Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 07:46 PM EDT

PDB ID	:	4B3U
Title	:	Pseudomonas aeruginosa RmlA in complex with allosteric inhibitor
Authors	:	Alphey, M.S.; Pirrie, L.; Torrie, L.S.; Gardiner, M.; Sarkar, A.; Brenk, R.; Westwood, N.J.; Gray, D.; Naismith, J.H.
Deposited on	:	2012-07-26
Resolution	:	1.80 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:

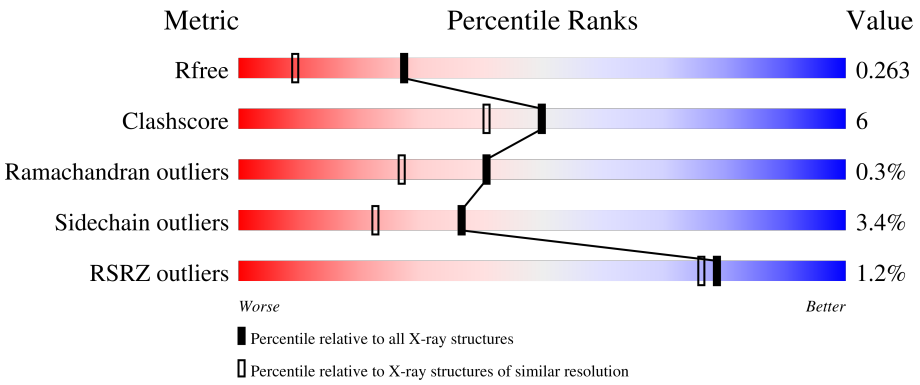
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	87% 11% •
1	B	303	% 86% 10% •
1	C	303	2% 85% 12% • •
1	D	303	2% 86% 10% • •

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	GOL	A	1295	-	-	X	-
4	GOL	C	1296	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10266 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
			Total	C	N	O	S			
1	A	299	2365	1511	406	443	5	0	2	0
1	B	293	2299	1471	387	436	5	0	1	0
1	C	298	2349	1501	402	441	5	0	1	0
1	D	293	2299	1471	387	436	5	0	1	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP Q9HU22
A	-8	HIS	-	expression tag	UNP Q9HU22
A	-7	HIS	-	expression tag	UNP Q9HU22
A	-6	HIS	-	expression tag	UNP Q9HU22
A	-5	HIS	-	expression tag	UNP Q9HU22
A	-4	HIS	-	expression tag	UNP Q9HU22
A	-3	GLY	-	expression tag	UNP Q9HU22
A	-2	SER	-	expression tag	UNP Q9HU22
A	-1	MET	-	expression tag	UNP Q9HU22
A	0	ALA	-	expression tag	UNP Q9HU22
B	-9	HIS	-	expression tag	UNP Q9HU22
B	-8	HIS	-	expression tag	UNP Q9HU22
B	-7	HIS	-	expression tag	UNP Q9HU22
B	-6	HIS	-	expression tag	UNP Q9HU22
B	-5	HIS	-	expression tag	UNP Q9HU22
B	-4	HIS	-	expression tag	UNP Q9HU22
B	-3	GLY	-	expression tag	UNP Q9HU22
B	-2	SER	-	expression tag	UNP Q9HU22
B	-1	MET	-	expression tag	UNP Q9HU22
B	0	ALA	-	expression tag	UNP Q9HU22

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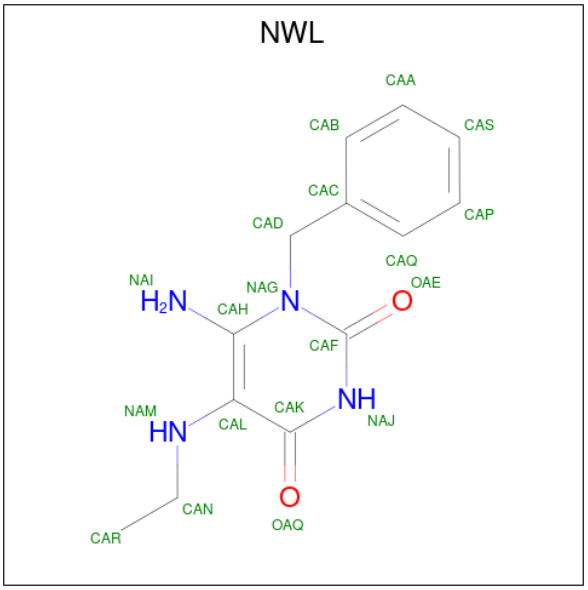
Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	HIS	-	expression tag	UNP Q9HU22
C	-8	HIS	-	expression tag	UNP Q9HU22
C	-7	HIS	-	expression tag	UNP Q9HU22
C	-6	HIS	-	expression tag	UNP Q9HU22
C	-5	HIS	-	expression tag	UNP Q9HU22
C	-4	HIS	-	expression tag	UNP Q9HU22
C	-3	GLY	-	expression tag	UNP Q9HU22
C	-2	SER	-	expression tag	UNP Q9HU22
C	-1	MET	-	expression tag	UNP Q9HU22
C	0	ALA	-	expression tag	UNP Q9HU22
D	-9	HIS	-	expression tag	UNP Q9HU22
D	-8	HIS	-	expression tag	UNP Q9HU22
D	-7	HIS	-	expression tag	UNP Q9HU22
D	-6	HIS	-	expression tag	UNP Q9HU22
D	-5	HIS	-	expression tag	UNP Q9HU22
D	-4	HIS	-	expression tag	UNP Q9HU22
D	-3	GLY	-	expression tag	UNP Q9HU22
D	-2	SER	-	expression tag	UNP Q9HU22
D	-1	MET	-	expression tag	UNP Q9HU22
D	0	ALA	-	expression tag	UNP Q9HU22

- Molecule 2 is 6-amino-1-benzyl-5-(ethylamino)pyrimidine-2,4(1H,3H)-dione (three-letter code: NWL) (formula: $C_{13}H_{16}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	19	13	4	2	0	0

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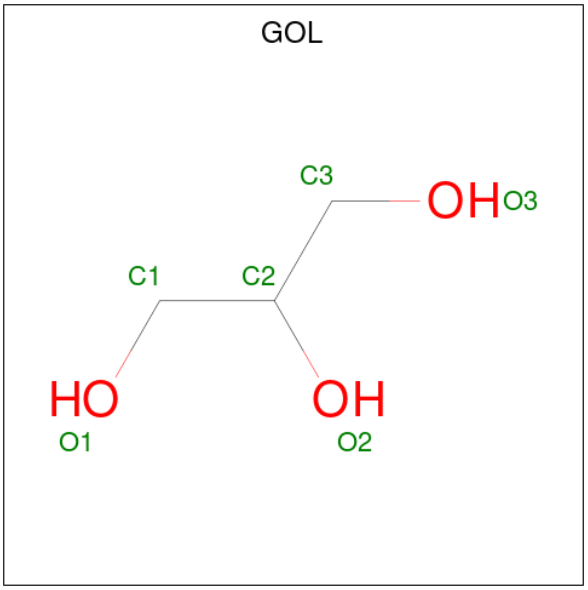
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	19	13	4	2	0	0
			Total	C	N	O		
2	C	1	19	13	4	2	0	0
			Total	C	N	O		
2	D	1	19	13	4	2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
			Total	Cl		
3	B	1	1	1	0	0
			Total	Cl		
3	C	1	1	1	0	0
			Total	Cl		
3	D	1	1	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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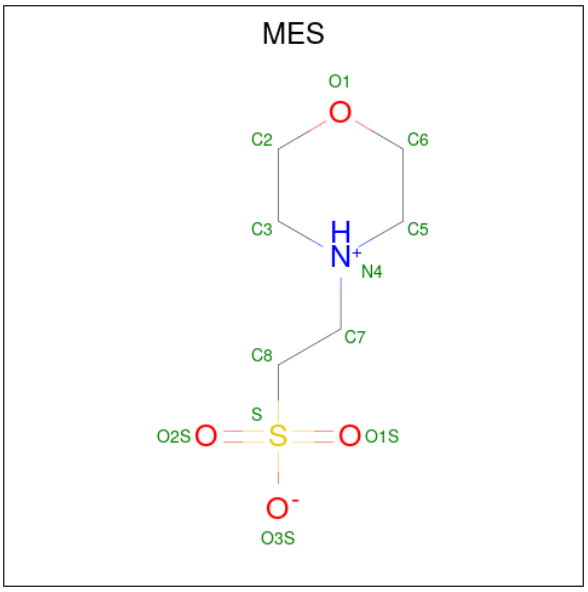
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	C	1	6	3	3	0	0
			Total	C	O		
4	D	1	6	3	3	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	236	236	236	0	0
			Total	O		
6	B	212	212	212	0	0
			Total	O		
6	C	203	203	203	0	0

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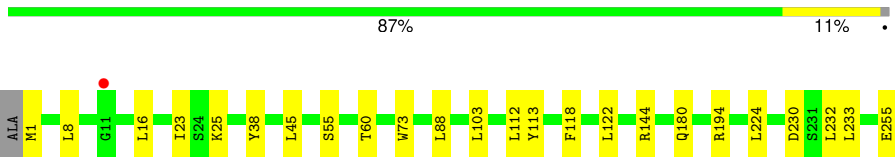
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	D	151	151	151	0	0

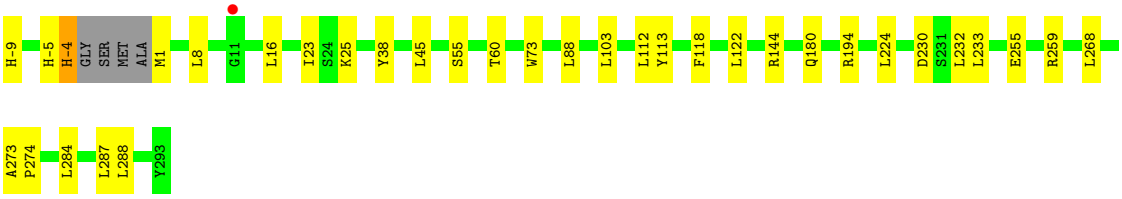
3 Residue-property plots (i)

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

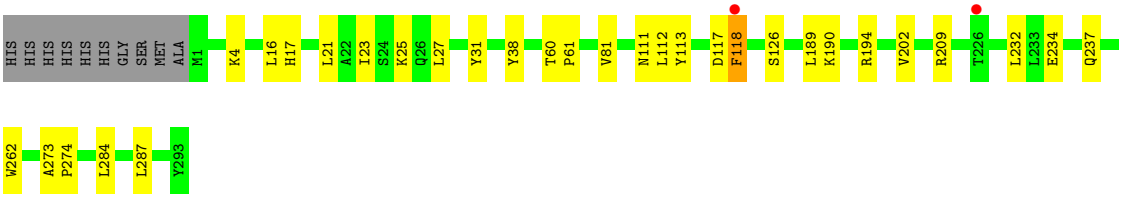
Chain A:





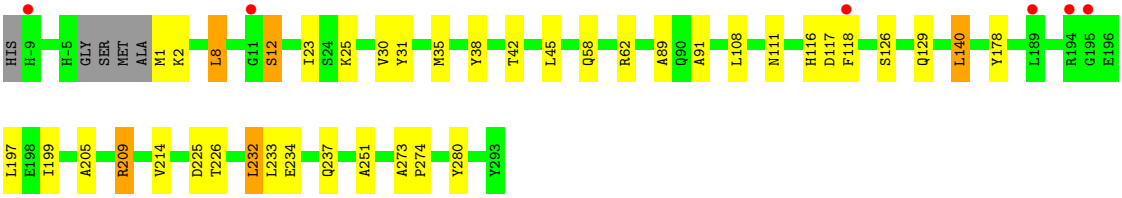
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain B:



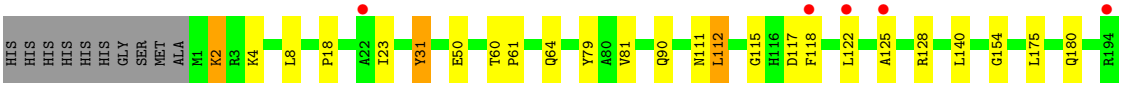
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain C:



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain D:



L197
E215
Y221
L233
Q237
A251
W262
Y293

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	64.21Å 154.58Å 134.03Å 90.00° 92.05° 90.00°	Depositor
Resolution (Å)	45.13 – 1.80 45.13 – 1.75	Depositor EDS
% Data completeness (in resolution range)	85.6 (45.13-1.80) 86.6 (45.13-1.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.218 , 0.262 0.222 , 0.263	Depositor DCC
R_{free} test set	5662 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 30.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.088 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10266	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: CL, NWL, GOL, 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	0.53	1/2426 (0.0%)	0.62	0/3289
1	B	0.48	1/2352 (0.0%)	0.62	0/3190
1	C	0.51	0/2406	0.62	1/3262 (0.0%)
1	D	0.46	1/2352 (0.0%)	0.59	0/3190
All	All	0.50	3/9536 (0.0%)	0.62	1/12931 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	262	TRP	CD2-CE2	5.22	1.47	1.41
1	D	262	TRP	CD2-CE2	5.04	1.47	1.41
1	A	73	TRP	CD2-CE2	5.00	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	140	LEU	CA-CB-CG	5.09	127.02	115.30

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	2365	0	2343	31	0
1	B	2299	0	2292	29	0
1	C	2349	0	2329	41	0
1	D	2299	0	2292	33	0
2	A	19	0	16	1	0
2	B	19	0	16	1	0
2	C	19	0	16	0	0
2	D	19	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
4	A	6	0	8	4	0
4	C	12	0	16	6	0
4	D	6	0	8	1	0
5	A	12	0	13	0	0
5	B	12	0	13	0	0
5	C	12	0	13	1	0
5	D	12	0	13	1	0
6	A	236	0	0	1	0
6	B	212	0	0	5	0
6	C	203	0	0	2	0
6	D	151	0	0	1	0
All	All	10266	0	9404	110	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 6.

All (110) 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:OE1	1:D:237[A]:GLN:OE1	1.68	1.10
1:C:226:THR:CG2	1:C:232:LEU:HG	1.89	1.01
1:C:226:THR:HG23	1:C:232:LEU:HG	1.49	0.94
1:C:23:ILE:CG2	1:D:23:ILE:HD12	2.04	0.88
1:A:45:LEU:HD12	4:A:1295:GOL:O3	1.77	0.83
1:A:118:PHE:CE2	1:A:122:LEU:HD11	2.18	0.78
1:A:23:ILE:CG2	1:B:23:ILE:HD13	2.13	0.78
4:C:1296:GOL:H32	1:D:31:TYR:O	1.87	0.75
1:A:233:LEU:HD21	1:B:237[A]:GLN:CG	2.18	0.73
1:B:113:TYR:HB3	1:B:118:PHE:CZ	2.24	0.71
1:C:237[A]:GLN:CD	1:D:237[A]:GLN:OE1	2.31	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ILE:HG23	1:B:23:ILE:HD13	1.74	0.69
1:A:23:ILE:HG23	1:B:23:ILE:CD1	2.25	0.66
1:C:23:ILE:HG21	1:D:23:ILE:HD12	1.75	0.65
1:A:233:LEU:HD11	1:B:237[A]:GLN:HG3	1.79	0.65
1:A:233:LEU:HD21	1:B:237[A]:GLN:HG2	1.81	0.62
1:A:23:ILE:HD13	1:B:23:ILE:HG21	1.81	0.62
1:A:23:ILE:HG21	1:B:23:ILE:HD13	1.81	0.62
1:D:251:ALA:HB2	4:D:1295:GOL:H31	1.83	0.61
1:A:23:ILE:CG2	1:B:23:ILE:CD1	2.79	0.61
1:C:89:ALA:HB3	1:C:197:LEU:HB3	1.83	0.60
1:C:1:MET:HB2	1:C:129:GLN:OE1	2.00	0.60
1:C:251:ALA:HB2	4:C:1295:GOL:H31	1.82	0.59
1:A:38:TYR:HB2	1:A:112:LEU:HD22	1.84	0.59
1:C:232:LEU:HD23	6:C:2023:HOH:O	2.02	0.58
1:C:232:LEU:HB3	4:C:1296:GOL:H2	1.85	0.58
1:C:23:ILE:HB	1:D:23:ILE:HD12	1.85	0.57
1:B:21:LEU:C	1:B:21:LEU:HD23	2.25	0.57
1:C:23:ILE:CB	1:D:23:ILE:HD12	2.34	0.57
1:C:35:MET:HE2	1:C:226:THR:HG21	1.87	0.56
1:C:35:MET:CE	1:C:226:THR:HG21	2.37	0.55
1:C:226:THR:CG2	1:C:232:LEU:CG	2.76	0.55
1:D:4:LYS:NZ	1:D:50:GLU:OE1	2.40	0.55
2:A:400:NWL:NAM	4:A:1295:GOL:H12	2.22	0.54
1:C:233:LEU:HD11	1:D:237[A]:GLN:HG3	1.90	0.53
1:A:233:LEU:HD21	1:B:237[A]:GLN:HG3	1.90	0.53
1:C:116:HIS:ND1	3:C:1294:CL:CL	2.73	0.53
1:A:38:TYR:CB	1:A:112:LEU:HD22	2.39	0.52
1:A:113:TYR:O	4:A:1295:GOL:H2	2.08	0.52
1:C:233:LEU:HD21	1:D:237[B]:GLN:HA	1.90	0.52
2:B:400:NWL:HARA	6:B:2176:HOH:O	2.10	0.52
1:B:287:LEU:HD23	6:B:2205:HOH:O	2.10	0.52
1:A:144:ARG:HD2	6:A:2131:HOH:O	2.09	0.52
1:A:55:SER:HG	1:A:60:THR:HG1	1.56	0.52
1:A:55:SER:OG	1:A:60:THR:OG1	2.27	0.51
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.93	0.51
1:C:108:LEU:HD12	6:C:2084:HOH:O	2.10	0.51
1:C:237[A]:GLN:CG	1:D:237[A]:GLN:OE1	2.59	0.51
1:B:209:ARG:NH1	6:B:2159:HOH:O	2.43	0.50
1:A:118:PHE:CE2	4:A:1295:GOL:H32	2.46	0.50
1:C:237[A]:GLN:HG2	1:D:237[A]:GLN:OE1	2.11	0.50
4:C:1296:GOL:C3	1:D:31:TYR:O	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:HG22	6:D:2041:HOH:O	2.11	0.50
1:C:233:LEU:HD21	1:D:237[A]:GLN:HA	1.92	0.50
1:C:226:THR:O	1:C:226:THR:HG22	2.11	0.49
1:D:64:GLN:HG2	1:D:79:TYR:CG	2.47	0.49
1:D:122:LEU:CD2	1:D:175:LEU:HD21	2.42	0.49
1:D:90:GLN:HG2	1:D:197:LEU:HD12	1.94	0.49
1:A:268:LEU:HD23	1:A:288:LEU:CD2	2.44	0.48
1:B:113:TYR:HB3	1:B:118:PHE:CE2	2.49	0.48
1:B:284:LEU:HA	1:B:287:LEU:HD12	1.96	0.48
1:A:233:LEU:HD21	1:B:237[B]:GLN:HA	1.96	0.47
1:A:16:LEU:HD12	1:A:25:LYS:HD3	1.96	0.47
1:D:64:GLN:HG2	1:D:79:TYR:CD2	2.49	0.47
1:B:81:VAL:HG22	6:B:2065:HOH:O	2.15	0.47
1:C:42:THR:HG23	1:C:118:PHE:HE2	1.80	0.47
1:A:233:LEU:HD21	1:B:237[A]:GLN:HA	1.96	0.46
1:A:118:PHE:CD2	1:A:122:LEU:HD11	2.50	0.46
1:C:226:THR:HG22	1:C:232:LEU:CD1	2.46	0.46
1:C:45:LEU:HD12	4:C:1295:GOL:H12	1.98	0.46
1:C:30:VAL:HB	1:C:38:TYR:CE1	2.51	0.46
1:C:232:LEU:HD22	4:C:1296:GOL:H2	1.98	0.46
1:C:226:THR:HG23	1:C:232:LEU:CG	2.33	0.45
1:C:214:VAL:O	5:C:1297:MES:H71	2.17	0.45
1:A:103:LEU:HD21	1:A:180:GLN:NE2	2.31	0.45
1:B:189:LEU:HD11	1:B:202:VAL:HG23	1.98	0.45
1:A:-4:HIS:ND1	1:A:-4:HIS:N	2.65	0.45
1:B:23:ILE:HD11	1:B:27:LEU:HD13	1.99	0.44
1:C:237[A]:GLN:HG3	1:D:233:LEU:HD11	1.99	0.44
1:D:122:LEU:HD21	1:D:175:LEU:HD21	1.99	0.44
1:C:234:GLU:HA	1:C:237[A]:GLN:NE2	2.32	0.44
1:D:118:PHE:CE2	1:D:122:LEU:HD11	2.52	0.44
1:D:60:THR:O	1:D:64:GLN:HG3	2.18	0.44
1:D:154:GLY:O	5:D:1296:MES:H32	2.17	0.44
1:B:60:THR:HB	1:B:61:PRO:HD3	2.00	0.43
1:D:125:ALA:HA	1:D:128:ARG:NH1	2.33	0.43
1:C:280:TYR:CD2	1:D:18:PRO:HD3	2.54	0.43
1:A:8:LEU:HD23	1:A:88:LEU:HD22	2.00	0.43
1:D:2:LYS:HD2	1:D:2:LYS:HA	1.92	0.42
1:D:128:ARG:NH2	1:D:215:GLU:OE2	2.52	0.42
1:A:284:LEU:HA	1:A:287:LEU:HD12	2.01	0.42
1:D:115:GLY:HA3	1:D:221:TYR:CD1	2.54	0.42
1:C:25:LYS:NZ	1:C:226:THR:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:CD2	1:C:91:ALA:HB2	2.49	0.42
1:D:60:THR:N	1:D:61:PRO:CD	2.83	0.42
1:D:112:LEU:HD12	1:D:112:LEU:C	2.40	0.42
1:A:194:ARG:HD2	1:A:194:ARG:N	2.35	0.42
1:B:4:LYS:NZ	6:B:2006:HOH:O	2.52	0.41
1:C:273:ALA:HB3	1:C:274:PRO:HD3	2.03	0.41
1:A:255:GLU:O	1:A:259:ARG:HG3	2.21	0.41
1:C:205:ALA:O	1:C:209:ARG:HD3	2.21	0.41
1:C:178:TYR:OH	1:C:199:ILE:HD11	2.21	0.41
1:B:21:LEU:HD23	1:B:21:LEU:O	2.20	0.41
1:B:113:TYR:HB3	1:B:118:PHE:HZ	1.80	0.41
1:B:16:LEU:HD12	1:B:25:LYS:HD3	2.02	0.41
1:B:38:TYR:HB2	1:B:112:LEU:HD22	2.03	0.41
1:B:273:ALA:HB3	1:B:274:PRO:HD3	2.03	0.40
1:C:237[A]:GLN:OE1	1:D:237[A]:GLN:CD	2.53	0.40
1:B:234:GLU:HA	1:B:237[A]:GLN:HE21	1.86	0.40
1:C:12:SER:HB3	1:C:25:LYS:HD3	2.04	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	297/303 (98%)	291 (98%)	6 (2%)	0	100	100
1	B	292/303 (96%)	287 (98%)	4 (1%)	1 (0%)	41	27
1	C	295/303 (97%)	288 (98%)	5 (2%)	2 (1%)	22	10
1	D	292/303 (96%)	285 (98%)	6 (2%)	1 (0%)	41	27
All	All	1176/1212 (97%)	1151 (98%)	21 (2%)	4 (0%)	41	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	31	TYR
1	D	31	TYR
1	B	31	TYR
1	C	12	SER

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	248/248 (100%)	241 (97%)	7 (3%)	43	30
1	B	241/248 (97%)	233 (97%)	8 (3%)	38	23
1	C	246/248 (99%)	235 (96%)	11 (4%)	27	13
1	D	241/248 (97%)	234 (97%)	7 (3%)	42	29
All	All	976/992 (98%)	943 (97%)	33 (3%)	37	22

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-9	HIS
1	A	-5	HIS
1	A	-4	HIS
1	A	1	MET
1	A	224	LEU
1	A	230	ASP
1	A	232	LEU
1	B	17	HIS
1	B	111	ASN
1	B	117	ASP
1	B	118	PHE
1	B	126	SER
1	B	190	LYS
1	B	194	ARG
1	B	232	LEU
1	C	2	LYS
1	C	8	LEU
1	C	58	GLN

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Mol	Chain	Res	Type
1	C	62	ARG
1	C	111	ASN
1	C	117	ASP
1	C	126	SER
1	C	140	LEU
1	C	209	ARG
1	C	225	ASP
1	C	232	LEU
1	D	2	LYS
1	D	8	LEU
1	D	111	ASN
1	D	112	LEU
1	D	117	ASP
1	D	140	LEU
1	D	180	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-9	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
5	MES	D	1296	-	12,12,12	1.82	1 (8%)	15,16,16	5.74	6 (40%)
4	GOL	A	1295	-	5,5,5	0.32	0	5,5,5	0.60	0
5	MES	B	1295	-	12,12,12	1.96	1 (8%)	15,16,16	5.95	8 (53%)
4	GOL	D	1295	-	5,5,5	0.46	0	5,5,5	0.64	0
5	MES	C	1297	-	12,12,12	1.93	1 (8%)	15,16,16	5.92	6 (40%)
2	NWL	C	400	-	20,20,20	0.69	0	22,27,27	1.77	5 (22%)
2	NWL	A	400	-	20,20,20	0.71	0	22,27,27	1.63	4 (18%)
2	NWL	D	400	-	20,20,20	0.80	0	22,27,27	1.90	8 (36%)
5	MES	A	1296	-	12,12,12	1.84	1 (8%)	15,16,16	5.72	6 (40%)
2	NWL	B	400	-	20,20,20	0.78	0	22,27,27	1.85	7 (31%)
4	GOL	C	1295	-	5,5,5	0.50	0	5,5,5	0.53	0
4	GOL	C	1296	-	5,5,5	0.42	0	5,5,5	0.97	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
5	MES	D	1296	-	-	4/6/14/14	0/1/1/1
4	GOL	A	1295	-	-	2/4/4/4	-
5	MES	B	1295	-	-	3/6/14/14	0/1/1/1
4	GOL	D	1295	-	-	3/4/4/4	-
5	MES	C	1297	-	-	2/6/14/14	0/1/1/1
2	NWL	C	400	-	-	3/7/7/7	0/2/2/2
2	NWL	A	400	-	-	2/7/7/7	0/2/2/2
2	NWL	D	400	-	-	3/7/7/7	0/2/2/2
5	MES	A	1296	-	-	2/6/14/14	0/1/1/1
2	NWL	B	400	-	-	3/7/7/7	0/2/2/2
4	GOL	C	1295	-	-	4/4/4/4	-
4	GOL	C	1296	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1295	MES	C8-S	-6.11	1.69	1.77
5	C	1297	MES	C8-S	-6.03	1.69	1.77
5	A	1296	MES	C8-S	-5.54	1.69	1.77
5	D	1296	MES	C8-S	-5.52	1.69	1.77

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1295	MES	O1S-S-C8	-13.52	86.30	106.73
5	C	1297	MES	O1S-S-C8	-13.05	87.01	106.73
5	A	1296	MES	O1S-S-C8	-12.15	88.37	106.73
5	C	1297	MES	O3S-S-O1S	-12.04	81.27	111.40
5	D	1296	MES	O1S-S-C8	-11.73	89.00	106.73
5	D	1296	MES	O3S-S-O1S	-11.29	83.16	111.40
5	A	1296	MES	O3S-S-O1S	-11.07	83.71	111.40
5	B	1295	MES	O3S-S-O1S	-10.76	84.47	111.40
5	C	1297	MES	O3S-S-C8	9.91	125.38	106.00
5	B	1295	MES	O2S-S-O1S	-9.76	82.08	113.82
5	A	1296	MES	O2S-S-O1S	-9.73	82.19	113.82
5	D	1296	MES	O2S-S-O1S	-9.64	82.48	113.82
5	D	1296	MES	O2S-S-C8	9.21	120.64	106.73
5	C	1297	MES	O2S-S-O1S	-8.77	85.31	113.82
5	A	1296	MES	O2S-S-C8	8.66	119.81	106.73
5	B	1295	MES	O2S-S-C8	8.18	119.09	106.73
5	B	1295	MES	O3S-S-C8	6.40	118.52	106.00
5	A	1296	MES	O3S-S-C8	6.06	117.86	106.00
5	D	1296	MES	O3S-S-C8	5.65	117.07	106.00
2	D	400	NWL	CAK-NAJ-CAF	-5.38	120.28	127.34
2	C	400	NWL	CAK-NAJ-CAF	-4.88	120.95	127.34
2	B	400	NWL	CAK-NAJ-CAF	-4.81	121.03	127.34
5	C	1297	MES	O2S-S-C8	4.81	113.99	106.73
2	A	400	NWL	CAK-NAJ-CAF	-4.37	121.61	127.34
5	D	1296	MES	O3S-S-O2S	3.40	119.91	111.40
5	A	1296	MES	O3S-S-O2S	3.37	119.83	111.40
5	B	1295	MES	O3S-S-O2S	3.21	119.44	111.40
2	B	400	NWL	CAL-CAK-NAJ	2.96	120.25	112.13
2	C	400	NWL	CAL-CAK-NAJ	2.82	119.87	112.13
2	D	400	NWL	NAJ-CAF-NAG	2.78	120.44	115.45
2	D	400	NWL	CAL-CAK-NAJ	2.65	119.40	112.13
2	D	400	NWL	OAQ-CAK-CAL	-2.65	120.88	127.26
2	A	400	NWL	CAL-CAK-NAJ	2.58	119.21	112.13
5	C	1297	MES	O3S-S-O2S	2.58	117.85	111.40
2	C	400	NWL	OAQ-CAK-CAL	-2.41	121.44	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	NWL	CAK-CAL-NAM	2.29	123.02	116.83
2	C	400	NWL	NAJ-CAF-NAG	2.28	119.54	115.45
2	B	400	NWL	CAD-NAG-CAF	2.26	119.64	117.05
2	C	400	NWL	CAD-NAG-CAF	2.23	119.60	117.05
5	B	1295	MES	C2-C3-N4	2.22	113.50	110.12
2	B	400	NWL	OAQ-CAK-CAL	-2.20	121.95	127.26
5	B	1295	MES	C6-C5-N4	2.20	113.47	110.12
2	A	400	NWL	NAJ-CAF-NAG	2.18	119.36	115.45
2	D	400	NWL	CAL-CAH-NAI	-2.14	119.17	123.34
2	A	400	NWL	OAQ-CAK-CAL	-2.11	122.18	127.26
2	D	400	NWL	OAE-CAF-NAG	-2.10	119.58	122.32
2	D	400	NWL	CAD-NAG-CAF	2.09	119.45	117.05
2	D	400	NWL	NAI-CAH-NAG	2.08	120.35	116.29
2	B	400	NWL	NAJ-CAF-NAG	2.04	119.12	115.45
2	B	400	NWL	CAL-CAH-NAI	-2.04	119.36	123.34

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	NWL	CAK-CAL-NAM-CAN
2	B	400	NWL	CAH-CAL-NAM-CAN
2	C	400	NWL	CAK-CAL-NAM-CAN
2	D	400	NWL	CAK-CAL-NAM-CAN
5	A	1296	MES	C7-C8-S-O2S
5	A	1296	MES	C7-C8-S-O3S
5	B	1295	MES	C8-C7-N4-C3
5	B	1295	MES	C7-C8-S-O1S
5	C	1297	MES	C7-C8-S-O3S
5	D	1296	MES	C8-C7-N4-C5
4	C	1295	GOL	O2-C2-C3-O3
5	B	1295	MES	C7-C8-S-O3S
4	A	1295	GOL	O1-C1-C2-C3
4	C	1295	GOL	O1-C1-C2-C3
4	C	1295	GOL	C1-C2-C3-O3
4	D	1295	GOL	C1-C2-C3-O3
4	C	1295	GOL	O1-C1-C2-O2
2	B	400	NWL	CAK-CAL-NAM-CAN
4	D	1295	GOL	O2-C2-C3-O3
2	A	400	NWL	CAH-CAL-NAM-CAN
2	C	400	NWL	CAH-CAL-NAM-CAN
2	D	400	NWL	CAH-CAL-NAM-CAN

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Mol	Chain	Res	Type	Atoms
5	C	1297	MES	C7-C8-S-O1S
5	D	1296	MES	C7-C8-S-O1S
5	D	1296	MES	C7-C8-S-O2S
4	D	1295	GOL	O1-C1-C2-C3
2	B	400	NWL	CAR-CAN-NAM-CAL
2	C	400	NWL	CAR-CAN-NAM-CAL
2	D	400	NWL	CAR-CAN-NAM-CAL
4	A	1295	GOL	O1-C1-C2-O2
5	D	1296	MES	C8-C7-N4-C3

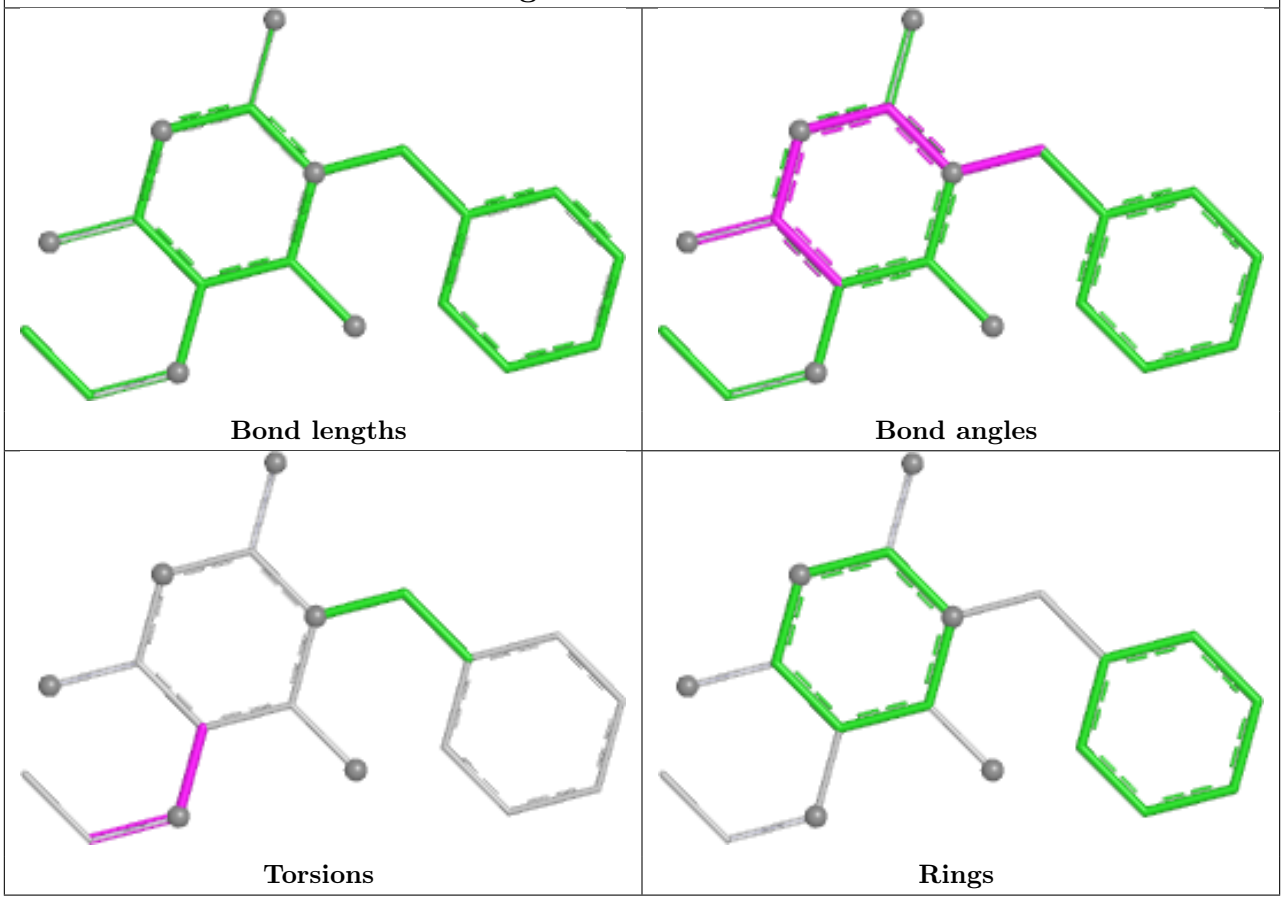
There are no ring outliers.

8 monomers are involved in 14 short contacts:

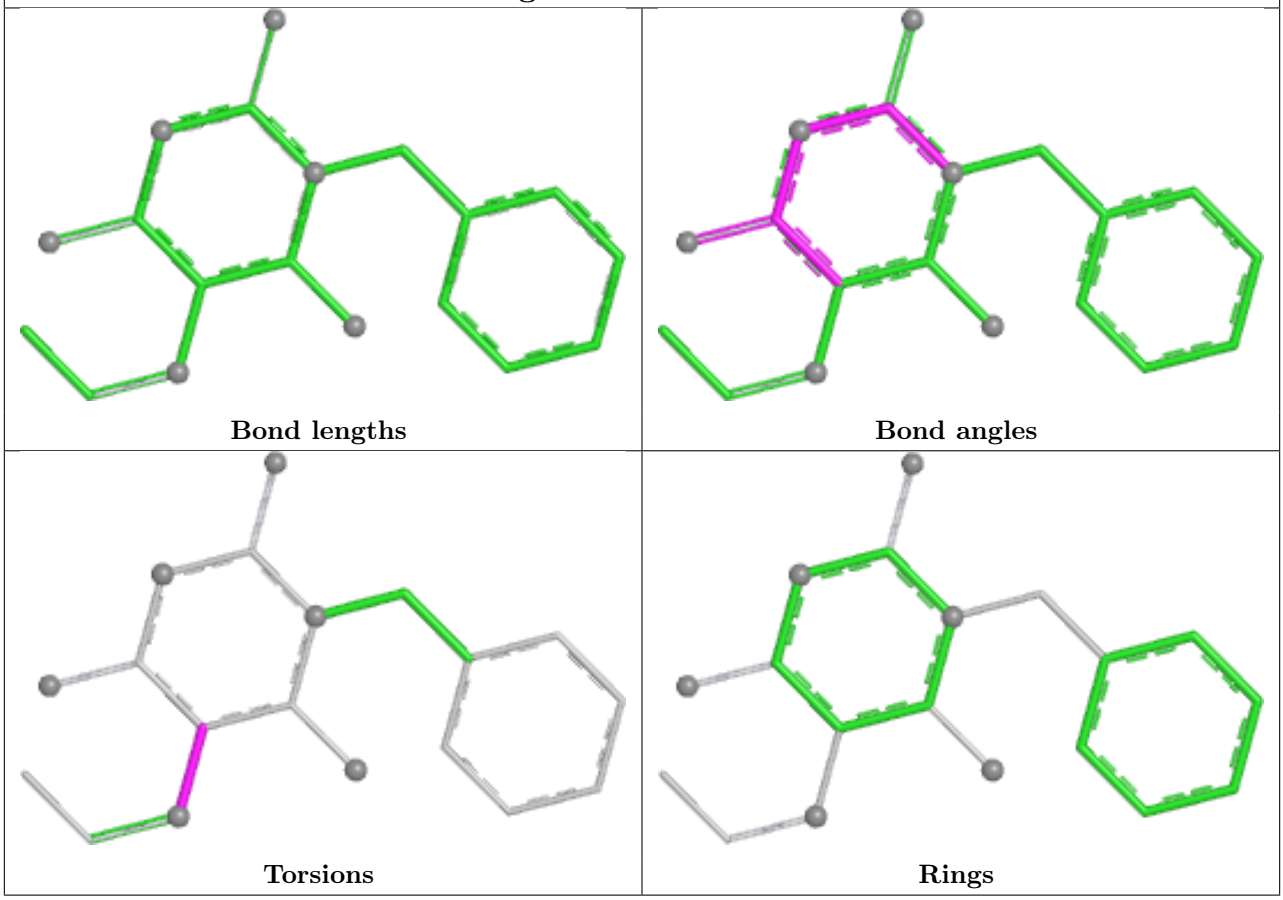
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1296	MES	1	0
4	A	1295	GOL	4	0
4	D	1295	GOL	1	0
5	C	1297	MES	1	0
2	A	400	NWL	1	0
2	B	400	NWL	1	0
4	C	1295	GOL	2	0
4	C	1296	GOL	4	0

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.

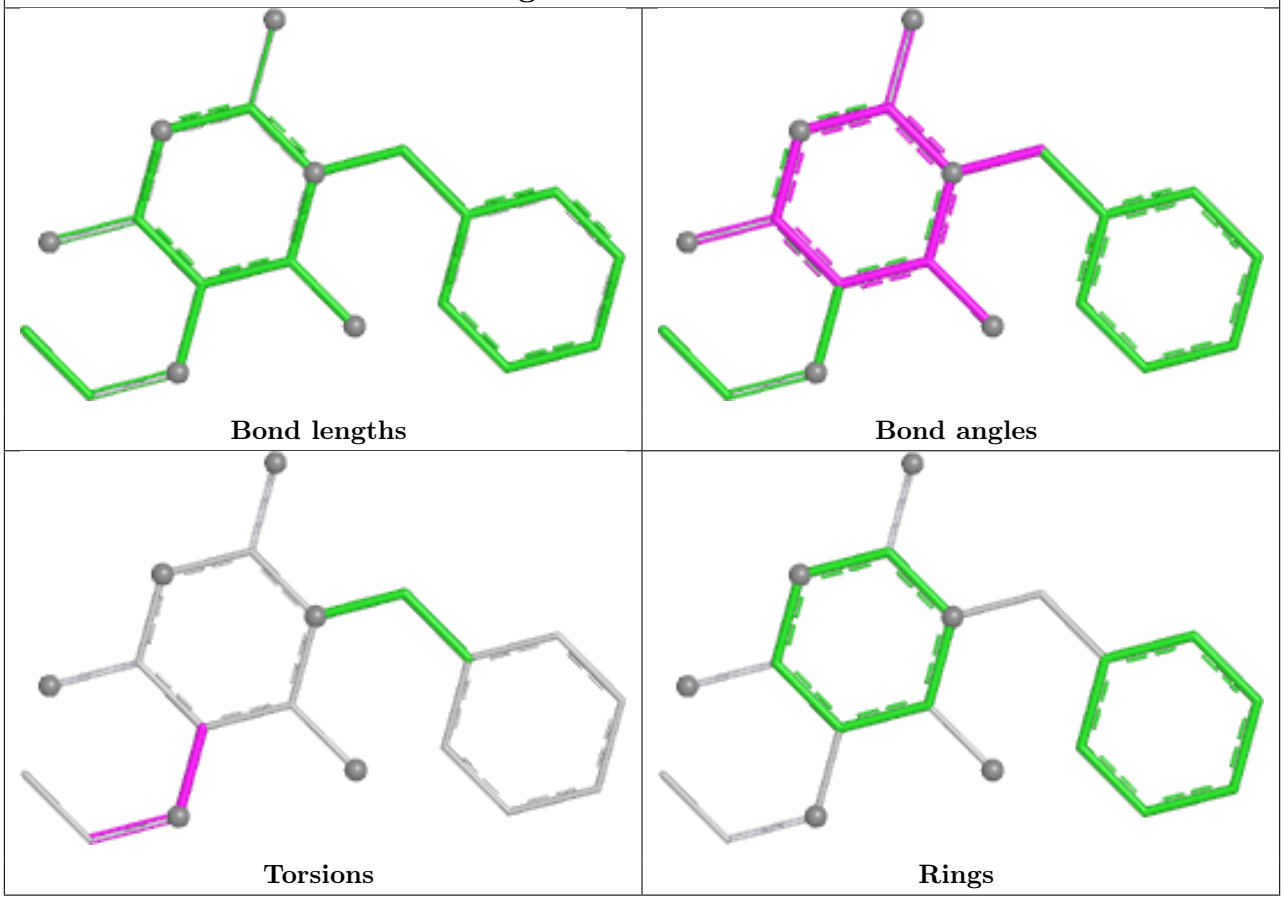
Ligand NWL C 400



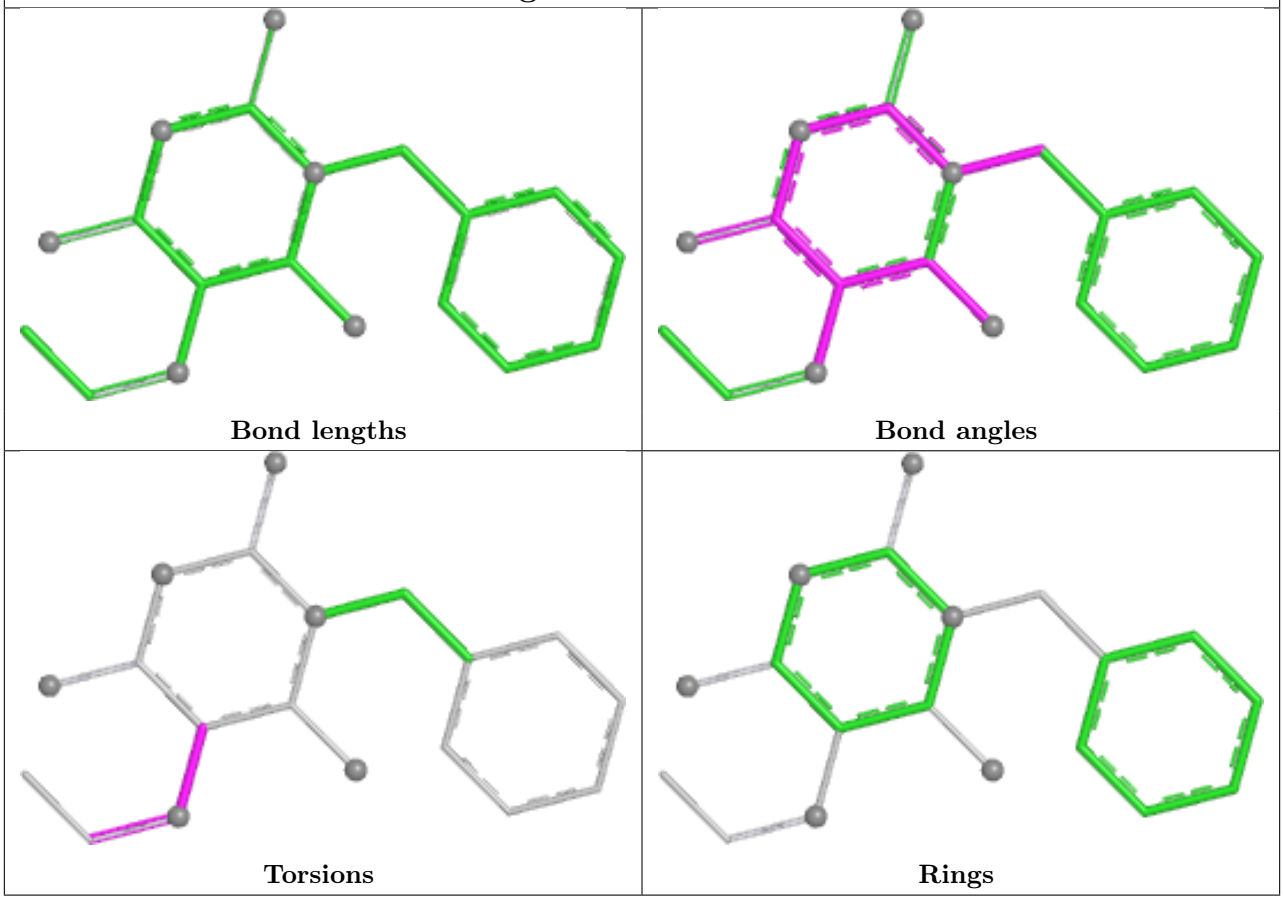
Ligand NWL A 400



Ligand NWL D 400



Ligand NWL B 400



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	299/303 (98%)	-0.38	1 (0%)	94	92	23, 34, 60, 85	0
1	B	293/303 (96%)	-0.39	2 (0%)	87	86	28, 38, 55, 79	0
1	C	298/303 (98%)	-0.28	6 (2%)	65	61	23, 37, 64, 102	1 (0%)
1	D	293/303 (96%)	-0.25	5 (1%)	70	66	27, 40, 63, 95	1 (0%)
All	All	1183/1212 (97%)	-0.33	14 (1%)	79	76	23, 37, 61, 102	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	189	LEU	5.0
1	A	11	GLY	3.5
1	C	194	ARG	3.5
1	C	11	GLY	3.2
1	C	195	GLY	3.1
1	D	194	ARG	2.9
1	D	22	ALA	2.9
1	C	-9	HIS	2.6
1	D	118	PHE	2.3
1	B	226	THR	2.1
1	C	118	PHE	2.1
1	B	118	PHE	2.1
1	D	125	ALA	2.0
1	D	122	LEU	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)

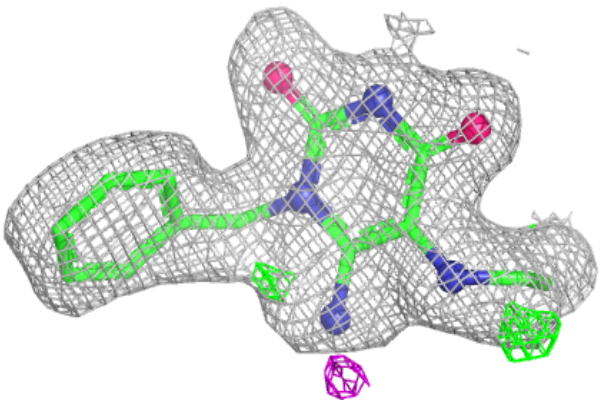
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

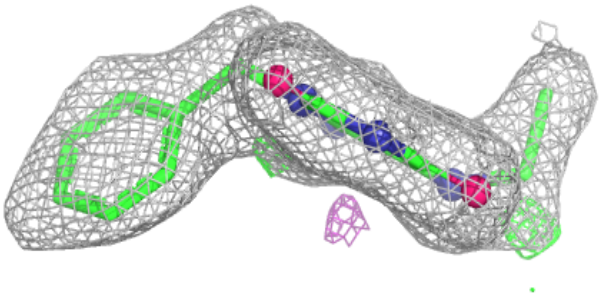
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	C	1295	6/6	0.79	0.19	42,44,46,46	0
4	GOL	C	1296	6/6	0.83	0.36	37,41,42,46	0
4	GOL	D	1295	6/6	0.83	0.27	37,38,41,43	0
5	MES	A	1296	12/12	0.86	0.30	65,69,75,79	0
5	MES	D	1296	12/12	0.88	0.15	59,67,69,70	0
4	GOL	A	1295	6/6	0.89	0.35	38,45,49,53	0
5	MES	B	1295	12/12	0.91	0.18	67,72,73,74	0
2	NWL	B	400	19/19	0.92	0.09	40,43,46,47	0
2	NWL	D	400	19/19	0.93	0.13	37,40,48,49	0
2	NWL	A	400	19/19	0.94	0.10	33,38,42,44	0
5	MES	C	1297	12/12	0.95	0.15	50,53,56,57	0
2	NWL	C	400	19/19	0.95	0.09	31,36,42,42	0
3	CL	C	1294	1/1	0.96	0.08	41,41,41,41	0
3	CL	B	1294	1/1	0.97	0.07	41,41,41,41	0
3	CL	A	1294	1/1	0.97	0.05	39,39,39,39	0
3	CL	D	1294	1/1	0.98	0.06	48,48,48,48	0

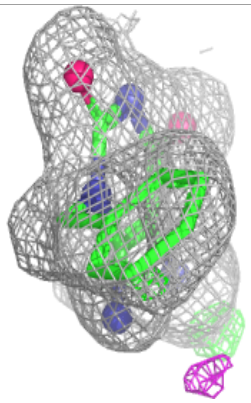
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NWL B 400:

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

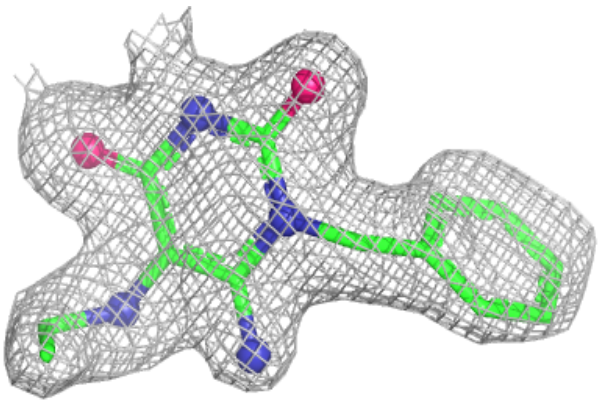


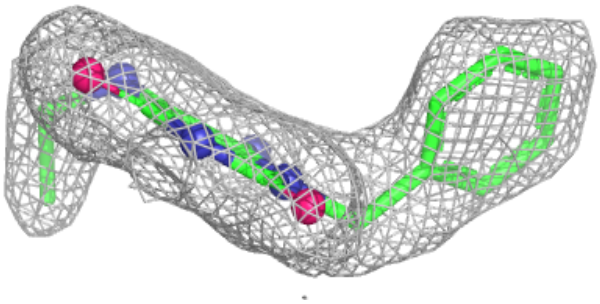


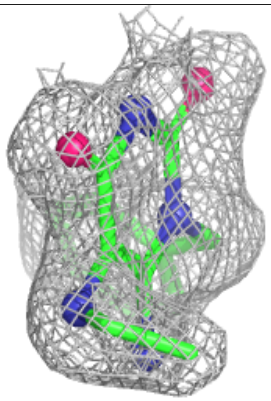


Electron density around NWL D 400:

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

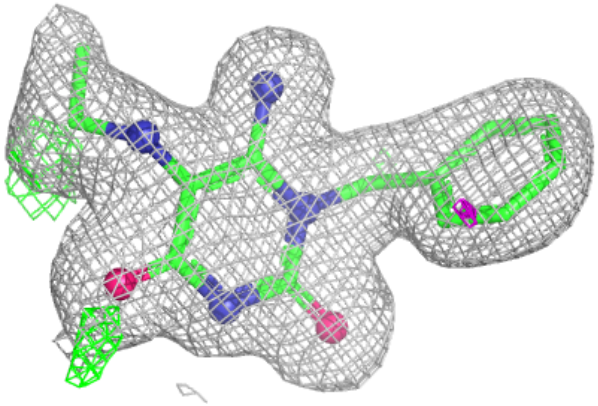


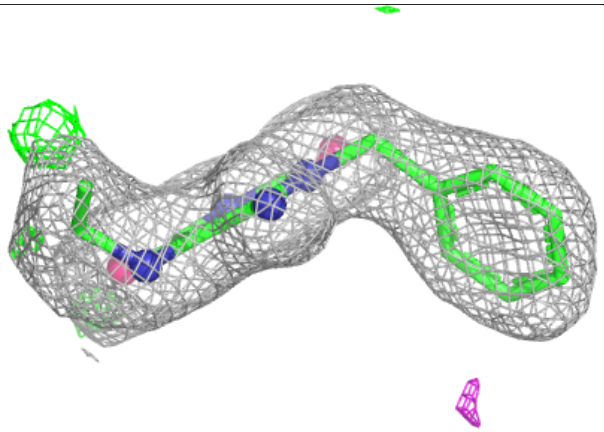


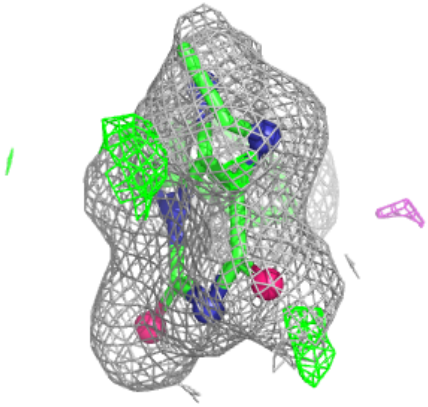


Electron density around NWL A 400:

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

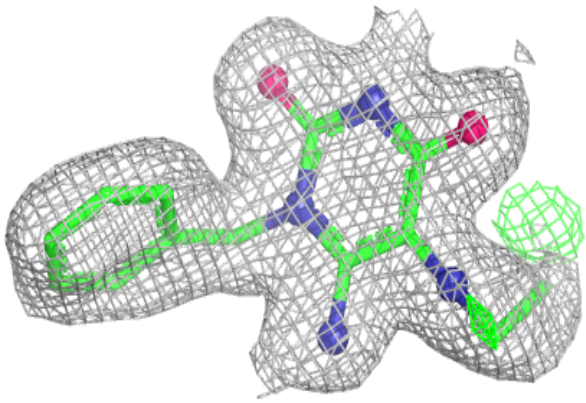


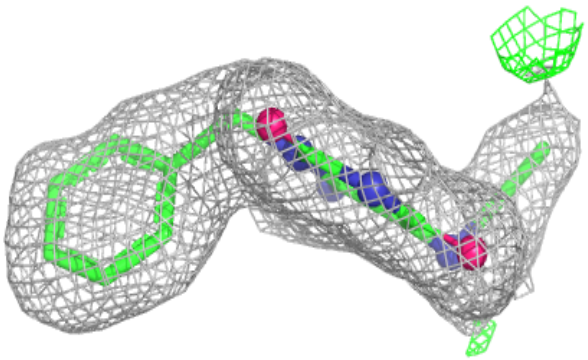


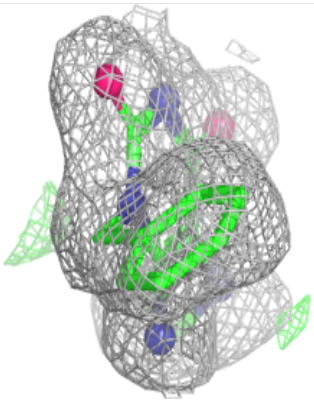


Electron density around NWL C 400:

$2mF_o$-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.