Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:31 AM BST

PDB ID	:	5CTC
Title	:	Humanized yeast ACC carboxyltransferase domain bound to tert-butyl 7-[(7-methyl-1H-indazol-5-yl)carbonyl]-2,7-diazaspiro[3.5]nonane-2-carboxylate
Authors	:	Vajdos, F.F.
Deposited on	:	2015-07-23
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:

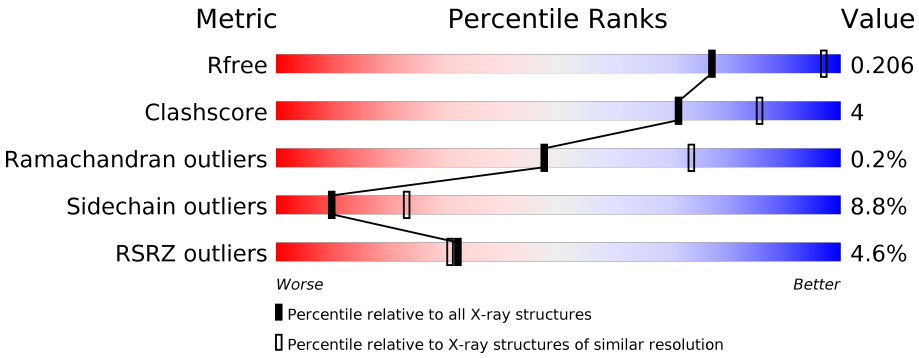
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.70 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 <=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	4% 77% 13% • 10%
1	B	769	5% 76% 12% • 11%
1	C	769	4% 74% 13% • 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	2303	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17404 atoms, of which 84 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	691	Total	C	N	O	S	0	1	0
			5521	3512	953	1039	17			
1	B	687	Total	C	N	O	S	0	0	0
			5482	3492	943	1030	17			
1	C	681	Total	C	N	O	S	0	0	0
			5433	3453	937	1026	17			

There are 60 discrepancies between the modelled and reference sequences:

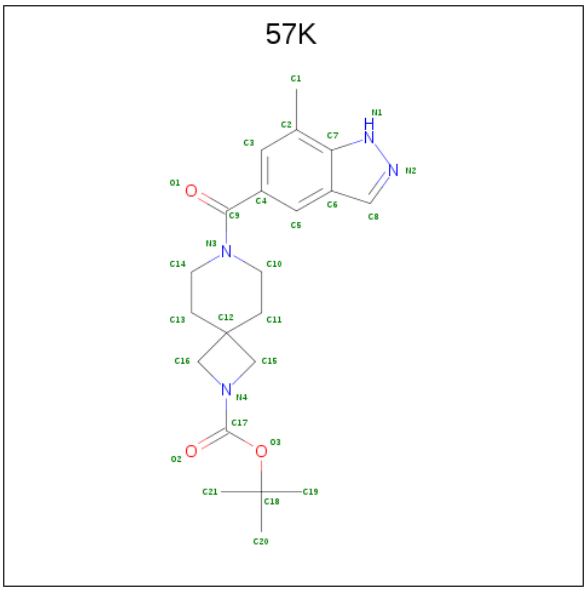
Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	expression tag	UNP Q00955
A	1474	ALA	-	expression tag	UNP Q00955
A	1475	SER	-	expression tag	UNP Q00955
A	1760	SER	PRO	engineered mutation	UNP Q00955
A	1762	LEU	ILE	engineered mutation	UNP Q00955
A	1765	VAL	MET	engineered mutation	UNP Q00955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

Continued on next page...

Continued from previous page...

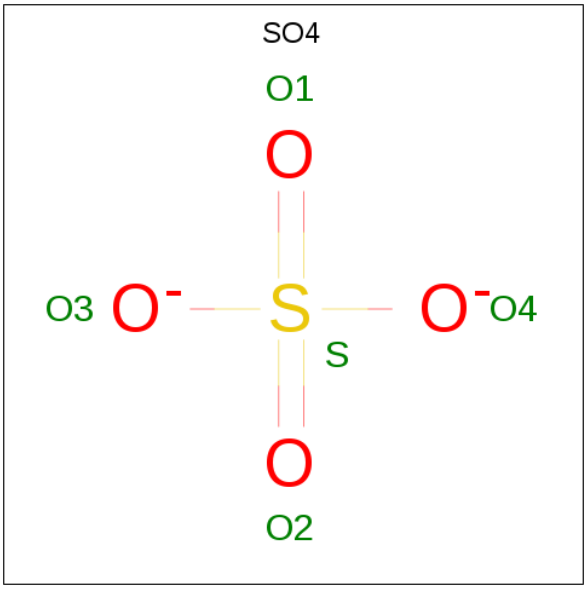
Chain	Residue	Modelled	Actual	Comment	Reference
B	1760	SER	PRO	engineered mutation	UNP Q00955
B	1762	LEU	ILE	engineered mutation	UNP Q00955
B	1765	VAL	MET	engineered mutation	UNP Q00955
B	1919	GLN	GLU	engineered mutation	UNP Q00955
B	1920	ALA	PRO	engineered mutation	UNP Q00955
B	1925	PHE	HIS	engineered 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 tert-butyl 7-[(7-methyl-1H-indazol-5-yl)carbonyl]-2,7-diazaspiro[3.5]nonane-2-carboxylate (three-letter code: 57K) (formula: $C_{21}H_{28}N_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			56	21	28	4	3		
2	B	1	Total	C	H	N	O	0	0
			56	21	28	4	3		
2	C	1	Total	C	H	N	O	0	0
			56	21	28	4	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

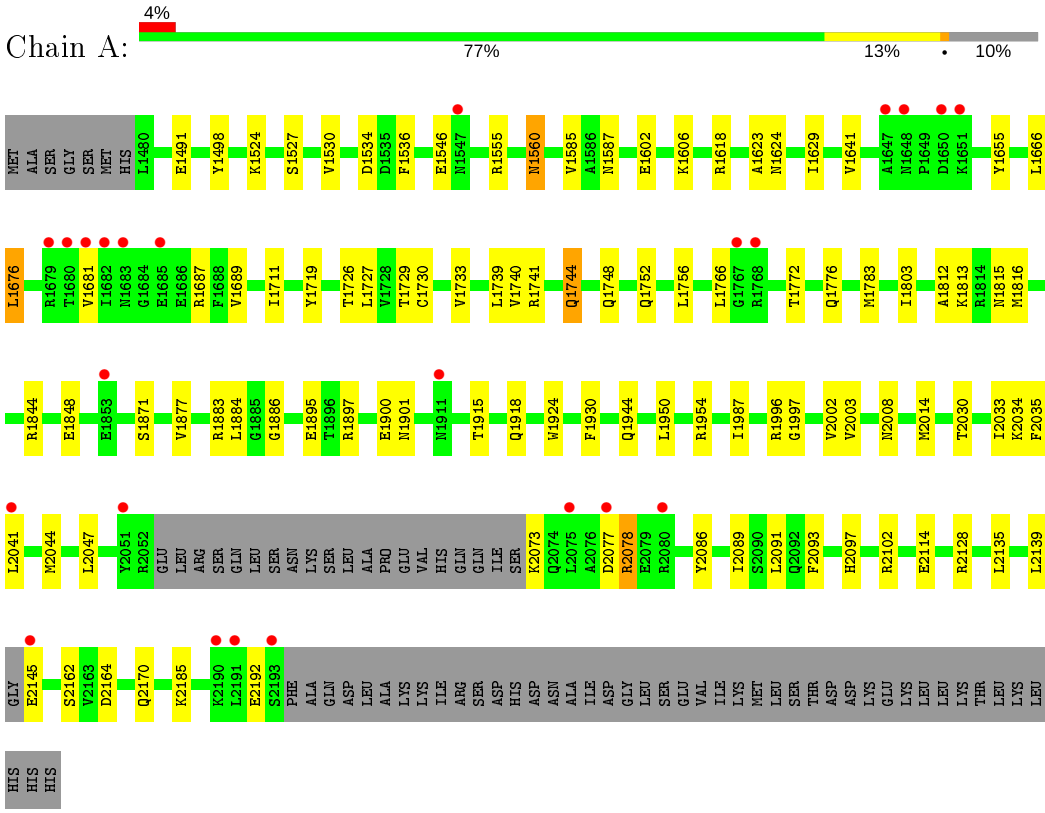
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	283	Total O 283 283	0	0
4	B	257	Total O 257 257	0	0
4	C	245	Total O 245 245	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

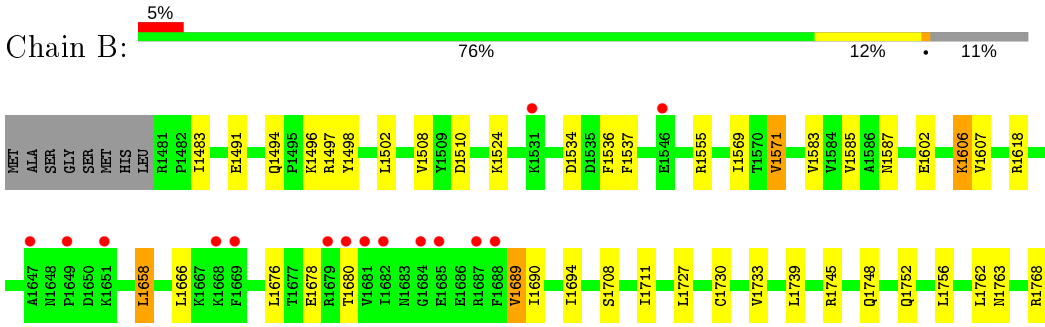
- Molecule 1: Acetyl-CoA carboxylase

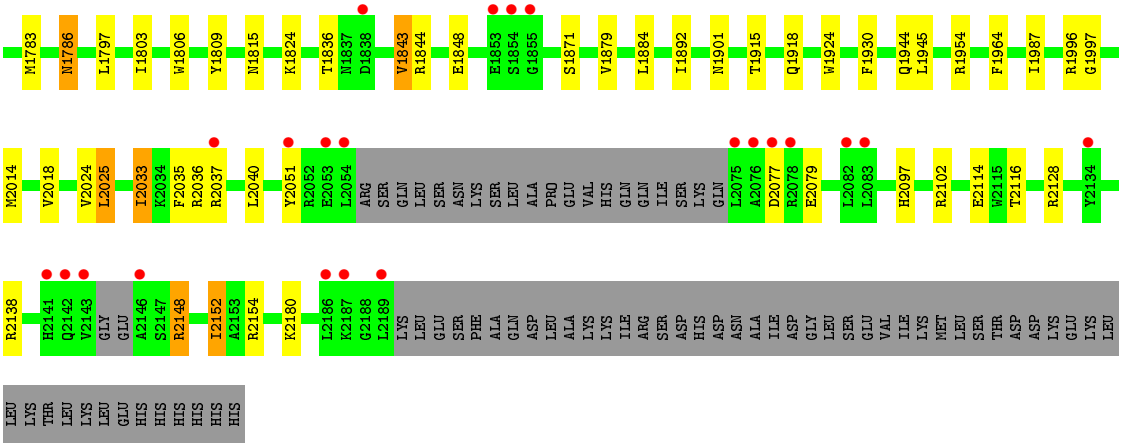
Chain A:



- Molecule 1: Acetyl-CoA carboxylase

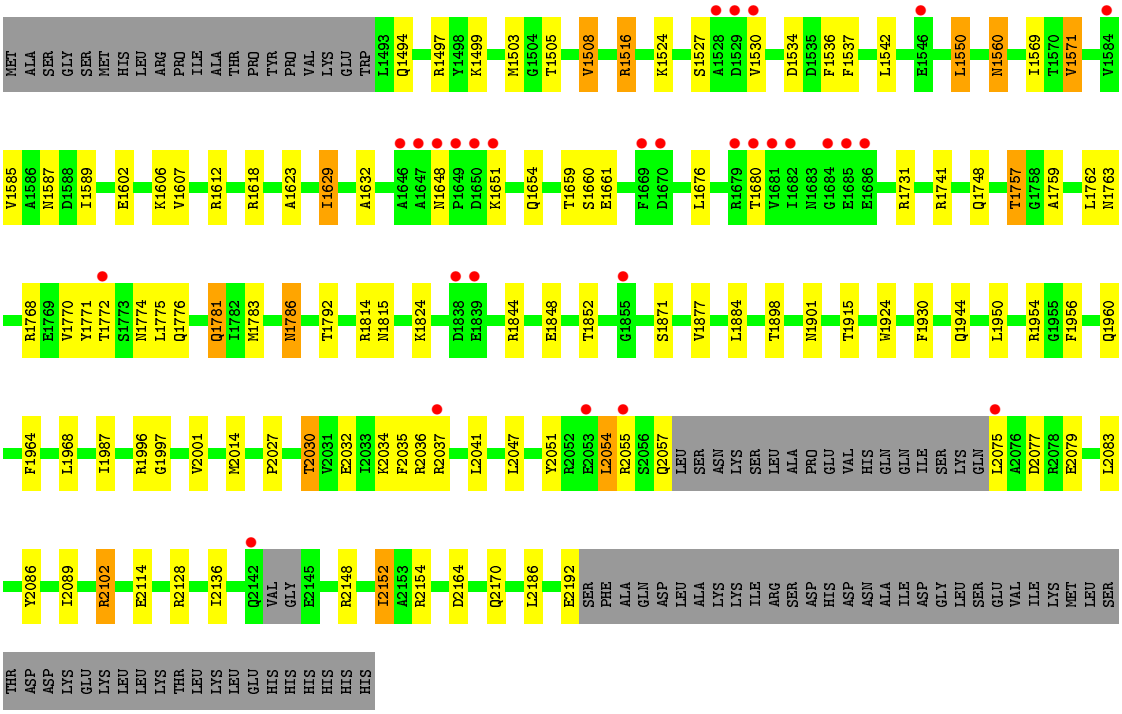
Chain B:





• 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	247.27Å 122.70Å 146.43Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	32.63 – 2.70 32.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (32.63-2.70) 96.2 (32.63-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.68Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.6	Depositor
R, R_{free}	0.173 , 0.201 0.179 , 0.206	Depositor DCC
R_{free} test set	11469 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 78.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17404	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 57K, 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	A	0.52	0/5647	0.71	0/7647
1	B	0.51	0/5601	0.71	0/7588
1	C	0.51	0/5546	0.71	0/7506
All	All	0.51	0/16794	0.71	0/22741

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	5521	0	5446	37	0
1	B	5482	0	5414	40	0
1	C	5433	0	5363	49	0
2	A	28	28	28	0	0
2	B	28	28	28	2	0
2	C	28	28	28	0	0
3	A	5	0	0	0	0
3	C	10	0	0	0	0
4	A	283	0	0	0	0
4	B	257	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	245	0	0	3	0
All	All	17320	84	16307	116	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 (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1629:ILE:CD1	1:C:1629:ILE:CG1	1.75	1.63
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.18	0.91
1:C:1763:ASN:HD21	1:C:1771:TYR:H	1.21	0.89
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.41	0.84
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.51	0.76
1:A:2078:ARG:HH11	1:A:2078:ARG:HA	1.49	0.76
1:A:1813:LYS:HG2	1:A:1816:MET:HE2	1.69	0.74
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.33	0.74
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.37	0.73
1:C:2136:ILE:HD11	1:C:2152:ILE:HG23	1.72	0.71
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.40	0.69
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.39	0.69
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.92	0.68
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.42	0.67
1:A:1900:GLU:HG2	1:A:1918:GLN:HG2	1.79	0.65
1:B:1606:LYS:HD3	4:B:2440:HOH:O	1.97	0.64
1:A:2162:SER:HB3	1:B:1797:LEU:HD23	1.80	0.63
1:C:1508:VAL:HG22	4:C:2477:HOH:O	1.97	0.63
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.63	0.63
1:A:1812:ALA:HB3	1:A:1816:MET:CE	2.29	0.63
1:C:1560:ASN:HD22	1:C:1560:ASN:H	1.47	0.62
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	1.98	0.62
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.65	0.61
1:A:1812:ALA:HB3	1:A:1816:MET:HE1	1.82	0.61
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.48	0.61
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.47	0.61
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.64	0.61
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.48	0.60
1:B:1497:ARG:HD3	1:B:1510:ASP:OD2	2.01	0.59
1:C:1648:ASN:HB3	1:C:1651:LYS:HD3	1.83	0.59
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.49	0.59
1:A:1813:LYS:HG2	1:A:1816:MET:CE	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.71	0.55
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.72	0.54
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.05	0.54
1:C:1852:THR:HG23	4:C:2632:HOH:O	2.08	0.53
1:B:1879:VAL:HG22	1:B:1892:ILE:HG12	1.90	0.53
1:C:1772:THR:H	1:C:1776:GLN:NE2	2.05	0.53
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.08	0.52
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.92	0.51
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.11	0.51
1:C:1527:SER:O	1:C:1530:VAL:HG22	2.11	0.51
1:A:2033:ILE:HG22	1:A:2034:LYS:HG2	1.93	0.50
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.46	0.50
1:B:1678:GLU:O	1:B:1689:VAL:HG13	2.11	0.50
1:A:1560:ASN:H	1:A:1560:ASN:ND2	2.08	0.50
1:C:2054:LEU:HB3	1:C:2075:LEU:HD12	1.93	0.49
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.10	0.49
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.10	0.49
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.62	0.48
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.61	0.48
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.42	0.48
1:B:2138:ARG:HD3	4:B:2429:HOH:O	2.13	0.47
1:C:1550:LEU:HD21	1:C:1607:VAL:HG22	1.97	0.47
1:B:1964:PHE:HA	1:C:1786:ASN:HD21	1.80	0.47
1:A:1987:ILE:HB	1:A:2014:MET:HG3	1.97	0.46
1:C:2041:LEU:HB3	1:C:2055:ARG:HH12	1.80	0.46
1:B:2033:ILE:HG12	1:C:1629:ILE:HD11	1.97	0.46
1:C:2051:TYR:HE2	1:C:2079:GLU:HG3	1.81	0.46
1:A:1726:THR:HG21	1:A:1740:VAL:HG22	1.97	0.46
1:C:1560:ASN:ND2	1:C:1560:ASN:H	2.13	0.45
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.65	0.45
1:B:1776:GLN:O	1:C:1960:GLN:HG3	2.17	0.45
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.97	0.45
1:C:1516:ARG:HD3	4:C:2636:HOH:O	2.16	0.45
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.63	0.45
1:A:1883[B]:ARG:NH1	1:A:1886:GLY:O	2.50	0.45
1:B:1987:ILE:HB	1:B:2014:MET:HG3	1.99	0.45
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.99	0.44
1:C:1569:ILE:HG22	1:C:1571:VAL:HG22	2.00	0.44
1:B:1786:ASN:HD21	1:C:1964:PHE:HA	1.82	0.44
1:C:1987:ILE:HB	1:C:2014:MET:HG3	1.99	0.44
1:A:1772:THR:H	1:A:1776:GLN:NE2	2.13	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1491:GLU:HB3	1:B:1498:TYR:HB2	2.00	0.44
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.18	0.44
1:C:1503:MET:HG3	1:C:1589:ILE:HG12	1.99	0.44
1:A:1844:ARG:O	1:A:1848:GLU:HG2	2.18	0.43
1:A:2093:PHE:O	1:A:2097:HIS:HD2	2.01	0.43
1:B:1954:ARG:O	1:B:1996:ARG:HB2	2.18	0.43
1:B:1658:LEU:HD13	1:B:1690:ILE:HD11	1.99	0.43
1:C:1844:ARG:O	1:C:1848:GLU:HG2	2.17	0.43
1:A:1954:ARG:O	1:A:1996:ARG:HB2	2.17	0.43
1:B:1776:GLN:HG2	1:C:1960:GLN:HE21	1.83	0.43
1:C:1954:ARG:O	1:C:1996:ARG:HB2	2.19	0.43
1:C:2032:GLU:O	1:C:2036:ARG:HD3	2.19	0.43
1:A:2093:PHE:O	1:A:2097:HIS:CD2	2.72	0.43
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	2.02	0.42
1:B:1809:TYR:O	1:B:1945:LEU:HD21	2.19	0.42
1:B:1756:LEU:HD13	1:C:1956:PHE:HB2	2.01	0.42
1:A:1676:LEU:HA	1:A:1676:LEU:HD12	1.85	0.42
1:C:1781:GLN:HE21	1:C:1781:GLN:H	1.68	0.42
1:C:2148:ARG:O	1:C:2152:ILE:HG13	2.20	0.42
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	2.00	0.42
2:B:2301:57K:H8	2:B:2301:57K:C3	2.49	0.42
1:C:1503:MET:HB2	1:C:1505:THR:HG22	2.01	0.42
1:C:1659:THR:OG1	1:C:1661:GLU:HG2	2.19	0.42
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.30	0.42
1:B:1708:SER:HB2	1:C:2001:VAL:HG12	2.01	0.41
1:A:1719:TYR:CE1	1:A:1744:GLN:HG3	2.55	0.41
1:A:2041:LEU:HA	1:A:2044:MET:HG3	2.02	0.41
1:A:1727:LEU:HB2	1:A:1803:ILE:HD11	2.02	0.41
1:B:1711:ILE:HD12	1:B:1739:LEU:HD11	2.03	0.41
1:A:1491:GLU:HB3	1:A:1498:TYR:HB2	2.01	0.41
1:B:2024:VAL:HG12	1:B:2025:LEU:HD13	2.03	0.41
2:B:2301:57K:H18	1:C:1757:THR:HG21	2.01	0.41
1:C:2027:PRO:HA	1:C:2030:THR:HG23	2.02	0.41
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.54	0.41
1:C:2086:TYR:HA	1:C:2089:ILE:HD12	2.02	0.41
1:B:2148:ARG:O	1:B:2152:ILE:HG13	2.20	0.41
1:B:1583:VAL:HG11	1:B:1607:VAL:HG13	2.02	0.40
1:A:1741:ARG:HA	1:A:1741:ARG:HD2	1.92	0.40
1:A:2078:ARG:HA	1:A:2078:ARG:NH1	2.26	0.40
1:B:1843:VAL:HG22	4:B:2406:HOH:O	2.22	0.40
1:B:2051:TYR:HE2	1:B:2079:GLU:HB2	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1655:TYR:CD1	1:A:1689:VAL:HG13	2.57	0.40
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.20	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	686/769 (89%)	659 (96%)	25 (4%)	2 (0%)	41	66
1	B	681/769 (89%)	652 (96%)	28 (4%)	1 (0%)	51	78
1	C	675/769 (88%)	648 (96%)	26 (4%)	1 (0%)	51	78
All	All	2042/2307 (88%)	1959 (96%)	79 (4%)	4 (0%)	47	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1997	GLY
1	B	1997	GLY
1	C	1997	GLY
1	A	1744	GLN

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	587/658 (89%)	539 (92%)	48 (8%)	11 26
1	B	582/658 (88%)	535 (92%)	47 (8%)	11 27
1	C	577/658 (88%)	519 (90%)	58 (10%)	7 17
All	All	1746/1974 (88%)	1593 (91%)	153 (9%)	10 23

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

Mol	Chain	Res	Type
1	A	1524	LYS
1	A	1534	ASP
1	A	1536	PHE
1	A	1546	GLU
1	A	1555	ARG
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	1666	LEU
1	A	1676	LEU
1	A	1681	VAL
1	A	1687	ARG
1	A	1729	THR
1	A	1756	LEU
1	A	1766	LEU
1	A	1826	THR
1	A	1871	SER
1	A	1877	VAL
1	A	1884	LEU
1	A	1901	ASN
1	A	1915	THR
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	2030	THR
1	A	2035	PHE
1	A	2036	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2038	GLU
1	A	2047	LEU
1	A	2073	LYS
1	A	2077	ASP
1	A	2078	ARG
1	A	2091	LEU
1	A	2102	ARG
1	A	2114	GLU
1	A	2128	ARG
1	A	2135	LEU
1	A	2139	LEU
1	A	2145	GLU
1	A	2185	LYS
1	A	2192	GLU
1	B	1483	ILE
1	B	1502	LEU
1	B	1508	VAL
1	B	1524	LYS
1	B	1534	ASP
1	B	1536	PHE
1	B	1555	ARG
1	B	1571	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1606	LYS
1	B	1618	ARG
1	B	1629	ILE
1	B	1658	LEU
1	B	1666	LEU
1	B	1676	LEU
1	B	1680	THR
1	B	1689	VAL
1	B	1762	LEU
1	B	1768	ARG
1	B	1786	ASN
1	B	1824	LYS
1	B	1836	THR
1	B	1843	VAL
1	B	1871	SER
1	B	1884	LEU
1	B	1901	ASN
1	B	1915	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1918	GLN
1	B	1924	TRP
1	B	1930	PHE
1	B	2018	VAL
1	B	2025	LEU
1	B	2033	ILE
1	B	2035	PHE
1	B	2036	ARG
1	B	2037	ARG
1	B	2040	LEU
1	B	2077	ASP
1	B	2102	ARG
1	B	2114	GLU
1	B	2116	THR
1	B	2128	ARG
1	B	2148	ARG
1	B	2152	ILE
1	B	2154	ARG
1	B	2180	LYS
1	C	1494	GLN
1	C	1497	ARG
1	C	1499	LYS
1	C	1508	VAL
1	C	1516	ARG
1	C	1524	LYS
1	C	1534	ASP
1	C	1536	PHE
1	C	1542	LEU
1	C	1550	LEU
1	C	1560	ASN
1	C	1571	VAL
1	C	1585	VAL
1	C	1602	GLU
1	C	1606	LYS
1	C	1618	ARG
1	C	1629	ILE
1	C	1654	GLN
1	C	1660	SER
1	C	1676	LEU
1	C	1680	THR
1	C	1731	ARG
1	C	1741	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1757	THR
1	C	1762	LEU
1	C	1768	ARG
1	C	1770	VAL
1	C	1775	LEU
1	C	1781	GLN
1	C	1786	ASN
1	C	1792	THR
1	C	1824	LYS
1	C	1871	SER
1	C	1877	VAL
1	C	1884	LEU
1	C	1898	THR
1	C	1901	ASN
1	C	1915	THR
1	C	1924	TRP
1	C	1930	PHE
1	C	1950	LEU
1	C	1968	LEU
1	C	2030	THR
1	C	2034	LYS
1	C	2035	PHE
1	C	2037	ARG
1	C	2047	LEU
1	C	2054	LEU
1	C	2057	GLN
1	C	2077	ASP
1	C	2083	LEU
1	C	2102	ARG
1	C	2114	GLU
1	C	2128	ARG
1	C	2152	ILE
1	C	2154	ARG
1	C	2186	LEU
1	C	2192	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1560	ASN
1	A	1587	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1605	ASN
1	A	1624	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1815	ASN
1	A	1837	ASN
1	A	1934	GLN
1	A	2008	ASN
1	A	2097	HIS
1	A	2131	ASN
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1786	ASN
1	B	1815	ASN
1	B	1934	GLN
1	B	1944	GLN
1	B	2097	HIS
1	B	2131	ASN
1	C	1494	GLN
1	C	1517	GLN
1	C	1522	GLN
1	C	1560	ASN
1	C	1587	ASN
1	C	1605	ASN
1	C	1748	GLN
1	C	1763	ASN
1	C	1774	ASN
1	C	1776	GLN
1	C	1781	GLN
1	C	1786	ASN
1	C	1815	ASN
1	C	1960	GLN
1	C	2011	GLN
1	C	2057	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2170	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

6 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	A	2302	-	4,4,4	0.14	0	6,6,6	0.19	0
2	57K	C	2301	-	31,31,31	1.57	7 (22%)	32,48,48	1.25	5 (15%)
2	57K	B	2301	-	31,31,31	1.58	7 (22%)	32,48,48	1.30	5 (15%)
2	57K	A	2301	-	31,31,31	1.56	7 (22%)	32,48,48	1.28	6 (18%)
3	SO4	C	2303	-	4,4,4	0.18	0	6,6,6	0.16	0
3	SO4	C	2302	-	4,4,4	0.19	0	6,6,6	0.12	0

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	57K	B	2301	-	-	1/17/39/39	0/4/4/4
2	57K	A	2301	-	-	1/17/39/39	0/4/4/4
2	57K	C	2301	-	-	1/17/39/39	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2301	57K	C17-N4	4.10	1.42	1.35
2	C	2301	57K	C17-N4	3.89	1.41	1.35
2	A	2301	57K	C17-N4	3.78	1.41	1.35
2	A	2301	57K	O3-C18	-3.33	1.42	1.48
2	B	2301	57K	O3-C18	-3.30	1.42	1.48
2	C	2301	57K	O3-C18	-3.25	1.42	1.48
2	A	2301	57K	C15-N4	3.01	1.51	1.47
2	B	2301	57K	C15-N4	3.00	1.51	1.47
2	B	2301	57K	C16-N4	2.97	1.50	1.47
2	C	2301	57K	C16-N4	2.81	1.50	1.47
2	C	2301	57K	C15-N4	2.70	1.50	1.47
2	A	2301	57K	C16-N4	2.67	1.50	1.47
2	C	2301	57K	C9-N3	2.58	1.40	1.34
2	A	2301	57K	C16-C12	2.47	1.56	1.54
2	C	2301	57K	C16-C12	2.38	1.56	1.54
2	B	2301	57K	C9-N3	2.27	1.39	1.34
2	A	2301	57K	C9-N3	2.14	1.39	1.34
2	C	2301	57K	C15-C12	2.11	1.56	1.54
2	B	2301	57K	C15-C12	2.10	1.56	1.54
2	A	2301	57K	C15-C12	2.07	1.56	1.54
2	B	2301	57K	C16-C12	2.04	1.56	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2301	57K	C16-N4-C17	-3.27	117.65	128.77
2	A	2301	57K	C16-N4-C17	-3.21	117.86	128.77
2	C	2301	57K	C16-N4-C17	-3.13	118.12	128.77
2	B	2301	57K	C15-N4-C16	-2.54	92.51	95.19
2	B	2301	57K	C4-C5-C6	-2.52	117.34	121.24
2	B	2301	57K	C15-N4-C17	-2.51	120.22	128.77
2	A	2301	57K	C4-C5-C6	-2.46	117.44	121.24
2	A	2301	57K	C1-C2-C3	2.43	124.29	120.74
2	C	2301	57K	C15-N4-C17	-2.38	120.68	128.77
2	C	2301	57K	C4-C5-C6	-2.33	117.65	121.24
2	C	2301	57K	C1-C2-C3	2.32	124.13	120.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2301	57K	C5-C4-C3	2.20	122.54	119.83
2	A	2301	57K	C15-N4-C17	-2.16	121.42	128.77
2	A	2301	57K	C5-C4-C3	2.14	122.47	119.83
2	A	2301	57K	C15-N4-C16	-2.14	92.93	95.19
2	C	2301	57K	C15-N4-C16	-2.07	93.01	95.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2301	57K	O3-C17-N4-C15
2	B	2301	57K	O2-C17-N4-C16
2	A	2301	57K	O2-C17-N4-C16

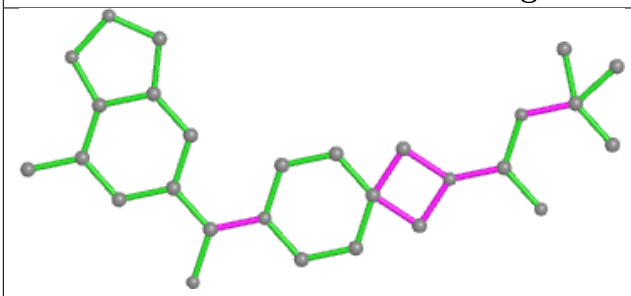
There are no ring outliers.

1 monomer is involved in 2 short contacts:

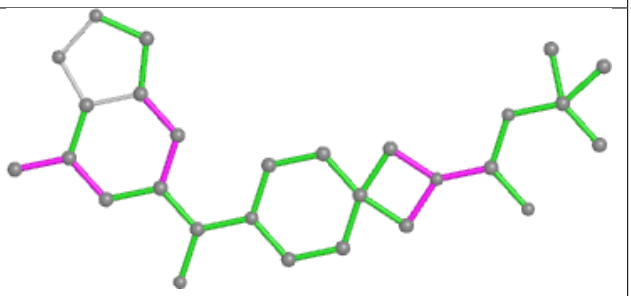
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2301	57K	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

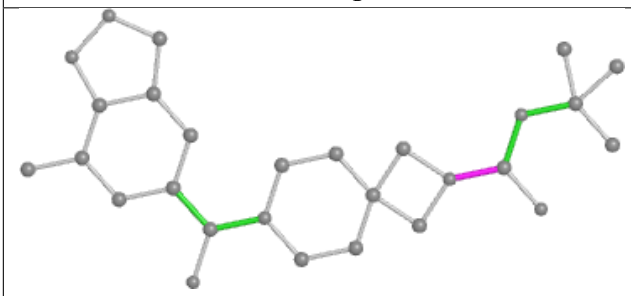
Ligand 57K C 2301



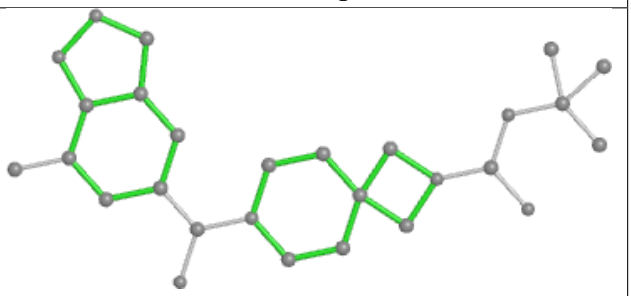
Bond lengths



Bond angles

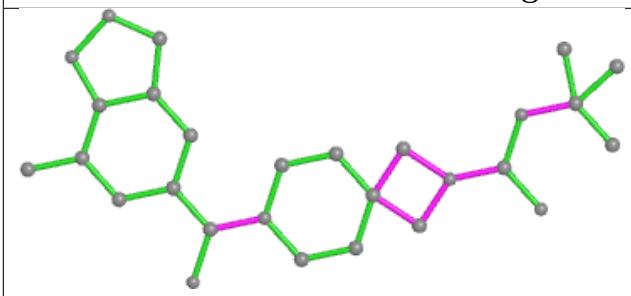


Torsions

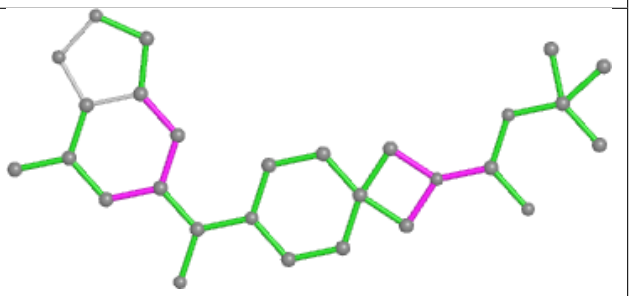


Rings

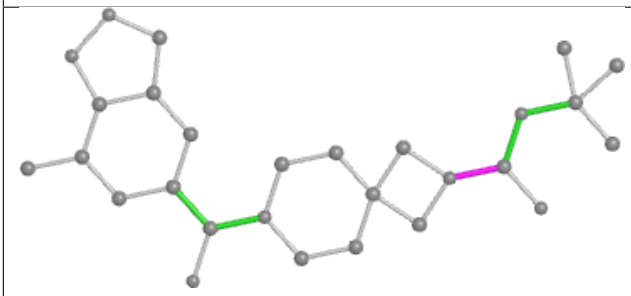
Ligand 57K B 2301



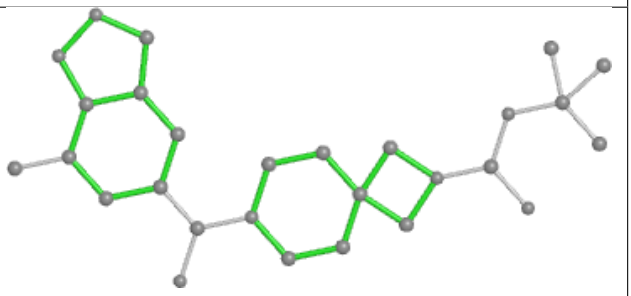
Bond lengths



Bond angles

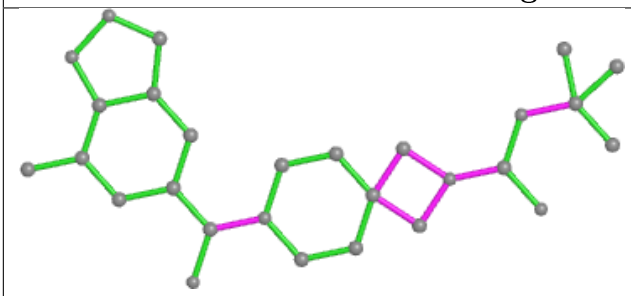


Torsions

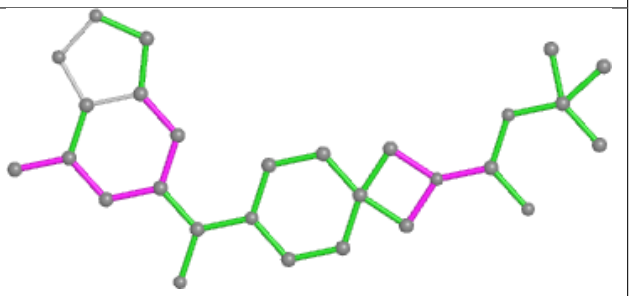


Rings

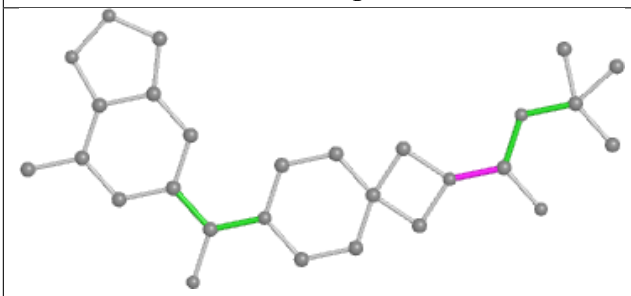
Ligand 57K A 2301



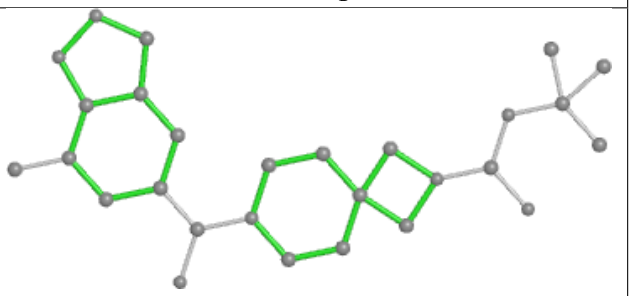
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	691/769 (89%)	-0.04	28 (4%)	37	36	34, 55, 104, 135	0
1	B	687/769 (89%)	0.07	37 (5%)	25	24	35, 59, 115, 144	0
1	C	681/769 (88%)	0.06	29 (4%)	35	33	35, 58, 111, 147	0
All	All	2059/2307 (89%)	0.03	94 (4%)	32	31	34, 57, 110, 147	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2075	LEU	8.3
1	B	2143	VAL	6.1
1	B	1682	ILE	4.9
1	B	2054	LEU	4.5
1	A	1669	PHE	4.4
1	B	2189	LEU	4.3
1	C	1679	ARG	4.3
1	A	1681	VAL	4.2
1	A	1651	LYS	4.1
1	B	2082	LEU	4.0
1	B	1649	PRO	4.0
1	C	1838	ASP	3.9
1	C	1682	ILE	3.8
1	C	1684	GLY	3.8
1	B	2077	ASP	3.7
1	A	1648	ASN	3.7
1	B	2187	LYS	3.7
1	A	2145	GLU	3.7
1	A	1838	ASP	3.7
1	B	2142	GLN	3.7
1	A	1682	ILE	3.5
1	A	2191	LEU	3.5
1	B	1680	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	2053	GLU	3.5
1	A	2075	LEU	3.4
1	C	1680	THR	3.4
1	B	1854	SER	3.3
1	B	1684	GLY	3.3
1	B	2053	GLU	3.3
1	C	1651	LYS	3.2
1	C	1669	PHE	3.2
1	B	2146	ALA	3.2
1	C	1685	GLU	3.2
1	B	2076	ALA	3.2
1	C	1647	ALA	3.1
1	C	1650	ASP	3.1
1	C	2055	ARG	3.1
1	C	1681	VAL	3.0
1	B	2083	LEU	3.0
1	B	1679	ARG	3.0
1	B	1685	GLU	2.9
1	A	2193	SER	2.9
1	A	1647	ALA	2.9
1	B	1853	GLU	2.8
1	B	1668	LYS	2.8
1	A	1839	GLU	2.7
1	A	2080	ARG	2.7
1	A	1911	ASN	2.7
1	C	1839	GLU	2.7
1	B	1687	ARG	2.6
1	B	2078	ARG	2.6
1	C	1646	ALA	2.6
1	A	2190	LYS	2.6
1	A	1685	GLU	2.5
1	B	1669	PHE	2.5
1	C	1530	VAL	2.5
1	A	2077	ASP	2.5
1	B	2051	TYR	2.5
1	A	1768	ARG	2.5
1	A	1679	ARG	2.4
1	A	1683	ASN	2.4
1	B	2134	TYR	2.4
1	C	1528	ALA	2.4
1	C	1584	VAL	2.4
1	C	2037	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2141	HIS	2.4
1	B	1647	ALA	2.4
1	A	1853	GLU	2.4
1	C	1855	GLY	2.4
1	A	1667	LYS	2.3
1	B	2037	ARG	2.3
1	B	1651	LYS	2.3
1	C	2075	LEU	2.3
1	B	1688	PHE	2.3
1	C	1649	PRO	2.3
1	B	2186	LEU	2.3
1	C	1546	GLU	2.2
1	B	1838	ASP	2.2
1	C	2142	GLN	2.2
1	C	1772	THR	2.2
1	C	1670	ASP	2.1
1	A	1650	ASP	2.1
1	B	1681	VAL	2.1
1	A	2051	TYR	2.1
1	B	1546	GLU	2.1
1	A	1680	THR	2.1
1	A	2041	LEU	2.1
1	B	1855	GLY	2.1
1	C	1529	ASP	2.1
1	A	1547	ASN	2.1
1	A	1767	GLY	2.1
1	B	1531	LYS	2.1
1	C	1648	ASN	2.0
1	C	1686	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)

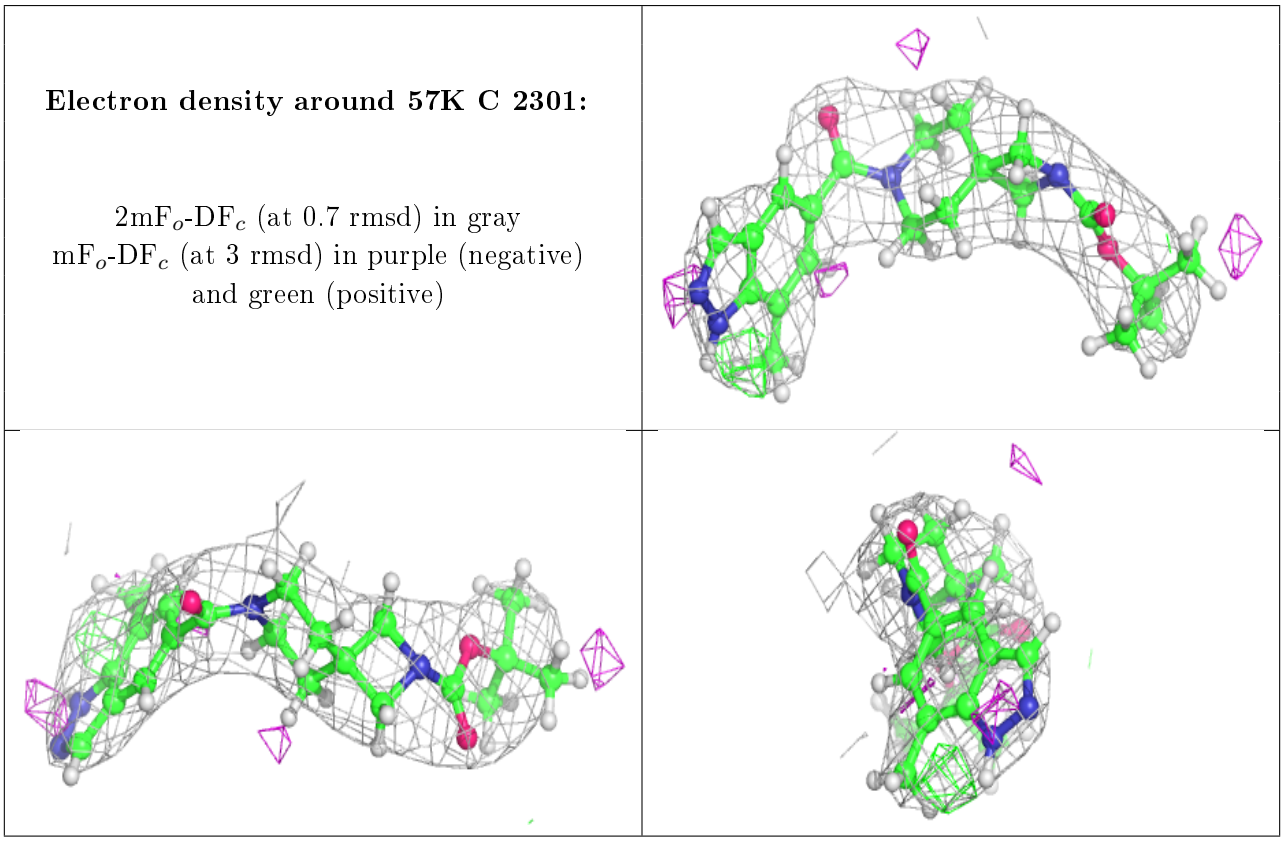
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	2303	5/5	0.78	0.68	180,181,181,182	0
3	SO4	A	2302	5/5	0.92	0.48	145,145,146,146	0
2	57K	C	2301	28/28	0.93	0.20	68,73,85,88	0
2	57K	A	2301	28/28	0.95	0.17	60,66,74,78	0
2	57K	B	2301	28/28	0.95	0.22	70,80,97,98	0
3	SO4	C	2302	5/5	0.96	0.18	109,109,109,109	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.

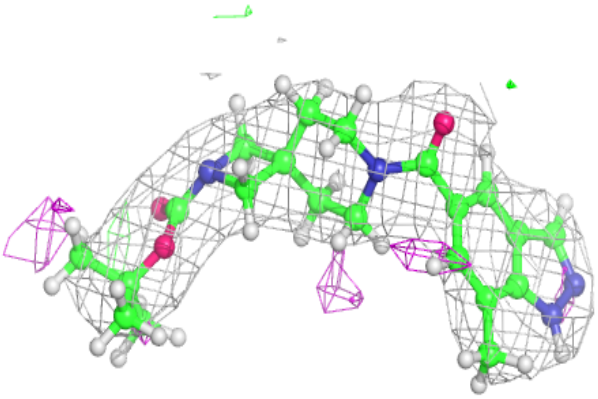
Electron density around 57K C 2301:

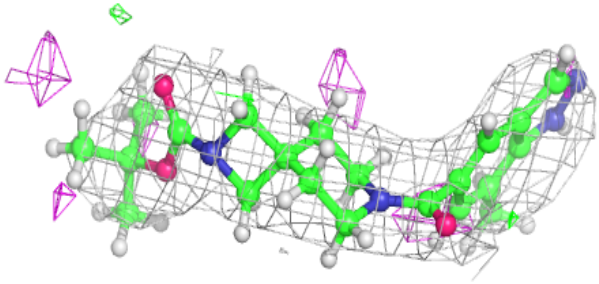
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

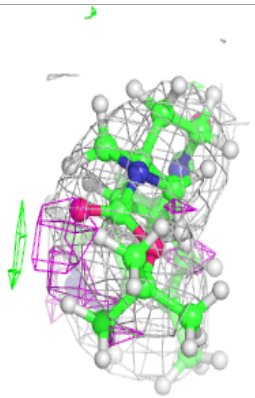


Electron density around 57K A 2301:

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

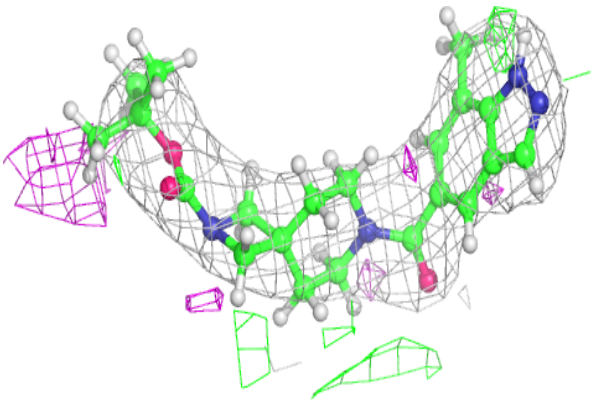


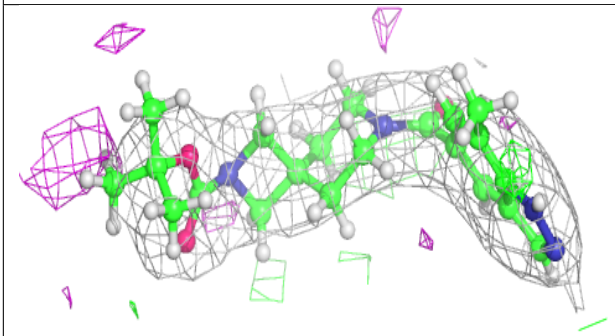


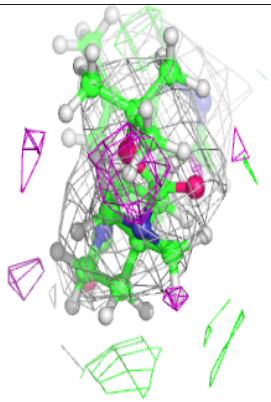


Electron density around 57K B 2301:

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







6.5 Other polymers (i)

There are no such residues in this entry.