



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:49 PM UTC

PDB ID : 8R3U / pdb_00008r3u
Title : Crystal structure of DHPS in complex with an inhibitor
Authors : Turnbull, A.P.
Deposited on : 2023-11-10
Resolution : 1.63 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

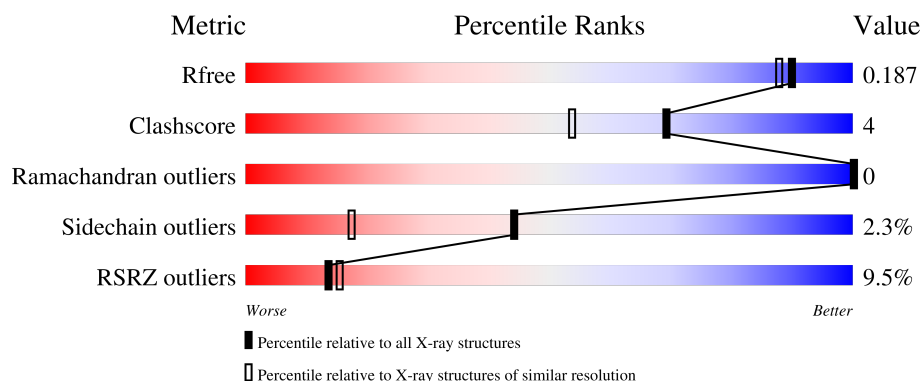
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	AAA	370	9% 75% 7% 17%
1	BBB	370	7% 77% 6% 16%
1	CCC	370	9% 79% 6% 15%
1	DDD	370	8% 76% 5% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	CCC	403	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10723 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.

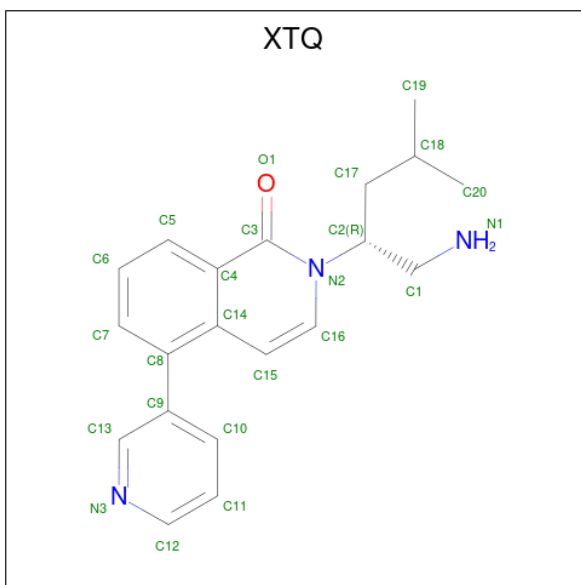
- Molecule 1 is a protein called Deoxyhypusine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	308	Total	C	N	O	S	0	4	0
			2411	1540	404	452	15			
1	BBB	311	Total	C	N	O	S	0	10	0
			2458	1571	413	460	14			
1	CCC	314	Total	C	N	O	S	0	2	0
			2423	1546	406	456	15			
1	DDD	300	Total	C	N	O	S	0	2	0
			2315	1484	384	433	14			

There are 8 discrepancies between the modelled and reference sequences:

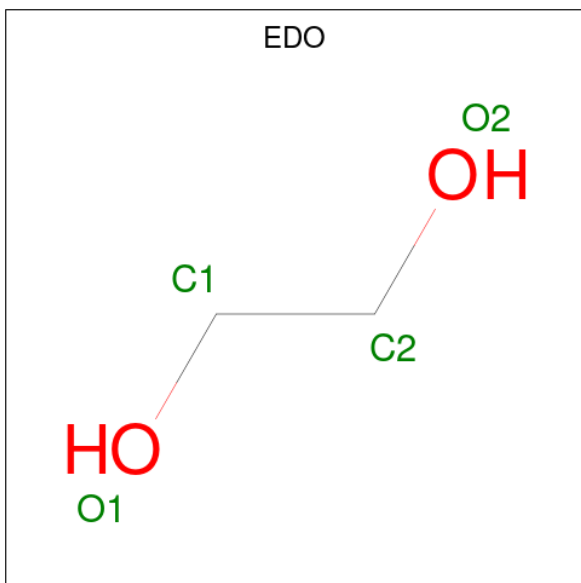
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	GLY	-	expression tag	UNP P49366
AAA	1	SER	-	expression tag	UNP P49366
BBB	0	GLY	-	expression tag	UNP P49366
BBB	1	SER	-	expression tag	UNP P49366
CCC	0	GLY	-	expression tag	UNP P49366
CCC	1	SER	-	expression tag	UNP P49366
DDD	0	GLY	-	expression tag	UNP P49366
DDD	1	SER	-	expression tag	UNP P49366

- Molecule 2 is 2-[(2 {R})-1-azanyl-4-methyl-pentan-2-yl]-5-pyridin-3-yl-isoquinolin-1-one (CCD ID: XTQ) (formula: C₂₀H₂₃N₃O) (labeled as "Ligand of Interest" by depositor).



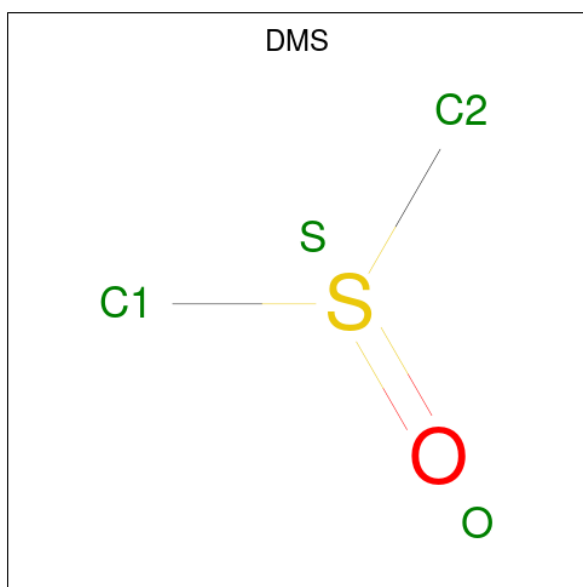
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			24	20	3	1		
2	BBB	1	Total	C	N	O	0	0
			24	20	3	1		
2	CCC	1	Total	C	N	O	0	0
			24	20	3	1		
2	DDD	1	Total	C	N	O	0	0
			24	20	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	DDD	1	Total C O 4 2 2	0	0
3	DDD	1	Total C O 4 2 2	0	0
3	DDD	1	Total C O 4 2 2	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	CCC	1	Total	C	O	S	0	0
			4	2	1	1		
4	DDD	1	Total	C	O	S	0	0
			4	2	1	1		

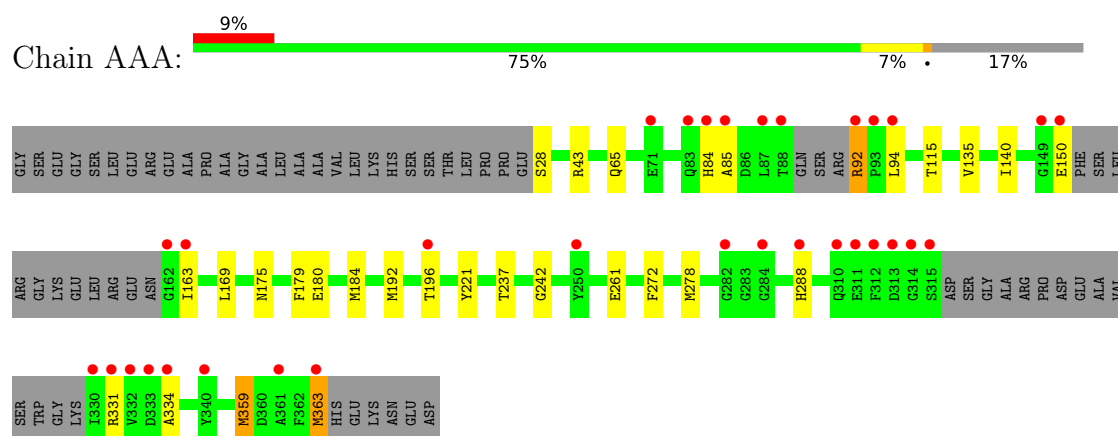
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	221	Total	O	0	0
			221	221		
5	BBB	267	Total	O	0	0
			267	267		
5	CCC	223	Total	O	0	0
			223	223		
5	DDD	229	Total	O	0	0
			229	229		

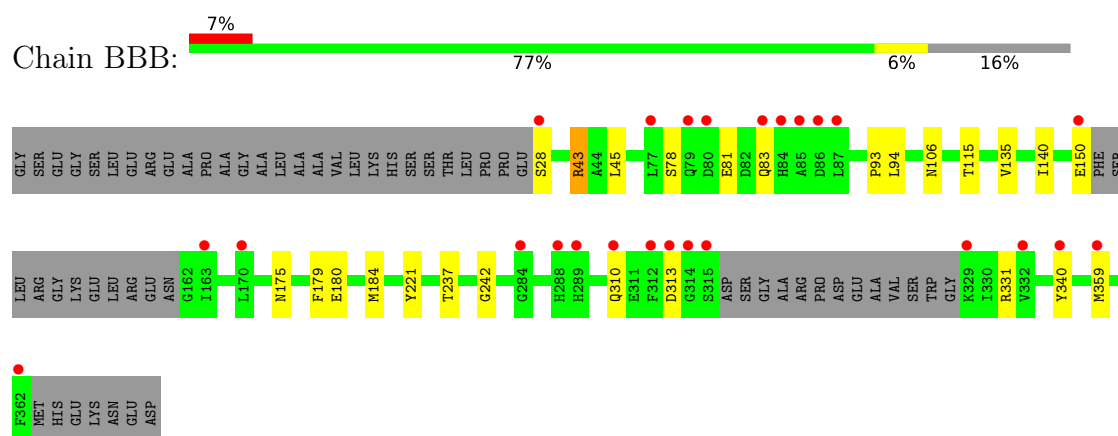
3 Residue-property plots [i](#)

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.

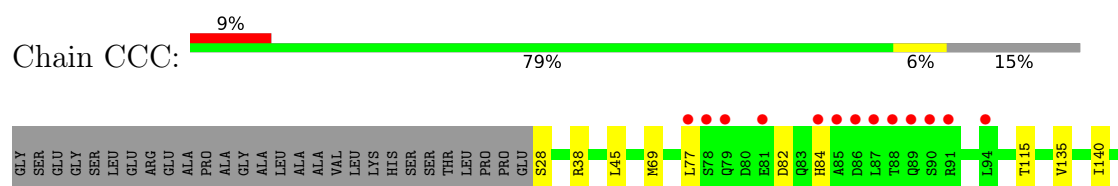
- Molecule 1: Deoxyhypusine synthase

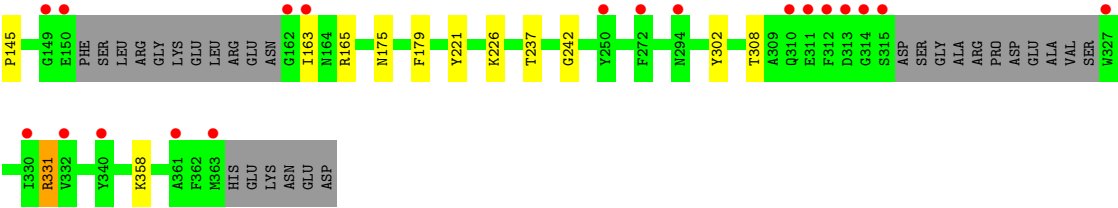


- Molecule 1: Deoxyhypusine synthase

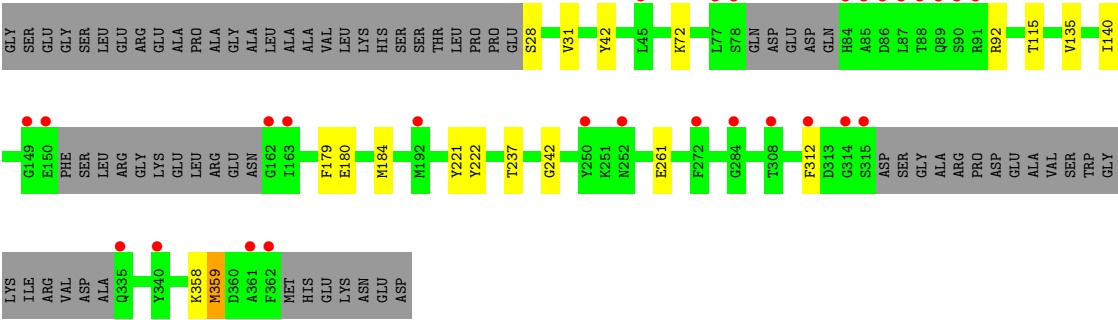
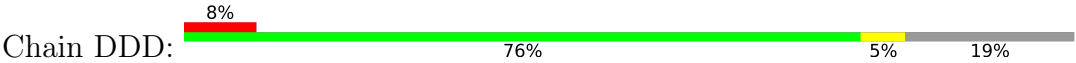


- Molecule 1: Deoxyhypusine synthase





● Molecule 1: Deoxyhypusine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.53Å 107.85Å 96.86Å 90.00° 93.13° 90.00°	Depositor
Resolution (Å)	72.00 – 1.63 72.00 – 1.63	Depositor EDS
% Data completeness (in resolution range)	97.9 (72.00-1.63) 97.9 (72.00-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.180 , 0.210 (Not available) , 0.187	Depositor DCC
R_{free} test set	1968 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10723	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XTQ, DMS, EDO

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	AAA	1.07	0/2466	1.20	5/3346 (0.1%)
1	BBB	1.04	0/2516	1.20	0/3411
1	CCC	1.06	0/2474	1.20	2/3360 (0.1%)
1	DDD	1.03	0/2367	1.19	0/3213
All	All	1.05	0/9823	1.20	7/13330 (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	CCC	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	363	MET	CA-C-O	-7.22	108.52	120.80
1	AAA	84	HIS	CA-C-N	5.16	127.19	120.28
1	AAA	84	HIS	C-N-CA	5.16	127.19	120.28
1	CCC	84	HIS	CA-C-N	5.09	127.11	120.28
1	CCC	84	HIS	C-N-CA	5.09	127.11	120.28
1	AAA	272	PHE	CA-CB-CG	-5.06	108.74	113.80
1	AAA	278	MET	CG-SD-CE	-5.04	89.81	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	77	LEU	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	AAA	2411	0	2369	21	0
1	BBB	2458	0	2432	20	0
1	CCC	2423	0	2361	14	0
1	DDD	2315	0	2265	19	0
2	AAA	24	0	0	0	0
2	BBB	24	0	0	0	0
2	CCC	24	0	0	0	0
2	DDD	24	0	0	0	0
3	AAA	20	0	30	0	0
3	BBB	16	0	24	0	0
3	CCC	24	0	36	6	0
3	DDD	12	0	18	0	0
4	CCC	4	0	6	3	0
4	DDD	4	0	6	2	0
5	AAA	221	0	0	4	0
5	BBB	267	0	0	4	0
5	CCC	223	0	0	2	0
5	DDD	229	0	0	5	0
All	All	10723	0	9547	68	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 4.

All (68) 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:BBB:340:TYR:CE1	1:DDD:312:PHE:CZ	2.49	1.01
1:AAA:85:ALA:HB1	1:AAA:94:LEU:CB	1.98	0.94
1:AAA:85:ALA:HB1	1:AAA:94:LEU:HB3	1.47	0.94
1:BBB:340:TYR:CD1	1:DDD:312:PHE:CZ	2.57	0.91
1:BBB:340:TYR:CD1	1:DDD:312:PHE:CE1	2.75	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:340:TYR:CE1	1:DDD:312:PHE:CE2	2.76	0.73
1:AAA:92:ARG:HD3	5:AAA:546:HOH:O	1.91	0.68
1:BBB:45[B]:LEU:HD23	1:BBB:45[B]:LEU:C	2.19	0.67
1:BBB:150:GLU:C	5:BBB:704:HOH:O	2.39	0.65
1:CCC:45:LEU:HD23	1:CCC:45:LEU:C	2.23	0.64
1:AAA:85:ALA:HB1	1:AAA:94:LEU:HB2	1.79	0.62
1:CCC:331:ARG:HH11	1:CCC:331:ARG:HB3	1.66	0.61
1:CCC:226:LYS:HE2	3:CCC:403:EDO:O1	2.01	0.59
1:AAA:85:ALA:HA	1:AAA:94:LEU:HD22	1.83	0.59
1:BBB:340:TYR:CZ	1:DDD:312:PHE:CE2	2.91	0.59
3:CCC:403:EDO:H12	4:CCC:407:DMS:H13	1.85	0.58
1:AAA:85:ALA:CB	1:AAA:94:LEU:HB3	2.29	0.57
3:CCC:403:EDO:C1	4:CCC:407:DMS:H13	2.35	0.56
1:BBB:180:GLU:HG3	1:BBB:184:MET:HE3	1.87	0.56
1:DDD:92:ARG:HD3	5:DDD:590:HOH:O	2.07	0.55
1:BBB:340:TYR:CD1	1:DDD:312:PHE:CE2	2.95	0.54
1:BBB:83:GLN:HE21	1:BBB:93:PRO:HA	1.71	0.54
1:AAA:261:GLU:HG2	5:AAA:578:HOH:O	2.08	0.53
1:CCC:165:ARG:CG	5:CCC:715:HOH:O	2.56	0.53
1:AAA:288:HIS:CE1	1:AAA:334:ALA:O	2.62	0.53
1:DDD:359:MET:HE2	5:DDD:549:HOH:O	2.08	0.52
1:AAA:180:GLU:HG3	1:AAA:184:MET:HE2	1.91	0.52
1:DDD:222:TYR:OH	4:DDD:405:DMS:C1	2.58	0.52
1:BBB:78:SER:HB3	1:BBB:81:GLU:OE2	2.10	0.51
1:CCC:145:PRO:HD3	3:CCC:405:EDO:H22	1.93	0.51
1:CCC:308:THR:HG21	1:DDD:312:PHE:CE1	2.47	0.50
1:AAA:359:MET:HE2	5:DDD:533:HOH:O	2.09	0.50
1:AAA:85:ALA:CB	1:AAA:94:LEU:HD22	2.42	0.50
1:BBB:83:GLN:NE2	1:BBB:94:LEU:H	2.10	0.49
1:DDD:261:GLU:HG2	5:DDD:570:HOH:O	2.13	0.48
1:CCC:140:ILE:HG12	1:CCC:179:PHE:HB2	1.95	0.47
1:DDD:140:ILE:HG12	1:DDD:179:PHE:HB2	1.96	0.47
1:AAA:85:ALA:CA	1:AAA:94:LEU:HD22	2.45	0.47
1:BBB:106:ASN:HB3	5:BBB:699:HOH:O	2.14	0.47
1:DDD:72:LYS:HD2	5:DDD:524:HOH:O	2.13	0.47
1:DDD:135:VAL:HA	1:DDD:221:TYR:CE2	2.51	0.46
1:AAA:65:GLN:OE1	5:AAA:501:HOH:O	2.21	0.45
1:AAA:135:VAL:HA	1:AAA:221:TYR:CE2	2.51	0.45
1:AAA:140:ILE:HG12	1:AAA:179:PHE:HB2	1.98	0.45
1:AAA:169:LEU:HD22	1:DDD:31:VAL:HG21	1.98	0.45
1:BBB:313:ASP:OD2	5:BBB:501:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:340:TYR:CD1	1:BBB:340:TYR:C	2.96	0.44
1:AAA:43:ARG:HD3	1:DDD:42:TYR:OH	2.18	0.44
1:BBB:135:VAL:HA	1:BBB:221:TYR:CE2	2.52	0.43
1:BBB:140:ILE:HG12	1:BBB:179:PHE:HB2	2.01	0.43
1:CCC:38:ARG:HD2	5:CCC:681:HOH:O	2.17	0.43
1:BBB:140:ILE:CG2	1:BBB:175:ASN:HB3	2.49	0.43
1:CCC:135:VAL:HA	1:CCC:221:TYR:CE2	2.54	0.42
1:BBB:43:ARG:NH2	5:BBB:518:HOH:O	2.51	0.42
3:CCC:403:EDO:O2	4:CCC:407:DMS:H13	2.19	0.42
1:DDD:222:TYR:OH	4:DDD:405:DMS:H13	2.18	0.42
1:CCC:140:ILE:CG2	1:CCC:175:ASN:HB3	2.49	0.42
1:CCC:45:LEU:C	1:CCC:45:LEU:CD2	2.92	0.42
1:CCC:69:MET:HG3	1:CCC:302:TYR:HB2	2.02	0.42
1:CCC:226:LYS:HE2	3:CCC:403:EDO:HO1	1.82	0.41
1:BBB:237:THR:O	1:BBB:242:GLY:HA3	2.19	0.41
1:DDD:180:GLU:HG3	1:DDD:184:MET:HE2	2.03	0.41
1:AAA:150:GLU:C	5:AAA:679:HOH:O	2.63	0.41
1:CCC:237:THR:O	1:CCC:242:GLY:HA3	2.20	0.41
1:AAA:237:THR:O	1:AAA:242:GLY:HA3	2.21	0.40
1:AAA:192:MET:HE3	1:AAA:196:THR:OG1	2.20	0.40
1:AAA:140:ILE:CG2	1:AAA:175:ASN:HB3	2.51	0.40
1:DDD:237:THR:O	1:DDD:242:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	304/370 (82%)	301 (99%)	3 (1%)	0	100	100
1	BBB	315/370 (85%)	309 (98%)	6 (2%)	0	100	100
1	CCC	310/370 (84%)	306 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DDD	294/370 (80%)	291 (99%)	3 (1%)	0	100	100
All	All	1223/1480 (83%)	1207 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	257/310 (83%)	250 (97%)	7 (3%)	39	13
1	BBB	261/310 (84%)	255 (98%)	6 (2%)	44	17
1	CCC	255/310 (82%)	249 (98%)	6 (2%)	43	15
1	DDD	245/310 (79%)	241 (98%)	4 (2%)	55	30
All	All	1018/1240 (82%)	995 (98%)	23 (2%)	44	17

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	28	SER
1	AAA	92	ARG
1	AAA	115	THR
1	AAA	163	ILE
1	AAA	331	ARG
1	AAA	359	MET
1	AAA	363	MET
1	BBB	28	SER
1	BBB	43	ARG
1	BBB	115	THR
1	BBB	310	GLN
1	BBB	331	ARG
1	BBB	359	MET
1	CCC	28	SER
1	CCC	82	ASP
1	CCC	115	THR

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Mol	Chain	Res	Type
1	CCC	163	ILE
1	CCC	331	ARG
1	CCC	358	LYS
1	DDD	28	SER
1	DDD	115	THR
1	DDD	358	LYS
1	DDD	359	MET

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	AAA	405	-	3,3,3	0.14	0	2,2,2	0.15	0
3	EDO	CCC	403	-	3,3,3	0.10	0	2,2,2	0.13	0
3	EDO	CCC	408	-	3,3,3	0.30	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XTQ	AAA	401	-	26,26,26	0.69	0	31,36,36	1.13	3 (9%)
3	EDO	DDD	402	-	3,3,3	0.23	0	2,2,2	0.26	0
3	EDO	AAA	406	-	3,3,3	0.21	0	2,2,2	0.22	0
4	DMS	DDD	405	-	3,3,3	0.18	0	3,3,3	0.23	0
3	EDO	AAA	403	-	3,3,3	0.23	0	2,2,2	0.04	0
3	EDO	BBB	402	-	3,3,3	0.13	0	2,2,2	0.09	0
2	XTQ	CCC	401	-	26,26,26	0.99	1 (3%)	31,36,36	1.27	4 (12%)
3	EDO	DDD	403	-	3,3,3	0.04	0	2,2,2	0.13	0
3	EDO	CCC	402	-	3,3,3	0.26	0	2,2,2	0.53	0
2	XTQ	DDD	401	-	26,26,26	0.90	1 (3%)	31,36,36	1.06	2 (6%)
3	EDO	AAA	404	-	3,3,3	0.04	0	2,2,2	0.05	0
2	XTQ	BBB	401	-	26,26,26	0.70	0	31,36,36	1.09	3 (9%)
3	EDO	BBB	405	-	3,3,3	0.20	0	2,2,2	0.11	0
3	EDO	AAA	402	-	3,3,3	0.04	0	2,2,2	0.11	0
3	EDO	CCC	405	-	3,3,3	0.15	0	2,2,2	0.20	0
3	EDO	CCC	406	-	3,3,3	0.02	0	2,2,2	0.13	0
3	EDO	BBB	404	-	3,3,3	0.20	0	2,2,2	0.09	0
3	EDO	CCC	404	-	3,3,3	0.26	0	2,2,2	0.20	0
3	EDO	BBB	403	-	3,3,3	0.05	0	2,2,2	0.23	0
4	DMS	CCC	407	-	3,3,3	0.21	0	3,3,3	0.13	0
3	EDO	DDD	404	-	3,3,3	0.09	0	2,2,2	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	AAA	405	-	-	1/1/1/1	-
3	EDO	CCC	403	-	-	0/1/1/1	-
3	EDO	CCC	408	-	-	0/1/1/1	-
2	XTQ	AAA	401	-	-	0/14/14/14	0/3/3/3
3	EDO	DDD	402	-	-	0/1/1/1	-
3	EDO	AAA	406	-	-	0/1/1/1	-
3	EDO	AAA	403	-	-	0/1/1/1	-
3	EDO	BBB	402	-	-	0/1/1/1	-
2	XTQ	CCC	401	-	-	0/14/14/14	0/3/3/3
3	EDO	DDD	403	-	-	1/1/1/1	-
3	EDO	CCC	402	-	-	1/1/1/1	-
2	XTQ	DDD	401	-	-	0/14/14/14	0/3/3/3
3	EDO	AAA	404	-	-	0/1/1/1	-
2	XTQ	BBB	401	-	-	0/14/14/14	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	BBB	405	-	-	1/1/1/1	-
3	EDO	AAA	402	-	-	0/1/1/1	-
3	EDO	CCC	405	-	-	1/1/1/1	-
3	EDO	CCC	406	-	-	0/1/1/1	-
3	EDO	BBB	404	-	-	1/1/1/1	-
3	EDO	CCC	404	-	-	1/1/1/1	-
3	EDO	BBB	403	-	-	1/1/1/1	-
3	EDO	DDD	404	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	401	XTQ	C1-C2	-3.86	1.49	1.53
2	DDD	401	XTQ	C1-C2	-3.18	1.50	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	401	XTQ	C14-C4-C3	-4.50	118.69	121.69
2	DDD	401	XTQ	C14-C4-C3	-3.62	119.27	121.69
2	AAA	401	XTQ	C14-C4-C3	-3.21	119.54	121.69
2	AAA	401	XTQ	C14-C8-C9	3.07	125.87	122.10
2	BBB	401	XTQ	C14-C4-C3	-3.05	119.65	121.69
2	CCC	401	XTQ	C16-N2-C3	3.05	124.38	122.22
2	BBB	401	XTQ	C14-C8-C9	2.97	125.75	122.10
2	CCC	401	XTQ	C14-C8-C9	2.75	125.48	122.10
2	DDD	401	XTQ	C14-C8-C9	2.33	124.96	122.10
2	BBB	401	XTQ	C16-N2-C3	2.13	123.73	122.22
2	CCC	401	XTQ	O1-C3-N2	-2.03	119.05	120.71
2	AAA	401	XTQ	C16-N2-C3	2.01	123.64	122.22

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	403	EDO	O1-C1-C2-O2
3	BBB	404	EDO	O1-C1-C2-O2
3	CCC	405	EDO	O1-C1-C2-O2
3	DDD	404	EDO	O1-C1-C2-O2
3	DDD	403	EDO	O1-C1-C2-O2
3	CCC	402	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	CCC	404	EDO	O1-C1-C2-O2
3	AAA	405	EDO	O1-C1-C2-O2
3	BBB	405	EDO	O1-C1-C2-O2

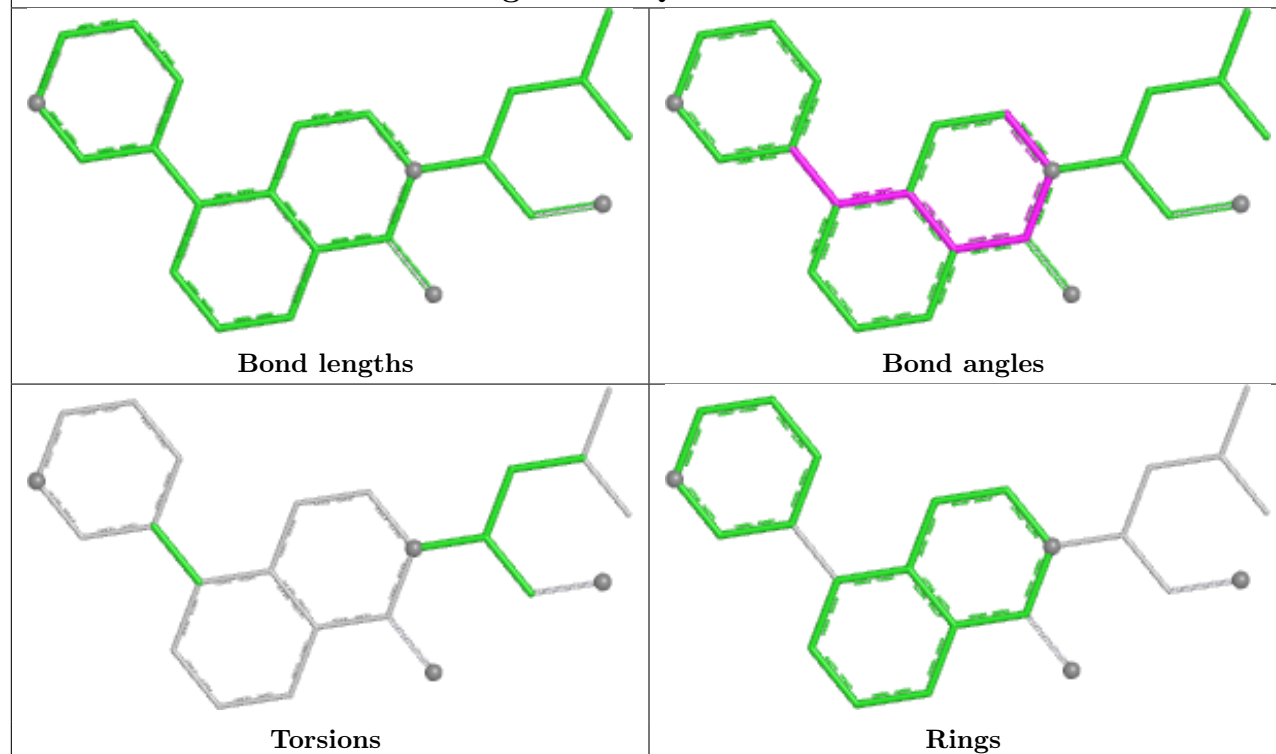
There are no ring outliers.

4 monomers are involved in 8 short contacts:

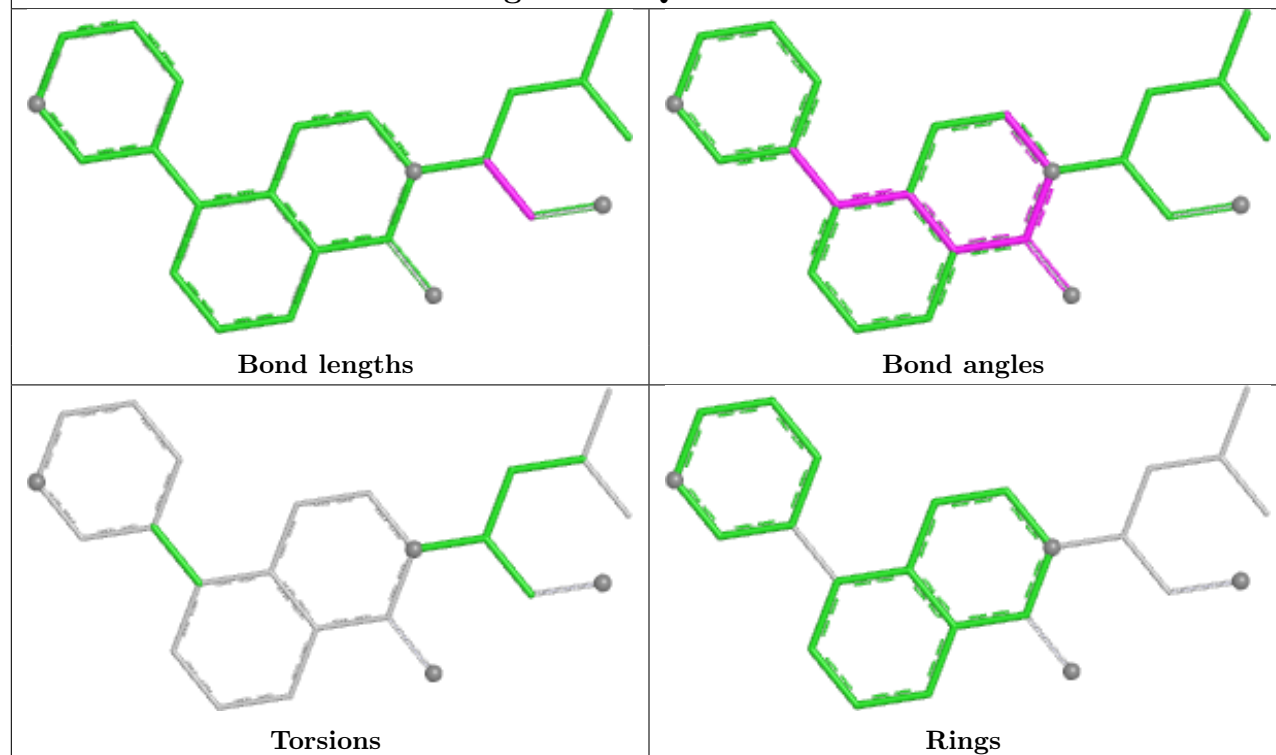
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	CCC	403	EDO	5	0
4	DDD	405	DMS	2	0
3	CCC	405	EDO	1	0
4	CCC	407	DMS	3	0

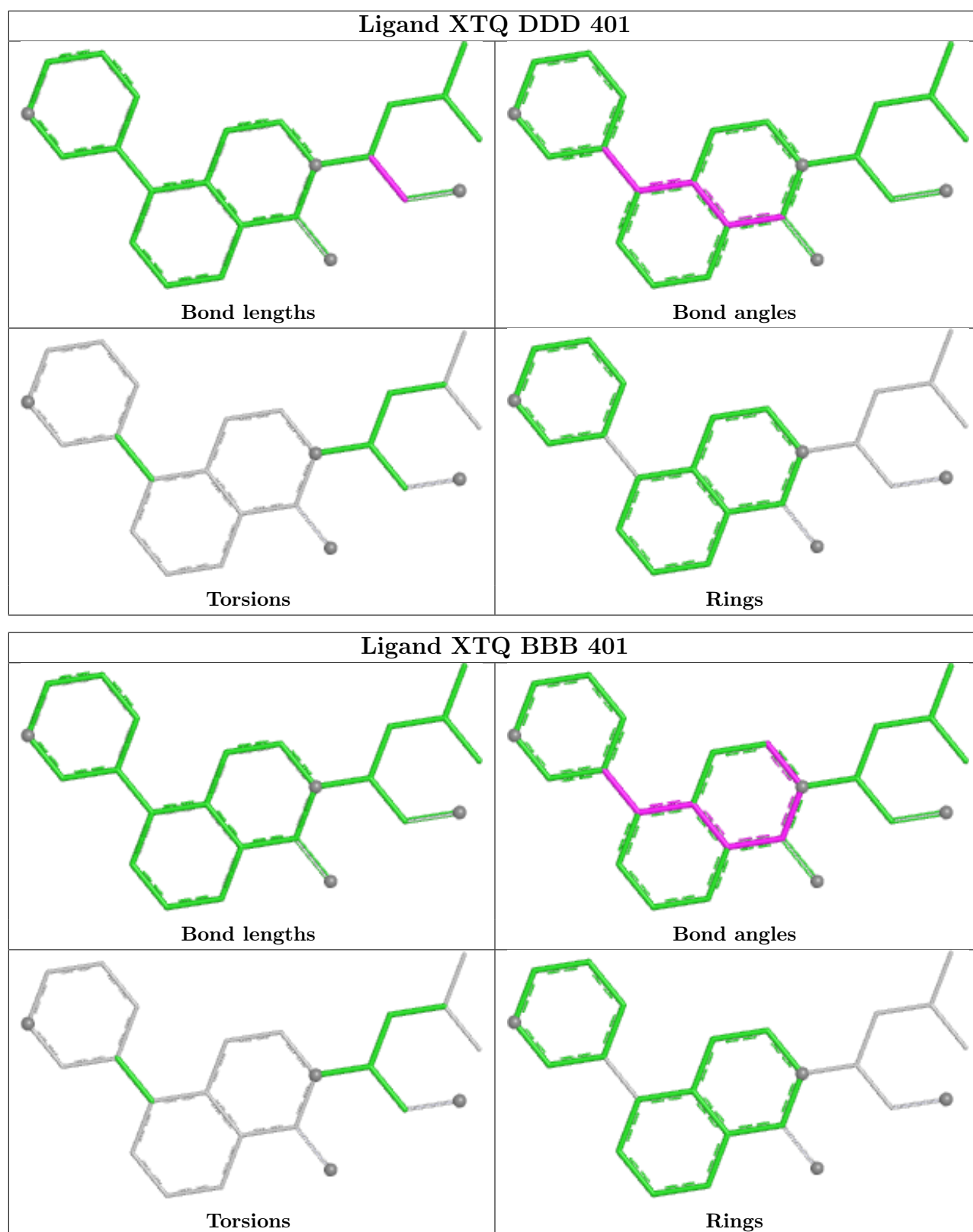
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 XTQ AAA 401



Ligand XTQ CCC 401





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	AAA	308/370 (83%)	0.46	32 (10%) 11 13	15, 36, 72, 105	4 (1%)
1	BBB	311/370 (84%)	0.30	25 (8%) 18 21	14, 33, 69, 104	10 (3%)
1	CCC	314/370 (84%)	0.50	32 (10%) 12 14	15, 37, 75, 136	2 (0%)
1	DDD	300/370 (81%)	0.58	28 (9%) 14 16	23, 39, 72, 118	2 (0%)
All	All	1233/1480 (83%)	0.46	117 (9%) 14 15	14, 36, 73, 136	18 (1%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	312	PHE	8.0
1	CCC	312	PHE	7.1
1	DDD	78	SER	6.0
1	BBB	312	PHE	6.0
1	DDD	87	LEU	5.8
1	CCC	85	ALA	5.8
1	CCC	87	LEU	5.5
1	CCC	327	TRP	5.5
1	AAA	330	ILE	5.3
1	DDD	312	PHE	5.2
1	DDD	88	THR	5.2
1	CCC	340	TYR	5.2
1	BBB	87	LEU	5.1
1	CCC	313	ASP	4.9
1	AAA	315	SER	4.9
1	AAA	85	ALA	4.8
1	BBB	313	ASP	4.6
1	AAA	84	HIS	4.5
1	DDD	150	GLU	4.5
1	CCC	88	THR	4.5
1	AAA	88	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	BBB	84	HIS	4.4
1	AAA	87	LEU	4.3
1	CCC	89	GLN	4.2
1	CCC	77	LEU	4.1
1	AAA	332	VAL	4.0
1	DDD	84	HIS	4.0
1	DDD	85	ALA	4.0
1	AAA	334	ALA	3.9
1	BBB	314	GLY	3.8
1	BBB	85	ALA	3.8
1	CCC	311	GLU	3.8
1	CCC	272	PHE	3.7
1	CCC	84	HIS	3.6
1	AAA	314	GLY	3.6
1	CCC	90	SER	3.6
1	CCC	310	GLN	3.5
1	BBB	77	LEU	3.5
1	BBB	340	TYR	3.5
1	BBB	150	GLU	3.4
1	BBB	284[A]	GLY	3.4
1	DDD	250	TYR	3.4
1	CCC	314	GLY	3.4
1	CCC	150	GLU	3.4
1	AAA	250	TYR	3.3
1	BBB	288	HIS	3.3
1	DDD	86	ASP	3.3
1	DDD	91	ARG	3.3
1	BBB	362	PHE	3.2
1	DDD	362	PHE	3.2
1	DDD	149	GLY	3.2
1	AAA	93	PRO	3.1
1	AAA	92	ARG	3.1
1	AAA	284	GLY	3.1
1	CCC	250	TYR	3.0
1	AAA	94	LEU	3.0
1	DDD	314	GLY	3.0
1	AAA	333	ASP	3.0
1	BBB	315	SER	3.0
1	CCC	78	SER	3.0
1	BBB	289	HIS	3.0
1	DDD	77	LEU	3.0
1	DDD	89	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	DDD	162	GLY	3.0
1	DDD	340	TYR	2.9
1	BBB	86	ASP	2.9
1	CCC	315	SER	2.9
1	DDD	163	ILE	2.9
1	CCC	162	GLY	2.8
1	AAA	150	GLU	2.8
1	AAA	313	ASP	2.8
1	CCC	361	ALA	2.8
1	AAA	163	ILE	2.8
1	DDD	272	PHE	2.7
1	DDD	308	THR	2.7
1	DDD	252	ASN	2.7
1	BBB	310	GLN	2.6
1	CCC	149	GLY	2.6
1	CCC	86	ASP	2.6
1	AAA	162	GLY	2.6
1	BBB	79	GLN	2.6
1	BBB	83	GLN	2.6
1	AAA	363	MET	2.6
1	DDD	284	GLY	2.5
1	AAA	340[A]	TYR	2.5
1	DDD	192	MET	2.5
1	DDD	315	SER	2.5
1	BBB	80	ASP	2.4
1	AAA	331	ARG	2.4
1	AAA	310	GLN	2.3
1	CCC	332	VAL	2.3
1	DDD	361	ALA	2.3
1	CCC	94	LEU	2.3
1	CCC	163	ILE	2.3
1	BBB	332	VAL	2.3
1	BBB	359	MET	2.3
1	BBB	170	LEU	2.2
1	AAA	149	GLY	2.2
1	AAA	83	GLN	2.2
1	CCC	330	ILE	2.2
1	BBB	329	LYS	2.2
1	AAA	311	GLU	2.1
1	CCC	81	GLU	2.1
1	AAA	288	HIS	2.1
1	DDD	45	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	DDD	90	SER	2.1
1	AAA	196	THR	2.1
1	DDD	335	GLN	2.1
1	AAA	361	ALA	2.1
1	AAA	71	GLU	2.1
1	BBB	28	SER	2.1
1	AAA	282	GLY	2.0
1	CCC	294	ASN	2.0
1	CCC	363	MET	2.0
1	CCC	79	GLN	2.0
1	BBB	163	ILE	2.0
1	CCC	91	ARG	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(Å ²)	Q<0.9
4	DMS	CCC	407	4/4	0.78	0.21	83,90,92,97	0
4	DMS	DDD	405	4/4	0.78	0.20	99,100,104,104	0
3	EDO	AAA	405	4/4	0.80	0.17	60,67,68,69	0
3	EDO	CCC	402	4/4	0.82	0.19	63,63,66,68	0
3	EDO	CCC	404	4/4	0.84	0.15	56,65,66,66	0
3	EDO	CCC	406	4/4	0.85	0.13	57,59,63,63	0
3	EDO	CCC	403	4/4	0.86	0.15	65,66,67,75	0
3	EDO	DDD	404	4/4	0.86	0.18	69,70,70,74	0
3	EDO	AAA	404	4/4	0.86	0.16	71,73,76,78	0
3	EDO	CCC	405	4/4	0.86	0.15	71,72,72,77	0
3	EDO	BBB	403	4/4	0.88	0.12	69,76,78,81	0

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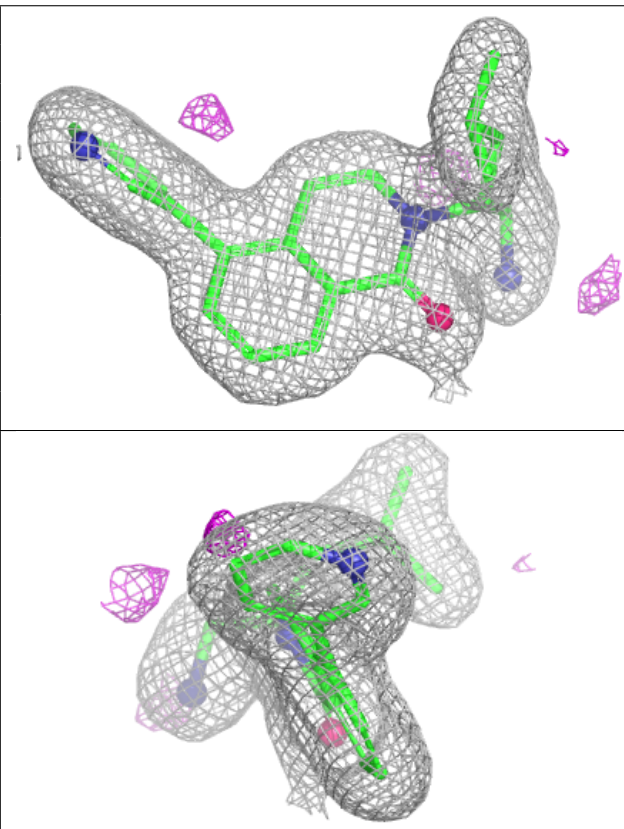
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	BBB	404	4/4	0.89	0.13	64,67,69,70	0
3	EDO	BBB	402	4/4	0.90	0.13	47,55,60,63	0
3	EDO	DDD	403	4/4	0.91	0.11	60,66,73,80	0
3	EDO	AAA	406	4/4	0.93	0.12	42,44,45,48	0
3	EDO	AAA	403	4/4	0.94	0.11	55,58,59,65	0
3	EDO	DDD	402	4/4	0.94	0.10	50,54,56,58	0
3	EDO	CCC	408	4/4	0.95	0.09	38,43,44,45	0
3	EDO	AAA	402	4/4	0.95	0.09	48,50,51,52	0
3	EDO	BBB	405	4/4	0.96	0.09	42,43,49,51	0
2	XTQ	DDD	401	24/24	0.97	0.06	30,33,37,40	0
2	XTQ	AAA	401	24/24	0.97	0.06	24,28,31,34	0
2	XTQ	CCC	401	24/24	0.97	0.06	27,29,33,35	0
2	XTQ	BBB	401	24/24	0.98	0.05	23,27,32,34	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.

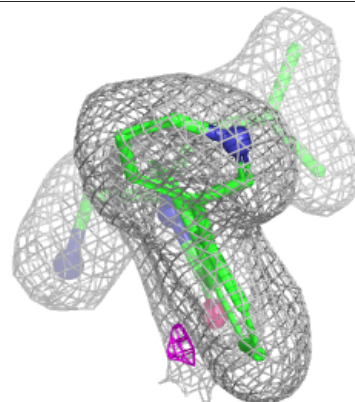
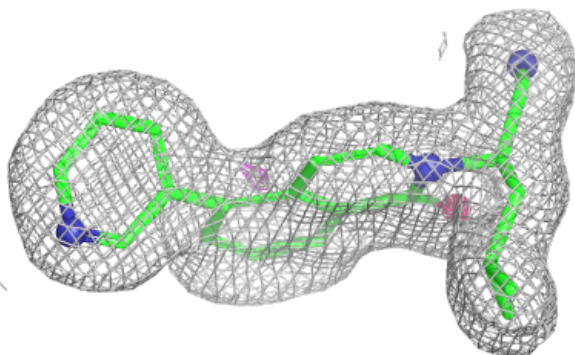
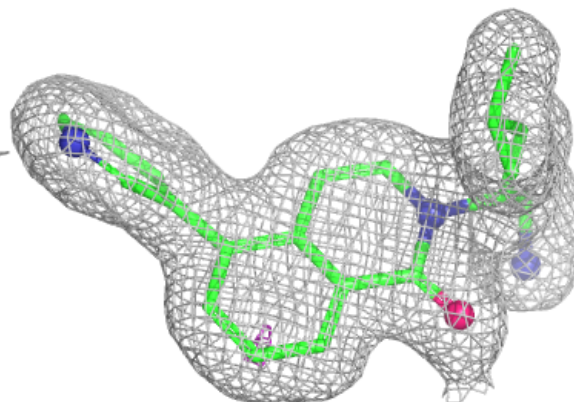
Electron density around XTQ DDD 401:

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

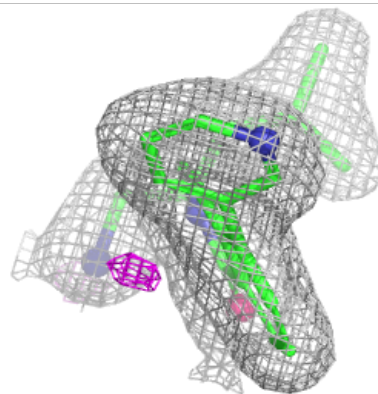
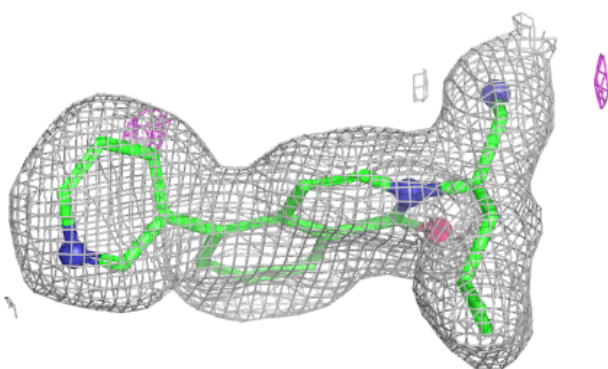
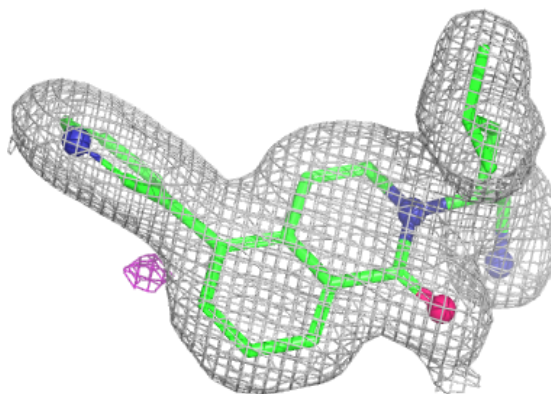


Electron density around XTQ AAA 401:

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

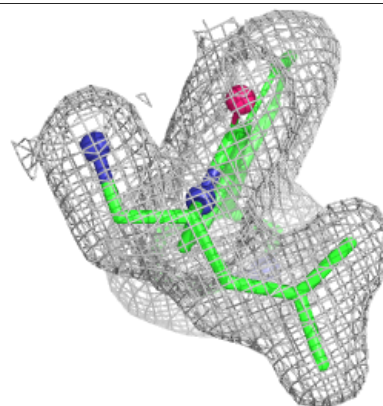
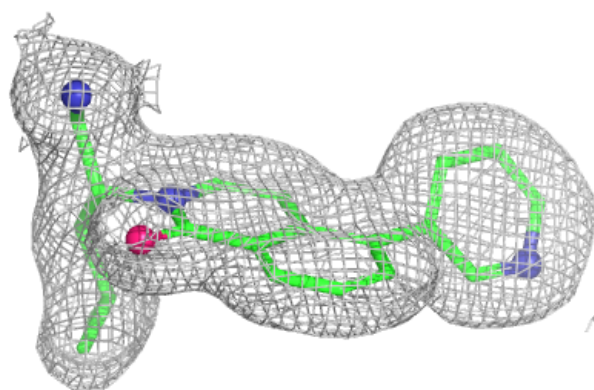
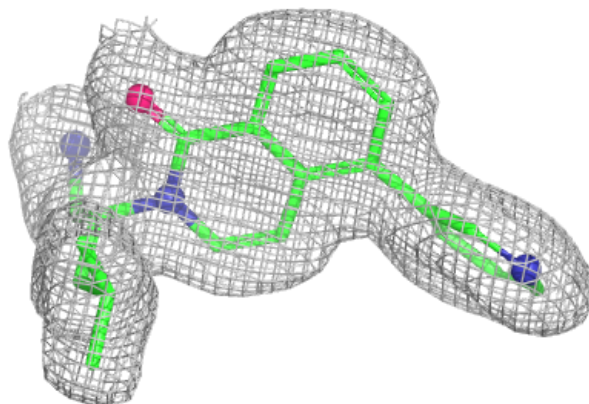
**Electron density around XTQ CCC 401:**

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



Electron density around XTQ BBB 401:

$2mF_o-DF_c$ (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.