



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:51 AM UTC

PDB ID : 8F97 / pdb_00008f97
Title : Compound 5 bound to procaspase-6
Authors : Fan, P.; Zhao, Y.; Renslo, A.R.; Arkin, M.R.
Deposited on : 2022-11-23
Resolution : 2.32 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

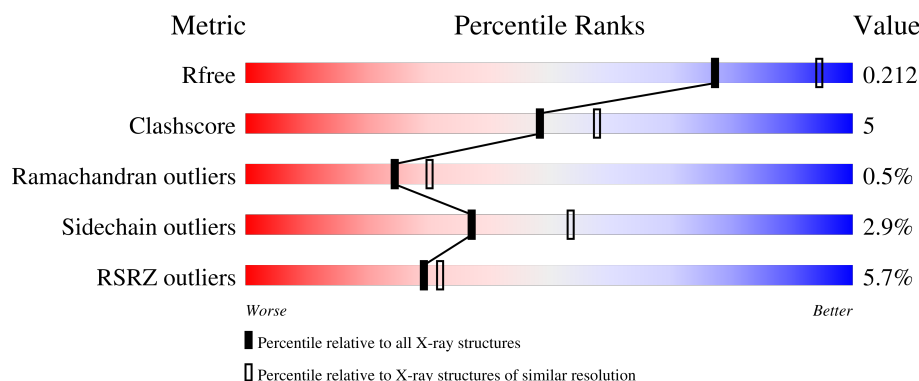
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	299	4% 71% 10% • 18%
1	B	299	4% 71% 10% • 18%
1	C	299	6% 75% 10% 15%
1	D	299	5% 74% 10% 15%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XM6	C	301[A]	-	-	-	X
2	XM6	C	301[B]	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8603 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 Procaspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	2	0
			1975	1260	342	357	16			
1	B	244	Total	C	N	O	S	0	2	0
			1967	1256	340	355	16			
1	C	254	Total	C	N	O	S	0	1	0
			2054	1309	358	373	14			
1	D	253	Total	C	N	O	S	0	0	0
			2042	1302	354	372	14			

There are 28 discrepancies between the modelled and reference sequences:

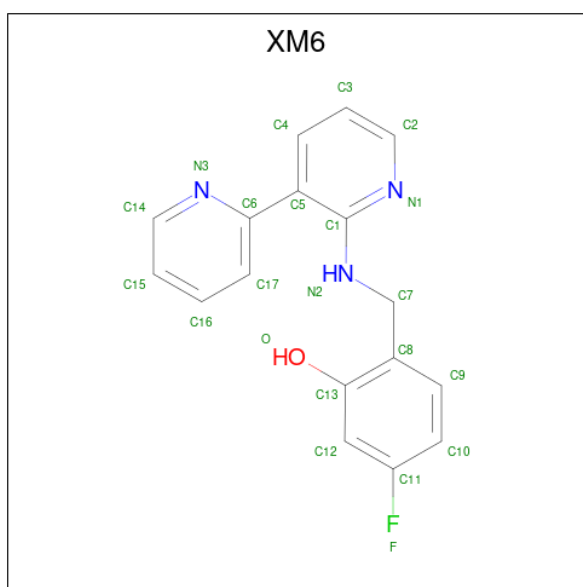
Chain	Residue	Modelled	Actual	Comment	Reference
A	163	ALA	CYS	conflict	UNP P55212
A	294	GLU	-	expression tag	UNP P55212
A	295	ASN	-	expression tag	UNP P55212
A	296	LEU	-	expression tag	UNP P55212
A	297	TYR	-	expression tag	UNP P55212
A	298	PHE	-	expression tag	UNP P55212
A	299	GLN	-	expression tag	UNP P55212
B	163	ALA	CYS	conflict	UNP P55212
B	294	GLU	-	expression tag	UNP P55212
B	295	ASN	-	expression tag	UNP P55212
B	296	LEU	-	expression tag	UNP P55212
B	297	TYR	-	expression tag	UNP P55212
B	298	PHE	-	expression tag	UNP P55212
B	299	GLN	-	expression tag	UNP P55212
C	163	ALA	CYS	conflict	UNP P55212
C	294	GLU	-	expression tag	UNP P55212
C	295	ASN	-	expression tag	UNP P55212
C	296	LEU	-	expression tag	UNP P55212
C	297	TYR	-	expression tag	UNP P55212
C	298	PHE	-	expression tag	UNP P55212
C	299	GLN	-	expression tag	UNP P55212

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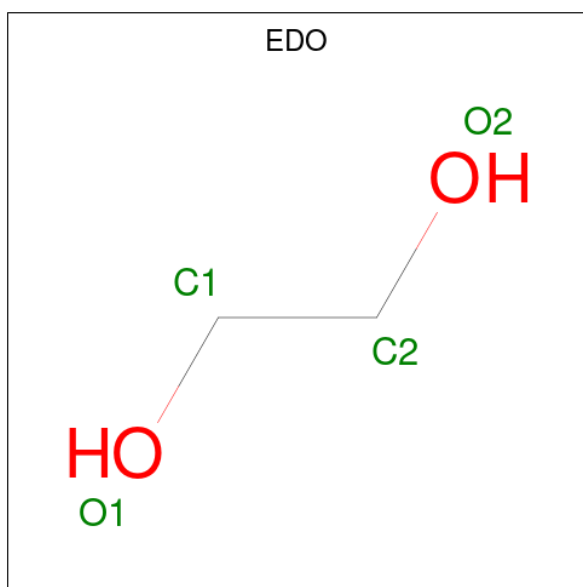
Chain	Residue	Modelled	Actual	Comment	Reference
D	163	ALA	CYS	conflict	UNP P55212
D	294	GLU	-	expression tag	UNP P55212
D	295	ASN	-	expression tag	UNP P55212
D	296	LEU	-	expression tag	UNP P55212
D	297	TYR	-	expression tag	UNP P55212
D	298	PHE	-	expression tag	UNP P55212
D	299	GLN	-	expression tag	UNP P55212

- Molecule 2 is 2-([[(2M)-[2,3'-bipyridin]-2'-yl]amino}methyl)-5-fluorophenol (CCD ID: XM6) (formula: C₁₇H₁₄FN₃O) (labeled as "Ligand of Interest" by depositor).



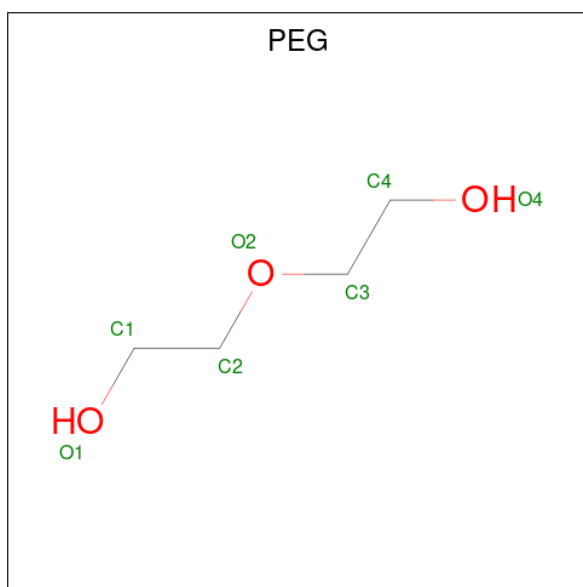
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	1
			44	34	2	6	2		
2	C	1	Total	C	F	N	O	0	1
			44	34	2	6	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

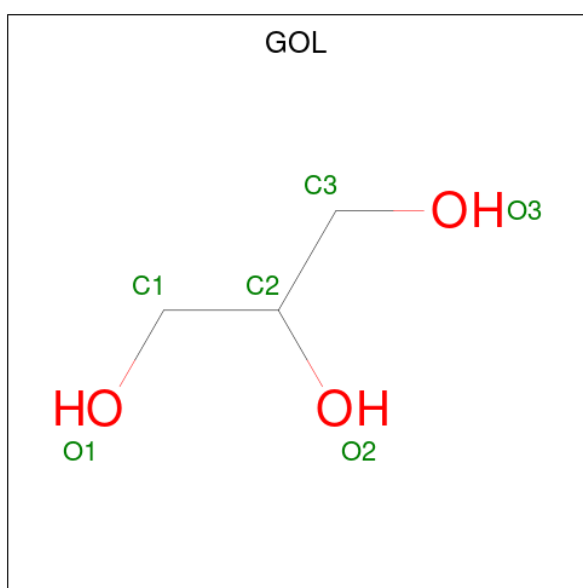


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		

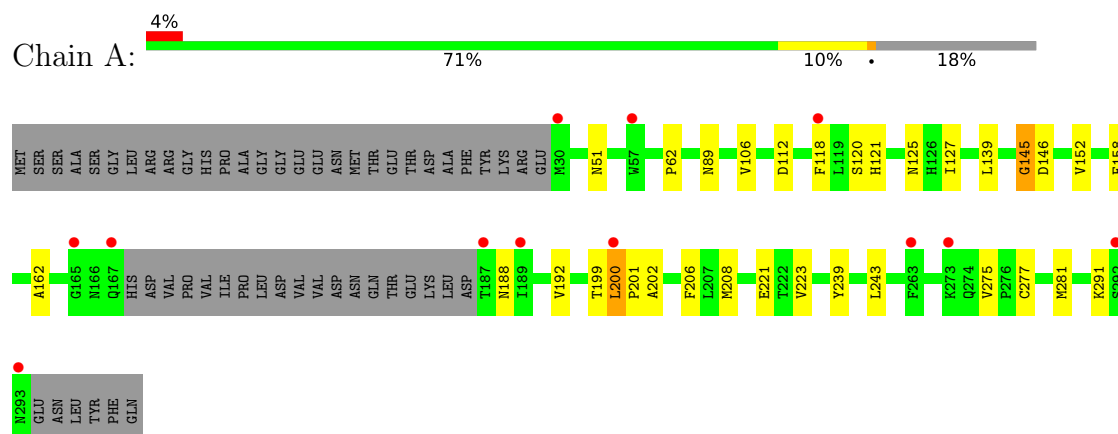
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	114	Total	O	0	0
			114	114		
7	B	109	Total	O	0	0
			109	109		
7	C	106	Total	O	0	0
			106	106		
7	D	106	Total	O	0	0
			106	106		

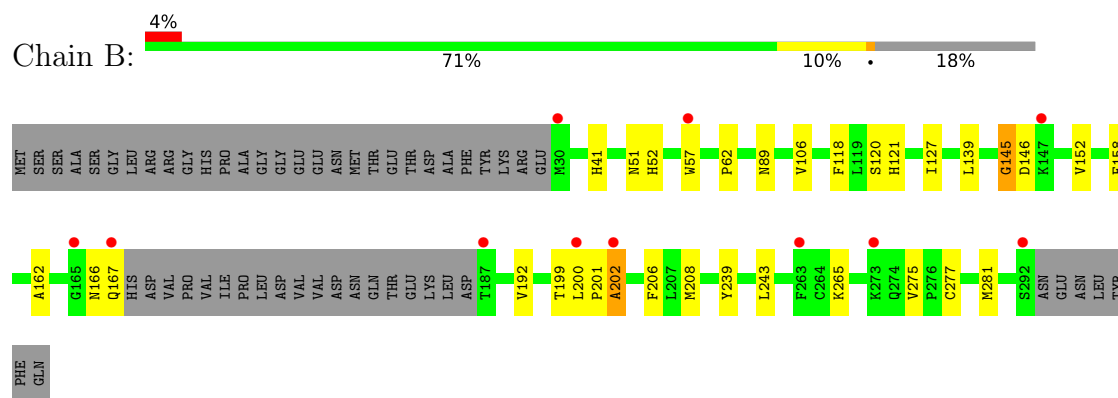
3 Residue-property plots [i](#)

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.

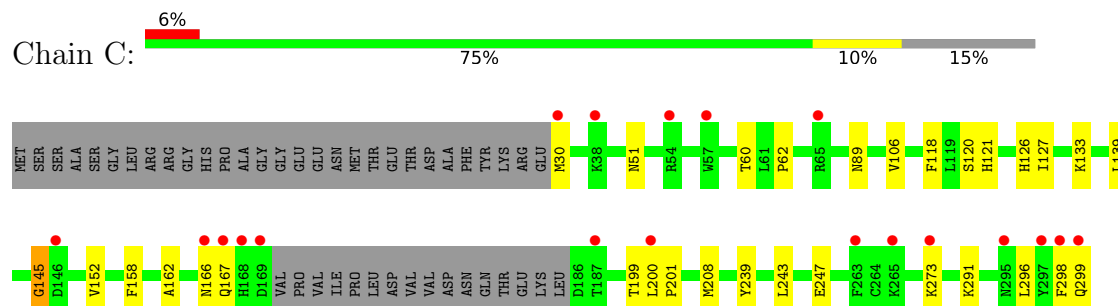
• Molecule 1: Procaspase-6



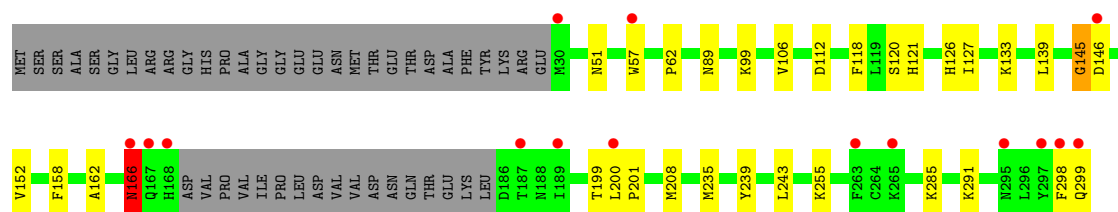
• Molecule 1: Procaspase-6



• Molecule 1: Procaspase-6



Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	102.66Å 102.66Å 322.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.96 – 2.32 48.96 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.96-2.32) 99.9 (48.96-2.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.179 , 0.210 0.184 , 0.212	Depositor DCC
R_{free} test set	4035 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.489 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8603	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: EDO, XM6, CL, GOL, PEG

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	0.98	0/2026	1.30	0/2727
1	B	0.98	0/2018	1.30	1/2716 (0.0%)
1	C	0.98	0/2105	1.32	0/2834
1	D	0.98	0/2090	1.31	0/2815
All	All	0.98	0/8239	1.30	1/11092 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ALA	CA-C-O	-5.98	116.36	119.77

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	1975	0	1950	33	0
1	B	1967	0	1944	27	0
1	C	2054	0	2010	16	0
1	D	2042	0	1996	22	0
2	A	44	0	0	2	0
2	C	44	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	6	0	0
3	B	8	0	12	1	0
3	C	12	0	18	1	0
3	D	4	0	6	1	0
4	B	7	0	10	0	0
5	D	1	0	0	0	0
6	D	6	0	8	2	0
7	A	114	0	0	2	0
7	B	109	0	0	2	0
7	C	106	0	0	0	0
7	D	106	0	0	2	0
All	All	8603	0	7960	88	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 5.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ASN:ND2	7:D:401:HOH:O	2.20	0.75
1:A:201:PRO:HB2	1:A:281[B]:MET:SD	2.29	0.72
1:B:201:PRO:HB2	1:B:281[B]:MET:SD	2.30	0.70
1:A:188:ASN:HD22	1:A:223:VAL:H	1.36	0.70
1:B:201:PRO:CB	1:B:281[B]:MET:SD	2.81	0.69
1:A:188:ASN:ND2	1:A:223:VAL:H	1.93	0.67
1:A:201:PRO:CB	1:A:281[B]:MET:SD	2.82	0.67
1:A:281[A]:MET:HE2	1:B:275:VAL:CG1	2.26	0.66
1:D:112:ASP:OD2	1:D:291:LYS:CE	2.44	0.66
1:A:112:ASP:OD2	1:A:291:LYS:CE	2.44	0.64
1:A:199:THR:OG1	1:B:201:PRO:HD3	1.98	0.63
1:D:145:GLY:HA2	1:D:152:VAL:HG22	1.81	0.62
1:A:112:ASP:OD2	1:A:291:LYS:HE2	1.99	0.62
1:C:145:GLY:HA2	1:C:152:VAL:HG22	1.80	0.62
1:A:281[A]:MET:HE2	1:B:275:VAL:HG11	1.80	0.62
1:A:201:PRO:HD3	1:B:199:THR:OG1	1.99	0.62
1:D:112:ASP:OD2	1:D:291:LYS:HE2	1.99	0.61
1:A:275:VAL:CG1	1:B:281[A]:MET:HE2	2.32	0.60
1:B:145:GLY:HA2	1:B:152:VAL:HG22	1.84	0.59
1:A:145:GLY:HA2	1:A:152:VAL:HG22	1.87	0.56
1:A:188:ASN:HD21	1:A:221:GLU:HB3	1.70	0.56
1:A:275:VAL:HG11	1:B:281[A]:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:HD2	7:A:494:HOH:O	1.89	0.55
1:D:51:ASN:HD22	1:D:89:ASN:HD22	1.56	0.54
1:C:51:ASN:HD22	1:C:89:ASN:HD22	1.56	0.54
1:A:202:ALA:H	1:A:281[B]:MET:HE3	1.72	0.54
1:D:57:TRP:HB3	3:D:301:EDO:H12	1.90	0.53
1:C:60:THR:O	1:C:167:GLN:HG2	2.09	0.53
1:C:247:GLU:OE2	1:D:285:LYS:HE3	2.10	0.52
1:A:281[A]:MET:CE	1:B:275:VAL:CG1	2.88	0.51
1:B:41:HIS:HE1	7:B:501:HOH:O	1.93	0.51
1:B:202:ALA:H	1:B:281[B]:MET:HE3	1.75	0.51
2:C:301[B]:XM6:N2	2:C:301[B]:XM6:N3	2.58	0.51
1:D:121:HIS:HD2	7:D:477:HOH:O	1.92	0.51
1:A:51:ASN:HD22	1:A:89:ASN:HD22	1.59	0.50
1:B:51:ASN:HD22	1:B:89:ASN:HD22	1.58	0.50
1:B:201:PRO:HB3	1:B:281[B]:MET:SD	2.52	0.49
1:C:62:PRO:O	1:C:121:HIS:HE1	1.95	0.49
1:D:298:PHE:O	1:D:299:GLN:HB2	2.12	0.49
1:D:291:LYS:NZ	6:D:303:GOL:H11	2.28	0.49
1:D:62:PRO:O	1:D:121:HIS:HE1	1.95	0.49
1:D:291:LYS:HZ2	6:D:303:GOL:H11	1.77	0.49
1:C:199:THR:OG1	1:D:201:PRO:HD3	2.13	0.49
1:C:291:LYS:NZ	3:C:304:EDO:H22	2.28	0.49
1:B:62:PRO:O	1:B:121:HIS:HE1	1.96	0.48
1:C:120:SER:O	1:C:162:ALA:HA	2.13	0.48
2:A:301[B]:XM6:N2	2:A:301[B]:XM6:N3	2.61	0.48
2:A:301[A]:XM6:N2	2:A:301[A]:XM6:N3	2.61	0.48
1:C:51:ASN:HD22	1:C:89:ASN:ND2	2.11	0.48
1:A:62:PRO:O	1:A:121:HIS:HE1	1.96	0.48
1:B:158:PHE:HB2	1:B:208:MET:SD	2.54	0.48
1:C:298:PHE:O	1:C:299:GLN:HB2	2.12	0.48
1:A:120:SER:O	1:A:162:ALA:HA	2.13	0.48
1:D:120:SER:O	1:D:162:ALA:HA	2.13	0.48
1:B:120:SER:O	1:B:162:ALA:HA	2.13	0.48
1:A:158:PHE:HB2	1:A:208:MET:SD	2.54	0.47
1:C:201:PRO:HD3	1:D:199:THR:OG1	2.14	0.47
1:D:51:ASN:HD22	1:D:89:ASN:ND2	2.11	0.47
1:D:158:PHE:HB2	1:D:208:MET:SD	2.55	0.47
1:C:158:PHE:HB2	1:C:208:MET:SD	2.55	0.47
1:A:201:PRO:HB3	1:A:281[B]:MET:SD	2.55	0.47
1:B:51:ASN:HD22	1:B:89:ASN:ND2	2.12	0.46
1:B:57:TRP:HB3	3:B:302:EDO:H22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301[A]:XM6:N2	2:C:301[A]:XM6:N3	2.62	0.46
1:A:51:ASN:HD22	1:A:89:ASN:ND2	2.13	0.46
1:B:206:PHE:O	1:B:281[B]:MET:HE2	2.17	0.45
1:D:99:LYS:HA	1:D:99:LYS:HE3	1.97	0.45
1:D:118:PHE:CZ	1:D:139:LEU:HD13	2.51	0.45
1:C:118:PHE:CZ	1:C:139:LEU:HD13	2.51	0.45
1:A:281[B]:MET:HG3	1:B:277:CYS:HB3	1.99	0.44
1:D:239:TYR:HB3	1:D:243:LEU:HD22	1.99	0.44
1:B:52:HIS:HD2	7:B:424:HOH:O	2.00	0.44
1:A:239:TYR:HB3	1:A:243:LEU:HD22	1.99	0.44
1:A:188:ASN:HD22	1:A:223:VAL:N	2.08	0.43
1:B:239:TYR:HB3	1:B:243:LEU:HD22	1.99	0.43
1:C:126:HIS:HB3	1:C:133:LYS:HB2	2.00	0.43
1:C:239:TYR:HB3	1:C:243:LEU:HD22	2.00	0.43
1:A:275:VAL:CG1	1:B:281[A]:MET:CE	2.96	0.43
1:A:281[A]:MET:CE	1:B:275:VAL:HG12	2.49	0.43
1:D:126:HIS:HB3	1:D:133:LYS:HB2	2.00	0.42
1:A:277:CYS:HB3	1:B:281[B]:MET:HG3	2.00	0.42
1:B:118:PHE:CZ	1:B:139:LEU:HD13	2.55	0.41
1:C:30:MET:HE2	1:C:30:MET:HB2	1.96	0.41
1:A:206:PHE:O	1:A:281[B]:MET:HE2	2.20	0.41
1:A:118:PHE:CZ	1:A:139:LEU:HD13	2.56	0.41
1:A:121:HIS:CD2	7:A:494:HOH:O	2.68	0.40
1:D:235:MET:HE3	1:D:255:LYS:HE3	2.03	0.40
1:A:200:LEU:H	1:A:200:LEU:HG	1.75	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	243/299 (81%)	233 (96%)	9 (4%)	1 (0%)	30 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	242/299 (81%)	232 (96%)	9 (4%)	1 (0%)	30	37
1	C	251/299 (84%)	240 (96%)	10 (4%)	1 (0%)	30	37
1	D	249/299 (83%)	239 (96%)	8 (3%)	2 (1%)	16	19
All	All	985/1196 (82%)	944 (96%)	36 (4%)	5 (0%)	24	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	GLY
1	C	145	GLY
1	D	145	GLY
1	A	145	GLY
1	D	166	ASN

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	215/260 (83%)	209 (97%)	6 (3%)	38	55
1	B	214/260 (82%)	206 (96%)	8 (4%)	30	44
1	C	222/260 (85%)	216 (97%)	6 (3%)	39	56
1	D	221/260 (85%)	216 (98%)	5 (2%)	44	62
All	All	872/1040 (84%)	847 (97%)	25 (3%)	37	53

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	VAL
1	A	125	ASN
1	A	127	ILE
1	A	146	ASP
1	A	192	VAL
1	A	200	LEU

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Mol	Chain	Res	Type
1	B	106	VAL
1	B	127	ILE
1	B	146	ASP
1	B	166	ASN
1	B	167	GLN
1	B	192	VAL
1	B	200	LEU
1	B	265	LYS
1	C	106	VAL
1	C	127	ILE
1	C	166	ASN
1	C	200	LEU
1	C	273	LYS
1	C	296	LEU
1	D	106	VAL
1	D	127	ILE
1	D	146	ASP
1	D	166	ASN
1	D	200	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	52	HIS
1	A	89	ASN
1	A	101	HIS
1	A	121	HIS
1	A	161	GLN
1	A	166	ASN
1	A	188	ASN
1	A	224	ASN
1	A	230	GLN
1	B	41	HIS
1	B	58	HIS
1	B	89	ASN
1	B	101	HIS
1	B	121	HIS
1	B	224	ASN
1	B	230	GLN
1	B	287	HIS
1	C	41	HIS

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Mol	Chain	Res	Type
1	C	89	ASN
1	C	101	HIS
1	C	121	HIS
1	C	167	GLN
1	C	224	ASN
1	C	230	GLN
1	C	293	ASN
1	C	295	ASN
1	D	41	HIS
1	D	52	HIS
1	D	89	ASN
1	D	121	HIS
1	D	166	ASN
1	D	230	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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
6	GOL	D	303	-	5,5,5	0.14	0	5,5,5	0.59	0
2	XM6	C	301[A]	-	24,24,24	1.57	3 (12%)	31,32,32	2.01	10 (32%)
3	EDO	B	301	-	3,3,3	0.05	0	2,2,2	0.17	0
3	EDO	C	304	-	3,3,3	0.23	0	2,2,2	0.78	0
3	EDO	C	303	-	3,3,3	0.12	0	2,2,2	0.15	0
3	EDO	D	301	-	3,3,3	0.04	0	2,2,2	0.21	0
2	XM6	A	301[B]	-	24,24,24	1.37	2 (8%)	31,32,32	1.90	8 (25%)
3	EDO	A	302	-	3,3,3	0.40	0	2,2,2	0.48	0
3	EDO	C	302	-	3,3,3	0.17	0	2,2,2	0.14	0
2	XM6	A	301[A]	-	24,24,24	1.43	2 (8%)	31,32,32	1.79	6 (19%)
3	EDO	B	302	-	3,3,3	0.09	0	2,2,2	0.21	0
4	PEG	B	303	-	6,6,6	0.30	0	5,5,5	0.23	0
2	XM6	C	301[B]	-	24,24,24	1.51	3 (12%)	31,32,32	1.88	7 (22%)

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
6	GOL	D	303	-	-	2/4/4/4	-
2	XM6	C	301[A]	-	-	0/9/9/9	0/3/3/3
3	EDO	B	301	-	-	1/1/1/1	-
3	EDO	C	304	-	-	1/1/1/1	-
3	EDO	C	303	-	-	0/1/1/1	-
3	EDO	D	301	-	-	1/1/1/1	-
2	XM6	A	301[B]	-	-	0/9/9/9	0/3/3/3
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	C	302	-	-	1/1/1/1	-
2	XM6	A	301[A]	-	-	0/9/9/9	0/3/3/3
3	EDO	B	302	-	-	1/1/1/1	-
4	PEG	B	303	-	-	1/4/4/4	-
2	XM6	C	301[B]	-	-	0/9/9/9	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[A]	XM6	C1-N2	4.65	1.41	1.34
2	C	301[A]	XM6	C1-N2	4.47	1.41	1.34
2	C	301[B]	XM6	C1-N2	4.44	1.41	1.34
2	A	301[B]	XM6	C1-N2	4.35	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[A]	XM6	C10-C11	3.95	1.44	1.37
2	C	301[B]	XM6	C10-C11	3.56	1.44	1.37
2	A	301[B]	XM6	C10-C11	2.91	1.42	1.37
2	C	301[A]	XM6	C9-C10	2.60	1.43	1.38
2	A	301[A]	XM6	C10-C11	2.30	1.41	1.37
2	C	301[B]	XM6	C9-C10	2.28	1.42	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301[A]	XM6	C5-C1-N2	-5.11	118.76	121.81
2	C	301[A]	XM6	F-C11-C10	5.10	126.73	118.55
2	A	301[B]	XM6	C5-C1-N2	-4.97	118.84	121.81
2	C	301[B]	XM6	C5-C1-N2	-4.62	119.06	121.81
2	C	301[A]	XM6	C5-C1-N2	-4.29	119.25	121.81
2	C	301[B]	XM6	F-C11-C10	3.68	124.45	118.55
2	A	301[B]	XM6	C14-N3-C6	3.60	122.28	117.24
2	A	301[B]	XM6	F-C11-C10	3.49	124.14	118.55
2	A	301[B]	XM6	F-C11-C12	-3.39	113.47	118.28
2	C	301[A]	XM6	C10-C11-C12	-3.38	118.77	123.23
2	C	301[B]	XM6	C7-N2-C1	-3.29	118.82	123.08
2	A	301[A]	XM6	C14-N3-C6	3.09	121.56	117.24
2	C	301[B]	XM6	C10-C11-C12	-3.01	119.26	123.23
2	C	301[A]	XM6	C4-C5-C1	2.79	119.43	117.46
2	C	301[B]	XM6	C4-C5-C1	2.74	119.39	117.46
2	A	301[B]	XM6	C9-C8-C13	2.73	121.12	118.16
2	C	301[A]	XM6	F-C11-C12	-2.66	114.50	118.28
2	C	301[A]	XM6	C14-N3-C6	2.64	120.93	117.24
2	A	301[A]	XM6	C15-C16-C17	-2.60	117.03	120.24
2	C	301[B]	XM6	C14-N3-C6	2.54	120.80	117.24
2	C	301[A]	XM6	C9-C10-C11	2.50	120.94	118.38
2	A	301[B]	XM6	C10-C9-C8	-2.47	118.16	121.39
2	C	301[B]	XM6	C15-C16-C17	-2.44	117.23	120.24
2	A	301[A]	XM6	C7-N2-C1	-2.35	120.04	123.08
2	A	301[B]	XM6	C15-C14-N3	-2.25	119.85	123.42
2	A	301[A]	XM6	F-C11-C12	-2.18	115.19	118.28
2	C	301[A]	XM6	C2-N1-C1	2.16	120.94	116.74
2	C	301[A]	XM6	C12-C13-C8	2.10	123.34	120.75
2	A	301[A]	XM6	C9-C8-C13	2.09	120.43	118.16
2	C	301[A]	XM6	C15-C16-C17	-2.08	117.68	120.24
2	A	301[B]	XM6	C2-N1-C1	2.02	120.66	116.74

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	303	GOL	C1-C2-C3-O3
4	B	303	PEG	O1-C1-C2-O2
6	D	303	GOL	O2-C2-C3-O3
3	B	302	EDO	O1-C1-C2-O2
3	D	301	EDO	O1-C1-C2-O2
3	C	304	EDO	O1-C1-C2-O2
3	B	301	EDO	O1-C1-C2-O2
3	C	302	EDO	O1-C1-C2-O2

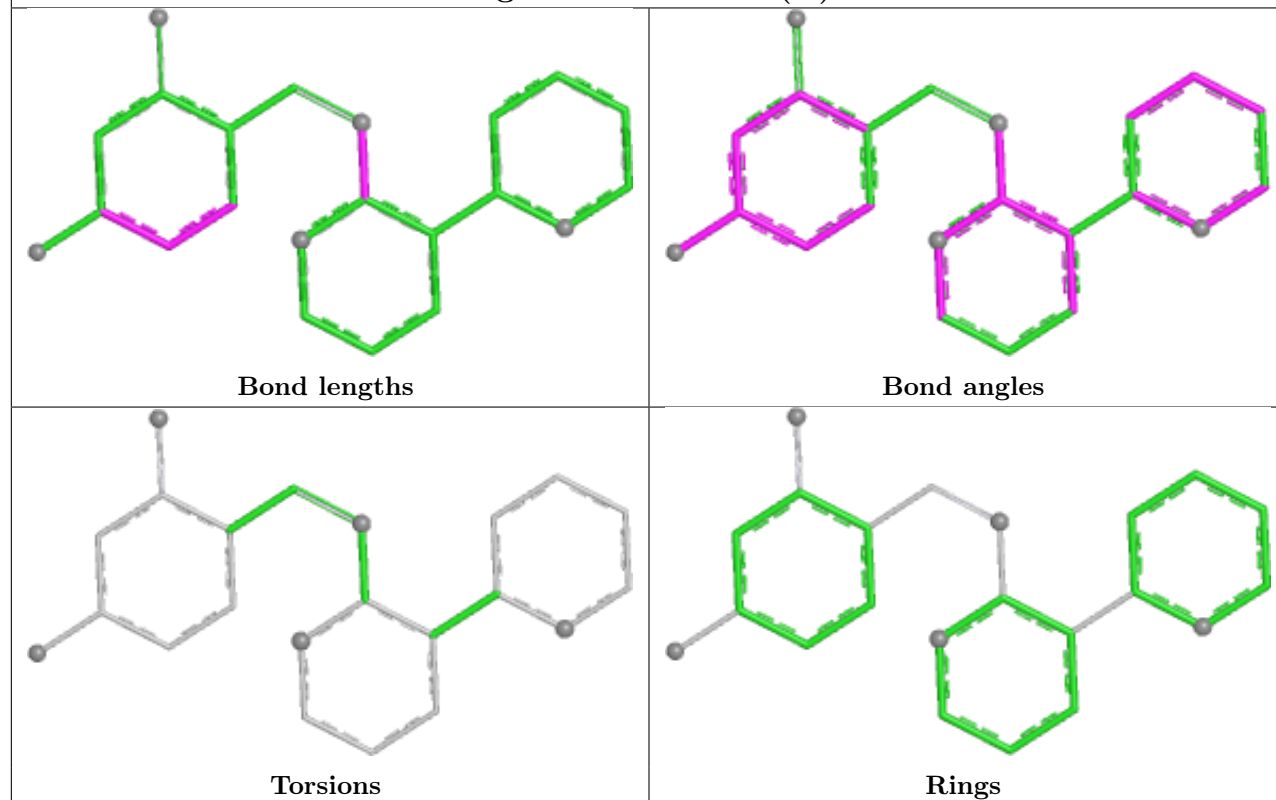
There are no ring outliers.

8 monomers are involved in 9 short contacts:

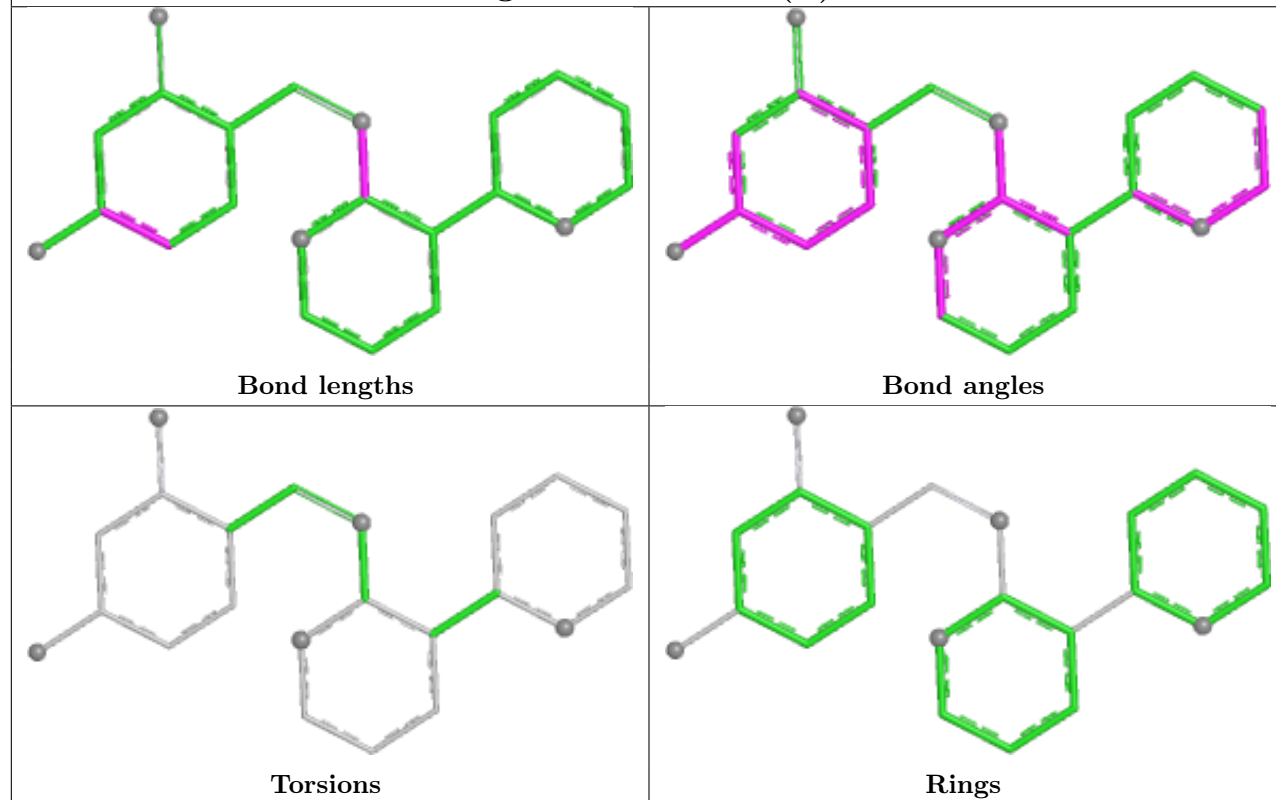
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	303	GOL	2	0
2	C	301[A]	XM6	1	0
3	C	304	EDO	1	0
3	D	301	EDO	1	0
2	A	301[B]	XM6	1	0
2	A	301[A]	XM6	1	0
3	B	302	EDO	1	0
2	C	301[B]	XM6	1	0

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.

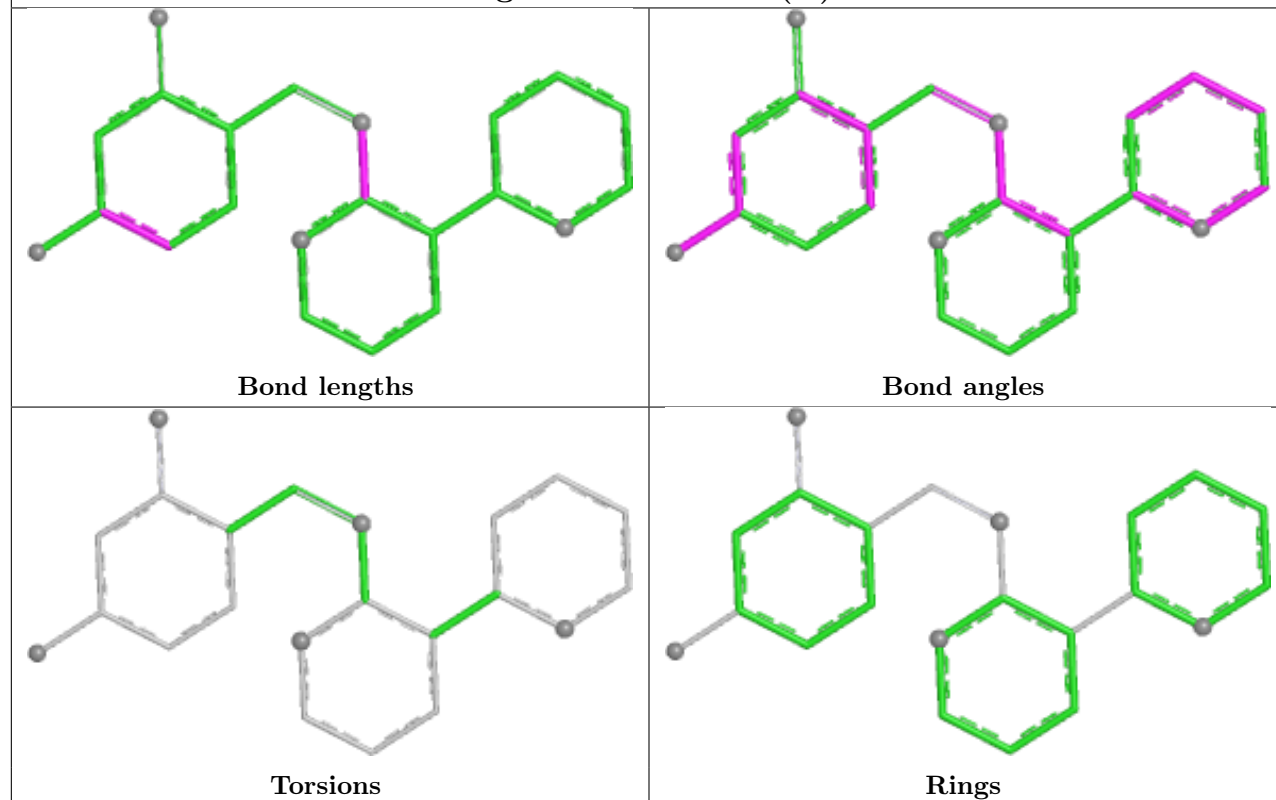
Ligand XM6 C 301 (A)



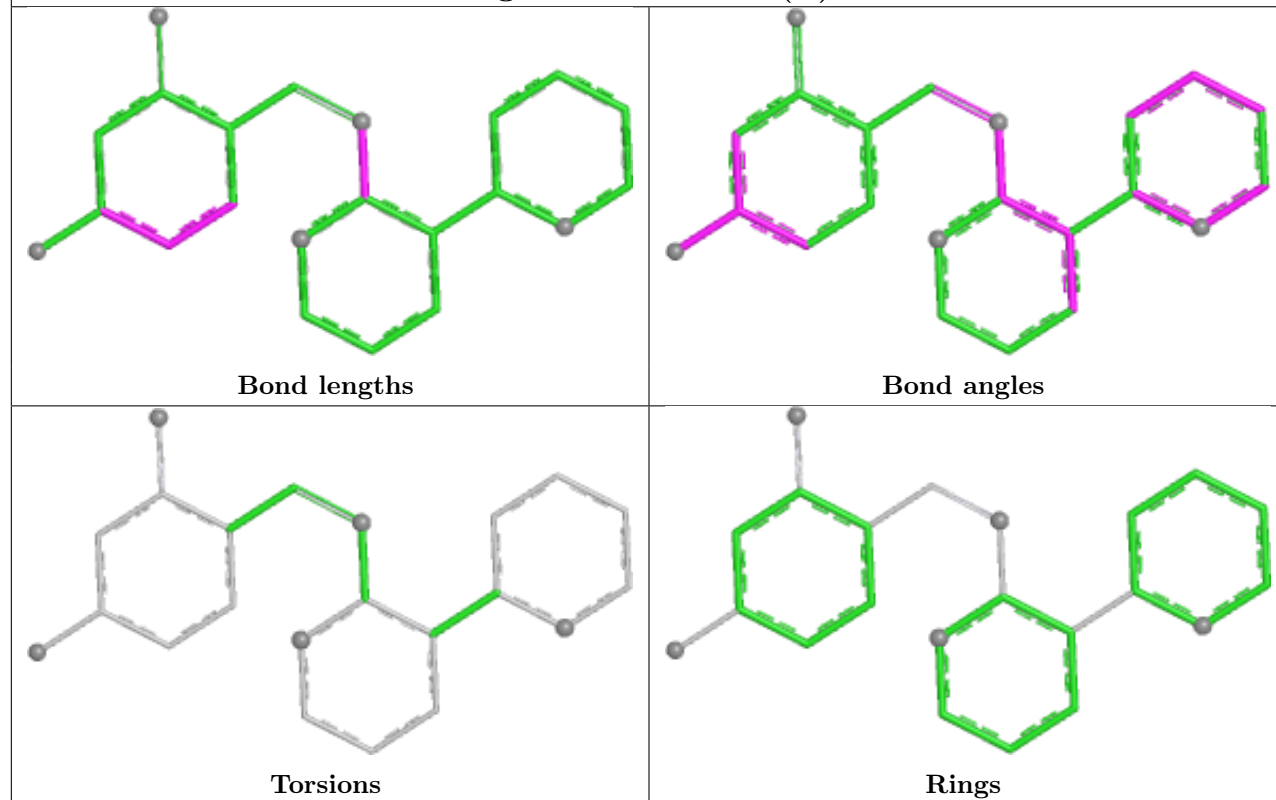
Ligand XM6 A 301 (B)



Ligand XM6 A 301 (A)



Ligand XM6 C 301 (B)



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	245/299 (81%)	0.18	12 (4%) 35 37	32, 61, 104, 152	2 (0%)
1	B	244/299 (81%)	0.16	11 (4%) 38 40	32, 61, 103, 140	2 (0%)
1	C	254/299 (84%)	0.25	19 (7%) 20 23	46, 62, 115, 179	1 (0%)
1	D	253/299 (84%)	0.21	15 (5%) 28 31	49, 62, 114, 172	0
All	All	996/1196 (83%)	0.20	57 (5%) 29 32	32, 61, 111, 179	5 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169	ASP	5.8
1	B	30	MET	5.3
1	D	168	HIS	4.9
1	C	200	LEU	4.8
1	A	30	MET	4.6
1	D	200	LEU	4.4
1	D	30	MET	4.4
1	A	187	THR	4.2
1	B	187	THR	4.1
1	C	30	MET	4.1
1	B	292	SER	4.0
1	D	298	PHE	3.9
1	C	168	HIS	3.9
1	A	263	PHE	3.8
1	C	298	PHE	3.6
1	D	263	PHE	3.6
1	B	57	TRP	3.5
1	B	200	LEU	3.5
1	D	187	THR	3.4
1	C	263	PHE	3.3
1	A	57	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	167	GLN	3.0
1	C	38	LYS	3.0
1	D	57	TRP	3.0
1	A	200	LEU	2.9
1	B	263	PHE	2.9
1	C	57	TRP	2.9
1	C	187	THR	2.9
1	D	189	ILE	2.8
1	D	265	LYS	2.8
1	A	273	LYS	2.7
1	D	299	GLN	2.7
1	A	167	GLN	2.7
1	D	295	ASN	2.5
1	C	167	GLN	2.5
1	B	165	GLY	2.4
1	A	292	SER	2.4
1	D	297	TYR	2.4
1	C	166	ASN	2.4
1	C	299	GLN	2.4
1	A	189	ILE	2.4
1	A	293	ASN	2.3
1	C	265	LYS	2.3
1	C	273	LYS	2.3
1	D	166	ASN	2.3
1	B	202	ALA	2.2
1	C	297	TYR	2.2
1	C	295	ASN	2.2
1	A	118	PHE	2.2
1	D	146	ASP	2.1
1	C	54[A]	ARG	2.1
1	B	147	LYS	2.1
1	C	146	ASP	2.1
1	B	273	LYS	2.1
1	C	65	ARG	2.0
1	A	165	GLY	2.0
1	D	167	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

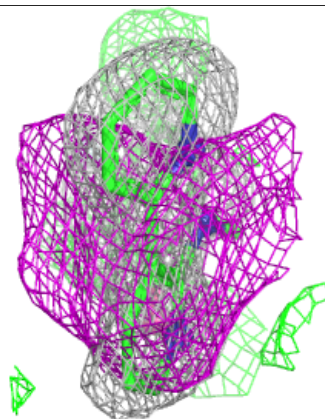
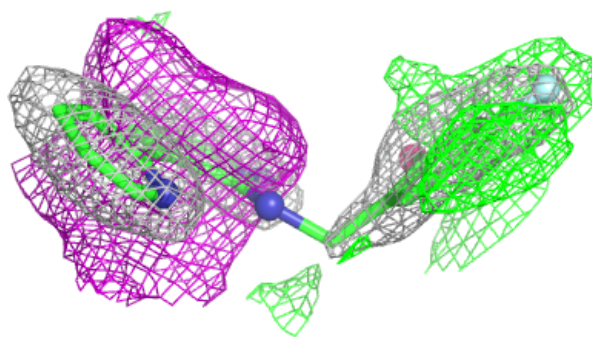
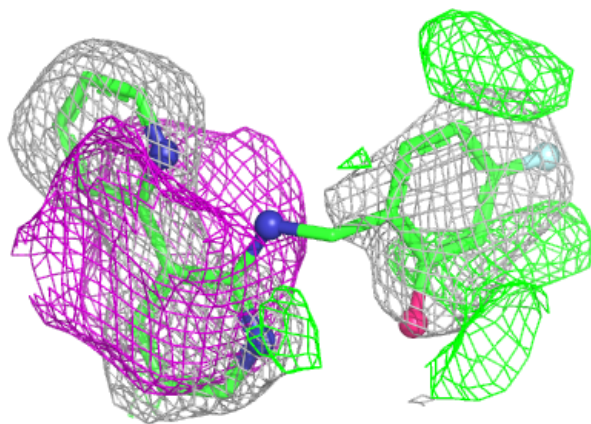
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	XM6	A	301[A]	22/22	0.64	0.36	45,64,73,75	22
2	XM6	A	301[B]	22/22	0.64	0.36	45,70,81,86	22
2	XM6	C	301[A]	22/22	0.64	0.42	47,96,114,119	22
2	XM6	C	301[B]	22/22	0.64	0.42	47,84,100,105	22
3	EDO	A	302	4/4	0.78	0.28	86,104,107,108	0
3	EDO	D	301	4/4	0.80	0.22	104,107,114,117	0
3	EDO	B	301	4/4	0.81	0.26	97,99,105,106	0
3	EDO	C	304	4/4	0.86	0.26	83,84,90,101	0
3	EDO	C	303	4/4	0.86	0.17	103,109,109,110	0
4	PEG	B	303	7/7	0.87	0.26	112,120,130,136	0
3	EDO	C	302	4/4	0.90	0.16	84,92,100,104	0
6	GOL	D	303	6/6	0.90	0.18	86,92,97,117	0
3	EDO	B	302	4/4	0.91	0.15	109,113,113,115	0
5	CL	D	302	1/1	0.94	0.10	86,86,86,86	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.

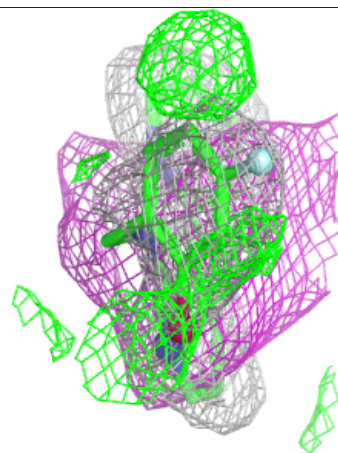
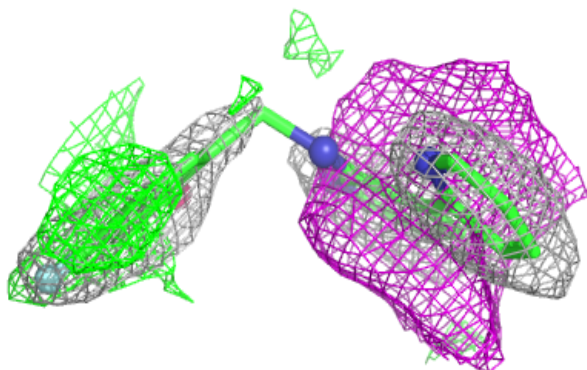
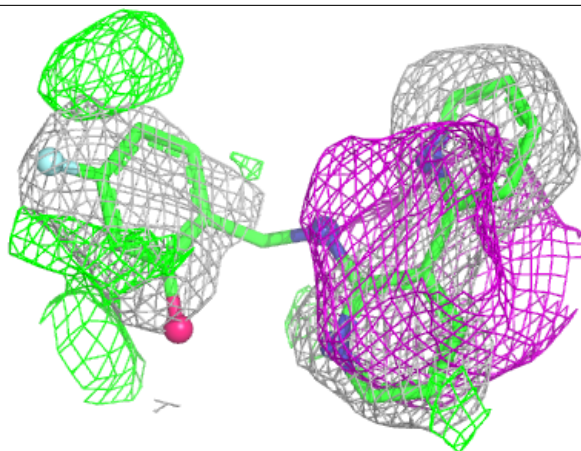
Electron density around XM6 A 301 (A):

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



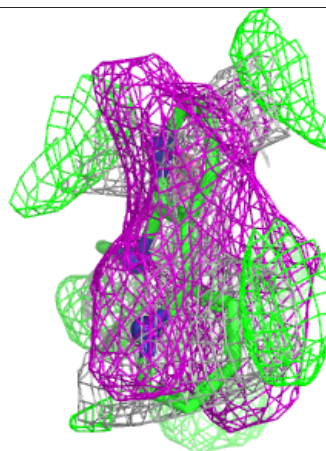
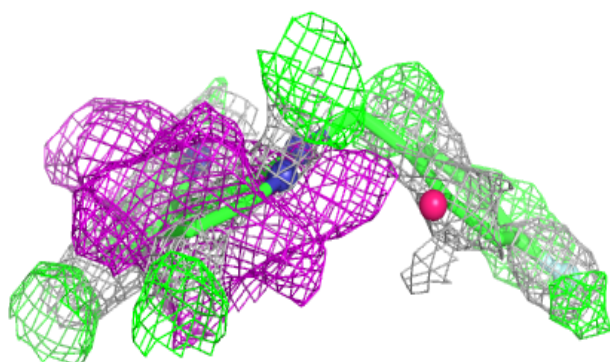
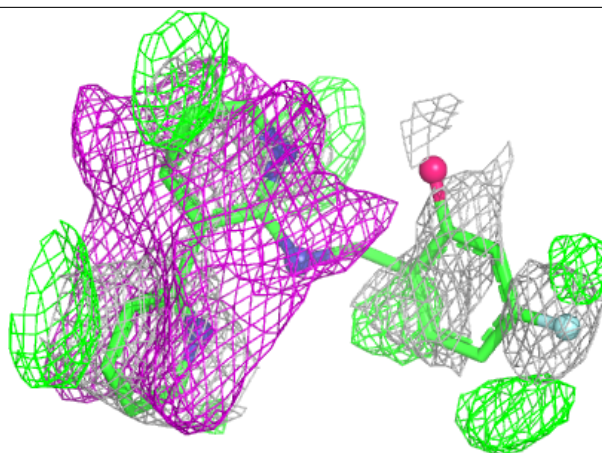
Electron density around XM6 A 301 (B):

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



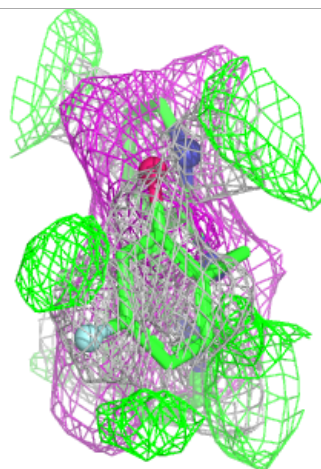
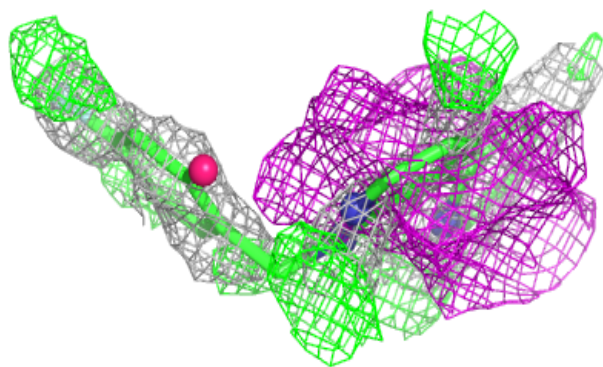
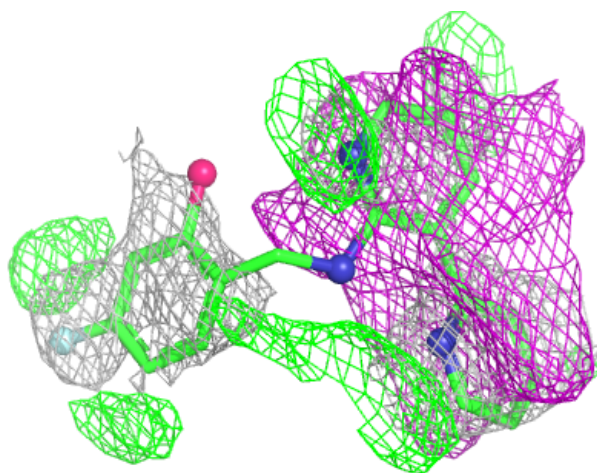
Electron density around XM6 C 301 (A):

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



Electron density around XM6 C 301 (B):

$2mF_o-DF_c$ (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.