



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:32 AM UTC

PDB ID : 6LE4 / pdb_00006le4
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

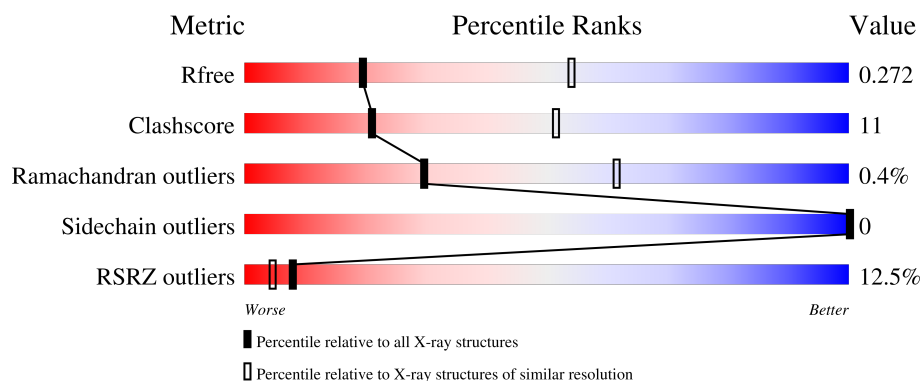
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	389	8% 76% 22% .
1	B	389	20% 72% 25% .
1	C	389	17% 74% 24% .
1	D	389	4% 74% 23% .
1	E	389	19% 74% 23% .

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Mol	Chain	Length	Quality of chain
1	F	389	6% 75% 23%

2 Entry composition

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
1	A	380	Total	C	N	O	S	0	0	0
			2867	1829	482	547	9			
1	B	380	Total	C	N	O	S	0	0	0
			2867	1829	482	547	9			
1	C	380	Total	C	N	O	S	0	0	0
			2867	1829	482	547	9			
1	D	380	Total	C	N	O	S	0	0	0
			2867	1829	482	547	9			
1	E	380	Total	C	N	O	S	0	0	0
			2867	1829	482	547	9			
1	F	380	Total	C	N	O	S	0	0	0
			2867	1829	482	547	9			

There are 54 discrepancies between the modelled and reference sequences:

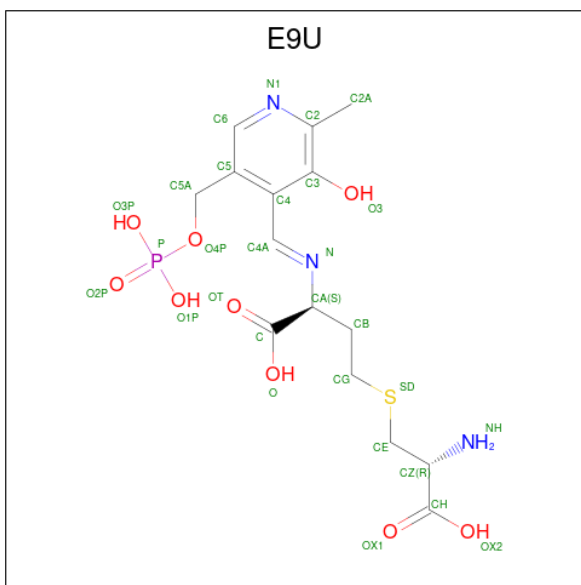
Chain	Residue	Modelled	Actual	Comment	Reference
A	194	ALA	LYS	engineered mutation	UNP A0A162EFJ4
A	382	LEU	-	expression tag	UNP A0A162EFJ4
A	383	GLU	-	expression tag	UNP A0A162EFJ4
A	384	HIS	-	expression tag	UNP A0A162EFJ4
A	385	HIS	-	expression tag	UNP A0A162EFJ4
A	386	HIS	-	expression tag	UNP A0A162EFJ4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

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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]methylenediamino]butanoic acid (CCD ID: E9U) (formula: C₁₅H₂₂N₃O₉PS) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

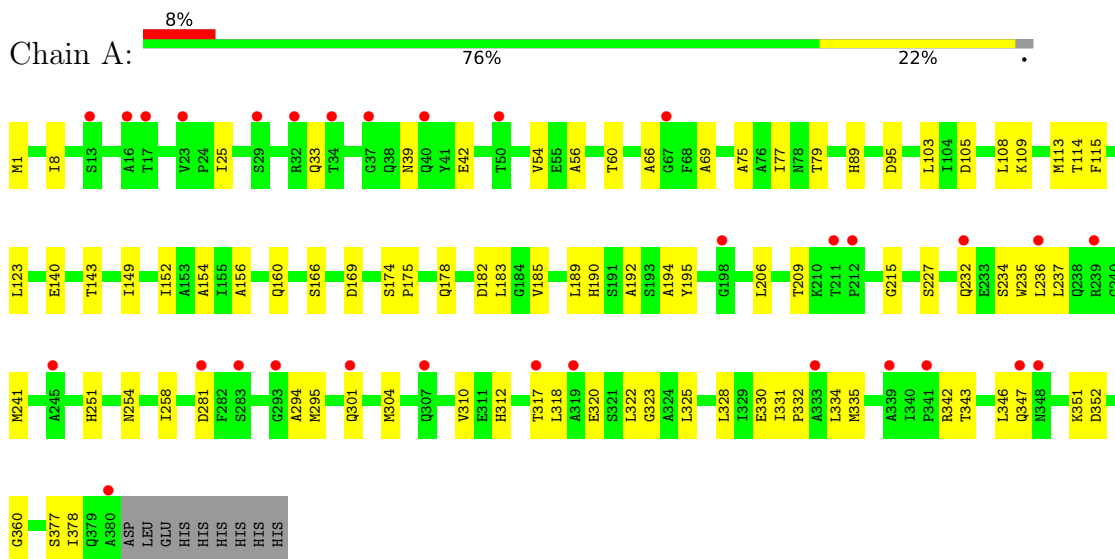
- Molecule 4 is water.

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

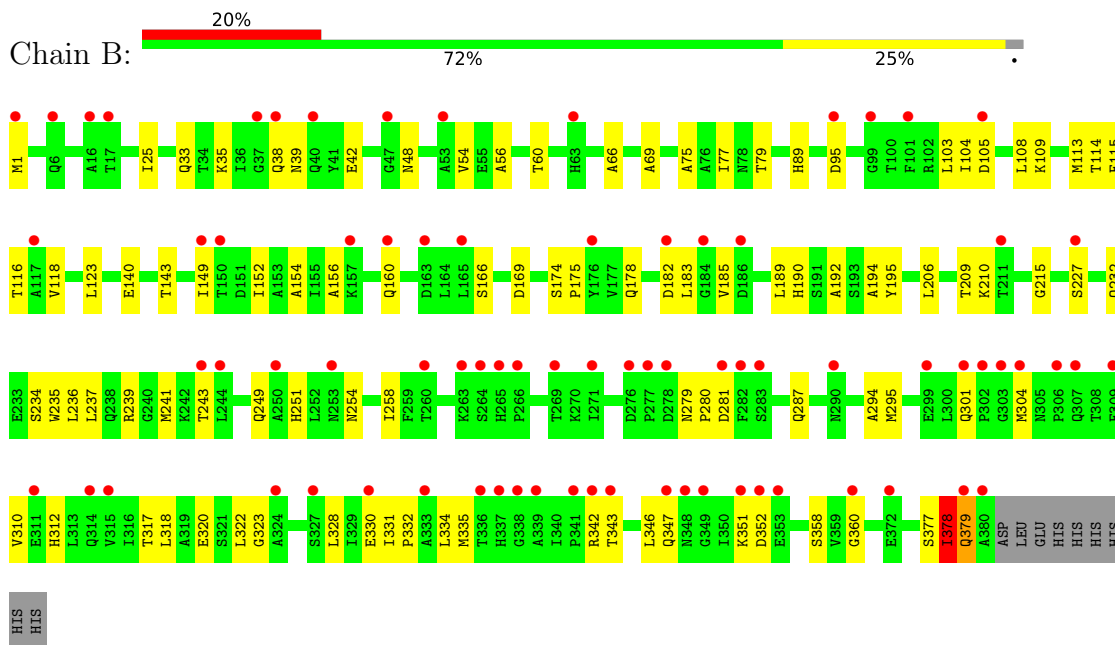
3 Residue-property plots

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

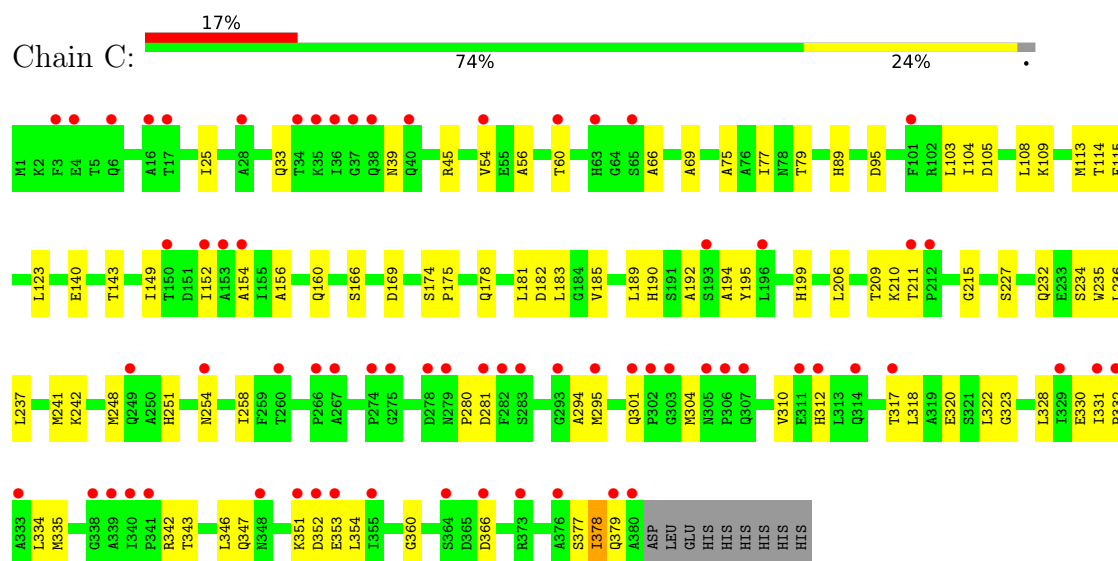
• Molecule 1: Cystathionine gamma-lyase



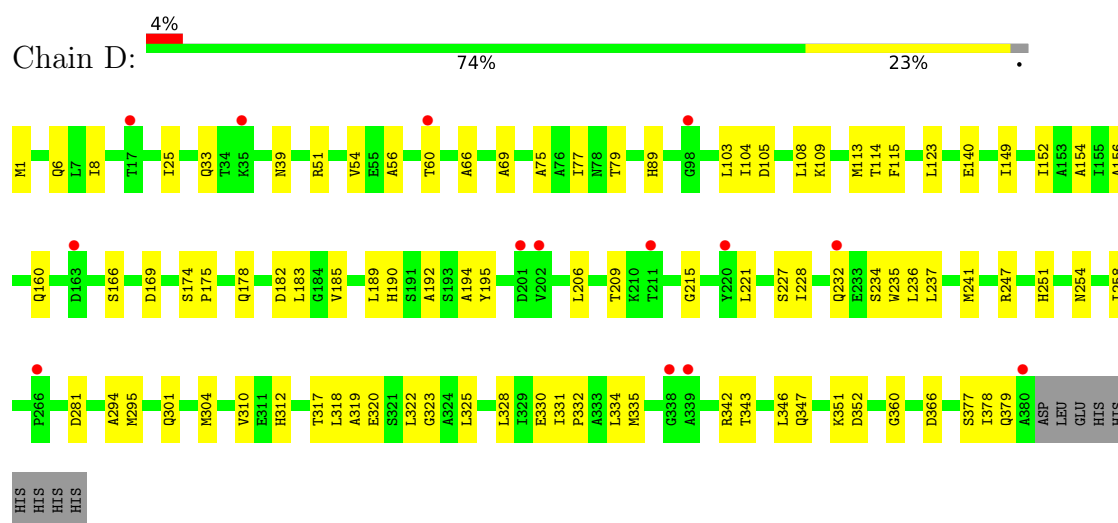
• Molecule 1: Cystathionine gamma-lyase



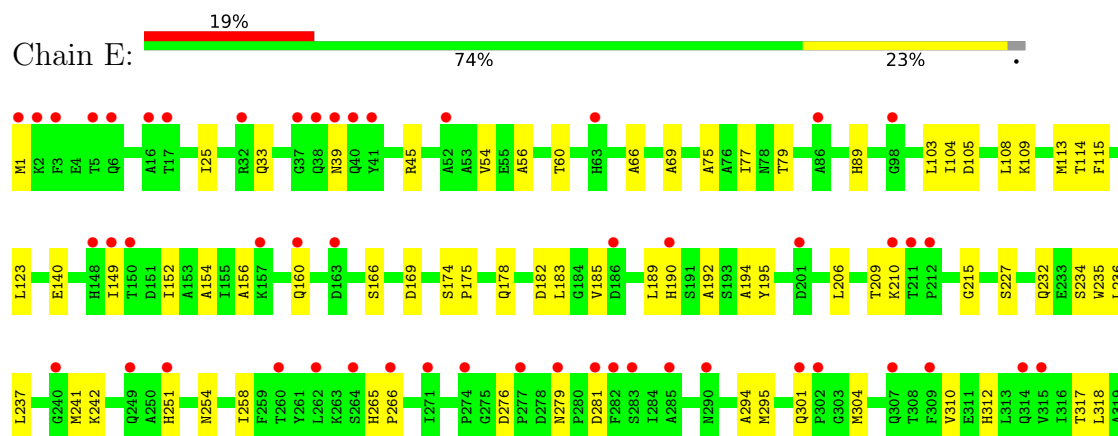
• Molecule 1: Cystathionine gamma-lyase

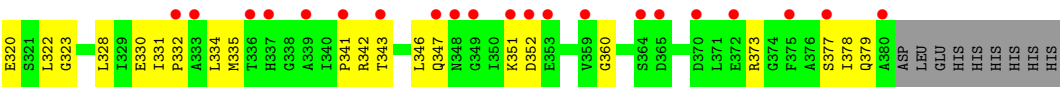


• Molecule 1: Cystathionine gamma-lyase

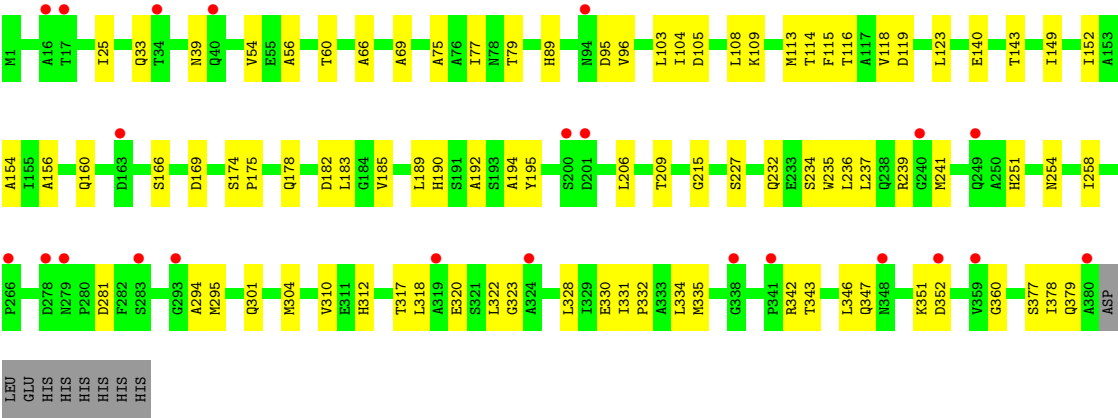


• Molecule 1: Cystathionine gamma-lyase





● Molecule 1: Cystathionine gamma-lyase



4 Data and refinement statistics

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 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.6 (36.26-3.10) 91.4 (36.26-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.06Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.246 , 0.273 0.246 , 0.272	Depositor DCC
R_{free} test set	3656 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	17687	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/2924	0.64	2/3978 (0.1%)
1	B	0.40	2/2924 (0.1%)	0.67	4/3978 (0.1%)
1	C	0.39	0/2924	0.65	2/3978 (0.1%)
1	D	0.37	0/2924	0.64	2/3978 (0.1%)
1	E	0.38	0/2924	0.64	2/3978 (0.1%)
1	F	0.37	0/2924	0.64	2/3978 (0.1%)
All	All	0.38	2/17544 (0.0%)	0.65	14/23868 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	GLN	CG-CD	5.01	1.64	1.52
1	B	379	GLN	N-CA	5.01	1.52	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	ILE	O-C-N	-11.13	107.78	122.03
1	A	378	ILE	CA-C-N	8.04	136.89	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ILE	C-N-CA	8.04	136.89	121.54
1	D	378	ILE	CA-C-N	7.70	136.24	121.54
1	D	378	ILE	C-N-CA	7.70	136.24	121.54
1	C	378	ILE	CA-C-N	7.66	136.17	121.54
1	C	378	ILE	C-N-CA	7.66	136.17	121.54
1	B	378	ILE	CA-C-N	-7.58	110.26	120.79
1	B	378	ILE	C-N-CA	-7.58	110.26	120.79
1	F	378	ILE	CA-C-N	7.18	135.26	121.54
1	F	378	ILE	C-N-CA	7.18	135.26	121.54
1	E	1	MET	CA-C-N	6.33	134.99	121.45
1	E	1	MET	C-N-CA	6.33	134.99	121.45
1	B	379	GLN	N-CA-C	5.20	117.37	111.02

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 ⓘ

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	63	0
1	B	2867	0	2883	74	0
1	C	2867	0	2883	70	0
1	D	2867	0	2883	68	0
1	E	2867	0	2883	64	0
1	F	2867	0	2883	61	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	0
4	C	71	0	0	9	0
4	D	41	0	0	4	0
4	E	68	0	0	5	0
4	F	33	0	0	3	0
All	All	17687	0	17298	380	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 11.

All (380) 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: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:D:295:MET:HE1	1:D:322:LEU:HB2	1.63	0.81
1:C:227:SER:HB3	1:D:227:SER:HB3	1.60	0.81
1:C:295:MET:HE1	1:C:322:LEU:HB2	1.63	0.81
1:B:237:LEU:HD22	1:B:241:MET:HE2	1.63	0.80
1:B:295:MET:HE1	1:B:322:LEU:HB2	1.63	0.80
1:E:295:MET:HE1	1:E:322:LEU:HB2	1.63	0.80
1:B:123:LEU:HD21	1:B:154:ALA:HB1	1.62	0.80
1:A:295:MET:HE1	1:A:322:LEU:HB2	1.63	0.79
1:C:237:LEU:HD22	1:C:241:MET:HE2	1.63	0.79
1:A:237:LEU:HD22	1:A:241:MET:HE2	1.63	0.79
1:A:123:LEU:HD21	1:A:154:ALA:HB1	1.62	0.79
1:E:237:LEU:HD22	1:E:241:MET:HE2	1.63	0.79
1:F:295:MET:HE1	1:F:322:LEU:HB2	1.63	0.79
1:D:237:LEU:HD22	1:D:241:MET:HE2	1.63	0.78
1:F:237:LEU:HD22	1:F:241:MET:HE2	1.63	0.77
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

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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:F:192:ALA:HB1	1:F:237:LEU:HD21	1.74	0.68
1:B:378:ILE:O	1:B:379:GLN:C	2.30	0.67
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:E:108:LEU:HD13	1:E:113:MET:HE1	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:HD13	1:B:113:MET:HE1	1.84	0.60
1:D:25:ILE:HG21	1:D:232:GLN:HE21	1.66	0.60
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:C:108:LEU:HD13	1:C:113:MET:HE1	1.84	0.59
1:E:209:THR:HG21	1:E:215:GLY:CA	2.31	0.59
1:F:108:LEU:HD13	1:F:113:MET:HE1	1.84	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:D:108:LEU:HD13	1:D:113:MET:HE1	1.84	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:A:108:LEU:HD13	1:A:113:MET:HE1	1.84	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:D:1:MET:HE3	1:D:6:GLN:HG2	1.85	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:251:HIS:CE1	1:B:360:GLY:HA2	2.42	0.55
1:F:251:HIS:CE1	1:F:360:GLY:HA2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:295:MET:CE	1:C:322:LEU:HB2	2.39	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:A:295:MET:CE	1:A:322:LEU:HB2	2.39	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:295:MET:CE	1:E:322:LEU:HB2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:MET:CE	1:D:322:LEU:HB2	2.39	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
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:B:358:SER:OG	4:B:1031:HOH:O	2.19	0.46
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:A:113:MET:HE2	1:A:115:PHE:HZ	1.81	0.45
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:D:113:MET:HE2	1:D:115:PHE:HZ	1.82	0.45
1:E:210:LYS:HB3	4:E:1201:HOH:O	2.15	0.45
1:F:295:MET:CE	1:F:322:LEU:HB2	2.39	0.45
1:F:113:MET:HE2	1:F:115:PHE:HZ	1.82	0.45
1:B:113:MET:HE2	1:B:115:PHE:HZ	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:MET:HE2	1:C:115:PHE:HZ	1.82	0.44
1:F:301:GLN:HB2	1:F:304:MET:SD	2.57	0.44
1:B:295:MET:CE	1:B:322:LEU:HB2	2.39	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:E:113:MET:HE2	1:E:115:PHE:HZ	1.82	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
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:B:334:LEU:C	1:B:335:MET:HG3	2.43	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:D:334:LEU:C	1:D:335:MET:HG3	2.43	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:C:334:LEU:C	1:C:335:MET:HG3	2.43	0.43
1:D:33:GLN:HA	1:D:39:ASN:OD1	2.18	0.43
1:A:334:LEU:C	1:A:335:MET:HG3	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:334:LEU:C	1:E:335:MET:HG3	2.43	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:F:334:LEU:C	1:F:335:MET:HG3	2.43	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
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:182:ASP:C	1:C:183:LEU:HD23	2.45	0.42
1:E:182:ASP:C	1:E:183:LEU:HD23	2.45	0.42
1:A:209:THR:HG21	1:A:215:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:379:GLN:CD	1:E:379:GLN:N	2.77	0.42
1:F:182:ASP:C	1:F:183:LEU:HD23	2.45	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:D:182:ASP:C	1:D:183:LEU:HD23	2.45	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:A:182:ASP:C	1:A:183:LEU:HD23	2.45	0.41
1:B:182:ASP:C	1:B:183:LEU:HD23	2.45	0.41
1:D:174:SER:HA	1:D:190:HIS:HE1	1.84	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:343:THR:O	1:E:347:GLN:HB2	2.21	0.40
1:B:209:THR:HG21	1:B:215:GLY:HA2	2.02	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
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/389 (97%)	362 (96%)	15 (4%)	1 (0%)	36	67
1	B	378/389 (97%)	364 (96%)	13 (3%)	1 (0%)	36	67
1	C	378/389 (97%)	363 (96%)	13 (3%)	2 (0%)	24	57
1	D	378/389 (97%)	363 (96%)	13 (3%)	2 (0%)	24	57
1	E	378/389 (97%)	363 (96%)	14 (4%)	1 (0%)	36	67
1	F	378/389 (97%)	362 (96%)	14 (4%)	2 (0%)	24	57
All	All	2268/2334 (97%)	2177 (96%)	82 (4%)	9 (0%)	30	61

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
1	F	194	ALA
1	C	379	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/312 (97%)	303 (100%)	0	100	100
1	B	303/312 (97%)	303 (100%)	0	100	100
1	C	303/312 (97%)	303 (100%)	0	100	100
1	D	303/312 (97%)	303 (100%)	0	100	100
1	E	303/312 (97%)	303 (100%)	0	100	100
1	F	303/312 (97%)	303 (100%)	0	100	100
All	All	1818/1872 (97%)	1818 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	148	HIS
1	A	232	GLN
1	A	290	ASN
1	A	312	HIS
1	B	232	GLN
1	B	290	ASN
1	B	312	HIS
1	B	379	GLN
1	C	38	GLN
1	C	148	HIS
1	C	232	GLN
1	C	290	ASN
1	C	312	HIS
1	D	232	GLN
1	D	290	ASN
1	D	312	HIS
1	E	9	HIS
1	E	232	GLN
1	E	290	ASN
1	E	312	HIS
1	F	232	GLN
1	F	290	ASN
1	F	312	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	E	505	-	28,29,29	1.21	2 (7%)	33,40,40	1.69	5 (15%)
3	PO4	B	701	-	4,4,4	0.69	0	6,6,6	0.70	0
3	PO4	C	703	-	4,4,4	0.76	0	6,6,6	1.08	0
2	E9U	A	501	-	28,29,29	1.20	2 (7%)	33,40,40	1.69	5 (15%)
2	E9U	D	504	-	28,29,29	1.20	2 (7%)	33,40,40	1.69	5 (15%)
2	E9U	C	503	-	28,29,29	1.20	2 (7%)	33,40,40	1.69	5 (15%)
2	E9U	F	506	-	28,29,29	1.21	2 (7%)	33,40,40	1.69	5 (15%)
3	PO4	B	702	-	4,4,4	1.07	0	6,6,6	0.89	0
2	E9U	B	502	-	28,29,29	1.20	2 (7%)	33,40,40	1.69	5 (15%)

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	E	505	-	-	9/26/26/26	0/1/1/1
2	E9U	A	501	-	-	9/26/26/26	0/1/1/1
2	E9U	D	504	-	-	9/26/26/26	0/1/1/1
2	E9U	C	503	-	-	9/26/26/26	0/1/1/1
2	E9U	F	506	-	-	9/26/26/26	0/1/1/1
2	E9U	B	502	-	-	9/26/26/26	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	3.55	1.32	1.22
2	C	503	E9U	OX1-CH	3.55	1.32	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	506	E9U	OX1-CH	3.55	1.32	1.22
2	A	501	E9U	OX1-CH	3.55	1.32	1.22
2	E	505	E9U	OX1-CH	3.54	1.32	1.22
2	B	502	E9U	OX1-CH	3.54	1.32	1.22
2	A	501	E9U	OX2-CH	-2.52	1.22	1.30
2	E	505	E9U	OX2-CH	-2.50	1.22	1.30
2	B	502	E9U	OX2-CH	-2.50	1.22	1.30
2	D	504	E9U	OX2-CH	-2.49	1.22	1.30
2	F	506	E9U	OX2-CH	-2.49	1.22	1.30
2	C	503	E9U	OX2-CH	-2.49	1.22	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	506	E9U	CA-N-C4A	6.30	126.12	116.77
2	A	501	E9U	CA-N-C4A	6.29	126.12	116.77
2	D	504	E9U	CA-N-C4A	6.29	126.11	116.77
2	E	505	E9U	CA-N-C4A	6.28	126.10	116.77
2	B	502	E9U	CA-N-C4A	6.28	126.09	116.77
2	C	503	E9U	CA-N-C4A	6.26	126.06	116.77
2	B	502	E9U	CE-SD-CG	4.01	114.16	102.26
2	C	503	E9U	CE-SD-CG	4.00	114.14	102.26
2	A	501	E9U	CE-SD-CG	4.00	114.13	102.26
2	D	504	E9U	CE-SD-CG	4.00	114.12	102.26
2	E	505	E9U	CE-SD-CG	3.99	114.12	102.26
2	F	506	E9U	CE-SD-CG	3.99	114.11	102.26
2	F	506	E9U	O-C-OT	-2.59	118.21	124.08
2	D	504	E9U	O-C-OT	-2.58	118.22	124.08
2	A	501	E9U	CB-CG-SD	-2.58	107.69	113.45
2	E	505	E9U	O-C-OT	-2.58	118.22	124.08
2	C	503	E9U	O-C-OT	-2.58	118.23	124.08
2	B	502	E9U	CB-CG-SD	-2.57	107.72	113.45
2	A	501	E9U	O-C-OT	-2.56	118.26	124.08
2	E	505	E9U	CB-CG-SD	-2.56	107.73	113.45
2	B	502	E9U	O-C-OT	-2.56	118.28	124.08
2	F	506	E9U	CB-CG-SD	-2.55	107.75	113.45
2	D	504	E9U	CB-CG-SD	-2.55	107.76	113.45
2	C	503	E9U	CB-CG-SD	-2.54	107.78	113.45
2	D	504	E9U	CB-CA-C	2.11	112.99	109.48
2	A	501	E9U	CB-CA-C	2.10	112.98	109.48
2	E	505	E9U	CB-CA-C	2.10	112.98	109.48
2	C	503	E9U	CB-CA-C	2.10	112.97	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	506	E9U	CB-CA-C	2.10	112.97	109.48
2	B	502	E9U	CB-CA-C	2.08	112.94	109.48

There are no chirality outliers.

All (54) 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
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	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	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	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

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Mol	Chain	Res	Type	Atoms
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
2	A	501	E9U	CZ-CE-SD-CG
2	B	502	E9U	CZ-CE-SD-CG
2	C	503	E9U	CZ-CE-SD-CG
2	D	504	E9U	CZ-CE-SD-CG
2	E	505	E9U	CZ-CE-SD-CG
2	F	506	E9U	CZ-CE-SD-CG

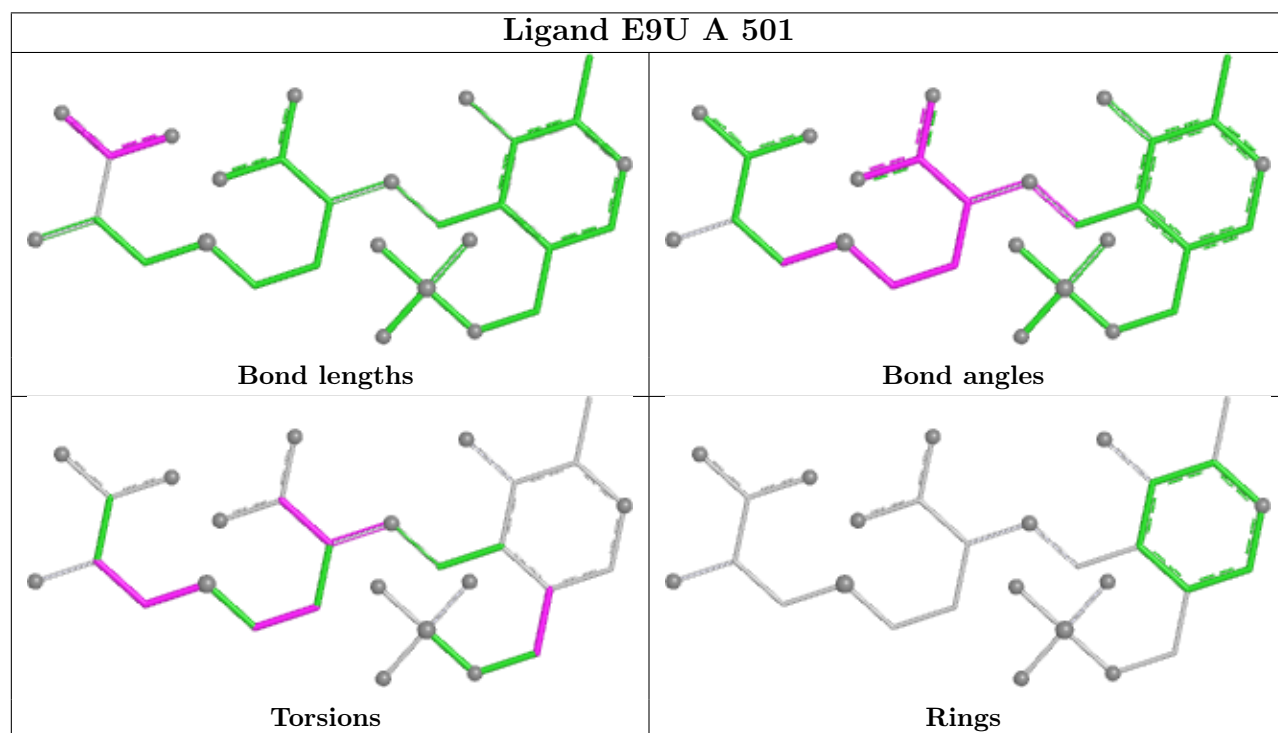
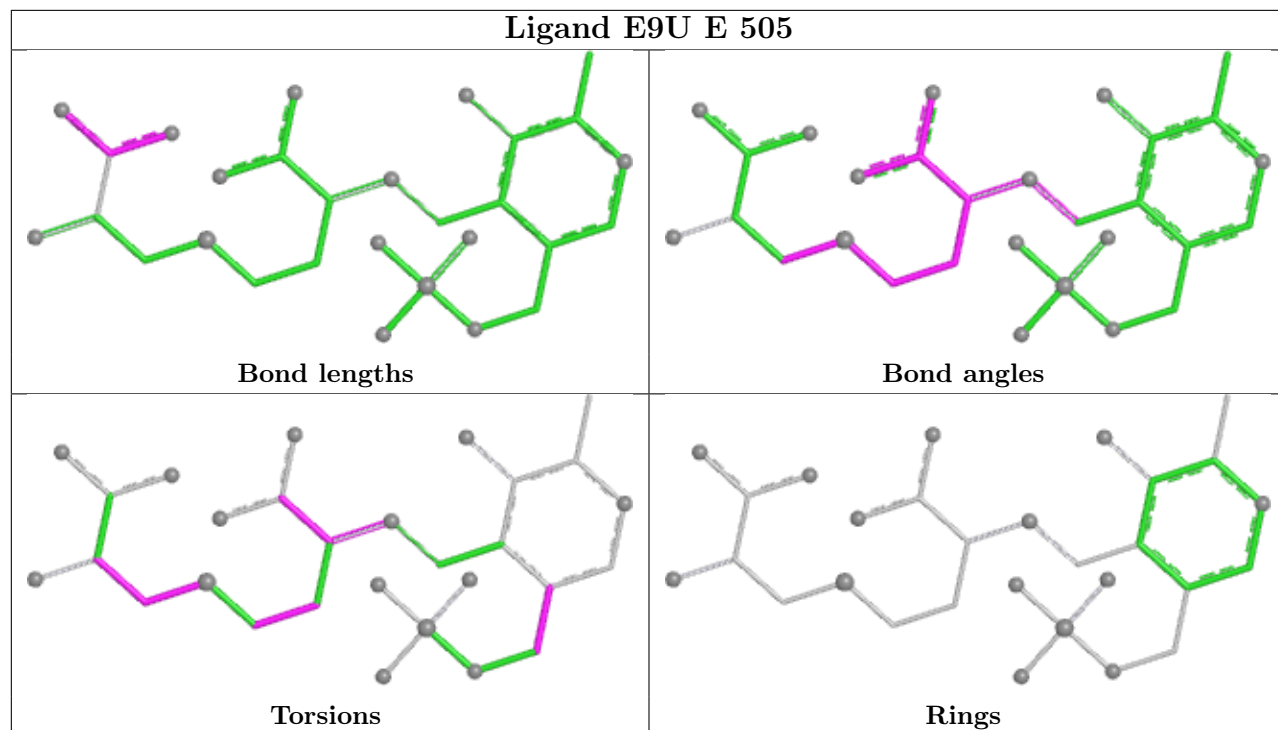
There are no ring outliers.

6 monomers are involved in 10 short contacts:

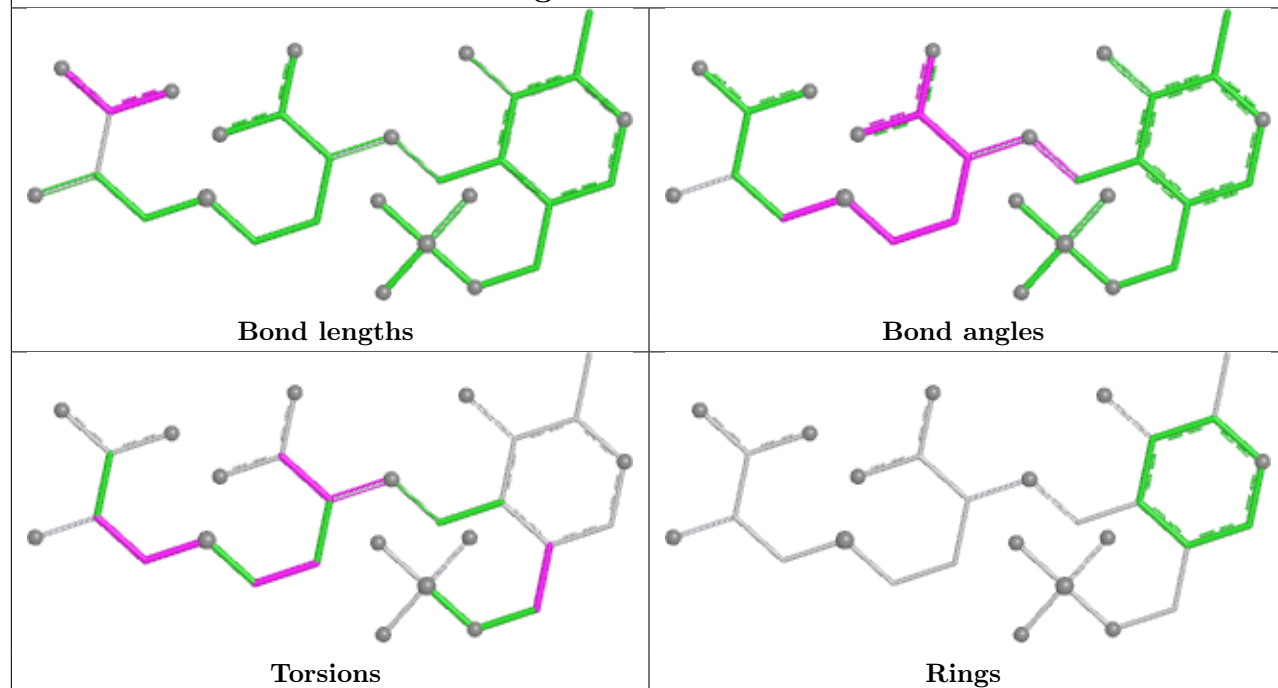
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	505	E9U	1	0
2	A	501	E9U	2	0
2	D	504	E9U	2	0
2	C	503	E9U	1	0
2	F	506	E9U	2	0
2	B	502	E9U	2	0

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

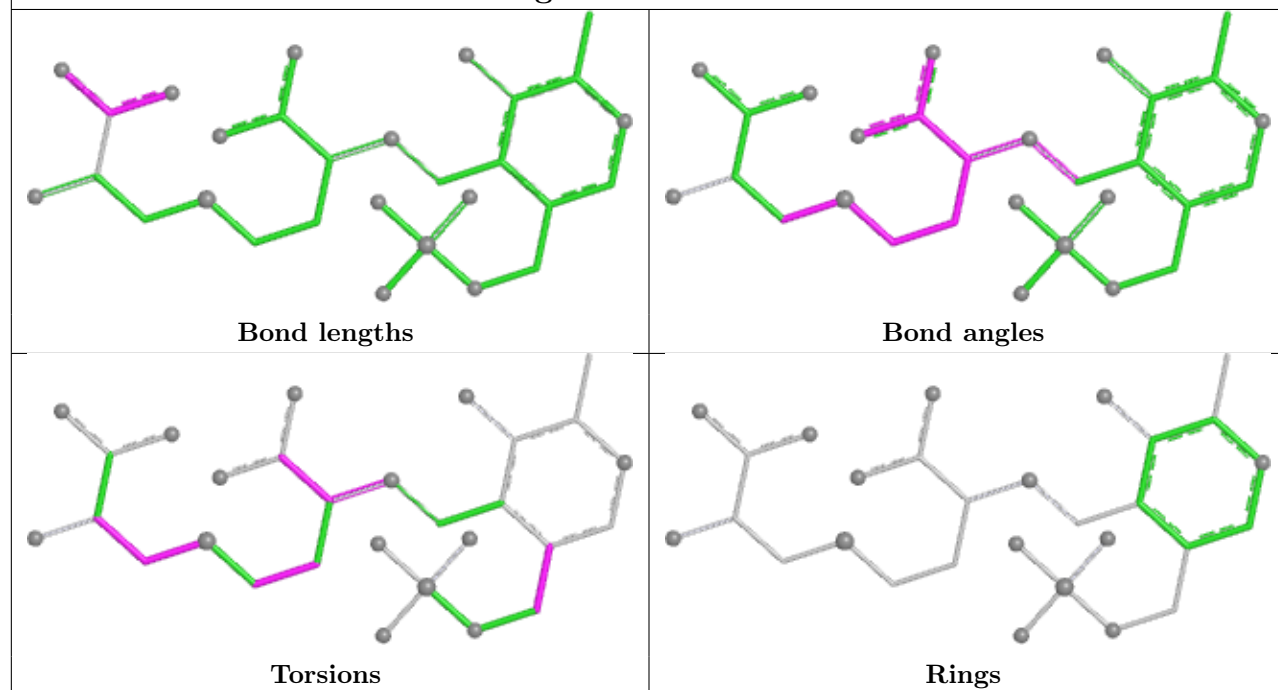
equivalents in the CSD to analyse the geometry.

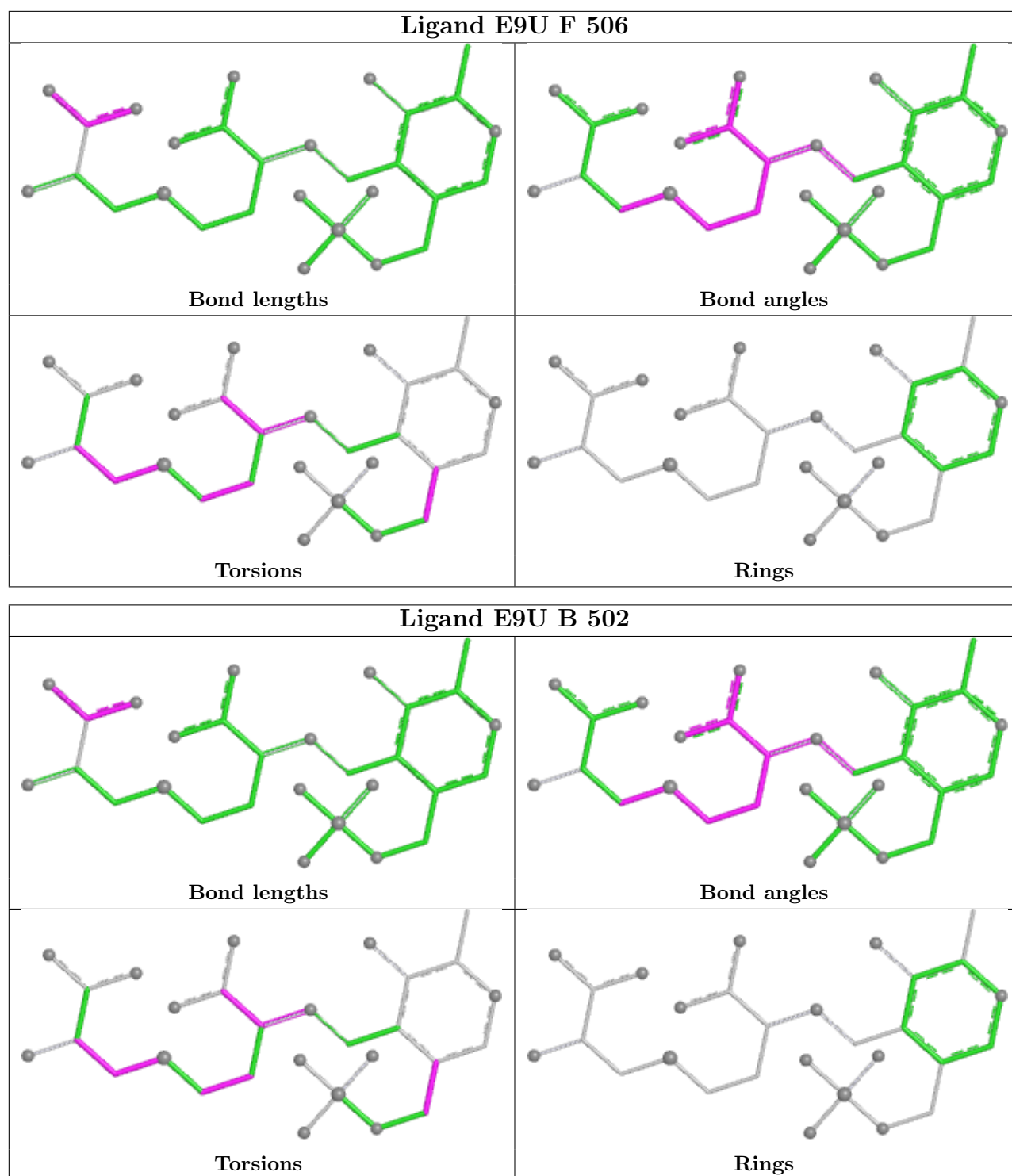


Ligand E9U D 504



Ligand E9U C 503





5.7 Other polymers [i](#)

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, 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%)	0.69	31 (8%) 17 10	17, 35, 66, 91	0
1	B	380/389 (97%)	1.23	77 (20%) 3 1	17, 35, 66, 86	0
1	C	380/389 (97%)	1.18	68 (17%) 3 1	17, 35, 65, 136	0
1	D	380/389 (97%)	0.67	14 (3%) 45 25	17, 35, 65, 104	0
1	E	380/389 (97%)	1.22	72 (18%) 3 1	17, 35, 66, 165	0
1	F	380/389 (97%)	0.69	23 (6%) 27 15	17, 35, 65, 131	0
All	All	2280/2334 (97%)	0.95	285 (12%) 8 5	17, 35, 66, 165	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	380	ALA	8.5
1	E	380	ALA	6.9
1	E	266	PRO	6.5
1	B	266	PRO	6.4
1	C	38	GLN	6.3
1	A	380	ALA	6.1
1	B	307	GLN	6.0
1	F	380	ALA	6.0
1	E	37	GLY	5.9
1	B	339	ALA	5.6
1	C	314	GLN	5.4
1	C	35	LYS	5.2
1	B	352	ASP	5.1
1	B	301	GLN	5.1
1	C	17	THR	5.0
1	C	37	GLY	5.0
1	E	38	GLN	4.9
1	E	339	ALA	4.8
1	E	352	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	34	THR	4.7
1	E	249	GLN	4.4
1	E	40	GLN	4.4
1	B	338	GLY	4.3
1	B	269	THR	4.3
1	E	260	THR	4.3
1	F	16	ALA	4.2
1	B	38	GLN	4.2
1	B	302	PRO	4.2
1	B	380	ALA	4.2
1	D	380	ALA	4.2
1	E	307	GLN	4.1
1	C	260	THR	4.1
1	C	307	GLN	4.1
1	C	301	GLN	4.1
1	B	16	ALA	4.0
1	E	52	ALA	4.0
1	C	366	ASP	3.9
1	E	1	MET	3.9
1	B	281	ASP	3.9
1	B	176	TYR	3.9
1	E	39	ASN	3.9
1	B	160	GLN	3.8
1	B	337	HIS	3.7
1	B	283	SER	3.7
1	C	339	ALA	3.7
1	B	37	GLY	3.7
1	E	41	TYR	3.6
1	E	283	SER	3.6
1	E	281	ASP	3.6
1	C	40	GLN	3.6
1	C	266	PRO	3.6
1	D	339	ALA	3.6
1	E	315	VAL	3.6
1	D	163	ASP	3.6
1	E	301	GLN	3.5
1	A	13	SER	3.5
1	F	201	ASP	3.5
1	B	150	THR	3.5
1	C	282	PHE	3.4
1	B	333	ALA	3.4
1	D	17	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	304	MET	3.3
1	B	260	THR	3.3
1	C	379	GLN	3.3
1	A	17	THR	3.3
1	B	253	ASN	3.3
1	B	379	GLN	3.3
1	C	312	HIS	3.3
1	E	5	THR	3.3
1	C	16	ALA	3.2
1	F	200	SER	3.2
1	B	182	ASP	3.2
1	C	352	ASP	3.2
1	E	160	GLN	3.2
1	A	211	THR	3.2
1	C	353	GLU	3.2
1	C	302	PRO	3.2
1	A	307	GLN	3.2
1	B	1	MET	3.2
1	E	375	PHE	3.1
1	E	17	THR	3.1
1	B	278	ASP	3.1
1	C	275	GLY	3.1
1	B	353	GLU	3.1
1	B	282	PHE	3.1
1	D	220	TYR	3.1
1	B	265	HIS	3.1
1	B	6	GLN	3.1
1	E	353	GLU	3.1
1	B	351	LYS	3.1
1	C	348	ASN	3.1
1	C	101	PHE	3.1
1	E	212	PRO	3.1
1	E	336	THR	3.0
1	E	279	ASN	3.0
1	E	264	SER	3.0
1	E	337	HIS	3.0
1	B	349	GLY	3.0
1	A	16	ALA	3.0
1	E	16	ALA	3.0
1	E	186	ASP	3.0
1	B	341	PRO	2.9
1	E	341	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	98	GLY	2.9
1	B	314	GLN	2.9
1	B	311	GLU	2.9
1	C	211	THR	2.9
1	C	333	ALA	2.9
1	B	303	GLY	2.9
1	B	244	LEU	2.9
1	E	290	ASN	2.9
1	C	54	VAL	2.9
1	B	342	ARG	2.9
1	B	336	THR	2.9
1	E	3	PHE	2.9
1	B	163	ASP	2.8
1	E	6	GLN	2.8
1	E	98	GLY	2.8
1	F	338	GLY	2.8
1	B	184	GLY	2.8
1	C	193	SER	2.8
1	A	232	GLN	2.8
1	F	348	ASN	2.7
1	B	157	LYS	2.7
1	E	377	SER	2.7
1	F	279	ASN	2.7
1	C	274	PRO	2.7
1	A	37	GLY	2.7
1	D	35	LYS	2.7
1	E	262	LEU	2.7
1	B	347	GLN	2.6
1	E	282	PHE	2.6
1	B	327	SER	2.6
1	E	86	ALA	2.6
1	E	314	GLN	2.6
1	D	202	VAL	2.6
1	A	348	ASN	2.6
1	C	249	GLN	2.6
1	C	311	GLU	2.6
1	B	211	THR	2.6
1	C	329	ILE	2.6
1	C	351	LYS	2.6
1	A	29	SER	2.6
1	A	341	PRO	2.6
1	F	341	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	40	GLN	2.6
1	A	236	LEU	2.6
1	E	157	LYS	2.6
1	A	34	THR	2.6
1	C	63	HIS	2.5
1	B	348	ASN	2.5
1	E	333	ALA	2.5
1	B	299	GLU	2.5
1	E	302	PRO	2.5
1	A	239	ARG	2.5
1	B	227	SER	2.5
1	E	364	SER	2.5
1	F	94	ASN	2.5
1	C	3	PHE	2.5
1	A	319	ALA	2.5
1	C	373	ARG	2.5
1	A	67	GLY	2.5
1	A	333	ALA	2.4
1	C	60	THR	2.4
1	D	266	PRO	2.4
1	B	360	GLY	2.4
1	B	40	GLN	2.4
1	B	263	LYS	2.4
1	E	309	PHE	2.4
1	C	278	ASP	2.4
1	C	212	PRO	2.4
1	F	359	VAL	2.4
1	B	149	ILE	2.4
1	B	324	ALA	2.4
1	E	211	THR	2.4
1	E	163	ASP	2.4
1	F	163	ASP	2.4
1	C	28	ALA	2.4
1	A	40	GLN	2.4
1	E	32	ARG	2.4
1	B	372	GLU	2.4
1	B	264	SER	2.4
1	C	153	ALA	2.4
1	C	267	ALA	2.4
1	C	376	ALA	2.4
1	F	324	ALA	2.4
1	A	347	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	283	SER	2.4
1	B	277	PRO	2.4
1	C	341	PRO	2.4
1	C	152	ILE	2.3
1	F	352	ASP	2.3
1	D	232	GLN	2.3
1	A	32	ARG	2.3
1	F	17	THR	2.3
1	B	95	ASP	2.3
1	C	338	GLY	2.3
1	E	149	ILE	2.3
1	E	271	ILE	2.3
1	A	50	THR	2.3
1	C	317	THR	2.3
1	C	196	LEU	2.3
1	E	370	ASP	2.3
1	C	36	ILE	2.3
1	C	293	GLY	2.3
1	A	283	SER	2.3
1	E	2	LYS	2.3
1	B	306	PRO	2.3
1	E	63	HIS	2.3
1	C	279	ASN	2.3
1	C	305	ASN	2.3
1	C	6	GLN	2.3
1	E	359	VAL	2.3
1	F	278	ASP	2.3
1	C	295	MET	2.2
1	B	276	ASP	2.2
1	B	271	ILE	2.2
1	B	53	ALA	2.2
1	A	317	THR	2.2
1	B	243	THR	2.2
1	E	351	LYS	2.2
1	F	249	GLN	2.2
1	C	4	GLU	2.2
1	A	245	ALA	2.2
1	F	319	ALA	2.2
1	D	211	THR	2.2
1	C	65	SER	2.2
1	E	347	GLN	2.2
1	E	348	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	372	GLU	2.2
1	B	47	GLY	2.2
1	C	303	GLY	2.2
1	E	274	PRO	2.2
1	B	17	THR	2.2
1	D	60	THR	2.2
1	F	34	THR	2.2
1	B	330	GLU	2.2
1	D	338	GLY	2.2
1	E	210	LYS	2.2
1	F	240	GLY	2.2
1	B	101	PHE	2.2
1	B	250	ALA	2.1
1	C	364	SER	2.1
1	A	293	GLY	2.1
1	E	240	GLY	2.1
1	F	266	PRO	2.1
1	F	293	GLY	2.1
1	B	63	HIS	2.1
1	C	150	THR	2.1
1	E	343	THR	2.1
1	E	349	GLY	2.1
1	A	281	ASP	2.1
1	B	315	VAL	2.1
1	C	281	ASP	2.1
1	E	201	ASP	2.1
1	B	165	LEU	2.1
1	C	340	ILE	2.1
1	C	355	ILE	2.1
1	A	301	GLN	2.1
1	E	332	PRO	2.1
1	C	254	ASN	2.1
1	B	343	THR	2.1
1	A	339	ALA	2.1
1	E	285	ALA	2.1
1	A	198	GLY	2.1
1	B	309	PHE	2.1
1	C	332	PRO	2.1
1	F	283	SER	2.1
1	B	290	ASN	2.1
1	E	190	HIS	2.1
1	B	186	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	201	ASP	2.1
1	C	306	PRO	2.1
1	A	23	VAL	2.0
1	C	154	ALA	2.0
1	A	212	PRO	2.0
1	E	277	PRO	2.0
1	C	331	ILE	2.0
1	E	148	HIS	2.0
1	E	251	HIS	2.0
1	B	117	ALA	2.0
1	E	150	THR	2.0
1	B	105	ASP	2.0
1	E	365	ASP	2.0
1	B	99	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

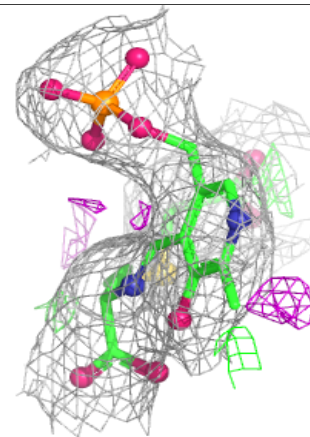
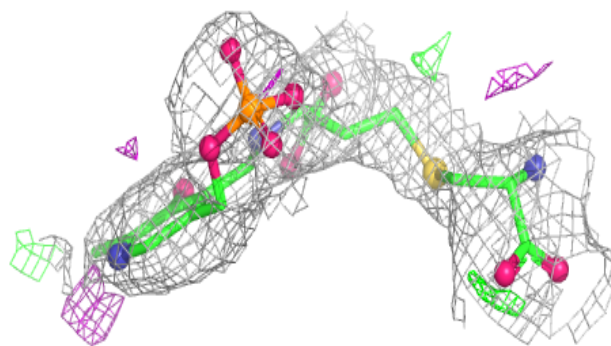
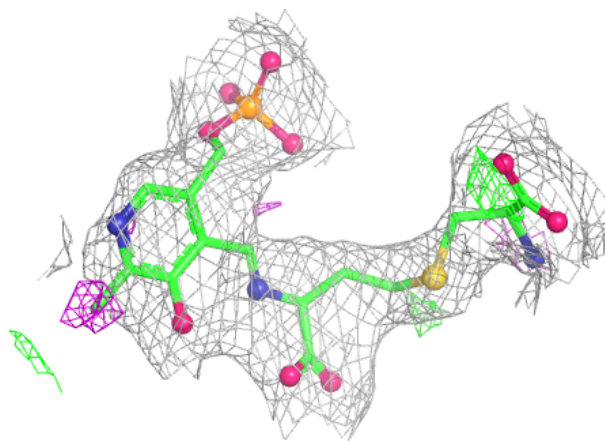
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	C	703	5/5	0.87	0.26	3,17,45,287	0
3	PO4	B	702	5/5	0.89	0.16	25,27,68,216	0
2	E9U	A	501	29/29	0.92	0.15	0,30,86,90	0
3	PO4	B	701	5/5	0.92	0.11	13,18,47,198	0
2	E9U	C	503	29/29	0.94	0.12	0,30,86,90	0
2	E9U	B	502	29/29	0.95	0.10	0,30,86,90	0
2	E9U	E	505	29/29	0.95	0.11	0,30,86,90	0
2	E9U	F	506	29/29	0.95	0.10	0,30,86,90	0
2	E9U	D	504	29/29	0.96	0.10	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.

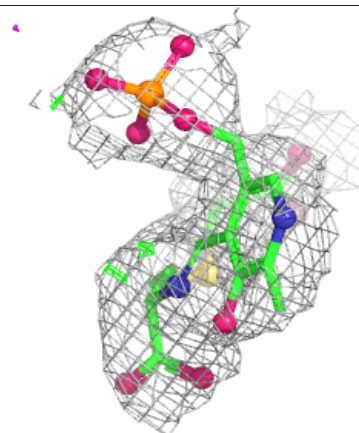
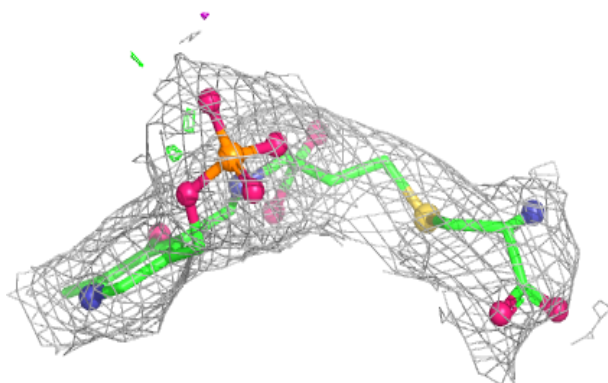
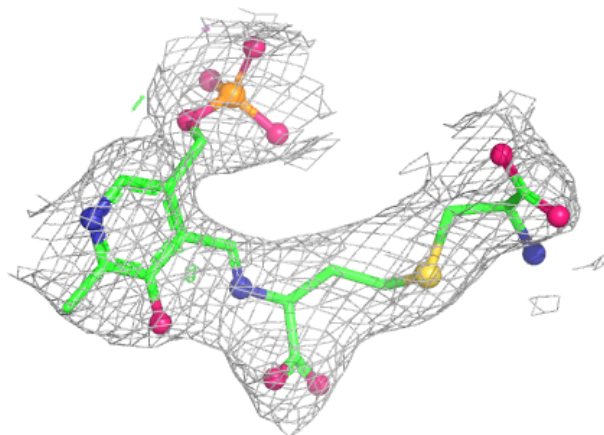
Electron density around E9U A 501:

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



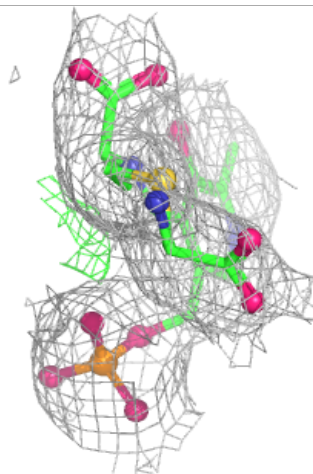
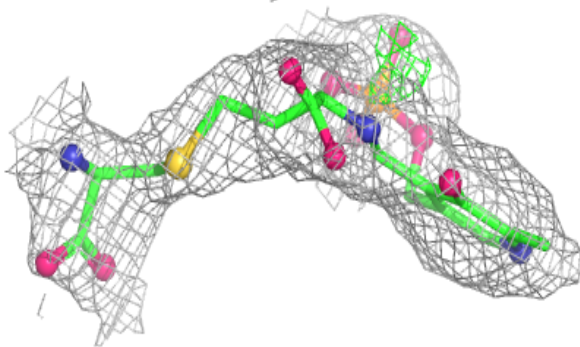
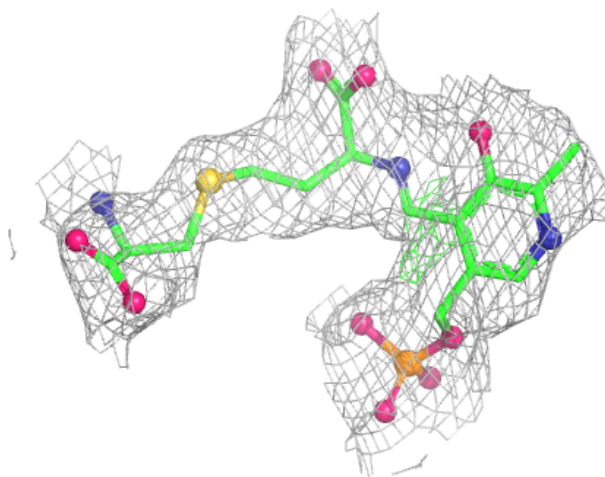
Electron density around E9U C 503:

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



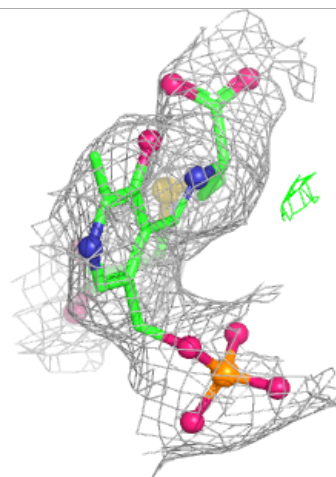
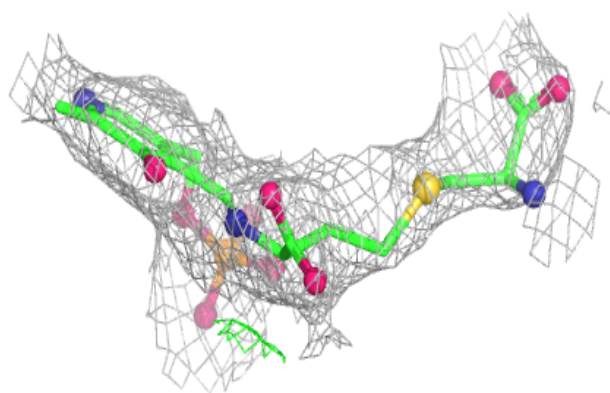
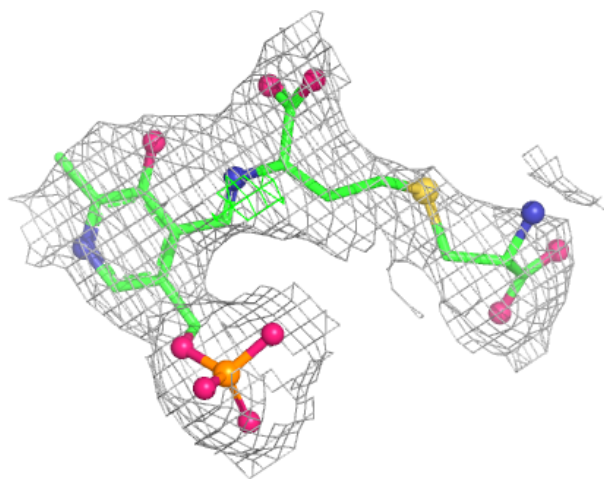
Electron density around E9U B 502:

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



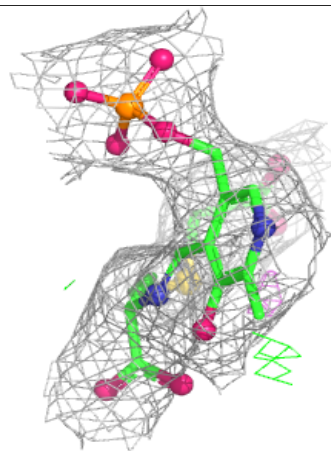
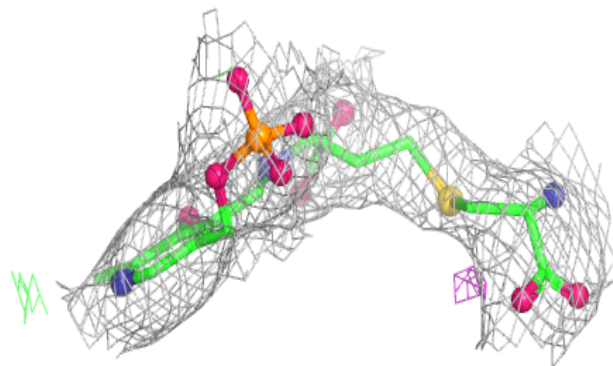
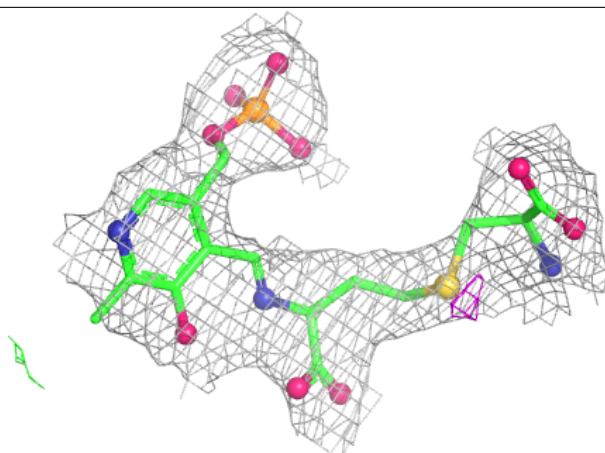
Electron density around E9U E 505:

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



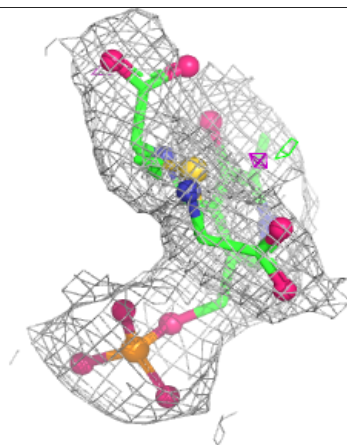
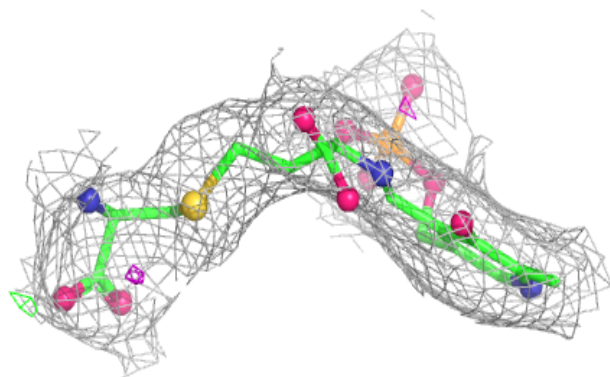
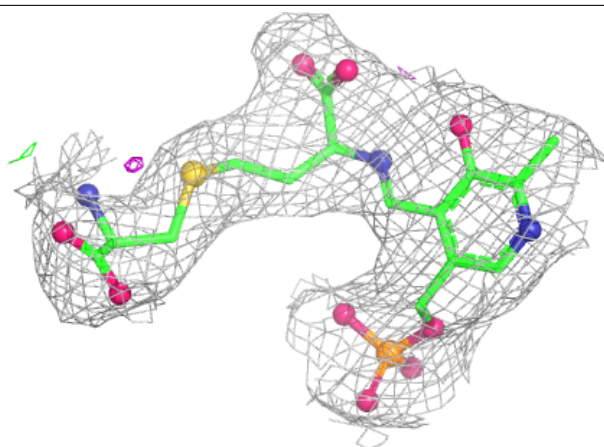
Electron density around E9U F 506:

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



Electron density around E9U 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.