Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:26 am BST

PDB ID	:	4BO2
Title	:	Crystal structure of 3-oxoacyl-(acyl-carrier-protein) reductase (FabG) from Pseudomonas aeruginosa in complex with 1-(1-ethylbenzimidazol-2- yl)-3-(2-methoxyphenyl)urea at 1.9A resolution
Authors	:	Cukier, C.D.; Schnell, R.; Lindqvist, Y.; Schneider, G.
Deposited on	:	2013-05-18
Resolution	:	1.90 Å(reported)

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

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

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

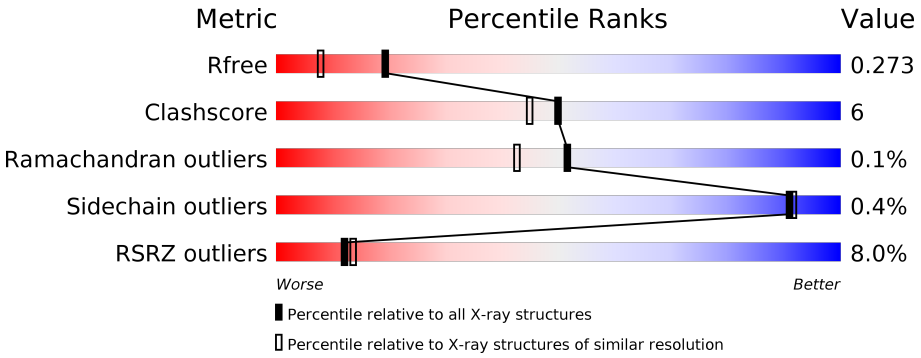
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	269	8% 78% 10% 12%
1	B	269	7% 78% 9% 13%
1	C	269	8% 83% 6% 11%
1	D	269	5% 86% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	36K	A	1248[A]	-	-	X	-
2	36K	A	1248[B]	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7250 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	3	0
			1740	1089	308	337	6			
1	B	235	Total	C	N	O	S	0	2	0
			1704	1066	304	329	5			
1	C	240	Total	C	N	O	S	0	1	0
			1745	1092	310	337	6			
1	D	245	Total	C	N	O	S	0	1	0
			1789	1117	319	346	7			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP O54438
A	-20	HIS	-	expression tag	UNP O54438
A	-19	HIS	-	expression tag	UNP O54438
A	-18	HIS	-	expression tag	UNP O54438
A	-17	HIS	-	expression tag	UNP O54438
A	-16	HIS	-	expression tag	UNP O54438
A	-15	HIS	-	expression tag	UNP O54438
A	-14	SER	-	expression tag	UNP O54438
A	-13	SER	-	expression tag	UNP O54438
A	-12	GLY	-	expression tag	UNP O54438
A	-11	VAL	-	expression tag	UNP O54438
A	-10	ASP	-	expression tag	UNP O54438
A	-9	LEU	-	expression tag	UNP O54438
A	-8	GLY	-	expression tag	UNP O54438
A	-7	THR	-	expression tag	UNP O54438
A	-6	GLU	-	expression tag	UNP O54438
A	-5	ASN	-	expression tag	UNP O54438
A	-4	LEU	-	expression tag	UNP O54438
A	-3	TYR	-	expression tag	UNP O54438
A	-2	PHE	-	expression tag	UNP O54438

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP O54438
A	0	SER	-	expression tag	UNP O54438
B	-21	MET	-	expression tag	UNP O54438
B	-20	HIS	-	expression tag	UNP O54438
B	-19	HIS	-	expression tag	UNP O54438
B	-18	HIS	-	expression tag	UNP O54438
B	-17	HIS	-	expression tag	UNP O54438
B	-16	HIS	-	expression tag	UNP O54438
B	-15	HIS	-	expression tag	UNP O54438
B	-14	SER	-	expression tag	UNP O54438
B	-13	SER	-	expression tag	UNP O54438
B	-12	GLY	-	expression tag	UNP O54438
B	-11	VAL	-	expression tag	UNP O54438
B	-10	ASP	-	expression tag	UNP O54438
B	-9	LEU	-	expression tag	UNP O54438
B	-8	GLY	-	expression tag	UNP O54438
B	-7	THR	-	expression tag	UNP O54438
B	-6	GLU	-	expression tag	UNP O54438
B	-5	ASN	-	expression tag	UNP O54438
B	-4	LEU	-	expression tag	UNP O54438
B	-3	TYR	-	expression tag	UNP O54438
B	-2	PHE	-	expression tag	UNP O54438
B	-1	GLN	-	expression tag	UNP O54438
B	0	SER	-	expression tag	UNP O54438
C	-21	MET	-	expression tag	UNP O54438
C	-20	HIS	-	expression tag	UNP O54438
C	-19	HIS	-	expression tag	UNP O54438
C	-18	HIS	-	expression tag	UNP O54438
C	-17	HIS	-	expression tag	UNP O54438
C	-16	HIS	-	expression tag	UNP O54438
C	-15	HIS	-	expression tag	UNP O54438
C	-14	SER	-	expression tag	UNP O54438
C	-13	SER	-	expression tag	UNP O54438
C	-12	GLY	-	expression tag	UNP O54438
C	-11	VAL	-	expression tag	UNP O54438
C	-10	ASP	-	expression tag	UNP O54438
C	-9	LEU	-	expression tag	UNP O54438
C	-8	GLY	-	expression tag	UNP O54438
C	-7	THR	-	expression tag	UNP O54438
C	-6	GLU	-	expression tag	UNP O54438
C	-5	ASN	-	expression tag	UNP O54438
C	-4	LEU	-	expression tag	UNP O54438

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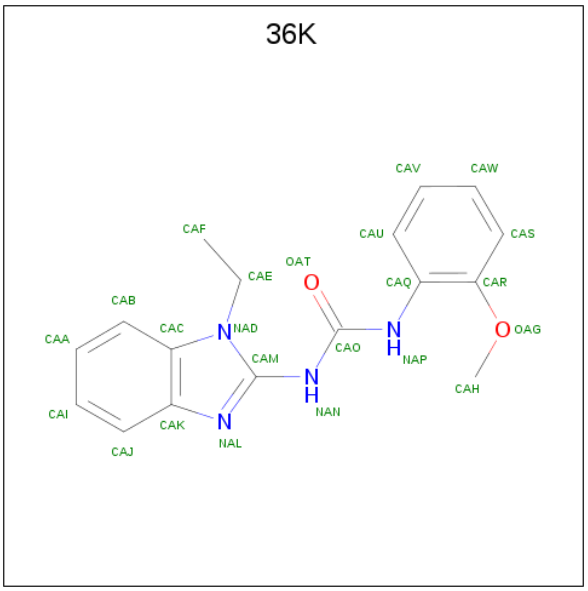
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP O54438
C	-2	PHE	-	expression tag	UNP O54438
C	-1	GLN	-	expression tag	UNP O54438
C	0	SER	-	expression tag	UNP O54438
D	-21	MET	-	expression tag	UNP O54438
D	-20	HIS	-	expression tag	UNP O54438
D	-19	HIS	-	expression tag	UNP O54438
D	-18	HIS	-	expression tag	UNP O54438
D	-17	HIS	-	expression tag	UNP O54438
D	-16	HIS	-	expression tag	UNP O54438
D	-15	HIS	-	expression tag	UNP O54438
D	-14	SER	-	expression tag	UNP O54438
D	-13	SER	-	expression tag	UNP O54438
D	-12	GLY	-	expression tag	UNP O54438
D	-11	VAL	-	expression tag	UNP O54438
D	-10	ASP	-	expression tag	UNP O54438
D	-9	LEU	-	expression tag	UNP O54438
D	-8	GLY	-	expression tag	UNP O54438
D	-7	THR	-	expression tag	UNP O54438
D	-6	GLU	-	expression tag	UNP O54438
D	-5	ASN	-	expression tag	UNP O54438
D	-4	LEU	-	expression tag	UNP O54438
D	-3	TYR	-	expression tag	UNP O54438
D	-2	PHE	-	expression tag	UNP O54438
D	-1	GLN	-	expression tag	UNP O54438
D	0	SER	-	expression tag	UNP O54438

- Molecule 2 is 1-(1-ethylbenzimidazol-2-yl)-3-(2-methoxyphenyl)urea (three-letter code: 36K) (formula: $C_{17}H_{18}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 46 34 8 4	0	1
2	C	1	Total C N O 23 17 4 2	0	0

- Molecule 3 is water.

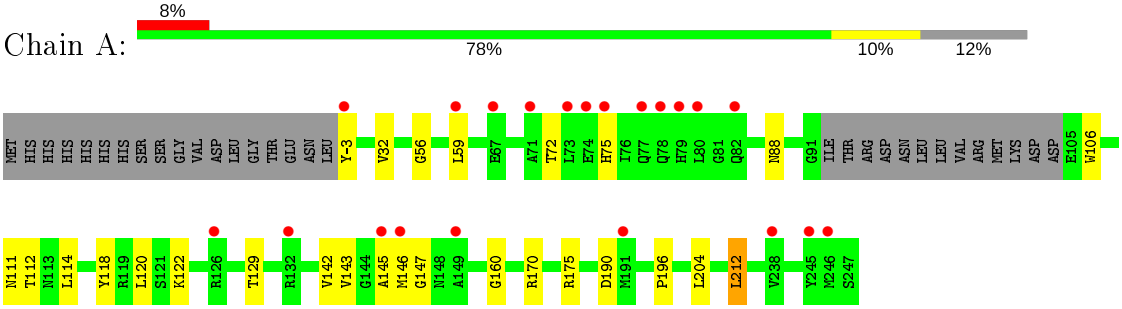
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	B	48	Total O 48 48	0	0
3	C	43	Total O 43 43	0	0
3	D	57	Total O 57 57	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

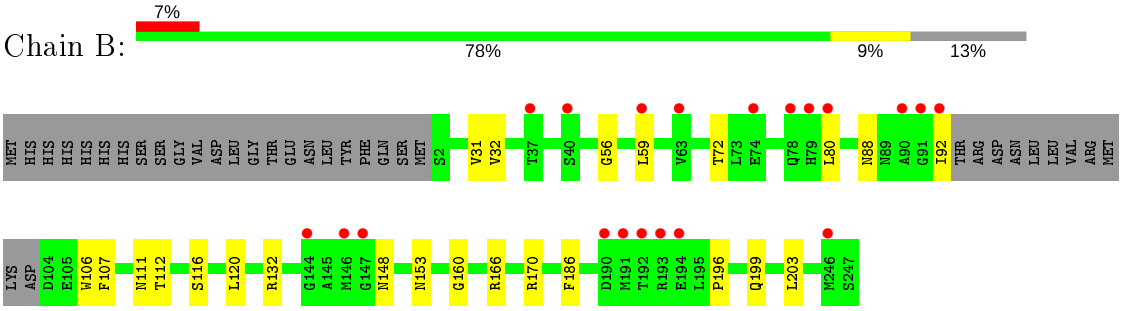
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG

Chain A:



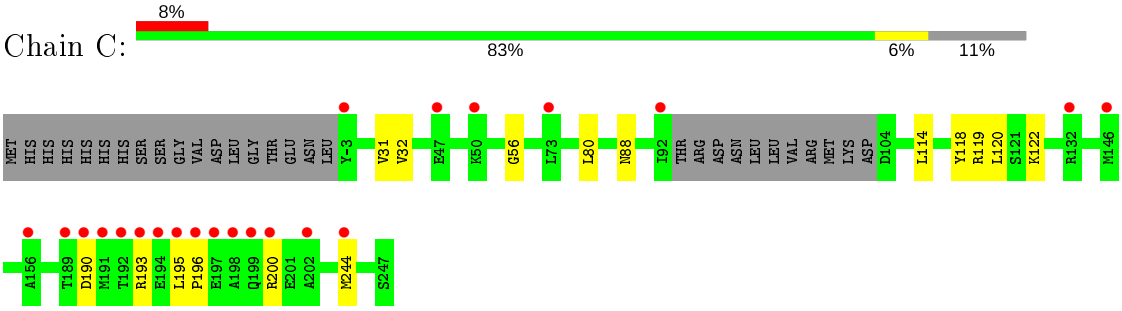
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG

Chain B:



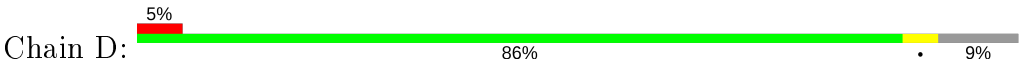
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG

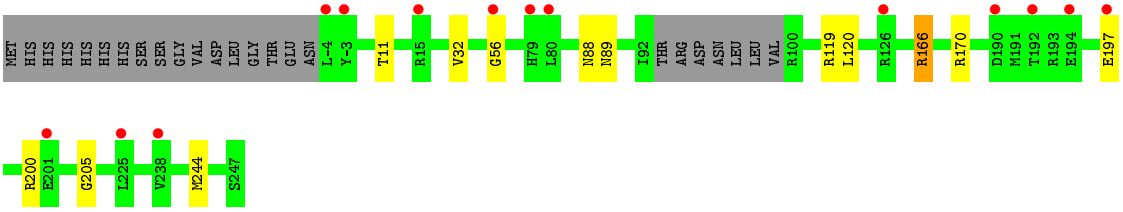
Chain C:



• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG

Chain D:




MET
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
VAL
ASP
LEU
GLY
THR
GLU
ASN
L-4
Y-3
T11
R15
V32
G56
H79
L80
N88
N89
I92
THR
ARG
ASP
ASN
LEU
LEU
VAL
R100
R119
L120
R126
R166
R170
D190
M191
T192
R193
E194
E197
R200
E201
G205
L225
V238
M244
S247

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.55Å 108.92Å 149.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.56 – 1.90 38.53 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.3 (38.56-1.90) 87.3 (38.53-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.235 , 0.269 0.240 , 0.273	Depositor DCC
R_{free} test set	3363 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7250	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 36K

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	0.80	0/1768	0.84	2/2392 (0.1%)
1	B	0.85	0/1727	0.87	2/2338 (0.1%)
1	C	0.82	0/1767	0.82	2/2391 (0.1%)
1	D	0.82	0/1811	0.87	4/2448 (0.2%)
All	All	0.82	0/7073	0.85	10/9569 (0.1%)

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	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	119	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	244	MET	CG-SD-CE	5.88	109.61	100.20
1	A	170	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	D	244	MET	CG-SD-CE	5.60	109.16	100.20
1	D	170	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	212	LEU	CB-CG-CD2	5.44	120.25	111.00
1	C	119	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	132	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	170	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	170	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1740	0	1775	22	0
1	B	1704	0	1748	19	0
1	C	1745	0	1780	11	0
1	D	1789	0	1823	6	0
2	A	46	0	36	31	0
2	C	23	0	18	5	0
3	A	55	0	0	3	0
3	B	48	0	0	1	0
3	C	43	0	0	0	0
3	D	57	0	0	0	0
All	All	7250	0	7180	82	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 (82) 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)
2:A:1248[B]:36K:HAP	2:A:1248[B]:36K:CAH	1.29	1.43
2:A:1248[B]:36K:HAB	2:A:1248[B]:36K:CAF	1.64	1.27
2:A:1248[B]:36K:CAU	2:A:1248[B]:36K:HAN	1.34	1.21
2:A:1248[A]:36K:HAN	2:A:1248[A]:36K:CAU	1.43	1.14
1:A:59[B]:LEU:HD21	1:A:72:THR:HG23	1.24	1.10
2:A:1248[B]:36K:HAU	2:A:1248[B]:36K:NAN	1.37	1.08
1:B:59[B]:LEU:HD21	1:B:72:THR:CG2	1.83	1.06
2:A:1248[B]:36K:HAF3	2:A:1248[B]:36K:HAB	1.36	1.06
2:A:1248[B]:36K:HAB	2:A:1248[B]:36K:HAF2	1.35	1.06
2:A:1248[B]:36K:HAH2	2:A:1248[B]:36K:HAP	0.92	1.04
2:A:1248[B]:36K:HAH2	2:A:1248[B]:36K:NAP	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59[B]:LEU:CD2	1:B:72:THR:HG23	1.88	1.02
2:A:1248[A]:36K:NAN	2:A:1248[A]:36K:HAU	1.51	1.02
2:A:1248[B]:36K:HAP	2:A:1248[B]:36K:HAH3	1.25	1.00
2:A:1248[A]:36K:HAF2	2:A:1248[A]:36K:OAT	1.62	1.00
2:A:1248[B]:36K:NAP	2:A:1248[B]:36K:CAH	2.00	0.99
1:A:59[B]:LEU:CD2	1:A:72:THR:HG23	1.92	0.99
2:A:1248[B]:36K:CAB	2:A:1248[B]:36K:CAF	2.35	0.90
1:B:59[B]:LEU:HD21	1:B:72:THR:HG23	0.93	0.88
2:A:1248[A]:36K:HAU	2:A:1248[A]:36K:HAN	0.66	0.83
2:A:1248[B]:36K:HAF2	2:A:1248[B]:36K:CAB	2.05	0.81
2:A:1248[A]:36K:CAF	2:A:1248[A]:36K:OAT	2.30	0.80
2:A:1248[B]:36K:NAP	2:A:1248[B]:36K:HAH3	1.87	0.78
2:A:1248[B]:36K:HAF3	2:A:1248[B]:36K:CAB	2.06	0.77
1:D:197:GLU:OE2	1:D:200:ARG:NH1	2.19	0.76
2:A:1248[B]:36K:HAN	2:A:1248[B]:36K:HAU	0.59	0.75
2:A:1248[A]:36K:CAE	2:A:1248[A]:36K:OAT	2.43	0.67
2:A:1248[A]:36K:HAH1	1:B:107:PHE:CE1	2.34	0.63
2:A:1248[B]:36K:CAU	2:A:1248[B]:36K:NAN	2.08	0.62
1:A:160:GLY:HA2	2:A:1248[B]:36K:HAE2	1.82	0.62
1:C:193:ARG:O	1:C:200:ARG:NH2	2.33	0.61
1:A:-3:TYR:CD2	3:A:2001:HOH:O	2.52	0.60
1:A:204:LEU:HD21	1:A:212:LEU:HD12	1.84	0.59
1:B:92:ILE:HG13	1:B:112:THR:HG22	1.82	0.59
2:A:1248[B]:36K:NAL	2:A:1248[B]:36K:OAT	2.26	0.58
1:A:118:TYR:OH	1:A:122:LYS:HE3	2.05	0.57
1:C:195:LEU:HG	1:C:196:PRO:HD2	1.85	0.57
1:B:148:ASN:ND2	1:D:205:GLY:O	2.26	0.55
2:A:1248[B]:36K:HAE1	1:B:160:GLY:HA2	1.90	0.54
1:A:114:LEU:HD13	2:A:1248[A]:36K:HAH2	1.90	0.52
1:A:112:THR:HG23	3:A:2018:HOH:O	2.09	0.52
1:A:190:ASP:OD1	1:A:190:ASP:N	2.43	0.52
1:A:112:THR:HA	3:A:2018:HOH:O	2.10	0.52
1:A:204:LEU:HD21	1:A:212:LEU:CD1	2.40	0.52
1:B:106:TRP:HB3	1:B:153:ASN:HD22	1.74	0.51
1:C:118:TYR:OH	1:C:122:LYS:HE2	2.10	0.51
1:C:190:ASP:OD1	1:C:190:ASP:N	2.44	0.50
1:C:114:LEU:HD12	2:C:1248:36K:NAN	2.27	0.49
1:A:32:VAL:O	1:A:56:GLY:HA3	2.13	0.49
1:D:32:VAL:O	1:D:56:GLY:HA3	2.11	0.49
2:A:1248[B]:36K:HAH1	1:B:111:ASN:HB2	1.96	0.48
1:B:196:PRO:HD2	1:B:199:GLN:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG11	1:B:80:LEU:HD22	1.96	0.48
1:A:106:TRP:CZ3	2:A:1248[B]:36K:HAI	2.50	0.47
1:C:32:VAL:O	1:C:56:GLY:HA3	2.14	0.47
1:A:160:GLY:CA	2:A:1248[B]:36K:HAE2	2.43	0.46
1:A:88:ASN:OD1	1:A:120:LEU:HD23	2.15	0.46
1:B:116:SER:HB2	3:B:2015:HOH:O	2.15	0.46
1:A:111:ASN:OD1	1:B:111:ASN:ND2	2.48	0.46
1:B:59[B]:LEU:CD2	1:B:72:THR:CG2	2.69	0.46
1:C:88:ASN:OD1	1:C:120:LEU:HD23	2.16	0.45
1:B:92:ILE:HG13	1:B:112:THR:CG2	2.47	0.45
2:C:1248:36K:NAL	2:C:1248:36K:NAP	2.61	0.45
1:B:88:ASN:OD1	1:B:120:LEU:HD23	2.17	0.44
1:D:88:ASN:OD1	1:D:120:LEU:HD23	2.18	0.43
1:B:186:PHE:CD2	1:B:203:LEU:HD11	2.53	0.43
1:B:32:VAL:O	1:B:56:GLY:HA3	2.19	0.43
1:D:11:THR:O	1:D:89:ASN:HB3	2.19	0.43
1:A:142:VAL:HG12	1:A:143:VAL:O	2.19	0.43
2:C:1248:36K:OAT	2:C:1248:36K:HAU	2.18	0.42
1:A:118:TYR:CZ	1:A:122:LYS:HE3	2.54	0.42
1:A:59[B]:LEU:HD23	1:A:72:THR:HG23	1.92	0.42
1:C:31:VAL:HG11	1:C:80:LEU:HD22	2.01	0.42
1:B:106:TRP:HB3	1:B:153:ASN:ND2	2.34	0.42
1:C:114:LEU:HD12	2:C:1248:36K:CAO	2.50	0.41
2:A:1248[A]:36K:HAE1	2:A:1248[A]:36K:OAT	2.19	0.41
1:C:114:LEU:CD1	2:C:1248:36K:CAM	2.99	0.41
1:A:129:THR:HG23	1:A:175:ARG:HD3	2.02	0.41
1:A:122:LYS:HA	1:A:122:LYS:HD3	1.76	0.41
1:A:146:MET:HE1	1:A:196:PRO:HD2	2.02	0.41
1:D:166:ARG:HD2	1:D:166:ARG:HH11	1.73	0.40
1:C:118:TYR:CZ	1:C:122:LYS:HE2	2.56	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	237/269 (88%)	232 (98%)	4 (2%)	1 (0%)	34 24
1	B	233/269 (87%)	230 (99%)	3 (1%)	0	100 100
1	C	237/269 (88%)	235 (99%)	2 (1%)	0	100 100
1	D	242/269 (90%)	239 (99%)	3 (1%)	0	100 100
All	All	949/1076 (88%)	936 (99%)	12 (1%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ALA

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	175/201 (87%)	174 (99%)	1 (1%)	86 87
1	B	171/201 (85%)	170 (99%)	1 (1%)	86 87
1	C	175/201 (87%)	175 (100%)	0	100 100
1	D	180/201 (90%)	179 (99%)	1 (1%)	86 87
All	All	701/804 (87%)	698 (100%)	3 (0%)	91 91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	B	166	ARG
1	D	166	ARG

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

Mol	Chain	Res	Type
1	A	151	GLN
1	A	214	GLN
1	B	153	ASN
1	B	214	GLN
1	C	19	GLN
1	C	206	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 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	36K	A	1248[A]	-	22,25,25	2.27	5 (22%)	27,34,34	3.02	5 (18%)
2	36K	C	1248	-	22,25,25	1.98	6 (27%)	27,34,34	2.78	8 (29%)
2	36K	A	1248[B]	-	22,25,25	2.15	6 (27%)	27,34,34	3.25	4 (14%)

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	36K	A	1248[A]	-	-	5/10/12/12	0/3/3/3
2	36K	C	1248	-	-	0/10/12/12	0/3/3/3
2	36K	A	1248[B]	-	-	7/10/12/12	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1248[B]	36K	CAJ-CAK	-6.46	1.30	1.41
2	A	1248[A]	36K	CAJ-CAK	-6.27	1.31	1.41
2	C	1248	36K	CAJ-CAK	-5.90	1.31	1.41
2	A	1248[A]	36K	CAB-CAC	-5.27	1.30	1.41
2	A	1248[B]	36K	CAB-CAC	-4.44	1.32	1.41
2	A	1248[A]	36K	CAQ-NAP	-4.14	1.33	1.41
2	A	1248[B]	36K	CAQ-NAP	-3.77	1.34	1.41
2	C	1248	36K	CAQ-NAP	-3.73	1.34	1.41
2	A	1248[B]	36K	CAC-CAK	-3.00	1.34	1.40
2	A	1248[A]	36K	CAC-CAK	-2.97	1.34	1.40
2	C	1248	36K	CAI-CAJ	2.88	1.43	1.36
2	A	1248[A]	36K	CAK-NAL	-2.85	1.29	1.38
2	C	1248	36K	CAO-NAP	2.62	1.42	1.37
2	C	1248	36K	CAC-CAK	-2.39	1.35	1.40
2	A	1248[B]	36K	CAO-NAP	-2.18	1.32	1.37
2	C	1248	36K	CAB-CAC	-2.16	1.36	1.41
2	A	1248[B]	36K	CAK-NAL	-2.07	1.32	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1248[B]	36K	CAM-NAN-CAO	-13.56	115.94	130.40
2	A	1248[A]	36K	CAE-NAD-CAM	10.06	136.52	127.06
2	A	1248[A]	36K	CAM-NAN-CAO	-8.12	121.74	130.40
2	C	1248	36K	CAM-NAN-CAO	-7.89	121.99	130.40
2	C	1248	36K	CAE-NAD-CAM	7.73	134.33	127.06
2	A	1248[B]	36K	CAE-NAD-CAM	7.06	133.70	127.06
2	A	1248[A]	36K	CAH-OAG-CAR	-6.64	107.51	117.53
2	C	1248	36K	OAT-CAO-NAN	-5.05	115.07	123.62
2	A	1248[B]	36K	CAQ-NAP-CAO	-4.68	115.01	125.39
2	C	1248	36K	NAP-CAO-NAN	4.02	119.51	112.49
2	C	1248	36K	CAH-OAG-CAR	3.51	122.83	117.53
2	A	1248[B]	36K	CAH-OAG-CAR	-3.51	112.24	117.53
2	A	1248[A]	36K	CAQ-NAP-CAO	-3.29	118.09	125.39
2	C	1248	36K	CAF-CAE-NAD	-2.96	106.49	111.49
2	A	1248[A]	36K	CAA-CAI-CAJ	-2.72	116.62	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1248	36K	CAI-CAA-CAB	-2.71	116.64	120.44
2	C	1248	36K	CAB-CAC-CAK	2.39	125.20	121.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1248[A]	36K	CAQ-CAR-OAG-CAH
2	A	1248[B]	36K	CAF-CAE-NAD-CAC
2	A	1248[B]	36K	CAF-CAE-NAD-CAM
2	A	1248[B]	36K	CAQ-CAR-OAG-CAH
2	A	1248[B]	36K	CAS-CAR-OAG-CAH
2	A	1248[A]	36K	CAS-CAR-OAG-CAH
2	A	1248[A]	36K	OAT-CAO-NAP-CAQ
2	A	1248[B]	36K	OAT-CAO-NAP-CAQ
2	A	1248[A]	36K	NAN-CAO-NAP-CAQ
2	A	1248[B]	36K	NAN-CAO-NAP-CAQ
2	A	1248[A]	36K	OAT-CAO-NAN-CAM
2	A	1248[B]	36K	OAT-CAO-NAN-CAM

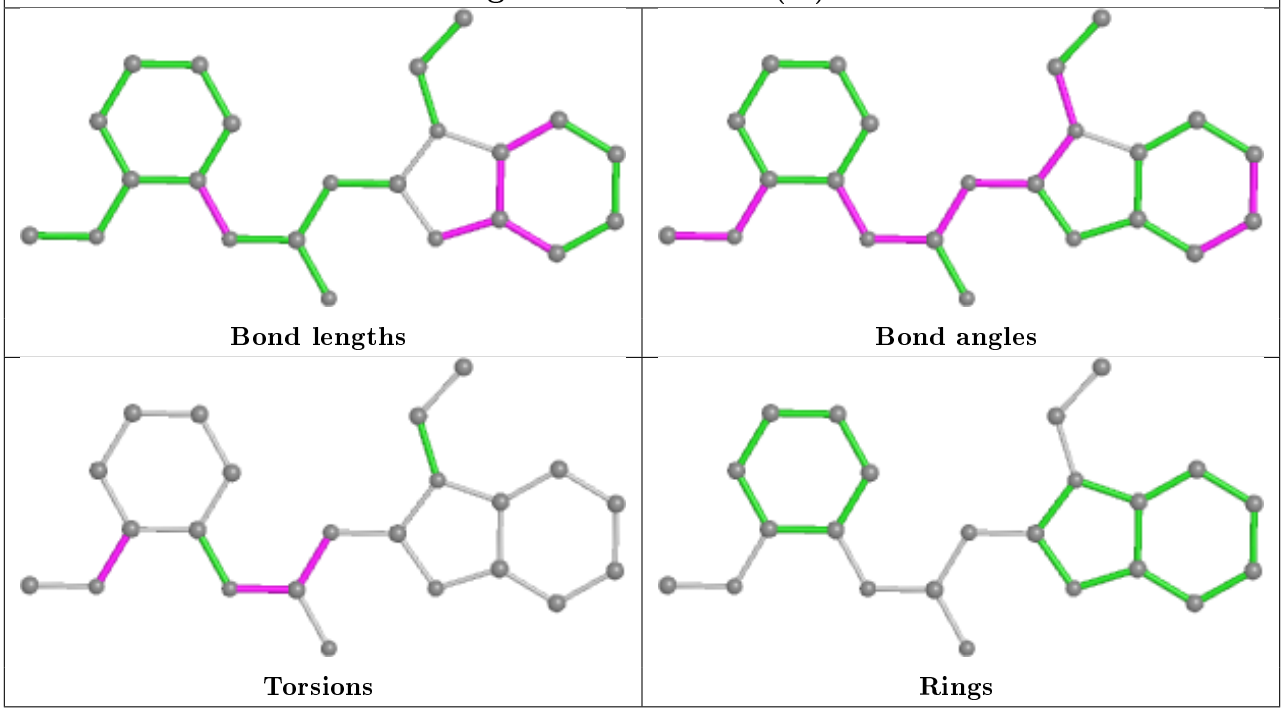
There are no ring outliers.

3 monomers are involved in 36 short contacts:

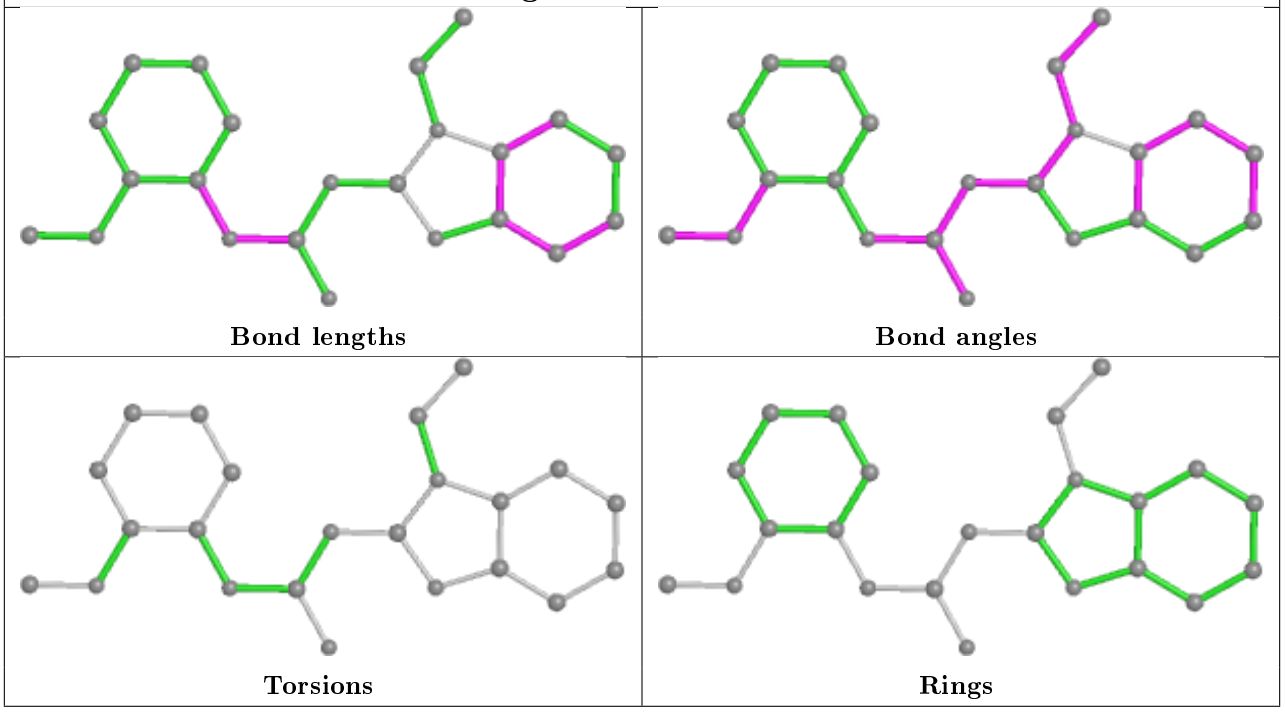
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1248[A]	36K	9	0
2	C	1248	36K	5	0
2	A	1248[B]	36K	22	0

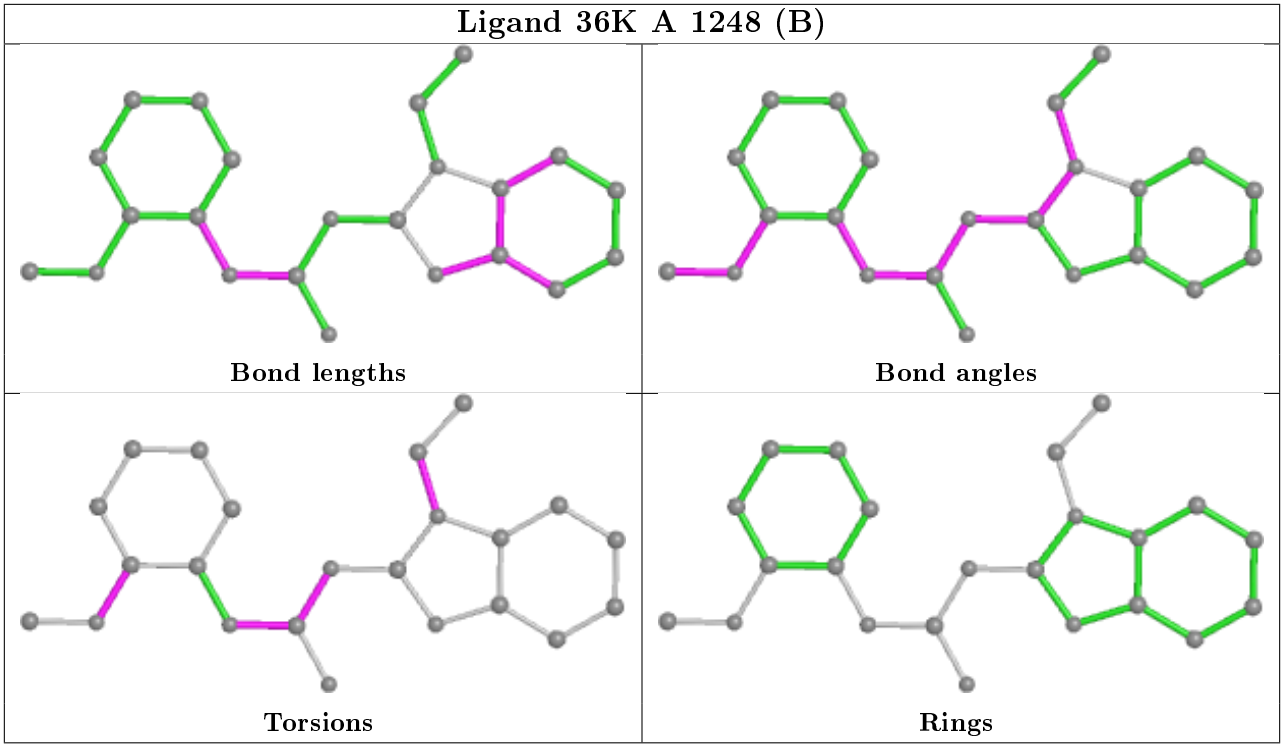
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 36K A 1248 (A)



Ligand 36K C 1248





5.7 Other polymers

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, 95^{th} 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	238/269 (88%)	0.65	21 (8%)	10 11	20, 36, 69, 91	0
1	B	235/269 (87%)	0.66	20 (8%)	10 12	20, 34, 72, 105	0
1	C	240/269 (89%)	0.62	22 (9%)	9 10	18, 33, 78, 114	0
1	D	245/269 (91%)	0.54	14 (5%)	23 26	19, 34, 66, 92	0
All	All	958/1076 (89%)	0.62	77 (8%)	12 13	18, 34, 71, 114	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	ILE	9.4
1	C	191	MET	7.4
1	B	191	MET	7.1
1	C	195	LEU	7.0
1	C	192	THR	5.7
1	A	80	LEU	5.6
1	C	92	ILE	5.5
1	C	193	ARG	5.4
1	A	146	MET	5.4
1	C	-3	TYR	5.2
1	B	144	GLY	4.8
1	C	190	ASP	4.8
1	B	59[A]	LEU	4.5
1	A	149	ALA	4.4
1	A	75	HIS	3.9
1	C	146	MET	3.7
1	B	192	THR	3.7
1	D	192	THR	3.7
1	D	-3	TYR	3.5
1	C	198	ALA	3.5
1	A	67	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	189	THR	3.4
1	A	77	GLN	3.4
1	B	147	GLY	3.4
1	D	56	GLY	3.4
1	D	201	GLU	3.2
1	A	-3	TYR	3.2
1	B	80	LEU	3.2
1	D	190	ASP	3.1
1	D	80	LEU	3.1
1	D	-4	LEU	3.1
1	C	194	GLU	3.0
1	C	199	GLN	3.0
1	B	90	ALA	3.0
1	C	73[A]	LEU	2.9
1	D	197	GLU	2.9
1	B	146	MET	2.9
1	A	78	GLN	2.8
1	A	59[A]	LEU	2.8
1	C	50	LYS	2.8
1	D	126	ARG	2.7
1	A	82	GLN	2.6
1	D	15	ARG	2.6
1	A	73	LEU	2.6
1	C	202	ALA	2.5
1	B	63	VAL	2.5
1	B	79	HIS	2.5
1	A	245	TYR	2.5
1	D	194	GLU	2.4
1	C	196	PRO	2.4
1	A	74	GLU	2.4
1	B	78	GLN	2.4
1	B	246	MET	2.4
1	C	47	GLU	2.3
1	B	194	GLU	2.3
1	A	246	MET	2.3
1	D	79	HIS	2.3
1	C	132	ARG	2.3
1	A	71	ALA	2.3
1	B	193	ARG	2.3
1	D	225	LEU	2.2
1	B	37	THR	2.2
1	B	91	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	40	SER	2.2
1	B	190	ASP	2.2
1	C	200	ARG	2.1
1	A	126	ARG	2.1
1	B	74	GLU	2.1
1	C	197	GLU	2.1
1	D	238	VAL	2.1
1	A	132	ARG	2.1
1	A	238	VAL	2.1
1	A	145	ALA	2.1
1	A	79	HIS	2.1
1	C	156	ALA	2.1
1	C	244	MET	2.0
1	A	191	MET	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 carbohydrates in this entry.

6.4 Ligands (i)

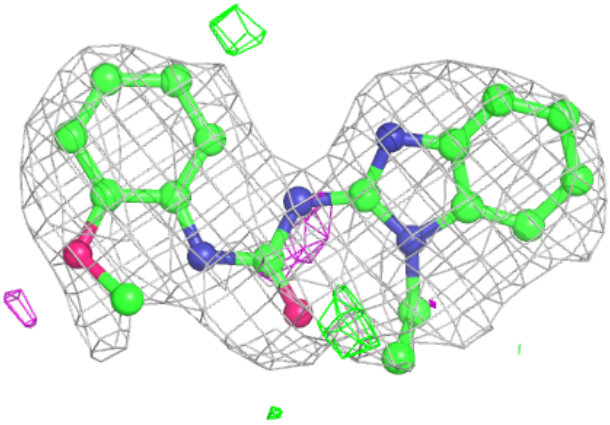
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

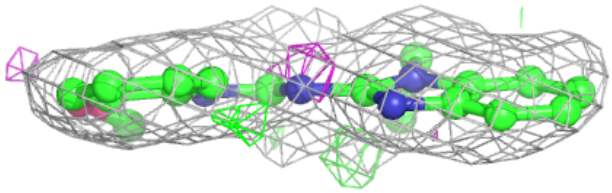
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	36K	A	1248[A]	23/23	0.90	0.18	22,34,44,44	23
2	36K	A	1248[B]	23/23	0.90	0.18	37,42,50,53	23
2	36K	C	1248	23/23	0.93	0.13	19,26,31,36	0

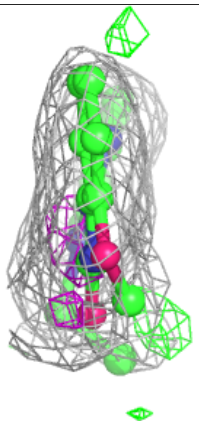
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 36K A 1248 (A):

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

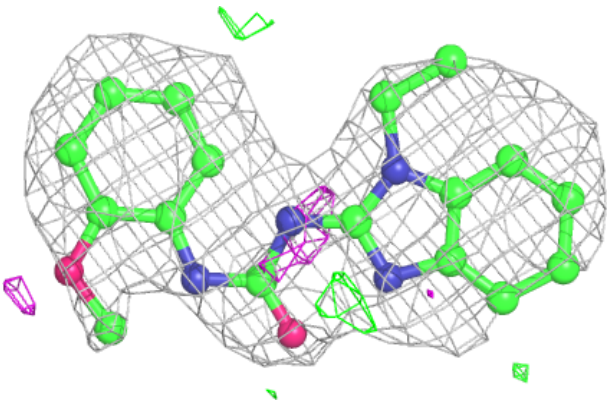


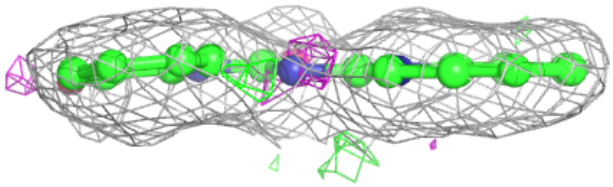


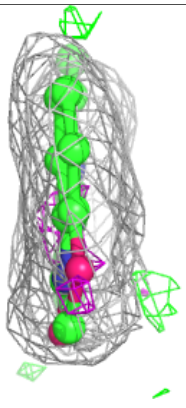


Electron density around 36K A 1248 (B):

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

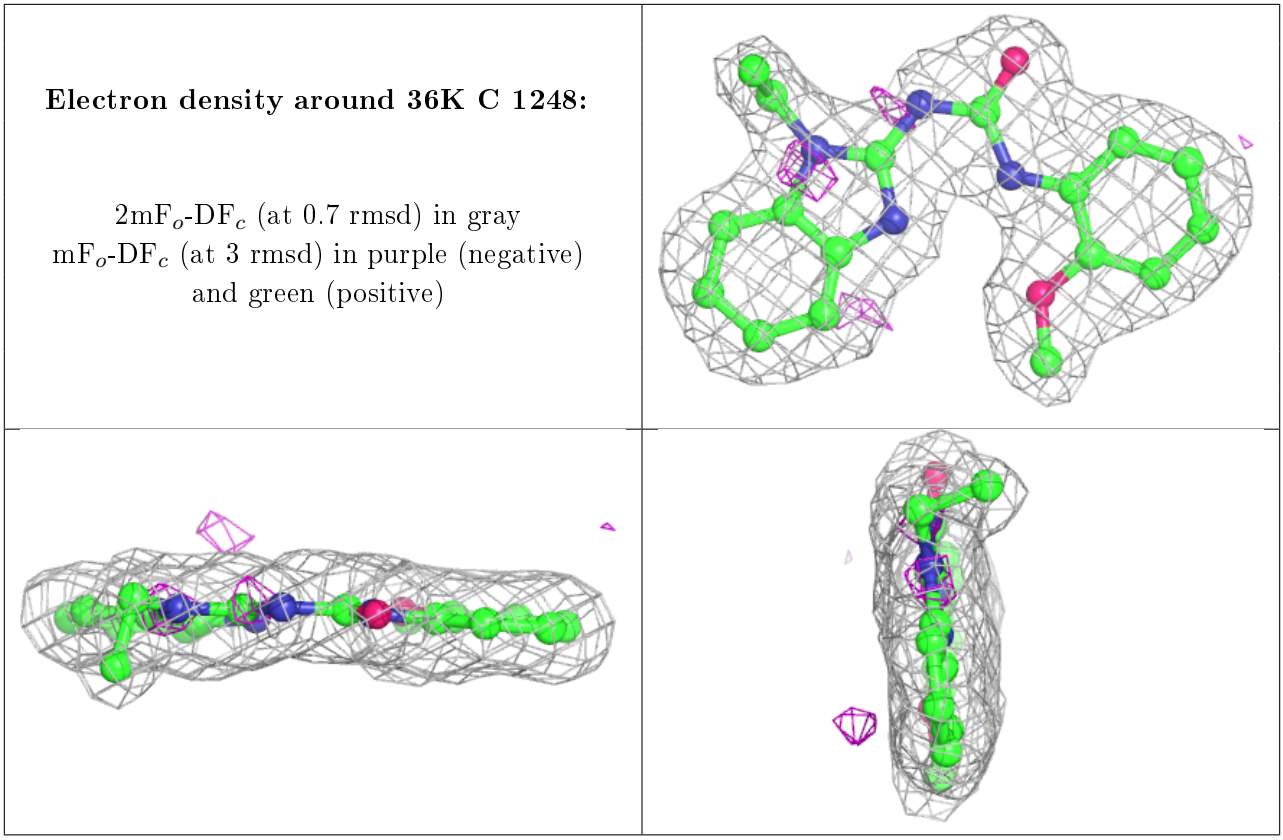






Electron density around 36K C 1248:

$2mF_o$-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

There are no such residues in this entry.