Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 02:22 pm BST

PDB ID	:	4D2P
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	:	2014-05-12
Resolution	:	2.55 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:

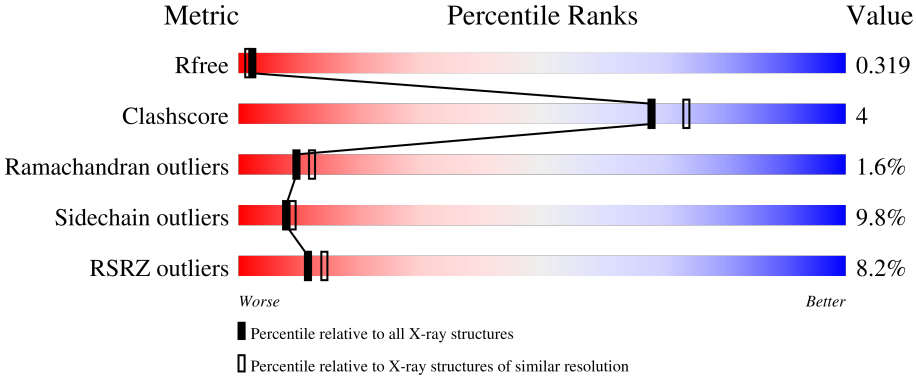
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	4% 74% 12% • 12%
1	B	356	9% 75% 14% • 9%
1	C	356	8% 73% 14% • 11%
1	D	356	8% 72% 15% • 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10948 atoms, of which 96 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	313	2550	1645	429	459	17	0	1	0
1	B	323	2611	1680	442	471	18	0	0	0
1	C	316	2565	1653	435	460	17	0	0	0
1	D	317	2567	1658	435	459	15	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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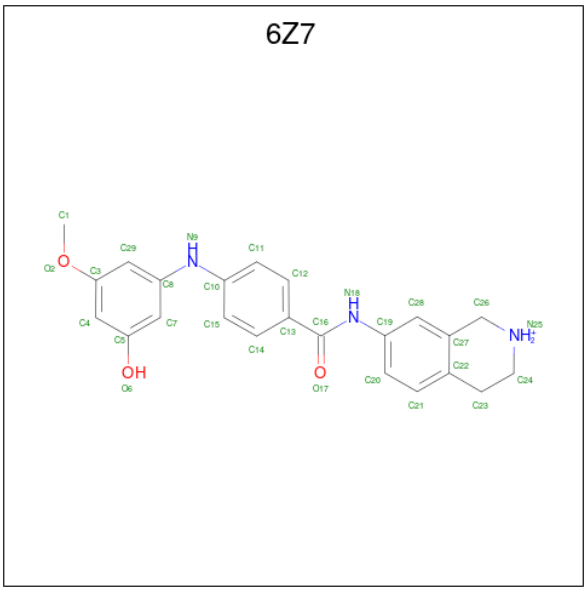
Chain	Residue	Modelled	Actual	Comment	Reference
D	215	ALA	MET	engineered mutation	UNP Q14680
D	218	VAL	TYR	engineered mutation	UNP Q14680
D	219	ALA	LYS	engineered mutation	UNP Q14680

- Molecule 2 is 7-({4-[(3-hydroxy-5-methoxyphenyl)amino]benzoyl}amino)-1,2,3,4-tetrahydroisoquinolinium (three-letter code: 6Z7) (formula: $C_{23}H_{24}N_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	53	23	24	3	3	0	0
2	B	1	53	23	24	3	3	0	0
2	C	1	53	23	24	3	3	0	0
2	D	1	53	23	24	3	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	126	126	126	0	0
3	B	111	111	111	0	0
3	C	93	93	93	0	0

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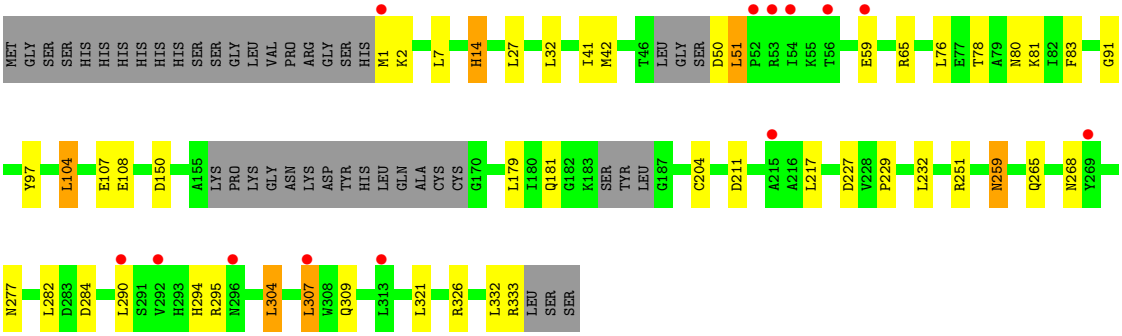
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	D	113	113	113	0	0

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.

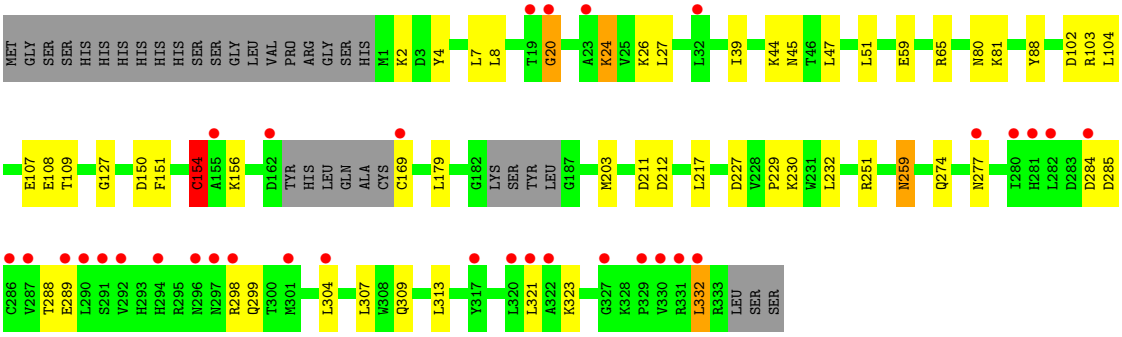
• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

Chain A:



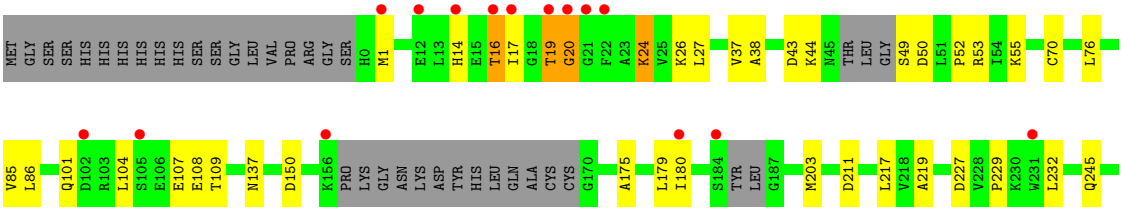
• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

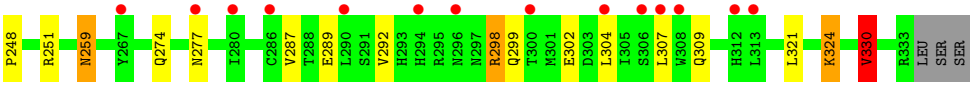
Chain B:



• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

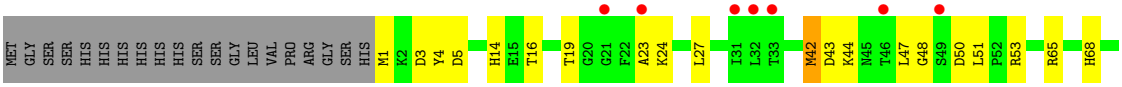
Chain C:

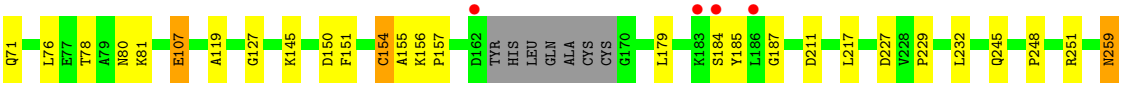


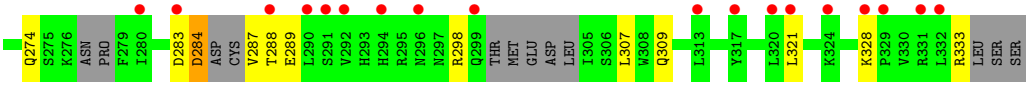


• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.28Å 76.03Å 78.60Å 85.86° 69.87° 90.17°	Depositor
Resolution (Å)	41.03 – 2.55 41.03 – 2.55	Depositor EDS
% Data completeness (in resolution range)	84.8 (41.03-2.55) 84.8 (41.03-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.234 , 0.312 0.239 , 0.319	Depositor DCC
R_{free} test set	2000 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	64.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 82.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10948	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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: 6Z7

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	0.55	0/2607	0.71	0/3525
1	B	0.54	0/2669	0.70	0/3607
1	C	0.52	0/2622	0.69	0/3542
1	D	0.54	0/2623	0.69	0/3541
All	All	0.54	0/10521	0.70	0/14215

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	155	ALA	Peptide

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	2550	0	2559	13	0
1	B	2611	0	2633	19	0
1	C	2565	0	2582	29	0
1	D	2567	0	2594	19	0
2	A	29	24	24	0	0
2	B	29	24	23	2	0
2	C	29	24	24	0	0
2	D	29	24	24	0	0
3	A	126	0	0	1	0
3	B	111	0	0	1	0
3	C	93	0	0	0	0
3	D	113	0	0	1	0
All	All	10852	96	10463	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:VAL:HG11	1:C:85:VAL:CG1	1.87	1.03
1:C:37:VAL:HG11	1:C:85:VAL:HG13	1.45	0.99
1:C:37:VAL:HG11	1:C:85:VAL:HG12	1.67	0.76
1:D:157:PRO:HB3	1:D:187:GLY:HA3	1.67	0.75
1:C:324:LYS:HG2	1:C:330:VAL:HG13	1.67	0.75
1:C:245:GLN:HB2	1:C:251:ARG:HG2	1.73	0.69
1:D:245:GLN:HB2	1:D:251:ARG:HG2	1.75	0.69
1:C:37:VAL:HG13	1:C:86:LEU:O	1.94	0.67
1:C:37:VAL:CG1	1:C:85:VAL:HG13	2.27	0.62
1:B:323:LYS:HD3	3:B:2105:HOH:O	2.01	0.60
1:C:16:THR:HA	1:C:26:LYS:HG2	1.83	0.60
1:C:175:ALA:CB	1:C:180:ILE:HD11	2.34	0.57
1:B:151:PHE:O	1:B:154:CYS:HB2	2.05	0.56
1:C:248:PRO:HA	1:C:251:ARG:HG3	1.88	0.56
1:B:20:GLY:HA3	1:C:20:GLY:HA3	1.87	0.55
1:D:248:PRO:HA	1:D:251:ARG:HG3	1.88	0.55
1:D:151:PHE:O	1:D:154:CYS:HB2	2.06	0.55
1:D:284:ASP:HB3	1:D:287:VAL:HB	1.89	0.54
1:B:45:ASN:HD21	1:B:80:ASN:HB3	1.73	0.54
1:A:41:ILE:HG12	1:A:83:PHE:CD2	2.42	0.54
1:D:5:ASP:HB2	3:D:2001:HOH:O	2.07	0.53
1:B:289:GLU:HG3	1:B:332:LEU:HD22	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:PRO:HD2	1:D:232:LEU:HD22	1.91	0.51
1:B:47:LEU:HD22	1:B:51:LEU:HA	1.93	0.51
1:B:307:LEU:HB3	1:B:309:GLN:HG3	1.93	0.51
1:D:65:ARG:HG3	1:D:71:GLN:HE22	1.76	0.51
1:B:24:LYS:HD2	1:B:26:LYS:HG3	1.93	0.51
1:C:287:VAL:HB	1:C:298:ARG:HH21	1.76	0.51
1:A:41:ILE:HG12	1:A:83:PHE:HD2	1.76	0.50
1:B:229:PRO:HD2	1:B:232:LEU:HD22	1.93	0.50
1:C:19:THR:HG23	1:C:24:LYS:HE3	1.93	0.50
1:D:259:ASN:HD22	1:D:259:ASN:H	1.60	0.50
1:B:88:TYR:CE1	2:B:1334:6Z7:H21	2.47	0.50
1:A:229:PRO:HD2	1:A:232:LEU:HD22	1.94	0.49
1:C:104:LEU:HB3	1:C:108:GLU:HB3	1.94	0.49
1:C:229:PRO:HD2	1:C:232:LEU:HD22	1.94	0.49
1:C:259:ASN:HD22	1:C:259:ASN:H	1.60	0.49
1:C:175:ALA:HB3	1:C:180:ILE:HD11	1.94	0.48
1:C:287:VAL:HG11	1:C:302:GLU:HG3	1.95	0.48
1:B:44:LYS:HA	1:B:47:LEU:HD12	1.95	0.48
1:A:91:GLY:O	1:A:97[B]:TYR:HE1	1.96	0.48
1:B:104:LEU:HB3	1:B:108:GLU:HB3	1.96	0.48
1:D:127:GLY:O	1:D:156:LYS:HA	2.14	0.48
1:A:307:LEU:HB3	1:A:309:GLN:HG3	1.96	0.47
1:D:47:LEU:HB2	1:D:50:ASP:HB2	1.95	0.47
1:C:289:GLU:O	1:C:292:VAL:HG12	2.15	0.47
1:B:127:GLY:O	1:B:156:LYS:HA	2.15	0.46
1:D:307:LEU:HB3	1:D:309:GLN:HG3	1.98	0.46
1:C:307:LEU:HB3	1:C:309:GLN:HG3	1.98	0.46
1:C:37:VAL:HG12	1:C:38:ALA:N	2.32	0.45
1:A:32:LEU:HD22	1:A:332:LEU:HG	1.97	0.45
1:D:23:ALA:HB2	1:D:42:MET:HG3	1.98	0.45
1:B:285:ASP:HA	1:B:288:THR:HG22	1.99	0.45
1:D:19:THR:HG23	1:D:24:LYS:HG3	1.99	0.45
1:B:259:ASN:H	1:B:259:ASN:HD22	1.64	0.44
1:C:219:ALA:HB1	1:D:107:GLU:HB2	2.00	0.44
1:A:259:ASN:HD22	1:A:259:ASN:H	1.66	0.44
1:C:16:THR:O	1:C:17:ILE:HG13	2.17	0.44
1:A:104:LEU:HB3	1:A:108:GLU:HB3	2.01	0.43
1:A:108:GLU:HG2	3:A:2046:HOH:O	2.18	0.43
1:A:204:CYS:SG	1:A:229:PRO:HG2	2.58	0.43
1:B:47:LEU:HB3	1:B:51:LEU:HB2	2.00	0.43
1:D:78:THR:OG1	1:D:81:LYS:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD11	1:B:39:ILE:HD13	2.00	0.42
1:B:4:TYR:HB3	1:B:8:LEU:HD12	2.01	0.42
1:C:52:PRO:HA	1:C:55:LYS:HB2	2.01	0.42
1:D:68:HIS:HB2	1:D:119:ALA:HB2	2.02	0.42
1:D:259:ASN:HD22	1:D:259:ASN:N	2.18	0.42
1:B:109:THR:HG21	1:B:203:MET:HG2	2.02	0.42
1:C:19:THR:HA	1:C:24:LYS:HD2	2.01	0.41
1:D:16:THR:HG21	1:D:24:LYS:HD3	2.03	0.41
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.95	0.41
1:C:109:THR:HG21	1:C:203:MET:HG3	2.02	0.41
1:C:175:ALA:HB1	1:C:180:ILE:HD11	2.02	0.41
2:B:1334:6Z7:H29	2:B:1334:6Z7:H11	2.01	0.41
1:A:78:THR:OG1	1:A:81:LYS:HB2	2.20	0.41
1:A:14:HIS:HB2	1:A:27:LEU:HB3	2.02	0.41
1:C:324:LYS:HD3	1:C:324:LYS:HA	1.84	0.40
1:C:137:ASN:HD22	1:C:137:ASN:HA	1.67	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	306/356 (86%)	284 (93%)	19 (6%)	3 (1%)	15 22
1	B	317/356 (89%)	295 (93%)	18 (6%)	4 (1%)	12 16
1	C	308/356 (86%)	283 (92%)	19 (6%)	6 (2%)	8 9
1	D	307/356 (86%)	279 (91%)	21 (7%)	7 (2%)	6 6
All	All	1238/1424 (87%)	1141 (92%)	77 (6%)	20 (2%)	9 12

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	GLY
1	B	102	ASP
1	A	268	ASN
1	C	1	MET
1	D	3	ASP
1	D	184	SER
1	A	150	ASP
1	B	150	ASP
1	C	150	ASP
1	C	298	ARG
1	C	330	VAL
1	D	4	TYR
1	D	150	ASP
1	C	16	THR
1	D	298	ARG
1	C	20	GLY
1	D	288	THR
1	A	51	LEU
1	B	154	CYS
1	D	48	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%)	245 (88%)	32 (12%)	5 5
1	B	285/314 (91%)	258 (90%)	27 (10%)	8 10
1	C	279/314 (89%)	254 (91%)	25 (9%)	9 11
1	D	278/314 (88%)	252 (91%)	26 (9%)	8 10
All	All	1119/1256 (89%)	1009 (90%)	110 (10%)	8 9

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS

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Mol	Chain	Res	Type
1	A	7	LEU
1	A	14	HIS
1	A	42	MET
1	A	50	ASP
1	A	51	LEU
1	A	59	GLU
1	A	65	ARG
1	A	76	LEU
1	A	80	ASN
1	A	104	LEU
1	A	107	GLU
1	A	179	LEU
1	A	181	GLN
1	A	211	ASP
1	A	217	LEU
1	A	227	ASP
1	A	251	ARG
1	A	259	ASN
1	A	265	GLN
1	A	277	ASN
1	A	282	LEU
1	A	284	ASP
1	A	290	LEU
1	A	294	HIS
1	A	295	ARG
1	A	304	LEU
1	A	307	LEU
1	A	321	LEU
1	A	326	ARG
1	A	333	ARG
1	B	2	LYS
1	B	24	LYS
1	B	27	LEU
1	B	59	GLU
1	B	65	ARG
1	B	81	LYS
1	B	103	ARG
1	B	107	GLU
1	B	154	CYS
1	B	169	CYS
1	B	179	LEU
1	B	211	ASP

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Mol	Chain	Res	Type
1	B	212	ASP
1	B	217	LEU
1	B	227	ASP
1	B	230	LYS
1	B	251	ARG
1	B	259	ASN
1	B	274	GLN
1	B	277	ASN
1	B	284	ASP
1	B	298	ARG
1	B	299	GLN
1	B	304	LEU
1	B	313	LEU
1	B	321	LEU
1	B	332	LEU
1	C	14	HIS
1	C	19	THR
1	C	24	LYS
1	C	27	LEU
1	C	43	ASP
1	C	44	LYS
1	C	49	SER
1	C	50	ASP
1	C	53	ARG
1	C	70	CYS
1	C	76	LEU
1	C	101	GLN
1	C	107	GLU
1	C	179	LEU
1	C	211	ASP
1	C	217	LEU
1	C	227	ASP
1	C	259	ASN
1	C	274	GLN
1	C	277	ASN
1	C	299	GLN
1	C	304	LEU
1	C	321	LEU
1	C	324	LYS
1	C	330	VAL
1	D	1	MET
1	D	14	HIS

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Mol	Chain	Res	Type
1	D	27	LEU
1	D	42	MET
1	D	43	ASP
1	D	44	LYS
1	D	51	LEU
1	D	53	ARG
1	D	76	LEU
1	D	80	ASN
1	D	107	GLU
1	D	145	LYS
1	D	154	CYS
1	D	179	LEU
1	D	185	TYR
1	D	211	ASP
1	D	217	LEU
1	D	227	ASP
1	D	259	ASN
1	D	274	GLN
1	D	283	ASP
1	D	284	ASP
1	D	289	GLU
1	D	321	LEU
1	D	328	LYS
1	D	333	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	181	GLN
1	A	256	ASN
1	A	259	ASN
1	A	277	ASN
1	B	45	ASN
1	B	137	ASN
1	B	181	GLN
1	B	256	ASN
1	B	259	ASN
1	B	277	ASN
1	B	312	HIS
1	C	71	GLN
1	C	137	ASN

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Mol	Chain	Res	Type
1	C	256	ASN
1	C	259	ASN
1	C	277	ASN
1	C	281	HIS
1	C	312	HIS
1	D	71	GLN
1	D	137	ASN
1	D	245	GLN
1	D	259	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	6Z7	C	1334	-	32,32,32	0.47	1 (3%)	41,44,44	0.85	1 (2%)
2	6Z7	A	1334	-	32,32,32	0.46	1 (3%)	41,44,44	0.76	0
2	6Z7	D	1334	-	32,32,32	0.50	1 (3%)	41,44,44	0.80	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	6Z7	B	1334	-	32,32,32	0.48	1 (3%)	41,44,44	0.89	1 (2%)

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	6Z7	C	1334	-	-	0/14/21/21	0/4/4/4
2	6Z7	A	1334	-	-	0/14/21/21	0/4/4/4
2	6Z7	D	1334	-	-	0/14/21/21	0/4/4/4
2	6Z7	B	1334	-	-	0/14/21/21	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1334	6Z7	C26-N25	2.37	1.49	1.46
2	C	1334	6Z7	C26-N25	2.31	1.49	1.46
2	B	1334	6Z7	C26-N25	2.10	1.49	1.46
2	A	1334	6Z7	C26-N25	2.09	1.49	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1334	6Z7	C10-N9-C8	2.68	135.90	128.30
2	D	1334	6Z7	C10-N9-C8	2.50	135.38	128.30
2	B	1334	6Z7	C27-C26-N25	-2.22	108.24	113.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

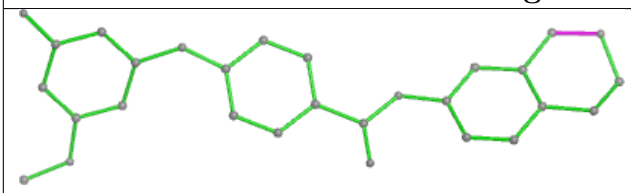
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1334	6Z7	2	0

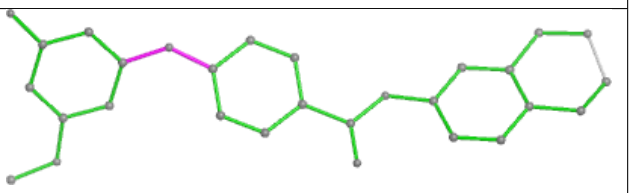
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

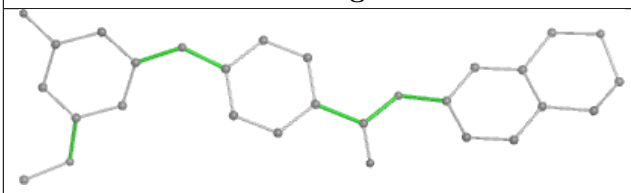
Ligand 6Z7 C 1334



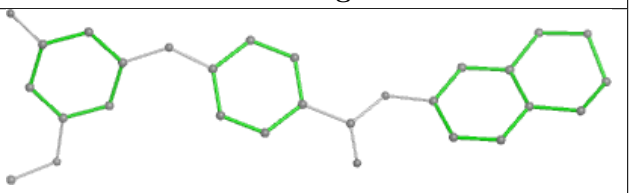
Bond lengths



Bond angles

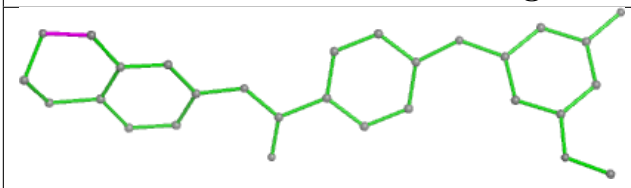


Torsions

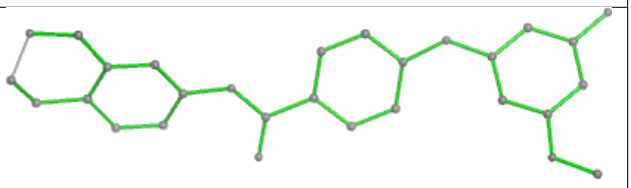


Rings

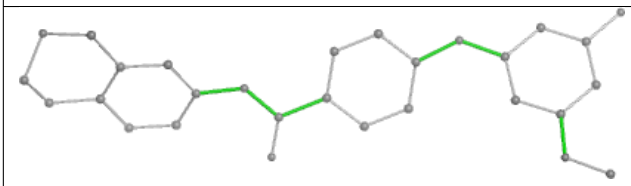
Ligand 6Z7 A 1334



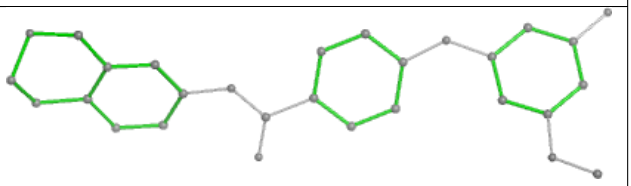
Bond lengths



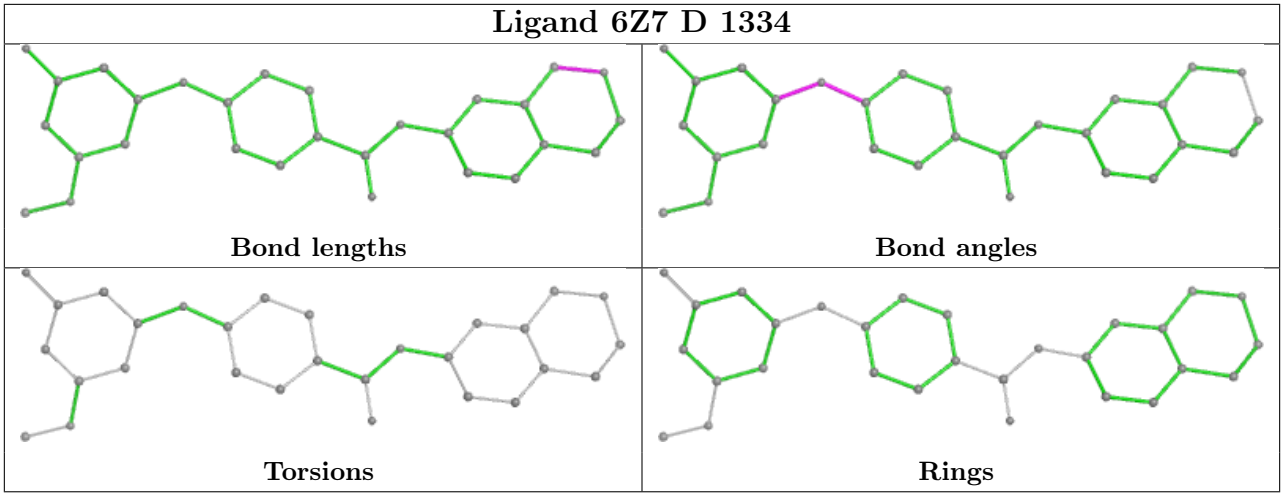
Bond angles

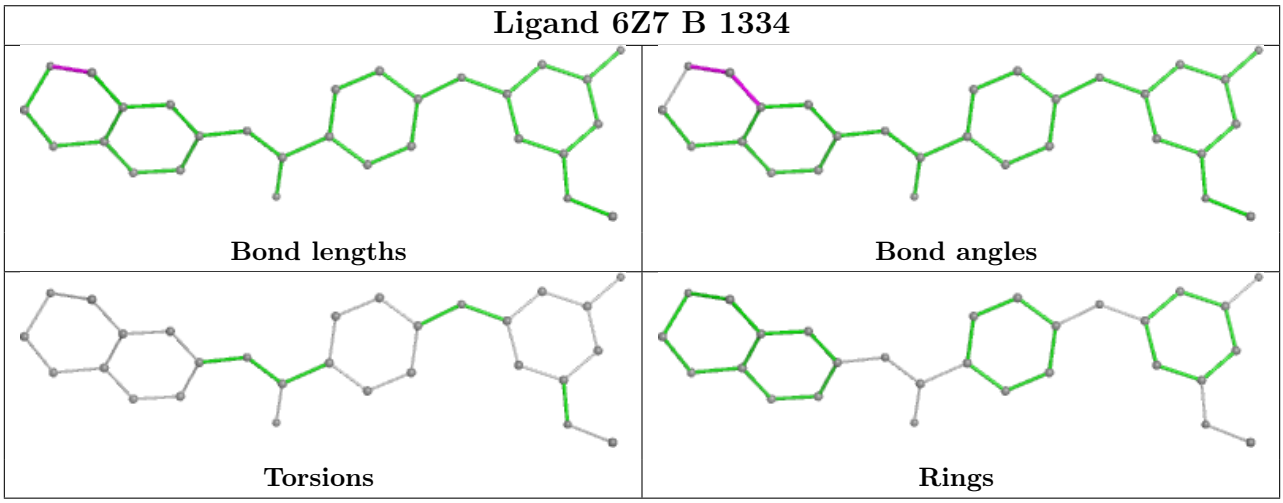


Torsions



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	313/356 (87%)	0.44	13 (4%)	36	42	44, 71, 104, 130	0
1	B	323/356 (90%)	0.56	33 (10%)	6	8	44, 72, 113, 134	0
1	C	316/356 (88%)	0.61	29 (9%)	9	10	49, 81, 119, 170	0
1	D	317/356 (89%)	0.70	29 (9%)	9	11	41, 75, 123, 161	0
All	All	1269/1424 (89%)	0.58	104 (8%)	11	14	41, 75, 117, 170	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	186	LEU	11.2
1	D	290	LEU	6.9
1	B	169	CYS	6.2
1	D	183	LYS	5.9
1	D	320	LEU	5.9
1	D	332	LEU	5.5
1	D	292	VAL	5.5
1	A	292	VAL	5.4
1	D	32	LEU	5.2
1	B	290	LEU	5.1
1	B	321	LEU	5.1
1	A	52	PRO	4.8
1	B	286	CYS	4.7
1	B	331	ARG	4.4
1	A	56	THR	4.3
1	D	317	TYR	4.3
1	B	296	ASN	4.0
1	D	313	LEU	3.9
1	D	329	PRO	3.9
1	D	31	ILE	3.9
1	B	330	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	33	THR	3.7
1	B	320	LEU	3.5
1	C	21	GLY	3.5
1	C	267	TYR	3.5
1	C	304	LEU	3.5
1	C	17	ILE	3.3
1	D	184	SER	3.3
1	C	280	ILE	3.1
1	C	184	SER	3.1
1	B	304	LEU	3.1
1	C	300	THR	3.1
1	D	291	SER	3.1
1	A	296	ASN	3.0
1	C	286	CYS	3.0
1	C	290	LEU	3.0
1	B	301	MET	2.9
1	C	312	HIS	2.9
1	D	324	LYS	2.9
1	D	296	ASN	2.8
1	B	298	ARG	2.8
1	D	162	ASP	2.7
1	D	288	THR	2.7
1	D	331	ARG	2.7
1	A	313	LEU	2.7
1	C	308	TRP	2.7
1	B	287	VAL	2.6
1	B	292	VAL	2.6
1	B	332	LEU	2.6
1	B	277	ASN	2.6
1	A	54	ILE	2.6
1	C	22	PHE	2.6
1	B	282	LEU	2.6
1	C	277	ASN	2.6
1	C	19	THR	2.6
1	D	23	ALA	2.6
1	C	105	SER	2.6
1	B	329	PRO	2.6
1	D	328	LYS	2.5
1	C	307	LEU	2.5
1	C	313	LEU	2.5
1	D	294	HIS	2.5
1	B	322	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.5
1	D	283	ASP	2.5
1	D	321	LEU	2.4
1	B	155	ALA	2.4
1	C	102	ASP	2.4
1	C	306	SER	2.4
1	B	20	GLY	2.4
1	D	280	ILE	2.4
1	C	231	TRP	2.4
1	D	46	THR	2.4
1	B	327	GLY	2.4
1	C	20	GLY	2.4
1	C	294	HIS	2.3
1	A	59	GLU	2.3
1	D	49	SER	2.3
1	B	289	GLU	2.3
1	A	307	LEU	2.3
1	B	281	HIS	2.3
1	B	317	TYR	2.3
1	B	32	LEU	2.3
1	C	1	MET	2.3
1	C	296	ASN	2.3
1	D	21	GLY	2.3
1	C	156	LYS	2.2
1	B	162	ASP	2.2
1	B	294	HIS	2.2
1	C	180	ILE	2.2
1	B	291	SER	2.2
1	A	215	ALA	2.2
1	C	16	THR	2.2
1	B	284	ASP	2.1
1	D	299	GLN	2.1
1	A	53	ARG	2.1
1	C	14	HIS	2.1
1	B	19	THR	2.1
1	A	269	TYR	2.1
1	A	290	LEU	2.1
1	C	12	GLU	2.1
1	B	297	ASN	2.1
1	B	280	ILE	2.0
1	B	23	ALA	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)

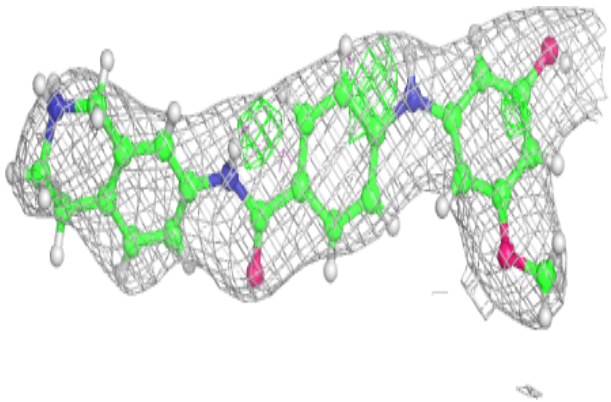
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

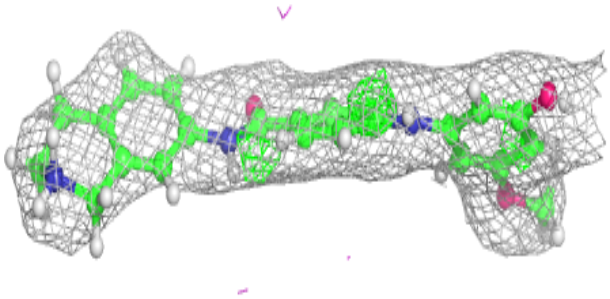
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6Z7	A	1334	29/29	0.92	0.36	25,36,58,59	53
2	6Z7	C	1334	29/29	0.92	0.32	42,52,61,61	53
2	6Z7	B	1334	29/29	0.94	0.21	50,58,85,86	53
2	6Z7	D	1334	29/29	0.94	0.26	26,38,62,63	53

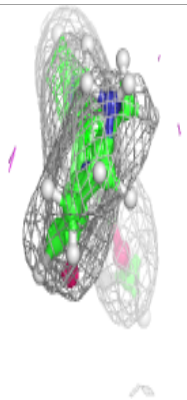
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6Z7 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)

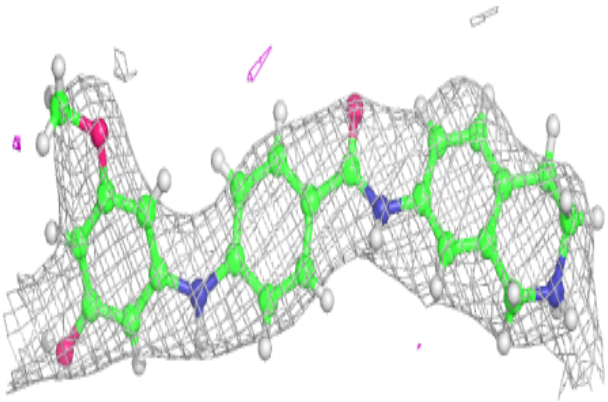


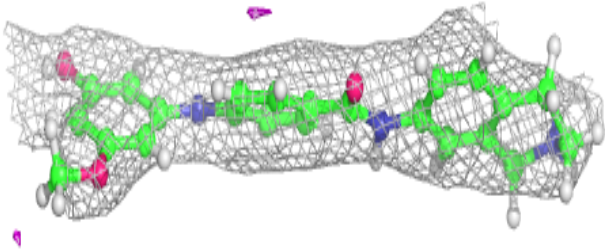


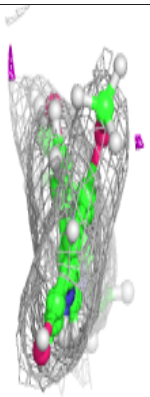


Electron density around 6Z7 C 1334:

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

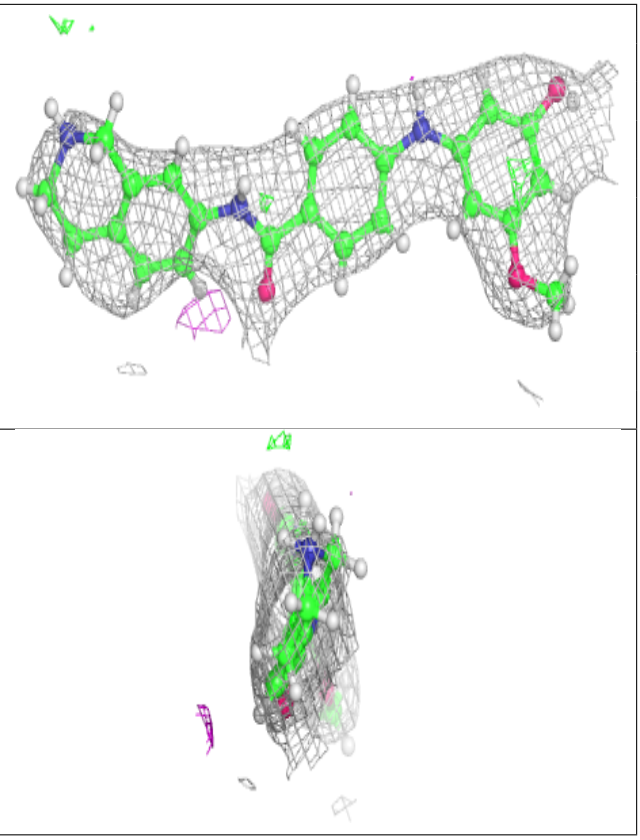






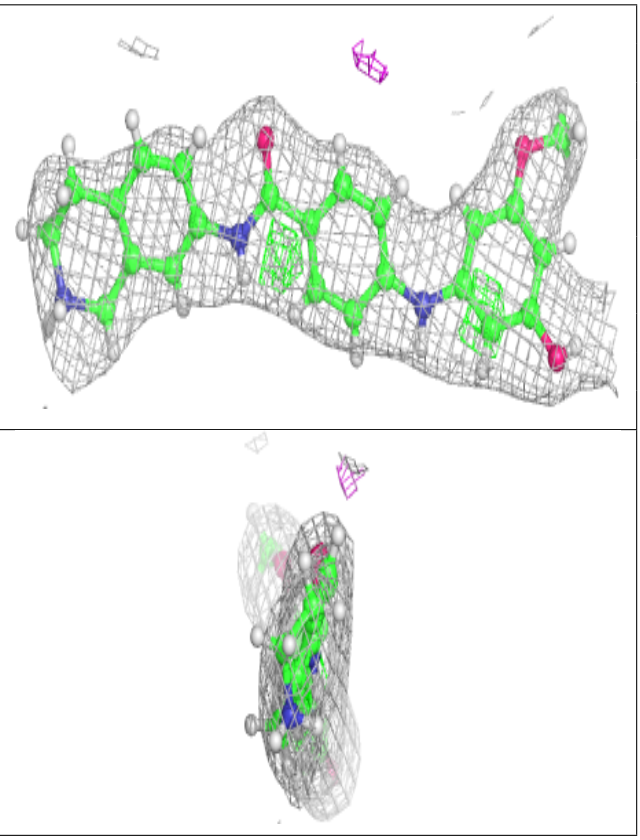
Electron density around 6Z7 B 1334:

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



Electron density around 6Z7 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.