Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2022 – 12:32 am GMT

PDB ID	:	6TQG
Title	:	Pseudomonas aeruginosa RmlA in complex with allosteric inhibitor
Authors	:	Alphey, M.S.; Xiao, G.; Westwood, J.N.
Deposited on	:	2019-12-16
Resolution	:	2.45 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 following versions of software and data (see references ⓘ) were used in the production of this report:

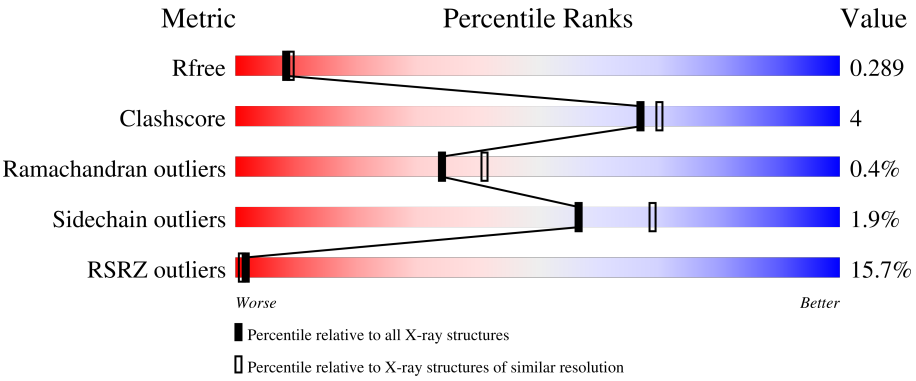
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	303	13% 85% 6% 8%
1	B	303	11% 81% 8% 11%
1	C	303	15% 80% • • 15%
1	D	303	17% 82% • • 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8599 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 Glucose-1-phosphate thymidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	1	0
			2173	1391	362	416	4			
1	B	271	Total	C	N	O	S	0	1	0
			2119	1361	352	402	4			
1	C	259	Total	C	N	O	S	0	1	0
			2000	1285	326	385	4			
1	D	261	Total	C	N	O	S	0	1	0
			2013	1292	331	386	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP G3XCK4
A	-8	HIS	-	expression tag	UNP G3XCK4
A	-7	HIS	-	expression tag	UNP G3XCK4
A	-6	HIS	-	expression tag	UNP G3XCK4
A	-5	HIS	-	expression tag	UNP G3XCK4
A	-4	HIS	-	expression tag	UNP G3XCK4
A	-3	GLY	-	expression tag	UNP G3XCK4
A	-2	SER	-	expression tag	UNP G3XCK4
A	-1	MET	-	expression tag	UNP G3XCK4
A	0	ALA	-	expression tag	UNP G3XCK4
B	-9	HIS	-	expression tag	UNP G3XCK4
B	-8	HIS	-	expression tag	UNP G3XCK4
B	-7	HIS	-	expression tag	UNP G3XCK4
B	-6	HIS	-	expression tag	UNP G3XCK4
B	-5	HIS	-	expression tag	UNP G3XCK4
B	-4	HIS	-	expression tag	UNP G3XCK4
B	-3	GLY	-	expression tag	UNP G3XCK4
B	-2	SER	-	expression tag	UNP G3XCK4
B	-1	MET	-	expression tag	UNP G3XCK4
B	0	ALA	-	expression tag	UNP G3XCK4
C	-9	HIS	-	expression tag	UNP G3XCK4

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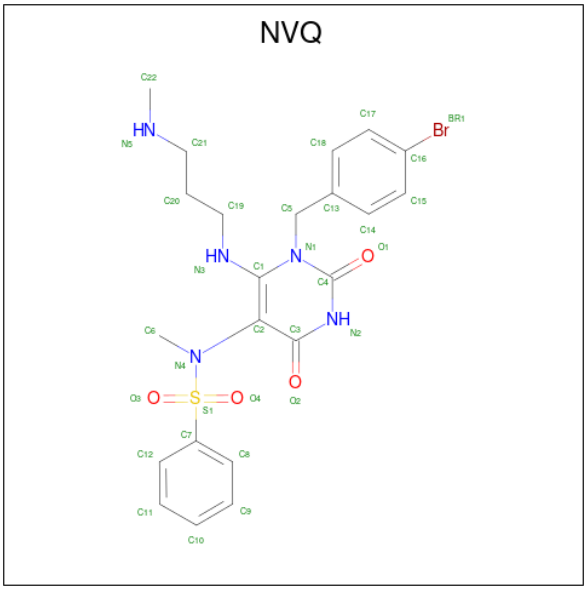
Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	HIS	-	expression tag	UNP G3XCK4
C	-7	HIS	-	expression tag	UNP G3XCK4
C	-6	HIS	-	expression tag	UNP G3XCK4
C	-5	HIS	-	expression tag	UNP G3XCK4
C	-4	HIS	-	expression tag	UNP G3XCK4
C	-3	GLY	-	expression tag	UNP G3XCK4
C	-2	SER	-	expression tag	UNP G3XCK4
C	-1	MET	-	expression tag	UNP G3XCK4
C	0	ALA	-	expression tag	UNP G3XCK4
D	-9	HIS	-	expression tag	UNP G3XCK4
D	-8	HIS	-	expression tag	UNP G3XCK4
D	-7	HIS	-	expression tag	UNP G3XCK4
D	-6	HIS	-	expression tag	UNP G3XCK4
D	-5	HIS	-	expression tag	UNP G3XCK4
D	-4	HIS	-	expression tag	UNP G3XCK4
D	-3	GLY	-	expression tag	UNP G3XCK4
D	-2	SER	-	expression tag	UNP G3XCK4
D	-1	MET	-	expression tag	UNP G3XCK4
D	0	ALA	-	expression tag	UNP G3XCK4

- Molecule 2 is {N}-[1-[(4-bromophenyl)methyl]-6-[3-(methylamino)propylamino]-2,4-bis(oxidanylidene)pyrimidin-5-yl]- {N}-methyl-benzenesulfonamide (three-letter code: NVQ) (formula: $C_{22}H_{26}BrN_5O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	0
			33	1	22	5	4	1		

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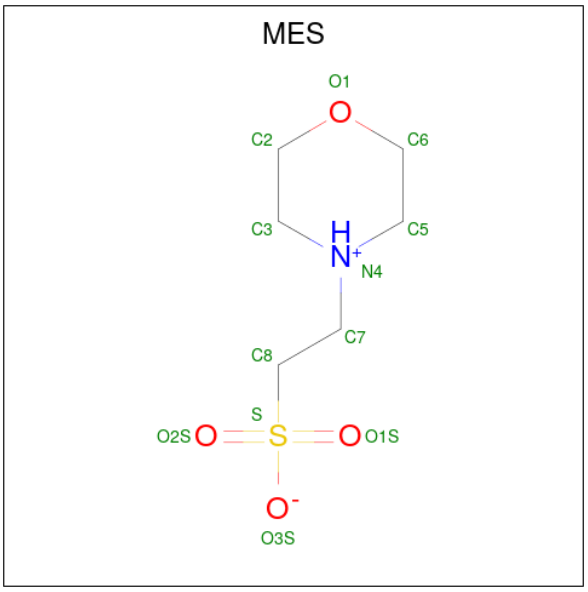
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	Br	C	N	O	S	0	0
			33	1	22	5	4	1		
2	C	1	Total	Br	C	N	O	S	0	0
			33	1	22	5	4	1		
2	D	1	Total	Br	C	N	O	S	0	0
			33	1	22	5	4	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		
4	B	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is water.

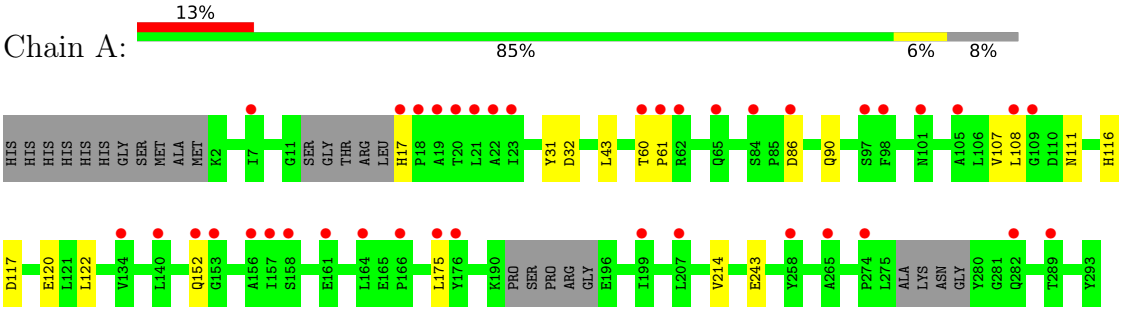
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	20	Total O 20 20	0	0
5	C	25	Total O 25 25	0	0
5	D	30	Total O 30 30	0	0

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.

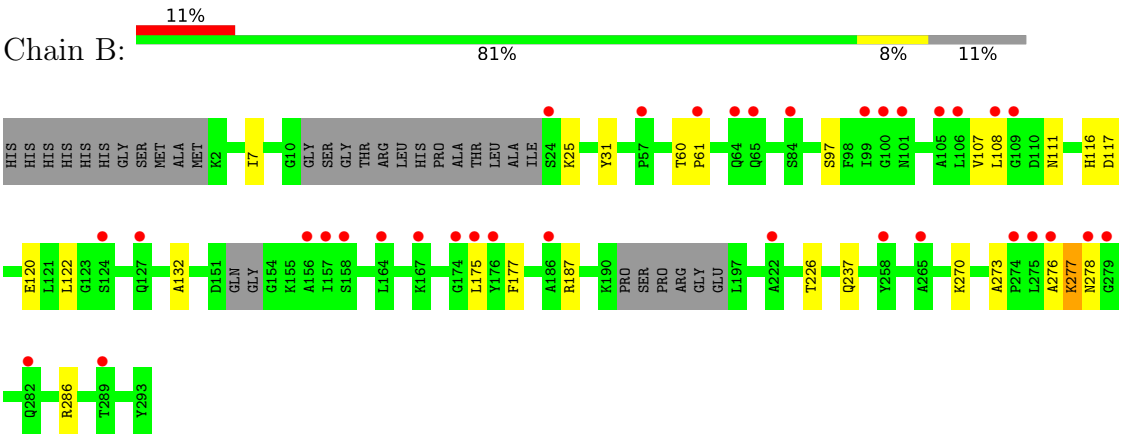
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain A:



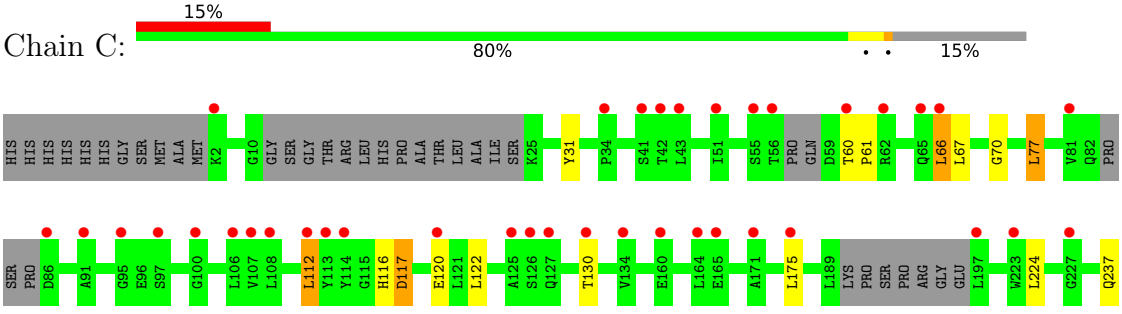
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

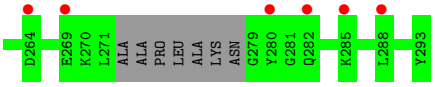
Chain B:



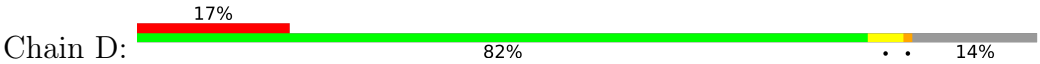
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

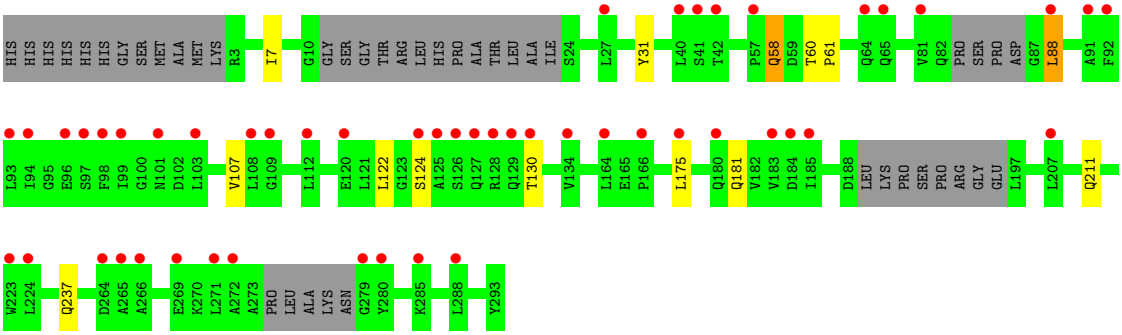
Chain C:





• Molecule 1: Glucose-1-phosphate thymidylyltransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.01Å 137.92Å 73.93Å 90.00° 102.98° 90.00°	Depositor
Resolution (Å)	29.57 – 2.45 29.57 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.4 (29.57-2.45) 95.4 (29.57-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.257 , 0.284 0.261 , 0.289	Depositor DCC
R_{free} test set	2551 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8599	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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: CL, NVQ, MES

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	0.65	0/2220	0.74	0/3011
1	B	0.65	0/2165	0.75	0/2936
1	C	0.66	0/2040	0.73	0/2765
1	D	0.65	0/2055	0.73	0/2789
All	All	0.66	0/8480	0.74	0/11501

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	2173	0	2129	11	0
1	B	2119	0	2077	14	0
1	C	2000	0	1912	28	0
1	D	2013	0	1932	25	0
2	A	33	0	0	1	0
2	B	33	0	0	0	0
2	C	33	0	0	1	0
2	D	33	0	0	1	0
3	A	12	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	13	0	0
3	C	12	0	13	0	0
3	D	12	0	13	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	0	0	0
5	B	20	0	0	1	0
5	C	25	0	0	0	0
5	D	30	0	0	0	0
All	All	8599	0	8102	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:C:237[A]:GLN:HE21	1:D:237[A]:GLN:NE2	1.30	1.26
1:C:237[A]:GLN:NE2	1:D:237[A]:GLN:HG2	1.77	1.00
1:C:237[A]:GLN:NE2	1:D:237[A]:GLN:NE2	2.12	0.96
1:C:237[A]:GLN:HE21	1:D:237[A]:GLN:CD	1.67	0.95
1:C:237[A]:GLN:HE21	1:D:237[A]:GLN:HE21	1.12	0.95
1:C:237[A]:GLN:HG2	1:D:237[A]:GLN:HE21	1.39	0.87
1:C:237[A]:GLN:NE2	1:D:237[A]:GLN:CG	2.42	0.82
1:C:237[A]:GLN:HG2	1:D:237[A]:GLN:NE2	1.94	0.82
1:B:237[B]:GLN:HG2	1:D:237[B]:GLN:HG2	1.62	0.81
1:C:237[A]:GLN:NE2	1:D:237[A]:GLN:HE21	1.73	0.81
1:C:237[A]:GLN:CG	1:D:237[A]:GLN:HE21	1.97	0.78
1:C:237[A]:GLN:HE21	1:D:237[A]:GLN:CG	2.01	0.69
1:C:112:LEU:HD21	1:C:224:LEU:HB2	1.75	0.67
1:A:107:VAL:HG12	1:A:175:LEU:HD13	1.76	0.66
1:A:86:ASP:HB2	1:A:90:GLN:OE1	1.97	0.65
1:C:237[A]:GLN:HE22	1:D:237[A]:GLN:HG2	1.58	0.64
1:A:108:LEU:HB2	1:A:111:ASN:ND2	2.13	0.64
1:C:237[A]:GLN:NE2	1:D:237[A]:GLN:CD	2.46	0.61
1:C:112:LEU:CD2	1:C:224:LEU:HB2	2.33	0.58
1:D:58:GLN:N	1:D:58:GLN:OE1	2.36	0.57
1:D:88:LEU:HD23	1:D:88:LEU:N	2.20	0.57
1:A:108:LEU:HB2	1:A:111:ASN:HD22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLN:H	1:D:58:GLN:CD	2.08	0.56
1:B:122:LEU:HD21	1:B:175:LEU:HD21	1.89	0.55
1:A:122:LEU:HD21	1:A:175:LEU:HD21	1.89	0.54
1:C:66:LEU:C	1:C:66:LEU:CD2	2.77	0.53
1:D:122:LEU:HD21	1:D:175:LEU:HD21	1.91	0.53
1:C:122:LEU:HD21	1:C:175:LEU:HD21	1.90	0.52
1:B:25:LYS:HE2	1:B:226:THR:O	2.10	0.51
1:D:88:LEU:N	1:D:88:LEU:CD2	2.74	0.51
1:C:70:GLY:CA	1:C:77:LEU:HD22	2.41	0.50
2:D:301:NVQ:C5	2:D:301:NVQ:C19	2.90	0.50
1:C:237[A]:GLN:CD	1:D:237[A]:GLN:HE21	2.14	0.49
1:C:66:LEU:CD2	1:C:66:LEU:O	2.61	0.48
1:A:43:LEU:HD21	1:A:107:VAL:HG13	1.96	0.48
1:C:66:LEU:C	1:C:66:LEU:HD22	2.33	0.48
1:B:117:ASP:HA	1:B:120:GLU:OE1	2.15	0.47
1:C:77:LEU:N	1:C:77:LEU:CD1	2.77	0.47
1:A:117:ASP:HA	1:A:120:GLU:OE1	2.15	0.46
1:C:116:HIS:O	1:C:117:ASP:HB2	2.15	0.46
1:B:108:LEU:HB2	1:B:111:ASN:ND2	2.30	0.46
1:A:214:VAL:O	3:A:302:MES:H71	2.17	0.44
1:A:60:THR:HB	1:A:61:PRO:HD3	2.00	0.44
1:B:60:THR:HB	1:B:61:PRO:HD3	1.99	0.44
1:B:237[B]:GLN:CG	1:D:237[B]:GLN:HG2	2.42	0.44
1:B:111:ASN:HB2	5:B:405:HOH:O	2.17	0.44
1:C:117:ASP:HA	1:C:120:GLU:OE1	2.17	0.44
1:D:58:GLN:N	1:D:58:GLN:CD	2.72	0.43
1:C:60:THR:HB	1:C:61:PRO:HD3	1.99	0.43
1:B:273:ALA:O	1:B:276:ALA:HB2	2.18	0.43
2:C:301:NVQ:C5	2:C:301:NVQ:C19	2.96	0.43
1:D:60:THR:HB	1:D:61:PRO:HD3	2.00	0.43
1:D:181:GLN:NE2	1:D:211:GLN:OE1	2.45	0.42
1:C:66:LEU:O	1:C:66:LEU:HD22	2.20	0.42
1:B:277:LYS:HD3	1:B:278:ASN:HB3	2.02	0.42
1:C:66:LEU:HD13	1:C:67:LEU:HG	2.02	0.42
1:A:116:HIS:O	1:A:117:ASP:HB2	2.20	0.42
1:C:70:GLY:HA3	1:C:77:LEU:HD22	2.01	0.41
1:B:116:HIS:O	1:B:117:ASP:HB2	2.21	0.41
2:A:301:NVQ:C19	2:A:301:NVQ:C5	2.99	0.41
1:B:7:ILE:HG12	1:B:107:VAL:CG1	2.50	0.41
1:A:32:ASP:OD2	1:A:243:GLU:OE1	2.39	0.40
1:B:132:ALA:HA	1:B:177:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:HB2	1:B:111:ASN:HD22	1.85	0.40
1:D:7:ILE:HG12	1:D:107:VAL:CG1	2.51	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	271/303 (89%)	267 (98%)	3 (1%)	1 (0%)	34	41
1	B	264/303 (87%)	261 (99%)	2 (1%)	1 (0%)	34	41
1	C	248/303 (82%)	245 (99%)	2 (1%)	1 (0%)	34	41
1	D	252/303 (83%)	250 (99%)	1 (0%)	1 (0%)	34	41
All	All	1035/1212 (85%)	1023 (99%)	8 (1%)	4 (0%)	34	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	TYR
1	D	31	TYR
1	B	31	TYR
1	C	31	TYR

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	225/248 (91%)	223 (99%)	2 (1%)	78	86
1	B	218/248 (88%)	213 (98%)	5 (2%)	50	63
1	C	200/248 (81%)	195 (98%)	5 (2%)	47	60
1	D	202/248 (82%)	198 (98%)	4 (2%)	55	67
All	All	845/992 (85%)	829 (98%)	16 (2%)	57	69

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	152	GLN
1	B	97	SER
1	B	187	ARG
1	B	270	LYS
1	B	277	LYS
1	B	286	ARG
1	C	66	LEU
1	C	77	LEU
1	C	112	LEU
1	C	117	ASP
1	C	130	THR
1	D	58	GLN
1	D	88	LEU
1	D	124	SER
1	D	130	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	169	ASN
1	B	101	ASN
1	C	127	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	MES	C	302	-	12,12,12	0.75	0	14,16,16	0.43	0
2	NVQ	C	301	-	32,35,35	1.16	3 (9%)	37,49,49	2.82	7 (18%)
2	NVQ	A	301	-	32,35,35	0.90	2 (6%)	37,49,49	2.81	6 (16%)
2	NVQ	B	301	-	32,35,35	1.04	4 (12%)	37,49,49	2.84	7 (18%)
3	MES	D	302	-	12,12,12	0.77	0	14,16,16	0.36	0
3	MES	A	302	-	12,12,12	0.74	0	14,16,16	0.38	0
2	NVQ	D	301	-	32,35,35	1.17	3 (9%)	37,49,49	2.99	8 (21%)
3	MES	B	302	-	12,12,12	0.76	0	14,16,16	0.42	0

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
3	MES	C	302	-	-	0/6/14/14	0/1/1/1
2	NVQ	C	301	-	-	9/26/26/26	0/3/3/3
2	NVQ	A	301	-	-	8/26/26/26	0/3/3/3
2	NVQ	B	301	-	-	10/26/26/26	0/3/3/3
3	MES	D	302	-	-	3/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	302	-	-	2/6/14/14	0/1/1/1
2	NVQ	D	301	-	-	8/26/26/26	0/3/3/3
3	MES	B	302	-	-	0/6/14/14	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NVQ	S1-N4	4.88	1.71	1.64
2	C	301	NVQ	S1-N4	4.62	1.71	1.64
2	D	301	NVQ	C3-N2	3.24	1.38	1.33
2	C	301	NVQ	C3-N2	3.17	1.38	1.33
2	A	301	NVQ	C3-N2	3.14	1.38	1.33
2	B	301	NVQ	C3-N2	3.13	1.38	1.33
2	B	301	NVQ	S1-N4	2.86	1.68	1.64
2	B	301	NVQ	C2-C1	2.80	1.45	1.41
2	C	301	NVQ	C2-C3	2.33	1.44	1.41
2	A	301	NVQ	C2-C1	2.28	1.44	1.41
2	B	301	NVQ	C2-C3	2.28	1.44	1.41
2	D	301	NVQ	C2-C3	2.00	1.44	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	NVQ	C4-N2-C3	13.38	126.44	115.14
2	A	301	NVQ	C4-N2-C3	13.17	126.26	115.14
2	D	301	NVQ	C4-N2-C3	13.01	126.12	115.14
2	C	301	NVQ	C4-N2-C3	12.99	126.11	115.14
2	D	301	NVQ	N3-C1-N1	8.73	122.77	116.65
2	C	301	NVQ	N3-C1-N1	6.84	121.45	116.65
2	D	301	NVQ	C1-C2-C3	6.45	119.48	114.44
2	A	301	NVQ	C1-C2-C3	6.43	119.47	114.44
2	B	301	NVQ	N3-C1-N1	6.09	120.92	116.65
2	C	301	NVQ	C1-C2-C3	5.88	119.04	114.44
2	B	301	NVQ	C1-C2-C3	5.72	118.91	114.44
2	A	301	NVQ	N3-C1-N1	5.42	120.45	116.65
2	B	301	NVQ	C13-C5-N1	4.06	118.94	112.63
2	A	301	NVQ	C13-C5-N1	3.93	118.73	112.63
2	A	301	NVQ	C2-C3-N2	-3.64	115.67	123.14
2	D	301	NVQ	C2-C3-N2	-3.63	115.68	123.14
2	B	301	NVQ	C2-C3-N2	-3.53	115.88	123.14
2	C	301	NVQ	C13-C5-N1	3.50	118.07	112.63
2	C	301	NVQ	C2-C3-N2	-3.44	116.07	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	NVQ	C13-C5-N1	2.79	116.95	112.63
2	D	301	NVQ	C19-N3-C1	2.72	130.00	124.60
2	A	301	NVQ	C19-N3-C1	2.71	129.99	124.60
2	B	301	NVQ	C19-N3-C1	2.52	129.60	124.60
2	C	301	NVQ	C19-N3-C1	2.41	129.40	124.60
2	C	301	NVQ	C5-N1-C4	-2.35	115.17	117.92
2	D	301	NVQ	C5-N1-C4	-2.23	115.32	117.92
2	B	301	NVQ	C5-N1-C4	-2.15	115.41	117.92
2	D	301	NVQ	C6-N4-S1	2.04	120.27	116.83

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NVQ	N1-C1-N3-C19
2	A	301	NVQ	C2-C1-N3-C19
2	A	301	NVQ	C6-N4-S1-O3
2	A	301	NVQ	C6-N4-S1-O4
2	B	301	NVQ	N1-C1-N3-C19
2	B	301	NVQ	C2-C1-N3-C19
2	B	301	NVQ	C6-N4-S1-O3
2	B	301	NVQ	C6-N4-S1-O4
2	C	301	NVQ	N1-C1-N3-C19
2	C	301	NVQ	C6-N4-S1-O3
2	C	301	NVQ	C6-N4-S1-O4
2	D	301	NVQ	N1-C1-N3-C19
2	D	301	NVQ	C6-N4-S1-O3
2	D	301	NVQ	C6-N4-S1-O4
2	C	301	NVQ	N3-C19-C20-C21
2	C	301	NVQ	C19-C20-C21-N5
3	D	302	MES	C7-C8-S-O3S
2	A	301	NVQ	C19-C20-C21-N5
2	C	301	NVQ	C2-C1-N3-C19
2	B	301	NVQ	C19-C20-C21-N5
2	D	301	NVQ	C20-C21-N5-C22
2	C	301	NVQ	C14-C13-C5-N1
2	B	301	NVQ	C14-C13-C5-N1
2	D	301	NVQ	C14-C13-C5-N1
2	A	301	NVQ	C14-C13-C5-N1
2	A	301	NVQ	C20-C19-N3-C1
2	B	301	NVQ	C18-C13-C5-N1
2	D	301	NVQ	C18-C13-C5-N1

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Mol	Chain	Res	Type	Atoms
2	A	301	NVQ	C18-C13-C5-N1
2	C	301	NVQ	C18-C13-C5-N1
3	A	302	MES	C7-C8-S-O2S
3	D	302	MES	C7-C8-S-O1S
3	D	302	MES	C7-C8-S-O2S
3	A	302	MES	C7-C8-S-O3S
2	B	301	NVQ	C20-C19-N3-C1
2	D	301	NVQ	C19-C20-C21-N5
2	B	301	NVQ	C20-C21-N5-C22
2	C	301	NVQ	C20-C21-N5-C22
2	B	301	NVQ	N3-C19-C20-C21
2	D	301	NVQ	C6-N4-S1-C7

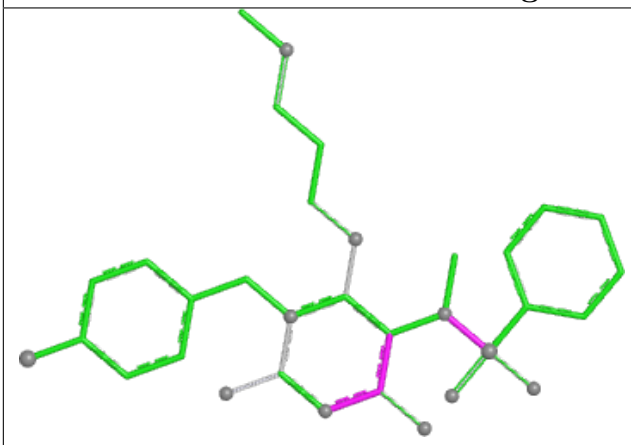
There are no ring outliers.

4 monomers are involved in 4 short contacts:

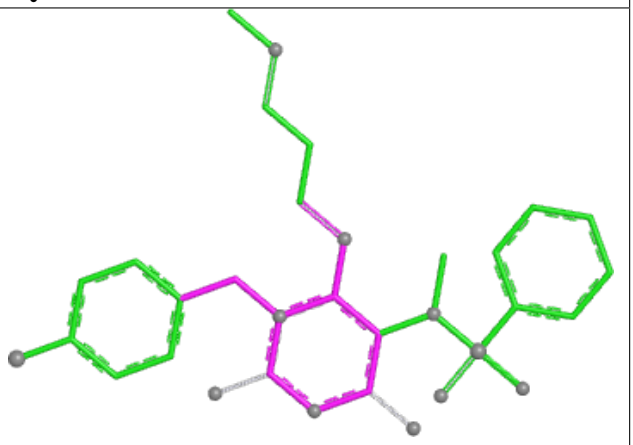
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	NVQ	1	0
2	A	301	NVQ	1	0
3	A	302	MES	1	0
2	D	301	NVQ	1	0

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.

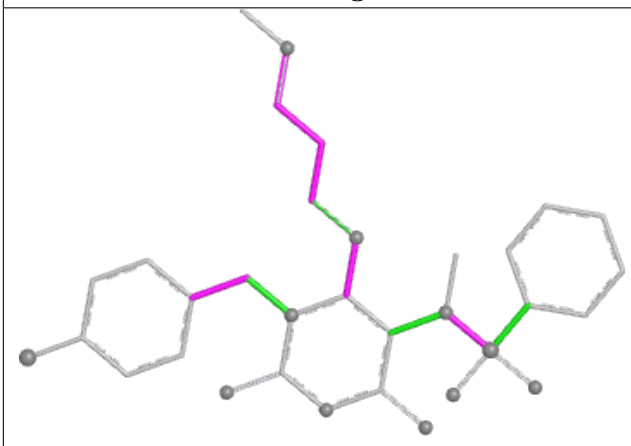
Ligand NVQ C 301



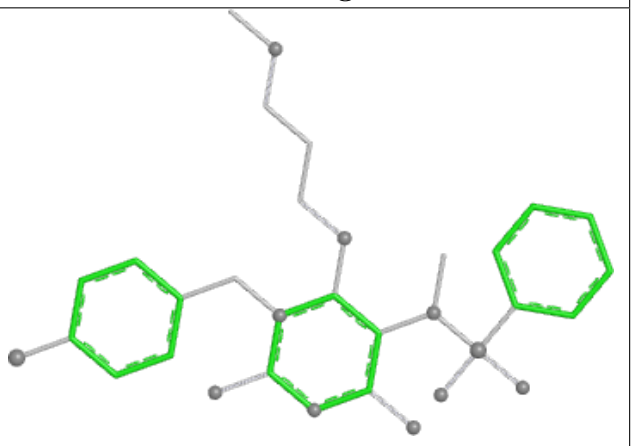
Bond lengths



Bond angles

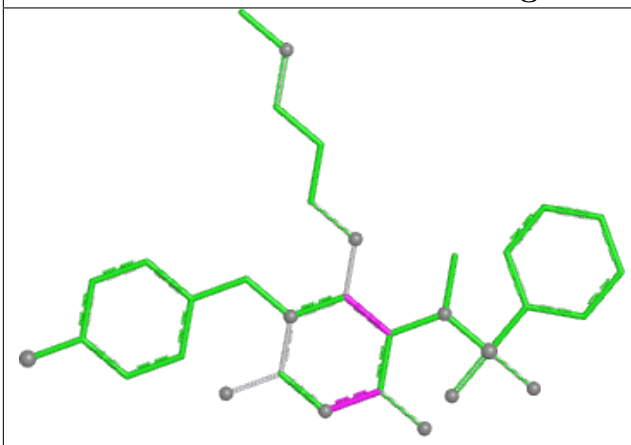


Torsions

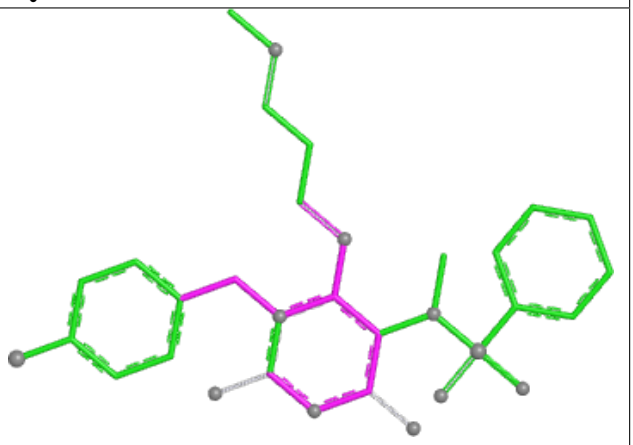


Rings

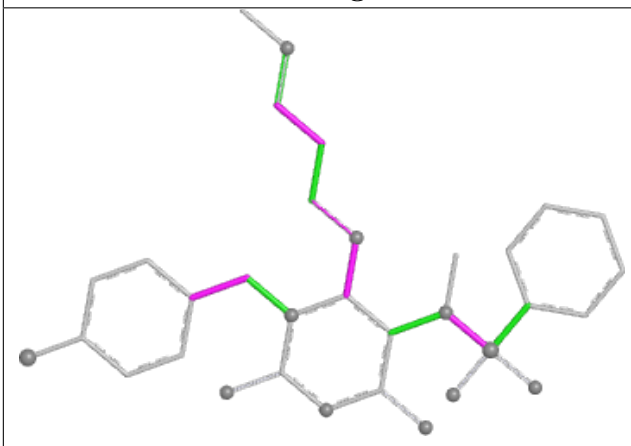
Ligand NVQ A 301



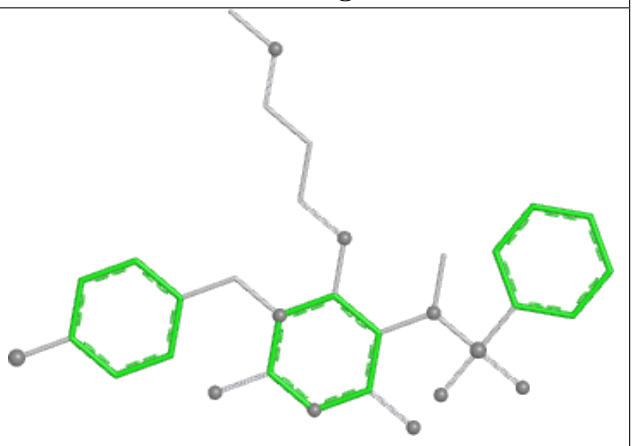
Bond lengths



Bond angles

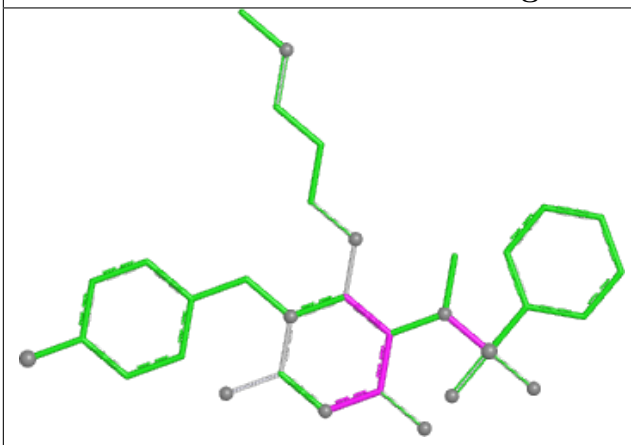


Torsions

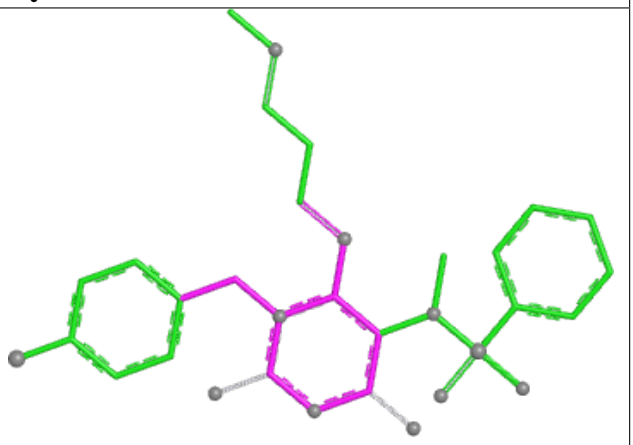


Rings

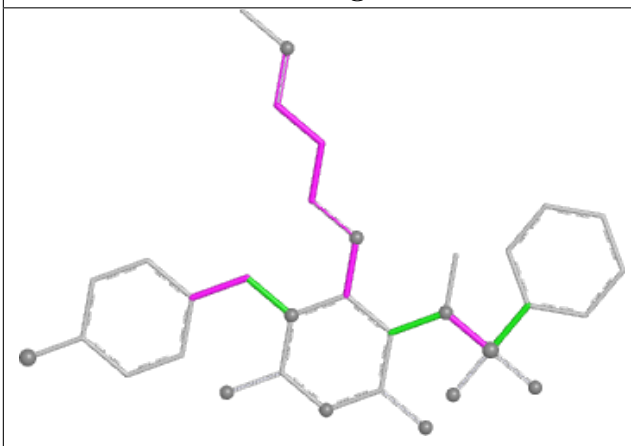
Ligand NVQ B 301



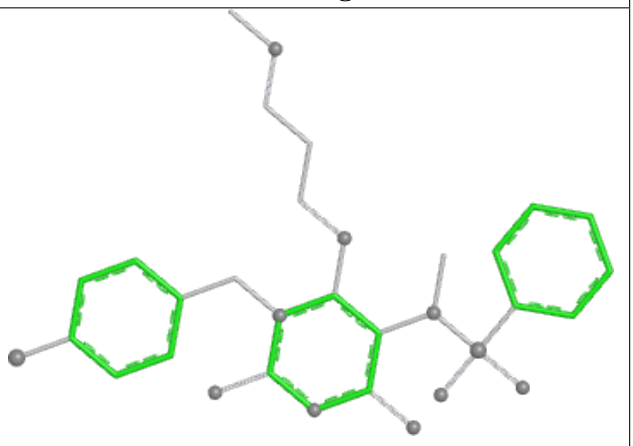
Bond lengths



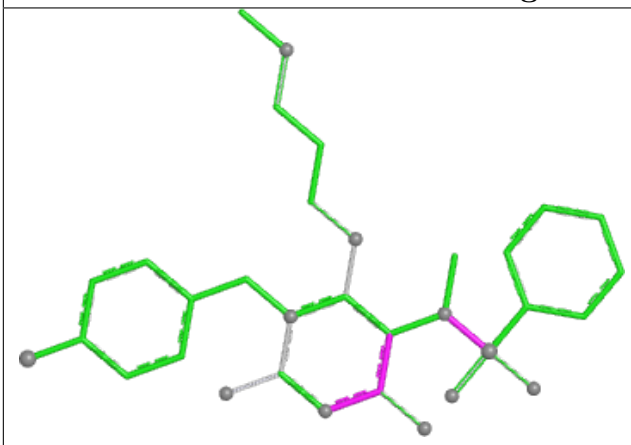
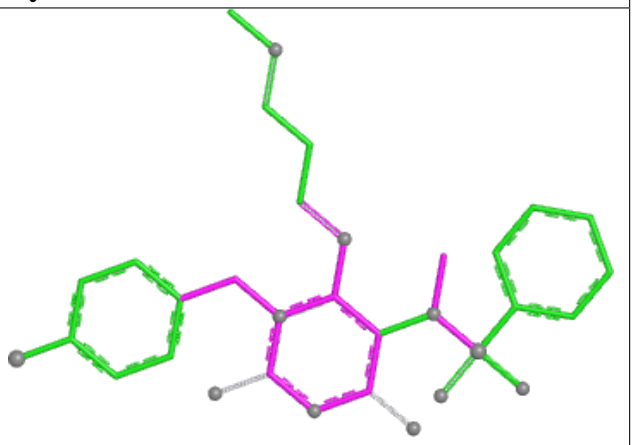
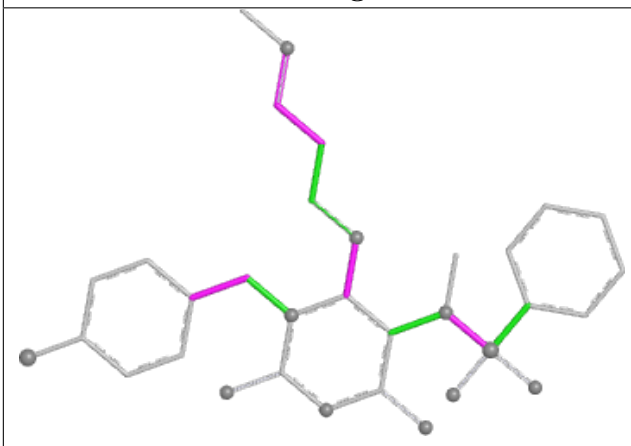
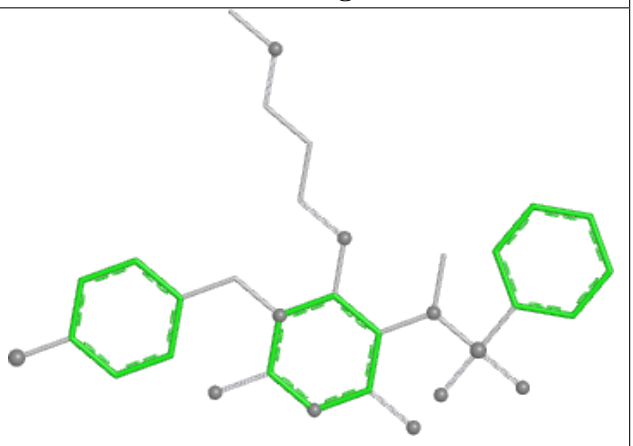
Bond angles



Torsions



Rings

Ligand NVQ D 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	278/303 (91%)	1.14	39 (14%)	2 1	29, 49, 67, 74	0
1	B	271/303 (89%)	1.08	34 (12%)	3 2	28, 46, 67, 75	0
1	C	259/303 (85%)	1.17	44 (16%)	1 1	29, 52, 78, 91	0
1	D	261/303 (86%)	1.23	51 (19%)	1 0	30, 53, 80, 90	0
All	All	1069/1212 (88%)	1.15	168 (15%)	2 1	28, 49, 73, 91	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	TYR	6.4
1	C	280	TYR	6.0
1	D	91	ALA	5.5
1	B	65	GLN	5.3
1	A	152	GLN	5.1
1	B	108	LEU	4.8
1	D	93	LEU	4.7
1	A	17	HIS	4.5
1	D	108	LEU	4.4
1	A	282	GLN	4.4
1	C	81	VAL	4.3
1	A	274	PRO	4.2
1	A	101	ASN	4.2
1	C	108	LEU	4.1
1	D	126	SER	4.0
1	A	289	THR	3.9
1	A	61	PRO	3.8
1	A	23	ILE	3.8
1	B	156	ALA	3.8
1	D	127	GLN	3.8
1	D	94	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	66	LEU	3.7
1	C	264	ASP	3.7
1	D	272	ALA	3.6
1	D	97	SER	3.6
1	D	224	LEU	3.6
1	C	60	THR	3.5
1	C	127	GLN	3.5
1	C	56	THR	3.4
1	B	176	TYR	3.3
1	D	184	ASP	3.3
1	C	126	SER	3.3
1	B	275	LEU	3.3
1	C	42	THR	3.2
1	D	109	GLY	3.2
1	A	164	LEU	3.2
1	D	264	ASP	3.1
1	D	112	LEU	3.1
1	A	18	PRO	3.1
1	A	20	THR	3.1
1	D	223	TRP	3.1
1	B	289	THR	3.1
1	C	112	LEU	3.1
1	D	271	LEU	3.1
1	C	43	LEU	3.1
1	C	285	LYS	3.0
1	B	157	ILE	3.0
1	D	96	GLU	3.0
1	B	24	SER	3.0
1	A	156	ALA	3.0
1	D	130	THR	3.0
1	A	97	SER	2.9
1	C	134	VAL	2.9
1	A	21	LEU	2.9
1	A	108	LEU	2.9
1	D	164	LEU	2.9
1	B	124	SER	2.9
1	A	175	LEU	2.9
1	A	84	SER	2.8
1	C	91	ALA	2.8
1	C	113	TYR	2.8
1	C	86	ASP	2.8
1	B	109	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	265	ALA	2.7
1	D	81	VAL	2.7
1	B	84	SER	2.7
1	C	55	SER	2.7
1	D	183	VAL	2.7
1	B	282	GLN	2.7
1	D	40	LEU	2.7
1	C	165	GLU	2.7
1	A	19	ALA	2.7
1	C	171	ALA	2.7
1	B	274	PRO	2.7
1	A	65	GLN	2.7
1	A	98	PHE	2.7
1	D	92	PHE	2.6
1	D	125	ALA	2.6
1	C	106	LEU	2.6
1	D	185	ILE	2.6
1	B	167	LYS	2.6
1	D	285	LYS	2.6
1	A	109	GLY	2.6
1	B	158	SER	2.6
1	A	62	ARG	2.6
1	B	106	LEU	2.5
1	D	65	GLN	2.5
1	D	129	GLN	2.5
1	B	61	PRO	2.5
1	A	199	ILE	2.5
1	D	64	GLN	2.5
1	D	120	GLU	2.5
1	A	157	ILE	2.5
1	D	124	SER	2.5
1	B	127	GLN	2.5
1	C	269	GLU	2.5
1	D	266	ALA	2.5
1	A	258	TYR	2.5
1	C	282	GLN	2.5
1	C	2	LYS	2.5
1	A	161	GLU	2.5
1	C	120	GLU	2.5
1	D	101	ASN	2.4
1	C	160	GLU	2.4
1	A	176	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	130	THR	2.4
1	D	175	LEU	2.4
1	B	64	GLN	2.4
1	B	99	ILE	2.4
1	D	57	PRO	2.4
1	A	105	ALA	2.4
1	B	164	LEU	2.4
1	D	279	GLY	2.4
1	B	186	ALA	2.4
1	D	128	ARG	2.4
1	C	223	TRP	2.4
1	C	41	SER	2.3
1	C	65	GLN	2.3
1	C	107	VAL	2.3
1	A	265	ALA	2.3
1	D	103	LEU	2.3
1	A	153	GLY	2.3
1	C	62	ARG	2.3
1	D	42	THR	2.3
1	C	197	LEU	2.3
1	D	88	LEU	2.3
1	D	99	ILE	2.3
1	A	22	ALA	2.3
1	B	258	TYR	2.3
1	B	278	ASN	2.2
1	D	134	VAL	2.2
1	A	60	THR	2.2
1	C	34	PRO	2.2
1	B	265	ALA	2.2
1	C	95	GLY	2.2
1	A	158	SER	2.2
1	D	98	PHE	2.2
1	A	140	LEU	2.2
1	C	100	GLY	2.2
1	B	57	PRO	2.2
1	D	288	LEU	2.2
1	C	97	SER	2.1
1	B	175	LEU	2.1
1	D	269	GLU	2.1
1	C	227	GLY	2.1
1	B	222	ALA	2.1
1	B	105	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	125	ALA	2.1
1	B	279	GLY	2.1
1	A	134	VAL	2.1
1	C	175	LEU	2.1
1	D	41	SER	2.1
1	B	101	ASN	2.1
1	B	276	ALA	2.1
1	B	174	GLY	2.1
1	A	166	PRO	2.0
1	D	166	PRO	2.0
1	A	7	ILE	2.0
1	C	164	LEU	2.0
1	C	288	LEU	2.0
1	D	180	GLN	2.0
1	A	207	LEU	2.0
1	D	27	LEU	2.0
1	D	207	LEU	2.0
1	A	86	ASP	2.0
1	B	100	GLY	2.0
1	C	51	ILE	2.0
1	C	114	TYR	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	MES	D	302	12/12	0.81	0.29	74,77,81,82	0
3	MES	C	302	12/12	0.84	0.30	70,72,75,76	0

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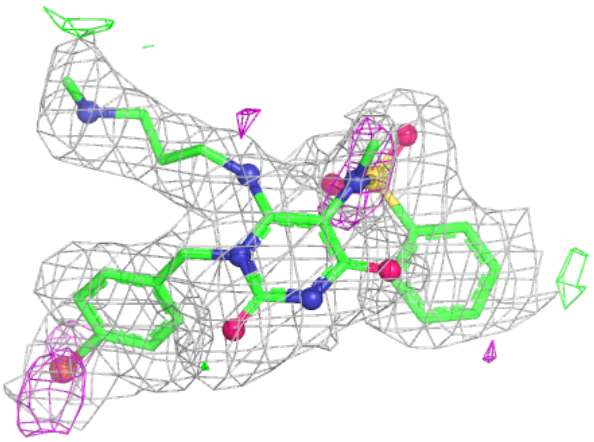
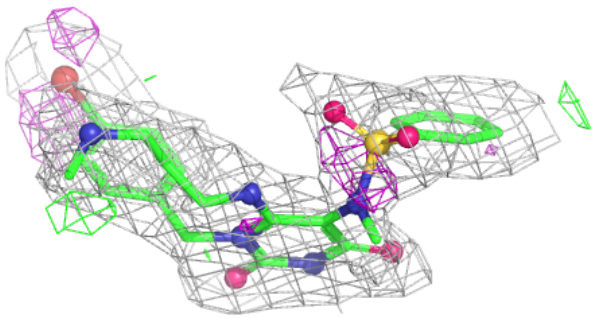
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NVQ	C	301	33/33	0.86	0.23	36,44,48,52	0
2	NVQ	D	301	33/33	0.87	0.23	35,39,46,55	0
2	NVQ	B	301	33/33	0.90	0.20	34,37,44,45	0
2	NVQ	A	301	33/33	0.91	0.21	32,37,41,45	0
3	MES	A	302	12/12	0.93	0.23	53,55,56,57	0
3	MES	B	302	12/12	0.94	0.25	45,47,49,50	0
4	CL	A	303	1/1	0.96	0.21	24,24,24,24	0
4	CL	B	303	1/1	0.96	0.27	32,32,32,32	0
4	CL	A	305	1/1	0.97	0.23	25,25,25,25	0
4	CL	B	304	1/1	0.97	0.26	28,28,28,28	0
4	CL	C	303	1/1	0.97	0.27	22,22,22,22	0
4	CL	B	305	1/1	0.98	0.25	21,21,21,21	0
4	CL	A	304	1/1	0.98	0.21	30,30,30,30	0
4	CL	D	303	1/1	0.98	0.28	21,21,21,21	0

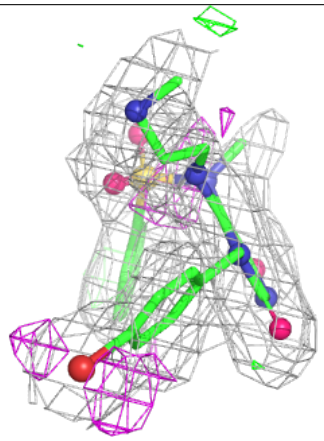
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NVQ C 301:

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

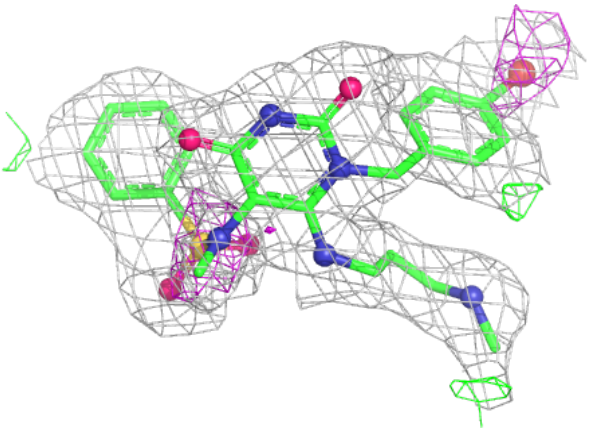


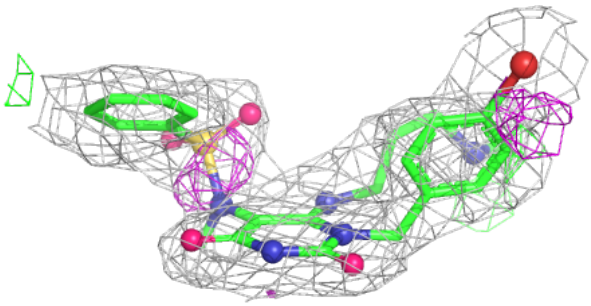


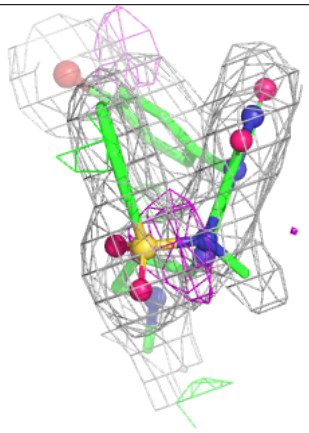


Electron density around NVQ D 301:

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

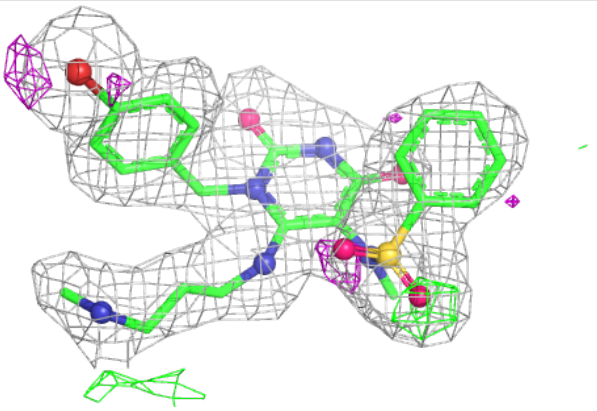


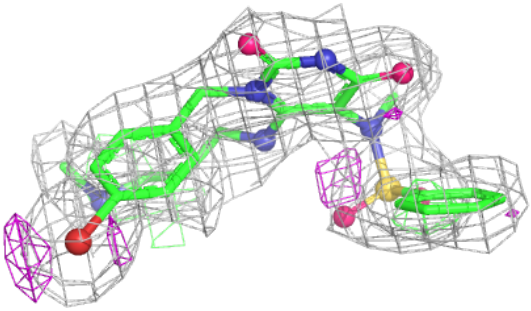


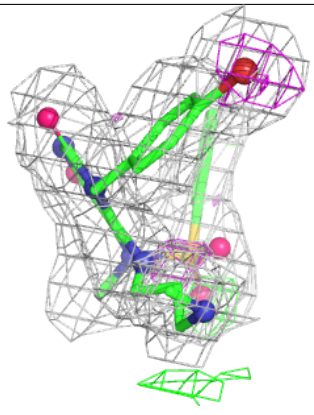


Electron density around NVQ B 301:

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

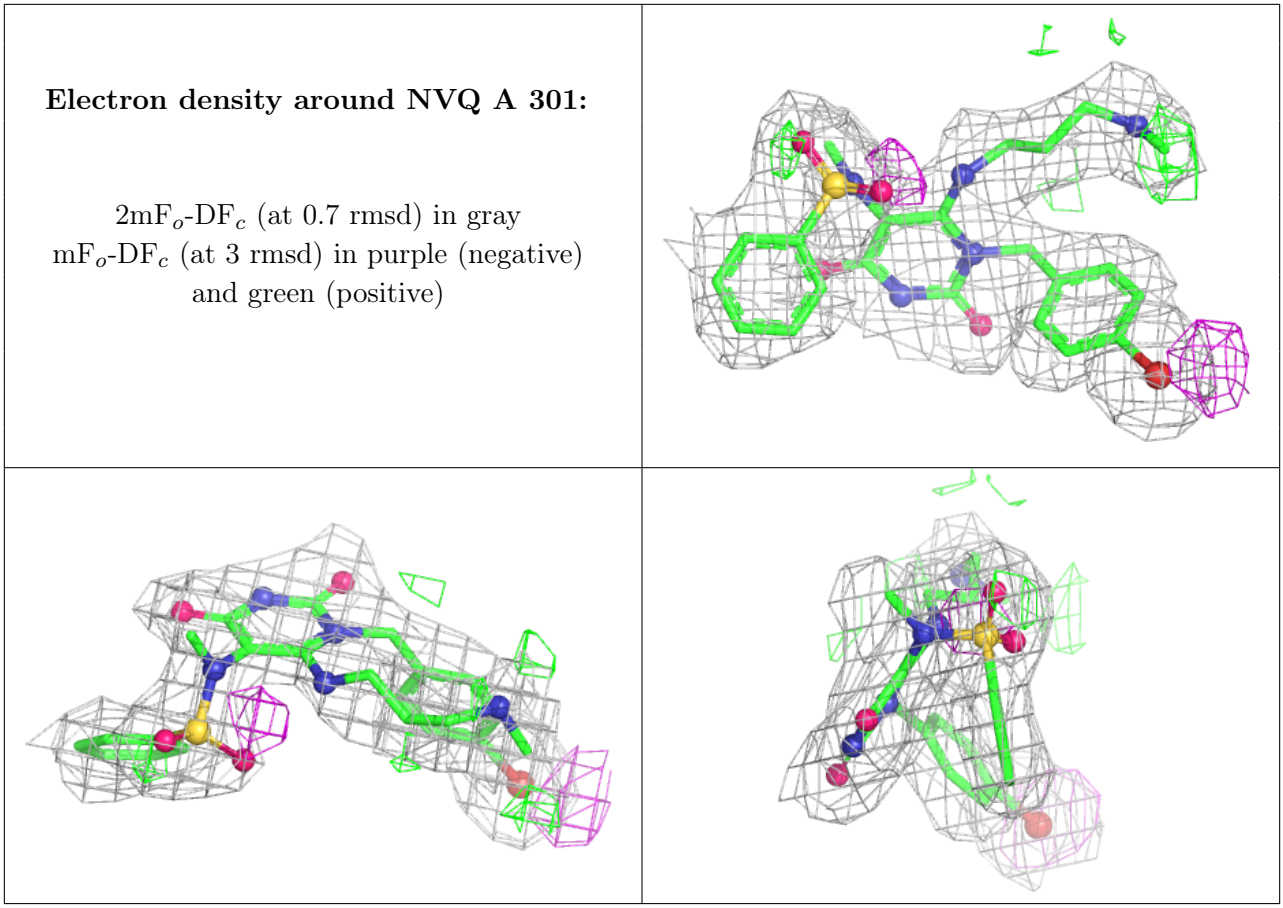






Electron density around NVQ A 301:

$2mF_o$-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

There are no such residues in this entry.