



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:58 AM UTC

PDB ID : 3I25 / pdb_00003i25
Title : Potent Beta-Secretase 1 hydroxyethylene Inhibitor
Authors : Lindberg, J.D.; Borkakoti, N.; Nystrom, S.
Deposited on : 2009-06-29
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

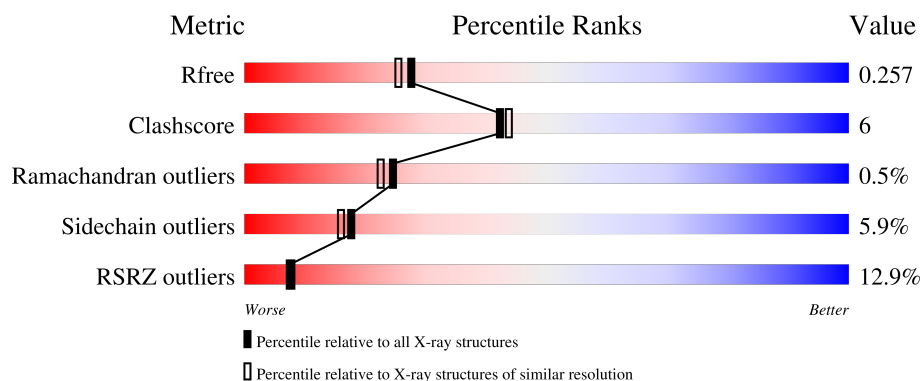
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	406	11% 76% 14% •• 8%
1	B	406	10% 75% 14% • 8%
1	C	406	15% 77% 13% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9203 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.

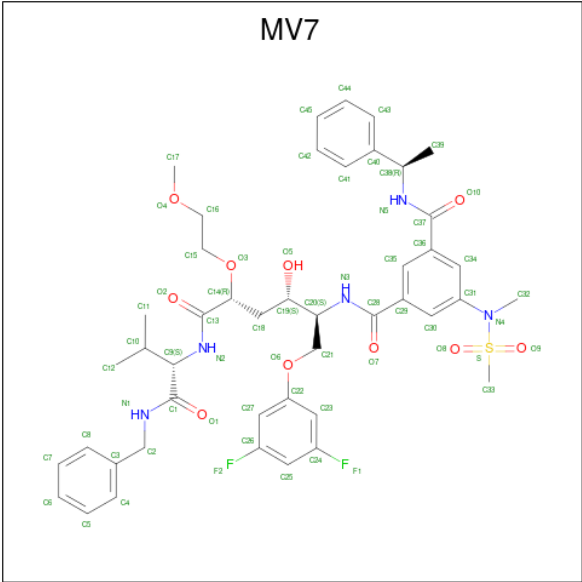
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2940	1882	489	555	14			
1	B	373	Total	C	N	O	S	0	0	0
			2940	1882	489	555	14			
1	C	373	Total	C	N	O	S	0	0	0
			2940	1882	489	555	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28P	MET	-	initiating methionine	UNP P56817
B	28P	MET	-	initiating methionine	UNP P56817
C	28P	MET	-	initiating methionine	UNP P56817

- Molecule 2 is N-[(2S,3S,5R)-1-(3,5-difluorophenoxy)-3-hydroxy-5-(2-methoxyethoxy)-6-[[[(2S)-3-methyl-1-oxo-1-(phenylmethylamino)butan-2-yl]amino]-6-oxo-hexan-2-yl]-5-(methylmethylsulfonyl-amino)-N'-[(1R)-1-phenylethyl]benzene-1,3-dicarboxamide (CCD ID: MV7) (formula: C₄₅H₅₅F₂N₅O₁₀S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			63	45	2	5	10	1		
2	B	1	Total	C	F	N	O	S	0	0
			63	45	2	5	10	1		
2	C	1	Total	C	F	N	O	S	0	0
			63	45	2	5	10	1		

- Molecule 3 is water.

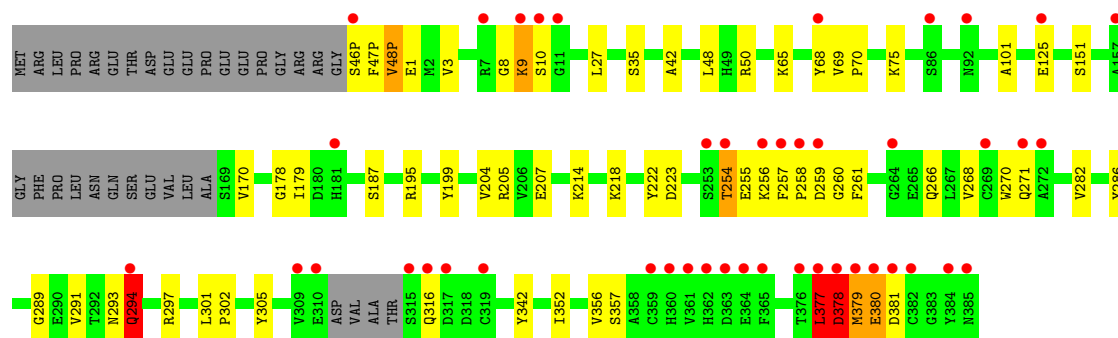
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total	O	0
			69	69	
3	B	67	Total	O	0
			67	67	
3	C	58	Total	O	0
			58	58	

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.

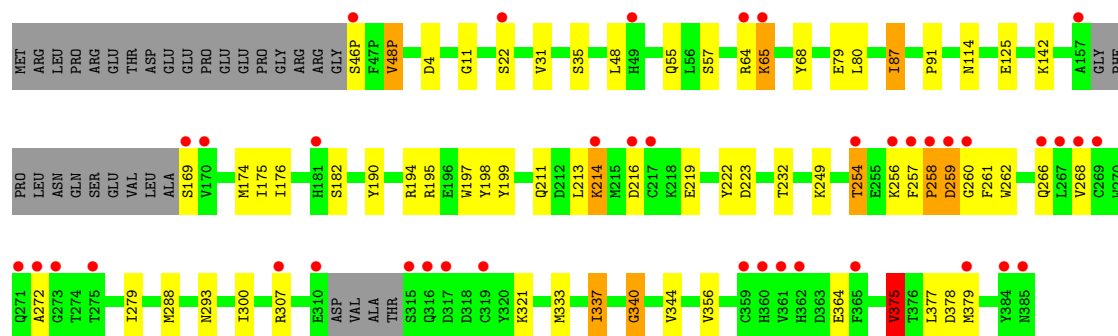
• Molecule 1: Beta-secretase 1

Chain A: 



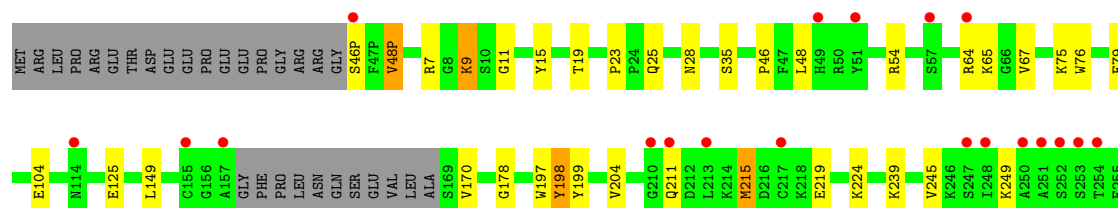
• Molecule 1: Beta-secretase 1

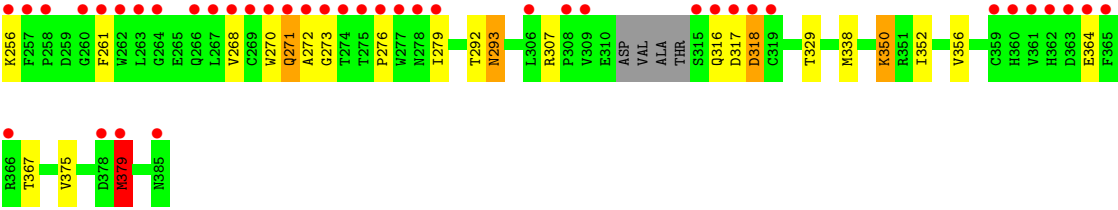
Chain B: 



• Molecule 1: Beta-secretase 1

Chain C: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.42Å 102.48Å 100.19Å 90.00° 103.53° 90.00°	Depositor
Resolution (Å)	79.16 – 2.10 79.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (79.16-2.10) 94.1 (79.16-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.238 (Not available) , 0.257	Depositor DCC
R_{free} test set	4449 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9203	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: MV7

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	1.08	3/3014 (0.1%)	1.10	8/4092 (0.2%)
1	B	1.08	5/3014 (0.2%)	1.09	9/4092 (0.2%)
1	C	1.03	2/3014 (0.1%)	1.06	13/4092 (0.3%)
All	All	1.06	10/9042 (0.1%)	1.08	30/12276 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	VAL	CA-CB	6.30	1.59	1.54
1	A	69	VAL	N-CA	5.86	1.50	1.45
1	B	175	ILE	CA-CB	5.75	1.60	1.54
1	B	344	VAL	CA-CB	5.69	1.60	1.54
1	C	48(P)	VAL	CA-CB	5.53	1.61	1.54
1	B	31	VAL	CA-CB	5.47	1.59	1.53
1	B	199	TYR	CA-C	-5.44	1.46	1.53
1	A	293	ASN	CA-C	5.08	1.60	1.53
1	B	232	THR	CA-CB	5.06	1.61	1.53
1	C	379	MET	CA-C	5.05	1.59	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48(P)	VAL	CB-CA-C	-9.93	99.04	112.04
1	A	378	ASP	CA-CB-CG	9.88	122.48	112.60
1	B	48(P)	VAL	CB-CA-C	-8.67	100.43	112.14
1	B	375	VAL	CB-CA-C	-8.29	99.29	110.98
1	A	48(P)	VAL	CB-CA-C	-8.26	100.99	112.14
1	B	87	ILE	CA-C-N	7.59	127.14	119.24
1	B	87	ILE	C-N-CA	7.59	127.14	119.24
1	A	377	LEU	CA-C-N	7.14	132.28	122.07
1	A	377	LEU	C-N-CA	7.14	132.28	122.07
1	B	337	ILE	N-CA-C	-6.73	105.19	111.45
1	A	48(P)	VAL	N-CA-CB	6.67	119.61	110.54
1	C	293	ASN	CA-C-N	-6.50	114.02	123.00
1	C	293	ASN	C-N-CA	-6.50	114.02	123.00
1	C	48(P)	VAL	N-CA-CB	6.28	118.32	110.47
1	C	170	VAL	N-CA-C	5.99	117.79	109.29
1	C	270	TRP	N-CA-C	-5.87	100.85	109.18
1	C	338	MET	N-CA-C	5.64	118.19	111.71
1	A	293	ASN	CA-CB-CG	5.52	118.12	112.60
1	B	340	GLY	N-CA-C	5.42	120.92	113.99
1	C	178	GLY	N-CA-C	5.29	118.26	110.80
1	C	198	TYR	N-CA-C	-5.27	102.19	110.36
1	B	48(P)	VAL	N-CA-CB	5.27	117.70	110.54
1	B	260	GLY	N-CA-C	-5.25	108.45	115.32
1	C	379	MET	N-CA-C	5.22	116.97	111.28
1	C	23	PRO	CA-C-N	5.13	126.25	119.84
1	C	23	PRO	C-N-CA	5.13	126.25	119.84
1	C	318	ASP	N-CA-C	5.08	121.63	110.80
1	A	294	GLN	CB-CA-C	-5.07	100.97	109.48
1	B	190	TYR	N-CA-C	5.05	117.71	109.59
1	A	214	LYS	N-CA-C	5.01	118.52	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	340	GLY	Peptide

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	2940	0	2849	46	0
1	B	2940	0	2849	35	1
1	C	2940	0	2849	31	1
2	A	63	0	55	1	0
2	B	63	0	55	2	0
2	C	63	0	55	6	0
3	A	69	0	0	0	0
3	B	67	0	0	1	0
3	C	58	0	0	1	0
All	All	9203	0	8712	112	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 6.

All (112) 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:378:ASP:HB3	1:A:380:GLU:OE2	1.38	1.19
1:A:289:GLY:HA3	1:A:294:GLN:HG3	1.31	1.11
1:A:378:ASP:CB	1:A:380:GLU:OE2	2.08	1.01
1:A:289:GLY:HA3	1:A:294:GLN:CG	1.93	0.98
1:C:271:GLN:HA	1:C:317:ASP:HB2	1.50	0.93
1:C:204:VAL:HG11	1:C:379:MET:HG2	1.52	0.91
1:C:224:LYS:HE2	2:C:531:MV7:H17	1.55	0.86
1:A:378:ASP:C	1:A:380:GLU:H	1.86	0.83
1:A:378:ASP:C	1:A:380:GLU:N	2.38	0.77
1:B:125:GLU:OE1	1:B:195:ARG:NH2	2.20	0.74
1:B:194:ARG:HE	1:B:379:MET:HE3	1.51	0.73
1:C:271:GLN:O	1:C:273:GLY:N	2.21	0.73
1:A:289:GLY:CA	1:A:294:GLN:HG3	2.17	0.73
1:A:257:PHE:HD2	1:A:268:VAL:HG11	1.55	0.71
1:C:215:MET:HE1	1:C:239:LYS:HG2	1.72	0.71
1:B:257:PHE:HD2	1:B:268:VAL:HG11	1.55	0.70
1:A:8:GLY:C	1:A:9:LYS:HE2	2.16	0.70
1:A:378:ASP:CA	1:A:380:GLU:OE2	2.45	0.65
1:A:378:ASP:HA	1:A:380:GLU:OE2	1.98	0.64
1:A:291:VAL:O	1:A:294:GLN:HB3	1.98	0.63
1:A:260:GLY:HA3	1:A:266:GLN:HE21	1.63	0.63
1:A:9:LYS:HE2	1:A:9:LYS:N	2.13	0.62
1:B:211:GLN:HG3	3:B:400:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:O	1:A:380:GLU:N	2.33	0.61
1:A:257:PHE:CD2	1:A:268:VAL:HG11	2.36	0.60
1:B:261:PHE:CE1	1:B:268:VAL:HG22	2.37	0.60
1:B:333:MET:HE3	1:B:337:ILE:HG21	1.82	0.60
1:C:9:LYS:HA	1:C:9:LYS:HE2	1.84	0.60
1:B:258:PRO:HB3	1:B:266:GLN:NE2	2.18	0.59
1:C:224:LYS:CE	2:C:531:MV7:H17	2.31	0.58
1:A:199:TYR:HB3	1:A:352:ILE:HD11	1.86	0.58
1:B:257:PHE:CD2	1:B:268:VAL:HG11	2.38	0.57
1:A:205:ARG:NH1	1:A:207:GLU:OE2	2.38	0.56
1:A:125:GLU:OE2	1:A:195:ARG:NH2	2.38	0.56
1:C:215:MET:HE2	1:C:219:GLU:HG3	1.89	0.54
1:A:204:VAL:HG11	1:A:379:MET:HG2	1.89	0.54
1:A:291:VAL:HG22	1:A:294:GLN:HB2	1.89	0.54
1:A:377:LEU:N	1:A:377:LEU:HD13	2.23	0.53
1:B:11:GLY:HA3	1:B:307:ARG:HH21	1.73	0.52
1:C:125:GLU:O	1:C:125:GLU:HG3	2.10	0.51
1:A:47(P):PHE:CZ	1:A:178:GLY:HA3	2.46	0.51
1:A:289:GLY:HA3	1:A:294:GLN:HG2	1.89	0.51
1:C:15:TYR:CD1	1:C:28:ASN:HB3	2.45	0.51
1:A:9:LYS:O	1:A:10:SER:C	2.54	0.50
1:B:11:GLY:HA3	1:B:307:ARG:NH2	2.27	0.50
1:B:65:LYS:HG2	1:B:80:LEU:HD12	1.94	0.50
1:B:11:GLY:CA	1:B:307:ARG:HH21	2.25	0.49
1:B:257:PHE:O	1:B:258:PRO:C	2.55	0.49
1:B:91:PRO:HD3	1:B:176:ILE:HB	1.94	0.49
1:B:258:PRO:O	1:B:259:ASP:HB3	2.13	0.49
1:A:254:THR:HG22	1:A:255:GLU:HG3	1.93	0.48
1:B:125:GLU:OE1	1:B:195:ARG:NE	2.46	0.48
1:B:259:ASP:OD2	1:B:266:GLN:NE2	2.46	0.48
1:C:292:THR:O	1:C:293:ASN:HB2	2.13	0.48
1:A:27:LEU:HD23	1:A:50:ARG:HG3	1.95	0.48
1:A:261:PHE:CD1	1:A:268:VAL:HG13	2.49	0.48
1:C:19:THR:HA	1:C:25:GLN:O	2.14	0.47
1:B:174:MET:HE2	1:B:176:ILE:HG12	1.96	0.47
1:A:68:TYR:OH	1:A:70:PRO:HB3	2.14	0.47
1:B:35:SER:HA	2:B:531:MV7:H11B	1.96	0.47
1:B:288:MET:HE2	1:B:378:ASP:HA	1.98	0.46
1:A:380:GLU:H	1:A:380:GLU:HG3	1.28	0.46
1:A:35:SER:HA	2:A:531:MV7:H11B	1.97	0.46
1:A:302:PRO:HA	1:A:305:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLU:OE1	1:C:239:LYS:HE3	2.16	0.45
1:B:197:TRP:CG	1:B:198:TYR:H	2.34	0.45
1:C:54:ARG:HH12	1:C:79:GLU:CD	2.24	0.45
1:B:213:LEU:O	1:B:214:LYS:CB	2.65	0.45
1:C:329:THR:CB	2:C:531:MV7:H17B	2.47	0.45
1:C:329:THR:HB	2:C:531:MV7:H17B	1.98	0.45
1:C:215:MET:HE2	1:C:215:MET:HB3	1.76	0.44
1:C:379:MET:HB2	3:C:399:HOH:O	2.16	0.44
1:B:216:ASP:HB3	1:B:219:GLU:HG2	1.98	0.44
1:B:258:PRO:HB3	1:B:266:GLN:CD	2.43	0.44
1:C:276:PRO:HB2	1:C:279:ILE:HG12	2.00	0.44
1:A:282:VAL:HG12	1:A:301:LEU:HD23	2.00	0.43
1:A:270:TRP:O	1:A:271:GLN:C	2.61	0.43
1:B:174:MET:HE2	1:B:176:ILE:CG1	2.49	0.43
1:B:288:MET:HE1	1:B:379:MET:HA	1.99	0.43
1:C:261:PHE:CD1	1:C:268:VAL:HG23	2.54	0.43
1:B:222:TYR:HA	1:B:223:ASP:HA	1.86	0.42
2:B:531:MV7:H17B	2:B:531:MV7:H15A	1.81	0.42
1:C:11:GLY:HA2	1:C:307:ARG:HH12	1.84	0.42
1:C:67:VAL:HG13	1:C:76:TRP:HZ3	1.85	0.42
1:A:8:GLY:C	1:A:170:VAL:HG22	2.44	0.42
1:A:378:ASP:HA	1:A:380:GLU:HG3	2.01	0.42
1:C:199:TYR:HB3	1:C:352:ILE:HD11	2.02	0.42
1:C:329:THR:OG1	2:C:531:MV7:H17B	2.20	0.42
1:B:321:LYS:HE3	1:B:321:LYS:HB2	1.88	0.42
1:A:294:GLN:HB2	1:A:294:GLN:HE21	1.62	0.42
1:B:55:GLN:H	1:B:55:GLN:CD	2.25	0.42
1:A:218:LYS:HG3	1:A:381:ASP:O	2.19	0.41
1:B:258:PRO:O	1:B:259:ASP:CB	2.68	0.41
1:B:293:ASN:HA	1:B:375:VAL:HA	2.02	0.41
1:A:222:TYR:HA	1:A:223:ASP:HA	1.73	0.41
1:B:254:THR:HG21	1:B:279:ILE:HG21	2.02	0.41
1:C:350:LYS:HB2	1:C:350:LYS:HE2	1.90	0.41
1:A:261:PHE:CE1	1:A:268:VAL:HG22	2.55	0.41
1:C:9:LYS:HE2	1:C:9:LYS:CA	2.48	0.41
1:C:271:GLN:CD	1:C:271:GLN:N	2.79	0.41
1:A:3:VAL:HG11	1:B:68:TYR:CZ	2.55	0.41
1:C:197:TRP:CG	1:C:198:TYR:H	2.38	0.41
1:A:257:PHE:HA	1:A:258:PRO:HD2	1.91	0.41
1:A:286:TYR:CZ	1:A:297:ARG:HD3	2.56	0.41
1:C:7:ARG:HA	1:C:7:ARG:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:VAL:HG12	1:C:249:LYS:HD3	2.04	0.40
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.86	0.40
1:B:22:SER:O	1:B:57:SER:HA	2.21	0.40
1:B:249:LYS:HG3	1:B:262:TRP:CZ2	2.56	0.40
1:C:35:SER:HA	2:C:531:MV7:H11B	2.04	0.40
1:A:46(P):SER:O	1:A:1:GLU:HB2	2.21	0.40
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.51	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:B:46(P):SER:OG	1:C:104:GLU:OE2[2_455]	2.13	0.07

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	367/406 (90%)	358 (98%)	8 (2%)	1 (0%)	36	36
1	B	367/406 (90%)	355 (97%)	9 (2%)	3 (1%)	16	12
1	C	367/406 (90%)	357 (97%)	8 (2%)	2 (0%)	24	22
All	All	1101/1218 (90%)	1070 (97%)	25 (2%)	6 (0%)	24	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	258	PRO
1	C	272	ALA
1	B	259	ASP
1	C	318	ASP
1	A	379	MET

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Mol	Chain	Res	Type
1	B	272	ALA

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	319/347 (92%)	302 (95%)	17 (5%)	20	19
1	B	319/347 (92%)	300 (94%)	19 (6%)	17	15
1	C	319/347 (92%)	299 (94%)	20 (6%)	16	14
All	All	957/1041 (92%)	901 (94%)	56 (6%)	18	16

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48(P)	VAL
1	A	9	LYS
1	A	48	LEU
1	A	65	LYS
1	A	75	LYS
1	A	151	SER
1	A	187	SER
1	A	254	THR
1	A	256	LYS
1	A	259	ASP
1	A	294	GLN
1	A	316	GLN
1	A	356	VAL
1	A	357	SER
1	A	377	LEU
1	A	378	ASP
1	A	380	GLU
1	B	48(P)	VAL
1	B	4	ASP
1	B	48	LEU
1	B	64	ARG

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Mol	Chain	Res	Type
1	B	65	LYS
1	B	79	GLU
1	B	87	ILE
1	B	114	ASN
1	B	142	LYS
1	B	169	SER
1	B	182	SER
1	B	214	LYS
1	B	254	THR
1	B	256	LYS
1	B	300	ILE
1	B	356	VAL
1	B	364	GLU
1	B	375	VAL
1	B	377	LEU
1	C	46(P)	SER
1	C	48(P)	VAL
1	C	9	LYS
1	C	46	PRO
1	C	48	LEU
1	C	64	ARG
1	C	65	LYS
1	C	75	LYS
1	C	149	LEU
1	C	211	GLN
1	C	215	MET
1	C	256	LYS
1	C	271	GLN
1	C	316	GLN
1	C	350	LYS
1	C	356	VAL
1	C	364	GLU
1	C	367	THR
1	C	375	VAL
1	C	379	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	53	GLN
1	A	89	HIS

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Mol	Chain	Res	Type
1	A	266	GLN
1	A	278	ASN
1	A	294	GLN
1	A	304	GLN
1	A	316	GLN
1	B	28	ASN
1	B	89	HIS
1	B	266	GLN
1	B	304	GLN
1	B	316	GLN
1	B	326	GLN
1	B	385	ASN
1	C	12	GLN
1	C	28	ASN
1	C	89	HIS
1	C	111	ASN
1	C	316	GLN
1	C	362	HIS

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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MV7	A	531	-	65,66,66	1.04	3 (4%)	85,91,91	1.83	18 (21%)
2	MV7	B	531	-	65,66,66	1.09	5 (7%)	85,91,91	1.67	14 (16%)
2	MV7	C	531	-	65,66,66	1.12	4 (6%)	85,91,91	1.70	17 (20%)

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	MV7	A	531	-	-	12/69/69/69	0/4/4/4
2	MV7	B	531	-	-	13/69/69/69	0/4/4/4
2	MV7	C	531	-	-	15/69/69/69	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	531	MV7	S-N4	-4.80	1.55	1.64
2	A	531	MV7	C33-S	-3.72	1.67	1.75
2	B	531	MV7	C33-S	-3.33	1.68	1.75
2	A	531	MV7	S-N4	-2.99	1.59	1.64
2	C	531	MV7	C33-S	-2.48	1.70	1.75
2	A	531	MV7	O9-S	-2.33	1.40	1.43
2	B	531	MV7	C25-C26	2.23	1.41	1.37
2	B	531	MV7	C23-C24	2.21	1.41	1.37
2	B	531	MV7	C23-C22	2.14	1.42	1.39
2	C	531	MV7	C27-C26	2.12	1.41	1.37
2	B	531	MV7	C18-C14	-2.11	1.49	1.53
2	C	531	MV7	C35-C36	-2.05	1.36	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	531	MV7	C10-C9-C1	-7.07	94.15	111.38
2	C	531	MV7	O8-S-N4	6.93	115.07	107.14
2	A	531	MV7	O6-C21-C20	6.09	118.29	108.13
2	B	531	MV7	O6-C21-C20	5.83	117.85	108.13
2	C	531	MV7	C10-C9-C1	-5.78	97.30	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	531	MV7	C10-C9-C1	-5.58	97.77	111.38
2	A	531	MV7	O9-S-C33	-5.02	101.41	108.30
2	A	531	MV7	C21-C20-N3	-4.67	103.02	109.66
2	A	531	MV7	C21-O6-C22	4.53	127.83	117.85
2	B	531	MV7	C11-C10-C9	3.52	120.83	111.16
2	A	531	MV7	O8-S-N4	3.39	111.02	107.14
2	A	531	MV7	C11-C10-C9	3.27	120.12	111.16
2	B	531	MV7	O8-S-N4	3.23	110.84	107.14
2	C	531	MV7	C21-O6-C22	3.22	124.95	117.85
2	B	531	MV7	C10-C9-N2	3.19	119.15	111.44
2	C	531	MV7	C35-C36-C34	3.09	123.26	119.65
2	C	531	MV7	O8-S-O9	-3.05	113.90	118.46
2	A	531	MV7	O8-S-O9	-3.01	113.95	118.46
2	B	531	MV7	C21-O6-C22	2.96	124.38	117.85
2	C	531	MV7	C11-C10-C9	2.91	119.15	111.16
2	A	531	MV7	O8-S-C33	2.89	112.26	108.30
2	C	531	MV7	C3-C2-N1	-2.79	107.18	113.07
2	C	531	MV7	O3-C15-C16	-2.78	100.25	109.67
2	B	531	MV7	O5-C19-C20	2.77	115.35	109.88
2	A	531	MV7	C2-N1-C1	2.70	126.00	122.29
2	B	531	MV7	C11-C10-C12	2.69	117.96	110.58
2	B	531	MV7	O3-C14-C13	-2.67	106.22	111.56
2	A	531	MV7	O9-S-N4	2.67	110.19	107.14
2	B	531	MV7	O2-C13-C14	-2.66	115.43	119.58
2	C	531	MV7	C19-C18-C14	-2.57	110.09	113.97
2	C	531	MV7	O6-C21-C20	2.56	112.40	108.13
2	A	531	MV7	C3-C2-N1	-2.49	107.83	113.07
2	C	531	MV7	C22-C23-C24	2.44	120.59	117.55
2	B	531	MV7	C32-N4-S	2.42	121.70	118.23
2	C	531	MV7	C19-C20-N3	2.41	114.49	109.97
2	A	531	MV7	C19-C18-C14	-2.30	110.50	113.97
2	C	531	MV7	O10-C37-C36	-2.26	116.42	120.90
2	B	531	MV7	C23-C24-C25	-2.24	120.78	123.50
2	B	531	MV7	O9-S-C33	-2.24	105.23	108.30
2	C	531	MV7	C23-C24-C25	-2.23	120.79	123.50
2	C	531	MV7	C10-C9-N2	2.21	116.78	111.44
2	C	531	MV7	C2-N1-C1	2.21	125.33	122.29
2	A	531	MV7	C23-C24-C25	-2.18	120.85	123.50
2	B	531	MV7	O2-C13-N2	2.18	126.86	122.96
2	A	531	MV7	C22-C23-C24	2.17	120.25	117.55
2	C	531	MV7	O8-S-C33	-2.14	105.36	108.30
2	A	531	MV7	C35-C36-C34	2.14	122.15	119.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	531	MV7	C29-C35-C36	-2.06	118.05	120.43
2	A	531	MV7	C8-C3-C4	2.04	121.26	118.23

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	531	MV7	C34-C31-N4-S
2	A	531	MV7	C30-C31-N4-S
2	A	531	MV7	C20-C21-O6-C22
2	B	531	MV7	C34-C31-N4-S
2	B	531	MV7	C30-C31-N4-S
2	B	531	MV7	N3-C20-C21-O6
2	B	531	MV7	C20-C21-O6-C22
2	C	531	MV7	C34-C31-N4-S
2	C	531	MV7	C30-C31-N4-S
2	C	531	MV7	N3-C20-C21-O6
2	C	531	MV7	C12-C10-C9-N2
2	C	531	MV7	C12-C10-C9-C1
2	A	531	MV7	C12-C10-C9-N2
2	B	531	MV7	C12-C10-C9-N2
2	B	531	MV7	C12-C10-C9-C1
2	A	531	MV7	C12-C10-C9-C1
2	A	531	MV7	C11-C10-C9-N2
2	B	531	MV7	C11-C10-C9-N2
2	C	531	MV7	C11-C10-C9-N2
2	B	531	MV7	C11-C10-C9-C1
2	A	531	MV7	O3-C15-C16-O4
2	C	531	MV7	C11-C10-C9-C1
2	A	531	MV7	C11-C10-C9-C1
2	B	531	MV7	O3-C15-C16-O4
2	B	531	MV7	C15-C16-O4-C17
2	C	531	MV7	C20-C21-O6-C22
2	C	531	MV7	O3-C15-C16-O4
2	C	531	MV7	C13-C14-O3-C15
2	C	531	MV7	C19-C20-C21-O6
2	C	531	MV7	C15-C16-O4-C17
2	A	531	MV7	C15-C16-O4-C17
2	A	531	MV7	O2-C13-C14-O3
2	A	531	MV7	N2-C13-C14-O3
2	B	531	MV7	O2-C13-C14-O3
2	B	531	MV7	N2-C13-C14-O3

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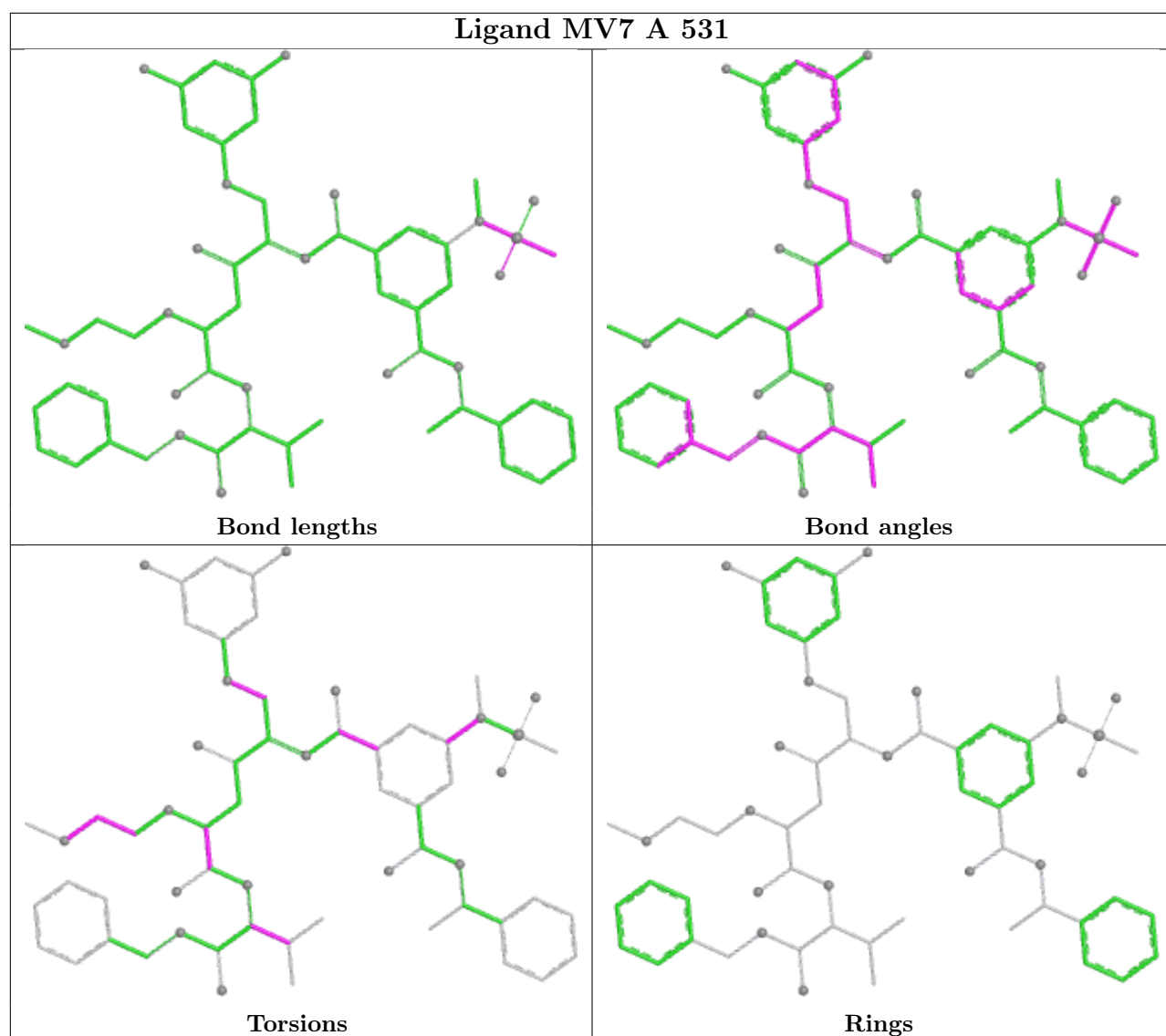
Mol	Chain	Res	Type	Atoms
2	C	531	MV7	O3-C14-C18-C19
2	C	531	MV7	O2-C13-C14-O3
2	C	531	MV7	N2-C13-C14-O3
2	B	531	MV7	C19-C20-C21-O6
2	A	531	MV7	O7-C28-C29-C35

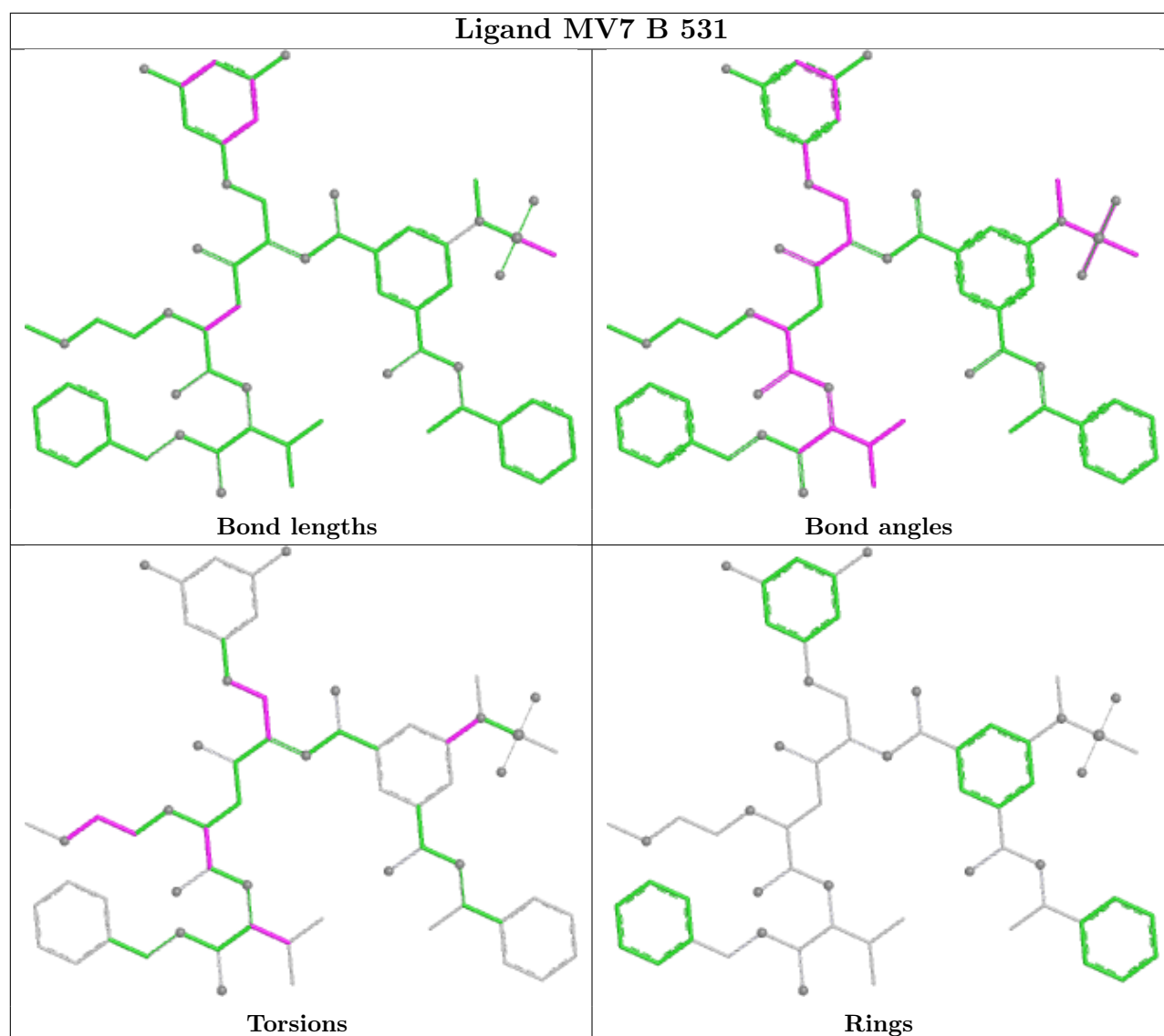
There are no ring outliers.

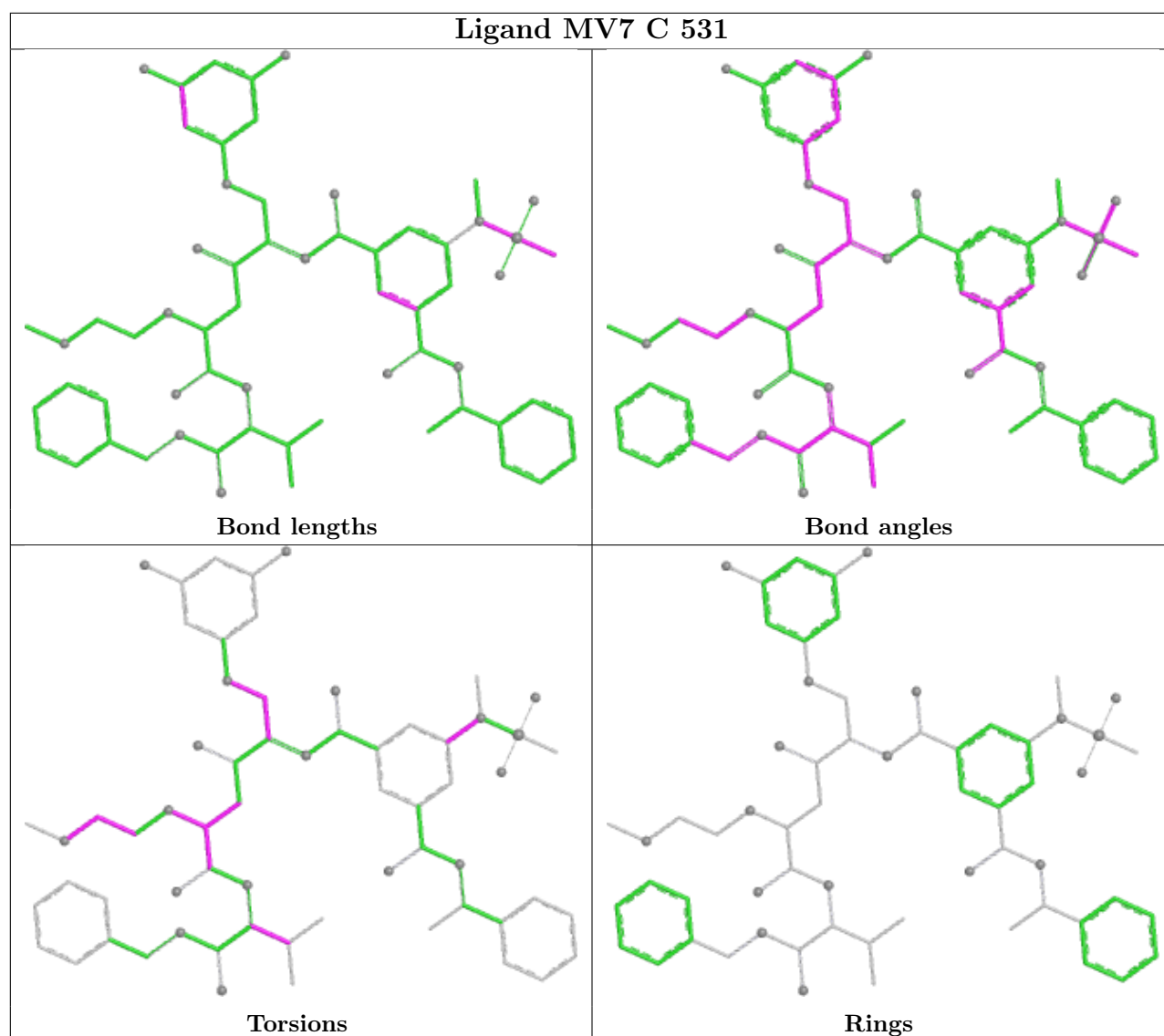
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	531	MV7	1	0
2	B	531	MV7	2	0
2	C	531	MV7	6	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	373/406 (91%)	0.63	44 (11%)	9 9	19, 36, 59, 77	0
1	B	373/406 (91%)	0.49	40 (10%)	11 11	20, 35, 57, 73	0
1	C	373/406 (91%)	0.76	60 (16%)	4 5	19, 38, 70, 83	0
All	All	1119/1218 (91%)	0.63	144 (12%)	7 8	19, 36, 64, 83	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	GLN	6.4
1	C	272	ALA	6.1
1	B	365	PHE	5.9
1	B	259	ASP	5.7
1	C	157	ALA	5.4
1	A	68	TYR	5.3
1	A	380	GLU	5.3
1	B	362	HIS	5.2
1	C	315	SER	5.1
1	A	381	ASP	5.1
1	A	365	PHE	4.9
1	C	361	VAL	4.9
1	A	315	SER	4.8
1	A	258	PRO	4.8
1	C	365	PHE	4.7
1	A	378	ASP	4.6
1	A	259	ASP	4.3
1	C	252	SER	4.2
1	C	258	PRO	4.1
1	B	258	PRO	4.1
1	B	315	SER	4.0
1	C	46(P)	SER	4.0
1	A	364	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	317	ASP	3.9
1	C	364	GLU	3.9
1	A	360	HIS	3.8
1	B	46(P)	SER	3.8
1	C	250	ALA	3.7
1	C	362	HIS	3.7
1	C	267	LEU	3.7
1	B	157	ALA	3.7
1	A	362	HIS	3.6
1	C	269	CYS	3.5
1	A	157	ALA	3.5
1	A	379	MET	3.5
1	C	264	GLY	3.4
1	C	64	ARG	3.4
1	B	254	THR	3.4
1	C	378	ASP	3.3
1	B	316	GLN	3.3
1	A	9	LYS	3.3
1	A	256	LYS	3.3
1	A	385	ASN	3.3
1	A	316	GLN	3.3
1	B	170	VAL	3.3
1	A	253	SER	3.2
1	A	7	ARG	3.2
1	C	256	LYS	3.2
1	C	278	ASN	3.2
1	C	260	GLY	3.2
1	C	319	CYS	3.2
1	C	316	GLN	3.2
1	A	319	CYS	3.2
1	C	251	ALA	3.1
1	A	384	TYR	3.1
1	B	384	TYR	3.1
1	A	46(P)	SER	3.1
1	B	385	ASN	3.1
1	C	273	GLY	3.0
1	A	309	VAL	3.0
1	B	271	GLN	3.0
1	B	256	LYS	2.9
1	C	359	CYS	2.9
1	B	275	THR	2.9
1	A	377	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	213	LEU	2.8
1	C	275	THR	2.8
1	A	257	PHE	2.8
1	C	263	LEU	2.8
1	C	211	GLN	2.8
1	C	210	GLY	2.8
1	C	279	ILE	2.7
1	B	169	SER	2.7
1	B	269	CYS	2.7
1	C	217	CYS	2.7
1	C	277	TRP	2.7
1	A	11	GLY	2.7
1	A	254	THR	2.7
1	A	10	SER	2.7
1	A	363	ASP	2.7
1	C	254	THR	2.6
1	B	319	CYS	2.6
1	C	266	GLN	2.6
1	B	268	VAL	2.6
1	C	385	ASN	2.6
1	C	318	ASP	2.6
1	C	270	TRP	2.6
1	A	376	THR	2.5
1	C	363	ASP	2.5
1	C	274	THR	2.5
1	B	65	LYS	2.5
1	B	273	GLY	2.5
1	B	310	GLU	2.5
1	A	86	SER	2.5
1	A	272	ALA	2.5
1	A	181	HIS	2.5
1	B	217	CYS	2.4
1	C	57	SER	2.4
1	B	360	HIS	2.4
1	B	257	PHE	2.4
1	B	361	VAL	2.4
1	C	155	CYS	2.4
1	C	308	PRO	2.4
1	C	271	GLN	2.4
1	C	309	VAL	2.4
1	B	317	ASP	2.3
1	B	64	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	247	SER	2.3
1	C	360	HIS	2.3
1	A	271	GLN	2.3
1	C	248	ILE	2.3
1	A	361	VAL	2.3
1	B	359	CYS	2.3
1	C	253	SER	2.3
1	B	307	ARG	2.3
1	B	260	GLY	2.3
1	A	125	GLU	2.2
1	C	276	PRO	2.2
1	A	92	ASN	2.2
1	B	216	ASP	2.2
1	A	264	GLY	2.2
1	B	272	ALA	2.2
1	A	269	CYS	2.2
1	C	306	LEU	2.2
1	C	268	VAL	2.2
1	C	257	PHE	2.1
1	B	181	HIS	2.1
1	B	267	LEU	2.1
1	B	22	SER	2.1
1	C	114	ASN	2.1
1	C	379	MET	2.1
1	B	49	HIS	2.1
1	A	317	ASP	2.1
1	B	266	GLN	2.1
1	C	49	HIS	2.1
1	C	261	PHE	2.1
1	C	262	TRP	2.1
1	A	359	CYS	2.1
1	C	51	TYR	2.1
1	B	214	LYS	2.1
1	A	310	GLU	2.0
1	B	379	MET	2.0
1	A	382	CYS	2.0
1	C	366	ARG	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 [i](#)

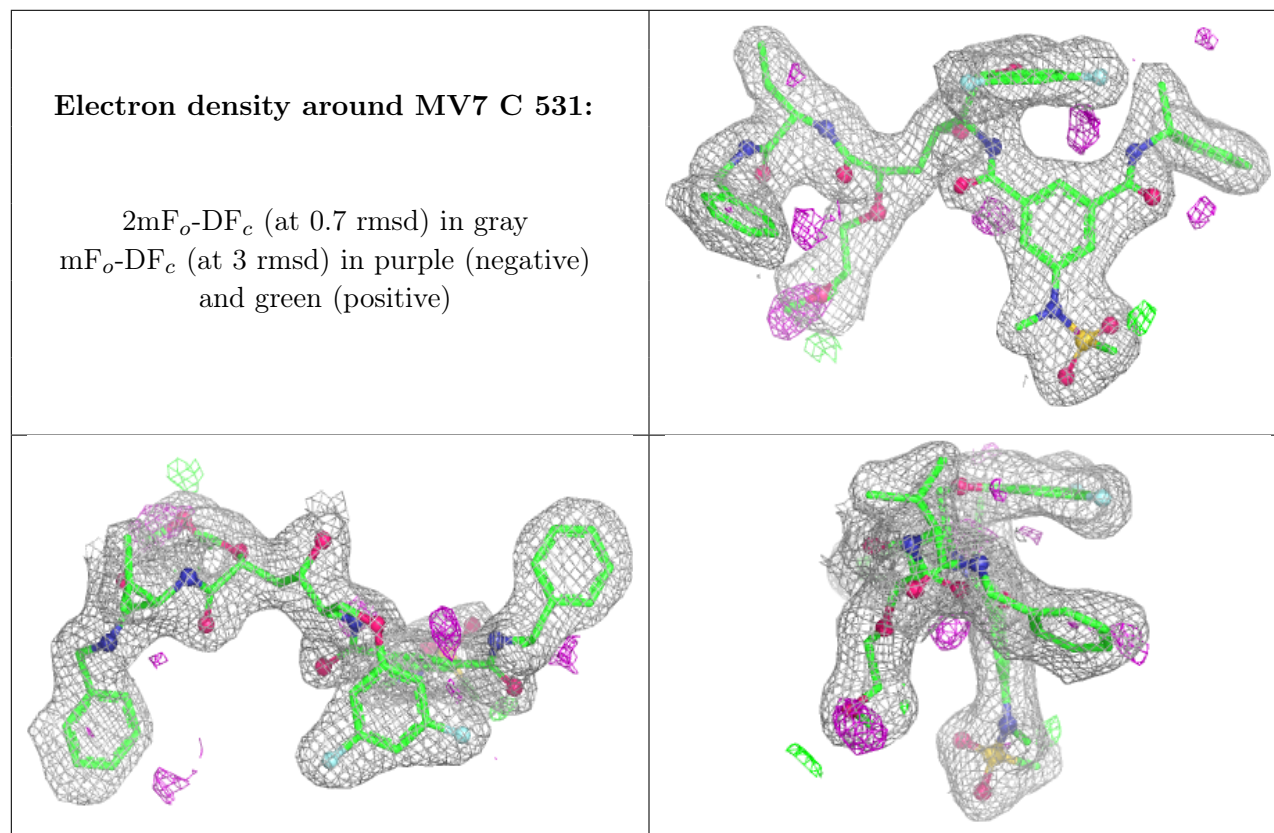
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

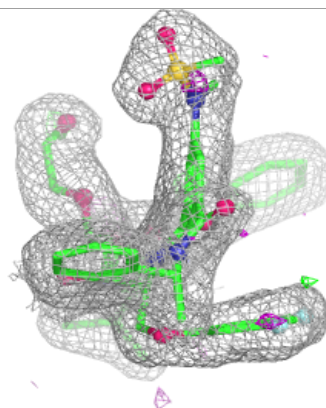
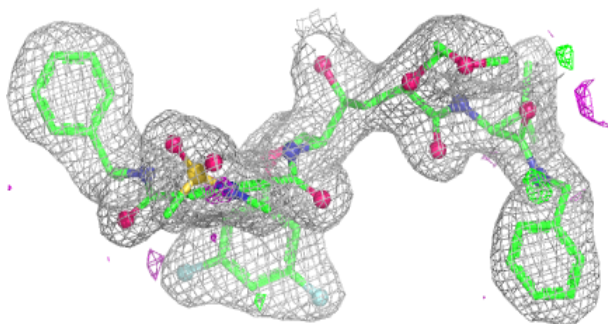
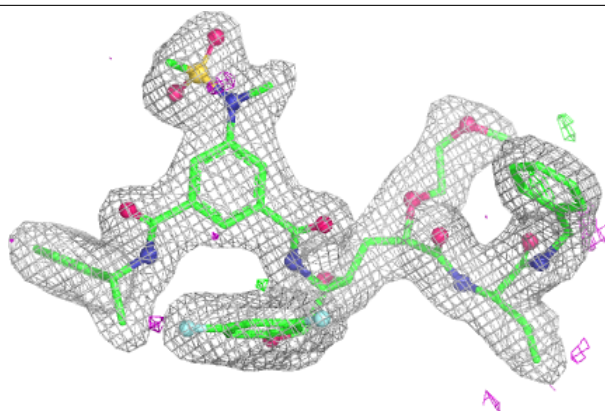
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MV7	C	531	63/63	0.94	0.09	25,32,41,45	0
2	MV7	B	531	63/63	0.96	0.07	22,28,40,46	0
2	MV7	A	531	63/63	0.96	0.08	26,32,49,53	0

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.

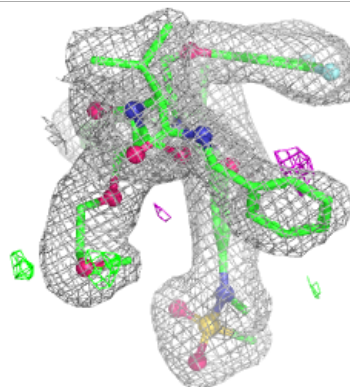
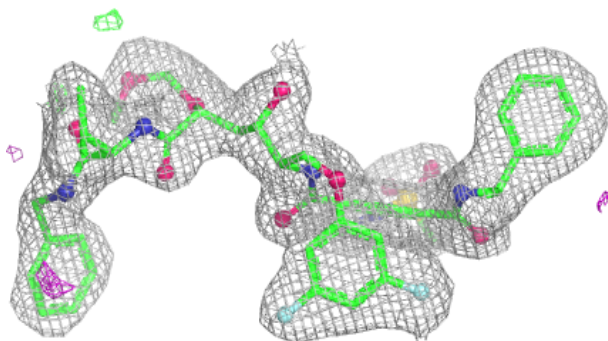
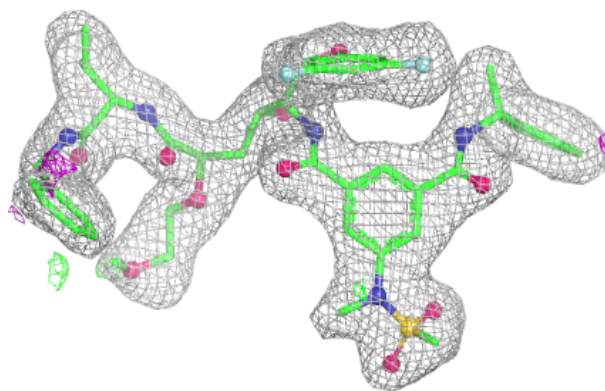


Electron density around MV7 B 531:

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

**Electron density around MV7 A 531:**

$2mF_o-DF_c$ (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.