27:PRO:HG3	1:E:95:TRP:CH2	2.56	0.40
1:F:243:ALA:HA	1:F:284:MET:CG	2.52	0.40
1:G:232:ARG:HD3	1:G:258:THR:HG23	2.04	0.40
1:J:298:PRO:O	1:J:301:ALA:HB3	2.21	0.40
1:J:76:ASP:O	1:J:77:VAL:C	2.59	0.40
1:K:249:ILE:HG12	1:K:250:ILE:N	2.36	0.40
1:K:263:LEU:HA	1:K:263:LEU:HD23	1.98	0.40
1:A:126:ILE:HG23	1:A:136:ILE:HD12	2.04	0.40
1:B:159:ASP:OD1	1:E:265:LYS:CE	2.69	0.40
1:B:59:GLN:O	1:B:79:VAL:CG1	2.66	0.40
1:E:27:PRO:HG3	1:E:95:TRP:CZ3	2.56	0.40
1:E:30:PHE:CE1	1:E:56:LEU:HD23	2.56	0.40
1:G:143:VAL:O	1:G:143:VAL:HG22	2.20	0.40
1:G:243:ALA:HA	1:G:284:MET:CG	2.50	0.40
1:H:277:GLU:O	1:H:277:GLU:HG2	2.21	0.40
1:I:371:ARG:NH2	3:I:626:HOH:O	2.54	0.40
1:D:101:VAL:HG21	1:D:145:ALA:HB3	2.03	0.40
1:F:155:HIS:HD2	1:F:181:ILE:HB	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:243:ALA:HA	1:I:284:MET:CG	2.52	0.40
1:K:97:LEU:HD11	1:K:145:ALA:HB3	2.04	0.40
1:K:236:GLY:HA3	1:K:306:MET:CE	2.52	0.40
1:L:252:ARG:O	1:L:253:ASN:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLU:OE1	1:I:46:LYS:NZ[1_666]	2.06	0.14

## 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	413/418 (99%)	396 (96%)	15 (4%)	2 (0%)	29	48
1	B	413/418 (99%)	400 (97%)	13 (3%)	0	100	100
1	C	413/418 (99%)	398 (96%)	15 (4%)	0	100	100
1	D	413/418 (99%)	397 (96%)	15 (4%)	1 (0%)	47	68
1	E	413/418 (99%)	396 (96%)	17 (4%)	0	100	100
1	F	413/418 (99%)	396 (96%)	16 (4%)	1 (0%)	47	68
1	G	413/418 (99%)	397 (96%)	16 (4%)	0	100	100
1	H	413/418 (99%)	397 (96%)	15 (4%)	1 (0%)	47	68
1	I	413/418 (99%)	394 (95%)	18 (4%)	1 (0%)	47	68
1	J	413/418 (99%)	368 (89%)	43 (10%)	2 (0%)	29	48
1	K	413/418 (99%)	378 (92%)	33 (8%)	2 (0%)	29	48
1	L	413/418 (99%)	397 (96%)	15 (4%)	1 (0%)	47	68
All	All	4956/5016 (99%)	4714 (95%)	231 (5%)	11 (0%)	47	68



All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	91	ARG
1	A	91	ARG
1	D	91	ARG
1	H	91	ARG
1	K	329	GLU
1	F	91	ARG
1	I	91	ARG
1	J	260	ASP
1	J	313	LEU
1	A	329	GLU
1	K	333	MET

### 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	329/329 (100%)	317 (96%)	12 (4%)	35	61
1	B	329/329 (100%)	317 (96%)	12 (4%)	35	61
1	C	329/329 (100%)	317 (96%)	12 (4%)	35	61
1	D	329/329 (100%)	317 (96%)	12 (4%)	35	61
1	E	329/329 (100%)	317 (96%)	12 (4%)	35	61
1	F	329/329 (100%)	317 (96%)	12 (4%)	35	61
1	G	329/329 (100%)	316 (96%)	13 (4%)	31	56
1	H	329/329 (100%)	316 (96%)	13 (4%)	31	56
1	I	329/329 (100%)	317 (96%)	12 (4%)	35	61
1	J	329/329 (100%)	304 (92%)	25 (8%)	13	25
1	K	329/329 (100%)	313 (95%)	16 (5%)	25	47
1	L	329/329 (100%)	316 (96%)	13 (4%)	31	56
All	All	3948/3948 (100%)	3784 (96%)	164 (4%)	30	54

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	86	LEU
1	A	111	LEU
1	A	143	VAL
1	A	193	ASP
1	A	212	ARG
1	A	229	LEU
1	A	258	THR
1	A	307	GLN
1	A	330	ASN
1	A	391	ARG
1	A	416	VAL
1	B	57	LEU
1	B	86	LEU
1	B	111	LEU
1	B	143	VAL
1	B	187	ARG
1	B	193	ASP
1	B	229	LEU
1	B	258	THR
1	B	307	GLN
1	B	330	ASN
1	B	391	ARG
1	B	416	VAL
1	C	57	LEU
1	C	86	LEU
1	C	111	LEU
1	C	143	VAL
1	C	193	ASP
1	C	210	THR
1	C	229	LEU
1	C	258	THR
1	C	300	PRO
1	C	330	ASN
1	C	391	ARG
1	C	416	VAL
1	D	57	LEU
1	D	86	LEU
1	D	111	LEU
1	D	143	VAL
1	D	193	ASP
1	D	212	ARG
1	D	229	LEU

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Mol	Chain	Res	Type
1	D	258	THR
1	D	307	GLN
1	D	330	ASN
1	D	391	ARG
1	D	416	VAL
1	E	10	THR
1	E	57	LEU
1	E	86	LEU
1	E	111	LEU
1	E	143	VAL
1	E	187	ARG
1	E	193	ASP
1	E	229	LEU
1	E	258	THR
1	E	330	ASN
1	E	391	ARG
1	E	416	VAL
1	F	10	THR
1	F	57	LEU
1	F	86	LEU
1	F	111	LEU
1	F	143	VAL
1	F	193	ASP
1	F	229	LEU
1	F	258	THR
1	F	307	GLN
1	F	330	ASN
1	F	391	ARG
1	F	416	VAL
1	G	10	THR
1	G	57	LEU
1	G	75	ARG
1	G	86	LEU
1	G	111	LEU
1	G	143	VAL
1	G	193	ASP
1	G	229	LEU
1	G	258	THR
1	G	300	PRO
1	G	330	ASN
1	G	391	ARG
1	G	416	VAL

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Mol	Chain	Res	Type
1	H	10	THR
1	H	15	GLU
1	H	57	LEU
1	H	86	LEU
1	H	111	LEU
1	H	143	VAL
1	H	187	ARG
1	H	193	ASP
1	H	229	LEU
1	H	258	THR
1	H	330	ASN
1	H	391	ARG
1	H	416	VAL
1	I	10	THR
1	I	57	LEU
1	I	86	LEU
1	I	111	LEU
1	I	143	VAL
1	I	193	ASP
1	I	229	LEU
1	I	258	THR
1	I	300	PRO
1	I	307	GLN
1	I	330	ASN
1	I	416	VAL
1	J	39	VAL
1	J	55	LYS
1	J	57	LEU
1	J	63	LYS
1	J	106	GLN
1	J	108	GLN
1	J	111	LEU
1	J	125	HIS
1	J	160	LYS
1	J	188	GLU
1	J	193	ASP
1	J	211	ASP
1	J	216	GLU
1	J	229	LEU
1	J	258	THR
1	J	265	LYS
1	J	275	VAL

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Mol	Chain	Res	Type
1	J	300	PRO
1	J	307	GLN
1	J	330	ASN
1	J	349	SER
1	J	354	CYS
1	J	360	LEU
1	J	414	GLU
1	J	416	VAL
1	K	3	LYS
1	K	34	LEU
1	K	39	VAL
1	K	47	LEU
1	K	57	LEU
1	K	59	GLN
1	K	86	LEU
1	K	111	LEU
1	K	160	LYS
1	K	211	ASP
1	K	219	GLU
1	K	229	LEU
1	K	248	LYS
1	K	307	GLN
1	K	359	LYS
1	K	416	VAL
1	L	10	THR
1	L	57	LEU
1	L	86	LEU
1	L	111	LEU
1	L	143	VAL
1	L	193	ASP
1	L	212	ARG
1	L	229	LEU
1	L	258	THR
1	L	307	GLN
1	L	330	ASN
1	L	391	ARG
1	L	416	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS

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Mol	Chain	Res	Type
1	C	155	HIS
1	E	106	GLN
1	F	155	HIS
1	G	155	HIS
1	H	155	HIS
1	I	155	HIS
1	K	307	GLN
1	L	155	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	IAS	L	67	1	4,7,8	0.49	0	2,8,10	1.37	0
1	QPA	J	115	1	8,15,16	3.77	3 (37%)	7,22,24	1.71	1 (14%)
1	QPA	L	115	1	8,15,16	3.58	3 (37%)	7,22,24	1.51	1 (14%)
1	IAS	A	67	1	4,7,8	0.62	0	2,8,10	1.39	0
1	IAS	I	67	1	4,7,8	1.65	1 (25%)	2,8,10	1.28	0
1	IAS	J	67	1	4,7,8	0.79	0	2,8,10	1.41	0
1	IAS	E	67	1	4,7,8	2.10	2 (50%)	2,8,10	1.69	0
1	IAS	C	67	1	4,7,8	0.76	0	2,8,10	1.39	0
1	QPA	I	115	1	8,15,16	4.16	3 (37%)	7,22,24	1.49	1 (14%)
1	IAS	F	67	1	4,7,8	1.78	1 (25%)	2,8,10	0.49	0
1	IAS	H	67	1	4,7,8	0.74	0	2,8,10	1.39	0
1	QPA	A	115	1	8,15,16	4.05	3 (37%)	7,22,24	1.67	1 (14%)
1	QPA	C	115	1	8,15,16	3.51	3 (37%)	7,22,24	1.48	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	IAS	K	67	1	4,7,8	2.41	2 (50%)	2,8,10	1.96	1 (50%)
1	QPA	K	115	1	8,15,16	3.84	4 (50%)	7,22,24	1.77	1 (14%)
1	IAS	D	67	1	4,7,8	0.91	0	2,8,10	1.18	0
1	QPA	D	115	1	8,15,16	3.90	4 (50%)	7,22,24	1.65	1 (14%)
1	IAS	B	67	1	4,7,8	0.49	0	2,8,10	1.28	0
1	IAS	G	67	1	4,7,8	0.68	0	2,8,10	1.31	0
1	QPA	E	115	1	8,15,16	3.84	3 (37%)	7,22,24	1.52	1 (14%)
1	QPA	G	115	1	8,15,16	3.55	4 (50%)	7,22,24	1.64	1 (14%)
1	QPA	F	115	1	8,15,16	3.85	3 (37%)	7,22,24	1.64	1 (14%)
1	QPA	H	115	1	8,15,16	3.57	3 (37%)	7,22,24	1.54	1 (14%)
1	QPA	B	115	1	8,15,16	3.73	3 (37%)	7,22,24	1.52	1 (14%)

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
1	IAS	L	67	1	-	0/3/7/8	-
1	QPA	J	115	1	-	1/7/20/22	-
1	QPA	L	115	1	-	0/7/20/22	-
1	IAS	A	67	1	-	0/3/7/8	-
1	IAS	I	67	1	-	2/3/7/8	-
1	IAS	J	67	1	-	0/3/7/8	-
1	IAS	E	67	1	-	1/3/7/8	-
1	IAS	C	67	1	-	0/3/7/8	-
1	QPA	I	115	1	-	1/7/20/22	-
1	IAS	F	67	1	-	1/3/7/8	-
1	IAS	H	67	1	-	0/3/7/8	-
1	QPA	A	115	1	-	1/7/20/22	-
1	QPA	C	115	1	-	1/7/20/22	-
1	IAS	K	67	1	-	1/3/7/8	-
1	QPA	K	115	1	-	0/7/20/22	-
1	IAS	D	67	1	-	0/3/7/8	-
1	QPA	D	115	1	-	1/7/20/22	-
1	IAS	B	67	1	-	0/3/7/8	-
1	IAS	G	67	1	-	0/3/7/8	-
1	QPA	E	115	1	-	1/7/20/22	-
1	QPA	G	115	1	-	1/7/20/22	-
1	QPA	F	115	1	-	1/7/20/22	-
1	QPA	H	115	1	-	1/7/20/22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	QPA	B	115	1	-	1/7/20/22	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	115	QPA	P2-O14	9.75	1.77	1.59
1	A	115	QPA	P2-O14	9.56	1.77	1.59
1	E	115	QPA	P2-O14	8.79	1.75	1.59
1	J	115	QPA	P2-O14	8.67	1.75	1.59
1	F	115	QPA	P2-O14	8.60	1.75	1.59
1	K	115	QPA	P2-O14	8.56	1.75	1.59
1	D	115	QPA	P2-O14	8.54	1.75	1.59
1	B	115	QPA	P2-O14	8.36	1.75	1.59
1	L	115	QPA	P2-O14	8.18	1.74	1.59
1	G	115	QPA	P2-O14	7.65	1.73	1.59
1	C	115	QPA	P2-O14	7.63	1.73	1.59
1	H	115	QPA	P2-O14	7.56	1.73	1.59
1	D	115	QPA	P2-O13	5.85	1.69	1.50
1	F	115	QPA	P2-O13	5.76	1.69	1.50
1	I	115	QPA	P2-O13	5.62	1.68	1.50
1	H	115	QPA	P2-O13	5.59	1.68	1.50
1	B	115	QPA	P2-O13	5.56	1.68	1.50
1	G	115	QPA	P2-O13	5.44	1.68	1.50
1	E	115	QPA	P2-O13	5.39	1.67	1.50
1	C	115	QPA	P2-O13	5.30	1.67	1.50
1	A	115	QPA	P2-O13	5.29	1.67	1.50
1	K	115	QPA	P2-O13	5.28	1.67	1.50
1	J	115	QPA	P2-O13	5.17	1.67	1.50
1	L	115	QPA	P2-O13	4.97	1.66	1.50
1	K	67	IAS	CB-CA	-3.64	1.45	1.54
1	H	115	QPA	P2-O11	3.44	1.68	1.54
1	E	67	IAS	CB-CA	-3.33	1.46	1.54
1	I	67	IAS	CB-CA	-3.18	1.46	1.54
1	K	67	IAS	CA-N	-3.15	1.40	1.47
1	K	115	QPA	P2-O11	3.14	1.66	1.54
1	J	115	QPA	P2-O11	3.14	1.66	1.54
1	E	115	QPA	P2-O11	3.13	1.66	1.54
1	F	115	QPA	P2-O11	3.02	1.66	1.54
1	B	115	QPA	P2-O11	2.99	1.66	1.54
1	A	115	QPA	P2-O11	2.94	1.66	1.54
1	D	115	QPA	P2-O11	2.93	1.66	1.54
1	F	67	IAS	CB-CA	-2.84	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	115	QPA	P2-O11	2.77	1.65	1.54
1	C	115	QPA	P2-O11	2.68	1.65	1.54
1	I	115	QPA	P2-O11	2.62	1.64	1.54
1	G	115	QPA	P2-O11	2.48	1.64	1.54
1	G	115	QPA	CB-CA	2.33	1.59	1.53
1	K	115	QPA	CB-CA	2.21	1.58	1.53
1	E	67	IAS	CA-N	-2.06	1.42	1.47
1	D	115	QPA	CB-CA	2.01	1.58	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	115	QPA	CB-SG-C8	4.37	112.98	103.27
1	A	115	QPA	CB-SG-C8	4.16	112.50	103.27
1	J	115	QPA	CB-SG-C8	4.10	112.38	103.27
1	D	115	QPA	CB-SG-C8	4.08	112.32	103.27
1	F	115	QPA	CB-SG-C8	4.07	112.30	103.27
1	G	115	QPA	CB-SG-C8	3.98	112.10	103.27
1	H	115	QPA	CB-SG-C8	3.82	111.76	103.27
1	B	115	QPA	CB-SG-C8	3.70	111.49	103.27
1	L	115	QPA	CB-SG-C8	3.68	111.44	103.27
1	E	115	QPA	CB-SG-C8	3.66	111.40	103.27
1	I	115	QPA	CB-SG-C8	3.66	111.39	103.27
1	C	115	QPA	CB-SG-C8	3.51	111.06	103.27
1	K	67	IAS	CA-CB-CG	-2.01	105.81	114.50

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	67	IAS	N-CA-CB-CG
1	I	115	QPA	C8-O14-P2-O11
1	A	115	QPA	C8-O14-P2-O11
1	C	115	QPA	C8-O14-P2-O11
1	D	115	QPA	C8-O14-P2-O11
1	E	115	QPA	C8-O14-P2-O11
1	I	67	IAS	C-CA-CB-CG
1	I	67	IAS	CA-CB-CG-OD1
1	K	67	IAS	CA-CB-CG-OD1
1	J	115	QPA	C8-O14-P2-O11
1	F	67	IAS	CA-CB-CG-OD1
1	G	115	QPA	C8-O14-P2-O11

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Mol	Chain	Res	Type	Atoms
1	F	115	QPA	C8-O14-P2-O11
1	H	115	QPA	C8-O14-P2-O11
1	B	115	QPA	C8-O14-P2-O11

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	115	QPA	1	0
1	I	67	IAS	8	0
1	F	67	IAS	3	0
1	K	67	IAS	5	0
1	K	115	QPA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EPZ	H	501	-	36,46,46	1.46	6 (16%)	46,69,69	1.23	3 (6%)
2	EPZ	J	501	-	36,46,46	1.38	7 (19%)	46,69,69	1.24	2 (4%)
2	EPZ	C	501	-	36,46,46	1.53	8 (22%)	46,69,69	1.33	5 (10%)
2	EPZ	E	501	-	36,46,46	1.49	6 (16%)	46,69,69	1.19	4 (8%)
2	EPZ	A	501	-	36,46,46	1.46	9 (25%)	46,69,69	1.23	3 (6%)
2	EPZ	K	501	-	36,46,46	1.55	7 (19%)	46,69,69	1.32	2 (4%)
2	EPZ	G	501	-	36,46,46	1.54	6 (16%)	46,69,69	1.19	2 (4%)
2	EPZ	I	501	-	36,46,46	1.44	7 (19%)	46,69,69	1.16	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EPZ	D	501	-	36,46,46	1.64	9 (25%)	46,69,69	1.37	5 (10%)
2	EPZ	F	501	-	36,46,46	1.67	9 (25%)	46,69,69	1.20	4 (8%)
2	EPZ	B	501	-	36,46,46	1.36	5 (13%)	46,69,69	1.33	6 (13%)
2	EPZ	L	501	-	36,46,46	1.45	6 (16%)	46,69,69	1.28	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPZ	H	501	-	-	9/28/71/71	0/3/3/3
2	EPZ	J	501	-	-	6/28/71/71	0/3/3/3
2	EPZ	C	501	-	-	6/28/71/71	0/3/3/3
2	EPZ	E	501	-	-	6/28/71/71	0/3/3/3
2	EPZ	A	501	-	-	7/28/71/71	0/3/3/3
2	EPZ	K	501	-	-	7/28/71/71	0/3/3/3
2	EPZ	G	501	-	-	5/28/71/71	0/3/3/3
2	EPZ	I	501	-	-	7/28/71/71	0/3/3/3
2	EPZ	D	501	-	-	7/28/71/71	0/3/3/3
2	EPZ	F	501	-	-	9/28/71/71	0/3/3/3
2	EPZ	B	501	-	-	7/28/71/71	0/3/3/3
2	EPZ	L	501	-	-	3/28/71/71	0/3/3/3

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	501	EPZ	C4U-N3U	4.62	1.41	1.33
2	F	501	EPZ	C4U-N3U	3.52	1.39	1.33
2	L	501	EPZ	C2D-C1D	-3.41	1.48	1.53
2	G	501	EPZ	C6U-N1U	3.26	1.39	1.35
2	D	501	EPZ	C4U-N3U	3.23	1.38	1.33
2	G	501	EPZ	C4U-N3U	3.23	1.38	1.33
2	D	501	EPZ	PB-O1B	-3.13	1.40	1.55
2	F	501	EPZ	PB-O1B	-3.13	1.40	1.55
2	B	501	EPZ	C4U-N3U	3.12	1.38	1.33
2	E	501	EPZ	C6U-N1U	3.06	1.39	1.35
2	L	501	EPZ	PB-O1B	-3.03	1.41	1.55
2	I	501	EPZ	O4D-C1D	3.01	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	EPZ	C4U-N3U	3.01	1.38	1.33
2	J	501	EPZ	C4U-N3U	2.99	1.38	1.33
2	F	501	EPZ	PB-O2B	-2.96	1.40	1.50
2	C	501	EPZ	O5D-C5D	-2.94	1.33	1.44
2	H	501	EPZ	PB-O1B	-2.93	1.41	1.55
2	L	501	EPZ	C4U-N3U	2.93	1.38	1.33
2	F	501	EPZ	C2D-C1D	-2.90	1.49	1.53
2	G	501	EPZ	PB-O1B	-2.89	1.41	1.55
2	I	501	EPZ	C4U-N3U	2.88	1.38	1.33
2	D	501	EPZ	PA-O1A	-2.75	1.41	1.50
2	A	501	EPZ	PB-O1B	-2.75	1.42	1.55
2	H	501	EPZ	C3-C2	2.73	1.57	1.53
2	F	501	EPZ	PA-O2A	-2.70	1.42	1.55
2	E	501	EPZ	PB-O1B	-2.69	1.42	1.55
2	C	501	EPZ	PB-O1B	-2.63	1.43	1.55
2	H	501	EPZ	C4U-N3U	2.61	1.37	1.33
2	E	501	EPZ	PB-O1	-2.61	1.53	1.60
2	A	501	EPZ	O4D-C1D	2.60	1.44	1.41
2	F	501	EPZ	PB-O1	-2.60	1.53	1.60
2	J	501	EPZ	PB-O1B	-2.60	1.43	1.55
2	I	501	EPZ	PB-O1B	-2.59	1.43	1.55
2	D	501	EPZ	C3-C2	2.59	1.57	1.53
2	D	501	EPZ	PB-O2B	-2.59	1.41	1.50
2	D	501	EPZ	C6U-N1U	2.58	1.39	1.35
2	B	501	EPZ	PB-O1B	-2.57	1.43	1.55
2	C	501	EPZ	PA-O2A	-2.57	1.43	1.55
2	G	501	EPZ	O5D-C5D	-2.57	1.34	1.44
2	F	501	EPZ	C3-C2	2.55	1.57	1.53
2	K	501	EPZ	PB-O1B	-2.52	1.43	1.55
2	H	501	EPZ	C2D-C1D	-2.51	1.50	1.53
2	C	501	EPZ	C4U-N3U	2.49	1.37	1.33
2	J	501	EPZ	O5D-C5D	-2.48	1.35	1.44
2	K	501	EPZ	PA-O2A	-2.44	1.43	1.55
2	L	501	EPZ	O4D-C1D	2.43	1.44	1.41
2	D	501	EPZ	PA-O2A	-2.42	1.44	1.55
2	I	501	EPZ	PB-O1	-2.39	1.54	1.60
2	C	501	EPZ	PB-O2B	-2.39	1.42	1.50
2	F	501	EPZ	O3-C3	-2.36	1.37	1.43
2	J	501	EPZ	O4-C4	-2.35	1.37	1.43
2	B	501	EPZ	O3-C3	-2.34	1.37	1.43
2	D	501	EPZ	O3-C3	-2.32	1.37	1.43
2	I	501	EPZ	O3-C3	-2.32	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	EPZ	PB-O2B	-2.31	1.42	1.50
2	F	501	EPZ	O2D-C2D	-2.30	1.37	1.43
2	B	501	EPZ	O5D-C5D	-2.28	1.36	1.44
2	L	501	EPZ	PA-O2A	-2.27	1.44	1.55
2	E	501	EPZ	O3-C3	-2.26	1.38	1.43
2	D	501	EPZ	O5D-C5D	-2.25	1.36	1.44
2	I	501	EPZ	PA-O2A	-2.24	1.44	1.55
2	A	501	EPZ	PA-O2A	-2.24	1.44	1.55
2	K	501	EPZ	C3-C2	2.23	1.56	1.53
2	E	501	EPZ	PA-O2A	-2.21	1.44	1.55
2	K	501	EPZ	PA-O1A	-2.20	1.43	1.50
2	B	501	EPZ	PA-O2A	-2.19	1.45	1.55
2	A	501	EPZ	C2D-C1D	-2.17	1.50	1.53
2	A	501	EPZ	PB-O2B	-2.17	1.43	1.50
2	J	501	EPZ	PA-O2A	-2.16	1.45	1.55
2	C	501	EPZ	C3-C2	2.15	1.56	1.53
2	H	501	EPZ	O5D-C5D	-2.14	1.36	1.44
2	E	501	EPZ	C4U-N3U	2.14	1.36	1.33
2	C	501	EPZ	C6U-N1U	2.11	1.38	1.35
2	G	501	EPZ	C2D-C1D	-2.11	1.50	1.53
2	K	501	EPZ	O5D-C5D	-2.11	1.36	1.44
2	J	501	EPZ	C2D-C1D	-2.10	1.50	1.53
2	L	501	EPZ	O2D-C2D	-2.09	1.38	1.43
2	A	501	EPZ	O2D-C2D	-2.07	1.38	1.43
2	A	501	EPZ	PB-O1	-2.07	1.55	1.60
2	K	501	EPZ	C2D-C1D	-2.05	1.50	1.53
2	A	501	EPZ	O3-C3	-2.05	1.38	1.43
2	J	501	EPZ	PB-O1	-2.04	1.55	1.60
2	C	501	EPZ	C6U-C5U	2.04	1.42	1.38
2	I	501	EPZ	O4-C4	-2.02	1.38	1.43
2	H	501	EPZ	PB-O1	-2.01	1.55	1.60

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	501	EPZ	O4D-C4D-C5D	-4.20	95.57	109.37
2	C	501	EPZ	O4D-C4D-C5D	-4.04	96.08	109.37
2	J	501	EPZ	O4D-C4D-C5D	-3.84	96.75	109.37
2	H	501	EPZ	O4D-C4D-C5D	-3.66	97.34	109.37
2	J	501	EPZ	O5D-C5D-C4D	3.56	121.23	108.99
2	D	501	EPZ	O4D-C4D-C5D	-3.55	97.69	109.37
2	A	501	EPZ	O4D-C4D-C5D	-3.55	97.70	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	EPZ	O4D-C4D-C5D	-3.50	97.87	109.37
2	B	501	EPZ	O5D-C5D-C4D	3.44	120.85	108.99
2	K	501	EPZ	O5D-C5D-C4D	3.39	120.66	108.99
2	F	501	EPZ	O4D-C4D-C5D	-3.33	98.43	109.37
2	B	501	EPZ	O4D-C4D-C5D	-3.22	98.77	109.37
2	A	501	EPZ	O5D-C5D-C4D	3.12	119.73	108.99
2	E	501	EPZ	O4D-C4D-C5D	-3.05	99.35	109.37
2	D	501	EPZ	O5D-C5D-C4D	3.00	119.30	108.99
2	I	501	EPZ	C3E-C2E-C1E	-2.89	109.62	113.35
2	D	501	EPZ	O5-C1-O1	-2.88	107.60	111.36
2	L	501	EPZ	O4D-C4D-C5D	-2.81	100.12	109.37
2	G	501	EPZ	O5D-C5D-C4D	2.78	118.54	108.99
2	E	501	EPZ	O5D-C5D-C4D	2.68	118.20	108.99
2	I	501	EPZ	O4D-C4D-C5D	-2.65	100.67	109.37
2	B	501	EPZ	C3E-C2E-C1E	-2.59	110.00	113.35
2	D	501	EPZ	C3E-C2E-C1E	-2.57	110.03	113.35
2	L	501	EPZ	O5D-C5D-C4D	2.51	117.64	108.99
2	I	501	EPZ	O5D-C5D-C4D	2.51	117.62	108.99
2	C	501	EPZ	C3D-C2D-C1D	2.50	104.74	100.98
2	C	501	EPZ	O5D-C5D-C4D	2.50	117.59	108.99
2	L	501	EPZ	C3E-C2E-C1E	-2.45	110.18	113.35
2	F	501	EPZ	C3D-C2D-C1D	2.44	104.65	100.98
2	C	501	EPZ	C3E-C2E-C1E	-2.42	110.23	113.35
2	A	501	EPZ	C3D-C2D-C1D	2.37	104.54	100.98
2	H	501	EPZ	O5D-C5D-C4D	2.35	117.06	108.99
2	H	501	EPZ	C3E-C2E-C1E	-2.26	110.42	113.35
2	B	501	EPZ	C3D-C2D-C1D	2.22	104.33	100.98
2	L	501	EPZ	O5-C1-O1	-2.14	108.56	111.36
2	B	501	EPZ	O3A-PB-O1	-2.14	98.16	102.48
2	B	501	EPZ	C6U-N1U-C2U	-2.14	117.80	121.20
2	D	501	EPZ	C3D-C2D-C1D	2.14	104.19	100.98
2	E	501	EPZ	O3D-C3D-C2D	-2.09	105.08	111.82
2	F	501	EPZ	C6U-N1U-C2U	-2.09	117.89	121.20
2	C	501	EPZ	O1-PB-O2B	-2.08	101.67	109.47
2	F	501	EPZ	O5D-C5D-C4D	2.02	115.96	108.99
2	E	501	EPZ	O5-C5-C6	2.02	111.47	106.44

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	501	EPZ	C3E-C2E-O3-C3

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Mol	Chain	Res	Type	Atoms
2	H	501	EPZ	C2D-C1D-N1U-C6U
2	H	501	EPZ	O4D-C1D-N1U-C6U
2	J	501	EPZ	C2D-C1D-N1U-C6U
2	J	501	EPZ	O4D-C1D-N1U-C6U
2	C	501	EPZ	C1E-C2E-O3-C3
2	C	501	EPZ	C3E-C2E-O3-C3
2	C	501	EPZ	O4D-C1D-N1U-C6U
2	E	501	EPZ	C2D-C1D-N1U-C6U
2	E	501	EPZ	O4D-C1D-N1U-C6U
2	A	501	EPZ	C2D-C1D-N1U-C6U
2	A	501	EPZ	O4D-C1D-N1U-C6U
2	K	501	EPZ	C2D-C1D-N1U-C6U
2	K	501	EPZ	O4D-C1D-N1U-C6U
2	I	501	EPZ	C2D-C1D-N1U-C6U
2	I	501	EPZ	O4D-C1D-N1U-C6U
2	D	501	EPZ	C3E-C2E-O3-C3
2	D	501	EPZ	C2D-C1D-N1U-C6U
2	D	501	EPZ	O4D-C1D-N1U-C6U
2	F	501	EPZ	C3E-C2E-O3-C3
2	F	501	EPZ	C2D-C1D-N1U-C6U
2	F	501	EPZ	O4D-C1D-N1U-C6U
2	F	501	EPZ	O4D-C4D-C5D-O5D
2	B	501	EPZ	C3E-C2E-O3-C3
2	H	501	EPZ	O4D-C4D-C5D-O5D
2	J	501	EPZ	O4D-C4D-C5D-O5D
2	C	501	EPZ	O4D-C4D-C5D-O5D
2	E	501	EPZ	O4D-C4D-C5D-O5D
2	A	501	EPZ	O4D-C4D-C5D-O5D
2	K	501	EPZ	O4D-C4D-C5D-O5D
2	G	501	EPZ	O4D-C4D-C5D-O5D
2	I	501	EPZ	O4D-C4D-C5D-O5D
2	D	501	EPZ	O4D-C4D-C5D-O5D
2	B	501	EPZ	O4D-C4D-C5D-O5D
2	L	501	EPZ	O4D-C4D-C5D-O5D
2	F	501	EPZ	C3D-C4D-C5D-O5D
2	I	501	EPZ	C4-C5-C6-O6
2	D	501	EPZ	C3D-C4D-C5D-O5D
2	I	501	EPZ	O5-C5-C6-O6
2	H	501	EPZ	C3D-C4D-C5D-O5D
2	H	501	EPZ	C4-C5-C6-O6
2	E	501	EPZ	C3D-C4D-C5D-O5D
2	G	501	EPZ	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	H	501	EPZ	C1E-C2E-O3-C3
2	G	501	EPZ	C1E-C2E-O3-C3
2	G	501	EPZ	C3E-C2E-O3-C3
2	D	501	EPZ	C1E-C2E-O3-C3
2	F	501	EPZ	C1E-C2E-O3-C3
2	B	501	EPZ	C1E-C2E-O3-C3
2	C	501	EPZ	C3D-C4D-C5D-O5D
2	A	501	EPZ	C3D-C4D-C5D-O5D
2	K	501	EPZ	C3D-C4D-C5D-O5D
2	J	501	EPZ	PB-O3A-PA-O1A
2	B	501	EPZ	PB-O3A-PA-O1A
2	H	501	EPZ	O5-C5-C6-O6
2	J	501	EPZ	C3E-C2E-O3-C3
2	K	501	EPZ	C1E-C2E-O3-C3
2	K	501	EPZ	C3E-C2E-O3-C3
2	I	501	EPZ	C3E-C2E-O3-C3
2	F	501	EPZ	C1-O1-PB-O3A
2	B	501	EPZ	C3D-C4D-C5D-O5D
2	A	501	EPZ	C1E-C2E-O3-C3
2	A	501	EPZ	C3E-C2E-O3-C3
2	E	501	EPZ	PA-O3A-PB-O2B
2	F	501	EPZ	PA-O3A-PB-O2B
2	B	501	EPZ	PB-O3A-PA-O2A
2	H	501	EPZ	C5D-O5D-PA-O1A
2	J	501	EPZ	C5D-O5D-PA-O1A
2	C	501	EPZ	C5D-O5D-PA-O1A
2	E	501	EPZ	C5D-O5D-PA-O1A
2	A	501	EPZ	C5D-O5D-PA-O1A
2	K	501	EPZ	C5D-O5D-PA-O1A
2	G	501	EPZ	C5D-O5D-PA-O1A
2	I	501	EPZ	C5D-O5D-PA-O1A
2	D	501	EPZ	C5D-O5D-PA-O1A
2	F	501	EPZ	C5D-O5D-PA-O1A
2	B	501	EPZ	C5D-O5D-PA-O1A
2	L	501	EPZ	C5D-O5D-PA-O1A
2	L	501	EPZ	C3D-C4D-C5D-O5D

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	501	EPZ	2	0

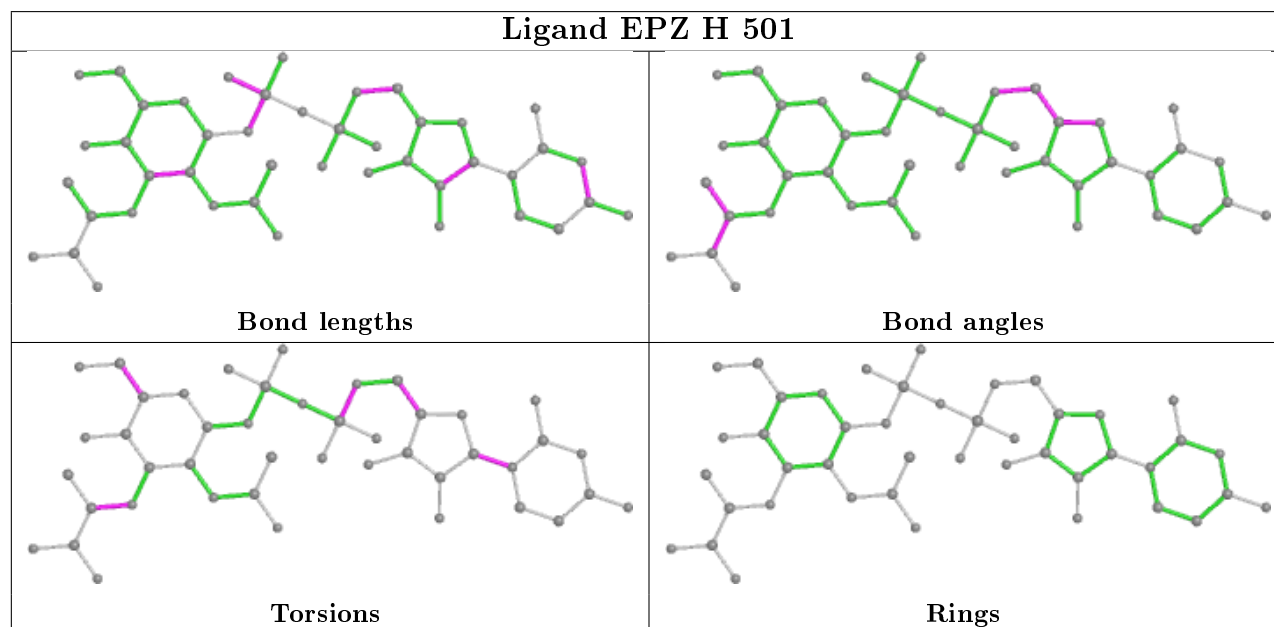
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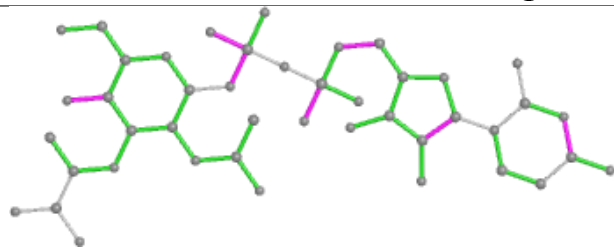
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	EPZ	1	0
2	K	501	EPZ	3	0
2	G	501	EPZ	1	0
2	I	501	EPZ	2	0
2	B	501	EPZ	2	0
2	L	501	EPZ	1	0

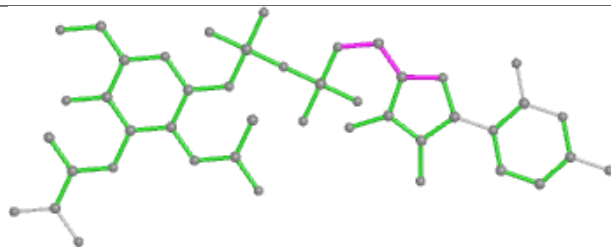
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



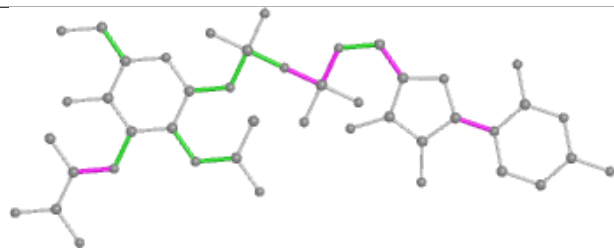
## Ligand EPZ J 501



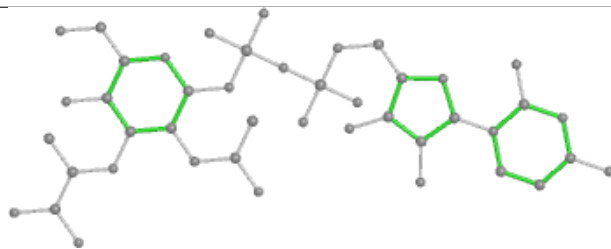
Bond lengths



Bond angles

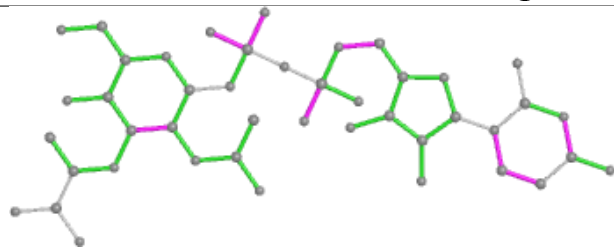


Torsions

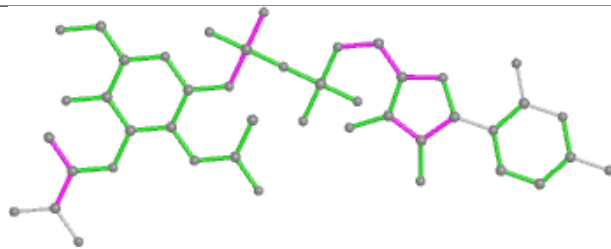


Rings

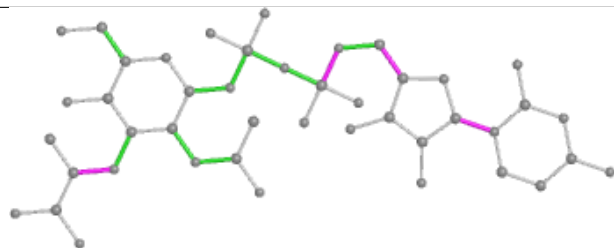
## Ligand EPZ C 501



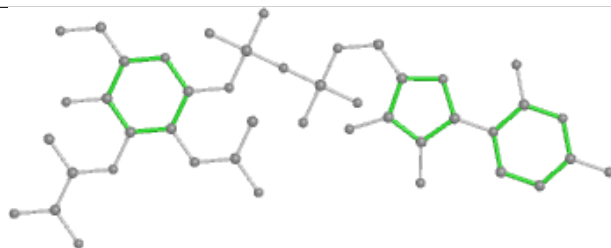
Bond lengths



Bond angles

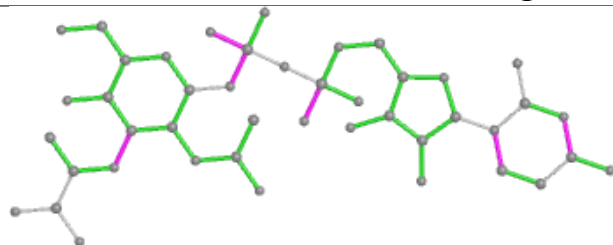


Torsions

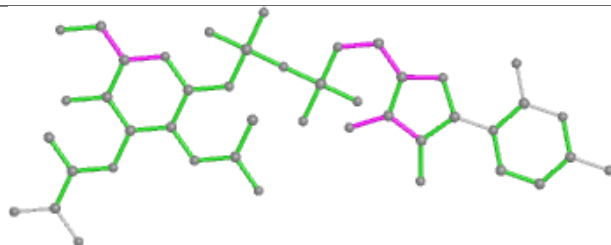


Rings

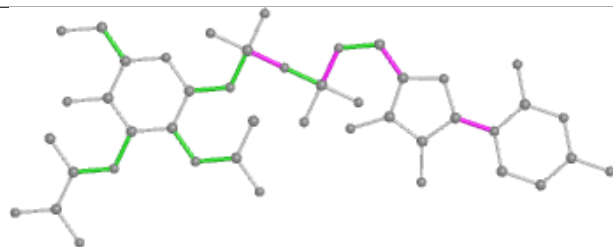
## Ligand EPZ E 501



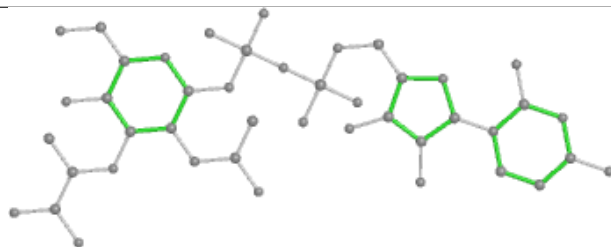
Bond lengths



Bond angles

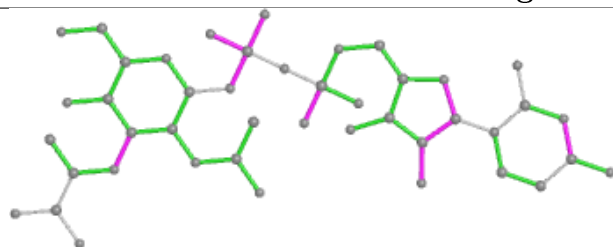


Torsions

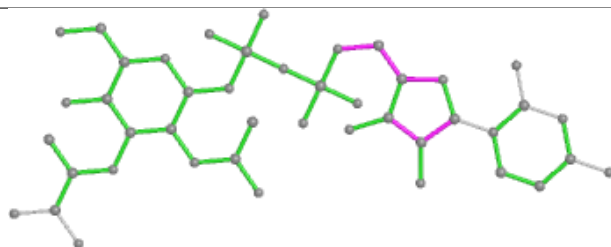


Rings

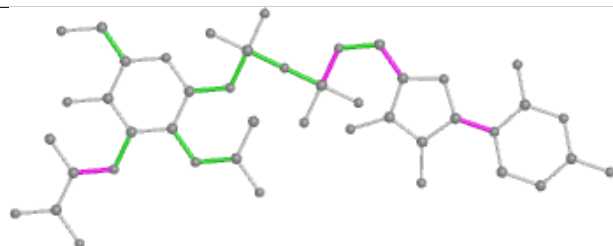
## Ligand EPZ A 501



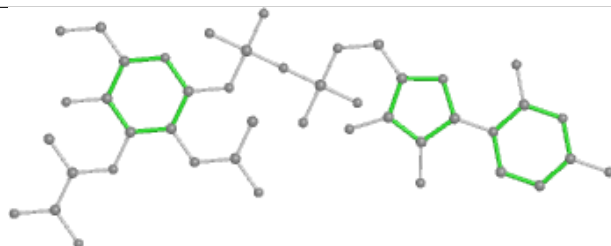
Bond lengths



Bond angles

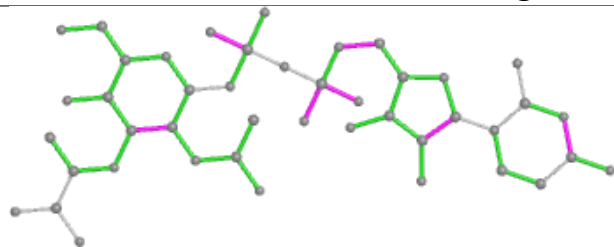


Torsions

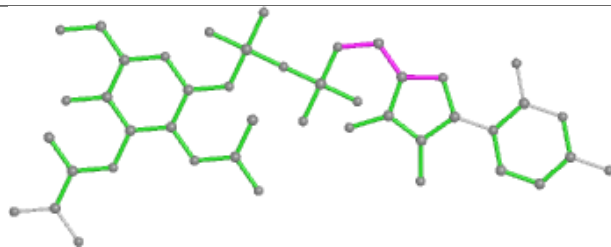


Rings

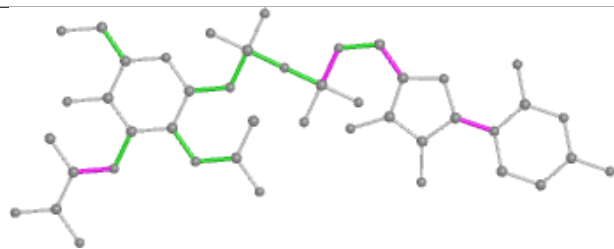
## Ligand EPZ K 501



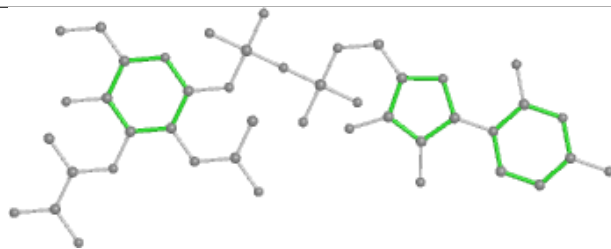
Bond lengths



Bond angles

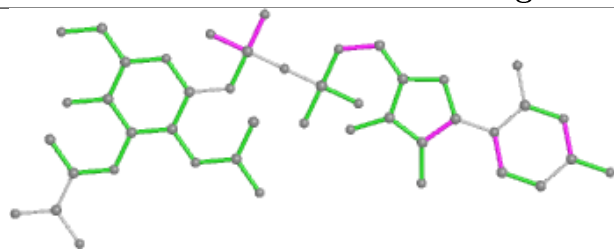


Torsions

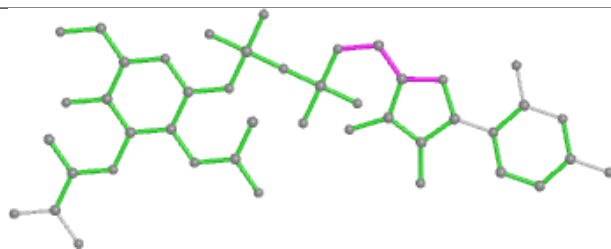


Rings

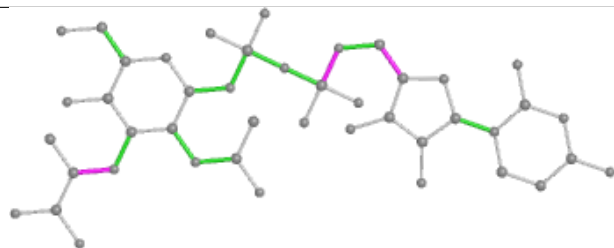
## Ligand EPZ G 501



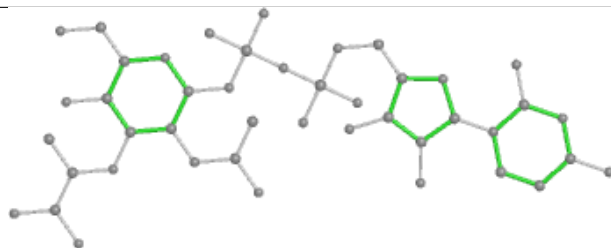
Bond lengths



Bond angles

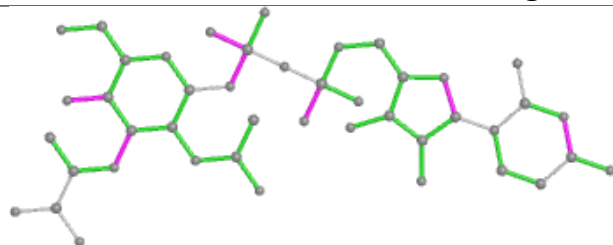


Torsions

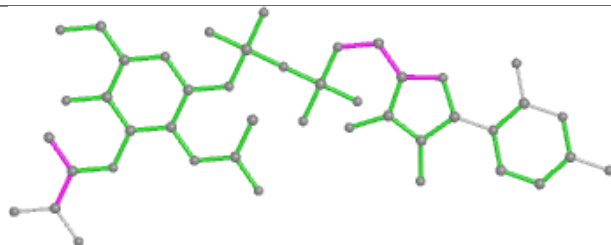


Rings

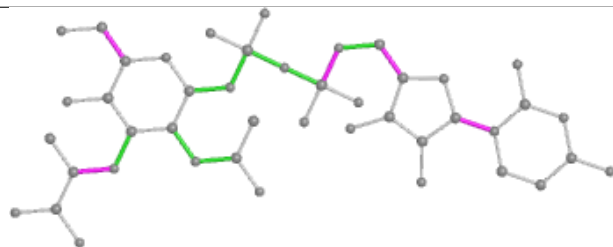
## Ligand EPZ I 501



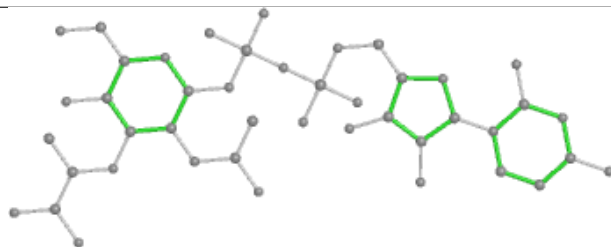
Bond lengths



Bond angles

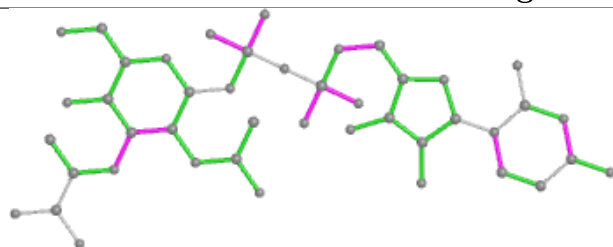


Torsions

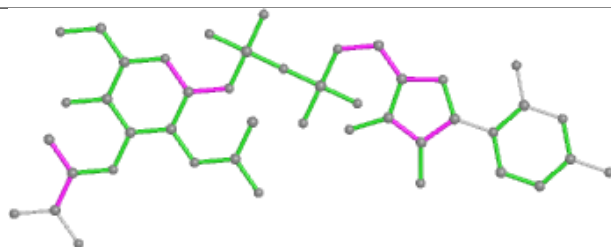


Rings

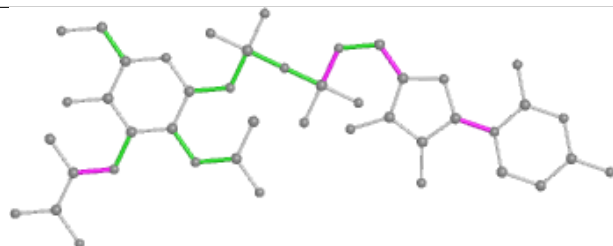
## Ligand EPZ D 501



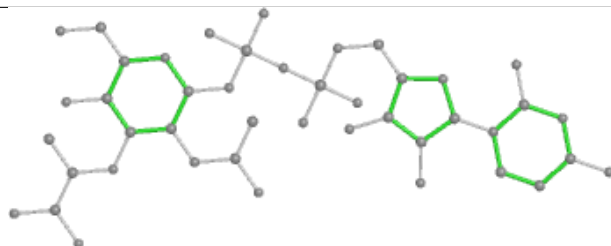
Bond lengths



Bond angles

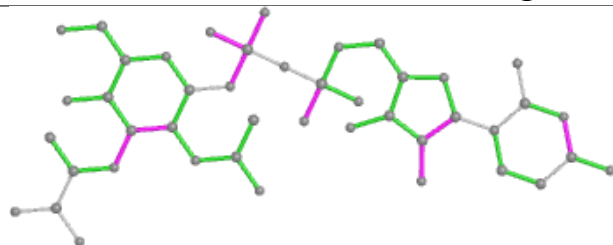


Torsions

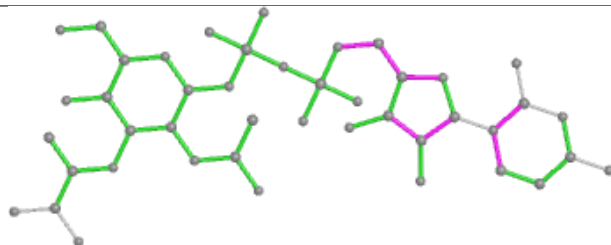


Rings

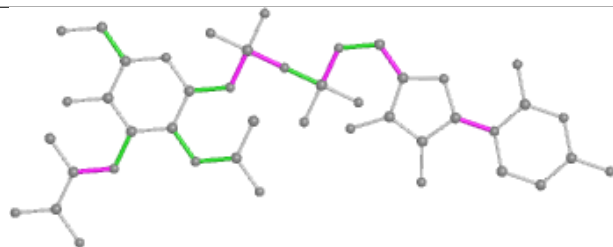
## Ligand EPZ F 501



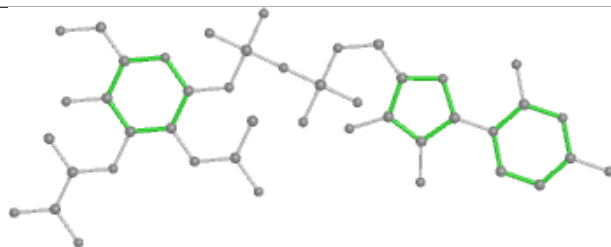
Bond lengths



Bond angles

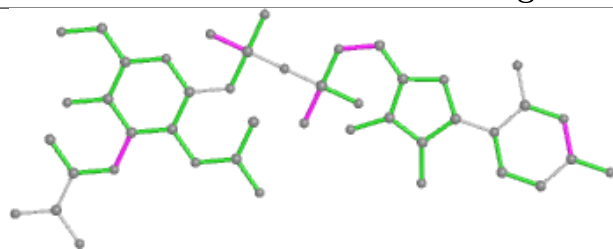


Torsions

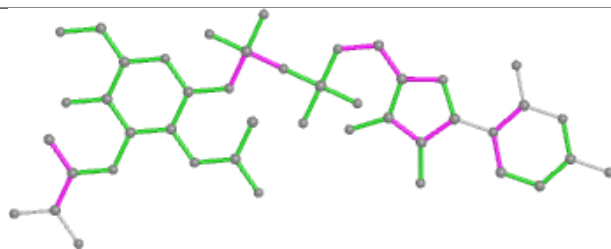


Rings

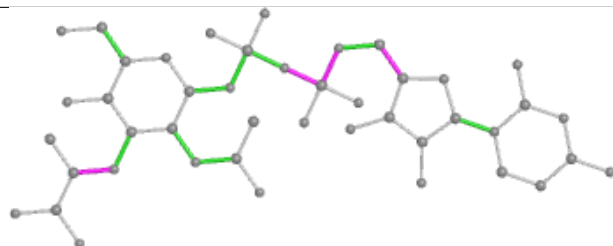
## Ligand EPZ B 501



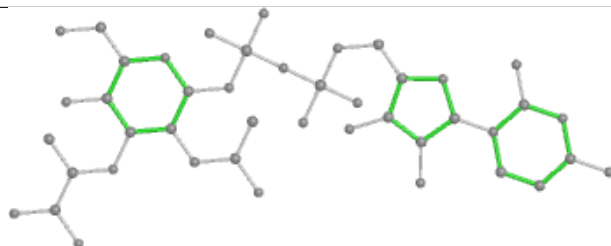
Bond lengths



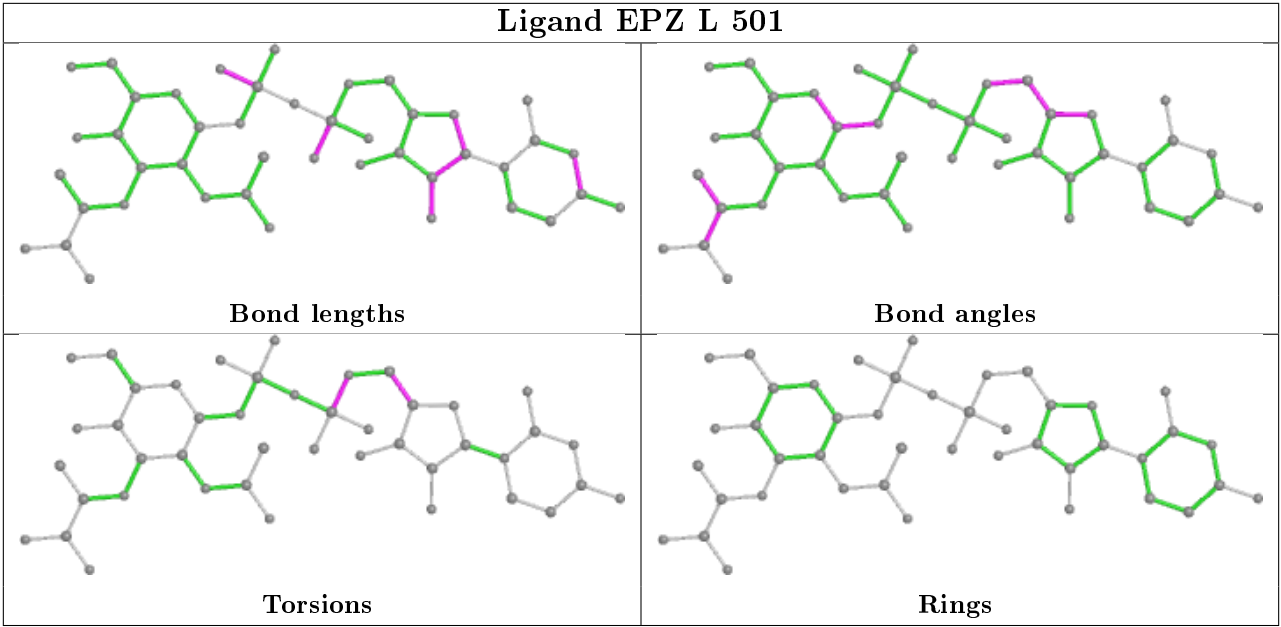
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	67:IAS	C	68:GLY	N	4.51
1	A	67:IAS	C	68:GLY	N	4.32

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	67:IAS	C	68:GLY	N	4.32
1	L	67:IAS	C	68:GLY	N	4.31
1	B	67:IAS	C	68:GLY	N	4.30
1	J	67:IAS	C	68:GLY	N	4.28
1	H	67:IAS	C	68:GLY	N	4.27
1	C	67:IAS	C	68:GLY	N	4.26
1	D	67:IAS	C	68:GLY	N	4.25
1	E	67:IAS	C	68:GLY	N	4.24
1	F	67:IAS	C	68:GLY	N	3.73
1	K	67:IAS	C	68:GLY	N	3.71



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	416/418 (99%)	-0.17	4 (0%) 82 84	36, 54, 76, 97	0
1	B	416/418 (99%)	0.23	18 (4%) 35 38	37, 61, 83, 100	0
1	C	416/418 (99%)	-0.23	1 (0%) 95 95	30, 47, 69, 95	0
1	D	416/418 (99%)	-0.31	0 100 100	25, 47, 68, 95	0
1	E	416/418 (99%)	-0.12	3 (0%) 87 89	30, 50, 72, 102	0
1	F	416/418 (99%)	-0.05	3 (0%) 87 89	29, 53, 77, 100	0
1	G	416/418 (99%)	0.11	13 (3%) 49 52	33, 60, 83, 104	0
1	H	416/418 (99%)	-0.24	3 (0%) 87 89	34, 50, 70, 95	0
1	I	416/418 (99%)	0.44	42 (10%) 7 6	39, 67, 93, 110	0
1	J	416/418 (99%)	-0.15	5 (1%) 79 80	37, 58, 79, 100	0
1	K	416/418 (99%)	-0.25	5 (1%) 79 80	29, 50, 73, 88	0
1	L	416/418 (99%)	0.69	55 (13%) 3 3	43, 72, 94, 120	0
All	All	4992/5016 (99%)	-0.00	152 (3%) 50 53	25, 55, 83, 120	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	221	LEU	8.8
1	L	222	GLY	8.2
1	L	215	ILE	7.0
1	I	215	ILE	6.8
1	I	81	CYS	5.8
1	I	216	GLU	5.5
1	L	205	ILE	5.5
1	B	395	ILE	5.1
1	I	134	ALA	5.0
1	B	418	GLY	5.0
1	L	37	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	L	39	VAL	4.9
1	I	99	PRO	4.9
1	I	177	GLU	4.9
1	L	216	GLU	4.8
1	I	181	ILE	4.7
1	L	213	ILE	4.6
1	L	12	LEU	4.5
1	L	277	GLU	4.5
1	L	201	LEU	4.2
1	G	56	LEU	4.0
1	I	136	ILE	4.0
1	H	418	GLY	4.0
1	L	38	PRO	4.0
1	G	59	GLN	3.9
1	I	152	LYS	3.8
1	I	148	ASP	3.8
1	E	57	LEU	3.8
1	B	273	ILE	3.7
1	I	132	LEU	3.7
1	L	204	LYS	3.7
1	J	273	ILE	3.6
1	B	86	LEU	3.6
1	I	248	LYS	3.5
1	B	146	SER	3.5
1	L	41	ILE	3.4
1	L	279	TRP	3.4
1	G	74	ALA	3.4
1	I	133	GLY	3.4
1	L	270	GLY	3.4
1	B	60	LEU	3.4
1	I	100	LEU	3.3
1	L	220	ARG	3.3
1	I	230	PRO	3.3
1	B	13	GLN	3.2
1	J	72	ILE	3.1
1	L	197	PHE	3.1
1	L	199	ILE	3.1
1	G	418	GLY	3.1
1	F	225	VAL	3.1
1	I	80	PHE	3.0
1	F	72	ILE	3.0
1	L	64	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	152	LYS	2.9
1	L	282	LEU	2.9
1	I	78	ASN	2.9
1	H	60	LEU	2.9
1	L	200	THR	2.8
1	L	272	ASP	2.8
1	L	70	VAL	2.8
1	I	154	ALA	2.8
1	B	244	ILE	2.7
1	L	175	LEU	2.7
1	I	74	ALA	2.7
1	L	26	LEU	2.7
1	L	44	VAL	2.7
1	A	147	VAL	2.6
1	I	171	CYS	2.6
1	L	225	VAL	2.6
1	I	135	THR	2.6
1	L	76	ASP	2.6
1	G	54	MET	2.6
1	I	102	ALA	2.6
1	I	86	LEU	2.6
1	J	201	LEU	2.6
1	I	349	SER	2.6
1	G	12	LEU	2.6
1	E	39	VAL	2.5
1	K	330	ASN	2.5
1	L	226	TYR	2.5
1	L	281	SER	2.5
1	L	117	ILE	2.5
1	G	79	VAL	2.4
1	K	349	SER	2.4
1	L	16	VAL	2.4
1	B	219	GLU	2.4
1	I	39	VAL	2.4
1	L	63	LYS	2.4
1	H	176	ALA	2.4
1	B	68	GLY	2.4
1	I	350	ASN	2.4
1	L	350	ASN	2.4
1	G	401	ARG	2.4
1	K	249	ILE	2.4
1	L	18	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	249	ILE	2.4
1	I	42	GLN	2.3
1	L	267	ARG	2.3
1	L	255	GLN	2.3
1	I	402	ILE	2.3
1	I	33	LEU	2.3
1	I	151	LEU	2.3
1	L	100	LEU	2.3
1	G	1	MET	2.3
1	B	35	ALA	2.3
1	I	198	LEU	2.3
1	B	272	ASP	2.3
1	I	194	THR	2.3
1	L	417	LYS	2.3
1	I	223	GLY	2.3
1	I	182	ILE	2.3
1	I	179	THR	2.3
1	G	37	GLU	2.3
1	L	351	THR	2.2
1	K	350	ASN	2.2
1	L	75	ARG	2.2
1	E	223	GLY	2.2
1	C	349	SER	2.2
1	G	326	THR	2.2
1	B	282	LEU	2.2
1	I	399	TYR	2.2
1	J	349	SER	2.2
1	I	64	VAL	2.2
1	L	126	ILE	2.2
1	L	191	ILE	2.2
1	B	350	ASN	2.2
1	B	61	GLY	2.2
1	L	362	GLY	2.2
1	L	246	ARG	2.2
1	A	9	PRO	2.1
1	B	99	PRO	2.1
1	F	177	GLU	2.1
1	J	74	ALA	2.1
1	L	194	THR	2.1
1	L	171	CYS	2.1
1	B	41	ILE	2.1
1	G	411	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	137	LYS	2.1
1	I	175	LEU	2.1
1	L	248	LYS	2.1
1	I	218	VAL	2.1
1	L	33	LEU	2.1
1	L	378	LEU	2.1
1	K	105	GLY	2.1
1	I	144	LYS	2.1
1	G	38	PRO	2.0
1	I	147	VAL	2.0
1	L	324	THR	2.0
1	A	133	GLY	2.0
1	A	418	GLY	2.0
1	B	34	LEU	2.0
1	L	280	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	IAS	I	67	8/9	0.65	0.27	79,89,111,120	0
1	IAS	L	67	8/9	0.82	0.26	81,89,99,102	0
1	IAS	A	67	8/9	0.89	0.15	50,56,66,69	0
1	IAS	G	67	8/9	0.90	0.18	64,67,75,77	0
1	QPA	B	115	16/17	0.91	0.12	46,64,92,95	0
1	IAS	D	67	8/9	0.92	0.15	42,54,62,62	0
1	IAS	C	67	8/9	0.92	0.15	61,69,72,72	0
1	QPA	A	115	16/17	0.92	0.22	49,62,92,92	0
1	IAS	F	67	8/9	0.93	0.13	52,64,76,80	0
1	IAS	B	67	8/9	0.93	0.19	66,72,84,90	0
1	QPA	I	115	16/17	0.93	0.15	46,65,92,92	0
1	QPA	E	115	16/17	0.93	0.15	42,62,77,80	0
1	QPA	F	115	16/17	0.93	0.20	41,60,80,86	0
1	IAS	K	67	8/9	0.93	0.14	59,61,65,71	0
1	QPA	L	115	16/17	0.94	0.15	50,65,81,85	0
1	QPA	H	115	16/17	0.94	0.17	40,63,76,77	0
1	IAS	H	67	8/9	0.94	0.20	53,66,80,88	0
1	QPA	K	115	16/17	0.95	0.18	36,57,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	IAS	J	67	8/9	0.95	0.13	53,75,79,84	0
1	QPA	C	115	16/17	0.95	0.19	38,62,79,83	0
1	IAS	E	67	8/9	0.95	0.08	41,53,62,78	0
1	QPA	G	115	16/17	0.96	0.15	41,58,76,79	0
1	QPA	D	115	16/17	0.96	0.17	30,51,68,68	0
1	QPA	J	115	16/17	0.98	0.15	37,55,84,103	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

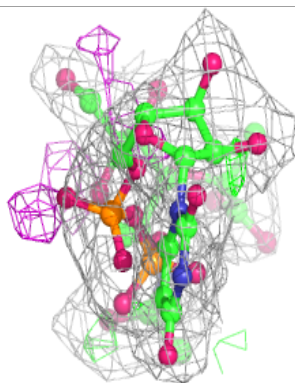
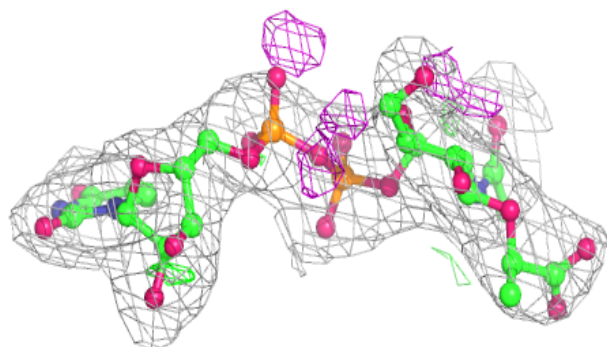
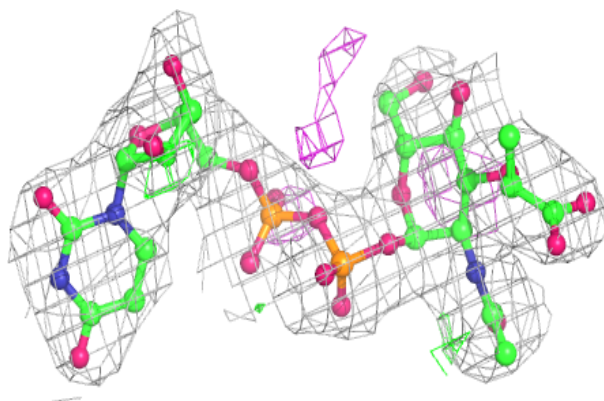
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EPZ	I	501	44/44	0.94	0.17	38,58,68,84	0
2	EPZ	G	501	44/44	0.96	0.18	31,48,65,67	0
2	EPZ	L	501	44/44	0.96	0.18	25,60,76,99	0
2	EPZ	A	501	44/44	0.97	0.17	28,46,60,63	0
2	EPZ	K	501	44/44	0.97	0.14	27,43,60,66	0
2	EPZ	H	501	44/44	0.97	0.14	27,44,58,66	0
2	EPZ	J	501	44/44	0.97	0.14	30,45,64,70	0
2	EPZ	D	501	44/44	0.97	0.14	25,43,58,70	0
2	EPZ	B	501	44/44	0.97	0.13	27,51,73,82	0
2	EPZ	C	501	44/44	0.97	0.16	28,40,57,66	0
2	EPZ	E	501	44/44	0.98	0.16	31,44,60,82	0
2	EPZ	F	501	44/44	0.98	0.16	20,38,59,78	0

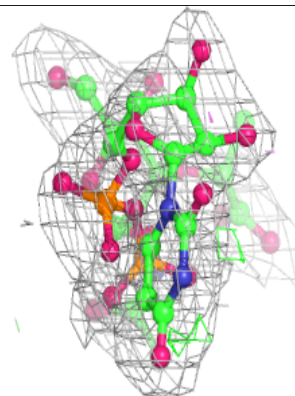
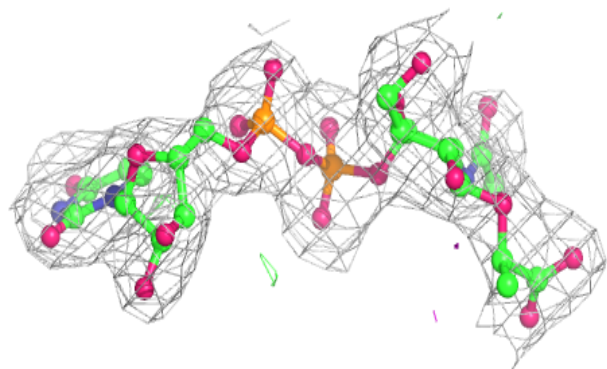
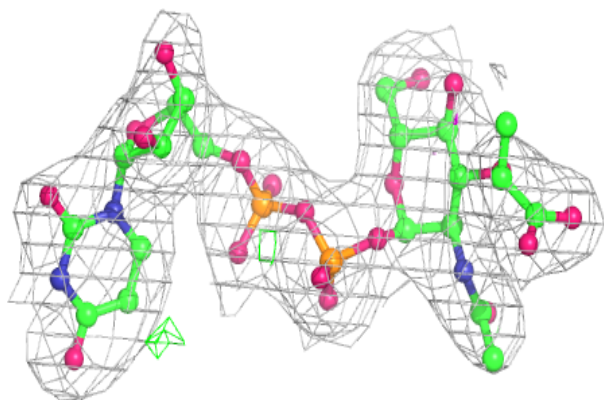
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around EPZ I 501:**

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

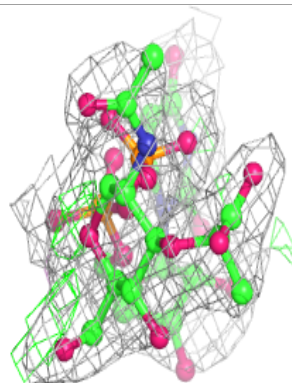
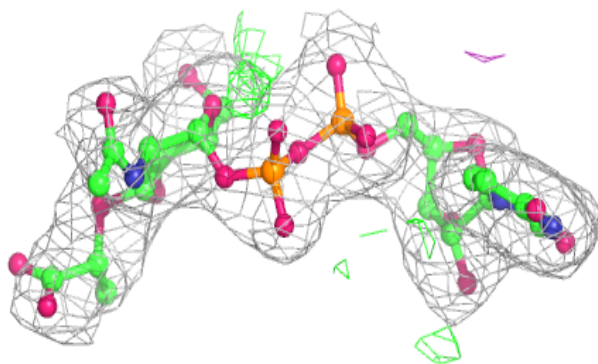
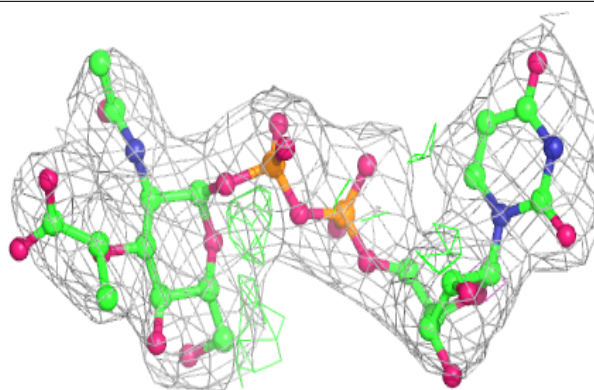
**Electron density around EPZ G 501:**

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

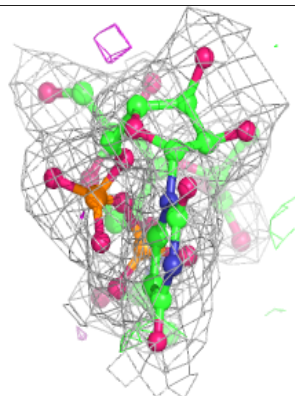
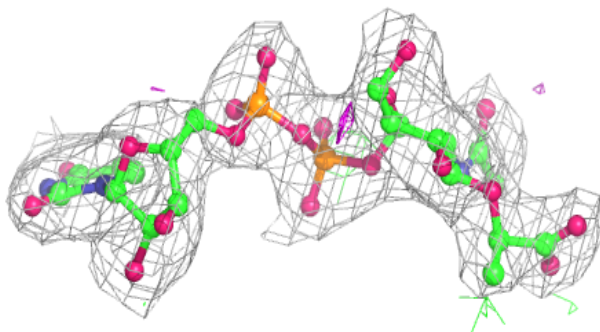
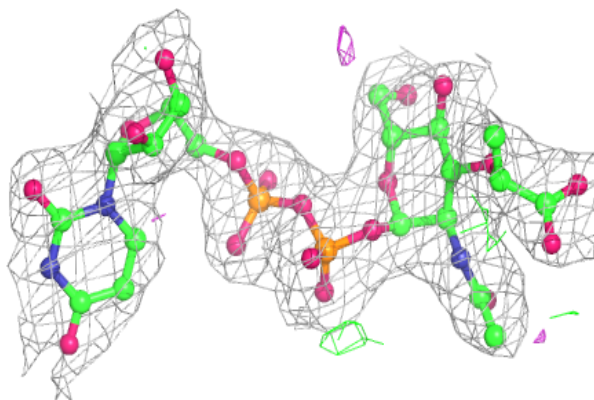


**Electron density around EPZ L 501:**

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

**Electron density around EPZ A 501:**

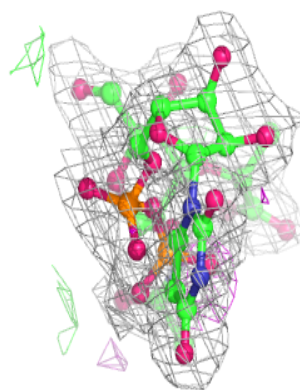
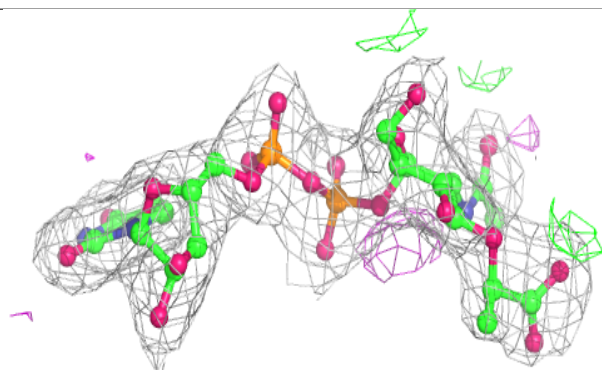
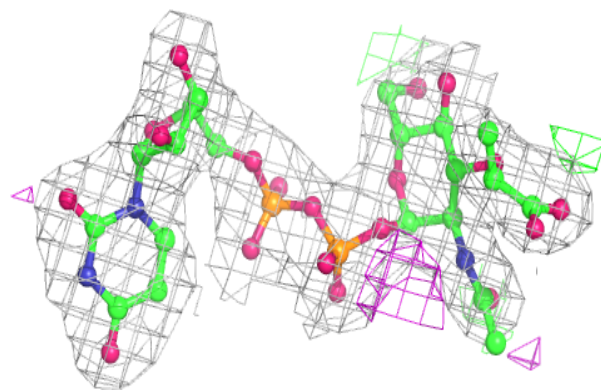
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



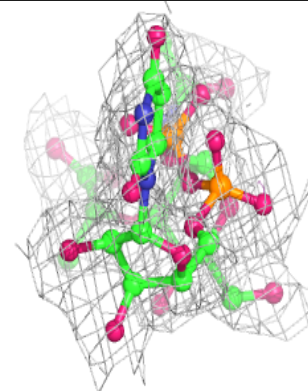
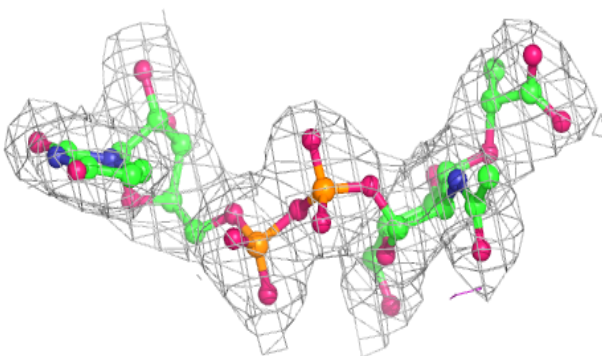
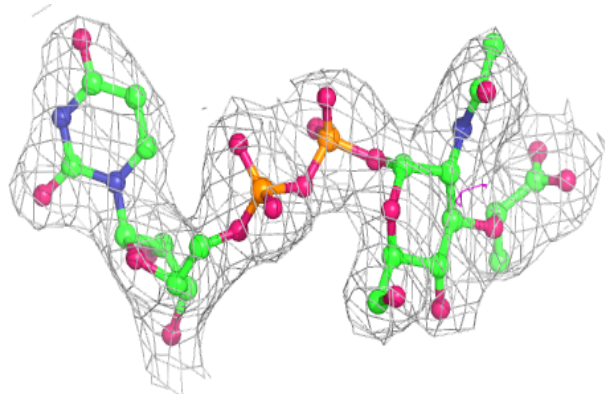


**Electron density around EPZ K 501:**

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

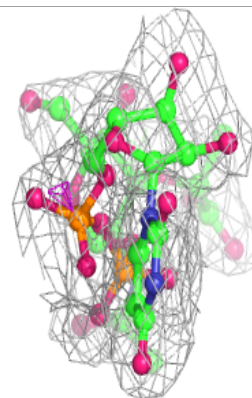
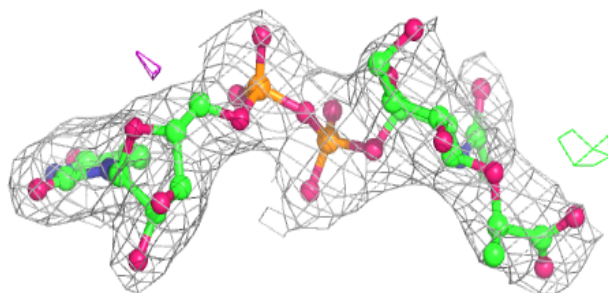
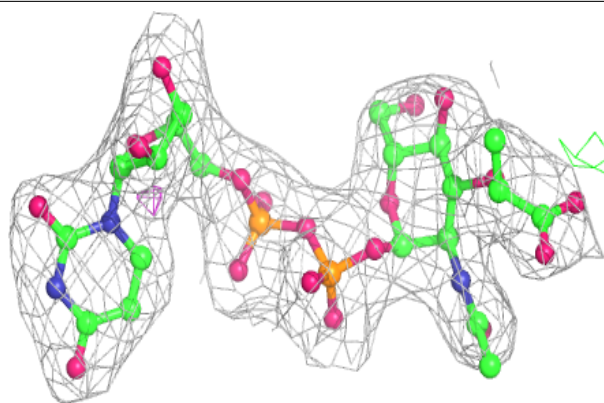
**Electron density around EPZ H 501:**

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

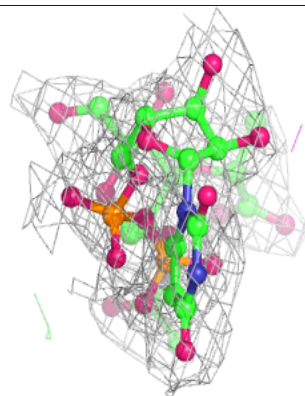
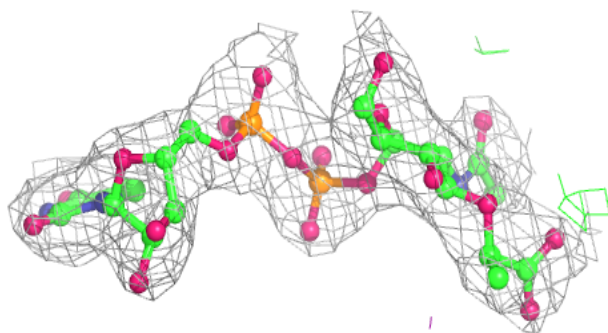
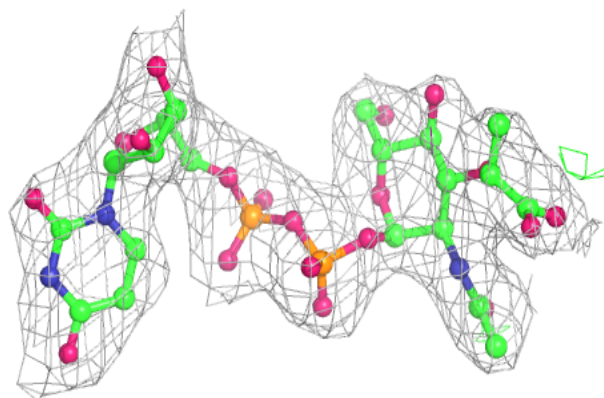


**Electron density around EPZ J 501:**

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

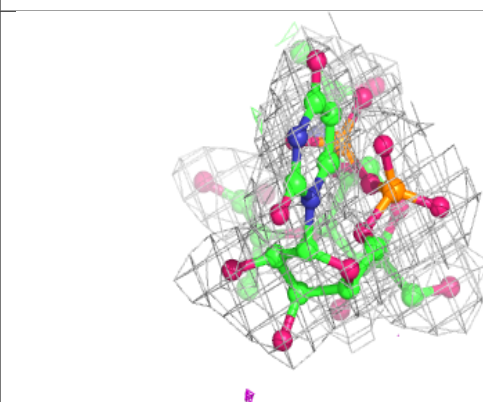
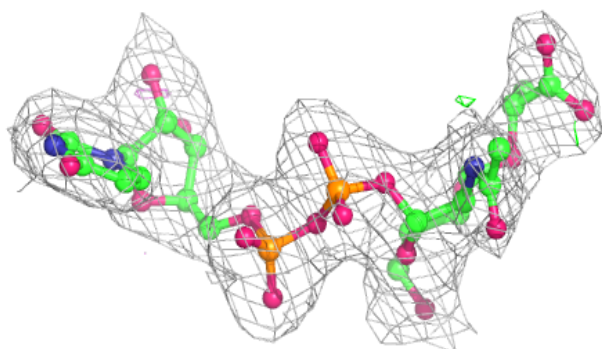
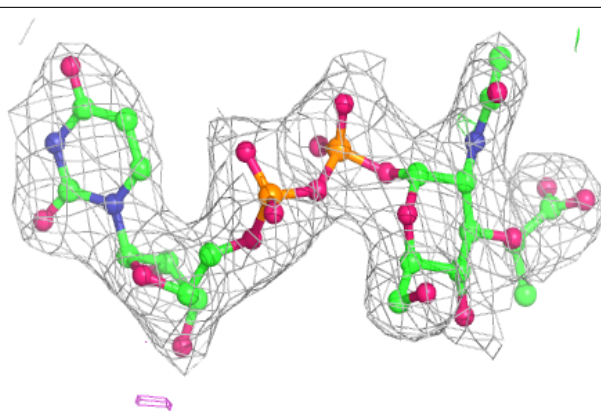
**Electron density around EPZ D 501:**

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

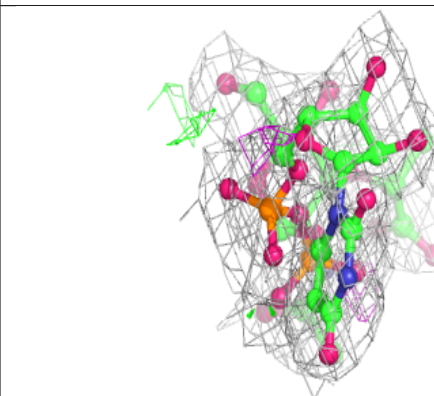
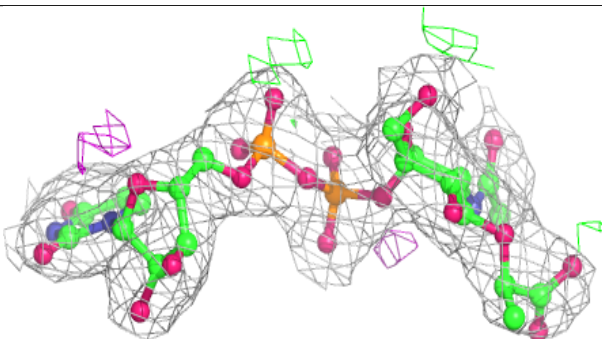
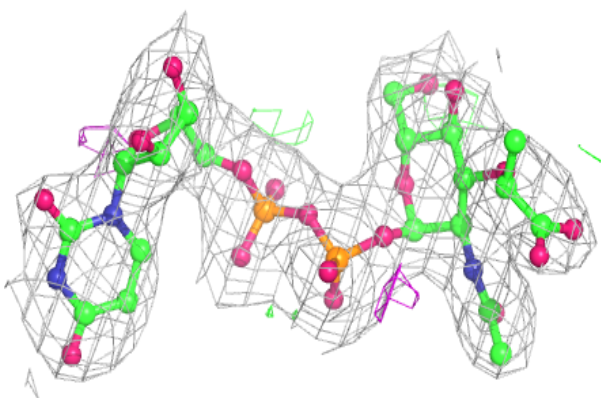


**Electron density around EPZ B 501:**

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

**Electron density around EPZ C 501:**

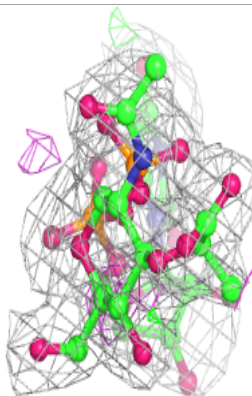
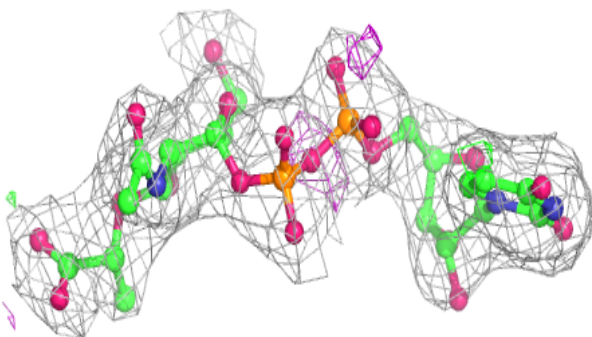
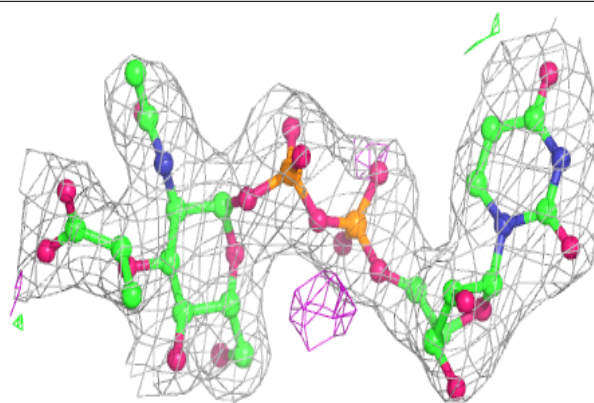
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



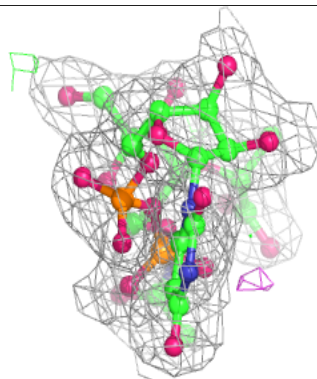
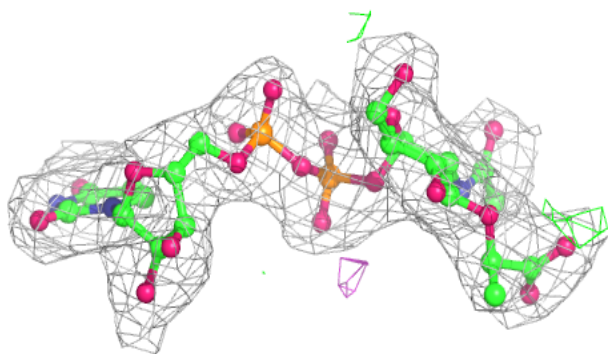
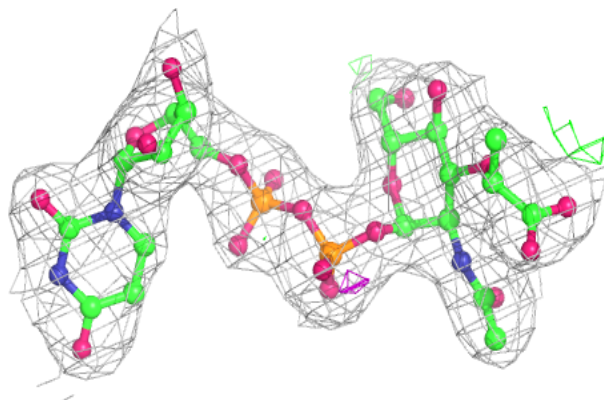


**Electron density around EPZ E 501:**

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

**Electron density around EPZ F 501:**

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



## 6.5 Other polymers

There are no such residues in this entry.