Full wwPDB X-ray Structure Validation Report (i)

Sep 4, 2023 – 07:16 PM EDT

PDB ID	:	3TVU
Title	:	Crystal Structure of the humanized carboxyltransferase domain of yeast Acetyl-coA caroxylase in complex with compound 3
Authors	:	Rajamohan, F.; Marr, E.; Reyes, A.; Landro, J.A.; Anderson, M.D.; Corbett, J.W.; Dirico, K.J.; Harwood, J.H.; Tu, M.; Vajdos, F.F.
Deposited on	:	2011-09-20
Resolution	:	2.40 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:

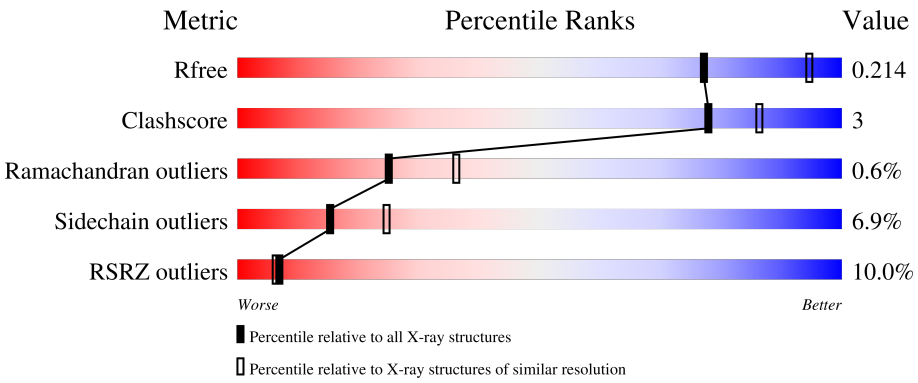
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	769	6% 80% 10% • 9%
1	B	769	11% 77% 11% • 10%
1	C	769	10% 76% 11% • 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17661 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 Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	696	5561	3539	960	1045	17	0	1	0
1	B	690	5513	3510	949	1037	17	0	0	0
1	C	681	5437	3454	939	1027	17	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	expression tag	UNP Q00955
A	1474	ALA	-	expression tag	UNP Q00955
A	1475	SER	-	expression tag	UNP Q00955
A	1760	SER	PRO	engineered mutation	UNP Q00955
A	1762	LEU	ILE	engineered mutation	UNP Q00955
A	1765	VAL	MET	engineered mutation	UNP Q00955
A	1919	GLN	GLU	engineered mutation	UNP Q00955
A	1920	ALA	PRO	engineered mutation	UNP Q00955
A	1925	PHE	HIS	engineered mutation	UNP Q00955
A	2028	GLU	GLN	engineered mutation	UNP Q00955
A	2030	THR	MET	engineered mutation	UNP Q00955
A	2032	GLU	GLY	engineered mutation	UNP Q00955
A	2234	LEU	-	expression tag	UNP Q00955
A	2235	GLU	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
A	2240	HIS	-	expression tag	UNP Q00955
A	2241	HIS	-	expression tag	UNP Q00955
B	1473	MET	-	expression tag	UNP Q00955
B	1474	ALA	-	expression tag	UNP Q00955
B	1475	SER	-	expression tag	UNP Q00955

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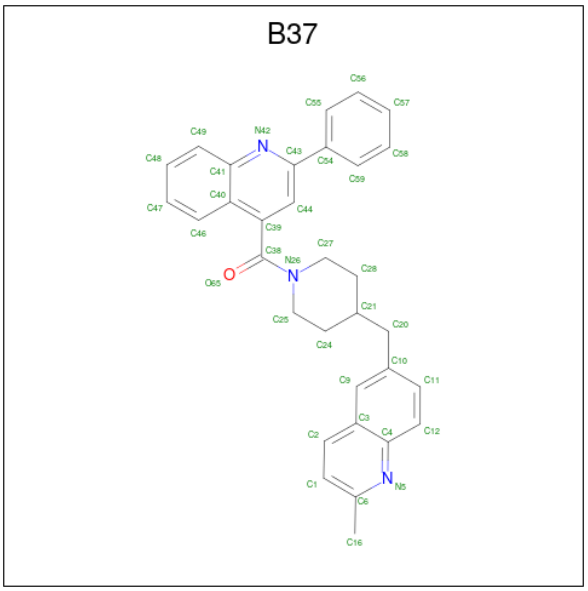
Chain	Residue	Modelled	Actual	Comment	Reference
B	1760	SER	PRO	engineered mutation	UNP Q00955
B	1762	LEU	ILE	engineered mutation	UNP Q00955
B	1765	VAL	MET	engineered mutation	UNP Q00955
B	1919	GLN	GLU	engineered mutation	UNP Q00955
B	1920	ALA	PRO	engineered mutation	UNP Q00955
B	1925	PHE	HIS	engineered mutation	UNP Q00955
B	2028	GLU	GLN	engineered mutation	UNP Q00955
B	2030	THR	MET	engineered mutation	UNP Q00955
B	2032	GLU	GLY	engineered mutation	UNP Q00955
B	2234	LEU	-	expression tag	UNP Q00955
B	2235	GLU	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955
B	2240	HIS	-	expression tag	UNP Q00955
B	2241	HIS	-	expression tag	UNP Q00955
C	1473	MET	-	expression tag	UNP Q00955
C	1474	ALA	-	expression tag	UNP Q00955
C	1475	SER	-	expression tag	UNP Q00955
C	1760	SER	PRO	engineered mutation	UNP Q00955
C	1762	LEU	ILE	engineered mutation	UNP Q00955
C	1765	VAL	MET	engineered mutation	UNP Q00955
C	1919	GLN	GLU	engineered mutation	UNP Q00955
C	1920	ALA	PRO	engineered mutation	UNP Q00955
C	1925	PHE	HIS	engineered mutation	UNP Q00955
C	2028	GLU	GLN	engineered mutation	UNP Q00955
C	2030	THR	MET	engineered mutation	UNP Q00955
C	2032	GLU	GLY	engineered mutation	UNP Q00955
C	2234	LEU	-	expression tag	UNP Q00955
C	2235	GLU	-	expression tag	UNP Q00955
C	2236	HIS	-	expression tag	UNP Q00955
C	2237	HIS	-	expression tag	UNP Q00955
C	2238	HIS	-	expression tag	UNP Q00955
C	2239	HIS	-	expression tag	UNP Q00955
C	2240	HIS	-	expression tag	UNP Q00955
C	2241	HIS	-	expression tag	UNP Q00955

- Molecule 2 is 4-({4-[(2-methylquinolin-6-yl)methyl]piperidin-1-yl}carbonyl)-2-phenylquinoline (three-letter code: B37) (formula: $C_{32}H_{29}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	32	3	1		
2	B	1	Total	C	N	O	0	0
			36	32	3	1		
2	C	1	Total	C	N	O	0	0
			36	32	3	1		

- Molecule 3 is water.

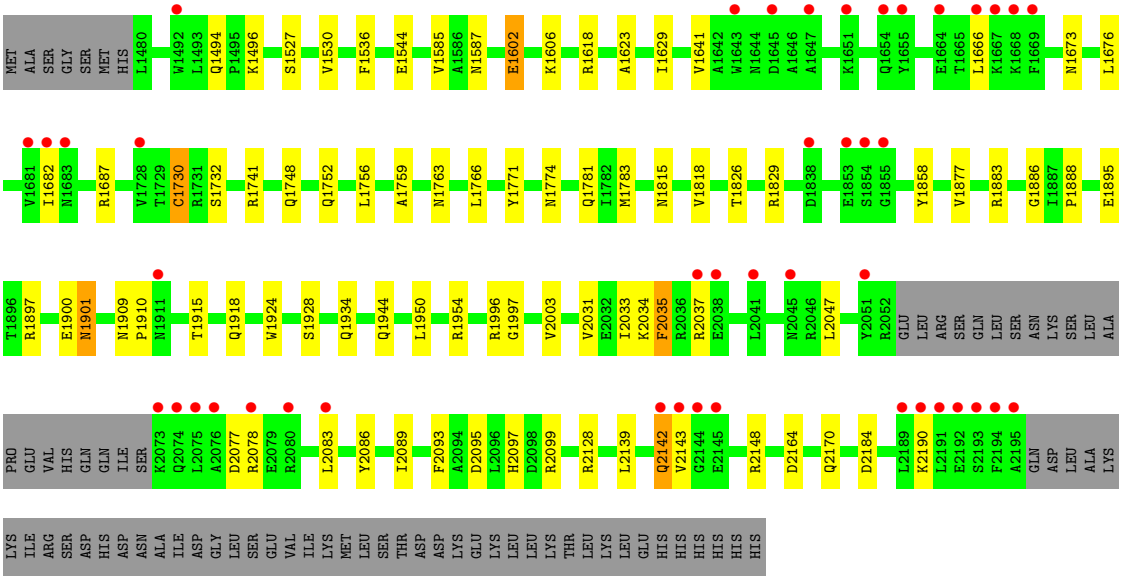
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	382	Total	O	0	0
			382	382		
3	B	339	Total	O	0	0
			339	339		
3	C	321	Total	O	0	0
			321	321		

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.

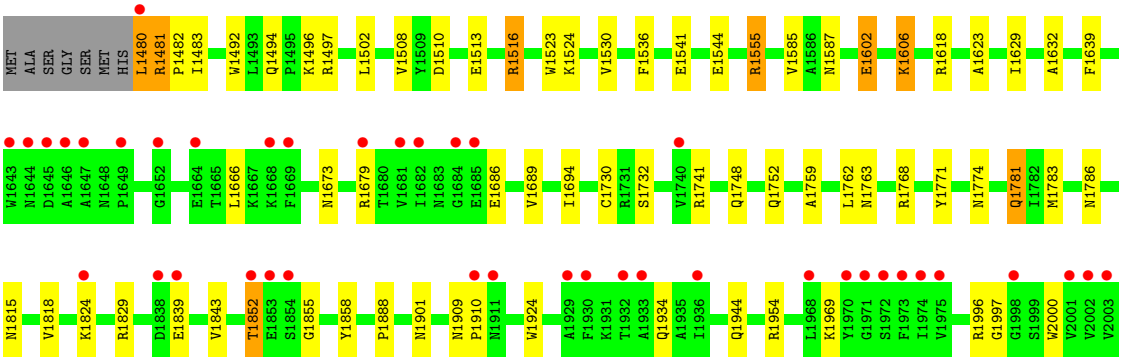
• Molecule 1: Acetyl-CoA carboxylase

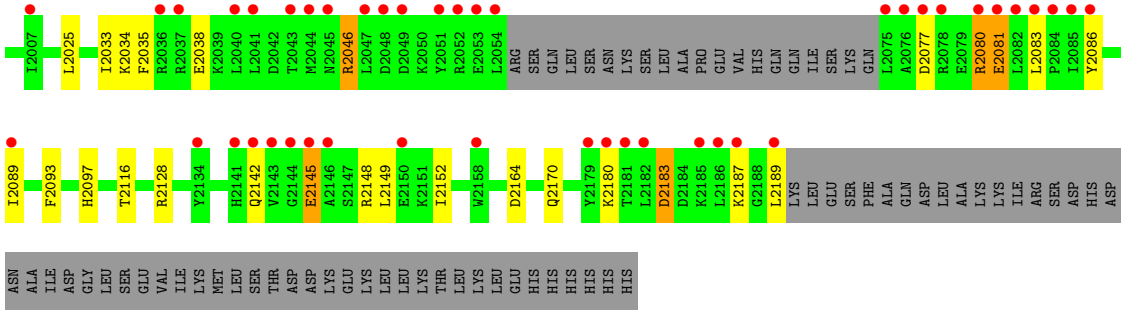
Chain A:



• Molecule 1: Acetyl-CoA carboxylase

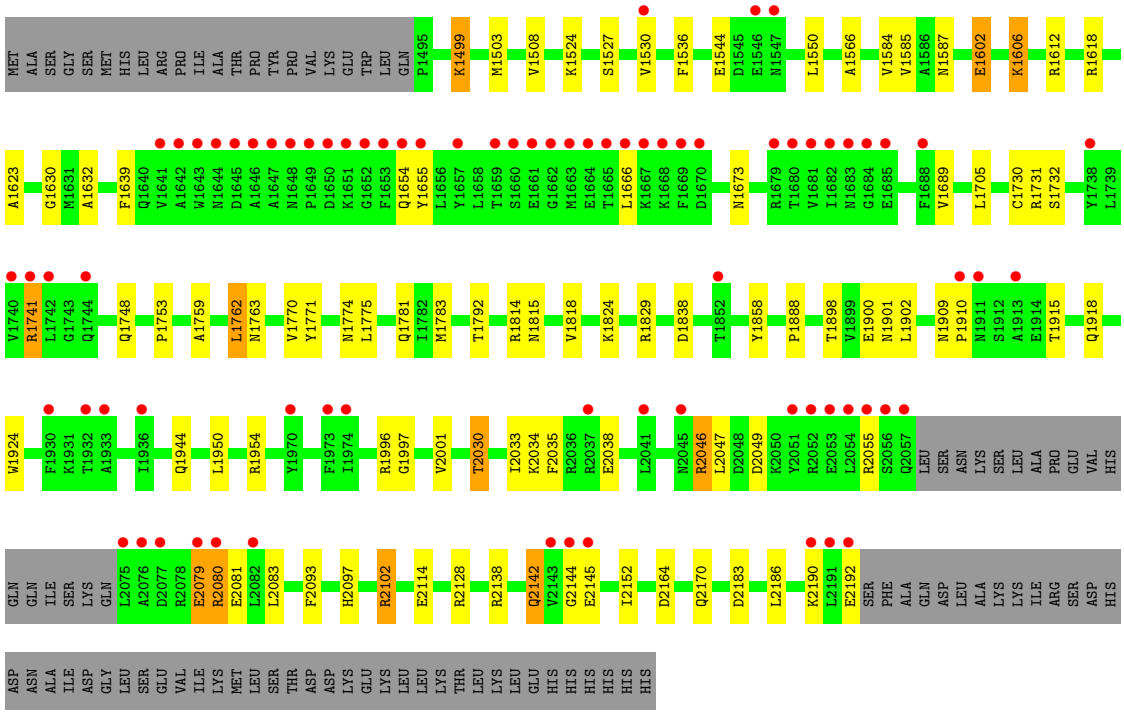
Chain B:





- Molecule 1: Acetyl-CoA carboxylase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	246.99Å 123.18Å 146.16Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	43.55 – 2.40 43.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.55-2.40) 96.4 (43.55-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.39Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.2, BUSTER 2.11.2	Depositor
R, R_{free}	0.202 , 0.223 0.191 , 0.214	Depositor DCC
R_{free} test set	16364 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 71.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17661	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: B37

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.51	0/5689	0.72	1/7704 (0.0%)
1	B	0.50	0/5633	0.73	2/7631 (0.0%)
1	C	0.50	0/5551	0.74	2/7512 (0.0%)
All	All	0.50	0/16873	0.73	5/22847 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2079	GLU	C-N-CA	7.22	139.75	121.70
1	B	2080	ARG	C-N-CA	7.14	139.56	121.70
1	C	2080	ARG	C-N-CA	6.11	136.99	121.70
1	B	1786	ASN	CB-CA-C	-5.87	98.65	110.40
1	A	1730	CYS	N-CA-C	-5.07	97.32	111.00

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	5561	0	5492	30	0
1	B	5513	0	5450	39	0
1	C	5437	0	5373	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	29	0	0
2	B	36	0	29	0	0
2	C	36	0	29	0	0
3	A	382	0	0	3	0
3	B	339	0	0	0	0
3	C	321	0	0	3	0
All	All	17661	0	16402	95	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 3.

All (95) 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:1815:ASN:H	1:B:1944:GLN:HE22	1.18	0.88
1:C:1815:ASN:H	1:C:1944:GLN:HE22	1.21	0.86
1:C:1763:ASN:HD21	1:C:1771:TYR:H	1.22	0.84
1:A:1763:ASN:HD21	1:A:1771:TYR:H	1.24	0.84
1:A:1815:ASN:H	1:A:1944:GLN:HE22	1.19	0.84
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.31	0.79
1:B:1632:ALA:H	1:C:2097:HIS:HE1	1.30	0.78
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	1.86	0.76
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.38	0.72
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.25	0.69
1:A:1877:VAL:HG23	1:A:1928:SER:HB2	1.73	0.69
1:B:1541:GLU:OE1	1:B:1555:ARG:HD3	1.94	0.66
1:B:2080:ARG:H	1:B:2081:GLU:HB2	1.59	0.65
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.81	0.63
1:A:2095:ASP:OD2	1:A:2099:ARG:NH1	2.33	0.62
1:A:1494:GLN:HE21	1:A:1496:LYS:H	1.47	0.61
1:C:1898:THR:HG22	3:C:142:HOH:O	2.00	0.61
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.49	0.59
1:B:2080:ARG:N	1:B:2081:GLU:HB2	2.18	0.59
1:B:2164:ASP:H	1:B:2170:GLN:NE2	2.02	0.58
1:A:1900:GLU:HG2	1:A:1918:GLN:HG2	1.85	0.57
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.70	0.57
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.70	0.57
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.68	0.57
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.05	0.56
1:C:1759:ALA:H	1:C:1774:ASN:ND2	2.05	0.55
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1759:ALA:H	1:A:1774:ASN:ND2	2.05	0.55
1:B:1759:ALA:H	1:B:1774:ASN:ND2	2.05	0.55
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.06	0.52
1:B:2046:ARG:NH2	1:C:1639:PHE:O	2.43	0.52
1:A:2184:ASP:OD2	1:B:1481:ARG:NH2	2.36	0.51
1:C:1900:GLU:HG2	1:C:1918:GLN:HG2	1.92	0.51
1:B:1969:LYS:HA	1:C:1741:ARG:HD2	1.93	0.50
1:C:2030:THR:HG21	3:C:955:HOH:O	2.10	0.49
1:B:1694:ILE:HA	1:C:2102:ARG:CD	2.42	0.49
1:B:2183:ASP:O	1:B:2187:LYS:HG2	2.12	0.49
1:A:2033:ILE:HG22	1:A:2034:LYS:HG2	1.95	0.49
1:B:1852:THR:HG22	1:B:1855:GLY:O	2.13	0.49
1:A:2142:GLN:O	1:A:2142:GLN:HG2	2.13	0.49
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.46	0.49
1:C:1527:SER:O	1:C:1530:VAL:HG22	2.13	0.49
1:C:2138:ARG:NH2	1:C:2183:ASP:OD1	2.47	0.48
1:C:1623:ALA:HA	1:C:1730:CYS:HB3	1.96	0.48
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.79	0.48
1:C:1499:LYS:O	1:C:1503:MET:HG2	2.15	0.47
1:C:1606:LYS:HD2	3:C:967:HOH:O	2.15	0.47
1:A:2031:VAL:HG13	1:A:2035:PHE:HB3	1.98	0.46
1:B:2034:LYS:HD2	1:C:1630:GLY:HA2	1.98	0.46
1:B:1497:ARG:HD3	1:B:1510:ASP:OD1	2.16	0.45
1:A:1877:VAL:CG2	1:A:1928:SER:HB2	2.43	0.45
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.13	0.45
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.98	0.45
1:C:1753:PRO:HB3	1:C:1775:LEU:HD13	1.99	0.44
1:B:1639:PHE:O	1:C:2046:ARG:NH2	2.50	0.44
1:A:1818:VAL:HB	1:A:1888:PRO:HG2	2.00	0.44
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.65	0.44
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.65	0.44
1:B:1606:LYS:HE3	1:B:1606:LYS:HB2	1.71	0.44
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	2.00	0.44
1:B:1480:LEU:HA	1:B:1492:TRP:CD1	2.53	0.43
1:B:1954:ARG:O	1:B:1996:ARG:HB2	2.18	0.43
1:A:1544:GLU:OE2	1:A:1602:GLU:OE1	2.37	0.43
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	2.01	0.43
1:C:2142:GLN:H	1:C:2142:GLN:HG2	1.73	0.43
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.17	0.42
1:B:1909:ASN:HD22	1:B:1910:PRO:HD2	1.84	0.42
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1523:TRP:HB3	1:B:1530:VAL:HG11	2.01	0.42
1:A:1954:ARG:O	1:A:1996:ARG:HB2	2.19	0.42
1:B:2086:TYR:HA	1:B:2089:ILE:HD12	2.01	0.42
1:A:1883[B]:ARG:NH1	1:A:1886:GLY:O	2.51	0.41
1:C:1655:TYR:CE1	1:C:1689:VAL:HG22	2.55	0.41
1:C:1762:LEU:HD12	1:C:1762:LEU:HA	1.92	0.41
1:A:2099:ARG:NH2	3:A:447:HOH:O	2.53	0.41
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.85	0.41
1:B:2093:PHE:O	1:B:2097:HIS:HD2	2.03	0.41
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.51	0.41
1:C:1566:ALA:HA	1:C:1584:VAL:O	2.21	0.41
1:B:1544:GLU:OE2	1:B:1602:GLU:OE1	2.38	0.41
1:B:1829:ARG:CZ	1:B:1858:TYR:HB3	2.50	0.41
1:C:1544:GLU:OE2	1:C:1602:GLU:OE1	2.38	0.41
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.50	0.41
1:C:2097:HIS:O	1:C:2102:ARG:HG3	2.20	0.41
1:C:1954:ARG:O	1:C:1996:ARG:HB2	2.21	0.41
1:A:2037:ARG:HG2	3:A:91:HOH:O	2.20	0.41
1:A:2093:PHE:O	1:A:2097:HIS:HD2	2.04	0.41
1:B:1481:ARG:HA	1:B:1482:PRO:HA	1.95	0.41
1:C:2093:PHE:O	1:C:2097:HIS:HD2	2.04	0.41
1:B:1781:GLN:NE2	1:B:1781:GLN:H	2.19	0.40
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.57	0.40
1:A:1901:ASN:ND2	3:A:960:HOH:O	2.53	0.40
1:C:1909:ASN:HD22	1:C:1910:PRO:HD2	1.85	0.40
1:A:1909:ASN:HD22	1:A:1910:PRO:HD2	1.85	0.40
1:B:2164:ASP:H	1:B:2170:GLN:HE22	1.68	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	693/769 (90%)	670 (97%)	21 (3%)	2 (0%)	41	55
1	B	686/769 (89%)	658 (96%)	23 (3%)	5 (1%)	22	32
1	C	677/769 (88%)	651 (96%)	20 (3%)	6 (1%)	17	25
All	All	2056/2307 (89%)	1979 (96%)	64 (3%)	13 (1%)	25	36

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2081	GLU
1	C	2144	GLY
1	A	1997	GLY
1	A	2143	VAL
1	B	1997	GLY
1	B	2046	ARG
1	B	2145	GLU
1	C	1997	GLY
1	C	2046	ARG
1	C	2080	ARG
1	C	2081	GLU
1	C	2145	GLU
1	B	1481	ARG

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	591/658 (90%)	559 (95%)	32 (5%)	22	36
1	B	586/658 (89%)	542 (92%)	44 (8%)	13	21
1	C	578/658 (88%)	533 (92%)	45 (8%)	12	19
All	All	1755/1974 (89%)	1634 (93%)	121 (7%)	15	25

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1536	PHE
1	A	1585	VAL
1	A	1602	GLU
1	A	1606	LYS
1	A	1618	ARG
1	A	1629	ILE
1	A	1641	VAL
1	A	1666	LEU
1	A	1673	ASN
1	A	1676	LEU
1	A	1682	ILE
1	A	1687	ARG
1	A	1732	SER
1	A	1756	LEU
1	A	1766	LEU
1	A	1781	GLN
1	A	1826	THR
1	A	1901	ASN
1	A	1915	THR
1	A	1924	TRP
1	A	1950	LEU
1	A	2003	VAL
1	A	2035	PHE
1	A	2047	LEU
1	A	2077	ASP
1	A	2078	ARG
1	A	2083	LEU
1	A	2128	ARG
1	A	2139	LEU
1	A	2142	GLN
1	A	2148	ARG
1	A	2190	LYS
1	B	1480	LEU
1	B	1483	ILE
1	B	1502	LEU
1	B	1508	VAL
1	B	1516	ARG
1	B	1524	LYS
1	B	1536	PHE
1	B	1555	ARG
1	B	1585	VAL
1	B	1602	GLU
1	B	1606	LYS

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Mol	Chain	Res	Type
1	B	1618	ARG
1	B	1629	ILE
1	B	1666	LEU
1	B	1673	ASN
1	B	1679	ARG
1	B	1686	GLU
1	B	1689	VAL
1	B	1732	SER
1	B	1762	LEU
1	B	1768	ARG
1	B	1781	GLN
1	B	1824	LYS
1	B	1839	GLU
1	B	1843	VAL
1	B	1852	THR
1	B	1901	ASN
1	B	1924	TRP
1	B	2025	LEU
1	B	2033	ILE
1	B	2035	PHE
1	B	2038	GLU
1	B	2077	ASP
1	B	2083	LEU
1	B	2116	THR
1	B	2128	ARG
1	B	2142	GLN
1	B	2145	GLU
1	B	2148	ARG
1	B	2149	LEU
1	B	2152	ILE
1	B	2180	LYS
1	B	2183	ASP
1	B	2189	LEU
1	C	1499	LYS
1	C	1508	VAL
1	C	1524	LYS
1	C	1536	PHE
1	C	1550	LEU
1	C	1585	VAL
1	C	1602	GLU
1	C	1606	LYS
1	C	1618	ARG

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Mol	Chain	Res	Type
1	C	1654	GLN
1	C	1666	LEU
1	C	1673	ASN
1	C	1731	ARG
1	C	1732	SER
1	C	1741	ARG
1	C	1762	LEU
1	C	1770	VAL
1	C	1781	GLN
1	C	1792	THR
1	C	1824	LYS
1	C	1838	ASP
1	C	1901	ASN
1	C	1902	LEU
1	C	1915	THR
1	C	1924	TRP
1	C	1950	LEU
1	C	2001	VAL
1	C	2030	THR
1	C	2033	ILE
1	C	2034	LYS
1	C	2035	PHE
1	C	2038	GLU
1	C	2047	LEU
1	C	2049	ASP
1	C	2055	ARG
1	C	2079	GLU
1	C	2083	LEU
1	C	2102	ARG
1	C	2114	GLU
1	C	2128	ARG
1	C	2142	GLN
1	C	2152	ILE
1	C	2186	LEU
1	C	2190	LYS
1	C	2192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1517	GLN

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Mol	Chain	Res	Type
1	A	1587	ASN
1	A	1605	ASN
1	A	1673	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1763	ASN
1	A	1774	ASN
1	A	1781	GLN
1	A	1815	ASN
1	A	1909	ASN
1	A	1934	GLN
1	A	1941	ASN
1	A	1944	GLN
1	A	2097	HIS
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1587	ASN
1	B	1605	ASN
1	B	1673	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1774	ASN
1	B	1781	GLN
1	B	1815	ASN
1	B	1909	ASN
1	B	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	2097	HIS
1	B	2170	GLN
1	C	1517	GLN
1	C	1587	ASN
1	C	1605	ASN
1	C	1748	GLN
1	C	1752	GLN
1	C	1763	ASN
1	C	1774	ASN
1	C	1781	GLN
1	C	1815	ASN
1	C	1909	ASN

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Mol	Chain	Res	Type
1	C	1941	ASN
1	C	1944	GLN
1	C	2045	ASN
1	C	2097	HIS
1	C	2142	GLN
1	C	2170	GLN

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)

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	B37	C	2242	-	40,41,41	1.13	4 (10%)	52,58,58	1.14	3 (5%)
2	B37	A	2242	-	40,41,41	1.21	5 (12%)	52,58,58	1.21	6 (11%)
2	B37	B	2242	-	40,41,41	1.14	1 (2%)	52,58,58	1.09	2 (3%)

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	B37	C	2242	-	-	0/12/26/26	0/6/6/6
2	B37	A	2242	-	-	0/12/26/26	0/6/6/6
2	B37	B	2242	-	-	0/12/26/26	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2242	B37	C44-C43	-2.40	1.38	1.41
2	B	2242	B37	C44-C43	-2.32	1.38	1.41
2	C	2242	B37	C39-C40	-2.21	1.38	1.43
2	A	2242	B37	C39-C40	-2.20	1.38	1.43
2	C	2242	B37	C38-N26	2.16	1.39	1.34
2	C	2242	B37	C44-C43	-2.13	1.38	1.41
2	A	2242	B37	C38-N26	2.08	1.39	1.34
2	A	2242	B37	C27-N26	-2.05	1.43	1.47
2	A	2242	B37	C40-C41	-2.03	1.39	1.42
2	C	2242	B37	C49-C41	-2.02	1.38	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2242	B37	C28-C27-N26	-2.89	106.43	110.82
2	C	2242	B37	C9-C3-C4	2.74	121.85	118.27
2	A	2242	B37	C9-C3-C4	2.67	121.75	118.27
2	B	2242	B37	C27-N26-C25	2.58	117.58	112.62
2	A	2242	B37	C44-C43-N42	2.41	124.01	121.83
2	C	2242	B37	C44-C43-N42	2.30	123.92	121.83
2	C	2242	B37	C27-N26-C25	2.23	116.92	112.62
2	A	2242	B37	O65-C38-N26	2.17	125.93	122.34
2	B	2242	B37	O65-C38-C39	-2.12	116.19	120.62
2	A	2242	B37	C27-N26-C25	2.09	116.65	112.62
2	A	2242	B37	C46-C40-C41	2.07	120.64	118.33

There are no chirality outliers.

There are no torsion outliers.

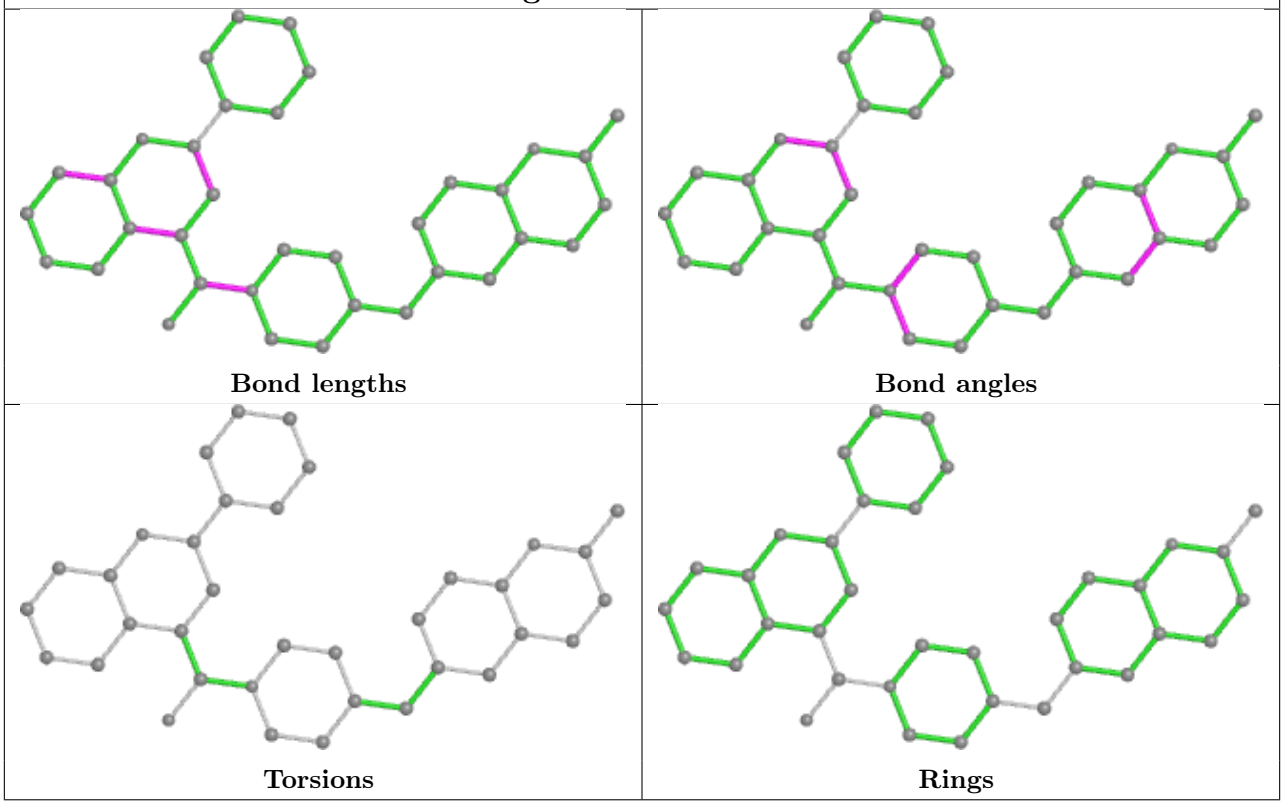
There are no ring outliers.

No monomer is involved in short contacts.

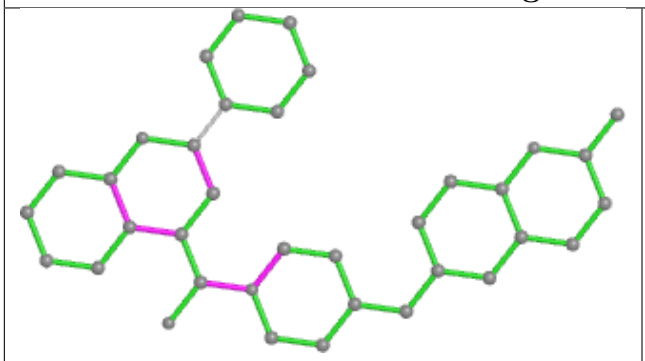
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

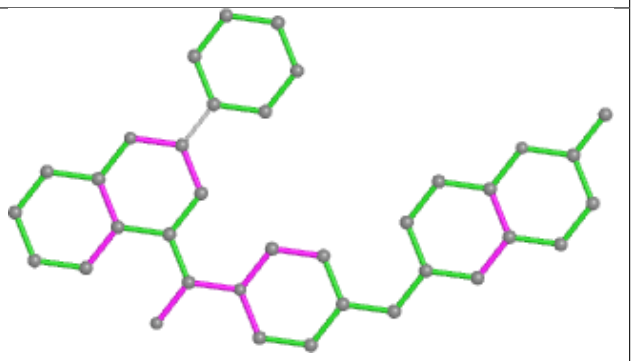
Ligand B37 C 2242



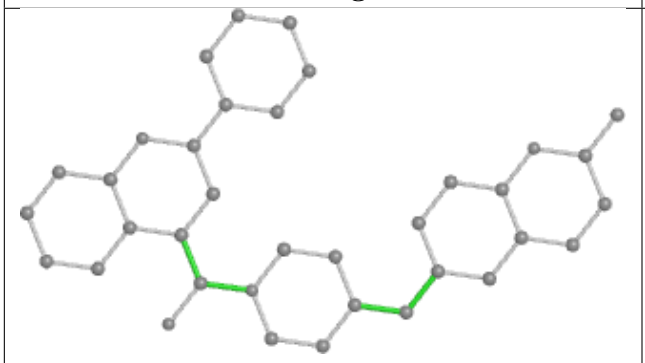
Ligand B37 A 2242



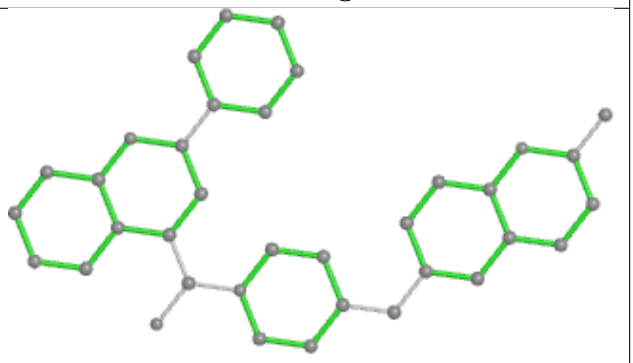
Bond lengths



Bond angles

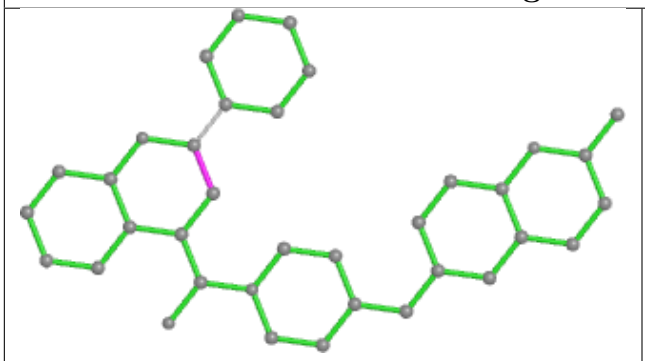


Torsions

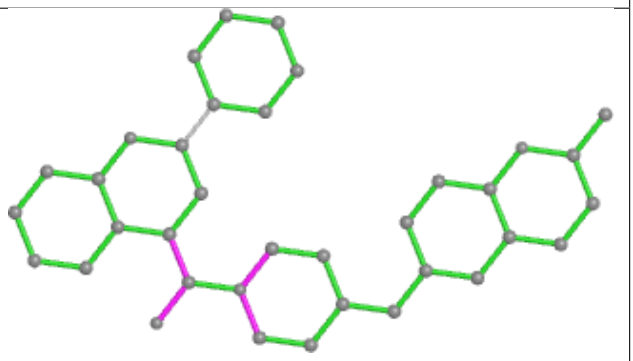


Rings

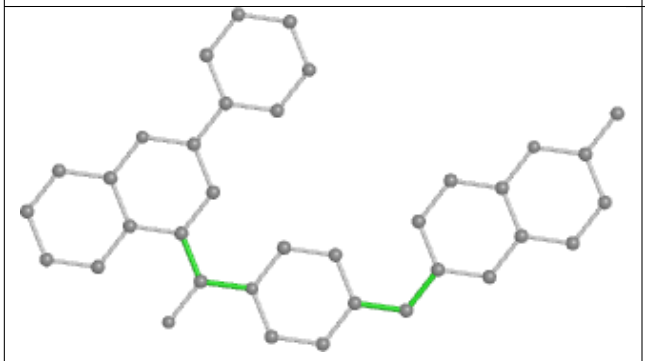
Ligand B37 B 2242



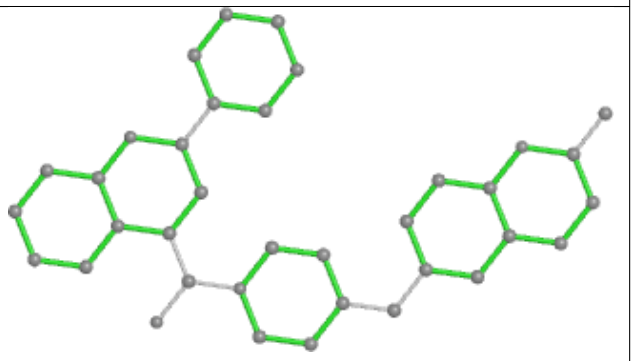
Bond lengths



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	696/769 (90%)	0.16	44 (6%)	20	18	38, 56, 111, 147	0
1	B	690/769 (89%)	0.39	85 (12%)	4	3	40, 61, 119, 159	0
1	C	681/769 (88%)	0.36	77 (11%)	5	4	38, 59, 123, 153	0
All	All	2067/2307 (89%)	0.30	206 (9%)	7	6	38, 58, 118, 159	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2144	GLY	9.9
1	B	2075	LEU	9.0
1	C	2144	GLY	8.2
1	A	2195	ALA	7.7
1	A	2194	PHE	7.3
1	B	2145	GLU	6.6
1	B	2179	TYR	6.4
1	C	2143	VAL	6.3
1	C	1649	PRO	6.3
1	B	1682	ILE	6.0
1	B	2082	LEU	6.0
1	C	1685	GLU	6.0
1	C	1682	ILE	5.9
1	A	2143	VAL	5.8
1	C	1669	PHE	5.7
1	C	1680	THR	5.6
1	B	2143	VAL	5.4
1	B	2186	LEU	5.4
1	C	1652	GLY	5.3
1	B	2086	TYR	5.2
1	A	1682	ILE	5.2
1	A	1669	PHE	4.9
1	B	2041	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	2080	ARG	4.7
1	C	1648	ASN	4.7
1	B	2085	ILE	4.7
1	C	2055	ARG	4.6
1	A	2193	SER	4.6
1	C	1647	ALA	4.5
1	C	1681	VAL	4.5
1	B	2083	LEU	4.5
1	C	1643	TRP	4.5
1	C	2054	LEU	4.4
1	B	2037	ARG	4.3
1	A	2192	GLU	4.3
1	B	2134	TYR	4.3
1	C	1655	TYR	4.2
1	B	1669	PHE	4.2
1	B	2051	TYR	4.1
1	B	2189	LEU	4.1
1	C	1679	ARG	4.1
1	C	2053	GLU	4.1
1	C	1650	ASP	4.0
1	C	1657	TYR	4.0
1	A	2075	LEU	4.0
1	C	2075	LEU	4.0
1	B	2144	GLY	3.9
1	B	2052	ARG	3.9
1	C	1651	LYS	3.8
1	B	2077	ASP	3.8
1	C	1646	ALA	3.7
1	A	2145	GLU	3.7
1	B	2043	THR	3.7
1	C	2191	LEU	3.7
1	B	2049	ASP	3.6
1	A	2142	GLN	3.6
1	A	2191	LEU	3.5
1	C	1641	VAL	3.5
1	C	1668	LYS	3.5
1	A	1683	ASN	3.5
1	B	2002	VAL	3.4
1	B	2182	LEU	3.4
1	A	1911	ASN	3.4
1	C	2082	LEU	3.4
1	C	2076	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1853	GLU	3.4
1	B	2054	LEU	3.3
1	B	2081	GLU	3.3
1	B	1685	GLU	3.3
1	B	1684	GLY	3.3
1	C	1644	ASN	3.3
1	C	1913	ALA	3.3
1	B	1973	PHE	3.2
1	C	1683	ASN	3.2
1	B	2044	MET	3.2
1	B	1972	SER	3.2
1	C	1684	GLY	3.2
1	A	2076	ALA	3.2
1	C	2145	GLU	3.2
1	B	2146	ALA	3.2
1	B	1910	PRO	3.2
1	C	1911	ASN	3.2
1	B	2187	LYS	3.1
1	B	2181	THR	3.1
1	B	2078	ARG	3.1
1	B	1974	ILE	3.0
1	B	1971	GLY	3.0
1	B	1933	ALA	3.0
1	B	2076	ALA	3.0
1	B	1649	PRO	3.0
1	C	2051	TYR	2.9
1	C	1547	ASN	2.9
1	C	1973	PHE	2.9
1	C	2192	GLU	2.9
1	B	1854	SER	2.9
1	B	1480	LEU	2.9
1	A	2190	LYS	2.9
1	B	1911	ASN	2.9
1	B	2053	GLU	2.9
1	C	2056	SER	2.9
1	A	1651	LYS	2.9
1	C	1645	ASP	2.8
1	B	1644	ASN	2.8
1	C	1666	LEU	2.8
1	C	1664	GLU	2.8
1	B	1645	ASP	2.8
1	A	2041	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	2057	GLN	2.8
1	B	2045	ASN	2.8
1	B	2001	VAL	2.7
1	A	1667	LYS	2.7
1	C	1659	THR	2.7
1	B	1681	VAL	2.7
1	B	2040	LEU	2.7
1	C	1738	TYR	2.7
1	A	2037	ARG	2.7
1	A	1645	ASP	2.7
1	C	1546	GLU	2.7
1	C	1642	ALA	2.7
1	B	2141	HIS	2.7
1	C	1670	ASP	2.7
1	C	2077	ASP	2.7
1	C	2079	GLU	2.6
1	B	2036	ARG	2.6
1	C	2080	ARG	2.6
1	C	1932	THR	2.6
1	B	1838	ASP	2.6
1	B	1932	THR	2.6
1	A	2189	LEU	2.6
1	A	2083	LEU	2.6
1	C	2037	ARG	2.6
1	C	1974	ILE	2.6
1	C	1742	LEU	2.6
1	B	2089	ILE	2.6
1	B	1668	LYS	2.6
1	A	2074	GLN	2.6
1	B	2142	GLN	2.6
1	B	1998	GLY	2.5
1	C	1930	PHE	2.5
1	A	1643	TRP	2.5
1	B	1970	TYR	2.5
1	A	1854	SER	2.5
1	A	1853	GLU	2.5
1	B	1647	ALA	2.5
1	B	2084	PRO	2.5
1	C	1654	GLN	2.5
1	A	1838	ASP	2.5
1	A	2045	ASN	2.5
1	C	1653	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1936	ILE	2.5
1	B	1930	PHE	2.5
1	B	1936	ILE	2.5
1	B	1929	ALA	2.5
1	C	1665	THR	2.4
1	B	1975	VAL	2.4
1	B	2003	VAL	2.4
1	C	1662	GLY	2.4
1	C	2045	ASN	2.4
1	A	2051	TYR	2.4
1	B	1652	GLY	2.4
1	C	1933	ALA	2.4
1	A	1855	GLY	2.3
1	C	1663	MET	2.3
1	B	1839	GLU	2.3
1	B	1679	ARG	2.3
1	C	2041	LEU	2.3
1	B	2048	ASP	2.3
1	C	1530	VAL	2.3
1	B	1824	LYS	2.3
1	B	1664	GLU	2.3
1	C	1661	GLU	2.3
1	B	1968	LEU	2.3
1	C	1741	ARG	2.3
1	C	1852	THR	2.3
1	A	1647	ALA	2.2
1	A	1492	TRP	2.2
1	B	2158	TRP	2.2
1	A	1681	VAL	2.2
1	A	2080	ARG	2.2
1	A	1664	GLU	2.2
1	C	1667	LYS	2.1
1	A	1655	TYR	2.1
1	C	1910	PRO	2.1
1	A	2073	LYS	2.1
1	B	2180	LYS	2.1
1	A	2078	ARG	2.1
1	B	2150	GLU	2.1
1	B	1852	THR	2.1
1	A	1666	LEU	2.1
1	B	1740	VAL	2.1
1	B	1643	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1654	GLN	2.1
1	C	1970	TYR	2.1
1	B	2185	LYS	2.1
1	C	1660	SER	2.1
1	A	1728	VAL	2.1
1	C	2052	ARG	2.1
1	C	2190	LYS	2.1
1	B	2007	ILE	2.0
1	B	1646	ALA	2.0
1	C	1744	GLN	2.0
1	A	1668	LYS	2.0
1	C	1688	PHE	2.0
1	C	1740	VAL	2.0
1	B	2047	LEU	2.0
1	A	2038	GLU	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)

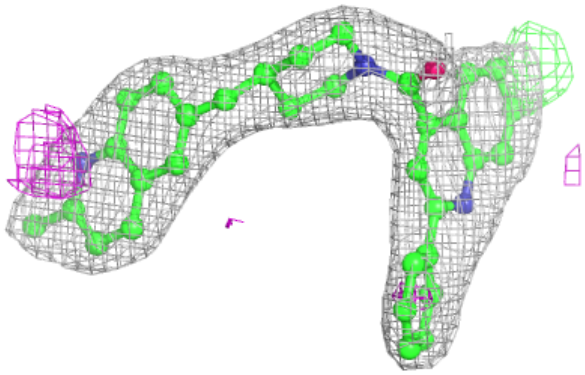
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

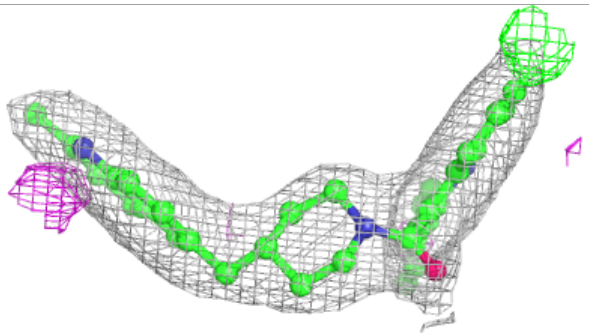
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	B37	B	2242	36/36	0.91	0.15	59,67,82,84	0
2	B37	C	2242	36/36	0.92	0.15	51,60,76,77	0
2	B37	A	2242	36/36	0.93	0.14	49,55,77,79	0

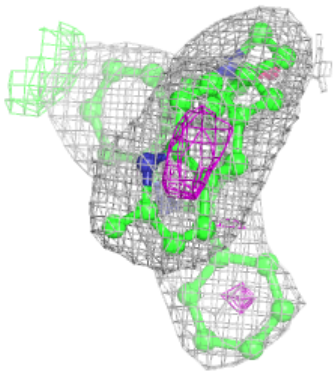
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B37 B 2242:

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

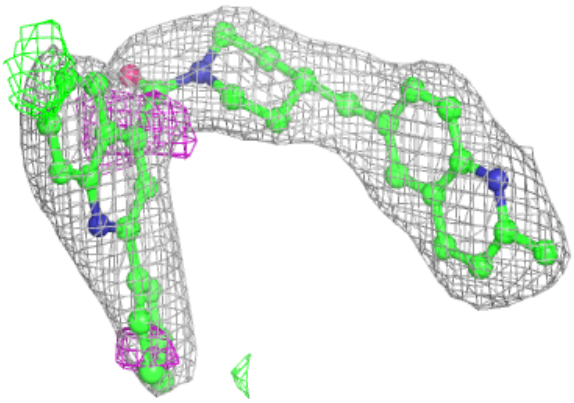


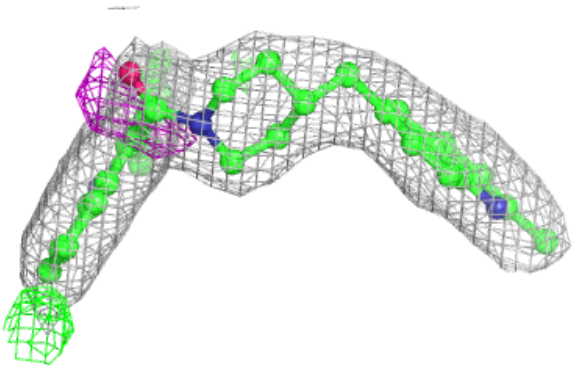


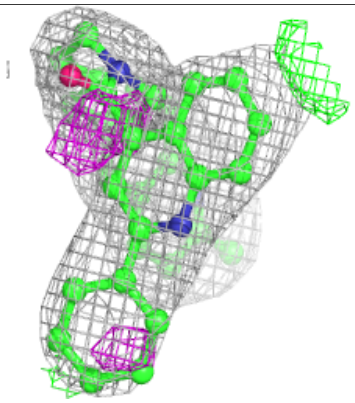


Electron density around B37 C 2242:

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

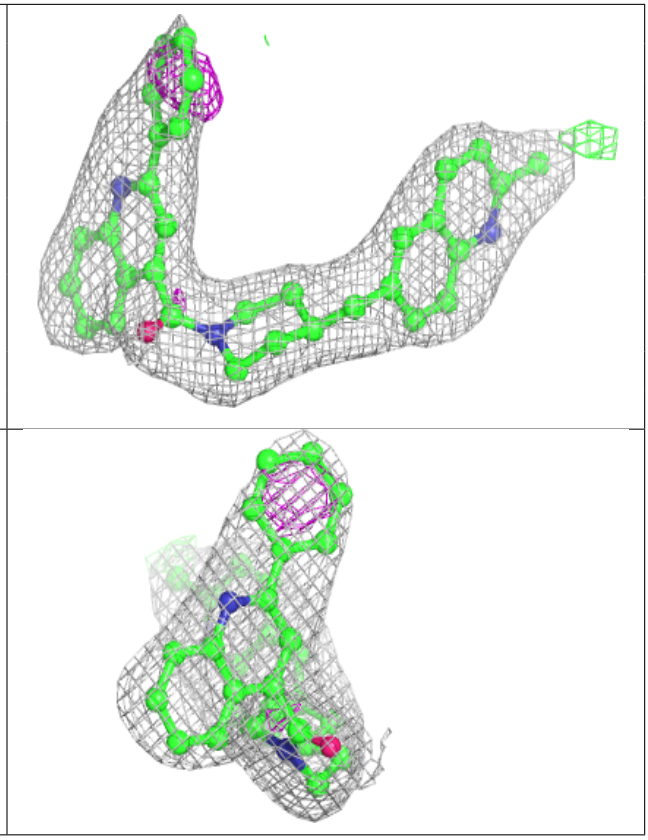






Electron density around B37 A 2242:

$2mF_o$-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.