Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 09:21 PM EDT

PDB ID	:	3QV7
Title	:	Crystal structure of Leishmania mexicana pyruvate kinase(LmPYK)in complex with ponceau S and acid blue 25.
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	:	2011-02-25
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

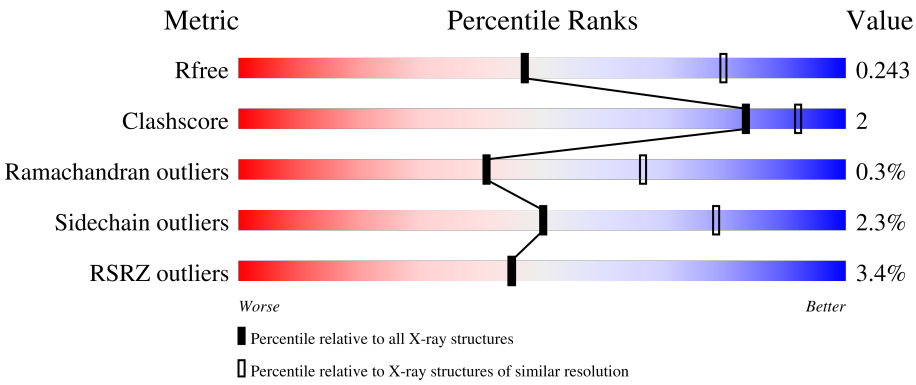
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	499	3% 91% 8% ••
1	B	499	% 75% 5% 20%
1	C	499	5% 74% 6% 20%
1	D	499	4% 93% 5% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	QV7	D	503	-	-	X	-

2 Entry composition (i)

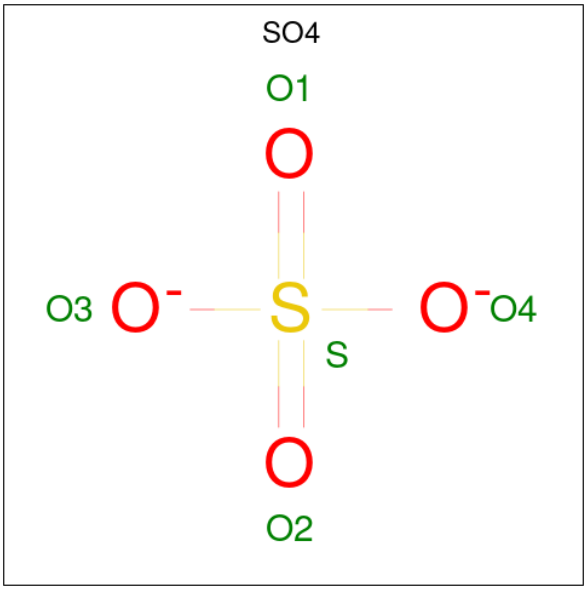
There are 6 unique types of molecules in this entry. The entry contains 14425 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	D	494	3793	2367	666	734	26	0	4	0
1	A	493	3774	2355	661	732	26	0	3	0
1	B	400	3051	1908	540	581	22	0	2	0
1	C	398	3032	1895	536	579	22	0	2	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	D	1	5	4	1	0	0
2	D	1	Total 5	O 4	S 1	0	0

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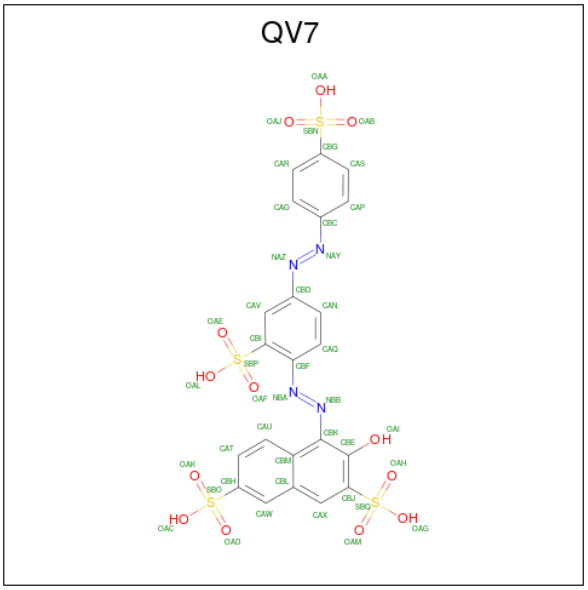
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	D	2	2	2	0	0
			Total	K		
3	A	2	2	2	0	0
			Total	K		
3	B	2	2	2	0	0
			Total	K		
3	C	2	2	2	0	0

- Molecule 4 is 3-hydroxy-4-[(E)-{2-sulfo-4-[(E)-(4-sulfophenyl)diazenyl]phenyl}diazenyl]naphthalene-2,7-disulfonic acid (three-letter code: QV7) (formula: $C_{22}H_{16}N_4O_{13}S_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	D	1	43	22	4	13	4	0	0
			Total	C	N	O	S		
4	A	1	43	22	4	13	4	0	0
			Total	C	N	O	S		
4	B	1	43	22	4	13	4	0	0

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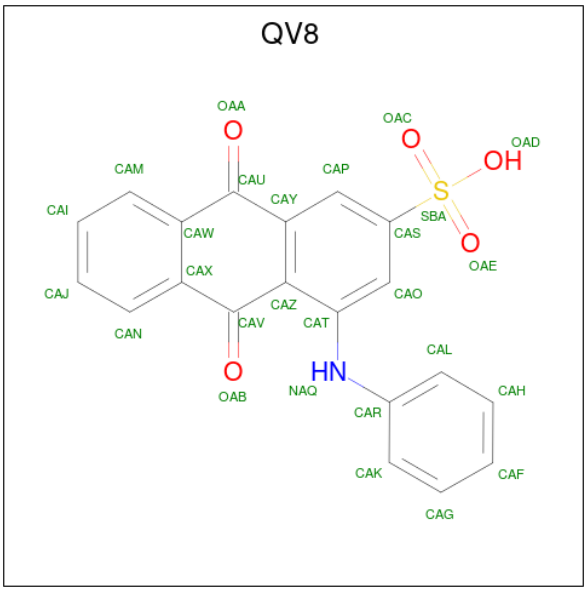
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	43	22	4	13	4	0	0
			Total	C	N	O	S		
4	B	1	43	22	4	13	4	0	0

- Molecule 5 is 9,10-dioxo-4-(phenylamino)-9,10-dihydroanthracene-2-sulfonic acid (three-letter code: QV8) (formula: $C_{20}H_{13}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	27	20	1	5	1	0	0

- Molecule 6 is water.

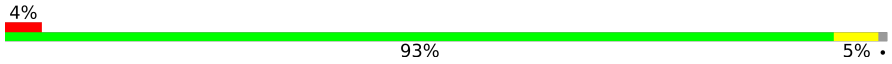
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	D	161	161	161	0	0
			Total	O		
6	A	167	167	167	0	0
			Total	O		
6	B	109	109	109	0	0
			Total	O		
6	C	68	68	68	0	0

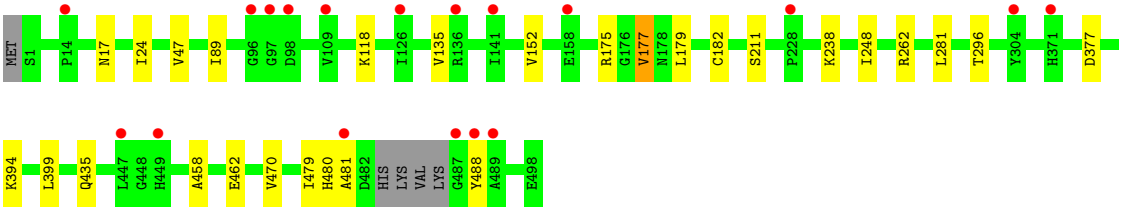
3 Residue-property plots (i)

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

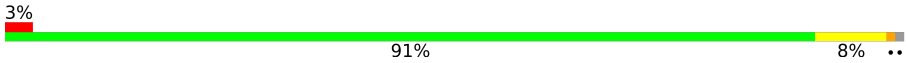
Chain D:

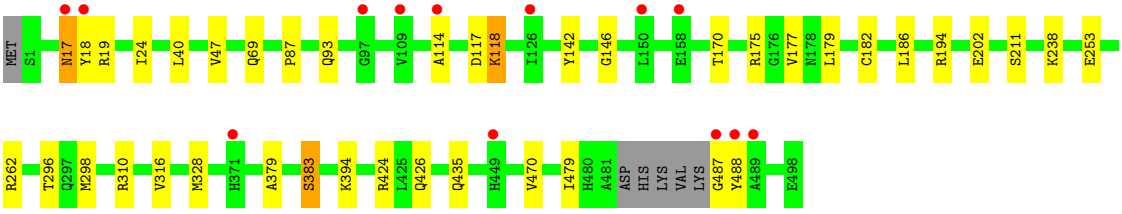




• Molecule 1: Pyruvate kinase

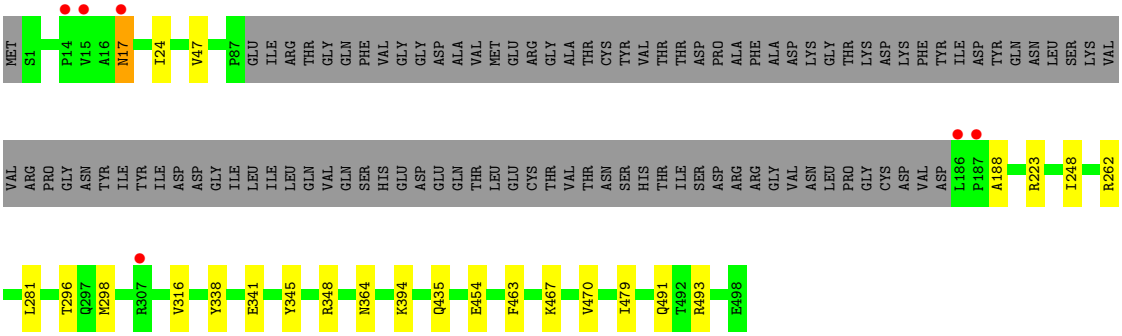
Chain A:





• Molecule 1: Pyruvate kinase

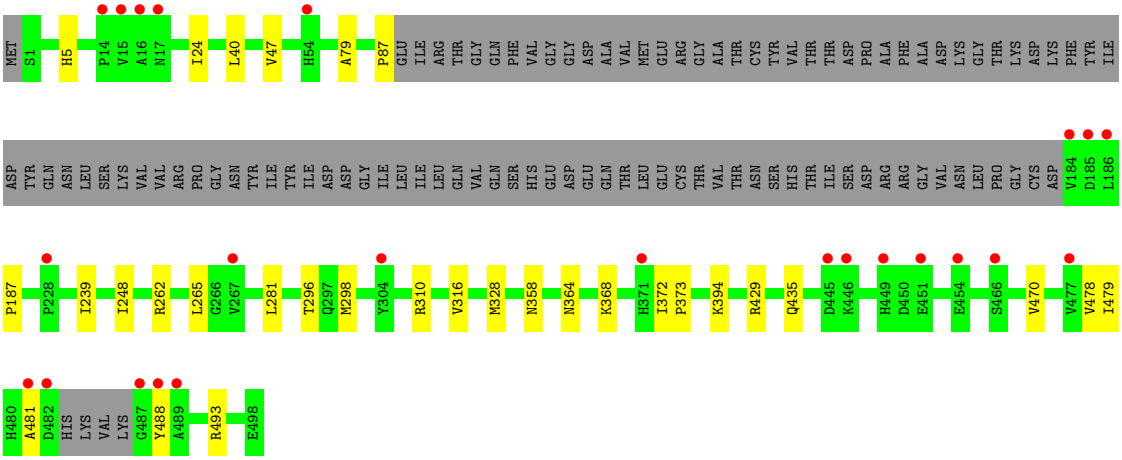
Chain B:



• Molecule 1: Pyruvate kinase

Chain C:

5%
74%
6%
20%


MET S1 H5 P14 V15 A16 N17 I24 L40 V47 H54 A79 P87 GLU ILE ARG THR GLY GLN PHE VAL GLY GLY ASP ALA VAL MET GLU ARG GLY ALA THR CYS TYR VAL THR THR ASP PRO ALA PHE ALA ASP LYS GLY THR LYS ASP LYS PHE TYR ILE
ASP TYR GLN ASN LEU SER LYS VAL VAL ARG PRO GLY ASN TYR ILE TYR ILE ASP ASP GLY ILE LEU ILE LEU GLN VAL GLN SER HIS GLU ASP GLU GLN THR LEU GLU CYS THR VAL THR ASN SER HIS THR ILE SER ASP ARG ARG GLY VAL ASN LEU PRO GLY CYS ASP V184 D185 L186
P187 P228 I239 I248 R262 L265 G266 V267 L281 T296 Q297 M298 Y304 R310 V316 M328 N358 N364 K368 H371 I372 P373 K394 R429 Q435 D445 K446 H449 D450 E451 E454 S466 V470 V477 V478 I479
H480 A481 D482 HIS LYS VAL LYS G487 Y488 A489 R493 E498

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.11Å 164.80Å 123.35Å 90.00° 115.80° 90.00°	Depositor
Resolution (Å)	21.14 – 2.70 21.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (21.14-2.70) 99.8 (21.14-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.215 , 0.244 0.215 , 0.243	Depositor DCC
R_{free} test set	4480 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14425	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: QV7, QV8, SO4, K

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	0.31	0/3839	0.46	0/5197
1	B	0.31	0/3101	0.45	0/4193
1	C	0.31	0/3081	0.44	0/4167
1	D	0.32	0/3863	0.45	0/5230
All	All	0.31	0/13884	0.45	0/18787

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 (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	3774	0	3775	16	0
1	B	3051	0	3087	11	0
1	C	3032	0	3058	13	0
1	D	3793	0	3788	11	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	43	0	14	0	0
4	B	129	0	42	1	0
4	D	43	0	14	10	0
5	B	27	0	13	5	0
6	A	167	0	0	0	0
6	B	109	0	0	1	0
6	C	68	0	0	0	0
6	D	161	0	0	0	0
All	All	14425	0	13791	67	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 2.

All (67) 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)
4:D:503:QV7:CAO	4:D:503:QV7:HAN	1.70	1.20
4:D:503:QV7:HAU	4:D:503:QV7:NBA	1.56	1.19
4:D:503:QV7:CAO	4:D:503:QV7:CAN	2.34	1.04
4:D:503:QV7:HAN	4:D:503:QV7:HAO	1.01	1.00
4:D:503:QV7:CAN	4:D:503:QV7:HAO	1.90	1.00
4:D:503:QV7:NBA	4:D:503:QV7:CAU	2.28	0.75
5:B:500:QV8:HAO	5:B:500:QV8:HAK	1.69	0.73
4:D:503:QV7:HAU	4:D:503:QV7:OAE	1.94	0.66
1:A:142:TYR:HB3	1:A:146:GLY:HA2	1.78	0.65
1:D:89:ILE:HG22	1:D:177:VAL:HG13	1.79	0.65
1:A:202[A]:GLU:HA	1:A:202[A]:GLU:OE1	1.99	0.63
5:B:500:QV8:HAK	5:B:500:QV8:CAO	2.29	0.62
1:A:298:MET:HE3	1:A:316:VAL:HG22	1.82	0.62
5:B:500:QV8:HAO	5:B:500:QV8:CAK	2.29	0.62
1:C:24:ILE:HB	1:C:328:MET:HG3	1.84	0.59
1:B:345:TYR:HD1	1:B:348:ARG:HH11	1.49	0.59
1:C:298:MET:HE3	1:C:316:VAL:HG22	1.86	0.57
4:D:503:QV7:CAN	4:D:503:QV7:CBC	2.82	0.57
4:D:503:QV7:CAU	4:D:503:QV7:OAE	2.53	0.56
1:B:394:LYS:HB2	1:B:470:VAL:HG12	1.88	0.54
1:A:114:ALA:O	1:A:118:LYS:HD3	2.10	0.52
1:C:5:HIS:HB2	1:C:358:ASN:HD22	1.75	0.51
1:B:223:ARG:HD2	6:B:592:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:500:QV8:CAO	5:B:500:QV8:CAK	2.88	0.50
1:B:24:ILE:HG12	1:B:47:VAL:HB	1.92	0.50
1:B:298:MET:HE3	1:B:316:VAL:HG22	1.94	0.49
1:C:372:ILE:HG13	1:C:373:PRO:HA	1.94	0.49
1:C:248:ILE:HG12	1:C:281:LEU:HD22	1.94	0.48
1:D:481:ALA:HB1	1:D:488:TYR:OH	2.13	0.48
1:A:394:LYS:HB2	1:A:470:VAL:HG12	1.96	0.48
1:C:394:LYS:HB2	1:C:470:VAL:HG12	1.95	0.48
1:D:248:ILE:HG12	1:D:281:LEU:HD22	1.96	0.47
1:D:394:LYS:HB2	1:D:470:VAL:HG12	1.96	0.47
4:B:501:QV7:NBA	4:B:501:QV7:HAU	2.28	0.47
1:A:18[B]:TYR:CG	1:A:19:ARG:N	2.83	0.47
1:A:379:ALA:O	1:A:383:SER:HB2	2.15	0.45
1:B:338:TYR:HB3	1:B:341:GLU:HB2	1.99	0.45
1:A:24:ILE:HB	1:A:328:MET:HG3	1.98	0.45
1:D:179:LEU:HB3	1:D:182:CYS:HB2	1.99	0.45
1:B:491:GLN:HE22	1:B:493:ARG:HH21	1.63	0.45
1:B:463:PHE:CZ	1:B:467:LYS:HE3	2.53	0.44
1:A:87:PRO:HB2	1:A:186:LEU:HD13	1.99	0.44
1:A:179:LEU:HB3	1:A:182:CYS:HB2	2.00	0.44
1:C:47:VAL:HG22	1:C:79:ALA:HB3	1.99	0.44
1:B:248:ILE:HG12	1:B:281:LEU:HD22	2.00	0.44
1:C:481:ALA:HB1	1:C:488:TYR:OH	2.17	0.44
1:C:239:ILE:HG22	1:C:265:LEU:HD21	2.01	0.43
1:A:93:GLN:HB2	1:A:117:ASP:HA	2.00	0.43
1:D:135:VAL:HG11	1:D:152:VAL:HG21	2.00	0.43
4:D:503:QV7:OAE	4:D:503:QV7:CAT	2.67	0.43
1:B:345:TYR:HD1	1:B:348:ARG:NH1	2.15	0.42
1:C:24:ILE:HG12	1:C:47:VAL:HB	2.01	0.42
1:A:211:SER:HA	1:A:238:LYS:HD3	2.01	0.42
1:D:24:ILE:HG12	1:D:47:VAL:HB	2.02	0.42
1:A:17:ASN:HD22	1:A:17:ASN:N	2.17	0.42
1:A:24:ILE:HG12	1:A:47:VAL:HB	2.01	0.42
1:C:87:PRO:HG2	1:C:187:PRO:O	2.19	0.42
1:A:487:GLY:HA2	1:A:488:TYR:HA	1.75	0.42
1:B:17:ASN:H	1:B:17:ASN:HD22	1.67	0.42
1:C:79:ALA:HB2	1:C:429:ARG:O	2.19	0.42
1:C:478:VAL:HB	1:C:493:ARG:HB2	2.01	0.42
1:D:211:SER:HA	1:D:238:LYS:HD3	2.02	0.41
1:D:377:ASP:HB3	1:D:488:TYR:CZ	2.55	0.41
5:B:500:QV8:OAB	5:B:500:QV8:NAQ	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:ALA:O	1:D:462[B]:GLU:HB2	2.21	0.41
1:D:399:LEU:HB2	1:D:480[B]:HIS:HD2	1.85	0.41
1:A:424:ARG:NH2	1:A:426:GLN:OE1	2.54	0.41

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	492/499 (99%)	483 (98%)	8 (2%)	1 (0%)	47	73
1	B	398/499 (80%)	389 (98%)	7 (2%)	2 (0%)	29	54
1	C	394/499 (79%)	383 (97%)	10 (2%)	1 (0%)	41	66
1	D	494/499 (99%)	480 (97%)	13 (3%)	1 (0%)	47	73
All	All	1778/1996 (89%)	1735 (98%)	38 (2%)	5 (0%)	41	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	296	THR
1	A	296	THR
1	C	296	THR
1	B	188	ALA
1	B	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	414/417 (99%)	400 (97%)	14 (3%)	37	66
1	B	333/417 (80%)	326 (98%)	7 (2%)	53	80
1	C	331/417 (79%)	324 (98%)	7 (2%)	53	80
1	D	416/417 (100%)	409 (98%)	7 (2%)	60	84
All	All	1494/1668 (90%)	1459 (98%)	35 (2%)	50	78

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	17	ASN
1	D	118	LYS
1	D	175	ARG
1	D	177	VAL
1	D	262	ARG
1	D	435	GLN
1	D	479	ILE
1	A	17	ASN
1	A	40	LEU
1	A	69	GLN
1	A	118	LYS
1	A	170	THR
1	A	175	ARG
1	A	177	VAL
1	A	194	ARG
1	A	253	GLU
1	A	262	ARG
1	A	310	ARG
1	A	383	SER
1	A	435	GLN
1	A	479	ILE
1	B	17	ASN
1	B	262	ARG
1	B	364	ASN
1	B	435	GLN
1	B	454[A]	GLU
1	B	454[B]	GLU
1	B	479	ILE
1	C	40	LEU
1	C	262	ARG

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Mol	Chain	Res	Type
1	C	310	ARG
1	C	364	ASN
1	C	368	LYS
1	C	435	GLN
1	C	479	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	17	ASN
1	D	65	ASN
1	D	286	ASN
1	D	305	ASN
1	D	322	ASN
1	D	471	GLN
1	A	17	ASN
1	A	54	HIS
1	A	155	HIS
1	A	286	ASN
1	A	305	ASN
1	A	471	GLN
1	B	17	ASN
1	B	286	ASN
1	B	322	ASN
1	B	386	ASN
1	B	471	GLN
1	B	491	GLN
1	C	17	ASN
1	C	65	ASN
1	C	286	ASN
1	C	305	ASN
1	C	435	GLN
1	C	491	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	QV7	B	499	-	44,46,46	1.16	3 (6%)	64,72,72	1.21	7 (10%)
2	SO4	D	500	-	4,4,4	0.14	0	6,6,6	0.09	0
4	QV7	D	503	-	44,46,46	1.20	4 (9%)	64,72,72	1.25	8 (12%)
5	QV8	B	500	-	30,30,30	1.56	5 (16%)	44,45,45	0.71	0
2	SO4	A	500	-	4,4,4	0.14	0	6,6,6	0.07	0
4	QV7	B	504	-	44,46,46	1.16	4 (9%)	64,72,72	1.30	7 (10%)
4	QV7	B	501	-	44,46,46	1.16	4 (9%)	64,72,72	1.83	6 (9%)
2	SO4	C	499	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	499	-	4,4,4	0.14	0	6,6,6	0.06	0
4	QV7	A	499	-	44,46,46	1.25	4 (9%)	64,72,72	1.11	5 (7%)

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
4	QV7	D	503	-	-	18/34/34/34	0/4/4/4
4	QV7	A	499	-	-	1/34/34/34	0/4/4/4
5	QV8	B	500	-	-	0/10/26/26	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	QV7	B	504	-	-	7/34/34/34	0/4/4/4
4	QV7	B	501	-	-	13/34/34/34	0/4/4/4
4	QV7	B	499	-	-	4/34/34/34	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	QV8	CAW-CAU	-4.12	1.39	1.48
4	A	499	QV7	CBF-NBA	-4.00	1.33	1.42
5	B	500	QV8	CAY-CAU	-3.97	1.40	1.48
5	B	500	QV8	CAX-CAV	-3.74	1.40	1.48
4	D	503	QV7	CBF-NBA	-3.62	1.34	1.42
4	B	499	QV7	CBF-NBA	-3.49	1.35	1.42
4	B	504	QV7	CBF-NBA	-3.40	1.35	1.42
4	B	501	QV7	CBF-NBA	-3.28	1.35	1.42
5	B	500	QV8	CAZ-CAV	-2.91	1.40	1.47
4	A	499	QV7	CAX-CBJ	2.86	1.40	1.37
5	B	500	QV8	CAR-NAQ	-2.63	1.34	1.40
4	B	501	QV7	CAX-CBJ	2.50	1.39	1.37
4	D	503	QV7	CBD-NAZ	-2.50	1.33	1.44
4	B	499	QV7	CBC-NAY	-2.47	1.33	1.44
4	A	499	QV7	CBD-NAZ	-2.46	1.33	1.44
4	B	499	QV7	CBD-NAZ	-2.45	1.33	1.44
4	A	499	QV7	CBC-NAY	-2.45	1.33	1.44
4	D	503	QV7	CBC-NAY	-2.44	1.33	1.44
4	B	501	QV7	CBD-NAZ	-2.38	1.34	1.44
4	B	504	QV7	CBD-NAZ	-2.37	1.34	1.44
4	B	501	QV7	CBC-NAY	-2.34	1.34	1.44
4	B	504	QV7	CAX-CBJ	2.32	1.39	1.37
4	D	503	QV7	CBK-CBM	-2.30	1.39	1.43
4	B	504	QV7	CBC-NAY	-2.28	1.34	1.44

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	QV7	CBI-CBF-NBA	8.67	127.21	117.56
4	B	501	QV7	CBF-NBA-NBB	6.71	130.06	114.56
4	B	501	QV7	CBF-CBI-SBP	5.05	125.26	120.85
4	D	503	QV7	CBI-CBF-NBA	4.71	122.81	117.56
4	B	499	QV7	CBI-CBF-NBA	4.25	122.29	117.56
4	B	504	QV7	CBF-NBA-NBB	3.93	123.64	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	499	QV7	CBK-NBB-NBA	3.90	126.35	117.04
4	A	499	QV7	CBK-NBB-NBA	3.88	126.29	117.04
4	B	504	QV7	CBI-CBF-NBA	3.42	121.36	117.56
4	D	503	QV7	CBF-NBA-NBB	3.41	122.44	114.56
4	B	501	QV7	CBD-CAV-CBI	3.35	121.94	119.21
4	A	499	QV7	CBI-CBF-NBA	2.89	120.77	117.56
4	B	504	QV7	CBF-CBI-SBP	2.83	123.33	120.85
4	D	503	QV7	CAU-CBM-CBK	-2.59	119.22	123.74
4	B	504	QV7	CBD-CAV-CBI	2.58	121.31	119.21
4	D	503	QV7	CBF-CBI-SBP	2.41	122.95	120.85
4	A	499	QV7	CAU-CBM-CBK	-2.38	119.59	123.74
4	B	504	QV7	OAH-SBQ-CBJ	2.27	110.35	106.51
4	B	501	QV7	OAF-SBP-CBI	2.27	110.35	106.51
4	B	504	QV7	CBK-NBB-NBA	2.22	122.33	117.04
4	B	504	QV7	CBM-CBK-NBB	2.19	120.91	115.81
4	D	503	QV7	CBC-NAY-NAZ	2.18	123.80	112.99
4	B	501	QV7	CBD-NAZ-NAY	2.17	123.79	112.99
4	B	499	QV7	OAH-SBQ-CBJ	2.15	110.14	106.51
4	D	503	QV7	CBD-CAV-CBI	2.13	120.94	119.21
4	B	499	QV7	OAM-SBQ-CBJ	2.11	110.07	106.51
4	D	503	QV7	CBD-NAZ-NAY	2.10	123.44	112.99
4	B	499	QV7	OAF-SBP-CBI	2.09	110.04	106.51
4	B	499	QV7	CBF-NBA-NBB	2.09	119.38	114.56
4	A	499	QV7	CBD-NAZ-NAY	2.04	123.14	112.99
4	B	499	QV7	CBC-NAY-NAZ	2.02	123.04	112.99
4	D	503	QV7	OAE-SBP-CBI	2.01	109.91	106.51
4	A	499	QV7	OAE-SBP-CBI	2.01	109.90	106.51

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	503	QV7	CBM-CBK-NBB-NBA
4	D	503	QV7	CAX-CBJ-SBQ-OAH
4	D	503	QV7	CAX-CBJ-SBQ-OAM
4	B	501	QV7	CBM-CBK-NBB-NBA
4	B	501	QV7	CAX-CBJ-SBQ-OAH
4	B	501	QV7	CAX-CBJ-SBQ-OAM
4	B	501	QV7	CBE-CBJ-SBQ-OAG
4	B	504	QV7	CBI-CBF-NBA-NBB
4	B	504	QV7	CAN-CBD-NAZ-NAY
4	B	499	QV7	CAV-CBD-NAZ-NAY

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Mol	Chain	Res	Type	Atoms
4	B	504	QV7	CAV-CBD-NAZ-NAY
4	B	499	QV7	CAN-CBD-NAZ-NAY
4	B	499	QV7	CAO-CBC-NAY-NAZ
4	D	503	QV7	CAP-CBC-NAY-NAZ
4	B	499	QV7	CAP-CBC-NAY-NAZ
4	D	503	QV7	CAO-CBC-NAY-NAZ
4	D	503	QV7	CAV-CBD-NAZ-NAY
4	D	503	QV7	CAN-CBD-NAZ-NAY
4	B	504	QV7	CAP-CBC-NAY-NAZ
4	D	503	QV7	CBE-CBJ-SBQ-OAH
4	D	503	QV7	CBE-CBJ-SBQ-OAM
4	B	501	QV7	CBE-CBJ-SBQ-OAH
4	B	501	QV7	CBE-CBJ-SBQ-OAM
4	B	501	QV7	CBE-CBK-NBB-NBA
4	B	504	QV7	CAO-CBC-NAY-NAZ
4	D	503	QV7	CAV-CBI-SBP-OAE
4	D	503	QV7	CBC-NAY-NAZ-CBD
4	B	501	QV7	CAP-CBC-NAY-NAZ
4	B	501	QV7	CAO-CBC-NAY-NAZ
4	B	504	QV7	CAQ-CBF-NBA-NBB
4	D	503	QV7	CAV-CBI-SBP-OAL
4	D	503	QV7	CBF-CBI-SBP-OAL
4	D	503	QV7	CAX-CBJ-SBQ-OAG
4	D	503	QV7	CBE-CBJ-SBQ-OAG
4	B	501	QV7	CAX-CBJ-SBQ-OAG
4	B	501	QV7	CAQ-CBF-NBA-NBB
4	B	501	QV7	CAV-CBD-NAZ-NAY
4	D	503	QV7	CBE-CBK-NBB-NBA
4	B	501	QV7	CAN-CBD-NAZ-NAY
4	A	499	QV7	CBM-CBK-NBB-NBA
4	B	504	QV7	CBE-CBK-NBB-NBA
4	D	503	QV7	CAR-CBG-SBN-OAA
4	D	503	QV7	CAT-CBH-SBO-OAC

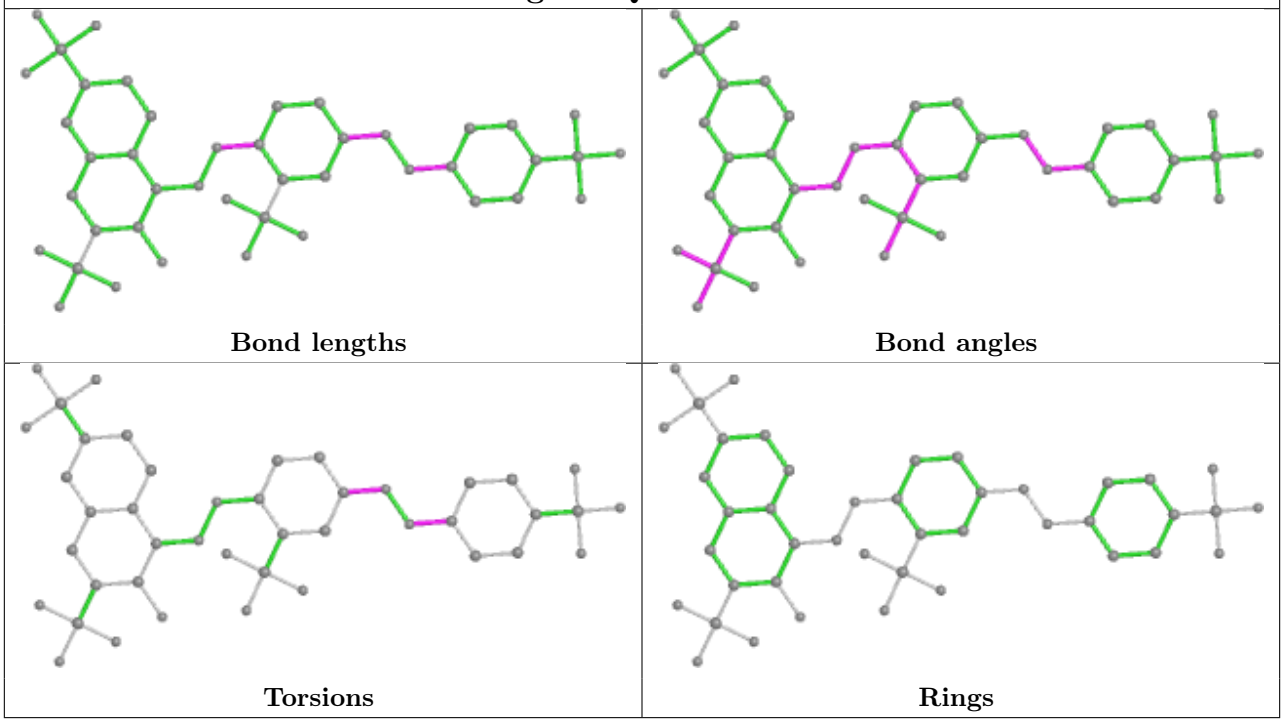
There are no ring outliers.

3 monomers are involved in 16 short contacts:

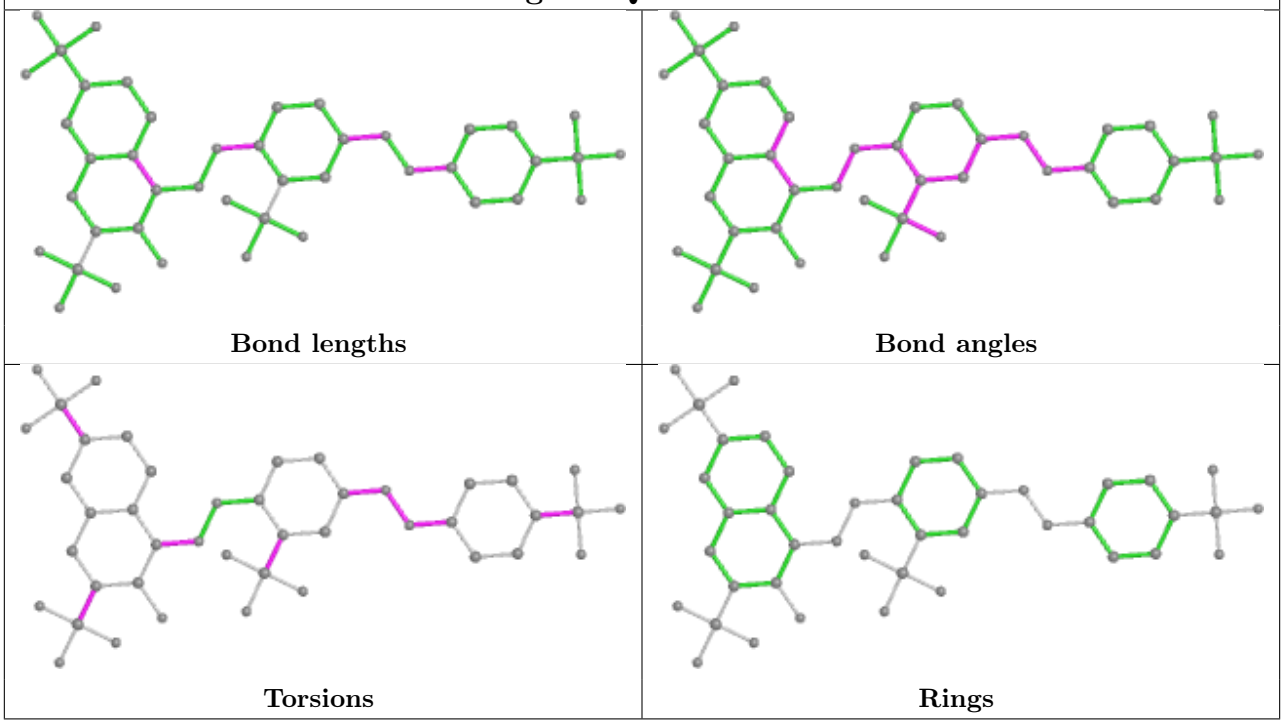
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	QV7	10	0
5	B	500	QV8	5	0
4	B	501	QV7	1	0

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

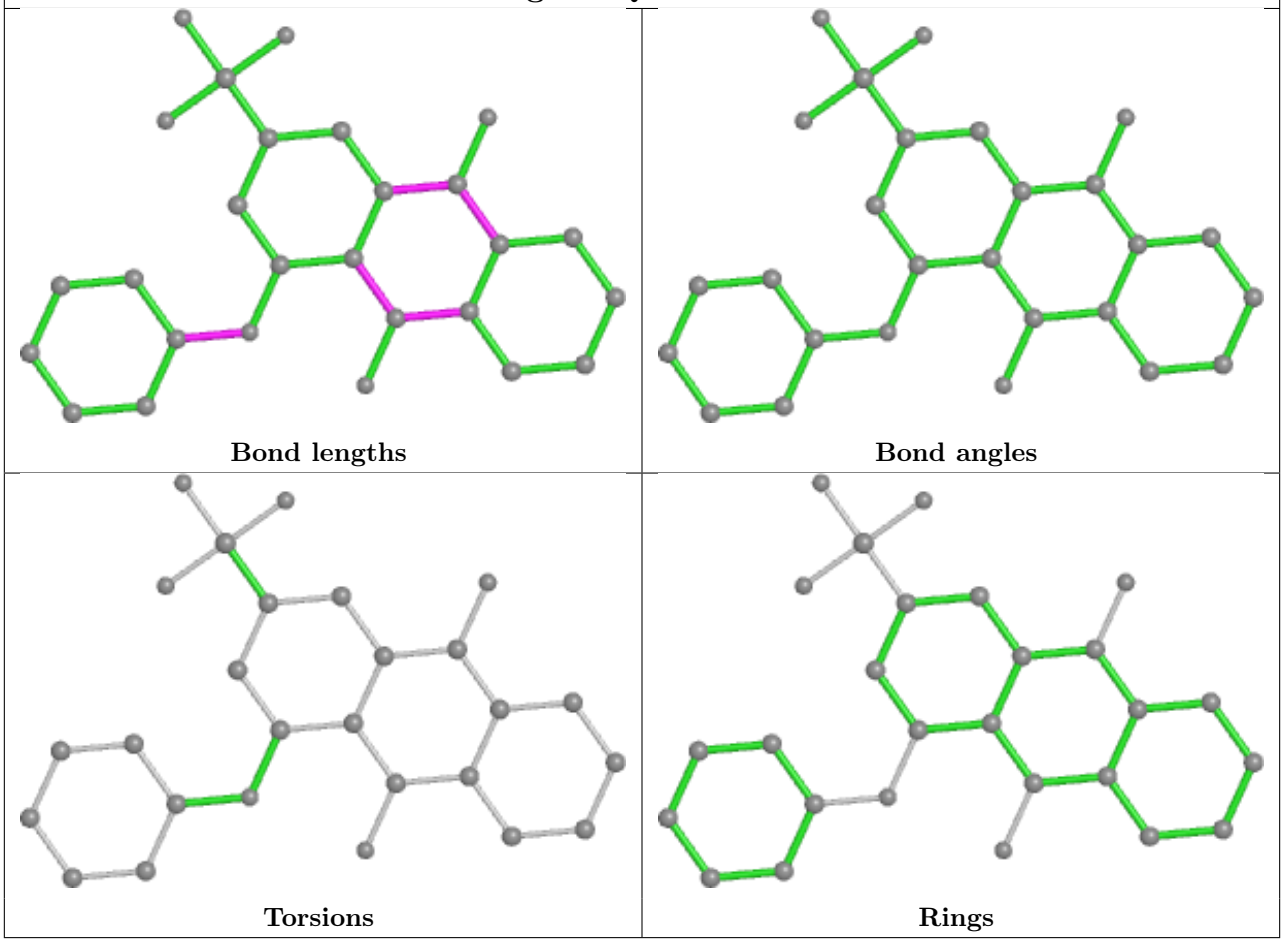
Ligand QV7 B 499



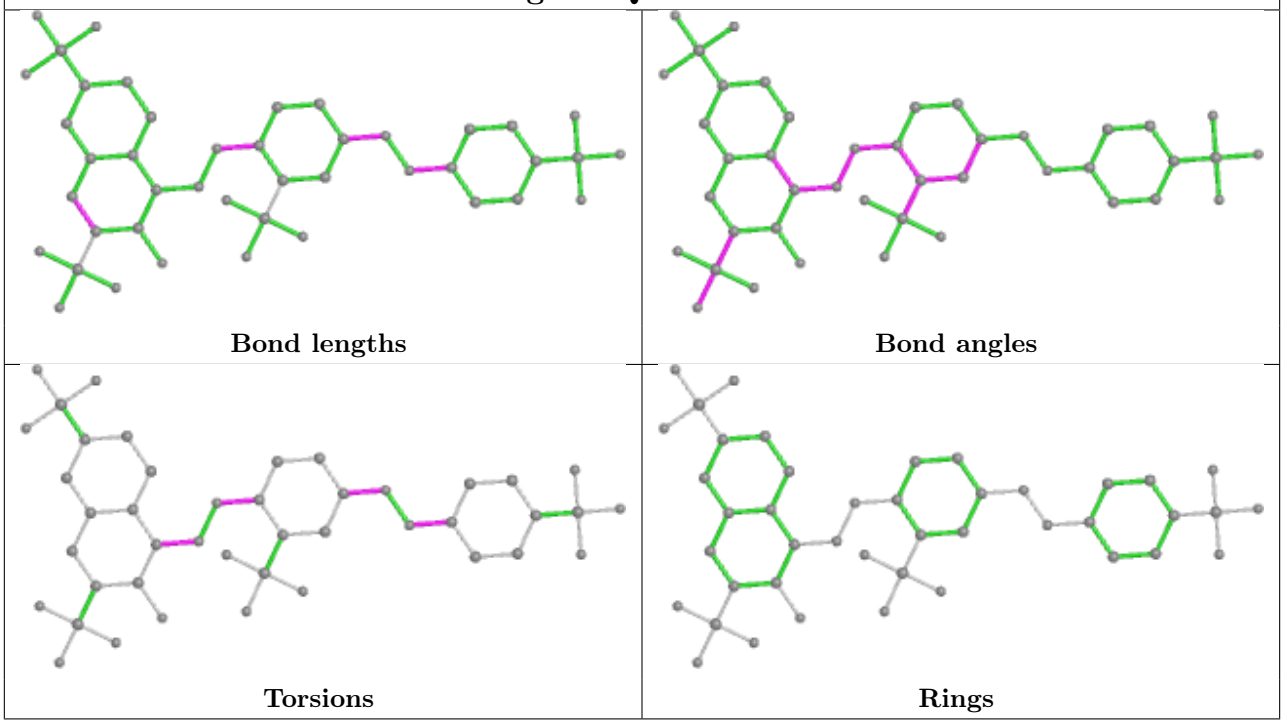
Ligand QV7 D 503



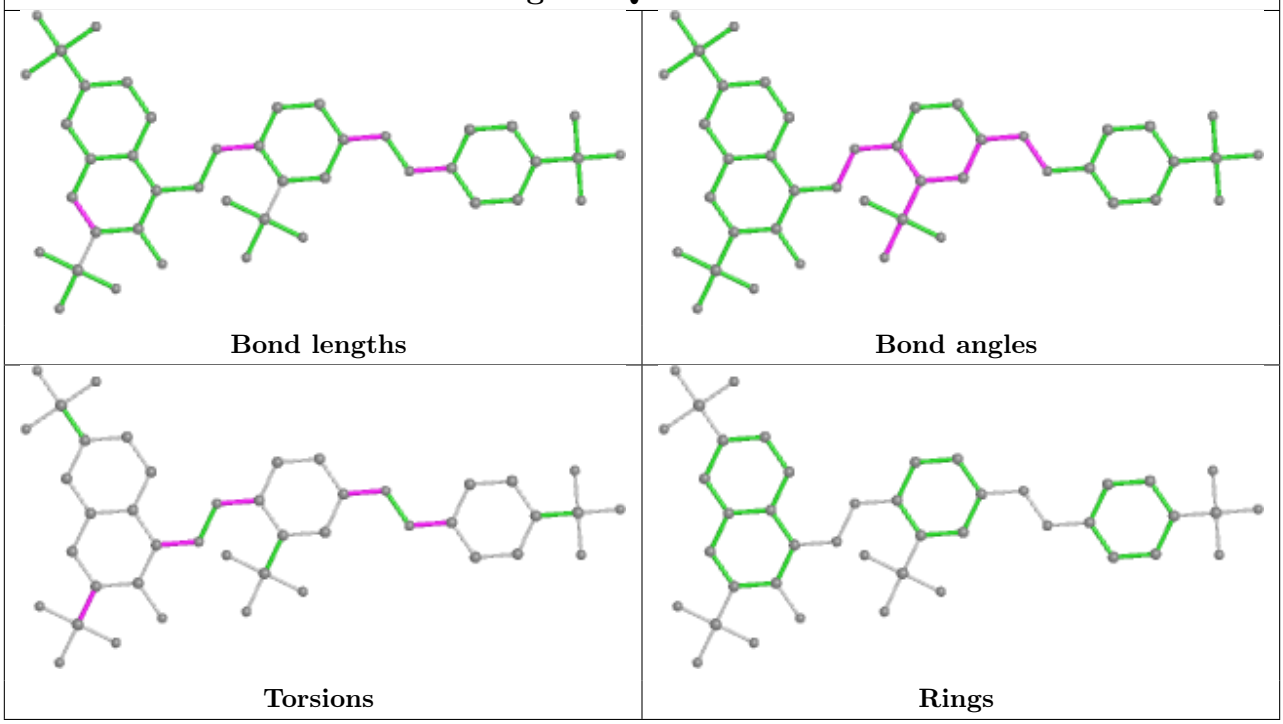
Ligand QV8 B 500



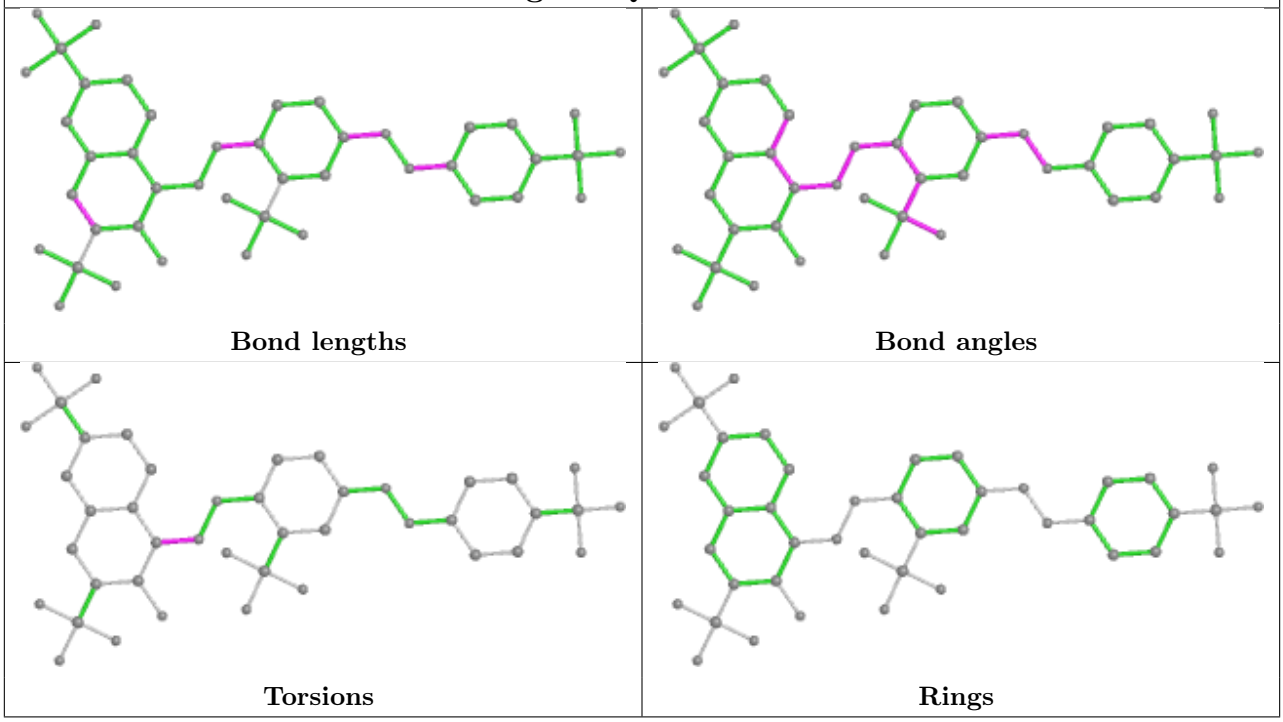
Ligand QV7 B 504



Ligand QV7 B 501



Ligand QV7 A 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	493/499 (98%)	-0.11	13 (2%)	56	57	27, 38, 59, 67	0
1	B	400/499 (80%)	-0.18	6 (1%)	73	76	30, 44, 54, 57	0
1	C	398/499 (79%)	0.10	24 (6%)	21	20	37, 51, 64, 71	0
1	D	494/499 (98%)	-0.02	18 (3%)	42	42	27, 41, 57, 62	0
All	All	1785/1996 (89%)	-0.05	61 (3%)	45	45	27, 44, 60, 71	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	488	TYR	5.0
1	C	14	PRO	4.3
1	D	449	HIS	4.0
1	A	487	GLY	3.7
1	D	109	VAL	3.6
1	A	109	VAL	3.3
1	C	17	ASN	3.3
1	C	449	HIS	3.2
1	D	228	PRO	3.2
1	C	184	VAL	3.1
1	B	17	ASN	3.1
1	C	489	ALA	3.1
1	C	15	VAL	3.1
1	A	17	ASN	3.0
1	C	304	TYR	3.0
1	A	488	TYR	3.0
1	C	481	ALA	2.9
1	D	371[A]	HIS	2.9
1	A	371	HIS	2.9
1	D	126	ILE	2.9
1	B	187	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	16	ALA	2.8
1	C	185	ASP	2.8
1	A	158	GLU	2.8
1	A	114	ALA	2.7
1	D	487	GLY	2.7
1	C	466	SER	2.7
1	C	186	LEU	2.6
1	D	304	TYR	2.6
1	C	228	PRO	2.6
1	D	97	GLY	2.6
1	D	96	GLY	2.6
1	C	445	ASP	2.6
1	C	488	TYR	2.5
1	D	481	ALA	2.5
1	C	451	GLU	2.5
1	C	267	VAL	2.5
1	B	186	LEU	2.5
1	A	449	HIS	2.5
1	A	489	ALA	2.5
1	B	307	ARG	2.4
1	D	447	LEU	2.4
1	D	158	GLU	2.3
1	B	15	VAL	2.3
1	C	487	GLY	2.3
1	D	14	PRO	2.3
1	C	54	HIS	2.3
1	D	136	ARG	2.3
1	C	371[A]	HIS	2.3
1	B	14	PRO	2.2
1	C	482	ASP	2.2
1	A	150	LEU	2.2
1	C	446	LYS	2.1
1	D	98	ASP	2.1
1	A	126	ILE	2.1
1	D	141	ILE	2.1
1	A	97	GLY	2.1
1	A	18[A]	TYR	2.0
1	C	477	VAL	2.0
1	D	489	ALA	2.0
1	C	454	GLU	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)

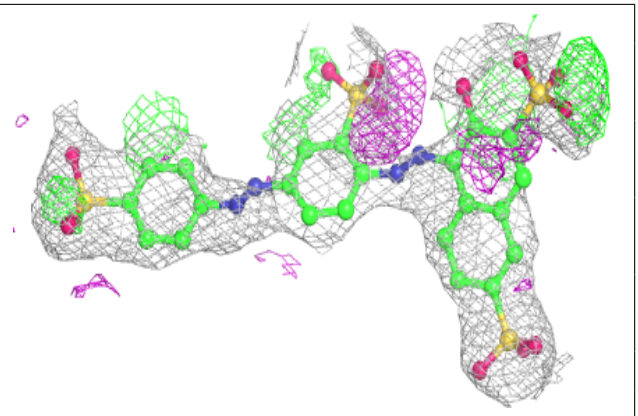
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

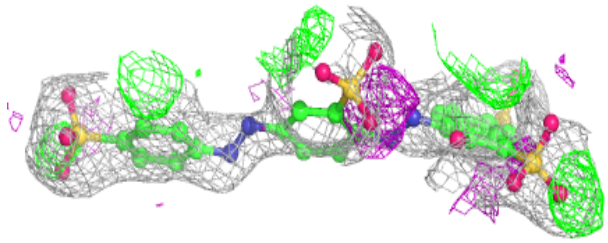
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	D	501	1/1	0.25	0.28	94,94,94,94	0
3	K	C	500	1/1	0.53	0.19	88,88,88,88	0
4	QV7	B	501	43/43	0.72	0.31	94,101,102,102	0
3	K	A	502	1/1	0.79	0.14	59,59,59,59	0
3	K	B	503	1/1	0.80	0.11	58,58,58,58	0
4	QV7	D	503	43/43	0.81	0.24	62,65,66,66	43
2	SO4	D	499	5/5	0.81	0.25	103,103,103,103	0
4	QV7	B	504	43/43	0.81	0.30	81,87,88,88	0
5	QV8	B	500	27/27	0.84	0.27	97,97,98,98	0
4	QV7	A	499	43/43	0.90	0.18	64,67,70,71	0
3	K	C	501	1/1	0.90	0.12	61,61,61,61	0
3	K	B	502	1/1	0.92	0.19	91,91,91,91	0
3	K	A	501	1/1	0.93	0.07	64,64,64,64	0
3	K	D	502	1/1	0.94	0.14	65,65,65,65	0
4	QV7	B	499	43/43	0.96	0.13	41,42,45,45	0
2	SO4	C	499	5/5	0.97	0.11	89,89,89,89	0
2	SO4	D	500	5/5	0.97	0.17	71,71,71,71	0
2	SO4	A	500	5/5	0.97	0.17	89,89,89,89	0

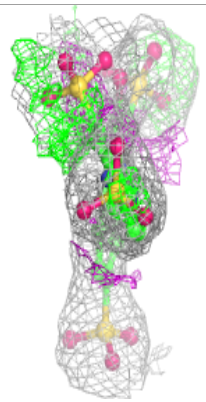
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QV7 B 501:

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

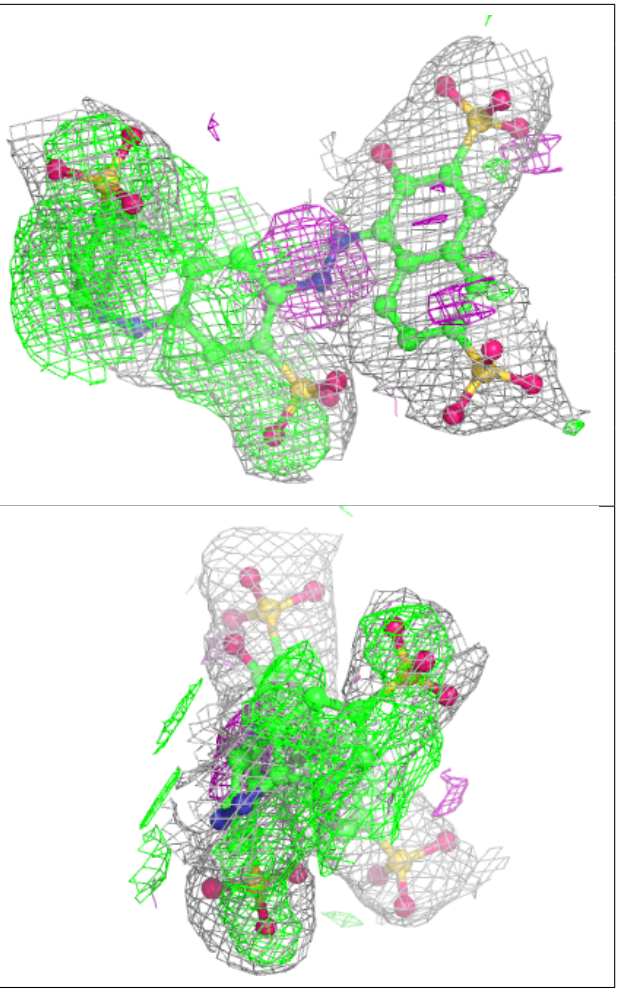






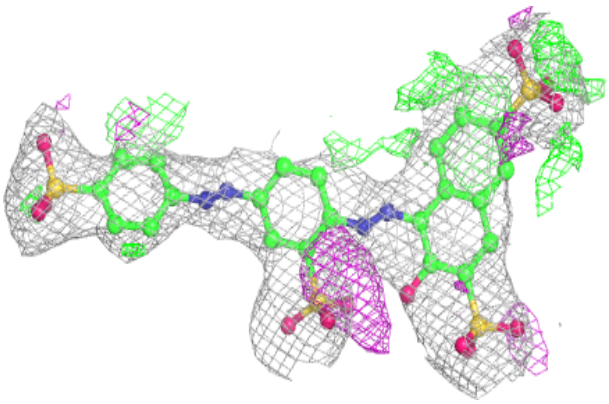
Electron density around QV7 D 503:

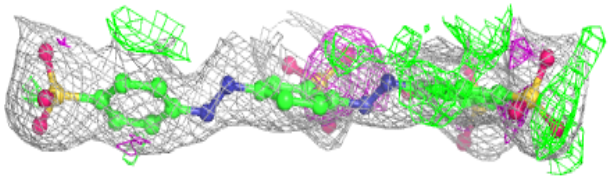
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

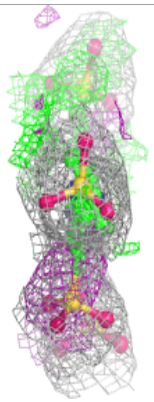


Electron density around QV7 B 504:

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

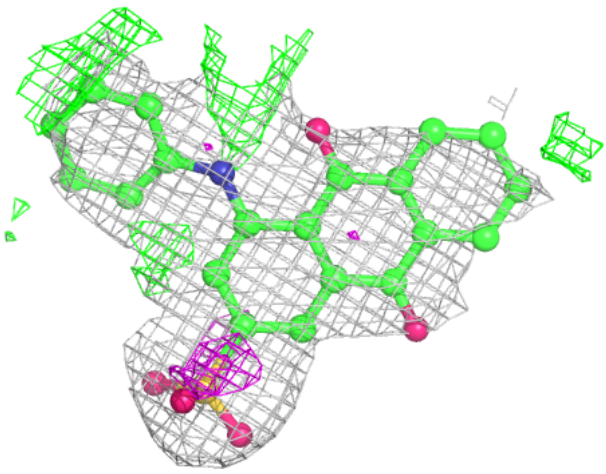


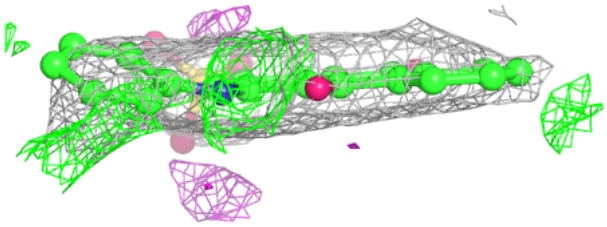


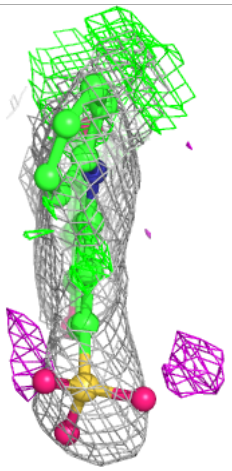


Electron density around QV8 B 500:

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

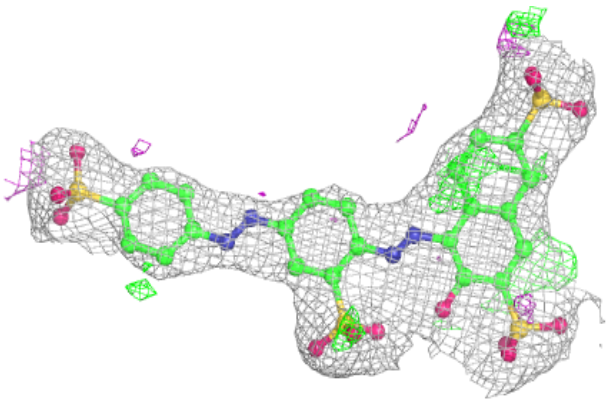


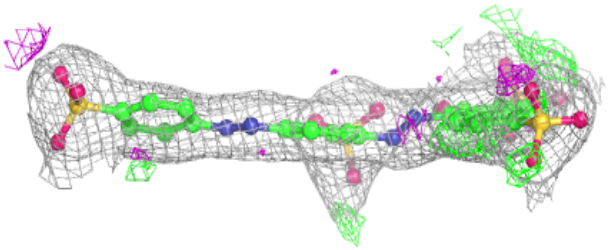


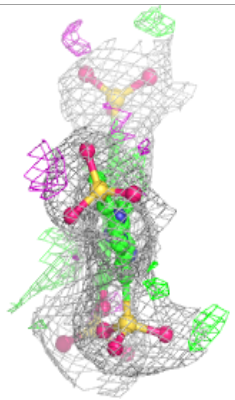


Electron density around QV7 A 499:

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

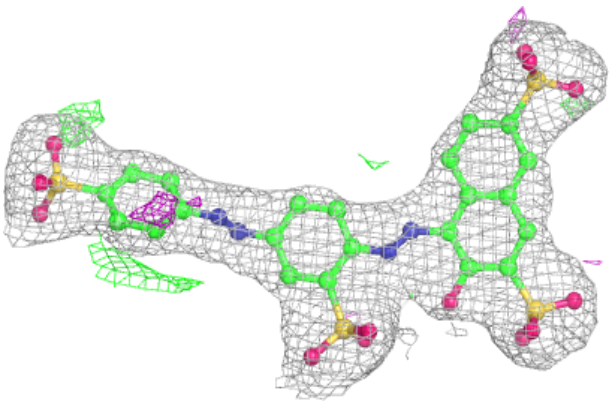


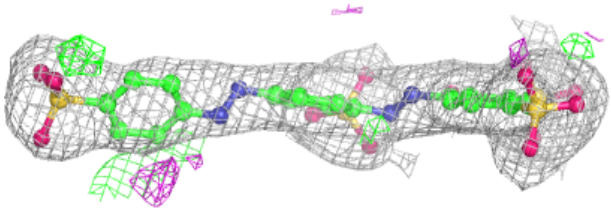


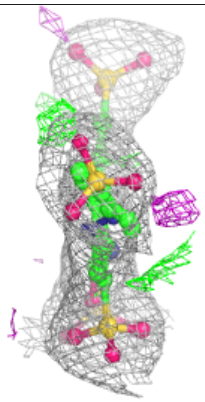


Electron density around QV7 B 499:

$2mF_o$-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.