



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:15 pm BST

PDB ID : 3TZ3
Title : Crystal Structure of the humanized carboxyltransferase domain of yeast Acetyl-coA carboxylase in complex with compound 2
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 : 2011-09-26
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

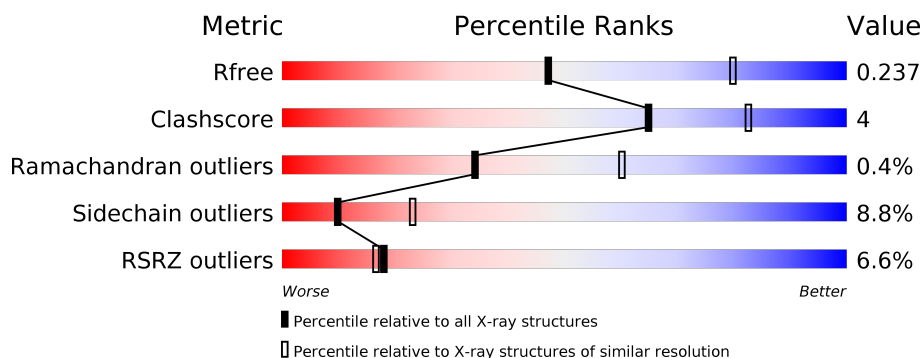
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	769	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>• 10%</div> </div> </div>
1	B	769	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>• 10%</div> </div> </div>
1	C	769	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>• 12%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17404 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
1	A	694	Total	C	N	O	S	0	0	0
			5541	3526	955	1043	17			
1	B	692	Total	C	N	O	S	0	0	0
			5519	3512	953	1037	17			
1	C	676	Total	C	N	O	S	0	0	0
			5384	3421	929	1017	17			

There are 60 discrepancies between the modelled and reference sequences:

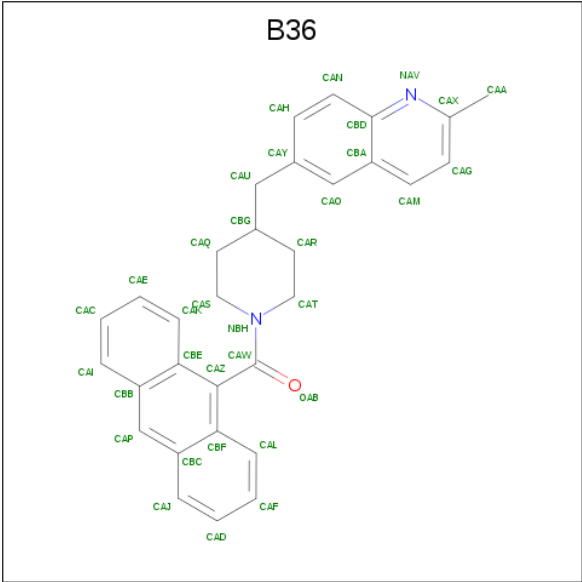
Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	EXPRESSION TAG	UNP Q00955
A	1474	ALA	-	EXPRESSION TAG	UNP Q00955
A	1475	SER	-	EXPRESSION TAG	UNP Q00955
A	1760	SER	PRO	ENGINEERED MUTATION	UNP Q00955
A	1762	LEU	ILE	ENGINEERED MUTATION	UNP Q00955
A	1765	VAL	MET	ENGINEERED MUTATION	UNP Q00955
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 6-([1-(anthracen-9-ylcarbonyl)piperidin-4-yl]methyl)-2-methylquinoline (three-letter code: B36) (formula: C₃₁H₂₈N₂O).



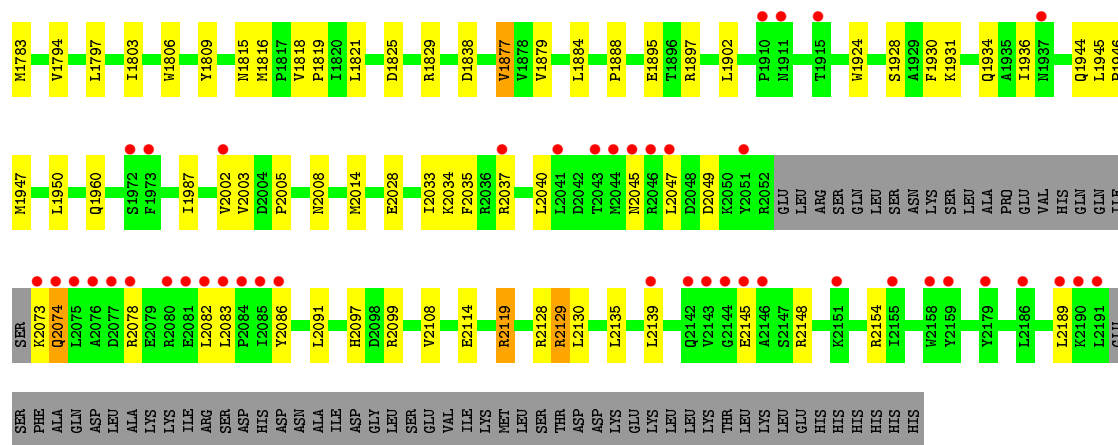
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	31	2	1		
2	B	1	Total	C	N	O	0	0
			34	31	2	1		
2	C	1	Total	C	N	O	0	0
			34	31	2	1		

- Molecule 3 is water.

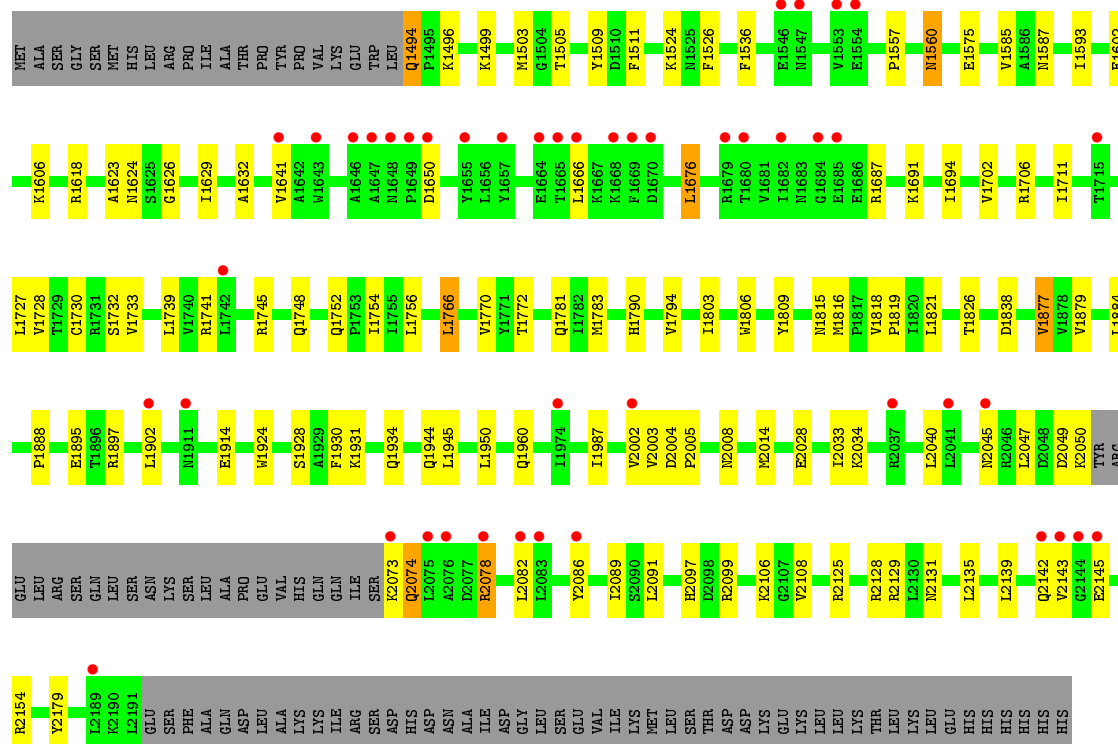
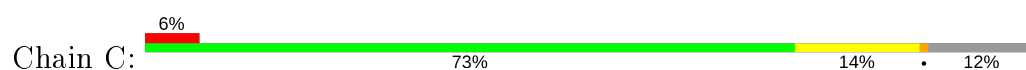
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	301	Total	O	0	0
			301	301		
3	B	266	Total	O	0	0
			266	266		
3	C	291	Total	O	0	0
			291	291		

- Molecule 1: Acetyl-CoA carboxylase





• Molecule 1: Acetyl-CoA carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.85Å 123.37Å 145.10Å 90.00° 94.41° 90.00°	Depositor
Resolution (Å)	44.75 – 2.70 44.75 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.4 (44.75-2.70) 92.4 (44.75-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.69Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.2, BUSTER 2.11.2	Depositor
R, R_{free}	0.206 , 0.238 0.205 , 0.237	Depositor DCC
R_{free} test set	10911 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17404	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B36

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	0/5661	0.74	0/7667
1	B	0.51	0/5638	0.73	0/7636
1	C	0.51	0/5497	0.74	0/7441
All	All	0.51	0/16796	0.73	0/22744

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5541	0	5477	48	0
1	B	5519	0	5459	44	0
1	C	5384	0	5318	50	0
2	A	34	0	28	0	0
2	B	34	0	28	0	0
2	C	34	0	28	0	0
3	A	301	0	0	6	0
3	B	266	0	0	2	0
3	C	291	0	0	5	0
All	All	17404	0	16338	134	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 (134) 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:A:2040:LEU:HD11	1:A:2086:TYR:HB3	1.61	0.83
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.39	0.70
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.57	0.68
1:B:1632:ALA:H	1:C:2097:HIS:HE1	1.40	0.67
1:A:2033:ILE:HG22	1:A:2034:LYS:HG2	1.77	0.66
1:B:1946:PRO:HG3	1:B:2130:LEU:HD21	1.75	0.66
1:C:2033:ILE:HG22	1:C:2034:LYS:HG2	1.77	0.65
1:B:2033:ILE:HG22	1:B:2034:LYS:HG2	1.78	0.64
1:C:2073:LYS:HB3	1:C:2074:GLN:HE21	1.64	0.63
1:B:2073:LYS:HB3	1:B:2074:GLN:HE21	1.64	0.62
1:B:1936:ILE:HG12	1:B:1947:MET:HE1	1.80	0.61
1:A:2073:LYS:HB3	1:A:2074:GLN:HE21	1.64	0.61
1:B:1936:ILE:HG12	1:B:1947:MET:CE	2.30	0.61
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.16	0.60
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.02	0.59
1:B:1815:ASN:ND2	1:B:1944:GLN:HE22	2.02	0.58
1:B:1895:GLU:OE1	1:B:1897:ARG:HD3	2.04	0.58
1:C:1895:GLU:OE1	1:C:1897:ARG:HD3	2.03	0.58
1:C:1575:GLU:HG3	1:C:1821:LEU:HD22	1.85	0.57
1:B:1766:LEU:HD23	1:B:1770:VAL:HG21	1.87	0.57
1:A:1883:ARG:NH1	3:A:354:HOH:O	2.36	0.56
1:B:2129:ARG:HD3	3:B:356:HOH:O	2.06	0.56
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.04	0.55
1:C:1560:ASN:HD22	1:C:1560:ASN:H	1.55	0.55
1:C:1494:GLN:HB3	3:C:351:HOH:O	2.07	0.55
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.55	0.54
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.73	0.54
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.73	0.54
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.05	0.54
1:A:2162:SER:HB3	1:B:1797:LEU:HD23	1.89	0.53
1:B:1657:TYR:CE2	1:B:1687:ARG:HD2	2.43	0.53
1:B:1560:ASN:HD22	1:B:1560:ASN:H	1.57	0.53
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.44	0.53
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.56	0.53
1:A:1624:ASN:HD22	1:A:1626:GLY:H	1.57	0.52
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.44	0.52
1:C:1624:ASN:HD22	1:C:1626:GLY:H	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2050:LYS:HB2	1:C:2078:ARG:HE	1.74	0.52
1:C:2143:VAL:HG22	1:C:2145:GLU:H	1.74	0.52
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.74	0.52
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.45	0.51
1:A:1766:LEU:HD23	1:A:1770:VAL:HG21	1.93	0.51
1:B:1706:ARG:HD2	1:C:2108:VAL:HG12	1.93	0.51
1:C:1727:LEU:HB2	1:C:1803:ILE:HD11	1.92	0.51
1:B:1829:ARG:HD2	1:B:2119:ARG:NH2	2.26	0.50
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.60	0.50
1:A:1526:PHE:CE2	1:A:1821:LEU:HD11	2.46	0.50
1:B:2108:VAL:HG12	1:C:1706:ARG:HD2	1.92	0.50
1:A:2099:ARG:NH2	3:A:348:HOH:O	2.41	0.50
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.60	0.49
1:A:1503:MET:HE1	3:A:562:HOH:O	2.12	0.49
1:A:2040:LEU:CD1	1:A:2086:TYR:HB3	2.38	0.49
1:C:1494:GLN:N	3:C:697:HOH:O	2.46	0.49
1:C:2005:PRO:HG3	1:C:2014:MET:HB2	1.95	0.49
1:A:1730:CYS:CA	1:A:1752:GLN:HE21	2.26	0.48
1:A:1987:ILE:HB	1:A:2014:MET:HG3	1.93	0.48
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	1.96	0.48
1:B:1623:ALA:HB2	1:B:1729:THR:HG23	1.95	0.48
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.11	0.48
1:C:1790:HIS:HD2	3:C:24:HOH:O	1.97	0.48
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.95	0.48
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	1.96	0.48
1:A:1496:LYS:O	1:A:1590:THR:HG21	2.13	0.48
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.62	0.48
1:C:1987:ILE:HB	1:C:2014:MET:HG3	1.95	0.48
1:B:1877:VAL:HG23	1:B:1931:LYS:HD3	1.95	0.48
1:C:1728:VAL:HG21	1:C:1754:ILE:HD11	1.96	0.47
1:C:1766:LEU:HD23	1:C:1770:VAL:HG21	1.96	0.47
1:C:1711:ILE:HD12	1:C:1739:LEU:HD11	1.97	0.47
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.63	0.47
1:C:1741:ARG:HH22	1:C:1934:GLN:NE2	2.12	0.47
1:C:2125:ARG:O	1:C:2129:ARG:HG3	2.15	0.47
1:B:1480:LEU:HA	1:B:1492:TRP:CD1	2.49	0.47
1:B:1987:ILE:HB	1:B:2014:MET:HG3	1.96	0.47
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.63	0.47
1:C:2028:GLU:HB2	3:C:84:HOH:O	2.15	0.47
1:B:1809:TYR:O	1:B:1945:LEU:HD21	2.15	0.47
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1818:VAL:HB	1:A:1888:PRO:HG2	1.97	0.46
1:A:1883:ARG:HD2	3:A:354:HOH:O	2.16	0.46
1:A:1877:VAL:HG23	1:A:1931:LYS:HD3	1.96	0.46
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.45	0.46
1:C:1509:TYR:CG	1:C:1557:PRO:HB3	2.51	0.46
1:B:1526:PHE:CE2	1:B:1821:LEU:HD11	2.51	0.46
1:A:1624:ASN:O	1:A:1731:ARG:HG3	2.15	0.45
1:B:2082:LEU:HD22	1:B:2086:TYR:HE1	1.81	0.45
1:B:1711:ILE:HD12	1:B:1739:LEU:HD11	1.99	0.45
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.14	0.45
1:C:1624:ASN:ND2	1:C:1733:VAL:H	2.14	0.45
1:C:1877:VAL:HG23	1:C:1931:LYS:HD3	1.98	0.44
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	1.99	0.44
1:A:1480:LEU:HA	1:A:1492:TRP:CD1	2.52	0.44
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	2.00	0.44
1:A:2148:ARG:HD3	3:A:66:HOH:O	2.17	0.44
1:B:1575:GLU:HB3	1:B:1819:PRO:HB2	2.00	0.44
1:C:1902:LEU:HD11	1:C:1914:GLU:CD	2.37	0.43
1:C:1526:PHE:CE2	1:C:1821:LEU:HD11	2.52	0.43
1:A:1809:TYR:O	1:A:1945:LEU:HD21	2.19	0.43
1:C:2131:ASN:ND2	1:C:2179:TYR:OH	2.49	0.43
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	2.01	0.43
1:C:1575:GLU:HB3	1:C:1819:PRO:HB2	2.00	0.43
1:A:1657:TYR:CD2	1:A:1687:ARG:HB3	2.54	0.43
1:A:1575:GLU:HB3	1:A:1819:PRO:HB2	2.00	0.43
1:C:1509:TYR:CB	1:C:1557:PRO:HB3	2.47	0.43
1:C:2040:LEU:HD22	1:C:2086:TYR:HB3	2.00	0.43
1:C:2086:TYR:HA	1:C:2089:ILE:HD12	2.00	0.43
1:B:2082:LEU:HD22	1:B:2086:TYR:CE1	2.54	0.43
1:B:2005:PRO:HG3	1:B:2014:MET:HB2	2.01	0.43
1:B:1706:ARG:HA	1:C:2004:ASP:OD1	2.19	0.43
1:A:1511:PHE:CZ	1:A:1729:THR:HG21	2.54	0.42
1:B:1676:LEU:HD22	1:B:1694:ILE:HD11	2.01	0.42
1:A:2131:ASN:HB3	1:A:2175:ILE:HG21	2.01	0.42
1:C:1730:CYS:HA	1:C:1752:GLN:HE21	1.84	0.42
1:C:2078:ARG:HD3	1:C:2082:LEU:HG	2.01	0.42
1:C:1809:TYR:O	1:C:1945:LEU:HD21	2.19	0.42
1:B:1702:VAL:HB	1:C:2108:VAL:HG21	2.02	0.42
1:A:1730:CYS:H	1:A:1752:GLN:HG3	1.85	0.41
1:A:1902:LEU:HD11	1:A:1914:GLU:OE1	2.19	0.41
1:B:2108:VAL:HG21	1:C:1702:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1827:TRP:CE2	1:A:1828:ASP:HB2	2.55	0.41
1:A:2079:GLU:HG2	1:A:2083:LEU:HD12	2.03	0.41
1:A:2019:ASN:HB3	3:A:570:HOH:O	2.19	0.41
1:A:1865:SER:HB2	1:A:1883:ARG:HG3	2.02	0.41
1:B:1566:ALA:HA	1:B:1584:VAL:O	2.20	0.41
1:A:1667:LYS:HA	1:A:1672:GLU:HG3	2.03	0.41
1:B:1496:LYS:O	1:B:1590:THR:HG21	2.21	0.41
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.18	0.41
1:C:1499:LYS:O	1:C:1503:MET:HG3	2.21	0.41
1:C:1505:THR:HB	1:C:1730:CYS:HB2	2.03	0.41
1:B:2028:GLU:HB2	3:B:216:HOH:O	2.21	0.40
1:C:1496:LYS:NZ	3:C:516:HOH:O	2.54	0.40
1:B:1825:ASP:OD1	1:B:2119:ARG:NH1	2.54	0.40
1:C:1676:LEU:HD22	1:C:1694:ILE:HD11	2.03	0.40
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.22	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	690/769 (90%)	658 (95%)	28 (4%)	4 (1%)	25	50
1	B	688/769 (90%)	653 (95%)	33 (5%)	2 (0%)	41	66
1	C	672/769 (87%)	646 (96%)	24 (4%)	2 (0%)	41	66
All	All	2050/2307 (89%)	1957 (96%)	85 (4%)	8 (0%)	34	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1731	ARG
1	A	2142	GLN

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Mol	Chain	Res	Type
1	B	1731	ARG
1	C	2142	GLN
1	A	1593	ILE
1	A	1997	GLY
1	B	1593	ILE
1	C	1593	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/658 (90%)	540 (92%)	49 (8%)	11	25
1	B	586/658 (89%)	530 (90%)	56 (10%)	8	19
1	C	572/658 (87%)	524 (92%)	48 (8%)	11	25
All	All	1747/1974 (88%)	1594 (91%)	153 (9%)	10	23

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1499	LYS
1	A	1524	LYS
1	A	1536	PHE
1	A	1560	ASN
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	1650	ASP
1	A	1666	LEU
1	A	1676	LEU
1	A	1687	ARG
1	A	1691	LYS
1	A	1731	ARG

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Mol	Chain	Res	Type
1	A	1732	SER
1	A	1756	LEU
1	A	1760	SER
1	A	1766	LEU
1	A	1772	THR
1	A	1781	GLN
1	A	1794	VAL
1	A	1816	MET
1	A	1838	ASP
1	A	1877	VAL
1	A	1879	VAL
1	A	1883	ARG
1	A	1884	LEU
1	A	1924	TRP
1	A	1930	PHE
1	A	1950	LEU
1	A	2002	VAL
1	A	2003	VAL
1	A	2008	ASN
1	A	2035	PHE
1	A	2040	LEU
1	A	2047	LEU
1	A	2074	GLN
1	A	2077	ASP
1	A	2083	LEU
1	A	2091	LEU
1	A	2099	ARG
1	A	2114	GLU
1	A	2128	ARG
1	A	2135	LEU
1	A	2139	LEU
1	A	2145	GLU
1	A	2192	GLU
1	B	1524	LYS
1	B	1536	PHE
1	B	1560	ASN
1	B	1585	VAL
1	B	1602	GLU
1	B	1606	LYS
1	B	1618	ARG
1	B	1629	ILE
1	B	1641	VAL

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Mol	Chain	Res	Type
1	B	1650	ASP
1	B	1666	LEU
1	B	1676	LEU
1	B	1687	ARG
1	B	1691	LYS
1	B	1732	SER
1	B	1756	LEU
1	B	1760	SER
1	B	1766	LEU
1	B	1772	THR
1	B	1781	GLN
1	B	1794	VAL
1	B	1816	MET
1	B	1838	ASP
1	B	1877	VAL
1	B	1879	VAL
1	B	1884	LEU
1	B	1902	LEU
1	B	1924	TRP
1	B	1928	SER
1	B	1930	PHE
1	B	1950	LEU
1	B	1960	GLN
1	B	2002	VAL
1	B	2003	VAL
1	B	2008	ASN
1	B	2035	PHE
1	B	2037	ARG
1	B	2040	LEU
1	B	2045	ASN
1	B	2047	LEU
1	B	2049	ASP
1	B	2074	GLN
1	B	2078	ARG
1	B	2083	LEU
1	B	2091	LEU
1	B	2099	ARG
1	B	2114	GLU
1	B	2119	ARG
1	B	2128	ARG
1	B	2129	ARG
1	B	2135	LEU

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Mol	Chain	Res	Type
1	B	2139	LEU
1	B	2145	GLU
1	B	2148	ARG
1	B	2154	ARG
1	B	2189	LEU
1	C	1494	GLN
1	C	1511	PHE
1	C	1524	LYS
1	C	1536	PHE
1	C	1560	ASN
1	C	1585	VAL
1	C	1602	GLU
1	C	1606	LYS
1	C	1618	ARG
1	C	1629	ILE
1	C	1641	VAL
1	C	1650	ASP
1	C	1666	LEU
1	C	1676	LEU
1	C	1687	ARG
1	C	1691	LYS
1	C	1732	SER
1	C	1756	LEU
1	C	1766	LEU
1	C	1772	THR
1	C	1781	GLN
1	C	1794	VAL
1	C	1816	MET
1	C	1826	THR
1	C	1838	ASP
1	C	1877	VAL
1	C	1879	VAL
1	C	1884	LEU
1	C	1924	TRP
1	C	1928	SER
1	C	1930	PHE
1	C	1950	LEU
1	C	1960	GLN
1	C	2002	VAL
1	C	2003	VAL
1	C	2008	ASN
1	C	2045	ASN

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Mol	Chain	Res	Type
1	C	2047	LEU
1	C	2049	ASP
1	C	2074	GLN
1	C	2078	ARG
1	C	2091	LEU
1	C	2099	ARG
1	C	2106	LYS
1	C	2128	ARG
1	C	2135	LEU
1	C	2139	LEU
1	C	2154	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1786	ASN
1	A	1815	ASN
1	A	1919	GLN
1	A	1934	GLN
1	A	2008	ASN
1	A	2074	GLN
1	A	2097	HIS
1	A	2131	ASN
1	A	2165	HIS
1	B	1522	GLN
1	B	1560	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1683	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1815	ASN
1	B	1919	GLN
1	B	1934	GLN

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Mol	Chain	Res	Type
1	B	2008	ASN
1	B	2074	GLN
1	B	2097	HIS
1	B	2131	ASN
1	B	2142	GLN
1	C	1522	GLN
1	C	1560	ASN
1	C	1587	ASN
1	C	1605	ASN
1	C	1624	ASN
1	C	1748	GLN
1	C	1752	GLN
1	C	1815	ASN
1	C	1919	GLN
1	C	1934	GLN
1	C	2008	ASN
1	C	2074	GLN
1	C	2097	HIS
1	C	2131	ASN
1	C	2165	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 carbohydrates 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	B36	A	2242	-	39,39,39	1.23	4 (10%)	56,56,56	1.62	9 (16%)
2	B36	C	2242	-	39,39,39	1.18	2 (5%)	56,56,56	1.25	5 (8%)
2	B36	B	2242	-	39,39,39	1.12	3 (7%)	56,56,56	1.42	4 (7%)

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	B36	A	2242	-	-	0/12/22/22	0/6/6/6
2	B36	C	2242	-	-	0/12/22/22	0/6/6/6
2	B36	B	2242	-	-	0/12/22/22	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2242	B36	CAW-NBH	2.64	1.40	1.34
2	A	2242	B36	CAW-NBH	2.52	1.40	1.34
2	B	2242	B36	CAW-NBH	2.39	1.40	1.34
2	A	2242	B36	CBE-CBB	-2.22	1.38	1.43
2	C	2242	B36	CBF-CBC	-2.09	1.39	1.43
2	B	2242	B36	CBE-CBB	-2.08	1.39	1.43
2	A	2242	B36	CAL-CBF	-2.07	1.38	1.42
2	B	2242	B36	CBF-CBC	-2.02	1.39	1.43
2	A	2242	B36	CBF-CBC	-2.00	1.39	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2242	B36	OAB-CAW-CAZ	-6.21	115.58	121.59
2	B	2242	B36	OAB-CAW-CAZ	-6.20	115.58	121.59
2	C	2242	B36	OAB-CAW-CAZ	-5.15	116.60	121.59
2	A	2242	B36	CAO-CBA-CBD	3.41	122.72	118.27
2	B	2242	B36	CAO-CBA-CBD	3.01	122.20	118.27
2	A	2242	B36	CBF-CAZ-CAW	2.85	121.95	119.28
2	A	2242	B36	CAK-CBE-CAZ	-2.84	120.14	122.90
2	A	2242	B36	CAM-CBA-CAO	-2.70	117.26	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2242	B36	CAN-CBD-CBA	-2.69	116.21	119.04
2	A	2242	B36	OAB-CAW-NBH	2.54	126.53	122.34
2	A	2242	B36	CAS-NBH-CAT	2.38	117.21	112.62
2	C	2242	B36	CAO-CBA-CBD	2.38	121.38	118.27
2	C	2242	B36	OAB-CAW-NBH	2.33	126.19	122.34
2	A	2242	B36	CAA-CAX-CAG	-2.33	116.86	121.63
2	B	2242	B36	CBF-CAZ-CAW	2.21	121.35	119.28
2	C	2242	B36	CAY-CAU-CBG	-2.20	110.38	114.50
2	C	2242	B36	CAT-CAR-CBG	-2.12	106.63	111.99
2	A	2242	B36	CAK-CBE-CBB	2.12	120.63	117.89

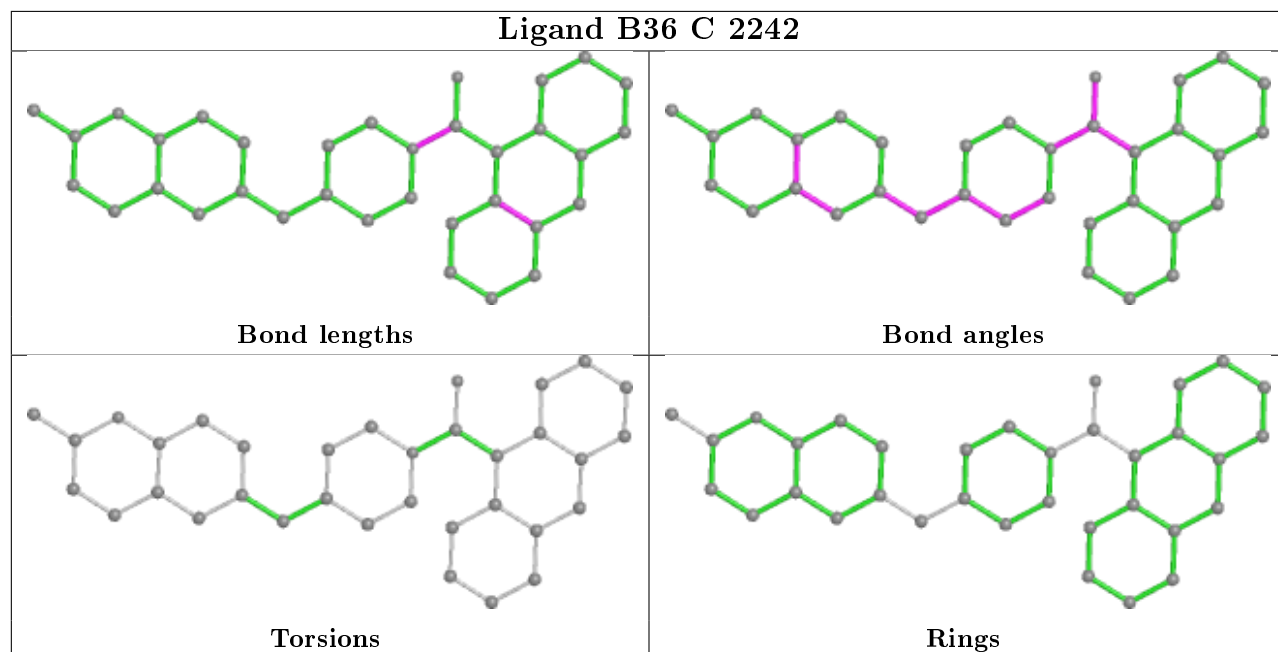
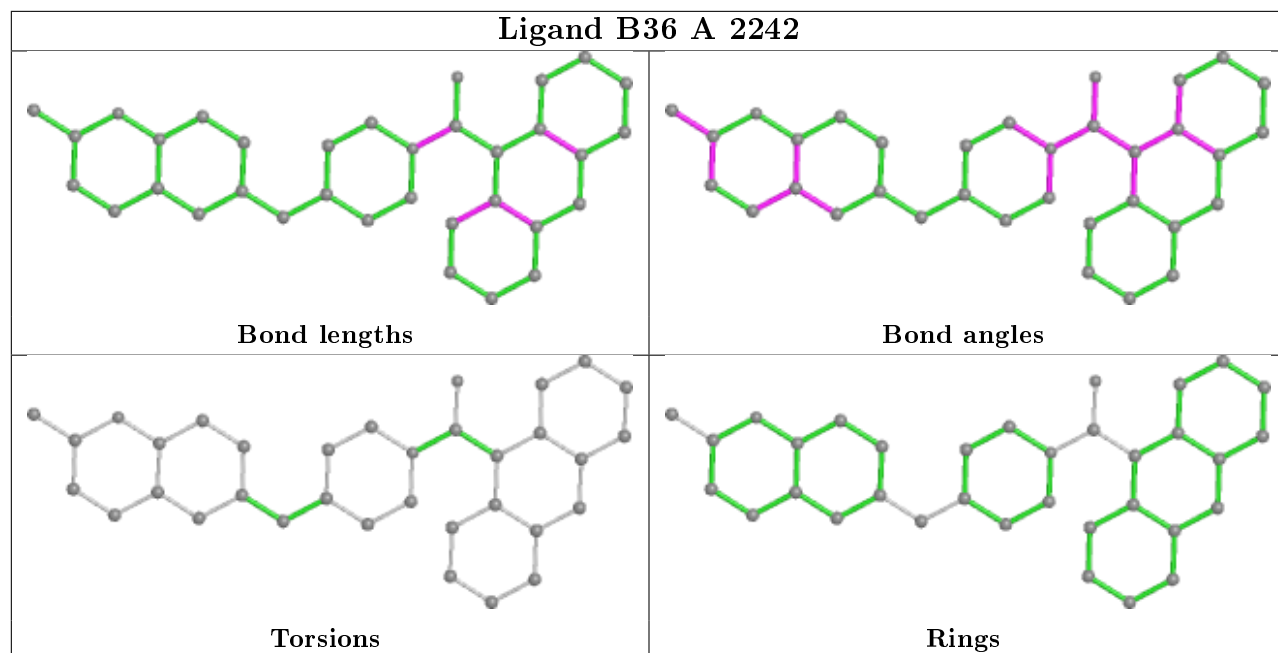
There are no chirality outliers.

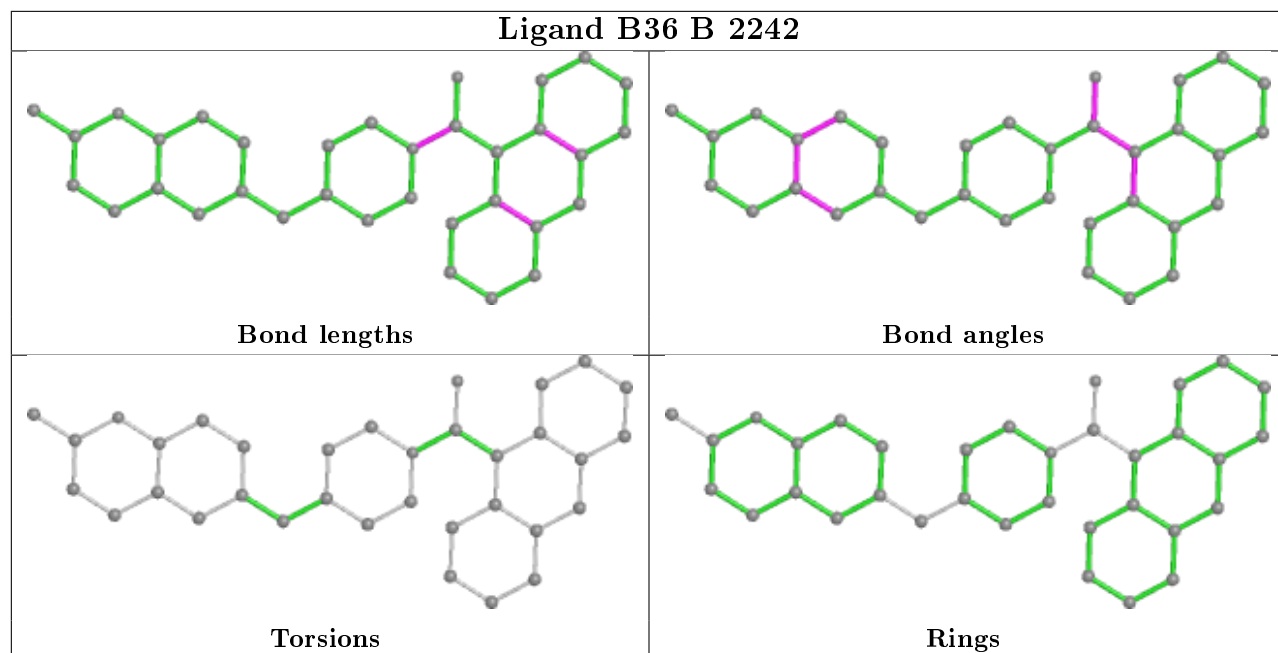
There are no torsion outliers.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	694/769 (90%)	0.13	25 (3%)	42 42	43, 63, 112, 147	1 (0%)
1	B	692/769 (89%)	0.41	66 (9%)	8 6	42, 67, 126, 184	1 (0%)
1	C	676/769 (87%)	0.33	45 (6%)	17 16	42, 66, 127, 169	1 (0%)
All	All	2062/2307 (89%)	0.29	136 (6%)	18 16	42, 65, 124, 184	3 (0%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2144	GLY	10.3
1	B	2082	LEU	6.9
1	C	2143	VAL	6.6
1	B	2190	LYS	5.9
1	B	2191	LEU	5.9
1	B	2075	LEU	5.7
1	B	2189	LEU	5.4
1	B	2144	GLY	5.3
1	A	1682	ILE	5.2
1	B	2143	VAL	4.9
1	C	1669	PHE	4.9
1	C	2082	LEU	4.5
1	B	2051	TYR	4.1
1	C	1666	LEU	4.0
1	C	2075	LEU	4.0
1	B	1682	ILE	3.9
1	B	2037	ARG	3.9
1	C	1650	ASP	3.9
1	C	1641	VAL	3.9
1	B	2077	ASP	3.7
1	C	1911	ASN	3.7
1	C	1668	LYS	3.7
1	C	1649	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	2193	SER	3.6
1	B	1669	PHE	3.6
1	B	1647	ALA	3.5
1	B	2158	TRP	3.5
1	A	1669	PHE	3.5
1	B	2086	TYR	3.5
1	B	1480	LEU	3.5
1	B	1668	LYS	3.4
1	C	1647	ALA	3.4
1	B	2078	ARG	3.4
1	B	2041	LEU	3.4
1	A	2189	LEU	3.4
1	B	2186	LEU	3.4
1	B	2145	GLU	3.3
1	C	2073	LYS	3.3
1	C	1680	THR	3.3
1	A	1911	ASN	3.3
1	B	2045	ASN	3.3
1	B	1651	LYS	3.3
1	C	2045	ASN	3.3
1	B	2080	ARG	3.3
1	C	1685	GLU	3.3
1	B	2084	PRO	3.3
1	C	2037	ARG	3.2
1	B	1637	PRO	3.2
1	B	2076	ALA	3.2
1	C	2145	GLU	3.1
1	A	2037	ARG	3.1
1	B	2047	LEU	3.1
1	C	2142	GLN	3.1
1	B	2073	LYS	3.1
1	B	1645	ASP	3.1
1	B	2179	TYR	3.0
1	B	1642	ALA	3.0
1	A	1637	PRO	3.0
1	B	2139	LEU	3.0
1	C	1665	THR	2.9
1	C	2041	LEU	2.9
1	B	1972	SER	2.9
1	C	1648	ASN	2.8
1	B	2085	ILE	2.8
1	B	1649	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	2044	MET	2.7
1	C	1902	LEU	2.7
1	C	1682	ILE	2.7
1	B	2081	GLU	2.7
1	A	1681	VAL	2.7
1	B	1648	ASN	2.7
1	C	1679	ARG	2.7
1	A	2145	GLU	2.7
1	B	2155	ILE	2.7
1	B	1646	ALA	2.6
1	B	1643	TRP	2.6
1	A	1916	LEU	2.6
1	A	2143	VAL	2.6
1	C	1646	ALA	2.6
1	A	1683	ASN	2.6
1	C	2086	TYR	2.6
1	B	1973	PHE	2.6
1	B	1666	LEU	2.6
1	B	2046	ARG	2.5
1	C	2083	LEU	2.5
1	B	1910	PRO	2.5
1	B	2083	LEU	2.5
1	C	1554	GLU	2.5
1	B	1688	PHE	2.5
1	C	2076	ALA	2.4
1	C	2189	LEU	2.4
1	B	1657	TYR	2.4
1	A	1933	ALA	2.4
1	B	1915	THR	2.4
1	C	1643	TRP	2.4
1	A	2041	LEU	2.4
1	B	2002	VAL	2.4
1	A	2075	LEU	2.4
1	B	1679	ARG	2.3
1	B	1670	ASP	2.3
1	C	1657	TYR	2.3
1	B	2043	THR	2.3
1	A	1666	LEU	2.3
1	B	2151	LYS	2.3
1	C	1655	TYR	2.3
1	C	1664	GLU	2.3
1	A	1483	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1670	ASP	2.2
1	B	2074	GLN	2.2
1	C	1547	ASN	2.2
1	A	2192	GLU	2.2
1	B	1667	LYS	2.2
1	A	1839	GLU	2.2
1	C	1546	GLU	2.2
1	B	2146	ALA	2.2
1	B	1658	LEU	2.1
1	A	1838	ASP	2.1
1	C	1684	GLY	2.1
1	C	2078	ARG	2.1
1	C	1715	THR	2.1
1	B	2142	GLN	2.1
1	C	1974	ILE	2.1
1	B	1911	ASN	2.1
1	A	1636	VAL	2.1
1	B	2159	TYR	2.1
1	C	1742	LEU	2.1
1	C	2002	VAL	2.1
1	B	1937	ASN	2.1
1	A	1855	GLY	2.1
1	A	2142	GLN	2.0
1	B	1650	ASP	2.0
1	B	1636	VAL	2.0
1	A	1977	ALA	2.0
1	B	1644	ASN	2.0
1	C	1553	VAL	2.0
1	A	1937	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

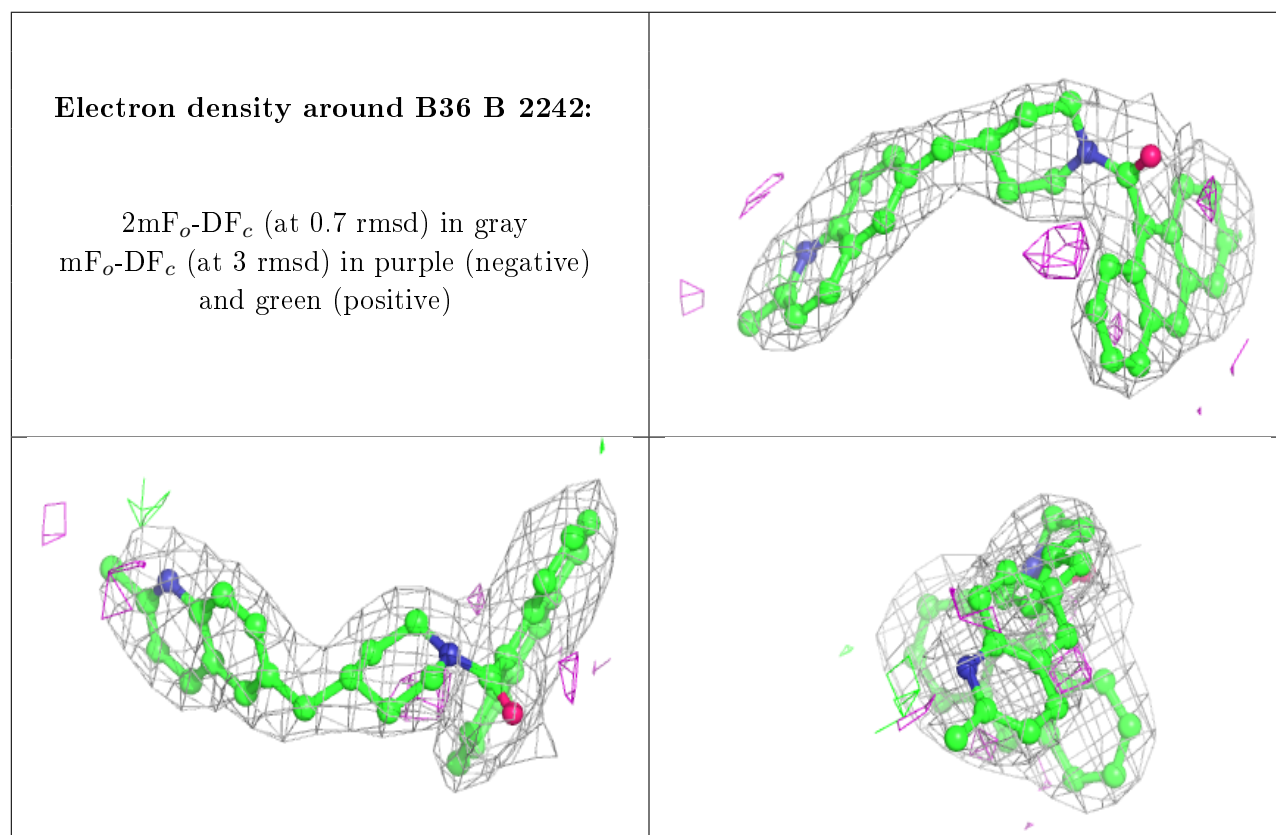
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

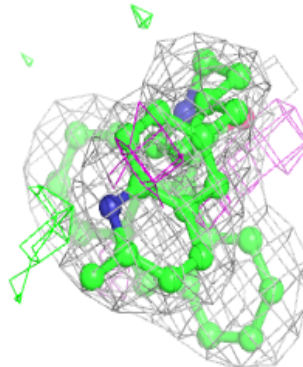
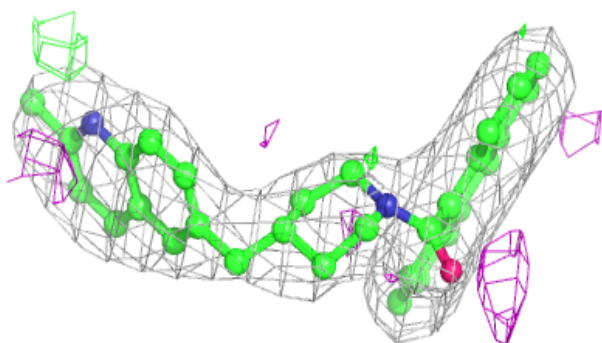
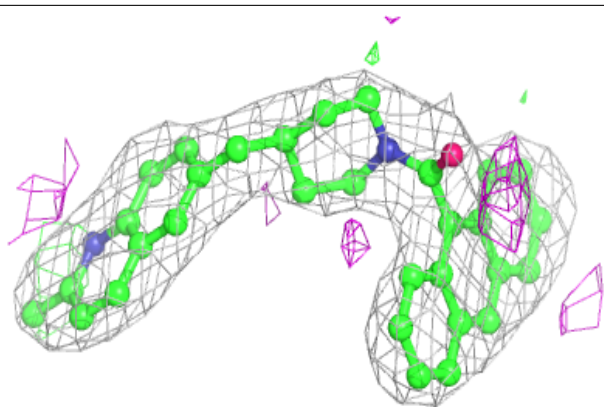
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	B36	B	2242	34/34	0.94	0.17	63,68,71,72	0
2	B36	C	2242	34/34	0.95	0.16	53,62,69,70	0
2	B36	A	2242	34/34	0.96	0.17	52,58,63,64	0

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.

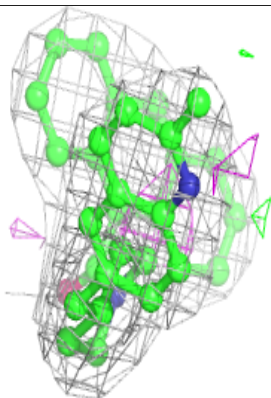
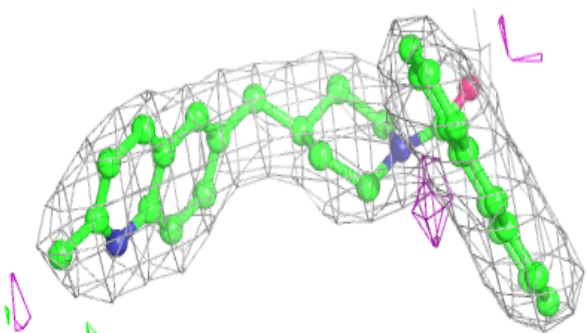
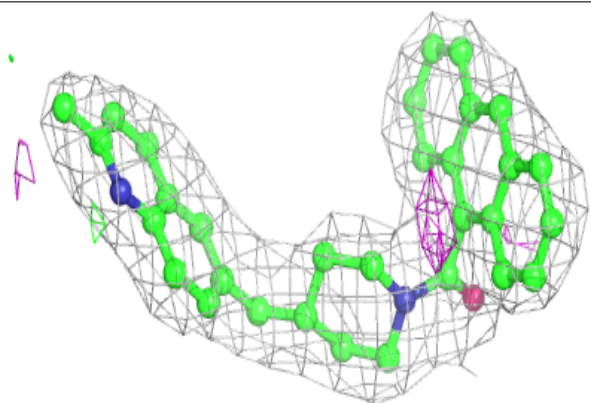


Electron density around B36 C 2242:

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

**Electron density around B36 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.