Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:16 pm BST

PDB ID	:	5CTB
Title	:	Humanized yeast ACC carboxyltransferase domain bound to 6,7-dimethyl-1'-[(7-methyl-1H-indazol-5-yl)carbonyl]spiro[chromene-2,4'-piperidin]-4(3H)-one
Authors	:	Vajdos, F.F.
Deposited on	:	2015-07-23
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

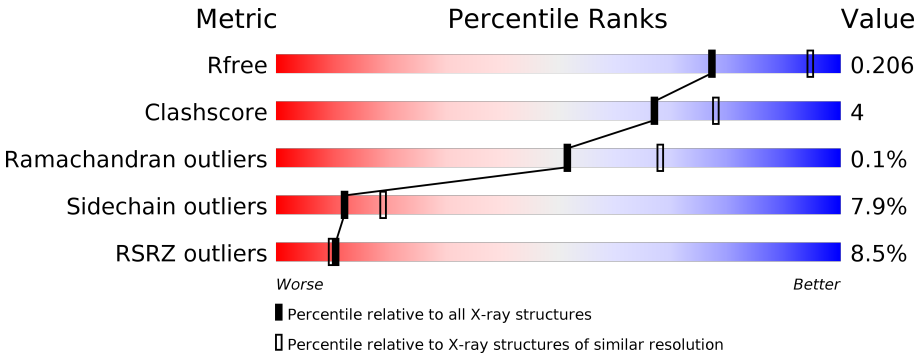
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	8% 78% 12% • 10%
1	B	769	7% 75% 11% • 12%
1	C	769	8% 75% 11% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17717 atoms, of which 75 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	695	Total	C	N	O	S	0	0	0
			5502	3506	945	1034	17			
1	B	673	Total	C	N	O	S	0	0	0
			5358	3417	918	1006	17			
1	C	672	Total	C	N	O	S	0	0	0
			5296	3374	910	995	17			

There are 60 discrepancies between the modelled and reference sequences:

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

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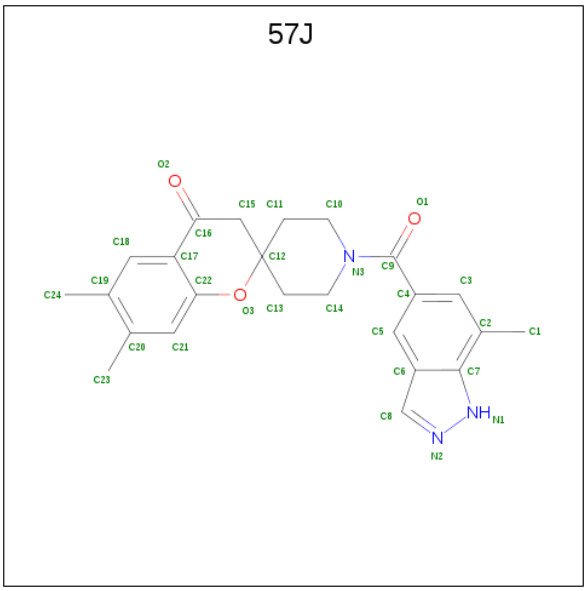
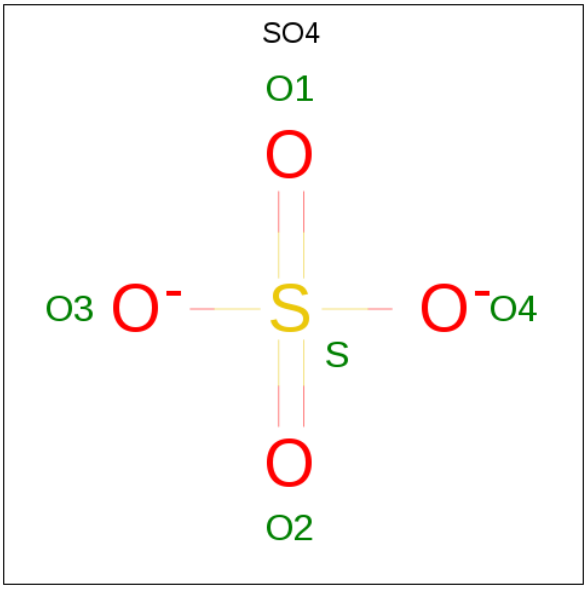
Chain	Residue	Modelled	Actual	Comment	Reference
B	1760	SER	PRO	engineered mutation	UNP Q00955
B	1762	LEU	ILE	engineered mutation	UNP Q00955
B	1765	VAL	MET	engineered mutation	UNP Q00955
B	1919	GLN	GLU	engineered mutation	UNP Q00955
B	1920	ALA	PRO	engineered mutation	UNP Q00955
B	1925	PHE	HIS	engineered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

- Molecule 2 is 6,7-dimethyl-1'-[(7-methyl-1H-indazol-5-yl)carbonyl]spiro[chromene-2,4'-piperidin]-4(3H)-one (three-letter code: 57J) (formula: $C_{24}H_{25}N_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			55	24	25	3	3		
2	B	1	Total	C	H	N	O	0	0
			55	24	25	3	3		
2	C	1	Total	C	H	N	O	0	0
			55	24	25	3	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		

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

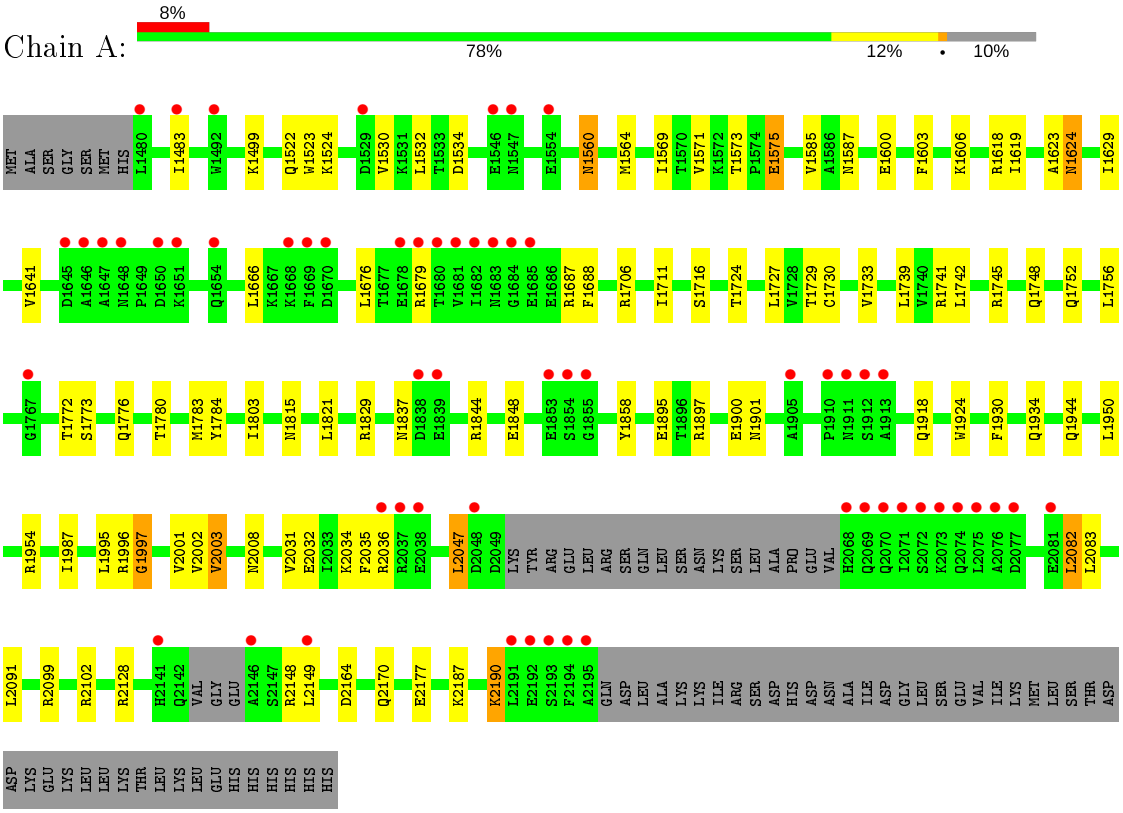
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	488	Total O 488 488	0	0
4	B	449	Total O 449 449	0	0
4	C	434	Total O 434 434	0	0

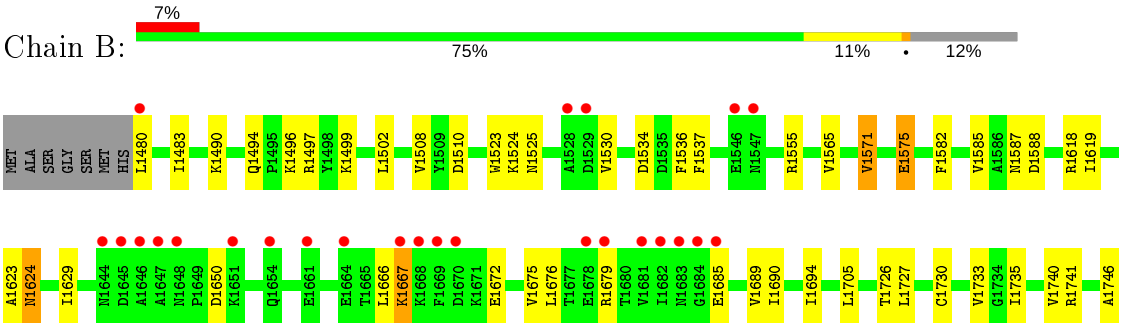
3 Residue-property plots (i)

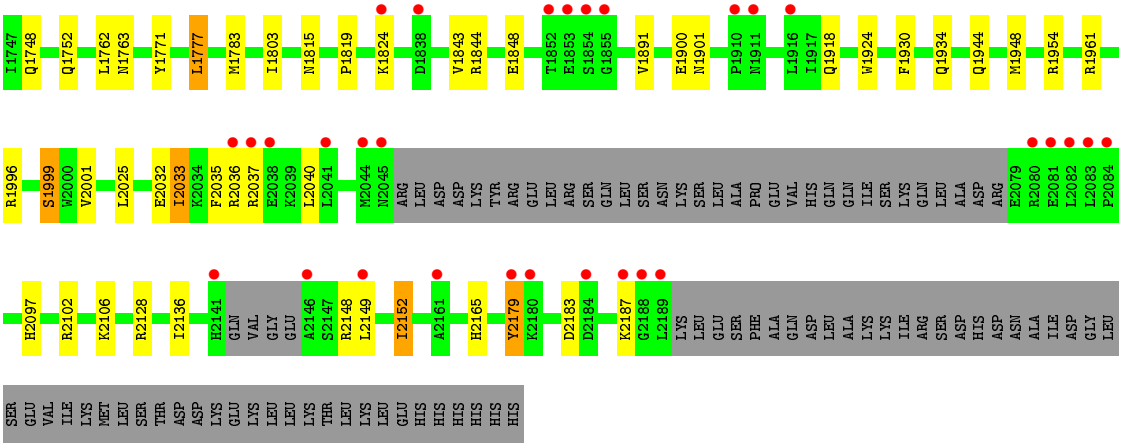
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



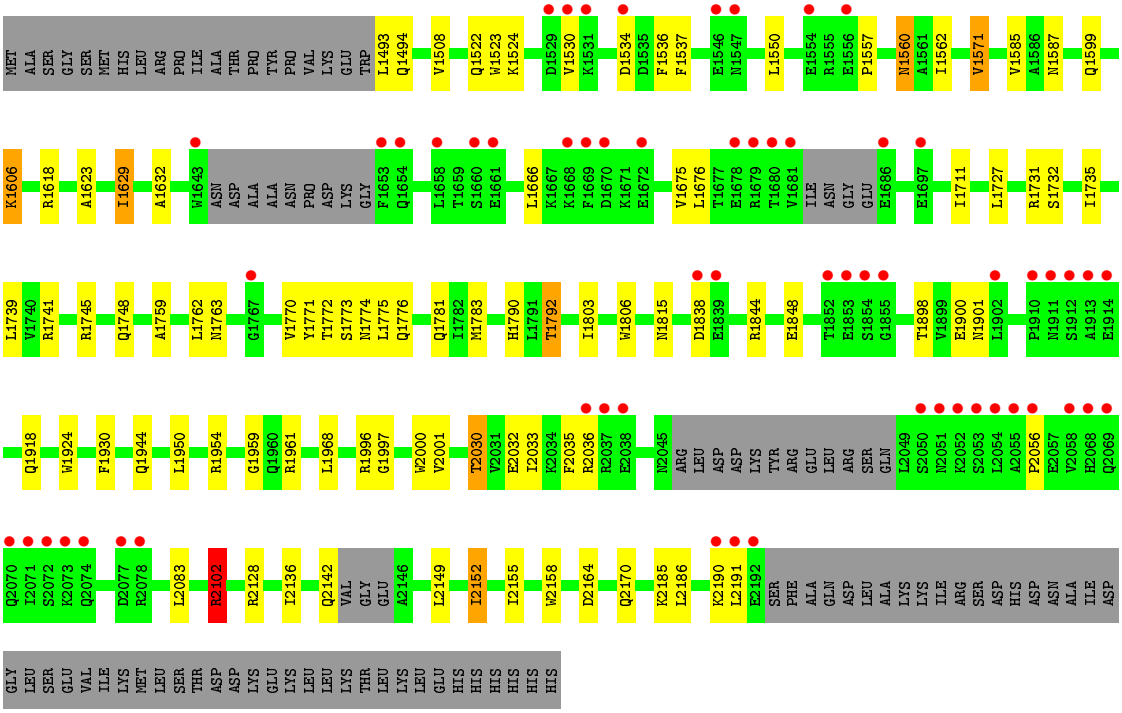
- Molecule 1: Acetyl-CoA carboxylase





• 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	245.85Å 124.38Å 145.67Å 90.00° 94.39° 90.00°	Depositor
Resolution (Å)	19.66 – 2.40 19.64 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.66-2.40) 98.5 (19.64-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.41Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.6	Depositor
R, R_{free}	0.172 , 0.199 0.178 , 0.206	Depositor DCC
R_{free} test set	16730 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.5	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	0.96	EDS
Total number of atoms	17717	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: 57J, 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	0.51	0/5621	0.70	0/7618
1	B	0.51	0/5476	0.70	0/7421
1	C	0.51	0/5404	0.71	2/7317 (0.0%)
All	All	0.51	0/16501	0.70	2/22356 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2056	PRO	N-CA-CB	6.05	110.56	103.30
1	C	2102	ARG	CB-CG-CD	5.15	124.99	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	5502	0	5403	44	0
1	B	5358	0	5291	46	0
1	C	5296	0	5179	43	0
2	A	30	25	25	0	0
2	B	30	25	25	0	0
2	C	30	25	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	0	0	0
3	C	15	0	0	0	0
4	A	488	0	0	12	0
4	B	449	0	0	11	0
4	C	434	0	0	11	0
All	All	17642	75	15948	124	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 (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1742:LEU:HD22	4:A:2412:HOH:O	1.57	1.03
1:B:1588:ASP:HB2	4:B:2736:HOH:O	1.63	0.98
1:A:1603:PHE:HB3	4:A:2446:HOH:O	1.65	0.95
1:A:1716:SER:HB2	4:A:2412:HOH:O	1.67	0.95
1:C:1599:GLN:HB2	4:C:2428:HOH:O	1.68	0.94
1:B:2033:ILE:HD11	1:C:1629:ILE:HD11	1.51	0.92
1:B:1565:VAL:HG13	4:B:2736:HOH:O	1.70	0.91
1:B:1891:VAL:HG22	4:B:2694:HOH:O	1.75	0.87
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.20	0.84
1:B:1948:MET:HB3	4:B:2694:HOH:O	1.79	0.82
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.27	0.79
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.27	0.79
1:B:1726:THR:HB	4:B:2493:HOH:O	1.84	0.77
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.32	0.76
1:A:1600:GLU:HA	4:A:2446:HOH:O	1.85	0.75
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.84	0.75
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.84	0.74
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.35	0.73
1:A:1564:MET:HB3	4:A:2446:HOH:O	1.89	0.72
1:A:2047:LEU:HD22	1:A:2082:LEU:HD11	1.73	0.70
1:C:1763:ASN:HD21	1:C:1771:TYR:H	1.36	0.70
1:C:1898:THR:HG22	4:C:2658:HOH:O	1.93	0.69
1:B:1675:VAL:HB	4:B:2410:HOH:O	1.96	0.66
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.60	0.66
1:A:1679:ARG:HG2	4:A:2462:HOH:O	1.95	0.66
1:B:1777:LEU:HG	4:C:2564:HOH:O	1.95	0.66
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.62	0.65
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1746:ALA:HB2	4:B:2493:HOH:O	1.97	0.64
1:C:2030:THR:HG21	4:C:2410:HOH:O	1.97	0.63
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.98	0.62
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.66	0.61
1:B:1900:GLU:HG2	1:B:1918:GLN:HG2	1.84	0.60
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.49	0.60
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.00	0.60
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.65	0.59
1:B:2179:TYR:HD1	1:B:2179:TYR:H	1.50	0.59
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.02	0.59
1:C:1560:ASN:HD22	1:C:1560:ASN:H	1.51	0.59
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.37	0.59
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.37	0.59
1:A:2164:ASP:H	1:A:2170:GLN:NE2	1.99	0.59
1:C:1959:GLY:HA2	4:C:2564:HOH:O	2.02	0.59
1:A:1900:GLU:HG2	1:A:1918:GLN:HG2	1.85	0.58
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.68	0.58
1:C:1900:GLU:HG2	1:C:1918:GLN:HG2	1.86	0.57
1:A:1575:GLU:HG3	4:A:2442:HOH:O	2.04	0.56
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.03	0.56
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.70	0.56
1:C:1790:HIS:HD2	4:C:2414:HOH:O	1.88	0.56
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.04	0.56
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.70	0.55
1:A:2177:GLU:HG3	1:B:1490:LYS:HE3	1.88	0.54
1:A:1997:GLY:O	1:A:2001:VAL:HG23	2.08	0.54
1:B:2001:VAL:HG21	1:C:1735:ILE:HD13	1.90	0.54
1:B:1667:LYS:HG2	1:B:1672:GLU:HG2	1.88	0.54
1:B:1497:ARG:HD3	1:B:1510:ASP:OD2	2.07	0.54
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.09	0.53
1:A:1724:THR:H	1:A:1745:ARG:HH21	1.56	0.53
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.57	0.53
1:C:1844:ARG:O	1:C:1848:GLU:HG2	2.08	0.53
1:A:1821:LEU:HD22	4:A:2442:HOH:O	2.08	0.52
1:B:1690:ILE:HG23	4:B:2410:HOH:O	2.08	0.52
1:B:1740:VAL:HG13	4:B:2493:HOH:O	2.08	0.52
1:C:2136:ILE:HD11	1:C:2152:ILE:HG23	1.91	0.52
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.58	0.52
1:B:1735:ILE:HD13	1:C:2001:VAL:HG21	1.92	0.51
1:C:2155:ILE:HG13	4:C:2635:HOH:O	2.10	0.51
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1844:ARG:O	1:A:1848:GLU:HG2	2.10	0.51
1:A:1523:TRP:CE3	1:A:1530:VAL:HG21	2.46	0.51
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.60	0.50
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.10	0.50
1:C:1954:ARG:O	1:C:1996:ARG:HB2	2.12	0.50
1:C:1606:LYS:HD2	4:C:2422:HOH:O	2.13	0.49
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.11	0.49
1:A:1729:THR:HB	4:A:2834:HOH:O	2.12	0.48
1:C:1792:THR:HG21	4:C:2749:HOH:O	2.13	0.48
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.60	0.48
1:C:1493:LEU:HD11	1:C:1557:PRO:HB2	1.95	0.48
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.21	0.47
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.12	0.47
1:A:1571:VAL:HG13	1:A:1573:THR:HG23	1.97	0.47
1:B:1705:LEU:HB3	1:C:2000:TRP:CD1	2.50	0.47
1:B:2106:LYS:HG3	4:C:2456:HOH:O	2.14	0.46
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.63	0.46
1:C:1727:LEU:HB2	1:C:1803:ILE:HD11	1.97	0.45
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.64	0.45
1:C:1562:ILE:HG22	4:C:2428:HOH:O	2.15	0.45
1:C:2164:ASP:H	1:C:2170:GLN:HE22	1.65	0.45
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.99	0.44
1:A:1954:ARG:O	1:A:1996:ARG:HB2	2.17	0.44
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.99	0.44
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.65	0.44
1:A:1569:ILE:HG22	4:A:2408:HOH:O	2.17	0.44
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.14	0.44
1:B:2179:TYR:HD1	1:B:2179:TYR:N	2.13	0.44
1:C:1523:TRP:CE3	1:C:1530:VAL:HG21	2.52	0.44
1:A:1995:LEU:HA	1:A:1995:LEU:HD12	1.91	0.43
1:A:2187:LYS:O	1:A:2190:LYS:HB2	2.19	0.43
1:C:1711:ILE:HD12	1:C:1739:LEU:HD11	2.00	0.43
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	1.99	0.43
1:A:1727:LEU:HB2	1:A:1803:ILE:HD11	2.01	0.43
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.65	0.43
1:A:1560:ASN:H	1:A:1560:ASN:ND2	2.16	0.43
1:B:2033:ILE:CD1	1:C:1629:ILE:HD11	2.36	0.43
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.54	0.42
1:A:1571:VAL:HG12	4:A:2408:HOH:O	2.19	0.42
1:A:1773:SER:HB2	4:A:2855:HOH:O	2.19	0.42
1:C:2158:TRP:CE2	1:C:2185:LYS:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1575:GLU:HB3	1:B:1819:PRO:HB2	2.02	0.42
1:A:1679:ARG:HG3	1:A:1688:PHE:CE2	2.55	0.41
1:A:1987:ILE:HD12	1:A:2003:VAL:HG22	2.02	0.41
1:B:1582:PHE:CD2	1:B:1619:ILE:HD12	2.56	0.41
1:B:2179:TYR:CD1	1:B:2179:TYR:N	2.85	0.41
1:B:1954:ARG:O	1:B:1996:ARG:HB2	2.20	0.41
1:C:1560:ASN:ND2	1:C:1560:ASN:H	2.18	0.41
1:B:2179:TYR:HB3	4:B:2796:HOH:O	2.20	0.40
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.21	0.40
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.52	0.40
1:B:1999:SER:HB3	4:B:2415:HOH:O	2.21	0.40
1:B:2136:ILE:HD11	1:B:2152:ILE:HG23	2.03	0.40
1:C:2142:GLN:HB3	1:C:2190:LYS:HG3	2.02	0.40
1:B:1523:TRP:CE3	1:B:1530:VAL:HG11	2.56	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	689/769 (90%)	665 (96%)	23 (3%)	1 (0%)	51 68
1	B	667/769 (87%)	643 (96%)	24 (4%)	0	100 100
1	C	660/769 (86%)	637 (96%)	22 (3%)	1 (0%)	47 62
All	All	2016/2307 (87%)	1945 (96%)	69 (3%)	2 (0%)	51 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1997	GLY
1	A	1997	GLY

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	578/658 (88%)	535 (93%)	43 (7%)	13	22
1	B	569/658 (86%)	521 (92%)	48 (8%)	11	16
1	C	552/658 (84%)	509 (92%)	43 (8%)	12	19
All	All	1699/1974 (86%)	1565 (92%)	134 (8%)	12	19

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1483	ILE
1	A	1499	LYS
1	A	1522	GLN
1	A	1524	LYS
1	A	1532	LEU
1	A	1534	ASP
1	A	1560	ASN
1	A	1575	GLU
1	A	1585	VAL
1	A	1606	LYS
1	A	1618	ARG
1	A	1619	ILE
1	A	1624	ASN
1	A	1629	ILE
1	A	1641	VAL
1	A	1666	LEU
1	A	1676	LEU
1	A	1687	ARG
1	A	1706	ARG
1	A	1756	LEU
1	A	1837	ASN
1	A	1901	ASN
1	A	1924	TRP
1	A	1930	PHE
1	A	1950	LEU
1	A	2002	VAL

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Mol	Chain	Res	Type
1	A	2003	VAL
1	A	2008	ASN
1	A	2031	VAL
1	A	2032	GLU
1	A	2034	LYS
1	A	2035	PHE
1	A	2036	ARG
1	A	2047	LEU
1	A	2082	LEU
1	A	2083	LEU
1	A	2091	LEU
1	A	2099	ARG
1	A	2102	ARG
1	A	2128	ARG
1	A	2148	ARG
1	A	2149	LEU
1	A	2190	LYS
1	B	1480	LEU
1	B	1483	ILE
1	B	1499	LYS
1	B	1502	LEU
1	B	1508	VAL
1	B	1524	LYS
1	B	1525	ASN
1	B	1534	ASP
1	B	1536	PHE
1	B	1555	ARG
1	B	1571	VAL
1	B	1575	GLU
1	B	1585	VAL
1	B	1618	ARG
1	B	1624	ASN
1	B	1629	ILE
1	B	1650	ASP
1	B	1666	LEU
1	B	1667	LYS
1	B	1676	LEU
1	B	1679	ARG
1	B	1685	GLU
1	B	1689	VAL
1	B	1762	LEU
1	B	1777	LEU

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Mol	Chain	Res	Type
1	B	1824	LYS
1	B	1843	VAL
1	B	1901	ASN
1	B	1924	TRP
1	B	1930	PHE
1	B	1961	ARG
1	B	1999	SER
1	B	2025	LEU
1	B	2032	GLU
1	B	2033	ILE
1	B	2035	PHE
1	B	2036	ARG
1	B	2037	ARG
1	B	2040	LEU
1	B	2102	ARG
1	B	2128	ARG
1	B	2148	ARG
1	B	2149	LEU
1	B	2152	ILE
1	B	2165	HIS
1	B	2179	TYR
1	B	2183	ASP
1	B	2187	LYS
1	C	1494	GLN
1	C	1508	VAL
1	C	1522	GLN
1	C	1524	LYS
1	C	1534	ASP
1	C	1536	PHE
1	C	1550	LEU
1	C	1560	ASN
1	C	1571	VAL
1	C	1585	VAL
1	C	1606	LYS
1	C	1618	ARG
1	C	1629	ILE
1	C	1666	LEU
1	C	1675	VAL
1	C	1676	LEU
1	C	1731	ARG
1	C	1732	SER
1	C	1741	ARG

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Mol	Chain	Res	Type
1	C	1762	LEU
1	C	1770	VAL
1	C	1775	LEU
1	C	1781	GLN
1	C	1792	THR
1	C	1838	ASP
1	C	1901	ASN
1	C	1924	TRP
1	C	1930	PHE
1	C	1950	LEU
1	C	1961	ARG
1	C	1968	LEU
1	C	2030	THR
1	C	2032	GLU
1	C	2033	ILE
1	C	2035	PHE
1	C	2036	ARG
1	C	2083	LEU
1	C	2102	ARG
1	C	2128	ARG
1	C	2149	LEU
1	C	2152	ILE
1	C	2186	LEU
1	C	2191	LEU

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

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1720	HIS
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1815	ASN
1	A	1901	ASN
1	A	1918	GLN
1	A	1934	GLN
1	A	2008	ASN

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Mol	Chain	Res	Type
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	1815	ASN
1	B	1901	ASN
1	B	1934	GLN
1	B	1944	GLN
1	B	2097	HIS
1	B	2131	ASN
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	1815	ASN
1	C	1901	ASN
1	C	1918	GLN
1	C	1919	GLN
1	C	2011	GLN
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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	2303	-	4,4,4	0.21	0	6,6,6	0.18	0
2	57J	B	2301	-	34,34,34	0.89	1 (2%)	36,52,52	0.91	2 (5%)
3	SO4	C	2304	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	C	2303	-	4,4,4	0.16	0	6,6,6	0.11	0
2	57J	C	2301	-	34,34,34	0.90	1 (2%)	36,52,52	0.96	2 (5%)
3	SO4	A	2302	-	4,4,4	0.10	0	6,6,6	0.12	0
2	57J	A	2301	-	34,34,34	0.88	1 (2%)	36,52,52	0.96	2 (5%)
3	SO4	C	2302	-	4,4,4	0.23	0	6,6,6	0.13	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	57J	B	2301	-	-	0/8/34/34	0/5/5/5
2	57J	C	2301	-	-	0/8/34/34	0/5/5/5
2	57J	A	2301	-	-	0/8/34/34	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2301	57J	C9-N3	2.53	1.40	1.34
2	B	2301	57J	C9-N3	2.32	1.39	1.34
2	A	2301	57J	C9-N3	2.23	1.39	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2301	57J	C4-C5-C6	-2.54	117.32	121.24
2	C	2301	57J	C4-C5-C6	-2.52	117.35	121.24
2	A	2301	57J	C4-C5-C6	-2.49	117.40	121.24
2	A	2301	57J	C5-C4-C3	2.17	122.51	119.83
2	C	2301	57J	C5-C4-C3	2.16	122.49	119.83
2	B	2301	57J	C5-C4-C3	2.13	122.45	119.83

There are no chirality outliers.

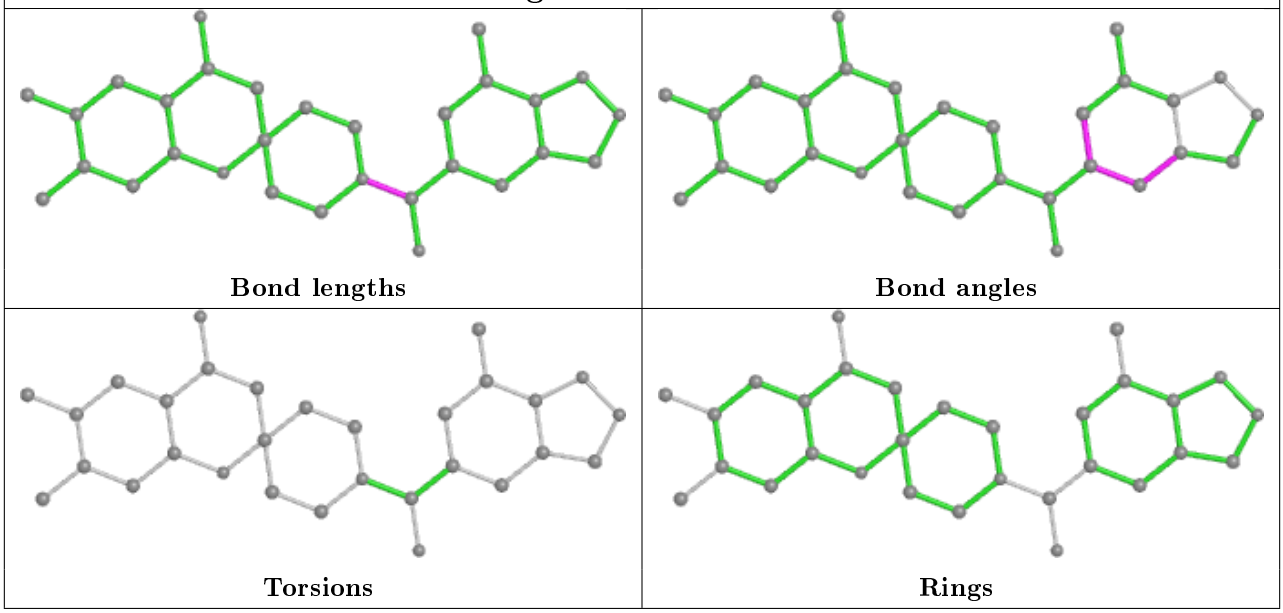
There are no torsion outliers.

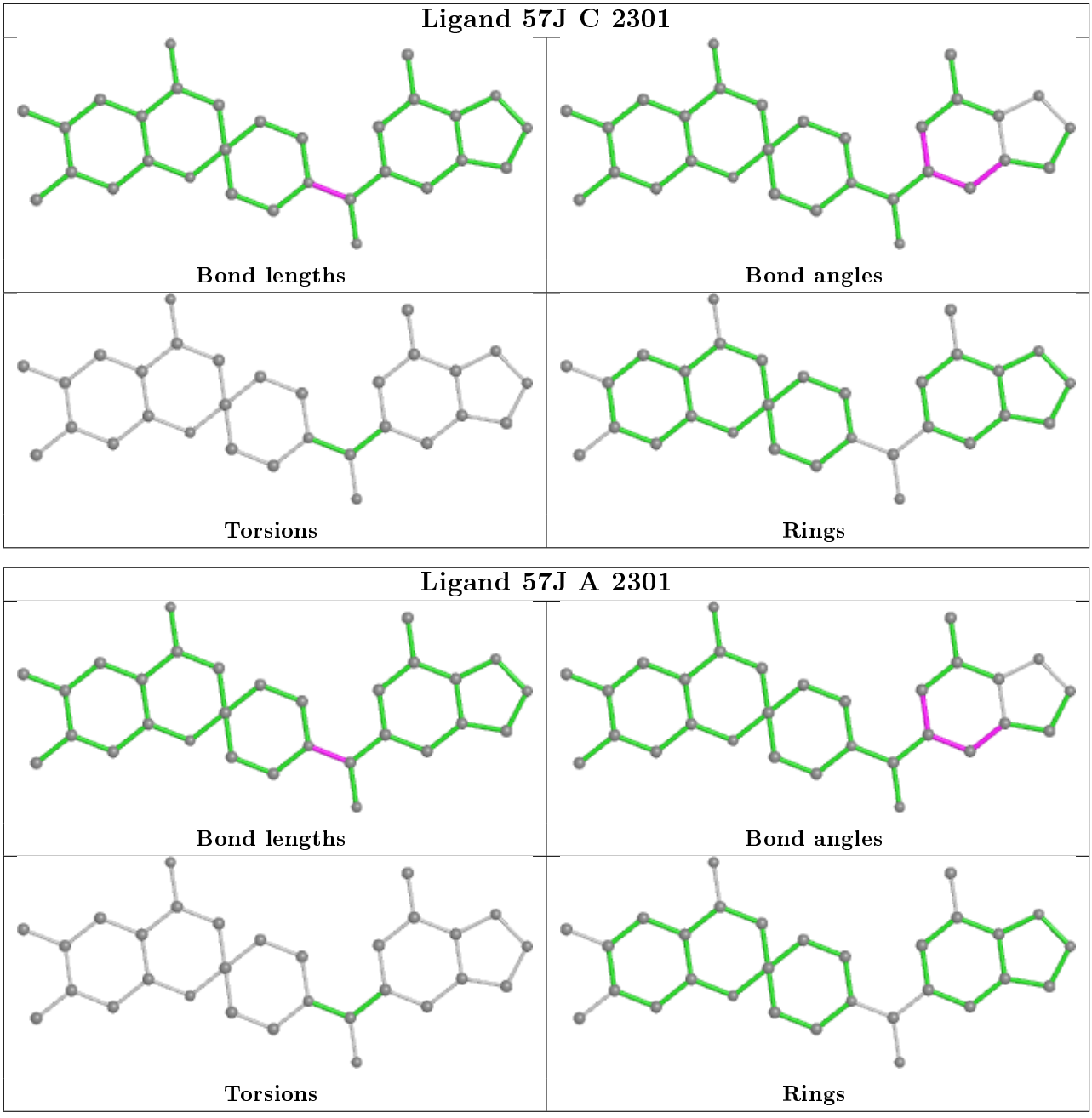
There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand 57J B 2301





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2058:VAL	C	2068:HIS	N	10.40

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	695/769 (90%)	-0.11	59 (8%)	10 10	25, 47, 102, 135	0
1	B	673/769 (87%)	-0.06	55 (8%)	11 10	28, 50, 104, 135	0
1	C	672/769 (87%)	-0.07	60 (8%)	9 9	27, 50, 105, 144	0
All	All	2040/2307 (88%)	-0.08	174 (8%)	10 10	25, 49, 104, 144	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2194	PHE	7.5
1	A	2068	HIS	6.5
1	A	2071	ILE	5.8
1	B	2082	LEU	5.8
1	C	2069	GLN	5.7
1	B	1682	ILE	5.7
1	B	2179	TYR	5.2
1	B	1684	GLY	5.1
1	A	1911	ASN	5.1
1	C	2068	HIS	5.0
1	B	1647	ALA	5.0
1	C	2071	ILE	4.9
1	C	2192	GLU	4.9
1	C	2056	PRO	4.9
1	A	2072	SER	4.9
1	C	2058	VAL	4.8
1	A	1669	PHE	4.7
1	C	2037	ARG	4.7
1	B	1911	ASN	4.7
1	B	1910	PRO	4.6
1	A	1648	ASN	4.6
1	C	2070	GLN	4.6
1	C	1654	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	1679	ARG	4.5
1	A	1647	ALA	4.5
1	C	1680	THR	4.5
1	B	1683	ASN	4.4
1	B	2189	LEU	4.3
1	A	1838	ASP	4.2
1	A	2069	GLN	4.2
1	C	1546	GLU	4.2
1	B	1854	SER	4.2
1	C	1838	ASP	4.1
1	B	2037	ARG	4.1
1	C	1681	VAL	4.1
1	A	2048	ASP	4.1
1	C	2072	SER	4.1
1	B	1645	ASP	4.0
1	B	1838	ASP	4.0
1	A	2195	ALA	4.0
1	B	1679	ARG	4.0
1	B	2188	GLY	4.0
1	C	1855	GLY	4.0
1	A	1651	LYS	4.0
1	B	1651	LYS	4.0
1	C	1668	LYS	3.9
1	A	1910	PRO	3.9
1	B	2187	LYS	3.9
1	C	1669	PHE	3.9
1	C	1670	ASP	3.8
1	A	2075	LEU	3.8
1	A	2191	LEU	3.8
1	B	2041	LEU	3.8
1	C	1911	ASN	3.8
1	C	2054	LEU	3.7
1	C	1913	ALA	3.7
1	A	1681	VAL	3.7
1	C	2191	LEU	3.7
1	C	1910	PRO	3.6
1	B	1546	GLU	3.4
1	B	1654	GLN	3.4
1	C	1853	GLU	3.4
1	B	1529	ASP	3.3
1	A	1853	GLU	3.3
1	B	1853	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	2074	GLN	3.3
1	B	1685	GLU	3.3
1	B	1648	ASN	3.3
1	A	1839	GLU	3.3
1	A	2070	GLN	3.3
1	B	2036	ARG	3.3
1	B	2083	LEU	3.3
1	C	2055	ALA	3.3
1	C	2051	ASN	3.3
1	A	1529	ASP	3.2
1	B	2038	GLU	3.2
1	A	1645	ASP	3.2
1	B	2081	GLU	3.2
1	C	1767	GLY	3.2
1	A	1684	GLY	3.1
1	C	1643	TRP	3.1
1	B	1644	ASN	3.1
1	A	1855	GLY	3.1
1	A	2038	GLU	3.0
1	B	1547	ASN	3.0
1	B	2141	HIS	3.0
1	A	2076	ALA	3.0
1	C	2050	SER	3.0
1	A	2077	ASP	3.0
1	B	1668	LYS	3.0
1	A	1683	ASN	3.0
1	C	2190	LYS	3.0
1	B	1669	PHE	2.9
1	B	2149	LEU	2.9
1	A	1483	ILE	2.9
1	A	2037	ARG	2.9
1	A	2192	GLU	2.9
1	C	1686	GLU	2.9
1	C	1653	PHE	2.8
1	C	2036	ARG	2.8
1	A	1668	LYS	2.8
1	A	1767	GLY	2.8
1	A	2141	HIS	2.8
1	B	2161	ALA	2.8
1	A	1912	SER	2.8
1	C	1914	GLU	2.8
1	B	2044	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	2077	ASP	2.8
1	C	1661	GLU	2.7
1	A	1546	GLU	2.7
1	B	2084	PRO	2.7
1	B	1852	THR	2.7
1	C	2073	LYS	2.7
1	A	1685	GLU	2.7
1	B	1824	LYS	2.7
1	A	2074	GLN	2.7
1	B	1681	VAL	2.7
1	B	2146	ALA	2.7
1	B	1480	LEU	2.7
1	A	2193	SER	2.6
1	C	2053	SER	2.6
1	A	1646	ALA	2.6
1	C	1529	ASP	2.6
1	C	1534	ASP	2.6
1	B	1916	LEU	2.5
1	B	1646	ALA	2.5
1	A	2036	ARG	2.5
1	A	1492	TRP	2.5
1	A	1670	ASP	2.5
1	A	1682	ILE	2.5
1	C	1902	LEU	2.4
1	C	1530	VAL	2.4
1	B	1670	ASP	2.4
1	C	1556	GLU	2.4
1	A	2073	LYS	2.4
1	C	1658	LEU	2.4
1	B	2045	ASN	2.4
1	B	1678	GLU	2.4
1	A	2146	ALA	2.4
1	B	1855	GLY	2.4
1	A	1854	SER	2.3
1	A	1654	GLN	2.3
1	C	1547	ASN	2.3
1	C	1854	SER	2.3
1	C	1672	GLU	2.3
1	B	2180	LYS	2.3
1	C	2038	GLU	2.3
1	A	1554	GLU	2.3
1	C	1531	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	1660	SER	2.2
1	B	2184	ASP	2.2
1	A	2081	GLU	2.2
1	C	2052	LYS	2.2
1	A	1905	ALA	2.2
1	A	1680	THR	2.2
1	A	2149	LEU	2.2
1	A	1678	GLU	2.2
1	B	1664	GLU	2.2
1	A	1913	ALA	2.2
1	A	1547	ASN	2.2
1	C	1678	GLU	2.2
1	B	1667	LYS	2.1
1	C	1839	GLU	2.1
1	B	2080	ARG	2.1
1	C	1554	GLU	2.1
1	C	2078	ARG	2.1
1	B	1528	ALA	2.1
1	A	1679	ARG	2.1
1	C	1912	SER	2.1
1	B	1661	GLU	2.1
1	C	1852	THR	2.0
1	A	1650	ASP	2.0
1	A	1480	LEU	2.0
1	C	1697	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 carbohydrates in this entry.

6.4 Ligands (i)

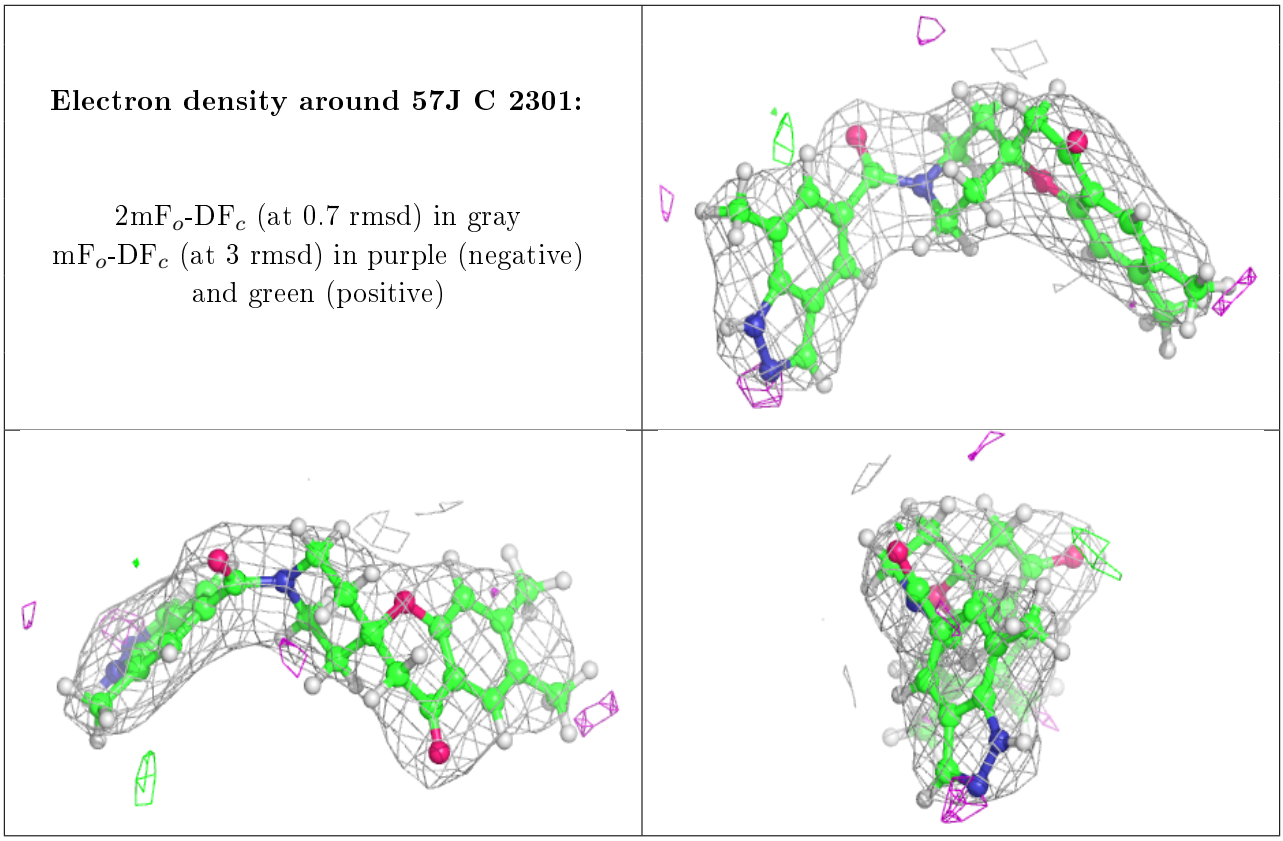
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	2304	5/5	0.83	0.46	143,144,144,145	0
3	SO4	C	2302	5/5	0.87	0.26	121,122,123,123	0
3	SO4	A	2303	5/5	0.94	0.34	121,121,122,122	0
2	57J	C	2301	30/30	0.95	0.11	48,56,65,68	0
2	57J	B	2301	30/30	0.95	0.15	53,61,74,75	0
2	57J	A	2301	30/30	0.96	0.14	46,51,61,63	0
3	SO4	A	2302	5/5	0.97	0.26	107,107,108,109	0
3	SO4	C	2303	5/5	0.98	0.24	101,101,101,101	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.

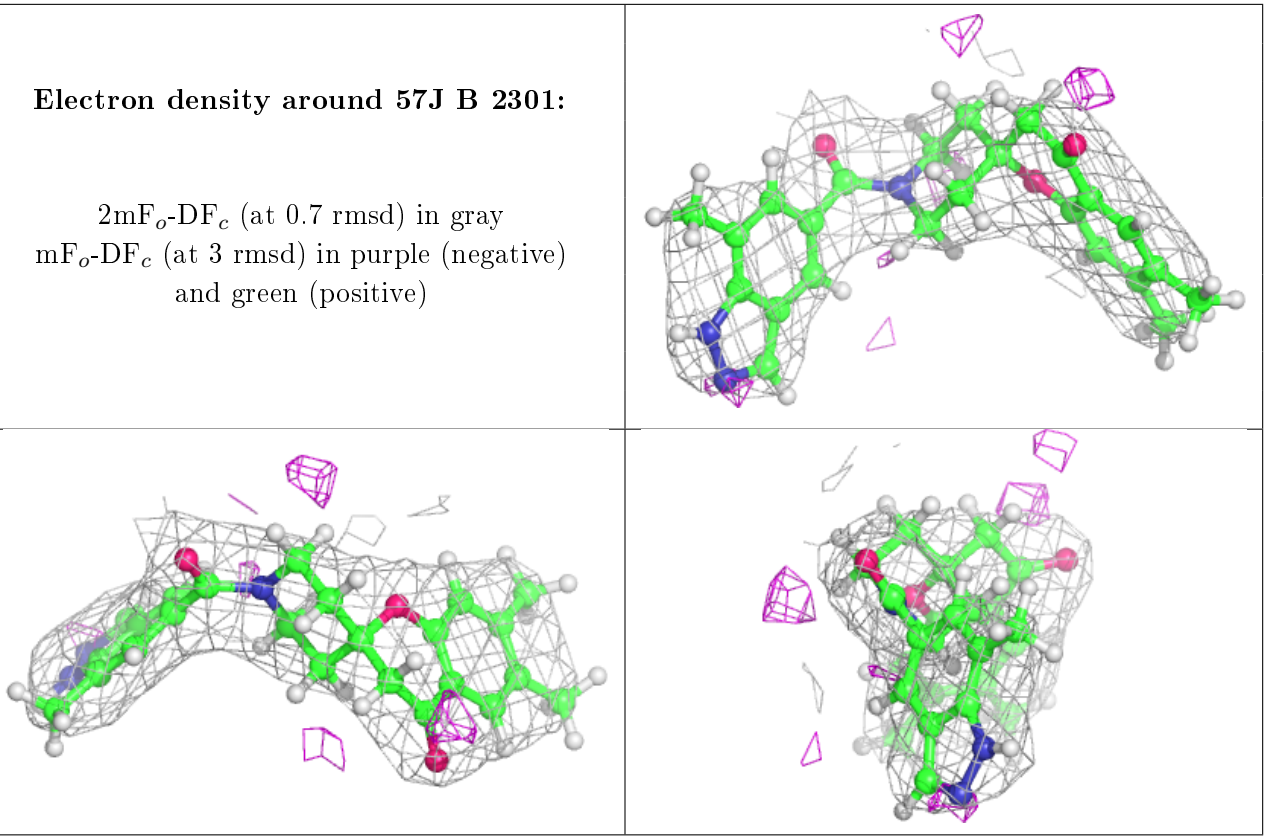
Electron density around 57J C 2301:

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



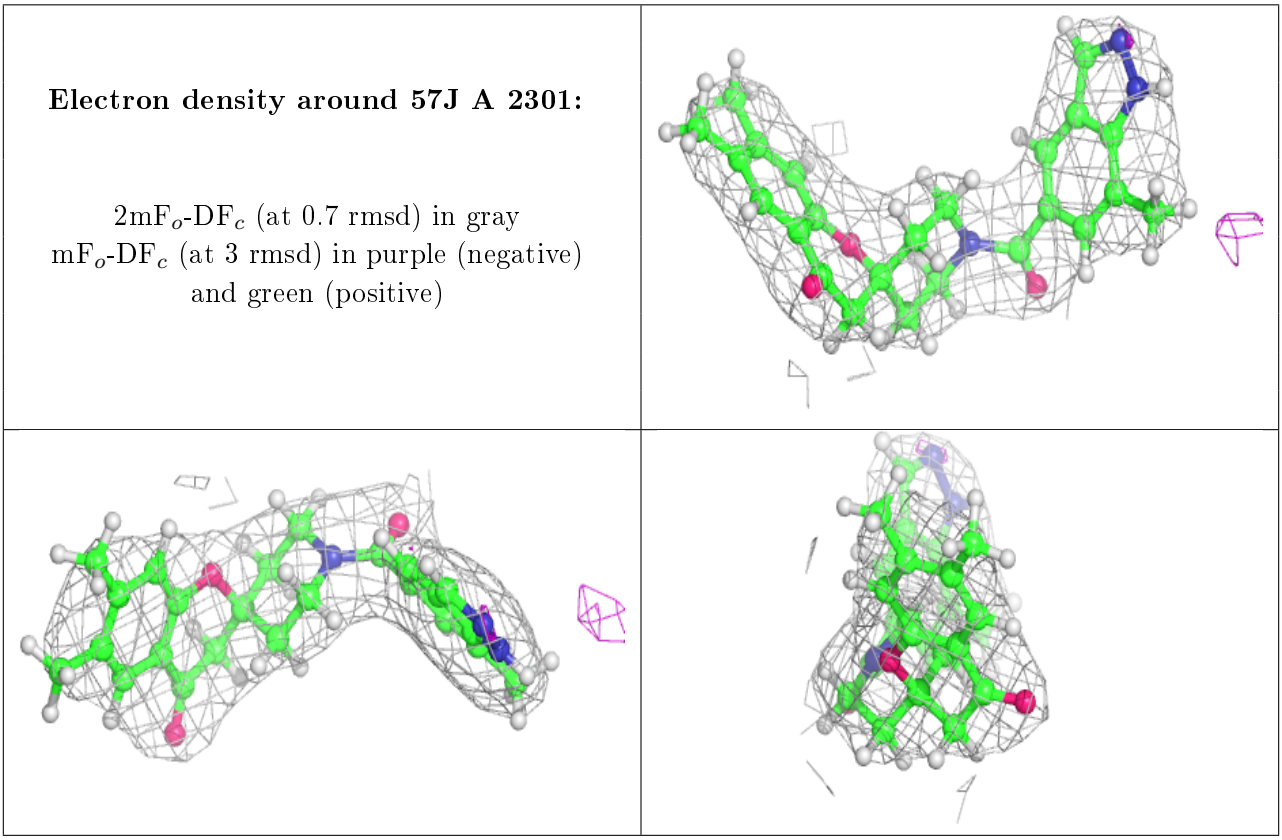
Electron density around 57J B 2301:

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



Electron density around 57J 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)



6.5 Other polymers (i)

There are no such residues in this entry.