



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:25 PM UTC

PDB ID : 3K8X / pdb_00003k8x
Title : Crystal structure of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in complex with tepraloxydim
Authors : Xiang, S.; Callaghan, M.M.; Watson, K.G.; Tong, L.
Deposited on : 2009-10-15
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

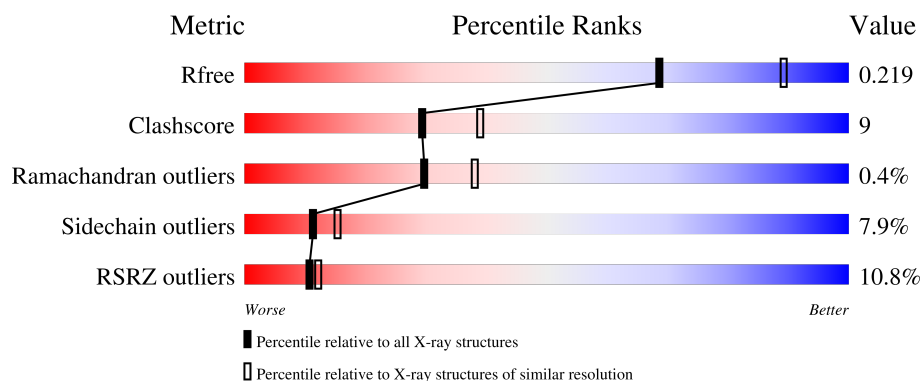
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	758	9% 75% 12% • 9%
1	B	758	11% 70% 16% • 10%
1	C	758	10% 72% 15% • 11%

2 Entry composition [i](#)

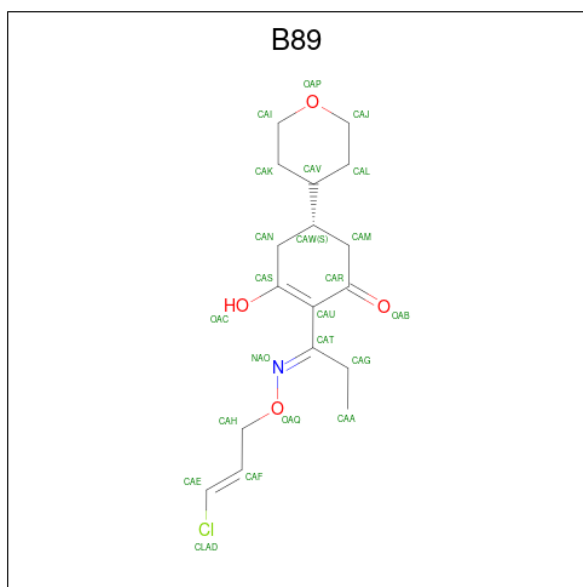
There are 3 unique types of molecules in this entry. The entry contains 17693 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	688	Total	C	N	O	S	0	0	0
			5491	3500	944	1028	19			
1	B	682	Total	C	N	O	S	0	0	0
			5443	3468	937	1019	19			
1	C	675	Total	C	N	O	S	0	0	0
			5387	3428	927	1013	19			

- Molecule 2 is (5S)-2-[(1E)-N-{[(2E)-3-chloroprop-2-en-1-yl]oxy}propanimidoyl]-3-hydroxy-5-(tetrahydro-2H-pyran-4-yl)cyclohex-2-en-1-one (CCD ID: B89) (formula: C₁₇H₂₄ClNO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			23	17	1	1	4		
2	B	1	Total	C	Cl	N	O	0	0
			23	17	1	1	4		
2	C	1	Total	C	Cl	N	O	0	0
			23	17	1	1	4		

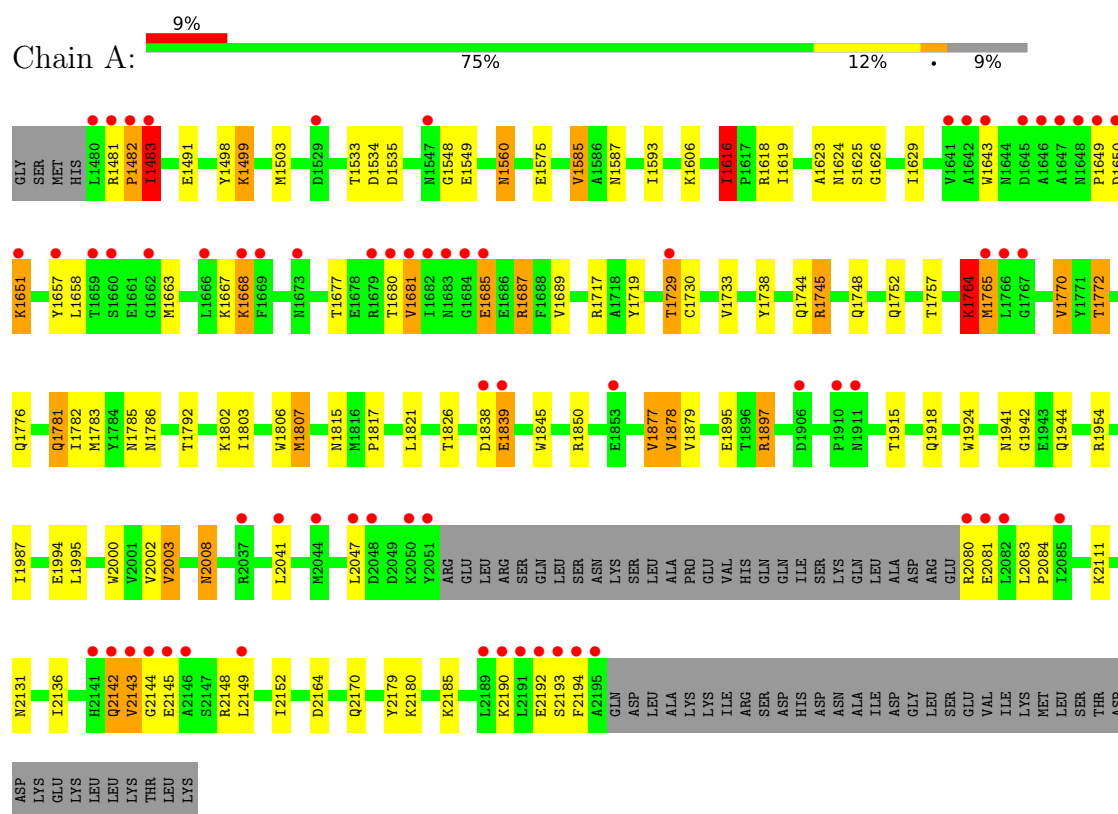
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	483	Total 483	O 483	0	0
3	B	415	Total 415	O 415	0	0
3	C	405	Total 405	O 405	0	0

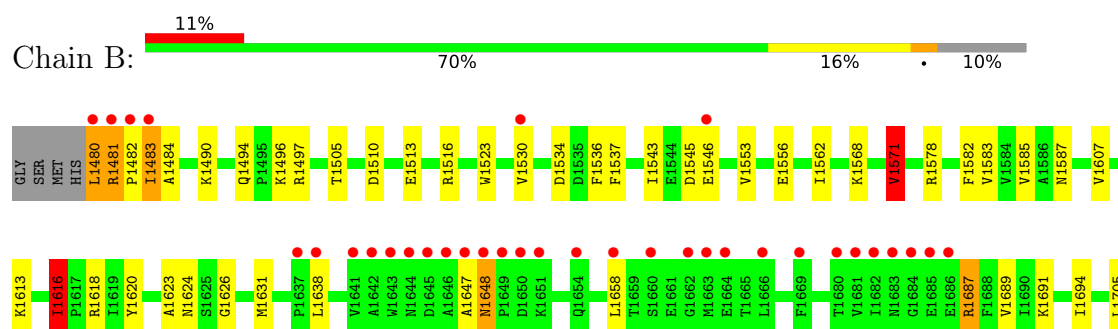
3 Residue-property plots [i](#)

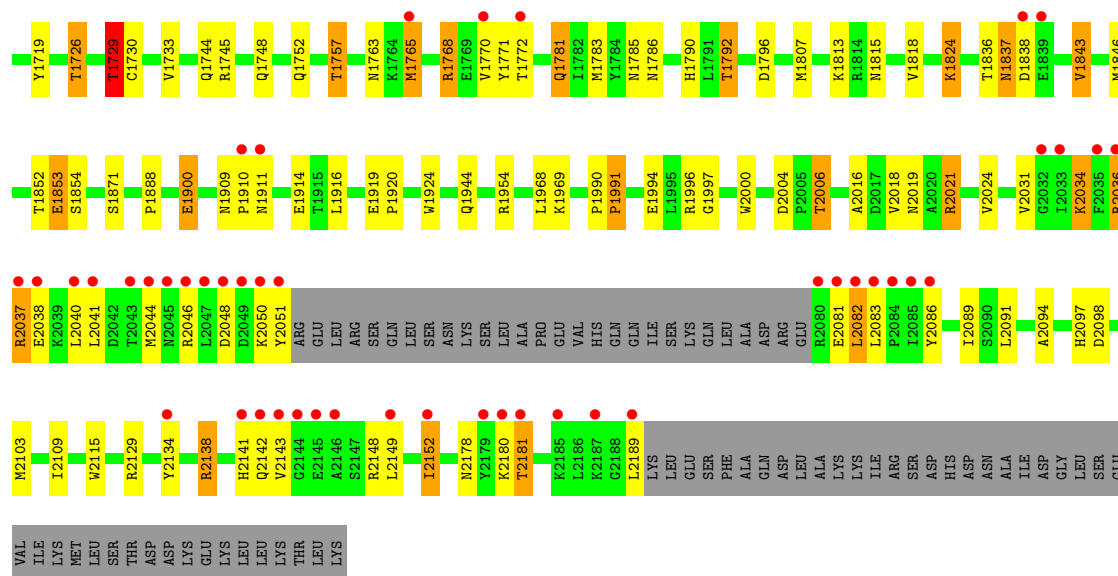
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

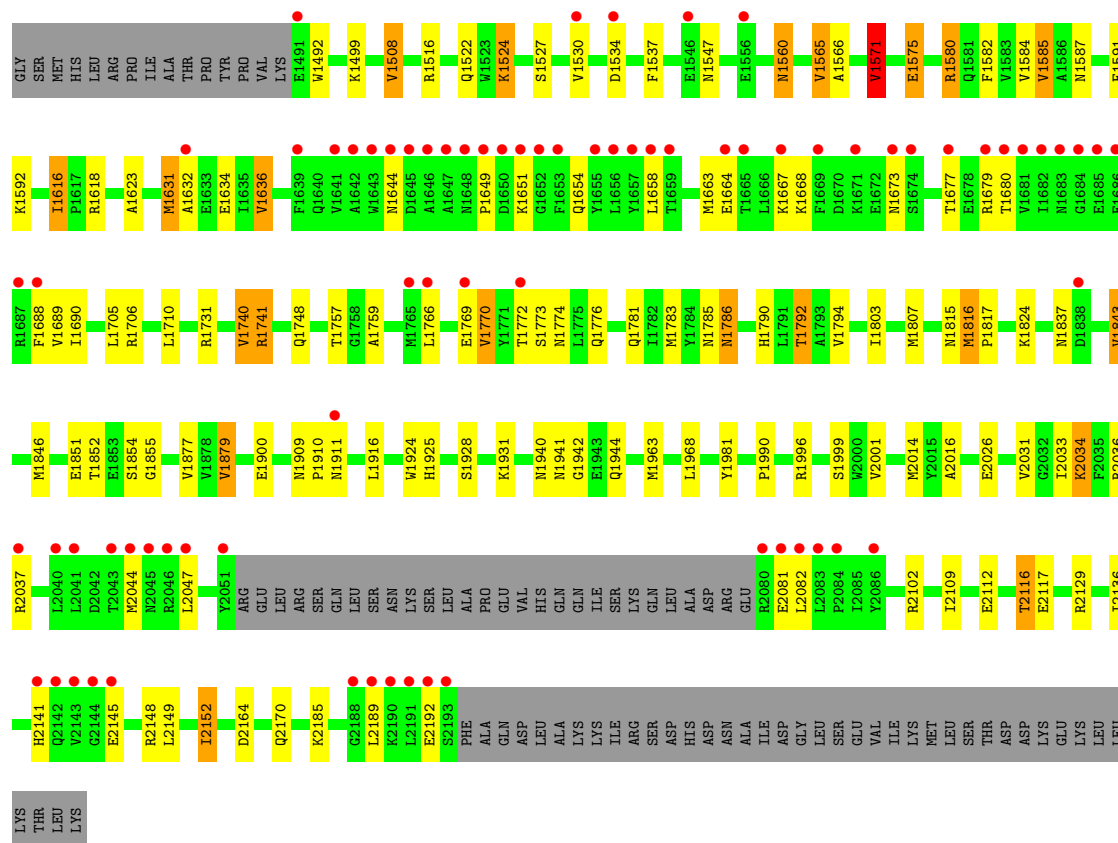


• Molecule 1: Acetyl-CoA carboxylase





• Molecule 1: Acetyl-CoA carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.30Å 124.80Å 145.37Å 90.00° 94.32° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.30) 98.7 (30.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.187 , 0.221 (Not available) , 0.219	Depositor DCC
R_{free} test set	9659 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17693	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B89

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	0.86	2/5614 (0.0%)	1.03	27/7605 (0.4%)
1	B	0.83	1/5565 (0.0%)	0.98	13/7540 (0.2%)
1	C	0.82	3/5505 (0.1%)	1.01	15/7454 (0.2%)
All	All	0.84	6/16684 (0.0%)	1.01	55/22599 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1942	GLY	N-CA	7.84	1.56	1.45
1	C	1942	GLY	N-CA	6.89	1.55	1.45
1	A	1786	ASN	CB-CG	-6.16	1.36	1.52
1	C	1636	VAL	CA-CB	5.42	1.57	1.53
1	B	1483	ILE	CA-CB	5.36	1.61	1.54
1	C	1565	VAL	CA-CB	5.07	1.62	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1941	ASN	CA-C-N	-10.95	99.95	121.41
1	A	1941	ASN	C-N-CA	-10.95	99.95	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1483	ILE	N-CA-C	9.52	124.19	111.44
1	C	1941	ASN	N-CA-C	9.18	120.97	110.97
1	C	1941	ASN	CA-C-N	-9.06	103.64	121.41
1	C	1941	ASN	C-N-CA	-9.06	103.64	121.41
1	A	1585	VAL	CB-CA-C	-8.76	97.57	110.62
1	B	1571	VAL	CB-CA-C	-8.57	97.86	110.62
1	C	1843	VAL	CB-CA-C	-8.22	100.05	112.05
1	C	1508	VAL	CB-CA-C	-8.17	101.43	111.88
1	A	1729	THR	N-CA-C	7.99	125.22	114.12
1	A	1941	ASN	O-C-N	-7.82	113.90	122.03
1	A	2081	GLU	N-CA-C	-7.75	103.14	112.59
1	B	1843	VAL	CB-CA-C	-7.59	100.97	112.05
1	B	1729	THR	CB-CA-C	-7.38	96.97	109.38
1	B	1745	ARG	NE-CZ-NH2	-7.29	112.64	119.20
1	B	1991	PRO	CA-C-N	-7.17	111.19	122.73
1	B	1991	PRO	C-N-CA	-7.17	111.19	122.73
1	C	1585	VAL	CB-CA-C	-7.07	99.56	110.95
1	C	1571	VAL	CB-CA-C	-7.00	100.18	110.62
1	A	1717	ARG	NE-CZ-NH2	-6.85	113.04	119.20
1	A	1786	ASN	CB-CA-C	-6.82	96.48	110.38
1	B	1786	ASN	CB-CA-C	-6.78	96.54	110.38
1	C	2081	GLU	N-CA-C	-6.77	103.04	112.25
1	C	1508	VAL	N-CA-CB	6.76	118.02	110.51
1	A	1481	ARG	CA-C-N	6.72	128.24	119.84
1	A	1481	ARG	C-N-CA	6.72	128.24	119.84
1	C	1941	ASN	O-C-N	-6.56	115.21	122.03
1	A	1941	ASN	N-CA-C	6.52	118.08	110.97
1	A	1616	ILE	CA-CB-CG2	6.43	121.44	110.50
1	B	1745	ARG	CG-CD-NE	-6.37	97.99	112.00
1	A	1717	ARG	CG-CD-NE	-6.34	98.05	112.00
1	C	1837	ASN	N-CA-C	6.31	118.97	111.33
1	B	1785	ASN	CA-C-N	6.03	130.93	120.68
1	B	1785	ASN	C-N-CA	6.03	130.93	120.68
1	B	1770	VAL	N-CA-C	5.95	116.13	110.53
1	A	1745	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	A	2145	GLU	N-CA-C	5.82	119.44	110.42
1	B	2143	VAL	N-CA-C	5.79	115.98	110.42
1	A	1785	ASN	CA-C-N	5.77	130.49	120.68
1	A	1785	ASN	C-N-CA	5.77	130.49	120.68
1	C	1928	SER	N-CA-CB	-5.60	101.86	110.20
1	A	1878	VAL	CB-CA-C	5.46	118.71	110.63
1	A	1877	VAL	CB-CA-C	-5.38	102.54	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2194	PHE	N-CA-C	-5.29	106.51	113.12
1	C	1785	ASN	CA-C-N	5.26	129.62	120.68
1	C	1785	ASN	C-N-CA	5.26	129.62	120.68
1	A	1483	ILE	CA-C-N	-5.22	113.94	123.34
1	A	1483	ILE	C-N-CA	-5.22	113.94	123.34
1	A	1745	ARG	CG-CD-NE	-5.18	100.59	112.00
1	B	1616	ILE	CA-CB-CG2	5.18	119.30	110.50
1	A	1685	GLU	N-CA-C	5.11	117.89	109.72
1	A	1770	VAL	N-CA-C	5.10	115.87	110.72
1	C	1740	VAL	N-CA-CB	5.07	117.44	110.54
1	A	2143	VAL	N-CA-C	5.02	116.12	111.45

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1482	PRO	Peptide
1	B	1481	ARG	Peptide

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	5491	0	5431	76	0
1	B	5443	0	5382	133	0
1	C	5387	0	5318	84	0
2	A	23	0	24	1	0
2	B	23	0	24	3	0
2	C	23	0	24	2	0
3	A	483	0	0	9	1
3	B	415	0	0	16	0
3	C	405	0	0	20	0
All	All	17693	0	16203	280	1

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 9.

All (280) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2016:ALA:CB	1:B:2103:MET:HE1	1.61	1.29
1:A:1482:PRO:HB2	3:A:1267:HOH:O	1.40	1.15
1:B:2024:VAL:HG13	3:C:266:HOH:O	1.54	1.06
1:B:2016:ALA:HB2	1:B:2103:MET:HE1	1.42	0.97
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.06	0.94
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.09	0.93
1:B:1757:THR:HG21	3:C:1242:HOH:O	1.67	0.93
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.16	0.93
1:B:1513:GLU:OE2	1:B:1516:ARG:NH1	2.04	0.91
1:B:2138:ARG:HG2	1:B:2138:ARG:HH11	1.36	0.91
1:C:2129:ARG:HD2	3:C:1240:HOH:O	1.70	0.91
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.18	0.89
1:B:1792:THR:HG22	3:B:195:HOH:O	1.72	0.89
1:B:2016:ALA:CB	1:B:2103:MET:CE	2.50	0.88
1:B:1480:LEU:C	1:B:1481:ARG:HG2	2.00	0.86
1:B:2004:ASP:OD2	1:B:2006:THR:HB	1.75	0.86
1:B:1480:LEU:O	1:B:1481:ARG:HG2	1.74	0.86
2:B:2:B89:HAJA	3:C:1276:HOH:O	1.74	0.86
1:B:1513:GLU:CD	1:B:1516:ARG:HH12	1.83	0.86
1:B:1513:GLU:CD	1:B:1516:ARG:NH1	2.35	0.85
1:B:2016:ALA:HB3	1:B:2103:MET:HE1	1.56	0.84
1:C:1852:THR:HG22	1:C:1854:SER:H	1.43	0.84
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.76	0.84
1:A:2142:GLN:HG2	1:A:2143:VAL:N	1.91	0.82
1:C:1644:ASN:HD21	1:C:1654:GLN:HG2	1.41	0.81
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.28	0.80
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.47	0.79
1:B:1729:THR:CG2	1:B:1796:ASP:OD1	2.30	0.79
1:A:1954:ARG:NH1	1:A:1994:GLU:OE1	2.15	0.79
1:B:1481:ARG:HG3	3:B:1309:HOH:O	1.82	0.79
1:C:1560:ASN:HD22	1:C:1560:ASN:H	1.32	0.78
1:A:1658:LEU:HB2	1:A:1663:MET:HE1	1.66	0.78
1:B:1483:ILE:HG13	3:B:382:HOH:O	1.83	0.78
1:B:1483:ILE:HA	3:B:1265:HOH:O	1.82	0.77
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.33	0.77
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.32	0.76
1:B:2103:MET:HE3	1:B:2109:ILE:HG21	1.67	0.75
1:C:2044:MET:HE2	1:C:2082:LEU:HB2	1.68	0.75
1:B:1729:THR:HG22	1:B:1796:ASP:OD1	1.87	0.75
1:C:1766:LEU:HD12	1:C:1770:VAL:HG11	1.69	0.74
1:B:1578:ARG:HD3	3:B:1013:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1631:MET:HE2	1:C:2034:LYS:HB3	1.71	0.73
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.87	0.72
1:B:2044:MET:SD	1:B:2082:LEU:HD21	2.30	0.72
1:B:2016:ALA:HB3	1:B:2103:MET:CE	2.20	0.71
1:B:1837:ASN:H	1:B:1837:ASN:ND2	1.86	0.71
1:B:1852:THR:HG22	3:B:520:HOH:O	1.89	0.71
1:B:1480:LEU:O	1:B:1481:ARG:CG	2.38	0.70
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.73	0.70
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.55	0.70
1:B:1726:THR:CG2	3:B:5:HOH:O	2.38	0.70
1:B:1781:GLN:H	1:B:1781:GLN:HE21	1.38	0.70
1:B:1781:GLN:H	1:B:1781:GLN:NE2	1.89	0.69
1:C:1580:ARG:HD3	3:C:36:HOH:O	1.92	0.68
1:C:2033:ILE:HG22	1:C:2034:LYS:HD3	1.75	0.68
1:A:1651:LYS:HD2	1:A:1651:LYS:O	1.93	0.68
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.75	0.68
1:B:2016:ALA:HB2	1:B:2103:MET:CE	2.20	0.67
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.43	0.67
1:C:1792:THR:HG23	3:C:317:HOH:O	1.94	0.67
1:B:2041:LEU:HA	1:B:2044:MET:HE2	1.75	0.66
1:C:1644:ASN:ND2	1:C:1654:GLN:HG2	2.10	0.66
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.44	0.65
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.32	0.65
1:A:1729:THR:O	1:A:1729:THR:OG1	2.15	0.64
1:B:1624:ASN:ND2	1:B:1733:VAL:H	1.95	0.64
1:B:2006:THR:HG23	1:C:1710:LEU:HA	1.79	0.64
1:C:1616:ILE:HD11	3:C:336:HOH:O	1.98	0.64
1:B:2040:LEU:HD11	1:B:2086:TYR:O	1.99	0.63
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.95	0.63
1:C:1792:THR:CG2	3:C:317:HOH:O	2.46	0.63
1:B:1494:GLN:NE2	1:B:1496:LYS:H	1.93	0.63
1:A:2111:LYS:HE3	3:A:1129:HOH:O	1.98	0.63
1:A:2164:ASP:H	1:A:2170:GLN:NE2	1.97	0.62
1:B:1726:THR:HG23	3:B:5:HOH:O	1.97	0.62
1:C:1560:ASN:H	1:C:1560:ASN:ND2	1.95	0.62
1:C:1663:MET:HE3	1:C:1688:PHE:CG	2.34	0.62
1:C:1644:ASN:HD21	1:C:1654:GLN:CG	2.13	0.61
1:A:1658:LEU:HB2	1:A:1663:MET:CE	2.30	0.61
1:A:2142:GLN:HG2	1:A:2143:VAL:H	1.66	0.61
1:B:1768:ARG:HH11	1:B:1768:ARG:CG	2.12	0.61
1:C:1772:THR:N	1:C:1776:GLN:HE22	1.95	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1768:ARG:HH11	1:B:1768:ARG:HB2	1.66	0.60
1:B:2016:ALA:HB1	1:B:2103:MET:HE1	1.76	0.60
1:B:1687:ARG:HG3	1:B:1687:ARG:HH11	1.65	0.60
1:C:1663:MET:HE3	1:C:1688:PHE:CB	2.32	0.60
1:A:1560:ASN:H	1:A:1560:ASN:ND2	1.96	0.59
1:A:2136:ILE:HD11	1:A:2152:ILE:HD13	1.85	0.59
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.04	0.58
1:B:1497:ARG:HD3	1:B:1510:ASP:OD1	2.03	0.58
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.50	0.58
1:C:1852:THR:HB	1:C:1855:GLY:O	2.03	0.58
1:C:1900:GLU:HB3	1:C:1916:LEU:HD11	1.84	0.58
1:C:1816:MET:HG3	1:C:1817:PRO:HD2	1.85	0.58
1:A:1776:GLN:O	1:A:1782:ILE:HD11	2.04	0.57
1:B:2021:ARG:HG3	1:B:2098:ASP:O	2.03	0.57
1:B:2103:MET:CE	1:B:2109:ILE:HD13	2.34	0.57
1:B:2048:ASP:OD2	1:B:2050:LYS:HG2	2.04	0.57
1:C:1706:ARG:HD3	3:C:361:HOH:O	2.03	0.57
1:A:2142:GLN:NE2	1:A:2144:GLY:O	2.38	0.57
1:B:1768:ARG:HH11	1:B:1768:ARG:CB	2.17	0.57
1:C:2129:ARG:CD	3:C:1240:HOH:O	2.41	0.57
1:C:1592:LYS:HE2	3:C:633:HOH:O	2.03	0.57
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.68	0.57
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.69	0.57
1:B:1638:LEU:HD12	1:B:1658:LEU:HD22	1.85	0.57
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.70	0.56
1:C:1772:THR:N	1:C:1776:GLN:NE2	2.53	0.56
1:B:1991:PRO:O	1:B:2019:ASN:O	2.23	0.56
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.71	0.56
1:B:1480:LEU:O	1:B:1481:ARG:CD	2.53	0.56
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.54	0.55
1:B:1900:GLU:HB3	1:B:1916:LEU:HD11	1.88	0.55
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.05	0.55
1:B:1494:GLN:HE21	1:B:1496:LYS:N	1.96	0.55
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.53	0.55
2:C:3:B89:HAAA	3:C:266:HOH:O	2.06	0.55
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.71	0.55
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.70	0.55
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.40	0.55
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.20	0.55
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.05	0.54
1:C:2136:ILE:HD11	1:C:2152:ILE:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.20	0.54
1:B:1783:MET:CE	1:C:1963:MET:HE3	2.37	0.54
1:B:2178:ASN:HD22	1:B:2181:THR:HG21	1.73	0.54
1:A:1624:ASN:HD22	1:A:1626:GLY:H	1.56	0.54
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.19	0.53
1:A:1499:LYS:HG3	1:A:1503:MET:HE2	1.89	0.53
1:B:1837:ASN:H	1:B:1837:ASN:HD22	1.57	0.53
1:B:2103:MET:HE3	1:B:2109:ILE:HD13	1.90	0.53
1:C:1996:ARG:O	1:C:1999:SER:HB2	2.09	0.53
1:C:2026:GLU:HB2	3:C:1197:HOH:O	2.10	0.52
1:C:1925:HIS:HD2	3:C:279:HOH:O	1.92	0.52
1:A:2190:LYS:C	1:A:2192:GLU:H	2.18	0.52
1:A:1483:ILE:HD12	3:A:662:HOH:O	2.09	0.52
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.57	0.52
3:B:1287:HOH:O	1:C:1649:PRO:HG2	2.10	0.52
1:B:1616:ILE:HD11	3:B:473:HOH:O	2.09	0.51
1:B:1954:ARG:NH1	1:B:1994:GLU:OE1	2.43	0.51
1:A:1845:TRP:CD2	1:A:1850:ARG:HD3	2.45	0.51
1:B:2082:LEU:H	1:B:2082:LEU:CD2	2.24	0.51
1:A:1821:LEU:HD22	3:A:1310:HOH:O	2.09	0.51
1:B:1768:ARG:HH11	1:B:1768:ARG:HG3	1.74	0.51
1:B:1997:GLY:HA2	3:C:266:HOH:O	2.11	0.50
1:C:1516:ARG:NH1	3:C:1112:HOH:O	2.44	0.50
1:B:1768:ARG:HB2	1:B:1768:ARG:NH1	2.26	0.50
1:C:2189:LEU:O	1:C:2192:GLU:HG3	2.12	0.50
1:C:1673:ASN:H	1:C:1673:ASN:ND2	2.10	0.50
1:A:1649:PRO:O	1:A:1651:LYS:N	2.44	0.50
1:A:1680:THR:HG22	1:A:1681:VAL:N	2.26	0.50
1:A:1730:CYS:CA	1:A:1752:GLN:HE21	2.23	0.49
1:C:1527:SER:O	1:C:1530:VAL:HG22	2.12	0.49
1:A:2180:LYS:HG2	1:B:1482:PRO:HD3	1.95	0.48
1:B:2138:ARG:HH11	1:B:2138:ARG:CG	2.17	0.48
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.49	0.48
1:C:1909:ASN:HD22	1:C:1910:PRO:HD2	1.79	0.48
1:B:1790:HIS:HD2	3:B:70:HOH:O	1.97	0.48
1:B:2134:TYR:CZ	1:B:2138:ARG:HD2	2.48	0.48
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.60	0.48
1:B:1505:THR:HB	1:B:1730:CYS:HB2	1.95	0.48
1:B:1545:ASP:OD2	1:B:1545:ASP:C	2.57	0.48
1:A:1533:THR:HG22	1:A:1535:ASP:H	1.79	0.47
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2044:MET:HE2	1:C:2082:LEU:CB	2.41	0.47
3:A:386:HOH:O	1:B:1490:LYS:HE2	2.13	0.47
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.11	0.47
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	1.96	0.47
1:A:1680:THR:HG22	1:A:1681:VAL:H	1.78	0.47
1:B:2006:THR:CG2	1:C:1710:LEU:HA	2.44	0.47
1:A:1772:THR:N	1:A:1776:GLN:NE2	2.56	0.47
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.25	0.47
1:C:1757:THR:HG22	2:C:3:B89:HAL	1.97	0.47
1:A:1764:LYS:O	1:A:1765:MET:C	2.56	0.47
1:C:1524:LYS:HA	1:C:1524:LYS:HD3	1.76	0.47
1:A:1772:THR:N	1:A:1776:GLN:HE22	1.91	0.47
1:B:2152:ILE:H	1:B:2152:ILE:HG13	1.58	0.47
1:B:1546:GLU:HG2	3:B:1288:HOH:O	2.14	0.46
1:B:1545:ASP:HB2	3:B:1288:HOH:O	2.15	0.46
1:B:2006:THR:CG2	1:C:1710:LEU:CA	2.93	0.46
1:C:1575:GLU:HG2	3:C:84:HOH:O	2.16	0.46
1:A:2142:GLN:CG	1:A:2143:VAL:N	2.70	0.46
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.14	0.46
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.63	0.46
1:A:1803:ILE:O	1:A:1807:MET:HG2	2.15	0.46
1:B:1687:ARG:HH11	1:B:1687:ARG:CG	2.29	0.46
1:A:1483:ILE:H	1:A:1483:ILE:CD1	2.28	0.46
1:A:2041:LEU:HD11	1:A:2080:ARG:HH21	1.80	0.45
1:B:1523:TRP:HB3	1:B:1530:VAL:HG11	1.97	0.45
1:B:1582:PHE:CD2	1:B:1807:MET:HE1	2.52	0.45
1:B:1990:PRO:HB2	1:B:1991:PRO:HD2	1.98	0.45
1:C:1537:PHE:HD2	1:C:1571:VAL:CG1	2.28	0.45
1:B:1969:LYS:HA	1:C:1741:ARG:HD2	1.98	0.45
1:A:1781:GLN:H	1:A:1781:GLN:HE21	1.65	0.45
1:B:2034:LYS:HA	1:B:2034:LYS:HD2	1.83	0.45
1:C:1783:MET:HA	1:C:1786:ASN:HB2	1.97	0.45
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.64	0.45
1:C:1846:MET:HE1	1:C:1990:PRO:HB2	1.97	0.45
1:B:2050:LYS:HG3	1:B:2051:TYR:N	2.31	0.45
1:B:2094:ALA:HB2	1:C:1631:MET:CE	2.47	0.45
2:B:2:B89:HAGA	1:C:2001:VAL:HG21	1.98	0.45
1:C:1566:ALA:HA	1:C:1584:VAL:O	2.17	0.45
1:A:1765:MET:HB3	1:A:1765:MET:HE2	1.67	0.45
1:A:2143:VAL:HB	1:A:2193:SER:HB3	1.98	0.45
1:A:1838:ASP:HB2	3:A:780:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1909:ASN:HD22	1:C:1910:PRO:CD	2.29	0.44
1:A:1629:ILE:O	1:A:1629:ILE:HG13	2.16	0.44
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.51	0.44
1:A:1560:ASN:ND2	1:A:1560:ASN:N	2.64	0.44
1:A:1593:ILE:HG22	1:A:1625:SER:OG	2.17	0.44
1:B:1480:LEU:O	1:B:1481:ARG:HD2	2.18	0.44
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.18	0.44
1:A:1987:ILE:HD12	1:A:2003:VAL:HG22	1.99	0.44
1:B:1768:ARG:CB	1:B:1768:ARG:NH1	2.79	0.44
1:B:2006:THR:HG21	1:C:1710:LEU:HB2	2.00	0.44
1:B:2129:ARG:NH2	3:B:597:HOH:O	2.42	0.44
1:B:1585:VAL:HB	1:B:1607:VAL:HG11	2.00	0.44
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.52	0.44
1:B:1919:GLU:HA	1:B:1920:PRO:HD2	1.89	0.44
1:B:2134:TYR:OH	1:B:2138:ARG:HD2	2.17	0.44
1:B:2138:ARG:HG2	1:B:2138:ARG:NH1	2.15	0.44
1:A:1838:ASP:O	1:A:1839:GLU:HB2	2.17	0.43
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	2.29	0.43
1:B:1647:ALA:O	1:B:1648:ASN:ND2	2.51	0.43
1:B:1852:THR:HG22	1:B:1853:GLU:N	2.33	0.43
1:A:1616:ILE:HD11	3:A:542:HOH:O	2.17	0.43
1:A:1575:GLU:OE1	3:A:1310:HOH:O	2.21	0.43
1:A:1677:THR:HA	1:A:1689:VAL:O	2.19	0.43
1:B:2000:TRP:CD1	1:B:2000:TRP:C	2.96	0.43
1:C:2148:ARG:HG3	3:C:1027:HOH:O	2.18	0.43
1:C:1790:HIS:HD2	3:C:32:HOH:O	2.02	0.43
1:B:2148:ARG:O	1:B:2152:ILE:HG13	2.19	0.43
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	2.00	0.43
1:A:1649:PRO:C	1:A:1651:LYS:H	2.27	0.42
1:C:1677:THR:HG22	1:C:1690:ILE:HD13	2.01	0.42
1:B:2036:ARG:O	1:B:2038:GLU:N	2.51	0.42
1:C:1879:VAL:HG13	1:C:1931:LYS:HE2	2.01	0.42
1:C:1582:PHE:CD2	1:C:1807:MET:HE1	2.54	0.42
1:C:1663:MET:HE1	1:C:1677:THR:HG21	2.00	0.42
1:C:1925:HIS:HE1	3:C:659:HOH:O	2.01	0.42
1:A:2083:LEU:HB2	1:A:2084:PRO:HD3	2.01	0.42
1:B:1647:ALA:C	1:B:1648:ASN:HD22	2.28	0.42
1:B:1824:LYS:HB2	3:B:799:HOH:O	2.19	0.42
1:C:2014:MET:CG	1:C:2109:ILE:HG22	2.50	0.42
1:B:1616:ILE:HD12	1:B:1813:LYS:HG2	2.02	0.42
1:C:2116:THR:HG22	1:C:2117:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1792:THR:O	1:A:1802:LYS:HE2	2.19	0.42
1:A:1995:LEU:HG	1:A:2000:TRP:HA	2.01	0.42
1:C:1677:THR:HA	1:C:1689:VAL:O	2.19	0.42
1:C:1786:ASN:HD22	1:C:1786:ASN:HA	1.37	0.42
1:A:1548:GLY:O	1:A:1606:LYS:HE2	2.20	0.42
1:C:1803:ILE:O	1:C:1807:MET:HG3	2.20	0.42
1:A:1668:LYS:HD3	1:A:1668:LYS:HA	1.83	0.41
1:B:2037:ARG:HB3	1:B:2037:ARG:NH1	2.35	0.41
1:B:1620:TYR:HB3	1:B:1726:THR:HB	2.02	0.41
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.66	0.41
1:B:1846:MET:HE1	1:B:1990:PRO:HB2	2.01	0.41
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	2.03	0.41
1:B:1694:ILE:HA	1:C:2102:ARG:CD	2.46	0.41
1:A:1575:GLU:HB3	3:A:1310:HOH:O	2.20	0.41
1:A:1738:TYR:CD1	2:A:1:B89:CAF	3.03	0.41
1:B:1909:ASN:HA	1:B:1910:PRO:HD3	1.91	0.41
1:B:1991:PRO:HG3	1:B:2115:TRP:CG	2.55	0.41
1:C:1940:ASN:HB2	1:C:1981:TYR:CE1	2.56	0.41
1:C:1591:PHE:C	1:C:1591:PHE:CD2	2.99	0.41
1:A:1491:GLU:HB3	1:A:1498:TYR:HB2	2.03	0.41
1:B:1705:LEU:HD23	2:B:2:B89:HAA	2.03	0.41
1:B:1996:ARG:O	1:B:1997:GLY:C	2.63	0.41
1:A:2000:TRP:CD1	1:A:2000:TRP:C	2.99	0.41
1:A:2008:ASN:C	1:A:2008:ASN:HD22	2.28	0.41
1:B:2031:VAL:HG21	1:B:2091:LEU:HD23	2.02	0.41
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.56	0.40
1:B:1480:LEU:C	1:B:1481:ARG:CG	2.77	0.40
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.55	0.40
1:B:1765:MET:HE2	1:B:1765:MET:HB3	1.92	0.40
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.56	0.40
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.57	0.40
1:B:1792:THR:HG21	3:B:859:HOH:O	2.21	0.40
1:C:2016:ALA:O	1:C:2112:GLU:HA	2.22	0.40
1:A:2142:GLN:CG	1:A:2143:VAL:H	2.32	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:241:HOH:O	3:A:1113:HOH:O[2_555]	2.19	0.01

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	684/758 (90%)	656 (96%)	24 (4%)	4 (1%)	21	27
1	B	678/758 (89%)	639 (94%)	36 (5%)	3 (0%)	30	38
1	C	671/758 (88%)	645 (96%)	24 (4%)	2 (0%)	36	46
All	All	2033/2274 (89%)	1940 (95%)	84 (4%)	9 (0%)	30	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1650	ASP
1	A	1764	LYS
1	B	2037	ARG
1	C	1492	TRP
1	C	2141	HIS
1	A	1765	MET
1	A	1839	GLU
1	B	2142	GLN
1	B	2141	HIS

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	584/648 (90%)	547 (94%)	37 (6%)	16	23
1	B	579/648 (89%)	529 (91%)	50 (9%)	10	13
1	C	573/648 (88%)	522 (91%)	51 (9%)	9	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1736/1944 (89%)	1598 (92%)	138 (8%)	11	15

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1483	ILE
1	A	1499	LYS
1	A	1534	ASP
1	A	1549	GLU
1	A	1560	ASN
1	A	1585	VAL
1	A	1616	ILE
1	A	1618	ARG
1	A	1619	ILE
1	A	1651	LYS
1	A	1667	LYS
1	A	1668	LYS
1	A	1681	VAL
1	A	1685	GLU
1	A	1687	ARG
1	A	1757	THR
1	A	1764	LYS
1	A	1770	VAL
1	A	1772	THR
1	A	1781	GLN
1	A	1807	MET
1	A	1826	THR
1	A	1877	VAL
1	A	1878	VAL
1	A	1879	VAL
1	A	1897	ARG
1	A	1915	THR
1	A	1918	GLN
1	A	1924	TRP
1	A	2002	VAL
1	A	2003	VAL
1	A	2008	ASN
1	A	2047	LEU
1	A	2142	GLN
1	A	2148	ARG
1	A	2149	LEU
1	A	2185	LYS

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Mol	Chain	Res	Type
1	B	1480	LEU
1	B	1534	ASP
1	B	1536	PHE
1	B	1556	GLU
1	B	1562	ILE
1	B	1568	LYS
1	B	1571	VAL
1	B	1583	VAL
1	B	1613	LYS
1	B	1616	ILE
1	B	1618	ARG
1	B	1648	ASN
1	B	1687	ARG
1	B	1689	VAL
1	B	1691	LYS
1	B	1726	THR
1	B	1729	THR
1	B	1757	THR
1	B	1765	MET
1	B	1768	ARG
1	B	1772	THR
1	B	1781	GLN
1	B	1792	THR
1	B	1824	LYS
1	B	1837	ASN
1	B	1843	VAL
1	B	1853	GLU
1	B	1854	SER
1	B	1871	SER
1	B	1900	GLU
1	B	1911	ASN
1	B	1914	GLU
1	B	1924	TRP
1	B	1968	LEU
1	B	2006	THR
1	B	2018	VAL
1	B	2021	ARG
1	B	2034	LYS
1	B	2036	ARG
1	B	2046	ARG
1	B	2081	GLU
1	B	2082	LEU

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Mol	Chain	Res	Type
1	B	2083	LEU
1	B	2089	ILE
1	B	2138	ARG
1	B	2149	LEU
1	B	2152	ILE
1	B	2180	LYS
1	B	2181	THR
1	B	2189	LEU
1	C	1499	LYS
1	C	1508	VAL
1	C	1522	GLN
1	C	1524	LYS
1	C	1534	ASP
1	C	1547	ASN
1	C	1560	ASN
1	C	1565	VAL
1	C	1571	VAL
1	C	1575	GLU
1	C	1580	ARG
1	C	1585	VAL
1	C	1616	ILE
1	C	1618	ARG
1	C	1631	MET
1	C	1634	GLU
1	C	1636	VAL
1	C	1651	LYS
1	C	1664	GLU
1	C	1667	LYS
1	C	1668	LYS
1	C	1679	ARG
1	C	1680	THR
1	C	1731	ARG
1	C	1740	VAL
1	C	1741	ARG
1	C	1769	GLU
1	C	1770	VAL
1	C	1781	GLN
1	C	1786	ASN
1	C	1792	THR
1	C	1794	VAL
1	C	1816	MET
1	C	1824	LYS

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Mol	Chain	Res	Type
1	C	1843	VAL
1	C	1851	GLU
1	C	1877	VAL
1	C	1879	VAL
1	C	1911	ASN
1	C	1924	TRP
1	C	1968	LEU
1	C	2031	VAL
1	C	2034	LYS
1	C	2036	ARG
1	C	2037	ARG
1	C	2047	LEU
1	C	2116	THR
1	C	2145	GLU
1	C	2149	LEU
1	C	2152	ILE
1	C	2185	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1644	ASN
1	A	1654	GLN
1	A	1673	ASN
1	A	1683	ASN
1	A	1744	GLN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1781	GLN
1	A	1790	HIS
1	A	1815	ASN
1	A	1837	ASN
1	A	1934	GLN
1	A	1965	ASN
1	A	2008	ASN
1	A	2092	GLN
1	A	2097	HIS

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Mol	Chain	Res	Type
1	A	2131	ASN
1	A	2142	GLN
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1522	GLN
1	B	1525	ASN
1	B	1587	ASN
1	B	1599	GLN
1	B	1624	ASN
1	B	1640	GLN
1	B	1644	ASN
1	B	1648	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1781	GLN
1	B	1790	HIS
1	B	1815	ASN
1	B	1837	ASN
1	B	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	1960	GLN
1	B	2097	HIS
1	B	2131	ASN
1	B	2178	ASN
1	C	1522	GLN
1	C	1560	ASN
1	C	1587	ASN
1	C	1605	ASN
1	C	1644	ASN
1	C	1648	ASN
1	C	1673	ASN
1	C	1683	ASN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1786	ASN
1	C	1790	HIS
1	C	1815	ASN
1	C	1909	ASN

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Mol	Chain	Res	Type
1	C	1911	ASN
1	C	1922	GLN
1	C	1937	ASN
1	C	2019	ASN
1	C	2045	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B89	C	3	-	22,24,24	2.01	7 (31%)	23,31,31	1.88	6 (26%)
2	B89	A	1	-	22,24,24	1.71	6 (27%)	23,31,31	2.01	5 (21%)
2	B89	B	2	-	22,24,24	1.78	8 (36%)	23,31,31	2.06	5 (21%)

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	B89	C	3	-	-	4/14/40/40	0/2/2/2
2	B89	A	1	-	-	6/14/40/40	0/2/2/2
2	B89	B	2	-	-	5/14/40/40	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	B89	CAT-NAO	4.99	1.33	1.28
2	B	2	B89	CAT-NAO	3.70	1.32	1.28
2	A	1	B89	OAB-CAR	3.47	1.30	1.23
2	C	3	B89	CAN-CAS	3.41	1.53	1.49
2	A	1	B89	OAQ-NAO	-3.29	1.36	1.42
2	B	2	B89	OAB-CAR	3.25	1.29	1.23
2	C	3	B89	OAQ-NAO	-3.22	1.36	1.42
2	C	3	B89	CAU-CAR	3.11	1.53	1.45
2	C	3	B89	OAB-CAR	3.06	1.29	1.23
2	A	1	B89	CAU-CAR	3.04	1.53	1.45
2	A	1	B89	CAT-NAO	2.73	1.31	1.28
2	B	2	B89	OAQ-NAO	-2.65	1.37	1.42
2	B	2	B89	CAU-CAR	2.63	1.52	1.45
2	C	3	B89	CAH-CAF	-2.53	1.39	1.49
2	B	2	B89	CAH-CAF	-2.52	1.39	1.49
2	B	2	B89	CAG-CAT	2.39	1.55	1.50
2	B	2	B89	OAC-CAS	2.31	1.39	1.32
2	A	1	B89	CAH-CAF	-2.20	1.40	1.49
2	B	2	B89	CAM-CAR	2.03	1.54	1.50
2	A	1	B89	CAG-CAT	2.02	1.54	1.50
2	C	3	B89	OAC-CAS	2.02	1.38	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	B89	CAH-OAQ-NAO	6.47	114.74	107.94
2	A	1	B89	CAH-OAQ-NAO	6.26	114.52	107.94
2	B	2	B89	CAS-CAU-CAT	-4.46	118.16	121.10
2	A	1	B89	OAP-CAJ-CAL	-4.38	104.17	111.74
2	C	3	B89	OAC-CAS-CAN	3.99	119.86	113.29
2	C	3	B89	CAH-OAQ-NAO	3.91	112.06	107.94
2	C	3	B89	CAS-CAU-CAT	-3.50	118.79	121.10
2	C	3	B89	OAQ-NAO-CAT	3.40	116.55	111.47
2	A	1	B89	CAJ-CAL-CAV	-2.97	106.90	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	B89	OAC-CAS-CAU	-2.72	116.61	121.95
2	C	3	B89	CAM-CAR-CAU	2.71	121.38	115.98
2	A	1	B89	CAS-CAU-CAT	-2.51	119.44	121.10
2	B	2	B89	CAM-CAR-CAU	2.48	120.92	115.98
2	B	2	B89	OAB-CAR-CAU	-2.43	118.82	122.77
2	A	1	B89	OAC-CAS-CAN	2.34	117.14	113.29
2	B	2	B89	OAC-CAS-CAN	2.19	116.90	113.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	B89	CAA-CAG-CAT-NAO
2	A	1	B89	CAG-CAT-CAU-CAR
2	A	1	B89	CAG-CAT-CAU-CAS
2	A	1	B89	NAO-CAT-CAU-CAS
2	B	2	B89	CAA-CAG-CAT-NAO
2	B	2	B89	CAG-CAT-CAU-CAR
2	B	2	B89	CAG-CAT-CAU-CAS
2	B	2	B89	NAO-CAT-CAU-CAS
2	C	3	B89	CAG-CAT-CAU-CAR
2	C	3	B89	CAG-CAT-CAU-CAS
2	C	3	B89	NAO-CAT-CAU-CAS
2	A	1	B89	CAA-CAG-CAT-CAU
2	B	2	B89	CAA-CAG-CAT-CAU
2	C	3	B89	CAF-CAH-OAQ-NAO
2	A	1	B89	CAF-CAH-OAQ-NAO

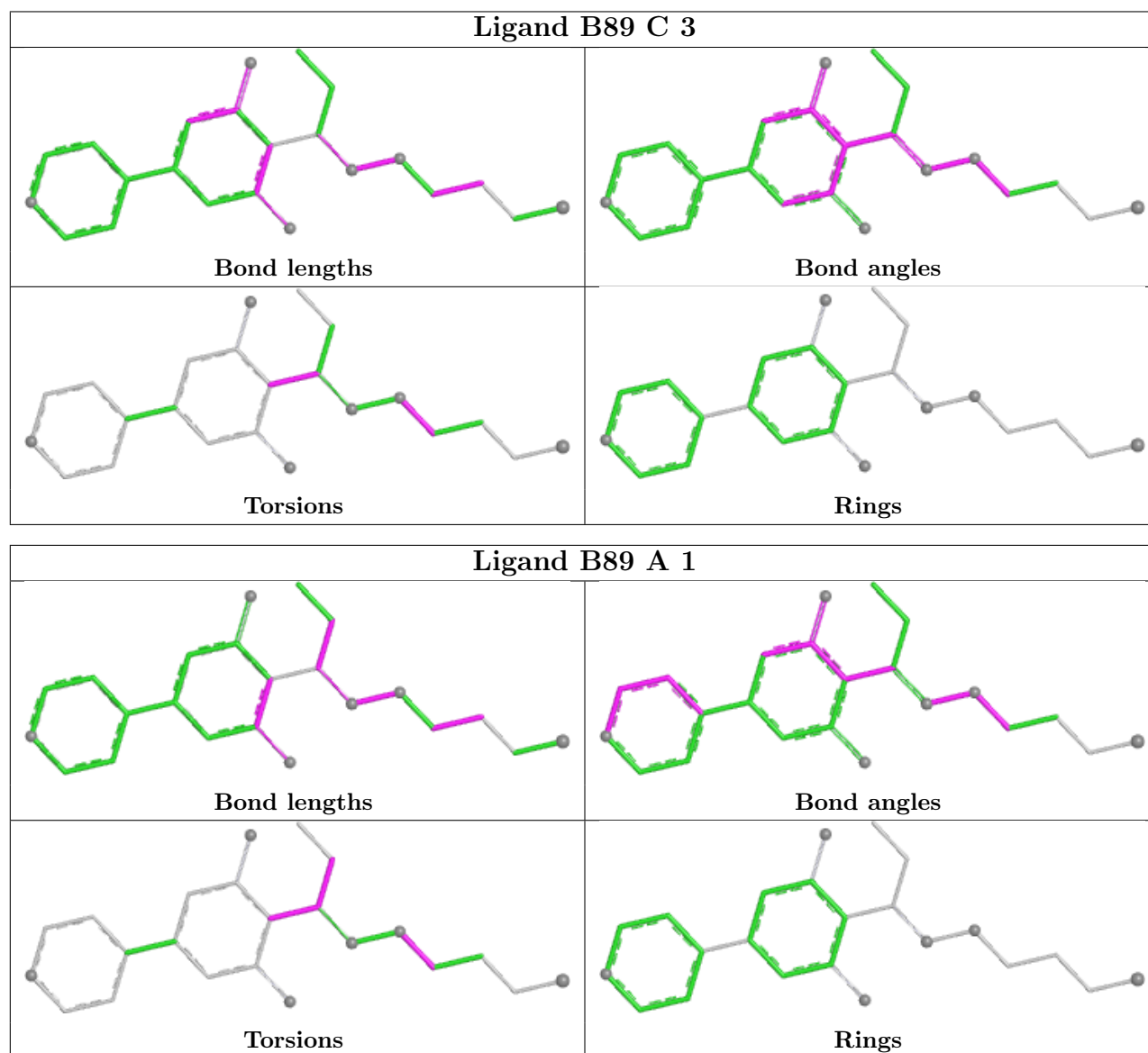
There are no ring outliers.

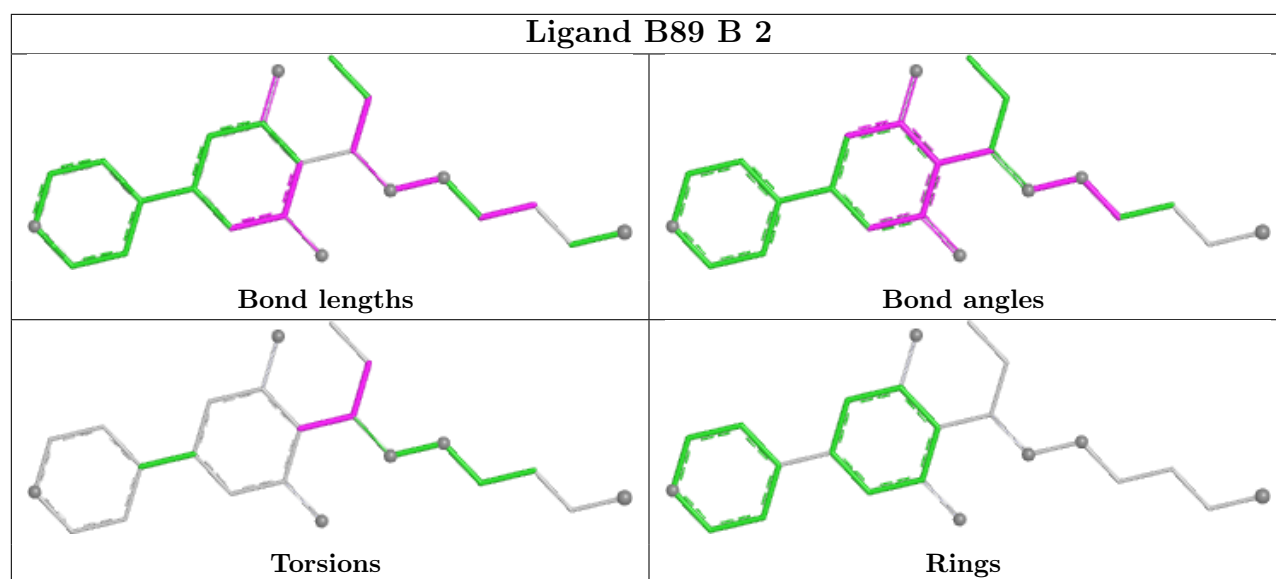
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	B89	2	0
2	A	1	B89	1	0
2	B	2	B89	3	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	688/758 (90%)	0.05	66 (9%)	13 15	17, 29, 75, 99	0
1	B	682/758 (89%)	0.25	80 (11%)	9 10	16, 33, 85, 103	0
1	C	675/758 (89%)	0.17	75 (11%)	10 11	17, 33, 83, 101	0
All	All	2045/2274 (89%)	0.16	221 (10%)	11 12	16, 31, 81, 103	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2143	VAL	8.6
1	A	2143	VAL	8.6
1	B	2143	VAL	8.2
1	B	1480	LEU	8.1
1	A	2195	ALA	7.4
1	B	2189	LEU	7.3
1	B	2051	TYR	7.1
1	B	2085	ILE	6.8
1	B	2144	GLY	6.4
1	A	2051	TYR	5.9
1	B	2083	LEU	5.9
1	C	2144	GLY	5.9
1	C	1681	VAL	5.9
1	A	2194	PHE	5.6
1	C	1647	ALA	5.6
1	B	2041	LEU	5.5
1	B	1483	ILE	5.5
1	A	1685	GLU	5.4
1	C	2191	LEU	5.3
1	A	1481	ARG	5.1
1	B	2082	LEU	5.0
1	A	2141	HIS	4.9
1	A	2144	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	1681	VAL	4.8
1	C	2051	TYR	4.8
1	B	1648	ASN	4.8
1	B	2045	ASN	4.7
1	C	2193	SER	4.7
1	B	1682	ILE	4.6
1	C	1682	ILE	4.6
1	A	1480	LEU	4.4
1	C	1646	ALA	4.4
1	B	2084	PRO	4.3
1	B	2050	LYS	4.2
1	C	2142	GLN	4.2
1	A	1482	PRO	4.1
1	B	1646	ALA	4.1
1	A	1680	THR	4.1
1	B	2043	THR	4.1
1	A	2190	LYS	4.1
1	A	2191	LEU	3.9
1	A	1838	ASP	3.9
1	B	1649	PRO	3.9
1	A	2082	LEU	3.9
1	B	1684	GLY	3.9
1	B	2080	ARG	3.8
1	C	2082	LEU	3.8
1	C	2041	LEU	3.8
1	B	1838	ASP	3.7
1	A	2050	LYS	3.7
1	A	2080	ARG	3.7
1	C	1679	ARG	3.7
1	C	1643	TRP	3.7
1	B	2081	GLU	3.6
1	C	2047	LEU	3.6
1	C	1648	ASN	3.6
1	C	2080	ARG	3.6
1	B	1647	ALA	3.6
1	B	1651	LYS	3.6
1	A	1684	GLY	3.6
1	B	1482	PRO	3.6
1	A	1651	LYS	3.6
1	C	2141	HIS	3.5
1	C	1657	TYR	3.5
1	C	1656	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1642	ALA	3.4
1	B	2040	LEU	3.4
1	B	2134	TYR	3.4
1	B	1681	VAL	3.4
1	C	1642	ALA	3.4
1	A	2047	LEU	3.3
1	A	1660	SER	3.3
1	A	1765	MET	3.3
1	A	1682	ILE	3.3
1	A	2041	LEU	3.3
1	A	2145	GLU	3.2
1	B	2047	LEU	3.2
1	A	1483	ILE	3.2
1	C	1669	PHE	3.2
1	C	1680	THR	3.2
1	C	2083	LEU	3.2
1	B	1481	ARG	3.1
1	A	2193	SER	3.1
1	C	1655	TYR	3.1
1	B	1772	THR	3.1
1	C	1651	LYS	3.1
1	B	1686	GLU	3.1
1	A	1648	ASN	3.1
1	C	2086	TYR	3.1
1	C	1659	THR	3.1
1	C	2192	GLU	3.1
1	C	1653	PHE	3.1
1	C	1644	ASN	3.1
1	B	2142	GLN	3.0
1	C	2046	ARG	3.0
1	A	1649	PRO	3.0
1	B	1664	GLU	3.0
1	C	1688	PHE	3.0
1	C	2045	ASN	3.0
1	A	1767	GLY	3.0
1	C	1546	GLU	2.9
1	A	1646	ALA	2.9
1	C	2040	LEU	2.9
1	C	1664	GLU	2.9
1	B	1669	PHE	2.9
1	C	1686	GLU	2.8
1	B	2086	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	2189	LEU	2.8
1	C	1639	PHE	2.8
1	A	1906	ASP	2.8
1	C	1673	ASN	2.8
1	A	2142	GLN	2.8
1	B	2145	GLU	2.8
1	C	1685	GLU	2.8
1	A	1647	ALA	2.8
1	C	1658	LEU	2.7
1	A	1657	TYR	2.7
1	B	2185	LYS	2.7
1	C	1671	LYS	2.7
1	C	2044	MET	2.7
1	A	1529	ASP	2.7
1	A	1650	ASP	2.7
1	B	2046	ARG	2.7
1	B	2187	LYS	2.7
1	B	2141	HIS	2.6
1	B	1530	VAL	2.6
1	A	2149	LEU	2.6
1	B	2149	LEU	2.6
1	B	1662	GLY	2.6
1	A	1910	PRO	2.6
1	B	1765	MET	2.6
1	C	1838	ASP	2.6
1	A	1669	PHE	2.6
1	B	1910	PRO	2.6
1	C	2189	LEU	2.6
1	C	1684	GLY	2.6
1	C	1641	VAL	2.6
1	A	1766	LEU	2.5
1	B	1644	ASN	2.5
1	C	1649	PRO	2.5
1	A	1683	ASN	2.5
1	B	1683	ASN	2.5
1	A	1668	LYS	2.5
1	C	1683	ASN	2.5
1	B	2036	ARG	2.5
1	B	1658	LEU	2.5
1	B	1645	ASP	2.5
1	A	2081	GLU	2.4
1	B	1685	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	2181	THR	2.4
1	C	2081	GLU	2.4
1	A	1641	VAL	2.4
1	A	1853	GLU	2.4
1	B	1680	THR	2.4
1	B	2035	PHE	2.4
1	C	2190	LYS	2.4
1	C	1765	MET	2.4
1	A	1645	ASP	2.4
1	A	1642	ALA	2.4
1	C	2043	THR	2.4
1	B	1666	LEU	2.4
1	A	1643	TRP	2.4
1	A	2037	ARG	2.4
1	B	2179	TYR	2.4
1	B	2049	ASP	2.4
1	C	1650	ASP	2.4
1	B	1660	SER	2.4
1	C	1674	SER	2.4
1	B	2152	ILE	2.4
1	C	1530	VAL	2.3
1	C	1556	GLU	2.3
1	B	2048	ASP	2.3
1	A	2146	ALA	2.3
1	C	1632	ALA	2.3
1	B	2033	ILE	2.3
1	B	1911	ASN	2.3
1	C	2084	PRO	2.3
1	C	2037	ARG	2.3
1	B	1654	GLN	2.3
1	C	2145	GLU	2.3
1	A	1673	ASN	2.2
1	A	2048	ASP	2.2
1	B	1637	PRO	2.2
1	B	2032	GLY	2.2
1	B	1770	VAL	2.2
1	B	1650	ASP	2.2
1	B	1663	MET	2.2
1	C	1687	ARG	2.2
1	A	1839	GLU	2.2
1	C	1772	THR	2.2
1	B	1643	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2037	ARG	2.2
1	B	1839	GLU	2.2
1	A	1666	LEU	2.1
1	A	1547	ASN	2.1
1	A	2044	MET	2.1
1	B	1546	GLU	2.1
1	B	2044	MET	2.1
1	A	1911	ASN	2.1
1	C	1645	ASP	2.1
1	A	1679	ARG	2.1
1	C	2188	GLY	2.1
1	A	1729	THR	2.1
1	C	1491	GLU	2.1
1	A	2085	ILE	2.1
1	A	1662	GLY	2.1
1	C	1652	GLY	2.1
1	B	2180	LYS	2.0
1	C	1665	THR	2.0
1	B	2038	GLU	2.0
1	C	1769	GLU	2.0
1	B	1638	LEU	2.0
1	C	1534	ASP	2.0
1	C	1766	LEU	2.0
1	B	1641	VAL	2.0
1	C	1667	LYS	2.0
1	A	1659	THR	2.0
1	A	2192	GLU	2.0
1	C	1677	THR	2.0
1	B	2146	ALA	2.0
1	C	1911	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

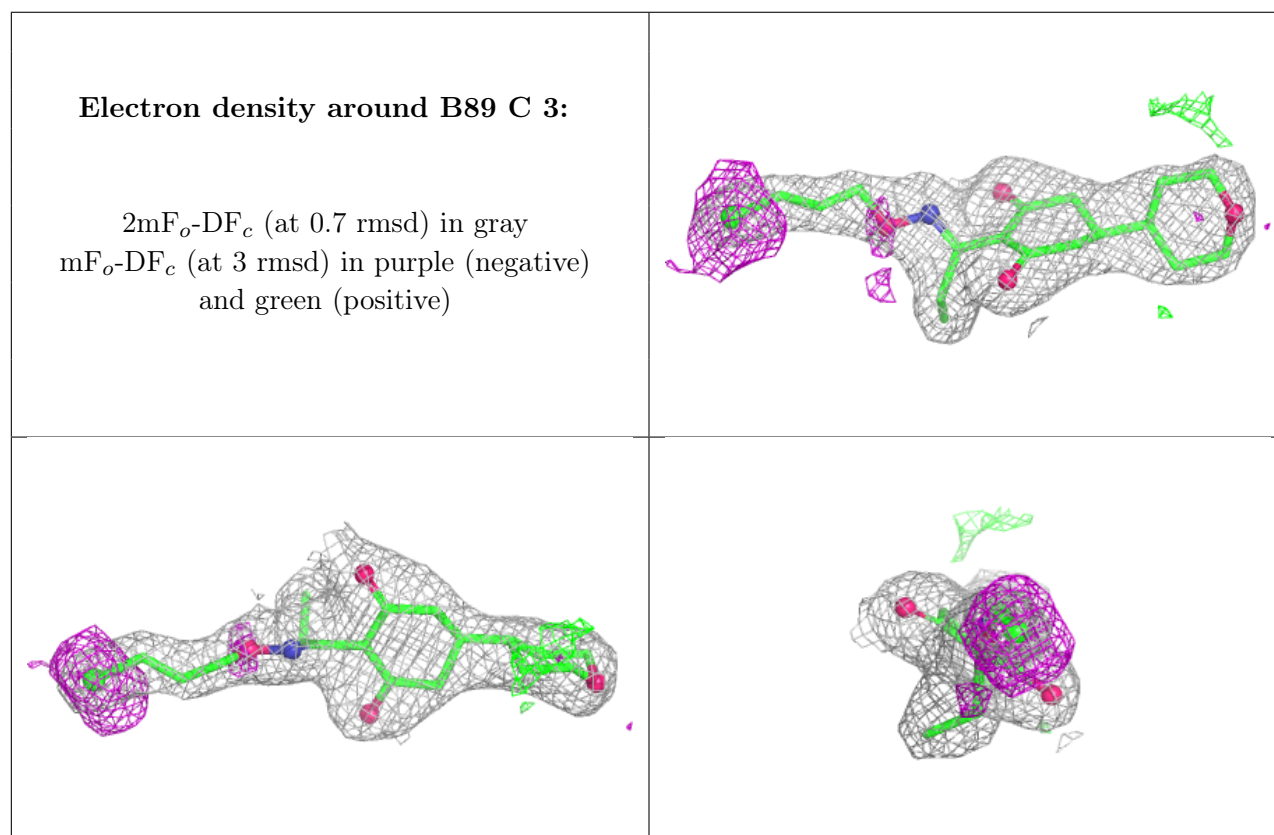
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

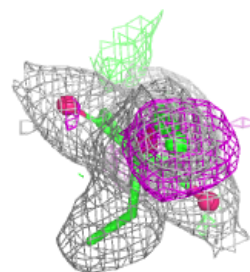
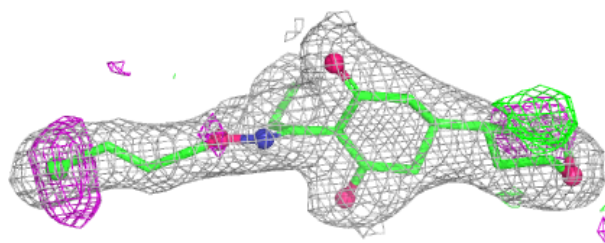
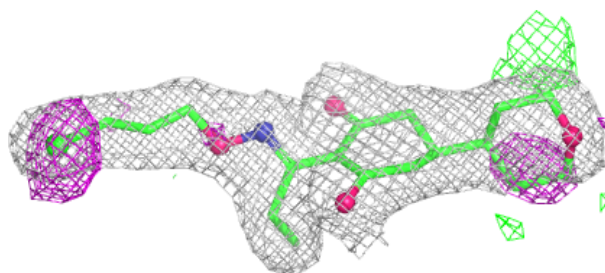
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B89	C	3	23/23	0.89	0.12	43,52,59,64	0
2	B89	A	1	23/23	0.90	0.12	29,38,49,52	0
2	B89	B	2	23/23	0.92	0.11	28,37,46,50	0

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.

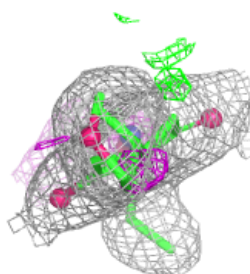
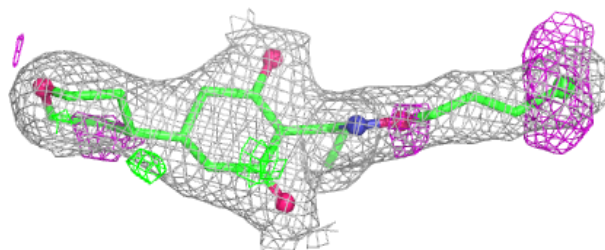
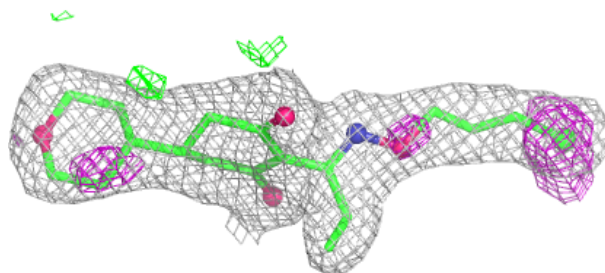


Electron density around B89 A 1:

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

**Electron density around B89 B 2:**

$2mF_o-DF_c$ (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.