Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 01:46 AM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

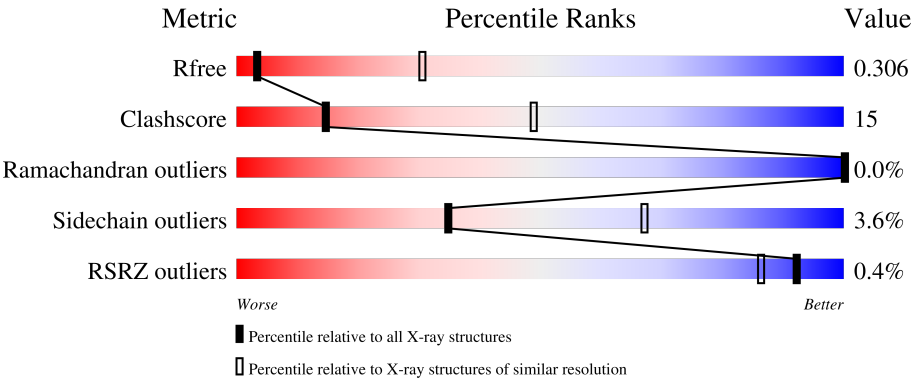
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (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 >=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 <=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	65% 32%
1	D	709	% 64% 32%
1	E	709	66% 31%
1	F	709	% 63% 34%
1	G	709	68% 29%

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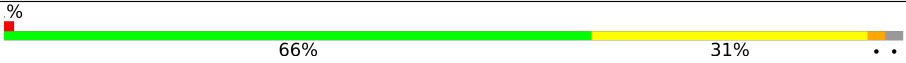
Mol	Chain	Length	Quality of chain
1	H	709	
1	I	709	
1	J	709	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A16	G	801	-	-	-	X

2 Entry composition (i)

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
D	192	ARG	LYS	conflict	UNP A0A5P2ALW6
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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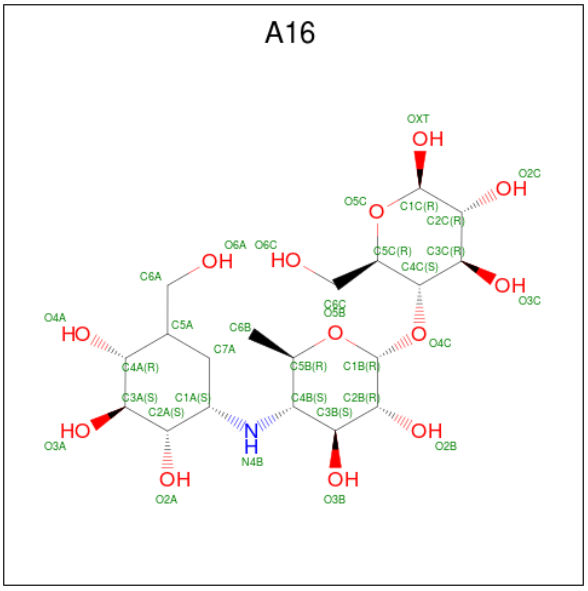
Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	SER	-	expression tag	UNP A0A5P2ALW6
I	0	HIS	-	expression tag	UNP A0A5P2ALW6
I	103	VAL	ILE	conflict	UNP A0A5P2ALW6
I	192	ARG	LYS	conflict	UNP A0A5P2ALW6
I	296	ALA	SER	conflict	UNP A0A5P2ALW6
I	297	ASP	ASN	conflict	UNP A0A5P2ALW6
I	303	MET	THR	conflict	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: $C_{19}H_{35}NO_{13}$) (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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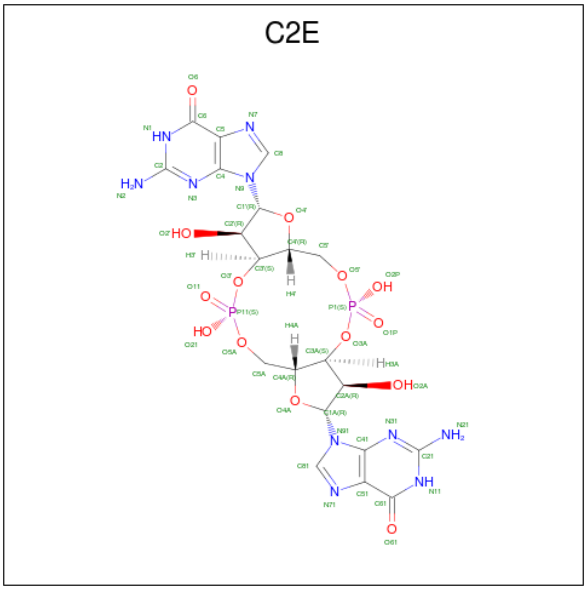
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			32	19	1	12		
2	F	1	Total	C	N	O	0	0
			32	19	1	12		
2	G	1	Total	C	N	O	0	0
			32	19	1	12		
2	H	1	Total	C	N	O	0	0
			32	19	1	12		
2	I	1	Total	C	N	O	0	0
			32	19	1	12		
2	J	1	Total	C	N	O	0	0
			32	19	1	12		

- 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: $C_{20}H_{24}N_{10}O_{14}P_2$).



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

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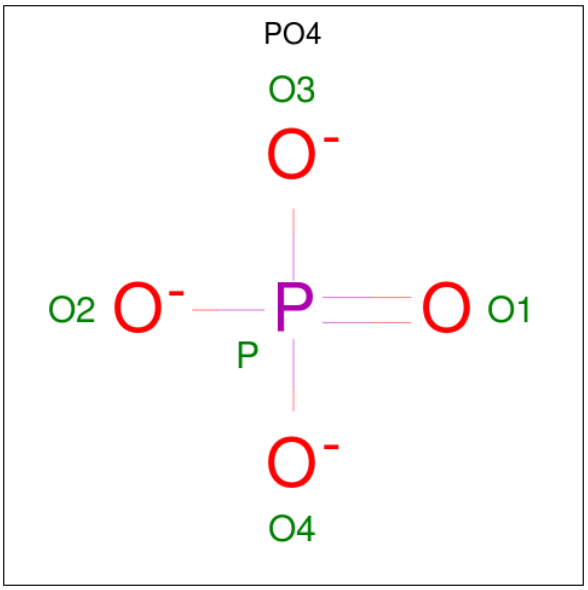
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	H	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	I	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	J	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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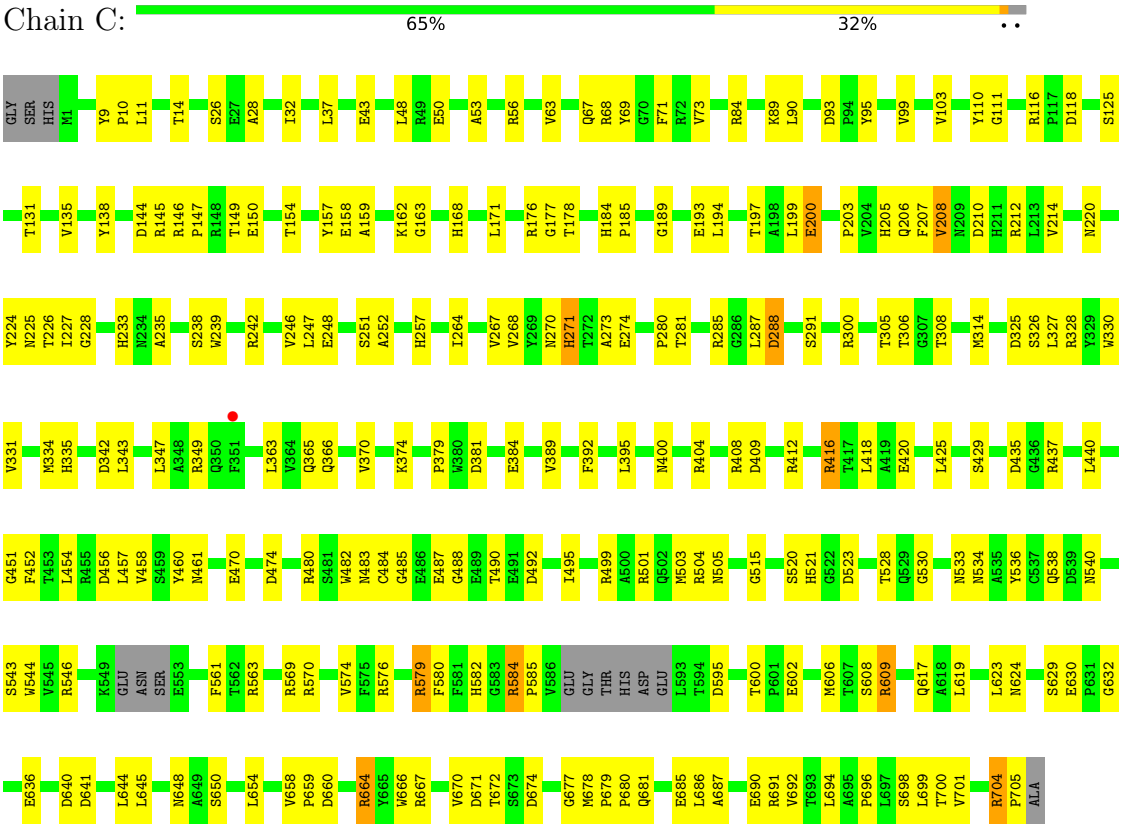
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	3	Total O 3 3	0	0
5	F	3	Total O 3 3	0	0
5	H	2	Total O 2 2	0	0
5	I	4	Total O 4 4	0	0

3 Residue-property plots (i)

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.

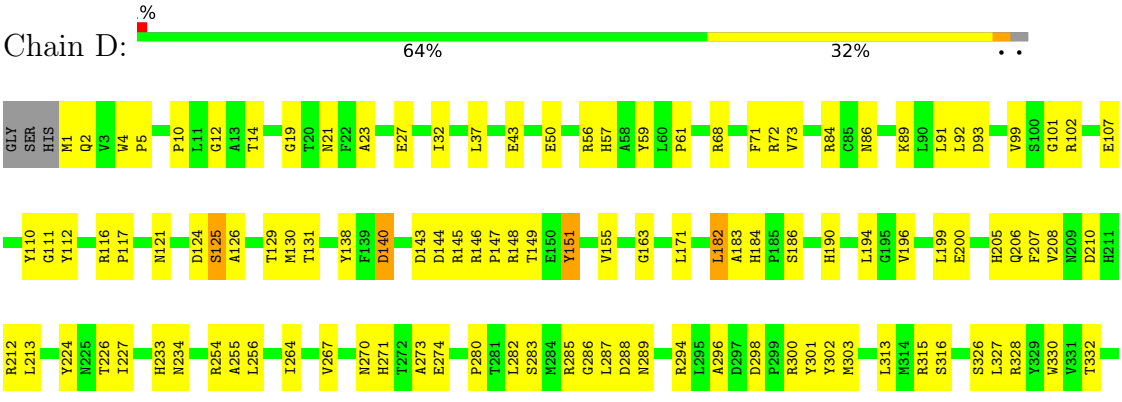
• Molecule 1: Glycogen debranching enzyme GlgX

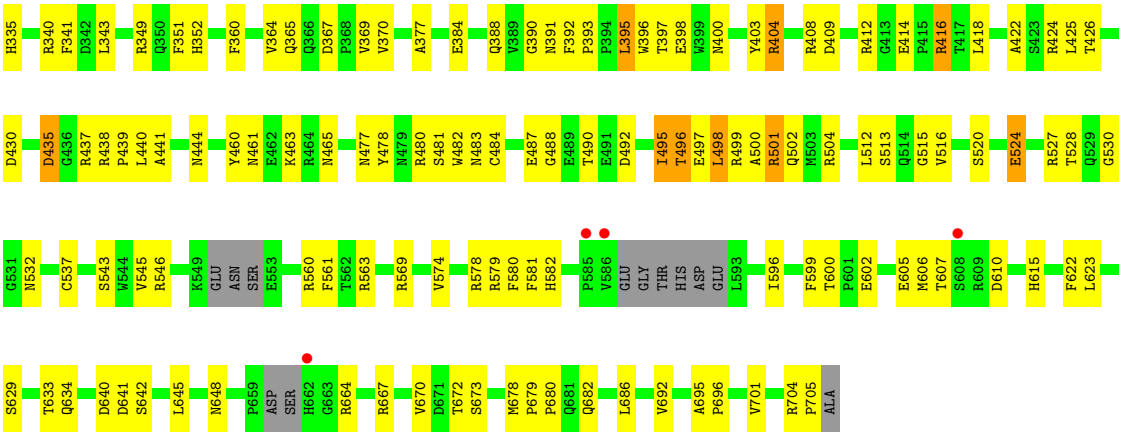
Chain C:



• Molecule 1: Glycogen debranching enzyme GlgX

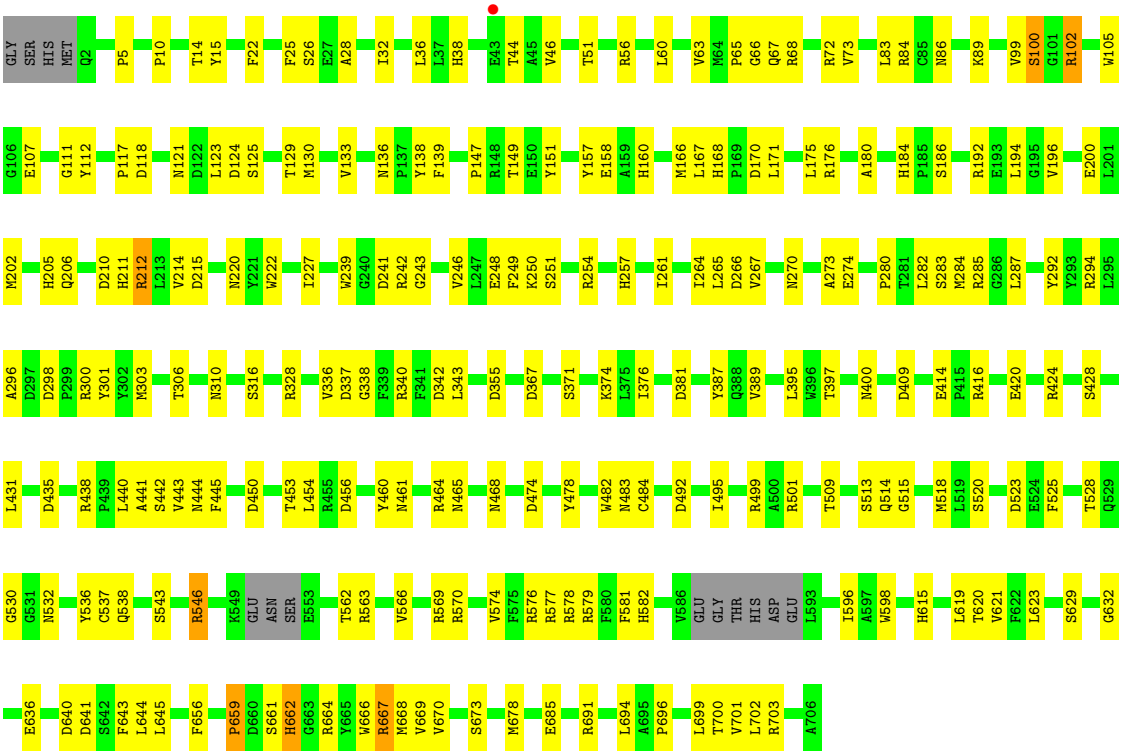
Chain D:





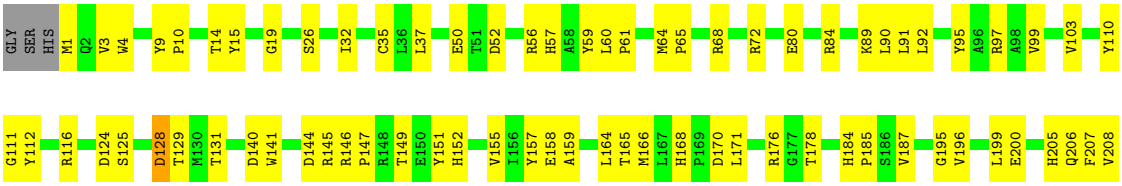
• Molecule 1: Glycogen debranching enzyme GlgX

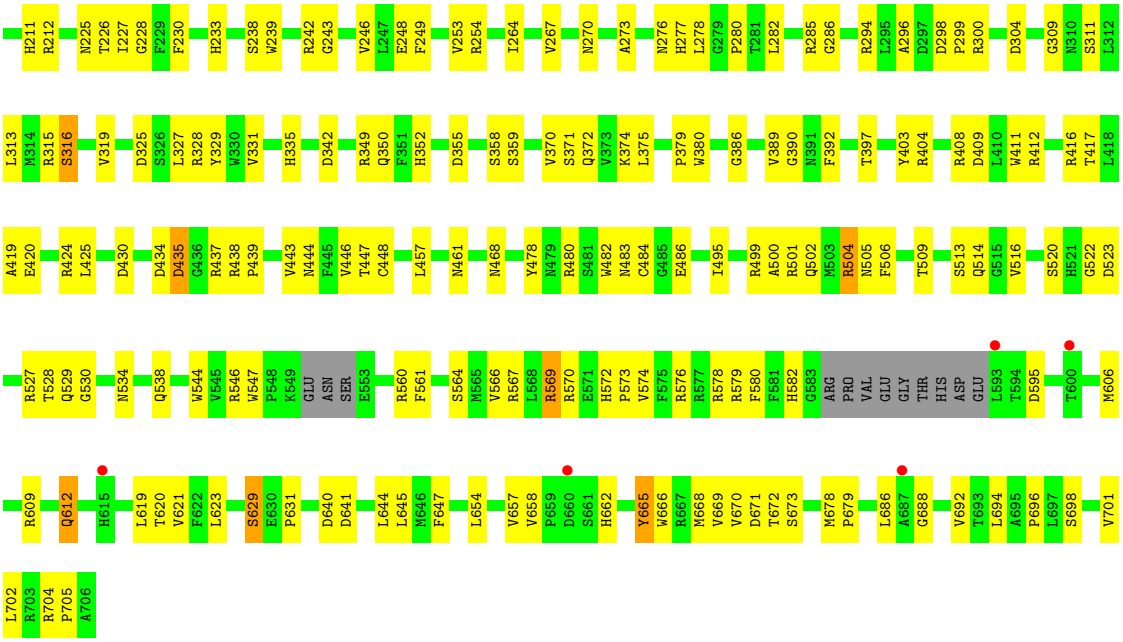
Chain E:



• Molecule 1: Glycogen debranching enzyme GlgX

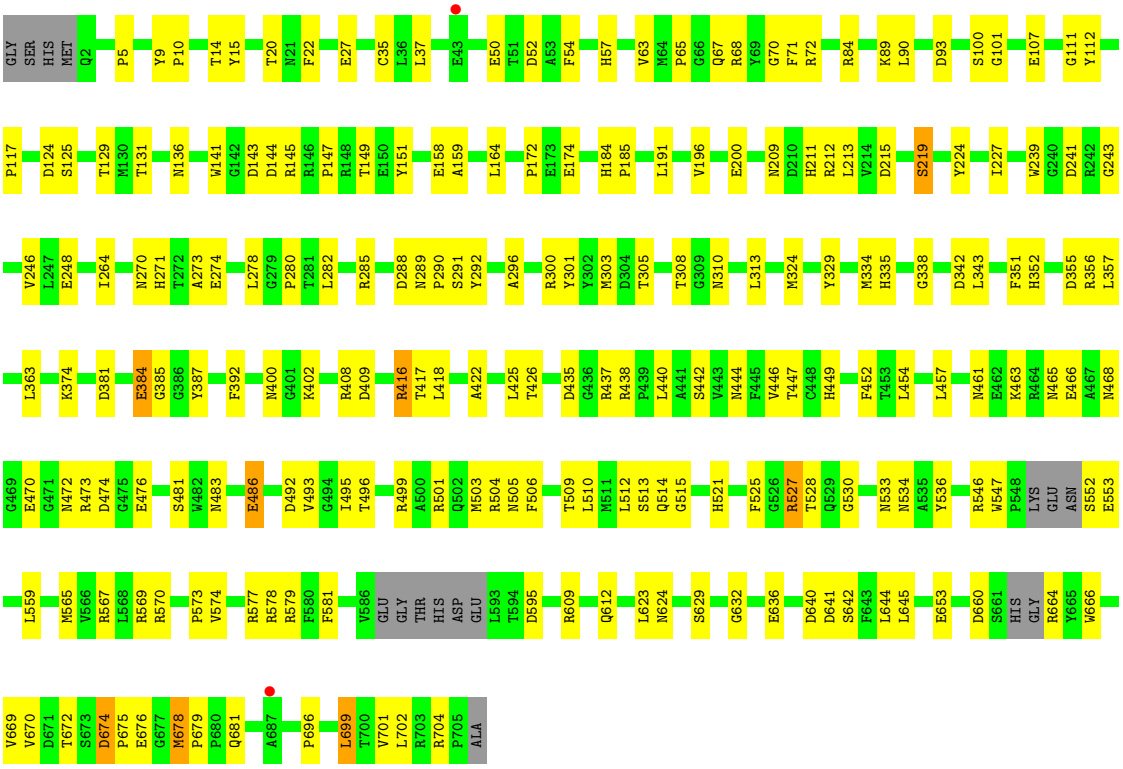
Chain F:





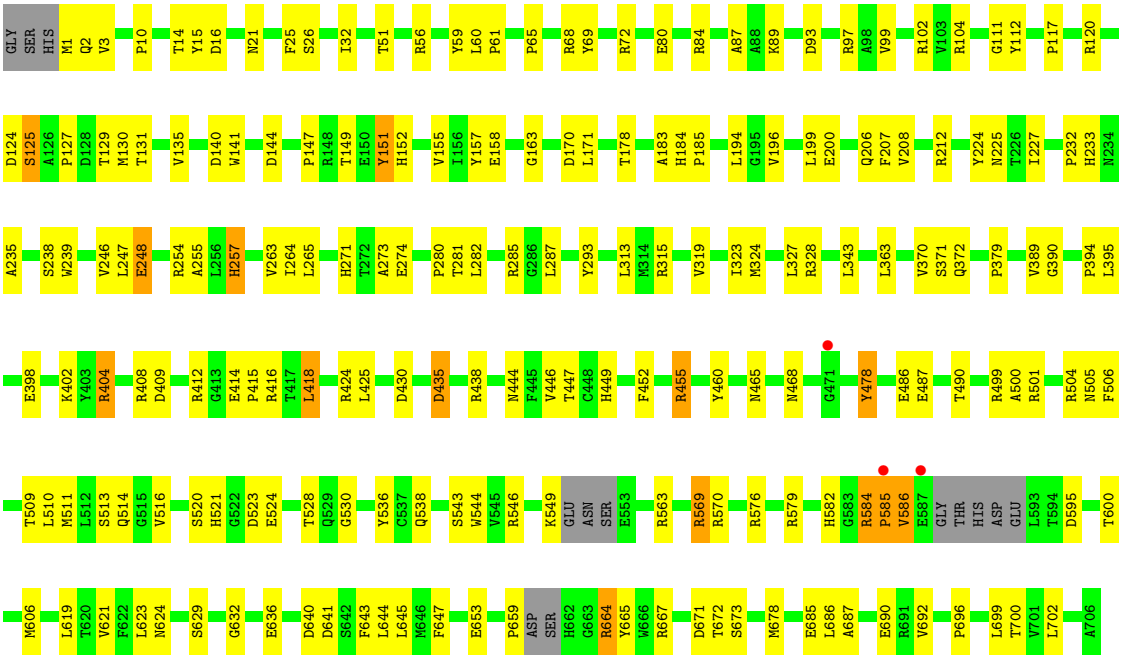
• Molecule 1: Glycogen debranching enzyme GlgX

Chain G:



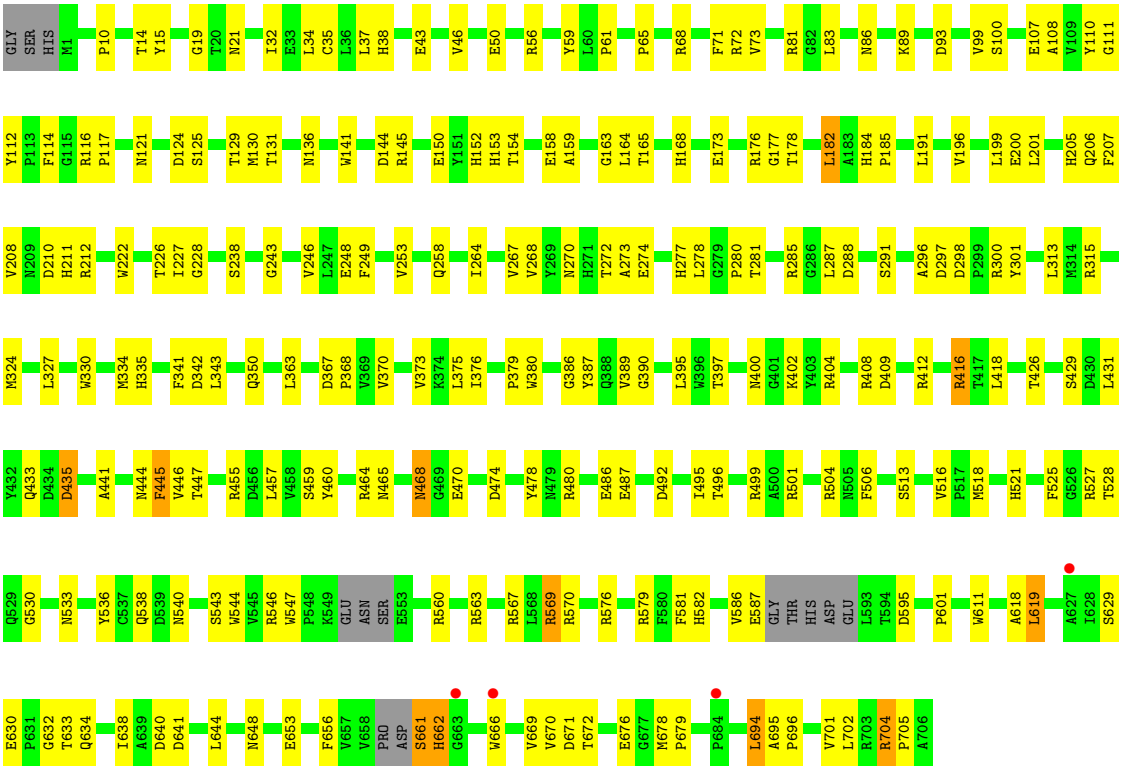
• Molecule 1: Glycogen debranching enzyme GlgX

Chain H:



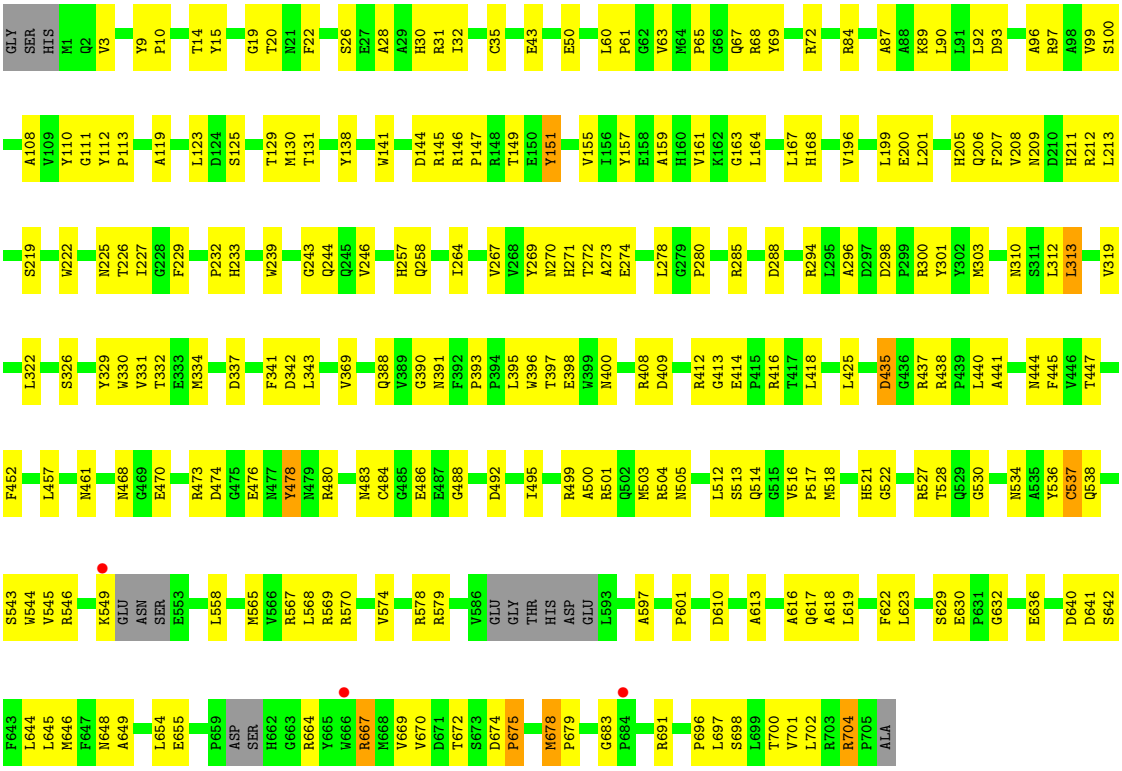
• Molecule 1: Glycogen debranching enzyme GlgX

Chain I:



• Molecule 1: Glycogen debranching enzyme GlgX

Chain J:


GLY SER HIS M1 Q2 V3 Y9 P10 T14 Y15 G19 T20 N21 F22 S26 E27 A28 A29 H30 R31 I32 C35 E43 E50 L60 P61 G62 V63 M64 P65 G66 Q67 R68 Y69 R72 R84 A87 A88 K89 L90 L91 L92 D93 A96 R97 A98 V99 S100
A108 V109 Y110 G111 Y112 P113 A119 L123 D124 S125 T129 M130 T131 Y138 W141 D144 R145 R146 P147 R148 T149 E150 Y151 V155 I156 Y157 E158 A159 H160 V161 K162 G163 L164 L167 H168 V196 L199 E200 L201 H205 Q206 F207 V208 N209 D210 H211 R212 L213
S219 W222 N225 T226 I227 G228 F229 P232 H233 W239 G243 Q244 Q245 V246 H257 Q258 I264 V267 V268 Y269 N270 H271 T272 A273 E274 L278 G279 P280 R285 D288 R294 L295 A296 D297 D298 P299 R300 Y301 Y302 M303 N310 S311 L312 L313 V319
L322 S326 Y329 W330 V331 T332 E333 M334 D337 F341 D342 L343 V369 Q388 V389 G390 N391 F392 P393 P394 L395 W396 T397 E398 W399 N400 R408 D409 R412 G413 E414 P415 R416 T417 L418 L425 D435 G436 R437 R438 P439 L440 A441 N444 F445 V446 T447
F452 L457 N461 N468 G469 E470 R473 D474 G475 E476 N477 Y478 N479 R480 N483 C484 G485 E486 E487 G488 D492 I495 R499 A500 R501 Q502 M503 R504 N505 L512 S513 Q514 G515 V516 P517 M518 H521 G522 R527 T528 Q529 G530 N534 A535 Y536 C537 Q538
S543 W544 V545 R546 K549 GLU ASN SER E553 L558 M565 V566 R567 L568 R569 R570 V574 R578 R579 V586 GLU GLY THR HIS ASP GLU L593 A597 P601 D610 A613 A616 Q617 A618 L619 F622 L623 S629 E630 P631 G632 E636 D640 D641 S642
F643 L644 L645 M646 F647 N648 A649 L654 E655 P659 ASP SER H662 G663 R664 Y665 W666 R667 H668 V669 V670 D671 T672 S673 D674 P675 M678 P679 G683 P684 R691 P696 L697 S698 L699 T700 V701 L702 R703 R704 P705 ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.84Å 185.59Å 184.67Å 90.00° 98.08° 90.00°	Depositor
Resolution (Å)	48.50 – 3.60 48.49 – 3.61	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.50-3.60) 98.2 (48.49-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.307 0.236 , 0.306	Depositor DCC
R_{free} test set	1986 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A16, PO4, C2E

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(^{o})	Ideal(^{o})
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%)	51	83
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 (i)

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%)	43	72
1	D	576/590 (98%)	548 (95%)	28 (5%)	25	59
1	E	577/590 (98%)	550 (95%)	27 (5%)	26	61
1	F	575/590 (98%)	557 (97%)	18 (3%)	40	71
1	G	575/590 (98%)	561 (98%)	14 (2%)	49	75
1	H	577/590 (98%)	554 (96%)	23 (4%)	31	65
1	I	574/590 (97%)	553 (96%)	21 (4%)	34	66
1	J	576/590 (98%)	556 (96%)	20 (4%)	36	68
All	All	4607/4720 (98%)	4440 (96%)	167 (4%)	35	67

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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	C2E	E	803	-	44,52,52	1.06	6 (13%)	52,82,82	1.12	4 (7%)
4	PO4	D	803	-	4,4,4	0.94	0	6,6,6	0.48	0
3	C2E	G	802	-	44,52,52	1.13	6 (13%)	52,82,82	1.02	2 (3%)
3	C2E	J	802	-	44,52,52	1.11	6 (13%)	52,82,82	1.13	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PO4	E	802	-	4,4,4	0.94	0	6,6,6	0.46	0
3	C2E	D	804	-	44,52,52	1.15	6 (13%)	52,82,82	1.35	7 (13%)
2	A16	F	801	-	33,34,35	0.79	1 (3%)	44,50,52	1.14	2 (4%)
3	C2E	F	802	-	44,52,52	1.22	6 (13%)	52,82,82	1.19	5 (9%)
2	A16	H	801	-	33,34,35	0.67	1 (3%)	44,50,52	1.53	6 (13%)
2	A16	G	801	1	33,34,35	0.57	0	44,50,52	1.15	5 (11%)
2	A16	C	801	-	33,34,35	0.49	0	44,50,52	1.07	2 (4%)
2	A16	J	801	-	33,34,35	0.57	0	44,50,52	1.14	3 (6%)
3	C2E	H	803	-	44,52,52	1.23	6 (13%)	52,82,82	1.26	5 (9%)
4	PO4	D	802	-	4,4,4	0.95	0	6,6,6	0.53	0
2	A16	I	801	-	33,34,35	0.62	1 (3%)	44,50,52	1.03	2 (4%)
3	C2E	I	802	-	44,52,52	1.14	6 (13%)	52,82,82	1.35	8 (15%)
3	C2E	C	802	-	44,52,52	1.15	6 (13%)	52,82,82	1.13	3 (5%)
2	A16	D	801	-	33,34,35	0.56	0	44,50,52	1.16	5 (11%)
2	A16	E	801	-	33,34,35	0.41	0	44,50,52	1.07	1 (2%)
4	PO4	H	802	-	4,4,4	0.94	0	6,6,6	0.44	0

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	E	803	-	-	5/22/62/62	0/6/7/7
3	C2E	F	802	-	-	6/22/62/62	0/6/7/7
3	C2E	H	803	-	-	10/22/62/62	0/6/7/7
2	A16	D	801	-	-	3/12/69/72	1/3/3/3
3	C2E	G	802	-	-	12/22/62/62	0/6/7/7
2	A16	H	801	-	-	4/12/69/72	0/3/3/3
3	C2E	J	802	-	-	5/22/62/62	0/6/7/7
2	A16	G	801	1	-	3/12/69/72	1/3/3/3
2	A16	C	801	-	-	5/12/69/72	1/3/3/3
2	A16	I	801	-	-	6/12/69/72	1/3/3/3
3	C2E	D	804	-	-	2/22/62/62	0/6/7/7
2	A16	E	801	-	-	5/12/69/72	1/3/3/3
2	A16	F	801	-	-	7/12/69/72	1/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C2E	I	802	-	-	13/22/62/62	0/6/7/7
3	C2E	C	802	-	-	7/22/62/62	0/6/7/7
2	A16	J	801	-	-	5/12/69/72	1/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	802	C2E	C51-C61	-3.39	1.40	1.47
3	I	802	C2E	C5-C6	-3.26	1.40	1.47
3	C	802	C2E	C51-C61	-3.23	1.40	1.47
3	D	804	C2E	C51-C61	-3.22	1.40	1.47
3	F	802	C2E	C5-C6	-3.16	1.41	1.47
3	J	802	C2E	C5-C6	-3.09	1.41	1.47
3	H	803	C2E	C51-C61	-3.08	1.41	1.47
2	F	801	A16	C2C-C3C	-3.05	1.48	1.52
3	J	802	C2E	C51-C61	-3.01	1.41	1.47
3	H	803	C2E	C5-C6	-3.00	1.41	1.47
3	G	802	C2E	C51-C61	-3.00	1.41	1.47
3	G	802	C2E	C5-C6	-2.99	1.41	1.47
3	C	802	C2E	C5-C6	-2.96	1.41	1.47
3	E	803	C2E	C51-C61	-2.77	1.41	1.47
3	E	803	C2E	C5-C6	-2.77	1.41	1.47
3	D	804	C2E	C5-C6	-2.68	1.42	1.47
3	G	802	C2E	C8-N7	-2.57	1.30	1.35
3	I	802	C2E	C51-C61	-2.56	1.42	1.47
3	J	802	C2E	C81-N71	-2.55	1.30	1.35
3	H	803	C2E	C81-N71	-2.52	1.30	1.35
3	C	802	C2E	C81-N71	-2.50	1.30	1.35
3	C	802	C2E	C51-C41	-2.50	1.36	1.43
3	I	802	C2E	C8-N7	-2.49	1.30	1.35
3	D	804	C2E	C81-N71	-2.45	1.30	1.35
3	I	802	C2E	C81-N71	-2.44	1.30	1.35
3	F	802	C2E	C51-C41	-2.44	1.36	1.43
3	F	802	C2E	C5-C4	-2.43	1.36	1.43
3	H	803	C2E	C5-C4	-2.42	1.36	1.43
3	H	803	C2E	C51-C41	-2.42	1.36	1.43
3	H	803	C2E	C8-N7	-2.39	1.30	1.35
3	F	802	C2E	C81-N71	-2.39	1.30	1.35
3	C	802	C2E	C5-C4	-2.39	1.37	1.43
3	I	802	C2E	C5-C4	-2.35	1.37	1.43
3	J	802	C2E	C51-C41	-2.34	1.37	1.43
3	C	802	C2E	C8-N7	-2.32	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	802	C2E	C5-C4	-2.32	1.37	1.43
3	G	802	C2E	C81-N71	-2.32	1.31	1.35
3	D	804	C2E	C51-C41	-2.31	1.37	1.43
3	E	803	C2E	C8-N7	-2.31	1.31	1.35
2	I	801	A16	C2C-C3C	-2.30	1.49	1.52
3	E	803	C2E	C51-C41	-2.30	1.37	1.43
3	F	802	C2E	C8-N7	-2.30	1.31	1.35
3	I	802	C2E	C51-C41	-2.28	1.37	1.43
3	D	804	C2E	C8-N7	-2.27	1.31	1.35
3	E	803	C2E	C5-C4	-2.25	1.37	1.43
3	J	802	C2E	C8-N7	-2.23	1.31	1.35
3	G	802	C2E	C51-C41	-2.22	1.37	1.43
3	J	802	C2E	C5-C4	-2.19	1.37	1.43
3	E	803	C2E	C81-N71	-2.19	1.31	1.35
3	D	804	C2E	C5-C4	-2.16	1.37	1.43
2	H	801	A16	C2C-C3C	-2.07	1.49	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	801	A16	C5A-C7A-C1A	7.04	117.32	108.49
2	C	801	A16	C1C-C2C-C3C	4.35	115.02	109.67
3	D	804	C2E	O2A-C2A-C1A	-4.31	94.92	110.85
3	J	802	C2E	P1-O3A-C3A	-4.16	104.27	119.41
2	J	801	A16	C5A-C7A-C1A	4.03	113.54	108.49
3	F	802	C2E	O2A-C2A-C1A	-3.96	96.22	110.85
3	H	803	C2E	O2'-C2'-C1'	-3.85	96.63	110.85
3	C	802	C2E	P11-O3'-C3'	-3.84	105.42	119.41
2	E	801	A16	C5A-C7A-C1A	3.78	113.22	108.49
2	F	801	A16	C5A-C7A-C1A	3.75	113.20	108.49
3	D	804	C2E	P11-O3'-C3'	-3.62	106.24	119.41
2	I	801	A16	C5A-C7A-C1A	3.61	113.02	108.49
3	I	802	C2E	P11-O3'-C3'	-3.58	106.36	119.41
3	I	802	C2E	O61-C61-C51	3.36	130.94	124.37
3	I	802	C2E	P1-O3A-C3A	-3.23	107.65	119.41
3	H	803	C2E	P1-O3A-C3A	-3.08	108.20	119.41
3	H	803	C2E	O2A-C2A-C1A	-2.98	99.85	110.85
2	H	801	A16	O5C-C1C-C2C	-2.89	106.31	110.77
2	F	801	A16	C2B-C3B-C4B	-2.85	106.17	110.34
2	I	801	A16	C5B-C4B-N4B	-2.78	104.10	111.74
3	F	802	C2E	P1-O3A-C3A	-2.77	109.31	119.41
3	C	802	C2E	C2A-C3A-C4A	-2.76	98.32	103.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	804	C2E	P1-O3A-C3A	-2.62	109.86	119.41
3	I	802	C2E	O21-P11-O3'	2.60	117.04	106.78
3	E	803	C2E	O2'-C2'-C1'	-2.58	101.34	110.85
3	I	802	C2E	O61-C61-N11	-2.49	117.70	120.65
3	I	802	C2E	O2'-C2'-C3'	-2.45	104.19	111.17
3	F	802	C2E	P11-O5A-C5A	-2.44	107.39	121.68
2	H	801	A16	O3B-C3B-C2B	-2.42	104.76	110.35
3	F	802	C2E	P11-O3'-C3'	-2.41	110.63	119.41
2	C	801	A16	C5A-C7A-C1A	2.41	111.51	108.49
2	D	801	A16	C1C-C2C-C3C	2.38	112.59	109.67
2	D	801	A16	O4A-C4A-C5A	2.37	114.09	110.08
2	G	801	A16	O4A-C4A-C5A	2.36	114.07	110.08
2	G	801	A16	C1C-C2C-C3C	2.36	112.56	109.67
3	D	804	C2E	O61-C61-C51	2.35	128.95	124.37
3	G	802	C2E	O3A-P1-O1P	2.34	118.26	109.47
3	I	802	C2E	O4A-C1A-C2A	-2.34	103.50	106.93
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
3	H	803	C2E	O3A-C3A-C4A	-2.30	101.77	110.08
3	E	803	C2E	O61-C61-C51	2.27	128.81	124.37
3	C	802	C2E	P1-O3A-C3A	-2.26	111.18	119.41
3	D	804	C2E	O3'-P11-O11	-2.25	101.03	109.47
3	J	802	C2E	O3'-P11-O11	-2.23	101.11	109.47
2	H	801	A16	C3A-C2A-C1A	2.22	114.28	111.02
3	I	802	C2E	C2'-C3'-C4'	-2.21	99.31	103.22
3	D	804	C2E	O21-P11-O11	2.19	123.07	112.24
3	E	803	C2E	O6-C6-C5	2.19	128.64	124.37
2	J	801	A16	O2C-C2C-C3C	2.16	114.47	110.14
3	D	804	C2E	O6-C6-C5	2.14	128.56	124.37
3	H	803	C2E	P11-O3'-C3'	-2.11	111.73	119.41
3	E	803	C2E	O2'-C2'-C3'	-2.08	105.27	111.17
2	D	801	A16	C7A-C5A-C6A	-2.07	108.10	111.86
3	G	802	C2E	P1-O3A-C3A	-2.07	111.86	119.41
2	J	801	A16	O4A-C4A-C3A	-2.07	105.56	110.35
2	D	801	A16	O6A-C6A-C5A	-2.06	106.62	111.36
2	G	801	A16	O6A-C6A-C5A	-2.06	106.62	111.36
2	G	801	A16	C7A-C5A-C6A	-2.05	108.14	111.86
3	F	802	C2E	C2A-C3A-C4A	-2.03	99.62	103.22
2	H	801	A16	O4C-C4C-C3C	2.03	112.69	107.28
2	H	801	A16	O2A-C2A-C3A	-2.03	105.66	110.35
3	J	802	C2E	C3'-C2'-C1'	2.02	104.37	99.89

There are no chirality outliers.

All (98) 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-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	O4'-C4'-C5'-O5'
3	G	802	C2E	C2A-C3A-O3A-P1
3	H	803	C2E	C5'-O5'-P1-O2P
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-O21
2	H	801	A16	C3C-C4C-O4C-C1B
3	I	802	C2E	C3'-C4'-C5'-O5'
2	E	801	A16	C5C-C4C-O4C-C1B
3	C	802	C2E	C3A-C4A-C5A-O5A
3	G	802	C2E	C3'-C4'-C5'-O5'
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
3	C	802	C2E	C5A-O5A-P11-O3'
3	I	802	C2E	C5A-O5A-P11-O3'
2	D	801	A16	C5C-C4C-O4C-C1B
2	G	801	A16	C5C-C4C-O4C-C1B
3	C	802	C2E	O4A-C4A-C5A-O5A
2	E	801	A16	C3C-C4C-O4C-C1B

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Mol	Chain	Res	Type	Atoms
2	I	801	A16	C5C-C4C-O4C-C1B
2	E	801	A16	C4C-C5C-C6C-O6C
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	D	801	A16	C3C-C4C-O4C-C1B
2	G	801	A16	C3C-C4C-O4C-C1B
2	C	801	A16	O5C-C5C-C6C-O6C
3	H	803	C2E	O4'-C4'-C5'-O5'
2	C	801	A16	C5C-C4C-O4C-C1B
3	H	803	C2E	C5'-O5'-P1-O3A
2	I	801	A16	C3C-C4C-O4C-C1B
2	C	801	A16	C3C-C4C-O4C-C1B
2	F	801	A16	C4C-C5C-C6C-O6C
3	G	802	C2E	C3A-O3A-P1-O5'
3	I	802	C2E	C3A-O3A-P1-O5'
2	J	801	A16	O5C-C5C-C6C-O6C
3	E	803	C2E	C4'-C3'-O3'-P11
3	J	802	C2E	C4A-C3A-O3A-P1
2	H	801	A16	C4A-C5A-C6A-O6A
3	F	802	C2E	C5'-O5'-P1-O3A
3	E	803	C2E	O4A-C4A-C5A-O5A
2	J	801	A16	C7A-C5A-C6A-O6A
3	C	802	C2E	C2A-C3A-O3A-P1
2	H	801	A16	C5C-C4C-O4C-C1B
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	F	802	C2E	C4'-C3'-O3'-P11
3	C	802	C2E	C5A-O5A-P11-O11
3	H	803	C2E	C5'-O5'-P1-O1P
3	H	803	C2E	C5A-O5A-P11-O11
3	I	802	C2E	C5A-O5A-P11-O11
2	F	801	A16	C3C-C4C-O4C-C1B
3	E	803	C2E	C2'-C3'-O3'-P11
3	F	802	C2E	C2'-C3'-O3'-P11
3	G	802	C2E	C4'-C3'-O3'-P11
3	G	802	C2E	C4A-C3A-O3A-P1
2	J	801	A16	C3C-C4C-O4C-C1B
3	G	802	C2E	C3A-O3A-P1-O2P

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Mol	Chain	Res	Type	Atoms
2	F	801	A16	C4A-C5A-C6A-O6A
3	F	802	C2E	C2A-C3A-O3A-P1
3	J	802	C2E	C2A-C3A-O3A-P1
3	J	802	C2E	C5A-O5A-P11-O3'
3	E	803	C2E	C4A-C3A-O3A-P1
3	D	804	C2E	O4A-C4A-C5A-O5A
2	I	801	A16	O5C-C5C-C6C-O6C
3	D	804	C2E	C5A-O5A-P11-O11
3	F	802	C2E	C5'-O5'-P1-O1P
3	J	802	C2E	C5A-O5A-P11-O11
3	J	802	C2E	O4A-C4A-C5A-O5A
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	E	803	C2E	5	0
3	G	802	C2E	5	0
3	J	802	C2E	4	0
3	D	804	C2E	18	0
2	F	801	A16	7	0
3	F	802	C2E	3	0
2	H	801	A16	5	0
2	G	801	A16	10	0
2	C	801	A16	5	0
2	J	801	A16	10	0
3	H	803	C2E	7	0
4	D	802	PO4	1	0
2	I	801	A16	5	0

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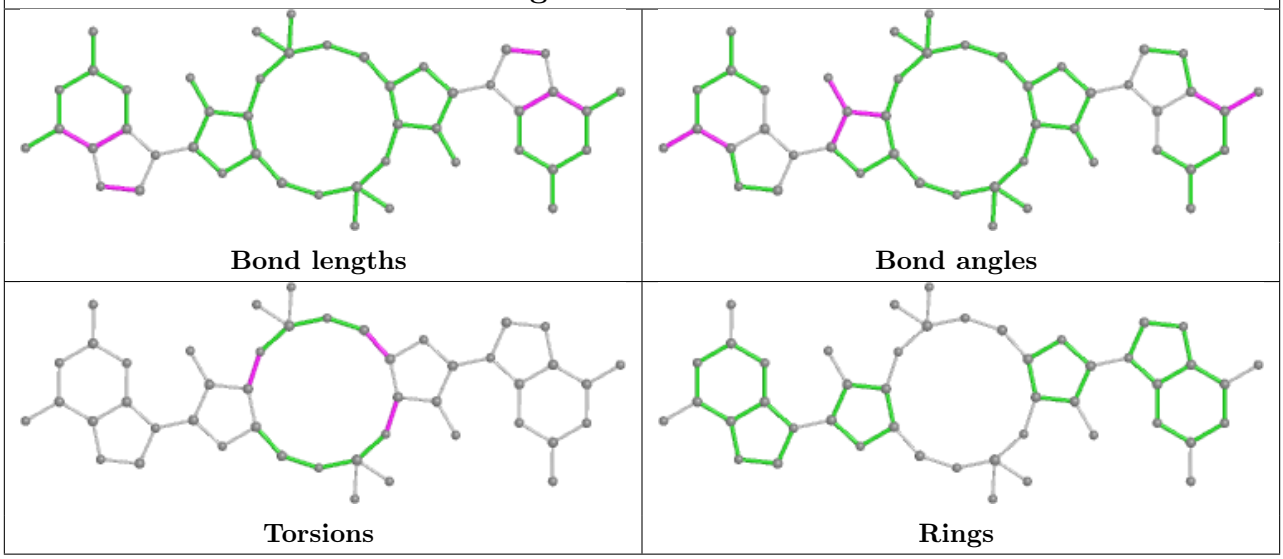
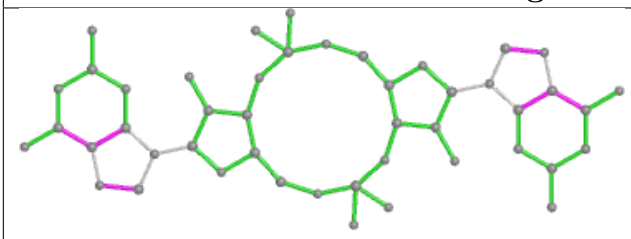
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	802	C2E	7	0
3	C	802	C2E	9	0
2	D	801	A16	7	0
2	E	801	A16	7	0

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 then 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.

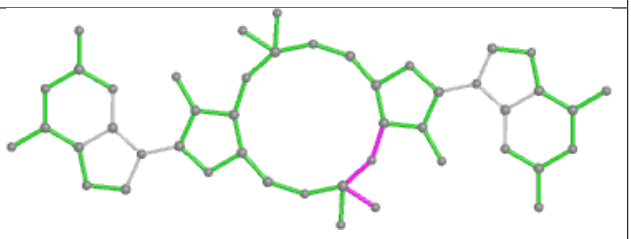
Ligand C2E E 803



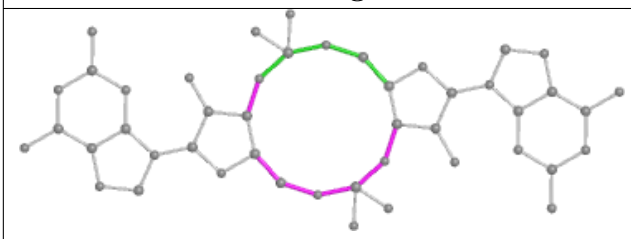
Ligand C2E G 802



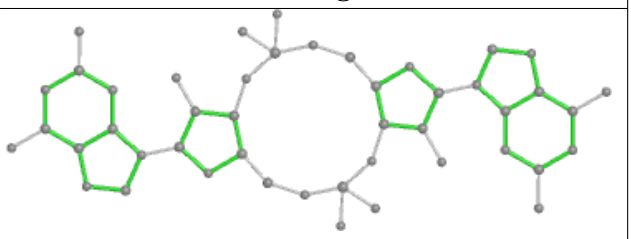
Bond lengths



Bond angles

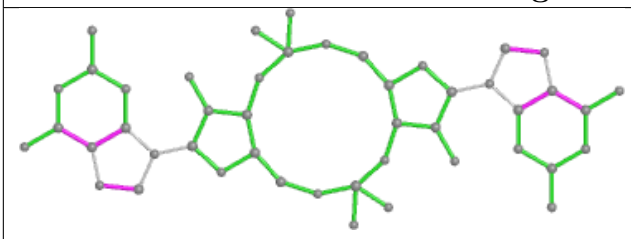


Torsions



Rings

Ligand C2E J 802



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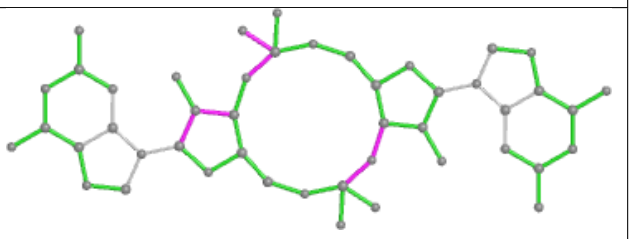
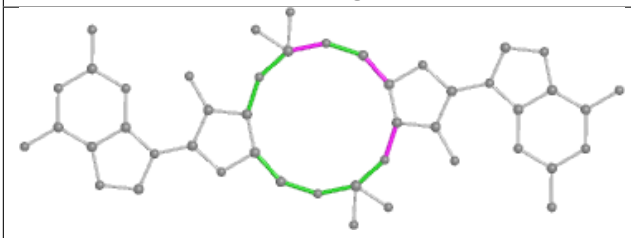


Bond angles



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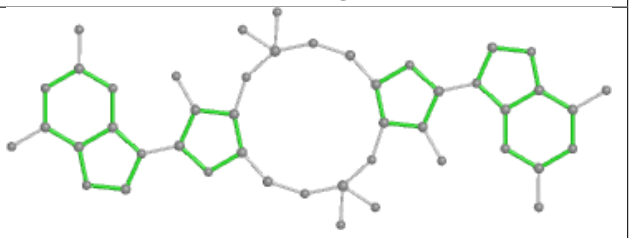
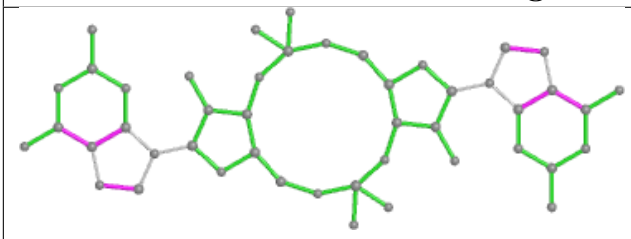


Rings

Ligand C2E D 804



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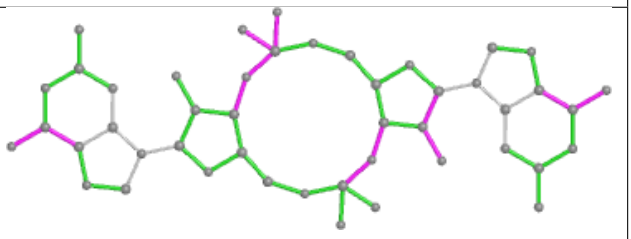
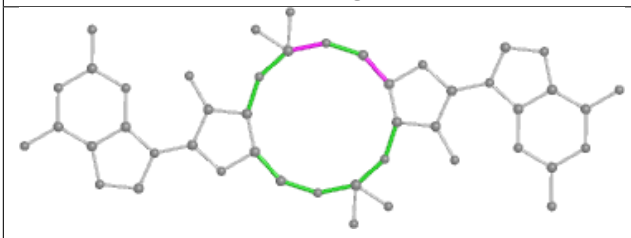


Bond angles



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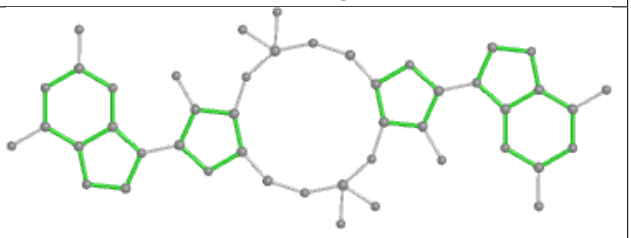
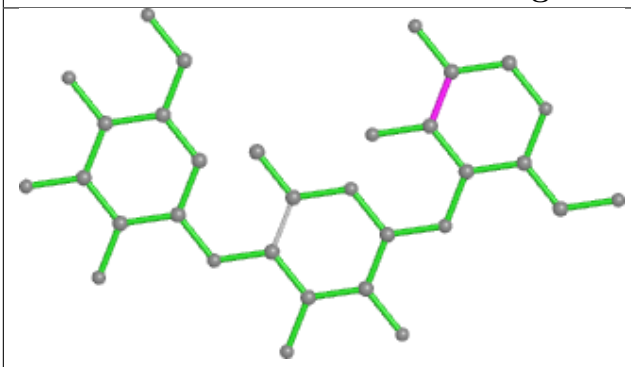


Rings

Ligand A16 F 801



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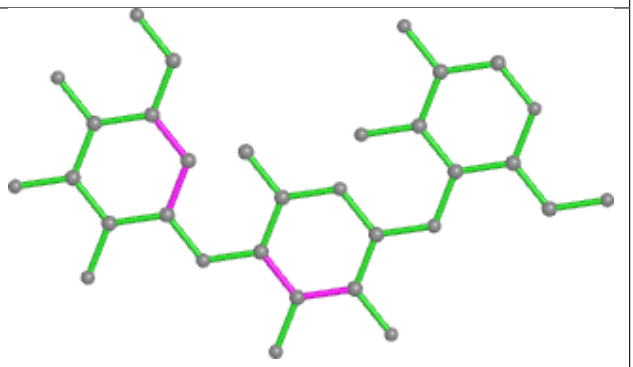

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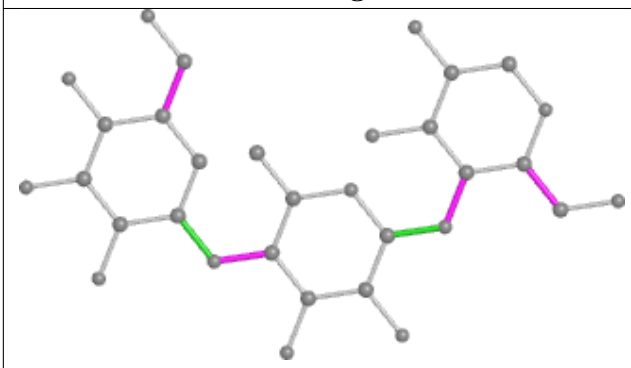

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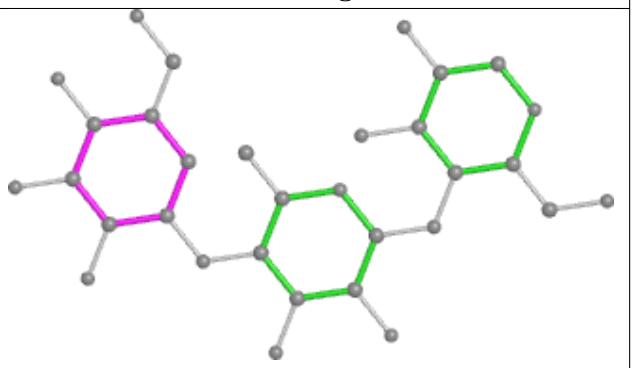
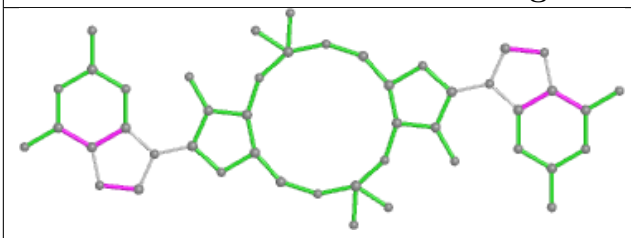


Rings

Ligand C2E F 802



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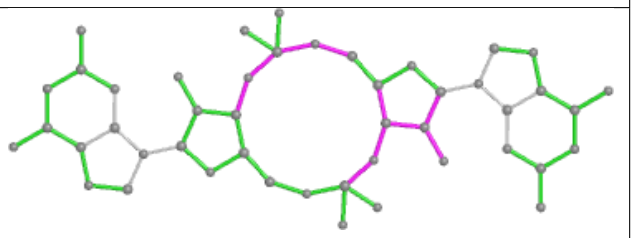

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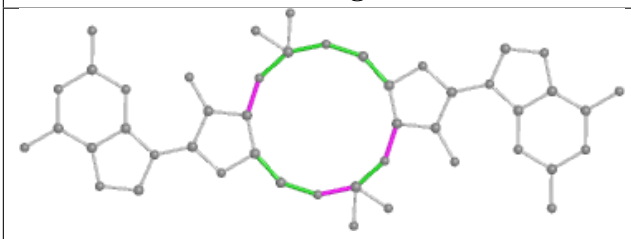

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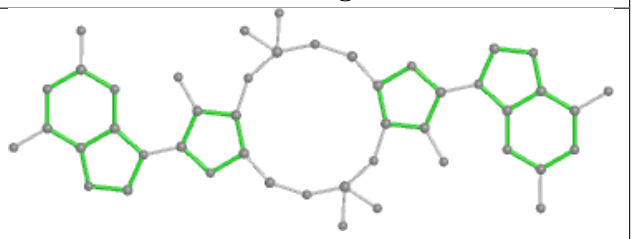

Rings

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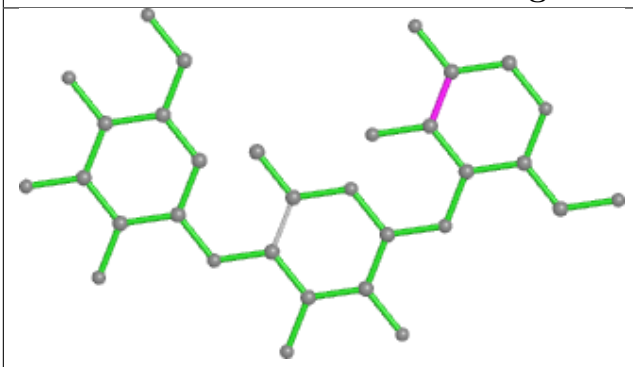

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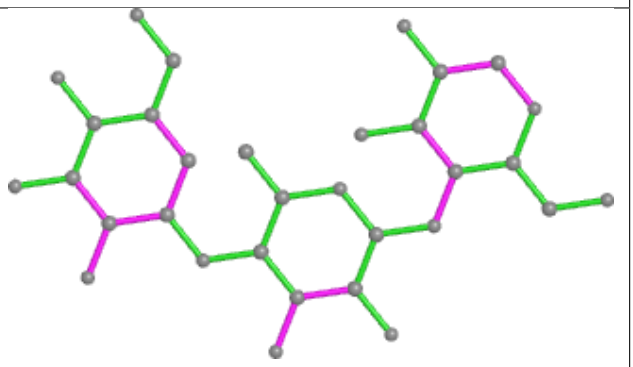

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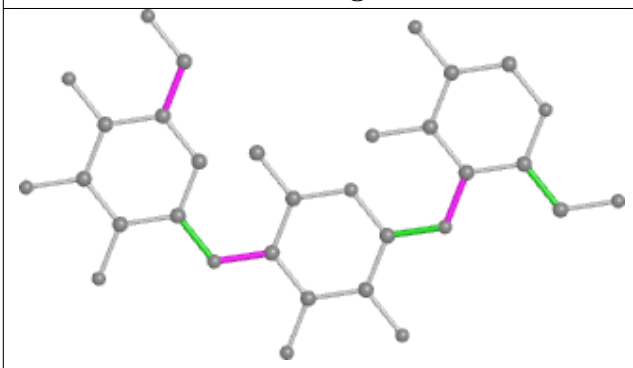

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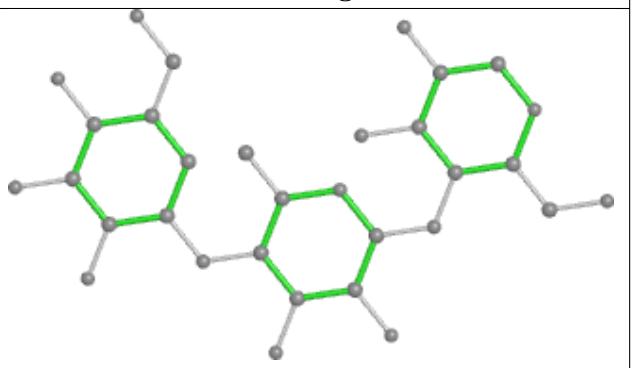

Rings

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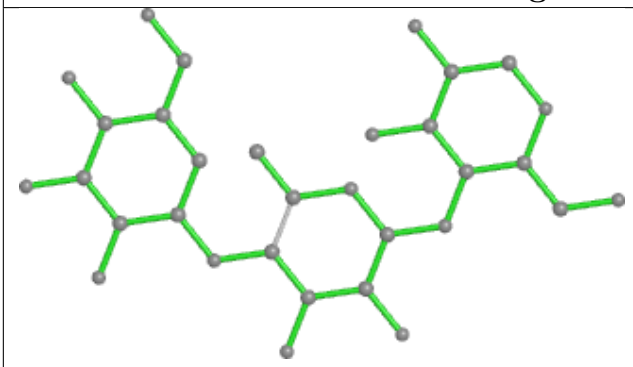

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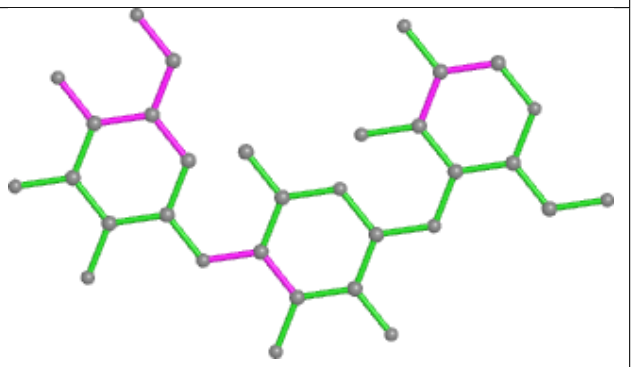

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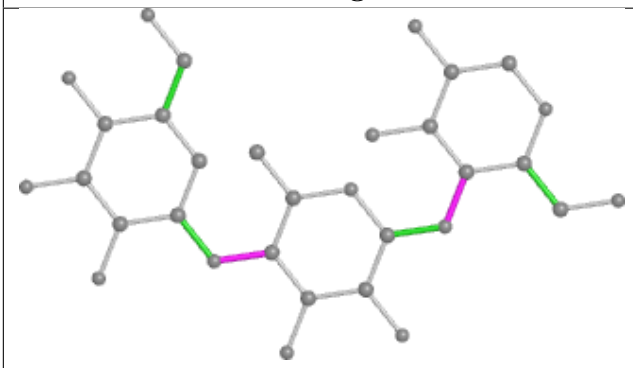

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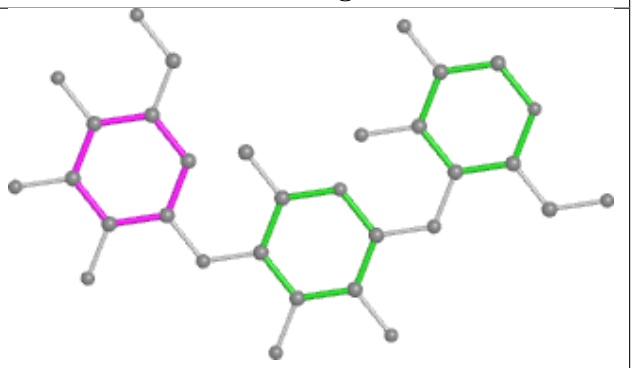
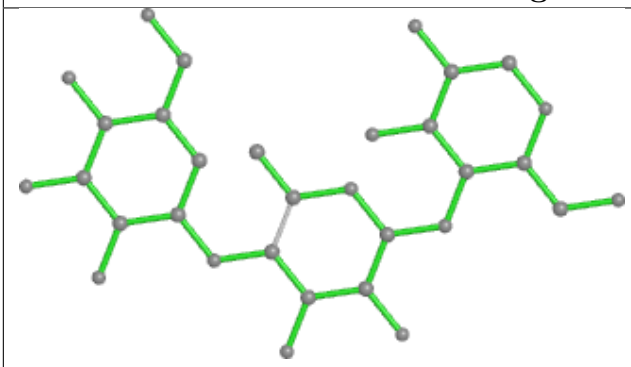


Rings

Ligand A16 C 801



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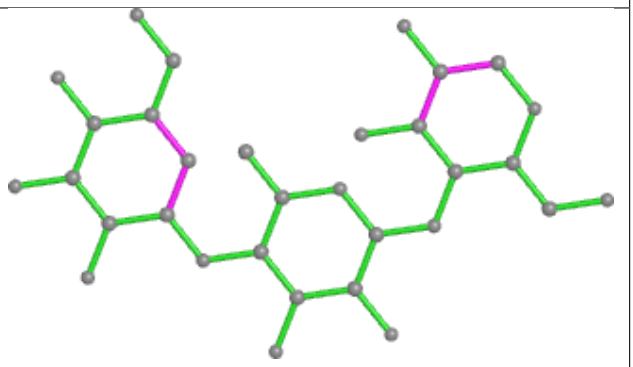

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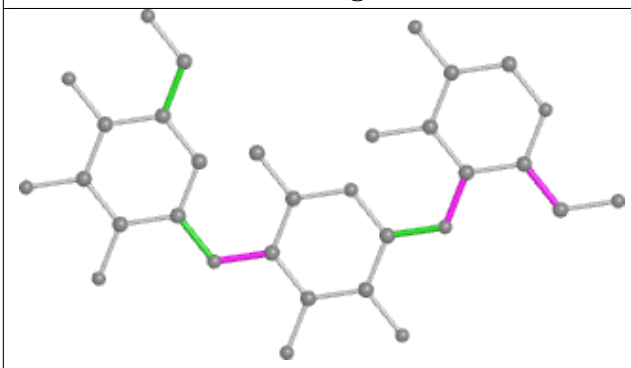

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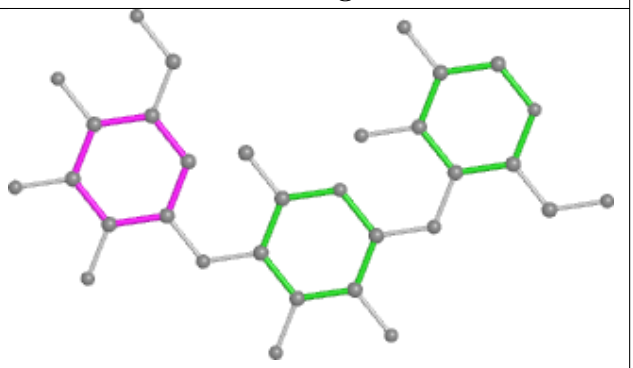
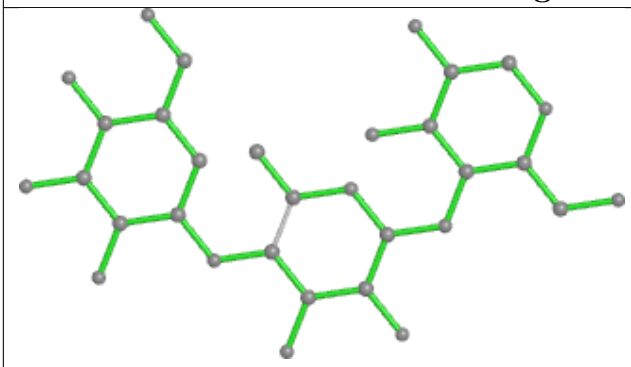


Rings

Ligand A16 J 801



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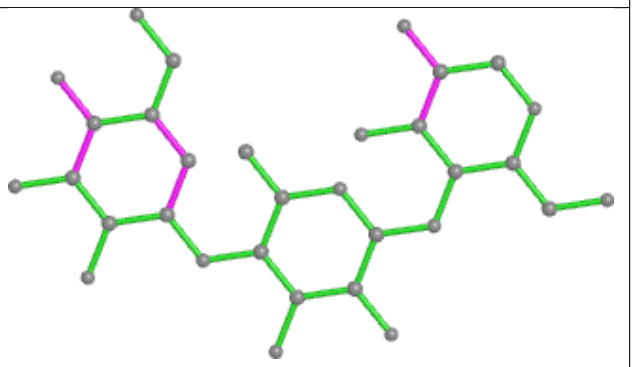

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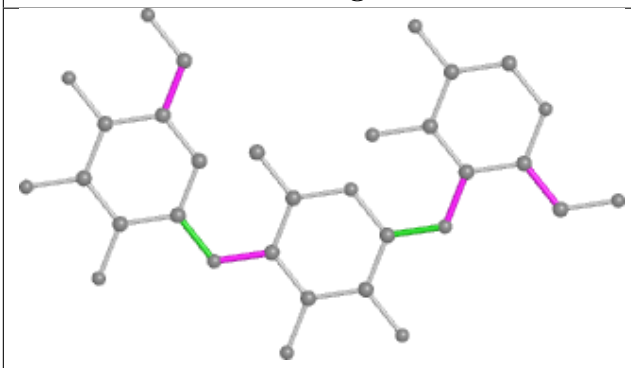

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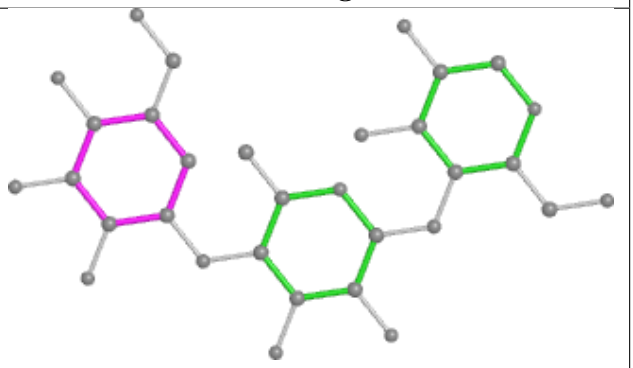
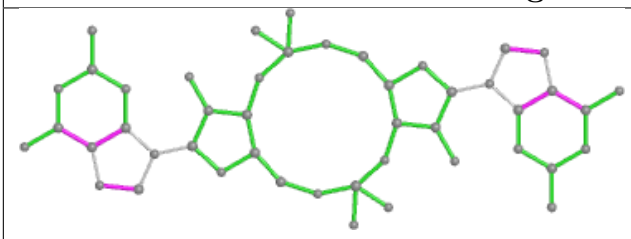


Rings

Ligand C2E H 803



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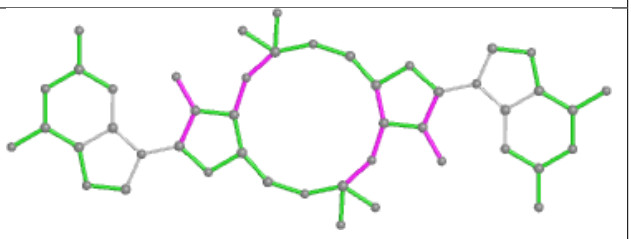

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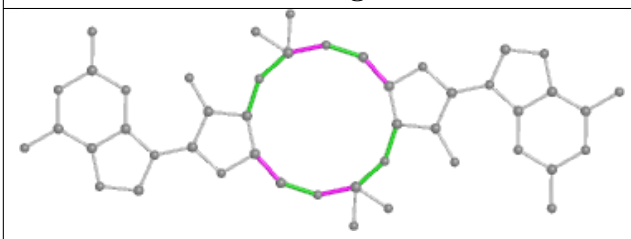

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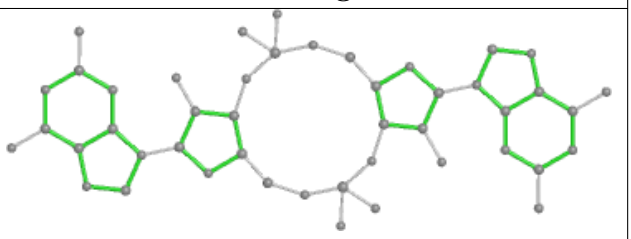
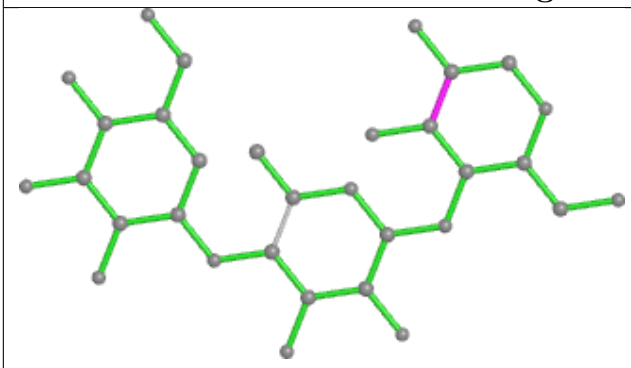


Rings

Ligand A16 I 801



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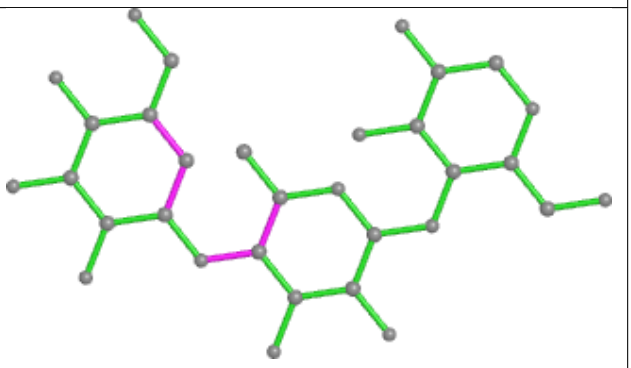
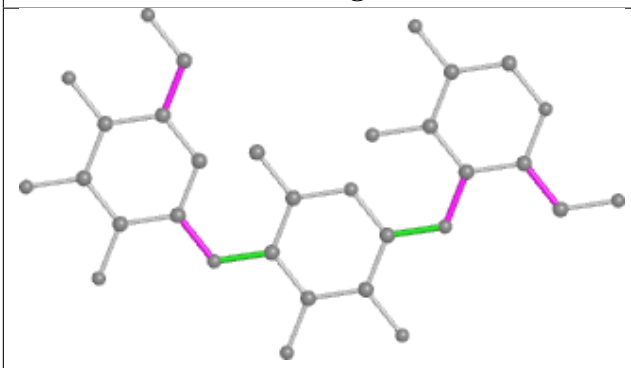


Bond angles



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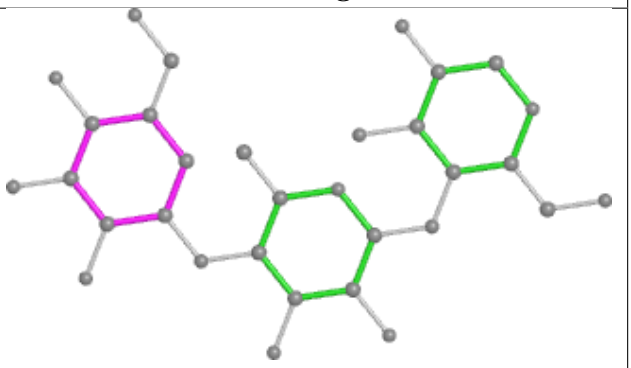
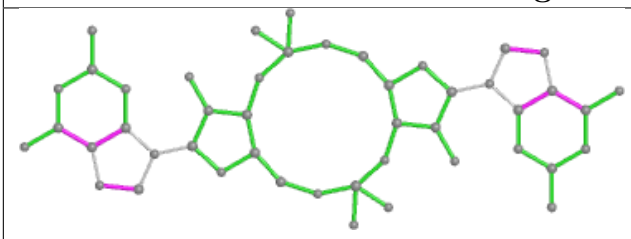
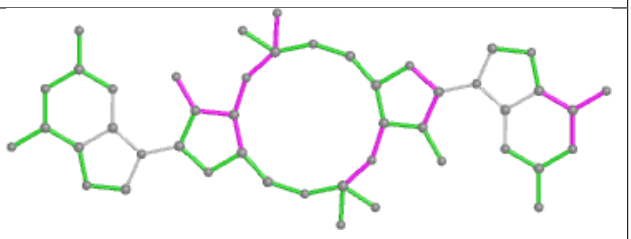


Rings

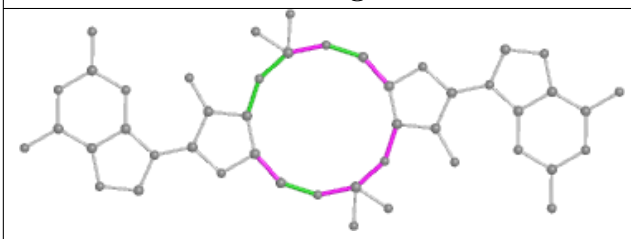
Ligand C2E I 802



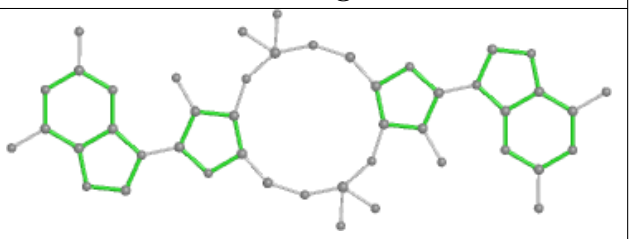
Bond lengths



Bond angles

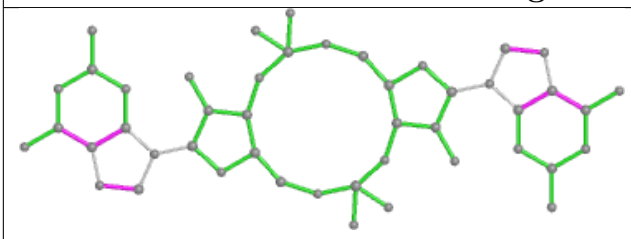


Torsions

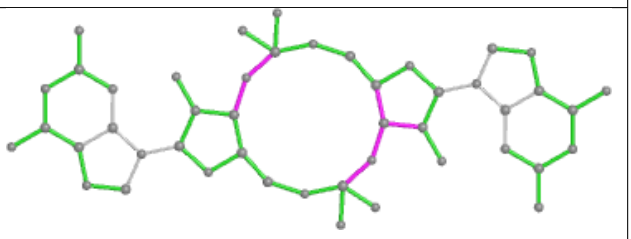


Rings

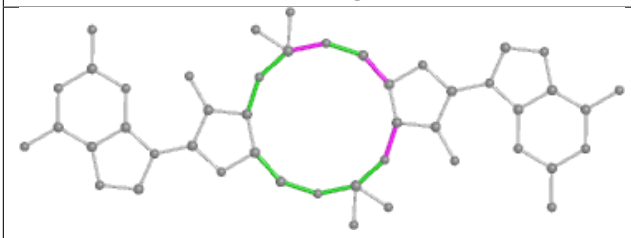
Ligand C2E C 802



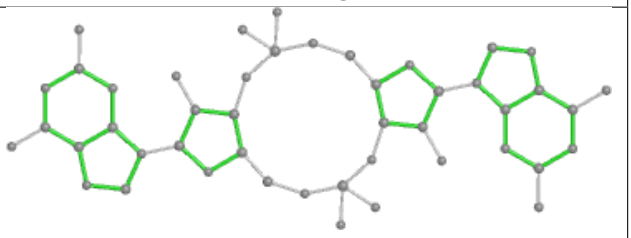
Bond lengths



Bond angles

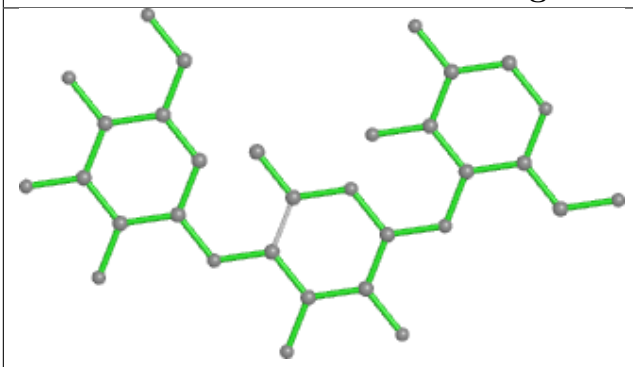


Torsions

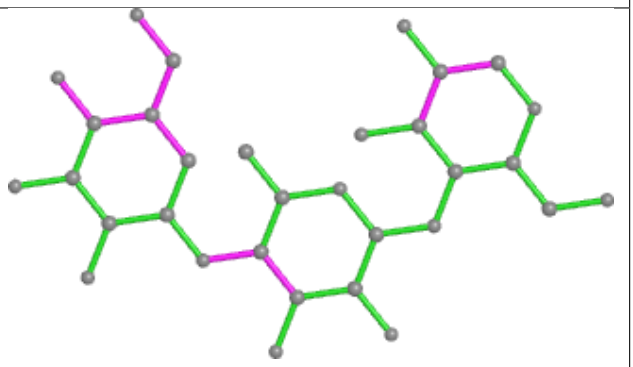


Rings

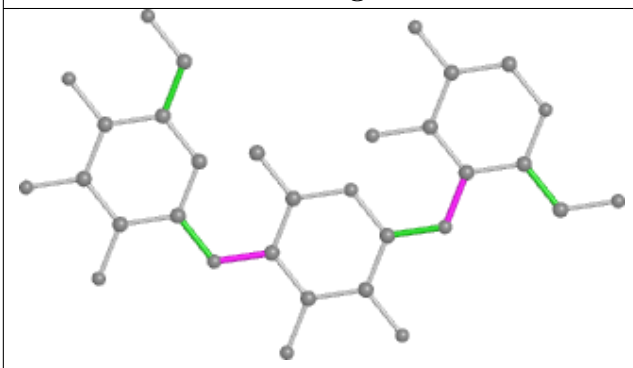
Ligand A16 D 801



Bond lengths



Bond angles



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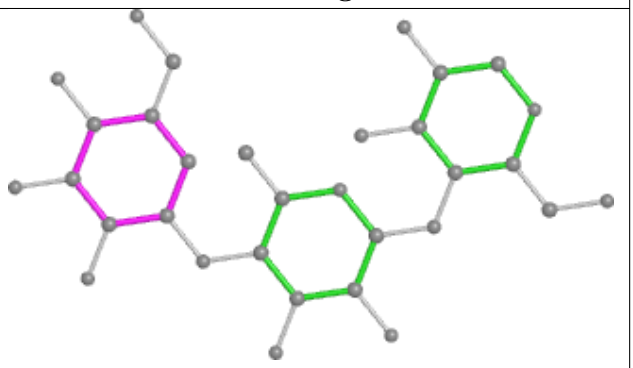
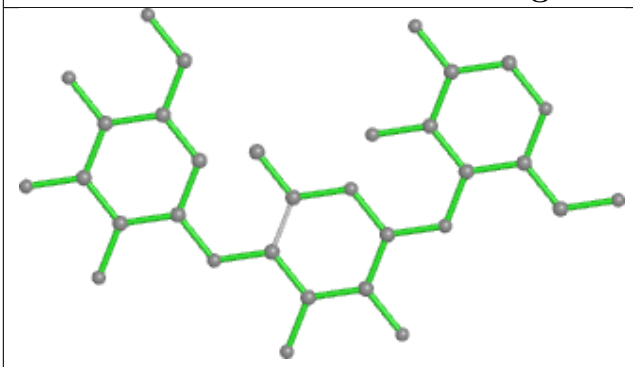
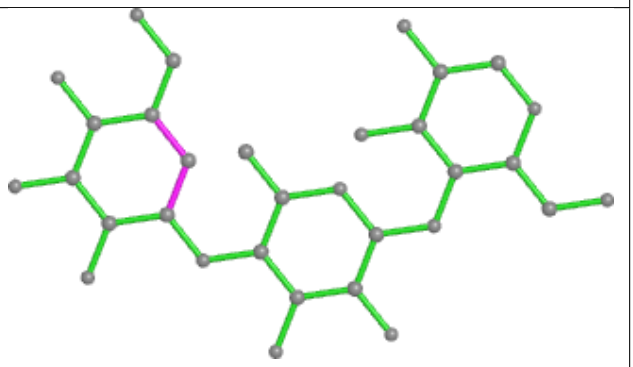


Rings

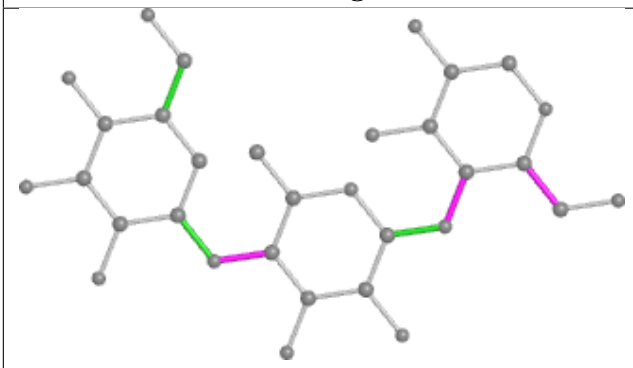
Ligand A16 E 801



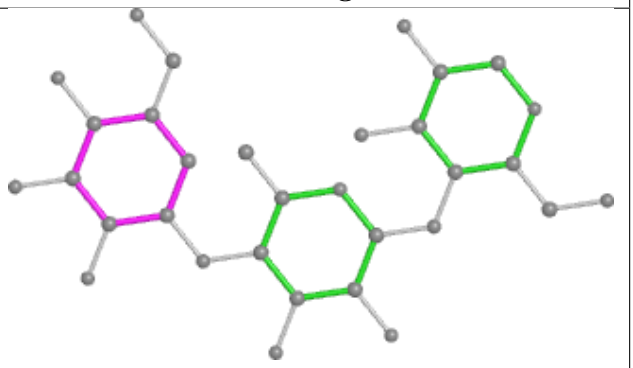
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	696/709 (98%)	-0.38	1 (0%)	95	93	23, 40, 64, 95	0
1	D	694/709 (97%)	-0.43	4 (0%)	89	81	19, 38, 66, 115	0
1	E	696/709 (98%)	-0.40	1 (0%)	95	93	22, 39, 62, 102	0
1	F	694/709 (97%)	-0.32	5 (0%)	87	78	17, 42, 67, 128	0
1	G	693/709 (97%)	-0.31	2 (0%)	94	88	23, 44, 75, 127	0
1	H	696/709 (98%)	-0.27	3 (0%)	92	86	24, 47, 76, 114	0
1	I	696/709 (98%)	-0.11	4 (0%)	89	81	23, 51, 80, 122	0
1	J	694/709 (97%)	-0.17	3 (0%)	92	86	23, 49, 83, 128	0
All	All	5559/5672 (98%)	-0.30	23 (0%)	92	86	17, 43, 74, 128	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	684	PRO	4.2
1	D	586	VAL	3.5
1	I	663	GLY	3.2
1	F	615	HIS	3.1
1	F	600	THR	3.0
1	F	593	LEU	2.7
1	J	666	TRP	2.7
1	I	666	TRP	2.3
1	H	587	GLU	2.3
1	D	585	PRO	2.3
1	F	660	ASP	2.3
1	E	43	GLU	2.2
1	J	684	PRO	2.2
1	G	43	GLU	2.2
1	H	585	PRO	2.2
1	H	471	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	687	ALA	2.1
1	C	351	PHE	2.1
1	D	608	SER	2.1
1	D	662	HIS	2.1
1	I	627	ALA	2.1
1	J	549	LYS	2.0
1	F	687	ALA	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A16	G	801	32/33	0.69	0.43	77,107,116,124	0
2	A16	I	801	32/33	0.74	0.32	77,107,116,124	0
2	A16	D	801	32/33	0.79	0.33	77,107,116,124	0
2	A16	J	801	32/33	0.79	0.33	78,107,116,124	0
2	A16	E	801	32/33	0.80	0.37	77,108,116,124	0
2	A16	H	801	32/33	0.83	0.28	78,107,120,124	0
4	PO4	D	802	5/5	0.84	0.41	70,72,82,88	0
2	A16	F	801	32/33	0.86	0.24	27,42,63,83	0
2	A16	C	801	32/33	0.87	0.28	70,82,105,114	0
4	PO4	D	803	5/5	0.88	0.24	66,70,75,84	0
3	C2E	D	804	46/46	0.89	0.24	96,101,117,122	0
3	C2E	E	803	46/46	0.92	0.22	39,47,59,66	0
3	C2E	G	802	46/46	0.93	0.19	28,49,58,65	0
3	C2E	I	802	46/46	0.93	0.22	38,46,55,59	0
4	PO4	E	802	5/5	0.93	0.24	44,45,61,76	0
3	C2E	J	802	46/46	0.94	0.20	29,49,60,63	0

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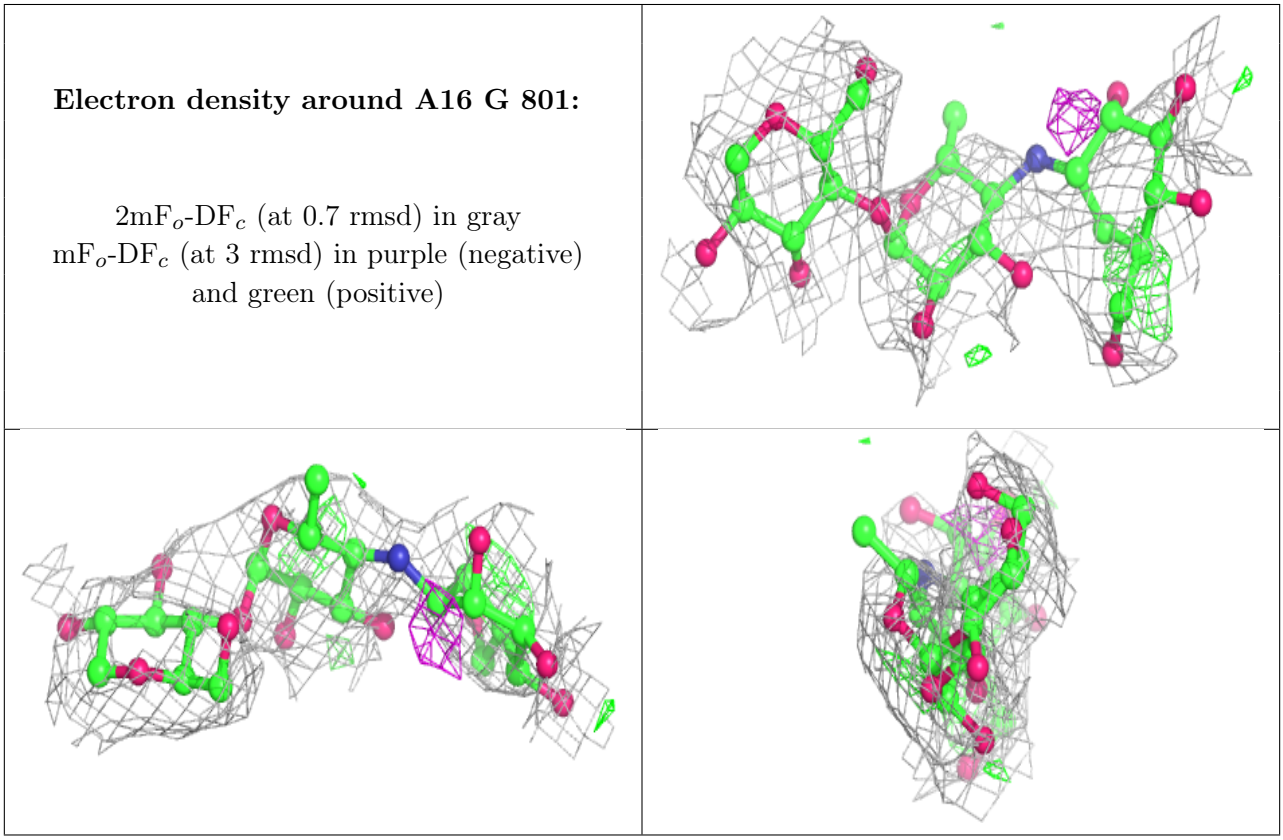
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	C2E	C	802	46/46	0.94	0.17	45,52,60,66	0
3	C2E	H	803	46/46	0.96	0.15	29,39,55,61	0
3	C2E	F	802	46/46	0.96	0.15	29,39,45,51	0
4	PO4	H	802	5/5	0.97	0.29	55,58,67,70	0

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.

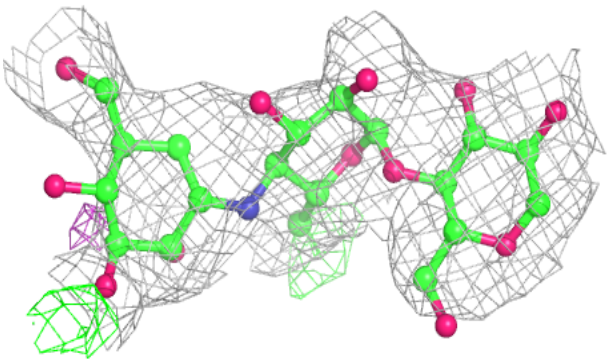
Electron density around A16 G 801:

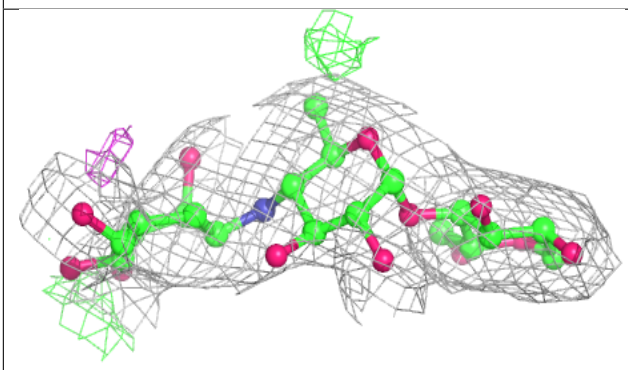
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

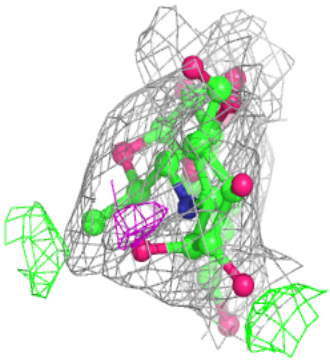


Electron density around A16 I 801:

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

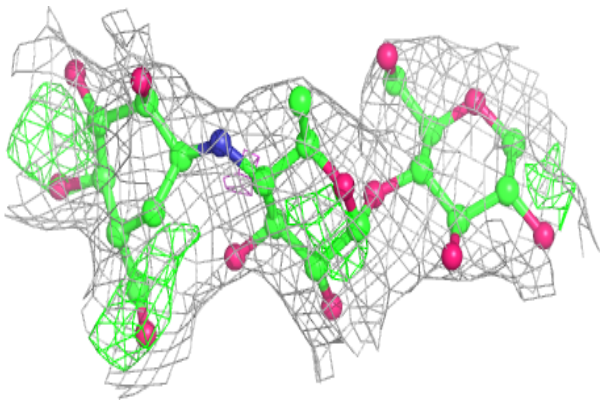


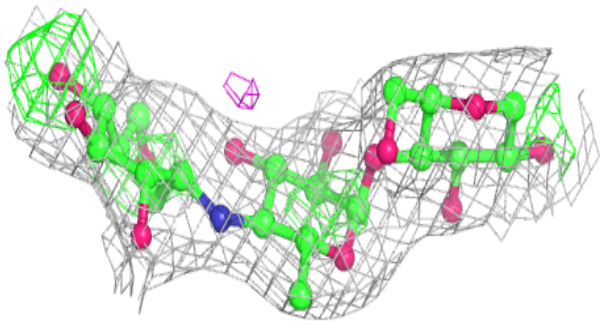


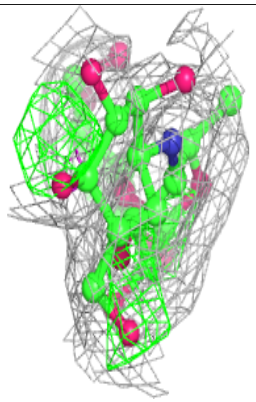


Electron density around A16 D 801:

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

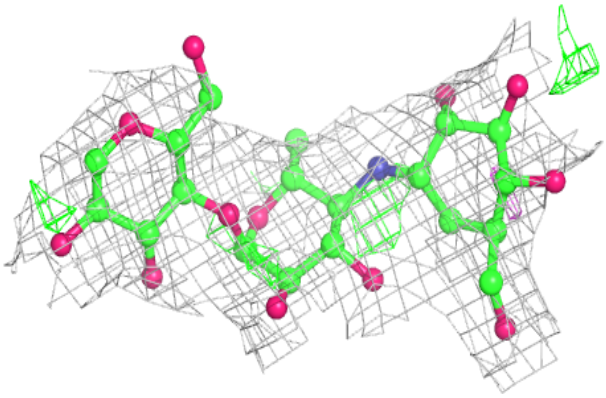


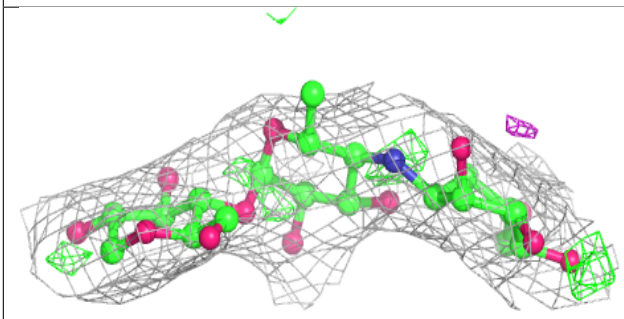


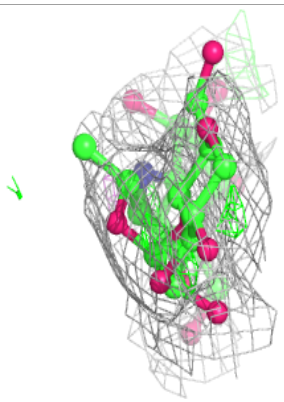


Electron density around A16 J 801:

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

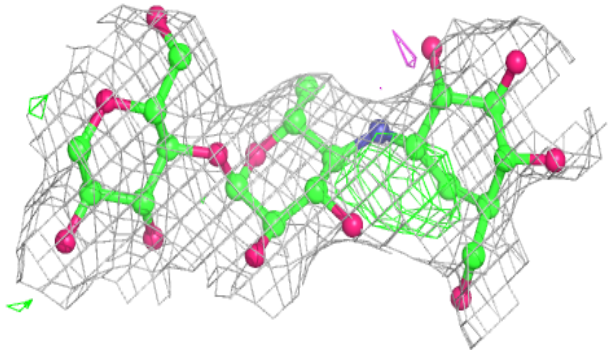


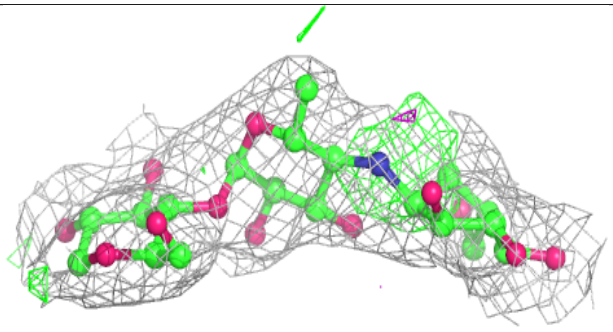


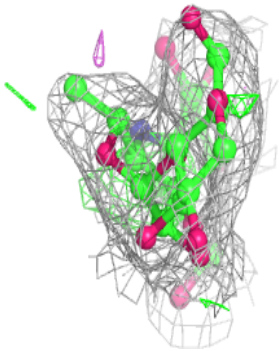


Electron density around A16 E 801:

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

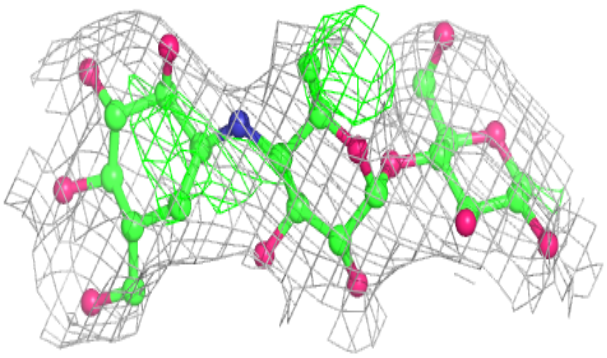


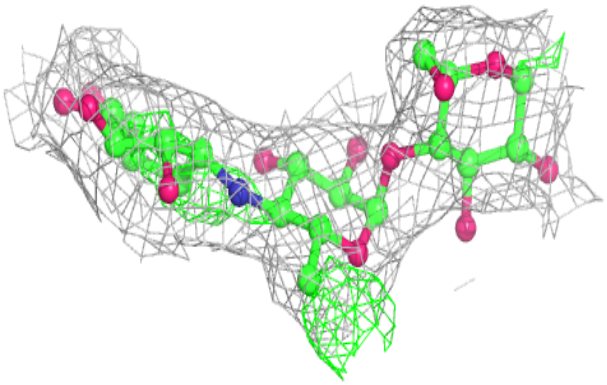


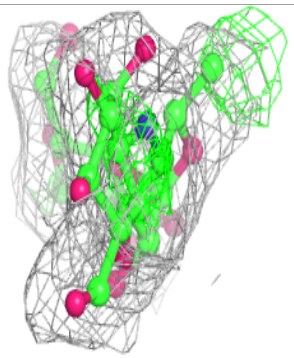


Electron density around A16 H 801:

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

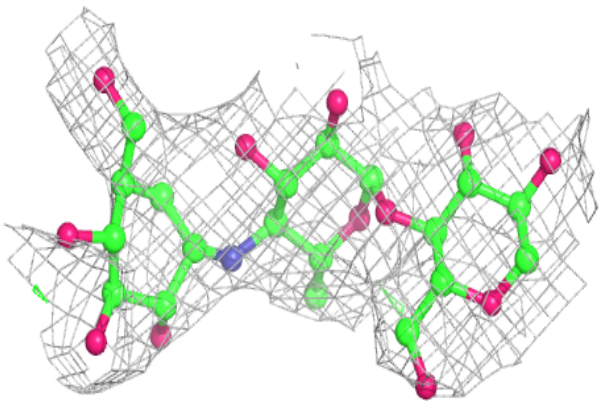


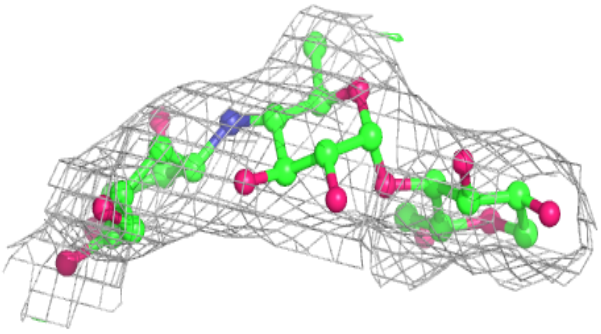


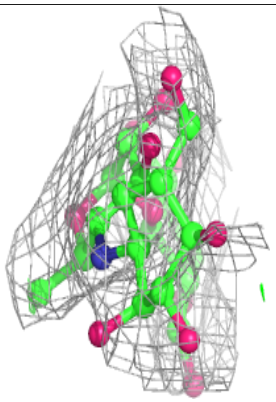


Electron density around A16 F 801:

$2mF_o$-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 C 801:

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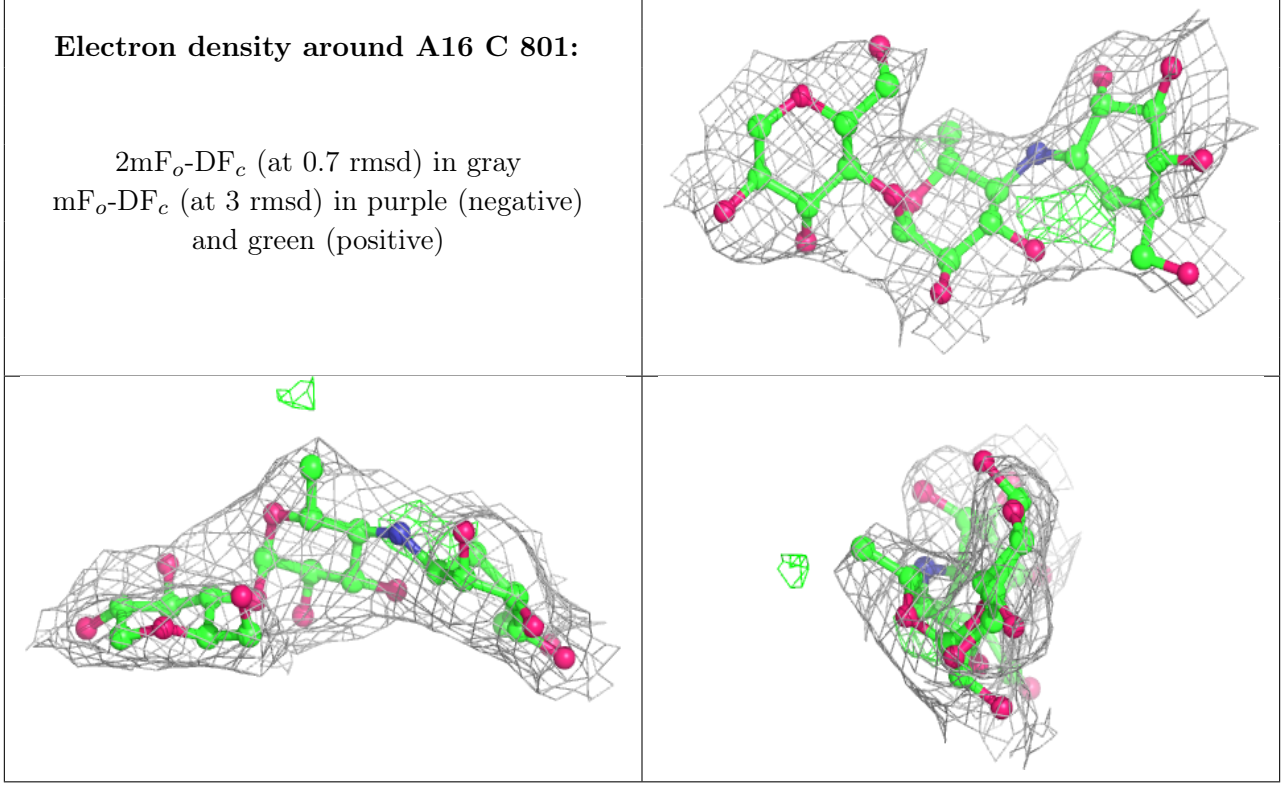
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around C2E D 804:

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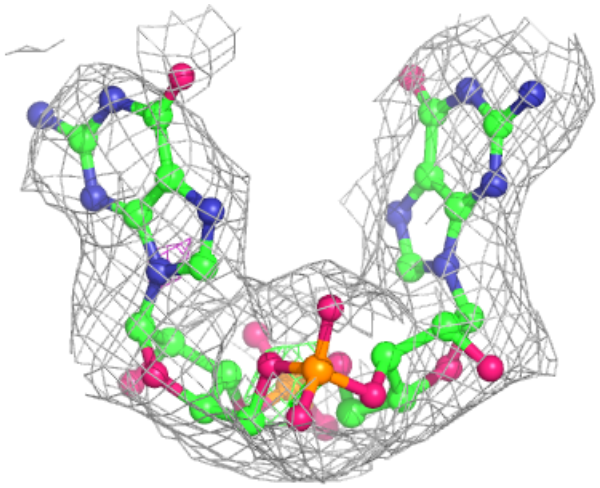
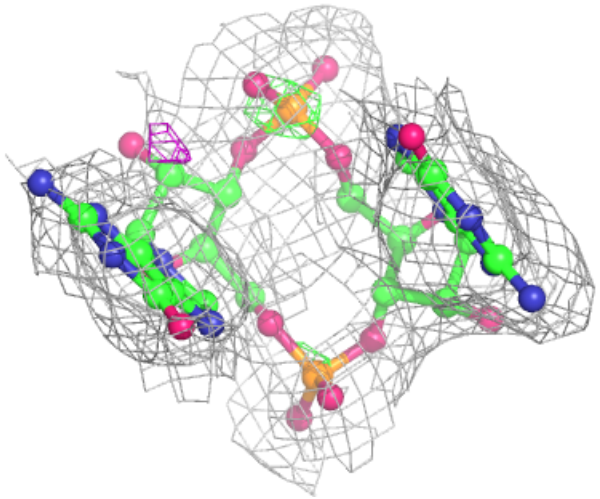
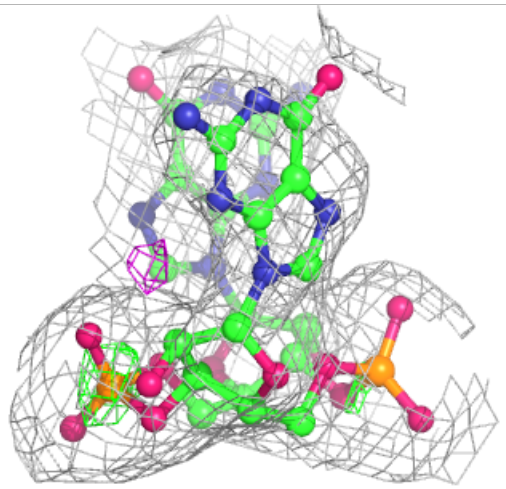
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

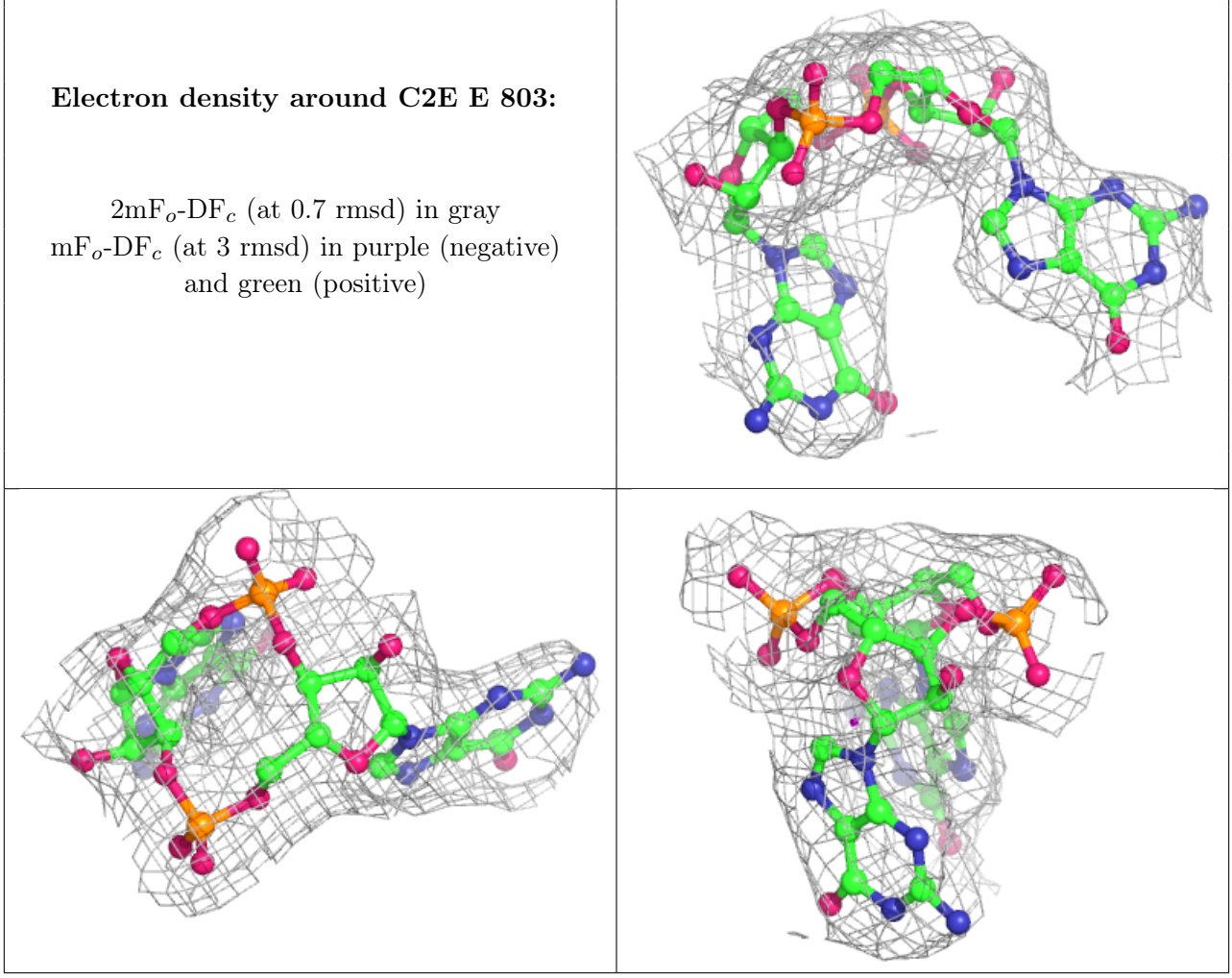






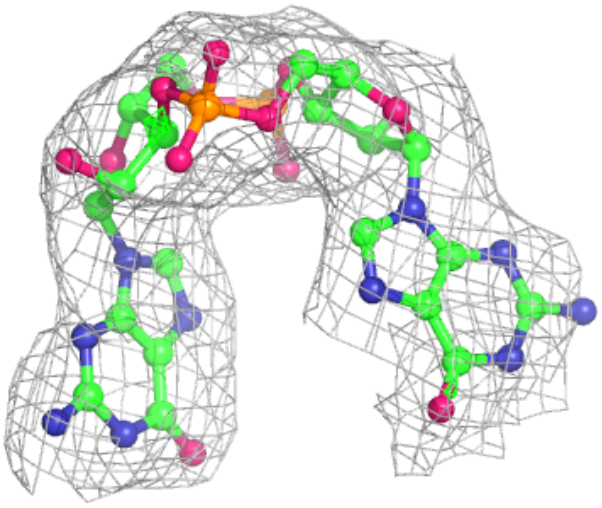
Electron density around C2E E 803:

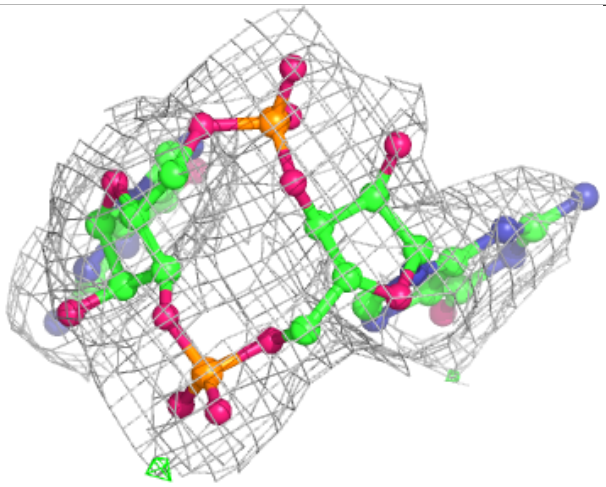
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

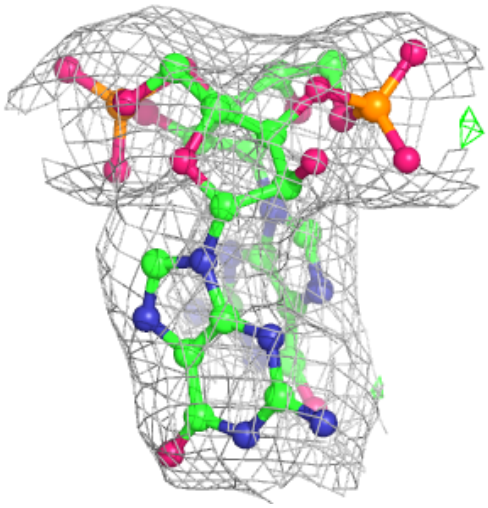


Electron density around C2E G 802:

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

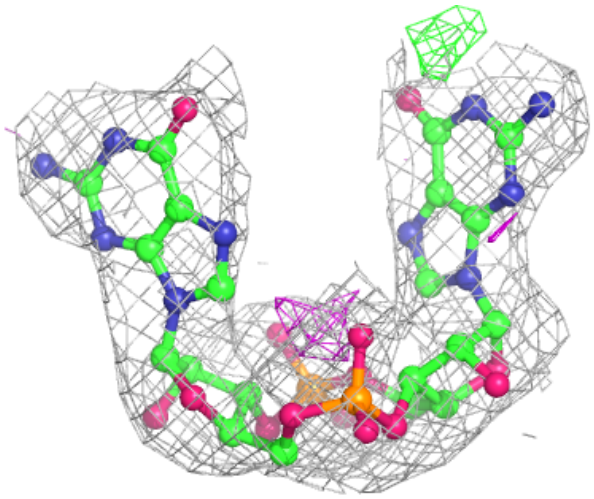


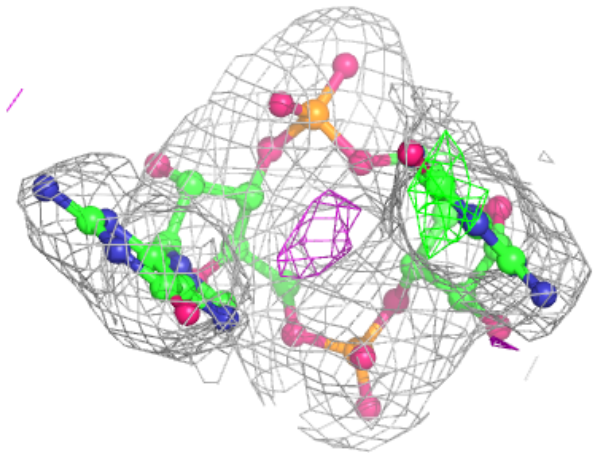


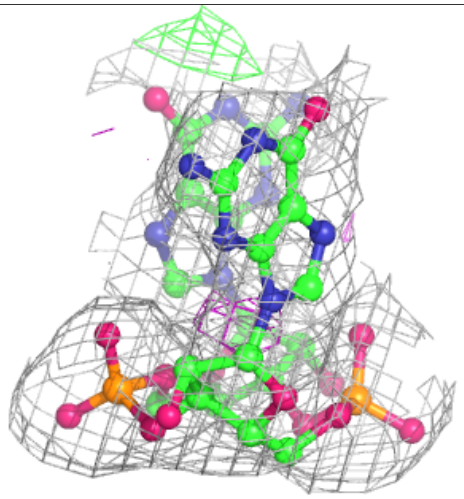


Electron density around C2E I 802:

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

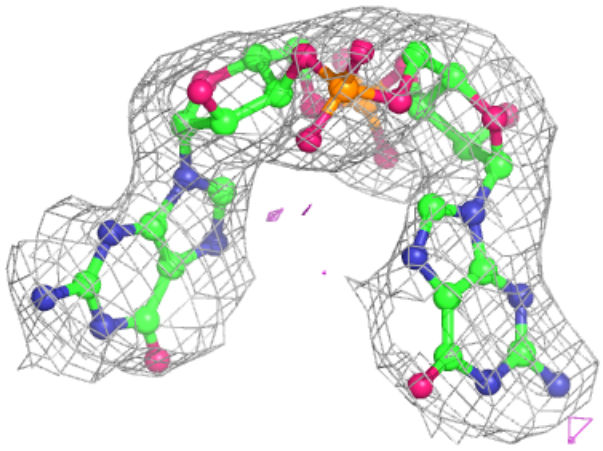


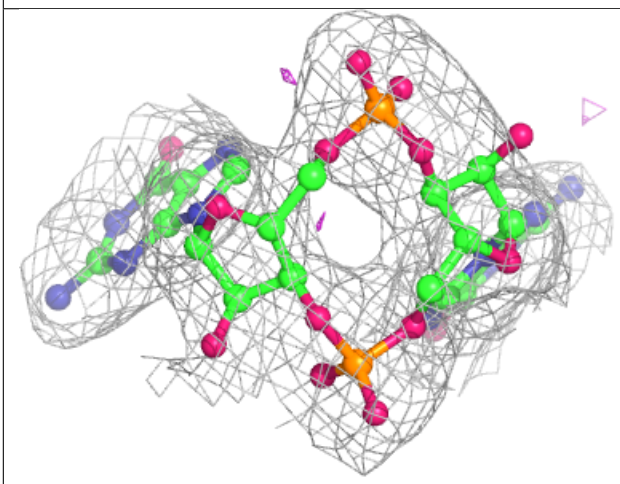


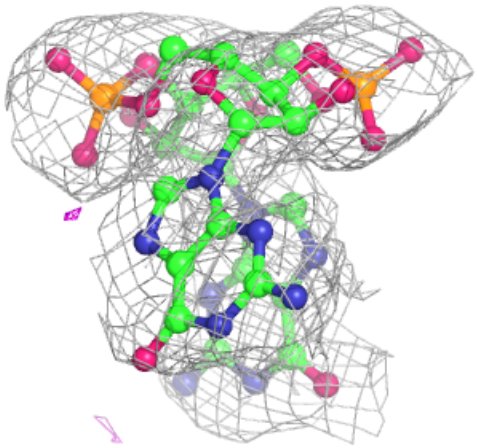


Electron density around C2E J 802:

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

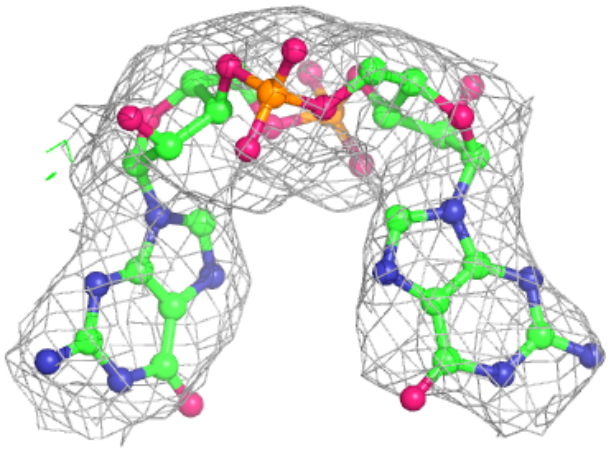


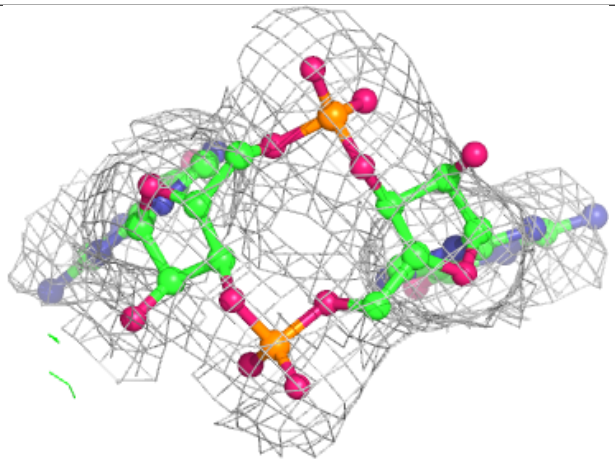


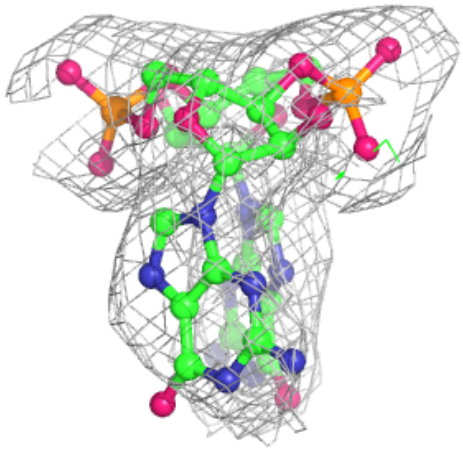


Electron density around C2E C 802:

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

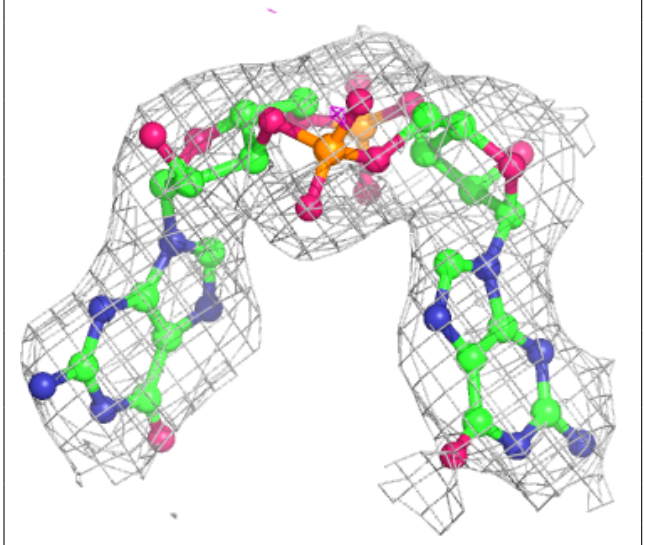


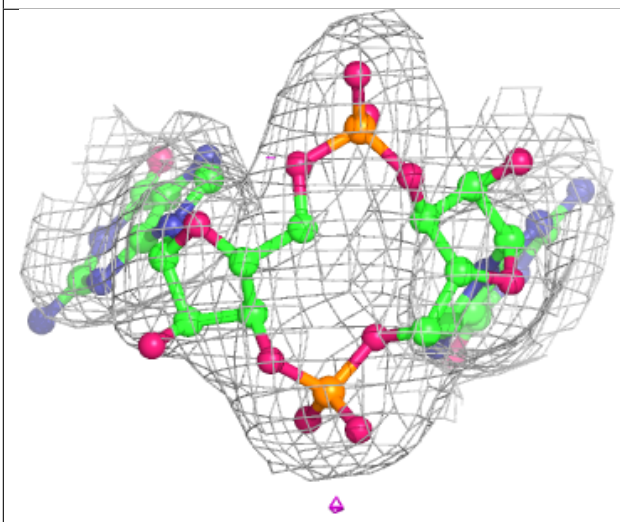


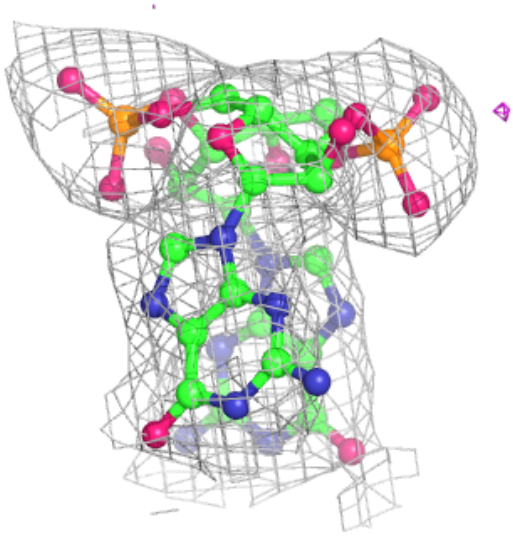


Electron density around C2E H 803:

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

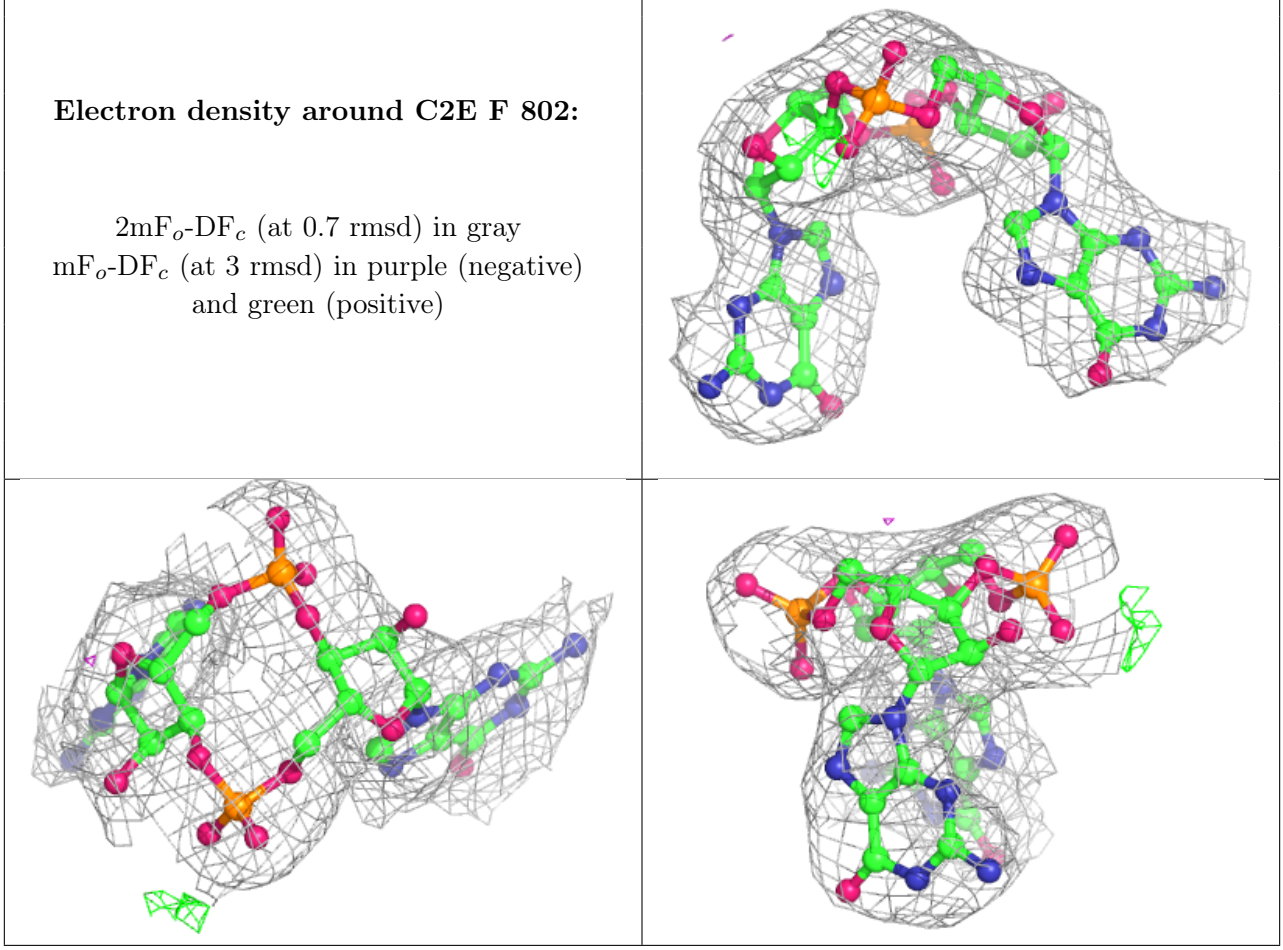






Electron density around C2E F 802:

$2mF_o$-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

There are no such residues in this entry.