



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 10:21 AM EDT

PDB ID : 6CN1
Title : 2.75 Angstrom Resolution Crystal Structure of UDP-N-acetylglucosamine 1-c arboxyvinyltransferase from Pseudomonas putida in Complex with Uridine-di phosphate-2(n-acetylglucosaminyl) butyric acid, (2R)-2-(phosphonoxy)prop anoic acid and Magnesium
Authors : Minasov, G.; Shuvalova, L.; Dubrovska, I.; Cardona-Correa, A.; Grimshaw, S.; Kwon, K.; Anderson, W.F.; Satchell, K.J.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2018-03-06
Resolution : 2.75 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)

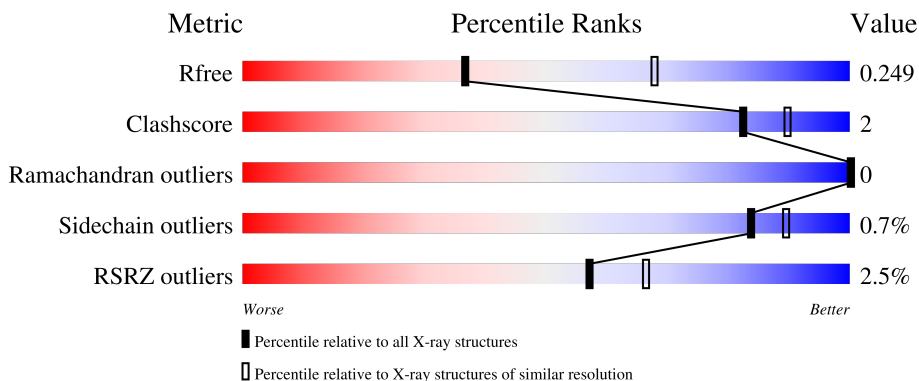
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

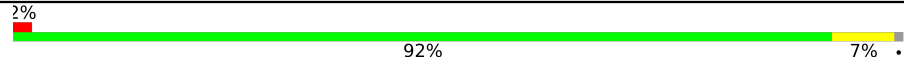
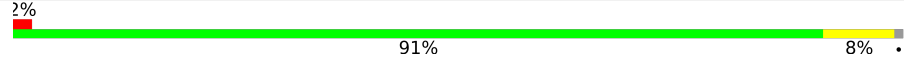
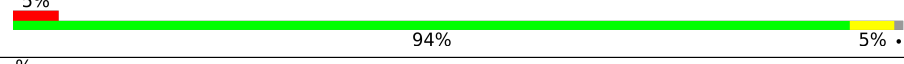
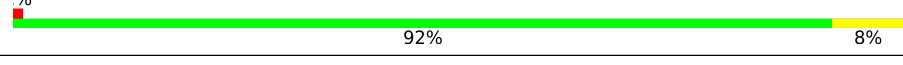
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	424	 4% 92% 7%
1	B	424	 2% 93% 6%
1	C	424	 2% 93% 6%

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
1	D	424	 2% 92% 7%
1	E	424	 2% 91% 8%
1	F	424	 2% 92% 7%
1	G	424	 5% 94% 5%
1	H	424	 2% 92% 8%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 25971 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	422	3156	1989	550	598	19	0	0	0
1	B	421	3151	1986	549	597	19	0	0	0
1	C	421	3151	1986	549	597	19	0	0	0
1	D	421	3151	1986	549	597	19	0	0	0
1	E	421	3151	1986	549	597	19	0	0	0
1	F	421	3151	1986	549	597	19	0	0	0
1	G	421	3151	1986	549	597	19	0	0	0
1	H	422	3167	1995	554	599	19	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

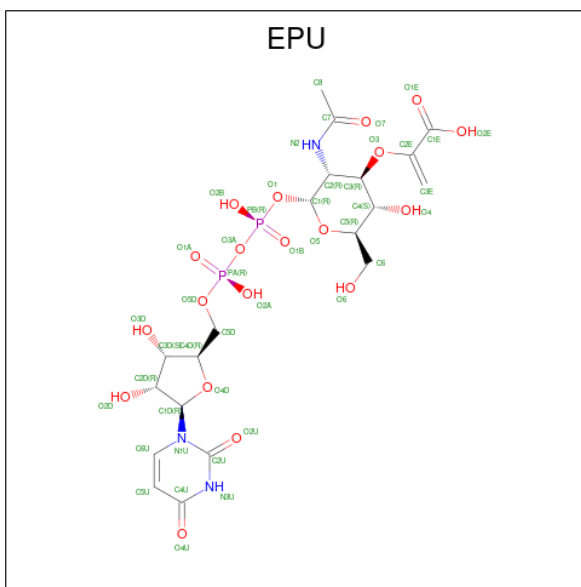
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q88P88
A	-1	ASN	-	expression tag	UNP Q88P88
A	0	ALA	-	expression tag	UNP Q88P88
B	-2	SER	-	expression tag	UNP Q88P88
B	-1	ASN	-	expression tag	UNP Q88P88
B	0	ALA	-	expression tag	UNP Q88P88
C	-2	SER	-	expression tag	UNP Q88P88
C	-1	ASN	-	expression tag	UNP Q88P88
C	0	ALA	-	expression tag	UNP Q88P88
D	-2	SER	-	expression tag	UNP Q88P88
D	-1	ASN	-	expression tag	UNP Q88P88
D	0	ALA	-	expression tag	UNP Q88P88
E	-2	SER	-	expression tag	UNP Q88P88

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q88P88
E	0	ALA	-	expression tag	UNP Q88P88
F	-2	SER	-	expression tag	UNP Q88P88
F	-1	ASN	-	expression tag	UNP Q88P88
F	0	ALA	-	expression tag	UNP Q88P88
G	-2	SER	-	expression tag	UNP Q88P88
G	-1	ASN	-	expression tag	UNP Q88P88
G	0	ALA	-	expression tag	UNP Q88P88
H	-2	SER	-	expression tag	UNP Q88P88
H	-1	ASN	-	expression tag	UNP Q88P88
H	0	ALA	-	expression tag	UNP Q88P88

- Molecule 2 is URIDINE-DIPHOSPHATE-2(N-ACETYLGLUCOSAMINYL) BUTYRIC ACID (three-letter code: EPU) (formula: C₂₀H₂₉N₃O₁₉P₂).



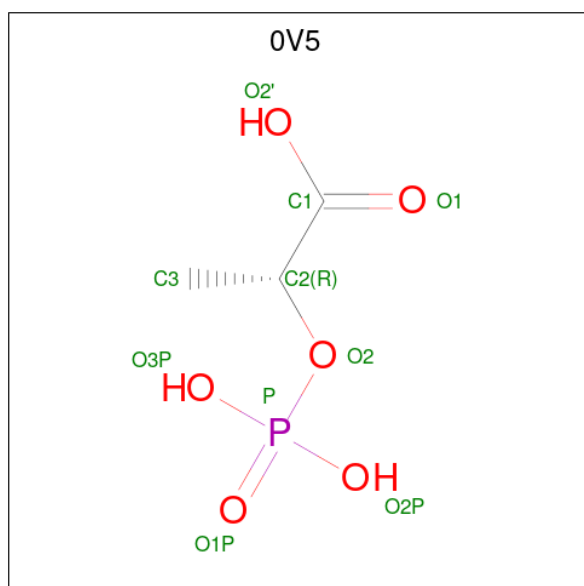
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
2	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
2	C	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
2	D	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
2	E	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

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

- Molecule 3 is (2R)-2-(phosphonoxy)propanoic acid (three-letter code: 0V5) (formula: C₃H₇O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		
3	E	1	Total	C	O	P	0	0
			10	3	6	1		
3	F	1	Total	C	O	P	0	0
			10	3	6	1		
3	G	1	Total	C	O	P	0	0
			10	3	6	1		
3	H	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	H	2	Total Cl 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	40	Total O 40 40	0	0
6	B	43	Total O 43 43	0	0
6	C	44	Total O 45 45	0	1
6	D	44	Total O 44 44	0	0
6	E	32	Total O 32 32	0	0

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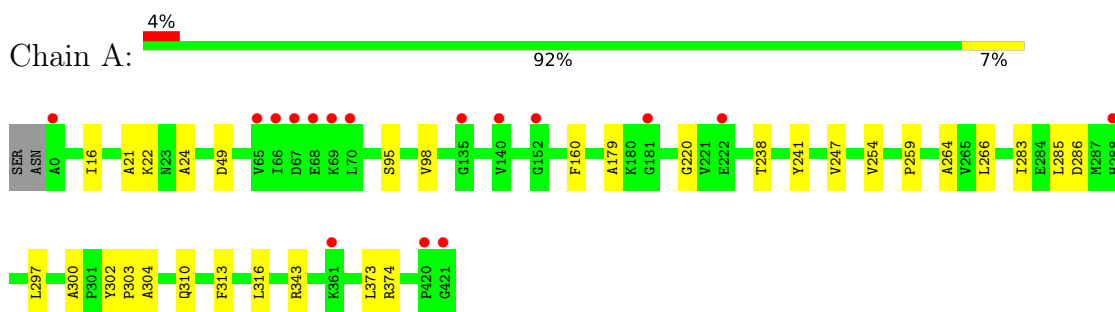
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	28	Total O 29 29	0	1
6	G	17	Total O 18 18	0	1
6	H	46	Total O 46 46	0	0

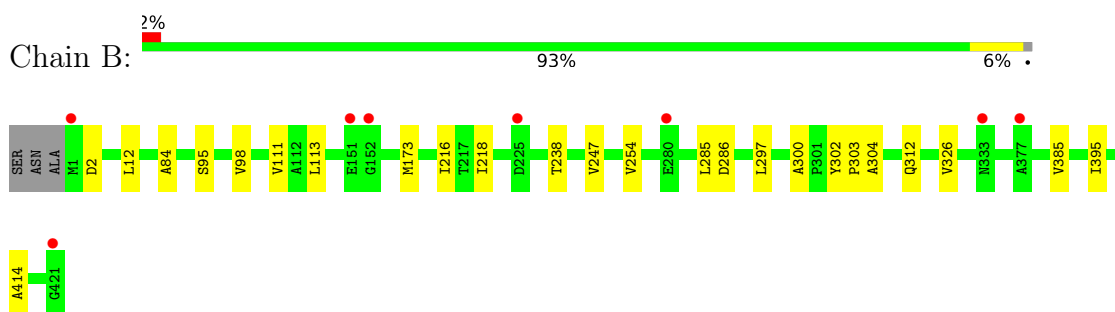
3 Residue-property plots [i](#)

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.

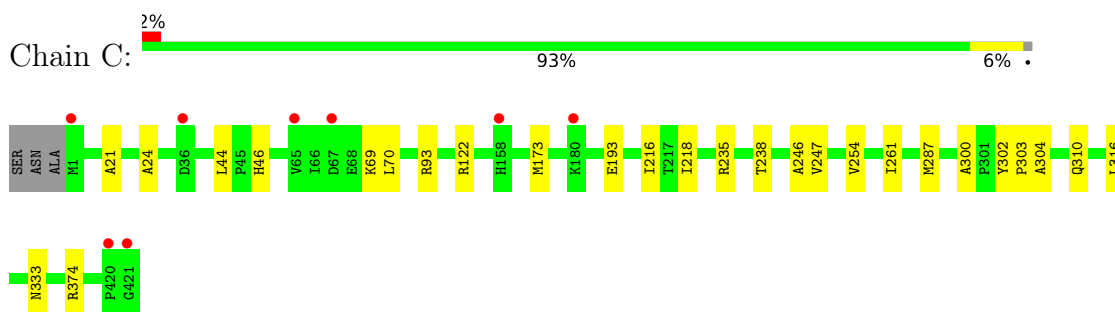
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



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

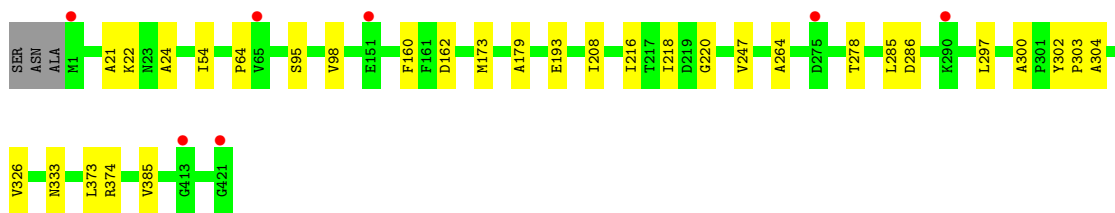


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

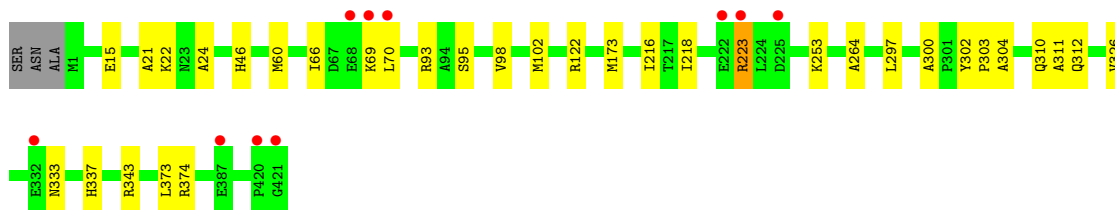
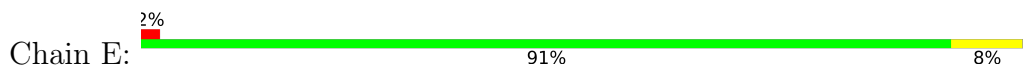


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

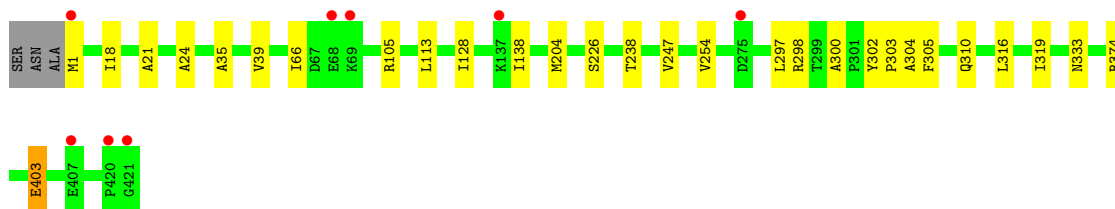
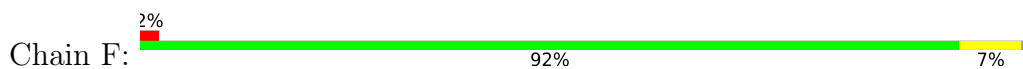




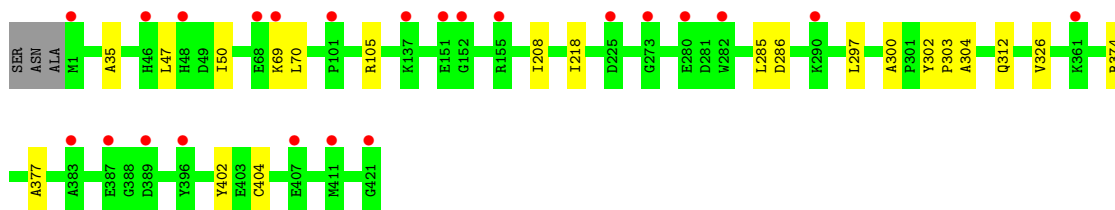
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



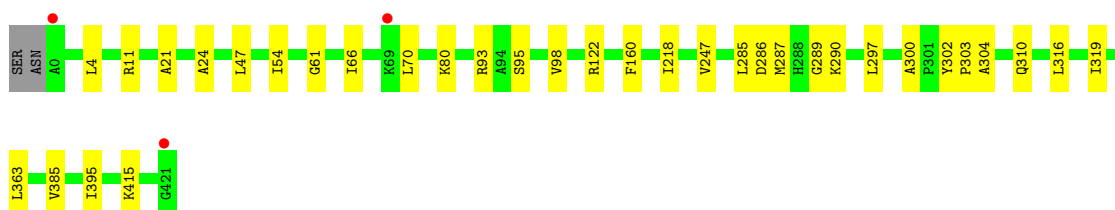
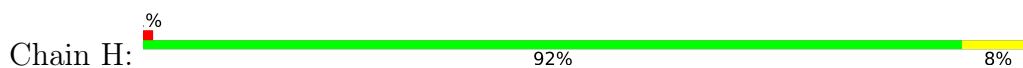
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.62Å 148.12Å 164.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 2.75 29.90 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.95-2.75) 99.4 (29.90-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.76Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.210 , 0.252 0.209 , 0.249	Depositor DCC
R_{free} test set	4127 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25971	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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: EPU, CL, MG, 0V5

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	0.34	0/3202	0.59	0/4335
1	B	0.34	0/3197	0.60	0/4328
1	C	0.35	0/3197	0.62	0/4328
1	D	0.34	0/3197	0.60	0/4328
1	E	0.34	0/3197	0.61	0/4328
1	F	0.34	0/3197	0.61	1/4328 (0.0%)
1	G	0.35	0/3197	0.60	1/4328 (0.0%)
1	H	0.35	0/3213	0.61	0/4349
All	All	0.34	0/25597	0.60	2/34652 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	403	GLU	CB-CA-C	-5.82	98.77	110.40
1	G	404	CYS	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3156	0	3236	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3151	0	3231	16	0
1	C	3151	0	3231	14	0
1	D	3151	0	3231	17	1
1	E	3151	0	3231	19	1
1	F	3151	0	3231	19	0
1	G	3151	0	3231	12	0
1	H	3167	0	3248	19	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
3	A	10	0	4	0	0
3	B	10	0	5	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
3	E	10	0	5	0	0
3	F	10	0	4	1	0
3	G	10	0	4	0	0
3	H	10	0	5	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	H	2	0	0	0	0
6	A	40	0	0	0	0
6	B	43	0	0	0	0
6	C	45	0	0	0	0
6	D	44	0	0	0	0
6	E	32	0	0	0	0
6	F	29	0	0	0	0
6	G	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	46	0	0	0	0
All	All	25971	0	26113	127	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:319:ILE:HD11	1:H:363:LEU:HG	1.72	0.71
1:F:403:GLU:O	1:F:403:GLU:HG2	1.95	0.67
3:F:502:OV5:O2P	3:F:502:OV5:H4	1.95	0.66
1:F:35:ALA:O	1:F:105:ARG:NH1	2.35	0.60
1:G:297:LEU:HD11	1:G:326:VAL:HG13	1.85	0.59
1:F:35:ALA:HB2	1:F:204:MET:HE1	1.86	0.57
1:E:343:ARG:HA	1:F:113:LEU:HD23	1.87	0.56
1:G:300:ALA:HB3	1:G:304:ALA:CB	2.36	0.56
1:A:302:TYR:CG	1:A:303:PRO:HA	2.42	0.54
1:F:39:VAL:HG12	1:F:226:SER:HA	1.90	0.54
1:G:35:ALA:O	1:G:105:ARG:NH1	2.40	0.54
1:F:247:VAL:HG12	1:F:316:LEU:HA	1.90	0.53
1:C:46:HIS:HB2	1:C:70:LEU:HD11	1.90	0.53
1:F:297:LEU:HD11	1:F:305:PHE:CZ	2.44	0.53
1:H:61:GLY:HA3	1:H:80:LYS:HG2	1.90	0.53
1:C:300:ALA:HB3	1:C:304:ALA:CB	2.39	0.53
1:H:247:VAL:HG12	1:H:316:LEU:HA	1.89	0.53
1:E:46:HIS:CE1	1:E:70:LEU:HD13	2.45	0.52
1:B:218:ILE:HD12	1:B:218:ILE:N	2.24	0.52
1:F:238:THR:HG23	1:F:254:VAL:HG11	1.91	0.52
1:H:319:ILE:HG13	1:H:385:VAL:HG21	1.92	0.52
1:H:218:ILE:HD12	1:H:218:ILE:N	2.25	0.51
1:G:218:ILE:HD12	1:G:218:ILE:N	2.25	0.51
1:H:70:LEU:HD12	1:H:70:LEU:N	2.27	0.50
1:A:300:ALA:HB3	1:A:304:ALA:CB	2.42	0.50
1:F:66:ILE:HD12	1:F:66:ILE:N	2.27	0.49
1:B:302:TYR:CG	1:B:303:PRO:HA	2.48	0.49
1:E:218:ILE:HD12	1:E:218:ILE:N	2.28	0.49
1:A:238:THR:HG23	1:A:254:VAL:HG11	1.95	0.49
1:B:95:SER:O	1:B:98:VAL:HG22	2.13	0.49
1:E:312:GLN:OE1	1:E:312:GLN:N	2.41	0.49
1:F:128:ILE:HG23	1:F:138:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:ASN:HB2	1:F:333:ASN:ND2	2.28	0.48
1:F:302:TYR:CG	1:F:303:PRO:HA	2.48	0.48
1:B:300:ALA:HB3	1:B:304:ALA:CB	2.43	0.48
1:D:297:LEU:HD11	1:D:326:VAL:HG13	1.95	0.48
1:E:21:ALA:HB3	1:E:24:ALA:HB3	1.96	0.48
1:A:247:VAL:HG12	1:A:316:LEU:HA	1.95	0.48
1:B:12:LEU:HD21	1:B:414:ALA:HB2	1.95	0.47
1:E:66:ILE:N	1:E:66:ILE:HD12	2.29	0.47
1:H:21:ALA:HB3	1:H:24:ALA:HB3	1.97	0.47
1:E:22:LYS:HE3	1:E:373:LEU:HD12	1.97	0.47
1:B:238:THR:HG23	1:B:254:VAL:HG11	1.96	0.47
1:B:247:VAL:HG12	1:B:385:VAL:CG1	2.45	0.47
1:H:319:ILE:HG22	1:H:319:ILE:O	2.16	0.46
1:B:297:LEU:HD11	1:B:326:VAL:HG13	1.98	0.46
1:E:95:SER:O	1:E:98:VAL:HG22	2.15	0.46
1:A:21:ALA:HB3	1:A:24:ALA:HB3	1.98	0.46
1:F:18:ILE:HD11	1:F:254:VAL:HG13	1.98	0.46
1:H:4:LEU:HG	1:H:395:ILE:HG21	1.98	0.46
1:G:69:LYS:C	1:G:70:LEU:HD12	2.36	0.46
1:H:54:ILE:HG21	1:H:66:ILE:HD11	1.97	0.46
1:C:44:LEU:O	1:C:70:LEU:HD13	2.16	0.46
1:C:238:THR:HG23	1:C:254:VAL:HG11	1.97	0.45
1:F:297:LEU:HD21	1:F:305:PHE:CD1	2.52	0.45
1:A:22:LYS:NZ	1:A:49:ASP:OD2	2.49	0.45
1:D:54:ILE:HG23	1:D:64:PRO:HG2	1.98	0.45
1:D:95:SER:O	1:D:98:VAL:HG22	2.16	0.45
1:E:93:ARG:NH2	1:E:122:ARG:O	2.50	0.45
1:E:264:ALA:HB2	1:H:160:PHE:CZ	2.52	0.45
1:H:300:ALA:HB3	1:H:304:ALA:CB	2.46	0.45
1:F:21:ALA:HB3	1:F:24:ALA:HB3	1.98	0.45
1:A:343:ARG:HA	1:B:113:LEU:HD23	1.99	0.45
1:F:300:ALA:HB3	1:F:304:ALA:CB	2.47	0.44
1:G:302:TYR:CG	1:G:303:PRO:HA	2.52	0.44
1:E:297:LEU:HD11	1:E:326:VAL:HG13	1.99	0.44
1:A:300:ALA:HB3	1:A:304:ALA:HB3	1.99	0.44
1:A:259:PRO:HA	1:A:283:ILE:HD11	2.00	0.44
1:C:302:TYR:CG	1:C:303:PRO:HA	2.52	0.44
1:H:285:LEU:HD23	1:H:286:ASP:N	2.33	0.44
1:A:285:LEU:HD23	1:A:286:ASP:N	2.33	0.44
1:E:302:TYR:CG	1:E:303:PRO:HA	2.53	0.44
1:E:311:ALA:HB2	1:E:337:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ALA:HB2	1:C:193:GLU:HG3	1.99	0.43
1:C:333:ASN:ND2	1:D:333:ASN:HB2	2.34	0.43
1:E:300:ALA:HB3	1:E:304:ALA:CB	2.47	0.43
1:D:247:VAL:HG12	1:D:385:VAL:HG11	2.01	0.43
1:C:93:ARG:NH2	1:C:122:ARG:O	2.50	0.43
1:C:235:ARG:HB3	1:C:261:ILE:HD12	2.01	0.43
1:A:179:ALA:O	1:A:220:GLY:HA3	2.17	0.43
1:E:60:MET:SD	1:E:102:MET:CE	3.07	0.43
1:A:16:ILE:HD11	1:A:241:TYR:CG	2.53	0.43
1:C:21:ALA:HB3	1:C:24:ALA:HB3	2.01	0.43
1:C:218:ILE:N	1:C:218:ILE:HD12	2.34	0.43
1:B:173:MET:CE	1:B:216:ILE:HD13	2.49	0.43
1:D:208:ILE:HG23	1:D:218:ILE:CD1	2.49	0.43
1:D:302:TYR:CG	1:D:303:PRO:HA	2.54	0.42
1:D:179:ALA:O	1:D:220:GLY:HA3	2.19	0.42
1:D:173:MET:CE	1:D:216:ILE:HD13	2.48	0.42
1:D:300:ALA:HB3	1:D:304:ALA:CB	2.49	0.42
1:F:297:LEU:HD23	1:F:298:ARG:N	2.35	0.42
1:D:24:ALA:HB2	1:D:193:GLU:HG3	2.02	0.42
1:B:247:VAL:HG12	1:B:385:VAL:HG11	2.00	0.42
1:E:15:GLU:HG2	1:E:253:LYS:HB3	2.00	0.42
1:D:297:LEU:C	1:D:297:LEU:HD12	2.40	0.42
1:F:297:LEU:HD11	1:F:305:PHE:CE1	2.55	0.42
1:G:47:LEU:HD12	1:G:50:ILE:HG12	2.02	0.42
1:B:285:LEU:HD23	1:B:286:ASP:N	2.35	0.41
1:C:173:MET:CE	1:C:216:ILE:HD13	2.50	0.41
1:D:285:LEU:HD23	1:D:286:ASP:N	2.35	0.41
1:G:297:LEU:HD12	1:G:297:LEU:C	2.40	0.41
1:A:297:LEU:HD11	1:A:313:PHE:CB	2.51	0.41
1:B:84:ALA:HB3	1:B:111:VAL:HG13	2.02	0.41
1:G:208:ILE:HG12	1:G:218:ILE:HG23	2.03	0.41
1:D:21:ALA:HB3	1:D:24:ALA:HB3	2.02	0.41
1:H:297:LEU:C	1:H:297:LEU:HD12	2.40	0.41
1:D:22:LYS:HE3	1:D:373:LEU:HD12	2.01	0.41
1:B:2:ASP:HB3	1:B:395:ILE:HD11	2.02	0.41
1:A:95:SER:O	1:A:98:VAL:HG22	2.21	0.41
1:C:246:ALA:HA	1:C:287:MET:HG3	2.03	0.41
1:A:266:LEU:HD21	1:A:283:ILE:HD13	2.03	0.41
1:H:302:TYR:CG	1:H:303:PRO:HA	2.56	0.41
1:C:247:VAL:HG12	1:C:316:LEU:HA	2.03	0.41
1:E:297:LEU:HD12	1:E:297:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:CD2	1:B:414:ALA:HB2	2.51	0.41
1:E:173:MET:CE	1:E:216:ILE:HD13	2.51	0.41
1:H:11:ARG:NH2	1:H:289:GLY:HA2	2.36	0.41
1:G:285:LEU:HD23	1:G:286:ASP:N	2.35	0.40
1:A:160:PHE:CZ	1:D:264:ALA:HB2	2.57	0.40
1:A:264:ALA:HB2	1:D:160:PHE:CZ	2.56	0.40
1:B:312:GLN:OE1	1:B:312:GLN:N	2.49	0.40
1:F:319:ILE:C	1:F:319:ILE:HD12	2.41	0.40
1:G:312:GLN:OE1	1:G:312:GLN:N	2.48	0.40
1:H:93:ARG:HD2	1:H:122:ARG:CZ	2.52	0.40
1:H:95:SER:O	1:H:98:VAL:HG22	2.21	0.40
1:H:287:MET:O	1:H:290:LYS:HG2	2.21	0.40
1:G:377:ALA:HB2	1:G:402:TYR:CE2	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:THR:OG1	1:E:223:ARG:NH1[1_554]	2.16	0.04

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	420/424 (99%)	403 (96%)	17 (4%)	0	100	100
1	B	419/424 (99%)	403 (96%)	16 (4%)	0	100	100
1	C	419/424 (99%)	406 (97%)	13 (3%)	0	100	100
1	D	419/424 (99%)	408 (97%)	11 (3%)	0	100	100
1	E	419/424 (99%)	406 (97%)	13 (3%)	0	100	100
1	F	419/424 (99%)	400 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	419/424 (99%)	404 (96%)	15 (4%)	0	100	100
1	H	421/424 (99%)	404 (96%)	17 (4%)	0	100	100
All	All	3355/3392 (99%)	3234 (96%)	121 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	327/329 (99%)	324 (99%)	3 (1%)	78	87
1	B	327/329 (99%)	327 (100%)	0	100	100
1	C	327/329 (99%)	324 (99%)	3 (1%)	78	87
1	D	327/329 (99%)	325 (99%)	2 (1%)	86	90
1	E	327/329 (99%)	323 (99%)	4 (1%)	71	82
1	F	327/329 (99%)	324 (99%)	3 (1%)	78	87
1	G	327/329 (99%)	326 (100%)	1 (0%)	92	95
1	H	328/329 (100%)	325 (99%)	3 (1%)	78	87
All	All	2617/2632 (99%)	2598 (99%)	19 (1%)	84	89

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	GLN
1	A	373	LEU
1	A	374	ARG
1	C	69	LYS
1	C	310	GLN
1	C	374	ARG
1	D	162	ASP
1	D	374	ARG
1	E	69	LYS

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Mol	Chain	Res	Type
1	E	223	ARG
1	E	310	GLN
1	E	374	ARG
1	F	1	MET
1	F	310	GLN
1	F	374	ARG
1	G	374	ARG
1	H	47	LEU
1	H	310	GLN
1	H	415	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 29 ligands modelled in this entry, 13 are monoatomic - leaving 16 for Mogul analysis.

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	EPU	A	501	-	43,46,46	1.12	4 (9%)	61,69,69	1.36	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EPU	B	500	-	43,46,46	1.15	5 (11%)	61,69,69	1.37	6 (9%)
3	OV5	H	502	4,1	8,9,9	1.08	0	11,13,13	0.77	0
2	EPU	D	500	-	43,46,46	1.10	4 (9%)	61,69,69	1.34	7 (11%)
3	OV5	D	501	4,1	8,9,9	0.97	0	11,13,13	0.63	0
2	EPU	E	500	-	43,46,46	1.11	4 (9%)	61,69,69	1.36	8 (13%)
3	OV5	E	501	4,1	8,9,9	1.02	0	11,13,13	0.74	0
3	OV5	F	502	4,1	8,9,9	0.98	0	11,13,13	0.66	0
2	EPU	F	501	-	43,46,46	1.13	4 (9%)	61,69,69	1.41	9 (14%)
3	OV5	B	501	4,1	8,9,9	1.02	0	11,13,13	0.69	0
2	EPU	C	501	-	43,46,46	1.11	4 (9%)	61,69,69	1.38	7 (11%)
3	OV5	C	502	4,1	8,9,9	1.00	0	11,13,13	0.81	0
3	OV5	G	501	4,1	8,9,9	1.03	0	11,13,13	0.67	0
2	EPU	H	501	-	43,46,46	1.12	4 (9%)	61,69,69	1.37	7 (11%)
2	EPU	G	500	-	43,46,46	1.11	4 (9%)	61,69,69	1.41	7 (11%)
3	OV5	A	502	4,1	8,9,9	0.96	0	11,13,13	0.64	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	EPU	A	501	-	-	7/32/71/71	0/3/3/3
2	EPU	B	500	-	-	8/32/71/71	0/3/3/3
3	OV5	H	502	4,1	-	3/9/9/9	-
2	EPU	D	500	-	-	7/32/71/71	0/3/3/3
3	OV5	D	501	4,1	-	2/9/9/9	-
2	EPU	E	500	-	-	7/32/71/71	0/3/3/3
3	OV5	E	501	4,1	-	5/9/9/9	-
3	OV5	F	502	4,1	-	2/9/9/9	-
2	EPU	F	501	-	-	7/32/71/71	0/3/3/3
3	OV5	B	501	4,1	-	2/9/9/9	-
2	EPU	C	501	-	-	7/32/71/71	0/3/3/3
3	OV5	C	502	4,1	-	4/9/9/9	-
3	OV5	G	501	4,1	-	4/9/9/9	-
2	EPU	H	501	-	-	7/32/71/71	0/3/3/3
2	EPU	G	500	-	-	7/32/71/71	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0V5	A	502	4,1	-	2/9/9/9	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	EPU	C2E-C1E	-3.33	1.46	1.49
2	A	501	EPU	O3-C2E	3.09	1.46	1.36
2	E	500	EPU	O3-C2E	3.09	1.46	1.36
2	F	501	EPU	C2E-C1E	-3.07	1.46	1.49
2	F	501	EPU	O3-C2E	3.06	1.46	1.36
2	H	501	EPU	C2E-C1E	-3.06	1.46	1.49
2	C	501	EPU	O3-C2E	3.06	1.46	1.36
2	H	501	EPU	O3-C2E	3.04	1.46	1.36
2	B	500	EPU	O3-C2E	3.02	1.46	1.36
2	D	500	EPU	O3-C2E	3.01	1.46	1.36
2	G	500	EPU	C2E-C1E	-2.97	1.46	1.49
2	G	500	EPU	O3-C2E	2.94	1.46	1.36
2	C	501	EPU	C2E-C1E	-2.90	1.46	1.49
2	A	501	EPU	C2E-C1E	-2.90	1.46	1.49
2	A	501	EPU	C2U-N1U	2.87	1.43	1.38
2	H	501	EPU	C2U-N1U	2.81	1.43	1.38
2	D	500	EPU	C2E-C1E	-2.79	1.46	1.49
2	E	500	EPU	C2U-N1U	2.76	1.42	1.38
2	C	501	EPU	C2U-N1U	2.71	1.42	1.38
2	E	500	EPU	C2E-C1E	-2.71	1.46	1.49
2	F	501	EPU	C2U-N1U	2.68	1.42	1.38
2	D	500	EPU	C2U-N1U	2.64	1.42	1.38
2	B	500	EPU	C2U-N1U	2.61	1.42	1.38
2	G	500	EPU	C2U-N1U	2.58	1.42	1.38
2	E	500	EPU	C4U-N3U	-2.24	1.34	1.38
2	C	501	EPU	C4U-N3U	-2.14	1.34	1.38
2	B	500	EPU	C4U-N3U	-2.13	1.34	1.38
2	F	501	EPU	C4U-N3U	-2.13	1.34	1.38
2	D	500	EPU	C4U-N3U	-2.12	1.34	1.38
2	G	500	EPU	C4U-N3U	-2.09	1.34	1.38
2	H	501	EPU	C4U-N3U	-2.06	1.34	1.38
2	A	501	EPU	C6U-C5U	2.02	1.39	1.35
2	B	500	EPU	C6U-C5U	2.00	1.39	1.35

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	EPU	C4U-N3U-C2U	-4.26	120.96	126.58
2	A	501	EPU	C4U-N3U-C2U	-4.20	121.04	126.58
2	G	500	EPU	C4U-N3U-C2U	-4.19	121.05	126.58
2	H	501	EPU	C4U-N3U-C2U	-4.19	121.06	126.58
2	B	500	EPU	C4U-N3U-C2U	-4.18	121.06	126.58
2	E	500	EPU	C4U-N3U-C2U	-4.16	121.09	126.58
2	F	501	EPU	C4U-N3U-C2U	-4.09	121.19	126.58
2	F	501	EPU	N3U-C2U-N1U	4.08	120.31	114.89
2	E	500	EPU	N3U-C2U-N1U	4.07	120.30	114.89
2	C	501	EPU	N3U-C2U-N1U	4.05	120.26	114.89
2	D	500	EPU	C4U-N3U-C2U	-4.01	121.30	126.58
2	A	501	EPU	N3U-C2U-N1U	4.00	120.19	114.89
2	G	500	EPU	N3U-C2U-N1U	3.99	120.19	114.89
2	B	500	EPU	N3U-C2U-N1U	3.90	120.07	114.89
2	D	500	EPU	N3U-C2U-N1U	3.87	120.03	114.89
2	H	501	EPU	N3U-C2U-N1U	3.84	119.99	114.89
2	G	500	EPU	PB-O3A-PA	-3.60	120.48	132.83
2	H	501	EPU	C5U-C4U-N3U	3.58	120.19	114.84
2	B	500	EPU	C5U-C4U-N3U	3.57	120.19	114.84
2	C	501	EPU	C5U-C4U-N3U	3.57	120.18	114.84
2	E	500	EPU	C5U-C4U-N3U	3.51	120.10	114.84
2	A	501	EPU	C5U-C4U-N3U	3.50	120.07	114.84
2	G	500	EPU	C5U-C4U-N3U	3.48	120.05	114.84
2	D	500	EPU	C5U-C4U-N3U	3.44	119.98	114.84
2	F	501	EPU	C5U-C4U-N3U	3.37	119.89	114.84
2	H	501	EPU	O4U-C4U-C5U	-3.26	119.43	125.16
2	F	501	EPU	PB-O3A-PA	-3.25	121.67	132.83
2	A	501	EPU	O4U-C4U-C5U	-3.18	119.57	125.16
2	B	500	EPU	O4U-C4U-C5U	-3.17	119.58	125.16
2	C	501	EPU	O4U-C4U-C5U	-3.14	119.64	125.16
2	G	500	EPU	O4U-C4U-C5U	-3.07	119.77	125.16
2	A	501	EPU	PB-O3A-PA	-3.05	122.36	132.83
2	C	501	EPU	PB-O3A-PA	-3.02	122.47	132.83
2	F	501	EPU	O4U-C4U-C5U	-3.01	119.86	125.16
2	D	500	EPU	O4U-C4U-C5U	-3.00	119.89	125.16
2	D	500	EPU	PB-O3A-PA	-2.99	122.57	132.83
2	B	500	EPU	PB-O3A-PA	-2.95	122.69	132.83
2	E	500	EPU	O4U-C4U-C5U	-2.93	120.00	125.16
2	E	500	EPU	PB-O3A-PA	-2.93	122.78	132.83
2	G	500	EPU	O2E-C1E-C2E	2.88	118.82	113.91
2	F	501	EPU	O2E-C1E-C2E	2.74	118.59	113.91
2	H	501	EPU	O2E-C1E-C2E	2.73	118.56	113.91
2	D	500	EPU	O2E-C1E-C2E	2.72	118.55	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	EPU	O2E-C1E-C2E	2.69	118.49	113.91
2	H	501	EPU	PB-O3A-PA	-2.59	123.93	132.83
2	A	501	EPU	O2E-C1E-C2E	2.57	118.30	113.91
2	B	500	EPU	O2E-C1E-C2E	2.54	118.24	113.91
2	E	500	EPU	O2E-C1E-C2E	2.46	118.11	113.91
2	H	501	EPU	C1D-N1U-C2U	2.28	121.70	117.57
2	F	501	EPU	C1D-N1U-C2U	2.16	121.49	117.57
2	E	500	EPU	C3D-C2D-C1D	2.15	105.51	101.43
2	G	500	EPU	C1D-N1U-C2U	2.15	121.46	117.57
2	F	501	EPU	C3D-C2D-C1D	2.13	105.48	101.43
2	C	501	EPU	C1D-N1U-C2U	2.08	121.34	117.57
2	D	500	EPU	C1D-N1U-C2U	2.05	121.29	117.57
2	E	500	EPU	C1D-N1U-C2U	2.03	121.25	117.57
2	F	501	EPU	O3-C3-C2	2.01	111.66	107.91
2	A	501	EPU	C3D-C2D-C1D	2.00	105.23	101.43

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	EPU	C5D-O5D-PA-O1A
2	A	501	EPU	C5D-O5D-PA-O2A
2	A	501	EPU	O1E-C1E-C2E-O3
2	A	501	EPU	O1E-C1E-C2E-C3E
2	A	501	EPU	O2E-C1E-C2E-O3
2	A	501	EPU	O2E-C1E-C2E-C3E
2	B	500	EPU	C5D-O5D-PA-O1A
2	B	500	EPU	C5D-O5D-PA-O2A
2	B	500	EPU	O1E-C1E-C2E-C3E
2	B	500	EPU	O2E-C1E-C2E-C3E
2	C	501	EPU	C5D-O5D-PA-O1A
2	C	501	EPU	C5D-O5D-PA-O2A
2	C	501	EPU	O1E-C1E-C2E-O3
2	C	501	EPU	O1E-C1E-C2E-C3E
2	C	501	EPU	O2E-C1E-C2E-O3
2	C	501	EPU	O2E-C1E-C2E-C3E
2	D	500	EPU	C5D-O5D-PA-O1A
2	D	500	EPU	C5D-O5D-PA-O2A
2	D	500	EPU	O1E-C1E-C2E-O3
2	D	500	EPU	O1E-C1E-C2E-C3E
2	D	500	EPU	O2E-C1E-C2E-O3
2	D	500	EPU	O2E-C1E-C2E-C3E

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Mol	Chain	Res	Type	Atoms
2	E	500	EPU	C5D-O5D-PA-O1A
2	E	500	EPU	C5D-O5D-PA-O2A
2	E	500	EPU	O1E-C1E-C2E-C3E
2	E	500	EPU	O2E-C1E-C2E-C3E
2	F	501	EPU	C5D-O5D-PA-O1A
2	F	501	EPU	C5D-O5D-PA-O2A
2	F	501	EPU	O1E-C1E-C2E-O3
2	F	501	EPU	O1E-C1E-C2E-C3E
2	F	501	EPU	O2E-C1E-C2E-O3
2	F	501	EPU	O2E-C1E-C2E-C3E
2	G	500	EPU	C5D-O5D-PA-O1A
2	G	500	EPU	C5D-O5D-PA-O2A
2	G	500	EPU	O1E-C1E-C2E-O3
2	G	500	EPU	O1E-C1E-C2E-C3E
2	G	500	EPU	O2E-C1E-C2E-O3
2	G	500	EPU	O2E-C1E-C2E-C3E
2	H	501	EPU	C5D-O5D-PA-O1A
2	H	501	EPU	C5D-O5D-PA-O2A
2	H	501	EPU	O1E-C1E-C2E-O3
2	H	501	EPU	O1E-C1E-C2E-C3E
2	H	501	EPU	O2E-C1E-C2E-O3
2	H	501	EPU	O2E-C1E-C2E-C3E
3	F	502	0V5	C3-C2-O2-P
3	B	501	0V5	O1-C1-C2-C3
3	B	501	0V5	O2'-C1-C2-C3
3	C	502	0V5	O1-C1-C2-C3
3	C	502	0V5	O2'-C1-C2-C3
3	H	502	0V5	O1-C1-C2-C3
3	H	502	0V5	O2'-C1-C2-C3
2	B	500	EPU	O1E-C1E-C2E-O3
2	E	500	EPU	O1E-C1E-C2E-O3
3	F	502	0V5	C2-O2-P-O1P
3	G	501	0V5	C2-O2-P-O1P
2	H	501	EPU	C5D-O5D-PA-O3A
3	E	501	0V5	O1-C1-C2-C3
3	E	501	0V5	O2'-C1-C2-C3
3	G	501	0V5	O1-C1-C2-C3
3	G	501	0V5	O2'-C1-C2-C3
2	B	500	EPU	C1-O1-PB-O3A
2	B	500	EPU	O2E-C1E-C2E-O3
2	E	500	EPU	O2E-C1E-C2E-O3
3	D	501	0V5	C3-C2-O2-P

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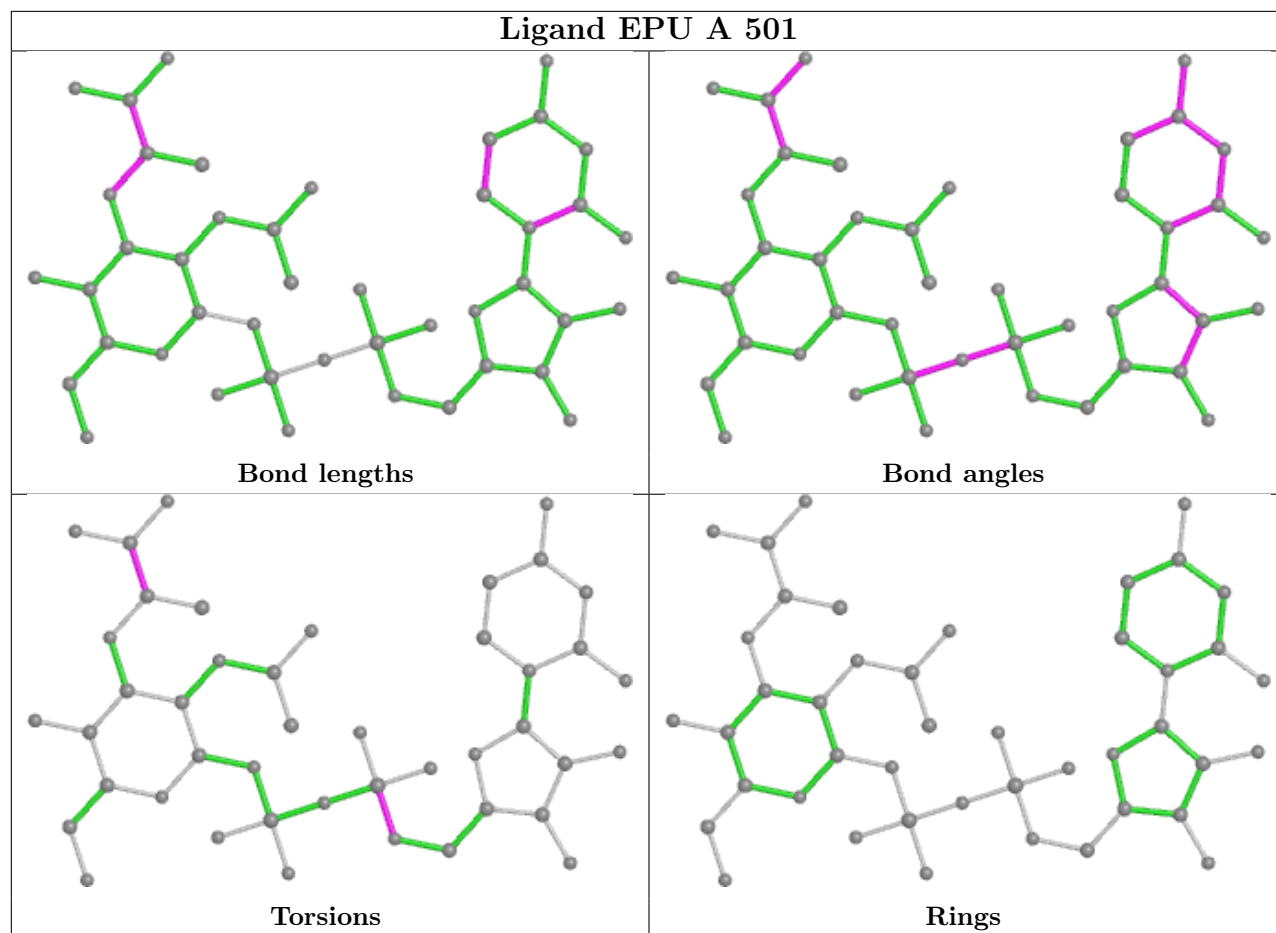
Mol	Chain	Res	Type	Atoms
3	A	502	0V5	C2-O2-P-O1P
3	E	501	0V5	C2-O2-P-O1P
3	H	502	0V5	C2-O2-P-O1P
2	A	501	EPU	C5D-O5D-PA-O3A
2	B	500	EPU	C5D-O5D-PA-O3A
2	C	501	EPU	C5D-O5D-PA-O3A
2	D	500	EPU	C5D-O5D-PA-O3A
2	E	500	EPU	C5D-O5D-PA-O3A
2	F	501	EPU	C5D-O5D-PA-O3A
2	G	500	EPU	C5D-O5D-PA-O3A
3	A	502	0V5	C2-O2-P-O2P
3	D	501	0V5	C2-O2-P-O3P
3	G	501	0V5	C2-O2-P-O2P
3	C	502	0V5	O1-C1-C2-O2
3	C	502	0V5	O2'-C1-C2-O2
3	E	501	0V5	O1-C1-C2-O2
3	E	501	0V5	O2'-C1-C2-O2

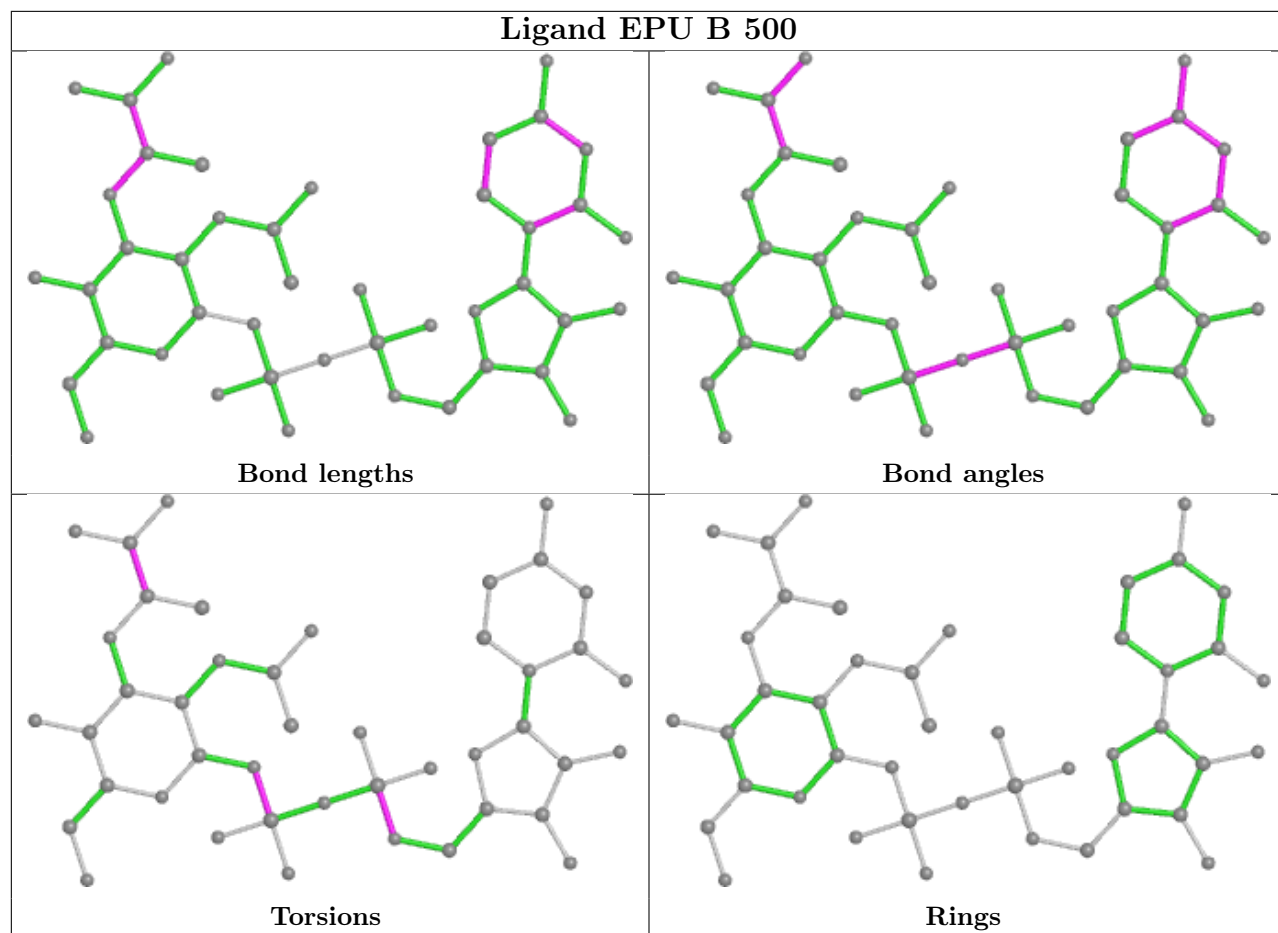
There are no ring outliers.

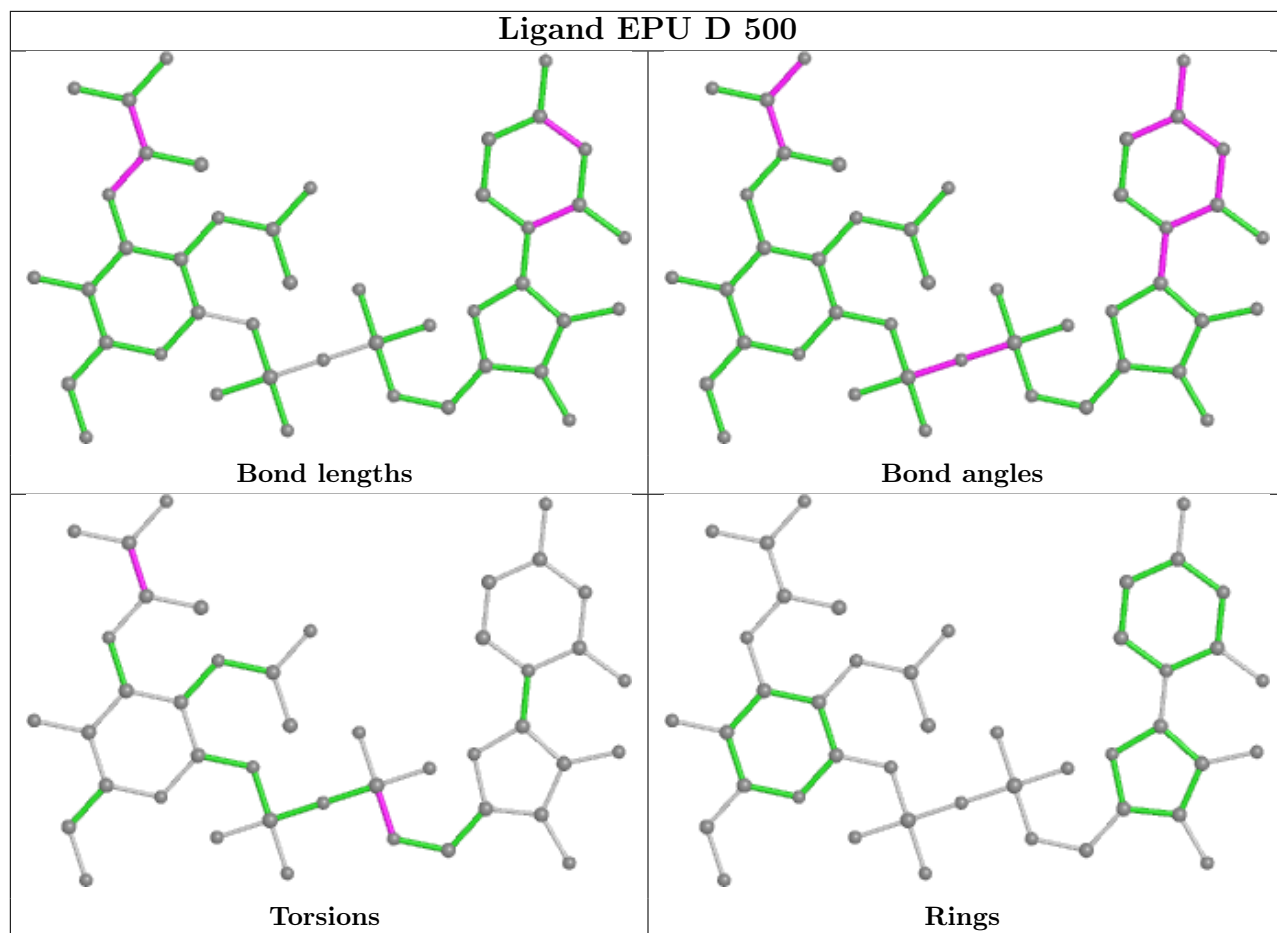
1 monomer is involved in 1 short contact:

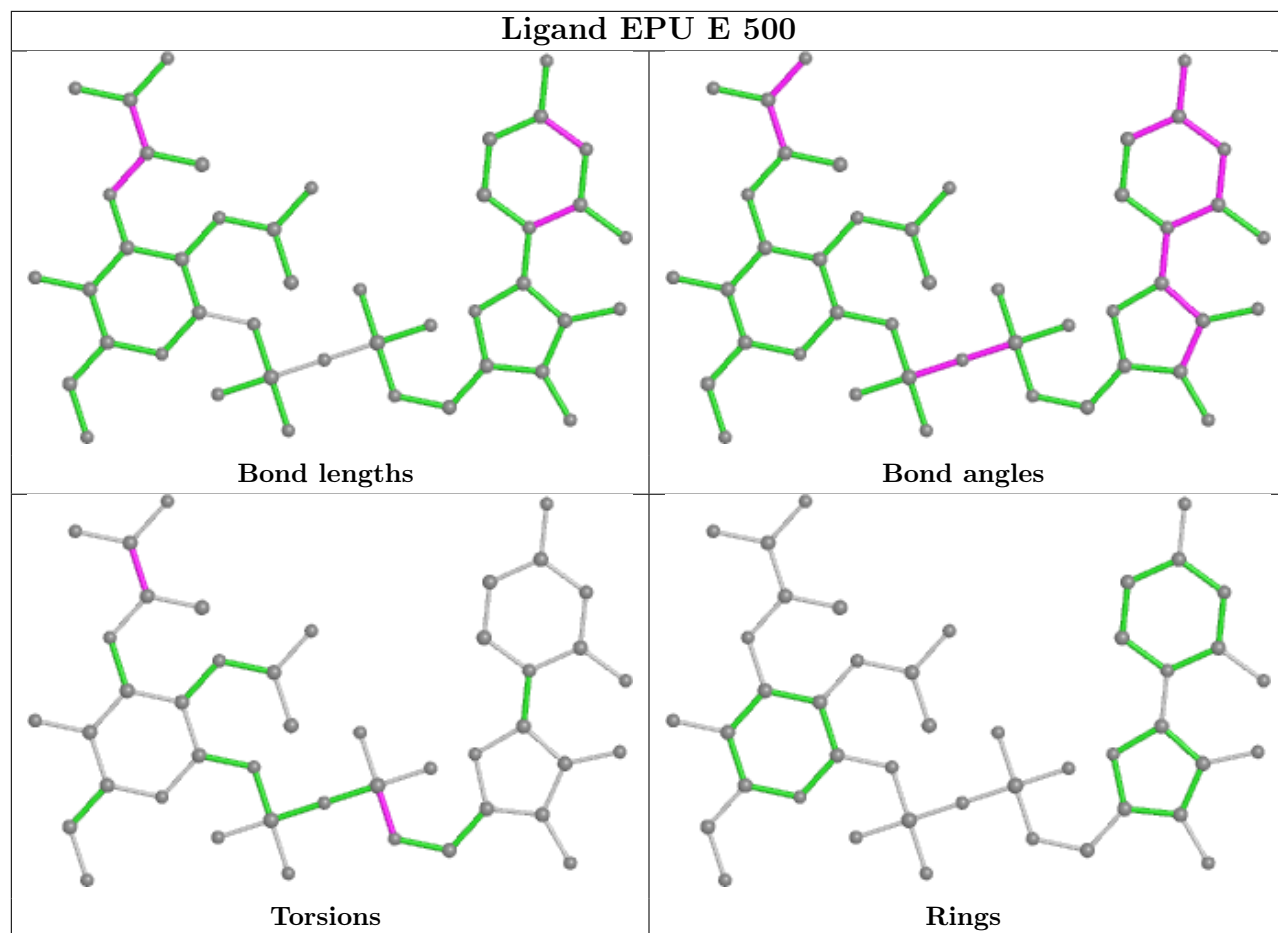
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	502	0V5	1	0

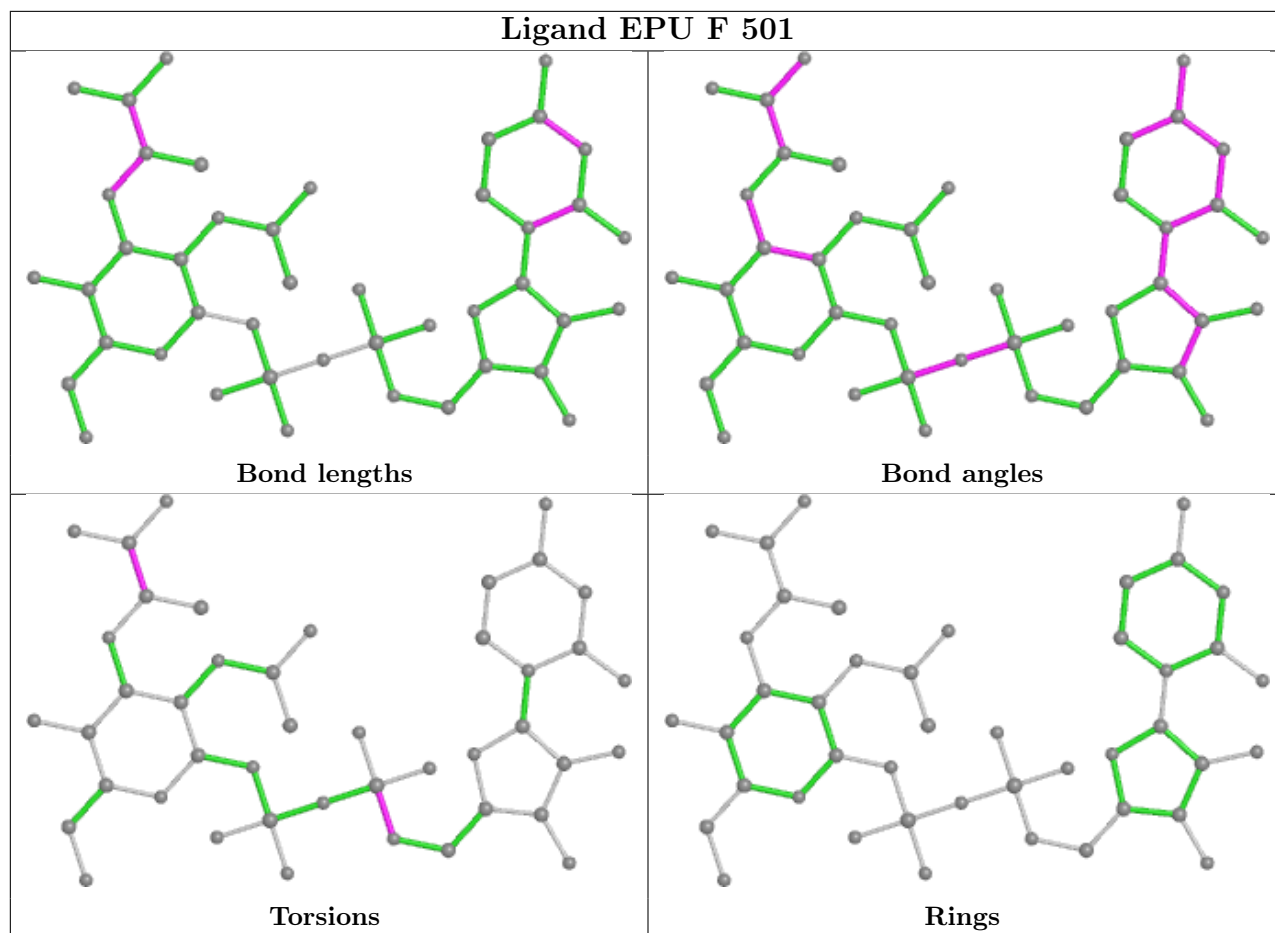
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

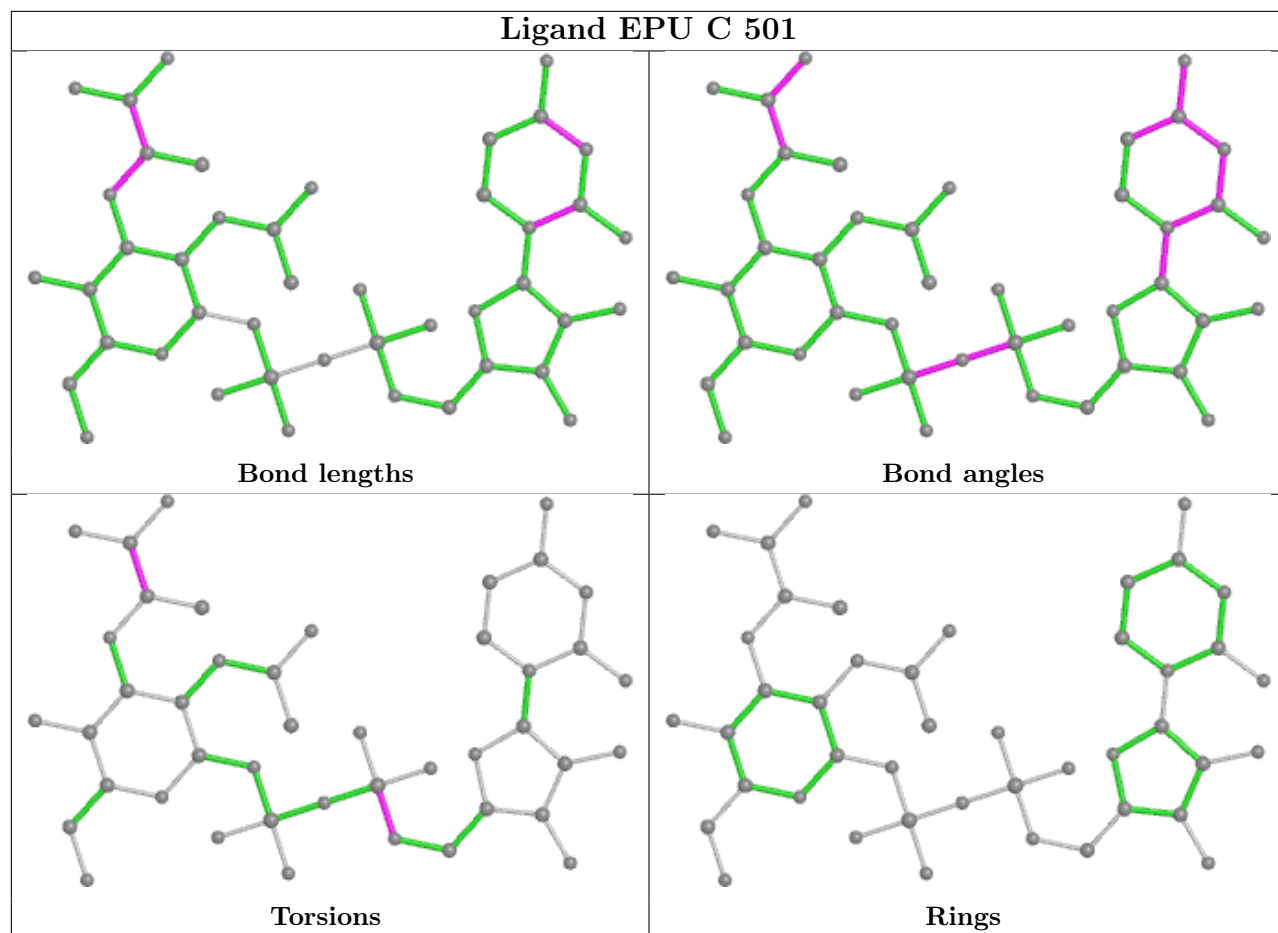


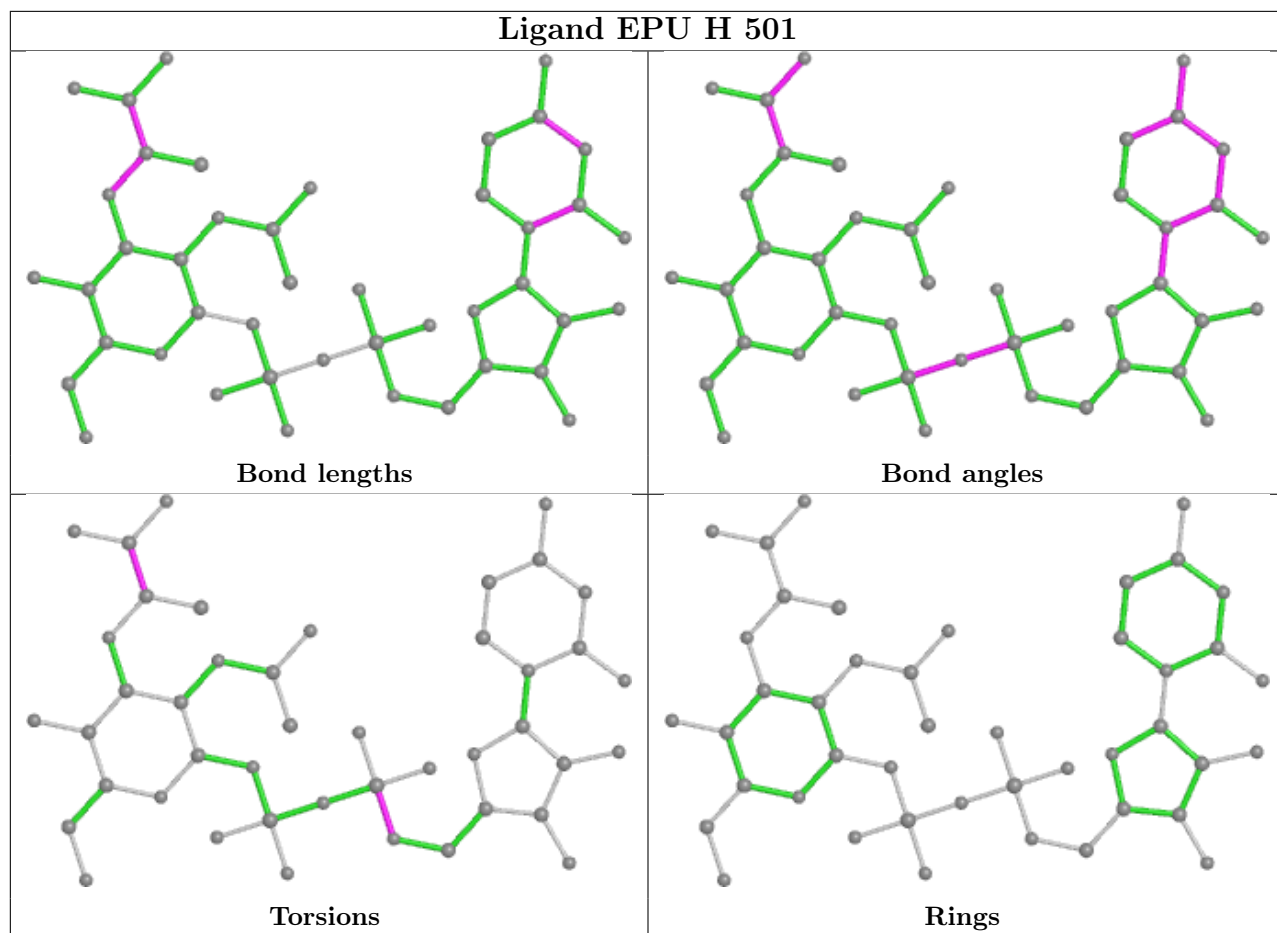


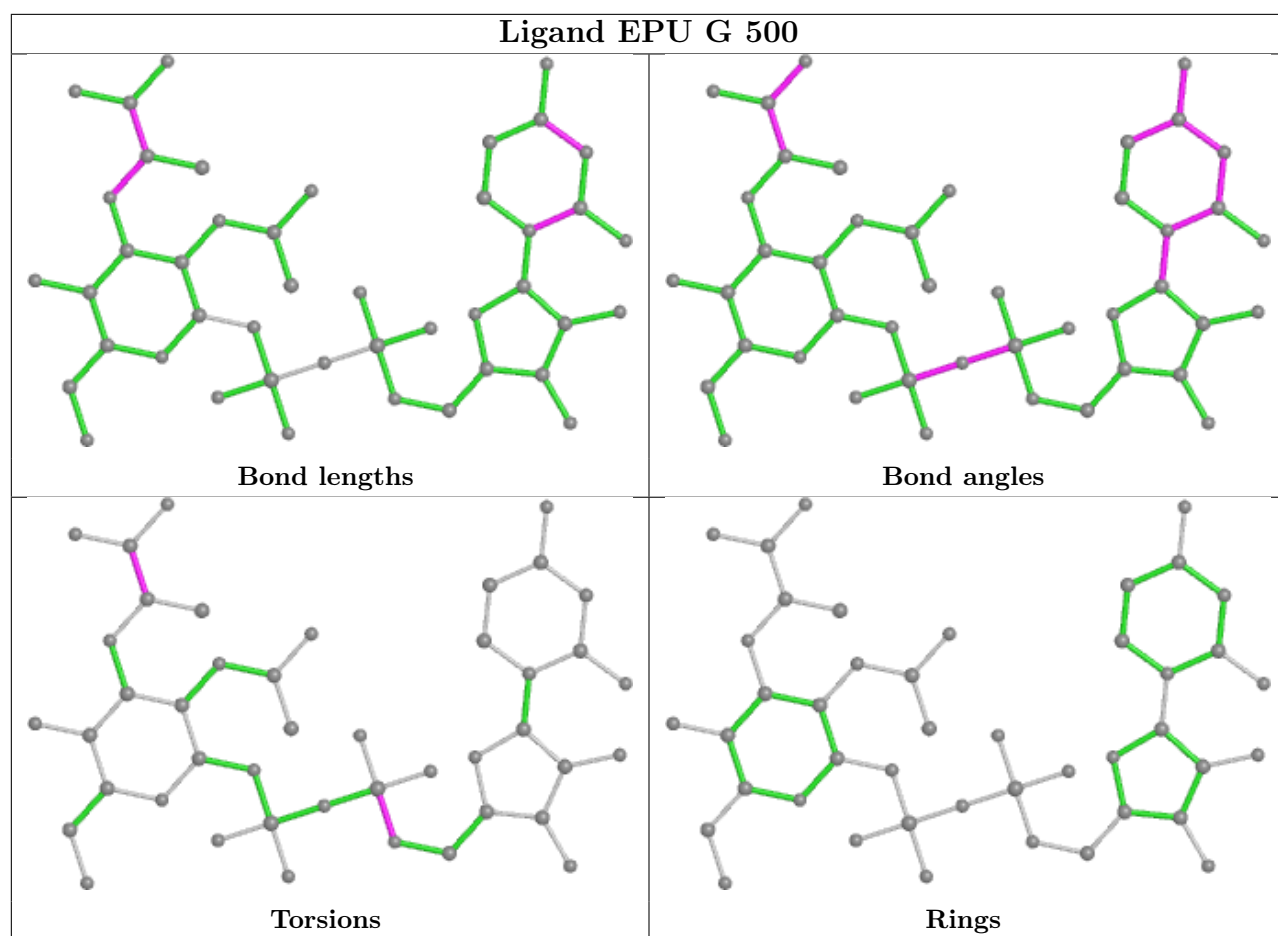












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	422/424 (99%)	0.20	16 (3%) 40 48	35, 53, 85, 109	0
1	B	421/424 (99%)	-0.07	8 (1%) 66 75	35, 48, 66, 98	0
1	C	421/424 (99%)	-0.06	8 (1%) 66 75	32, 45, 68, 97	0
1	D	421/424 (99%)	-0.06	7 (1%) 70 78	34, 46, 66, 86	0
1	E	421/424 (99%)	-0.04	10 (2%) 59 68	36, 47, 66, 105	0
1	F	421/424 (99%)	-0.03	8 (1%) 66 75	34, 47, 66, 111	0
1	G	421/424 (99%)	0.32	23 (5%) 25 30	41, 63, 90, 121	0
1	H	422/424 (99%)	-0.08	3 (0%) 87 91	32, 47, 69, 102	0
All	All	3370/3392 (99%)	0.02	83 (2%) 57 66	32, 49, 77, 121	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	421	GLY	5.8
1	F	68	GLU	5.4
1	A	69	LYS	5.2
1	B	421	GLY	4.9
1	G	69	LYS	4.8
1	C	421	GLY	4.7
1	A	152	GLY	4.7
1	F	421	GLY	4.3
1	A	65	VAL	4.3
1	A	67	ASP	4.3
1	D	421	GLY	4.1
1	E	68	GLU	4.1
1	A	222	GLU	4.0
1	G	155	ARG	3.9
1	D	275	ASP	3.9
1	G	387	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	68	GLU	3.8
1	E	70	LEU	3.7
1	H	421	GLY	3.5
1	C	1	MET	3.5
1	F	1	MET	3.4
1	A	0	ALA	3.3
1	G	421	GLY	3.3
1	G	151	GLU	3.2
1	G	46	HIS	3.2
1	C	67	ASP	3.2
1	H	0	ALA	3.1
1	F	69	LYS	3.1
1	A	66	ILE	3.0
1	A	420	PRO	3.0
1	G	1	MET	3.0
1	A	140	VAL	3.0
1	G	411	MET	2.9
1	E	222	GLU	2.9
1	A	68	GLU	2.9
1	E	223	ARG	2.9
1	G	48	HIS	2.8
1	A	70	LEU	2.8
1	G	225	ASP	2.8
1	G	361	LYS	2.8
1	C	36	ASP	2.7
1	D	1	MET	2.7
1	C	420	PRO	2.7
1	B	151	GLU	2.7
1	B	225	ASP	2.7
1	E	69	LYS	2.6
1	A	421	GLY	2.6
1	G	383	ALA	2.6
1	E	225	ASP	2.5
1	E	420	PRO	2.5
1	F	420	PRO	2.5
1	G	101	PRO	2.5
1	A	135	GLY	2.5
1	G	290	LYS	2.5
1	B	377	ALA	2.4
1	A	181	GLY	2.4
1	C	65	VAL	2.4
1	D	65	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	158	HIS	2.3
1	G	137	LYS	2.3
1	G	282	TRP	2.3
1	E	387	GLU	2.3
1	C	180	LYS	2.3
1	E	332	GLU	2.3
1	B	333	ASN	2.3
1	F	407	GLU	2.3
1	G	152	GLY	2.2
1	H	69	LYS	2.2
1	D	290	LYS	2.2
1	G	389	ASP	2.2
1	G	407	GLU	2.2
1	D	413	GLY	2.2
1	B	280	GLU	2.2
1	D	151	GLU	2.1
1	B	152	GLY	2.1
1	G	273	GLY	2.1
1	G	396	TYR	2.1
1	F	275	ASP	2.1
1	F	137	LYS	2.1
1	A	288	HIS	2.1
1	A	361	LYS	2.1
1	B	1	MET	2.1
1	G	280	GLU	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](#)

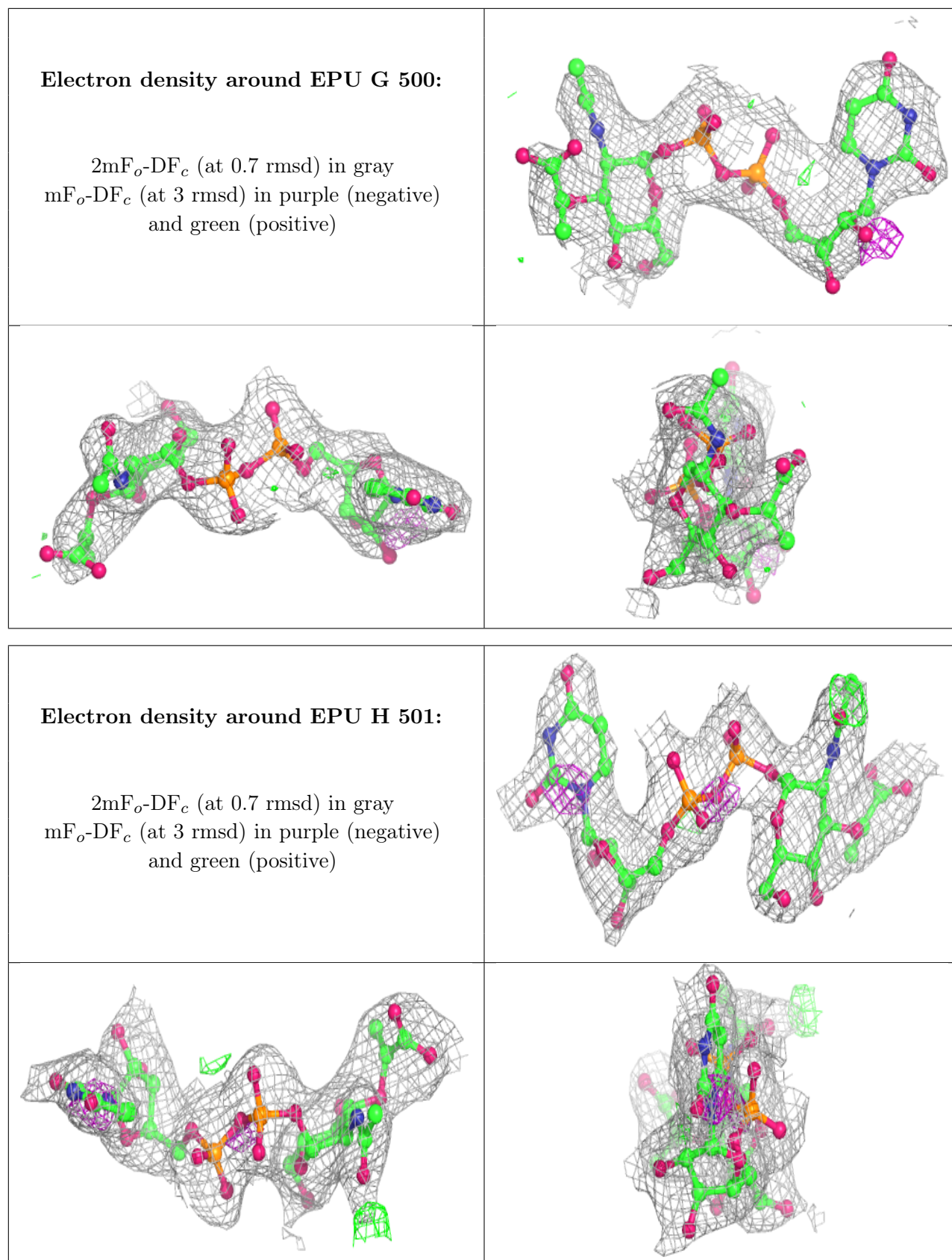
There are no monosaccharides in this entry.

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.

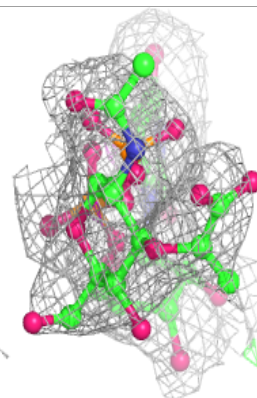
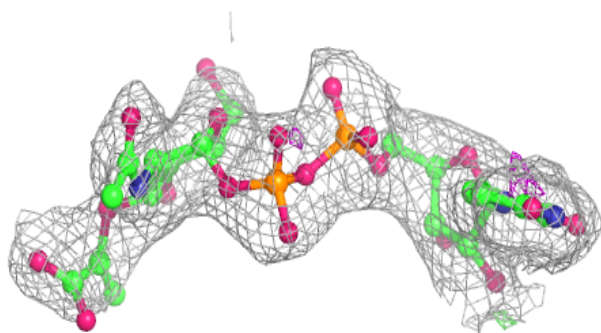
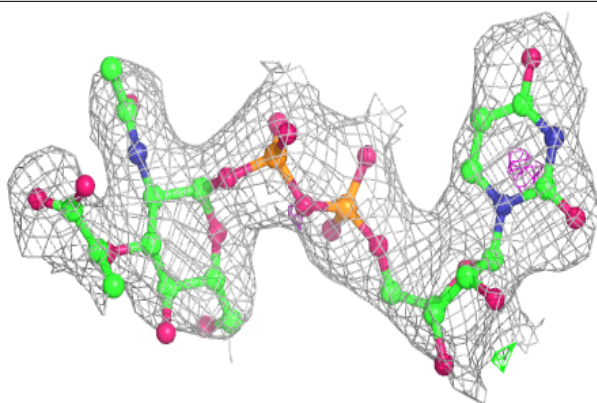
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	E	502	1/1	0.79	0.08	44,44,44,44	0
4	MG	H	503	1/1	0.79	0.08	47,47,47,47	0
4	MG	G	502	1/1	0.83	0.12	52,52,52,52	0
5	CL	H	504	1/1	0.85	0.37	69,69,69,69	0
5	CL	C	504	1/1	0.86	0.16	51,51,51,51	0
4	MG	C	503	1/1	0.89	0.06	41,41,41,41	0
3	OV5	G	501	10/10	0.92	0.16	50,53,55,56	0
2	EPU	G	500	44/44	0.92	0.18	50,55,64,70	0
3	OV5	F	502	10/10	0.92	0.14	46,47,48,48	0
4	MG	F	503	1/1	0.92	0.05	46,46,46,46	0
2	EPU	H	501	44/44	0.93	0.16	43,48,53,55	0
3	OV5	C	502	10/10	0.93	0.16	39,42,46,46	0
3	OV5	D	501	10/10	0.93	0.14	36,39,43,47	0
2	EPU	A	501	44/44	0.93	0.16	48,52,61,61	0
4	MG	D	502	1/1	0.94	0.08	39,39,39,39	0
2	EPU	E	500	44/44	0.94	0.16	46,50,60,66	0
2	EPU	F	501	44/44	0.94	0.16	44,50,57,59	0
3	OV5	H	502	10/10	0.94	0.14	48,49,51,53	0
4	MG	A	503	1/1	0.94	0.19	48,48,48,48	0
4	MG	B	502	1/1	0.94	0.07	47,47,47,47	0
5	CL	F	504	1/1	0.94	0.17	43,43,43,43	0
2	EPU	D	500	44/44	0.94	0.17	39,43,50,52	0
5	CL	H	505	1/1	0.94	0.15	53,53,53,53	0
3	OV5	E	501	10/10	0.95	0.14	46,46,48,50	0
3	OV5	A	502	10/10	0.95	0.12	47,50,51,52	0
2	EPU	C	501	44/44	0.95	0.15	39,45,52,52	0
2	EPU	B	500	44/44	0.95	0.14	38,45,52,54	0
3	OV5	B	501	10/10	0.96	0.12	47,48,50,51	0
5	CL	A	504	1/1	0.96	0.17	58,58,58,58	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.

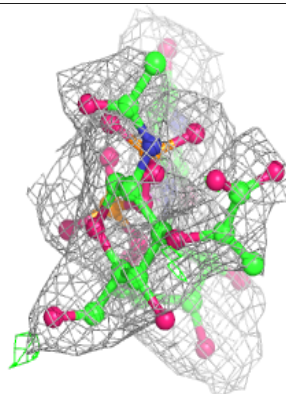
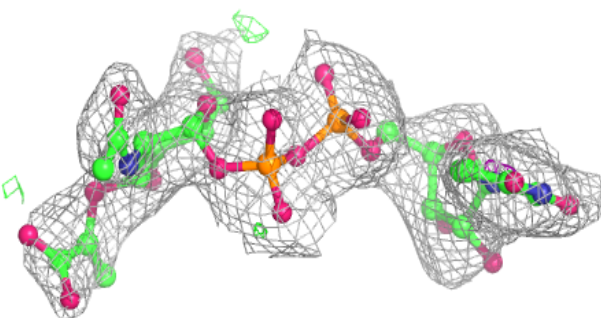
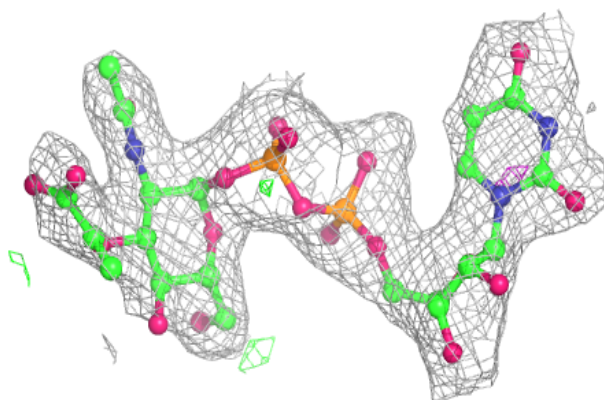


Electron density around EPU A 501:

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

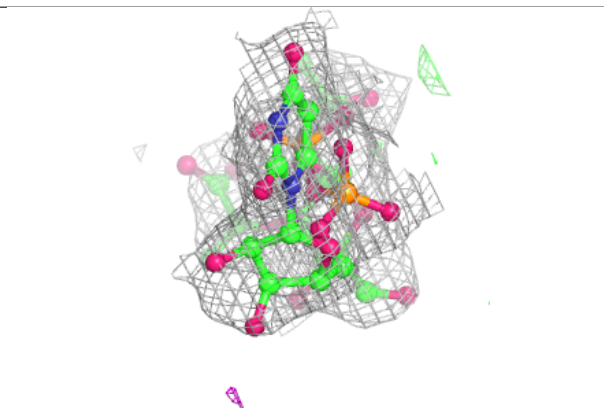
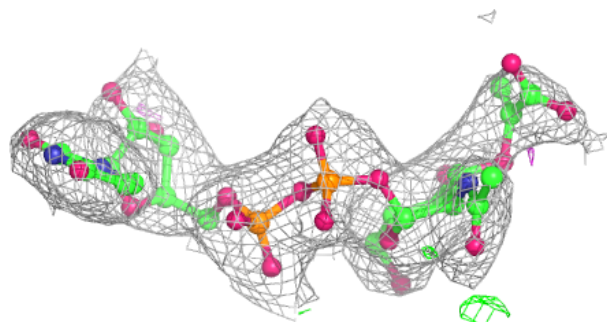
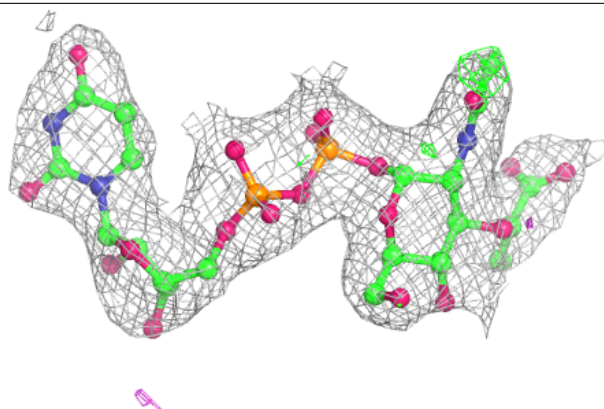
**Electron density around EPU E 500:**

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

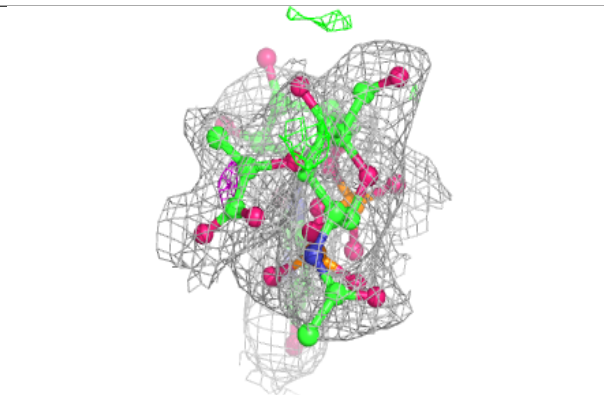
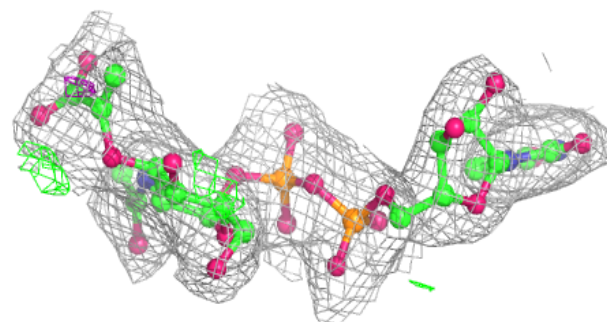
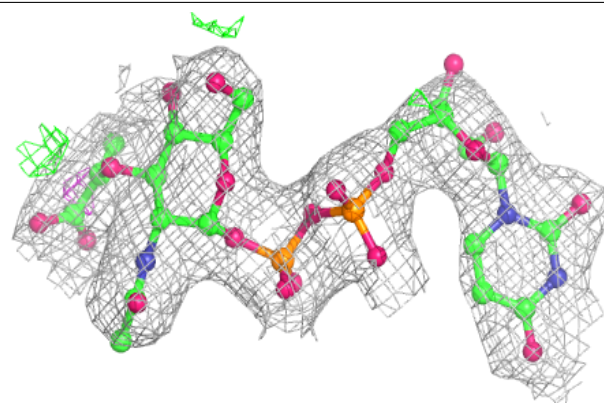


Electron density around EPU F 501:

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

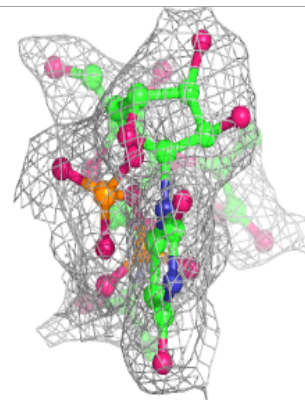
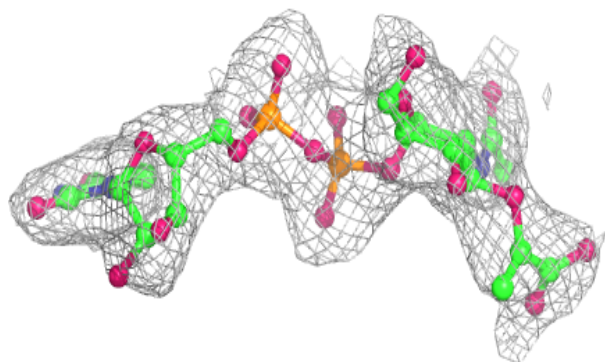
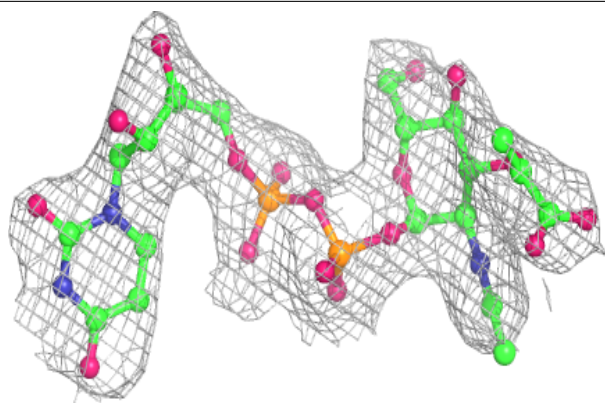
**Electron density around EPU D 500:**

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

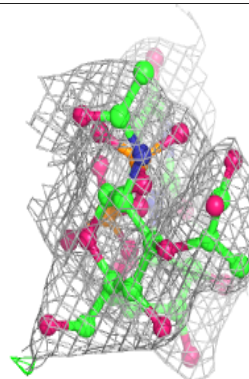
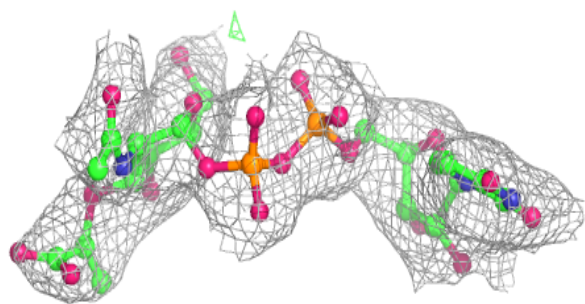
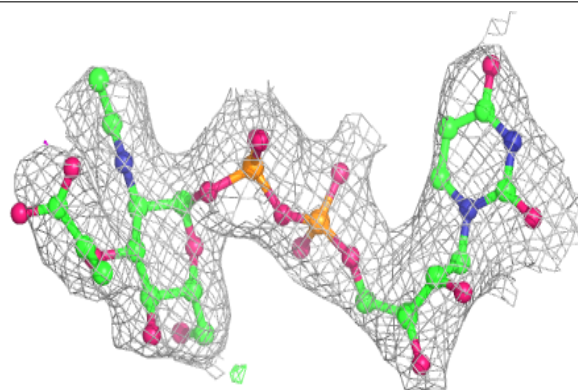


Electron density around EPU C 501:

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

**Electron density around EPU B 500:**

$2mF_o-DF_c$ (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.