



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 01:10 am BST

PDB ID : 4B42
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 : 2012-07-27
Resolution : 2.50 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

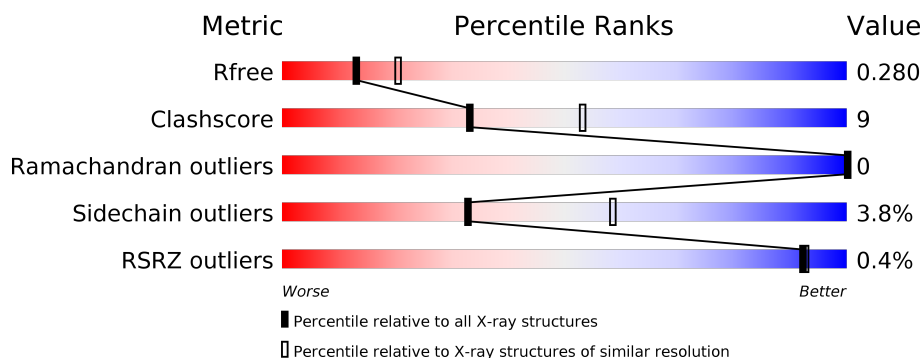
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	
1	B	303	
1	C	303	
1	D	303	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9527 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	293	Total	C	N	O	S	0	1	0
			2299	1471	387	436	5			
1	B	291	Total	C	N	O	S	0	1	0
			2283	1460	384	434	5			
1	C	293	Total	C	N	O	S	0	1	0
			2299	1471	387	436	5			
1	D	291	Total	C	N	O	S	0	1	0
			2284	1463	382	434	5			

There are 40 discrepancies between the modelled and reference sequences:

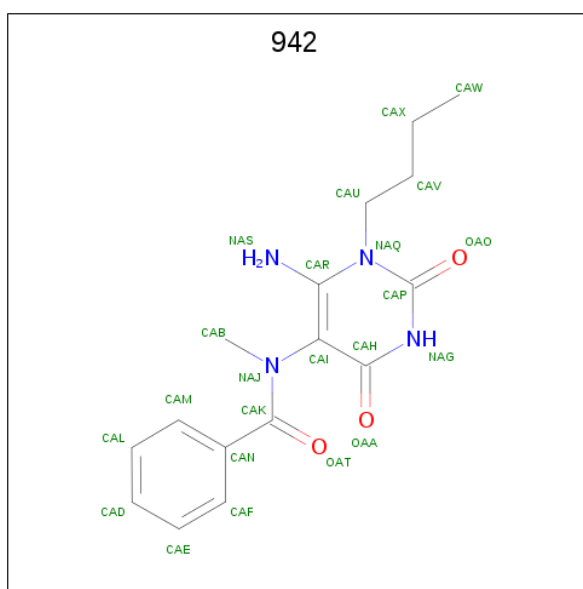
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP G3XCK4
A	-8	HIS	-	expression tag	UNP G3XCK4
A	-7	HIS	-	expression tag	UNP G3XCK4
A	-6	HIS	-	expression tag	UNP G3XCK4
A	-5	HIS	-	expression tag	UNP G3XCK4
A	-4	HIS	-	expression tag	UNP G3XCK4
A	-3	GLY	-	expression tag	UNP G3XCK4
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	HIS	-	expression tag	UNP G3XCK4
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-[6-azanyl-1-butyl-2,4-bis(oxidanylidene)pyrimidin-5-yl]-N-methyl-benzamide (three-letter code: 942) (formula: C₁₆H₂₀N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	16	4	3		

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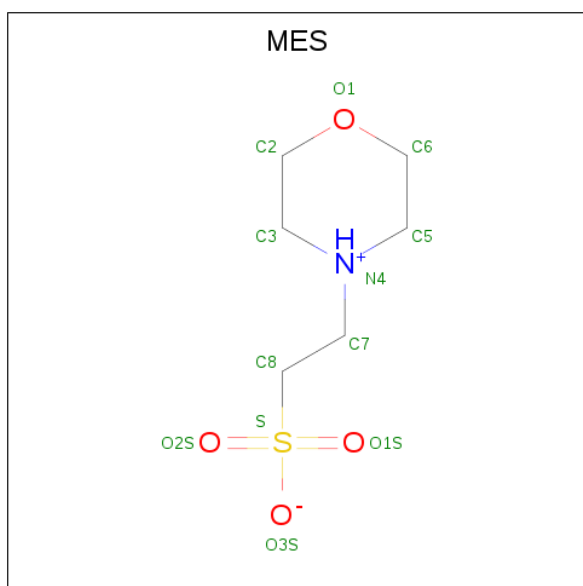
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			23	16	4	3		
2	C	1	Total	C	N	O	0	0
			23	16	4	3		
2	D	1	Total	C	N	O	0	0
			23	16	4	3		

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

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	64	Total	O	0	0
			64	64		
5	B	55	Total	O	0	0
			55	55		
5	C	56	Total	O	0	0
			56	56		
5	D	43	Total	O	0	0
			43	43		

- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



S192	P193	ARG	GLY	E196	L233	E234	Q237	A240	L286	R259	A276	K285	R286	L287	Y293
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.15Å 153.40Å 134.67Å 90.00° 92.54° 90.00°	Depositor
Resolution (Å)	34.79 – 2.50 34.79 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.2 (34.79-2.50) 97.2 (34.79-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.283 0.222 , 0.280	Depositor DCC
R_{free} test set	2181 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 18.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9527	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 942, MES, CL

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	0.81	0/2352	0.92	9/3190 (0.3%)
1	B	0.80	0/2334	0.88	3/3164 (0.1%)
1	C	0.72	2/2352 (0.1%)	0.87	3/3190 (0.1%)
1	D	0.72	0/2336	0.82	3/3168 (0.1%)
All	All	0.76	2/9374 (0.0%)	0.87	18/12712 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	262	TRP	CD2-CE2	5.23	1.47	1.41
1	C	73	TRP	CD2-CE2	5.12	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	LEU	CA-CB-CG	8.99	135.97	115.30
1	C	62	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	275	LEU	CB-CG-CD1	-6.64	99.71	111.00
1	A	62	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	62	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	D	112	LEU	CA-CB-CG	6.16	129.48	115.30
1	A	224	LEU	CB-CG-CD2	6.00	121.20	111.00
1	C	112	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	88	LEU	CB-CG-CD2	5.75	120.77	111.00
1	A	128	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	232	LEU	CB-CG-CD1	-5.68	101.35	111.00
1	D	143	GLU	CB-CA-C	-5.54	99.32	110.40
1	A	225	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	D	21	LEU	CA-CB-CG	5.27	127.42	115.30
1	B	209	ARG	NE-CZ-NH1	5.21	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LEU	CB-CG-CD1	5.18	119.81	111.00
1	B	3	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	143	GLU	CB-CA-C	-5.00	100.39	110.40

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	2299	0	2292	40	0
1	B	2283	0	2271	59	0
1	C	2299	0	2292	49	0
1	D	2284	0	2275	55	0
2	A	23	0	20	5	0
2	B	23	0	20	1	0
2	C	23	0	20	3	0
2	D	23	0	20	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	13	0	0
4	B	12	0	13	1	0
4	C	12	0	13	4	0
4	D	12	0	13	2	0
5	A	64	0	0	1	0
5	B	55	0	0	3	0
5	C	56	0	0	2	0
5	D	43	0	0	2	0
All	All	9527	0	9262	160	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 9.

All (160) 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:A:237[A]:GLN:OE1	1:C:237[A]:GLN:NE2	1.95	0.97
1:B:23:ILE:CD1	1:D:23:ILE:HD12	1.96	0.95
1:B:237[A]:GLN:OE1	1:D:237[A]:GLN:OE1	1.85	0.95
1:B:23:ILE:HD12	1:D:23:ILE:CD1	1.99	0.92
1:B:23:ILE:CD1	1:D:23:ILE:CD1	2.48	0.92
1:B:23:ILE:HG21	1:D:23:ILE:HD12	1.54	0.90
1:B:237[A]:GLN:OE1	1:D:237[A]:GLN:HG2	1.76	0.86
1:B:287:LEU:HD23	5:B:2054:HOH:O	1.79	0.82
1:A:237[A]:GLN:OE1	1:C:237[A]:GLN:HG2	1.82	0.79
1:A:256:ILE:HD11	2:A:1294:942:HAE	1.66	0.77
1:B:23:ILE:HD12	1:D:23:ILE:HD12	1.60	0.77
1:B:23:ILE:HG21	1:D:23:ILE:CD1	2.13	0.77
1:A:237[A]:GLN:CD	1:C:237[A]:GLN:HE21	1.87	0.76
1:C:154:GLY:O	4:C:1296:MES:H32	1.88	0.73
2:A:1294:942:HAF	2:A:1294:942:CAI	2.19	0.73
1:B:237[A]:GLN:OE1	1:D:237[A]:GLN:CG	2.37	0.72
1:B:23:ILE:HD13	1:D:23:ILE:CD1	2.18	0.72
1:A:237[A]:GLN:HG2	1:C:237[A]:GLN:NE2	2.03	0.72
1:A:17:HIS:CD2	1:A:21:LEU:HD13	2.25	0.72
1:B:237[A]:GLN:HG2	1:D:237[A]:GLN:OE1	1.90	0.71
1:B:23:ILE:CG2	1:D:23:ILE:HD12	2.18	0.71
1:C:186:ALA:HA	1:C:189:LEU:HD12	1.73	0.70
1:D:154:GLY:O	4:D:1296:MES:C7	2.40	0.70
1:A:144:ARG:NH2	5:A:2029:HOH:O	2.24	0.70
1:B:23:ILE:HD12	1:D:23:ILE:HG21	1.73	0.70
1:B:23:ILE:CD1	1:D:23:ILE:HG21	2.22	0.69
1:B:23:ILE:HD12	1:D:23:ILE:CB	2.23	0.69
1:D:154:GLY:O	4:D:1296:MES:H72	1.93	0.68
1:B:23:ILE:CD1	1:D:23:ILE:HD13	2.24	0.67
1:A:23:ILE:HB	1:C:23:ILE:HD13	1.76	0.67
1:A:256:ILE:CD1	2:A:1294:942:HAE	2.25	0.66
1:C:53:ILE:HD12	1:C:53:ILE:N	2.11	0.66
1:D:127:GLN:O	1:D:129:GLN:NE2	2.27	0.66
1:C:154:GLY:O	4:C:1296:MES:C3	2.44	0.65
1:C:53:ILE:CD1	1:C:53:ILE:N	2.60	0.65
1:C:86:ASP:HB2	1:C:90:GLN:OE1	1.97	0.65
1:B:112:LEU:CD1	1:B:226:THR:HG21	2.26	0.64
1:B:154:GLY:O	4:B:1296:MES:H32	1.97	0.64
1:B:23:ILE:HD12	1:D:23:ILE:CG2	2.28	0.64
1:B:237[A]:GLN:CG	1:D:237[A]:GLN:OE1	2.46	0.63
1:B:41:SER:HB3	1:B:256:ILE:HD12	1.79	0.63
1:A:237[A]:GLN:CG	1:C:237[A]:GLN:NE2	2.61	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:HB3	1:A:256:ILE:HD12	1.81	0.62
1:B:23:ILE:HD13	1:D:23:ILE:HD13	1.81	0.62
1:C:284:LEU:HA	1:C:287:LEU:HD12	1.82	0.62
1:B:237[A]:GLN:OE1	1:D:237[A]:GLN:CD	2.37	0.61
1:B:41:SER:HB3	1:B:256:ILE:CD1	2.30	0.61
1:B:23:ILE:HD13	1:D:23:ILE:HD12	1.81	0.61
1:B:22:ALA:O	1:D:62:ARG:NH2	2.34	0.60
1:D:86:ASP:HB2	1:D:90:GLN:OE1	2.01	0.60
1:A:23:ILE:HD13	1:C:23:ILE:HB	1.83	0.60
2:A:1294:942:CAF	2:A:1294:942:CAI	2.79	0.59
1:B:23:ILE:CB	1:D:23:ILE:HD12	2.32	0.59
1:B:233:LEU:HD21	1:D:237[B]:GLN:HA	1.85	0.59
1:A:237[A]:GLN:OE1	1:C:237[A]:GLN:CG	2.49	0.58
1:A:31:TYR:CD1	1:A:240:ALA:HB2	2.38	0.58
1:C:41:SER:HB3	1:C:256:ILE:CD1	2.33	0.58
1:D:41:SER:HB3	1:D:256:ILE:HD12	1.85	0.58
1:A:256:ILE:HD11	2:A:1294:942:CAE	2.33	0.58
1:A:237[A]:GLN:CD	1:C:237[A]:GLN:NE2	2.51	0.58
1:C:41:SER:HB3	1:C:256:ILE:HD12	1.86	0.57
1:B:237[A]:GLN:HG3	1:D:233:LEU:HD11	1.87	0.56
1:D:17:HIS:CD2	1:D:21:LEU:HD13	2.41	0.56
1:B:237[A]:GLN:CD	1:D:237[A]:GLN:OE1	2.43	0.56
1:A:27:LEU:HD13	1:C:22:ALA:HB1	1.88	0.55
1:A:24:SER:HB3	1:A:59:ASP:OD2	2.06	0.55
1:B:111:ASN:ND2	1:B:174:GLY:HA3	2.22	0.55
1:C:189:LEU:HD11	1:C:202:VAL:HG22	1.88	0.55
1:D:259:ARG:HD2	2:D:1294:942:HAV2	1.89	0.55
1:D:26:GLN:NE2	5:D:2007:HOH:O	2.34	0.55
1:B:189:LEU:HD11	1:B:202:VAL:HG22	1.89	0.54
1:A:61:PRO:HD3	1:B:64:GLN:NE2	2.22	0.54
1:C:24:SER:HB3	1:C:59:ASP:OD2	2.07	0.54
1:D:41:SER:HB3	1:D:256:ILE:CD1	2.38	0.54
1:B:112:LEU:CD1	1:B:226:THR:CG2	2.86	0.54
1:C:25:LYS:NZ	1:C:226:THR:O	2.40	0.54
1:B:23:ILE:HD12	1:D:23:ILE:HB	1.89	0.53
1:C:51:ILE:HG22	1:C:53:ILE:HD12	1.90	0.53
1:A:76:ASP:OD1	1:D:58:GLN:HA	2.09	0.53
1:B:233:LEU:HD21	1:D:237[A]:GLN:HA	1.89	0.52
1:D:276:ALA:HB2	1:D:285:LYS:HZ1	1.73	0.52
1:A:31:TYR:CG	1:A:240:ALA:HB2	2.45	0.51
1:D:234:GLU:HA	1:D:237[A]:GLN:HE21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:HD21	1:C:237[B]:GLN:HA	1.93	0.50
1:B:25:LYS:NZ	1:B:227:GLY:HA2	2.26	0.50
1:B:194:ARG:NH1	1:B:198:GLU:OE2	2.44	0.50
1:A:22:ALA:CB	1:C:27:LEU:HD22	2.41	0.50
1:C:45:LEU:CD1	2:C:1294:942:HAW2	2.41	0.50
2:C:1294:942:CAI	2:C:1294:942:CAF	2.89	0.50
1:B:192:SER:HB2	1:B:193:PRO:HD2	1.94	0.49
1:D:24:SER:HB3	1:D:59:ASP:OD1	2.12	0.49
1:D:16:LEU:HD12	1:D:25:LYS:HD3	1.95	0.49
1:D:234:GLU:HA	1:D:237[A]:GLN:NE2	2.26	0.49
1:C:214:VAL:O	4:C:1296:MES:H82	2.13	0.49
1:D:189:LEU:HD23	5:D:2031:HOH:O	2.13	0.49
1:C:31:TYR:CD1	1:C:240:ALA:HB2	2.48	0.48
1:A:25:LYS:NZ	1:A:226:THR:O	2.43	0.48
1:D:31:TYR:CD1	1:D:240:ALA:HB2	2.48	0.48
2:D:1294:942:CAI	2:D:1294:942:CAF	2.91	0.48
1:C:172:VAL:HG12	1:C:173:THR:O	2.15	0.47
2:C:1294:942:CAI	2:C:1294:942:HAF	2.44	0.47
1:A:62:ARG:NH1	1:C:62:ARG:HD2	2.30	0.47
1:A:189:LEU:HD11	1:A:202:VAL:HG22	1.97	0.47
1:A:233:LEU:HD21	1:C:237[A]:GLN:HA	1.97	0.47
1:A:192:SER:HB2	1:A:193:PRO:HD2	1.96	0.47
1:B:152:GLN:HB2	5:B:2030:HOH:O	2.14	0.47
1:B:111:ASN:HD21	1:B:174:GLY:HA3	1.80	0.46
1:C:189:LEU:HD11	1:C:202:VAL:CG2	2.45	0.46
1:B:112:LEU:HD13	1:B:226:THR:CG2	2.46	0.46
1:B:134:VAL:HG13	1:B:212:LEU:HD11	1.98	0.46
1:B:189:LEU:HD21	1:B:201:ASP:HB3	1.98	0.46
2:D:1294:942:HAF	2:D:1294:942:CAR	2.46	0.46
1:B:186:ALA:HA	1:B:189:LEU:HD12	1.97	0.46
1:C:192:SER:HB2	1:C:193:PRO:HD2	1.98	0.45
1:D:1:MET:HE2	1:D:129:GLN:HG2	1.98	0.45
1:B:16:LEU:HD12	1:B:25:LYS:HD3	1.99	0.44
1:A:265:ALA:HB1	1:A:288:LEU:HD22	1.99	0.44
1:D:259:ARG:NH2	1:D:287:LEU:HD22	2.33	0.44
1:D:276:ALA:HB2	1:D:285:LYS:NZ	2.33	0.44
1:C:209:ARG:NE	5:C:2039:HOH:O	2.51	0.44
1:C:23:ILE:HD11	1:C:27:LEU:HD13	1.99	0.44
1:B:265:ALA:HB1	1:B:288:LEU:HD22	2.00	0.43
1:C:224:LEU:HD11	1:C:238:PHE:CD1	2.52	0.43
1:B:23:ILE:HD12	1:D:23:ILE:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:SER:HB3	1:B:59:ASP:OD1	2.18	0.43
1:A:237[A]:GLN:HG2	1:C:237[A]:GLN:HE22	1.81	0.43
1:A:60:THR:N	1:A:61:PRO:HD2	2.34	0.43
1:B:237[B]:GLN:HA	1:D:233:LEU:HD21	2.00	0.43
1:A:29:PRO:HA	1:A:34:PRO:HA	2.00	0.42
1:D:148:VAL:HA	1:D:159:LEU:HD23	2.00	0.42
1:B:25:LYS:HZ3	1:B:227:GLY:HA2	1.84	0.42
1:A:22:ALA:HB1	1:C:27:LEU:HD13	2.00	0.42
1:C:130:THR:HG22	1:C:131:GLY:N	2.34	0.42
1:C:154:GLY:O	4:C:1296:MES:H31	2.16	0.42
1:A:88:LEU:HD13	1:A:108:LEU:HD21	2.01	0.42
1:B:136:ALA:HB3	1:B:216:ILE:HD13	2.02	0.42
1:C:29:PRO:HA	1:C:34:PRO:HA	2.00	0.42
1:D:29:PRO:HA	1:D:34:PRO:HA	2.01	0.42
1:A:23:ILE:HD13	1:C:23:ILE:CD1	2.49	0.42
1:B:29:PRO:HA	1:B:34:PRO:HA	2.00	0.42
1:C:81:VAL:HG22	5:C:2016:HOH:O	2.20	0.42
2:D:1294:942:CAI	2:D:1294:942:HAF	2.49	0.42
1:D:16:LEU:CD1	1:D:25:LYS:HD3	2.49	0.42
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.75	0.42
1:A:22:ALA:HB2	1:C:27:LEU:HD22	2.02	0.42
1:C:38:TYR:CD1	1:C:251:ALA:HB3	2.54	0.42
1:B:127:GLN:O	1:B:129:GLN:HG2	2.20	0.41
1:C:122:LEU:CD2	1:C:175:LEU:HD21	2.50	0.41
1:C:41:SER:CB	1:C:256:ILE:HD12	2.50	0.41
1:D:192:SER:HB2	1:D:193:PRO:HD2	2.02	0.41
1:B:16:LEU:CD1	1:B:25:LYS:HD2	2.51	0.41
1:B:112:LEU:HD11	1:B:226:THR:HG21	2.00	0.41
1:A:103:LEU:HD11	1:A:129:GLN:HG3	2.02	0.41
1:A:40:LEU:CD1	1:A:51:ILE:HD13	2.51	0.41
2:B:1294:942:HAL	5:B:2007:HOH:O	2.19	0.41
1:B:41:SER:CB	1:B:256:ILE:HD12	2.50	0.40
1:C:46:ALA:HB2	1:C:122:LEU:HD13	2.03	0.40
1:A:17:HIS:CG	1:A:21:LEU:HD13	2.57	0.40
1:C:122:LEU:HD21	1:C:175:LEU:HD21	2.03	0.40
1:B:237[A]:GLN:HA	1:D:233:LEU:HD21	2.02	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	292/303 (96%)	284 (97%)	8 (3%)	0	100	100
1	B	288/303 (95%)	277 (96%)	11 (4%)	0	100	100
1	C	292/303 (96%)	282 (97%)	10 (3%)	0	100	100
1	D	288/303 (95%)	277 (96%)	11 (4%)	0	100	100
All	All	1160/1212 (96%)	1120 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	241/248 (97%)	227 (94%)	14 (6%)	20	38
1	B	239/248 (96%)	233 (98%)	6 (2%)	47	73
1	C	241/248 (97%)	232 (96%)	9 (4%)	34	60
1	D	240/248 (97%)	233 (97%)	7 (3%)	42	69
All	All	961/992 (97%)	925 (96%)	36 (4%)	33	60

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	21	LEU

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Mol	Chain	Res	Type
1	A	23	ILE
1	A	58	GLN
1	A	97	SER
1	A	112	LEU
1	A	117	ASP
1	A	126	SER
1	A	129	GLN
1	A	155	LYS
1	A	173	THR
1	A	194	ARG
1	A	232	LEU
1	A	275	LEU
1	B	21	LEU
1	B	24	SER
1	B	97	SER
1	B	117	ASP
1	B	126	SER
1	B	155	LYS
1	C	21	LEU
1	C	23	ILE
1	C	53	ILE
1	C	97	SER
1	C	117	ASP
1	C	127	GLN
1	C	143	GLU
1	C	232	LEU
1	C	275	LEU
1	D	21	LEU
1	D	97	SER
1	D	112	LEU
1	D	117	ASP
1	D	127	GLN
1	D	129	GLN
1	D	143	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	129	GLN
1	B	111	ASN
1	C	111	ASN

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Mol	Chain	Res	Type
1	C	119	HIS
1	D	17	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 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
2	942	D	1294	-	21,24,24	2.60	6 (28%)	21,33,33	2.59	8 (38%)
2	942	B	1294	-	21,24,24	2.37	4 (19%)	21,33,33	2.60	9 (42%)
4	MES	C	1296	-	12,12,12	2.14	2 (16%)	14,16,16	1.86	3 (21%)
4	MES	D	1296	-	12,12,12	2.31	1 (8%)	14,16,16	2.58	4 (28%)
4	MES	A	1296	-	12,12,12	1.86	1 (8%)	14,16,16	2.76	5 (35%)
4	MES	B	1296	-	12,12,12	2.04	1 (8%)	14,16,16	3.11	5 (35%)
2	942	A	1294	-	21,24,24	2.29	3 (14%)	21,33,33	2.16	8 (38%)
2	942	C	1294	-	21,24,24	2.23	5 (23%)	21,33,33	2.79	9 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	942	D	1294	-	-	4/16/16/16	0/2/2/2
2	942	B	1294	-	-	2/16/16/16	0/2/2/2
4	MES	C	1296	-	-	3/6/14/14	0/1/1/1
4	MES	D	1296	-	-	5/6/14/14	0/1/1/1
4	MES	A	1296	-	-	3/6/14/14	0/1/1/1
4	MES	B	1296	-	-	2/6/14/14	0/1/1/1
2	942	A	1294	-	-	7/16/16/16	0/2/2/2
2	942	C	1294	-	-	1/16/16/16	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1294	942	CAI-NAJ	-7.59	1.31	1.44
4	D	1296	MES	C8-S	-7.15	1.67	1.77
4	C	1296	MES	C8-S	-6.78	1.67	1.77
2	D	1294	942	CAI-NAJ	-6.77	1.33	1.44
2	A	1294	942	CAN-CAK	-6.67	1.39	1.50
4	B	1296	MES	C8-S	-6.46	1.68	1.77
2	D	1294	942	CAN-CAK	-6.44	1.39	1.50
4	A	1296	MES	C8-S	-5.85	1.69	1.77
2	C	1294	942	CAN-CAK	-5.84	1.40	1.50
2	D	1294	942	CAH-NAG	4.97	1.41	1.33
2	A	1294	942	CAH-NAG	4.95	1.41	1.33
2	C	1294	942	CAI-NAJ	-4.77	1.36	1.44
2	A	1294	942	CAI-NAJ	-4.73	1.36	1.44
2	B	1294	942	CAN-CAK	-4.65	1.42	1.50
2	C	1294	942	CAH-NAG	4.63	1.41	1.33
2	B	1294	942	CAH-NAG	4.06	1.40	1.33
2	C	1294	942	CAB-NAJ	3.09	1.51	1.46
2	D	1294	942	CAK-NAJ	-2.99	1.30	1.36
2	C	1294	942	CAH-CAI	-2.82	1.37	1.41
2	D	1294	942	CAH-CAI	-2.51	1.38	1.41
2	B	1294	942	CAB-NAJ	2.27	1.50	1.46
4	C	1296	MES	O2S-S	2.16	1.51	1.45
2	D	1294	942	CAI-CAR	-2.11	1.38	1.41

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1294	942	CAH-NAG-CAP	8.56	122.37	115.14
4	A	1296	MES	O1S-S-C8	8.46	117.10	106.92
4	D	1296	MES	O2S-S-C8	7.08	115.44	106.92
2	D	1294	942	CAH-NAG-CAP	6.57	120.69	115.14
4	B	1296	MES	C2-C3-N4	6.55	120.04	110.10
2	B	1294	942	CAH-NAG-CAP	6.35	120.51	115.14
2	D	1294	942	CAH-CAI-CAR	5.99	120.22	114.57
2	A	1294	942	CAH-CAI-CAR	5.69	119.93	114.57
4	B	1296	MES	O1S-S-C8	5.40	113.42	106.92
2	B	1294	942	CAH-CAI-CAR	5.29	119.56	114.57
4	B	1296	MES	O2S-S-C8	5.21	113.19	106.92
2	C	1294	942	CAH-CAI-CAR	5.08	119.36	114.57
4	C	1296	MES	O2S-S-C8	5.04	112.99	106.92
4	B	1296	MES	O2S-S-O1S	-4.09	99.79	113.95
2	A	1294	942	CAB-NAJ-CAK	-3.63	111.57	118.71
2	D	1294	942	NAS-CAR-NAQ	3.60	124.98	120.12
2	A	1294	942	CAH-NAG-CAP	3.52	118.11	115.14
2	B	1294	942	OAT-CAK-NAJ	-3.49	116.15	121.47
2	B	1294	942	CAN-CAK-NAJ	3.48	123.86	118.61
2	C	1294	942	OAT-CAK-NAJ	-3.44	116.23	121.47
2	D	1294	942	CAU-NAQ-CAR	-3.37	115.78	121.39
2	C	1294	942	CAB-NAJ-CAK	-3.34	112.13	118.71
4	D	1296	MES	O3S-S-C8	3.32	111.14	105.77
4	A	1296	MES	C2-C3-N4	3.15	114.89	110.10
4	D	1296	MES	O1S-S-C8	-3.15	103.12	106.92
2	B	1294	942	CAI-CAH-NAG	-3.13	116.71	123.14
4	A	1296	MES	O2S-S-O1S	-3.05	103.40	113.95
2	B	1294	942	CAB-NAJ-CAK	-2.78	113.23	118.71
4	D	1296	MES	C2-C3-N4	2.78	114.33	110.10
2	C	1294	942	CAI-CAH-NAG	-2.76	117.47	123.14
4	A	1296	MES	O2S-S-C8	-2.70	103.67	106.92
2	D	1294	942	CAI-CAH-NAG	-2.66	117.67	123.14
4	C	1296	MES	O1-C2-C3	-2.49	106.32	111.80
2	B	1294	942	CAE-CAF-CAN	2.48	123.28	120.34
2	B	1294	942	CAI-NAJ-CAK	2.45	128.93	122.87
2	A	1294	942	NAS-CAR-NAQ	2.41	123.38	120.12
4	C	1296	MES	C6-C5-N4	2.30	113.59	110.10
2	D	1294	942	CAF-CAN-CAK	2.28	126.06	120.29
2	D	1294	942	CAB-NAJ-CAK	-2.22	114.35	118.71
4	A	1296	MES	O3S-S-C8	2.17	109.27	105.77
2	A	1294	942	CAD-CAL-CAM	2.14	123.45	120.19
2	C	1294	942	CAB-NAJ-CAI	2.14	120.72	115.25
2	A	1294	942	CAI-NAJ-CAK	2.11	128.07	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1294	942	OAT-CAK-NAJ	-2.10	118.28	121.47
2	A	1294	942	CAU-NAQ-CAR	-2.09	117.90	121.39
2	B	1294	942	CAL-CAM-CAN	2.09	122.82	120.34
2	C	1294	942	CAU-NAQ-CAR	-2.09	117.91	121.39
2	C	1294	942	NAS-CAR-NAQ	2.09	122.94	120.12
2	D	1294	942	OAT-CAK-NAJ	-2.05	118.35	121.47
4	B	1296	MES	O1-C2-C3	2.03	116.26	111.80
2	C	1294	942	CAL-CAM-CAN	2.02	122.73	120.34

There are no chirality outliers.

All (27) torsion outliers are listed below:

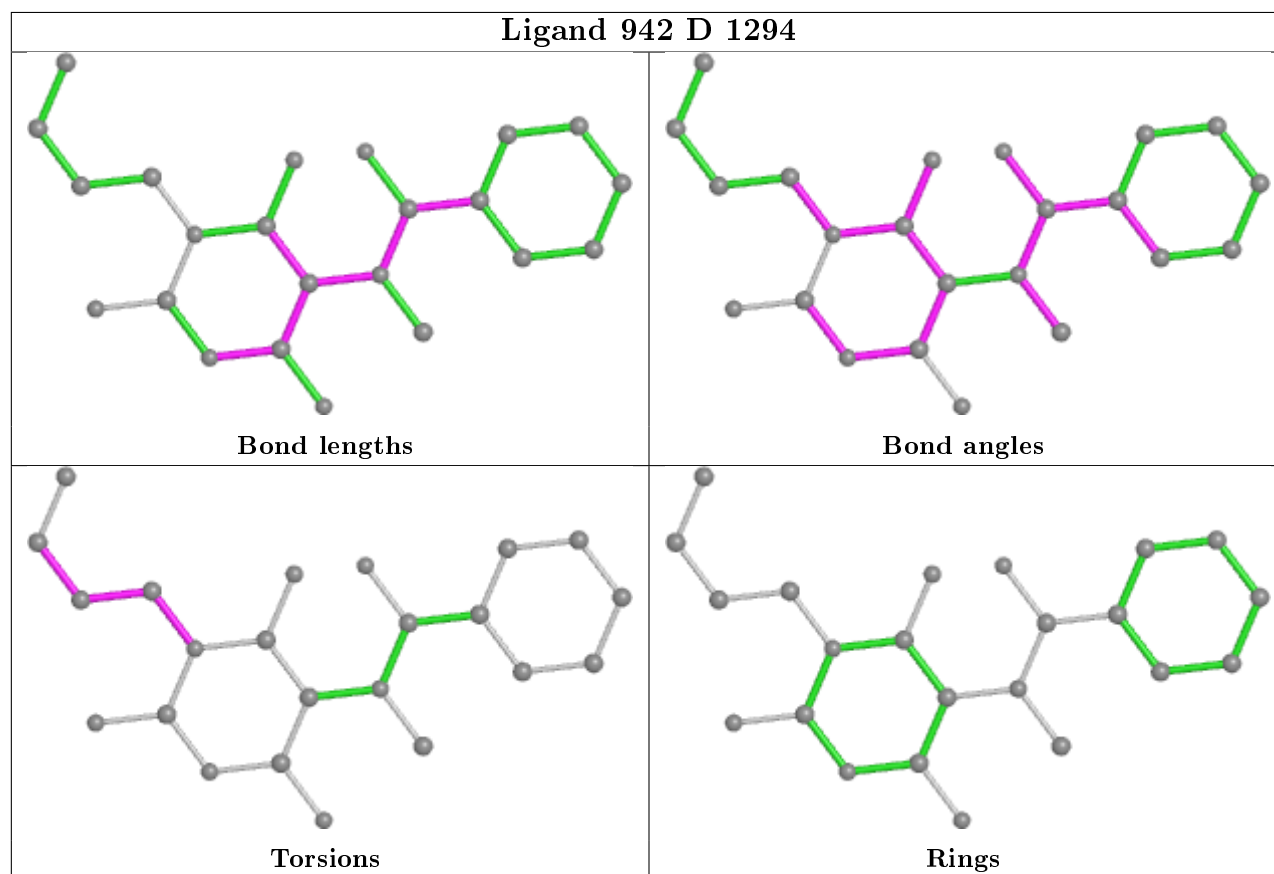
Mol	Chain	Res	Type	Atoms
2	D	1294	942	CAV-CAU-NAQ-CAR
2	D	1294	942	CAV-CAU-NAQ-CAP
4	B	1296	MES	N4-C7-C8-S
2	B	1294	942	CAR-CAI-NAJ-CAK
4	C	1296	MES	N4-C7-C8-S
4	D	1296	MES	C8-C7-N4-C3
4	D	1296	MES	C7-C8-S-O1S
4	D	1296	MES	C7-C8-S-O3S
2	C	1294	942	NAQ-CAU-CAV-CAX
4	A	1296	MES	C7-C8-S-O3S
2	D	1294	942	NAQ-CAU-CAV-CAX
2	D	1294	942	CAU-CAV-CAX-CAW
4	B	1296	MES	C8-C7-N4-C3
4	C	1296	MES	C8-C7-N4-C3
4	C	1296	MES	C8-C7-N4-C5
4	D	1296	MES	C8-C7-N4-C5
2	A	1294	942	NAQ-CAU-CAV-CAX
2	B	1294	942	CAV-CAU-NAQ-CAR
2	A	1294	942	NAJ-CAK-CAN-CAM
2	A	1294	942	NAJ-CAK-CAN-CAF
2	A	1294	942	CAV-CAU-NAQ-CAP
4	D	1296	MES	C7-C8-S-O2S
4	A	1296	MES	C7-C8-S-O1S
4	A	1296	MES	C7-C8-S-O2S
2	A	1294	942	CAU-CAV-CAX-CAW
2	A	1294	942	CAV-CAU-NAQ-CAR
2	A	1294	942	CAR-CAI-NAJ-CAK

There are no ring outliers.

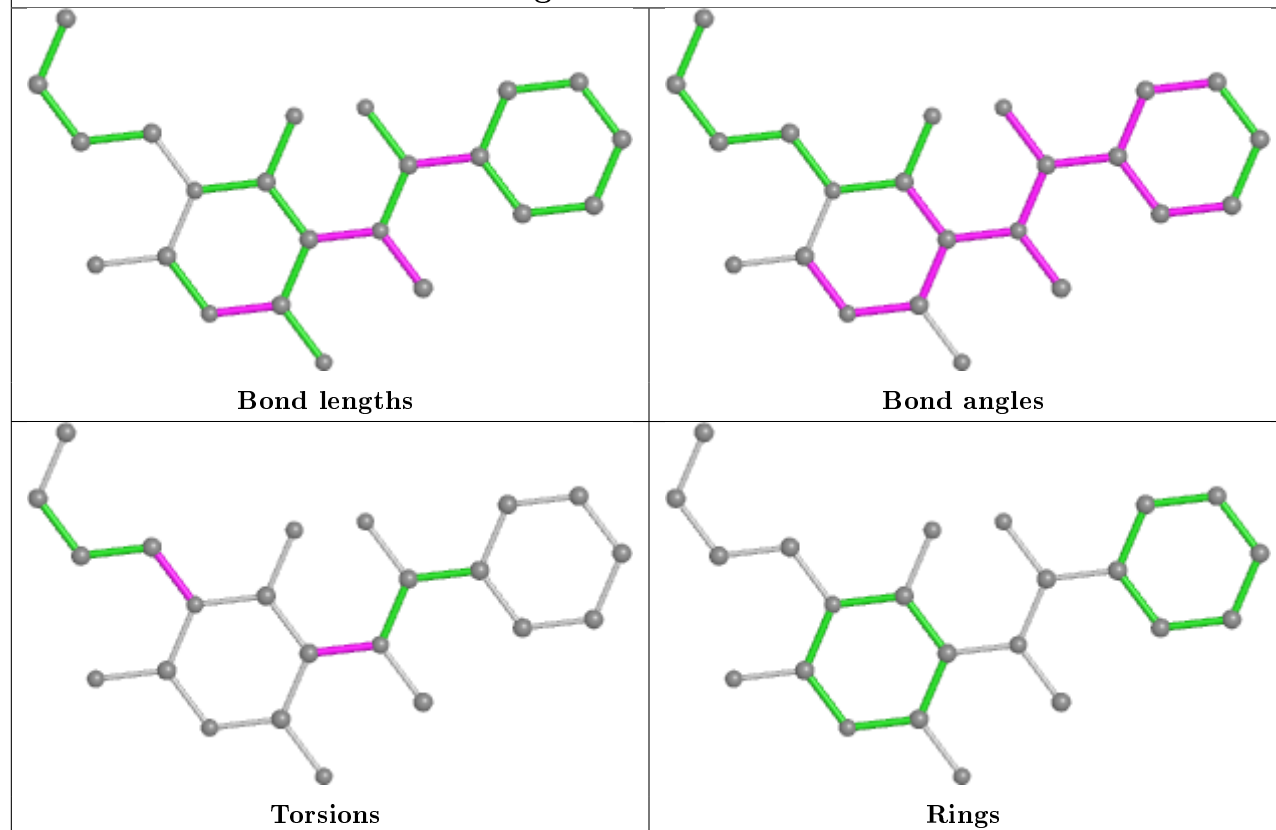
7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1294	942	4	0
2	B	1294	942	1	0
4	C	1296	MES	4	0
4	D	1296	MES	2	0
4	B	1296	MES	1	0
2	A	1294	942	5	0
2	C	1294	942	3	0

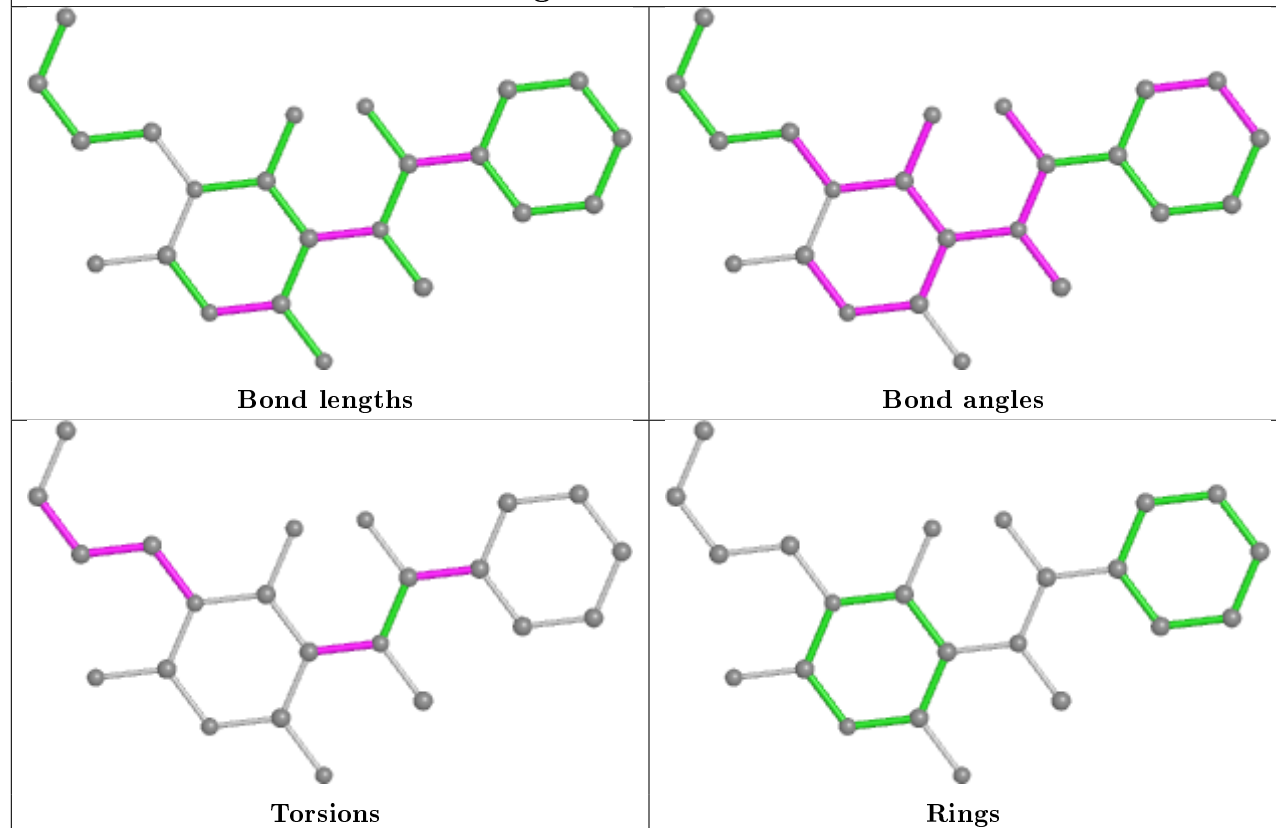
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

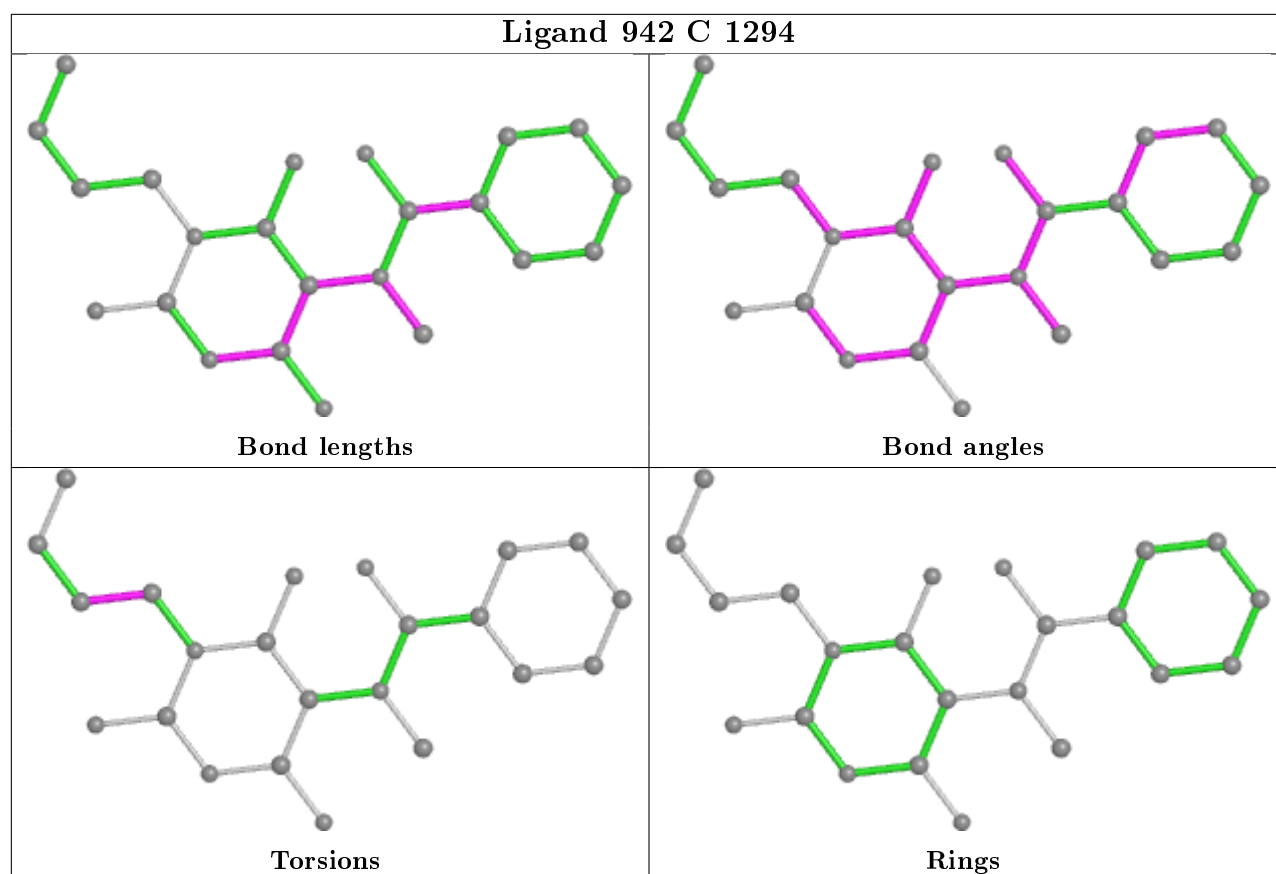


Ligand 942 B 1294



Ligand 942 A 1294





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	293/303 (96%)	-0.60	0	100 100	21, 38, 66, 81	3 (1%)
1	B	291/303 (96%)	-0.51	1 (0%)	94 94	19, 40, 74, 103	3 (1%)
1	C	293/303 (96%)	-0.40	1 (0%)	94 94	29, 46, 74, 88	4 (1%)
1	D	291/303 (96%)	-0.37	3 (1%)	82 84	26, 52, 79, 110	3 (1%)
All	All	1168/1212 (96%)	-0.47	5 (0%)	92 93	19, 44, 74, 110	13 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	3.7
1	D	23	ILE	3.2
1	B	23	ILE	3.0
1	D	191	PRO	2.8
1	C	193	PRO	2.4

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 carbohydrates 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,

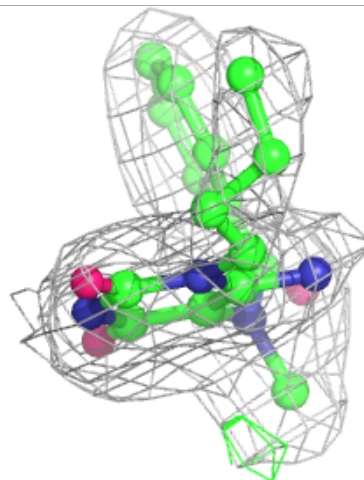
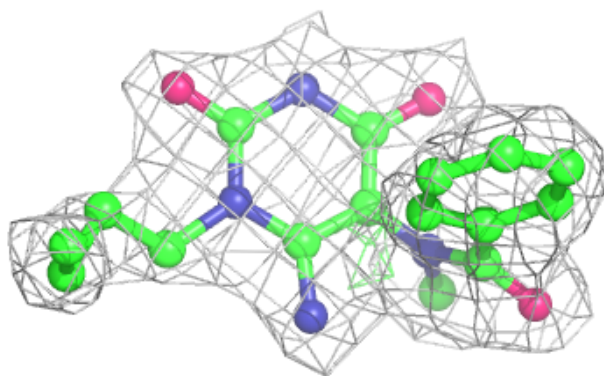
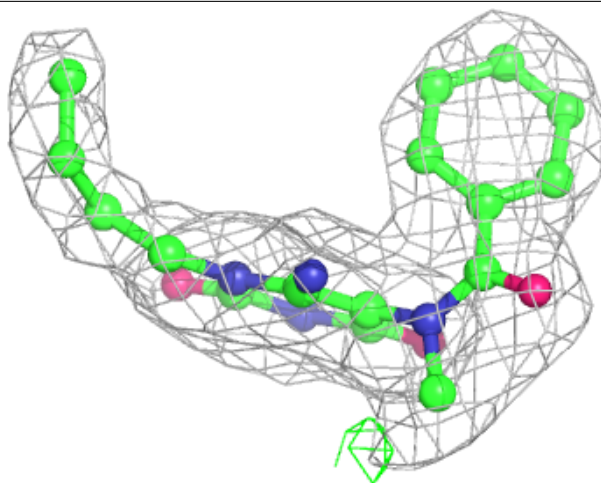
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MES	C	1296	12/12	0.88	0.17	58,73,87,90	0
4	MES	D	1296	12/12	0.92	0.16	49,56,59,67	0
3	CL	B	1295	1/1	0.93	0.18	43,43,43,43	0
2	942	D	1294	23/23	0.95	0.15	36,41,48,49	0
2	942	C	1294	23/23	0.96	0.13	32,41,49,51	0
4	MES	A	1296	12/12	0.96	0.13	39,45,57,57	0
4	MES	B	1296	12/12	0.97	0.13	44,57,61,64	0
3	CL	C	1295	1/1	0.97	0.08	62,62,62,62	0
2	942	A	1294	23/23	0.97	0.10	23,33,40,43	0
2	942	B	1294	23/23	0.97	0.10	24,29,36,37	0
3	CL	A	1295	1/1	0.97	0.09	44,44,44,44	0
3	CL	D	1295	1/1	0.98	0.08	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.

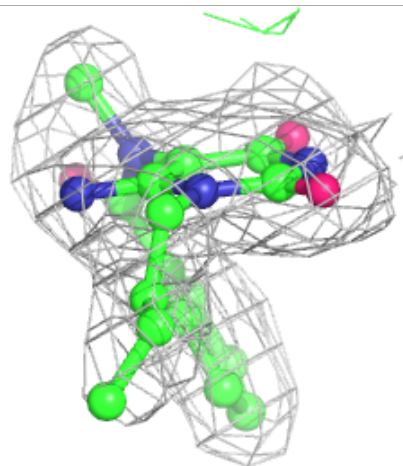
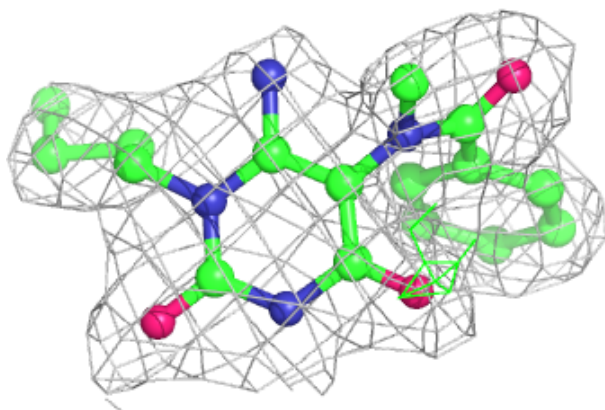
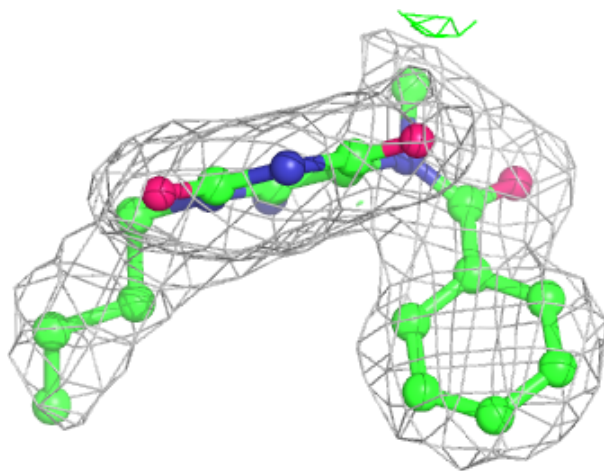
Electron density around 942 D 1294:

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



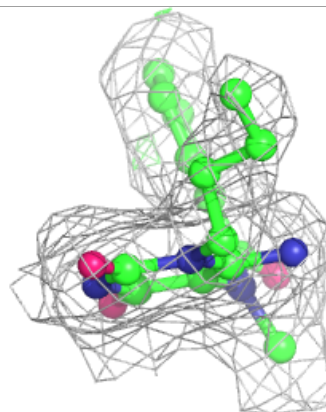
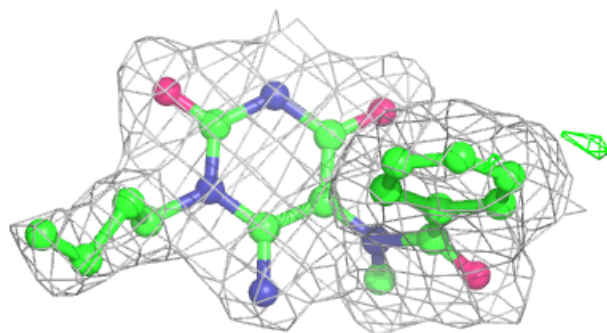
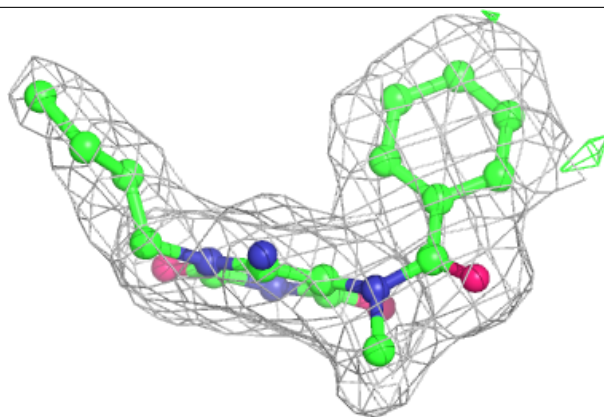
Electron density around 942 C 1294:

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

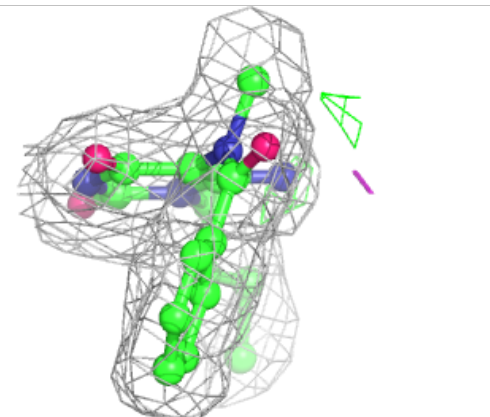
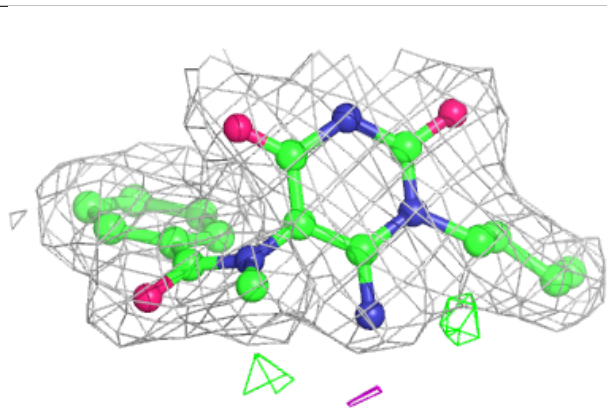
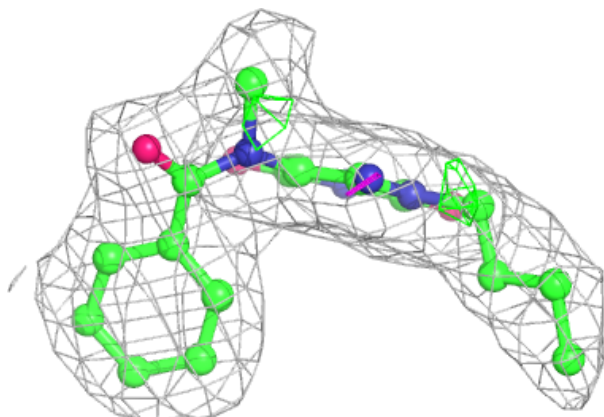


Electron density around 942 A 1294:

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

**Electron density around 942 B 1294:**

$2mF_o-DF_c$ (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.