



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:05 PM UTC

PDB ID : 6PKC / pdb_00006pkc
Title : Inhibition of Human Menin by VTP-50469
Authors : McKeever, B.M.; Chen, G.; Van Orton, R.
Deposited on : 2019-06-29
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

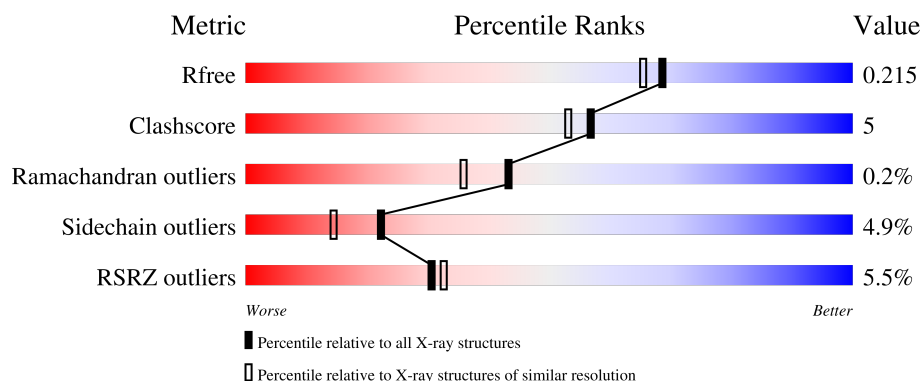
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	490	5% 82% 10% 6%
1	B	490	6% 76% 17% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8097 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.

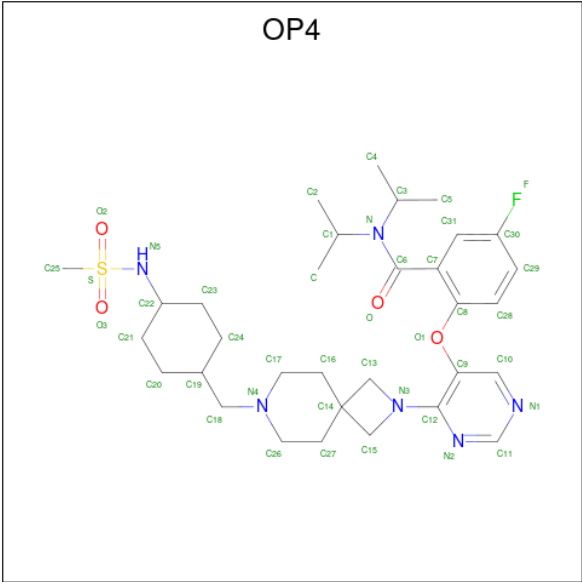
- Molecule 1 is a protein called Menin,Menin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	7	0
			3708	2371	634	687	16			
1	B	461	Total	C	N	O	S	0	10	0
			3729	2381	640	692	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O00255
A	1	SER	-	expression tag	UNP O00255
A	5	THR	ALA	engineered mutation	UNP O00255
B	0	GLY	-	expression tag	UNP O00255
B	1	SER	-	expression tag	UNP O00255
B	5	THR	ALA	engineered mutation	UNP O00255

- Molecule 2 is 5-fluoro-2-({4-[7-({trans-4-[(methylsulfonyl)amino]cyclohexyl)methyl]-2,7-diazaspiro[3.5]nonan-2-yl}pyrimidin-5-yl}oxy)-N,N-di(propan-2-yl)benzamide (CCD ID: OP4) (formula: C₃₂H₄₇FN₆O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			44	32	1	6	4	1		
2	B	1	Total	C	F	N	O	S	0	0
			44	32	1	6	4	1		

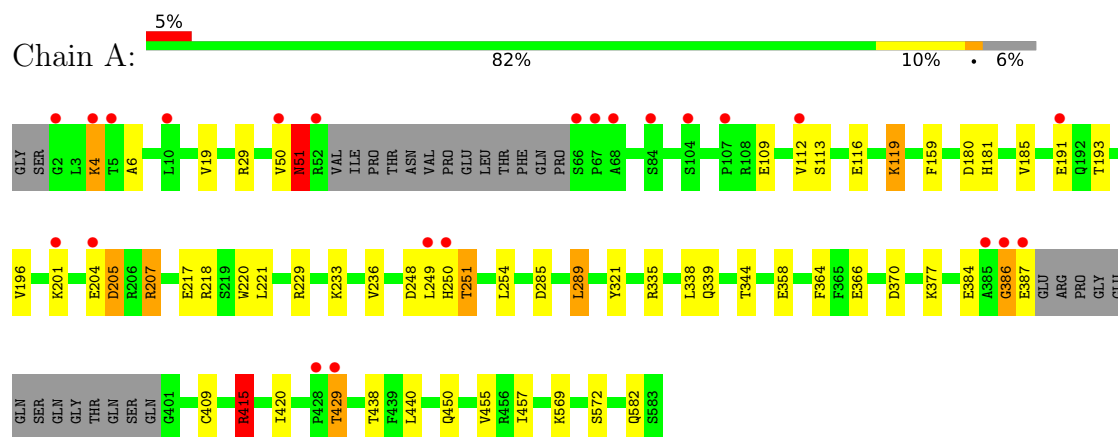
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	289	Total	O	0	0
			289	289		
3	B	283	Total	O	0	0
			283	283		

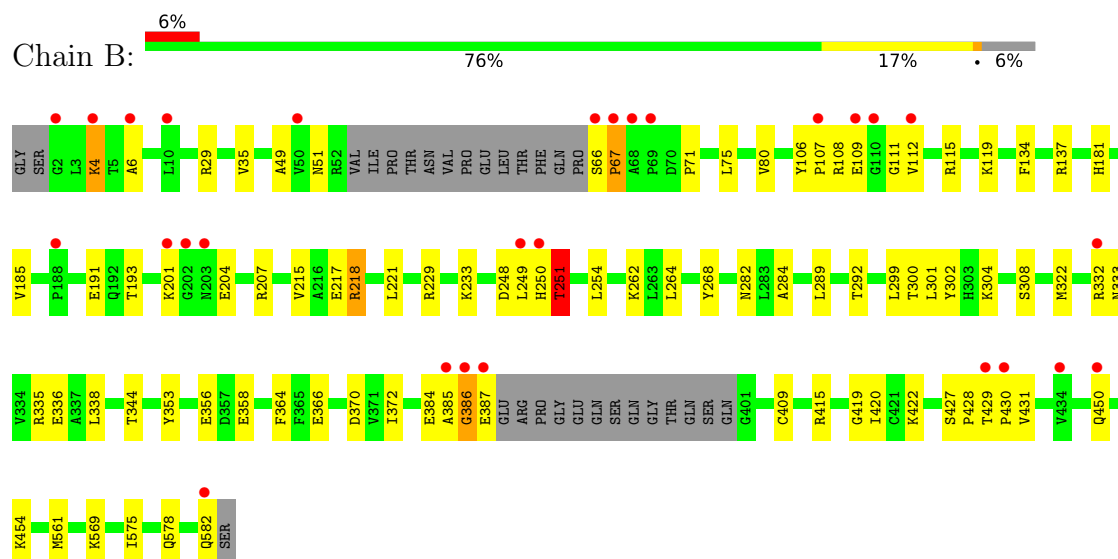
3 Residue-property plots [i](#)

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: Menin,Menin



• Molecule 1: Menin,Menin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.97Å 86.08Å 202.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 1.90 48.65 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.65-1.90) 99.9 (48.65-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.93 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.168 , 0.206 0.179 , 0.215	Depositor DCC
R_{free} test set	4146 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	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	0.96	EDS
Total number of atoms	8097	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: OP4

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	1.33	13/3791 (0.3%)	1.12	13/5141 (0.3%)
1	B	1.29	13/3812 (0.3%)	1.17	15/5168 (0.3%)
All	All	1.31	26/7603 (0.3%)	1.15	28/10309 (0.3%)

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	A	0	2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	GLY	C-N	13.27	1.51	1.33
1	A	572	SER	CA-C	-8.23	1.42	1.52
1	B	386	GLY	C-N	7.60	1.44	1.33
1	B	207	ARG	CD-NE	-7.31	1.36	1.46
1	B	262	LYS	CA-C	-6.57	1.44	1.52
1	A	415	ARG	CD-NE	-6.42	1.37	1.46
1	B	292	THR	CA-C	6.24	1.59	1.52
1	A	217	GLU	CA-C	6.04	1.61	1.52
1	A	440	LEU	N-CA	5.98	1.53	1.46
1	A	159	PHE	N-CA	-5.91	1.39	1.46
1	A	207	ARG	CD-NE	-5.78	1.38	1.46
1	A	113	SER	CA-C	-5.53	1.45	1.52
1	A	289	LEU	C-O	-5.42	1.17	1.24
1	A	236	VAL	N-CA	-5.40	1.40	1.46
1	B	299	LEU	CA-C	-5.40	1.45	1.52
1	B	308	SER	C-O	5.40	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ASP	CA-C	5.38	1.59	1.52
1	B	80	VAL	CA-CB	5.35	1.60	1.54
1	A	429	THR	CA-C	5.22	1.58	1.52
1	B	49	ALA	C-O	-5.18	1.17	1.24
1	B	419	GLY	C-O	-5.17	1.17	1.23
1	B	215	VAL	C-O	5.12	1.29	1.24
1	B	575	ILE	CA-C	-5.06	1.46	1.52
1	B	264	LEU	CA-C	5.05	1.59	1.52
1	B	134	PHE	C-O	-5.03	1.18	1.23
1	A	19	VAL	N-CA	5.01	1.52	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	GLY	CA-C-N	-14.62	95.38	121.70
1	B	386	GLY	C-N-CA	-14.62	95.38	121.70
1	B	386	GLY	O-C-N	13.84	140.69	122.70
1	A	415	ARG	CD-NE-CZ	10.12	138.56	124.40
1	B	207	ARG	NE-CZ-NH2	-9.61	110.55	119.20
1	A	207	ARG	NE-CZ-NH2	-9.60	110.56	119.20
1	A	415	ARG	NE-CZ-NH1	-9.19	112.31	121.50
1	B	207	ARG	NE-CZ-NH1	7.64	129.14	121.50
1	A	207	ARG	NE-CZ-NH1	7.18	128.68	121.50
1	A	358	GLU	CA-CB-CG	7.06	128.23	114.10
1	A	415	ARG	CG-CD-NE	6.65	126.64	112.00
1	A	51	ASN	N-CA-C	6.51	119.37	111.82
1	A	218	ARG	NE-CZ-NH2	-6.34	113.49	119.20
1	B	431	VAL	N-CA-C	-6.33	106.61	111.62
1	B	218	ARG	NE-CZ-NH2	-6.04	113.76	119.20
1	A	218	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	B	67	PRO	CA-N-CD	-5.95	103.67	112.00
1	B	372	ILE	O-C-N	5.79	124.12	120.42
1	A	386	GLY	O-C-N	-5.79	115.18	122.70
1	B	137	ARG	NE-CZ-NH2	-5.67	114.09	119.20
1	B	229	ARG	CG-CD-NE	-5.52	99.86	112.00
1	B	251	THR	N-CA-C	5.51	118.40	108.48
1	B	35	VAL	N-CA-C	5.39	115.59	110.42
1	A	205	ASP	CB-CA-C	5.31	118.58	109.51
1	B	218	ARG	CG-CD-NE	-5.24	100.47	112.00
1	A	358	GLU	N-CA-CB	-5.22	101.89	110.14
1	B	218	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	A	218	ARG	CG-CD-NE	-5.00	101.00	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	386	GLY	Mainchain
1	A	415	ARG	Sidechain

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	3708	0	3671	26	1
1	B	3729	0	3684	44	1
2	A	44	0	0	0	0
2	B	44	0	0	0	0
3	A	289	0	0	3	0
3	B	283	0	0	4	0
All	All	8097	0	7355	69	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 5.

All (69) 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:B:429:THR:HG22	1:B:430:PRO:HD2	1.24	1.16
1:B:429:THR:CG2	1:B:430:PRO:HD2	1.90	1.01
1:B:335:ARG:HG2	1:B:409[C]:CYS:SG	2.08	0.93
1:B:384:GLU:O	1:B:387:GLU:HG2	1.69	0.93
1:B:385:ALA:C	1:B:387:GLU:H	1.79	0.89
1:B:353:TYR:O	1:B:428:PRO:HD2	1.74	0.86
1:B:384:GLU:O	1:B:387:GLU:CG	2.29	0.81
1:A:338:LEU:HD12	1:A:409[B]:CYS:SG	2.23	0.79
1:B:66:SER:N	1:B:67:PRO:HD3	1.99	0.76
1:A:338:LEU:CD1	1:A:409[B]:CYS:SG	2.74	0.76
1:B:429:THR:HG22	1:B:430:PRO:CD	2.12	0.75
1:B:385:ALA:C	1:B:387:GLU:N	2.44	0.74
1:B:338:LEU:HD12	1:B:409[B]:CYS:SG	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:SER:N	1:B:67:PRO:CD	2.56	0.67
1:A:455[A]:VAL:CG1	1:A:457:ILE:HD12	2.26	0.66
1:B:338:LEU:CD1	1:B:409[B]:CYS:SG	2.84	0.65
1:A:321:TYR:HB2	1:A:344:THR:HG22	1.81	0.62
1:A:438[B]:THR:HG21	1:B:358:GLU:OE1	2.00	0.61
1:A:455[A]:VAL:HG11	1:A:457:ILE:HD12	1.82	0.61
1:A:335:ARG:HG2	1:A:409[C]:CYS:SG	2.42	0.60
1:B:384:GLU:O	1:B:387:GLU:CB	2.50	0.59
1:B:268:TYR:OH	1:B:304:LYS:HE3	2.03	0.58
1:A:455[A]:VAL:CG1	1:A:457:ILE:CD1	2.80	0.58
1:B:429:THR:CG2	1:B:430:PRO:CD	2.76	0.57
1:A:377:LYS:HE2	3:B:769:HOH:O	2.04	0.56
1:B:385:ALA:O	1:B:387:GLU:N	2.38	0.55
1:A:229:ARG:NH1	3:A:703:HOH:O	2.38	0.55
1:B:282:ASN:HB2	3:B:719:HOH:O	2.06	0.55
1:A:366[A]:GLU:OE2	1:A:370:ASP:OD2	2.24	0.54
1:A:4:LYS:HE3	1:A:6:ALA:HB3	1.90	0.53
1:B:422:LYS:HE3	3:B:937:HOH:O	2.09	0.53
1:B:217:GLU:OE1	1:B:356:GLU:OE1	2.27	0.52
1:B:4:LYS:HE3	1:B:6:ALA:HB3	1.91	0.52
1:B:71:PRO:HG2	1:B:75:LEU:HG	1.91	0.51
1:B:300:THR:O	1:B:304:LYS:HG3	2.10	0.51
1:B:115:ARG:HG2	1:B:119:LYS:HD2	1.93	0.51
1:B:106:TYR:O	1:B:108:ARG:N	2.46	0.49
1:A:51:ASN:O	1:A:51:ASN:ND2	2.45	0.49
1:A:455[A]:VAL:HG13	1:A:457:ILE:CD1	2.43	0.48
1:B:332:ARG:NH2	3:B:704:HOH:O	2.44	0.48
1:B:384:GLU:O	1:B:387:GLU:N	2.48	0.47
1:B:284:ALA:HB3	1:B:302:TYR:CE1	2.50	0.47
1:A:364:PHE:CD1	1:A:420[A]:ILE:HD11	2.50	0.47
1:A:384:GLU:O	1:A:387:GLU:HG3	2.15	0.46
1:B:322[A]:MET:HE2	1:B:344:THR:HG21	1.97	0.46
1:A:4:LYS:CE	1:A:6:ALA:HB3	2.45	0.46
1:B:4:LYS:CE	1:B:6:ALA:HB3	2.45	0.46
1:B:561:MET:HB3	1:B:578[A]:GLN:HG2	1.96	0.46
1:B:185:VAL:HG12	1:B:193:THR:HG22	1.97	0.46
1:B:384:GLU:O	1:B:387:GLU:HB3	2.16	0.45
1:B:364:PHE:CD1	1:B:420[A]:ILE:HD11	2.52	0.44
1:B:366:GLU:OE2	1:B:370:ASP:OD2	2.36	0.43
1:A:338:LEU:HD13	1:A:409[B]:CYS:SG	2.57	0.43
1:A:248:ASP:OD2	1:A:251:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:SER:HB3	1:B:428:PRO:HD2	2.01	0.43
1:B:248:ASP:OD2	1:B:251:THR:HG23	2.19	0.43
1:B:29:ARG:O	1:B:233:LYS:NZ	2.53	0.42
1:A:29:ARG:O	1:A:233:LYS:NZ	2.53	0.42
1:B:301:LEU:HD23	1:B:304:LYS:HD2	2.02	0.41
1:B:300:THR:HG22	1:B:304:LYS:HE2	2.02	0.41
1:B:333:ASN:HB3	1:B:336:GLU:OE2	2.20	0.41
1:A:119:LYS:CE	3:A:835:HOH:O	2.67	0.41
1:B:181:HIS:HB2	1:B:221:LEU:HD11	2.02	0.41
1:A:185:VAL:HG12	1:A:193:THR:HG22	2.01	0.41
1:B:429:THR:HG23	1:B:430:PRO:HD2	1.94	0.40
1:A:180:ASP:HB2	1:A:220:TRP:CH2	2.56	0.40
1:A:181:HIS:HB2	1:A:221:LEU:HD11	2.03	0.40
1:A:196:VAL:O	1:A:207:ARG:HD2	2.20	0.40
1:A:116:GLU:HB2	3:A:800:HOH:O	2.21	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:A:109:GLU:OE1	1:B:111:GLY:N[1_445]	1.83	0.37

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/490 (94%)	455 (98%)	8 (2%)	0	100	100
1	B	465/490 (95%)	454 (98%)	9 (2%)	2 (0%)	30	22
All	All	928/980 (95%)	909 (98%)	17 (2%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	107	PRO
1	B	386	GLY

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	395/413 (96%)	374 (95%)	21 (5%)	20	12
1	B	397/413 (96%)	377 (95%)	20 (5%)	22	14
All	All	792/826 (96%)	751 (95%)	41 (5%)	22	13

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	50	VAL
1	A	51	ASN
1	A	112	VAL
1	A	119	LYS
1	A	191	GLU
1	A	201	LYS
1	A	204	GLU
1	A	205	ASP
1	A	249	LEU
1	A	250	HIS
1	A	251	THR
1	A	254[A]	LEU
1	A	254[B]	LEU
1	A	289	LEU
1	A	339	GLN
1	A	415	ARG
1	A	429	THR
1	A	450	GLN
1	A	569	LYS
1	A	582	GLN
1	B	4	LYS

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Mol	Chain	Res	Type
1	B	51	ASN
1	B	109	GLU
1	B	112	VAL
1	B	191	GLU
1	B	201	LYS
1	B	204	GLU
1	B	218	ARG
1	B	249	LEU
1	B	250	HIS
1	B	251	THR
1	B	254[A]	LEU
1	B	254[B]	LEU
1	B	289	LEU
1	B	415[A]	ARG
1	B	415[B]	ARG
1	B	450	GLN
1	B	454	LYS
1	B	569	LYS
1	B	582	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	209	GLN
1	A	282	ASN
1	A	442	GLN
1	A	450	GLN
1	B	96	GLN
1	B	203	ASN
1	B	260	GLN
1	B	333	ASN
1	B	450	GLN

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](#)

2 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	OP4	A	601	-	48,48,48	1.73	12 (25%)	61,71,71	2.26	17 (27%)
2	OP4	B	601	-	48,48,48	2.13	13 (27%)	61,71,71	1.92	13 (21%)

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	OP4	A	601	-	-	2/29/65/65	0/5/5/5
2	OP4	B	601	-	-	2/29/65/65	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	OP4	C25-S	-8.69	1.55	1.75
2	A	601	OP4	C25-S	-4.59	1.65	1.75
2	B	601	OP4	C9-C12	4.54	1.45	1.40
2	A	601	OP4	C7-C8	4.22	1.48	1.40
2	B	601	OP4	O2-S	3.91	1.49	1.43
2	B	601	OP4	O3-S	3.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	OP4	C15-C14	-3.50	1.51	1.54
2	A	601	OP4	C6-N	-3.43	1.29	1.35
2	A	601	OP4	C31-C30	3.26	1.43	1.37
2	B	601	OP4	C3-N	-3.03	1.44	1.48
2	B	601	OP4	C22-N5	3.00	1.52	1.47
2	B	601	OP4	C7-C8	2.97	1.46	1.40
2	A	601	OP4	C29-C30	2.85	1.42	1.37
2	B	601	OP4	O1-C8	-2.83	1.33	1.39
2	B	601	OP4	C29-C30	2.80	1.42	1.37
2	B	601	OP4	C1-N	2.67	1.53	1.48
2	A	601	OP4	C15-N3	-2.66	1.44	1.48
2	A	601	OP4	C26-N4	2.55	1.53	1.46
2	A	601	OP4	C11-N1	-2.45	1.28	1.33
2	A	601	OP4	O1-C8	-2.42	1.34	1.39
2	B	601	OP4	S-N5	-2.38	1.57	1.62
2	B	601	OP4	C31-C7	-2.16	1.36	1.39
2	A	601	OP4	O-C6	2.14	1.26	1.22
2	A	601	OP4	C9-C12	2.12	1.43	1.40
2	A	601	OP4	C5-C3	2.00	1.57	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	OP4	O3-S-O2	-10.33	105.02	118.87
2	B	601	OP4	O3-S-O2	-5.12	112.01	118.87
2	B	601	OP4	C9-C12-N2	-4.94	117.22	124.58
2	A	601	OP4	C9-C12-N2	-4.93	117.23	124.58
2	B	601	OP4	O-C6-C7	-4.79	110.65	120.06
2	A	601	OP4	O2-S-C25	4.39	115.21	108.26
2	A	601	OP4	C11-N2-C12	4.06	121.75	111.83
2	B	601	OP4	C8-C7-C6	-4.03	115.28	122.26
2	B	601	OP4	C7-C6-N	4.01	124.02	118.77
2	B	601	OP4	C10-N1-C11	4.01	120.53	115.80
2	A	601	OP4	C10-N1-C11	3.56	120.00	115.80
2	B	601	OP4	C16-C17-N4	3.45	114.68	111.16
2	A	601	OP4	C8-C7-C6	-3.39	116.39	122.26
2	B	601	OP4	C11-N2-C12	3.37	120.05	111.83
2	A	601	OP4	C19-C18-N4	-3.32	108.79	114.06
2	B	601	OP4	C9-C10-N1	-3.23	118.75	122.83
2	A	601	OP4	C7-C6-N	3.21	122.97	118.77
2	A	601	OP4	O-C6-C7	-3.13	113.91	120.06
2	A	601	OP4	C23-C22-N5	-3.08	104.93	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	OP4	C25-S-N5	3.03	113.52	106.83
2	B	601	OP4	C23-C22-N5	-2.87	105.31	110.47
2	A	601	OP4	C13-N3-C12	2.74	133.31	125.20
2	A	601	OP4	C24-C23-C22	2.58	114.33	111.49
2	A	601	OP4	C9-C10-N1	-2.53	119.64	122.83
2	A	601	OP4	C4-C3-N	-2.39	108.18	111.78
2	A	601	OP4	N1-C11-N2	-2.37	123.30	127.33
2	A	601	OP4	C26-N4-C18	-2.35	104.84	111.35
2	B	601	OP4	C13-N3-C15	2.19	97.78	93.99
2	B	601	OP4	C31-C7-C6	2.14	124.65	118.57
2	B	601	OP4	C5-C3-N	-2.14	108.56	111.78

There are no chirality outliers.

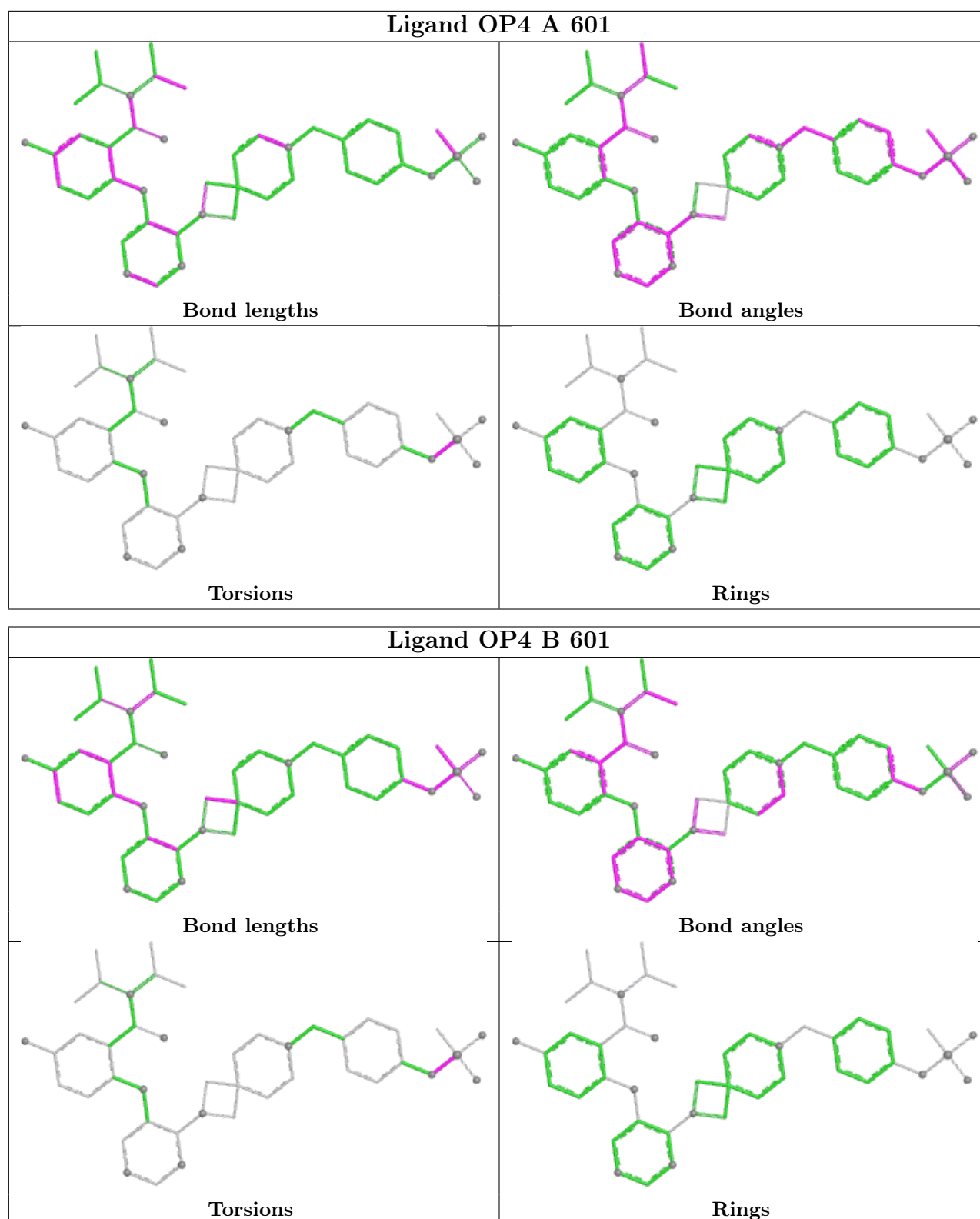
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	OP4	C22-N5-S-O3
2	B	601	OP4	C22-N5-S-O3
2	A	601	OP4	C22-N5-S-C25
2	B	601	OP4	C22-N5-S-C25

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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	462/490 (94%)	0.07	23 (4%) 34 36	9, 26, 55, 88	7 (1%)
1	B	461/490 (94%)	0.09	28 (6%) 27 29	9, 25, 60, 99	10 (2%)
All	All	923/980 (94%)	0.08	51 (5%) 30 32	9, 25, 58, 99	17 (1%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	SER	5.1
1	B	429	THR	4.4
1	A	249	LEU	4.2
1	A	50	VAL	4.2
1	B	430	PRO	4.1
1	B	386	GLY	4.0
1	B	67	PRO	3.9
1	B	201	LYS	3.9
1	B	202	GLY	3.9
1	B	387	GLU	3.8
1	B	249	LEU	3.8
1	B	250	HIS	3.6
1	B	68	ALA	3.5
1	A	250	HIS	3.5
1	A	387	GLU	3.5
1	A	4	LYS	3.4
1	B	203	ASN	3.4
1	B	582	GLN	3.3
1	A	67	PRO	3.2
1	B	110	GLY	2.8
1	B	385	ALA	2.8
1	B	112	VAL	2.7
1	B	2	GLY	2.7
1	A	10	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	68	ALA	2.6
1	A	107	PRO	2.6
1	A	66	SER	2.6
1	B	188	PRO	2.5
1	A	112	VAL	2.5
1	B	450	GLN	2.4
1	B	332	ARG	2.4
1	B	107	PRO	2.4
1	B	109	GLU	2.3
1	A	386	GLY	2.3
1	A	84	SER	2.3
1	B	6	ALA	2.3
1	A	429	THR	2.3
1	A	385	ALA	2.2
1	B	50	VAL	2.2
1	B	4	LYS	2.2
1	A	52	ARG	2.2
1	A	191	GLU	2.2
1	A	2	GLY	2.2
1	B	434	VAL	2.1
1	A	201	LYS	2.1
1	A	5	THR	2.1
1	A	104	SER	2.1
1	A	428	PRO	2.1
1	B	10	LEU	2.0
1	A	204	GLU	2.0
1	B	69	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

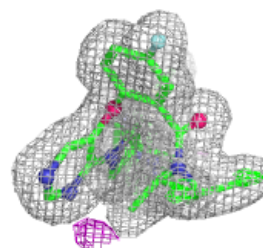
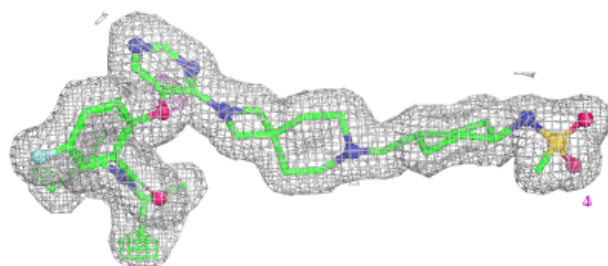
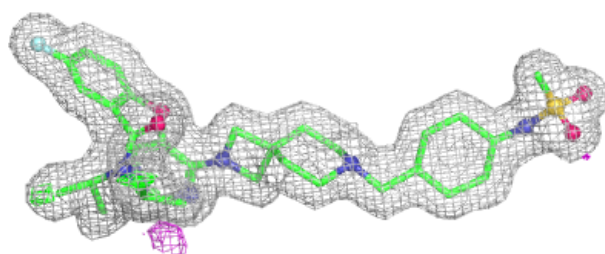
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OP4	A	601	44/44	0.97	0.06	15,18,25,26	0
2	OP4	B	601	44/44	0.98	0.05	14,16,22,30	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.

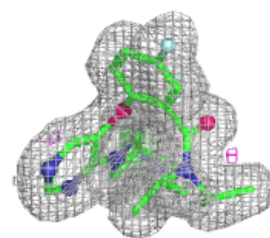
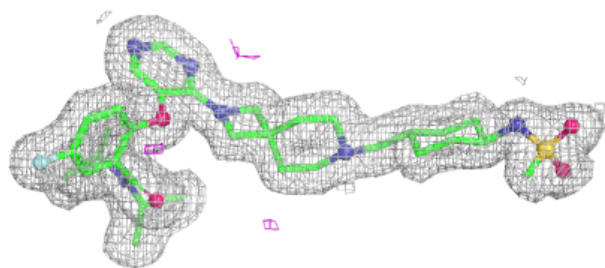
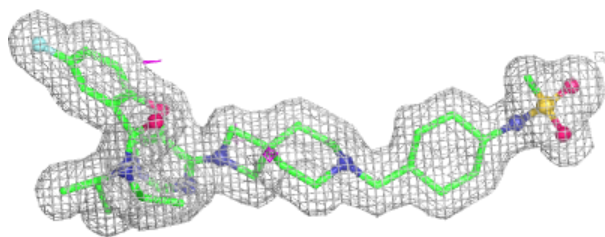
Electron density around OP4 A 601:

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 OP4 B 601:

$2mF_o-DF_c$ (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.