



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:34 PM UTC

PDB ID : 6GO5 / pdb_00006go5
Title : TdT chimera (Loop1 of pol mu) - Ternary complex with 1-nt gapped DNA substrate
Authors : Loc'h, J.; Gerodimos, C.A.; Rosario, S.; Lieber, M.R.; Delarue, M.
Deposited on : 2018-06-01
Resolution : 2.35 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

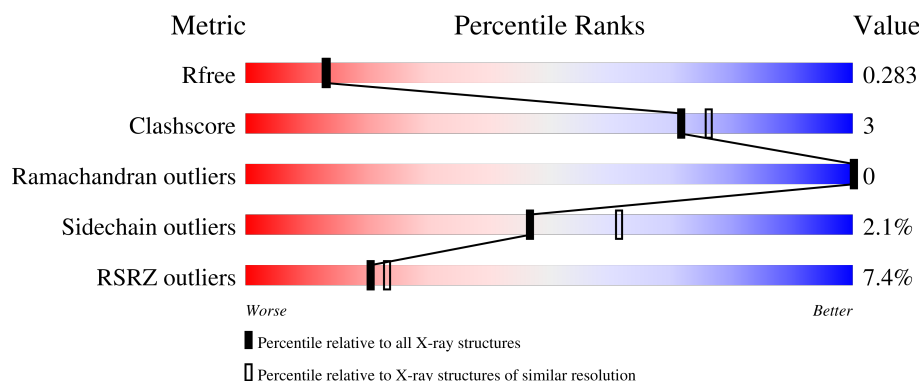
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	401	9% 76% 9% 14%
1	B	401	4% 75% 8% 16%
2	H	12	75% 25%
2	N	12	75% 25%
3	F	6	100%

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Mol	Chain	Length	Quality of chain
3	L	6	 100%
4	G	6	 17% 67% 33%
4	M	6	 67% 33%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6542 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 DNA nucleotidylexotransferase,DNA-directed DNA/RNA polymerase mu,DNA nucleotidylexotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2621	1667	453	485	16			
1	B	335	Total	C	N	O	S	0	1	0
			2598	1656	450	477	15			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	MET	-	initiating methionine	UNP P09838
A	112	GLY	-	expression tag	UNP P09838
A	113	SER	-	expression tag	UNP P09838
A	114	SER	-	expression tag	UNP P09838
A	115	HIS	-	expression tag	UNP P09838
A	116	HIS	-	expression tag	UNP P09838
A	117	HIS	-	expression tag	UNP P09838
A	118	HIS	-	expression tag	UNP P09838
A	119	HIS	-	expression tag	UNP P09838
A	120	HIS	-	expression tag	UNP P09838
A	121	SER	-	expression tag	UNP P09838
A	122	SER	-	expression tag	UNP P09838
A	123	GLY	-	expression tag	UNP P09838
A	124	LEU	-	expression tag	UNP P09838
A	125	VAL	-	expression tag	UNP P09838
A	126	PRO	-	expression tag	UNP P09838
A	127	ARG	-	expression tag	UNP P09838
A	128	GLY	-	expression tag	UNP P09838
A	129	SER	-	expression tag	UNP P09838
A	130	HIS	-	expression tag	UNP P09838
A	131	MET	-	expression tag	UNP P09838
A	401	VAL	ALA	conflict	UNP Q9JIW4
B	111	MET	-	initiating methionine	UNP P09838
B	112	GLY	-	expression tag	UNP P09838

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Chain	Residue	Modelled	Actual	Comment	Reference
B	113	SER	-	expression tag	UNP P09838
B	114	SER	-	expression tag	UNP P09838
B	115	HIS	-	expression tag	UNP P09838
B	116	HIS	-	expression tag	UNP P09838
B	117	HIS	-	expression tag	UNP P09838
B	118	HIS	-	expression tag	UNP P09838
B	119	HIS	-	expression tag	UNP P09838
B	120	HIS	-	expression tag	UNP P09838
B	121	SER	-	expression tag	UNP P09838
B	122	SER	-	expression tag	UNP P09838
B	123	GLY	-	expression tag	UNP P09838
B	124	LEU	-	expression tag	UNP P09838
B	125	VAL	-	expression tag	UNP P09838
B	126	PRO	-	expression tag	UNP P09838
B	127	ARG	-	expression tag	UNP P09838
B	128	GLY	-	expression tag	UNP P09838
B	129	SER	-	expression tag	UNP P09838
B	130	HIS	-	expression tag	UNP P09838
B	131	MET	-	expression tag	UNP P09838
B	401	VAL	ALA	conflict	UNP Q9JIW4

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*CP*TP*GP*GP*CP*AP*AP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	12	Total	C	N	O	P	0	0	0
			243	116	49	67	11			
2	N	12	Total	C	N	O	P	0	0	0
			243	116	49	67	11			

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*GP*TP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	6	Total	C	N	O	P	0	0	0
			121	60	18	38	5			
3	L	6	Total	C	N	O	P	0	0	0
			121	60	18	38	5			

- Molecule 4 is a DNA chain called DNA (5'-D(*AP*CP*AP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	6	Total 104	C 48	N 21	O 30	P 5	0	0	1
4	M	6	Total 104	C 48	N 21	O 30	P 5	0	0	1

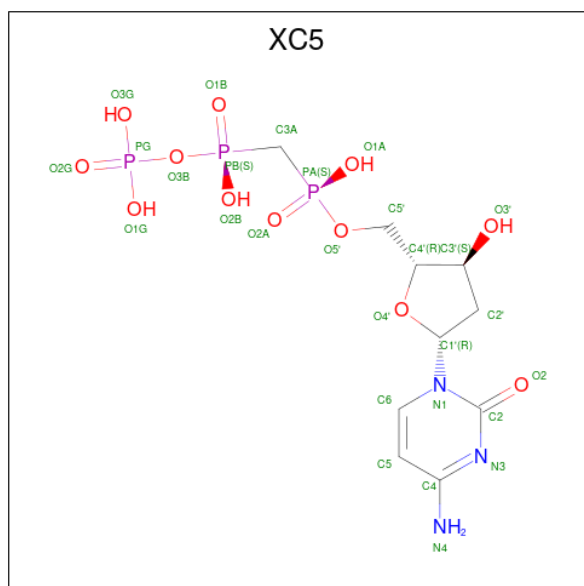
- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is 2'-deoxy-5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}p hosphoryl]cytidine (CCD ID: XC5) (formula: C₁₀H₁₈N₃O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			28	10	3	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			28	10	3	12	3		

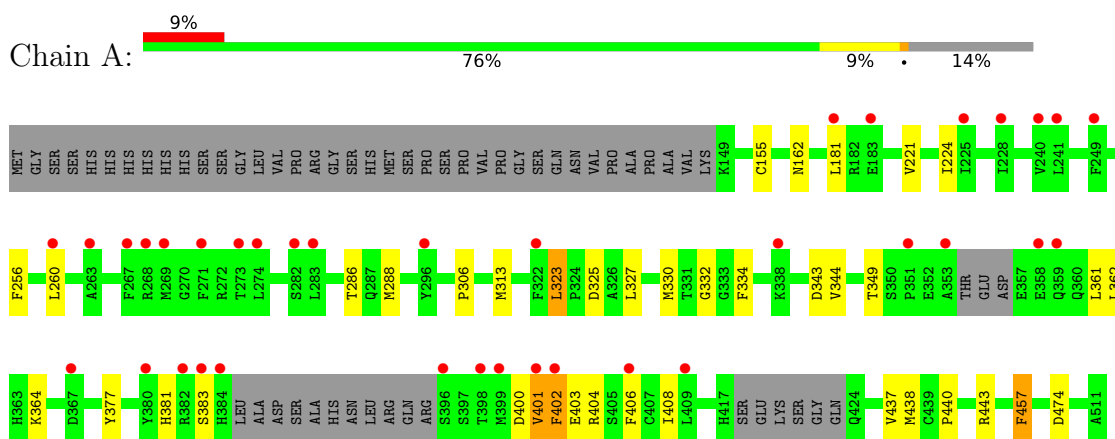
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	137	Total	O	0	0
			137	137		
8	B	131	Total	O	0	0
			131	131		
8	H	13	Total	O	0	0
			13	13		
8	F	3	Total	O	0	0
			3	3		
8	G	10	Total	O	0	0
			10	10		
8	L	7	Total	O	0	0
			7	7		
8	N	18	Total	O	0	0
			18	18		
8	M	8	Total	O	0	0
			8	8		

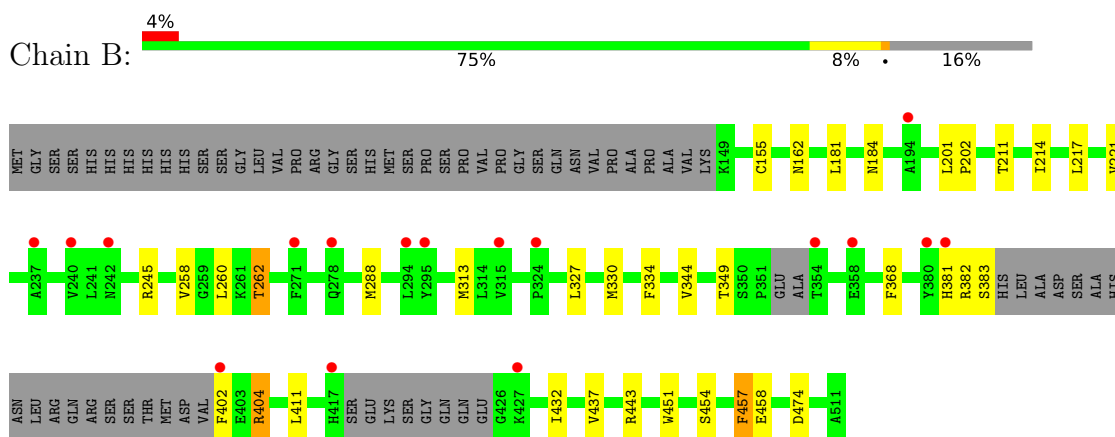
3 Residue-property plots [i](#)

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.

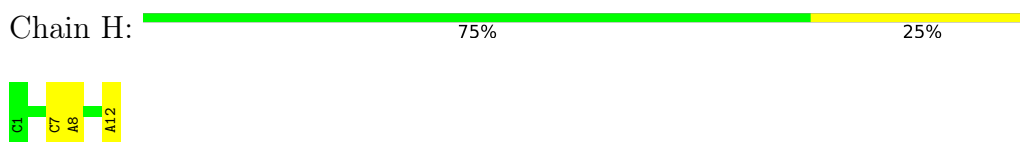
- Molecule 1: DNA nucleotidylexotransferase,DNA-directed DNA/RNA polymerase mu,DNA nucleotidylexotransferase



- Molecule 1: DNA nucleotidylexotransferase,DNA-directed DNA/RNA polymerase mu,DNA nucleotidylexotransferase



- Molecule 2: DNA (5'-D(*CP*GP*CP*TP*GP*GP*CP*AP*AP*AP*CP*A)-3')



- Molecule 2: DNA (5'-D(*CP*GP*CP*TP*GP*GP*CP*AP*AP*AP*CP*A)-3')

Chain N:  75% 25%

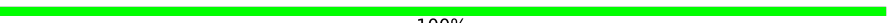


- Molecule 3: DNA (5'-D(*TP*GP*TP*TP*TP*G)-3')

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(*TP*GP*TP*TP*TP*G)-3')

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(*AP*CP*AP*GP*CP*G)-3')

Chain G:  17% 67% 33%



- Molecule 4: DNA (5'-D(*AP*CP*AP*GP*CP*G)-3')

Chain M:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	234.18Å 69.25Å 59.69Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	44.86 – 2.35 44.86 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (44.86-2.35) 98.3 (44.86-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.218 , 0.265 0.231 , 0.283	Depositor DCC
R_{free} test set	1961 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 80.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6542	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.13% 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: MG, NA, XC5

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	0.84	0/2675	1.45	22/3615 (0.6%)
1	B	0.82	0/2653	1.40	11/3578 (0.3%)
2	H	0.47	0/273	0.60	0/419
2	N	0.52	0/273	0.67	0/419
3	F	0.47	0/134	0.69	0/206
3	L	0.55	0/134	0.74	0/206
4	G	0.47	0/116	0.47	0/178
4	M	0.41	0/116	0.43	0/178
All	All	0.79	0/6374	1.32	33/8799 (0.4%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	VAL	CA-C-N	9.80	135.91	121.31
1	A	401	VAL	C-N-CA	9.80	135.91	121.31
1	B	162	ASN	CA-CB-CG	8.45	121.05	112.60
1	A	402	PHE	N-CA-C	7.13	120.33	110.35
1	A	474	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	400	ASP	N-CA-C	6.36	118.53	110.33
1	B	184	ASN	CA-C-N	6.08	128.43	120.28
1	B	184	ASN	C-N-CA	6.08	128.43	120.28
1	A	162	ASN	CA-CB-CG	6.06	118.66	112.60
1	B	368	PHE	CA-CB-CG	5.70	119.50	113.80
1	A	364	LYS	CA-C-N	5.68	128.24	120.46
1	A	364	LYS	C-N-CA	5.68	128.24	120.46
1	A	443	ARG	CA-C-N	5.63	127.76	120.44
1	A	443	ARG	C-N-CA	5.63	127.76	120.44
1	B	443	ARG	CA-C-N	5.59	127.71	120.44
1	B	443	ARG	C-N-CA	5.59	127.71	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	457	PHE	CA-C-N	5.35	127.88	120.29
1	B	457	PHE	C-N-CA	5.35	127.88	120.29
1	A	457	PHE	CA-C-N	5.32	127.68	120.44
1	A	457	PHE	C-N-CA	5.32	127.68	120.44
1	B	313	MET	CA-C-N	5.25	127.26	120.44
1	B	313	MET	C-N-CA	5.25	127.26	120.44
1	A	332	GLY	CA-C-N	5.17	125.72	119.98
1	A	332	GLY	C-N-CA	5.17	125.72	119.98
1	B	474	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	325	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	313	MET	CA-C-N	5.09	127.05	120.44
1	A	313	MET	C-N-CA	5.09	127.05	120.44
1	A	400	ASP	CA-C-N	5.08	131.11	121.97
1	A	400	ASP	C-N-CA	5.08	131.11	121.97
1	A	306	PRO	CA-C-N	5.07	127.33	120.44
1	A	306	PRO	C-N-CA	5.07	127.33	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2621	0	2439	14	0
1	B	2598	0	2458	19	0
2	H	243	0	135	2	0
2	N	243	0	135	2	0
3	F	121	0	72	0	0
3	L	121	0	72	0	0
4	G	104	0	56	1	0
4	M	104	0	56	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	28	0	0	0	0
7	B	28	0	0	0	0
8	A	137	0	0	0	0
8	B	131	0	0	0	0
8	F	3	0	0	0	0
8	G	10	0	0	0	0
8	H	13	0	0	0	0
8	L	7	0	0	0	0
8	M	8	0	0	0	0
8	N	18	0	0	0	0
All	All	6542	0	5423	38	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 3.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:HIS:HB2	1:A:404:ARG:HB3	1.71	0.71
1:B:217:LEU:HA	1:B:221:VAL:CG2	2.28	0.64
2:N:7:DC:H2'	2:N:8:DA:C8	2.35	0.61
2:H:7:DC:H2'	2:H:8:DA:C8	2.35	0.61
1:B:217:LEU:HA	1:B:221:VAL:HG21	1.82	0.59
1:A:401:VAL:HB	1:A:440:PRO:HG3	1.85	0.59
1:B:404:ARG:HG3	1:B:437:VAL:HG22	1.85	0.59
1:B:402:PHE:CE2	1:B:404:ARG:HB2	2.40	0.56
1:A:383:SER:HB3	1:A:402:PHE:HB3	1.88	0.55
1:B:381:HIS:HB2	1:B:404:ARG:HB3	1.89	0.54
1:B:382:ARG:HG3	1:B:383:SER:H	1.73	0.52
1:B:155:CYS:HA	1:B:457:PHE:CE1	2.45	0.51
1:B:330:MET:HE3	1:B:334:PHE:HB3	1.92	0.50
1:B:258:VAL:HG13	1:B:262:THR:HB	1.93	0.50
2:N:6:DG:H2''	2:N:7:DC:O5'	2.14	0.48
1:A:286:THR:HG22	2:H:12:DA:H5''	1.96	0.48
1:A:404:ARG:HG3	1:A:437:VAL:HG22	1.95	0.48
1:A:221:VAL:HA	1:A:224:ILE:HD12	1.96	0.47
1:A:361:LEU:HB3	1:A:438:MET:SD	2.54	0.47
1:B:454:SER:O	1:B:458:GLU:HG2	2.14	0.47
1:A:362:LEU:HD12	1:A:403:GLU:HB3	1.97	0.47
1:A:323:LEU:HD12	1:A:361:LEU:HD13	1.96	0.46
1:A:181:LEU:HA	1:A:260:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:THR:HA	1:B:214:ILE:HD12	1.99	0.45
1:B:402:PHE:HE2	1:B:404:ARG:HB2	1.79	0.45
1:B:181:LEU:HA	1:B:260:LEU:HD13	1.99	0.44
1:B:181:LEU:HD21	1:B:245:ARG:HG2	2.00	0.44
1:B:382:ARG:HG3	1:B:383:SER:N	2.32	0.44
1:B:411:LEU:HD22	1:B:432:ILE:HD12	2.00	0.43
4:M:5:DC:H2"	4:M:6:DG:C8	2.54	0.43
4:G:5:DC:H2"	4:G:6:DG:C8	2.55	0.42
1:B:382:ARG:CG	1:B:383:SER:H	2.32	0.42
1:B:404:ARG:HH22	1:B:451:TRP:HE1	1.68	0.41
1:A:256:PHE:CZ	1:A:406:PHE:HE2	2.39	0.41
1:A:377:TYR:HB3	1:A:408:ILE:HB	2.04	0.41
1:A:330:MET:HE3	1:A:334:PHE:HB3	2.02	0.40
1:A:155:CYS:HA	1:A:457:PHE:CE2	2.57	0.40
1:B:201:LEU:HA	1:B:202:PRO:HD3	1.99	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	335/401 (84%)	323 (96%)	12 (4%)	0	100	100
1	B	328/401 (82%)	323 (98%)	5 (2%)	0	100	100
All	All	663/802 (83%)	646 (97%)	17 (3%)	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	A	258/350 (74%)	253 (98%)	5 (2%)	50	65
1	B	257/350 (73%)	251 (98%)	6 (2%)	44	58
All	All	515/700 (74%)	504 (98%)	11 (2%)	47	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	MET
1	A	323	LEU
1	A	327	LEU
1	A	344	VAL
1	A	349	THR
1	B	262	THR
1	B	288	MET
1	B	327	LEU
1	B	344	VAL
1	B	349	THR
1	B	404	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	287	GLN
1	A	413	HIS
1	B	178	ASN
1	B	184	ASN
1	B	287	GLN
1	B	372	GLN
1	B	413	HIS

5.3.3 RNA ⓘ

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
7	XC5	A	603	6	25,29,29	1.17	3 (12%)	37,45,45	0.71	1 (2%)
7	XC5	B	603	6	25,29,29	1.14	1 (4%)	37,45,45	0.73	2 (5%)

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
7	XC5	A	603	6	-	2/19/34/34	0/2/2/2
7	XC5	B	603	6	-	3/19/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	603	XC5	PA-O1A	-4.20	1.46	1.56
7	A	603	XC5	PA-O1A	-3.27	1.48	1.56
7	A	603	XC5	PA-O2A	2.51	1.57	1.51
7	A	603	XC5	PB-O2B	-2.01	1.51	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	603	XC5	O1G-PG-O3B	2.94	114.49	104.64
7	B	603	XC5	O1G-PG-O3B	2.54	113.16	104.64
7	B	603	XC5	O1A-PA-C3A	2.01	115.05	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

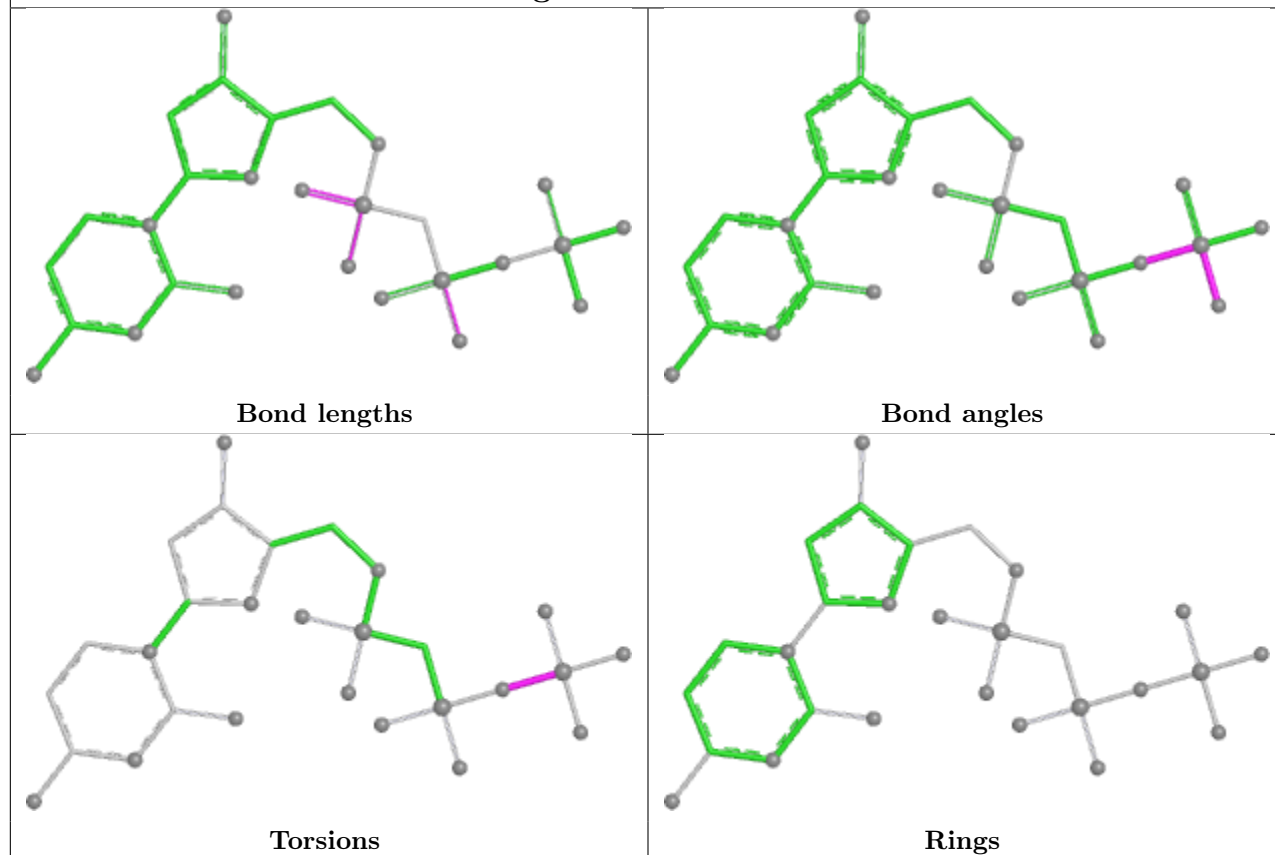
Mol	Chain	Res	Type	Atoms
7	A	603	XC5	PB-O3B-PG-O1G
7	B	603	XC5	PA-C3A-PB-O1B
7	B	603	XC5	PA-C3A-PB-O2B
7	B	603	XC5	PA-C3A-PB-O3B
7	A	603	XC5	PB-O3B-PG-O2G

There are no ring outliers.

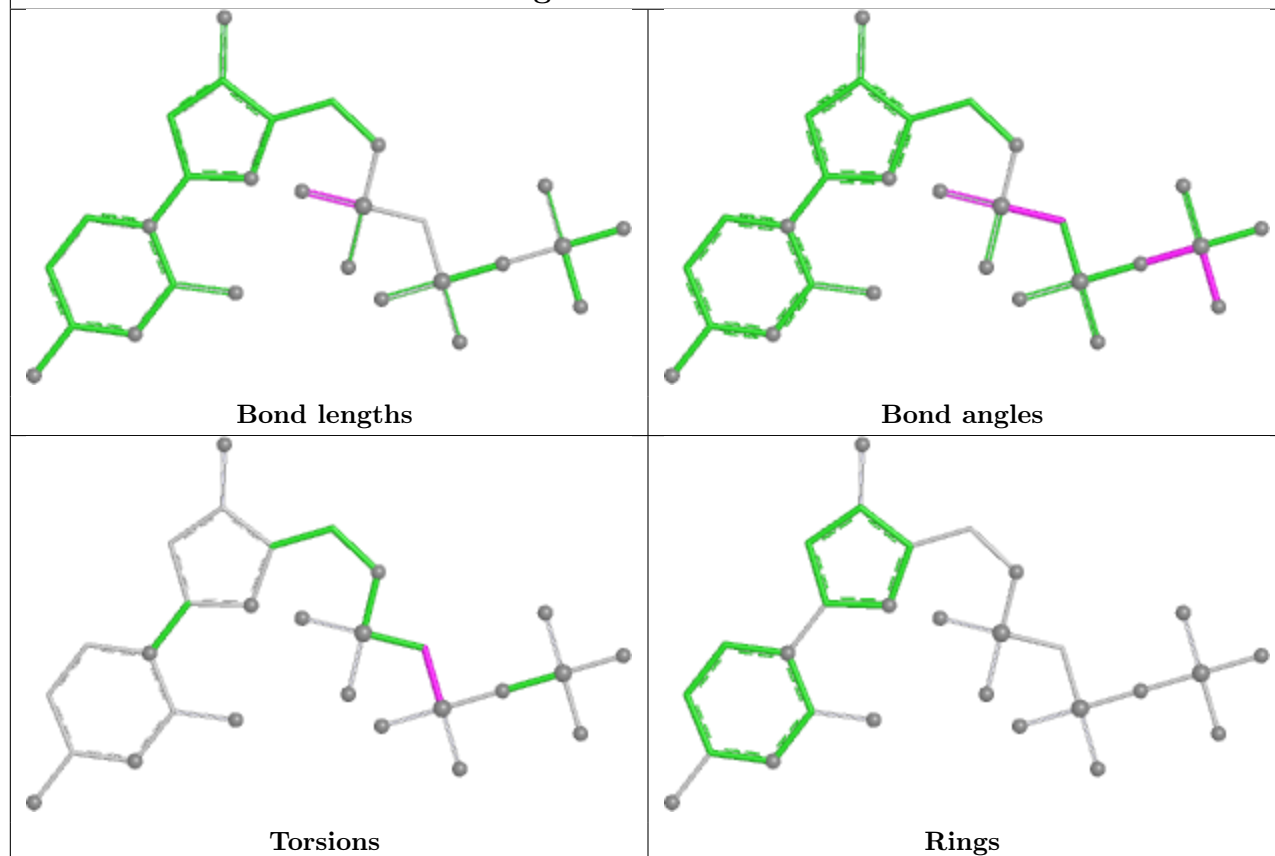
No monomer is involved in short contacts.

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 XC5 A 603



Ligand XC5 B 603



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	343/401 (85%)	0.91	36 (10%) 11 13	43, 71, 107, 130	0
1	B	335/401 (83%)	0.78	17 (5%) 33 39	44, 67, 94, 124	1 (0%)
2	H	12/12 (100%)	0.23	0 100 100	62, 85, 118, 129	0
2	N	12/12 (100%)	0.18	0 100 100	59, 77, 102, 115	0
3	F	6/6 (100%)	0.07	0 100 100	65, 69, 80, 91	0
3	L	6/6 (100%)	0.13	0 100 100	61, 65, 77, 94	0
4	G	6/6 (100%)	0.46	1 (16%) 4 4	73, 78, 85, 87	0
4	M	6/6 (100%)	0.18	0 100 100	71, 77, 84, 85	0
All	All	726/850 (85%)	0.81	54 (7%) 20 23	43, 69, 102, 130	1 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	GLN	4.7
1	B	402	PHE	4.0
1	B	381	HIS	3.7
1	A	228	ILE	3.6
1	A	260	LEU	3.5
1	A	402	PHE	3.5
1	A	241	LEU	3.3
1	B	417	HIS	3.3
1	A	353	ALA	3.2
1	A	384	HIS	3.1
1	A	273	THR	3.1
1	B	240	VAL	3.1
1	A	225	ILE	3.0
1	A	358	GLU	3.0
1	A	268	ARG	2.9
1	A	367	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	282	SER	2.8
1	B	294	LEU	2.7
1	B	271	PHE	2.7
1	B	324	PRO	2.7
1	A	401	VAL	2.6
1	A	322	PHE	2.6
1	A	269	MET	2.6
4	G	1	DA	2.5
1	A	283	LEU	2.5
1	A	399	MET	2.5
1	B	358	GLU	2.5
1	A	181	LEU	2.4
1	B	380	TYR	2.4
1	B	237	ALA	2.4
1	A	249	PHE	2.4
1	A	406	PHE	2.4
1	A	398	THR	2.3
1	B	354	THR	2.3
1	A	351	PRO	2.3
1	A	382	ARG	2.3
1	B	427	LYS	2.3
1	A	296	TYR	2.3
1	A	183	GLU	2.3
1	A	240	VAL	2.3
1	B	295	TYR	2.2
1	A	274	LEU	2.2
1	A	263	ALA	2.2
1	A	409	LEU	2.2
1	B	315	VAL	2.2
1	A	383	SER	2.1
1	A	380	TYR	2.1
1	A	271	PHE	2.1
1	A	267	PHE	2.1
1	A	338	LYS	2.1
1	B	242	ASN	2.1
1	A	396	SER	2.0
1	B	194	ALA	2.0
1	B	278	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

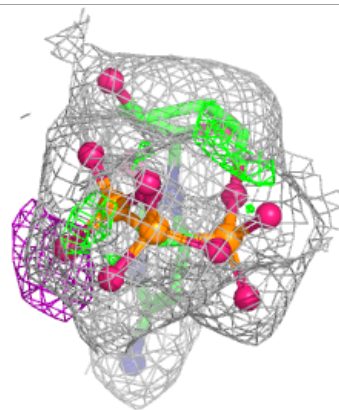
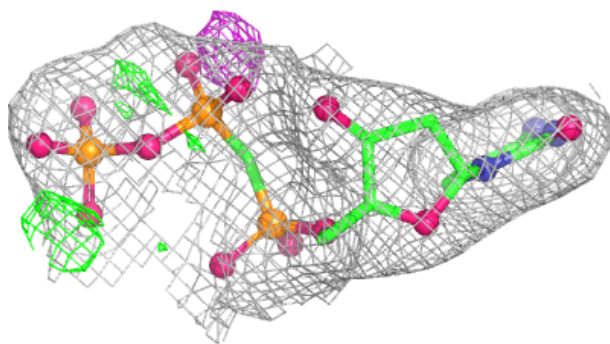
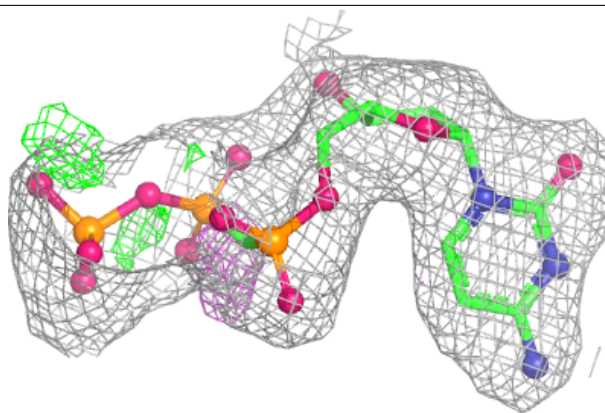
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	A	601	1/1	0.78	0.11	72,72,72,72	0
5	NA	B	602	1/1	0.91	0.06	55,55,55,55	0
7	XC5	A	603	28/28	0.94	0.10	45,52,72,75	0
6	MG	A	602	1/1	0.95	0.12	52,52,52,52	0
7	XC5	B	603	28/28	0.95	0.08	43,50,59,63	0
6	MG	B	601	1/1	0.97	0.04	51,51,51,51	0

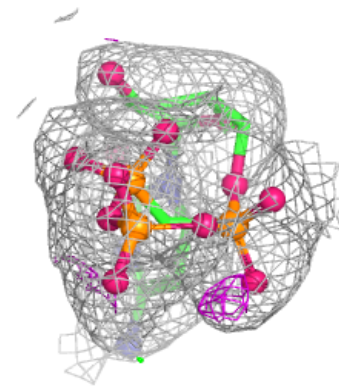
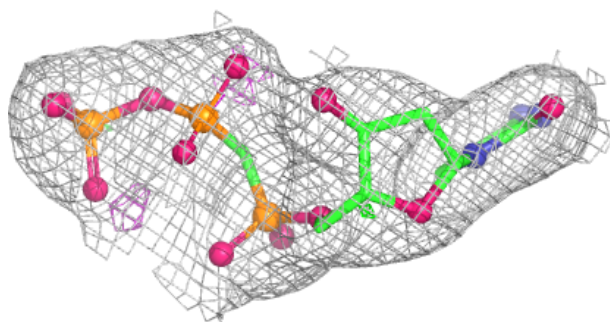
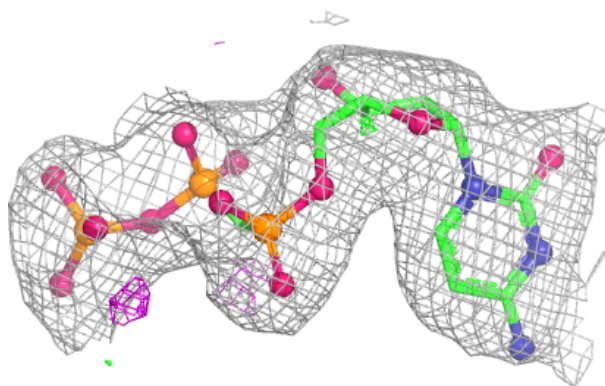
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around XC5 A 603:

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

**Electron density around XC5 B 603:**

$2mF_o-DF_c$ (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.