Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2023 – 11:15 PM EDT

PDB ID	:	3TVW
Title	:	Crystal Structure of the humanized carboxyltransferase domain of yeast Acetyl-coA caroxylase in complex with compound 4
Authors	:	Rajamohan, F.; Marr, E.; Reyes, A.; Landro, J.A.; Anderson, M.D.; Corbett, J.W.; Dirico, K.J.; Harwood, J.H.; Tu, M.; Vajdos, F.F.
Deposited on	:	2011-09-20
Resolution	:	2.80 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:

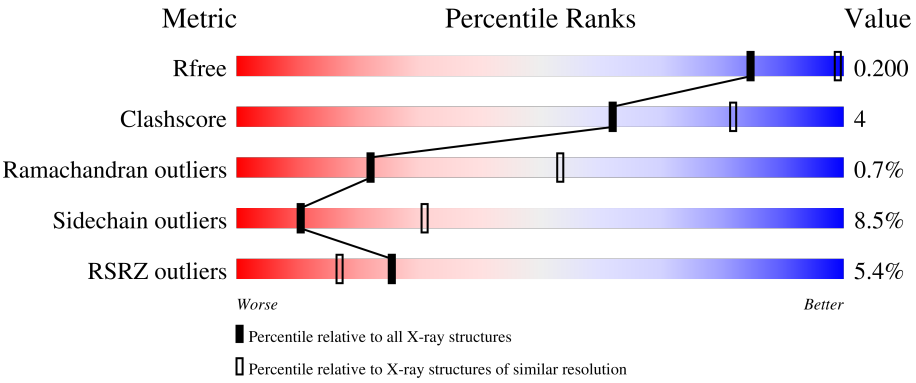
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	769	3% 78% 13% • 8%
1	B	769	6% 76% 15% • 8%
1	C	769	5% 75% 13% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17526 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	711	Total	C	N	O	S	0	1	0
			5586	3554	963	1052	17			
1	B	705	Total	C	N	O	S	0	0	0
			5535	3522	953	1043	17			
1	C	693	Total	C	N	O	S	0	0	0
			5437	3455	937	1028	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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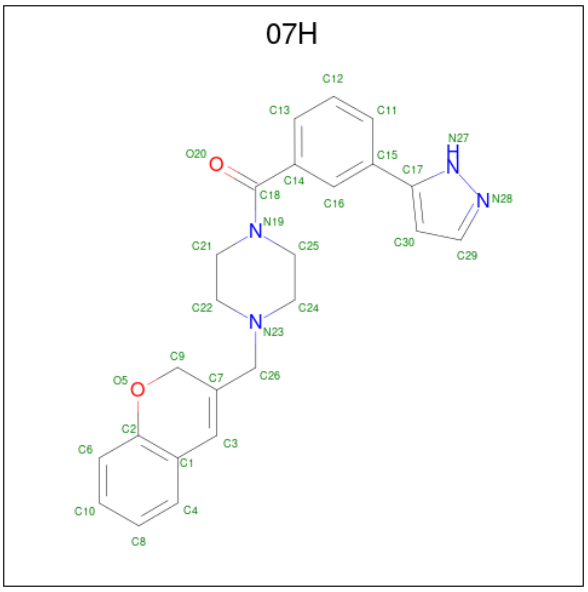
Chain	Residue	Modelled	Actual	Comment	Reference
B	1760	SER	PRO	engineered mutation	UNP Q00955
B	1762	LEU	ILE	engineered mutation	UNP Q00955
B	1765	VAL	MET	engineered mutation	UNP Q00955
B	1919	GLN	GLU	engineered mutation	UNP Q00955
B	1920	ALA	PRO	engineered mutation	UNP Q00955
B	1925	PHE	HIS	engineered 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 [4-(2H-chromen-3-ylmethyl)piperazin-1-yl]-[3-(1H-pyrazol-5-yl)phenyl]methanone (three-letter code: 07H) (formula: $C_{24}H_{24}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 30 24 4 2	0	0
2	B	1	Total C N O 30 24 4 2	0	0
2	C	1	Total C N O 30 24 4 2	0	0

- Molecule 3 is water.

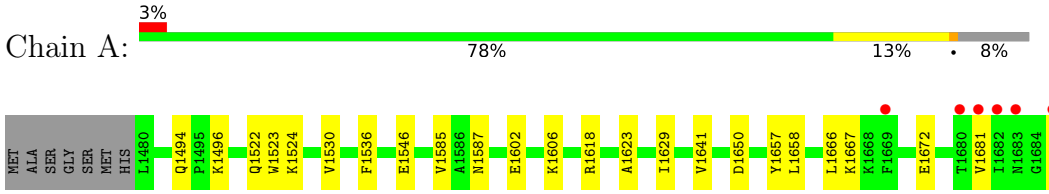
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	301	Total O 301 301	0	0
3	B	286	Total O 286 286	0	0
3	C	291	Total O 291 291	0	0

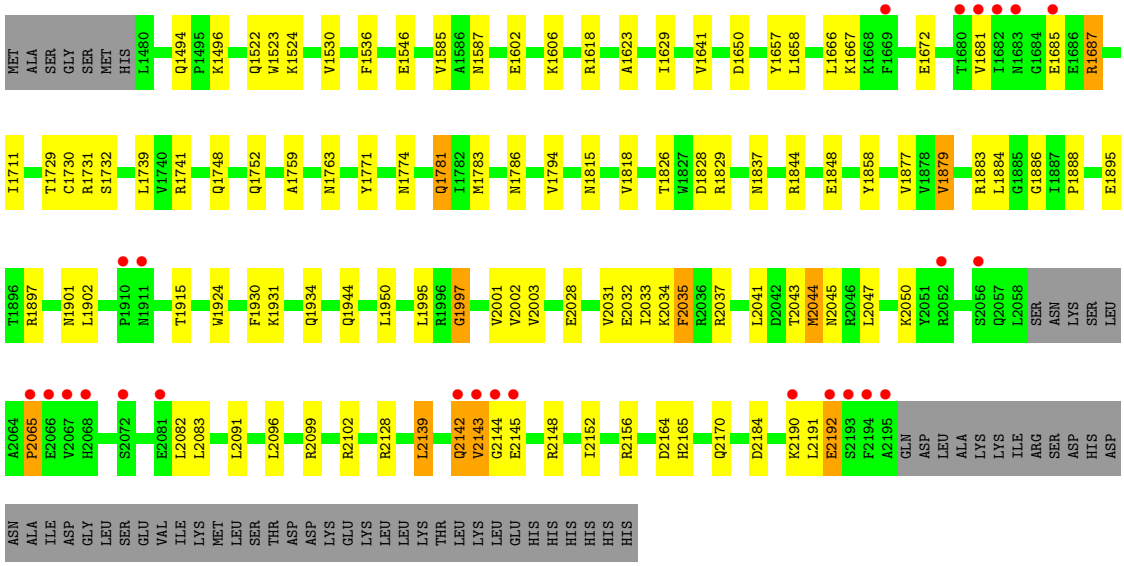
3 Residue-property plots

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

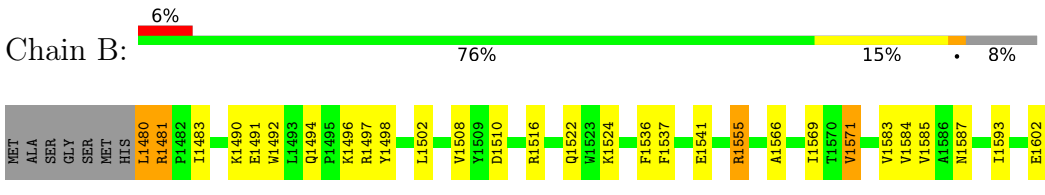
Chain A:

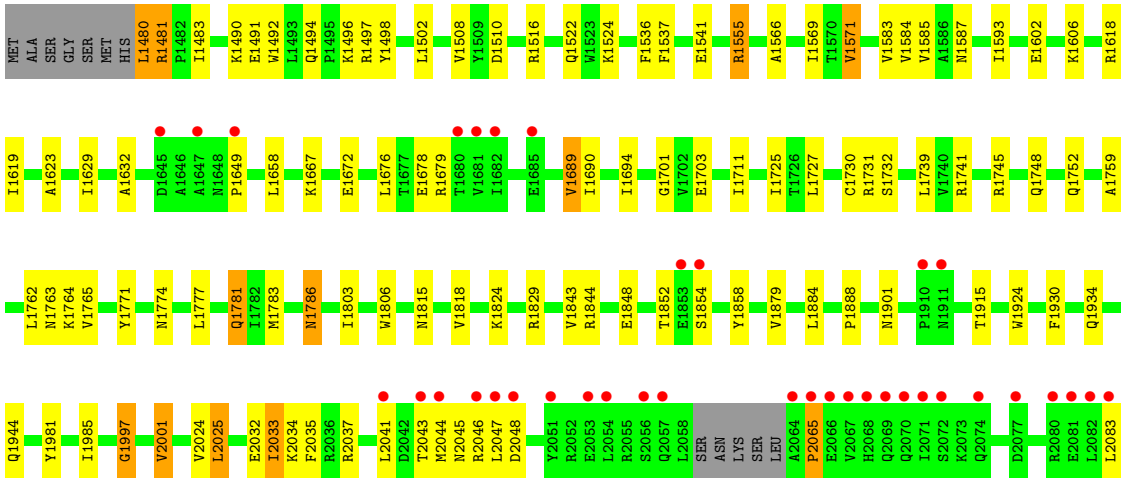


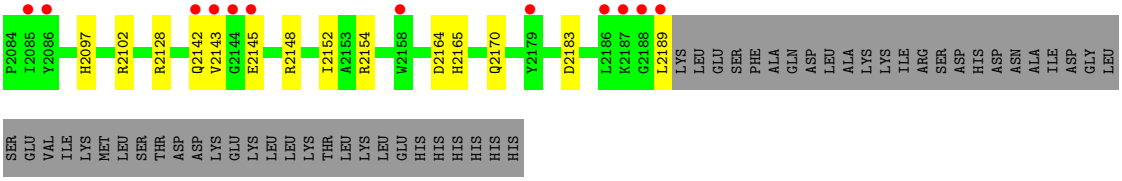


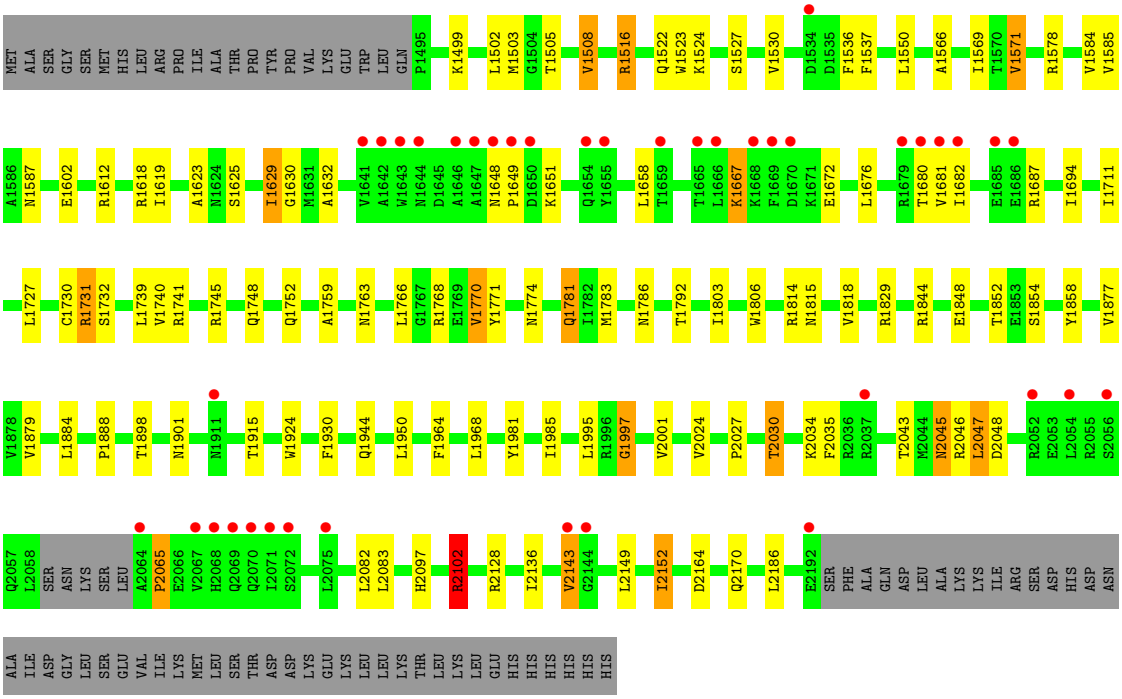
• Molecule 1: Acetyl-CoA carboxylase

Chain B:









• Molecule 1: Acetyl-CoA carboxylase

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	246.96Å 122.86Å 146.07Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	46.96 – 2.80 41.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.96-2.80) 99.7 (41.10-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.3, BUSTER 2.11.2	Depositor
R, R_{free}	0.176 , 0.205 0.171 , 0.200	Depositor DCC
R_{free} test set	10676 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 76.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17526	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: 07H

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	0/5713	0.74	1/7747 (0.0%)
1	B	0.51	0/5654	0.73	1/7670 (0.0%)
1	C	0.51	0/5550	0.74	2/7521 (0.0%)
All	All	0.51	0/16917	0.73	4/22938 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2065	PRO	N-CA-CB	6.00	110.50	103.30
1	C	2065	PRO	N-CA-CB	5.95	110.44	103.30
1	A	2065	PRO	N-CA-CB	5.94	110.43	103.30
1	C	2102	ARG	CB-CG-CD	5.53	125.98	111.60

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	5586	0	5439	43	0
1	B	5535	0	5390	55	0
1	C	5437	0	5298	58	0
2	A	30	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	30	0	24	0	0
2	C	30	0	24	1	0
3	A	301	0	0	4	0
3	B	286	0	0	1	0
3	C	291	0	0	4	0
All	All	17526	0	16199	145	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 (145) 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	1.74	1.65
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.21	0.88
1:B:2047:LEU:HG	1:B:2048:ASP:HB2	1.54	0.87
1:A:2047:LEU:HD22	1:A:2082:LEU:HD11	1.63	0.80
1:C:1763:ASN:HD21	1:C:1771:TYR:H	1.30	0.76
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.35	0.75
1:A:1763:ASN:HD21	1:A:1771:TYR:H	1.35	0.74
1:B:1632:ALA:H	1:C:2097:HIS:HE1	1.34	0.74
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.56	0.71
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.37	0.71
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	1.91	0.70
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.24	0.70
1:A:1815:ASN:H	1:A:1944:GLN:HE22	1.38	0.70
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.91	0.68
1:A:2047:LEU:HD23	1:A:2050:LYS:H	1.58	0.68
1:B:1759:ALA:H	1:B:1774:ASN:ND2	1.92	0.67
1:C:1815:ASN:H	1:C:1944:GLN:HE22	1.40	0.67
1:A:1759:ALA:H	1:A:1774:ASN:ND2	1.93	0.66
1:C:1625:SER:HB3	1:C:1731:ARG:HH21	1.61	0.65
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.79	0.65
1:A:2033:ILE:HG22	1:A:2034:LYS:HG2	1.79	0.64
1:A:1494:GLN:HE21	1:A:1496:LYS:H	1.48	0.62
1:C:1997:GLY:O	1:C:2001:VAL:HG13	2.01	0.61
1:B:1606:LYS:HD3	3:B:712:HOH:O	2.01	0.60
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.66	0.60
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.50	0.60
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.49	0.60
1:C:1766:LEU:CD1	1:C:1770:VAL:HG11	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1516:ARG:HD3	3:C:653:HOH:O	2.02	0.59
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.67	0.59
1:B:2164:ASP:H	1:B:2170:GLN:NE2	2.01	0.59
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.49	0.59
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.49	0.58
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.39	0.58
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.68	0.57
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.69	0.57
1:B:1649:PRO:HG2	1:C:2047:LEU:HD11	1.86	0.57
1:B:2033:ILE:HG12	1:C:1629:ILE:HD11	1.85	0.57
1:A:1826:THR:HG22	1:A:1828:ASP:H	1.70	0.56
1:A:2047:LEU:HD23	1:A:2050:LYS:N	2.20	0.56
1:B:1764:LYS:HG3	2:C:1:07H:H21	1.88	0.56
1:C:1766:LEU:HD13	1:C:1770:VAL:HG11	1.88	0.56
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.71	0.56
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.71	0.55
1:B:1759:ALA:H	1:B:1774:ASN:HD21	1.54	0.55
1:A:1523:TRP:CE3	1:A:1530:VAL:HG21	2.43	0.54
1:A:2041:LEU:HA	1:A:2044:MET:HG3	1.88	0.54
1:C:1730:CYS:HA	1:C:1752:GLN:HE21	1.71	0.54
1:A:2142:GLN:O	1:A:2144:GLY:N	2.41	0.54
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.43	0.53
1:A:1759:ALA:H	1:A:1774:ASN:HD21	1.55	0.53
1:B:1676:LEU:HG	1:B:1694:ILE:HD11	1.90	0.53
1:B:2047:LEU:HD23	1:C:1649:PRO:HG3	1.91	0.53
1:B:1497:ARG:HD3	1:B:1510:ASP:OD1	2.07	0.53
1:A:2043:THR:C	1:A:2045:ASN:H	2.12	0.52
1:C:1629:ILE:CD1	1:C:1629:ILE:CB	2.80	0.52
1:C:2045:ASN:C	1:C:2045:ASN:HD22	2.12	0.52
1:C:1667:LYS:HA	1:C:1672:GLU:HG2	1.91	0.52
1:A:2031:VAL:HG13	1:A:2035:PHE:HB3	1.91	0.52
1:C:1503:MET:HB2	1:C:1505:THR:HG22	1.92	0.52
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.46	0.51
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.56	0.51
1:A:1606:LYS:HD3	3:A:56:HOH:O	2.11	0.50
1:A:2047:LEU:HD21	3:A:864:HOH:O	2.11	0.50
1:C:1711:ILE:HD12	1:C:1739:LEU:HD11	1.94	0.50
1:C:1676:LEU:HG	1:C:1694:ILE:HD11	1.94	0.50
1:C:1898:THR:HG22	3:C:437:HOH:O	2.11	0.50
1:A:1530:VAL:HG23	3:A:108:HOH:O	2.12	0.49
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.11	0.49
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.11	0.49
1:C:2027:PRO:HA	1:C:2030:THR:HG23	1.95	0.49
1:B:2034:LYS:HD2	1:C:1630:GLY:HA2	1.95	0.48
1:B:1711:ILE:HD12	1:B:1739:LEU:HD11	1.95	0.48
1:C:1523:TRP:CE3	1:C:1530:VAL:HG21	2.49	0.48
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.11	0.48
1:A:2032:GLU:HG2	2:A:1:07H:N28	2.29	0.48
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.95	0.48
1:C:1569:ILE:HG22	1:C:1571:VAL:HG22	1.96	0.48
1:A:2028:GLU:OE1	2:A:1:07H:H20	2.14	0.48
1:B:1997:GLY:O	1:B:2001:VAL:HG13	2.14	0.47
1:C:1578:ARG:HB2	3:C:171:HOH:O	2.14	0.47
1:B:1703:GLU:OE2	1:C:2102:ARG:NH2	2.47	0.47
1:B:1541:GLU:OE1	1:B:1555:ARG:HD3	2.15	0.47
1:C:1527:SER:O	1:C:1530:VAL:HG22	2.16	0.46
1:A:1667:LYS:HA	1:A:1672:GLU:HG2	1.98	0.46
1:B:1480:LEU:HB3	1:B:1481:ARG:H	1.60	0.46
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.98	0.46
1:C:1682:ILE:HB	1:C:1687:ARG:HD2	1.97	0.46
1:A:2143:VAL:HA	1:A:2192:GLU:HG2	1.98	0.46
1:B:1480:LEU:HA	1:B:1492:TRP:NE1	2.31	0.46
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.51	0.46
1:B:1619:ILE:HG13	1:B:1725:ILE:CG2	2.46	0.46
1:C:2047:LEU:HD22	1:C:2082:LEU:HD11	1.97	0.46
1:B:1667:LYS:HA	1:B:1672:GLU:HG2	1.99	0.45
1:A:2096:LEU:HA	1:A:2099:ARG:NH2	2.32	0.45
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.14	0.45
1:A:2184:ASP:OD2	1:B:1481:ARG:NH2	2.50	0.44
1:C:1763:ASN:HD22	1:C:1770:VAL:HG13	1.81	0.44
1:C:1981:TYR:CG	1:C:1985:ILE:HD11	2.53	0.44
1:C:2136:ILE:HD11	1:C:2152:ILE:HG23	2.00	0.44
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.47	0.44
1:A:1883[B]:ARG:NH1	1:A:1886:GLY:O	2.49	0.44
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.48	0.44
1:C:1852:THR:HG22	1:C:1854:SER:H	1.81	0.44
1:C:1766:LEU:HD12	1:C:1770:VAL:HG11	1.99	0.43
1:A:1995:LEU:HD12	1:A:1995:LEU:HA	1.95	0.43
1:A:1997:GLY:O	1:A:2001:VAL:HG23	2.18	0.43
1:C:1727:LEU:HB2	1:C:1803:ILE:HD11	2.00	0.43
1:B:1852:THR:HG22	1:B:1854:SER:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2024:VAL:HG12	1:B:2025:LEU:HD13	2.00	0.43
1:C:1763:ASN:ND2	1:C:1770:VAL:HG13	2.34	0.43
1:B:1786:ASN:ND2	1:C:1964:PHE:O	2.50	0.42
1:C:1844:ARG:O	1:C:1848:GLU:HG2	2.19	0.42
1:B:1781:GLN:HE21	1:B:1781:GLN:H	1.67	0.42
1:B:1829:ARG:CZ	1:B:1858:TYR:HB3	2.49	0.42
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.54	0.42
1:C:2043:THR:C	1:C:2045:ASN:H	2.22	0.42
1:A:1844:ARG:O	1:A:1848:GLU:HG2	2.19	0.42
1:C:1566:ALA:HA	1:C:1584:VAL:O	2.20	0.42
1:B:1762:LEU:HA	1:B:1765:VAL:HG22	2.02	0.42
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	2.02	0.42
1:B:1658:LEU:HD12	1:B:1690:ILE:HG12	2.02	0.42
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.19	0.42
1:A:1530:VAL:CG2	3:A:108:HOH:O	2.66	0.42
1:B:2041:LEU:HA	1:B:2044:MET:HG3	2.01	0.42
1:C:1781:GLN:HE21	1:C:1781:GLN:H	1.67	0.42
1:A:2152:ILE:O	1:A:2156:ARG:HG3	2.19	0.42
1:C:1995:LEU:HD12	1:C:1995:LEU:HA	1.96	0.42
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	2.02	0.41
1:B:2043:THR:C	1:B:2045:ASN:H	2.22	0.41
1:C:1508:VAL:HG22	3:C:309:HOH:O	2.20	0.41
1:A:2139:LEU:HD23	1:A:2139:LEU:HA	1.86	0.41
1:B:1781:GLN:H	1:B:1781:GLN:NE2	2.19	0.41
1:C:1623:ALA:HA	1:C:1730:CYS:HB3	2.02	0.41
1:B:1678:GLU:O	1:B:1689:VAL:HG13	2.21	0.41
1:B:1701:GLY:HA2	1:C:2024:VAL:HG23	2.02	0.41
1:A:1781:GLN:H	1:A:1781:GLN:HE21	1.68	0.41
1:A:1818:VAL:HB	1:A:1888:PRO:HG2	2.03	0.41
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.28	0.41
1:B:1491:GLU:HB3	1:B:1498:TYR:HB2	2.03	0.40
1:B:1566:ALA:HA	1:B:1584:VAL:O	2.22	0.40
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	2.02	0.40
1:A:1879:VAL:HG13	1:A:1931:LYS:HE2	2.03	0.40
1:B:1658:LEU:HD12	1:B:1690:ILE:CG1	2.52	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	708/769 (92%)	678 (96%)	25 (4%)	5 (1%)	22	53
1	B	701/769 (91%)	670 (96%)	25 (4%)	6 (1%)	17	46
1	C	689/769 (90%)	663 (96%)	23 (3%)	3 (0%)	34	66
All	All	2098/2307 (91%)	2011 (96%)	73 (4%)	14 (1%)	22	53

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2065	PRO
1	B	2065	PRO
1	B	2143	VAL
1	C	2065	PRO
1	A	2044	MET
1	C	2143	VAL
1	A	1731	ARG
1	B	1731	ARG
1	A	2143	VAL
1	B	1481	ARG
1	A	1997	GLY
1	B	1997	GLY
1	C	1997	GLY
1	B	1593	ILE

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	580/658 (88%)	534 (92%)	46 (8%)	12 34
1	B	574/658 (87%)	526 (92%)	48 (8%)	11 31
1	C	564/658 (86%)	512 (91%)	52 (9%)	9 27
All	All	1718/1974 (87%)	1572 (92%)	146 (8%)	10 31

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1524	LYS
1	A	1536	PHE
1	A	1546	GLU
1	A	1585	VAL
1	A	1602	GLU
1	A	1618	ARG
1	A	1629	ILE
1	A	1641	VAL
1	A	1650	ASP
1	A	1658	LEU
1	A	1666	LEU
1	A	1681	VAL
1	A	1685	GLU
1	A	1687	ARG
1	A	1729	THR
1	A	1732	SER
1	A	1781	GLN
1	A	1786	ASN
1	A	1794	VAL
1	A	1837	ASN
1	A	1877	VAL
1	A	1879	VAL
1	A	1884	LEU
1	A	1901	ASN
1	A	1902	LEU
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	2035	PHE
1	A	2037	ARG

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Mol	Chain	Res	Type
1	A	2083	LEU
1	A	2091	LEU
1	A	2102	ARG
1	A	2128	ARG
1	A	2139	LEU
1	A	2142	GLN
1	A	2145	GLU
1	A	2148	ARG
1	A	2165	HIS
1	A	2190	LYS
1	A	2191	LEU
1	A	2192	GLU
1	B	1480	LEU
1	B	1483	ILE
1	B	1490	LYS
1	B	1502	LEU
1	B	1508	VAL
1	B	1516	ARG
1	B	1522	GLN
1	B	1524	LYS
1	B	1536	PHE
1	B	1555	ARG
1	B	1571	VAL
1	B	1583	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1618	ARG
1	B	1629	ILE
1	B	1679	ARG
1	B	1689	VAL
1	B	1732	SER
1	B	1777	LEU
1	B	1781	GLN
1	B	1786	ASN
1	B	1824	LYS
1	B	1843	VAL
1	B	1879	VAL
1	B	1884	LEU
1	B	1901	ASN
1	B	1915	THR
1	B	1924	TRP
1	B	1930	PHE

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Mol	Chain	Res	Type
1	B	2001	VAL
1	B	2025	LEU
1	B	2032	GLU
1	B	2033	ILE
1	B	2035	PHE
1	B	2037	ARG
1	B	2046	ARG
1	B	2083	LEU
1	B	2102	ARG
1	B	2128	ARG
1	B	2142	GLN
1	B	2145	GLU
1	B	2148	ARG
1	B	2152	ILE
1	B	2154	ARG
1	B	2165	HIS
1	B	2183	ASP
1	B	2189	LEU
1	C	1499	LYS
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	1550	LEU
1	C	1571	VAL
1	C	1585	VAL
1	C	1602	GLU
1	C	1618	ARG
1	C	1619	ILE
1	C	1629	ILE
1	C	1648	ASN
1	C	1651	LYS
1	C	1658	LEU
1	C	1667	LYS
1	C	1680	THR
1	C	1681	VAL
1	C	1731	ARG
1	C	1732	SER
1	C	1740	VAL
1	C	1741	ARG

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Mol	Chain	Res	Type
1	C	1768	ARG
1	C	1770	VAL
1	C	1781	GLN
1	C	1786	ASN
1	C	1792	THR
1	C	1877	VAL
1	C	1879	VAL
1	C	1884	LEU
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	2045	ASN
1	C	2046	ARG
1	C	2047	LEU
1	C	2048	ASP
1	C	2083	LEU
1	C	2102	ARG
1	C	2128	ARG
1	C	2143	VAL
1	C	2149	LEU
1	C	2152	ILE
1	C	2186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1517	GLN
1	A	1587	ASN
1	A	1605	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1763	ASN
1	A	1774	ASN
1	A	1781	GLN
1	A	1786	ASN

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Mol	Chain	Res	Type
1	A	1815	ASN
1	A	1934	GLN
1	A	1941	ASN
1	A	1944	GLN
1	A	2097	HIS
1	A	2142	GLN
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1587	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1774	ASN
1	B	1781	GLN
1	B	1786	ASN
1	B	1815	ASN
1	B	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	2097	HIS
1	B	2170	GLN
1	C	1517	GLN
1	C	1587	ASN
1	C	1605	ASN
1	C	1748	GLN
1	C	1752	GLN
1	C	1763	ASN
1	C	1774	ASN
1	C	1781	GLN
1	C	1786	ASN
1	C	1815	ASN
1	C	1934	GLN
1	C	1941	ASN
1	C	1944	GLN
1	C	2045	ASN
1	C	2097	HIS
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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	07H	A	1	-	33,34,34	0.87	1 (3%)	39,47,47	1.55	6 (15%)
2	07H	B	1	-	33,34,34	0.89	1 (3%)	39,47,47	1.47	5 (12%)
2	07H	C	1	-	33,34,34	0.87	1 (3%)	39,47,47	1.63	6 (15%)

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	07H	A	1	-	-	0/15/35/35	0/5/5/5
2	07H	B	1	-	-	0/15/35/35	0/5/5/5
2	07H	C	1	-	-	0/15/35/35	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	07H	C1-C3	2.59	1.49	1.43
2	A	1	07H	C1-C3	2.41	1.48	1.43
2	C	1	07H	C1-C3	2.18	1.48	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	07H	C26-N23-C22	-4.64	103.90	111.09
2	A	1	07H	C30-C17-C15	-4.14	124.90	128.77
2	C	1	07H	C30-C17-C15	-3.97	125.06	128.77
2	C	1	07H	C26-N23-C24	-3.91	105.03	111.09
2	A	1	07H	C15-C17-N27	3.82	127.07	120.96
2	C	1	07H	C15-C17-N27	3.75	126.95	120.96
2	B	1	07H	C15-C17-N27	3.59	126.70	120.96
2	B	1	07H	C30-C17-C15	-3.32	125.67	128.77
2	A	1	07H	C26-N23-C22	-3.20	106.14	111.09
2	B	1	07H	C14-C18-N19	2.84	122.32	118.72
2	A	1	07H	C16-C15-C17	-2.63	116.77	120.59
2	C	1	07H	C25-N19-C21	2.63	117.68	112.62
2	C	1	07H	C14-C18-N19	2.60	122.02	118.72
2	A	1	07H	C25-N19-C21	2.44	117.33	112.62
2	C	1	07H	C16-C15-C17	-2.41	117.09	120.59
2	B	1	07H	C30-C17-N27	-2.21	107.62	110.42
2	A	1	07H	C14-C18-N19	2.16	121.46	118.72

There are no chirality outliers.

There are no torsion outliers.

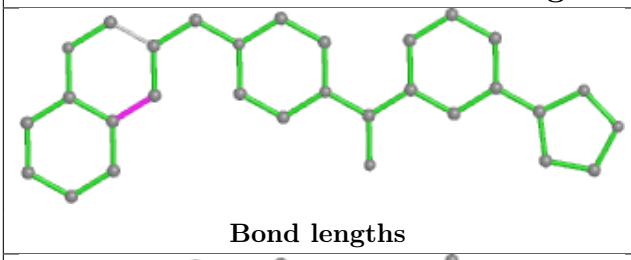
There are no ring outliers.

2 monomers are involved in 3 short contacts:

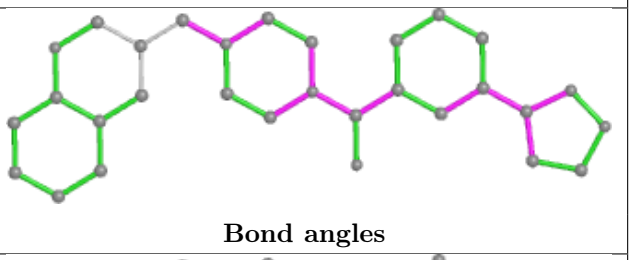
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	07H	2	0
2	C	1	07H	1	0

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.

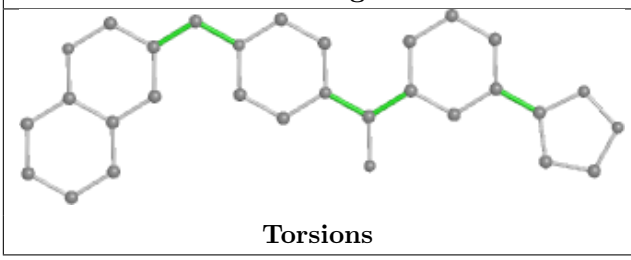
Ligand 07H A 1



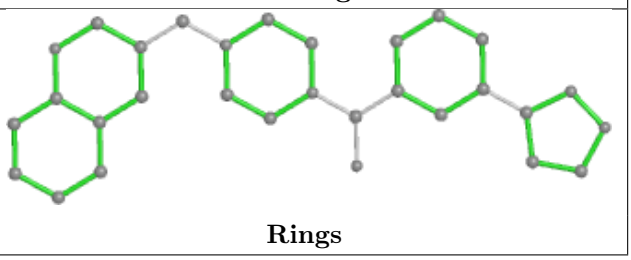
Bond lengths



Bond angles

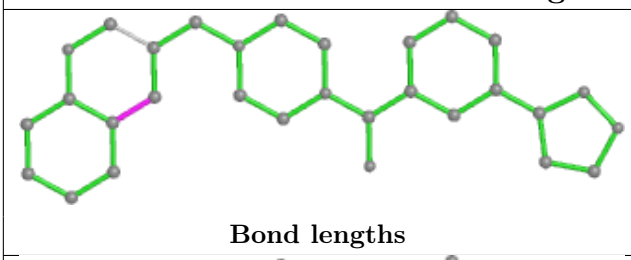


Torsions

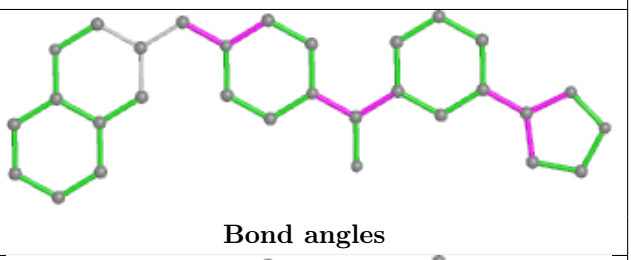


Rings

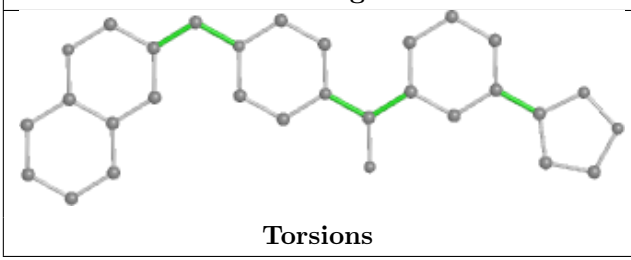
Ligand 07H B 1



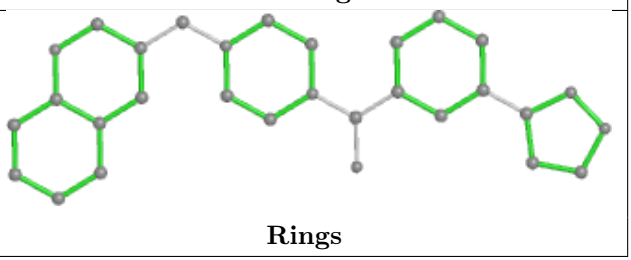
Bond lengths



Bond angles

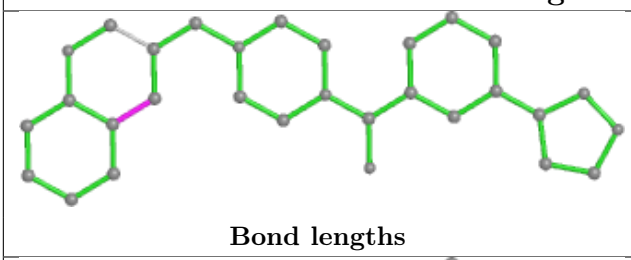


Torsions

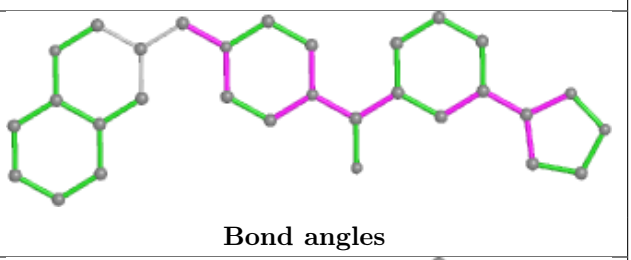


Rings

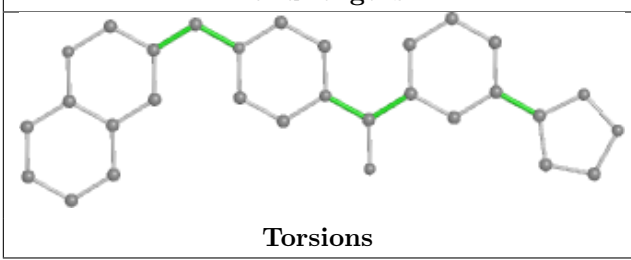
Ligand 07H C 1



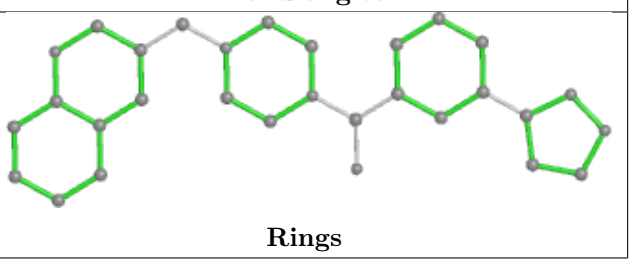
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	711/769 (92%)	-0.24	25 (3%)	44	34	26, 45, 115, 169	0
1	B	705/769 (91%)	-0.09	49 (6%)	16	9	26, 51, 126, 255	0
1	C	693/769 (90%)	-0.13	40 (5%)	23	15	24, 49, 125, 188	0
All	All	2109/2307 (91%)	-0.15	114 (5%)	25	17	24, 48, 123, 255	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2064	ALA	7.0
1	B	2069	GLN	5.6
1	C	1685	GLU	5.3
1	B	2082	LEU	5.1
1	B	2065	PRO	5.0
1	C	2143	VAL	4.9
1	B	2143	VAL	4.8
1	B	2066	GLU	4.8
1	A	2194	PHE	4.5
1	B	1682	ILE	4.5
1	B	2186	LEU	4.5
1	A	2142	GLN	4.4
1	C	1647	ALA	4.1
1	C	1646	ALA	4.1
1	C	1680	THR	3.9
1	B	2057	GLN	3.9
1	C	2068	HIS	3.9
1	A	1682	ILE	3.9
1	A	2195	ALA	3.7
1	B	2068	HIS	3.6
1	A	1911	ASN	3.6
1	C	1669	PHE	3.4
1	C	2144	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	2071	ILE	3.4
1	B	1911	ASN	3.4
1	A	2065	PRO	3.2
1	A	1669	PHE	3.2
1	B	2179	TYR	3.2
1	C	1643	TRP	3.2
1	C	1655	TYR	3.1
1	C	1681	VAL	3.1
1	A	2067	VAL	3.1
1	B	1910	PRO	3.1
1	B	2145	GLU	3.0
1	A	2068	HIS	3.0
1	C	2037	ARG	2.9
1	B	2047	LEU	2.9
1	B	2142	GLN	2.9
1	A	1683	ASN	2.9
1	B	2041	LEU	2.9
1	B	2144	GLY	2.8
1	B	1685	GLU	2.8
1	B	2085	ILE	2.8
1	B	2158	TRP	2.8
1	C	1682	ILE	2.8
1	B	1681	VAL	2.8
1	A	2144	GLY	2.7
1	A	2145	GLU	2.7
1	B	2081	GLU	2.7
1	B	2077	ASP	2.7
1	C	1666	LEU	2.7
1	C	2072	SER	2.7
1	C	1679	ARG	2.7
1	B	2054	LEU	2.7
1	B	2083	LEU	2.7
1	C	2069	GLN	2.7
1	C	1668	LYS	2.7
1	B	2189	LEU	2.6
1	A	2193	SER	2.6
1	B	2067	VAL	2.6
1	A	2056	SER	2.6
1	B	2056	SER	2.6
1	C	1649	PRO	2.6
1	A	1680	THR	2.6
1	A	2066	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1649	PRO	2.6
1	C	1911	ASN	2.6
1	A	1681	VAL	2.6
1	A	2192	GLU	2.6
1	B	2086	TYR	2.5
1	C	2067	VAL	2.5
1	B	2043	THR	2.5
1	B	1645	ASP	2.5
1	B	2070	GLN	2.5
1	C	1665	THR	2.5
1	C	2192	GLU	2.5
1	A	1685	GLU	2.4
1	C	2071	ILE	2.4
1	A	2072	SER	2.4
1	C	2070	GLN	2.4
1	B	2044	MET	2.4
1	C	2054	LEU	2.4
1	A	2143	VAL	2.4
1	C	2056	SER	2.3
1	A	2081	GLU	2.3
1	C	1654	GLN	2.3
1	B	2051	TYR	2.3
1	B	1853	GLU	2.3
1	B	1854	SER	2.3
1	C	1650	ASP	2.3
1	C	1659	THR	2.3
1	B	2072	SER	2.3
1	C	1686	GLU	2.3
1	B	2048	ASP	2.2
1	C	2052	ARG	2.2
1	B	2187	LYS	2.2
1	C	1534	ASP	2.2
1	B	1647	ALA	2.2
1	C	1642	ALA	2.2
1	B	2080	ARG	2.2
1	B	2188	GLY	2.2
1	C	1648	ASN	2.2
1	B	2074	GLN	2.1
1	A	2052	ARG	2.1
1	B	2053	GLU	2.1
1	A	1910	PRO	2.1
1	B	2046	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2190	LYS	2.1
1	C	2075	LEU	2.1
1	C	1641	VAL	2.1
1	C	1644	ASN	2.0
1	C	1670	ASP	2.0
1	C	2064	ALA	2.0
1	B	1680	THR	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)

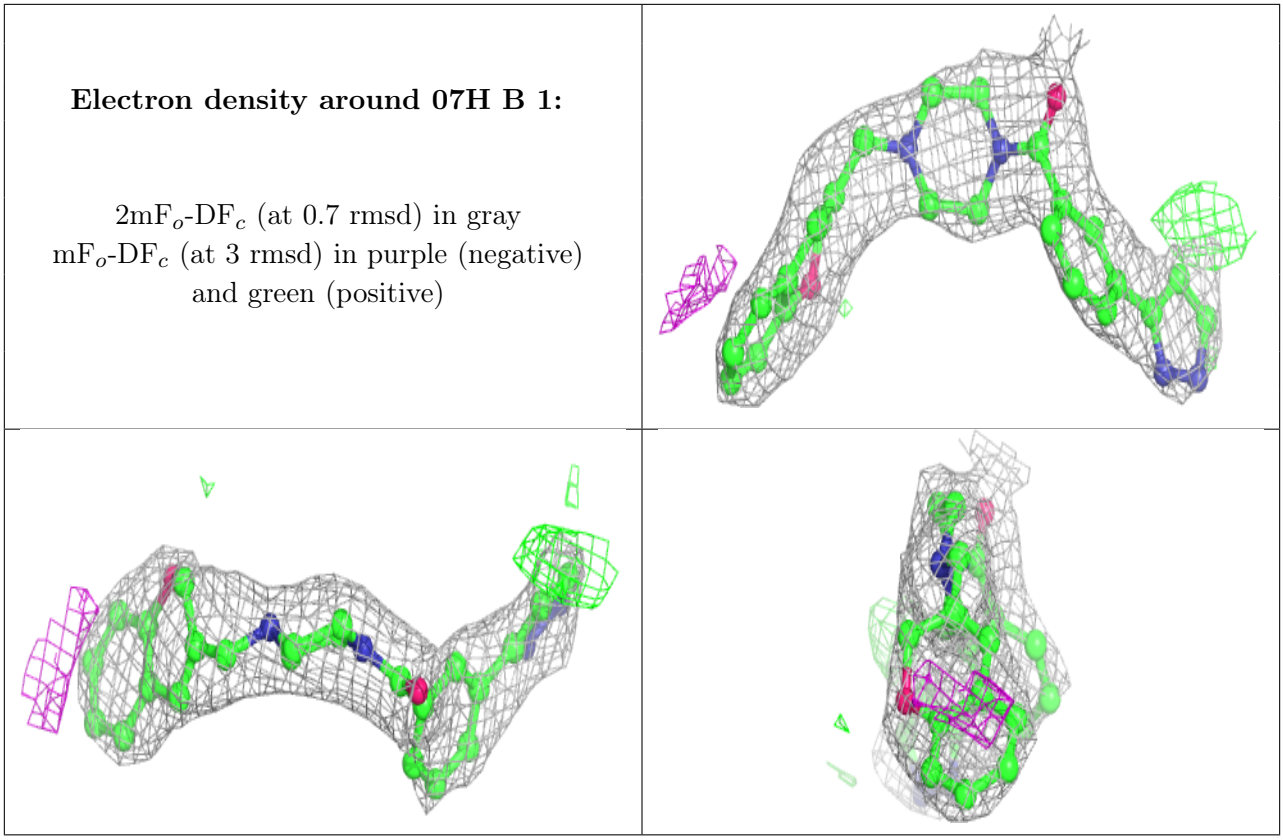
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	07H	B	1	30/30	0.90	0.25	77,84,108,109	0
2	07H	A	1	30/30	0.92	0.19	61,68,100,102	0
2	07H	C	1	30/30	0.92	0.21	66,73,93,93	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.

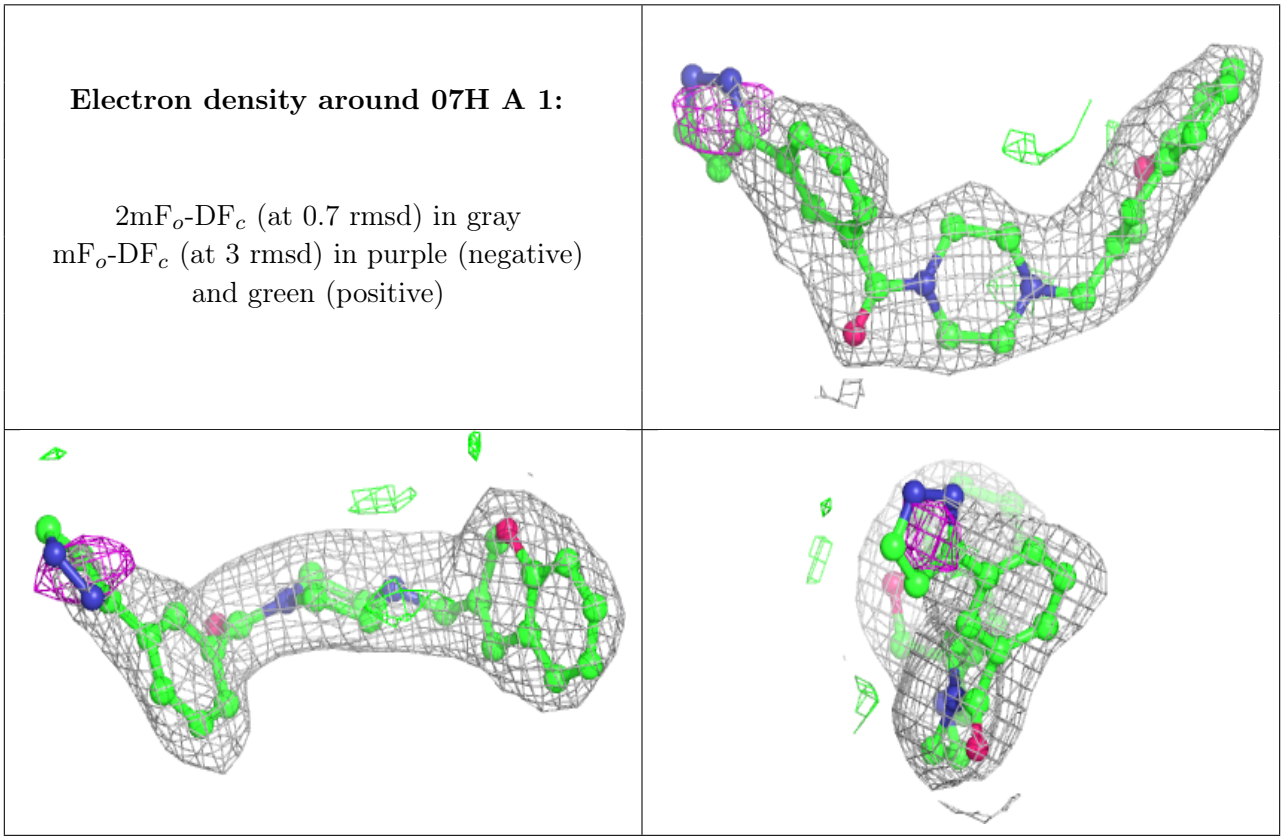
Electron density around 07H B 1:

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



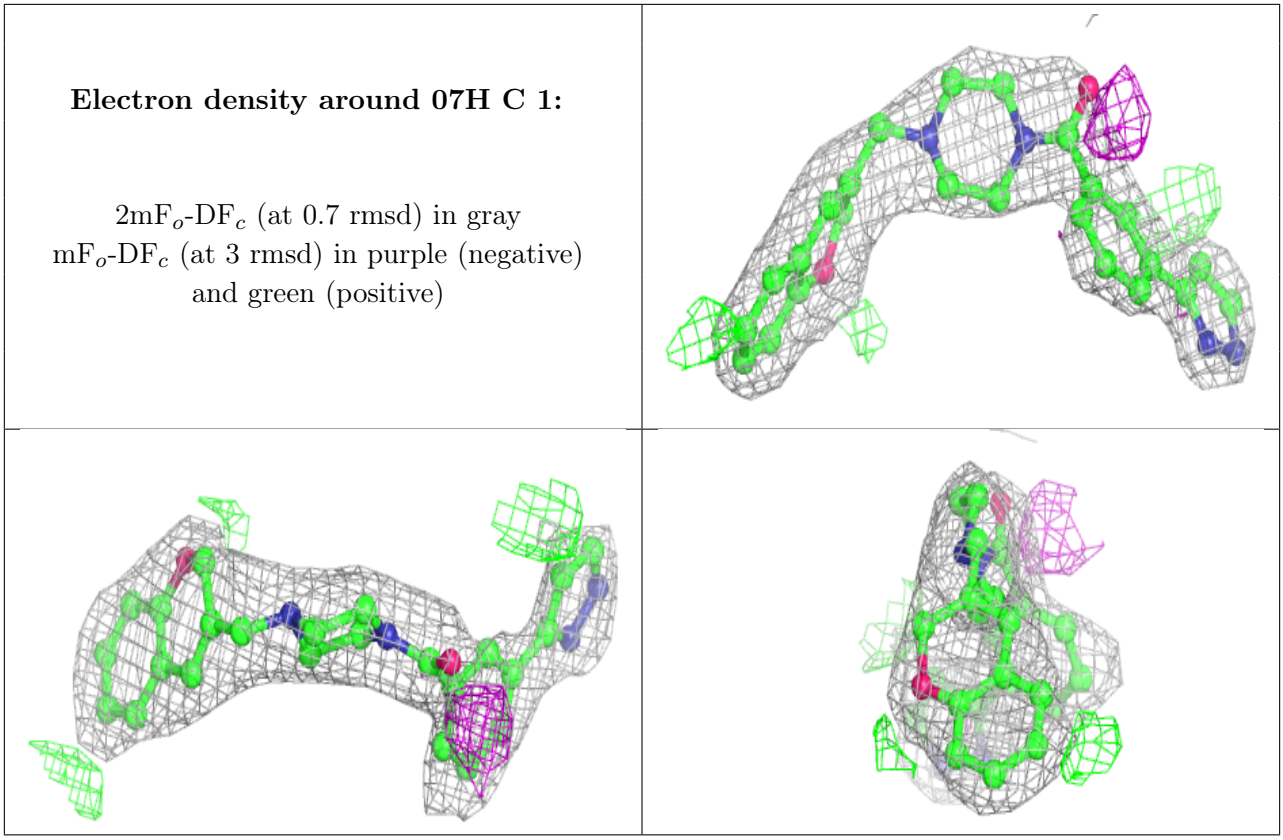
Electron density around 07H A 1:

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



Electron density around 07H C 1:

$2mF_o$-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.