Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 08:38 AM JST

PDB ID	:	6LE4
Title	:	Crystal structure of cystathionine gamma-lyase from Lactobacillus plantarum complexed with cystathionine
Authors	:	Oda, K.; Matoba, Y.
Deposited on	:	2019-11-24
Resolution	:	3.10 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:

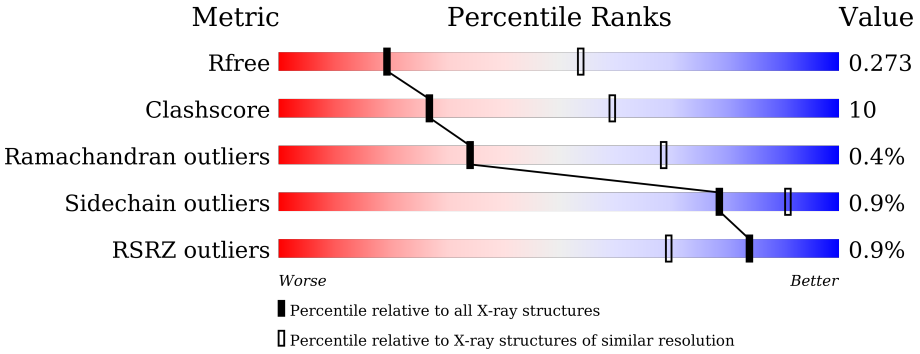
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	A	389	77% 20% • •
1	B	389	2% 74% 22% • •
1	C	389	% 74% 23% • •
1	D	389	76% 21% • •
1	E	389	2% 75% 22% • •
1	F	389	% 76% 21% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17687 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 Cystathionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	380	2867	1829	482	547	9	0	0	0
1	B	380	2867	1829	482	547	9	0	0	0
1	C	380	2867	1829	482	547	9	0	0	0
1	D	380	2867	1829	482	547	9	0	0	0
1	E	380	2867	1829	482	547	9	0	0	0
1	F	380	2867	1829	482	547	9	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

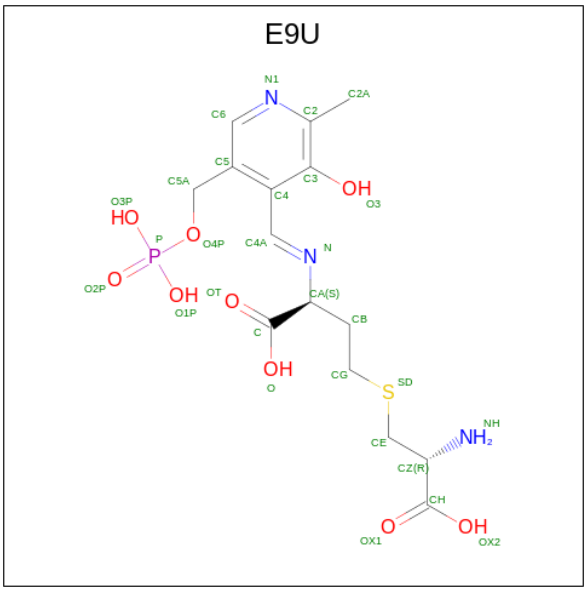
Chain	Residue	Modelled	Actual	Comment	Reference
A	194	ALA	LYS	engineered mutation	UNP A0A162EFJ4
A	382	LEU	-	expression tag	UNP A0A162EFJ4
A	383	GLU	-	expression tag	UNP A0A162EFJ4
A	384	HIS	-	expression tag	UNP A0A162EFJ4
A	385	HIS	-	expression tag	UNP A0A162EFJ4
A	386	HIS	-	expression tag	UNP A0A162EFJ4
A	387	HIS	-	expression tag	UNP A0A162EFJ4
A	388	HIS	-	expression tag	UNP A0A162EFJ4
A	389	HIS	-	expression tag	UNP A0A162EFJ4
B	194	ALA	LYS	engineered mutation	UNP A0A162EFJ4
B	382	LEU	-	expression tag	UNP A0A162EFJ4
B	383	GLU	-	expression tag	UNP A0A162EFJ4
B	384	HIS	-	expression tag	UNP A0A162EFJ4
B	385	HIS	-	expression tag	UNP A0A162EFJ4
B	386	HIS	-	expression tag	UNP A0A162EFJ4
B	387	HIS	-	expression tag	UNP A0A162EFJ4
B	388	HIS	-	expression tag	UNP A0A162EFJ4

Continued on next page...

Continued from previous page...

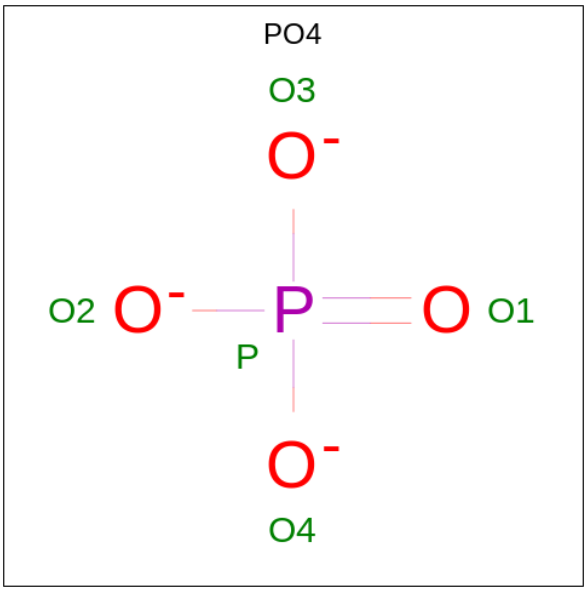
Chain	Residue	Modelled	Actual	Comment	Reference
B	389	HIS	-	expression tag	UNP A0A162EFJ4
C	194	ALA	LYS	engineered mutation	UNP A0A162EFJ4
C	382	LEU	-	expression tag	UNP A0A162EFJ4
C	383	GLU	-	expression tag	UNP A0A162EFJ4
C	384	HIS	-	expression tag	UNP A0A162EFJ4
C	385	HIS	-	expression tag	UNP A0A162EFJ4
C	386	HIS	-	expression tag	UNP A0A162EFJ4
C	387	HIS	-	expression tag	UNP A0A162EFJ4
C	388	HIS	-	expression tag	UNP A0A162EFJ4
C	389	HIS	-	expression tag	UNP A0A162EFJ4
D	194	ALA	LYS	engineered mutation	UNP A0A162EFJ4
D	382	LEU	-	expression tag	UNP A0A162EFJ4
D	383	GLU	-	expression tag	UNP A0A162EFJ4
D	384	HIS	-	expression tag	UNP A0A162EFJ4
D	385	HIS	-	expression tag	UNP A0A162EFJ4
D	386	HIS	-	expression tag	UNP A0A162EFJ4
D	387	HIS	-	expression tag	UNP A0A162EFJ4
D	388	HIS	-	expression tag	UNP A0A162EFJ4
D	389	HIS	-	expression tag	UNP A0A162EFJ4
E	194	ALA	LYS	engineered mutation	UNP A0A162EFJ4
E	382	LEU	-	expression tag	UNP A0A162EFJ4
E	383	GLU	-	expression tag	UNP A0A162EFJ4
E	384	HIS	-	expression tag	UNP A0A162EFJ4
E	385	HIS	-	expression tag	UNP A0A162EFJ4
E	386	HIS	-	expression tag	UNP A0A162EFJ4
E	387	HIS	-	expression tag	UNP A0A162EFJ4
E	388	HIS	-	expression tag	UNP A0A162EFJ4
E	389	HIS	-	expression tag	UNP A0A162EFJ4
F	194	ALA	LYS	engineered mutation	UNP A0A162EFJ4
F	382	LEU	-	expression tag	UNP A0A162EFJ4
F	383	GLU	-	expression tag	UNP A0A162EFJ4
F	384	HIS	-	expression tag	UNP A0A162EFJ4
F	385	HIS	-	expression tag	UNP A0A162EFJ4
F	386	HIS	-	expression tag	UNP A0A162EFJ4
F	387	HIS	-	expression tag	UNP A0A162EFJ4
F	388	HIS	-	expression tag	UNP A0A162EFJ4
F	389	HIS	-	expression tag	UNP A0A162EFJ4

- Molecule 2 is (2 {S})-4-[(2 {R})-2-azanyl-3-oxidanyl-3-oxidanylidene-propyl]sulfanyl-2-[({E})-[2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]methylideneamino]butanoic acid (three-letter code: E9U) (formula: $C_{15}H_{22}N_3O_9PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	29	15	3	9	1	1	0	0
			Total	C	N	O	P	S		
2	B	1	29	15	3	9	1	1	0	0
			Total	C	N	O	P	S		
2	C	1	29	15	3	9	1	1	0	0
			Total	C	N	O	P	S		
2	D	1	29	15	3	9	1	1	0	0
			Total	C	N	O	P	S		
2	E	1	29	15	3	9	1	1	0	0
			Total	C	N	O	P	S		
2	F	1	29	15	3	9	1	1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

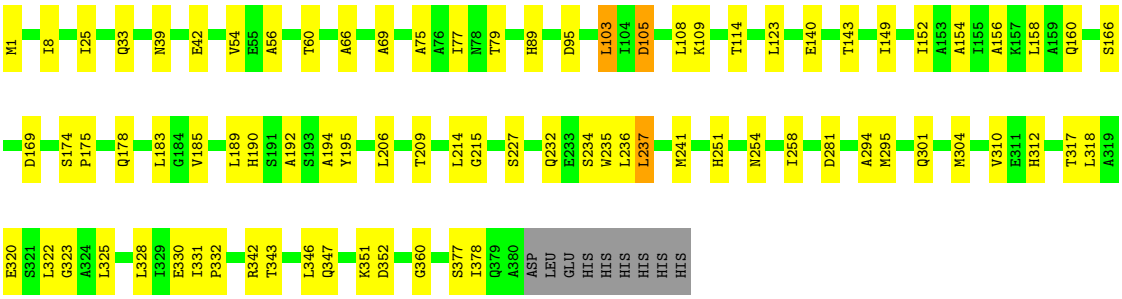
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	64	Total O 64 64	0	0
4	C	71	Total O 71 71	0	0
4	D	41	Total O 41 41	0	0
4	E	68	Total O 68 68	0	0
4	F	33	Total O 33 33	0	0

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.

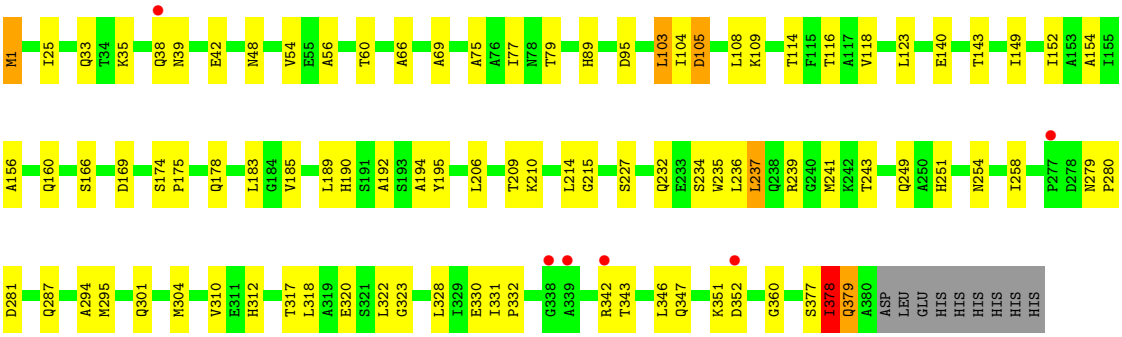
• Molecule 1: Cystathionine gamma-lyase

Chain A:



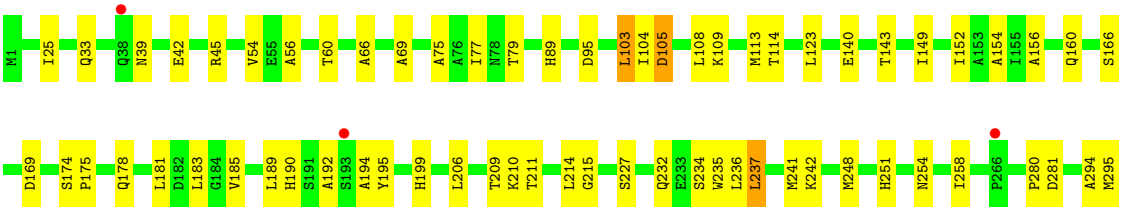
• Molecule 1: Cystathionine gamma-lyase

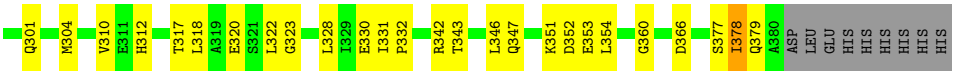
Chain B:



• Molecule 1: Cystathionine gamma-lyase

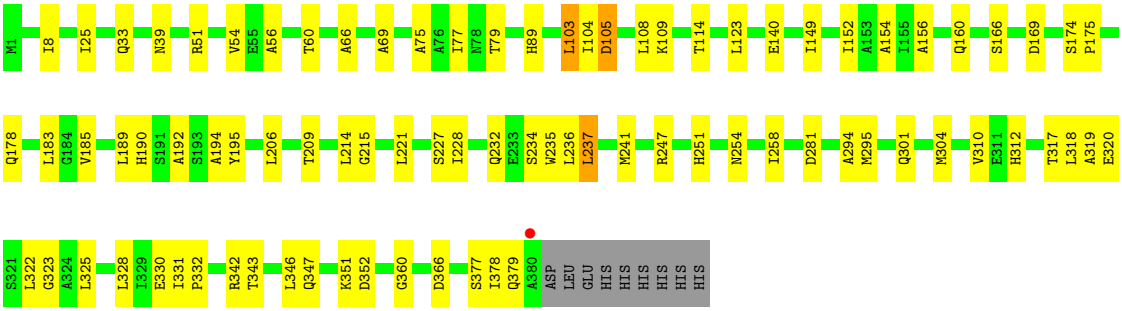
Chain C:





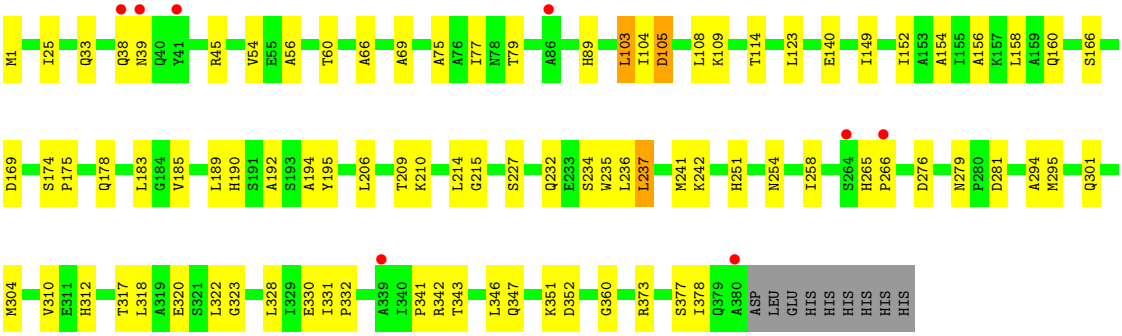
• Molecule 1: Cystathionine gamma-lyase

Chain D:



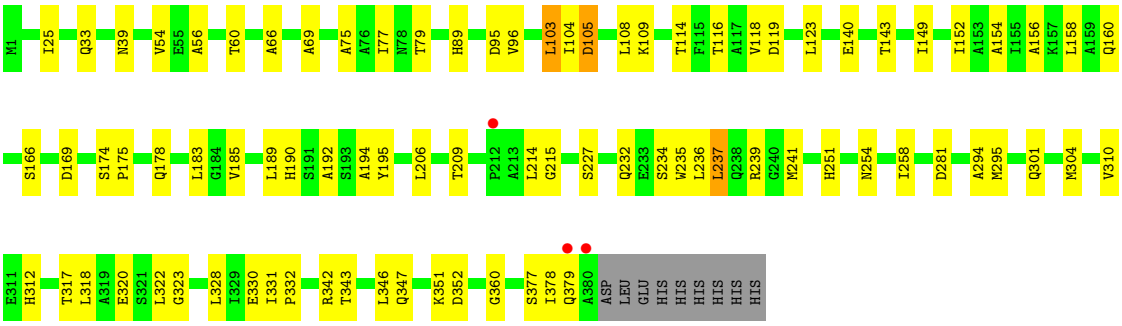
• Molecule 1: Cystathionine gamma-lyase

Chain E:



• Molecule 1: Cystathionine gamma-lyase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	216.57Å 200.74Å 114.88Å 90.00° 117.21° 90.00°	Depositor
Resolution (Å)	36.26 – 3.10 36.26 – 3.08	Depositor EDS
% Data completeness (in resolution range)	90.6 (36.26-3.10) 90.6 (36.26-3.08)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.246 , 0.273 0.246 , 0.273	Depositor DCC
R_{free} test set	3656 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	17687	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8703e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, E9U

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.41	0/2924	0.66	3/3978 (0.1%)
1	B	0.43	1/2924 (0.0%)	0.68	5/3978 (0.1%)
1	C	0.44	0/2924	0.66	4/3978 (0.1%)
1	D	0.41	0/2924	0.65	3/3978 (0.1%)
1	E	0.42	0/2924	0.66	3/3978 (0.1%)
1	F	0.41	0/2924	0.66	3/3978 (0.1%)
All	All	0.42	1/17544 (0.0%)	0.66	21/23868 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	E	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	GLN	CG-CD	5.88	1.64	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	378	ILE	O-C-N	-9.32	107.78	122.70
1	B	378	ILE	CA-C-N	6.47	131.44	117.20
1	A	378	ILE	C-N-CA	6.08	136.89	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	103	LEU	CA-CB-CG	5.92	128.93	115.30
1	B	103	LEU	CA-CB-CG	5.91	128.89	115.30
1	E	103	LEU	CA-CB-CG	5.90	128.87	115.30
1	A	103	LEU	CA-CB-CG	5.90	128.86	115.30
1	D	103	LEU	CA-CB-CG	5.90	128.86	115.30
1	C	103	LEU	CA-CB-CG	5.88	128.82	115.30
1	D	378	ILE	C-N-CA	5.82	136.24	121.70
1	C	378	ILE	C-N-CA	5.79	136.17	121.70
1	B	214	LEU	CA-CB-CG	5.77	128.56	115.30
1	F	214	LEU	CA-CB-CG	5.76	128.56	115.30
1	E	214	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	214	LEU	CA-CB-CG	5.75	128.54	115.30
1	D	214	LEU	CA-CB-CG	5.75	128.53	115.30
1	C	214	LEU	CA-CB-CG	5.75	128.52	115.30
1	B	1	MET	CG-SD-CE	5.74	109.39	100.20
1	F	378	ILE	C-N-CA	5.42	135.26	121.70
1	C	42	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	E	1	MET	C-N-CA	5.32	134.99	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	378	ILE	Mainchain
1	C	378	ILE	Mainchain
1	E	378	ILE	Mainchain,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	A	2867	0	2883	59	0
1	B	2867	0	2883	69	0
1	C	2867	0	2883	66	0
1	D	2867	0	2883	63	0
1	E	2867	0	2883	59	0
1	F	2867	0	2883	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	29	0	0	2	0
2	B	29	0	0	2	0
2	C	29	0	0	1	0
2	D	29	0	0	2	0
2	E	29	0	0	1	0
2	F	29	0	0	2	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
4	A	19	0	0	0	0
4	B	64	0	0	7	0
4	C	71	0	0	9	0
4	D	41	0	0	5	0
4	E	68	0	0	5	0
4	F	33	0	0	3	0
All	All	17687	0	17298	352	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 10.

All (352) 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:D:295:MET:HE1	1:D:322:LEU:HB2	1.46	0.98
1:E:295:MET:HE1	1:E:322:LEU:HB2	1.46	0.98
1:C:295:MET:HE1	1:C:322:LEU:HB2	1.46	0.96
1:A:295:MET:HE1	1:A:322:LEU:HB2	1.46	0.95
1:F:295:MET:HE1	1:F:322:LEU:HB2	1.46	0.95
1:B:295:MET:HE1	1:B:322:LEU:HB2	1.46	0.95
1:A:227:SER:HB3	1:B:227:SER:HB3	1.59	0.85
1:E:227:SER:HB3	1:F:227:SER:HB3	1.59	0.83
1:D:123:LEU:HD21	1:D:154:ALA:HB1	1.62	0.82
1:E:123:LEU:HD21	1:E:154:ALA:HB1	1.62	0.82
1:C:123:LEU:HD21	1:C:154:ALA:HB1	1.62	0.81
1:F:123:LEU:HD21	1:F:154:ALA:HB1	1.62	0.81
1:C:227:SER:HB3	1:D:227:SER:HB3	1.60	0.81
1:B:123:LEU:HD21	1:B:154:ALA:HB1	1.62	0.80
1:A:123:LEU:HD21	1:A:154:ALA:HB1	1.62	0.79
1:C:248:MET:SD	4:C:1121:HOH:O	2.42	0.77
1:B:312:HIS:HD2	1:B:377:SER:HB2	1.53	0.74
1:E:312:HIS:HD2	1:E:377:SER:HB2	1.53	0.74
1:C:312:HIS:HD2	1:C:377:SER:HB2	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:HIS:HD2	1:D:377:SER:HB2	1.53	0.73
1:A:312:HIS:HD2	1:A:377:SER:HB2	1.53	0.72
1:F:312:HIS:HD2	1:F:377:SER:HB2	1.53	0.72
1:B:280:PRO:HD2	4:B:1067:HOH:O	1.91	0.70
1:E:266:PRO:HD2	4:E:1245:HOH:O	1.90	0.70
1:D:192:ALA:HB1	1:D:237:LEU:HD21	1.74	0.70
1:E:192:ALA:HB1	1:E:237:LEU:HD21	1.74	0.69
1:B:192:ALA:HB1	1:B:237:LEU:HD21	1.74	0.69
1:C:192:ALA:HB1	1:C:237:LEU:HD21	1.74	0.69
1:A:192:ALA:HB1	1:A:237:LEU:HD21	1.74	0.68
1:B:378:ILE:O	1:B:379:GLN:C	2.30	0.68
1:F:192:ALA:HB1	1:F:237:LEU:HD21	1.74	0.68
1:C:354:LEU:HB2	4:C:1117:HOH:O	1.98	0.64
1:F:25:ILE:HD13	1:F:232:GLN:NE2	2.15	0.62
1:B:25:ILE:HD13	1:B:232:GLN:NE2	2.14	0.62
1:D:25:ILE:HD13	1:D:232:GLN:NE2	2.14	0.62
1:E:25:ILE:HD13	1:E:232:GLN:NE2	2.14	0.62
1:A:25:ILE:HD13	1:A:232:GLN:NE2	2.15	0.62
1:C:25:ILE:HD13	1:C:232:GLN:NE2	2.14	0.62
2:A:501:E9U:NH	1:B:42:GLU:OE2	2.33	0.61
1:C:89:HIS:HD2	1:C:114:THR:HB	1.66	0.61
1:B:140:GLU:HG2	1:B:169:ASP:HB3	1.83	0.61
1:C:280:PRO:HD3	4:C:1136:HOH:O	2.00	0.61
1:F:89:HIS:HD2	1:F:114:THR:HB	1.66	0.61
1:A:42:GLU:OE2	2:B:502:E9U:NH	2.33	0.61
1:C:351:LYS:N	4:C:1117:HOH:O	2.29	0.61
1:E:89:HIS:HD2	1:E:114:THR:HB	1.65	0.61
1:E:373:ARG:NH2	4:E:1260:HOH:O	2.23	0.61
1:A:25:ILE:HG21	1:A:232:GLN:HE21	1.66	0.61
1:A:89:HIS:HD2	1:A:114:THR:HB	1.65	0.61
1:A:140:GLU:HG2	1:A:169:ASP:HB3	1.83	0.61
1:F:209:THR:HG21	1:F:215:GLY:CA	2.31	0.61
1:F:25:ILE:HG21	1:F:232:GLN:HE21	1.66	0.60
1:F:140:GLU:HG2	1:F:169:ASP:HB3	1.83	0.60
1:A:209:THR:HG21	1:A:215:GLY:CA	2.31	0.60
1:C:140:GLU:HG2	1:C:169:ASP:HB3	1.83	0.60
1:C:25:ILE:HG21	1:C:232:GLN:HE21	1.66	0.60
1:C:209:THR:HG21	1:C:215:GLY:CA	2.31	0.60
1:D:89:HIS:HD2	1:D:114:THR:HB	1.66	0.60
1:D:209:THR:HG21	1:D:215:GLY:CA	2.31	0.60
1:D:25:ILE:HG21	1:D:232:GLN:HE21	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:HIS:HD2	1:B:114:THR:HB	1.66	0.60
1:E:25:ILE:HG21	1:E:232:GLN:HE21	1.66	0.60
1:A:1:MET:HB3	1:D:366:ASP:OD2	2.02	0.60
1:E:140:GLU:HG2	1:E:169:ASP:HB3	1.83	0.60
1:E:209:THR:HG21	1:E:215:GLY:CA	2.31	0.59
1:D:140:GLU:HG2	1:D:169:ASP:HB3	1.83	0.59
1:B:342:ARG:NH1	1:B:352:ASP:OD2	2.35	0.59
1:A:342:ARG:NH1	1:A:352:ASP:OD2	2.35	0.59
1:B:25:ILE:HG21	1:B:232:GLN:HE21	1.66	0.59
1:C:353:GLU:HB2	4:C:1125:HOH:O	2.02	0.59
1:D:312:HIS:CD2	1:D:377:SER:HB2	2.37	0.59
1:B:312:HIS:CD2	1:B:377:SER:HB2	2.37	0.59
1:C:312:HIS:CD2	1:C:377:SER:HB2	2.37	0.59
1:B:209:THR:HG21	1:B:215:GLY:CA	2.31	0.59
1:C:342:ARG:NH1	1:C:352:ASP:OD2	2.35	0.59
1:D:342:ARG:NH1	1:D:352:ASP:OD2	2.35	0.59
1:E:342:ARG:NH1	1:E:352:ASP:OD2	2.35	0.59
1:E:317:THR:HG23	1:E:328:LEU:HD23	1.86	0.58
1:F:342:ARG:NH1	1:F:352:ASP:OD2	2.35	0.58
1:A:312:HIS:CD2	1:A:377:SER:HB2	2.37	0.58
1:A:105:ASP:HA	1:A:109:LYS:HD2	1.86	0.57
1:F:105:ASP:HA	1:F:109:LYS:HD2	1.86	0.57
1:F:237:LEU:HD22	1:F:241:MET:HE2	1.85	0.57
1:B:317:THR:HG23	1:B:328:LEU:HD23	1.86	0.57
1:D:105:ASP:HA	1:D:109:LYS:HD2	1.86	0.57
1:C:105:ASP:HA	1:C:109:LYS:HD2	1.86	0.57
1:A:317:THR:HG23	1:A:328:LEU:HD23	1.86	0.56
1:B:105:ASP:HA	1:B:109:LYS:HD2	1.86	0.56
1:D:317:THR:HG23	1:D:328:LEU:HD23	1.86	0.56
1:E:105:ASP:HA	1:E:109:LYS:HD2	1.86	0.56
1:F:317:THR:HG23	1:F:328:LEU:HD23	1.86	0.56
1:C:317:THR:HG23	1:C:328:LEU:HD23	1.86	0.56
1:C:237:LEU:HD22	1:C:241:MET:HE2	1.87	0.56
1:C:312:HIS:HD2	1:C:377:SER:CB	2.19	0.56
1:A:312:HIS:HD2	1:A:377:SER:CB	2.19	0.56
1:B:312:HIS:HD2	1:B:377:SER:CB	2.19	0.56
1:D:237:LEU:HD22	1:D:241:MET:HE2	1.88	0.55
1:D:312:HIS:HD2	1:D:377:SER:CB	2.19	0.55
1:E:312:HIS:CD2	1:E:377:SER:HB2	2.37	0.55
1:E:312:HIS:HD2	1:E:377:SER:CB	2.19	0.55
1:B:210:LYS:HD3	4:B:1080:HOH:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:HIS:CE1	1:B:360:GLY:HA2	2.42	0.55
1:A:237:LEU:HD22	1:A:241:MET:HE2	1.90	0.54
1:F:251:HIS:CE1	1:F:360:GLY:HA2	2.42	0.54
1:B:237:LEU:HD22	1:B:241:MET:HE2	1.88	0.54
1:B:75:ALA:O	1:B:79:THR:HG23	2.08	0.54
1:D:77:ILE:HG12	1:D:189:LEU:HD11	1.90	0.54
1:F:312:HIS:CD2	1:F:377:SER:HB2	2.37	0.54
1:A:251:HIS:CE1	1:A:360:GLY:HA2	2.42	0.54
1:C:77:ILE:HG12	1:C:189:LEU:HD11	1.90	0.54
1:F:75:ALA:O	1:F:79:THR:HG23	2.08	0.54
1:B:320:GLU:HG3	4:B:1022:HOH:O	2.07	0.54
1:D:251:HIS:CE1	1:D:360:GLY:HA2	2.42	0.54
1:E:75:ALA:O	1:E:79:THR:HG23	2.08	0.54
1:F:312:HIS:HD2	1:F:377:SER:CB	2.19	0.54
1:E:251:HIS:CE1	1:E:360:GLY:HA2	2.42	0.54
1:A:25:ILE:HB	1:C:25:ILE:HB	1.90	0.53
1:A:75:ALA:O	1:A:79:THR:HG23	2.08	0.53
1:C:251:HIS:CE1	1:C:360:GLY:HA2	2.42	0.53
1:F:310:VAL:HG11	1:F:318:LEU:HD13	1.90	0.53
1:E:254:ASN:O	1:E:258:ILE:HG12	2.09	0.53
1:F:77:ILE:HG12	1:F:189:LEU:HD11	1.90	0.53
1:D:310:VAL:HG11	1:D:318:LEU:HD13	1.90	0.53
1:E:310:VAL:HG11	1:E:318:LEU:HD13	1.90	0.53
1:F:254:ASN:O	1:F:258:ILE:HG12	2.09	0.53
1:B:1:MET:HB3	1:C:366:ASP:OD2	2.09	0.53
1:C:149:ILE:HG12	4:C:1142:HOH:O	2.09	0.53
1:E:341:PRO:HA	4:E:1214:HOH:O	2.08	0.53
1:B:77:ILE:HG12	1:B:189:LEU:HD11	1.90	0.53
1:D:75:ALA:O	1:D:79:THR:HG23	2.08	0.53
1:A:77:ILE:HG12	1:A:189:LEU:HD11	1.90	0.53
1:C:75:ALA:O	1:C:79:THR:HG23	2.08	0.53
1:C:254:ASN:O	1:C:258:ILE:HG12	2.09	0.53
1:E:77:ILE:HG12	1:E:189:LEU:HD11	1.90	0.53
1:A:310:VAL:HG11	1:A:318:LEU:HD13	1.90	0.53
1:B:287:GLN:HG2	4:B:1079:HOH:O	2.09	0.53
1:C:242:LYS:HE2	4:C:1143:HOH:O	2.08	0.52
1:D:149:ILE:HB	1:D:281:ASP:HB3	1.92	0.52
1:D:254:ASN:O	1:D:258:ILE:HG12	2.09	0.52
1:B:149:ILE:HB	1:B:281:ASP:HB3	1.91	0.52
1:B:310:VAL:HG11	1:B:318:LEU:HD13	1.90	0.52
1:B:254:ASN:O	1:B:258:ILE:HG12	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:VAL:HG11	1:C:318:LEU:HD13	1.90	0.52
1:A:254:ASN:O	1:A:258:ILE:HG12	2.09	0.52
1:F:103:LEU:HD13	1:F:108:LEU:HG	1.92	0.52
1:A:103:LEU:HD13	1:A:108:LEU:HG	1.92	0.52
1:E:103:LEU:HD13	1:E:108:LEU:HG	1.92	0.52
1:A:149:ILE:HB	1:A:281:ASP:HB3	1.91	0.51
1:F:149:ILE:HB	1:F:281:ASP:HB3	1.92	0.51
1:C:103:LEU:HD13	1:C:108:LEU:HG	1.92	0.51
1:B:103:LEU:HD13	1:B:108:LEU:HG	1.92	0.51
1:E:149:ILE:HB	1:E:281:ASP:HB3	1.91	0.50
1:C:149:ILE:HB	1:C:281:ASP:HB3	1.92	0.50
1:F:330:GLU:OE1	1:F:332:PRO:HA	2.12	0.50
1:A:227:SER:CB	1:B:227:SER:HB3	2.39	0.50
1:D:330:GLU:OE1	1:D:332:PRO:HA	2.12	0.50
1:D:103:LEU:HD13	1:D:108:LEU:HG	1.92	0.50
1:C:330:GLU:OE1	1:C:332:PRO:HA	2.12	0.50
1:B:330:GLU:OE1	1:B:332:PRO:HA	2.12	0.50
1:E:227:SER:HB3	1:F:227:SER:CB	2.39	0.50
1:E:330:GLU:OE1	1:E:332:PRO:HA	2.12	0.50
1:A:330:GLU:OE1	1:A:332:PRO:HA	2.12	0.50
1:D:51:ARG:NH1	4:D:1159:HOH:O	2.33	0.49
1:E:237:LEU:HD22	1:E:241:MET:HE2	1.94	0.49
1:D:54:VAL:HG21	1:D:234:SER:HB3	1.95	0.49
1:F:54:VAL:HG21	1:F:234:SER:HB3	1.95	0.48
1:E:54:VAL:HG21	1:E:234:SER:HB3	1.96	0.48
1:E:69:ALA:HA	1:E:206:LEU:HD23	1.96	0.48
1:F:69:ALA:HA	1:F:206:LEU:HD23	1.96	0.48
1:B:54:VAL:HG21	1:B:234:SER:HB3	1.95	0.48
1:B:35:LYS:HD2	1:B:38:GLN:HE21	1.79	0.48
1:B:156:ALA:O	1:B:160:GLN:HG3	2.14	0.48
1:B:69:ALA:HA	1:B:206:LEU:HD23	1.96	0.47
1:C:54:VAL:HG21	1:C:234:SER:HB3	1.95	0.47
1:A:54:VAL:HG21	1:A:234:SER:HB3	1.95	0.47
1:D:156:ALA:O	1:D:160:GLN:HG3	2.14	0.47
1:A:320:GLU:OE1	2:A:501:E9U:NH	2.48	0.47
1:B:320:GLU:OE1	2:B:502:E9U:NH	2.48	0.47
1:C:156:ALA:O	1:C:160:GLN:HG3	2.14	0.47
1:A:152:ILE:HB	1:A:183:LEU:HD12	1.97	0.47
1:B:152:ILE:HB	1:B:183:LEU:HD12	1.97	0.47
1:C:320:GLU:OE1	2:C:503:E9U:NH	2.48	0.47
1:D:69:ALA:HA	1:D:206:LEU:HD23	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ILE:HB	1:D:183:LEU:HD12	1.97	0.47
1:E:156:ALA:O	1:E:160:GLN:HG3	2.14	0.47
1:F:320:GLU:OE1	2:F:506:E9U:NH	2.48	0.47
1:A:156:ALA:O	1:A:160:GLN:HG3	2.14	0.47
1:A:69:ALA:HA	1:A:206:LEU:HD23	1.96	0.47
1:C:69:ALA:HA	1:C:206:LEU:HD23	1.96	0.47
1:D:320:GLU:OE1	2:D:504:E9U:NH	2.48	0.46
1:E:320:GLU:OE1	2:E:505:E9U:NH	2.48	0.46
1:F:156:ALA:O	1:F:160:GLN:HG3	2.14	0.46
1:B:169:ASP:HA	1:B:189:LEU:HD23	1.98	0.46
1:C:152:ILE:HB	1:C:183:LEU:HD12	1.97	0.46
1:A:169:ASP:HA	1:A:189:LEU:HD23	1.98	0.46
1:F:152:ILE:HB	1:F:183:LEU:HD12	1.97	0.46
1:F:169:ASP:HA	1:F:189:LEU:HD23	1.98	0.46
1:E:242:LYS:NZ	4:E:1247:HOH:O	2.41	0.45
1:C:211:THR:HG22	4:C:1090:HOH:O	2.15	0.45
1:D:169:ASP:HA	1:D:189:LEU:HD23	1.98	0.45
1:E:75:ALA:HB1	1:E:227:SER:HB2	1.99	0.45
1:F:75:ALA:HB1	1:F:227:SER:HB2	1.99	0.45
1:B:75:ALA:HB1	1:B:227:SER:HB2	1.99	0.45
1:C:75:ALA:HB1	1:C:227:SER:HB2	1.99	0.45
1:D:75:ALA:HB1	1:D:227:SER:HB2	1.99	0.45
1:E:152:ILE:HB	1:E:183:LEU:HD12	1.97	0.45
1:A:346:LEU:HD23	1:A:351:LYS:HA	1.99	0.45
1:D:175:PRO:HA	1:D:178:GLN:O	2.17	0.45
1:E:169:ASP:HA	1:E:189:LEU:HD23	1.98	0.45
1:D:346:LEU:HD23	1:D:351:LYS:HA	1.99	0.45
1:A:175:PRO:HA	1:A:178:GLN:O	2.17	0.45
1:B:279:ASN:OD1	4:B:1067:HOH:O	2.21	0.45
1:E:210:LYS:HB3	4:E:1201:HOH:O	2.15	0.45
1:F:301:GLN:HB2	1:F:304:MET:SD	2.57	0.44
1:C:175:PRO:HA	1:C:178:GLN:O	2.17	0.44
1:C:195:TYR:CE1	1:C:323:GLY:HA2	2.53	0.44
1:E:301:GLN:HB2	1:E:304:MET:SD	2.57	0.44
1:F:175:PRO:HA	1:F:178:GLN:O	2.17	0.44
1:A:75:ALA:HB1	1:A:227:SER:HB2	1.99	0.44
1:B:301:GLN:HB2	1:B:304:MET:SD	2.57	0.44
1:C:227:SER:HB3	1:D:227:SER:CB	2.39	0.44
1:D:56:ALA:O	1:D:60:THR:HG23	2.18	0.44
1:A:108:LEU:HA	1:A:108:LEU:HD23	1.65	0.44
1:B:346:LEU:HD23	1:B:351:LYS:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LEU:HD21	1:C:235:TRP:CZ3	2.53	0.44
1:B:239:ARG:NH2	1:C:199:HIS:HB2	2.33	0.44
1:C:56:ALA:O	1:C:60:THR:HG23	2.18	0.44
1:C:169:ASP:HA	1:C:189:LEU:HD23	1.98	0.44
1:E:56:ALA:O	1:E:60:THR:HG23	2.18	0.44
1:E:175:PRO:HA	1:E:178:GLN:O	2.17	0.44
1:E:346:LEU:HD23	1:E:351:LYS:HA	1.99	0.44
1:E:195:TYR:CE1	1:E:323:GLY:HA2	2.53	0.44
1:A:56:ALA:O	1:A:60:THR:HG23	2.18	0.44
1:D:301:GLN:HB2	1:D:304:MET:SD	2.57	0.44
1:A:227:SER:HB3	1:B:227:SER:CB	2.39	0.43
1:B:175:PRO:HA	1:B:178:GLN:O	2.17	0.43
1:B:195:TYR:CE1	1:B:323:GLY:HA2	2.53	0.43
1:D:195:TYR:CE1	1:D:323:GLY:HA2	2.53	0.43
1:B:33:GLN:HA	1:B:39:ASN:OD1	2.18	0.43
1:C:301:GLN:HB2	1:C:304:MET:SD	2.57	0.43
1:F:195:TYR:CE1	1:F:323:GLY:HA2	2.53	0.43
1:A:195:TYR:CE1	1:A:323:GLY:HA2	2.53	0.43
1:D:33:GLN:HA	1:D:39:ASN:OD1	2.18	0.43
1:C:33:GLN:HA	1:C:39:ASN:OD1	2.18	0.43
1:A:33:GLN:HA	1:A:39:ASN:OD1	2.18	0.43
1:B:56:ALA:O	1:B:60:THR:HG23	2.18	0.43
1:F:56:ALA:O	1:F:60:THR:HG23	2.18	0.43
1:F:346:LEU:HD23	1:F:351:LYS:HA	1.99	0.43
1:F:239:ARG:NH1	4:F:1286:HOH:O	2.51	0.43
1:A:236:LEU:HD21	1:D:235:TRP:CZ3	2.54	0.43
1:F:96:VAL:HG12	4:F:1275:HOH:O	2.18	0.43
1:A:301:GLN:HB2	1:A:304:MET:SD	2.57	0.43
1:C:25:ILE:HD13	1:C:232:GLN:HE22	1.83	0.43
1:F:166:SER:OG	1:F:185:VAL:HA	2.19	0.43
1:B:249:GLN:HG2	4:B:1057:HOH:O	2.18	0.43
1:C:346:LEU:HD23	1:C:351:LYS:HA	1.99	0.43
1:F:25:ILE:HD13	1:F:232:GLN:HE22	1.83	0.43
1:A:235:TRP:CZ3	1:D:236:LEU:HD21	2.54	0.42
1:A:330:GLU:HG2	1:A:331:ILE:N	2.34	0.42
1:C:237:LEU:O	1:C:241:MET:HG3	2.19	0.42
1:A:25:ILE:HD13	1:A:232:GLN:HE22	1.83	0.42
1:C:330:GLU:HG2	1:C:331:ILE:N	2.34	0.42
1:E:33:GLN:HA	1:E:39:ASN:OD1	2.18	0.42
1:E:166:SER:OG	1:E:185:VAL:HA	2.19	0.42
1:F:33:GLN:HA	1:F:39:ASN:OD1	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:LEU:O	1:F:241:MET:HG3	2.19	0.42
1:B:235:TRP:CZ3	1:C:236:LEU:HD21	2.55	0.42
1:E:330:GLU:HG2	1:E:331:ILE:N	2.34	0.42
1:A:174:SER:HA	1:A:190:HIS:HE1	1.84	0.42
1:A:237:LEU:O	1:A:241:MET:HG3	2.19	0.42
1:A:325:LEU:HB3	1:D:8:ILE:HD12	2.01	0.42
1:B:166:SER:OG	1:B:185:VAL:HA	2.19	0.42
1:D:319:ALA:O	4:D:1180:HOH:O	2.21	0.42
1:F:330:GLU:HG2	1:F:331:ILE:N	2.34	0.42
1:C:66:ALA:HB3	1:C:209:THR:HG22	2.01	0.42
1:C:166:SER:OG	1:C:185:VAL:HA	2.19	0.42
1:D:237:LEU:O	1:D:241:MET:HG3	2.19	0.42
1:C:108:LEU:HA	1:C:108:LEU:HD23	1.65	0.42
1:B:237:LEU:O	1:B:241:MET:HG3	2.19	0.42
1:D:66:ALA:HB3	1:D:209:THR:HG22	2.01	0.42
1:D:221:LEU:HD23	1:D:221:LEU:HA	1.87	0.42
1:E:237:LEU:O	1:E:241:MET:HG3	2.19	0.42
1:A:66:ALA:HB3	1:A:209:THR:HG22	2.01	0.42
1:C:108:LEU:HB3	1:C:113:MET:HE2	2.02	0.42
1:A:209:THR:HG21	1:A:215:GLY:HA2	2.02	0.42
1:C:45:ARG:NH1	2:D:504:E9U:O1P	2.53	0.42
1:E:235:TRP:HE3	1:E:236:LEU:HD12	1.85	0.42
1:A:166:SER:OG	1:A:185:VAL:HA	2.19	0.42
1:A:251:HIS:HB3	1:A:294:ALA:CB	2.50	0.42
1:D:330:GLU:HG2	1:D:331:ILE:N	2.34	0.42
1:F:66:ALA:HB3	1:F:209:THR:HG22	2.01	0.42
1:D:166:SER:OG	1:D:185:VAL:HA	2.19	0.41
1:F:251:HIS:HB3	1:F:294:ALA:CB	2.50	0.41
1:A:8:ILE:HD12	1:D:325:LEU:HB3	2.02	0.41
1:B:235:TRP:HE3	1:B:236:LEU:HD12	1.85	0.41
1:B:330:GLU:HG2	1:B:331:ILE:N	2.34	0.41
1:C:174:SER:HA	1:C:190:HIS:HE1	1.84	0.41
1:C:343:THR:O	1:C:347:GLN:HB2	2.21	0.41
1:F:343:THR:O	1:F:347:GLN:HB2	2.20	0.41
1:B:25:ILE:HD13	1:B:232:GLN:HE22	1.83	0.41
1:E:265:HIS:HA	1:E:266:PRO:HD3	1.96	0.41
1:C:251:HIS:HB3	1:C:294:ALA:CB	2.50	0.41
1:D:209:THR:HG21	1:D:215:GLY:HA2	2.02	0.41
1:F:119:ASP:OD2	4:F:1280:HOH:O	2.22	0.41
1:D:174:SER:HA	1:D:190:HIS:HE1	1.84	0.41
1:D:295:MET:HE2	4:D:1193:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:SER:HA	1:E:190:HIS:HE1	1.84	0.41
1:F:174:SER:HA	1:F:190:HIS:HE1	1.84	0.41
1:C:95:ASP:O	1:C:143:THR:HB	2.21	0.41
1:F:95:ASP:O	1:F:143:THR:HB	2.21	0.41
1:F:235:TRP:HE3	1:F:236:LEU:HD12	1.85	0.41
1:A:343:THR:O	1:A:347:GLN:HB2	2.21	0.41
1:B:48:ASN:N	4:B:1076:HOH:O	2.52	0.41
1:C:104:ILE:HA	1:C:108:LEU:HB2	2.03	0.41
1:D:104:ILE:HA	1:D:108:LEU:HB2	2.03	0.41
1:D:228:ILE:HD13	4:D:1159:HOH:O	2.21	0.41
1:E:45:ARG:NH1	2:F:506:E9U:O1P	2.54	0.41
1:A:95:ASP:O	1:A:143:THR:HB	2.21	0.41
1:B:66:ALA:HB3	1:B:209:THR:HG22	2.01	0.41
1:B:343:THR:O	1:B:347:GLN:HB2	2.20	0.41
1:C:227:SER:CB	1:D:227:SER:HB3	2.42	0.41
1:D:25:ILE:HD13	1:D:232:GLN:HE22	1.83	0.41
1:D:235:TRP:HE3	1:D:236:LEU:HD12	1.85	0.41
1:D:251:HIS:HB3	1:D:294:ALA:CB	2.50	0.41
1:E:66:ALA:HB3	1:E:209:THR:HG22	2.01	0.41
1:F:108:LEU:HD23	1:F:108:LEU:HA	1.65	0.41
1:F:209:THR:HG21	1:F:215:GLY:HA2	2.02	0.41
1:B:95:ASP:O	1:B:143:THR:HB	2.21	0.41
1:B:243:THR:OG1	4:C:1120:HOH:O	2.21	0.41
1:B:251:HIS:HB3	1:B:294:ALA:CB	2.50	0.41
1:D:247:ARG:HD2	4:D:1182:HOH:O	2.20	0.41
1:D:343:THR:O	1:D:347:GLN:HB2	2.21	0.41
1:E:25:ILE:HD13	1:E:232:GLN:HE22	1.83	0.40
1:E:104:ILE:HA	1:E:108:LEU:HB2	2.03	0.40
1:A:235:TRP:HE3	1:A:236:LEU:HD12	1.85	0.40
1:B:25:ILE:HB	1:D:25:ILE:HB	2.03	0.40
1:B:116:THR:HG22	1:B:118:VAL:HG23	2.04	0.40
1:B:174:SER:HA	1:B:190:HIS:HE1	1.84	0.40
1:E:227:SER:CB	1:F:227:SER:HB3	2.40	0.40
1:E:237:LEU:HD22	1:E:241:MET:CE	2.51	0.40
1:E:343:THR:O	1:E:347:GLN:HB2	2.21	0.40
1:A:237:LEU:HD22	1:A:241:MET:CE	2.51	0.40
1:B:209:THR:HG21	1:B:215:GLY:HA2	2.02	0.40
1:B:237:LEU:HD22	1:B:241:MET:CE	2.51	0.40
1:C:181:LEU:HD22	1:C:210:LYS:HB2	2.04	0.40
1:E:276:ASP:HB3	1:E:279:ASN:HB2	2.03	0.40
1:B:104:ILE:HA	1:B:108:LEU:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:VAL:HG12	1:D:318:LEU:HD22	2.04	0.40
1:E:251:HIS:HB3	1:E:294:ALA:CB	2.50	0.40
1:E:310:VAL:HG12	1:E:318:LEU:HD22	2.04	0.40
1:F:104:ILE:HA	1:F:108:LEU:HB2	2.03	0.40
1:F:116:THR:HG22	1:F:118:VAL:HG23	2.04	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	A	378/389 (97%)	362 (96%)	15 (4%)	1 (0%)	41	73
1	B	378/389 (97%)	364 (96%)	13 (3%)	1 (0%)	41	73
1	C	378/389 (97%)	363 (96%)	13 (3%)	2 (0%)	29	64
1	D	378/389 (97%)	363 (96%)	13 (3%)	2 (0%)	29	64
1	E	378/389 (97%)	363 (96%)	14 (4%)	1 (0%)	41	73
1	F	378/389 (97%)	362 (96%)	14 (4%)	2 (0%)	29	64
All	All	2268/2334 (97%)	2177 (96%)	82 (4%)	9 (0%)	34	69

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	379	GLN
1	F	379	GLN
1	A	194	ALA
1	B	194	ALA
1	C	194	ALA
1	D	194	ALA
1	E	194	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	194	ALA
1	C	379	GLN

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	A	303/312 (97%)	300 (99%)	3 (1%)	76	90
1	B	303/312 (97%)	301 (99%)	2 (1%)	84	93
1	C	303/312 (97%)	301 (99%)	2 (1%)	84	93
1	D	303/312 (97%)	301 (99%)	2 (1%)	84	93
1	E	303/312 (97%)	299 (99%)	4 (1%)	69	87
1	F	303/312 (97%)	300 (99%)	3 (1%)	76	90
All	All	1818/1872 (97%)	1802 (99%)	16 (1%)	78	91

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASP
1	A	158	LEU
1	A	237	LEU
1	B	105	ASP
1	B	237	LEU
1	C	105	ASP
1	C	237	LEU
1	D	105	ASP
1	D	237	LEU
1	E	38	GLN
1	E	105	ASP
1	E	158	LEU
1	E	237	LEU
1	F	105	ASP
1	F	158	LEU
1	F	237	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	GLN
1	A	312	HIS
1	B	232	GLN
1	B	312	HIS
1	C	232	GLN
1	C	312	HIS
1	D	232	GLN
1	D	312	HIS
1	E	232	GLN
1	E	312	HIS
1	F	232	GLN
1	F	312	HIS

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)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	E9U	C	503	-	28,29,29	1.18	2 (7%)	34,40,40	1.64	5 (14%)
2	E9U	A	501	-	28,29,29	1.18	2 (7%)	34,40,40	1.65	5 (14%)
3	PO4	B	702	-	4,4,4	1.01	0	6,6,6	0.86	0
2	E9U	D	504	-	28,29,29	1.18	2 (7%)	34,40,40	1.65	5 (14%)
2	E9U	F	506	-	28,29,29	1.19	2 (7%)	34,40,40	1.65	5 (14%)
2	E9U	E	505	-	28,29,29	1.19	2 (7%)	34,40,40	1.65	5 (14%)
2	E9U	B	502	-	28,29,29	1.18	2 (7%)	34,40,40	1.64	5 (14%)
3	PO4	B	701	-	4,4,4	0.64	0	6,6,6	0.67	0
3	PO4	C	703	-	4,4,4	0.72	0	6,6,6	1.04	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
2	E9U	C	503	-	-	8/26/26/26	0/1/1/1
2	E9U	A	501	-	-	8/26/26/26	0/1/1/1
2	E9U	D	504	-	-	8/26/26/26	0/1/1/1
2	E9U	F	506	-	-	8/26/26/26	0/1/1/1
2	E9U	E	505	-	-	8/26/26/26	0/1/1/1
2	E9U	B	502	-	-	8/26/26/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	E9U	OX1-CH	3.44	1.32	1.22
2	C	503	E9U	OX1-CH	3.44	1.32	1.22
2	F	506	E9U	OX1-CH	3.43	1.32	1.22
2	A	501	E9U	OX1-CH	3.43	1.32	1.22
2	E	505	E9U	OX1-CH	3.43	1.32	1.22
2	B	502	E9U	OX1-CH	3.42	1.32	1.22
2	A	501	E9U	OX2-CH	-2.42	1.22	1.30
2	E	505	E9U	OX2-CH	-2.41	1.22	1.30
2	B	502	E9U	OX2-CH	-2.40	1.22	1.30
2	D	504	E9U	OX2-CH	-2.40	1.22	1.30
2	F	506	E9U	OX2-CH	-2.39	1.22	1.30
2	C	503	E9U	OX2-CH	-2.39	1.22	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	506	E9U	CA-N-C4A	6.10	126.12	117.31
2	A	501	E9U	CA-N-C4A	6.10	126.12	117.31
2	D	504	E9U	CA-N-C4A	6.10	126.11	117.31
2	E	505	E9U	CA-N-C4A	6.09	126.10	117.31
2	B	502	E9U	CA-N-C4A	6.09	126.09	117.31
2	C	503	E9U	CA-N-C4A	6.06	126.06	117.31
2	B	502	E9U	CE-SD-CG	3.96	114.16	102.27
2	C	503	E9U	CE-SD-CG	3.96	114.14	102.27
2	A	501	E9U	CE-SD-CG	3.96	114.13	102.27
2	D	504	E9U	CE-SD-CG	3.95	114.12	102.27
2	E	505	E9U	CE-SD-CG	3.95	114.12	102.27
2	F	506	E9U	CE-SD-CG	3.95	114.11	102.27
2	F	506	E9U	O-C-OT	-2.59	118.21	124.09
2	D	504	E9U	O-C-OT	-2.59	118.22	124.09
2	E	505	E9U	O-C-OT	-2.58	118.22	124.09
2	C	503	E9U	O-C-OT	-2.58	118.23	124.09
2	A	501	E9U	O-C-OT	-2.57	118.26	124.09
2	B	502	E9U	O-C-OT	-2.56	118.28	124.09
2	A	501	E9U	CB-CG-SD	-2.51	107.69	113.31
2	B	502	E9U	CB-CG-SD	-2.49	107.72	113.31
2	E	505	E9U	CB-CG-SD	-2.49	107.73	113.31
2	F	506	E9U	CB-CG-SD	-2.48	107.75	113.31
2	D	504	E9U	CB-CG-SD	-2.47	107.76	113.31
2	C	503	E9U	CB-CG-SD	-2.47	107.78	113.31
2	C	503	E9U	OX2-CH-CZ	2.11	120.57	113.38
2	F	506	E9U	OX2-CH-CZ	2.11	120.56	113.38
2	E	505	E9U	OX2-CH-CZ	2.11	120.56	113.38
2	A	501	E9U	OX2-CH-CZ	2.10	120.55	113.38
2	D	504	E9U	OX2-CH-CZ	2.10	120.55	113.38
2	B	502	E9U	OX2-CH-CZ	2.09	120.51	113.38

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	E9U	CB-CA-N-C4A
2	A	501	E9U	SD-CE-CZ-CH
2	A	501	E9U	SD-CE-CZ-NH
2	B	502	E9U	CB-CA-N-C4A
2	B	502	E9U	SD-CE-CZ-CH
2	B	502	E9U	SD-CE-CZ-NH
2	C	503	E9U	CB-CA-N-C4A
2	C	503	E9U	SD-CE-CZ-CH

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	503	E9U	SD-CE-CZ-NH
2	D	504	E9U	CB-CA-N-C4A
2	D	504	E9U	SD-CE-CZ-CH
2	D	504	E9U	SD-CE-CZ-NH
2	E	505	E9U	CB-CA-N-C4A
2	E	505	E9U	SD-CE-CZ-CH
2	E	505	E9U	SD-CE-CZ-NH
2	F	506	E9U	CB-CA-N-C4A
2	F	506	E9U	SD-CE-CZ-CH
2	F	506	E9U	SD-CE-CZ-NH
2	A	501	E9U	CA-CB-CG-SD
2	B	502	E9U	CA-CB-CG-SD
2	C	503	E9U	CA-CB-CG-SD
2	D	504	E9U	CA-CB-CG-SD
2	E	505	E9U	CA-CB-CG-SD
2	F	506	E9U	CA-CB-CG-SD
2	A	501	E9U	OT-C-CA-CB
2	B	502	E9U	OT-C-CA-CB
2	C	503	E9U	OT-C-CA-CB
2	D	504	E9U	OT-C-CA-CB
2	E	505	E9U	OT-C-CA-CB
2	F	506	E9U	OT-C-CA-CB
2	A	501	E9U	C4-C5-C5A-O4P
2	B	502	E9U	C4-C5-C5A-O4P
2	C	503	E9U	C4-C5-C5A-O4P
2	D	504	E9U	C4-C5-C5A-O4P
2	E	505	E9U	C4-C5-C5A-O4P
2	F	506	E9U	C4-C5-C5A-O4P
2	A	501	E9U	O-C-CA-CB
2	B	502	E9U	O-C-CA-CB
2	C	503	E9U	O-C-CA-CB
2	D	504	E9U	O-C-CA-CB
2	E	505	E9U	O-C-CA-CB
2	F	506	E9U	O-C-CA-CB
2	A	501	E9U	C6-C5-C5A-O4P
2	B	502	E9U	C6-C5-C5A-O4P
2	C	503	E9U	C6-C5-C5A-O4P
2	D	504	E9U	C6-C5-C5A-O4P
2	E	505	E9U	C6-C5-C5A-O4P
2	F	506	E9U	C6-C5-C5A-O4P

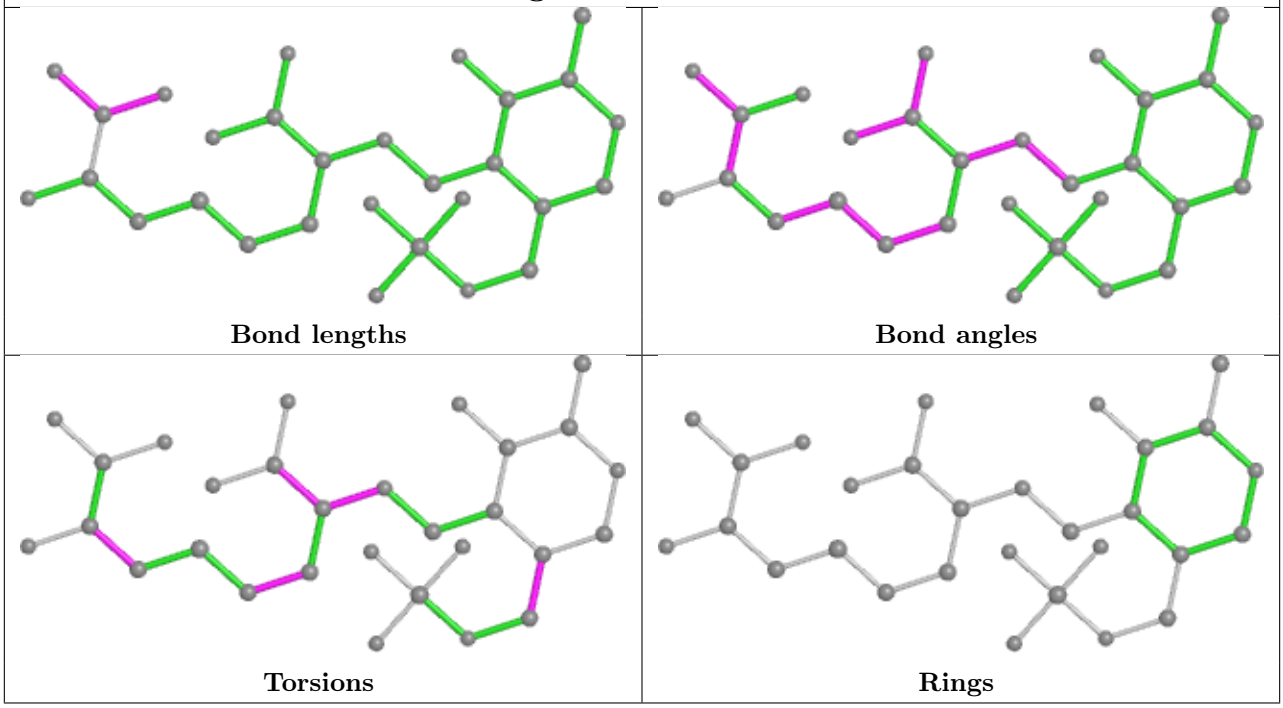
There are no ring outliers.

6 monomers are involved in 10 short contacts:

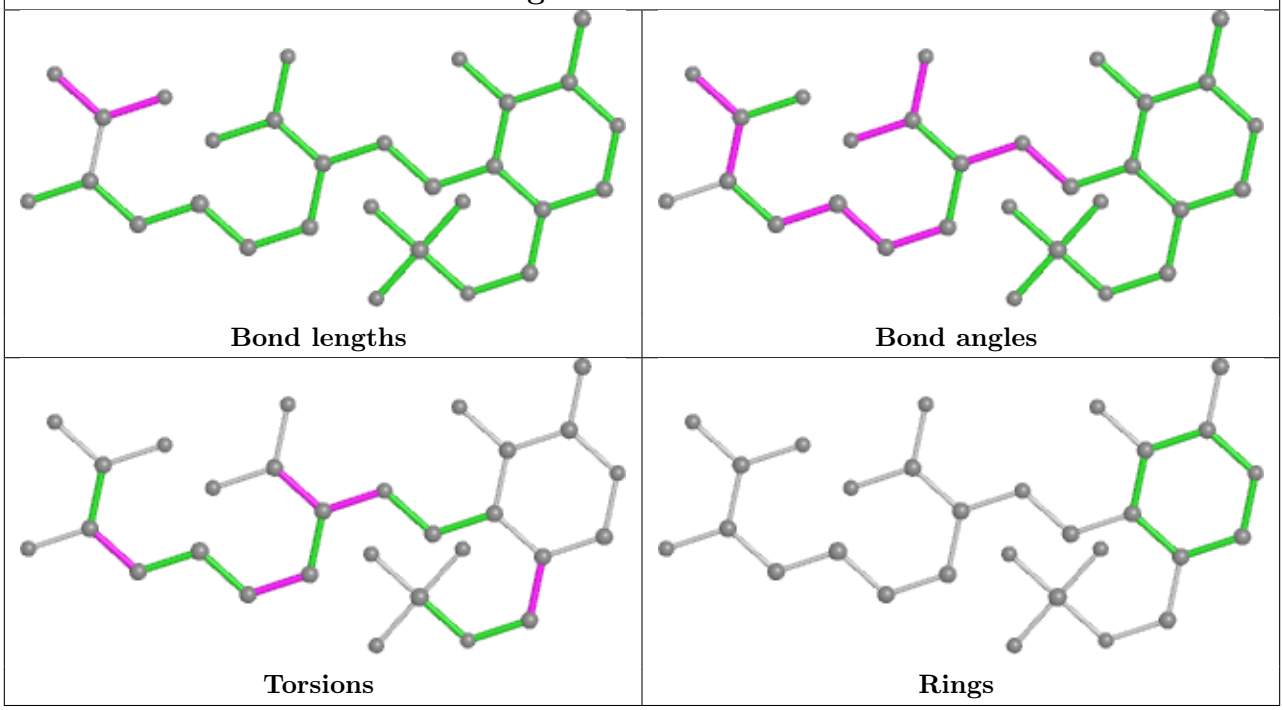
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	503	E9U	1	0
2	A	501	E9U	2	0
2	D	504	E9U	2	0
2	F	506	E9U	2	0
2	E	505	E9U	1	0
2	B	502	E9U	2	0

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

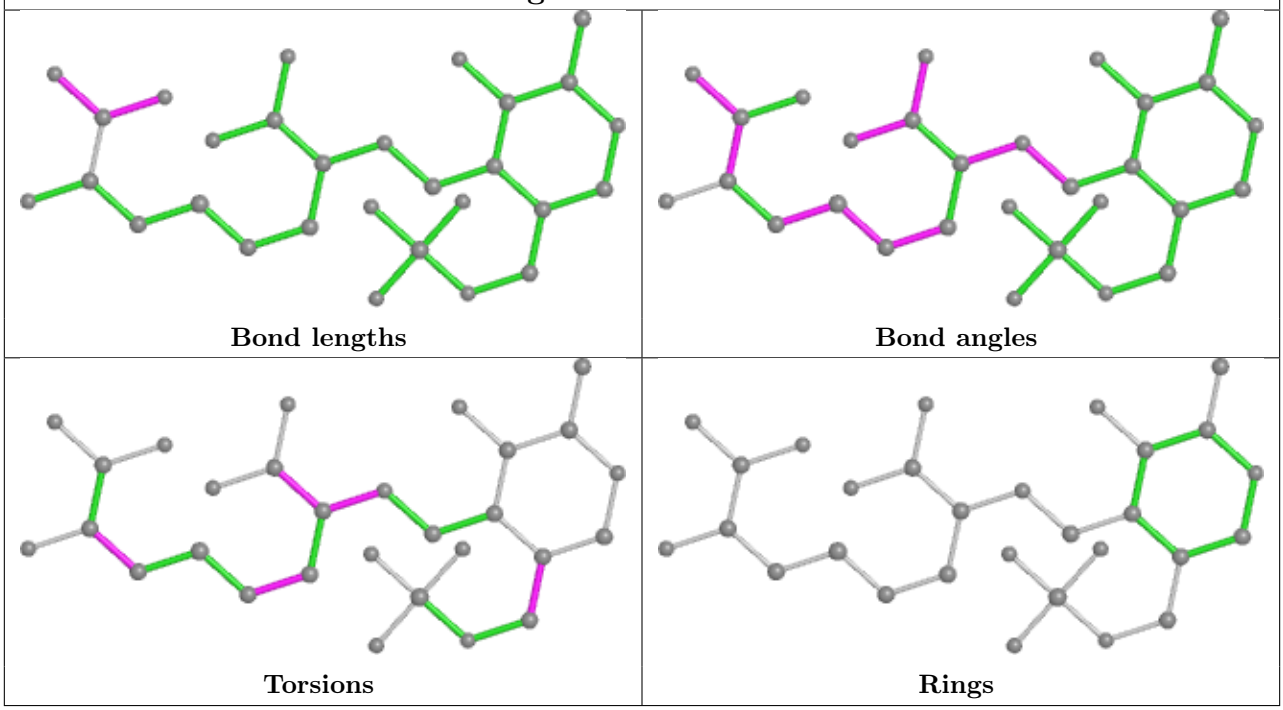
Ligand E9U C 503



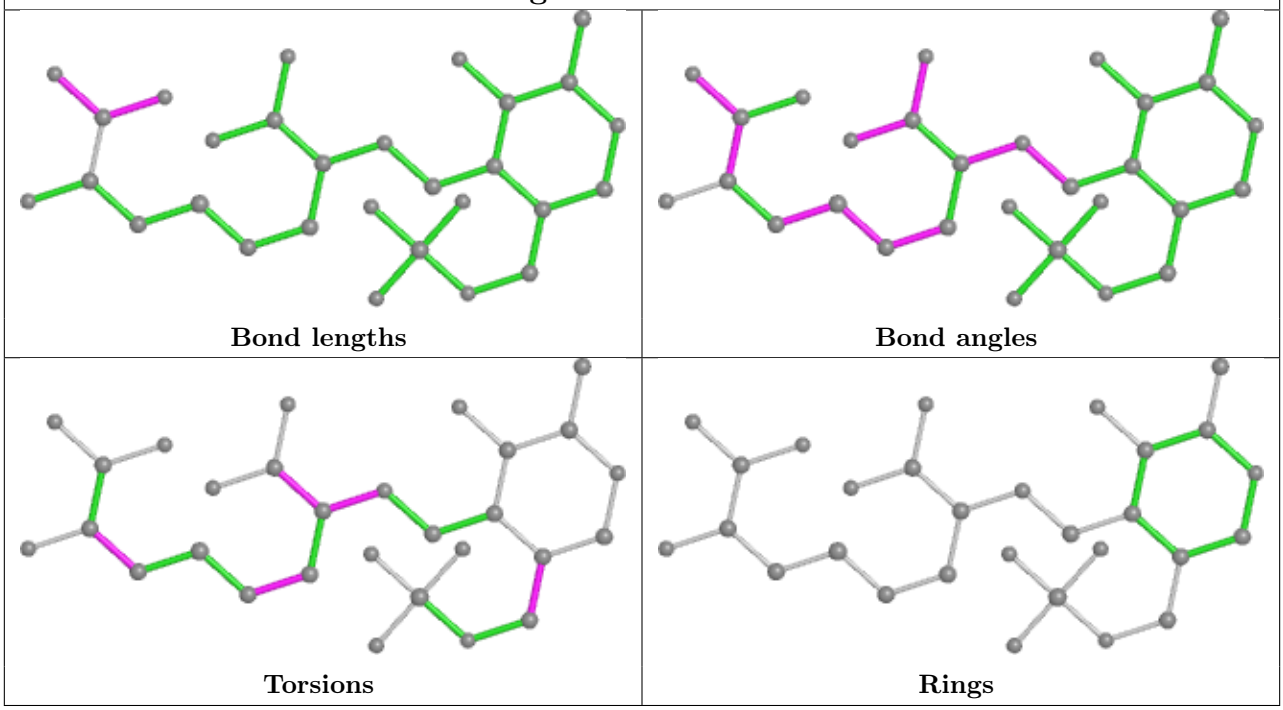
Ligand E9U A 501



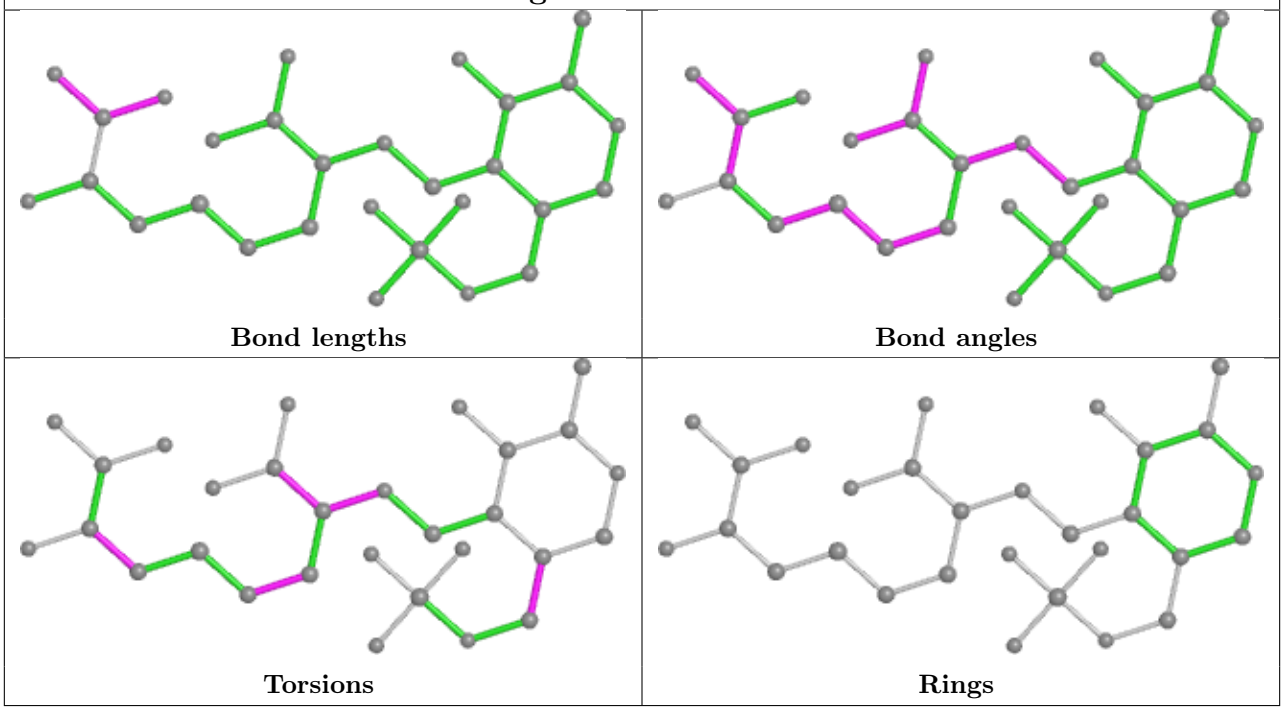
Ligand E9U D 504



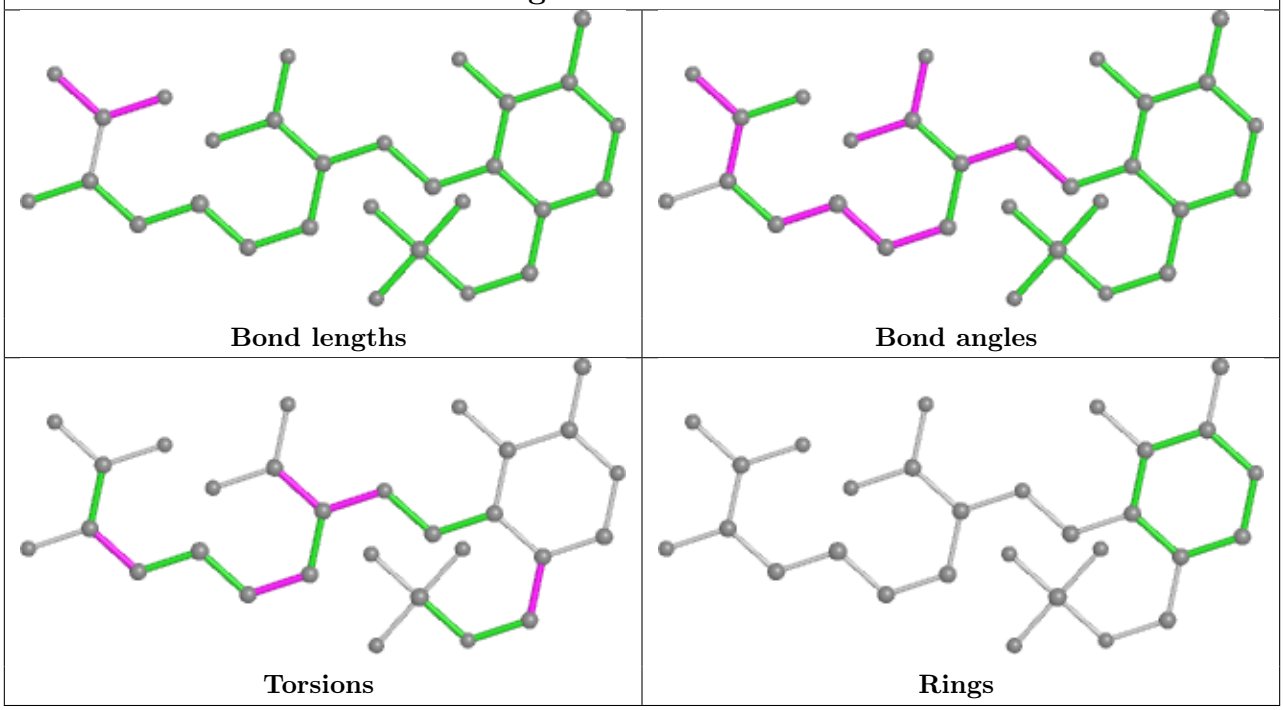
Ligand E9U F 506



Ligand E9U E 505



Ligand E9U B 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	380/389 (97%)	-0.38	0	100	100	17, 35, 66, 91	0
1	B	380/389 (97%)	-0.13	6 (1%)	72	51	17, 35, 66, 86	0
1	C	380/389 (97%)	-0.15	3 (0%)	86	72	17, 35, 65, 136	0
1	D	380/389 (97%)	-0.33	1 (0%)	94	88	17, 35, 65, 104	0
1	E	380/389 (97%)	-0.08	8 (2%)	63	43	17, 35, 66, 165	0
1	F	380/389 (97%)	-0.37	3 (0%)	86	72	17, 35, 65, 131	0
All	All	2280/2334 (97%)	-0.24	21 (0%)	84	69	17, 35, 66, 165	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	339	ALA	4.5
1	E	380	ALA	4.1
1	F	380	ALA	3.8
1	B	352	ASP	3.3
1	C	38	GLN	3.1
1	E	38	GLN	3.1
1	E	266	PRO	2.8
1	E	39	ASN	2.7
1	D	380	ALA	2.6
1	C	266	PRO	2.6
1	C	193	SER	2.4
1	B	338	GLY	2.4
1	B	342	ARG	2.4
1	E	339	ALA	2.4
1	B	38	GLN	2.4
1	E	41	TYR	2.4
1	F	379	GLN	2.2
1	B	277	PRO	2.2
1	E	264	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	212	PRO	2.1
1	E	86	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)

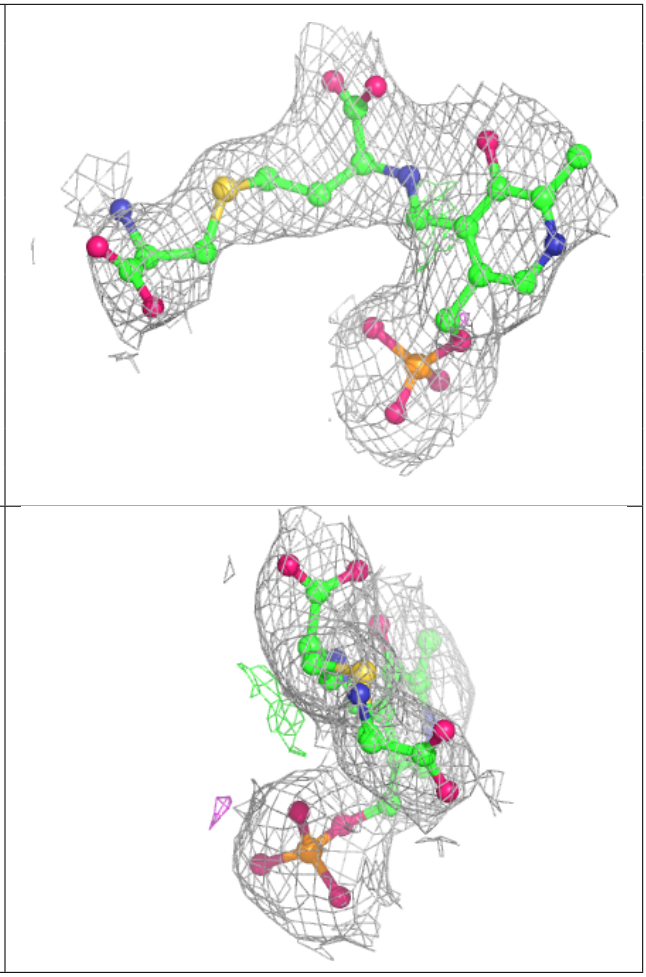
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	B	702	5/5	0.90	0.18	25,27,68,216	0
3	PO4	B	701	5/5	0.91	0.14	13,18,47,198	0
3	PO4	C	703	5/5	0.93	0.22	3,17,45,287	0
2	E9U	B	502	29/29	0.94	0.20	0,30,86,90	0
2	E9U	A	501	29/29	0.95	0.22	0,30,86,90	0
2	E9U	F	506	29/29	0.96	0.16	0,30,86,90	0
2	E9U	C	503	29/29	0.96	0.18	0,30,86,90	0
2	E9U	D	504	29/29	0.96	0.17	0,30,86,90	0
2	E9U	E	505	29/29	0.96	0.16	0,30,86,90	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.

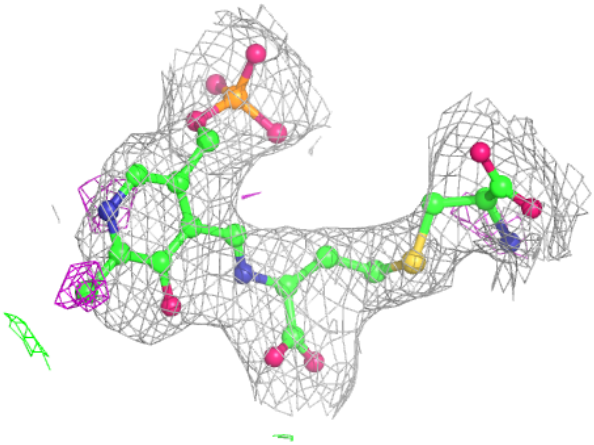
Electron density around E9U B 502:

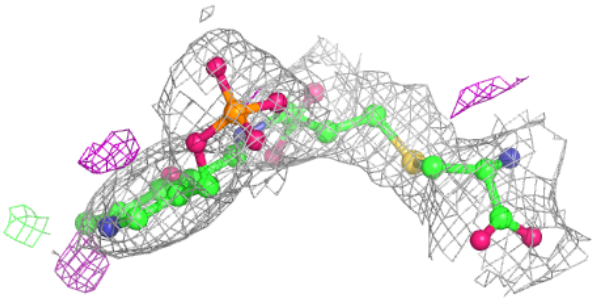
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

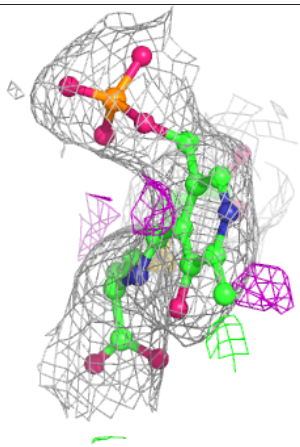


Electron density around E9U A 501:

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

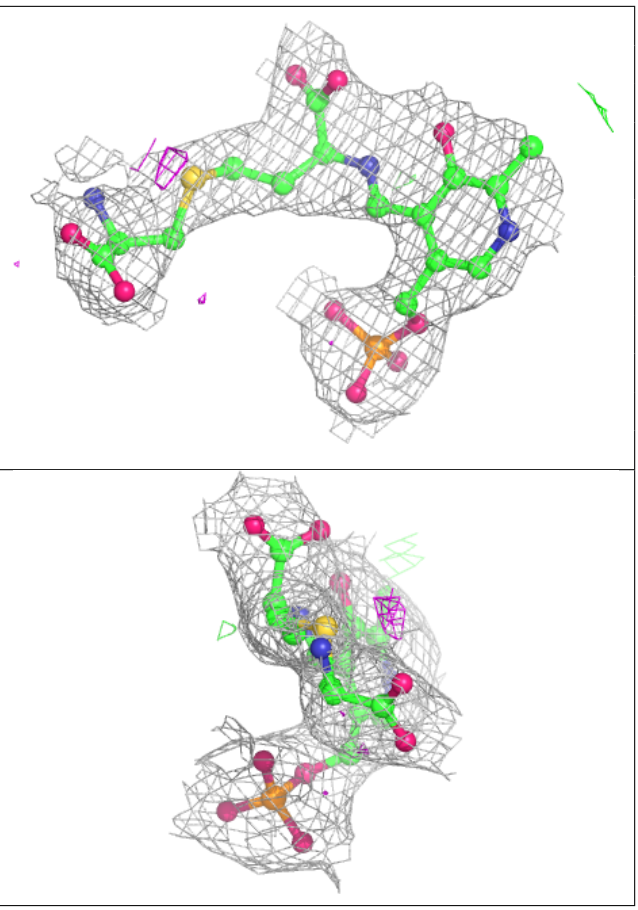






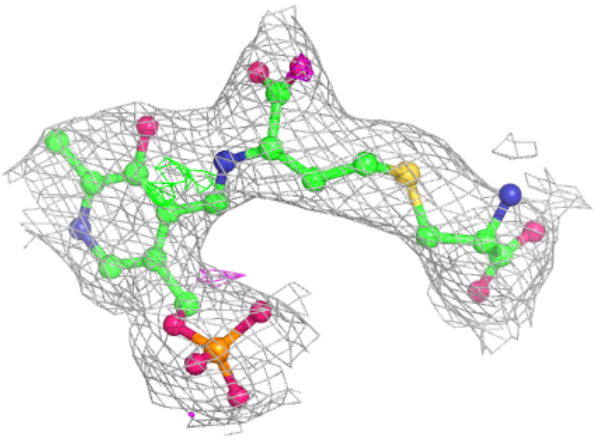
Electron density around E9U F 506:

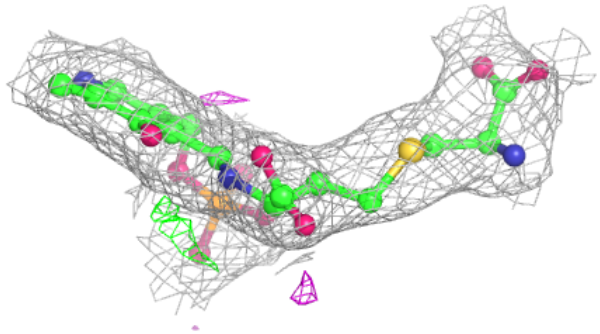
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

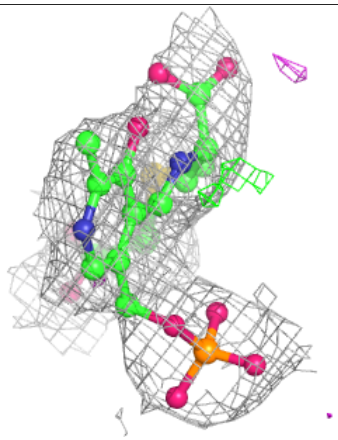


Electron density around E9U C 503:

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

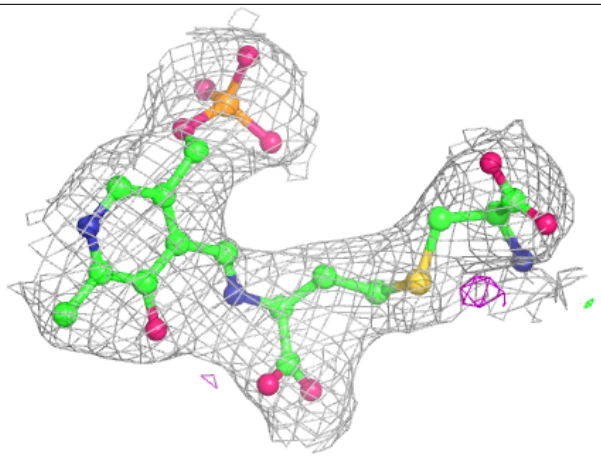


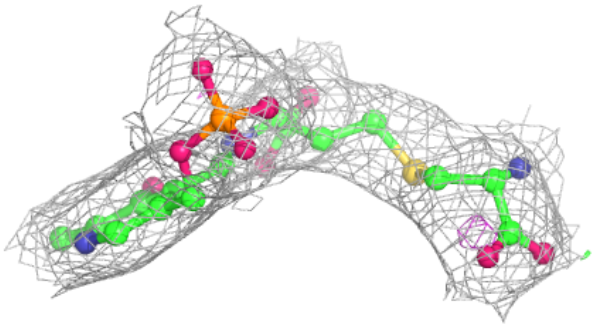


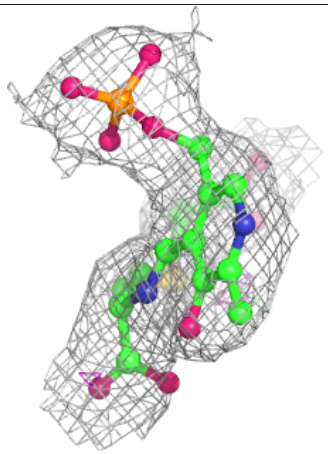


Electron density around E9U D 504:

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

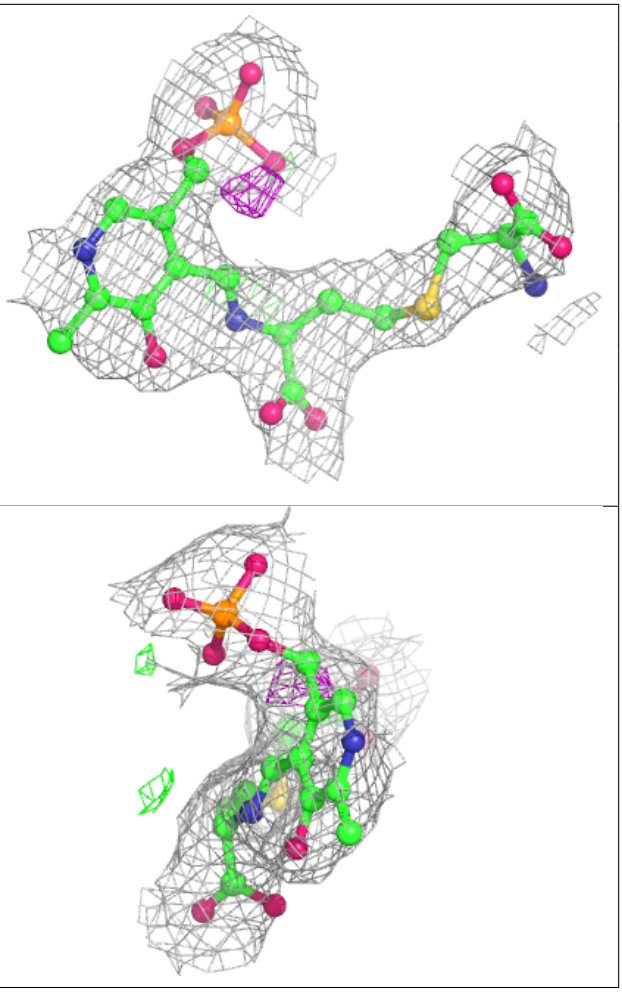






Electron density around E9U E 505:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.