Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 09:20 am BST

PDB ID	:	4D2T
Title	:	Structure of MELK in complex with inhibitors
Authors	:	Johnson, C.N.; Berdini, V.; Beke, L.; Bonnet, P.; Brehmer, D.; Coyle, J.E.; Day, P.J.; Frederickson, M.; Freyne, E.J.E.; Gilissen, R.A.H.J.; Hamlett, C.C.F.; Howard, S.; Meerpoel, L.; McMenamin, R.; Patel, S.; Rees, D.C.; Sharff, A.; Sommen, F.; Wu, T.; Linders, J.T.M.
Deposited on	:	2014-05-13
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

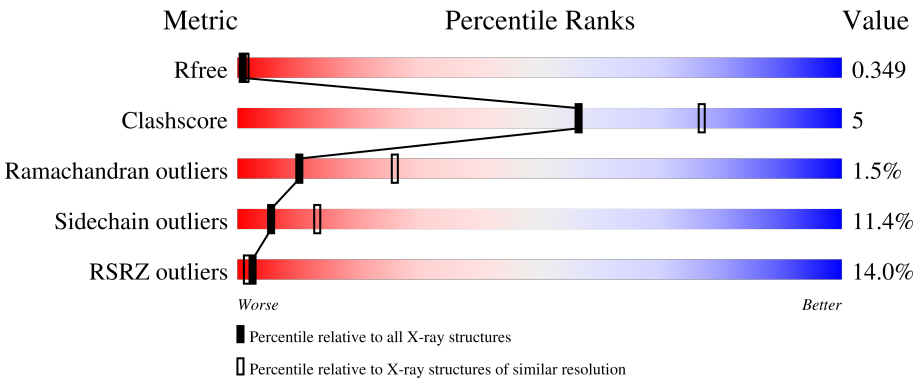
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	356	17% 71% 16% • 11%
1	B	356	7% 74% 16% • 9%
1	C	356	20% 66% 19% • • 12%
1	D	356	6% 70% 16% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10865 atoms, of which 84 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 MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2554	1645	431	460	18	0	0	0
1	B	323	2610	1677	444	471	18	0	0	0
1	C	313	2544	1641	429	457	17	0	1	0
1	D	319	2577	1666	430	465	16	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q14680
A	-18	GLY	-	expression tag	UNP Q14680
A	-17	SER	-	expression tag	UNP Q14680
A	-16	SER	-	expression tag	UNP Q14680
A	-15	HIS	-	expression tag	UNP Q14680
A	-14	HIS	-	expression tag	UNP Q14680
A	-13	HIS	-	expression tag	UNP Q14680
A	-12	HIS	-	expression tag	UNP Q14680
A	-11	HIS	-	expression tag	UNP Q14680
A	-10	HIS	-	expression tag	UNP Q14680
A	-9	SER	-	expression tag	UNP Q14680
A	-8	SER	-	expression tag	UNP Q14680
A	-7	GLY	-	expression tag	UNP Q14680
A	-6	LEU	-	expression tag	UNP Q14680
A	-5	VAL	-	expression tag	UNP Q14680
A	-4	PRO	-	expression tag	UNP Q14680
A	-3	ARG	-	expression tag	UNP Q14680
A	-2	GLY	-	expression tag	UNP Q14680
A	-1	SER	-	expression tag	UNP Q14680
A	0	HIS	-	expression tag	UNP Q14680
A	167	ALA	THR	engineered mutation	UNP Q14680

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Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	SER	engineered mutation	UNP Q14680
A	213	THR	ASN	engineered mutation	UNP Q14680
A	214	ALA	VAL	engineered mutation	UNP Q14680
A	215	ALA	MET	engineered mutation	UNP Q14680
A	218	VAL	TYR	engineered mutation	UNP Q14680
A	219	ALA	LYS	engineered mutation	UNP Q14680
B	-19	MET	-	expression tag	UNP Q14680
B	-18	GLY	-	expression tag	UNP Q14680
B	-17	SER	-	expression tag	UNP Q14680
B	-16	SER	-	expression tag	UNP Q14680
B	-15	HIS	-	expression tag	UNP Q14680
B	-14	HIS	-	expression tag	UNP Q14680
B	-13	HIS	-	expression tag	UNP Q14680
B	-12	HIS	-	expression tag	UNP Q14680
B	-11	HIS	-	expression tag	UNP Q14680
B	-10	HIS	-	expression tag	UNP Q14680
B	-9	SER	-	expression tag	UNP Q14680
B	-8	SER	-	expression tag	UNP Q14680
B	-7	GLY	-	expression tag	UNP Q14680
B	-6	LEU	-	expression tag	UNP Q14680
B	-5	VAL	-	expression tag	UNP Q14680
B	-4	PRO	-	expression tag	UNP Q14680
B	-3	ARG	-	expression tag	UNP Q14680
B	-2	GLY	-	expression tag	UNP Q14680
B	-1	SER	-	expression tag	UNP Q14680
B	0	HIS	-	expression tag	UNP Q14680
B	167	ALA	THR	engineered mutation	UNP Q14680
B	171	ALA	SER	engineered mutation	UNP Q14680
B	213	THR	ASN	engineered mutation	UNP Q14680
B	214	ALA	VAL	engineered mutation	UNP Q14680
B	215	ALA	MET	engineered mutation	UNP Q14680
B	218	VAL	TYR	engineered mutation	UNP Q14680
B	219	ALA	LYS	engineered mutation	UNP Q14680
C	-19	MET	-	expression tag	UNP Q14680
C	-18	GLY	-	expression tag	UNP Q14680
C	-17	SER	-	expression tag	UNP Q14680
C	-16	SER	-	expression tag	UNP Q14680
C	-15	HIS	-	expression tag	UNP Q14680
C	-14	HIS	-	expression tag	UNP Q14680
C	-13	HIS	-	expression tag	UNP Q14680
C	-12	HIS	-	expression tag	UNP Q14680
C	-11	HIS	-	expression tag	UNP Q14680

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	expression tag	UNP Q14680
C	-9	SER	-	expression tag	UNP Q14680
C	-8	SER	-	expression tag	UNP Q14680
C	-7	GLY	-	expression tag	UNP Q14680
C	-6	LEU	-	expression tag	UNP Q14680
C	-5	VAL	-	expression tag	UNP Q14680
C	-4	PRO	-	expression tag	UNP Q14680
C	-3	ARG	-	expression tag	UNP Q14680
C	-2	GLY	-	expression tag	UNP Q14680
C	-1	SER	-	expression tag	UNP Q14680
C	0	HIS	-	expression tag	UNP Q14680
C	167	ALA	THR	engineered mutation	UNP Q14680
C	171	ALA	SER	engineered mutation	UNP Q14680
C	213	THR	ASN	engineered mutation	UNP Q14680
C	214	ALA	VAL	engineered mutation	UNP Q14680
C	215	ALA	MET	engineered mutation	UNP Q14680
C	218	VAL	TYR	engineered mutation	UNP Q14680
C	219	ALA	LYS	engineered mutation	UNP Q14680
D	-19	MET	-	expression tag	UNP Q14680
D	-18	GLY	-	expression tag	UNP Q14680
D	-17	SER	-	expression tag	UNP Q14680
D	-16	SER	-	expression tag	UNP Q14680
D	-15	HIS	-	expression tag	UNP Q14680
D	-14	HIS	-	expression tag	UNP Q14680
D	-13	HIS	-	expression tag	UNP Q14680
D	-12	HIS	-	expression tag	UNP Q14680
D	-11	HIS	-	expression tag	UNP Q14680
D	-10	HIS	-	expression tag	UNP Q14680
D	-9	SER	-	expression tag	UNP Q14680
D	-8	SER	-	expression tag	UNP Q14680
D	-7	GLY	-	expression tag	UNP Q14680
D	-6	LEU	-	expression tag	UNP Q14680
D	-5	VAL	-	expression tag	UNP Q14680
D	-4	PRO	-	expression tag	UNP Q14680
D	-3	ARG	-	expression tag	UNP Q14680
D	-2	GLY	-	expression tag	UNP Q14680
D	-1	SER	-	expression tag	UNP Q14680
D	0	HIS	-	expression tag	UNP Q14680
D	167	ALA	THR	engineered mutation	UNP Q14680
D	171	ALA	SER	engineered mutation	UNP Q14680
D	213	THR	ASN	engineered mutation	UNP Q14680
D	214	ALA	VAL	engineered mutation	UNP Q14680

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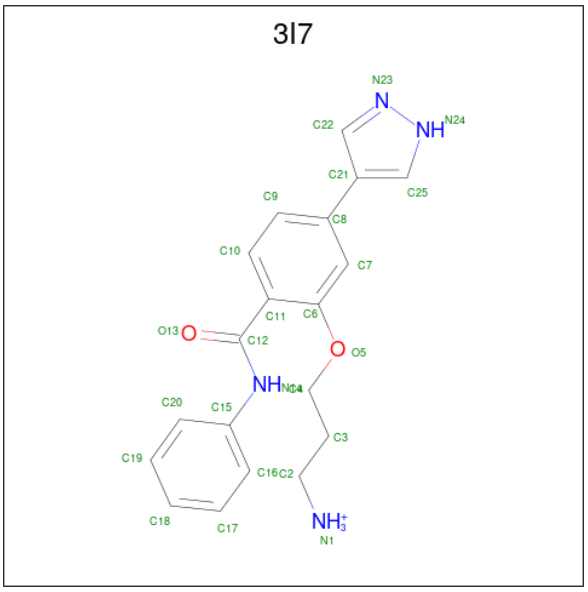
Chain	Residue	Modelled	Actual	Comment	Reference
D	215	ALA	MET	engineered mutation	UNP Q14680
D	218	VAL	TYR	engineered mutation	UNP Q14680
D	219	ALA	LYS	engineered mutation	UNP Q14680

- Molecule 2 is 3-[2-(phenylcarbamoyl)-5-(1H-pyrazol-4-yl)phenoxy]propan-1-aminium (three-letter code: 3I7) (formula: $C_{19}H_{21}N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	46	19	21	4	2	0	0
2	B	1	46	19	21	4	2	0	0
2	C	1	46	19	21	4	2	0	0
2	D	1	46	19	21	4	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	93	93	93	0	0
3	B	126	126	126	0	0
3	C	76	76	76	0	0

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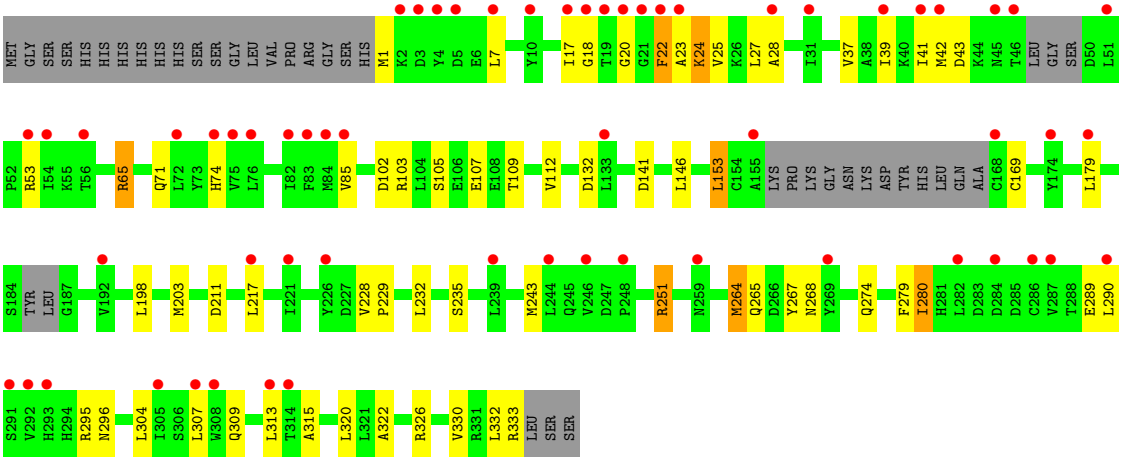
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	D	101	101	101	0	0

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.

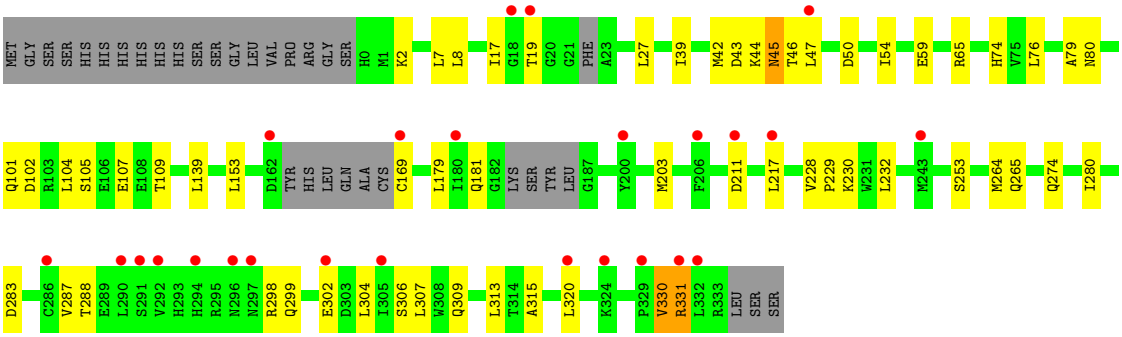
• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

Chain A:



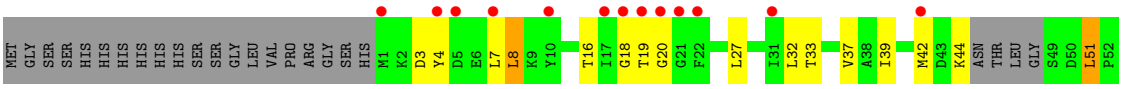
• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

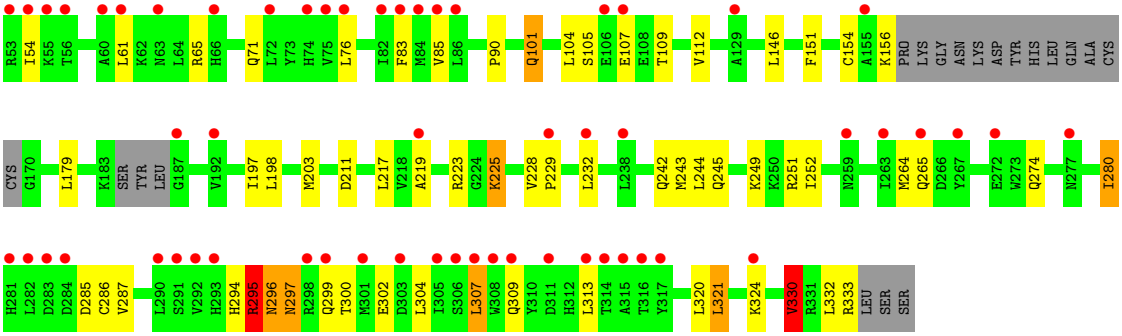
Chain B:



• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

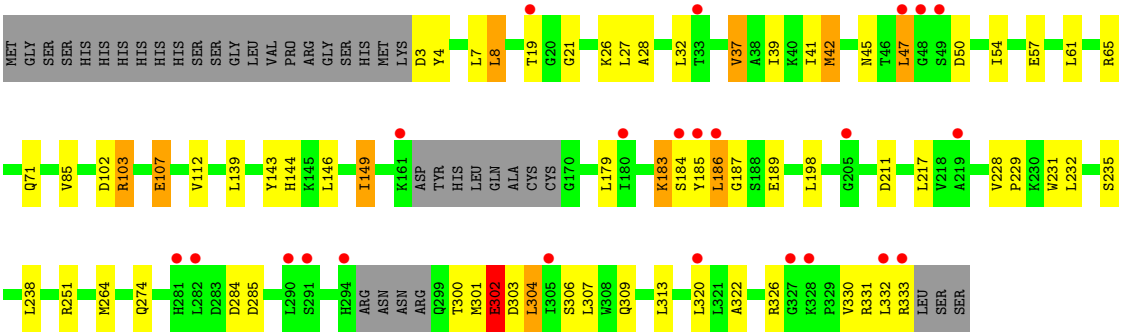
Chain C:





• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.53Å 75.41Å 79.74Å 86.03° 69.05° 90.03°	Depositor
Resolution (Å)	48.54 – 2.70 48.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (48.54-2.70) 93.1 (48.54-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.270 , 0.340 0.272 , 0.349	Depositor DCC
R_{free} test set	1870 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 95.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10865	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: 3I7

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	0.51	0/2610	0.68	0/3529
1	B	0.52	0/2667	0.68	0/3603
1	C	0.49	0/2603	0.66	0/3517
1	D	0.52	0/2636	0.70	0/3565
All	All	0.51	0/10516	0.68	0/14214

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2554	0	2560	26	0
1	B	2610	0	2630	19	0
1	C	2544	0	2564	36	0
1	D	2577	0	2599	25	0
2	A	25	21	21	1	0
2	B	25	21	21	0	0
2	C	25	21	21	1	0
2	D	25	21	21	0	0
3	A	93	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	126	0	0	2	0
3	C	76	0	0	0	0
3	D	101	0	0	0	0
All	All	10781	84	10437	105	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 5.

All (105) 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:D:302:GLU:HA	1:D:303:ASP:HB2	1.71	0.73
1:A:132:ASP:HB2	1:A:153:LEU:HD12	1.72	0.71
1:D:57:GLU:HG3	1:D:61:LEU:HD23	1.73	0.71
1:B:7:LEU:HD11	1:B:39:ILE:HD13	1.73	0.70
1:D:302:GLU:HB2	1:D:304:LEU:N	2.07	0.70
1:D:302:GLU:HB2	1:D:304:LEU:H	1.56	0.69
1:D:32:LEU:HD22	1:D:332:LEU:HG	1.74	0.69
1:A:25:VAL:HG21	2:A:1334:3I7:H3	1.77	0.67
1:B:47:LEU:HB3	1:B:50:ASP:HB2	1.79	0.65
1:D:7:LEU:HD11	1:D:39:ILE:HD13	1.80	0.64
1:B:109:THR:HG21	1:B:203:MET:HG2	1.80	0.63
1:A:22:PHE:HB2	1:A:42:MET:HA	1.80	0.63
1:A:109:THR:HG21	1:A:203:MET:HG2	1.81	0.63
1:C:76:LEU:HB3	1:C:83:PHE:HB2	1.81	0.62
1:B:104:LEU:HB2	1:B:109:THR:HG22	1.79	0.62
1:A:264:MET:O	1:A:267:TYR:O	2.17	0.61
1:C:105:SER:O	1:C:109:THR:HG23	2.01	0.60
1:B:105:SER:O	1:B:109:THR:HG23	2.01	0.60
1:C:109:THR:HG21	1:C:203:MET:HG2	1.83	0.60
1:A:22:PHE:C	1:A:24:LYS:H	2.06	0.59
1:B:45:ASN:HD21	1:B:80:ASN:HB3	1.66	0.59
1:D:185:TYR:HD2	1:D:187:GLY:HA2	1.68	0.58
1:B:50:ASP:O	1:B:54:ILE:HG12	2.04	0.57
1:A:105:SER:O	1:A:109:THR:HG23	2.04	0.57
1:C:104:LEU:HB2	1:C:109:THR:HG22	1.87	0.56
1:C:324:LYS:HD3	1:C:330:VAL:HG22	1.87	0.56
1:C:243:MET:HG3	1:C:252:ILE:HD11	1.88	0.56
1:C:296:ASN:HD22	1:C:297:ASN:H	1.53	0.56
1:D:322:ALA:O	1:D:326:ARG:HG3	2.06	0.55
1:C:197:ILE:HD13	1:C:244:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ASP:O	1:D:54:ILE:HG12	2.09	0.52
1:A:22:PHE:CD2	1:A:42:MET:HG3	2.44	0.52
1:C:39:ILE:HG12	1:C:85:VAL:HG22	1.93	0.51
1:D:28:ALA:HB3	1:D:37:VAL:HG12	1.92	0.51
1:D:320:LEU:HD22	1:D:330:VAL:HG13	1.93	0.51
1:C:219:ALA:HB1	1:D:107:GLU:HB2	1.93	0.51
1:A:18:GLY:HA3	1:A:25:VAL:H	1.77	0.50
1:C:242:GLN:HB3	1:C:252:ILE:HD13	1.93	0.50
1:C:242:GLN:HE21	1:C:252:ILE:HG21	1.75	0.50
1:B:288:THR:HB	1:B:298:ARG:HH12	1.76	0.50
1:C:61:LEU:HD11	1:C:151:PHE:CD1	2.46	0.50
1:C:229:PRO:HD2	1:C:232:LEU:HD22	1.94	0.50
1:B:283:ASP:O	1:B:287:VAL:HG23	2.12	0.49
1:A:65:ARG:HH21	1:A:279:PHE:HA	1.77	0.49
1:C:32:LEU:HB3	1:C:332:LEU:HD23	1.94	0.49
1:C:65:ARG:HG3	1:C:71:GLN:HE22	1.77	0.49
1:D:65:ARG:HG3	1:D:71:GLN:HE22	1.77	0.48
1:A:65:ARG:HG3	1:A:71:GLN:HE22	1.78	0.48
1:A:229:PRO:HD2	1:A:232:LEU:HD22	1.95	0.48
1:A:28:ALA:HB3	1:A:37:VAL:HG23	1.94	0.47
1:B:104:LEU:HB2	1:B:109:THR:CG2	2.45	0.47
1:D:229:PRO:HD2	1:D:232:LEU:HD22	1.96	0.47
1:A:320:LEU:HD22	1:A:330:VAL:HG13	1.96	0.47
1:D:143:TYR:OH	1:D:326:ARG:HG2	2.14	0.47
1:C:294:HIS:O	1:C:295:ARG:HB2	2.15	0.47
1:A:24:LYS:HD2	1:A:41:ILE:HB	1.97	0.47
1:C:280:ILE:H	1:C:280:ILE:HG13	1.59	0.47
1:A:289:GLU:HG3	1:A:332:LEU:HD22	1.97	0.46
1:C:243:MET:O	1:C:251:ARG:HD2	2.15	0.46
1:B:153:LEU:HD22	1:B:169:CYS:HB2	1.98	0.46
1:B:229:PRO:HD2	1:B:232:LEU:HD22	1.96	0.46
1:C:90:PRO:HA	2:C:1334:3I7:C17	2.47	0.45
1:C:104:LEU:HB2	1:C:109:THR:CG2	2.46	0.45
1:C:286:CYS:SG	1:C:321:LEU:HD12	2.57	0.45
1:C:324:LYS:HB2	1:C:330:VAL:HG13	2.00	0.44
1:B:307:LEU:HB3	1:B:309:GLN:HG3	1.99	0.44
1:C:42:MET:HG2	1:C:54:ILE:HG13	1.99	0.44
1:C:307:LEU:HB3	1:C:309:GLN:HG3	2.00	0.44
1:C:101:GLN:H	1:C:101:GLN:HG2	1.65	0.44
1:B:320:LEU:HD22	1:B:330:VAL:HG13	1.99	0.43
1:C:285:ASP:HB3	1:C:330:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:HB2	1:A:153:LEU:CD1	2.46	0.43
1:C:297:ASN:HD22	1:C:299:GLN:HB3	1.83	0.43
1:D:39:ILE:HG12	1:D:85:VAL:HG22	2.01	0.43
1:A:74:HIS:HB2	1:A:315:ALA:HB2	2.00	0.43
1:B:253:SER:HB2	3:B:2100:HOH:O	2.18	0.43
1:B:2:LYS:HG2	3:B:2003:HOH:O	2.18	0.43
1:C:33:THR:HG22	1:C:320:LEU:HG	2.01	0.43
1:D:183:LYS:O	1:D:185:TYR:HD1	2.01	0.43
1:A:22:PHE:CG	1:A:42:MET:HG3	2.54	0.42
1:C:7:LEU:HD11	1:C:39:ILE:HD13	2.01	0.42
1:A:280:ILE:H	1:A:280:ILE:HG13	1.62	0.42
1:B:331:ARG:HH11	1:B:331:ARG:HA	1.84	0.42
1:C:242:GLN:NE2	1:C:252:ILE:HG21	2.34	0.42
1:A:65:ARG:HB2	1:A:279:PHE:CE2	2.55	0.42
1:B:44:LYS:HE3	1:B:79:ALA:O	2.19	0.42
1:D:42:MET:HB3	1:D:47:LEU:HD13	2.02	0.41
1:A:112:VAL:HG13	1:A:146:LEU:HD11	2.03	0.41
1:A:322:ALA:O	1:A:326:ARG:HG3	2.20	0.41
1:D:307:LEU:HB3	1:D:309:GLN:HG3	2.02	0.41
1:C:4:TYR:HB3	1:C:8:LEU:HD12	2.03	0.41
1:D:139:LEU:HD12	1:D:149:ILE:CD1	2.51	0.41
1:A:39:ILE:HG12	1:A:85:VAL:HG22	2.02	0.41
1:D:4:TYR:HB3	1:D:8:LEU:HD12	2.03	0.41
1:C:243:MET:CG	1:C:252:ILE:HD11	2.51	0.41
1:A:243:MET:O	1:A:251:ARG:HD2	2.21	0.41
1:D:112:VAL:HG13	1:D:146:LEU:HD11	2.03	0.41
1:C:287:VAL:HG11	1:C:302:GLU:HG2	2.02	0.40
1:D:103:ARG:HD3	1:D:231:TRP:CE2	2.56	0.40
1:D:186:LEU:HB3	1:D:189:GLU:OE2	2.21	0.40
1:C:112:VAL:HG13	1:C:146:LEU:HD11	2.04	0.40
1:A:307:LEU:HB3	1:A:309:GLN:HG3	2.03	0.40
1:C:197:ILE:CD1	1:C:244:LEU:HD21	2.51	0.40
1:B:74:HIS:HB2	1:B:315:ALA:HB2	2.02	0.40
1:D:26:LYS:HE2	1:D:41:ILE:HD13	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	308/356 (86%)	285 (92%)	21 (7%)	2 (1%)	25 50
1	B	315/356 (88%)	296 (94%)	17 (5%)	2 (1%)	25 50
1	C	306/356 (86%)	280 (92%)	19 (6%)	7 (2%)	6 16
1	D	313/356 (88%)	285 (91%)	21 (7%)	7 (2%)	6 17
All	All	1242/1424 (87%)	1146 (92%)	78 (6%)	18 (1%)	10 28

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	THR
1	C	295	ARG
1	D	183	LYS
1	D	302	GLU
1	A	23	ALA
1	D	21	GLY
1	D	184	SER
1	C	265	GLN
1	C	330	VAL
1	D	304	LEU
1	C	225	LYS
1	D	306	SER
1	B	330	VAL
1	C	18	GLY
1	D	19	THR
1	C	51	LEU
1	A	20	GLY
1	C	20	GLY

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	277/314 (88%)	244 (88%)	33 (12%)	5 12
1	B	285/314 (91%)	255 (90%)	30 (10%)	7 16
1	C	277/314 (88%)	243 (88%)	34 (12%)	4 11
1	D	281/314 (90%)	250 (89%)	31 (11%)	6 14
All	All	1120/1256 (89%)	992 (89%)	128 (11%)	5 13

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	LEU
1	A	17	ILE
1	A	22	PHE
1	A	24	LYS
1	A	27	LEU
1	A	43	ASP
1	A	53	ARG
1	A	65	ARG
1	A	102	ASP
1	A	103	ARG
1	A	107	GLU
1	A	141	ASP
1	A	153	LEU
1	A	169	CYS
1	A	179	LEU
1	A	198	LEU
1	A	211	ASP
1	A	217	LEU
1	A	228	VAL
1	A	235	SER
1	A	251	ARG
1	A	264	MET
1	A	265	GLN

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Mol	Chain	Res	Type
1	A	268	ASN
1	A	274	GLN
1	A	280	ILE
1	A	290	LEU
1	A	295	ARG
1	A	296	ASN
1	A	304	LEU
1	A	313	LEU
1	A	333	ARG
1	B	8	LEU
1	B	17	ILE
1	B	27	LEU
1	B	42	MET
1	B	43	ASP
1	B	45	ASN
1	B	46	THR
1	B	59	GLU
1	B	65	ARG
1	B	76	LEU
1	B	101	GLN
1	B	102	ASP
1	B	107	GLU
1	B	139	LEU
1	B	179	LEU
1	B	181	GLN
1	B	211	ASP
1	B	217	LEU
1	B	228	VAL
1	B	230	LYS
1	B	264	MET
1	B	265	GLN
1	B	274	GLN
1	B	280	ILE
1	B	299	GLN
1	B	302	GLU
1	B	304	LEU
1	B	306	SER
1	B	313	LEU
1	B	331	ARG
1	C	3	ASP
1	C	8	LEU
1	C	16	THR

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Mol	Chain	Res	Type
1	C	19	THR
1	C	27	LEU
1	C	37	VAL
1	C	44	LYS
1	C	51	LEU
1	C	101	GLN
1	C	107	GLU
1	C	154	CYS
1	C	156	LYS
1	C	179	LEU
1	C	198	LEU
1	C	211	ASP
1	C	217	LEU
1	C	223	ARG
1	C	225	LYS
1	C	228	VAL
1	C	245	GLN
1	C	249	LYS
1	C	264	MET
1	C	274	GLN
1	C	280	ILE
1	C	295	ARG
1	C	296	ASN
1	C	297	ASN
1	C	300	THR
1	C	304	LEU
1	C	307	LEU
1	C	313	LEU
1	C	321	LEU
1	C	330	VAL
1	C	333	ARG
1	D	3	ASP
1	D	8	LEU
1	D	27	LEU
1	D	37	VAL
1	D	42	MET
1	D	45	ASN
1	D	47	LEU
1	D	102	ASP
1	D	103	ARG
1	D	107	GLU
1	D	144	HIS

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Mol	Chain	Res	Type
1	D	149	ILE
1	D	179	LEU
1	D	186	LEU
1	D	198	LEU
1	D	211	ASP
1	D	217	LEU
1	D	228	VAL
1	D	235	SER
1	D	238	LEU
1	D	251	ARG
1	D	264	MET
1	D	274	GLN
1	D	284	ASP
1	D	285	ASP
1	D	300	THR
1	D	301	MET
1	D	302	GLU
1	D	313	LEU
1	D	331	ARG
1	D	333	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	137	ASN
1	A	181	GLN
1	A	277	ASN
1	A	309	GLN
1	A	312	HIS
1	B	45	ASN
1	B	137	ASN
1	B	245	GLN
1	B	277	ASN
1	B	299	GLN
1	B	312	HIS
1	C	71	GLN
1	C	137	ASN
1	C	241	GLN
1	C	242	GLN
1	C	245	GLN
1	C	260	HIS

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Mol	Chain	Res	Type
1	C	296	ASN
1	C	297	ASN
1	C	312	HIS
1	D	71	GLN
1	D	137	ASN
1	D	245	GLN
1	D	277	ASN
1	D	312	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)

4 ligands are modelled in this entry.

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	3I7	D	1334	-	25,27,27	0.43	0	31,35,35	0.51	0
2	3I7	C	1334	-	25,27,27	0.43	0	31,35,35	0.49	0
2	3I7	B	1334	-	25,27,27	0.50	0	31,35,35	0.61	0
2	3I7	A	1334	-	25,27,27	0.39	0	31,35,35	0.50	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
2	3I7	D	1334	-	-	7/17/17/17	0/3/3/3
2	3I7	C	1334	-	-	6/17/17/17	0/3/3/3
2	3I7	B	1334	-	-	1/17/17/17	0/3/3/3
2	3I7	A	1334	-	-	2/17/17/17	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1334	3I7	C2-C3-C4-O5
2	B	1334	3I7	C2-C3-C4-O5
2	C	1334	3I7	C2-C3-C4-O5
2	D	1334	3I7	N1-C2-C3-C4
2	D	1334	3I7	C3-C4-O5-C6
2	C	1334	3I7	C20-C15-N14-C12
2	C	1334	3I7	C16-C15-N14-C12
2	D	1334	3I7	C16-C15-N14-C12
2	D	1334	3I7	C20-C15-N14-C12
2	C	1334	3I7	C6-C11-C12-O13
2	D	1334	3I7	C6-C11-C12-O13
2	C	1334	3I7	C6-C11-C12-N14
2	C	1334	3I7	C3-C4-O5-C6
2	D	1334	3I7	C6-C11-C12-N14
2	A	1334	3I7	C7-C6-O5-C4
2	D	1334	3I7	C7-C6-O5-C4

There are no ring outliers.

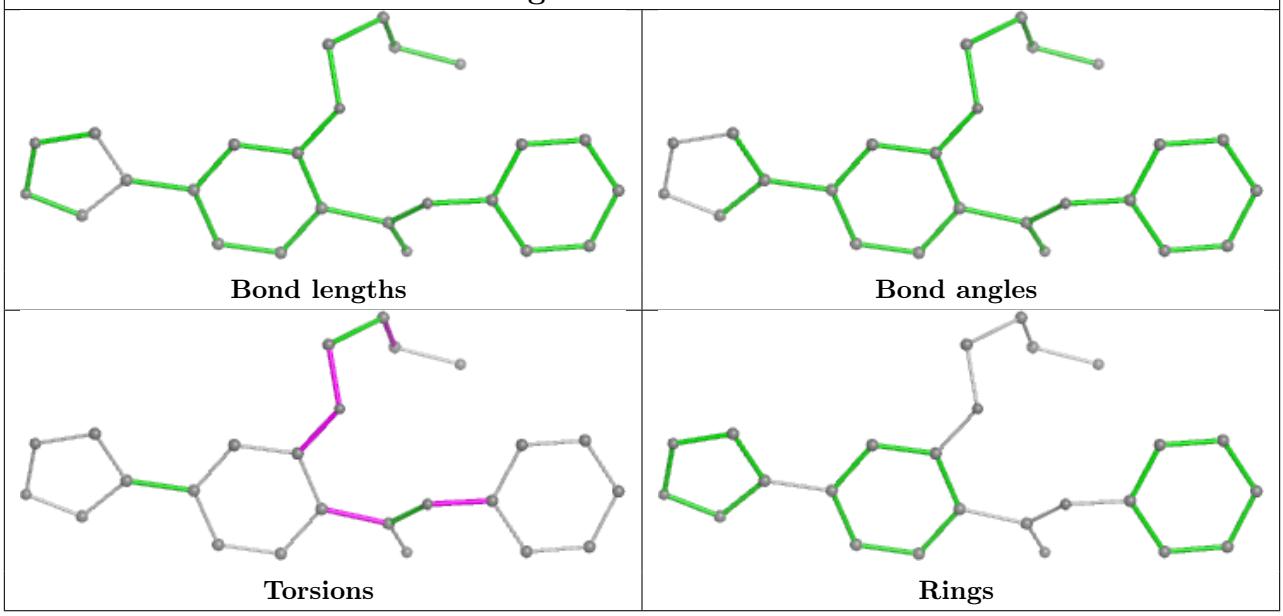
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1334	3I7	1	0
2	A	1334	3I7	1	0

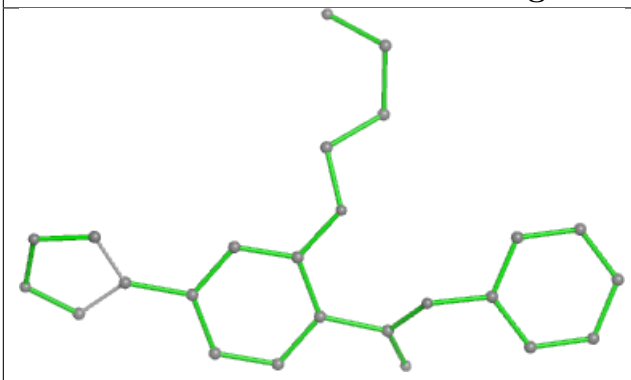
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

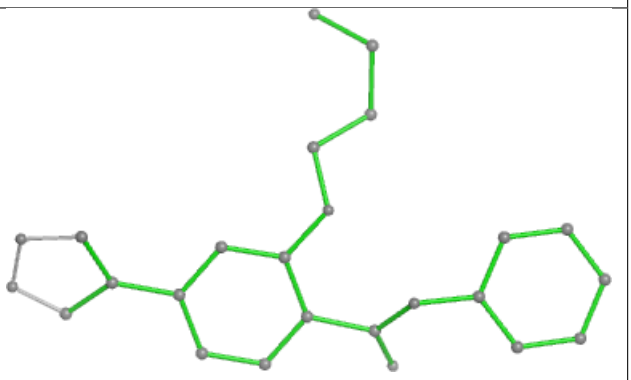
Ligand 3I7 D 1334



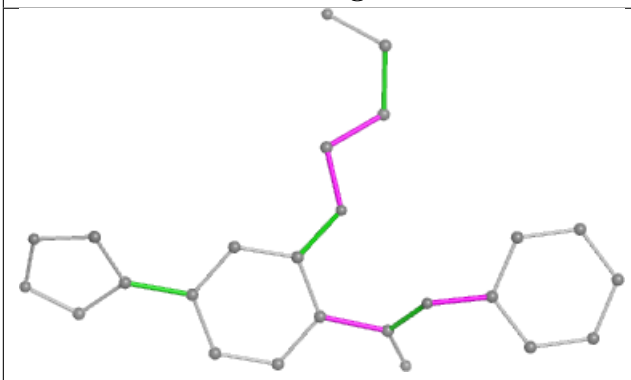
Ligand 3I7 C 1334



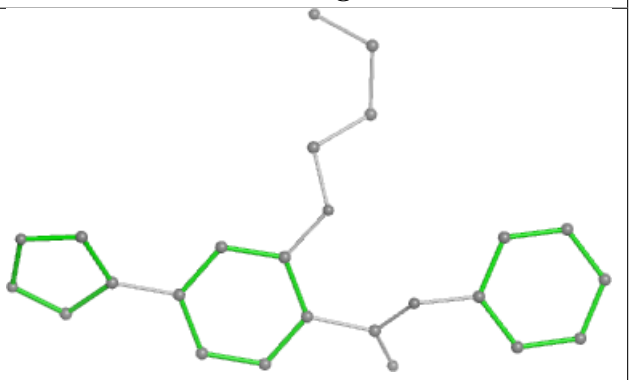
Bond lengths



Bond angles

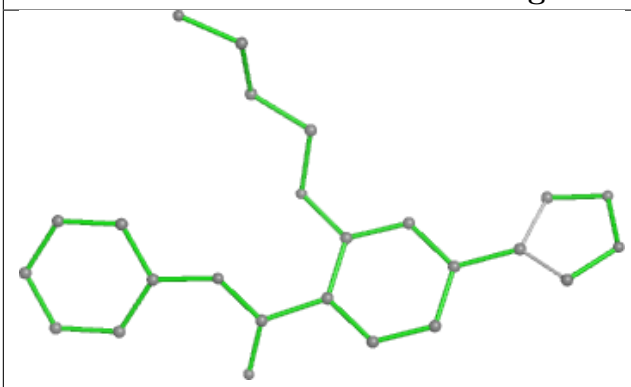


Torsions

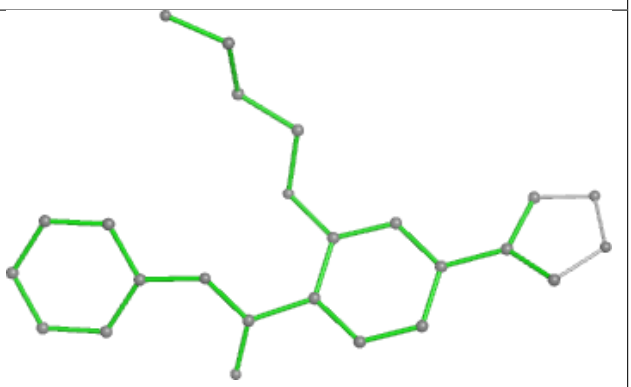


Rings

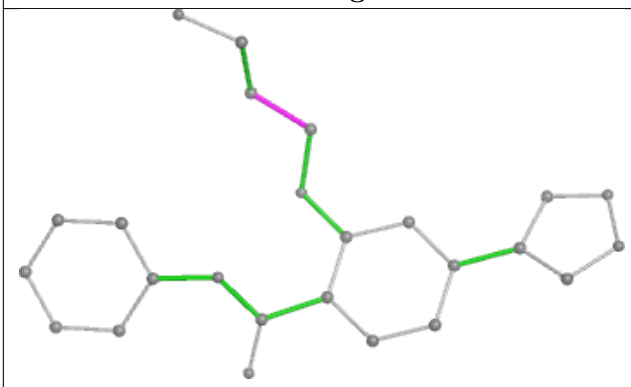
Ligand 3I7 B 1334



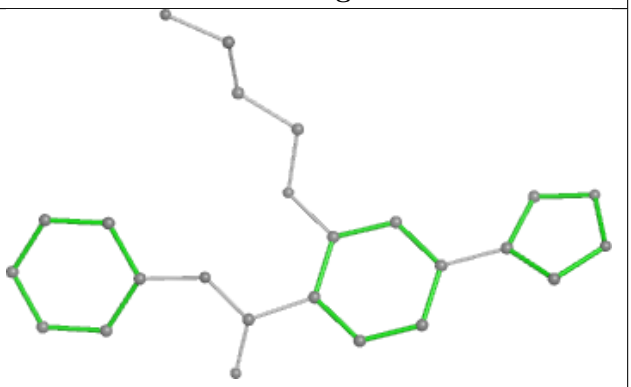
Bond lengths



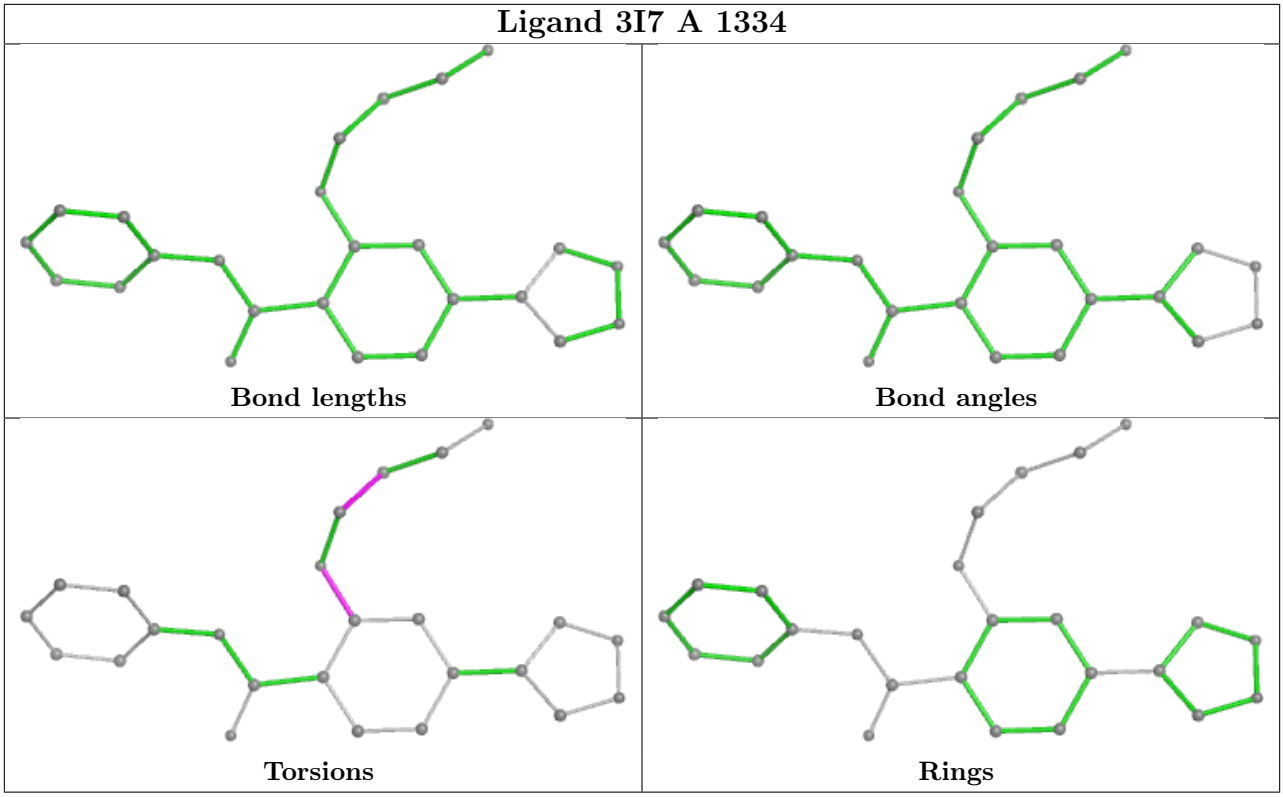
Bond angles



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 (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	316/356 (88%)	1.06	60 (18%) 1 0	47, 90, 135, 151	0
1	B	323/356 (90%)	0.61	25 (7%) 13 11	44, 80, 116, 139	0
1	C	313/356 (87%)	1.35	70 (22%) 0 0	53, 101, 142, 154	0
1	D	319/356 (89%)	0.63	23 (7%) 15 13	46, 82, 127, 164	0
All	All	1271/1424 (89%)	0.91	178 (14%) 2 1	44, 88, 132, 164	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	307	LEU	8.3
1	C	18	GLY	7.0
1	A	4	TYR	7.0
1	A	21	GLY	6.8
1	C	290	LEU	6.5
1	A	82	ILE	6.1
1	A	23	ALA	6.0
1	A	282	LEU	5.4
1	C	292	VAL	5.4
1	C	10	TYR	5.4
1	D	332	LEU	5.4
1	C	305	ILE	5.3
1	C	84	MET	5.1
1	C	303	ASP	5.1
1	C	74	HIS	4.9
1	A	18	GLY	4.8
1	C	229	PRO	4.8
1	C	267	TYR	4.8
1	A	75	VAL	4.7
1	C	298	ARG	4.7
1	A	53	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	18	GLY	4.5
1	C	60	ALA	4.5
1	C	82	ILE	4.4
1	A	290	LEU	4.3
1	C	72	LEU	4.3
1	C	293	HIS	4.2
1	A	7	LEU	4.2
1	B	162	ASP	4.1
1	A	314	THR	4.1
1	C	21	GLY	3.9
1	D	290	LEU	3.9
1	D	186	LEU	3.9
1	C	324	LYS	3.8
1	C	75	VAL	3.8
1	C	283	ASP	3.8
1	C	308	TRP	3.8
1	D	328	LYS	3.8
1	A	292	VAL	3.8
1	A	155	ALA	3.7
1	C	155	ALA	3.7
1	A	168	CYS	3.7
1	B	296	ASN	3.6
1	A	76	LEU	3.6
1	A	84	MET	3.6
1	A	179	LEU	3.6
1	A	17	ILE	3.6
1	A	46	THR	3.6
1	A	10	TYR	3.6
1	C	306	SER	3.5
1	C	85	VAL	3.5
1	A	293	HIS	3.5
1	C	313	LEU	3.5
1	A	286	CYS	3.4
1	D	281	HIS	3.4
1	C	301	MET	3.4
1	C	56	THR	3.4
1	A	5	ASP	3.3
1	C	107	GLU	3.3
1	C	63	ASN	3.3
1	C	291	SER	3.3
1	C	309	GLN	3.3
1	A	305	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	83	PHE	3.2
1	C	31	ILE	3.2
1	C	76	LEU	3.2
1	A	244	LEU	3.1
1	C	232	LEU	3.1
1	A	192	VAL	3.1
1	A	313	LEU	3.1
1	C	7	LEU	3.0
1	C	61	LEU	3.0
1	D	49	SER	3.0
1	C	17	ILE	3.0
1	A	307	LEU	3.0
1	D	180	ILE	3.0
1	C	284	ASP	2.9
1	D	320	LEU	2.9
1	D	294	HIS	2.9
1	C	282	LEU	2.9
1	B	290	LEU	2.9
1	C	315	ALA	2.8
1	A	248	PRO	2.8
1	C	4	TYR	2.8
1	A	85	VAL	2.8
1	B	286	CYS	2.8
1	C	53	ARG	2.8
1	A	42	MET	2.7
1	B	243	MET	2.7
1	C	66	HIS	2.7
1	C	54	ILE	2.7
1	C	281	HIS	2.7
1	B	206	PHE	2.7
1	D	19	THR	2.7
1	D	291	SER	2.7
1	C	192	VAL	2.7
1	C	259	ASN	2.7
1	C	106	GLU	2.7
1	A	2	LYS	2.7
1	C	5	ASP	2.6
1	A	41	ILE	2.6
1	B	331	ARG	2.6
1	A	74	HIS	2.6
1	A	22	PHE	2.6
1	B	180	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	277	ASN	2.6
1	B	292	VAL	2.6
1	D	48	GLY	2.6
1	D	205	GLY	2.5
1	C	1	MET	2.5
1	A	308	TRP	2.5
1	B	332	LEU	2.5
1	B	291	SER	2.5
1	A	284	ASP	2.5
1	B	297	ASN	2.5
1	A	287	VAL	2.5
1	D	33	THR	2.5
1	C	311	ASP	2.5
1	C	86	LEU	2.4
1	C	219	ALA	2.4
1	A	45	ASN	2.4
1	A	54	ILE	2.4
1	A	31	ILE	2.4
1	D	185	TYR	2.4
1	A	19	THR	2.3
1	A	217	LEU	2.3
1	C	22	PHE	2.3
1	B	305	ILE	2.3
1	A	51	LEU	2.3
1	B	302	GLU	2.3
1	C	272	GLU	2.3
1	C	20	GLY	2.3
1	B	324	LYS	2.3
1	C	187	GLY	2.3
1	B	47	LEU	2.3
1	A	269	TYR	2.3
1	D	161	LYS	2.3
1	C	238	LEU	2.3
1	C	299	GLN	2.3
1	A	20	GLY	2.3
1	C	265	GLN	2.3
1	A	39	ILE	2.3
1	C	19	THR	2.2
1	C	317	TYR	2.2
1	B	211	ASP	2.2
1	D	305	ILE	2.2
1	A	72	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	282	LEU	2.2
1	A	174	TYR	2.2
1	C	263	ILE	2.2
1	B	320	LEU	2.2
1	D	47	LEU	2.2
1	C	42	MET	2.2
1	D	219	ALA	2.2
1	C	55	LYS	2.2
1	A	291	SER	2.2
1	D	333	ARG	2.2
1	B	294	HIS	2.2
1	A	226	TYR	2.2
1	A	239	LEU	2.2
1	C	316	THR	2.2
1	A	28	ALA	2.2
1	A	246	VAL	2.1
1	A	133	LEU	2.1
1	C	129	ALA	2.1
1	A	56	THR	2.1
1	A	259	ASN	2.1
1	B	169	CYS	2.1
1	B	329	PRO	2.1
1	B	19	THR	2.1
1	A	221	ILE	2.1
1	C	314	THR	2.1
1	B	200	TYR	2.1
1	D	184	SER	2.1
1	C	83	PHE	2.1
1	B	217	LEU	2.0
1	A	3	ASP	2.0
1	D	327	GLY	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)

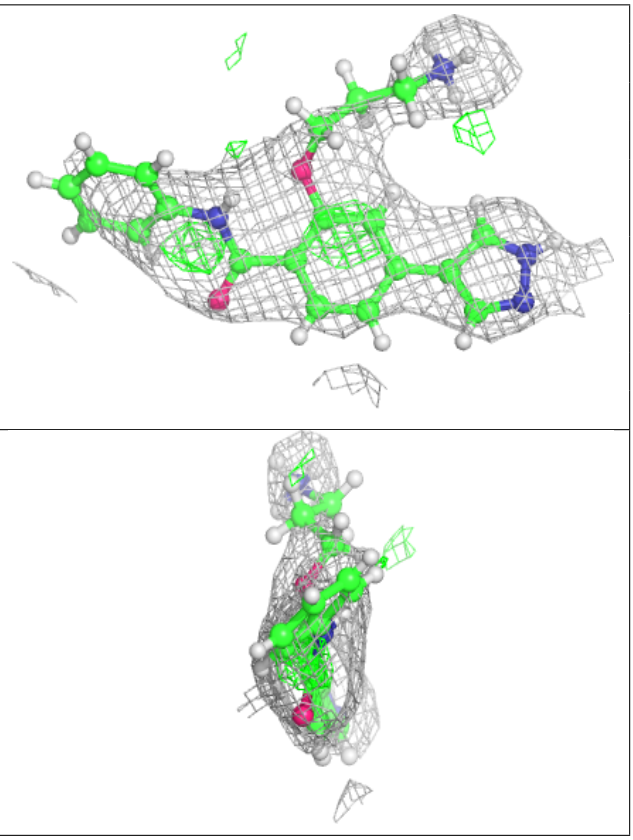
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	3I7	A	1334	25/25	0.86	0.30	68,86,98,98	46
2	3I7	C	1334	25/25	0.88	0.37	64,76,93,93	46
2	3I7	B	1334	25/25	0.89	0.21	49,76,94,94	0
2	3I7	D	1334	25/25	0.89	0.23	49,83,94,95	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.

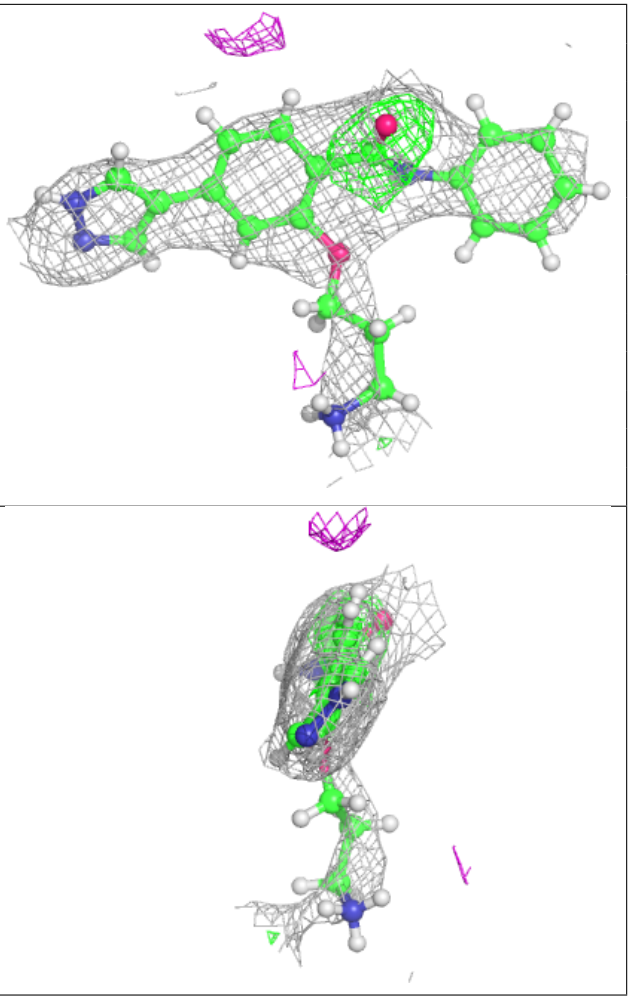
Electron density around 3I7 A 1334:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



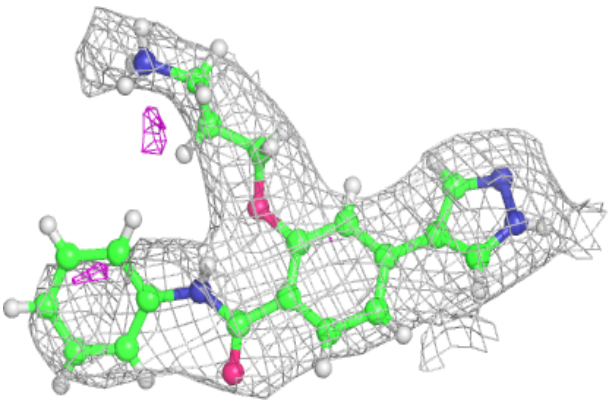
Electron density around 3I7 C 1334:

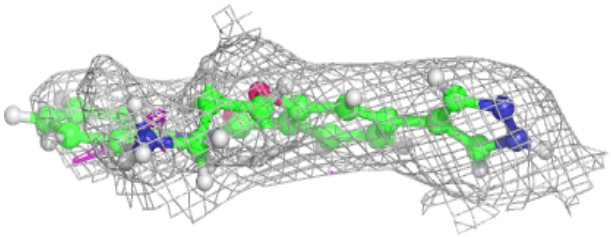
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

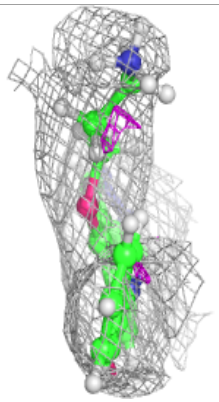


Electron density around 3I7 B 1334:

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

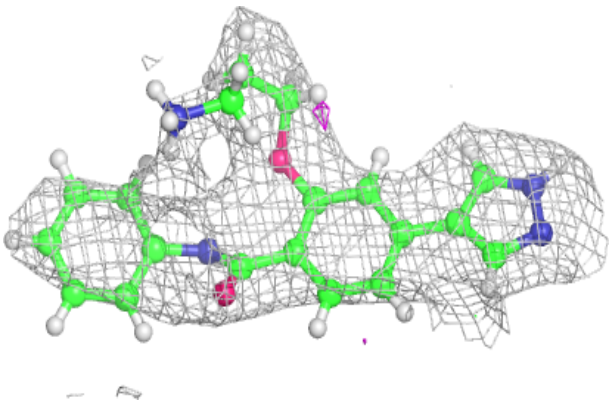


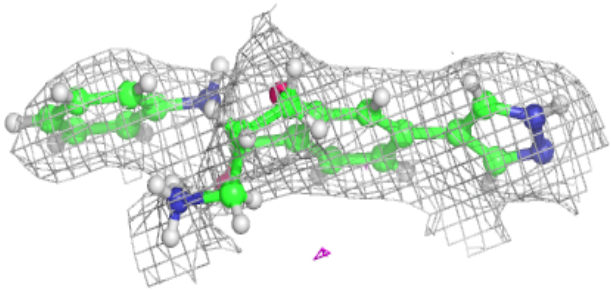


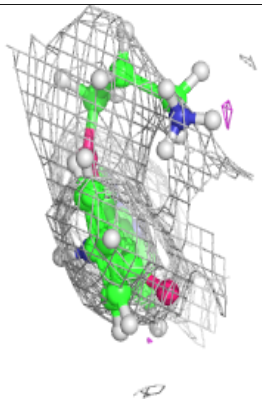


Electron density around 3I7 D 1334:

$2mF_o$-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.