



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2024 – 03:39 AM EST

PDB ID : 7U3B  
Title : Structure of *S. venezuelae* GlgX bound to c-di-GMP and acarbose (pH 8.5)  
Authors : Schumacher, M.A.; Tschowri, N.  
Deposited on : 2022-02-26  
Resolution : 3.60 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

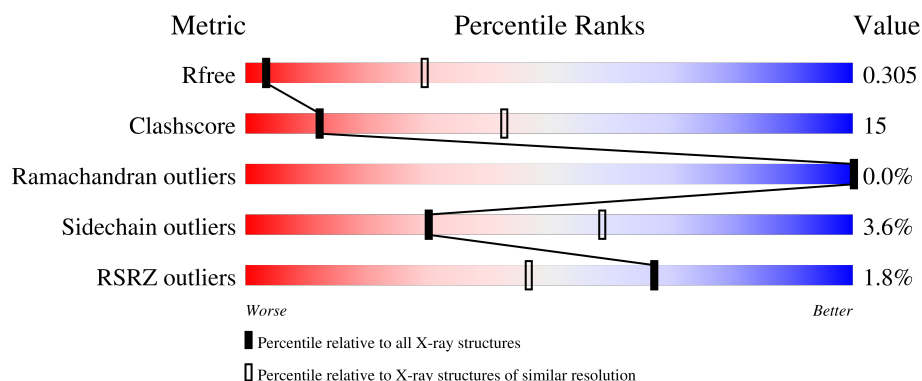
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	C	709	<div> <div>2%</div> <div>65% 32% ..</div> </div>
1	D	709	<div> <div>2%</div> <div>64% 32% ..</div> </div>
1	E	709	<div> <div>2%</div> <div>66% 31% ..</div> </div>
1	F	709	<div> <div>0%</div> <div>63% 34% ..</div> </div>
1	G	709	<div> <div>2%</div> <div>68% 29% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	709	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>70%27%</div><div>••</div></div></div>
1	I	709	<div><div><div>2%</div><div><div></div><div></div><div></div></div><div>66%31%</div><div>••</div></div></div>
1	J	709	<div><div><div>2%</div><div><div></div><div></div><div></div></div><div>64%32%</div><div>••</div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 44957 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 Glycogen debranching enzyme GlgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	696	Total	C	N	O	S	0	0	0
			5547	3485	1005	1033	24			
1	D	694	Total	C	N	O	S	0	0	0
			5535	3480	1003	1028	24			
1	E	696	Total	C	N	O	S	0	0	0
			5545	3484	1005	1033	23			
1	F	694	Total	C	N	O	S	0	0	0
			5529	3474	1000	1031	24			
1	G	693	Total	C	N	O	S	0	0	0
			5518	3468	996	1031	23			
1	H	696	Total	C	N	O	S	0	0	0
			5549	3488	1005	1032	24			
1	I	696	Total	C	N	O	S	0	0	0
			5535	3478	1002	1031	24			
1	J	694	Total	C	N	O	S	0	0	0
			5535	3480	1003	1028	24			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A5P2ALW6
C	-1	SER	-	expression tag	UNP A0A5P2ALW6
C	0	HIS	-	expression tag	UNP A0A5P2ALW6
C	103	VAL	ILE	conflict	UNP A0A5P2ALW6
C	192	ARG	LYS	conflict	UNP A0A5P2ALW6
C	296	ALA	SER	conflict	UNP A0A5P2ALW6
C	297	ASP	ASN	conflict	UNP A0A5P2ALW6
C	303	MET	THR	conflict	UNP A0A5P2ALW6
C	682	GLN	GLU	conflict	UNP A0A5P2ALW6
D	-2	GLY	-	expression tag	UNP A0A5P2ALW6
D	-1	SER	-	expression tag	UNP A0A5P2ALW6
D	0	HIS	-	expression tag	UNP A0A5P2ALW6
D	103	VAL	ILE	conflict	UNP A0A5P2ALW6

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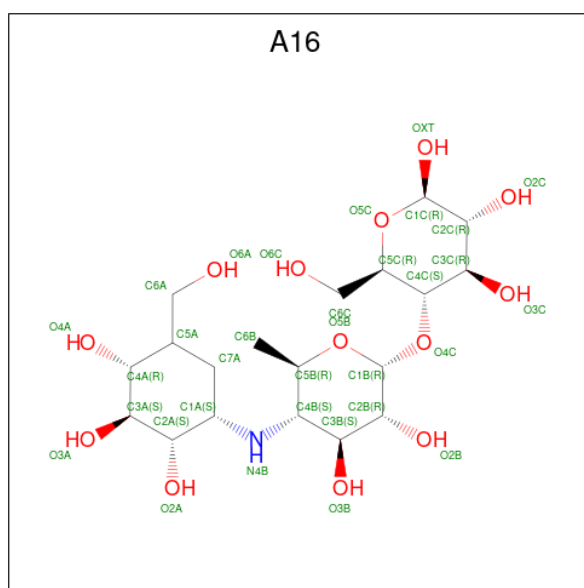
Chain	Residue	Modelled	Actual	Comment	Reference
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D	296	ALA	SER	conflict	UNP A0A5P2ALW6
D	297	ASP	ASN	conflict	UNP A0A5P2ALW6
D	303	MET	THR	conflict	UNP A0A5P2ALW6
D	682	GLN	GLU	conflict	UNP A0A5P2ALW6
E	-2	GLY	-	expression tag	UNP A0A5P2ALW6
E	-1	SER	-	expression tag	UNP A0A5P2ALW6
E	0	HIS	-	expression tag	UNP A0A5P2ALW6
E	103	VAL	ILE	conflict	UNP A0A5P2ALW6
E	192	ARG	LYS	conflict	UNP A0A5P2ALW6
E	296	ALA	SER	conflict	UNP A0A5P2ALW6
E	297	ASP	ASN	conflict	UNP A0A5P2ALW6
E	303	MET	THR	conflict	UNP A0A5P2ALW6
E	682	GLN	GLU	conflict	UNP A0A5P2ALW6
F	-2	GLY	-	expression tag	UNP A0A5P2ALW6
F	-1	SER	-	expression tag	UNP A0A5P2ALW6
F	0	HIS	-	expression tag	UNP A0A5P2ALW6
F	103	VAL	ILE	conflict	UNP A0A5P2ALW6
F	192	ARG	LYS	conflict	UNP A0A5P2ALW6
F	296	ALA	SER	conflict	UNP A0A5P2ALW6
F	297	ASP	ASN	conflict	UNP A0A5P2ALW6
F	303	MET	THR	conflict	UNP A0A5P2ALW6
F	682	GLN	GLU	conflict	UNP A0A5P2ALW6
G	-2	GLY	-	expression tag	UNP A0A5P2ALW6
G	-1	SER	-	expression tag	UNP A0A5P2ALW6
G	0	HIS	-	expression tag	UNP A0A5P2ALW6
G	103	VAL	ILE	conflict	UNP A0A5P2ALW6
G	192	ARG	LYS	conflict	UNP A0A5P2ALW6
G	296	ALA	SER	conflict	UNP A0A5P2ALW6
G	297	ASP	ASN	conflict	UNP A0A5P2ALW6
G	303	MET	THR	conflict	UNP A0A5P2ALW6
G	682	GLN	GLU	conflict	UNP A0A5P2ALW6
H	-2	GLY	-	expression tag	UNP A0A5P2ALW6
H	-1	SER	-	expression tag	UNP A0A5P2ALW6
H	0	HIS	-	expression tag	UNP A0A5P2ALW6
H	103	VAL	ILE	conflict	UNP A0A5P2ALW6
H	192	ARG	LYS	conflict	UNP A0A5P2ALW6
H	296	ALA	SER	conflict	UNP A0A5P2ALW6
H	297	ASP	ASN	conflict	UNP A0A5P2ALW6
H	303	MET	THR	conflict	UNP A0A5P2ALW6
H	682	GLN	GLU	conflict	UNP A0A5P2ALW6
I	-2	GLY	-	expression tag	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	SER	-	expression tag	UNP A0A5P2ALW6
I	0	HIS	-	expression tag	UNP A0A5P2ALW6
I	103	VAL	ILE	conflict	UNP A0A5P2ALW6
I	192	ARG	LYS	conflict	UNP A0A5P2ALW6
I	296	ALA	SER	conflict	UNP A0A5P2ALW6
I	297	ASP	ASN	conflict	UNP A0A5P2ALW6
I	303	MET	THR	conflict	UNP A0A5P2ALW6
I	682	GLN	GLU	conflict	UNP A0A5P2ALW6
J	-2	GLY	-	expression tag	UNP A0A5P2ALW6
J	-1	SER	-	expression tag	UNP A0A5P2ALW6
J	0	HIS	-	expression tag	UNP A0A5P2ALW6
J	103	VAL	ILE	conflict	UNP A0A5P2ALW6
J	192	ARG	LYS	conflict	UNP A0A5P2ALW6
J	296	ALA	SER	conflict	UNP A0A5P2ALW6
J	297	ASP	ASN	conflict	UNP A0A5P2ALW6
J	303	MET	THR	conflict	UNP A0A5P2ALW6
J	682	GLN	GLU	conflict	UNP A0A5P2ALW6

- Molecule 2 is 4-O-(4,6-dideoxy-4-[[[(1S,2S,3S,4R,5S)-2,3,4-trihydroxy-5-(hydroxymethyl)cyclohexyl]amino}-alpha-D-glucopyranosyl)-beta-D-glucopyranose (three-letter code: A16) (formula: C<sub>19</sub>H<sub>35</sub>NO<sub>13</sub>) (labeled as "Ligand of Interest" by depositor).



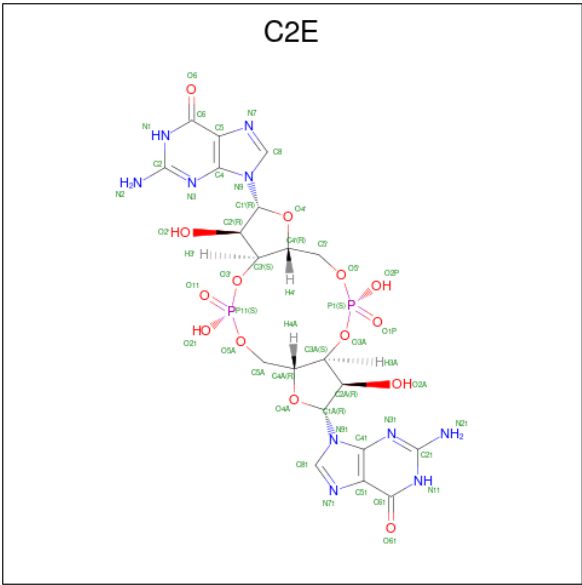
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			32	19	1	12		
2	D	1	Total	C	N	O	0	0
			32	19	1	12		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			32	19	1	12		
2	F	1	Total	C	N	O	0	0
			32	19	1	12		
2	G	1	Total	C	N	O	0	0
			32	19	1	12		
2	H	1	Total	C	N	O	0	0
			32	19	1	12		
2	I	1	Total	C	N	O	0	0
			32	19	1	12		
2	J	1	Total	C	N	O	0	0
			32	19	1	12		

- Molecule 3 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>14</sub>P<sub>2</sub>).



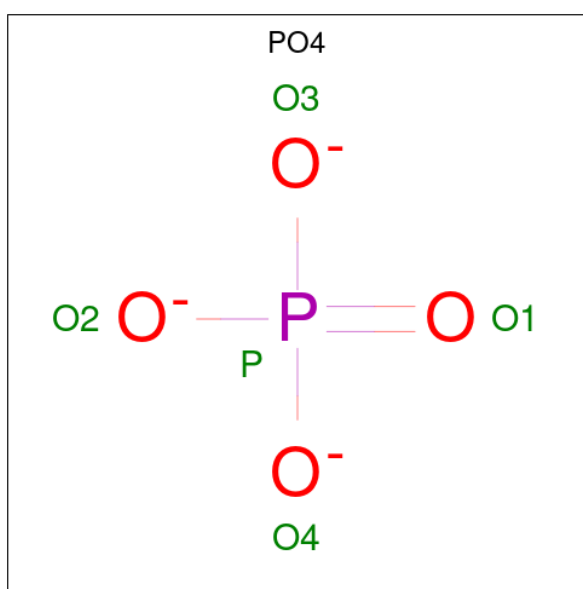
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0
			46	20	10	14	2	
3	D	1	Total	C	N	O	P	0
			46	20	10	14	2	
3	E	1	Total	C	N	O	P	0
			46	20	10	14	2	
3	F	1	Total	C	N	O	P	0
			46	20	10	14	2	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	H	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	I	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	J	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	8	Total	O	0	0
			8	8		

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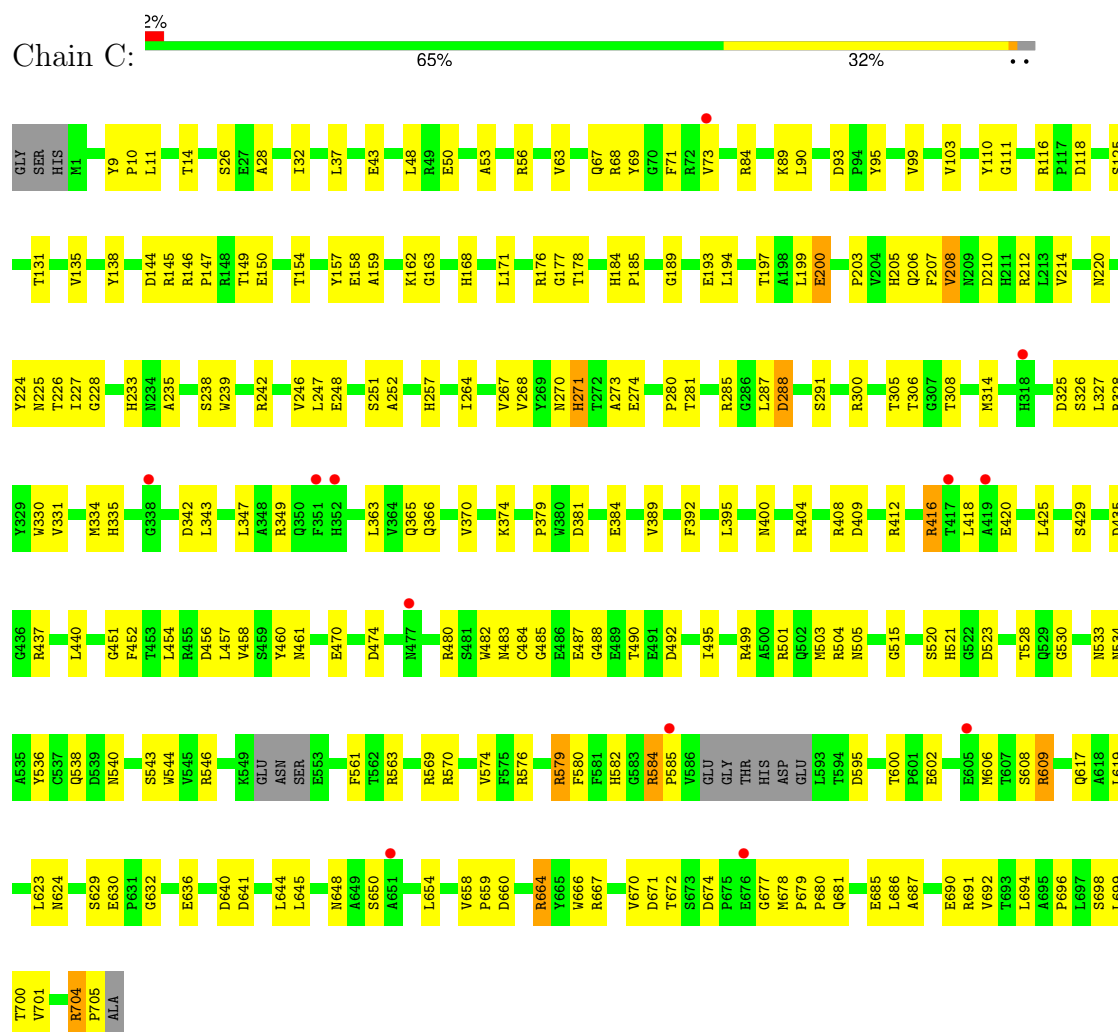
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	3	Total 3	O 3	0	0
5	F	3	Total 3	O 3	0	0
5	H	2	Total 2	O 2	0	0
5	I	4	Total 4	O 4	0	0

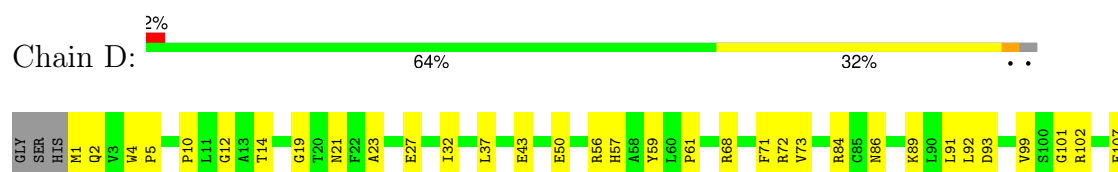
### 3 Residue-property plots

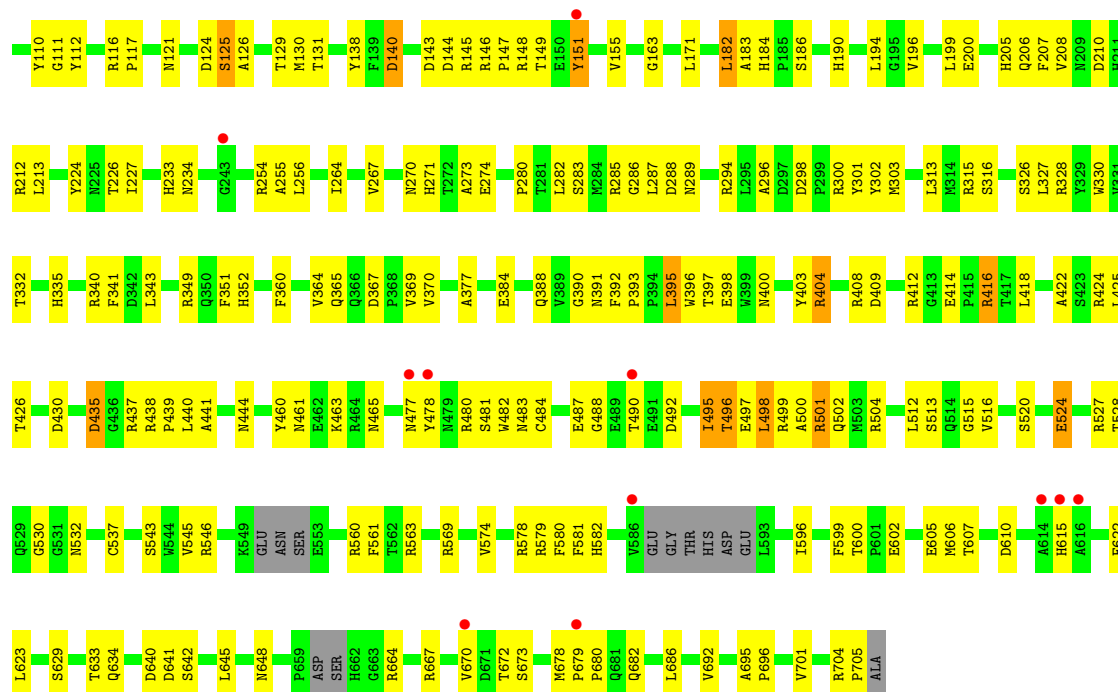
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Glycogen debranching enzyme GlgX

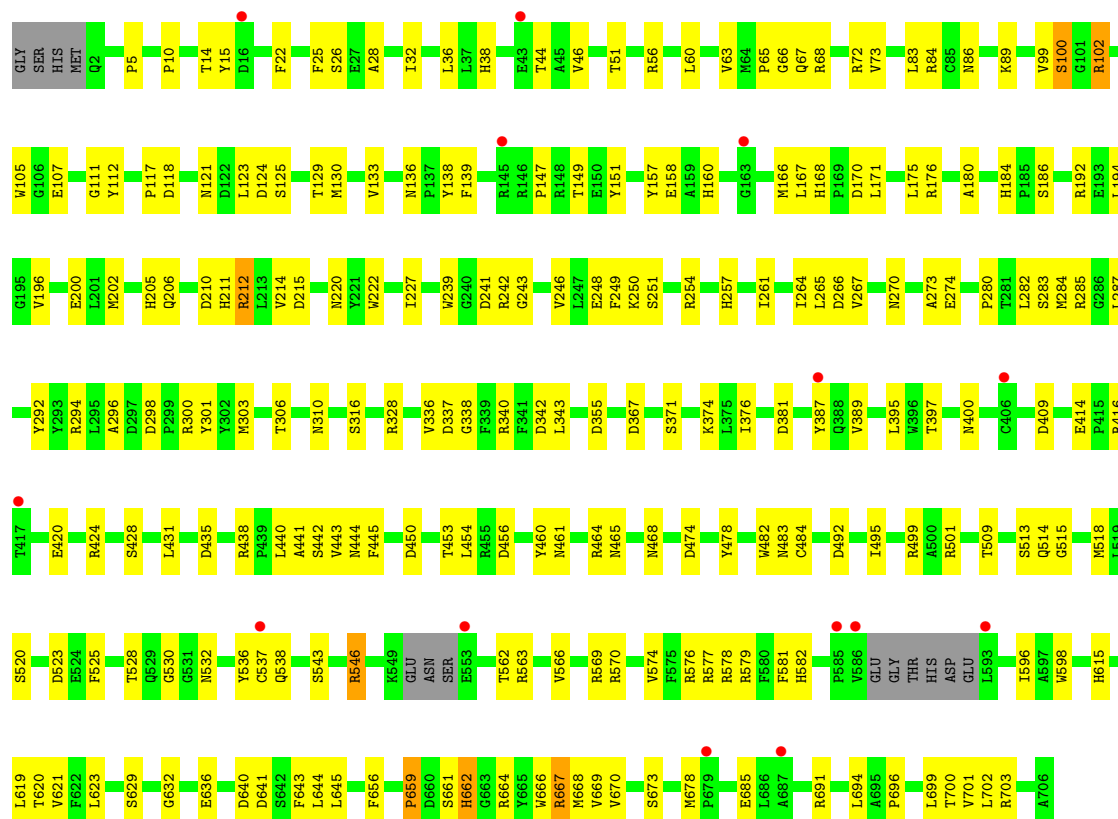


#### • Molecule 1: Glycogen debranching enzyme GlgX



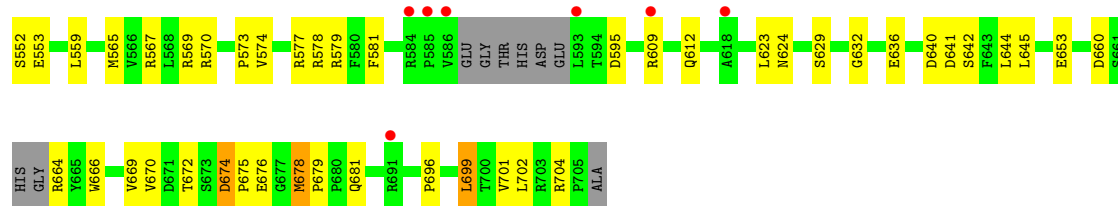


• Molecule 1: Glycogen debranching enzyme GlgX

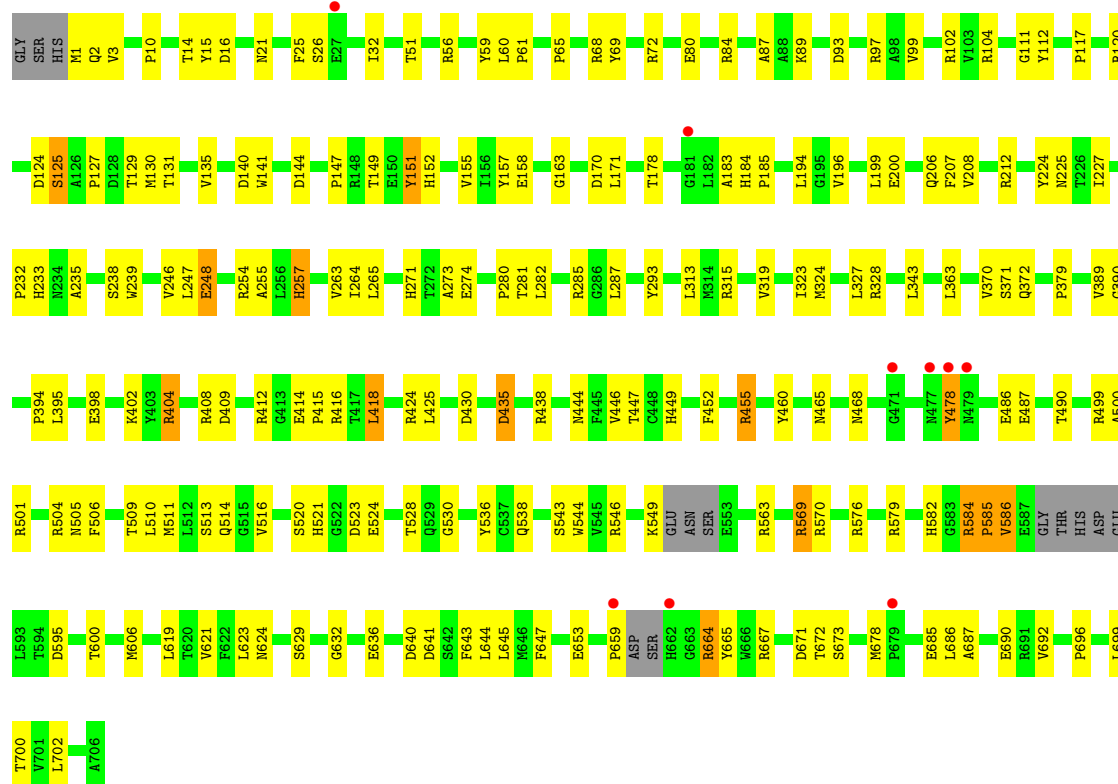


• Molecule 1: Glycogen debranching enzyme GlgX

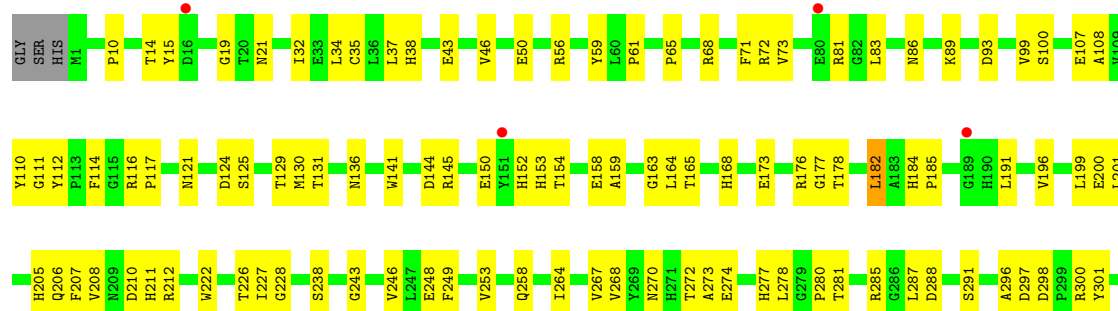


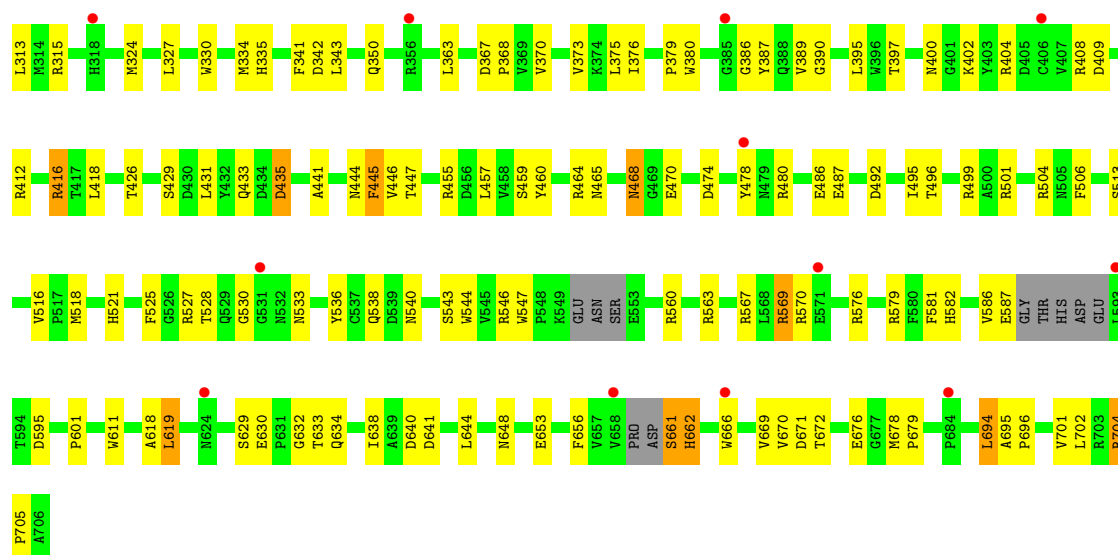


• Molecule 1: Glycogen debranching enzyme GlgX

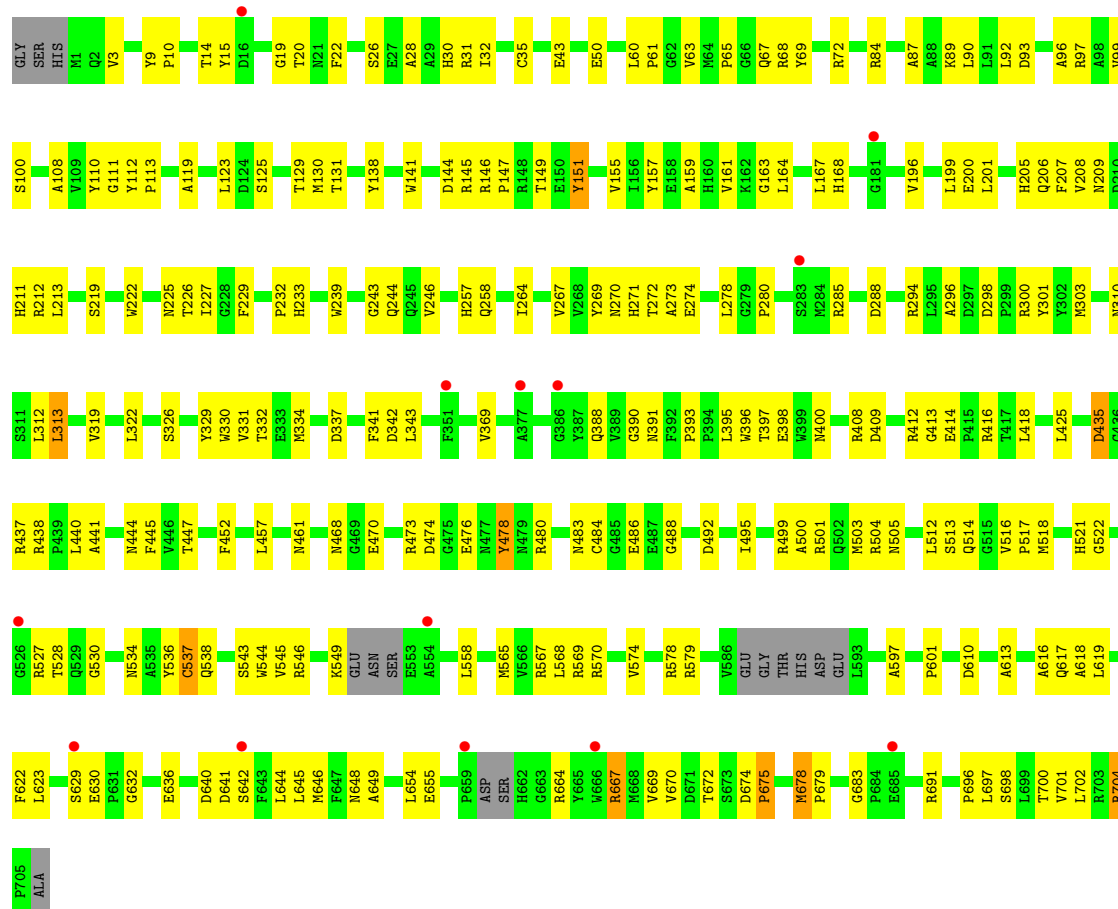


• Molecule 1: Glycogen debranching enzyme GlgX





• Molecule 1: Glycogen debranching enzyme GlgX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.84Å 185.59Å 184.67Å 90.00° 98.08° 90.00°	Depositor
Resolution (Å)	48.50 – 3.60 48.50 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.50-3.60) 98.1 (48.50-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.237 , 0.307 0.238 , 0.305	Depositor DCC
$R_{free}$ test set	82295 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	44957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.08% 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: PO4, C2E, A16

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	C	0.28	1/5699 (0.0%)	0.51	3/7750 (0.0%)
1	D	0.27	0/5686	0.49	3/7731 (0.0%)
1	E	0.33	1/5697 (0.0%)	0.50	2/7748 (0.0%)
1	F	0.30	2/5680 (0.0%)	0.49	1/7724 (0.0%)
1	G	0.26	0/5668	0.48	1/7710 (0.0%)
1	H	0.32	2/5700 (0.0%)	0.52	4/7750 (0.1%)
1	I	0.26	0/5684	0.48	2/7727 (0.0%)
1	J	0.32	2/5686 (0.0%)	0.49	2/7731 (0.0%)
All	All	0.29	8/45500 (0.0%)	0.50	18/61871 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	J	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	659	PRO	N-CA	13.08	1.69	1.47
1	J	675	PRO	N-CA	12.54	1.68	1.47
1	H	585	PRO	N-CA	12.40	1.68	1.47
1	C	208	VAL	C-N	7.28	1.50	1.34
1	F	657	VAL	C-N	6.49	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	606	MET	CG-SD	5.58	1.95	1.81
1	H	584	ARG	C-N	5.42	1.44	1.34
1	J	674	ASP	C-N	5.42	1.44	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	GLU	O-C-N	8.06	135.59	122.70
1	J	675	PRO	CA-N-CD	-7.29	101.30	111.50
1	H	585	PRO	CA-N-CD	-6.86	101.90	111.50
1	C	200	GLU	CA-C-N	-6.80	102.23	117.20
1	E	659	PRO	CA-N-CD	-6.74	102.07	111.50
1	I	661	SER	CB-CA-C	6.44	122.33	110.10
1	D	496	THR	CA-CB-OG1	-6.35	95.66	109.00
1	H	585	PRO	N-CA-C	-6.11	96.23	112.10
1	D	673	SER	C-N-CA	-5.51	107.93	121.70
1	H	586	VAL	C-N-CA	5.49	135.42	121.70
1	J	435	ASP	CB-CG-OD2	5.26	123.03	118.30
1	E	435	ASP	CB-CG-OD2	5.25	123.02	118.30
1	F	435	ASP	CB-CG-OD2	5.22	123.00	118.30
1	H	435	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	435	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	435	ASP	CB-CG-OD2	5.17	122.96	118.30
1	G	435	ASP	CB-CG-OD2	5.17	122.95	118.30
1	I	435	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	678	MET	Peptide
1	E	678	MET	Peptide
1	G	678	MET	Peptide
1	H	678	MET	Peptide
1	J	678	MET	Peptide

## 5.2 Too-close contacts [i](#)

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	C	5547	0	5252	177	0
1	D	5535	0	5249	173	0
1	E	5545	0	5251	144	0
1	F	5529	0	5235	194	0
1	G	5518	0	5217	157	0
1	H	5549	0	5260	140	0
1	I	5535	0	5236	157	0
1	J	5535	0	5249	169	0
2	C	32	0	33	5	0
2	D	32	0	33	7	0
2	E	32	0	33	7	0
2	F	32	0	33	7	0
2	G	32	0	33	10	0
2	H	32	0	33	5	0
2	I	32	0	32	5	0
2	J	32	0	33	10	0
3	C	46	0	22	9	0
3	D	46	0	22	18	0
3	E	46	0	22	5	0
3	F	46	0	22	3	0
3	G	46	0	22	5	0
3	H	46	0	22	7	0
3	I	46	0	22	7	0
3	J	46	0	22	4	0
4	D	10	0	0	1	0
4	E	5	0	0	0	0
4	H	5	0	0	0	0
5	C	8	0	0	0	0
5	E	3	0	0	0	0
5	F	3	0	0	0	0
5	H	2	0	0	0	0
5	I	4	0	0	0	0
All	All	44957	0	42388	1335	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1335) 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:H:585:PRO:N	1:H:585:PRO:CA	1.68	1.47
1:J:675:PRO:N	1:J:675:PRO:CA	1.68	1.44
1:E:659:PRO:N	1:E:659:PRO:CA	1.69	1.37
1:F:411:TRP:CD1	1:F:506:PHE:CE1	2.12	1.37
1:F:500:ALA:O	1:F:504:ARG:NH1	1.62	1.32
1:F:411:TRP:CG	1:F:506:PHE:HE1	1.47	1.32
1:D:212:ARG:NH2	2:D:801:A16:H7A1	1.44	1.31
1:F:342:ASP:OD1	2:F:801:A16:C1C	1.90	1.18
1:F:411:TRP:CD1	1:F:506:PHE:HE1	1.58	1.14
1:D:484:CYS:O	1:D:495:ILE:CG2	1.98	1.12
1:H:51:THR:O	3:H:803:C2E:N11	1.83	1.09
1:F:411:TRP:CG	1:F:506:PHE:CE1	2.39	1.05
1:D:579:ARG:CD	3:D:804:C2E:N71	2.22	1.02
1:D:579:ARG:HD3	3:D:804:C2E:C81	1.91	1.01
1:D:579:ARG:HD3	3:D:804:C2E:N71	1.78	0.98
1:J:536:TYR:CD2	2:J:801:A16:H2B	1.99	0.98
1:E:222:TRP:HZ3	2:E:801:A16:O3C	1.47	0.96
3:I:802:C2E:C5A	3:I:802:C2E:H81	1.94	0.96
1:D:212:ARG:NH2	2:D:801:A16:C7A	2.30	0.93
1:F:505:ASN:OD1	1:F:672:THR:HG21	1.70	0.91
1:D:484:CYS:O	1:D:495:ILE:HG21	1.68	0.91
1:E:51:THR:N	3:E:803:C2E:O61	2.02	0.91
1:E:38:HIS:HE2	1:E:44:THR:HG1	1.20	0.90
1:C:227:ILE:HG23	1:C:273:ALA:HB3	1.55	0.89
1:F:411:TRP:CB	1:F:506:PHE:HE1	1.86	0.88
1:F:411:TRP:HD1	1:F:506:PHE:CE1	1.90	0.88
1:H:449:HIS:NE2	2:H:801:A16:O2C	2.08	0.87
3:J:802:C2E:H81	3:J:802:C2E:O5A	1.74	0.87
1:E:222:TRP:CZ3	2:E:801:A16:O3C	2.27	0.86
3:D:804:C2E:H512	3:D:804:C2E:H5'2	1.55	0.86
1:F:505:ASN:OD1	1:F:672:THR:OG1	1.93	0.86
3:H:803:C2E:H512	3:H:803:C2E:H3'	1.58	0.86
1:F:500:ALA:C	1:F:504:ARG:NH1	2.29	0.85
3:D:804:C2E:O5'	3:D:804:C2E:H8	1.76	0.85
1:E:619:LEU:HD23	1:E:620:THR:N	1.90	0.85
1:J:246:VAL:CG2	1:J:334:MET:HE3	2.07	0.84
1:F:411:TRP:CB	1:F:506:PHE:CE1	2.61	0.83
1:F:505:ASN:OD1	1:F:672:THR:CG2	2.27	0.83
1:C:501:ARG:NH2	1:C:696:PRO:O	2.12	0.83
1:D:501:ARG:NH2	1:D:696:PRO:O	2.12	0.83
1:J:470:GLU:OE1	2:J:801:A16:O6A	1.97	0.83
1:C:584:ARG:HB3	1:C:585:PRO:HD3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:ILE:HG23	1:H:273:ALA:HB3	1.61	0.83
3:F:802:C2E:O5'	3:F:802:C2E:H8	1.78	0.83
1:H:501:ARG:NH2	1:H:696:PRO:O	2.13	0.82
1:J:246:VAL:HG23	1:J:334:MET:HE3	1.63	0.81
1:F:505:ASN:O	1:F:509:THR:OG1	1.98	0.81
1:J:10:PRO:HG2	1:J:14:THR:HG21	1.61	0.81
1:C:461:ASN:OD1	1:C:483:ASN:ND2	2.14	0.81
1:E:438:ARG:NH2	1:I:50:GLU:OE1	2.14	0.80
1:F:501:ARG:NH2	1:F:696:PRO:O	2.12	0.80
1:J:246:VAL:CG2	1:J:334:MET:CE	2.58	0.80
1:F:501:ARG:HA	1:F:504:ARG:HG3	1.62	0.80
1:F:110:TYR:OH	1:F:211:HIS:ND1	2.16	0.79
3:H:803:C2E:H512	3:H:803:C2E:C3'	2.13	0.79
1:F:411:TRP:HB2	1:F:506:PHE:CZ	2.18	0.79
1:F:227:ILE:HG23	1:F:273:ALA:HB3	1.64	0.79
1:J:579:ARG:HD2	1:J:630:GLU:HG2	1.63	0.79
1:C:212:ARG:NH2	1:C:470:GLU:OE1	2.16	0.78
1:H:600:THR:HG23	1:H:606:MET:HG3	1.65	0.78
1:E:51:THR:O	3:E:803:C2E:N11	2.16	0.78
1:G:212:ARG:NH2	1:G:536:TYR:OH	2.17	0.78
1:G:660:ASP:OD2	1:G:666:TRP:NE1	2.17	0.78
1:J:667:ARG:NH2	1:J:683:GLY:O	2.16	0.78
1:G:501:ARG:NH2	1:G:696:PRO:O	2.16	0.78
1:C:288:ASP:OD2	1:C:291:SER:OG	2.02	0.78
1:F:411:TRP:HB2	1:F:506:PHE:CE1	2.18	0.78
1:I:501:ARG:NH2	1:I:696:PRO:O	2.17	0.77
3:E:803:C2E:O5'	3:E:803:C2E:H8	1.84	0.77
1:H:513:SER:O	1:H:569:ARG:NH2	2.17	0.77
1:J:501:ARG:NH2	1:J:696:PRO:O	2.18	0.77
1:H:212:ARG:NH2	1:H:536:TYR:OH	2.17	0.77
1:C:144:ASP:OD2	1:C:335:HIS:ND1	2.18	0.77
1:D:579:ARG:NE	3:D:804:C2E:N71	2.31	0.77
1:E:619:LEU:HD23	1:E:620:THR:H	1.46	0.77
1:F:520:SER:OG	1:F:523:ASP:OD2	2.03	0.76
1:J:239:TRP:O	1:J:244:GLN:NE2	2.17	0.76
1:H:585:PRO:N	1:H:585:PRO:C	2.39	0.76
1:J:468:ASN:ND2	1:J:534:ASN:O	2.17	0.76
1:I:492:ASP:OD2	1:I:495:ILE:HD12	1.85	0.76
3:C:802:C2E:O5'	3:C:802:C2E:H8	1.84	0.76
1:J:579:ARG:NH1	1:J:629:SER:O	2.19	0.76
1:J:246:VAL:HG22	1:J:334:MET:CE	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:TYR:HH	1:J:211:HIS:HD1	1.32	0.75
2:H:801:A16:O3C	2:H:801:A16:H1B	1.83	0.75
3:I:802:C2E:H81	3:I:802:C2E:O5A	1.84	0.75
2:H:801:A16:H7A2	2:H:801:A16:O3B	1.86	0.75
1:F:144:ASP:OD2	1:F:335:HIS:ND1	2.18	0.75
1:G:227:ILE:HG23	1:G:273:ALA:HB3	1.69	0.75
1:H:343:LEU:HD11	2:H:801:A16:H6C2	1.68	0.75
1:C:212:ARG:NH2	1:C:536:TYR:OH	2.16	0.75
1:F:207:PHE:HB3	1:F:226:THR:HG22	1.69	0.75
1:J:444:ASN:ND2	1:J:514:GLN:O	2.20	0.75
1:D:89:LYS:HE3	1:D:111:GLY:HA2	1.68	0.75
1:D:579:ARG:NH1	1:D:629:SER:O	2.20	0.75
1:C:686:LEU:HD13	1:C:692:VAL:HG21	1.67	0.74
1:G:84:ARG:HD2	1:G:285:ARG:HD2	1.69	0.74
1:D:513:SER:O	1:D:569:ARG:NH2	2.20	0.74
1:E:227:ILE:HG23	1:E:273:ALA:HB3	1.69	0.74
3:D:804:C2E:H81	3:D:804:C2E:O5A	1.88	0.73
1:E:444:ASN:ND2	1:E:514:GLN:O	2.21	0.73
1:G:224:TYR:O	2:G:801:A16:H6B1	1.89	0.73
1:F:146:ARG:NH2	1:F:331:VAL:O	2.21	0.73
1:G:579:ARG:NH1	1:G:629:SER:O	2.21	0.73
1:J:413:GLY:O	1:J:617:GLN:NE2	2.21	0.73
1:J:461:ASN:OD1	1:J:483:ASN:ND2	2.21	0.73
1:G:669:VAL:HG13	1:G:670:VAL:HG23	1.71	0.73
1:C:528:THR:HG22	1:C:530:GLY:H	1.54	0.72
1:G:246:VAL:HG23	1:G:334:MET:HE3	1.71	0.72
1:F:409:ASP:HB3	1:F:416:ARG:HG3	1.70	0.72
1:C:50:GLU:OE1	1:H:438:ARG:NH2	2.23	0.72
1:I:144:ASP:OD2	1:I:335:HIS:ND1	2.17	0.72
1:D:212:ARG:HH22	2:D:801:A16:H7A1	1.51	0.72
1:G:676:GLU:CB	1:G:681:GLN:HE22	2.03	0.72
1:D:490:THR:HG22	1:D:492:ASP:H	1.54	0.72
1:H:178:THR:HG21	1:H:238:SER:HB3	1.72	0.72
1:H:528:THR:HG22	1:H:530:GLY:H	1.55	0.72
1:F:212:ARG:HH22	2:F:801:A16:H7A1	1.54	0.72
3:C:802:C2E:H81	3:C:802:C2E:H3A	1.72	0.71
1:J:418:LEU:HD13	1:J:619:LEU:HG	1.73	0.71
1:E:284:MET:HB3	1:E:292:TYR:HD1	1.56	0.71
2:J:801:A16:O3B	2:J:801:A16:H7A2	1.89	0.71
1:D:206:GLN:HG3	1:D:233:HIS:HA	1.73	0.71
1:D:607:THR:H	1:D:610:ASP:HB2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:802:C2E:H81	3:I:802:C2E:H511	1.73	0.70
2:E:801:A16:O3C	2:E:801:A16:H1B	1.90	0.70
1:F:444:ASN:ND2	1:F:514:GLN:O	2.25	0.70
1:E:270:ASN:ND2	1:E:342:ASP:O	2.23	0.70
1:H:579:ARG:NH1	1:H:629:SER:O	2.25	0.70
1:J:670:VAL:HB	1:J:701:VAL:HB	1.72	0.70
1:E:468:ASN:OD1	1:E:538:GLN:NE2	2.24	0.70
1:F:461:ASN:OD1	1:F:483:ASN:ND2	2.25	0.70
3:H:803:C2E:O5'	3:H:803:C2E:H8	1.90	0.70
1:C:671:ASP:HB3	1:C:678:MET:HG2	1.74	0.70
1:J:274:GLU:O	1:J:285:ARG:NH2	2.24	0.70
1:C:609:ARG:HH12	1:D:68:ARG:HH22	1.39	0.70
1:D:212:ARG:CZ	2:D:801:A16:H7A1	2.19	0.69
1:E:492:ASP:O	1:E:495:ILE:HG13	1.93	0.69
1:I:130:MET:SD	1:I:206:GLN:NE2	2.65	0.69
1:G:50:GLU:OE1	1:J:438:ARG:NH2	2.25	0.69
1:I:640:ASP:OD2	1:I:641:ASP:N	2.26	0.69
1:G:125:SER:HG	1:G:129:THR:HG1	1.37	0.69
1:G:470:GLU:HG2	1:G:473:ARG:HE	1.57	0.69
1:J:212:ARG:NH2	2:J:801:A16:H7A1	2.07	0.69
1:I:68:ARG:HB3	1:I:131:THR:HG21	1.73	0.69
1:J:468:ASN:ND2	1:J:474:ASP:OD2	2.26	0.69
1:F:505:ASN:OD1	1:F:672:THR:CB	2.42	0.68
1:F:686:LEU:HD13	1:F:692:VAL:HG21	1.73	0.68
3:D:804:C2E:H512	3:D:804:C2E:C5'	2.23	0.68
2:I:801:A16:H7A2	2:I:801:A16:O3B	1.94	0.68
1:J:146:ARG:NH2	1:J:331:VAL:O	2.27	0.68
1:D:579:ARG:CD	3:D:804:C2E:C81	2.63	0.68
1:G:72:ARG:NH2	1:G:124:ASP:OD1	2.26	0.68
1:G:409:ASP:HB3	1:G:416:ARG:HG3	1.76	0.68
1:F:411:TRP:CD1	1:F:506:PHE:CD1	2.78	0.68
1:I:86:ASN:ND2	1:I:121:ASN:O	2.23	0.68
1:I:227:ILE:HG23	1:I:273:ALA:HB3	1.75	0.68
1:D:409:ASP:OD2	1:D:480:ARG:NH1	2.25	0.67
1:E:461:ASN:ND2	1:E:483:ASN:OD1	2.27	0.67
1:D:227:ILE:HG23	1:D:273:ALA:HB3	1.76	0.67
1:C:68:ARG:HB3	1:C:131:THR:HG21	1.75	0.67
1:D:600:THR:HG23	1:D:606:MET:HG2	1.76	0.67
1:I:10:PRO:HG2	1:I:14:THR:HG21	1.75	0.67
1:I:468:ASN:ND2	1:I:474:ASP:OD2	2.28	0.67
1:J:528:THR:HG22	1:J:530:GLY:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:PRO:HG2	1:G:14:THR:HG21	1.77	0.67
1:G:440:LEU:HD21	1:G:578:ARG:HA	1.76	0.67
1:H:379:PRO:HG2	1:H:389:VAL:HG22	1.76	0.67
2:D:801:A16:H1B	2:D:801:A16:O3C	1.95	0.67
1:D:579:ARG:HD3	3:D:804:C2E:H81	1.73	0.67
1:D:130:MET:HE3	1:D:208:VAL:HG22	1.75	0.67
1:F:325:ASP:OD2	1:F:328:ARG:NH2	2.28	0.66
1:F:609:ARG:HG2	1:H:127:PRO:HB3	1.77	0.66
1:C:538:GLN:O	1:C:543:SER:OG	2.13	0.66
1:J:246:VAL:HG22	1:J:334:MET:HE1	1.76	0.66
1:G:144:ASP:OD2	1:G:335:HIS:ND1	2.28	0.66
1:E:528:THR:HG22	1:E:530:GLY:H	1.61	0.66
1:F:206:GLN:HG3	1:F:233:HIS:HA	1.78	0.66
1:J:227:ILE:HG23	1:J:273:ALA:HB3	1.78	0.66
1:J:644:LEU:HD23	1:J:702:LEU:HD12	1.76	0.66
1:D:528:THR:HG22	1:D:530:GLY:H	1.60	0.66
1:J:159:ALA:HB1	1:J:164:LEU:HG	1.77	0.66
1:I:212:ARG:NH2	1:I:536:TYR:OH	2.29	0.65
1:E:194:LEU:HD12	1:E:563:ARG:HG3	1.79	0.65
1:E:632:GLY:HA3	1:E:636:GLU:HG3	1.77	0.65
2:G:801:A16:O3C	2:G:801:A16:H1B	1.95	0.65
1:H:274:GLU:OE1	1:H:293:TYR:OH	2.09	0.65
1:I:212:ARG:NH2	2:I:801:A16:H5A	2.12	0.65
1:H:194:LEU:HA	1:H:563:ARG:HG2	1.78	0.65
1:J:89:LYS:HE3	1:J:111:GLY:HA2	1.78	0.65
1:D:461:ASN:ND2	1:D:483:ASN:OD1	2.30	0.65
1:F:409:ASP:OD1	1:F:412:ARG:NH1	2.30	0.65
1:C:579:ARG:HD3	1:C:630:GLU:HG2	1.78	0.65
1:G:270:ASN:ND2	1:G:342:ASP:O	2.30	0.65
1:G:200:GLU:HA	1:G:264:ILE:O	1.96	0.65
1:D:497:GLU:O	1:D:500:ALA:N	2.29	0.64
1:H:584:ARG:O	1:H:584:ARG:HG3	1.96	0.64
2:J:801:A16:O3C	2:J:801:A16:H1B	1.98	0.64
1:C:379:PRO:HG2	1:C:389:VAL:HG22	1.78	0.64
1:F:212:ARG:NH2	2:F:801:A16:H7A1	2.12	0.64
1:D:686:LEU:HD13	1:D:692:VAL:HG21	1.79	0.64
1:C:617:GLN:HE21	1:C:650:SER:HA	1.63	0.64
1:E:222:TRP:HZ3	2:E:801:A16:HG	1.27	0.64
1:F:4:TRP:HB2	1:F:59:TYR:HB3	1.79	0.64
1:D:110:TYR:HA	1:D:280:PRO:HA	1.80	0.64
1:I:178:THR:HG21	1:I:238:SER:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:GLN:HG3	1:C:233:HIS:HA	1.79	0.63
1:D:640:ASP:OD2	1:D:641:ASP:N	2.31	0.63
1:F:504:ARG:CG	1:F:504:ARG:HH11	2.11	0.63
1:H:486:GLU:O	1:H:499:ARG:NH2	2.31	0.63
1:D:343:LEU:HD11	2:D:801:A16:H6C2	1.81	0.63
1:I:644:LEU:HD23	1:I:702:LEU:HD12	1.81	0.63
1:E:640:ASP:OD2	1:E:641:ASP:N	2.32	0.63
1:C:308:THR:HG21	2:C:801:A16:C6C	2.27	0.63
1:F:10:PRO:HG2	1:F:14:THR:HG21	1.81	0.63
1:G:504:ARG:HB2	1:G:672:THR:HG23	1.81	0.63
1:C:664:ARG:HG2	1:C:704:ARG:NH2	2.13	0.63
1:H:158:GLU:HA	1:H:200:GLU:HB3	1.79	0.63
1:E:453:THR:OG1	1:E:456:ASP:OD1	2.16	0.63
1:G:486:GLU:O	1:G:499:ARG:NH2	2.32	0.63
1:E:296:ALA:HA	1:E:303:MET:HG2	1.81	0.63
1:H:281:THR:HG23	1:H:285:ARG:HB3	1.81	0.63
1:H:447:THR:OG1	1:H:452:PHE:O	2.17	0.63
1:J:110:TYR:OH	1:J:211:HIS:ND1	2.26	0.63
2:C:801:A16:O3C	2:C:801:A16:H1B	1.97	0.62
3:J:802:C2E:O5'	3:J:802:C2E:H8	1.99	0.62
1:C:460:TYR:HA	1:C:487:GLU:HG3	1.81	0.62
1:C:365:GLN:HG3	1:C:395:LEU:HD12	1.80	0.62
1:D:84:ARG:HD2	1:D:285:ARG:HD2	1.81	0.62
1:D:328:ARG:NH1	1:D:367:ASP:OD1	2.32	0.62
1:F:276:ASN:ND2	1:F:277:HIS:O	2.33	0.62
1:I:671:ASP:H	1:I:678:MET:HB3	1.64	0.62
1:F:125:SER:OG	1:F:129:THR:OG1	2.16	0.62
1:H:89:LYS:HA	1:H:125:SER:HB3	1.80	0.62
1:G:509:THR:O	1:G:513:SER:OG	2.18	0.62
1:C:138:TYR:HB2	1:E:138:TYR:HB2	1.82	0.62
1:D:89:LYS:HA	1:D:125:SER:HB3	1.81	0.62
1:F:89:LYS:HE3	1:F:111:GLY:HA2	1.81	0.62
1:I:409:ASP:HB3	1:I:416:ARG:HG3	1.82	0.62
1:J:26:SER:HB3	1:J:32:ILE:HD11	1.82	0.62
1:E:468:ASN:ND2	1:E:474:ASP:OD2	2.31	0.62
1:G:387:TYR:HE2	1:G:402:LYS:HE3	1.65	0.62
1:G:640:ASP:OD2	1:G:641:ASP:N	2.33	0.62
1:H:408:ARG:NH1	1:H:446:VAL:O	2.33	0.62
1:H:520:SER:OG	1:H:523:ASP:OD2	2.12	0.62
1:D:426:THR:HG23	1:D:581:PHE:HD1	1.64	0.62
1:G:246:VAL:CG2	1:G:334:MET:HE1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:20:THR:OG1	1:J:63:VAL:O	2.16	0.61
1:D:194:LEU:HA	1:D:563:ARG:HG2	1.81	0.61
1:D:484:CYS:O	1:D:495:ILE:HG23	1.95	0.61
1:G:329:TYR:CE2	1:G:334:MET:HE2	2.34	0.61
1:J:294:ARG:HA	1:J:313:LEU:HG	1.81	0.61
1:C:200:GLU:HA	1:C:264:ILE:O	2.01	0.61
1:I:32:ILE:H	1:I:56:ARG:NH1	1.98	0.61
1:H:68:ARG:HB3	1:H:131:THR:HG21	1.83	0.61
1:G:246:VAL:CG2	1:G:334:MET:CE	2.79	0.61
1:H:89:LYS:HE3	1:H:111:GLY:HA2	1.83	0.61
1:F:392:PHE:O	1:F:437:ARG:NH2	2.34	0.61
1:G:158:GLU:HA	1:G:200:GLU:HB3	1.83	0.61
1:G:296:ALA:HA	1:G:303:MET:HG3	1.83	0.61
1:E:492:ASP:HB3	1:E:495:ILE:HG12	1.82	0.60
1:F:294:ARG:HA	1:F:313:LEU:HG	1.83	0.60
1:G:418:LEU:O	1:G:422:ALA:N	2.31	0.60
1:G:664:ARG:HB2	1:G:704:ARG:HE	1.66	0.60
1:C:205:HIS:NE2	1:C:267:VAL:HG12	2.16	0.60
1:F:486:GLU:O	1:F:499:ARG:NH2	2.34	0.60
1:H:430:ASP:OD1	1:H:430:ASP:N	2.34	0.60
1:C:670:VAL:HB	1:C:701:VAL:HB	1.84	0.60
1:H:685:GLU:OE1	1:H:685:GLU:N	2.31	0.60
1:F:125:SER:O	1:F:129:THR:OG1	2.13	0.60
1:I:418:LEU:HD13	1:I:619:LEU:HG	1.84	0.60
1:J:669:VAL:HG13	1:J:670:VAL:HG23	1.84	0.60
1:D:144:ASP:OD2	1:D:335:HIS:ND1	2.34	0.60
1:F:158:GLU:HA	1:F:200:GLU:HB3	1.82	0.60
2:F:801:A16:H7A2	2:F:801:A16:O3B	2.01	0.60
1:F:408:ARG:HG2	1:F:457:LEU:HD21	1.84	0.60
1:C:10:PRO:HG2	1:C:14:THR:HG21	1.83	0.60
1:E:139:PHE:HE2	1:E:254:ARG:HD3	1.65	0.60
1:G:288:ASP:OD2	1:G:291:SER:OG	2.19	0.60
1:C:207:PHE:HB3	1:C:226:THR:HG22	1.82	0.60
1:F:350:GLN:NE2	1:F:359:SER:OG	2.34	0.59
1:G:246:VAL:HG23	1:G:334:MET:CE	2.31	0.59
1:I:32:ILE:HB	1:I:56:ARG:HD3	1.82	0.59
1:J:486:GLU:O	1:J:499:ARG:NH2	2.35	0.59
1:J:527:ARG:NH1	1:J:543:SER:O	2.34	0.59
1:D:84:ARG:NH2	1:D:300:ARG:O	2.35	0.59
1:F:26:SER:HB3	1:F:32:ILE:HD11	1.83	0.59
1:E:343:LEU:HD22	1:E:381:ASP:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:LEU:CD2	1:E:620:THR:N	2.63	0.59
1:F:171:LEU:HB2	1:F:176:ARG:HG2	1.85	0.59
1:I:141:TRP:HB3	1:I:144:ASP:HB2	1.85	0.59
3:D:804:C2E:O6	1:F:56:ARG:NH1	2.34	0.59
1:E:570:ARG:O	1:E:576:ARG:NH2	2.35	0.59
1:F:468:ASN:ND2	1:F:534:ASN:O	2.34	0.59
1:G:141:TRP:HB3	1:G:144:ASP:HB2	1.85	0.59
1:D:409:ASP:HB3	1:D:416:ARG:HG3	1.83	0.59
1:F:504:ARG:HB3	1:F:561:PHE:CE2	2.37	0.59
1:J:22:PHE:HZ	1:J:63:VAL:HG11	1.68	0.59
1:J:270:ASN:ND2	1:J:343:LEU:HB2	2.18	0.59
1:C:145:ARG:HH22	1:I:258:GLN:HG2	1.67	0.59
1:C:194:LEU:HA	1:C:563:ARG:HG2	1.85	0.59
1:D:145:ARG:HG3	1:G:143:ASP:HB3	1.84	0.59
1:G:264:ILE:HD11	1:G:374:LYS:HD2	1.84	0.59
1:H:206:GLN:HG3	1:H:233:HIS:HA	1.84	0.59
1:H:404:ARG:HG2	1:H:408:ARG:HD2	1.83	0.59
1:I:274:GLU:HB2	1:I:285:ARG:HH21	1.67	0.59
1:D:112:TYR:CD1	1:D:117:PRO:HA	2.38	0.59
1:E:257:HIS:NE2	1:E:337:ASP:OD2	2.36	0.59
1:H:501:ARG:HG3	1:H:672:THR:HG22	1.85	0.59
2:I:801:A16:H1B	2:I:801:A16:O3C	2.03	0.59
1:D:351:PHE:O	1:D:352:HIS:ND1	2.36	0.59
1:F:19:GLY:HA3	1:F:61:PRO:HA	1.83	0.59
1:I:455:ARG:HD2	1:I:528:THR:OG1	2.03	0.59
1:I:528:THR:HG22	1:I:530:GLY:H	1.68	0.59
1:J:409:ASP:HB3	1:J:416:ARG:HG3	1.83	0.59
3:C:802:C2E:H3A	3:C:802:C2E:C81	2.33	0.58
1:D:648:ASN:ND2	1:D:695:ALA:O	2.36	0.58
1:F:669:VAL:HG13	1:F:670:VAL:HG23	1.85	0.58
1:G:37:LEU:HD11	1:G:90:LEU:HD21	1.84	0.58
1:J:246:VAL:CG2	1:J:334:MET:HE1	2.30	0.58
1:J:246:VAL:HG22	1:J:334:MET:HE3	1.82	0.58
1:D:21:ASN:HB2	1:D:59:TYR:HD1	1.68	0.58
1:D:430:ASP:N	1:D:430:ASP:OD1	2.36	0.58
1:I:330:TRP:CE3	1:I:334:MET:HG3	2.38	0.58
1:F:379:PRO:HG2	1:F:389:VAL:HG22	1.86	0.58
1:J:483:ASN:OD1	1:J:486:GLU:N	2.36	0.58
3:D:804:C2E:H512	3:D:804:C2E:C3'	2.32	0.58
1:E:669:VAL:HG13	1:E:670:VAL:HG23	1.85	0.58
1:F:567:ARG:HG2	1:F:570:ARG:HH21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:THR:OG1	1:G:63:VAL:O	2.20	0.58
3:G:802:C2E:H3A	3:G:802:C2E:H3'	1.85	0.58
1:G:243:GLY:O	1:G:246:VAL:HG12	2.03	0.58
1:J:397:THR:HG23	1:J:441:ALA:HA	1.85	0.58
1:J:167:LEU:HD11	1:J:544:TRP:HE3	1.69	0.58
1:J:243:GLY:O	1:J:246:VAL:HG12	2.04	0.58
1:E:184:HIS:ND1	1:E:186:SER:OG	2.36	0.58
1:I:89:LYS:HE3	1:I:111:GLY:HA2	1.84	0.58
1:I:513:SER:O	1:I:569:ARG:NH2	2.36	0.58
1:D:190:HIS:NE2	1:D:524:GLU:OE1	2.37	0.58
1:F:349:ARG:NH1	1:F:352:HIS:O	2.37	0.58
1:F:579:ARG:NH1	1:F:629:SER:O	2.37	0.58
1:G:513:SER:O	1:G:569:ARG:NH2	2.37	0.58
1:G:426:THR:HG23	1:G:581:PHE:HD1	1.68	0.57
1:I:19:GLY:HA3	1:I:61:PRO:HA	1.86	0.57
1:I:669:VAL:HG13	1:I:670:VAL:HG23	1.86	0.57
1:J:409:ASP:OD2	1:J:480:ARG:NH1	2.37	0.57
1:E:579:ARG:NH1	1:E:629:SER:O	2.36	0.57
1:I:130:MET:HE3	1:I:227:ILE:HD11	1.86	0.57
1:C:343:LEU:HD22	1:C:381:ASP:HA	1.85	0.57
1:D:579:ARG:CG	3:D:804:C2E:N71	2.67	0.57
1:E:668:MET:HA	1:E:702:LEU:HD23	1.85	0.57
1:I:65:PRO:HG2	1:I:136:ASN:HB2	1.86	0.57
1:J:597:ALA:HB3	1:J:622:PHE:HB3	1.85	0.57
1:C:37:LEU:HD11	1:C:90:LEU:HD21	1.86	0.57
1:C:404:ARG:HE	1:C:408:ARG:NH1	2.03	0.57
1:F:151:TYR:HD2	1:F:516:VAL:HG21	1.70	0.57
1:H:379:PRO:HG3	1:H:398:GLU:HB3	1.87	0.57
1:I:445:PHE:HB3	1:I:518:MET:HB3	1.85	0.57
1:G:676:GLU:CB	1:G:681:GLN:NE2	2.66	0.57
1:I:409:ASP:OD2	1:I:480:ARG:NH1	2.37	0.57
1:J:63:VAL:HG13	1:J:67:GLN:HG2	1.85	0.57
1:E:194:LEU:HA	1:E:563:ARG:HG2	1.87	0.57
1:D:579:ARG:CG	3:D:804:C2E:C81	2.83	0.57
1:F:327:LEU:HD13	1:F:370:VAL:HG11	1.87	0.57
1:H:184:HIS:CG	1:H:185:PRO:HD2	2.40	0.57
1:H:686:LEU:HD13	1:H:692:VAL:HG21	1.86	0.57
2:E:801:A16:O3B	2:E:801:A16:H1A	2.04	0.57
1:H:460:TYR:HA	1:H:487:GLU:HG3	1.87	0.57
1:D:642:SER:N	1:D:704:ARG:O	2.38	0.57
1:E:509:THR:O	1:E:513:SER:OG	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ILE:HD12	1:C:228:GLY:N	2.19	0.56
1:F:621:VAL:HB	1:F:645:LEU:HB2	1.86	0.56
1:H:274:GLU:O	1:H:285:ARG:NH2	2.38	0.56
1:J:470:GLU:O	1:J:470:GLU:HG2	2.04	0.56
1:C:363:LEU:HD23	1:H:363:LEU:HD23	1.87	0.56
1:F:200:GLU:HA	1:F:264:ILE:O	2.05	0.56
1:H:644:LEU:HD21	1:H:659:PRO:HD2	1.87	0.56
1:D:496:THR:HG22	1:D:496:THR:O	2.06	0.56
1:E:86:ASN:HB3	1:E:89:LYS:HG2	1.87	0.56
1:F:424:ARG:NH2	1:F:430:ASP:OD2	2.39	0.56
1:H:125:SER:O	1:H:129:THR:OG1	2.21	0.56
1:I:644:LEU:HB3	1:I:702:LEU:HB2	1.86	0.56
1:D:171:LEU:HD22	1:D:184:HIS:CG	2.40	0.56
1:G:191:LEU:HD22	1:G:196:VAL:HG21	1.86	0.56
1:G:512:LEU:HD13	1:G:645:LEU:HD22	1.87	0.56
1:H:125:SER:OG	1:H:129:THR:OG1	2.23	0.56
1:H:671:ASP:OD1	1:H:673:SER:OG	2.19	0.56
1:J:227:ILE:CG2	1:J:273:ALA:HB3	2.35	0.56
1:C:89:LYS:HE3	1:C:111:GLY:HA2	1.88	0.56
1:E:243:GLY:O	1:E:246:VAL:HG12	2.06	0.56
1:F:145:ARG:HD2	1:J:145:ARG:HB2	1.87	0.56
1:I:150:GLU:O	1:I:154:THR:OG1	2.24	0.56
1:D:68:ARG:HB3	1:D:131:THR:HG21	1.88	0.56
1:I:238:SER:N	1:I:248:GLU:OE2	2.39	0.56
1:J:601:PRO:HG3	1:J:618:ALA:HB3	1.86	0.56
1:J:675:PRO:N	1:J:675:PRO:C	2.55	0.56
1:F:403:TYR:CD1	1:F:424:ARG:HB3	2.40	0.56
1:F:403:TYR:HD1	1:F:424:ARG:HB3	1.71	0.56
1:G:159:ALA:HB1	1:G:164:LEU:HD12	1.88	0.56
1:G:644:LEU:HB2	1:G:666:TRP:CZ3	2.40	0.56
1:I:470:GLU:OE2	2:I:801:A16:H6A2	2.05	0.56
1:D:207:PHE:HA	1:D:226:THR:HA	1.87	0.56
1:D:267:VAL:HG23	1:D:341:PHE:HA	1.87	0.56
1:I:486:GLU:O	1:I:499:ARG:NH2	2.38	0.56
1:J:207:PHE:HA	1:J:226:THR:HA	1.88	0.56
1:D:404:ARG:HG2	1:D:408:ARG:HD2	1.86	0.56
1:I:21:ASN:HB2	1:I:59:TYR:HD1	1.70	0.56
1:D:50:GLU:OE1	1:F:578:ARG:NH2	2.39	0.55
1:D:463:LYS:HE2	1:D:477:ASN:HA	1.89	0.55
1:F:570:ARG:O	1:F:576:ARG:NH2	2.39	0.55
1:G:22:PHE:HZ	1:G:63:VAL:HG11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:VAL:HG11	1:C:246:VAL:HG11	1.88	0.55
1:C:264:ILE:HD11	1:C:374:LYS:HD2	1.89	0.55
1:C:595:ASP:HA	1:C:624:ASN:HB3	1.88	0.55
1:E:440:LEU:HA	1:E:515:GLY:HA2	1.88	0.55
1:J:640:ASP:OD2	1:J:641:ASP:N	2.39	0.55
1:F:420:GLU:O	1:F:424:ARG:HG2	2.06	0.55
1:D:32:ILE:HD12	1:D:56:ARG:HD2	1.89	0.55
1:D:424:ARG:NH2	1:D:430:ASP:OD2	2.39	0.55
1:E:270:ASN:ND2	1:E:343:LEU:HB2	2.21	0.55
1:G:300:ARG:HH11	1:G:301:TYR:HE1	1.53	0.55
1:H:84:ARG:HD2	1:H:285:ARG:HD2	1.87	0.55
1:J:30:HIS:HB3	1:J:31:ARG:HH11	1.72	0.55
1:J:43:GLU:OE2	1:J:72:ARG:NH1	2.40	0.55
1:D:440:LEU:HA	1:D:515:GLY:HA2	1.88	0.55
1:F:270:ASN:ND2	1:F:342:ASP:O	2.40	0.55
1:H:409:ASP:OD1	1:H:412:ARG:NH1	2.39	0.55
1:I:601:PRO:HG3	1:I:618:ALA:HB3	1.88	0.55
1:D:210:ASP:OD2	1:D:212:ARG:NH1	2.39	0.55
1:D:270:ASN:ND2	1:D:343:LEU:HB2	2.21	0.55
1:F:640:ASP:OD2	1:F:641:ASP:N	2.40	0.55
1:H:687:ALA:HB3	1:H:690:GLU:HB3	1.87	0.55
1:I:418:LEU:HB3	1:I:611:TRP:HZ3	1.72	0.55
1:J:89:LYS:NZ	1:J:108:ALA:O	2.30	0.55
1:C:281:THR:HG23	1:C:285:ARG:HB3	1.89	0.55
3:C:802:C2E:C81	3:C:802:C2E:C3A	2.85	0.55
1:D:664:ARG:HB2	1:D:704:ARG:HE	1.72	0.55
1:F:629:SER:O	1:F:629:SER:OG	2.19	0.55
1:G:528:THR:HG22	1:G:530:GLY:H	1.70	0.55
1:G:574:VAL:HG11	1:G:623:LEU:HB3	1.89	0.55
1:G:461:ASN:ND2	1:G:483:ASN:OD1	2.40	0.55
1:I:397:THR:HG23	1:I:441:ALA:HA	1.89	0.55
1:J:68:ARG:HB3	1:J:131:THR:HG21	1.89	0.55
1:H:586:VAL:HG12	1:H:586:VAL:O	2.07	0.54
1:J:130:MET:HE1	1:J:208:VAL:HG22	1.89	0.54
1:J:504:ARG:HB2	1:J:672:THR:HG23	1.89	0.54
1:E:73:VAL:HG21	1:E:287:LEU:HA	1.88	0.54
1:C:648:ASN:HB3	1:C:694:LEU:HD22	1.89	0.54
1:D:397:THR:HG23	1:D:441:ALA:HA	1.89	0.54
1:E:63:VAL:HG13	1:E:67:GLN:HG2	1.89	0.54
1:F:145:ARG:HB3	1:J:145:ARG:HH11	1.72	0.54
1:G:632:GLY:HA3	1:G:636:GLU:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:653:GLU:HG3	1:I:696:PRO:HD3	1.89	0.54
1:F:430:ASP:OD1	1:F:430:ASP:N	2.40	0.54
1:G:525:PHE:HE2	1:G:559:LEU:HD22	1.71	0.54
1:I:379:PRO:HG2	1:I:389:VAL:HG22	1.90	0.54
1:C:490:THR:HG22	1:C:492:ASP:H	1.73	0.54
1:D:327:LEU:HD13	1:D:370:VAL:HG11	1.90	0.54
1:F:184:HIS:CG	1:F:185:PRO:HD2	2.43	0.54
1:F:500:ALA:C	1:F:504:ARG:HH12	2.02	0.54
2:C:801:A16:H7A2	2:C:801:A16:O3B	2.07	0.54
1:F:438:ARG:HG2	3:F:802:C2E:C21	2.38	0.54
1:F:574:VAL:HG11	1:F:623:LEU:HB3	1.89	0.54
1:H:200:GLU:HA	1:H:264:ILE:O	2.07	0.54
1:J:35:CYS:SG	1:J:72:ARG:HG3	2.48	0.54
1:C:145:ARG:HD2	1:I:145:ARG:HG2	1.89	0.54
1:C:327:LEU:O	1:C:331:VAL:HG23	2.08	0.54
1:D:12:GLY:N	1:D:23:ALA:O	2.39	0.54
1:I:633:THR:HG22	1:I:634:GLN:HG3	1.90	0.54
1:C:146:ARG:NH2	1:C:331:VAL:O	2.40	0.54
1:C:617:GLN:NE2	1:C:650:SER:HA	2.22	0.54
1:I:465:ASN:ND2	1:I:533:ASN:OD1	2.30	0.54
1:C:118:ASP:OD2	1:C:300:ARG:NH1	2.41	0.54
1:C:63:VAL:HG13	1:C:67:GLN:HG2	1.90	0.53
1:C:648:ASN:HD21	1:C:696:PRO:HA	1.72	0.53
1:F:578:ARG:NH1	1:F:631:PRO:O	2.41	0.53
1:J:151:TYR:CD2	1:J:516:VAL:HG21	2.43	0.53
1:J:398:GLU:OE2	1:J:437:ARG:NH2	2.39	0.53
3:C:802:C2E:H81	3:C:802:C2E:C3A	2.36	0.53
1:F:513:SER:O	1:F:569:ARG:NH2	2.39	0.53
1:G:211:HIS:NE2	1:G:215:ASP:OD2	2.41	0.53
1:J:147:PRO:O	1:J:149:THR:N	2.38	0.53
1:D:125:SER:O	1:D:129:THR:OG1	2.23	0.53
1:F:505:ASN:CG	1:F:672:THR:HG21	2.28	0.53
1:F:225:ASN:ND2	1:F:273:ALA:HA	2.24	0.53
1:F:155:VAL:HB	1:F:196:VAL:HA	1.91	0.53
1:J:93:ASP:HB3	1:J:96:ALA:HB2	1.89	0.53
1:C:632:GLY:HA3	1:C:636:GLU:HG3	1.90	0.53
1:E:66:GLY:HA2	1:E:242:ARG:HG2	1.89	0.53
3:F:802:C2E:O1P	3:F:802:C2E:H2A	2.08	0.53
1:C:90:LEU:H	1:C:125:SER:HB3	1.74	0.53
1:C:210:ASP:OD1	1:C:220:ASN:ND2	2.38	0.53
2:D:801:A16:H7A2	2:D:801:A16:O3B	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:658:VAL:CG1	1:F:688:GLY:HA2	2.39	0.53
1:F:671:ASP:N	1:F:678:MET:HG2	2.24	0.53
2:G:801:A16:H7A2	2:G:801:A16:O3B	2.09	0.53
1:D:210:ASP:HB2	1:D:213:LEU:HD22	1.89	0.53
1:I:112:TYR:CD1	1:I:117:PRO:HA	2.43	0.53
1:D:73:VAL:HG21	1:D:287:LEU:HA	1.91	0.53
1:F:84:ARG:HD2	1:F:285:ARG:HD2	1.89	0.53
1:F:645:LEU:HD22	1:F:701:VAL:HG22	1.91	0.53
1:H:640:ASP:OD2	1:H:641:ASP:N	2.42	0.53
1:I:270:ASN:ND2	1:I:343:LEU:HB2	2.23	0.53
1:J:536:TYR:CE2	2:J:801:A16:H2B	2.43	0.53
1:E:659:PRO:N	1:E:659:PRO:C	2.56	0.53
1:C:84:ARG:NH2	1:C:300:ARG:O	2.43	0.52
1:E:699:LEU:HD23	1:E:700:THR:H	1.74	0.52
1:E:644:LEU:HB2	1:E:666:TRP:CZ3	2.45	0.52
1:C:147:PRO:O	1:C:149:THR:N	2.41	0.52
1:E:501:ARG:NH2	1:E:696:PRO:O	2.39	0.52
1:F:411:TRP:HB2	1:F:506:PHE:HZ	1.72	0.52
1:G:27:GLU:HA	1:G:54:PHE:HB3	1.91	0.52
1:I:125:SER:O	1:I:129:THR:OG1	2.27	0.52
1:I:538:GLN:O	1:I:543:SER:OG	2.26	0.52
1:J:141:TRP:HB3	1:J:144:ASP:HB2	1.90	0.52
1:C:150:GLU:O	1:C:154:THR:OG1	2.28	0.52
1:C:574:VAL:HG23	1:C:640:ASP:HB3	1.92	0.52
1:F:527:ARG:NH2	1:F:529:GLN:OE1	2.42	0.52
2:F:801:A16:O3C	2:F:801:A16:H1B	2.09	0.52
1:J:296:ALA:HA	1:J:303:MET:HG2	1.91	0.52
1:C:203:PRO:HG3	1:C:224:TYR:CE2	2.44	0.52
1:H:152:HIS:O	1:H:576:ARG:HD2	2.09	0.52
1:H:486:GLU:HB3	1:H:490:THR:HG21	1.91	0.52
1:J:3:VAL:HG22	1:J:60:LEU:HD22	1.91	0.52
1:J:267:VAL:HG23	1:J:341:PHE:HA	1.90	0.52
3:J:802:C2E:H2A	3:J:802:C2E:O1P	2.10	0.52
1:F:502:GLN:OE1	1:F:502:GLN:HA	2.09	0.52
1:I:298:ASP:O	1:I:300:ARG:N	2.43	0.52
1:C:26:SER:HB3	1:C:32:ILE:HD11	1.91	0.52
1:C:225:ASN:OD1	1:C:273:ALA:HA	2.10	0.52
1:C:474:ASP:OD1	1:C:474:ASP:N	2.43	0.52
1:F:504:ARG:NH1	1:F:504:ARG:CG	2.71	0.52
1:F:671:ASP:OD1	1:F:673:SER:OG	2.27	0.52
1:I:207:PHE:HA	1:I:226:THR:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:THR:HG22	1:J:130:MET:N	2.25	0.52
1:J:670:VAL:HA	1:J:678:MET:O	2.10	0.52
1:D:200:GLU:HA	1:D:264:ILE:O	2.10	0.52
1:D:390:GLY:O	1:D:435:ASP:OD2	2.27	0.52
1:H:151:TYR:CE2	1:H:516:VAL:HG21	2.45	0.52
1:H:632:GLY:HA3	1:H:636:GLU:HG3	1.92	0.52
1:I:72:ARG:NH2	1:I:124:ASP:OD1	2.43	0.52
1:J:212:ARG:HH22	2:J:801:A16:H7A1	1.73	0.52
1:J:470:GLU:HG2	1:J:473:ARG:HB2	1.92	0.52
1:D:205:HIS:NE2	1:D:267:VAL:HG12	2.25	0.52
1:E:125:SER:O	1:E:129:THR:OG1	2.17	0.52
1:F:249:PHE:O	1:F:253:VAL:HG23	2.10	0.52
1:G:270:ASN:ND2	1:G:343:LEU:HB2	2.25	0.52
1:I:89:LYS:HZ1	1:I:111:GLY:H	1.58	0.52
1:I:315:ARG:HG2	1:I:350:GLN:HG3	1.91	0.52
1:I:446:VAL:HG21	1:I:506:PHE:HB3	1.92	0.52
1:I:538:GLN:HG3	1:I:540:ASN:OD1	2.10	0.52
1:J:15:TYR:CD1	1:J:65:PRO:HD3	2.45	0.52
1:J:501:ARG:HG3	1:J:672:THR:HG22	1.92	0.52
1:D:670:VAL:HB	1:D:701:VAL:HB	1.91	0.52
1:E:205:HIS:NE2	1:E:267:VAL:HG12	2.24	0.52
1:H:509:THR:O	1:H:513:SER:OG	2.16	0.52
1:C:248:GLU:O	1:C:252:ALA:N	2.38	0.51
3:C:802:C2E:H2A	3:C:802:C2E:O1P	2.09	0.51
1:G:209:ASN:HD21	1:G:219:SER:HB2	1.75	0.51
1:D:504:ARG:HB2	1:D:672:THR:HG23	1.92	0.51
1:E:147:PRO:O	1:E:149:THR:N	2.42	0.51
1:G:447:THR:OG1	1:G:452:PHE:O	2.20	0.51
1:C:157:TYR:CE2	1:C:159:ALA:HB2	2.45	0.51
1:C:184:HIS:CG	1:C:185:PRO:HD2	2.46	0.51
1:G:164:LEU:HD23	1:G:547:TRP:HZ2	1.75	0.51
1:F:157:TYR:CE2	1:F:159:ALA:HB2	2.45	0.51
1:I:281:THR:HG23	1:I:285:ARG:HB3	1.92	0.51
1:E:192:ARG:HG3	1:E:261:ILE:HD11	1.91	0.51
1:E:249:PHE:HZ	1:E:265:LEU:HD23	1.76	0.51
1:F:370:VAL:HG12	1:F:375:LEU:HD21	1.92	0.51
1:F:448:CYS:HA	1:F:520:SER:HB3	1.92	0.51
1:G:35:CYS:SG	1:G:72:ARG:NH1	2.78	0.51
1:G:440:LEU:HA	1:G:515:GLY:HA2	1.93	0.51
1:H:155:VAL:HB	1:H:196:VAL:HA	1.92	0.51
1:J:388:GLN:OE1	1:J:391:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:TRP:CE3	1:C:334:MET:HG3	2.46	0.51
1:C:484:CYS:O	1:C:495:ILE:HD12	2.10	0.51
1:F:573:PRO:HD2	1:F:640:ASP:HB2	1.92	0.51
1:G:212:ARG:HG2	1:G:213:LEU:HD12	1.92	0.51
1:H:414:GLU:HG3	1:H:415:PRO:HD2	1.92	0.51
3:I:802:C2E:H81	3:I:802:C2E:C4A	2.40	0.51
1:D:579:ARG:HG2	3:D:804:C2E:N71	2.25	0.51
1:F:239:TRP:N	1:F:248:GLU:OE2	2.44	0.51
1:F:342:ASP:OD1	2:F:801:A16:O5C	2.26	0.51
1:H:623:LEU:HD11	1:H:645:LEU:HD11	1.93	0.51
1:I:165:THR:HG21	1:I:182:LEU:HA	1.92	0.51
1:I:324:MET:HG3	1:I:363:LEU:HD23	1.93	0.51
1:G:147:PRO:O	1:G:149:THR:N	2.43	0.51
3:H:803:C2E:H8	3:H:803:C2E:C5'	2.40	0.51
1:I:563:ARG:HH21	1:I:567:ARG:HH22	1.57	0.51
1:F:166:MET:HA	1:F:176:ARG:HB3	1.93	0.51
1:G:444:ASN:ND2	1:G:514:GLN:O	2.44	0.51
1:I:567:ARG:HG2	1:I:570:ARG:NH2	2.26	0.51
1:I:595:ASP:OD1	1:I:595:ASP:N	2.42	0.51
1:J:326:SER:O	1:J:330:TRP:HD1	1.94	0.51
1:F:165:THR:HG22	1:F:187:VAL:HG21	1.92	0.51
1:F:390:GLY:O	1:F:435:ASP:OD2	2.29	0.51
1:F:528:THR:HG22	1:F:530:GLY:H	1.76	0.51
1:G:68:ARG:HB3	1:G:131:THR:HG21	1.93	0.51
1:G:644:LEU:HD23	1:G:702:LEU:HD12	1.93	0.51
1:J:167:LEU:HD11	1:J:544:TRP:CE3	2.45	0.51
1:E:397:THR:HG23	1:E:441:ALA:HA	1.93	0.50
1:G:351:PHE:O	1:G:352:HIS:ND1	2.44	0.50
1:G:417:THR:HG21	1:G:612:GLN:HA	1.92	0.50
1:G:660:ASP:HB2	1:G:664:ARG:HE	1.76	0.50
1:C:159:ALA:HA	1:C:521:HIS:CD2	2.46	0.50
1:C:305:THR:HG21	1:C:349:ARG:HD2	1.92	0.50
1:C:451:GLY:C	1:C:533:ASN:HB2	2.32	0.50
1:C:501:ARG:HB2	1:C:504:ARG:HH11	1.76	0.50
1:G:470:GLU:OE1	1:G:474:ASP:HB3	2.12	0.50
1:J:646:MET:N	1:J:700:THR:O	2.43	0.50
1:E:667:ARG:NH1	1:E:685:GLU:HB3	2.26	0.50
1:G:653:GLU:HG3	1:G:696:PRO:HD3	1.94	0.50
1:H:194:LEU:HD11	1:H:524:GLU:HG2	1.93	0.50
1:H:233:HIS:CD2	1:H:235:ALA:HB3	2.46	0.50
1:I:227:ILE:HG22	1:I:272:THR:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:267:VAL:HB	1:J:269:TYR:CE1	2.47	0.50
1:J:390:GLY:O	1:J:435:ASP:OD2	2.28	0.50
1:J:425:LEU:HD23	1:J:513:SER:HA	1.94	0.50
1:D:4:TRP:HB3	1:D:5:PRO:HD2	1.92	0.50
1:I:89:LYS:HA	1:I:125:SER:HB3	1.93	0.50
1:C:99:VAL:HB	1:C:206:GLN:OE1	2.11	0.50
1:E:409:ASP:HB3	1:E:416:ARG:HG3	1.93	0.50
1:F:15:TYR:HE1	1:F:64:MET:HG2	1.76	0.50
1:G:408:ARG:HA	1:G:506:PHE:HE2	1.76	0.50
1:I:567:ARG:HG2	1:I:570:ARG:HH21	1.76	0.50
1:J:155:VAL:HG13	1:J:517:PRO:HG2	1.93	0.50
1:J:229:PHE:CD2	1:J:322:LEU:HD21	2.46	0.50
1:C:314:MET:SD	1:C:347:LEU:HA	2.51	0.50
1:D:147:PRO:O	1:D:149:THR:N	2.43	0.50
1:E:112:TYR:CD1	1:E:117:PRO:HA	2.47	0.50
3:G:802:C2E:H511	1:J:579:ARG:HB3	1.93	0.50
1:J:492:ASP:HB3	1:J:495:ILE:HG12	1.92	0.50
1:G:90:LEU:H	1:G:125:SER:HB3	1.77	0.50
1:I:110:TYR:OH	1:I:211:HIS:ND1	2.30	0.50
1:D:574:VAL:HG11	1:D:623:LEU:HB3	1.94	0.50
1:E:632:GLY:HA3	1:E:636:GLU:CG	2.42	0.50
1:F:315:ARG:HB3	1:F:350:GLN:HG3	1.94	0.50
1:J:113:PRO:HD2	1:J:119:ALA:HB3	1.93	0.50
1:C:325:ASP:OD2	1:C:328:ARG:NH2	2.45	0.50
3:I:802:C2E:O1P	3:I:802:C2E:H2A	2.12	0.49
1:J:488:GLY:O	1:J:499:ARG:NH2	2.40	0.49
1:D:403:TYR:CE2	1:D:444:ASN:HB3	2.47	0.49
1:E:338:GLY:HA3	1:E:374:LYS:HB2	1.94	0.49
1:F:484:CYS:O	1:F:495:ILE:HG23	2.11	0.49
1:F:704:ARG:HG2	1:F:705:PRO:HD2	1.94	0.49
1:H:140:ASP:O	1:H:254:ARG:NH2	2.45	0.49
1:H:424:ARG:NH2	1:H:430:ASP:OD2	2.44	0.49
1:J:225:ASN:OD1	1:J:273:ALA:HA	2.12	0.49
1:C:68:ARG:HB3	1:C:131:THR:CG2	2.42	0.49
1:C:158:GLU:HA	1:C:200:GLU:HB3	1.94	0.49
1:C:233:HIS:CE1	1:C:235:ALA:HB3	2.47	0.49
1:D:151:TYR:CE2	1:D:516:VAL:HG21	2.48	0.49
1:E:298:ASP:O	1:E:300:ARG:N	2.45	0.49
1:E:598:TRP:CE3	1:E:619:LEU:HD11	2.47	0.49
1:F:68:ARG:HD3	1:F:242:ARG:CZ	2.42	0.49
1:H:69:TYR:OH	1:H:93:ASP:OD2	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:444:ASN:ND2	1:H:514:GLN:O	2.45	0.49
1:I:73:VAL:HG21	1:I:287:LEU:HA	1.93	0.49
1:J:342:ASP:OD1	2:J:801:A16:C1C	2.60	0.49
1:D:294:ARG:HA	1:D:313:LEU:HG	1.94	0.49
1:G:442:SER:OG	1:G:444:ASN:OD1	2.25	0.49
1:E:51:THR:HB	3:E:803:C2E:C61	2.43	0.49
1:F:397:THR:HG22	1:F:443:VAL:HG23	1.94	0.49
1:H:72:ARG:HD3	1:H:87:ALA:O	2.12	0.49
1:H:327:LEU:HD13	1:H:370:VAL:HG11	1.94	0.49
1:I:152:HIS:O	1:I:576:ARG:HD2	2.12	0.49
1:I:504:ARG:HB2	1:I:672:THR:HG23	1.93	0.49
1:E:105:TRP:CD1	1:E:214:VAL:HG11	2.48	0.49
1:E:266:ASP:OD2	1:E:340:ARG:NH1	2.46	0.49
1:F:238:SER:N	1:F:248:GLU:OE2	2.45	0.49
1:J:408:ARG:HG2	1:J:457:LEU:HD21	1.95	0.49
1:C:629:SER:O	1:C:629:SER:OG	2.31	0.49
1:D:71:PHE:HE1	1:D:93:ASP:HB2	1.78	0.49
1:E:211:HIS:NE2	1:E:215:ASP:OD2	2.46	0.49
1:C:110:TYR:HA	1:C:280:PRO:HA	1.94	0.49
1:D:2:GLN:HB3	1:D:61:PRO:HG2	1.94	0.49
1:D:86:ASN:ND2	1:D:121:ASN:O	2.26	0.49
1:I:300:ARG:HB3	1:I:301:TYR:CD1	2.47	0.49
1:I:464:ARG:NH2	1:I:487:GLU:HG2	2.27	0.49
1:D:205:HIS:HE1	1:D:330:TRP:NE1	2.11	0.49
1:E:89:LYS:HE3	1:E:111:GLY:HA2	1.95	0.49
1:F:72:ARG:NH2	1:F:124:ASP:OD1	2.46	0.49
1:F:157:TYR:HE2	1:F:159:ALA:HB2	1.76	0.49
1:F:207:PHE:HA	1:F:226:THR:HA	1.93	0.49
1:G:70:GLY:HA3	1:G:90:LEU:HD11	1.95	0.49
1:G:239:TRP:CD2	1:G:248:GLU:HG2	2.48	0.49
1:G:492:ASP:OD2	1:G:495:ILE:HD12	2.13	0.49
1:J:522:GLY:HA3	1:J:527:ARG:HB2	1.95	0.49
1:E:328:ARG:HD3	1:E:367:ASP:OD1	2.13	0.49
1:H:163:GLY:HA2	1:H:544:TRP:CE3	2.48	0.49
1:I:402:LYS:HD2	1:I:431:LEU:HD11	1.95	0.49
1:J:225:ASN:O	1:J:225:ASN:ND2	2.46	0.49
1:J:644:LEU:HB3	1:J:702:LEU:HB2	1.94	0.49
1:D:163:GLY:O	1:D:545:VAL:HG22	2.12	0.48
1:D:184:HIS:ND1	1:D:186:SER:OG	2.43	0.48
1:E:420:GLU:O	1:E:424:ARG:HG2	2.13	0.48
1:F:371:SER:OG	1:F:372:GLN:OE1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:TYR:CD1	1:G:117:PRO:HA	2.48	0.48
1:I:446:VAL:HG23	1:I:447:THR:HG22	1.94	0.48
1:I:662:HIS:ND1	1:I:662:HIS:N	2.60	0.48
1:C:458:VAL:HG21	1:C:503:MET:HG3	1.96	0.48
1:I:173:GLU:HA	1:I:176:ARG:HG3	1.95	0.48
1:D:498:LEU:CD2	1:D:502:GLN:HG2	2.43	0.48
1:E:428:SER:HB3	1:E:431:LEU:HD12	1.94	0.48
1:F:99:VAL:O	1:F:206:GLN:NE2	2.43	0.48
1:G:184:HIS:CG	1:G:185:PRO:HD2	2.47	0.48
1:E:239:TRP:CD2	1:E:248:GLU:HG2	2.48	0.48
1:G:212:ARG:HH22	2:G:801:A16:H7A1	1.77	0.48
1:H:412:ARG:NH2	1:H:478:TYR:HE1	2.11	0.48
1:J:212:ARG:NH2	2:J:801:A16:C7A	2.75	0.48
1:C:579:ARG:CD	1:C:630:GLU:HG2	2.43	0.48
1:E:86:ASN:ND2	1:E:121:ASN:O	2.44	0.48
1:F:97:ARG:HD3	1:F:329:TYR:CE1	2.49	0.48
1:F:665:TYR:HD2	1:F:666:TRP:H	1.62	0.48
1:G:158:GLU:OE2	1:G:449:HIS:ND1	2.31	0.48
1:G:172:PRO:HB2	1:G:174:GLU:OE1	2.14	0.48
1:J:92:LEU:CD2	1:J:227:ILE:HD13	2.43	0.48
1:J:205:HIS:HE1	1:J:267:VAL:HG12	1.77	0.48
1:J:632:GLY:HA3	1:J:636:GLU:HG3	1.95	0.48
1:C:408:ARG:HG2	1:C:457:LEU:HD21	1.95	0.48
1:C:99:VAL:HB	1:C:206:GLN:CD	2.34	0.48
1:C:203:PRO:CG	1:C:224:TYR:CE2	2.96	0.48
1:C:570:ARG:O	1:C:576:ARG:NH2	2.35	0.48
1:F:145:ARG:HH22	1:J:258:GLN:HG2	1.79	0.48
1:I:200:GLU:HA	1:I:264:ILE:O	2.13	0.48
1:I:470:GLU:OE2	2:I:801:A16:C6A	2.62	0.48
1:J:332:THR:HG23	1:J:369:VAL:HG11	1.96	0.48
1:C:32:ILE:HB	1:C:56:ARG:HD2	1.95	0.48
1:C:667:ARG:HA	1:C:685:GLU:HA	1.96	0.48
1:D:43:GLU:CD	1:D:72:ARG:HH12	2.16	0.48
1:D:360:PHE:O	1:D:364:VAL:HG23	2.14	0.48
1:F:522:GLY:HA3	1:F:527:ARG:HG3	1.94	0.48
1:J:512:LEU:HD13	1:J:645:LEU:HD22	1.95	0.48
1:D:125:SER:O	1:D:125:SER:OG	2.32	0.48
1:F:509:THR:O	1:F:513:SER:OG	2.25	0.48
1:H:238:SER:N	1:H:248:GLU:OE2	2.41	0.48
1:I:184:HIS:CG	1:I:185:PRO:HD2	2.49	0.48
1:J:232:PRO:HG2	1:J:246:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ASP:O	1:D:300:ARG:N	2.47	0.48
1:F:166:MET:O	1:F:176:ARG:HD3	2.14	0.48
1:G:356:ARG:HG3	1:G:357:LEU:HD13	1.95	0.48
1:I:408:ARG:HG2	1:I:457:LEU:HD21	1.96	0.48
1:C:144:ASP:OD1	1:C:257:HIS:ND1	2.47	0.47
1:E:520:SER:OG	1:E:523:ASP:OD2	2.21	0.47
1:F:694:LEU:HD23	1:F:698:SER:HB3	1.96	0.47
1:G:465:ASN:ND2	1:G:533:ASN:OD1	2.38	0.47
1:H:26:SER:HB3	1:H:32:ILE:HD11	1.96	0.47
1:I:89:LYS:NZ	1:I:108:ALA:O	2.46	0.47
1:C:154:THR:HA	1:C:197:THR:OG1	2.14	0.47
1:I:199:LEU:HD22	1:I:201:LEU:HD12	1.95	0.47
1:I:474:ASP:OD1	1:I:474:ASP:N	2.46	0.47
1:C:440:LEU:HA	1:C:515:GLY:HA2	1.96	0.47
1:G:89:LYS:HA	1:G:125:SER:HB2	1.96	0.47
1:G:642:SER:N	1:G:704:ARG:O	2.47	0.47
1:H:207:PHE:HB2	1:H:225:ASN:O	2.15	0.47
1:H:504:ARG:HB2	1:H:672:THR:HG23	1.96	0.47
1:I:641:ASP:HB3	1:I:705:PRO:HA	1.94	0.47
1:J:125:SER:OG	1:J:129:THR:OG1	2.27	0.47
1:G:89:LYS:HE3	1:G:111:GLY:HA2	1.96	0.47
1:G:521:HIS:CD2	1:G:527:ARG:HH12	2.33	0.47
1:C:9:TYR:CG	1:C:10:PRO:HA	2.49	0.47
1:C:672:THR:HB	1:C:699:LEU:H	1.79	0.47
1:D:488:GLY:O	1:D:499:ARG:NH2	2.37	0.47
1:E:15:TYR:CE1	1:E:65:PRO:HD3	2.49	0.47
1:E:32:ILE:HD12	1:E:56:ARG:HG3	1.96	0.47
1:H:130:MET:HE1	1:H:208:VAL:HG22	1.97	0.47
1:J:200:GLU:HA	1:J:264:ILE:O	2.14	0.47
1:C:584:ARG:CB	1:C:585:PRO:HD3	2.39	0.47
1:E:656:PHE:O	1:E:691:ARG:HA	2.14	0.47
1:G:501:ARG:HG3	1:G:672:THR:HG22	1.97	0.47
1:H:163:GLY:HA2	1:H:544:TRP:HE3	1.79	0.47
1:I:222:TRP:CD2	1:I:536:TYR:HA	2.50	0.47
1:D:21:ASN:HB2	1:D:59:TYR:CD1	2.49	0.47
1:D:289:ASN:OD1	1:D:302:TYR:OH	2.25	0.47
1:D:392:PHE:O	1:D:437:ARG:NH2	2.47	0.47
1:F:298:ASP:O	1:F:300:ARG:N	2.48	0.47
1:G:468:ASN:ND2	1:G:534:ASN:O	2.47	0.47
1:G:644:LEU:O	1:G:701:VAL:HA	2.15	0.47
1:H:32:ILE:HD12	1:H:56:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:LEU:HD22	1:H:184:HIS:CG	2.50	0.47
1:H:416:ARG:O	1:H:416:ARG:NH1	2.48	0.47
1:J:213:LEU:HD21	1:J:537:CYS:HB3	1.97	0.47
1:J:267:VAL:HB	1:J:269:TYR:HE1	1.79	0.47
1:J:296:ALA:C	1:J:298:ASP:H	2.18	0.47
1:J:642:SER:N	1:J:704:ARG:O	2.48	0.47
1:J:649:ALA:HA	1:J:697:LEU:HD23	1.97	0.47
1:C:178:THR:HG21	1:C:238:SER:HB3	1.94	0.47
1:F:80:GLU:O	1:F:299:PRO:HG2	2.13	0.47
1:F:149:THR:O	1:F:374:LYS:NZ	2.32	0.47
1:F:168:HIS:HB3	1:F:171:LEU:HG	1.96	0.47
1:G:446:VAL:HG11	1:G:506:PHE:HB3	1.97	0.47
1:G:672:THR:HB	1:G:699:LEU:H	1.79	0.47
1:H:418:LEU:HA	1:H:418:LEU:HD23	1.70	0.47
1:I:297:ASP:OD2	1:I:297:ASP:N	2.44	0.47
1:J:99:VAL:HB	1:J:206:GLN:OE1	2.15	0.47
1:C:89:LYS:HA	1:C:125:SER:HB2	1.97	0.47
1:D:349:ARG:NH1	1:D:384:GLU:O	2.47	0.47
1:E:581:PHE:CD2	1:E:596:ILE:HB	2.50	0.47
1:E:274:GLU:O	1:E:285:ARG:NH2	2.48	0.47
1:F:243:GLY:O	1:F:246:VAL:HG12	2.15	0.47
1:H:425:LEU:HD11	1:H:647:PHE:CZ	2.50	0.47
1:J:9:TYR:CD1	1:J:10:PRO:HA	2.50	0.47
1:G:100:SER:HA	1:G:241:ASP:HB2	1.96	0.46
1:G:552:SER:OG	1:G:553:GLU:N	2.48	0.46
1:H:225:ASN:ND2	1:H:273:ALA:HA	2.30	0.46
3:H:803:C2E:C3'	3:H:803:C2E:C5A	2.89	0.46
1:J:438:ARG:HG2	1:J:578:ARG:O	2.16	0.46
1:C:32:ILE:HD12	1:C:56:ARG:HG3	1.97	0.46
1:C:145:ARG:HB2	1:I:145:ARG:HG3	1.96	0.46
1:C:163:GLY:HA2	1:C:544:TRP:CE3	2.50	0.46
1:C:194:LEU:HD12	1:C:563:ARG:HG3	1.97	0.46
1:F:205:HIS:NE2	1:F:267:VAL:HG12	2.30	0.46
1:G:305:THR:HB	1:G:381:ASP:OD1	2.15	0.46
1:I:412:ARG:HH11	1:I:480:ARG:HA	1.79	0.46
1:I:560:ARG:NH2	1:I:676:GLU:O	2.48	0.46
1:C:429:SER:HA	1:C:580:PHE:CE2	2.50	0.46
1:D:101:GLY:O	1:D:234:ASN:ND2	2.47	0.46
1:E:440:LEU:HD21	1:E:578:ARG:HA	1.98	0.46
1:J:112:TYR:CZ	1:J:278:LEU:HA	2.50	0.46
1:J:272:THR:HG22	1:J:273:ALA:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:VAL:HB	1:C:206:GLN:NE2	2.31	0.46
1:D:27:GLU:N	1:D:288:ASP:OD1	2.46	0.46
1:E:72:ARG:NH2	1:E:124:ASP:OD1	2.49	0.46
1:F:380:TRP:HA	1:F:386:GLY:O	2.15	0.46
1:G:271:HIS:HB2	1:G:310:ASN:OD1	2.16	0.46
1:G:308:THR:HA	2:G:801:A16:H2A	1.98	0.46
1:H:257:HIS:HE1	1:H:263:VAL:HG23	1.79	0.46
1:I:380:TRP:HA	1:I:386:GLY:O	2.15	0.46
1:J:484:CYS:O	1:J:495:ILE:HG23	2.16	0.46
1:C:694:LEU:HD23	1:C:698:SER:HB3	1.98	0.46
1:J:151:TYR:CE2	1:J:516:VAL:HG21	2.51	0.46
1:J:167:LEU:HD13	1:J:544:TRP:HB3	1.96	0.46
1:J:222:TRP:CZ3	2:J:801:A16:O3C	2.69	0.46
1:D:10:PRO:HG2	1:D:14:THR:HG21	1.97	0.46
1:D:512:LEU:HD13	1:D:645:LEU:HD22	1.98	0.46
1:D:633:THR:HG22	1:D:634:GLN:HG3	1.98	0.46
1:E:460:TYR:CE2	1:E:464:ARG:HD2	2.51	0.46
1:F:91:LEU:HD11	1:F:286:GLY:HA3	1.97	0.46
1:F:644:LEU:HD23	1:F:702:LEU:HD12	1.97	0.46
1:I:264:ILE:HG21	1:I:376:ILE:HD12	1.96	0.46
1:I:387:TYR:HE2	1:I:402:LYS:HE3	1.79	0.46
1:J:205:HIS:CE1	1:J:267:VAL:HG12	2.51	0.46
1:F:296:ALA:C	1:F:298:ASP:H	2.19	0.46
1:H:141:TRP:HB3	1:H:144:ASP:HB2	1.98	0.46
1:I:130:MET:CE	1:I:227:ILE:HD11	2.46	0.46
1:I:288:ASP:OD2	1:I:291:SER:OG	2.30	0.46
1:J:69:TYR:OH	1:J:93:ASP:OD2	2.27	0.46
1:J:648:ASN:OD1	1:J:654:LEU:HD13	2.16	0.46
1:C:327:LEU:HD13	1:C:370:VAL:HG11	1.97	0.46
1:C:488:GLY:O	1:C:499:ARG:NH2	2.32	0.46
1:D:390:GLY:N	1:D:398:GLU:OE1	2.45	0.46
1:F:32:ILE:HD12	1:F:56:ARG:HG3	1.97	0.46
1:G:280:PRO:HB2	1:G:282:LEU:HG	1.97	0.46
3:G:802:C2E:O1P	3:G:802:C2E:H2A	2.16	0.46
1:H:10:PRO:HG2	1:H:14:THR:HG21	1.97	0.46
1:H:212:ARG:HH22	2:H:801:A16:H7A1	1.81	0.46
1:I:227:ILE:HG13	1:I:228:GLY:H	1.81	0.46
1:I:268:VAL:HG13	1:I:342:ASP:OD2	2.16	0.46
1:I:277:HIS:O	1:I:278:LEU:HB2	2.16	0.46
1:D:294:ARG:HG2	1:D:303:MET:HB2	1.98	0.46
1:D:377:ALA:N	1:D:397:THR:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:602:GLU:H	1:D:602:GLU:HG3	1.46	0.46
1:E:460:TYR:HE2	1:E:464:ARG:HD2	1.81	0.46
1:F:195:GLY:HA3	1:F:566:VAL:HG11	1.98	0.46
1:F:425:LEU:O	1:F:514:GLN:HG2	2.16	0.46
1:J:9:TYR:CG	1:J:10:PRO:HA	2.50	0.46
1:E:200:GLU:HA	1:E:264:ILE:O	2.16	0.46
1:E:212:ARG:NH2	1:E:536:TYR:OH	2.49	0.46
1:E:239:TRP:CE3	1:E:248:GLU:HG2	2.50	0.46
1:F:446:VAL:HG23	1:F:447:THR:H	1.81	0.46
1:G:71:PHE:HE1	1:G:93:ASP:HB2	1.81	0.46
1:G:274:GLU:O	1:G:285:ARG:NH2	2.49	0.46
1:H:446:VAL:HG11	1:H:506:PHE:HB3	1.98	0.46
1:D:296:ALA:HA	1:D:303:MET:HG2	1.98	0.45
1:F:668:MET:HG2	1:F:678:MET:HE2	1.97	0.45
1:D:439:PRO:HG3	1:D:580:PHE:CD2	2.51	0.45
1:F:439:PRO:HG3	1:F:580:PHE:CD2	2.52	0.45
1:G:68:ARG:HB3	1:G:131:THR:CG2	2.46	0.45
1:C:157:TYR:HE2	1:C:159:ALA:HB2	1.81	0.45
1:C:212:ARG:HH22	1:C:536:TYR:HH	1.56	0.45
1:C:677:GLY:O	1:C:681:GLN:HB3	2.17	0.45
1:D:460:TYR:HA	1:D:487:GLU:HG3	1.99	0.45
1:E:26:SER:HB3	1:E:32:ILE:HD11	1.99	0.45
1:E:36:LEU:HD11	1:E:60:LEU:HD12	1.97	0.45
1:F:9:TYR:CG	1:F:10:PRO:HA	2.51	0.45
1:F:178:THR:HG21	1:F:238:SER:HB3	1.98	0.45
1:F:417:THR:HG22	1:F:419:ALA:H	1.80	0.45
1:H:324:MET:HB3	1:H:328:ARG:NH1	2.31	0.45
1:J:161:VAL:HG22	1:J:201:LEU:HG	1.99	0.45
1:D:495:ILE:H	1:D:495:ILE:HG13	1.50	0.45
1:D:579:ARG:HG2	3:D:804:C2E:C81	2.47	0.45
1:E:210:ASP:CG	1:E:220:ASN:HD22	2.19	0.45
1:F:103:VAL:HG21	1:F:208:VAL:HG13	1.98	0.45
1:F:522:GLY:C	1:F:527:ARG:HB2	2.36	0.45
1:G:5:PRO:HB3	1:G:50:GLU:HG3	1.98	0.45
1:G:454:LEU:HG	1:G:503:MET:HG2	1.98	0.45
1:H:313:LEU:HD22	1:H:315:ARG:HG2	1.97	0.45
1:C:68:ARG:HD3	1:C:242:ARG:CZ	2.46	0.45
1:C:409:ASP:OD1	1:C:412:ARG:NH1	2.49	0.45
1:C:505:ASN:ND2	1:C:672:THR:HG21	2.31	0.45
1:C:699:LEU:HD23	1:C:700:THR:H	1.81	0.45
1:G:505:ASN:ND2	1:G:672:THR:HG21	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:445:PHE:HB3	1:J:518:MET:HB3	1.99	0.45
1:C:664:ARG:HG2	1:C:704:ARG:HH21	1.81	0.45
1:C:671:ASP:HB3	1:C:678:MET:CG	2.46	0.45
1:D:424:ARG:HA	1:D:424:ARG:HD3	1.83	0.45
1:H:412:ARG:NH1	1:H:414:GLU:OE1	2.50	0.45
1:I:492:ASP:O	1:I:496:THR:OG1	2.24	0.45
1:J:97:ARG:HD3	1:J:329:TYR:CE1	2.51	0.45
1:C:103:VAL:HG21	1:C:208:VAL:HG13	1.98	0.45
1:D:393:PRO:HB2	1:D:396:TRP:HD1	1.82	0.45
1:D:641:ASP:HA	1:D:705:PRO:HA	1.99	0.45
1:E:166:MET:O	1:E:176:ARG:HD3	2.17	0.45
1:F:37:LEU:HD11	1:F:90:LEU:HD21	1.98	0.45
1:G:408:ARG:HG2	1:G:457:LEU:HD21	1.99	0.45
1:H:2:GLN:HB3	1:H:61:PRO:HG2	1.98	0.45
1:J:19:GLY:HA3	1:J:61:PRO:HA	1.98	0.45
1:G:84:ARG:NH2	1:G:300:ARG:O	2.49	0.45
1:I:99:VAL:HB	1:I:206:GLN:OE1	2.17	0.45
1:I:586:VAL:O	1:I:587:GLU:HB2	2.17	0.45
1:C:418:LEU:HD13	1:C:619:LEU:HG	1.99	0.45
1:D:484:CYS:O	1:D:495:ILE:HG22	2.04	0.45
1:G:573:PRO:HD2	1:G:640:ASP:HB2	1.98	0.45
1:H:585:PRO:O	1:H:585:PRO:HG2	2.16	0.45
1:D:155:VAL:HB	1:D:196:VAL:HA	1.99	0.45
1:F:654:LEU:HA	1:F:654:LEU:HD23	1.79	0.45
1:H:72:ARG:NH2	1:H:124:ASP:OD1	2.49	0.45
1:I:163:GLY:HA2	1:I:544:TRP:HE3	1.82	0.45
1:C:482:TRP:CZ3	1:C:484:CYS:HA	2.52	0.44
3:D:804:C2E:C3'	3:D:804:C2E:C5A	2.91	0.44
1:F:304:ASP:OD2	1:F:309:GLY:N	2.49	0.44
1:H:183:ALA:HB1	1:H:255:ALA:HB3	1.98	0.44
1:I:327:LEU:HD13	1:I:370:VAL:HG11	1.98	0.44
1:J:28:ALA:N	1:J:288:ASP:OD1	2.47	0.44
1:E:157:TYR:HB2	1:E:196:VAL:HG11	1.99	0.44
1:F:3:VAL:HG13	1:F:60:LEU:HD21	1.99	0.44
1:F:461:ASN:ND2	1:F:482:TRP:HA	2.33	0.44
1:G:425:LEU:HD23	1:G:425:LEU:HA	1.84	0.44
1:H:3:VAL:HG22	1:H:60:LEU:HD22	1.98	0.44
1:H:455:ARG:NE	1:H:528:THR:OG1	2.49	0.44
1:H:653:GLU:HG3	1:H:696:PRO:HD3	1.99	0.44
1:I:579:ARG:NH1	1:I:629:SER:O	2.49	0.44
1:J:206:GLN:HA	1:J:233:HIS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLY:O	1:C:193:GLU:N	2.45	0.44
1:D:129:THR:HG23	1:D:282:LEU:HD22	1.98	0.44
1:E:175:LEU:HD22	1:E:180:ALA:HB3	1.99	0.44
1:E:283:SER:O	1:E:287:LEU:HG	2.17	0.44
1:F:92:LEU:HD22	1:F:227:ILE:HD13	1.99	0.44
1:F:171:LEU:HD12	1:F:176:ARG:HA	2.00	0.44
1:F:355:ASP:HB3	1:F:358:SER:HB3	1.98	0.44
1:H:15:TYR:CE1	1:H:65:PRO:HD3	2.52	0.44
1:I:168:HIS:HA	1:I:547:TRP:CD1	2.52	0.44
1:I:648:ASN:HB2	1:I:656:PHE:CE1	2.52	0.44
1:J:163:GLY:O	1:J:545:VAL:HG22	2.17	0.44
1:J:390:GLY:N	1:J:398:GLU:OE1	2.45	0.44
1:J:567:ARG:HG2	1:J:570:ARG:HH21	1.83	0.44
1:C:48:LEU:HD11	1:C:71:PHE:HE2	1.81	0.44
1:C:238:SER:N	1:C:248:GLU:OE2	2.51	0.44
1:C:600:THR:HG23	1:C:606:MET:HG2	2.00	0.44
1:C:699:LEU:HD23	1:C:700:THR:N	2.33	0.44
1:D:91:LEU:HD11	1:D:286:GLY:HA3	1.99	0.44
1:E:171:LEU:HD22	1:E:184:HIS:CG	2.52	0.44
1:F:504:ARG:NH1	1:F:504:ARG:HG2	2.32	0.44
1:H:621:VAL:O	1:H:644:LEU:HD12	2.17	0.44
1:I:130:MET:HE1	1:I:208:VAL:HG22	1.98	0.44
1:I:694:LEU:HD23	1:I:695:ALA:O	2.17	0.44
1:C:274:GLU:O	1:C:285:ARG:NH2	2.50	0.44
1:C:660:ASP:CG	1:C:666:TRP:HE1	2.20	0.44
1:D:117:PRO:HG2	4:D:802:PO4:O3	2.17	0.44
1:D:438:ARG:NH1	1:F:52:ASP:OD2	2.50	0.44
1:F:99:VAL:HB	1:F:206:GLN:OE1	2.18	0.44
1:G:313:LEU:HD23	1:G:313:LEU:HA	1.84	0.44
1:G:426:THR:HG23	1:G:581:PHE:CD1	2.49	0.44
1:H:319:VAL:O	1:H:323:ILE:HG13	2.18	0.44
1:H:699:LEU:HD23	1:H:700:THR:N	2.32	0.44
1:C:162:LYS:HA	1:C:177:GLY:HA2	1.99	0.44
1:D:99:VAL:CG1	1:D:130:MET:HB3	2.48	0.44
1:D:504:ARG:HD3	1:D:561:PHE:CE2	2.53	0.44
1:F:95:TYR:HA	1:F:230:PHE:CD1	2.52	0.44
1:I:375:LEU:HD12	1:I:395:LEU:HD22	1.98	0.44
1:J:157:TYR:HB2	1:J:196:VAL:HG11	1.99	0.44
1:C:540:ASN:N	1:C:540:ASN:OD1	2.50	0.44
1:D:2:GLN:O	1:D:61:PRO:HD2	2.18	0.44
1:D:599:PHE:CE2	1:D:605:GLU:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:LEU:HD22	1:E:621:VAL:CG2	2.47	0.44
3:H:803:C2E:O11	3:H:803:C2E:H2'	2.18	0.44
1:J:412:ARG:NH2	1:J:414:GLU:OE2	2.51	0.44
1:C:483:ASN:OD1	1:C:485:GLY:N	2.46	0.44
1:D:72:ARG:NH2	1:D:124:ASP:OD1	2.51	0.44
1:D:92:LEU:HD21	1:D:130:MET:HB2	1.99	0.44
1:E:699:LEU:HD23	1:E:700:THR:N	2.33	0.44
1:H:402:LYS:HB3	1:H:424:ARG:NH1	2.33	0.44
1:I:141:TRP:HH2	1:I:253:VAL:HB	1.83	0.44
1:I:444:ASN:N	1:I:516:VAL:O	2.45	0.44
1:J:474:ASP:OD2	1:J:534:ASN:HB3	2.18	0.44
1:C:69:TYR:OH	1:C:93:ASP:OD2	2.31	0.44
1:D:37:LEU:HD23	1:D:43:GLU:HG3	1.99	0.44
1:D:143:ASP:O	1:G:145:ARG:NE	2.40	0.44
1:E:246:VAL:HG22	1:E:250:LYS:HE3	1.99	0.44
1:E:562:THR:O	1:E:566:VAL:HG23	2.18	0.44
1:G:452:PHE:CD2	1:G:533:ASN:HB3	2.53	0.44
1:I:38:HIS:O	1:I:68:ARG:NH2	2.32	0.44
1:C:342:ASP:OD1	2:C:801:A16:C1C	2.66	0.43
1:E:450:ASP:HB2	2:E:801:A16:O2C	2.18	0.43
1:G:289:ASN:N	1:G:290:PRO:HD2	2.33	0.43
1:G:440:LEU:HD22	1:G:440:LEU:H	1.82	0.43
1:G:493:VAL:HA	1:G:496:THR:HB	2.00	0.43
1:I:426:THR:HG23	1:I:581:PHE:HD1	1.83	0.43
1:J:90:LEU:H	1:J:125:SER:HB3	1.83	0.43
1:C:660:ASP:HB2	1:C:664:ARG:NH2	2.32	0.43
1:D:622:PHE:HE1	1:D:642:SER:HB3	1.83	0.43
1:E:65:PRO:HG2	1:E:136:ASN:HB2	1.98	0.43
1:E:102:ARG:HA	1:E:130:MET:HG2	1.99	0.43
1:H:665:TYR:HA	1:H:687:ALA:O	2.18	0.43
1:I:267:VAL:HG23	1:I:341:PHE:HA	1.99	0.43
1:C:73:VAL:HG21	1:C:287:LEU:HA	1.99	0.43
3:C:802:C2E:O11	3:C:802:C2E:H2'	2.18	0.43
1:H:26:SER:OG	1:H:287:LEU:O	2.34	0.43
1:D:274:GLU:O	1:D:285:ARG:NH2	2.48	0.43
1:I:205:HIS:NE2	1:I:267:VAL:HG12	2.33	0.43
1:I:648:ASN:ND2	1:I:696:PRO:HA	2.33	0.43
1:C:145:ARG:HB2	1:I:145:ARG:CG	2.49	0.43
1:D:527:ARG:NH1	1:D:543:SER:O	2.49	0.43
1:D:579:ARG:HG2	3:D:804:C2E:C51	2.49	0.43
1:E:662:HIS:ND1	1:E:662:HIS:C	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ARG:HB2	1:J:145:ARG:HD2	2.00	0.43
1:F:171:LEU:HD22	1:F:184:HIS:CG	2.53	0.43
1:F:567:ARG:HG2	1:F:570:ARG:NH2	2.34	0.43
1:I:159:ALA:HA	1:I:521:HIS:HB3	1.99	0.43
3:I:802:C2E:C4A	3:I:802:C2E:C81	2.97	0.43
1:C:268:VAL:HG13	1:C:342:ASP:OD2	2.19	0.43
1:C:454:LEU:HD12	1:C:454:LEU:HA	1.80	0.43
1:E:409:ASP:HB3	1:E:416:ARG:CG	2.49	0.43
1:F:168:HIS:CE1	1:F:170:ASP:HB2	2.53	0.43
1:F:425:LEU:HD23	1:F:425:LEU:HA	1.83	0.43
1:G:578:ARG:NH2	1:J:50:GLU:OE2	2.44	0.43
1:I:296:ALA:C	1:I:298:ASP:H	2.22	0.43
1:J:312:LEU:HD23	1:J:319:VAL:HG13	2.01	0.43
1:C:171:LEU:HD22	1:C:184:HIS:CG	2.54	0.43
1:C:203:PRO:HG3	1:C:224:TYR:CD2	2.54	0.43
1:C:608:SER:HB2	1:D:126:ALA:HB3	2.01	0.43
1:C:609:ARG:NH1	1:D:68:ARG:HH22	2.13	0.43
1:C:654:LEU:HD23	1:C:654:LEU:HA	1.83	0.43
1:C:677:GLY:C	1:C:680:PRO:HD2	2.39	0.43
1:F:141:TRP:HB3	1:F:144:ASP:HB2	2.00	0.43
1:F:280:PRO:HB2	1:F:282:LEU:HG	2.00	0.43
1:G:63:VAL:HG13	1:G:67:GLN:HG2	2.00	0.43
1:G:112:TYR:CZ	1:G:278:LEU:HA	2.54	0.43
1:I:579:ARG:HG3	1:I:630:GLU:HG2	2.00	0.43
1:J:300:ARG:HH11	1:J:301:TYR:HE1	1.66	0.43
1:J:655:GLU:HG3	1:J:691:ARG:HH11	1.84	0.43
1:D:313:LEU:HD22	1:D:315:ARG:HG2	2.00	0.43
1:D:365:GLN:HG3	1:D:395:LEU:HD12	2.00	0.43
1:D:440:LEU:HD22	1:D:440:LEU:H	1.82	0.43
1:E:28:ALA:HB1	1:E:83:LEU:HD22	2.00	0.43
1:E:84:ARG:NH2	1:E:300:ARG:O	2.51	0.43
1:E:99:VAL:HB	1:E:206:GLN:NE2	2.33	0.43
1:E:465:ASN:OD1	1:E:532:ASN:HA	2.18	0.43
1:E:574:VAL:HG11	1:E:623:LEU:HB3	2.01	0.43
1:G:384:GLU:OE1	1:G:385:GLY:N	2.52	0.43
1:G:392:PHE:HB2	1:G:437:ARG:HH22	1.83	0.43
1:H:274:GLU:HB3	1:H:285:ARG:NH2	2.34	0.43
1:H:549:LYS:HD2	1:H:549:LYS:HA	1.85	0.43
1:I:632:GLY:HA2	1:I:638:ILE:HD11	2.00	0.43
1:C:171:LEU:HB2	1:C:176:ARG:HG2	2.01	0.43
1:C:644:LEU:HD21	1:C:659:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:ARG:H	1:D:664:ARG:HG2	1.65	0.43
1:G:65:PRO:HG2	1:G:136:ASN:HB2	2.00	0.43
1:G:417:THR:CG2	1:G:612:GLN:HA	2.49	0.43
1:G:636:GLU:H	1:G:636:GLU:HG2	1.57	0.43
1:H:224:TYR:O	1:H:271:HIS:NE2	2.46	0.43
1:D:37:LEU:HD12	1:D:131:THR:HG21	2.01	0.43
1:E:306:THR:OG1	1:E:310:ASN:O	2.30	0.43
1:E:328:ARG:NH2	1:I:368:PRO:HD3	2.33	0.43
1:G:574:VAL:O	1:G:577:ARG:HG3	2.18	0.43
3:G:802:C2E:O1P	3:G:802:C2E:C2A	2.67	0.43
1:I:249:PHE:O	1:I:253:VAL:HG23	2.19	0.43
1:I:460:TYR:HA	1:I:487:GLU:HG3	2.00	0.43
1:C:602:GLU:OE2	1:C:691:ARG:NH1	2.48	0.42
1:D:146:ARG:O	1:D:148:ARG:N	2.52	0.42
1:E:100:SER:HA	1:E:241:ASP:HB2	2.00	0.42
1:E:105:TRP:HD1	1:E:214:VAL:HG11	1.83	0.42
1:E:160:HIS:CD2	1:E:202:MET:HB2	2.54	0.42
1:F:89:LYS:HA	1:F:125:SER:HB3	2.00	0.42
1:F:207:PHE:HB2	1:F:225:ASN:O	2.19	0.42
1:H:1:MET:O	1:H:1:MET:HG3	2.19	0.42
1:I:666:TRP:CE3	1:I:704:ARG:HB2	2.54	0.42
1:C:99:VAL:O	1:C:206:GLN:NE2	2.49	0.42
1:G:9:TYR:CG	1:G:10:PRO:HA	2.54	0.42
1:C:409:ASP:HB3	1:C:416:ARG:HG3	2.00	0.42
1:D:138:TYR:HB2	1:J:138:TYR:HB2	2.01	0.42
1:D:183:ALA:HB1	1:D:255:ALA:HB3	2.02	0.42
1:E:445:PHE:HB3	1:E:518:MET:HB3	2.00	0.42
1:I:563:ARG:HH21	1:I:567:ARG:NH2	2.16	0.42
1:J:123:LEU:HD23	1:J:123:LEU:HA	1.89	0.42
1:J:164:LEU:HD23	1:J:164:LEU:HA	1.89	0.42
1:J:492:ASP:HB3	1:J:495:ILE:CG1	2.49	0.42
1:D:465:ASN:OD1	1:D:532:ASN:HA	2.18	0.42
1:F:504:ARG:O	1:F:561:PHE:CZ	2.73	0.42
1:F:560:ARG:O	1:F:564:SER:OG	2.22	0.42
1:G:212:ARG:NH2	1:G:536:TYR:HH	2.17	0.42
1:G:595:ASP:HA	1:G:624:ASN:HB3	2.00	0.42
1:H:135:VAL:HG11	1:H:246:VAL:HG11	2.01	0.42
1:I:164:LEU:O	1:I:164:LEU:HD23	2.19	0.42
1:J:110:TYR:HA	1:J:280:PRO:HA	2.01	0.42
1:C:515:GLY:O	1:C:569:ARG:NH2	2.49	0.42
1:C:658:VAL:HA	1:C:659:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:GLU:OE2	1:D:283:SER:N	2.47	0.42
1:D:596:ILE:HG13	1:D:623:LEU:HD23	2.02	0.42
1:E:100:SER:HB2	1:E:241:ASP:OD1	2.19	0.42
1:E:265:LEU:HD21	1:E:336:VAL:HG21	2.02	0.42
1:F:239:TRP:CG	1:F:248:GLU:HG3	2.54	0.42
1:I:313:LEU:HD23	1:I:313:LEU:HA	1.87	0.42
1:D:140:ASP:O	1:D:254:ARG:NH1	2.51	0.42
1:D:412:ARG:NH1	1:D:414:GLU:OE2	2.53	0.42
1:D:574:VAL:HG23	1:D:640:ASP:OD1	2.19	0.42
1:D:578:ARG:NH2	1:F:50:GLU:OE1	2.52	0.42
1:E:139:PHE:CE2	1:E:254:ARG:HD3	2.50	0.42
1:E:495:ILE:O	1:E:499:ARG:HG3	2.20	0.42
1:G:438:ARG:HH22	1:G:578:ARG:HH21	1.68	0.42
1:H:80:GLU:H	1:H:80:GLU:CD	2.23	0.42
1:H:194:LEU:HD12	1:H:563:ARG:HG3	2.01	0.42
1:H:510:LEU:HG	1:H:511:MET:HE2	2.02	0.42
1:I:37:LEU:HD23	1:I:37:LEU:HA	1.78	0.42
1:I:666:TRP:CZ3	1:I:704:ARG:HB2	2.54	0.42
1:C:168:HIS:HB3	1:C:171:LEU:HG	2.00	0.42
1:D:440:LEU:HD21	1:D:578:ARG:HA	2.01	0.42
1:F:164:LEU:HD23	1:F:547:TRP:HZ2	1.85	0.42
1:F:165:THR:HB	1:F:171:LEU:HD11	2.02	0.42
1:F:270:ASN:O	1:F:311:SER:HA	2.20	0.42
1:H:112:TYR:CD1	1:H:117:PRO:HA	2.55	0.42
1:H:147:PRO:O	1:H:149:THR:N	2.47	0.42
1:H:257:HIS:CE1	1:H:263:VAL:HG23	2.54	0.42
1:H:595:ASP:HA	1:H:624:ASN:HB3	2.02	0.42
1:J:478:TYR:HD2	1:J:478:TYR:HA	1.78	0.42
1:C:326:SER:O	1:C:330:TRP:HD1	2.02	0.42
1:D:200:GLU:OE2	1:D:340:ARG:HD2	2.20	0.42
1:D:224:TYR:O	1:D:271:HIS:NE2	2.49	0.42
1:D:300:ARG:HH11	1:D:301:TYR:HE1	1.66	0.42
1:E:376:ILE:HA	1:E:397:THR:O	2.19	0.42
1:F:140:ASP:O	1:F:254:ARG:NH1	2.53	0.42
1:F:152:HIS:O	1:F:576:ARG:HD2	2.19	0.42
1:I:387:TYR:OH	1:I:402:LYS:HG3	2.20	0.42
1:I:390:GLY:O	1:I:435:ASP:OD2	2.38	0.42
1:J:440:LEU:HD21	1:J:578:ARG:HA	2.01	0.42
1:C:210:ASP:O	1:C:214:VAL:HG23	2.20	0.42
1:C:270:ASN:OD1	1:C:306:THR:HG21	2.20	0.42
1:C:561:PHE:CE2	1:C:679:PRO:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:TRP:CZ3	1:D:484:CYS:HA	2.55	0.42
1:E:38:HIS:CE1	1:E:44:THR:HG1	2.32	0.42
1:E:158:GLU:HA	1:E:200:GLU:HB3	2.01	0.42
1:E:303:MET:HE2	1:E:303:MET:HB3	1.95	0.42
1:F:619:LEU:HD23	1:F:620:THR:N	2.34	0.42
1:G:100:SER:OG	1:G:101:GLY:N	2.53	0.42
1:G:324:MET:HG3	1:G:363:LEU:HD22	2.02	0.42
1:G:664:ARG:CB	1:G:704:ARG:HE	2.31	0.42
1:I:404:ARG:HG2	1:I:408:ARG:HD3	2.02	0.42
1:I:408:ARG:O	1:I:412:ARG:HB2	2.19	0.42
1:C:452:PHE:HB3	1:C:456:ASP:HB2	2.01	0.42
1:D:403:TYR:CD1	1:D:424:ARG:HB3	2.55	0.42
1:F:572:HIS:HA	1:F:573:PRO:HD3	1.89	0.42
1:G:446:VAL:HG22	1:G:510:LEU:HD22	2.01	0.42
1:H:247:LEU:HD21	1:I:15:TYR:OH	2.20	0.42
1:I:15:TYR:CD1	1:I:65:PRO:HD3	2.55	0.42
1:I:205:HIS:HE1	1:I:330:TRP:NE1	2.17	0.42
1:I:429:SER:O	1:I:433:GLN:HB3	2.19	0.42
1:J:408:ARG:O	1:J:412:ARG:HB2	2.20	0.42
1:J:447:THR:OG1	1:J:452:PHE:O	2.27	0.42
1:J:503:MET:HE1	1:J:558:LEU:HD21	2.01	0.42
1:C:640:ASP:OD2	1:C:641:ASP:N	2.53	0.41
1:C:687:ALA:HB3	1:C:690:GLU:HB3	2.01	0.41
1:E:10:PRO:HG2	1:E:14:THR:HG21	2.03	0.41
1:E:454:LEU:HD12	1:E:454:LEU:HA	1.86	0.41
1:F:572:HIS:HB3	1:F:640:ASP:OD1	2.20	0.41
1:G:264:ILE:HG23	1:G:338:GLY:C	2.40	0.41
1:G:670:VAL:HA	1:G:678:MET:O	2.20	0.41
1:I:37:LEU:HD12	1:I:131:THR:HG21	2.02	0.41
1:I:81:ARG:HH21	1:I:83:LEU:HD11	1.85	0.41
1:I:158:GLU:HB2	1:I:518:MET:HE2	2.00	0.41
1:J:613:ALA:HB3	1:J:616:ALA:HB2	2.01	0.41
1:C:11:LEU:HD12	1:C:95:TYR:CZ	2.56	0.41
1:C:704:ARG:HA	1:C:705:PRO:HD3	1.86	0.41
1:E:538:GLN:O	1:E:543:SER:OG	2.25	0.41
1:E:694:LEU:HD11	1:E:700:THR:HB	2.01	0.41
1:F:125:SER:HG	1:F:129:THR:HG1	1.56	0.41
1:G:224:TYR:O	2:G:801:A16:C6B	2.66	0.41
1:G:457:LEU:HD12	1:G:481:SER:HB2	2.03	0.41
1:G:466:GLU:HG3	1:G:472:ASN:HB2	2.01	0.41
3:G:802:C2E:O2A	3:G:802:C2E:P1	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:ASN:HB2	1:H:59:TYR:HD1	1.85	0.41
1:H:274:GLU:OE2	1:H:282:LEU:N	2.36	0.41
3:J:802:C2E:O1P	3:J:802:C2E:C2A	2.68	0.41
1:C:574:VAL:HG11	1:C:623:LEU:HB3	2.01	0.41
3:C:802:C2E:O11	3:C:802:C2E:C2'	2.68	0.41
1:D:182:LEU:CD2	1:D:256:LEU:HD11	2.51	0.41
1:E:280:PRO:HB2	1:E:282:LEU:HG	2.02	0.41
1:E:387:TYR:CE2	1:E:389:VAL:HB	2.56	0.41
1:G:5:PRO:O	1:G:57:HIS:ND1	2.54	0.41
1:G:50:GLU:HB3	1:G:57:HIS:CE1	2.55	0.41
1:G:212:ARG:NH2	2:G:801:A16:H7A1	2.36	0.41
1:G:465:ASN:N	1:G:472:ASN:OD1	2.54	0.41
1:H:390:GLY:O	1:H:435:ASP:OD2	2.38	0.41
1:H:664:ARG:H	1:H:664:ARG:HG2	1.62	0.41
1:C:203:PRO:CG	1:C:224:TYR:CD2	3.03	0.41
1:C:392:PHE:O	1:C:437:ARG:NH2	2.42	0.41
1:C:533:ASN:OD1	1:C:534:ASN:N	2.53	0.41
1:D:19:GLY:HA3	1:D:61:PRO:HA	2.02	0.41
1:D:438:ARG:HH22	1:D:578:ARG:HH21	1.67	0.41
1:E:167:LEU:HD23	1:E:546:ARG:HD2	2.02	0.41
1:F:35:CYS:SG	1:F:72:ARG:HG3	2.61	0.41
1:F:110:TYR:HB3	1:F:112:TYR:CE2	2.56	0.41
1:G:570:ARG:HE	1:G:570:ARG:HB2	1.69	0.41
1:H:99:VAL:HB	1:H:206:GLN:NE2	2.35	0.41
1:H:232:PRO:HG2	1:H:246:VAL:HA	2.03	0.41
1:H:500:ALA:O	1:H:504:ARG:HG3	2.20	0.41
1:J:271:HIS:HB2	1:J:310:ASN:OD1	2.20	0.41
1:C:239:TRP:CD2	1:C:248:GLU:HG2	2.55	0.41
1:C:363:LEU:O	1:C:366:GLN:HG3	2.20	0.41
1:C:694:LEU:HD11	1:C:700:THR:HB	2.01	0.41
1:E:643:PHE:CE2	1:E:703:ARG:HB2	2.56	0.41
1:F:50:GLU:HB2	1:F:57:HIS:CE1	2.55	0.41
1:F:425:LEU:HD11	1:F:647:PHE:CZ	2.55	0.41
1:F:595:ASP:N	1:F:595:ASP:OD1	2.49	0.41
1:I:107:GLU:HG3	1:I:114:PHE:CG	2.55	0.41
1:C:416:ARG:HD3	1:C:420:GLU:HG2	2.03	0.41
1:D:129:THR:HG22	1:D:130:MET:H	1.86	0.41
1:E:5:PRO:HG3	1:I:632:GLY:O	2.21	0.41
1:E:300:ARG:HD2	1:E:301:TYR:CE1	2.56	0.41
1:E:513:SER:O	1:E:569:ARG:NH2	2.49	0.41
2:G:801:A16:O3B	2:G:801:A16:C7A	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:TYR:HA	1:I:280:PRO:HA	2.02	0.41
1:J:257:HIS:NE2	1:J:337:ASP:OD2	2.53	0.41
1:D:143:ASP:HB3	1:G:145:ARG:HG3	2.03	0.41
1:D:332:THR:H	1:D:332:THR:HG1	1.63	0.41
1:E:118:ASP:CG	1:E:300:ARG:HE	2.24	0.41
1:F:227:ILE:HD12	1:F:228:GLY:N	2.36	0.41
1:G:674:ASP:HA	1:G:675:PRO:HD3	1.96	0.41
1:J:72:ARG:HD3	1:J:87:ALA:O	2.21	0.41
1:J:84:ARG:HD2	1:J:285:ARG:HD2	2.03	0.41
1:J:393:PRO:HB2	1:J:396:TRP:HD1	1.86	0.41
1:J:565:MET:HG2	1:J:679:PRO:HG3	2.02	0.41
1:C:224:TYR:O	1:C:271:HIS:NE2	2.53	0.41
1:C:674:ASP:OD2	1:C:678:MET:N	2.54	0.41
1:E:46:VAL:HG11	1:E:60:LEU:HD21	2.02	0.41
1:E:123:LEU:HD23	1:E:123:LEU:HA	1.93	0.41
1:H:371:SER:OG	1:H:372:GLN:NE2	2.51	0.41
1:H:586:VAL:O	1:H:586:VAL:CG1	2.67	0.41
1:I:165:THR:O	1:I:177:GLY:N	2.54	0.41
1:I:670:VAL:HB	1:I:701:VAL:HB	2.03	0.41
1:C:53:ALA:HA	1:H:394:PRO:HB2	2.02	0.41
1:C:454:LEU:HG	1:C:503:MET:HG2	2.03	0.41
1:C:584:ARG:HB3	1:C:585:PRO:CD	2.41	0.41
1:C:584:ARG:HD2	1:C:584:ARG:HA	1.77	0.41
1:D:125:SER:OG	1:D:129:THR:OG1	2.32	0.41
1:D:679:PRO:N	1:D:680:PRO:HD2	2.36	0.41
1:E:51:THR:O	3:E:803:C2E:C61	2.69	0.41
1:E:397:THR:HG22	1:E:443:VAL:HG23	2.03	0.41
1:E:416:ARG:HH21	1:E:420:GLU:HB2	1.86	0.41
1:E:645:LEU:HD23	1:E:701:VAL:HG13	2.03	0.41
1:F:112:TYR:CZ	1:F:278:LEU:HA	2.56	0.41
1:G:15:TYR:CE1	1:G:65:PRO:HD3	2.56	0.41
1:G:574:VAL:HG23	1:G:640:ASP:OD1	2.21	0.41
1:H:16:ASP:HB2	1:H:59:TYR:HE1	1.86	0.41
1:H:538:GLN:O	1:H:543:SER:OG	2.39	0.41
1:H:643:PHE:HA	1:H:702:LEU:O	2.21	0.41
1:I:71:PHE:HE1	1:I:93:ASP:HB2	1.86	0.41
1:I:468:ASN:OD1	1:I:468:ASN:N	2.53	0.41
1:J:500:ALA:O	1:J:504:ARG:HG3	2.20	0.41
1:J:549:LYS:HD2	1:J:549:LYS:HA	1.95	0.41
1:C:28:ALA:N	1:C:288:ASP:OD1	2.52	0.41
1:C:366:GLN:OE1	1:H:328:ARG:NH2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:ASP:OD2	1:C:480:ARG:NH1	2.46	0.41
1:C:520:SER:OG	1:C:523:ASP:OD2	2.33	0.41
1:D:112:TYR:HD1	1:D:117:PRO:HA	1.85	0.41
1:D:388:GLN:HB3	1:D:391:ASN:HB2	2.03	0.41
1:F:128:ASP:N	1:F:128:ASP:OD1	2.54	0.41
1:F:434:ASP:OD2	1:H:120:ARG:HD3	2.21	0.41
1:G:567:ARG:HG2	1:G:570:ARG:NH2	2.36	0.41
1:H:125:SER:HG	1:H:129:THR:HG1	1.63	0.41
1:H:157:TYR:CZ	1:H:521:HIS:HA	2.56	0.41
1:H:280:PRO:HB2	1:H:282:LEU:HG	2.03	0.41
1:H:505:ASN:ND2	1:H:672:THR:HG21	2.35	0.41
1:I:243:GLY:O	1:I:246:VAL:HG12	2.21	0.41
1:I:455:ARG:O	1:I:459:SER:OG	2.16	0.41
1:J:655:GLU:HG3	1:J:691:ARG:NH1	2.36	0.41
3:C:802:C2E:O1P	3:C:802:C2E:C2A	2.69	0.40
1:D:5:PRO:O	1:D:57:HIS:ND1	2.48	0.40
1:E:482:TRP:CH2	1:E:484:CYS:HA	2.57	0.40
1:F:316:SER:OG	1:F:319:VAL:HG23	2.21	0.40
1:F:612:GLN:OE1	1:H:127:PRO:HD2	2.22	0.40
1:F:678:MET:N	1:F:679:PRO:HD2	2.36	0.40
1:G:224:TYR:HB2	2:G:801:A16:H6B1	2.04	0.40
1:G:449:HIS:NE2	2:G:801:A16:O2C	2.42	0.40
1:J:505:ASN:ND2	1:J:672:THR:HG21	2.35	0.40
1:C:308:THR:HG21	2:C:801:A16:H6C1	2.02	0.40
1:C:645:LEU:HD22	1:C:701:VAL:HG22	2.02	0.40
1:D:151:TYR:CD2	1:D:516:VAL:HG21	2.57	0.40
1:D:328:ARG:HG2	1:D:369:VAL:HB	2.02	0.40
1:D:418:LEU:O	1:D:422:ALA:N	2.49	0.40
2:E:801:A16:O3B	2:E:801:A16:C1A	2.68	0.40
1:G:288:ASP:O	1:G:292:TYR:HD1	2.04	0.40
1:G:699:LEU:HD23	1:G:699:LEU:HA	1.93	0.40
1:H:158:GLU:OE2	1:H:449:HIS:ND1	2.54	0.40
1:H:239:TRP:CD2	1:H:248:GLU:HG2	2.56	0.40
1:C:247:LEU:O	1:C:251:SER:OG	2.31	0.40
1:D:326:SER:O	1:D:330:TRP:HD1	2.04	0.40
1:D:409:ASP:HA	1:D:412:ARG:HB3	2.03	0.40
1:D:425:LEU:HD23	1:D:513:SER:HA	2.04	0.40
1:E:22:PHE:HZ	1:E:63:VAL:HG11	1.87	0.40
1:E:501:ARG:HD2	1:E:673:SER:HA	2.04	0.40
1:F:15:TYR:CD1	1:F:65:PRO:HD3	2.56	0.40
1:F:68:ARG:HB3	1:F:131:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:329:TYR:HE2	1:G:334:MET:HE2	1.82	0.40
1:G:565:MET:HG2	1:G:679:PRO:HG3	2.03	0.40
1:I:56:ARG:NH2	3:I:802:C2E:O6	2.54	0.40
1:I:191:LEU:HB3	1:I:196:VAL:HG22	2.02	0.40
1:J:209:ASN:OD1	1:J:219:SER:HB2	2.20	0.40
1:E:662:HIS:C	1:E:662:HIS:HD1	2.24	0.40
1:F:147:PRO:O	1:F:149:THR:N	2.52	0.40
2:F:801:A16:O3B	2:F:801:A16:C7A	2.68	0.40
1:G:52:ASP:OD2	1:J:438:ARG:NH1	2.54	0.40
1:H:224:TYR:HH	1:H:449:HIS:CD2	2.39	0.40
1:H:425:LEU:HD11	1:H:647:PHE:CE1	2.56	0.40
1:H:465:ASN:HB3	1:H:468:ASN:ND2	2.37	0.40
1:H:686:LEU:HD23	1:H:686:LEU:HA	1.88	0.40
1:I:370:VAL:O	1:I:373:VAL:HG22	2.20	0.40
1:J:574:VAL:HG11	1:J:623:LEU:HB3	2.03	0.40
1:C:671:ASP:H	1:C:678:MET:HB3	1.85	0.40
1:E:68:ARG:HG2	1:E:133:VAL:HG22	2.04	0.40
1:E:414:GLU:O	1:E:416:ARG:N	2.55	0.40
1:G:463:LYS:HB3	1:G:533:ASN:ND2	2.36	0.40
1:I:34:LEU:N	1:I:46:VAL:O	2.51	0.40
1:I:35:CYS:HB3	1:I:43:GLU:OE2	2.22	0.40
1:I:125:SER:OG	1:I:129:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	690/709 (97%)	630 (91%)	60 (9%)	0	100	100
1	D	686/709 (97%)	637 (93%)	49 (7%)	0	100	100
1	E	690/709 (97%)	638 (92%)	52 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	688/709 (97%)	635 (92%)	53 (8%)	0	100	100
1	G	685/709 (97%)	629 (92%)	56 (8%)	0	100	100
1	H	688/709 (97%)	639 (93%)	49 (7%)	0	100	100
1	I	688/709 (97%)	628 (91%)	59 (9%)	1 (0%)	48	79
1	J	686/709 (97%)	641 (93%)	45 (7%)	0	100	100
All	All	5501/5672 (97%)	5077 (92%)	423 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	679	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	577/590 (98%)	561 (97%)	16 (3%)	38	64
1	D	576/590 (98%)	548 (95%)	28 (5%)	21	50
1	E	577/590 (98%)	550 (95%)	27 (5%)	22	51
1	F	575/590 (98%)	557 (97%)	18 (3%)	35	62
1	G	575/590 (98%)	561 (98%)	14 (2%)	44	67
1	H	577/590 (98%)	554 (96%)	23 (4%)	27	56
1	I	574/590 (97%)	553 (96%)	21 (4%)	29	58
1	J	576/590 (98%)	556 (96%)	20 (4%)	31	60
All	All	4607/4720 (98%)	4440 (96%)	167 (4%)	30	59

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	43	GLU
1	C	116	ARG

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Mol	Chain	Res	Type
1	C	199	LEU
1	C	271	HIS
1	C	288	ASP
1	C	384	GLU
1	C	400	ASN
1	C	416	ARG
1	C	425	LEU
1	C	546	ARG
1	C	579	ARG
1	C	582	HIS
1	C	584	ARG
1	C	609	ARG
1	C	664	ARG
1	C	704	ARG
1	D	1	MET
1	D	102	ARG
1	D	107	GLU
1	D	116	ARG
1	D	125	SER
1	D	140	ASP
1	D	151	TYR
1	D	182	LEU
1	D	199	LEU
1	D	316	SER
1	D	395	LEU
1	D	400	ASN
1	D	404	ARG
1	D	416	ARG
1	D	478	TYR
1	D	481	SER
1	D	495	ILE
1	D	498	LEU
1	D	501	ARG
1	D	520	SER
1	D	524	GLU
1	D	537	CYS
1	D	546	ARG
1	D	560	ARG
1	D	582	HIS
1	D	615	HIS
1	D	667	ARG
1	D	682	GLN

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Mol	Chain	Res	Type
1	E	25	PHE
1	E	100	SER
1	E	102	ARG
1	E	107	GLU
1	E	151	TYR
1	E	168	HIS
1	E	170	ASP
1	E	212	ARG
1	E	251	SER
1	E	294	ARG
1	E	316	SER
1	E	355	ASP
1	E	371	SER
1	E	395	LEU
1	E	400	ASN
1	E	442	SER
1	E	478	TYR
1	E	525	PHE
1	E	537	CYS
1	E	546	ARG
1	E	577	ARG
1	E	582	HIS
1	E	615	HIS
1	E	661	SER
1	E	662	HIS
1	E	664	ARG
1	E	667	ARG
1	F	1	MET
1	F	116	ARG
1	F	128	ASP
1	F	199	LEU
1	F	316	SER
1	F	404	ARG
1	F	478	TYR
1	F	480	ARG
1	F	504	ARG
1	F	538	GLN
1	F	544	TRP
1	F	546	ARG
1	F	569	ARG
1	F	582	HIS
1	F	612	GLN

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Mol	Chain	Res	Type
1	F	629	SER
1	F	662	HIS
1	F	665	TYR
1	G	107	GLU
1	G	151	TYR
1	G	219	SER
1	G	355	ASP
1	G	384	GLU
1	G	400	ASN
1	G	416	ARG
1	G	476	GLU
1	G	486	GLU
1	G	527	ARG
1	G	546	ARG
1	G	609	ARG
1	G	674	ASP
1	G	699	LEU
1	H	25	PHE
1	H	97	ARG
1	H	102	ARG
1	H	104	ARG
1	H	125	SER
1	H	151	TYR
1	H	170	ASP
1	H	199	LEU
1	H	248	GLU
1	H	257	HIS
1	H	265	LEU
1	H	395	LEU
1	H	404	ARG
1	H	418	LEU
1	H	455	ARG
1	H	478	TYR
1	H	546	ARG
1	H	569	ARG
1	H	570	ARG
1	H	582	HIS
1	H	619	LEU
1	H	664	ARG
1	H	667	ARG
1	I	100	SER
1	I	116	ARG

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Mol	Chain	Res	Type
1	I	153	HIS
1	I	182	LEU
1	I	210	ASP
1	I	367	ASP
1	I	400	ASN
1	I	416	ARG
1	I	445	PHE
1	I	468	ASN
1	I	478	TYR
1	I	525	PHE
1	I	527	ARG
1	I	546	ARG
1	I	569	ARG
1	I	582	HIS
1	I	619	LEU
1	I	661	SER
1	I	662	HIS
1	I	694	LEU
1	I	704	ARG
1	J	100	SER
1	J	151	TYR
1	J	168	HIS
1	J	199	LEU
1	J	313	LEU
1	J	395	LEU
1	J	400	ASN
1	J	476	GLU
1	J	478	TYR
1	J	521	HIS
1	J	537	CYS
1	J	538	GLN
1	J	546	ARG
1	J	568	LEU
1	J	569	ARG
1	J	610	ASP
1	J	664	ARG
1	J	667	ARG
1	J	698	SER
1	J	704	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:



Mol	Chain	Res	Type
1	C	233	HIS
1	C	521	HIS
1	C	617	GLN
1	E	538	GLN
1	G	205	HIS
1	G	681	GLN
1	H	257	HIS
1	H	350	GLN
1	J	205	HIS
1	J	681	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

20 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	$\# Z  > 2$
4	PO4	E	802	-	4,4,4	0.98	0	6,6,6	0.49	0
3	C2E	F	802	-	44,52,52	1.28	7 (15%)	50,82,82	1.02	2 (4%)
2	A16	I	801	-	33,34,35	0.60	1 (3%)	46,50,52	1.16	3 (6%)
2	A16	D	801	-	33,34,35	0.54	0	46,50,52	1.32	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	C2E	D	804	-	44,52,52	1.20	7 (15%)	50,82,82	1.09	5 (10%)
4	PO4	H	802	-	4,4,4	0.99	0	6,6,6	0.48	0
2	A16	E	801	-	33,34,35	0.40	0	46,50,52	1.29	2 (4%)
2	A16	H	801	-	33,34,35	0.65	0	46,50,52	1.75	6 (13%)
4	PO4	D	802	-	4,4,4	1.00	0	6,6,6	0.57	0
2	A16	F	801	-	33,34,35	0.77	1 (3%)	46,50,52	1.27	3 (6%)
2	A16	G	801	-	33,34,35	0.55	0	46,50,52	1.32	7 (15%)
2	A16	C	801	-	33,34,35	0.49	0	46,50,52	1.11	3 (6%)
3	C2E	G	802	-	44,52,52	1.22	8 (18%)	50,82,82	0.99	1 (2%)
3	C2E	I	802	-	44,52,52	1.21	7 (15%)	50,82,82	1.15	6 (12%)
3	C2E	H	803	-	44,52,52	1.27	7 (15%)	50,82,82	0.97	1 (2%)
3	C2E	J	802	-	44,52,52	1.19	6 (13%)	50,82,82	1.08	3 (6%)
3	C2E	C	802	-	44,52,52	1.22	6 (13%)	50,82,82	0.96	1 (2%)
3	C2E	E	803	-	44,52,52	1.11	6 (13%)	50,82,82	1.07	5 (10%)
4	PO4	D	803	-	4,4,4	0.98	0	6,6,6	0.51	0
2	A16	J	801	-	33,34,35	0.56	0	46,50,52	1.27	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
3	C2E	F	802	-	-	6/22/62/62	0/6/7/7
2	A16	E	801	-	-	5/12/69/72	1/3/3/3
2	A16	I	801	-	-	6/12/69/72	1/3/3/3
3	C2E	G	802	-	-	13/22/62/62	0/6/7/7
2	A16	F	801	-	-	7/12/69/72	1/3/3/3
2	A16	H	801	-	-	4/12/69/72	0/3/3/3
2	A16	D	801	-	-	3/12/69/72	1/3/3/3
3	C2E	D	804	-	-	1/22/62/62	0/6/7/7
3	C2E	I	802	-	-	14/22/62/62	0/6/7/7
3	C2E	H	803	-	-	10/22/62/62	0/6/7/7
3	C2E	J	802	-	-	3/22/62/62	0/6/7/7
3	C2E	C	802	-	-	7/22/62/62	0/6/7/7
2	A16	G	801	-	-	3/12/69/72	1/3/3/3
3	C2E	E	803	-	-	5/22/62/62	0/6/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A16	C	801	-	-	5/12/69/72	1/3/3/3
2	A16	J	801	-	-	5/12/69/72	1/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	802	C2E	C51-C61	-3.50	1.40	1.47
3	I	802	C2E	C5-C6	-3.37	1.40	1.47
3	C	802	C2E	C51-C61	-3.34	1.40	1.47
3	D	804	C2E	C51-C61	-3.32	1.40	1.47
3	F	802	C2E	C5-C6	-3.26	1.41	1.47
3	J	802	C2E	C5-C6	-3.19	1.41	1.47
3	H	803	C2E	C51-C61	-3.18	1.41	1.47
3	J	802	C2E	C51-C61	-3.11	1.41	1.47
3	H	803	C2E	C5-C6	-3.10	1.41	1.47
3	G	802	C2E	C51-C61	-3.10	1.41	1.47
3	G	802	C2E	C5-C6	-3.09	1.41	1.47
3	C	802	C2E	C5-C6	-3.06	1.41	1.47
2	F	801	A16	C2C-C3C	-2.91	1.48	1.52
3	E	803	C2E	C51-C61	-2.86	1.41	1.47
3	E	803	C2E	C5-C6	-2.86	1.41	1.47
3	D	804	C2E	C5-C6	-2.76	1.42	1.47
3	G	802	C2E	C8-N7	-2.68	1.30	1.34
3	J	802	C2E	C81-N71	-2.66	1.30	1.34
3	I	802	C2E	C51-C61	-2.65	1.42	1.47
3	H	803	C2E	C81-N71	-2.62	1.30	1.34
3	C	802	C2E	C81-N71	-2.61	1.30	1.34
3	I	802	C2E	C8-N7	-2.59	1.30	1.34
3	C	802	C2E	C51-C41	-2.59	1.36	1.43
3	D	804	C2E	C81-N71	-2.55	1.30	1.34
3	I	802	C2E	C81-N71	-2.54	1.30	1.34
3	F	802	C2E	C51-C41	-2.52	1.36	1.43
3	F	802	C2E	C5-C4	-2.52	1.36	1.43
3	H	803	C2E	C5-C4	-2.51	1.36	1.43
3	H	803	C2E	C51-C41	-2.51	1.36	1.43
3	H	803	C2E	C8-N7	-2.49	1.30	1.34
3	F	802	C2E	C81-N71	-2.49	1.30	1.34
3	C	802	C2E	C5-C4	-2.48	1.37	1.43
3	I	802	C2E	C5-C4	-2.44	1.37	1.43
3	J	802	C2E	C51-C41	-2.42	1.37	1.43
3	C	802	C2E	C8-N7	-2.41	1.31	1.34
3	G	802	C2E	C5-C4	-2.41	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	802	C2E	C81-N71	-2.41	1.31	1.34
3	E	803	C2E	C8-N7	-2.40	1.31	1.34
3	D	804	C2E	C51-C41	-2.39	1.37	1.43
3	F	802	C2E	C8-N7	-2.38	1.31	1.34
3	E	803	C2E	C51-C41	-2.38	1.37	1.43
3	I	802	C2E	C51-C41	-2.36	1.37	1.43
3	D	804	C2E	C8-N7	-2.36	1.31	1.34
3	E	803	C2E	C5-C4	-2.33	1.37	1.43
3	J	802	C2E	C8-N7	-2.31	1.31	1.34
3	G	802	C2E	C51-C41	-2.31	1.37	1.43
3	J	802	C2E	C5-C4	-2.27	1.37	1.43
3	E	803	C2E	C81-N71	-2.27	1.31	1.34
3	D	804	C2E	C5-C4	-2.25	1.37	1.43
3	D	804	C2E	C1A-N91	-2.23	1.44	1.50
2	I	801	A16	C2C-C3C	-2.20	1.49	1.52
3	F	802	C2E	C1A-N91	-2.17	1.44	1.50
3	I	802	C2E	C1A-N91	-2.16	1.44	1.50
3	G	802	C2E	C1'-N9	-2.14	1.44	1.50
3	H	803	C2E	C1A-N91	-2.10	1.44	1.50
3	G	802	C2E	C1A-N91	-2.05	1.44	1.50

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	A16	C5A-C7A-C1A	6.80	117.32	108.53
2	H	801	A16	C1A-N4B-C4B	6.64	127.19	116.13
2	E	801	A16	C1A-N4B-C4B	5.24	124.85	116.13
2	G	801	A16	C1A-N4B-C4B	4.59	123.77	116.13
2	D	801	A16	C1A-N4B-C4B	4.57	123.73	116.13
2	J	801	A16	C1A-N4B-C4B	4.53	123.67	116.13
2	F	801	A16	C1A-N4B-C4B	4.23	123.18	116.13
2	I	801	A16	C1A-N4B-C4B	4.04	122.86	116.13
2	J	801	A16	C5A-C7A-C1A	3.88	113.54	108.53
2	C	801	A16	C1C-C2C-C3C	3.69	115.02	109.64
2	E	801	A16	C5A-C7A-C1A	3.64	113.22	108.53
2	F	801	A16	C5A-C7A-C1A	3.61	113.20	108.53
2	C	801	A16	C1A-N4B-C4B	3.53	122.01	116.13
2	I	801	A16	C5A-C7A-C1A	3.47	113.02	108.53
3	I	802	C2E	O61-C61-C51	3.34	130.94	124.32
2	F	801	A16	C2B-C3B-C4B	-2.91	106.17	110.40
3	C	802	C2E	C2A-C3A-C4A	-2.81	98.32	103.24
2	I	801	A16	C5B-C4B-N4B	-2.78	104.10	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	804	C2E	O3'-P11-O11	-2.74	101.03	109.81
3	J	802	C2E	O3'-P11-O11	-2.72	101.11	109.81
3	G	802	C2E	O3A-P1-O1P	2.64	118.26	109.81
3	I	802	C2E	O21-P11-O3'	2.54	117.04	106.70
3	J	802	C2E	O4'-C1'-N9	-2.53	105.39	108.75
3	I	802	C2E	O2'-C2'-C3'	-2.50	104.19	111.19
3	I	802	C2E	O61-C61-N11	-2.46	117.70	120.62
2	D	801	A16	O4A-C4A-C5A	2.44	114.09	110.01
3	F	802	C2E	P11-O5A-C5A	-2.44	107.39	121.35
2	G	801	A16	O4A-C4A-C5A	2.43	114.07	110.01
2	H	801	A16	O3B-C3B-C2B	-2.38	104.76	110.38
3	E	803	C2E	C4A-O4A-C1A	-2.37	107.75	109.92
3	H	803	C2E	O3A-C3A-C4A	-2.34	101.77	110.03
3	D	804	C2E	O61-C61-C51	2.34	128.95	124.32
2	D	801	A16	C3B-C4B-N4B	2.33	118.16	111.49
2	G	801	A16	C3B-C4B-N4B	2.31	118.13	111.49
2	C	801	A16	C5A-C7A-C1A	2.31	111.51	108.53
3	D	804	C2E	O21-P11-O11	2.28	123.07	112.44
3	E	803	C2E	O61-C61-C51	2.27	128.81	124.32
3	I	802	C2E	C2'-C3'-C4'	-2.24	99.31	103.24
2	H	801	A16	C3A-C2A-C1A	2.22	114.28	111.02
3	E	803	C2E	O6-C6-C5	2.18	128.64	124.32
2	H	801	A16	O4C-C4C-C3C	2.15	112.69	107.23
3	D	804	C2E	O6-C6-C5	2.14	128.56	124.32
3	E	803	C2E	O2'-C2'-C3'	-2.11	105.27	111.19
2	J	801	A16	O2C-C2C-C3C	2.09	114.47	110.15
2	D	801	A16	C7A-C5A-C6A	-2.07	108.10	111.86
3	F	802	C2E	C2A-C3A-C4A	-2.07	99.62	103.24
3	D	804	C2E	O2P-P1-O1P	2.06	122.04	112.44
2	G	801	A16	C7A-C5A-C6A	-2.05	108.14	111.86
3	I	802	C2E	O4A-C1A-N91	-2.05	106.03	108.75
2	J	801	A16	O4A-C4A-C3A	-2.04	105.56	110.38
3	J	802	C2E	C3'-C2'-C1'	2.04	104.37	99.89
2	D	801	A16	O6A-C6A-C5A	-2.03	106.62	111.26
2	G	801	A16	O6A-C6A-C5A	-2.03	106.62	111.26
2	D	801	A16	C1C-C2C-C3C	2.03	112.59	109.64
2	G	801	A16	O4C-C4C-C3C	2.02	112.37	107.23
2	D	801	A16	O4C-C4C-C3C	2.02	112.36	107.23
3	E	803	C2E	C2A-C3A-C4A	-2.01	99.72	103.24
2	G	801	A16	C1C-C2C-C3C	2.00	112.56	109.64
2	H	801	A16	O2A-C2A-C3A	-2.00	105.66	110.38

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	A16	C3B-C4B-N4B-C1A
2	D	801	A16	C3B-C4B-N4B-C1A
2	E	801	A16	C3B-C4B-N4B-C1A
2	F	801	A16	C3B-C4B-N4B-C1A
2	F	801	A16	C7A-C5A-C6A-O6A
2	G	801	A16	C3B-C4B-N4B-C1A
2	H	801	A16	C3B-C4B-N4B-C1A
2	I	801	A16	C7A-C1A-N4B-C4B
2	I	801	A16	C4A-C5A-C6A-O6A
2	I	801	A16	C7A-C5A-C6A-O6A
2	J	801	A16	C3B-C4B-N4B-C1A
3	C	802	C2E	C5A-O5A-P11-O3'
3	C	802	C2E	C5A-O5A-P11-O21
3	G	802	C2E	C5'-O5'-P1-O2P
3	G	802	C2E	C5'-O5'-P1-O1P
3	G	802	C2E	C5'-O5'-P1-O3A
3	G	802	C2E	C3A-O3A-P1-O1P
3	G	802	C2E	C3A-O3A-P1-O5'
3	G	802	C2E	O4'-C4'-C5'-O5'
3	G	802	C2E	C2A-C3A-O3A-P1
3	H	803	C2E	C5'-O5'-P1-O2P
3	H	803	C2E	C5'-O5'-P1-O3A
3	H	803	C2E	C5A-O5A-P11-O3'
3	H	803	C2E	C5A-O5A-P11-O21
3	H	803	C2E	O4A-C4A-C5A-O5A
3	H	803	C2E	C3A-C4A-C5A-O5A
3	I	802	C2E	C5'-O5'-P1-O2P
3	I	802	C2E	C5'-O5'-P1-O1P
3	I	802	C2E	C5'-O5'-P1-O3A
3	I	802	C2E	O4'-C4'-C5'-O5'
3	I	802	C2E	C5A-O5A-P11-O3'
3	I	802	C2E	C5A-O5A-P11-O21
2	H	801	A16	C3C-C4C-O4C-C1B
2	E	801	A16	C5C-C4C-O4C-C1B
3	C	802	C2E	C3A-C4A-C5A-O5A
3	I	802	C2E	O4A-C4A-C5A-O5A
3	I	802	C2E	C3A-C4A-C5A-O5A
2	F	801	A16	O5C-C5C-C6C-O6C
3	I	802	C2E	C2A-C3A-O3A-P1
2	D	801	A16	C5C-C4C-O4C-C1B
2	E	801	A16	C3C-C4C-O4C-C1B
2	G	801	A16	C5C-C4C-O4C-C1B

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Mol	Chain	Res	Type	Atoms
3	C	802	C2E	O4A-C4A-C5A-O5A
3	I	802	C2E	C3'-C4'-C5'-O5'
2	I	801	A16	C5C-C4C-O4C-C1B
2	E	801	A16	C4C-C5C-C6C-O6C
2	D	801	A16	C3C-C4C-O4C-C1B
2	G	801	A16	C3C-C4C-O4C-C1B
3	G	802	C2E	C3'-C4'-C5'-O5'
3	C	802	C2E	C4A-C3A-O3A-P1
3	F	802	C2E	C4A-C3A-O3A-P1
3	I	802	C2E	C4A-C3A-O3A-P1
2	E	801	A16	O5C-C5C-C6C-O6C
2	C	801	A16	C4C-C5C-C6C-O6C
2	C	801	A16	O5C-C5C-C6C-O6C
3	H	803	C2E	O4'-C4'-C5'-O5'
2	C	801	A16	C5C-C4C-O4C-C1B
2	I	801	A16	C3C-C4C-O4C-C1B
2	C	801	A16	C3C-C4C-O4C-C1B
2	J	801	A16	O5C-C5C-C6C-O6C
2	F	801	A16	C4C-C5C-C6C-O6C
3	E	803	C2E	C4'-C3'-O3'-P11
3	J	802	C2E	C4A-C3A-O3A-P1
3	E	803	C2E	O4A-C4A-C5A-O5A
2	H	801	A16	C4A-C5A-C6A-O6A
2	H	801	A16	C5C-C4C-O4C-C1B
2	J	801	A16	C7A-C5A-C6A-O6A
3	H	803	C2E	C3'-C4'-C5'-O5'
2	J	801	A16	C5C-C4C-O4C-C1B
2	F	801	A16	C5C-C4C-O4C-C1B
3	C	802	C2E	C2A-C3A-O3A-P1
2	F	801	A16	C3C-C4C-O4C-C1B
3	F	802	C2E	C4'-C3'-O3'-P11
3	E	803	C2E	C2'-C3'-O3'-P11
3	F	802	C2E	C2'-C3'-O3'-P11
2	J	801	A16	C3C-C4C-O4C-C1B
3	C	802	C2E	C5A-O5A-P11-O11
3	F	802	C2E	C5'-O5'-P1-O3A
3	H	803	C2E	C5'-O5'-P1-O1P
3	H	803	C2E	C5A-O5A-P11-O11
3	I	802	C2E	C5A-O5A-P11-O11
3	G	802	C2E	C4'-C3'-O3'-P11
3	G	802	C2E	C4A-C3A-O3A-P1
2	F	801	A16	C4A-C5A-C6A-O6A

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Mol	Chain	Res	Type	Atoms
3	F	802	C2E	C2A-C3A-O3A-P1
3	J	802	C2E	C2A-C3A-O3A-P1
3	D	804	C2E	O4A-C4A-C5A-O5A
3	E	803	C2E	C4A-C3A-O3A-P1
2	I	801	A16	O5C-C5C-C6C-O6C
3	J	802	C2E	O4A-C4A-C5A-O5A
3	F	802	C2E	C3A-O3A-P1-O2P
3	G	802	C2E	C3A-O3A-P1-O2P
3	I	802	C2E	C3A-O3A-P1-O2P
3	I	802	C2E	C3A-O3A-P1-O1P
3	E	803	C2E	C2A-C3A-O3A-P1
3	G	802	C2E	C2'-C3'-O3'-P11
3	G	802	C2E	C4'-C5'-O5'-P1

All (7) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	J	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	F	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	I	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	C	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	G	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	D	801	A16	C1A-C2A-C3A-C4A-C5A-C7A

17 monomers are involved in 115 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	802	C2E	3	0
2	I	801	A16	5	0
2	D	801	A16	7	0
3	D	804	C2E	18	0
2	E	801	A16	7	0
2	H	801	A16	5	0
4	D	802	PO4	1	0
2	F	801	A16	7	0
2	G	801	A16	10	0
2	C	801	A16	5	0
3	G	802	C2E	5	0
3	I	802	C2E	7	0
3	H	803	C2E	7	0
3	J	802	C2E	4	0

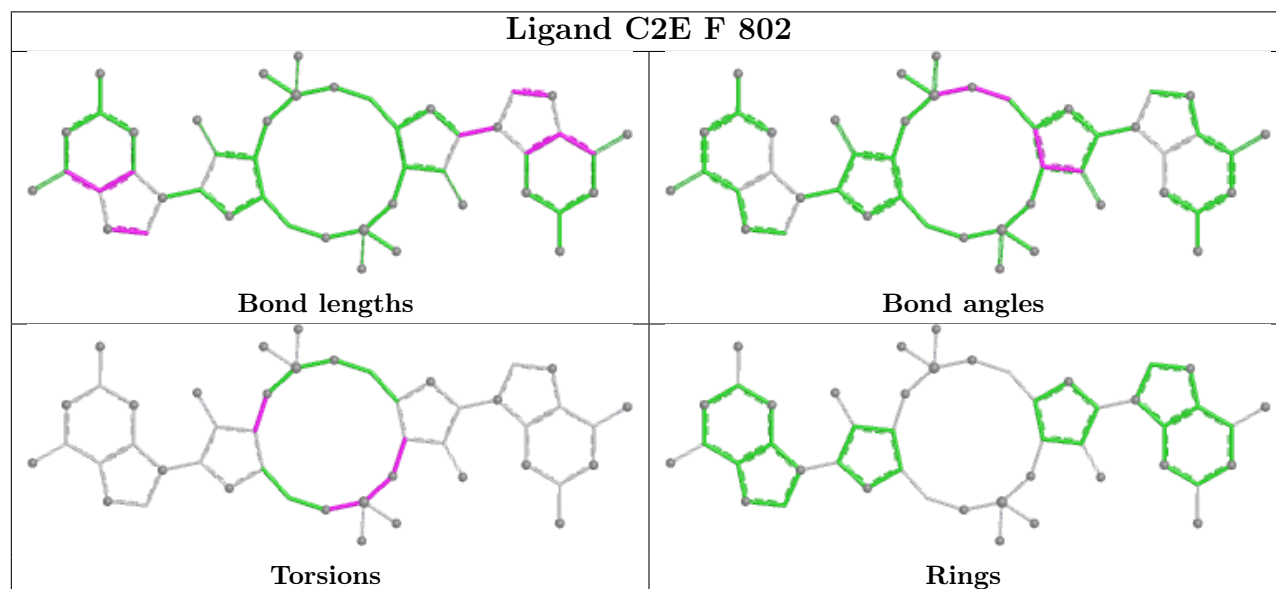
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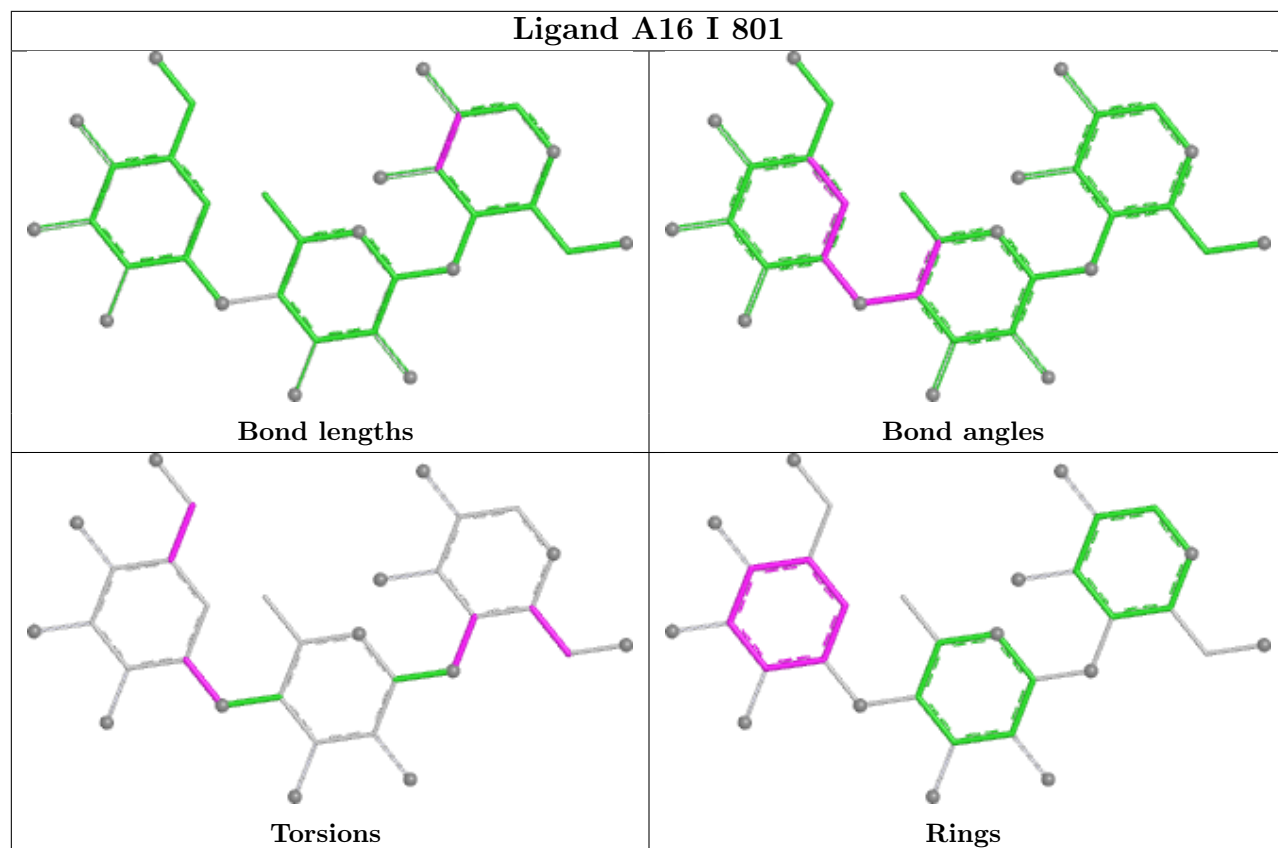
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	C2E	9	0
3	E	803	C2E	5	0
2	J	801	A16	10	0

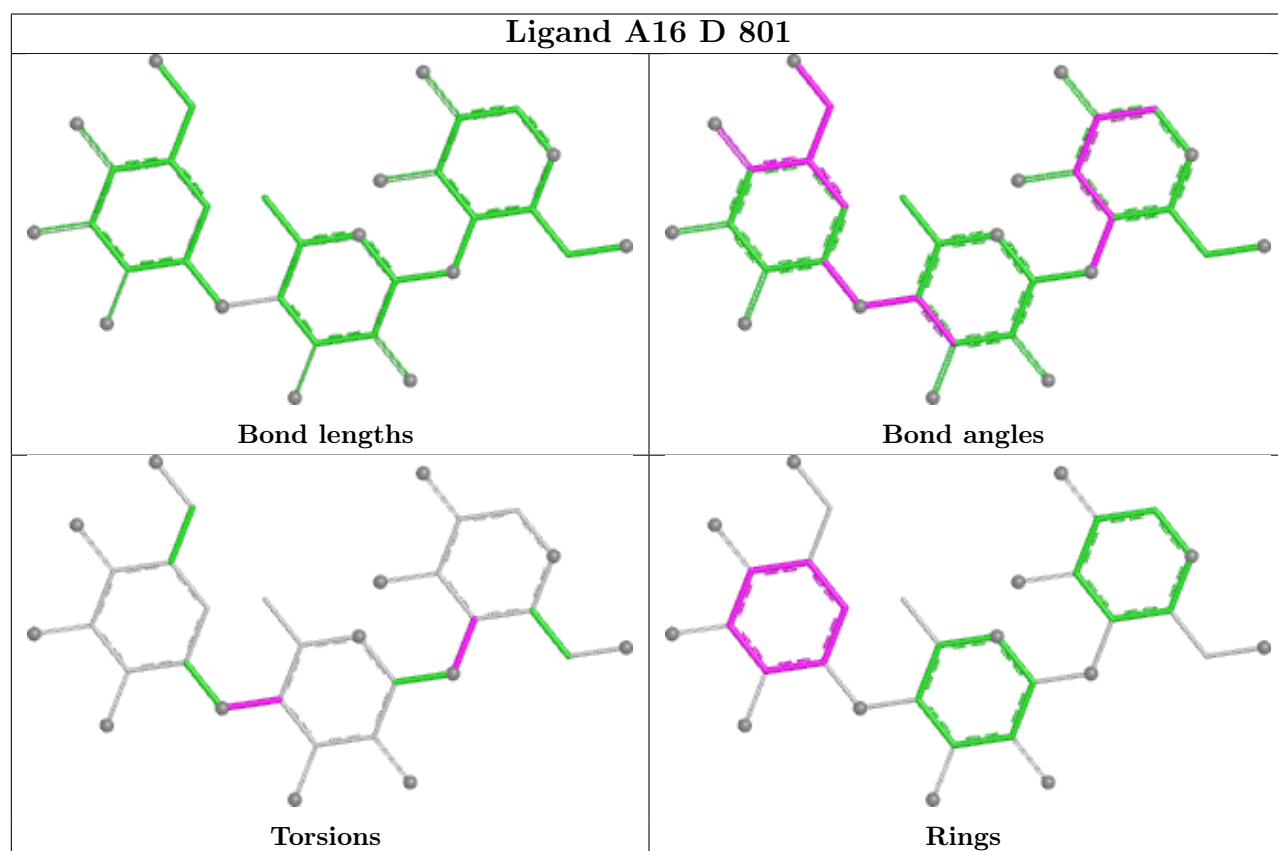
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



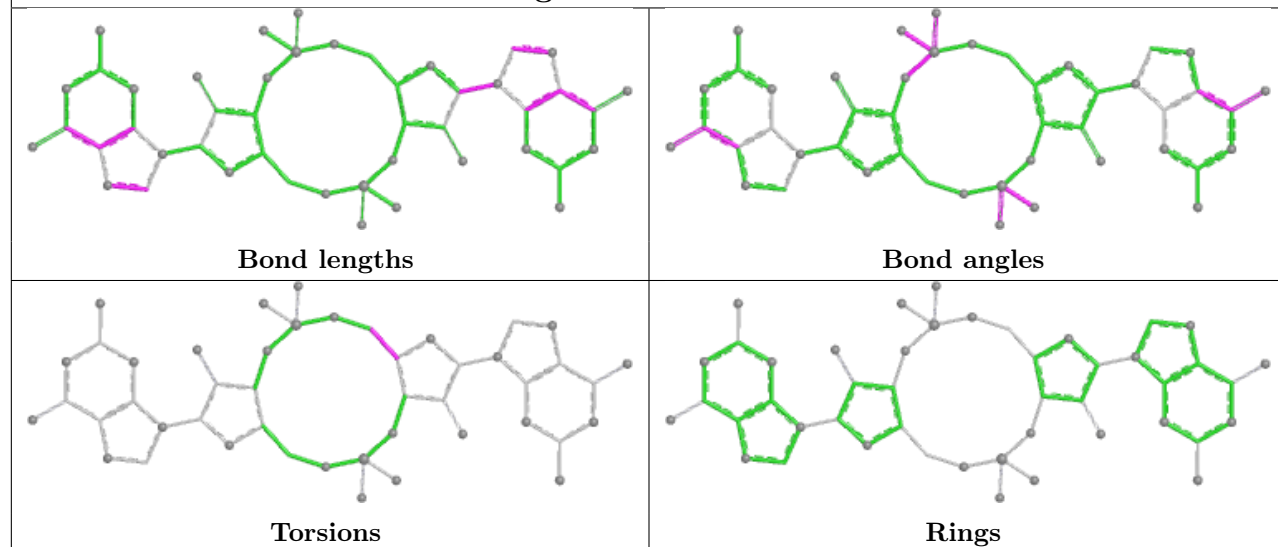
## Ligand A16 I 801



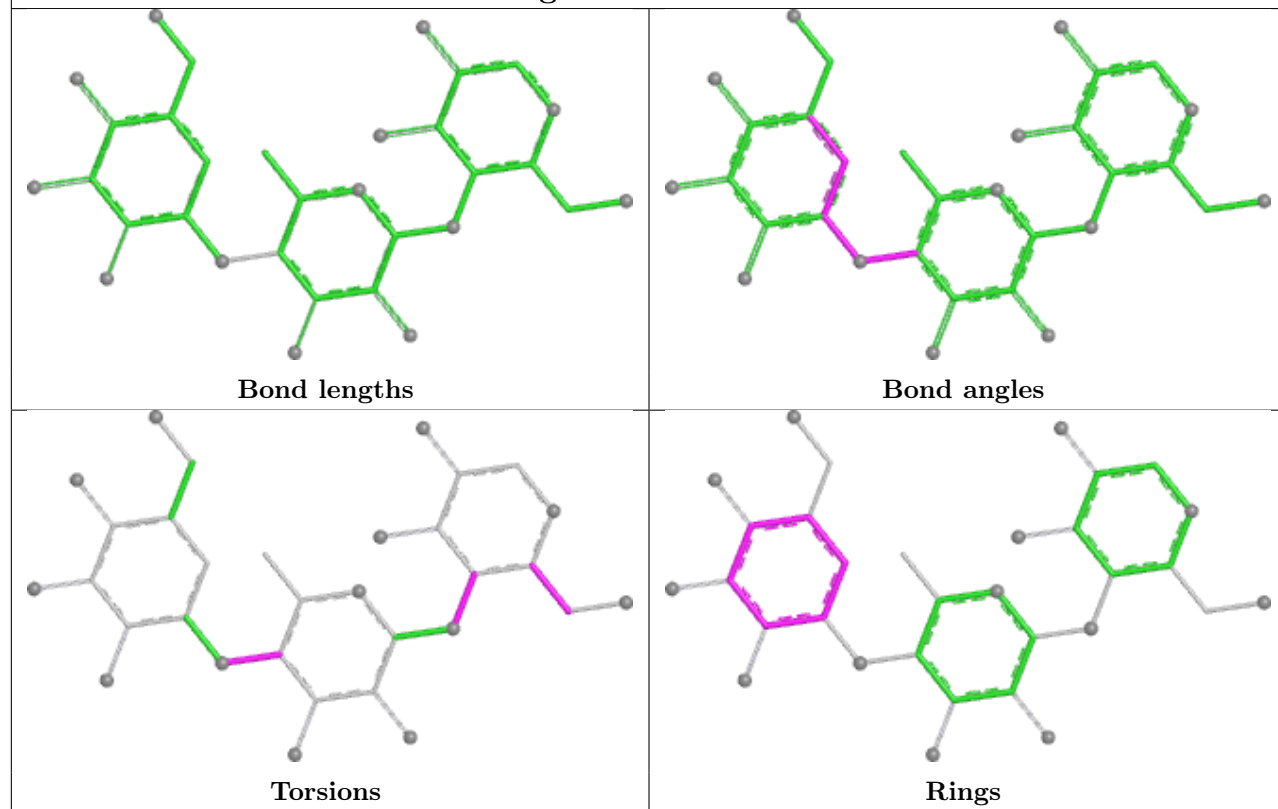
## Ligand A16 D 801



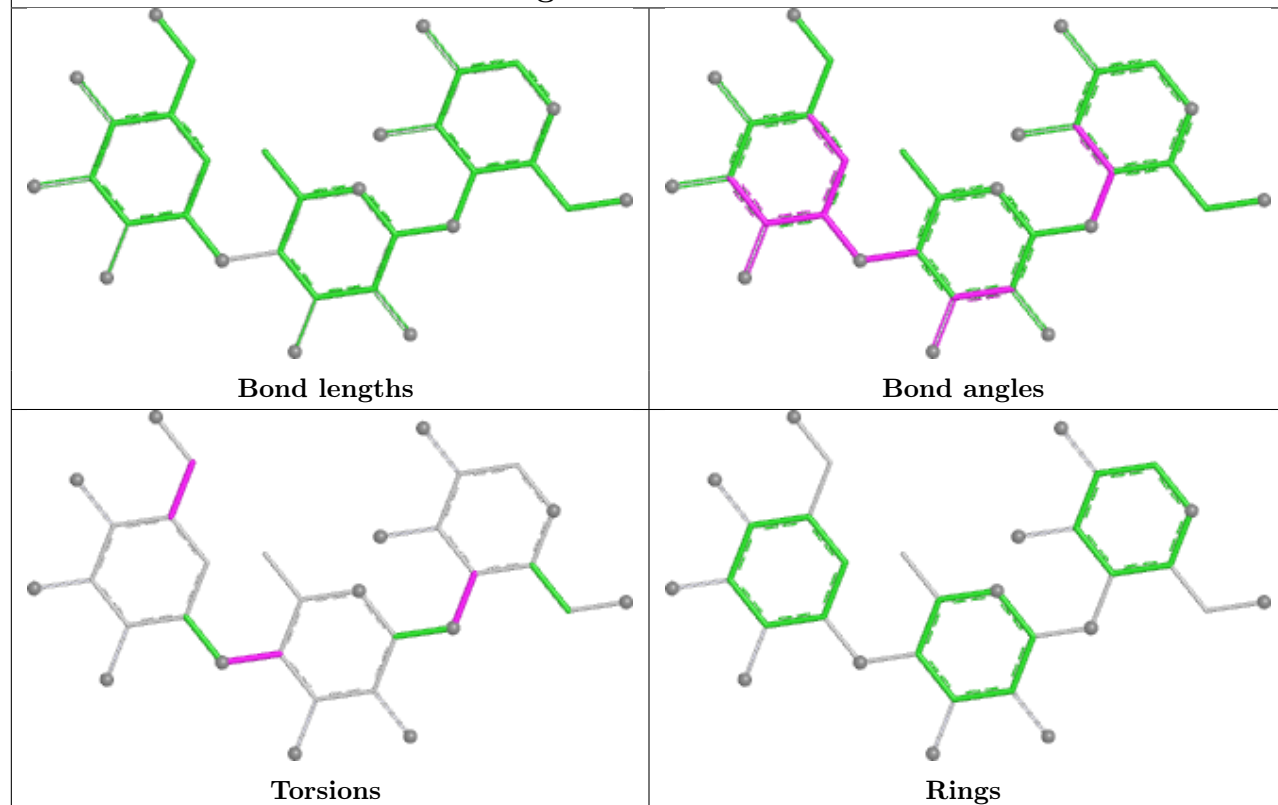
## Ligand C2E D 804



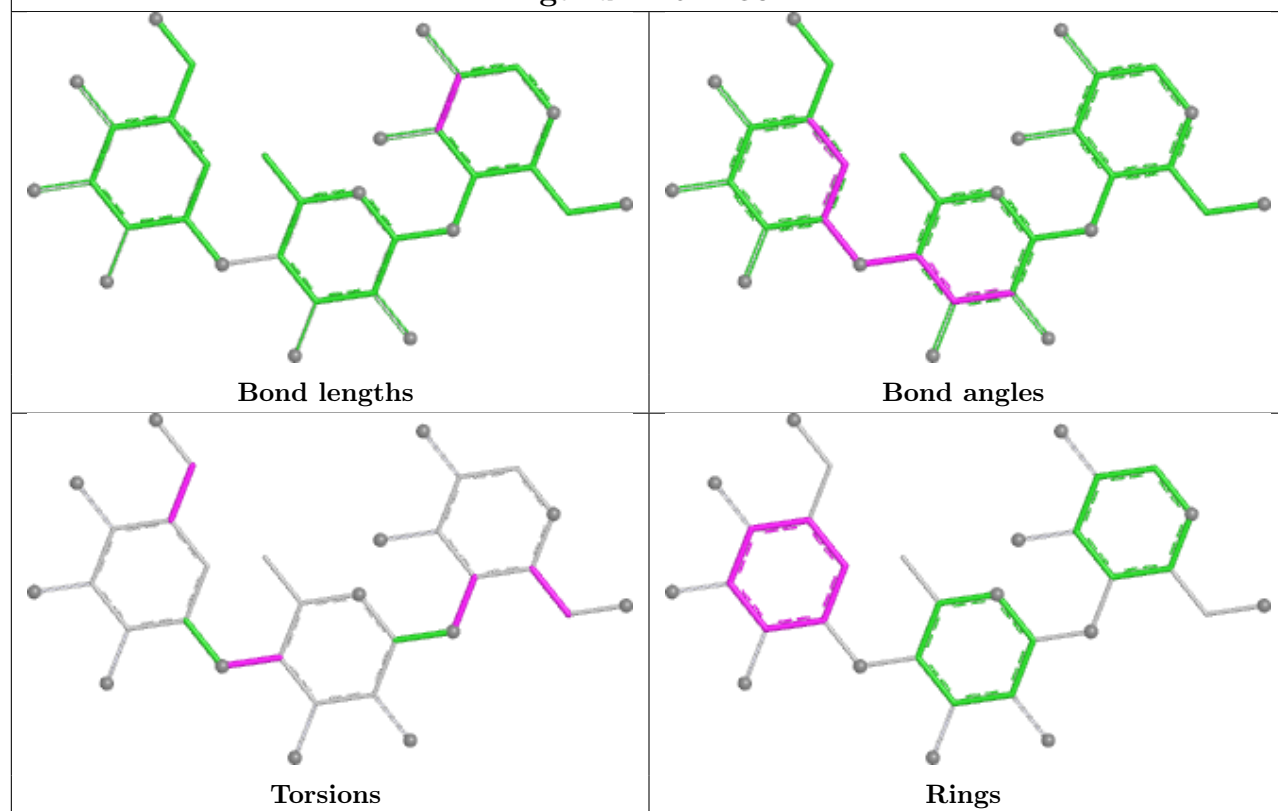
## Ligand A16 E 801



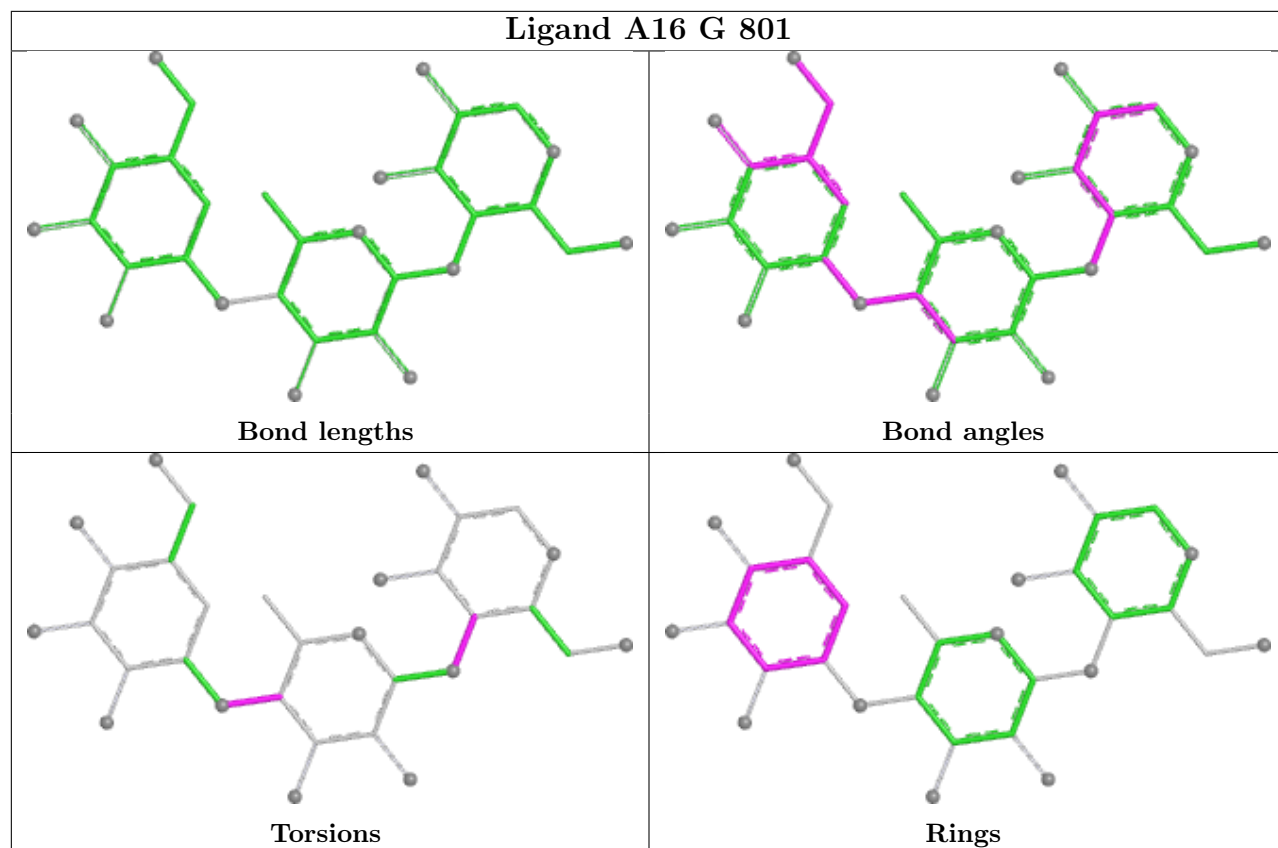
## Ligand A16 H 801



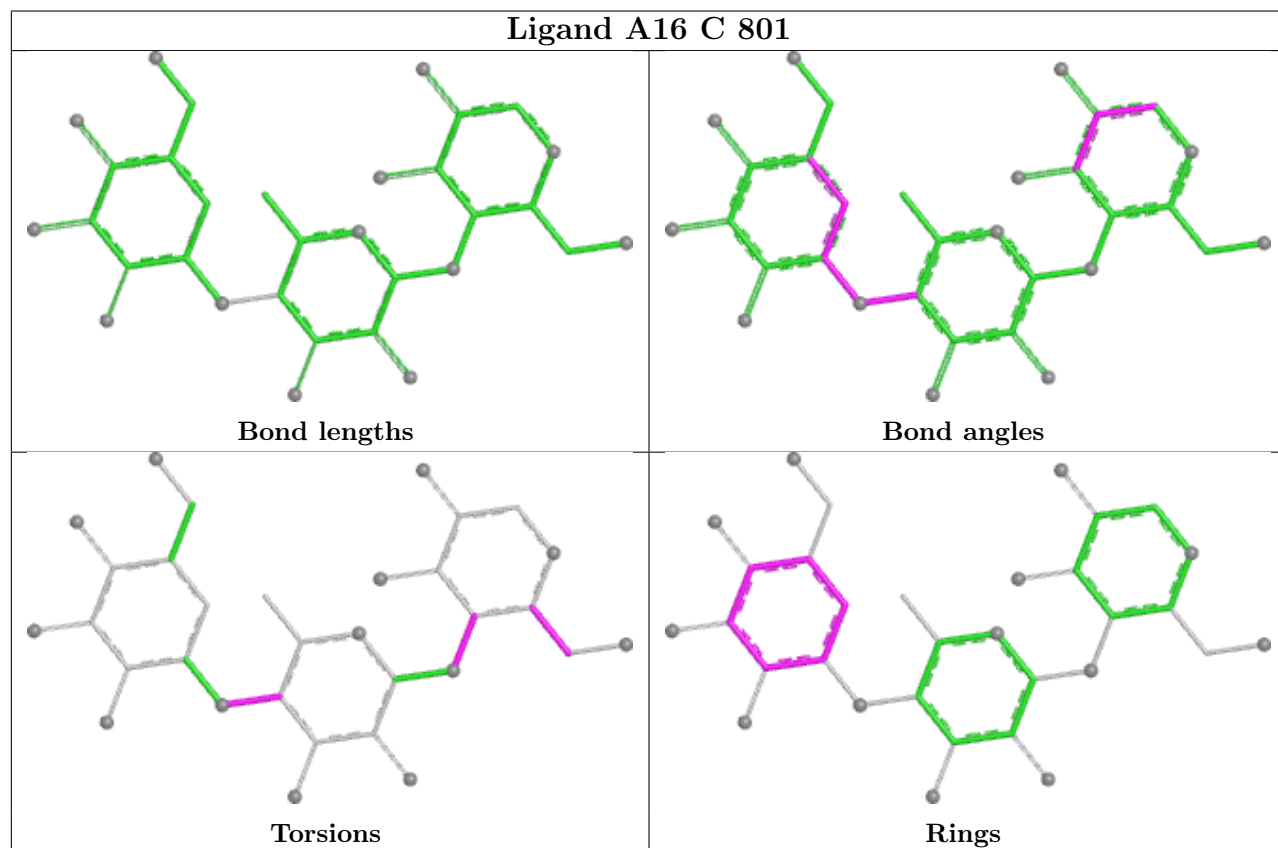
## Ligand A16 F 801



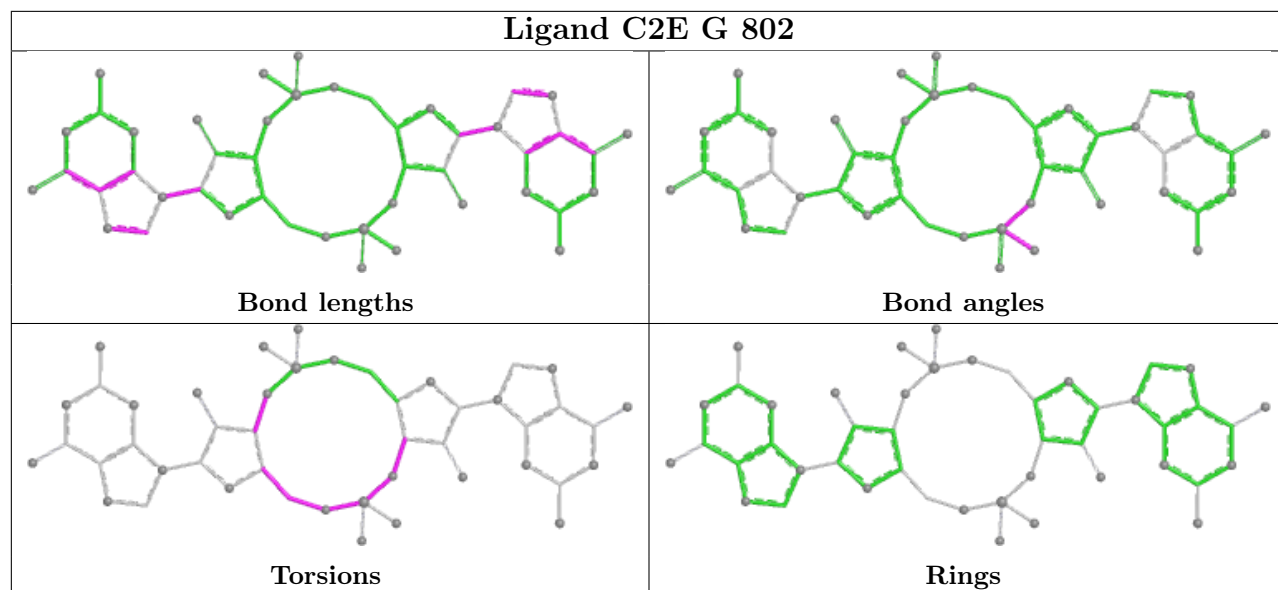
## Ligand A16 G 801



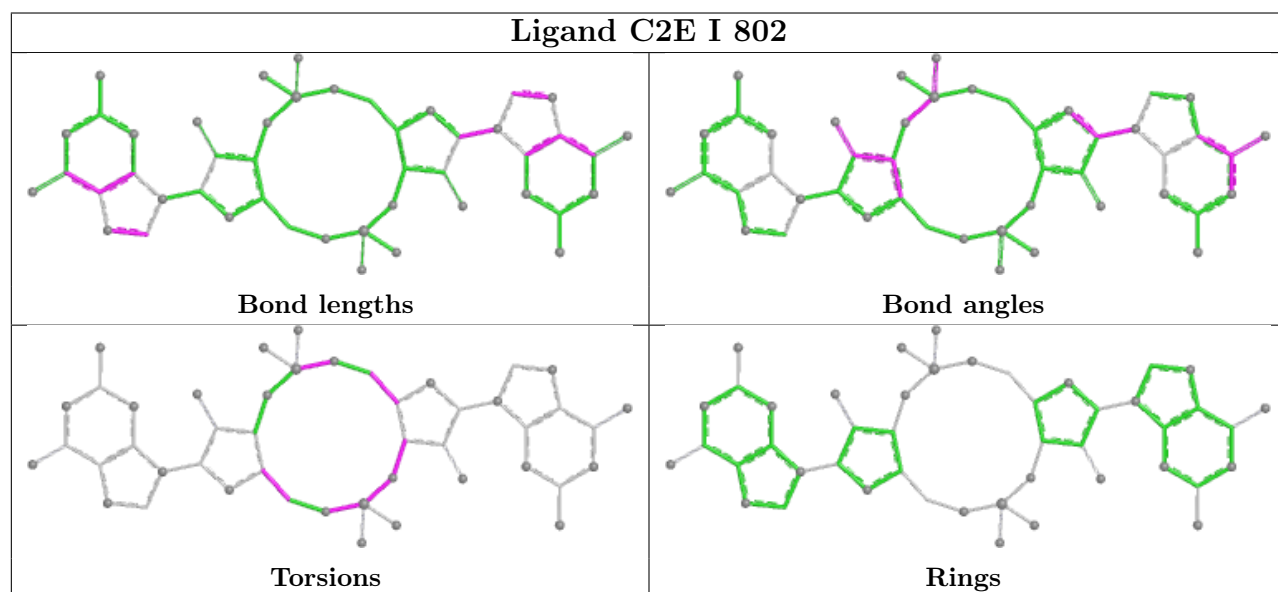
## Ligand A16 C 801



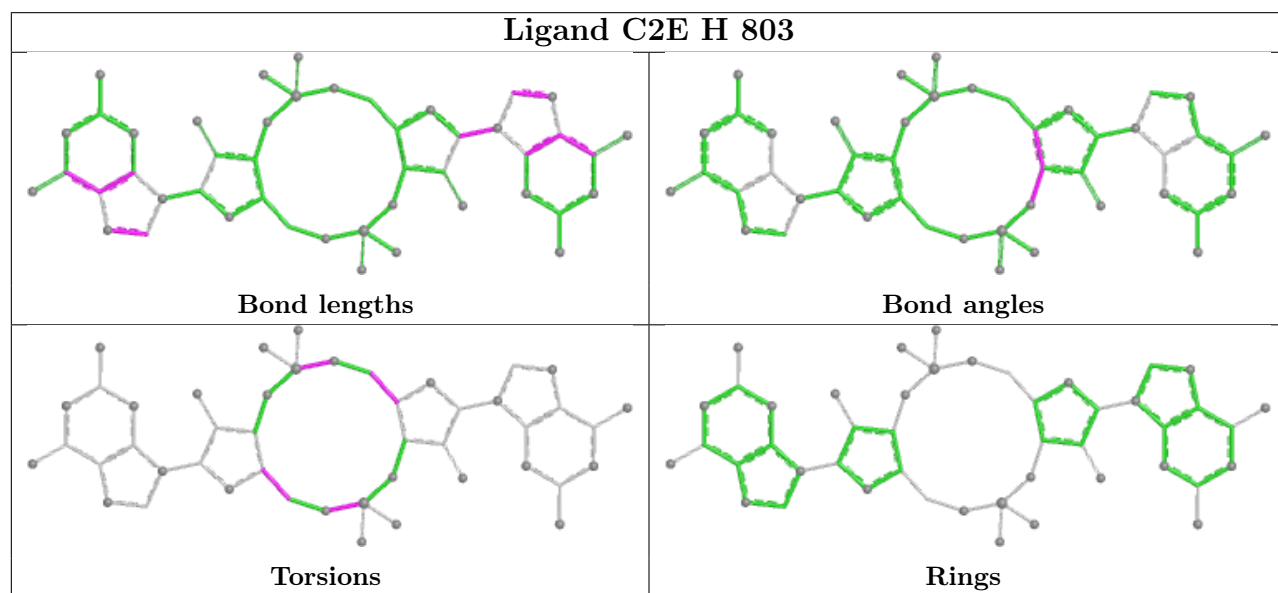
## Ligand C2E G 802



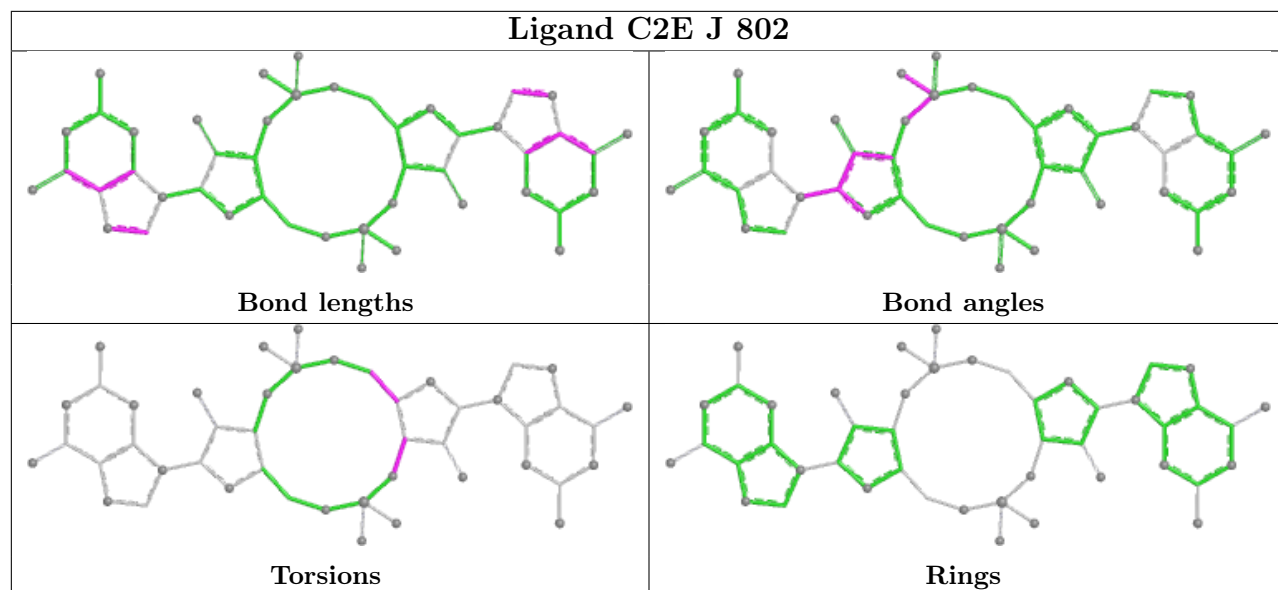
## Ligand C2E I 802



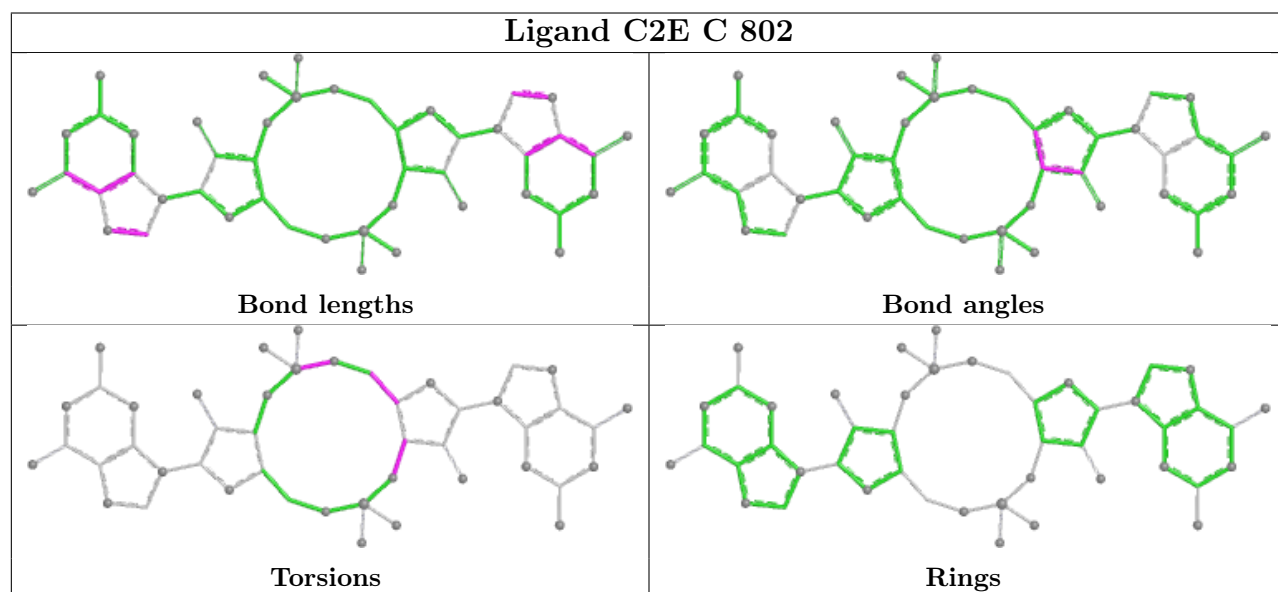
## Ligand C2E H 803



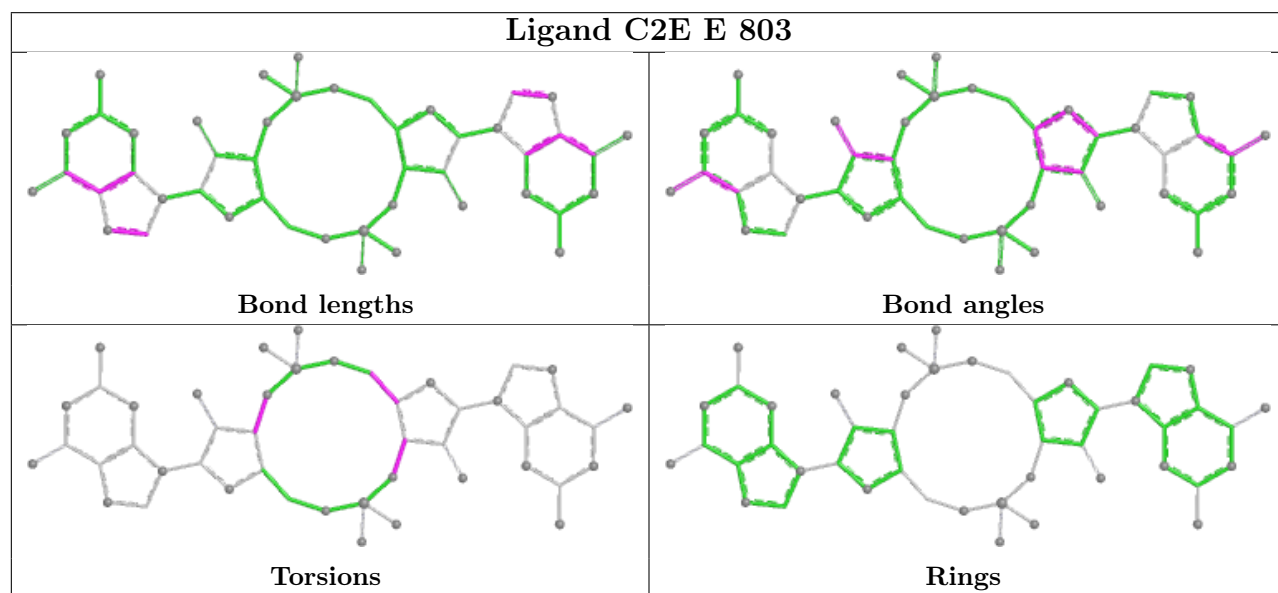
## Ligand C2E J 802

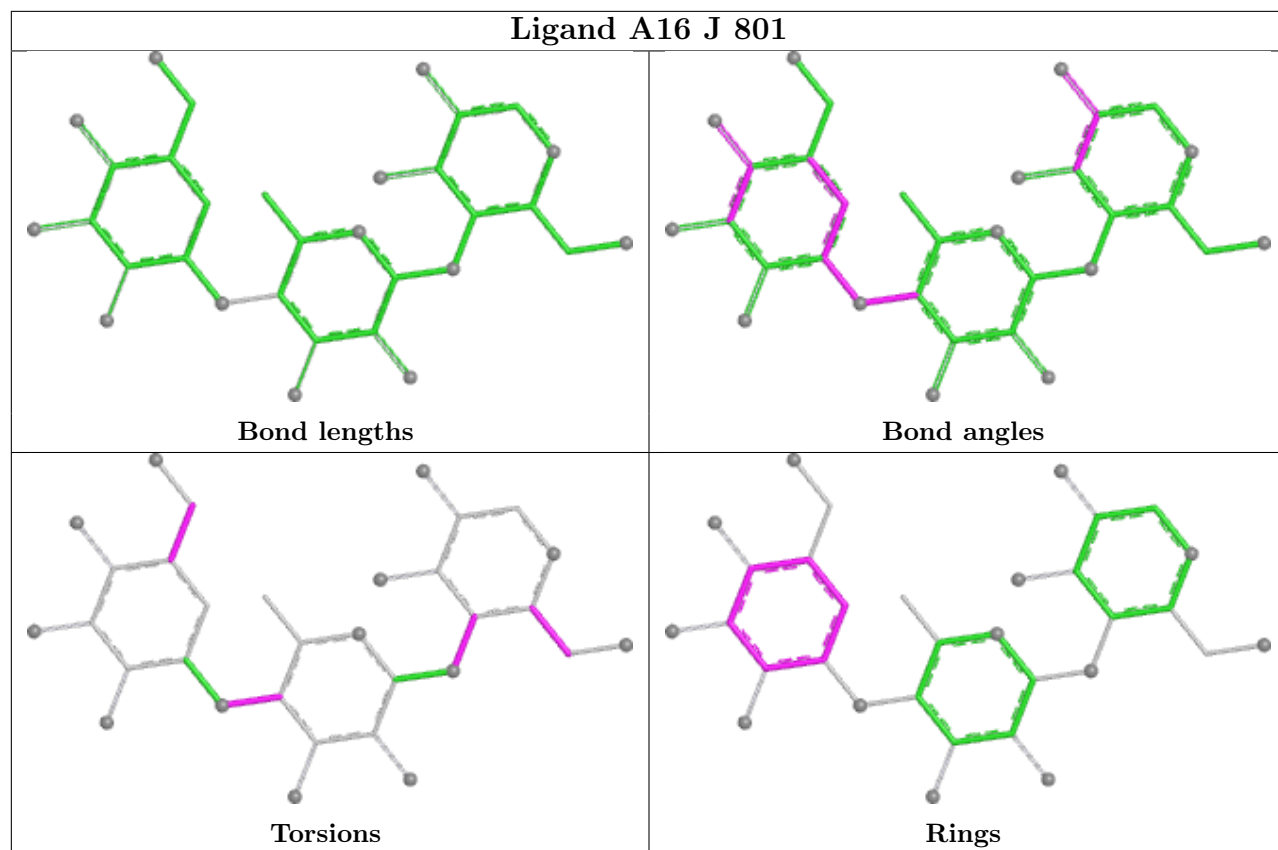


## Ligand C2E C 802



## Ligand C2E E 803





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	696/709 (98%)	0.30	12 (1%) 69 48	23, 40, 64, 95	0
1	D	694/709 (97%)	0.18	11 (1%) 70 49	19, 38, 66, 115	0
1	E	696/709 (98%)	0.28	14 (2%) 64 44	22, 39, 62, 102	0
1	F	694/709 (97%)	0.29	9 (1%) 74 53	17, 42, 67, 128	0
1	G	693/709 (97%)	0.33	14 (2%) 64 44	23, 44, 75, 127	0
1	H	696/709 (98%)	0.32	9 (1%) 74 53	24, 47, 76, 114	0
1	I	696/709 (98%)	0.39	16 (2%) 61 41	23, 51, 80, 122	0
1	J	694/709 (97%)	0.36	13 (1%) 66 45	23, 49, 83, 128	0
All	All	5559/5672 (98%)	0.31	98 (1%) 67 46	17, 43, 74, 128	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	215	ASP	4.2
1	I	684	PRO	4.1
1	H	27	GLU	4.0
1	E	586	VAL	3.7
1	J	377	ALA	3.6
1	J	526	GLY	3.6
1	C	338	GLY	3.5
1	F	659	PRO	3.4
1	F	660	ASP	3.3
1	F	417	THR	3.3
1	I	80	GLU	3.3
1	F	600	THR	3.2
1	E	687	ALA	3.2
1	H	679	PRO	3.2
1	J	629	SER	3.1
1	D	616	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	479	ASN	3.1
1	G	214	VAL	3.1
1	C	651	ALA	3.0
1	I	385	GLY	3.0
1	G	216	ALA	3.0
1	J	386	GLY	3.0
1	G	584	ARG	3.0
1	I	16	ASP	3.0
1	F	687	ALA	2.9
1	E	43	GLU	2.9
1	I	406	CYS	2.8
1	I	189	GLY	2.8
1	F	101	GLY	2.8
1	D	477	ASN	2.7
1	D	243	GLY	2.7
1	H	478	TYR	2.7
1	E	417	THR	2.6
1	I	531	GLY	2.6
1	C	351	PHE	2.6
1	D	478	TYR	2.6
1	I	593	LEU	2.6
1	I	318	HIS	2.6
1	C	417	THR	2.6
1	F	186	SER	2.6
1	D	586	VAL	2.5
1	G	609	ARG	2.5
1	E	679	PRO	2.5
1	F	615	HIS	2.5
1	E	537	CYS	2.5
1	G	585	PRO	2.5
1	C	419	ALA	2.4
1	E	593	LEU	2.4
1	E	387	TYR	2.4
1	D	614	ALA	2.4
1	J	659	PRO	2.4
1	G	691	ARG	2.4
1	H	477	ASN	2.4
1	D	670	VAL	2.4
1	C	73	VAL	2.3
1	C	585	PRO	2.3
1	H	659	PRO	2.3
1	D	615	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	244	GLN	2.3
1	D	151	TYR	2.3
1	J	181	GLY	2.3
1	D	490	THR	2.3
1	I	666	TRP	2.2
1	J	351	PHE	2.2
1	J	685	GLU	2.2
1	H	471	GLY	2.2
1	J	554	ALA	2.2
1	D	679	PRO	2.2
1	I	658	VAL	2.2
1	E	16	ASP	2.2
1	G	131	THR	2.2
1	F	679	PRO	2.1
1	C	477	ASN	2.1
1	C	676	GLU	2.1
1	E	553	GLU	2.1
1	G	32	ILE	2.1
1	H	662	HIS	2.1
1	G	593	LEU	2.1
1	J	666	TRP	2.1
1	E	163	GLY	2.1
1	J	283	SER	2.1
1	I	478	TYR	2.1
1	G	618	ALA	2.1
1	G	417	THR	2.1
1	C	605	GLU	2.1
1	I	571	GLU	2.1
1	C	352	HIS	2.1
1	E	145	ARG	2.1
1	I	356	ARG	2.1
1	I	151	TYR	2.1
1	E	406	CYS	2.1
1	J	642	SER	2.1
1	E	585	PRO	2.0
1	G	586	VAL	2.0
1	I	624	ASN	2.0
1	H	181	GLY	2.0
1	C	318	HIS	2.0
1	J	16	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

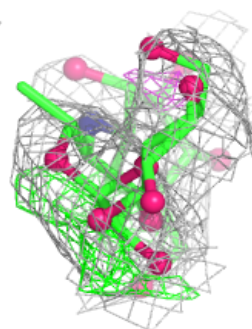
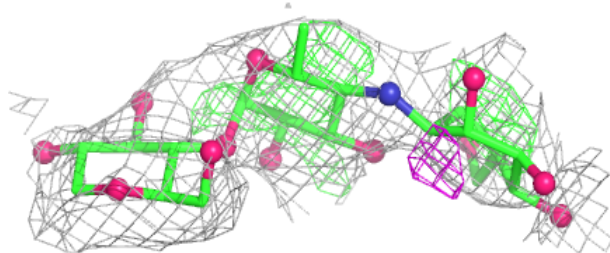
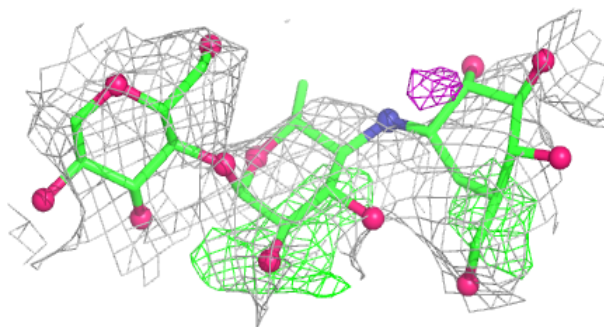
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	A16	G	801	32/33	0.70	0.31	77,107,116,124	0
2	A16	I	801	32/33	0.73	0.23	77,107,116,124	0
2	A16	H	801	32/33	0.77	0.27	78,107,120,124	0
2	A16	J	801	32/33	0.77	0.26	78,107,116,124	0
2	A16	E	801	32/33	0.79	0.28	77,108,116,124	0
4	PO4	D	802	5/5	0.79	0.21	70,72,82,88	0
4	PO4	E	802	5/5	0.80	0.19	44,45,61,76	0
2	A16	C	801	32/33	0.81	0.23	70,82,105,114	0
4	PO4	D	803	5/5	0.81	0.17	66,70,75,84	0
2	A16	F	801	32/33	0.81	0.16	27,42,63,83	0
2	A16	D	801	32/33	0.82	0.30	77,107,116,124	0
3	C2E	D	804	46/46	0.86	0.18	96,101,117,122	0
3	C2E	E	803	46/46	0.88	0.10	39,47,59,66	0
3	C2E	G	802	46/46	0.89	0.10	28,49,58,65	0
4	PO4	H	802	5/5	0.89	0.18	55,58,67,70	0
3	C2E	I	802	46/46	0.90	0.11	38,46,55,59	0
3	C2E	J	802	46/46	0.90	0.11	29,49,60,63	0
3	C2E	H	803	46/46	0.93	0.09	29,39,55,61	0
3	C2E	C	802	46/46	0.94	0.08	45,52,60,66	0
3	C2E	F	802	46/46	0.94	0.09	29,39,45,51	0

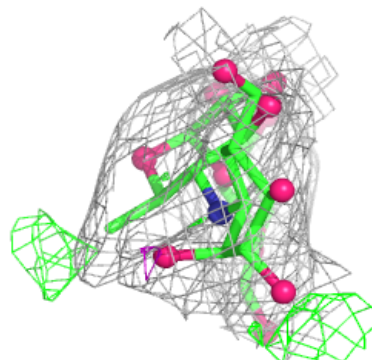
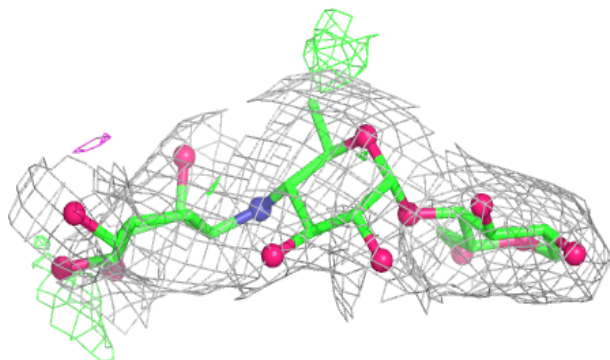
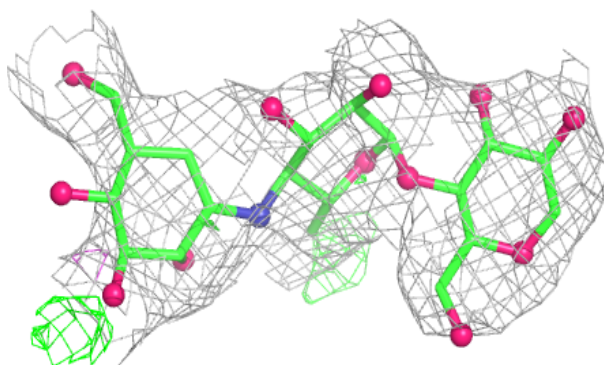
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A16 G 801:**

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

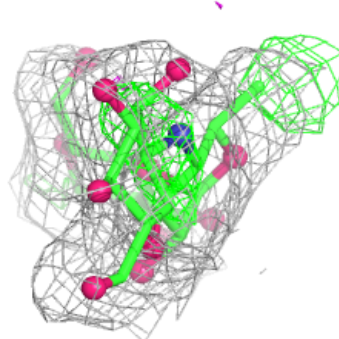
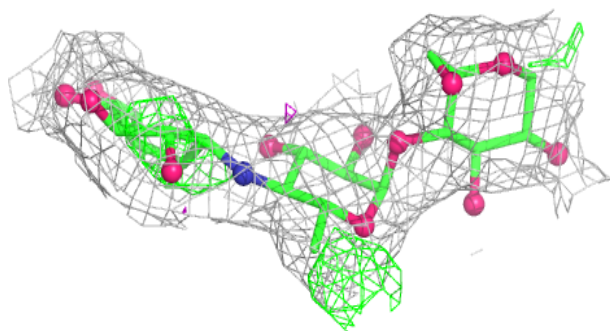
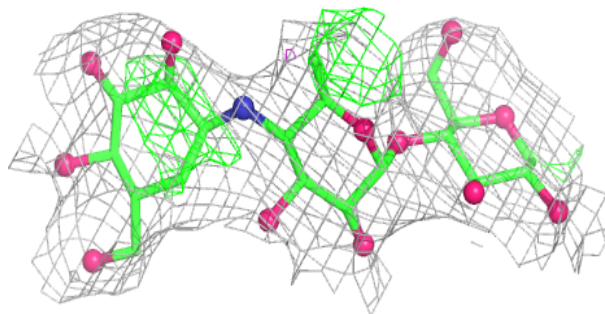
**Electron density around A16 I 801:**

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

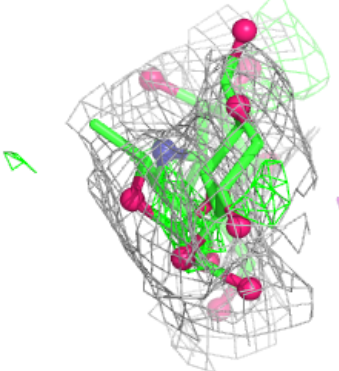
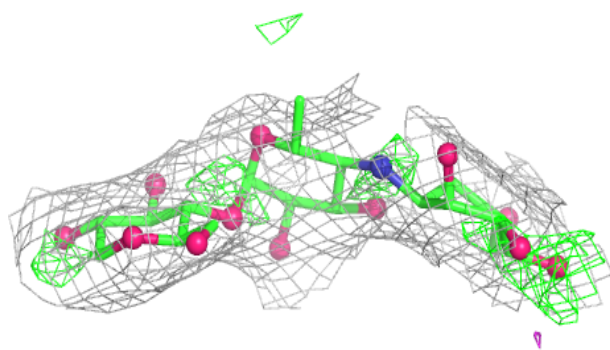
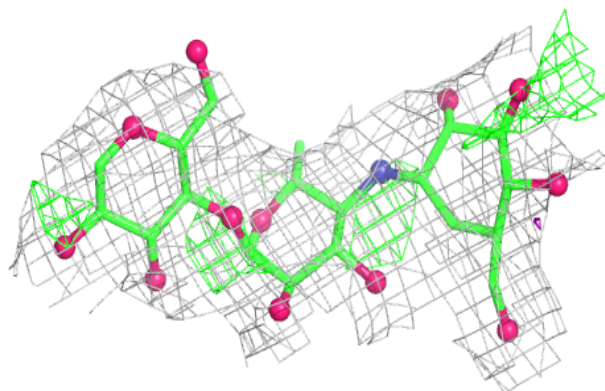


**Electron density around A16 H 801:**

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

**Electron density around A16 J 801:**

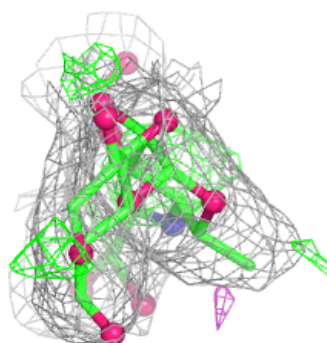
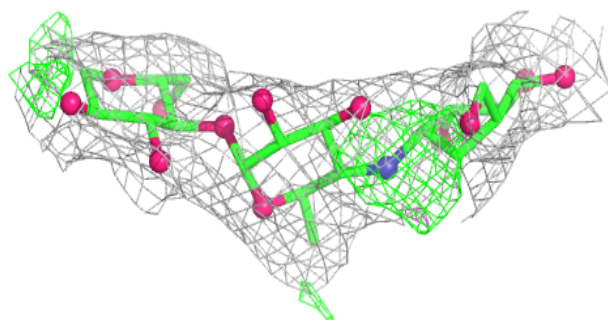
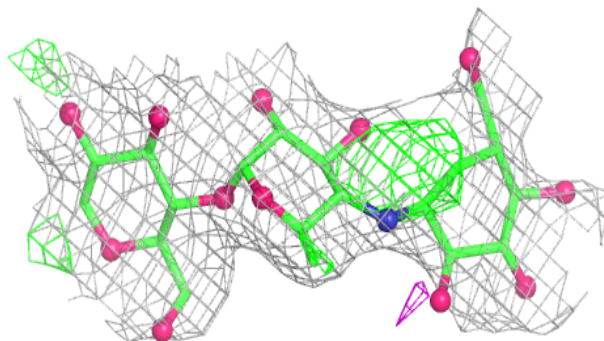
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



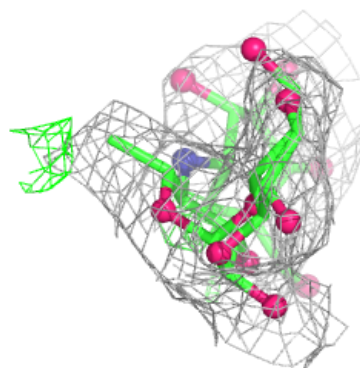
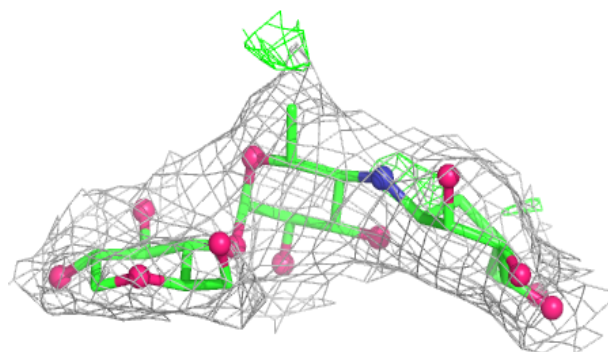
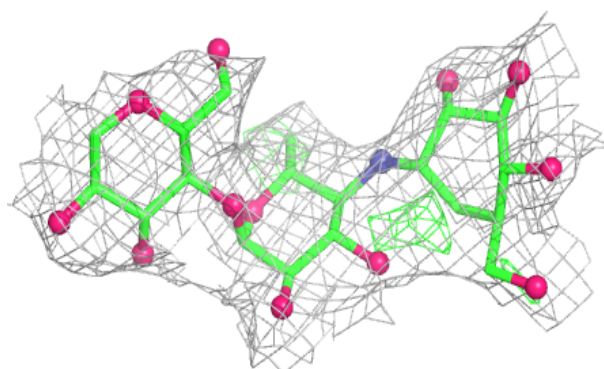


**Electron density around A16 E 801:**

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

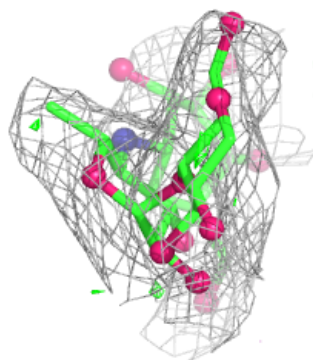
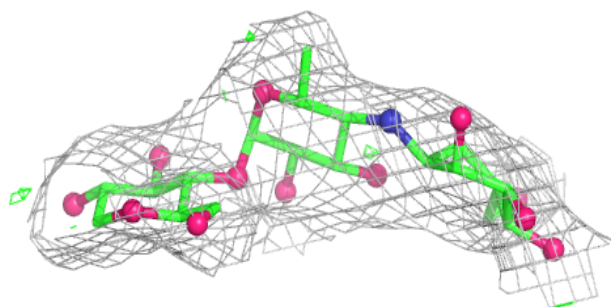
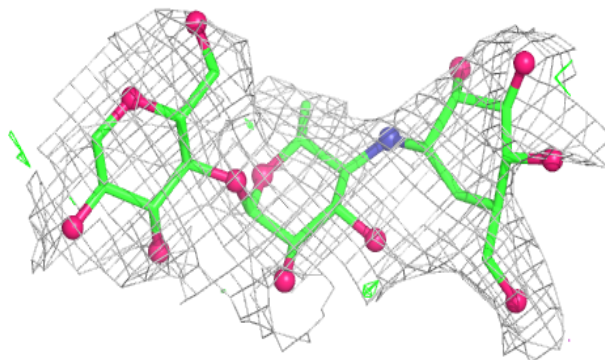
**Electron density around A16 C 801:**

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

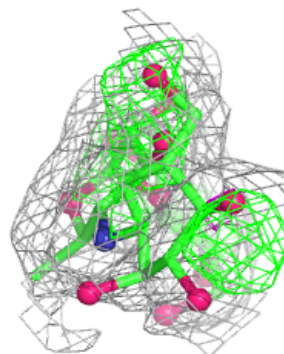
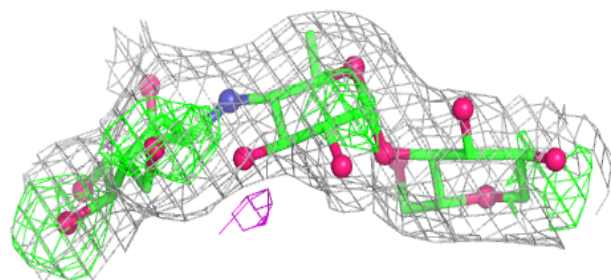
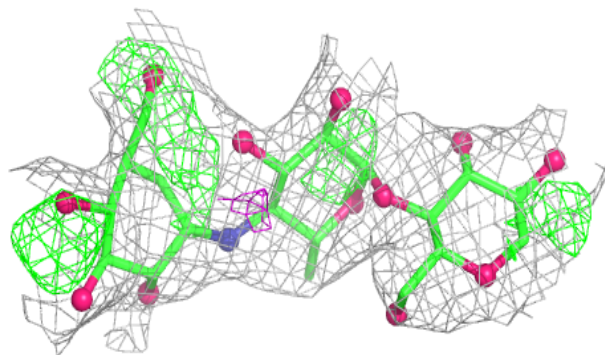


**Electron density around A16 F 801:**

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

**Electron density around A16 D 801:**

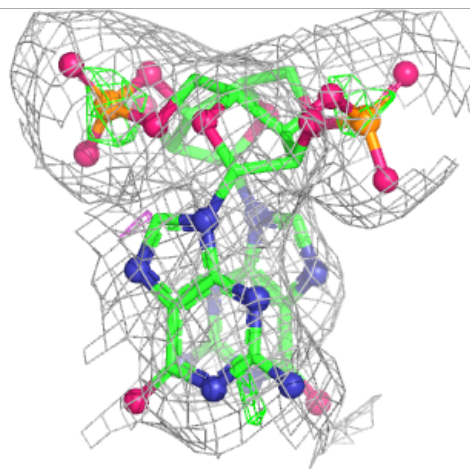
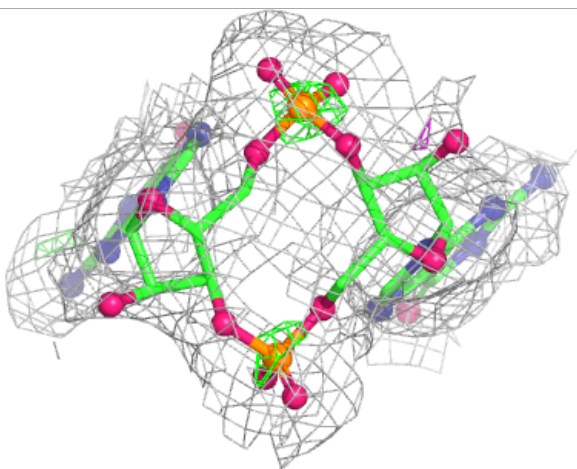
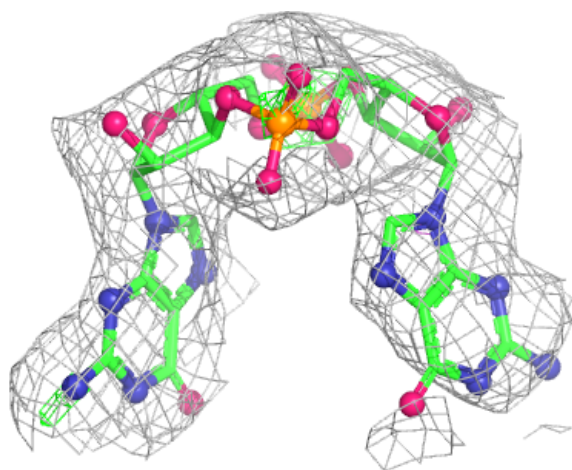
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





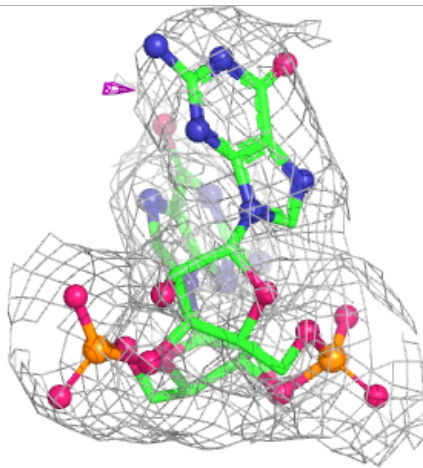
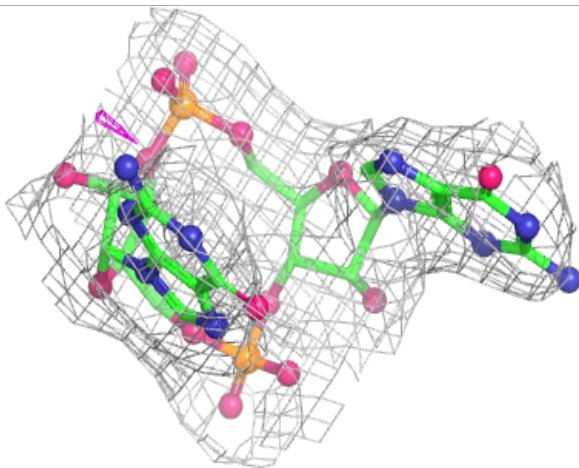
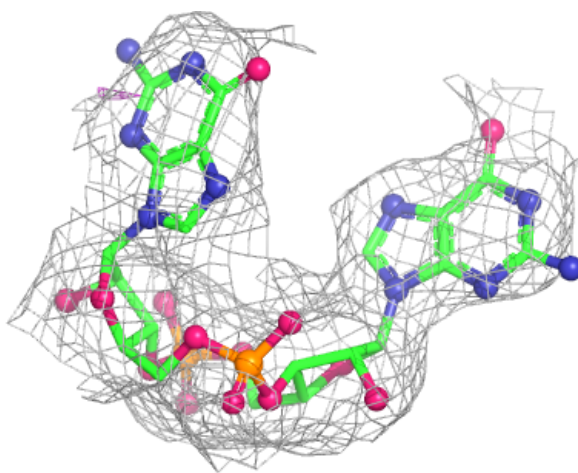
**Electron density around C2E D 804:**

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



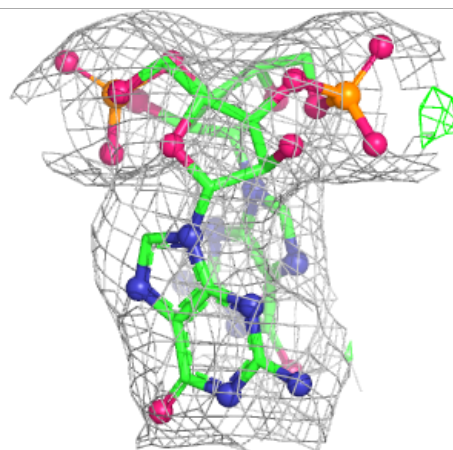
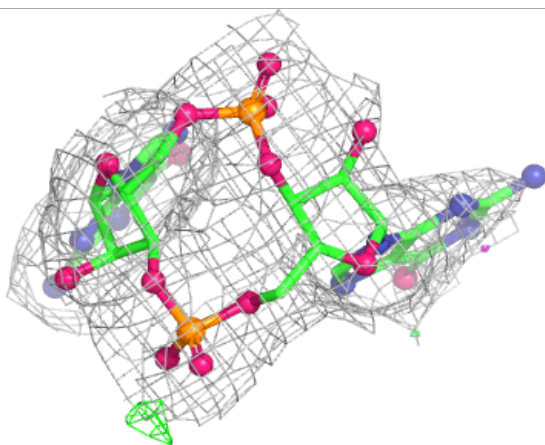
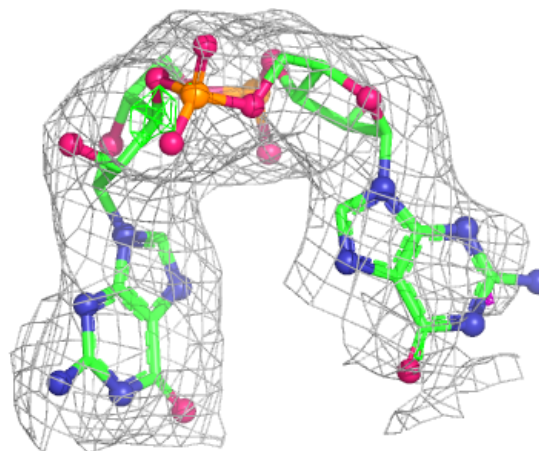
**Electron density around C2E E 803:**

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



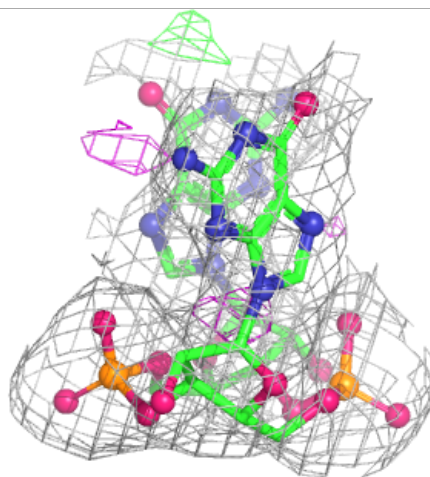
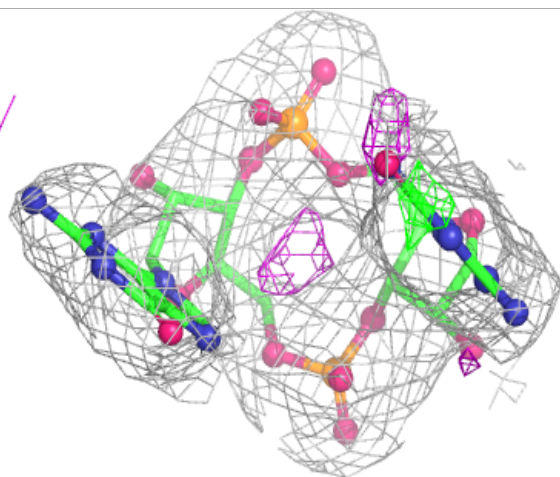
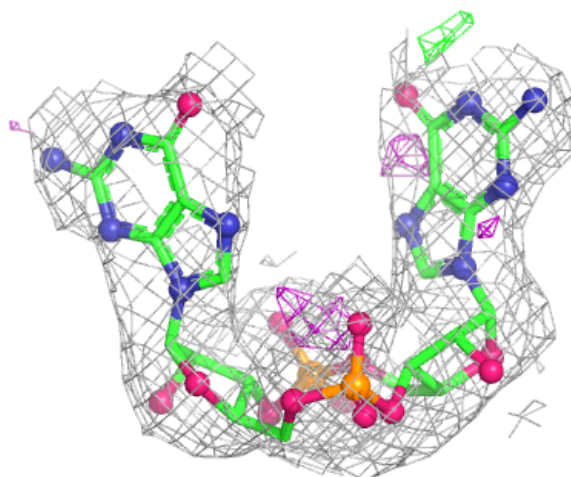
**Electron density around C2E G 802:**

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



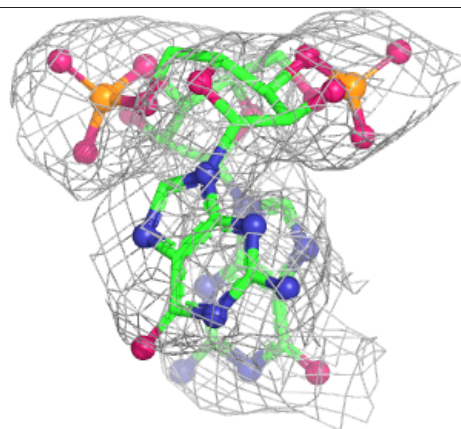
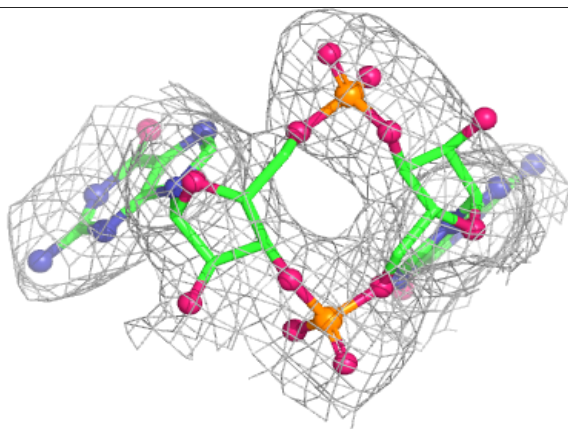
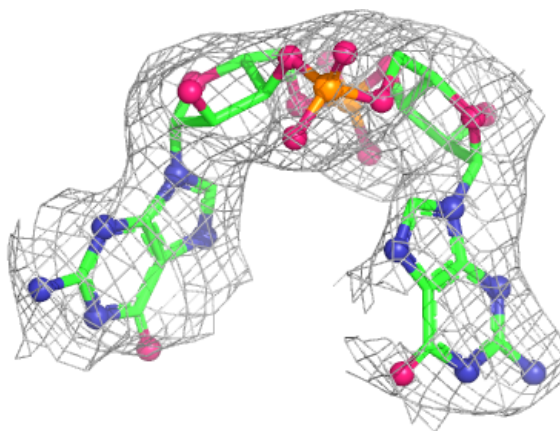
**Electron density around C2E I 802:**

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



**Electron density around C2E J 802:**

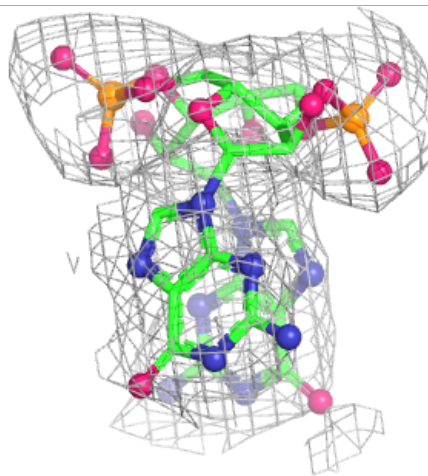
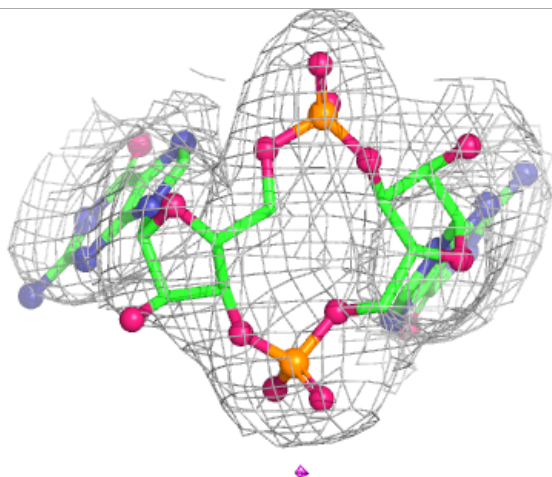
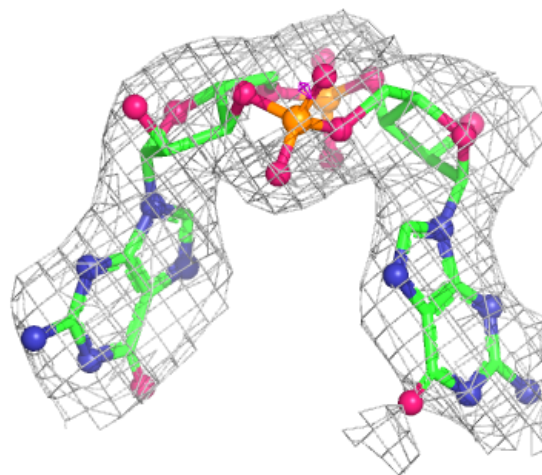
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





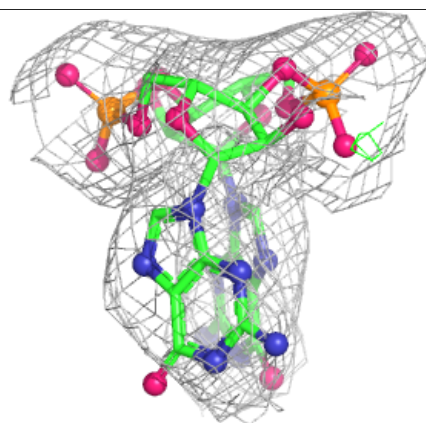
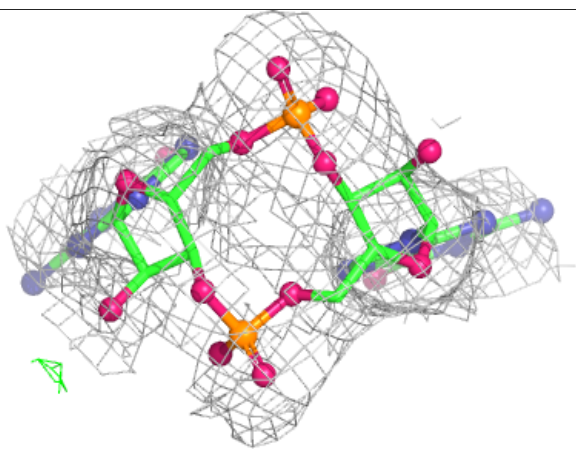
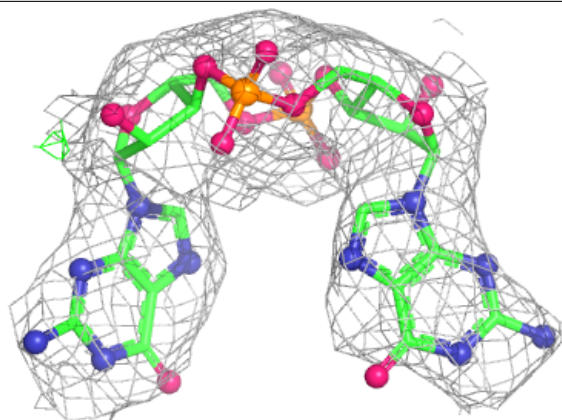
**Electron density around C2E H 803:**

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



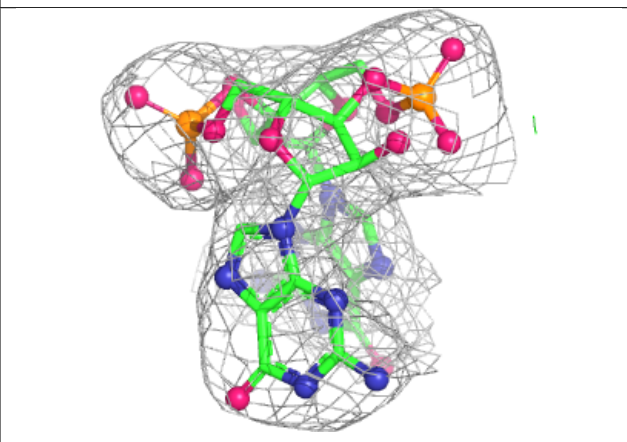
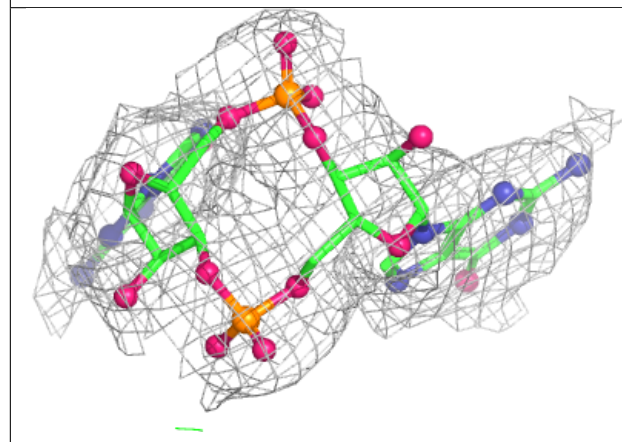
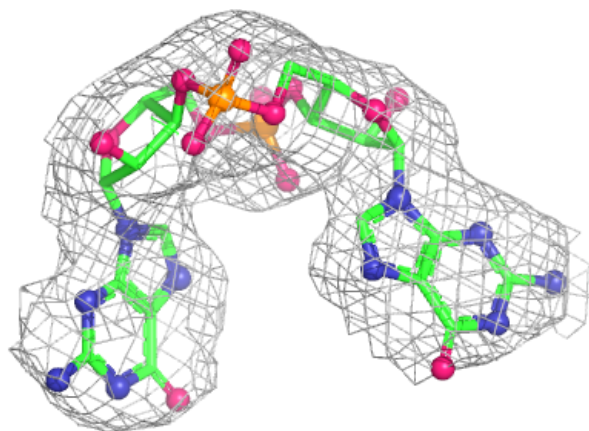
**Electron density around C2E C 802:**

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



**Electron density around C2E F 802:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.