



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:17 PM UTC

PDB ID : 5CTE / pdb_00005cte
Title : Humanized yeast ACC carboxyltransferase domain bound to 2,2-dimethylpropyl (1S)-1-methyl-8-[(7-methyl-1H-indazol-5-yl)carbonyl]-2,8-diazaspiro[4.5]decane-2-carboxylate
Authors : Vajdos, F.F.
Deposited on : 2015-07-23
Resolution : 2.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

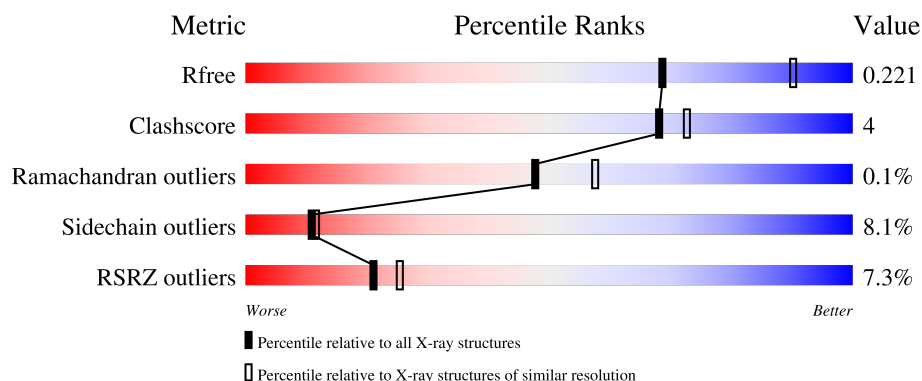
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	769	
1	C	769	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12599 atoms, of which 68 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	B	728	Total	C	N	O	S	0	1	0
			5796	3687	1000	1092	17			
1	C	721	Total	C	N	O	S	0	0	0
			5731	3638	990	1085	18			

There are 40 discrepancies between the modelled and reference sequences:

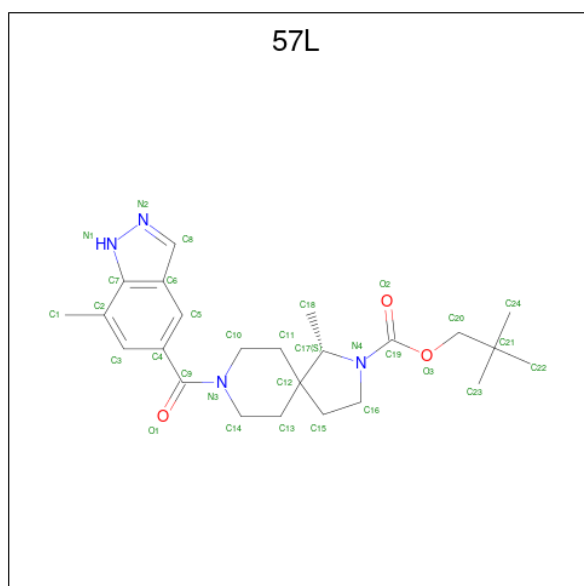
Chain	Residue	Modelled	Actual	Comment	Reference
B	1473	MET	-	expression tag	UNP Q00955
B	1474	ALA	-	expression tag	UNP Q00955
B	1475	SER	-	expression tag	UNP Q00955
B	1760	SER	PRO	engineered mutation	UNP Q00955
B	1762	LEU	ILE	engineered mutation	UNP Q00955
B	1765	VAL	MET	engineered mutation	UNP Q00955
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 2,2-dimethylpropyl (1S)-1-methyl-8-[(7-methyl-1H-indazol-5-yl)carbonyl]-2,8-diazaspiro[4.5]decane-2-carboxylate (CCD ID: 57L) (formula: C₂₄H₃₄N₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			65	24	34	4	3		
2	C	1	Total	C	H	N	O	0	0
			65	24	34	4	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		

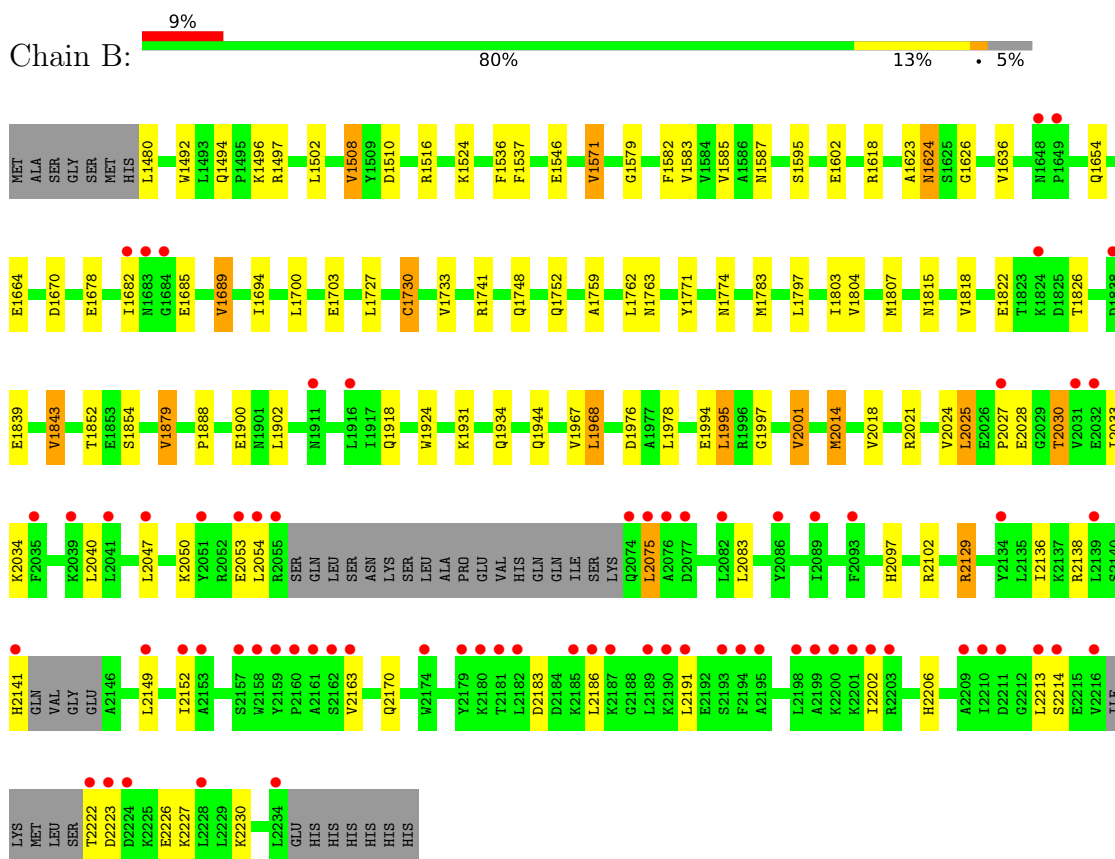
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	462	Total	O	0	0
			462	462		
4	C	475	Total	O	0	0
			475	475		

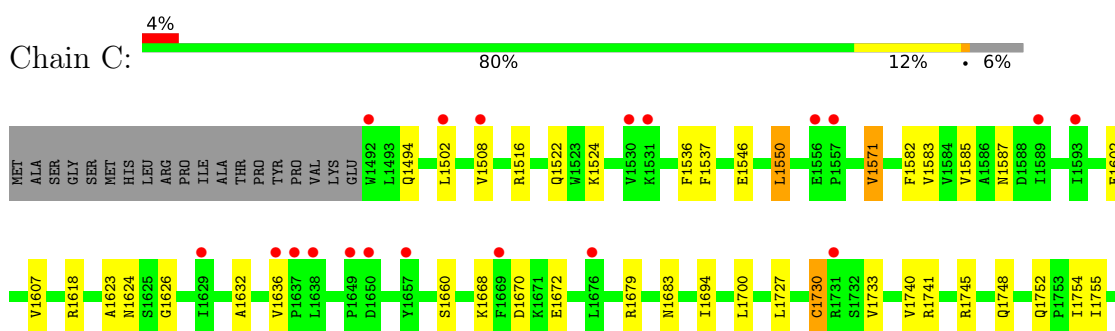
3 Residue-property plots

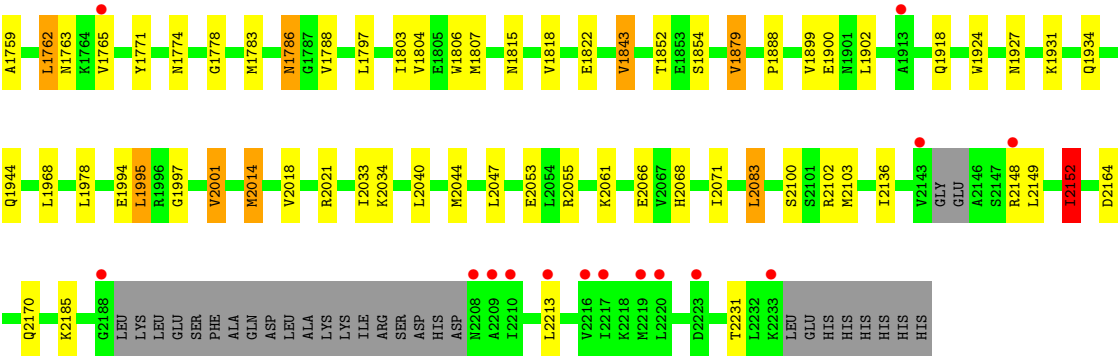
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Acetyl-CoA carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.34Å 138.12Å 185.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.05 – 2.34 42.05 – 2.34	Depositor EDS
% Data completeness (in resolution range)	92.4 (42.05-2.34) 92.5 (42.05-2.34)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.34Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.6	Depositor
R, R_{free}	0.185 , 0.217 0.186 , 0.221	Depositor DCC
R_{free} test set	4686 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12599	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: 57L, SO4

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	B	0.83	2/5919 (0.0%)	1.28	10/8013 (0.1%)
1	C	0.84	3/5848 (0.1%)	1.27	9/7916 (0.1%)
All	All	0.84	5/11767 (0.0%)	1.28	19/15929 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2014	MET	SD-CE	-7.54	1.60	1.79
1	B	2014	MET	SD-CE	-6.29	1.63	1.79
1	C	1636	VAL	CA-C	6.03	1.58	1.52
1	B	1636	VAL	CA-CB	5.94	1.57	1.54
1	C	1636	VAL	CA-CB	5.26	1.57	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1683	ASN	CA-CB-CG	7.33	119.93	112.60
1	C	2152	ILE	N-CA-CB	6.83	120.83	110.58
1	B	1689	VAL	N-CA-CB	5.89	117.55	110.31
1	B	1730	CYS	N-CA-C	-5.88	101.05	108.45
1	C	1730	CYS	N-CA-C	-5.69	101.28	108.45
1	B	1839	GLU	CA-C-N	5.64	128.72	120.71
1	B	1839	GLU	C-N-CA	5.64	128.72	120.71
1	B	1976	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	1508	VAL	N-CA-CB	5.45	117.28	110.47
1	C	2071	ILE	CA-C-N	5.30	127.38	120.28
1	C	2071	ILE	C-N-CA	5.30	127.38	120.28
1	B	1843	VAL	CB-CA-C	-5.24	104.41	112.05
1	C	1843	VAL	CB-CA-C	-5.15	104.53	112.05
1	B	1624	ASN	N-CA-C	5.11	115.28	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1492	TRP	N-CA-C	-5.11	106.74	113.12
1	B	2183	ASP	N-CA-C	-5.05	105.85	111.36
1	C	1927	ASN	CA-CB-CG	5.04	117.64	112.60
1	C	1660	SER	CA-C-N	5.01	126.95	120.44
1	C	1660	SER	C-N-CA	5.01	126.95	120.44

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	B	5796	0	5716	47	0
1	C	5731	0	5653	40	0
2	B	31	34	34	0	0
2	C	31	34	34	0	0
3	C	5	0	0	0	0
4	B	462	0	0	7	0
4	C	475	0	0	3	0
All	All	12531	68	11437	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 4.

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)
1:B:1595:SER:HB3	4:B:2406:HOH:O	1.64	0.94
1:B:2129:ARG:HG2	1:B:2129:ARG:HH11	1.39	0.86
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.27	0.79
1:C:1763:ASN:HD21	1:C:1771:TYR:H	1.29	0.78
1:C:1730:CYS:HA	1:C:1752:GLN:HE21	1.48	0.77
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.49	0.76
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.34	0.74
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1672:GLU:HG3	4:C:2590:HOH:O	1.99	0.62
1:C:1899:VAL:HB	4:C:2576:HOH:O	2.00	0.60
1:B:2163:VAL:HA	1:B:2170:GLN:NE2	2.16	0.60
1:B:1759:ALA:H	1:B:1774:ASN:ND2	2.00	0.60
1:C:1759:ALA:H	1:C:1774:ASN:ND2	2.01	0.59
1:B:2129:ARG:HH11	1:B:2129:ARG:CG	2.13	0.59
1:C:1900:GLU:HB3	1:C:1918:GLN:HE21	1.68	0.58
1:B:1900:GLU:HB3	1:B:1918:GLN:HE21	1.67	0.58
1:B:2163:VAL:HG12	4:B:2475:HOH:O	2.02	0.58
1:B:2040:LEU:HD21	4:B:2415:HOH:O	2.02	0.58
1:C:1754:ILE:O	1:C:1778:GLY:HA3	2.05	0.57
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.50	0.57
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.02	0.57
1:B:1497:ARG:HD3	1:B:1510:ASP:OD2	2.06	0.56
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.72	0.55
1:B:2136:ILE:HD11	1:B:2152:ILE:HG22	1.88	0.54
1:B:1815:ASN:ND2	1:B:1944:GLN:HE22	2.05	0.53
1:C:1624:ASN:HD21	1:C:1733:VAL:H	1.57	0.53
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.44	0.52
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.74	0.52
1:B:1968:LEU:HD13	4:B:2526:HOH:O	2.10	0.52
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.07	0.52
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.75	0.51
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.75	0.50
1:C:1624:ASN:ND2	1:C:1733:VAL:H	2.10	0.50
1:B:2054:LEU:HB3	1:B:2075:LEU:HG	1.94	0.49
1:B:2027:PRO:HA	1:B:2030:THR:HG23	1.94	0.49
1:C:1762:LEU:HA	1:C:1765:VAL:HG22	1.94	0.49
1:C:2033:ILE:HG22	1:C:2034:LYS:HG2	1.95	0.49
1:C:2136:ILE:HD11	1:C:2152:ILE:HG23	1.94	0.49
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.60	0.48
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.11	0.48
1:C:1550:LEU:HD21	1:C:1607:VAL:HG22	1.96	0.47
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.33	0.47
1:C:1995:LEU:HD23	1:C:2014:MET:HE1	1.95	0.47
1:B:1703:GLU:OE1	1:C:2102:ARG:NH2	2.47	0.47
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.61	0.47
1:C:1741:ARG:HH22	1:C:1934:GLN:NE2	2.13	0.47
1:C:1786:ASN:C	1:C:1786:ASN:HD22	2.20	0.47
1:B:1995:LEU:HD23	1:B:2014:MET:HE1	1.97	0.47
1:B:2050:LYS:HB3	4:B:2746:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2044:MET:HE1	1:C:2083:LEU:HD13	1.96	0.46
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.51	0.45
1:B:2033:ILE:HG22	1:B:2034:LYS:HG2	1.98	0.44
1:C:1727:LEU:HB2	1:C:1803:ILE:HD11	1.99	0.44
1:B:1582:PHE:CD1	1:B:1807:MET:HE1	2.53	0.44
1:C:1624:ASN:HD22	1:C:1626:GLY:H	1.66	0.44
1:C:1879:VAL:HG13	1:C:1931:LYS:HE2	2.00	0.44
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	2.00	0.44
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.65	0.44
1:C:1997:GLY:O	1:C:2001:VAL:HG12	2.18	0.44
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.52	0.43
1:B:2214:SER:CB	1:C:2231:THR:HG21	2.48	0.43
1:B:1967:VAL:CG1	4:B:2526:HOH:O	2.67	0.43
1:B:1826:THR:HA	4:B:2447:HOH:O	2.19	0.43
1:C:2068:HIS:HE1	4:C:2429:HOH:O	2.00	0.43
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	2.01	0.42
1:B:2102:ARG:HD2	1:C:1694:ILE:HA	1.99	0.42
1:B:1879:VAL:HG13	1:B:1931:LYS:HE2	2.00	0.42
1:B:2222:THR:HG23	1:B:2223:ASP:H	1.84	0.42
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.18	0.42
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	2.01	0.42
1:C:1786:ASN:ND2	1:C:1788:VAL:H	2.17	0.42
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.20	0.41
1:B:1997:GLY:O	1:B:2001:VAL:HG12	2.20	0.41
1:B:2024:VAL:HG12	1:B:2025:LEU:HD13	2.01	0.41
1:C:2100:SER:HA	1:C:2103:MET:HE3	2.03	0.41
1:B:1694:ILE:HA	1:C:2102:ARG:HD2	2.03	0.41
1:B:2227:LYS:HA	1:B:2230:LYS:HE3	2.01	0.41
1:C:1994:GLU:HA	1:C:2021:ARG:O	2.21	0.41
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.20	0.40
1:B:1494:GLN:NE2	1:B:1496:LYS:HB2	2.37	0.40
1:C:1582:PHE:CD1	1:C:1807:MET:HE1	2.56	0.40
1:B:2129:ARG:CG	1:B:2129:ARG:NH1	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	721/769 (94%)	703 (98%)	17 (2%)	1 (0%)	48	57
1	C	715/769 (93%)	696 (97%)	19 (3%)	0	100	100
All	All	1436/1538 (93%)	1399 (97%)	36 (2%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2206	HIS

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	B	612/658 (93%)	560 (92%)	52 (8%)	10	10
1	C	609/658 (93%)	561 (92%)	48 (8%)	11	12
All	All	1221/1316 (93%)	1121 (92%)	100 (8%)	11	11

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1480	LEU
1	B	1502	LEU
1	B	1508	VAL
1	B	1516	ARG
1	B	1524	LYS

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Mol	Chain	Res	Type
1	B	1536	PHE
1	B	1546	GLU
1	B	1571	VAL
1	B	1583	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1618	ARG
1	B	1654	GLN
1	B	1664	GLU
1	B	1670	ASP
1	B	1678	GLU
1	B	1682	ILE
1	B	1685	GLU
1	B	1689	VAL
1	B	1700	LEU
1	B	1762	LEU
1	B	1797	LEU
1	B	1804	VAL
1	B	1822	GLU
1	B	1843	VAL
1	B	1852	THR
1	B	1854	SER
1	B	1879	VAL
1	B	1902	LEU
1	B	1924	TRP
1	B	1968	LEU
1	B	1978	LEU
1	B	1995	LEU
1	B	2001	VAL
1	B	2018	VAL
1	B	2025	LEU
1	B	2028[A]	GLU
1	B	2028[B]	GLU
1	B	2030	THR
1	B	2047	LEU
1	B	2053	GLU
1	B	2075	LEU
1	B	2083	LEU
1	B	2129	ARG
1	B	2138	ARG
1	B	2141	HIS
1	B	2149	LEU

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Mol	Chain	Res	Type
1	B	2186	LEU
1	B	2191	LEU
1	B	2202	ILE
1	B	2213	LEU
1	B	2226	GLU
1	C	1494	GLN
1	C	1502	LEU
1	C	1508	VAL
1	C	1516	ARG
1	C	1522	GLN
1	C	1524	LYS
1	C	1536	PHE
1	C	1546	GLU
1	C	1550	LEU
1	C	1571	VAL
1	C	1583	VAL
1	C	1585	VAL
1	C	1602	GLU
1	C	1618	ARG
1	C	1668	LYS
1	C	1670	ASP
1	C	1679	ARG
1	C	1700	LEU
1	C	1740	VAL
1	C	1755	ILE
1	C	1762	LEU
1	C	1786	ASN
1	C	1797	LEU
1	C	1804	VAL
1	C	1822	GLU
1	C	1843	VAL
1	C	1852	THR
1	C	1854	SER
1	C	1879	VAL
1	C	1902	LEU
1	C	1924	TRP
1	C	1968	LEU
1	C	1978	LEU
1	C	1995	LEU
1	C	2001	VAL
1	C	2018	VAL
1	C	2040	LEU

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Mol	Chain	Res	Type
1	C	2047	LEU
1	C	2053	GLU
1	C	2055	ARG
1	C	2061	LYS
1	C	2066	GLU
1	C	2083	LEU
1	C	2148	ARG
1	C	2149	LEU
1	C	2152	ILE
1	C	2185	LYS
1	C	2213	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1494	GLN
1	B	1587	ASN
1	B	1599	GLN
1	B	1605	ASN
1	B	1624	ASN
1	B	1640	GLN
1	B	1648	ASN
1	B	1654	GLN
1	B	1673	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1774	ASN
1	B	1815	ASN
1	B	1918	GLN
1	B	1934	GLN
1	B	2019	ASN
1	B	2092	GLN
1	B	2097	HIS
1	C	1587	ASN
1	C	1605	ASN
1	C	1624	ASN
1	C	1673	ASN
1	C	1683	ASN
1	C	1748	GLN
1	C	1752	GLN
1	C	1763	ASN

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Mol	Chain	Res	Type
1	C	1774	ASN
1	C	1786	ASN
1	C	1815	ASN
1	C	1918	GLN
1	C	1934	GLN
1	C	2070	GLN
1	C	2165	HIS
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 oligosaccharides 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	$\# Z > 2$
3	SO4	C	2302	-	4,4,4	0.32	0	6,6,6	0.27	0
2	57L	C	2301	-	33,34,34	1.46	3 (9%)	44,52,52	1.26	7 (15%)
2	57L	B	2301	-	33,34,34	1.49	4 (12%)	44,52,52	1.21	6 (13%)

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	57L	C	2301	-	-	0/18/46/46	0/4/4/4
2	57L	B	2301	-	-	0/18/46/46	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2301	57L	C7-N1	4.71	1.39	1.36
2	C	2301	57L	C7-N1	4.57	1.39	1.36
2	C	2301	57L	C8-N2	4.53	1.35	1.32
2	B	2301	57L	C8-N2	4.52	1.35	1.32
2	B	2301	57L	C9-N3	2.49	1.40	1.34
2	C	2301	57L	C9-N3	2.30	1.39	1.34
2	B	2301	57L	C19-N4	2.07	1.38	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2301	57L	C7-C6-C8	3.02	105.48	103.94
2	B	2301	57L	C7-C6-C8	2.87	105.40	103.94
2	B	2301	57L	C5-C4-C3	2.59	122.69	119.65
2	C	2301	57L	C5-C4-C3	2.55	122.63	119.65
2	C	2301	57L	C6-C5-C4	-2.54	117.32	121.32
2	B	2301	57L	C6-C5-C4	-2.51	117.38	121.32
2	C	2301	57L	C6-C8-N2	-2.43	109.91	111.68
2	B	2301	57L	C6-C8-N2	-2.34	109.97	111.68
2	B	2301	57L	C1-C2-C3	2.30	123.62	119.57
2	B	2301	57L	C8-N2-N1	2.27	107.21	106.02
2	C	2301	57L	C8-N2-N1	2.27	107.21	106.02
2	C	2301	57L	C1-C2-C3	2.17	123.39	119.57
2	C	2301	57L	O3-C19-N4	2.02	113.36	111.02

There are no chirality outliers.

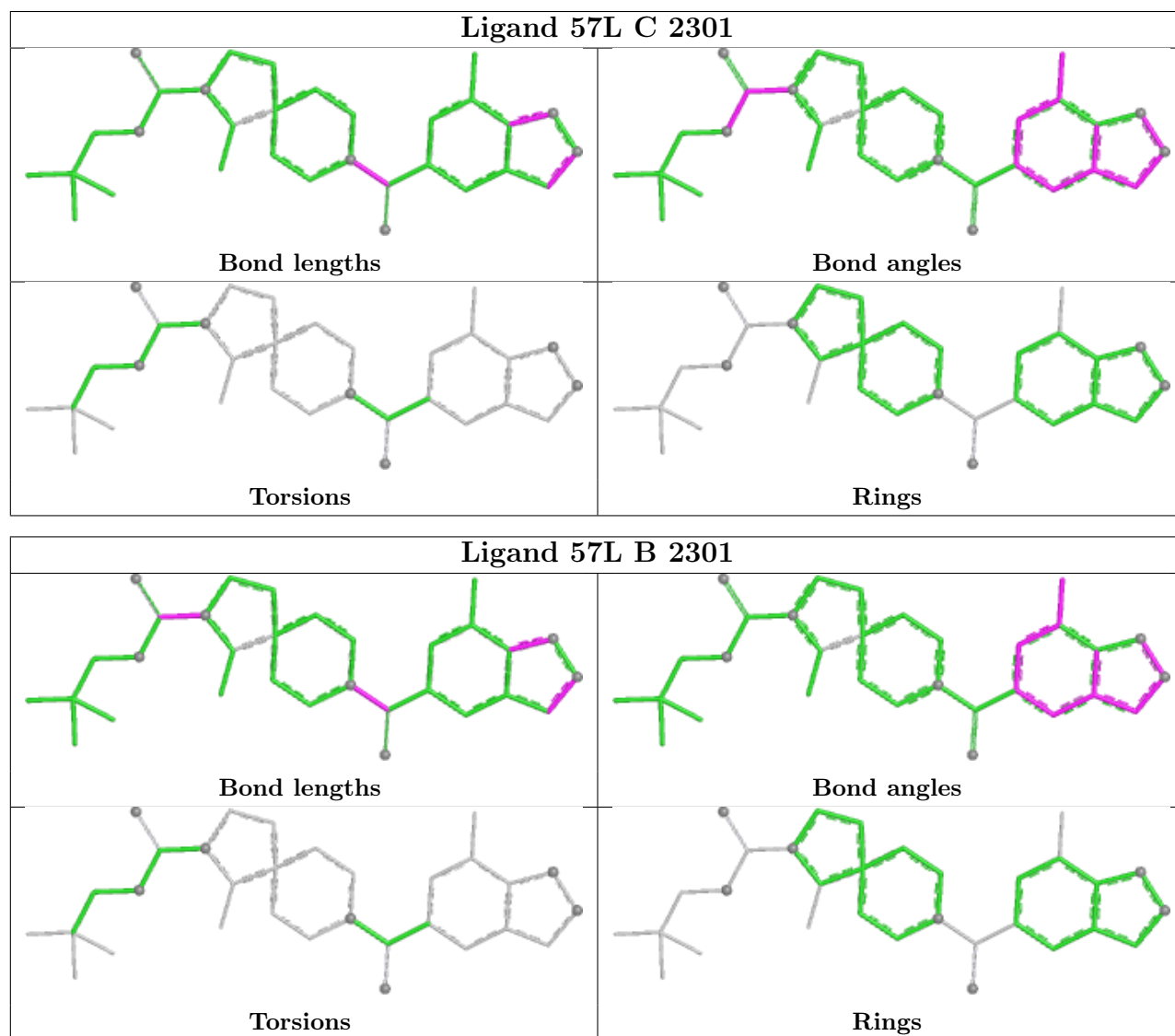
There are no torsion outliers.

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 ⓘ

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	B	728/769 (94%)	0.36	72 (9%)	13 15	32, 53, 125, 152	1 (0%)
1	C	721/769 (93%)	0.32	34 (4%)	36 42	30, 55, 97, 126	0
All	All	1449/1538 (94%)	0.34	106 (7%)	21 25	30, 54, 110, 152	1 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2216	VAL	6.4
1	B	2186	LEU	5.3
1	B	2234	LEU	5.2
1	B	2213	LEU	5.2
1	B	2202	ILE	4.9
1	B	2163	VAL	4.6
1	B	2179	TYR	4.6
1	B	2199	ALA	4.4
1	B	2152	ILE	4.3
1	C	1492	TRP	4.2
1	C	2188	GLY	4.2
1	B	2139	LEU	4.2
1	C	2208	ASN	4.1
1	B	2075	LEU	4.1
1	B	2153	ALA	3.9
1	B	2162	SER	3.9
1	B	2210	ILE	3.8
1	C	2213	LEU	3.8
1	B	2161	ALA	3.7
1	B	2194	PHE	3.7
1	B	2054	LEU	3.5
1	B	2195	ALA	3.5
1	C	2217	ILE	3.5
1	B	2189	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	2222	THR	3.4
1	C	2233	LYS	3.4
1	C	2143	VAL	3.4
1	B	2198	LEU	3.3
1	B	2086	TYR	3.3
1	B	2141	HIS	3.2
1	C	2216	VAL	3.2
1	B	1684	GLY	3.0
1	B	2160	PRO	3.0
1	B	2191	LEU	3.0
1	C	1629	ILE	3.0
1	C	1508	VAL	2.9
1	B	1682	ILE	2.9
1	B	2159	TYR	2.9
1	C	1556	GLU	2.9
1	B	2223	ASP	2.9
1	C	2223	ASP	2.9
1	C	2209	ALA	2.9
1	B	2158	TRP	2.9
1	B	2055	ARG	2.8
1	C	1530	VAL	2.8
1	C	1765	VAL	2.8
1	B	1683	ASN	2.8
1	B	2211	ASP	2.8
1	C	1557	PRO	2.8
1	B	2190	LYS	2.8
1	B	2047	LEU	2.8
1	B	2228	LEU	2.8
1	B	2076	ALA	2.8
1	C	1669	PHE	2.8
1	B	2180	LYS	2.7
1	B	2041	LEU	2.7
1	B	2134	TYR	2.7
1	B	2182	LEU	2.7
1	B	2185	LYS	2.6
1	C	1913	ALA	2.5
1	C	1637	PRO	2.5
1	B	2077	ASP	2.5
1	B	2174	TRP	2.5
1	B	2149	LEU	2.5
1	C	1650	ASP	2.5
1	C	2220	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	2157	SER	2.4
1	C	2210	ILE	2.4
1	B	2032	GLU	2.4
1	B	2051	TYR	2.3
1	B	2224	ASP	2.3
1	C	1593	ILE	2.3
1	B	2089	ILE	2.3
1	B	2093	PHE	2.3
1	B	2082	LEU	2.3
1	B	2039	LYS	2.3
1	C	1657	TYR	2.3
1	B	2074	GLN	2.2
1	B	2181	THR	2.2
1	C	1502	LEU	2.2
1	B	1648	ASN	2.2
1	B	1911	ASN	2.2
1	B	2027	PRO	2.2
1	B	1824	LYS	2.2
1	B	2209	ALA	2.2
1	B	2214	SER	2.2
1	C	1636	VAL	2.2
1	C	1649	PRO	2.2
1	B	2187	LYS	2.2
1	B	2203	ARG	2.2
1	C	2148	ARG	2.2
1	C	1531	LYS	2.2
1	B	2193	SER	2.2
1	C	1731	ARG	2.1
1	C	2219	MET	2.1
1	B	2031	VAL	2.1
1	B	2035	PHE	2.1
1	B	1916	LEU	2.1
1	B	2201	LYS	2.1
1	B	1649	PRO	2.1
1	B	2053	GLU	2.1
1	C	1676	LEU	2.1
1	B	1838	ASP	2.1
1	B	2200	LYS	2.0
1	C	1589	ILE	2.0
1	C	1638	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

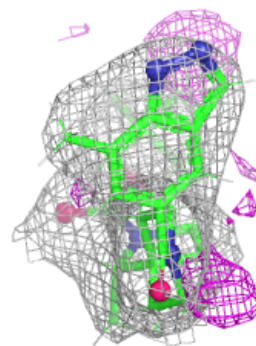
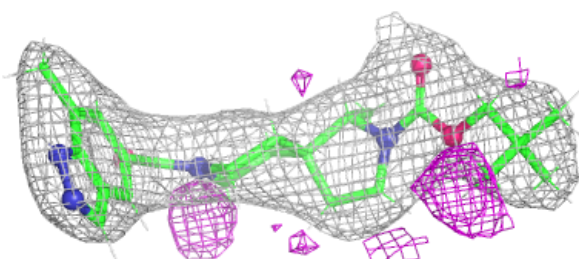
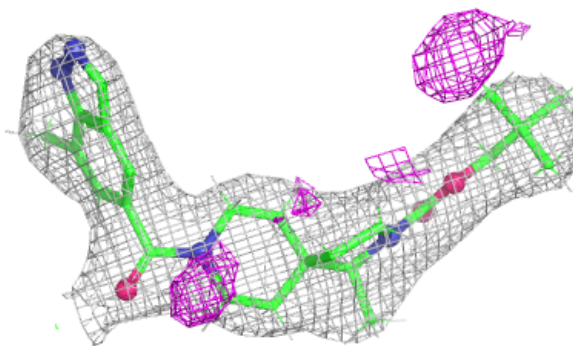
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	57L	B	2301	31/31	0.93	0.10	46,57,76,79	0
2	57L	C	2301	31/31	0.96	0.08	39,48,54,60	0
3	SO4	C	2302	5/5	0.96	0.05	83,85,86,87	0

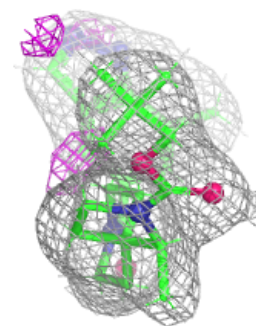
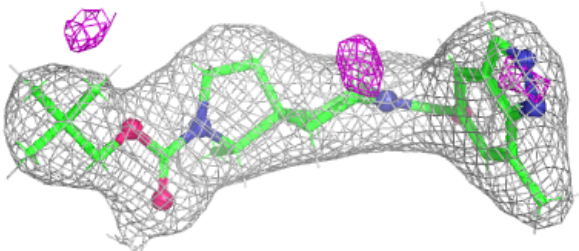
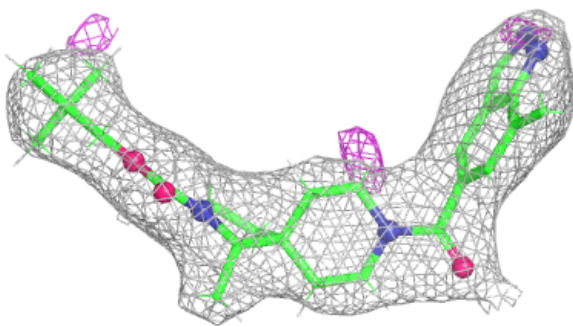
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 57L B 2301:

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

**Electron density around 57L C 2301:**

$2mF_o-DF_c$ (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.