Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 06:27 AM EDT

PDB ID	:	3PP7
Title	:	Crystal structure of Leishmania mexicana pyruvate kinase in complex with the drug suramin, an inhibitor of glycolysis.
Authors	:	Morgan, H.P.; Auld, D.S.; McNae, I.W.; Nowicki, M.W.; Michels, P.A.M.; Fothergill-Gilmore, L.A.; Walkinshaw, M.D.
Deposited on	:	2010-11-24
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:

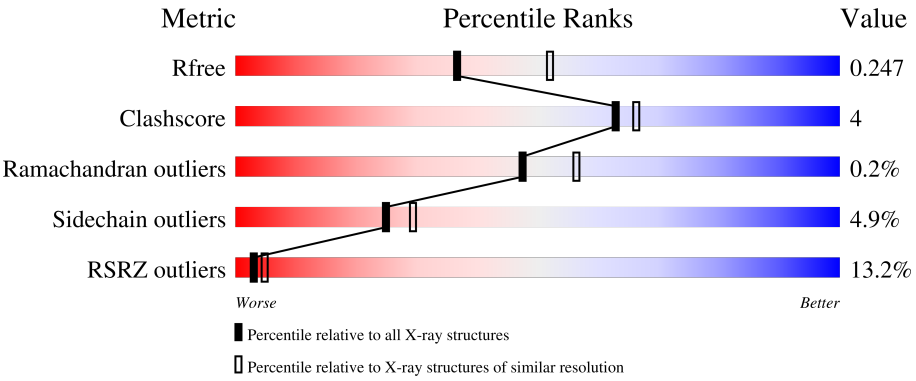
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 <=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	498	3% 89% 9% ··
1	B	498	23% 87% 11% ··

2 Entry composition

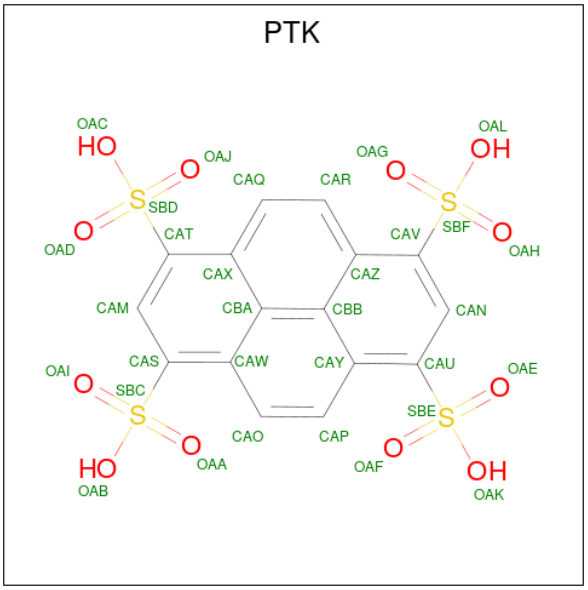
There are 6 unique types of molecules in this entry. The entry contains 8054 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate kinase.

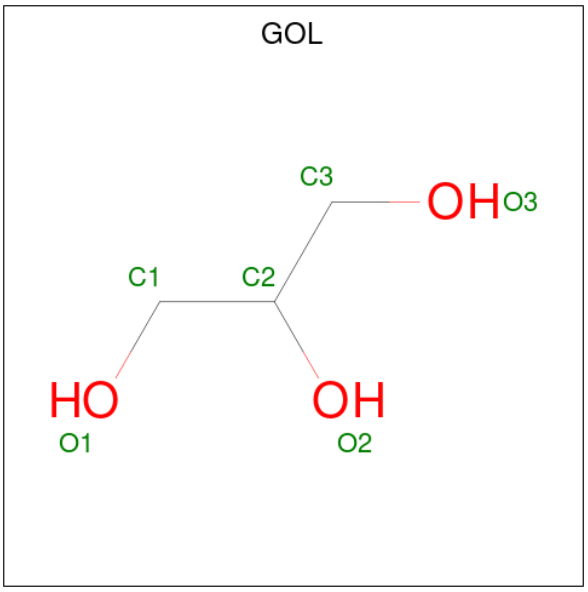
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	1	0
			3763	2345	663	729	26			
1	B	494	Total	C	N	O	S	0	0	0
			3766	2347	663	730	26			

- Molecule 2 is pyrene-1,3,6,8-tetrasulfonic acid (three-letter code: PTK) (formula: $C_{16}H_{10}O_{12}S_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			32	16	12	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

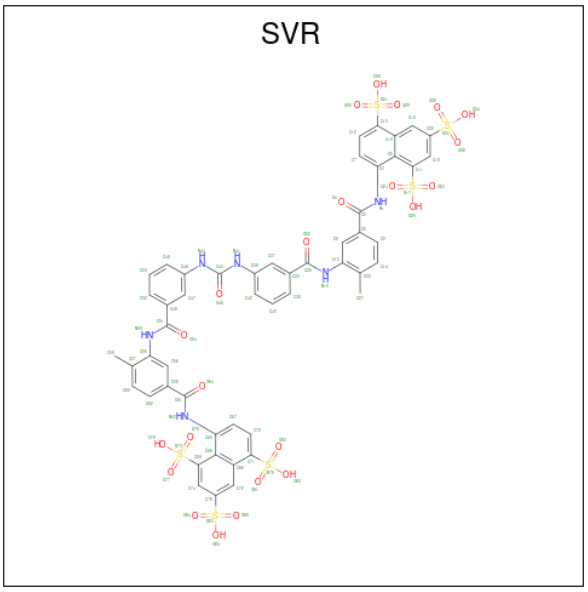


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total K 2 2	0	0
4	B	2	Total K 2 2	0	0

- Molecule 5 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFON IC ACID (three-letter code: SVR) (formula: $C_{51}H_{40}N_6O_{23}S_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			41	25	2	11	3		

- Molecule 6 is water.

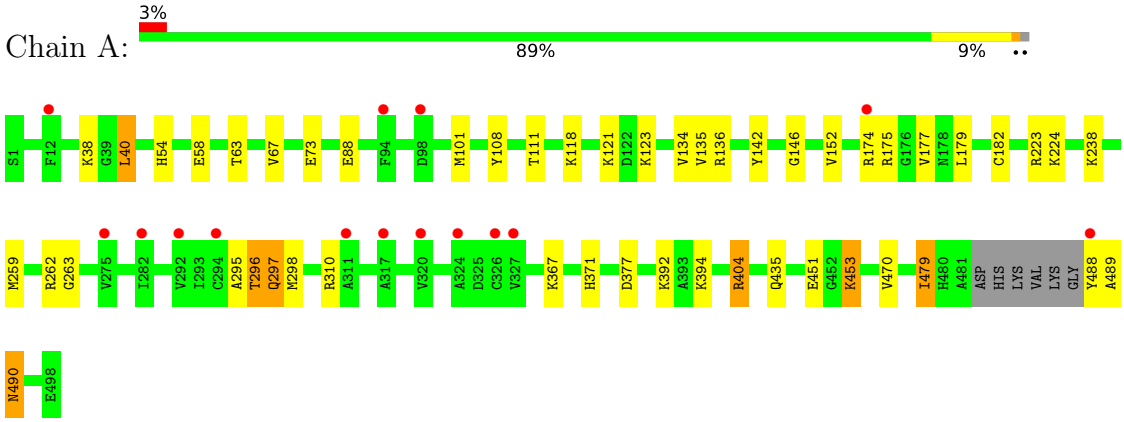
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	236	Total	O	0	0
			236	236		
6	B	200	Total	O	0	0
			200	200		

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.

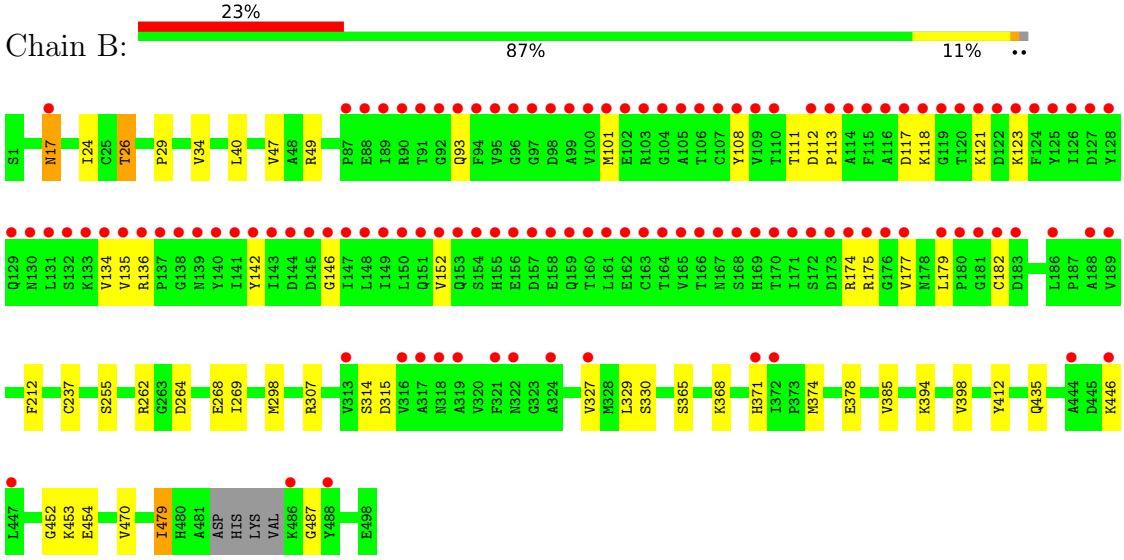
• Molecule 1: Pyruvate kinase

Chain A:



• Molecule 1: Pyruvate kinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.77Å 129.48Å 165.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.73 – 2.35 44.73 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (44.73-2.35) 98.0 (44.73-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.02	Depositor
$< I/\sigma(I) >$ [1]	4.55 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.191 , 0.231 0.208 , 0.247	Depositor DCC
R_{free} test set	2761 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8054	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: K, GOL, PTK, SVR

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	0.42	0/3819	0.55	0/5169
1	B	0.42	0/3821	0.56	0/5170
All	All	0.42	0/7640	0.55	0/10339

There are no bond length outliers.

There are no bond angle outliers.

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	3763	0	3758	32	0
1	B	3766	0	3768	33	0
2	A	32	0	8	0	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	B	41	0	18	3	0
6	A	236	0	0	2	0
6	B	200	0	0	1	0
All	All	8054	0	7568	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (65) 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:26:THR:HG21	1:B:49:ARG:HH11	1.38	0.87
1:A:263:GLY:H	1:A:296:THR:HG21	1.39	0.85
1:B:26:THR:HG23	1:B:330:SER:HA	1.62	0.81
1:A:479:ILE:HD11	1:A:489:ALA:CB	2.13	0.78
1:B:26:THR:HG21	1:B:49:ARG:NH1	2.00	0.74
1:A:295:ALA:O	1:A:296:THR:HB	1.85	0.74
1:B:26:THR:CG2	1:B:330:SER:HA	2.18	0.73
1:B:29:PRO:HG3	5:B:499:SVR:H56	1.71	0.72
1:A:223:ARG:HD2	6:A:609:HOH:O	1.90	0.71
1:A:263:GLY:N	1:A:296:THR:HG21	2.06	0.70
1:B:268:GLU:HG2	6:B:624:HOH:O	1.91	0.69
1:A:101:MET:HE1	1:A:121:LYS:HA	1.77	0.67
1:B:26:THR:CG2	1:B:49:ARG:HH11	2.08	0.67
1:A:377:ASP:HB3	1:A:488:TYR:CD2	2.30	0.65
1:B:135:VAL:HG11	1:B:152:VAL:HG21	1.81	0.63
1:A:135:VAL:HG11	1:A:152:VAL:HG21	1.84	0.59
1:B:101:MET:HE1	1:B:121:LYS:HA	1.86	0.57
1:A:296:THR:HG22	1:A:297:GLN:HG3	1.86	0.57
1:B:298:MET:HE3	1:B:327:VAL:HB	1.86	0.56
1:B:26:THR:CG2	1:B:329:LEU:O	2.53	0.56
1:A:404:ARG:CG	1:A:404:ARG:HH21	2.19	0.55
5:B:499:SVR:S73	5:B:499:SVR:N63	2.73	0.55
1:A:108:TYR:O	1:A:123:LYS:HA	2.09	0.53
1:B:108:TYR:O	1:B:123:LYS:HA	2.08	0.53
1:B:268:GLU:HG3	1:B:269:ILE:HG13	1.91	0.52
1:B:374:MET:CE	1:B:378:GLU:HG3	2.40	0.52
1:A:54[B]:HIS:C	1:A:54[B]:HIS:CD2	2.84	0.51
1:A:263:GLY:CA	1:A:296:THR:HG21	2.41	0.51
1:B:237:CYS:SG	1:B:255:SER:HB3	2.51	0.50
1:B:398:VAL:HG13	1:B:479:ILE:HG12	1.92	0.50
1:A:479:ILE:HD11	1:A:489:ALA:HB1	1.90	0.49
1:B:26:THR:HG23	1:B:329:LEU:O	2.12	0.49
1:A:392:LYS:O	1:A:394:LYS:HE3	2.12	0.48
1:B:394:LYS:HB2	1:B:470:VAL:HG12	1.95	0.48
1:A:88:GLU:HA	3:A:500:GOL:H2	1.95	0.48
1:B:29:PRO:CG	5:B:499:SVR:H56	2.42	0.48
1:A:263:GLY:HA3	1:A:296:THR:HG21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LYS:HB2	1:A:470:VAL:HG12	1.97	0.47
1:A:404:ARG:HH21	1:A:404:ARG:HG3	1.79	0.46
1:B:142:TYR:HB3	1:B:146:GLY:HA2	1.98	0.46
1:B:26:THR:HG22	1:B:329:LEU:O	2.15	0.46
1:A:142:TYR:HB3	1:A:146:GLY:HA2	1.98	0.45
1:B:112:ASP:HA	1:B:113:PRO:HD3	1.86	0.45
1:B:365:SER:HA	1:B:368:LYS:HE3	1.98	0.45
1:A:404:ARG:CG	1:A:404:ARG:NH2	2.79	0.44
1:B:298:MET:CE	1:B:327:VAL:HB	2.45	0.44
1:B:17:ASN:N	1:B:17:ASN:HD22	2.15	0.44
1:B:134:VAL:CG1	1:B:182:CYS:HB3	2.47	0.44
1:B:17:ASN:HD22	1:B:17:ASN:H	1.66	0.43
1:B:385:VAL:HG21	1:B:412:TYR:HB2	1.99	0.43
1:B:374:MET:HE2	1:B:378:GLU:HG3	2.00	0.43
1:A:134:VAL:CG1	1:A:182:CYS:HB3	2.48	0.43
1:A:263:GLY:H	1:A:296:THR:CG2	2.20	0.42
1:A:490:ASN:N	1:A:490:ASN:HD22	2.18	0.42
1:A:58:GLU:HB2	6:A:529:HOH:O	2.19	0.42
1:A:38:LYS:CE	1:A:73:GLU:OE1	2.69	0.41
1:A:377:ASP:HB3	1:A:488:TYR:CE2	2.56	0.41
1:B:452:GLY:O	1:B:453:LYS:HB2	2.20	0.41
1:B:24:ILE:HG12	1:B:47:VAL:HB	2.03	0.41
1:A:451:GLU:O	1:A:453:LYS:HE2	2.21	0.41
1:A:310:ARG:NH2	1:B:315:ASP:OD1	2.55	0.40
1:B:93:GLN:HB2	1:B:117:ASP:HA	2.02	0.40
1:A:238:LYS:HG2	1:A:259:MET:SD	2.62	0.40
1:A:40:LEU:HD12	1:A:40:LEU:HA	1.95	0.40
1:A:63:THR:O	1:A:67:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	489/498 (98%)	479 (98%)	9 (2%)	1 (0%)	47 56
1	B	490/498 (98%)	477 (97%)	12 (2%)	1 (0%)	47 56
All	All	979/996 (98%)	956 (98%)	21 (2%)	2 (0%)	47 56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	487	GLY
1	A	296	THR

5.3.2 Protein sidechains (i)

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	412/416 (99%)	393 (95%)	19 (5%)	27 32
1	B	412/416 (99%)	391 (95%)	21 (5%)	24 27
All	All	824/832 (99%)	784 (95%)	40 (5%)	25 29

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	111	THR
1	A	118	LYS
1	A	136	ARG
1	A	174	ARG
1	A	175	ARG
1	A	177	VAL
1	A	179	LEU
1	A	224	LYS
1	A	262	ARG
1	A	297	GLN
1	A	298	MET
1	A	367	LYS
1	A	371	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	404	ARG
1	A	435	GLN
1	A	453	LYS
1	A	479	ILE
1	A	490	ASN
1	B	17	ASN
1	B	26	THR
1	B	34	VAL
1	B	40	LEU
1	B	111	THR
1	B	118	LYS
1	B	136	ARG
1	B	174	ARG
1	B	175	ARG
1	B	177	VAL
1	B	179	LEU
1	B	212	PHE
1	B	262	ARG
1	B	264	ASP
1	B	307	ARG
1	B	314	SER
1	B	371	HIS
1	B	435	GLN
1	B	446	LYS
1	B	454	GLU
1	B	479	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	178	ASN
1	A	490	ASN
1	B	17	ASN
1	B	242	HIS
1	B	305	ASN
1	B	364	ASN
1	B	455	HIS
1	B	471	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	PTK	A	499	-	31,35,35	1.37	4 (12%)	48,60,60	1.13	4 (8%)
3	GOL	A	500	-	5,5,5	0.29	0	5,5,5	0.58	0
3	GOL	B	502	-	5,5,5	0.31	0	5,5,5	0.35	0
5	SVR	B	499	-	42,44,93	1.24	4 (9%)	60,68,145	1.04	6 (10%)

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	PTK	A	499	-	-	0/24/24/24	0/4/4/4
3	GOL	A	500	-	-	2/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
5	SVR	B	499	-	-	6/34/34/76	0/4/4/8

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	499	SVR	C58-C61	3.08	1.56	1.50
5	B	499	SVR	C55-N53	-3.02	1.36	1.41
5	B	499	SVR	C49-C51	2.72	1.55	1.50
2	A	499	PTK	CAV-CAZ	-2.49	1.39	1.43
2	A	499	PTK	CAT-CAX	-2.46	1.39	1.43
5	B	499	SVR	C70-C71	2.14	1.40	1.37
2	A	499	PTK	CAS-CAW	-2.09	1.39	1.43
2	A	499	PTK	CAU-CAY	-2.02	1.39	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	499	PTK	CAQ-CAX-CAT	-3.34	119.22	123.60
2	A	499	PTK	CAR-CAZ-CAV	-3.01	119.65	123.60
5	B	499	SVR	C70-C71-C68	-2.47	118.52	121.00
5	B	499	SVR	C60-C57-C55	2.47	119.76	117.44
2	A	499	PTK	CAO-CAW-CAS	-2.47	120.37	123.60
5	B	499	SVR	C57-C55-N53	2.34	122.46	118.81
2	A	499	PTK	CAP-CAY-CAU	-2.30	120.58	123.60
5	B	499	SVR	C71-C68-C66	2.12	121.41	118.01
5	B	499	SVR	C67-C65-C66	-2.05	118.12	120.27
5	B	499	SVR	C72-C76-C74	-2.02	118.79	120.97

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	GOL	O1-C1-C2-O2
3	B	502	GOL	O1-C1-C2-C3
5	B	499	SVR	C62-C58-C61-O64
5	B	499	SVR	C56-C58-C61-N63
5	B	499	SVR	C62-C58-C61-N63
5	B	499	SVR	C56-C58-C61-O64
3	A	500	GOL	O1-C1-C2-C3
3	A	500	GOL	O1-C1-C2-O2
5	B	499	SVR	C56-C55-N53-C51
5	B	499	SVR	C57-C55-N53-C51

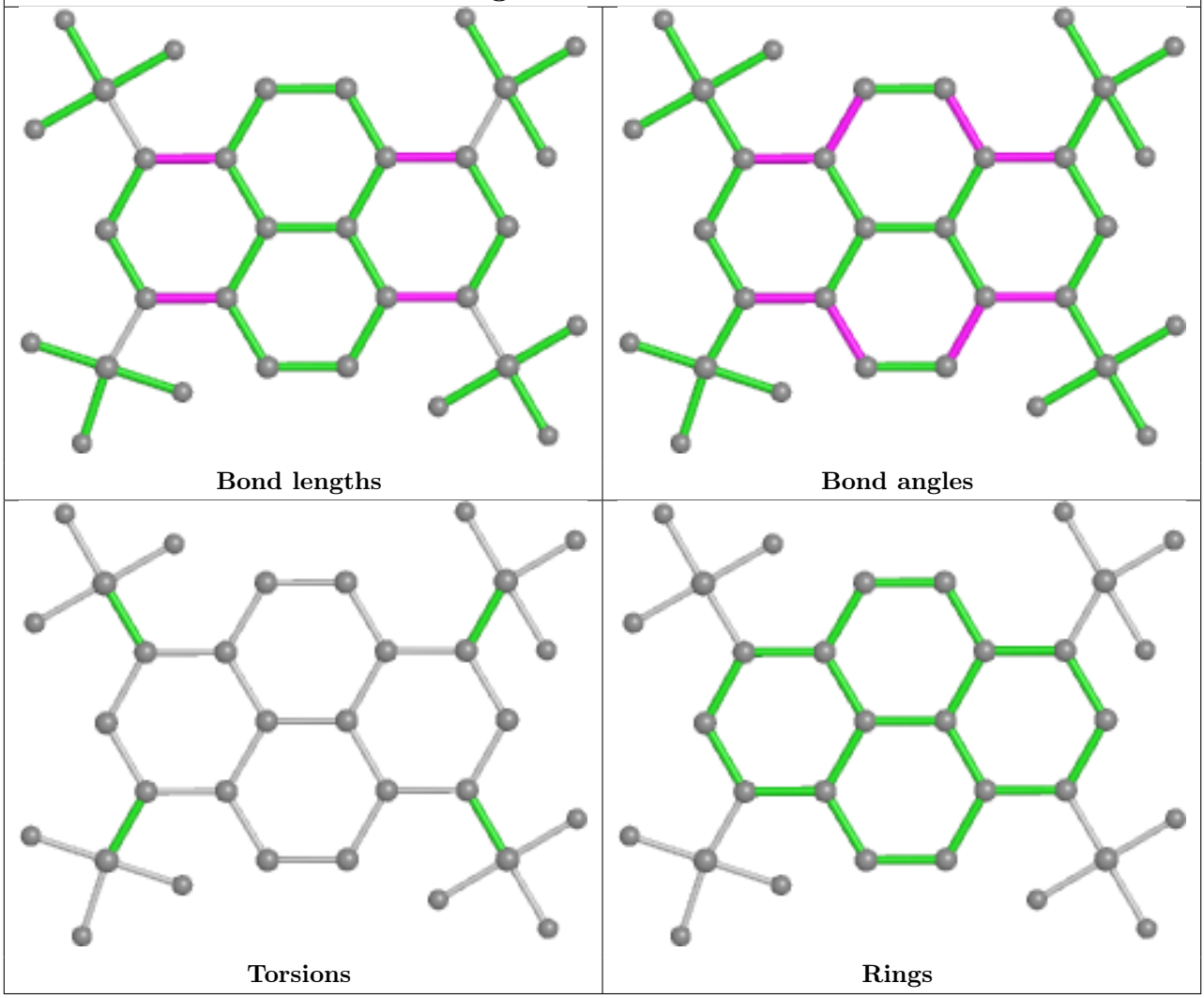
There are no ring outliers.

2 monomers are involved in 4 short contacts:

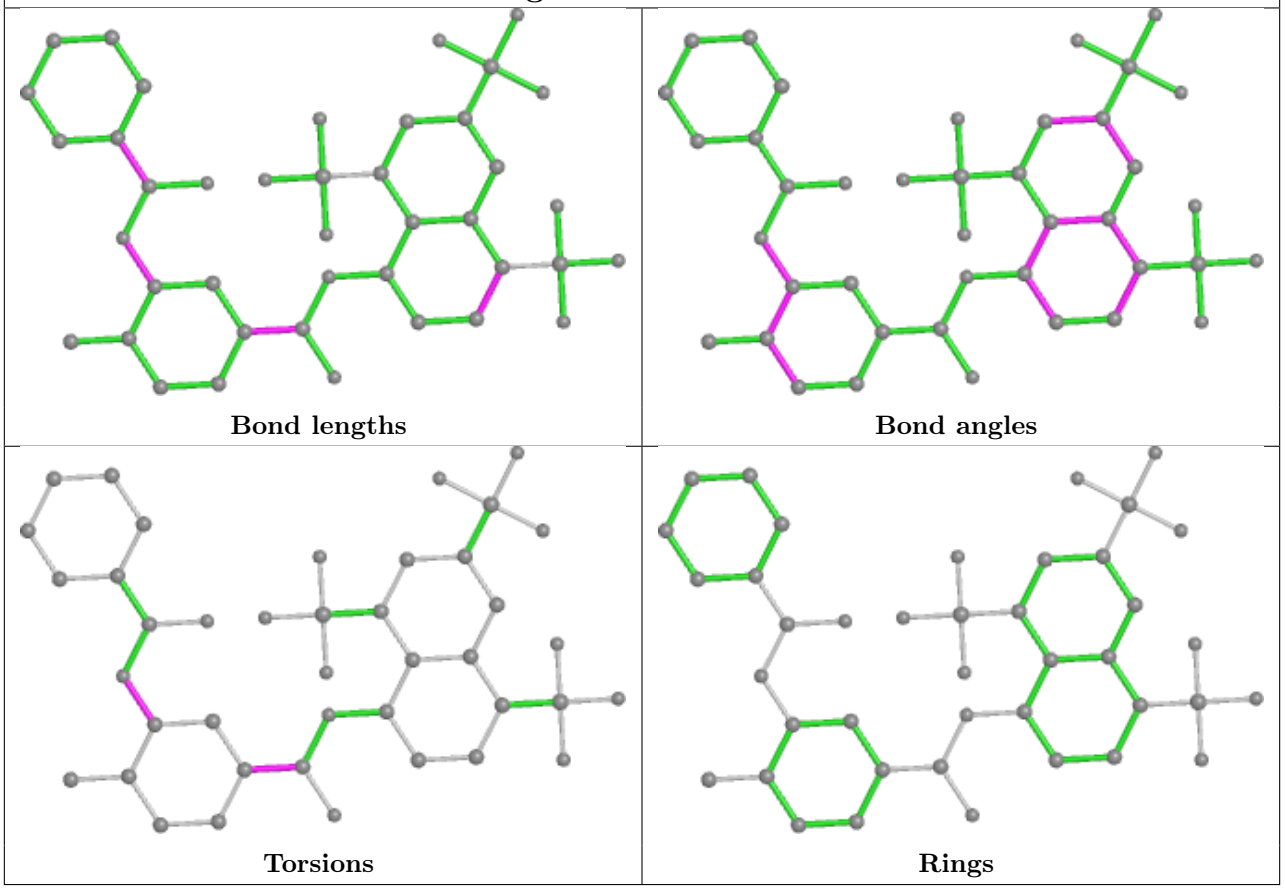
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	GOL	1	0
5	B	499	SVR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 PTK A 499



Ligand SVR B 499



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, 95^{th} 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	492/498 (98%)	0.35	15 (3%) 50 61	38, 55, 94, 109	0
1	B	494/498 (99%)	1.69	115 (23%) 0 1	37, 56, 215, 243	0
All	All	986/996 (98%)	1.02	130 (13%) 3 5	37, 55, 196, 243	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	VAL	22.1
1	B	171	ILE	21.5
1	B	124	PHE	17.4
1	B	126	ILE	17.2
1	B	172	SER	15.9
1	B	170	THR	14.9
1	B	92	GLY	14.7
1	B	94	PHE	14.6
1	B	106	THR	13.8
1	B	104	GLY	13.3
1	B	95	VAL	12.0
1	B	138	GLY	11.8
1	B	169	HIS	11.6
1	B	108	TYR	10.7
1	B	137	PRO	10.5
1	B	89	ILE	10.4
1	B	91	THR	9.5
1	B	107	CYS	9.2
1	B	175	ARG	9.2
1	B	164	THR	9.1
1	B	163	CYS	9.1
1	B	119	GLY	9.0
1	B	149	ILE	9.0
1	B	93	GLN	8.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	105	ALA	8.8
1	B	165	VAL	8.7
1	B	142	TYR	8.7
1	B	101	MET	8.6
1	B	167	ASN	8.5
1	B	143	ILE	8.4
1	B	122	ASP	8.0
1	B	103	ARG	8.0
1	B	99	ALA	8.0
1	B	90	ARG	7.9
1	B	133	LYS	7.9
1	B	152	VAL	7.7
1	B	150	LEU	7.6
1	B	134	VAL	7.6
1	B	125	TYR	7.5
1	B	140	TYR	7.4
1	B	96	GLY	7.2
1	B	181	GLY	7.2
1	B	168	SER	7.1
1	B	156	GLU	7.1
1	B	161	LEU	7.0
1	B	151	GLN	6.9
1	B	131	LEU	6.9
1	B	139	ASN	6.8
1	B	148	LEU	6.8
1	B	102	GLU	6.6
1	B	136	ARG	6.5
1	B	160	THR	6.4
1	B	141	ILE	6.4
1	B	173	ASP	6.2
1	B	135	VAL	6.2
1	B	162	GLU	6.2
1	B	153	GLN	6.0
1	B	121	LYS	5.9
1	B	155	HIS	5.9
1	B	166	THR	5.7
1	B	158	GLU	5.7
1	B	154	SER	5.7
1	B	146	GLY	5.6
1	B	157	ASP	5.6
1	B	100	VAL	5.6
1	B	115	PHE	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	113	PRO	5.3
1	B	110	THR	5.2
1	B	174	ARG	5.2
1	B	114	ALA	5.0
1	B	117	ASP	4.8
1	B	182	CYS	4.8
1	B	177	VAL	4.8
1	B	116	ALA	4.8
1	B	179	LEU	4.6
1	B	132	SER	4.5
1	B	159	GLN	4.3
1	B	97	GLY	4.3
1	B	180	PRO	4.3
1	B	147	ILE	4.1
1	B	98	ASP	3.9
1	B	188	ALA	3.7
1	B	129	GLN	3.7
1	B	120	THR	3.7
1	B	488	TYR	3.6
1	B	118	LYS	3.5
1	B	189	VAL	3.5
1	B	144	ASP	3.3
1	B	123	LYS	3.2
1	B	130	ASN	3.2
1	B	88	GLU	3.1
1	B	447	LEU	2.9
1	A	488	TYR	2.9
1	B	319	ALA	2.9
1	B	183	ASP	2.9
1	B	128	TYR	2.8
1	B	372	ILE	2.8
1	B	316	VAL	2.8
1	B	112	ASP	2.7
1	A	282	ILE	2.7
1	B	317	ALA	2.7
1	B	127	ASP	2.6
1	B	444	ALA	2.6
1	A	98	ASP	2.5
1	A	12	PHE	2.4
1	A	327	VAL	2.4
1	B	327	VAL	2.4
1	A	317	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	176	GLY	2.4
1	B	313	VAL	2.4
1	B	145	ASP	2.4
1	A	292	VAL	2.4
1	A	326	CYS	2.4
1	A	94	PHE	2.3
1	B	371	HIS	2.3
1	B	318	ASN	2.3
1	A	311	ALA	2.3
1	A	294	CYS	2.3
1	B	486	LYS	2.2
1	A	275	VAL	2.2
1	B	87	PRO	2.2
1	B	321	PHE	2.2
1	B	324	ALA	2.1
1	A	324	ALA	2.1
1	B	186	LEU	2.1
1	A	320	VAL	2.1
1	A	174	ARG	2.1
1	B	446	LYS	2.0
1	B	322	ASN	2.0
1	B	17	ASN	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 monosaccharides 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, 95^{th} 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
3	GOL	A	500	6/6	0.72	0.25	61,62,62,62	0

Continued on next page...

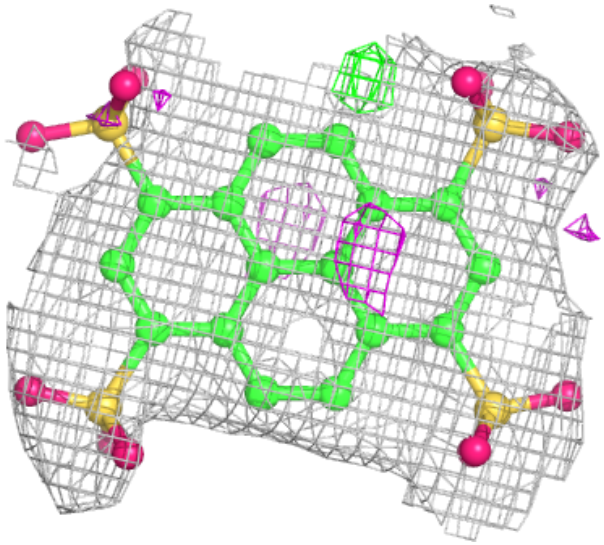
Continued from previous page...

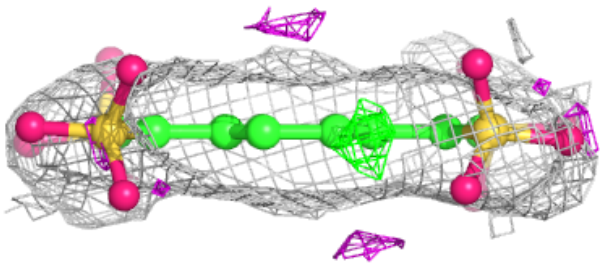
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	502	6/6	0.73	0.25	80,81,82,82	0
2	PTK	A	499	32/32	0.78	0.20	118,118,119,119	32
5	SVR	B	499	41/86	0.79	0.26	104,106,108,108	0
4	K	A	502	1/1	0.88	0.11	81,81,81,81	0
4	K	A	501	1/1	0.94	0.06	55,55,55,55	0
4	K	B	500	1/1	0.96	0.10	66,66,66,66	0
4	K	B	501	1/1	0.99	0.05	58,58,58,58	0

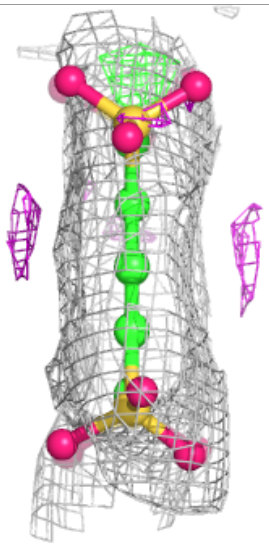
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTK A 499:

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

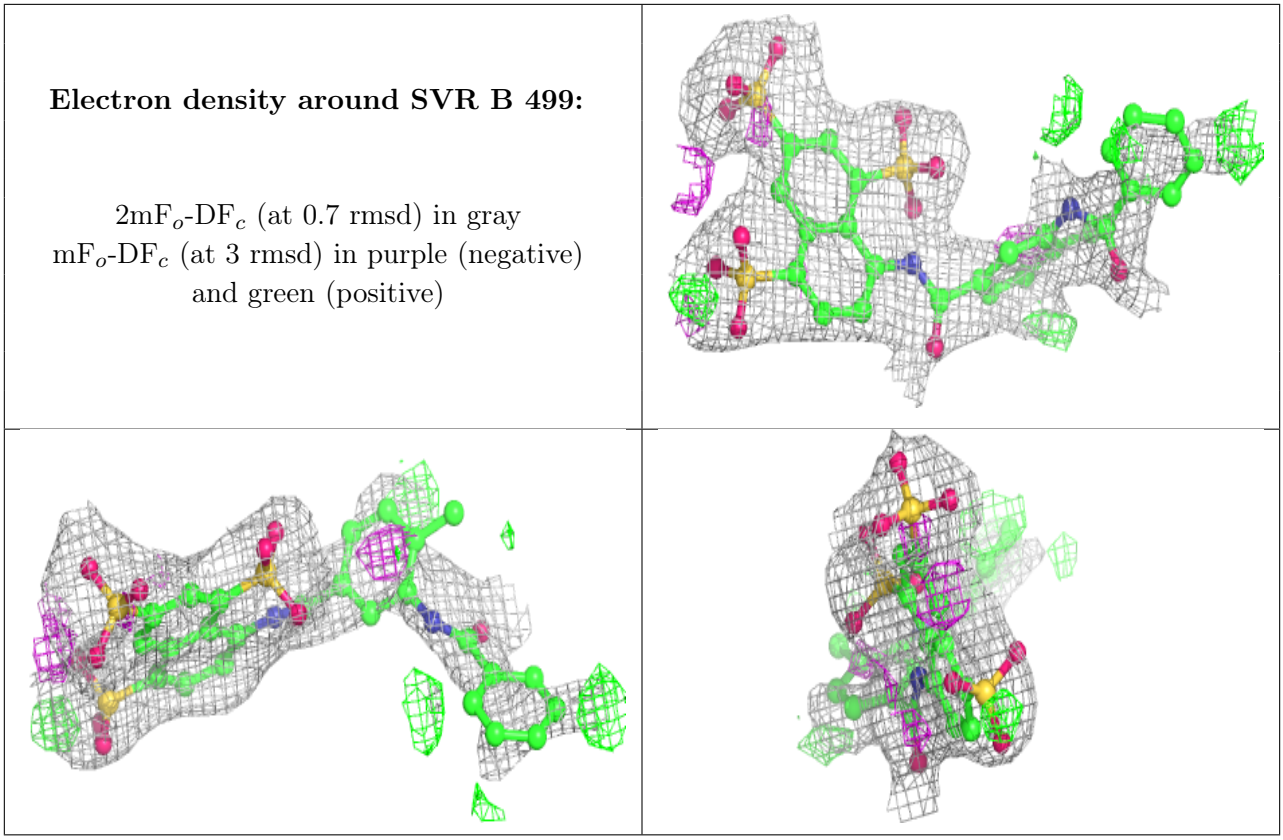






Electron density around SVR B 499:

$2mF_o$-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.