



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:59 AM UTC

PDB ID : 4D2T / pdb_00004d2t
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.; McMenemy, 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 ⓘ 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

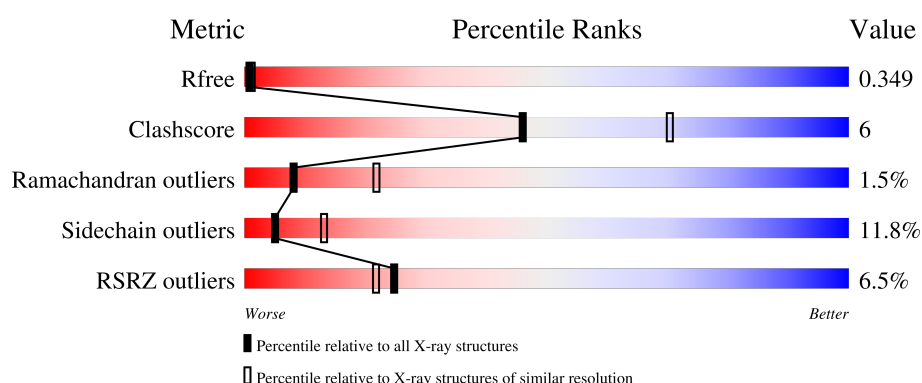
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	356	4% 68% 17% • 11%
1	B	356	3% 69% 19% • 9%
1	C	356	11% 64% 20% • • 12%
1	D	356	4% 68% 18% • • 10%

2 Entry composition

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

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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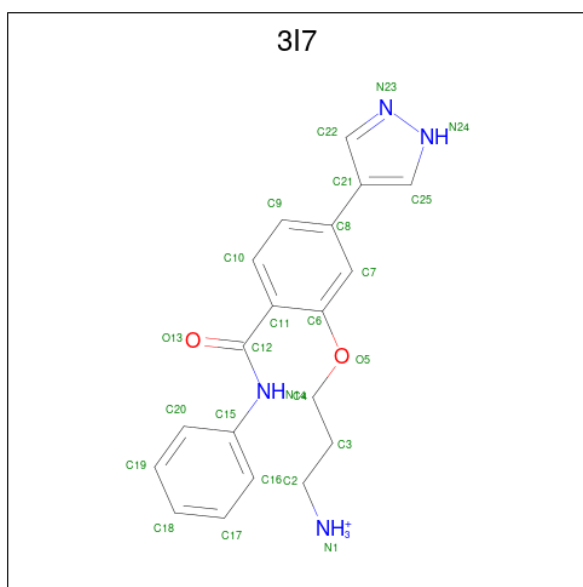
Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	expression tag	UNP Q14680
C	-9	SER	-	expression tag	UNP Q14680
C	-8	SER	-	expression tag	UNP Q14680
C	-7	GLY	-	expression tag	UNP Q14680
C	-6	LEU	-	expression tag	UNP Q14680
C	-5	VAL	-	expression tag	UNP Q14680
C	-4	PRO	-	expression tag	UNP 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 (CCD ID: 3I7) (formula: C₁₉H₂₁N₄O₂).



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

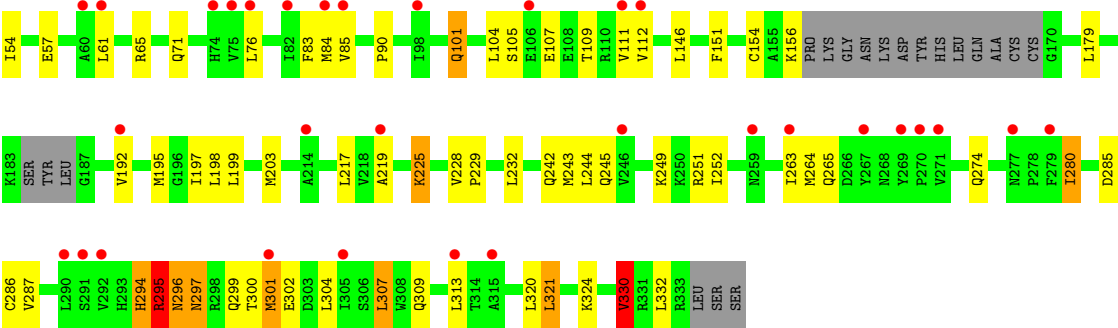
- Molecule 3 is water.

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

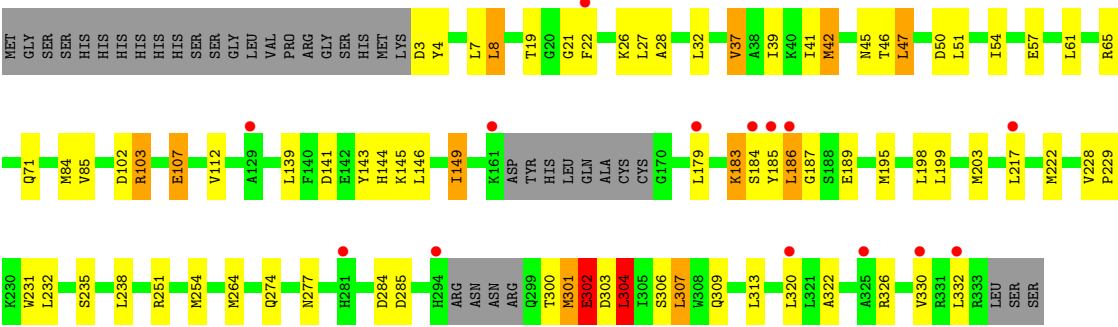
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	101	Total	O	0	0
			101	101		



● Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.34 , 129.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	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.*

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: 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	0.91	0/2610	1.38	14/3529 (0.4%)
1	B	0.92	0/2667	1.36	20/3603 (0.6%)
1	C	0.88	0/2603	1.35	9/3517 (0.3%)
1	D	0.92	0/2636	1.38	9/3565 (0.3%)
All	All	0.91	0/10516	1.37	52/14214 (0.4%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	PHE	CA-CB-CG	8.92	122.72	113.80
1	D	22	PHE	CA-CB-CG	6.96	120.76	113.80
1	D	302	GLU	CA-C-N	6.94	134.20	121.70
1	D	302	GLU	C-N-CA	6.94	134.20	121.70
1	A	222	MET	CA-C-N	6.63	129.71	120.29
1	A	222	MET	C-N-CA	6.63	129.71	120.29
1	D	277	ASN	CA-CB-CG	6.49	119.09	112.60
1	A	102	ASP	CA-CB-CG	6.41	119.01	112.60
1	D	301	MET	CA-C-N	6.38	133.72	121.54
1	D	301	MET	C-N-CA	6.38	133.72	121.54
1	B	277	ASN	CA-CB-CG	6.36	118.96	112.60
1	D	141	ASP	CA-CB-CG	6.25	118.85	112.60
1	B	141	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	277	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	267	TYR	CA-C-N	-6.06	112.13	122.56
1	A	267	TYR	C-N-CA	-6.06	112.13	122.56
1	B	59	GLU	CB-CG-CD	5.95	122.71	112.60
1	B	83	PHE	CA-CB-CG	5.91	119.71	113.80
1	B	53	ARG	CA-C-N	5.74	127.79	120.56
1	B	53	ARG	C-N-CA	5.74	127.79	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	222	MET	CA-C-N	5.64	128.30	120.29
1	D	222	MET	C-N-CA	5.64	128.30	120.29
1	B	18	GLY	CA-C-N	5.63	132.29	121.54
1	B	18	GLY	C-N-CA	5.63	132.29	121.54
1	C	22	PHE	CA-CB-CG	5.59	119.39	113.80
1	C	263	ILE	CA-C-N	5.58	128.21	120.29
1	C	263	ILE	C-N-CA	5.58	128.21	120.29
1	A	296	ASN	CA-CB-CG	5.42	118.02	112.60
1	C	294	HIS	CA-C-N	5.33	131.72	121.54
1	C	294	HIS	C-N-CA	5.33	131.72	121.54
1	C	301	MET	CA-C-N	5.31	127.65	120.38
1	C	301	MET	C-N-CA	5.31	127.65	120.38
1	A	313	LEU	CA-C-N	5.30	127.39	120.28
1	A	313	LEU	C-N-CA	5.30	127.39	120.28
1	B	14	HIS	CA-C-N	5.24	128.20	120.82
1	B	14	HIS	C-N-CA	5.24	128.20	120.82
1	B	254	MET	CA-C-N	5.22	127.28	120.28
1	B	254	MET	C-N-CA	5.22	127.28	120.28
1	B	279	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	43	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	111	VAL	CA-C-N	5.09	127.08	120.56
1	C	111	VAL	C-N-CA	5.09	127.08	120.56
1	A	141	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	50	ASP	CA-C-N	5.08	126.44	120.09
1	B	50	ASP	C-N-CA	5.08	126.44	120.09
1	B	162	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	160	ASN	CA-C-N	5.04	128.48	121.02
1	B	160	ASN	C-N-CA	5.04	128.48	121.02
1	A	111	VAL	CA-C-N	5.04	127.01	120.56
1	A	111	VAL	C-N-CA	5.04	127.01	120.56
1	B	57	GLU	CA-C-N	5.03	127.09	120.60
1	B	57	GLU	C-N-CA	5.03	127.09	120.60

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	31	0
1	B	2610	0	2630	23	0
1	C	2544	0	2564	40	0
1	D	2577	0	2599	28	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
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	121	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 (121) 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:B:195:MET:HE1	1:B:254:MET:HE1	1.57	0.87
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:A:22:PHE:C	1:A:24:LYS:H	2.06	0.64
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:B:57:GLU:HG2	1:B:84:MET:HE1	1.82	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASN:HD21	1:B:80:ASN:HB3	1.66	0.59
1:C:40:LYS:HB3	1:C:42:MET:HE1	1.84	0.59
1:D:57:GLU:HG2	1:D:84:MET:HE1	1.86	0.58
1:D:185:TYR:HD2	1:D:187:GLY:HA2	1.68	0.58
1:C:57:GLU:HG2	1:C:84:MET:HE1	1.85	0.57
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:A:57:GLU:HG2	1:A:84:MET:HE1	1.88	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:294:HIS:O	1:C:295:ARG:HB2	2.15	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
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:A:192:VAL:HA	1:A:195:MET:HE3	2.00	0.43
1:B:2:LYS:HG2	3:B:2003:HOH:O	2.18	0.43
1:B:199:LEU:HG	1:B:203:MET:HE2	2.01	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:B:192:VAL:HA	1:B:195:MET:HE3	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:D:199:LEU:HG	1:D:203:MET:HE2	2.02	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:C:199:LEU:HG	1:C:203:MET:HE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:C	1:A:24:LYS:N	2.75	0.41
1:D:4:TYR:HB3	1:D:8:LEU:HD12	2.03	0.41
1:A:199:LEU:HG	1:A:203:MET:HE2	2.01	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:192:VAL:HA	1:C:195:MET:HE3	2.02	0.40
1:C:197:ILE:CD1	1:C:244:LEU:HD21	2.51	0.40
1:D:195:MET:HE1	1:D:254:MET:HE1	2.02	0.40
1:A:195:MET:HE1	1:A:254:MET:HE1	2.03	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

5.3.1 Protein backbone

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%)	21	44
1	B	315/356 (88%)	296 (94%)	17 (5%)	2 (1%)	21	44
1	C	306/356 (86%)	280 (92%)	19 (6%)	7 (2%)	5	13
1	D	313/356 (88%)	285 (91%)	21 (7%)	7 (2%)	5	14
All	All	1242/1424 (87%)	1146 (92%)	78 (6%)	18 (1%)	8	23

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 ⓘ

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	13
1	B	285/314 (91%)	252 (88%)	33 (12%)	5	13
1	C	277/314 (88%)	244 (88%)	33 (12%)	5	13
1	D	281/314 (90%)	248 (88%)	33 (12%)	5	13
All	All	1120/1256 (89%)	988 (88%)	132 (12%)	5	13

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	17	ILE
1	A	22	PHE
1	A	24	LYS

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Mol	Chain	Res	Type
1	A	27	LEU
1	A	43	ASP
1	A	53	ARG
1	A	65	ARG
1	A	102	ASP
1	A	107	GLU
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
1	A	268	ASN
1	A	274	GLN
1	A	280	ILE
1	A	282	LEU
1	A	290	LEU
1	A	295	ARG
1	A	296	ASN
1	A	301	MET
1	A	304	LEU
1	A	307	LEU
1	A	313	LEU
1	A	333	ARG
1	B	8	LEU
1	B	17	ILE
1	B	27	LEU
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

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Mol	Chain	Res	Type
1	B	179	LEU
1	B	181	GLN
1	B	198	LEU
1	B	211	ASP
1	B	217	LEU
1	B	228	VAL
1	B	230	LYS
1	B	251	ARG
1	B	264	MET
1	B	274	GLN
1	B	280	ILE
1	B	282	LEU
1	B	299	GLN
1	B	301	MET
1	B	302	GLU
1	B	304	LEU
1	B	306	SER
1	B	307	LEU
1	B	313	LEU
1	B	331	ARG
1	C	3	ASP
1	C	8	LEU
1	C	16	THR
1	C	17	ILE
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	217	LEU
1	C	225	LYS
1	C	228	VAL
1	C	245	GLN
1	C	249	LYS
1	C	264	MET
1	C	274	GLN

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Mol	Chain	Res	Type
1	C	280	ILE
1	C	295	ARG
1	C	296	ASN
1	C	297	ASN
1	C	300	THR
1	C	301	MET
1	C	304	LEU
1	C	307	LEU
1	C	313	LEU
1	C	321	LEU
1	C	330	VAL
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	46	THR
1	D	47	LEU
1	D	51	LEU
1	D	102	ASP
1	D	103	ARG
1	D	107	GLU
1	D	144	HIS
1	D	145	LYS
1	D	149	ILE
1	D	179	LEU
1	D	186	LEU
1	D	198	LEU
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	304	LEU

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Mol	Chain	Res	Type
1	D	307	LEU
1	D	313	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) 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	293	HIS
1	A	309	GLN
1	A	312	HIS
1	B	45	ASN
1	B	80	ASN
1	B	101	GLN
1	B	137	ASN
1	B	181	GLN
1	B	277	ASN
1	B	299	GLN
1	B	312	HIS
1	C	71	GLN
1	C	80	ASN
1	C	101	GLN
1	C	137	ASN
1	C	241	GLN
1	C	242	GLN
1	C	245	GLN
1	C	296	ASN
1	C	297	ASN
1	C	312	HIS
1	D	71	GLN
1	D	137	ASN
1	D	265	GLN
1	D	277	ASN
1	D	312	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	1334	-	27,27,27	0.51	0	35,35,35	0.64	0
2	3I7	A	1334	-	27,27,27	0.40	0	35,35,35	0.56	0
2	3I7	C	1334	-	27,27,27	0.39	0	35,35,35	0.53	0
2	3I7	D	1334	-	27,27,27	0.38	0	35,35,35	0.57	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	B	1334	-	-	1/17/17/17	0/3/3/3
2	3I7	A	1334	-	-	2/17/17/17	0/3/3/3
2	3I7	C	1334	-	-	6/17/17/17	0/3/3/3
2	3I7	D	1334	-	-	7/17/17/17	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	C	1334	3I7	C2-C3-C4-O5
2	B	1334	3I7	C2-C3-C4-O5
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	N1-C2-C3-C4
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	C3-C4-O5-C6
2	C	1334	3I7	C6-C11-C12-N14
2	A	1334	3I7	C7-C6-O5-C4
2	D	1334	3I7	C6-C11-C12-N14
2	D	1334	3I7	C7-C6-O5-C4

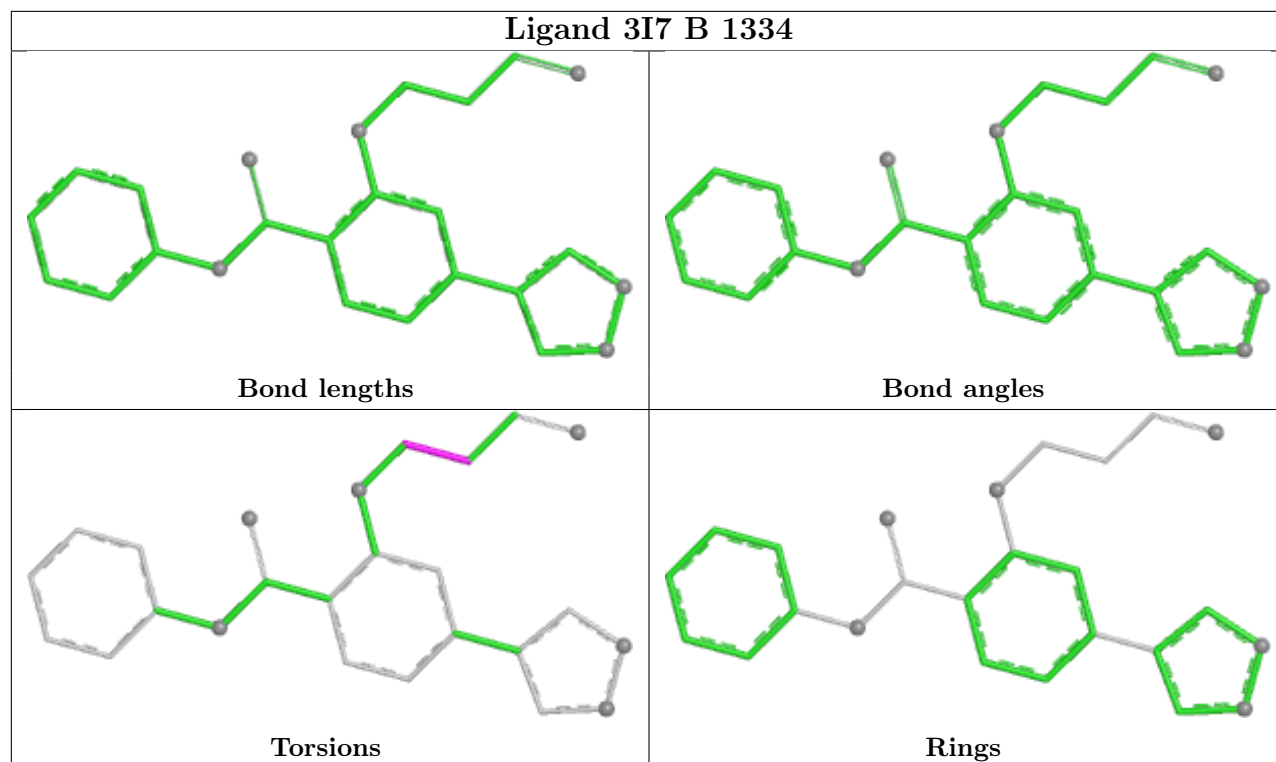
There are no ring outliers.

2 monomers are involved in 2 short contacts:

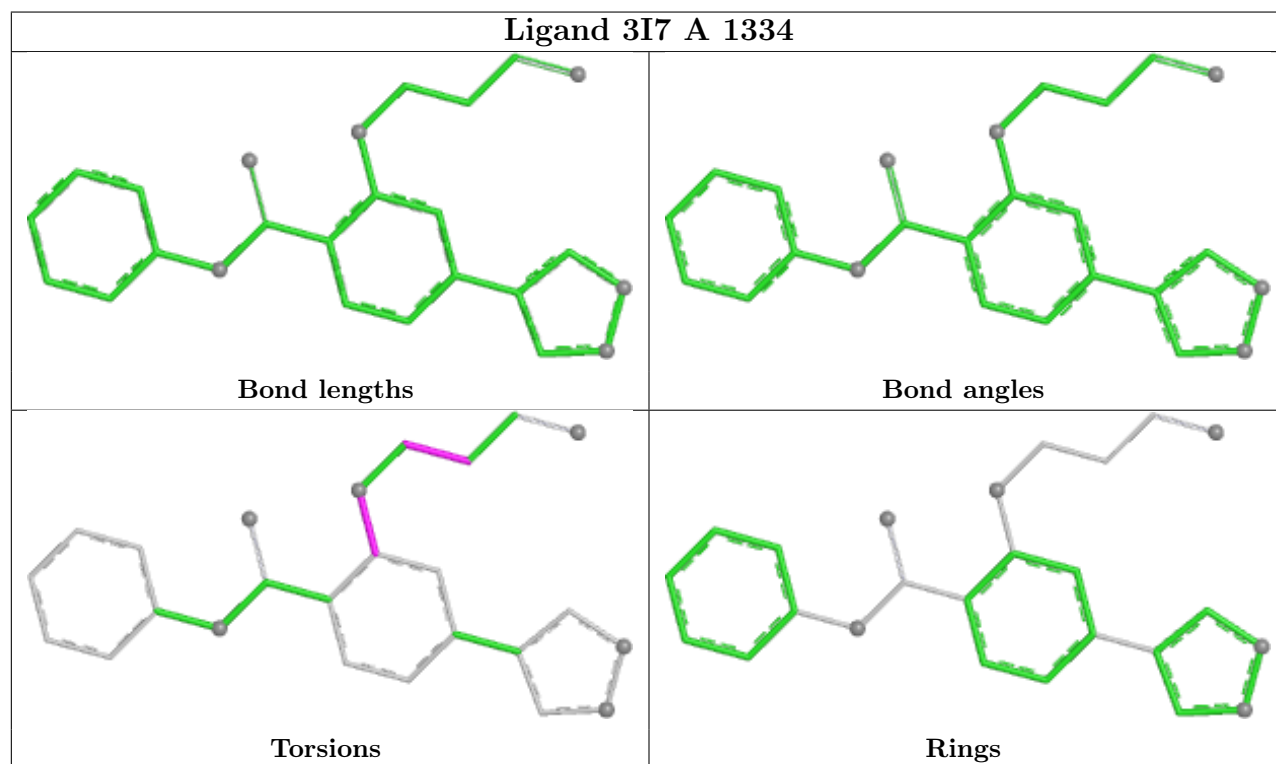
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1334	3I7	1	0
2	C	1334	3I7	1	0

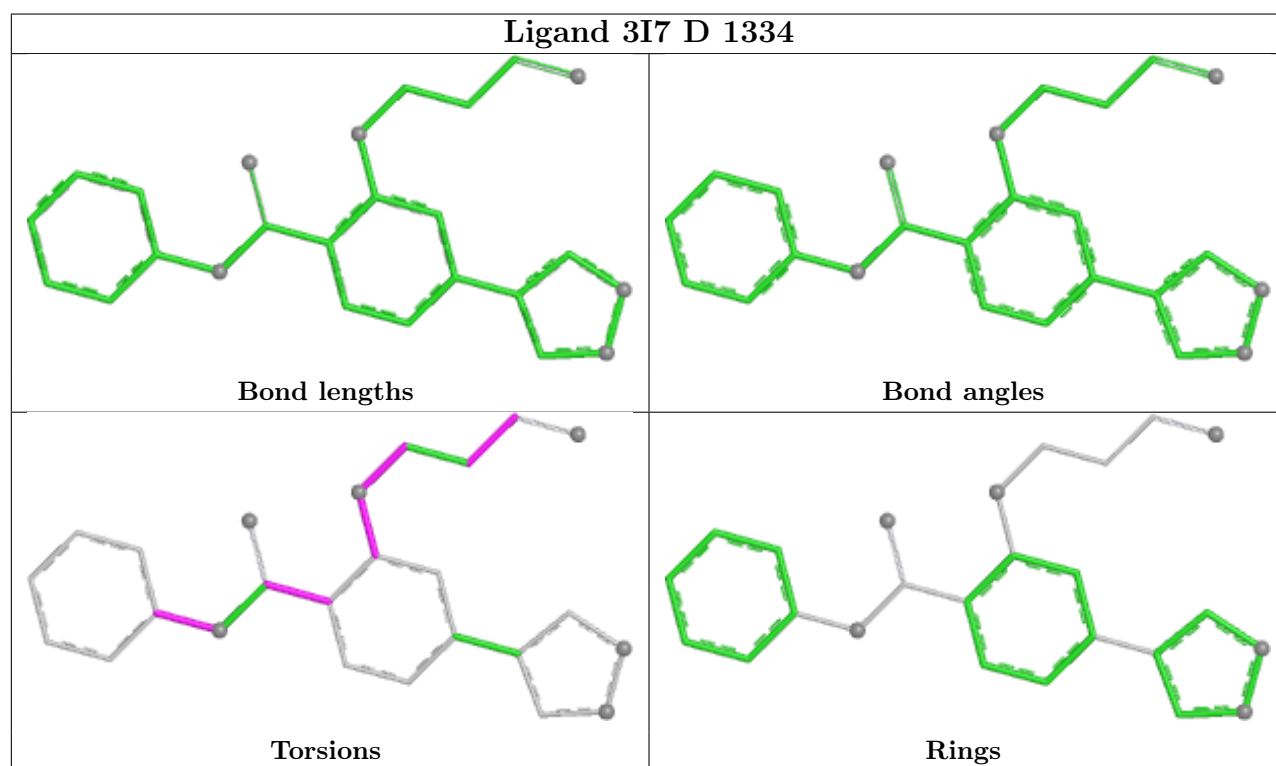
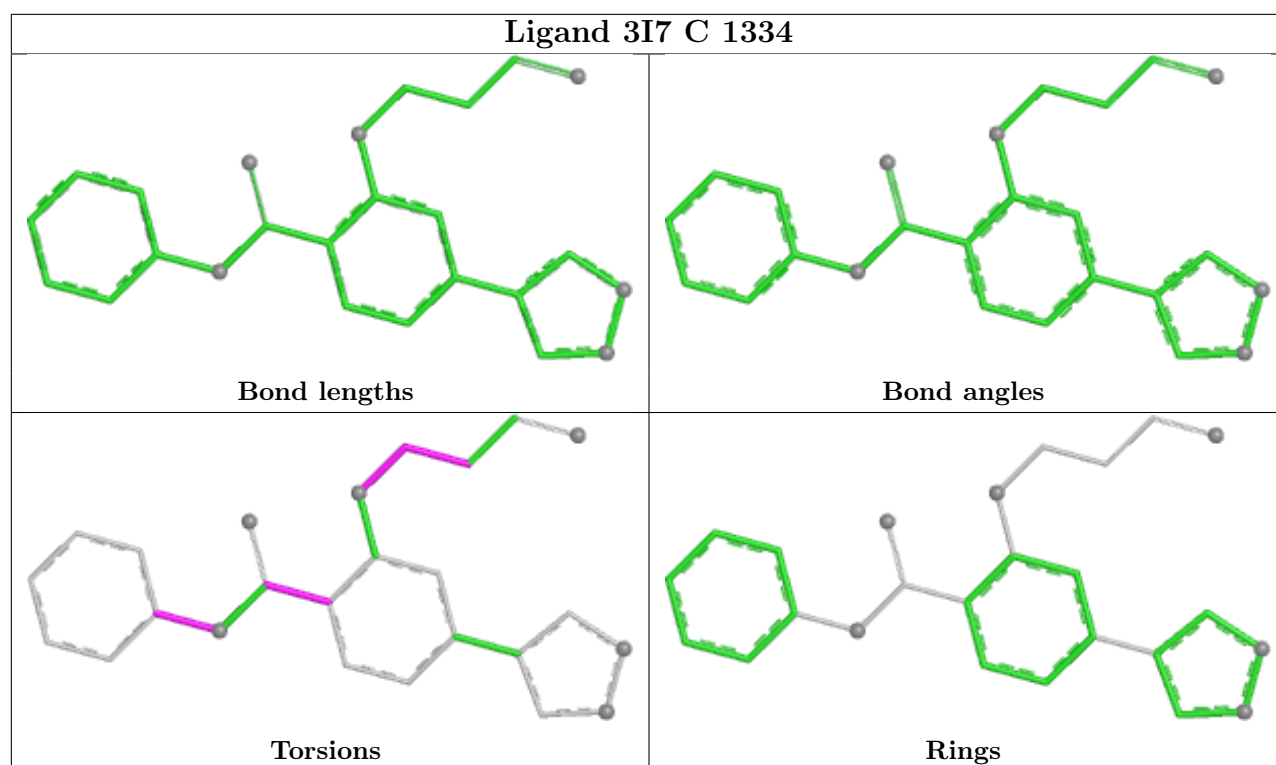
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 3I7 B 1334



Ligand 3I7 A 1334





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.83	16 (5%) 33 29	47, 90, 135, 151	0
1	B	323/356 (90%)	0.68	12 (3%) 45 41	44, 80, 116, 139	0
1	C	313/356 (87%)	1.16	40 (12%) 7 6	53, 101, 142, 154	1 (0%)
1	D	319/356 (89%)	0.73	14 (4%) 39 35	46, 82, 127, 164	0
All	All	1271/1424 (89%)	0.85	82 (6%) 25 22	44, 88, 132, 164	1 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	ALA	4.6
1	C	17	ILE	3.6
1	B	206	PHE	3.6
1	B	129	ALA	3.4
1	C	305	ILE	3.3
1	B	18	GLY	3.3
1	C	74	HIS	3.2
1	A	168	CYS	3.2
1	A	4	TYR	3.2
1	A	155	ALA	3.1
1	C	214	ALA	3.1
1	B	47	LEU	3.0
1	C	85	VAL	3.0
1	D	320	LEU	3.0
1	D	186	LEU	2.9
1	A	7	LEU	2.9
1	A	17	ILE	2.9
1	C	82	ILE	2.8
1	C	267	TYR	2.8
1	A	184	SER	2.8
1	C	4	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	192	VAL	2.8
1	C	270	PRO	2.8
1	C	61	LEU	2.8
1	C	84	MET	2.8
1	C	315	ALA	2.8
1	C	263	ILE	2.7
1	A	100	SER	2.7
1	A	85	VAL	2.7
1	C	259	ASN	2.7
1	D	161	LYS	2.7
1	D	332	LEU	2.6
1	C	7	LEU	2.6
1	C	18	GLY	2.6
1	C	76	LEU	2.6
1	C	75	VAL	2.6
1	C	313	LEU	2.5
1	D	184	SER	2.5
1	A	292	VAL	2.5
1	C	23	ALA	2.5
1	C	301	MET	2.4
1	D	281	HIS	2.4
1	C	192	VAL	2.4
1	B	155	ALA	2.4
1	C	1	MET	2.4
1	C	271	VAL	2.4
1	D	179	LEU	2.3
1	C	98	ILE	2.3
1	D	294	HIS	2.3
1	C	277	ASN	2.3
1	A	16	THR	2.3
1	A	25	VAL	2.3
1	C	246	VAL	2.3
1	D	22	PHE	2.3
1	C	219	ALA	2.2
1	C	3	ASP	2.2
1	B	187	GLY	2.2
1	B	179	LEU	2.2
1	B	290	LEU	2.2
1	C	106	GLU	2.2
1	D	330	VAL	2.2
1	A	76	LEU	2.2
1	C	291	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	325	ALA	2.2
1	C	13	LEU	2.2
1	C	269	TYR	2.1
1	C	290	LEU	2.1
1	B	218	VAL	2.1
1	C	279	PHE	2.1
1	D	129	ALA	2.1
1	C	19	THR	2.1
1	B	330	VAL	2.1
1	A	82	ILE	2.1
1	C	111	VAL	2.1
1	B	46	THR	2.0
1	B	243	MET	2.0
1	D	217	LEU	2.0
1	C	292	VAL	2.0
1	D	185	TYR	2.0
1	C	60	ALA	2.0
1	A	75	VAL	2.0
1	C	112	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

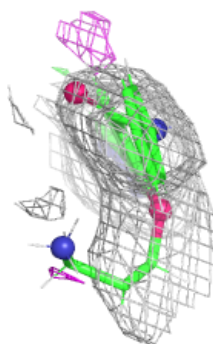
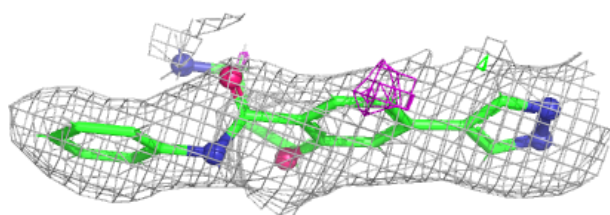
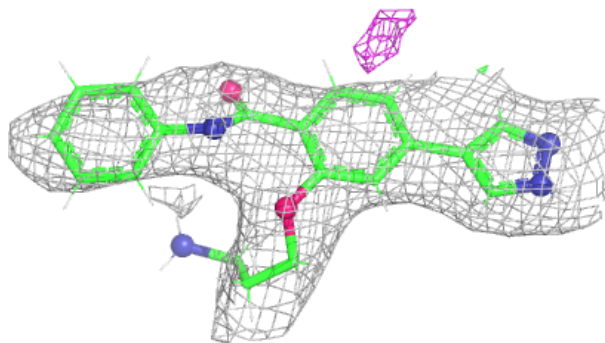
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D	1334	25/25	0.86	0.12	49,83,94,95	0
2	3I7	A	1334	25/25	0.87	0.21	68,86,98,98	46
2	3I7	B	1334	25/25	0.88	0.12	49,76,94,94	0
2	3I7	C	1334	25/25	0.91	0.20	64,76,93,93	46

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.

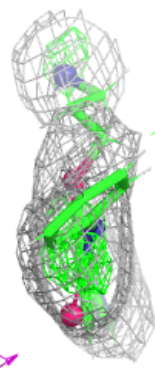
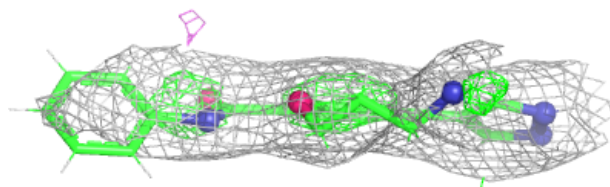
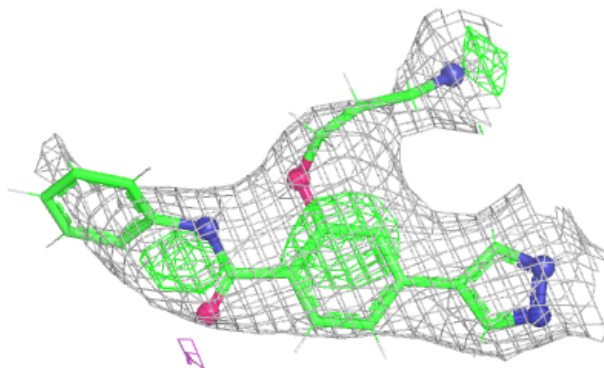
Electron density around 3I7 D 1334:

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

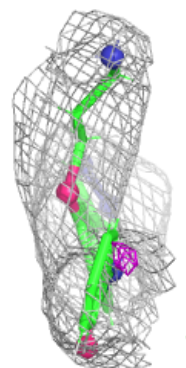
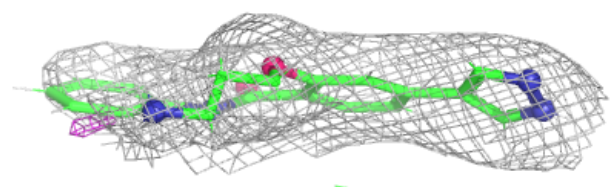
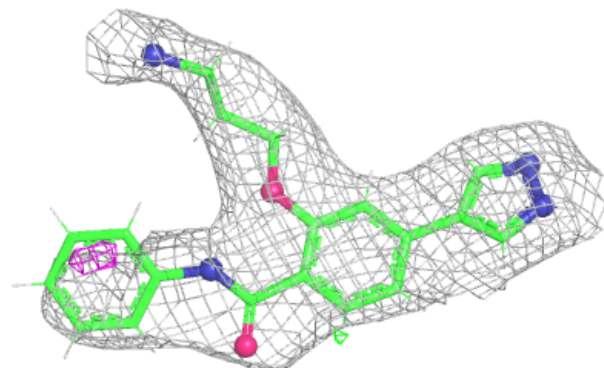


Electron density around 3I7 A 1334:

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

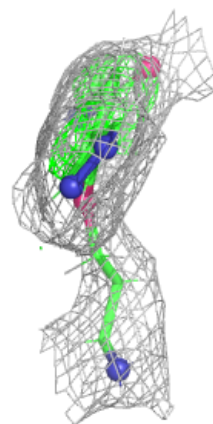
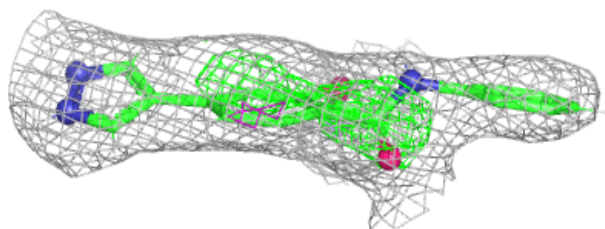
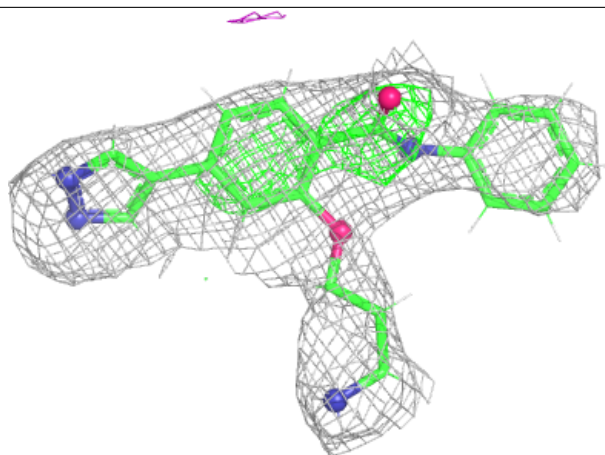
**Electron density around 3I7 B 1334:**

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



Electron density around 3I7 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.