



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:43 PM UTC

PDB ID : 1UYR / pdb_00001uyr
Title : Acetyl-CoA Carboxylase Carboxyltransferase Domain in complex with inhibitor Diclofop
Authors : Zhang, H.; Tweel, B.; Tong, L.
Deposited on : 2004-03-02
Resolution : 2.50 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

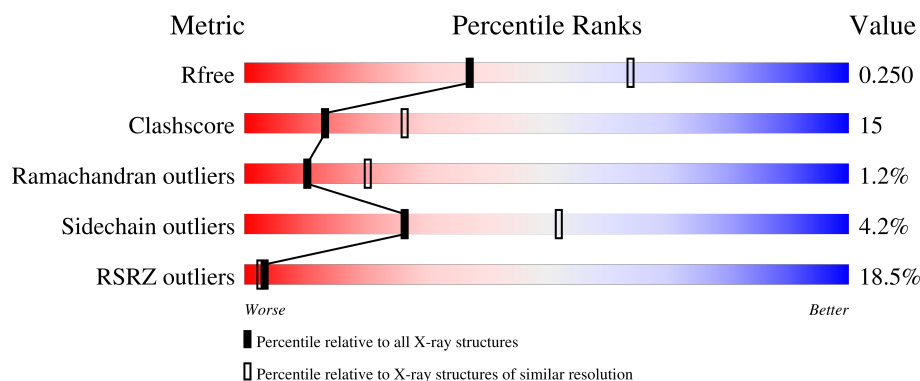
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	737	18% 67% 24% • 5%
1	B	737	17% 64% 27% • 6%

2 Entry composition [i](#)

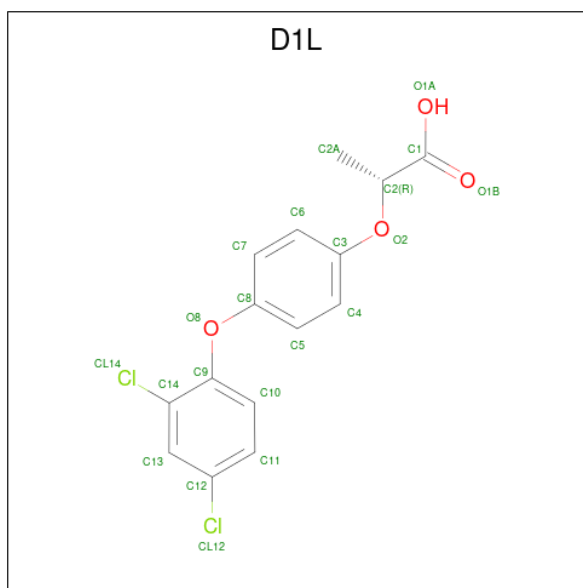
There are 3 unique types of molecules in this entry. The entry contains 11229 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	698	Total	C	N	O	S	0	0	0
			5515	3514	949	1034	18			
1	B	695	Total	C	N	O	S	0	0	0
			5495	3498	947	1032	18			

- Molecule 2 is 2-[4-(2,4-DICHLOROPHENOXY)PHENOXY]PROPANOIC ACID (CCD ID: D1L) (formula: C₁₅H₁₂Cl₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			21	15	2	4		
2	B	1	Total	C	Cl	O	0	0
			21	15	2	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total 92	O 92	0	0
3	B	85	Total 85	O 85	0	0

3 Residue-property plots

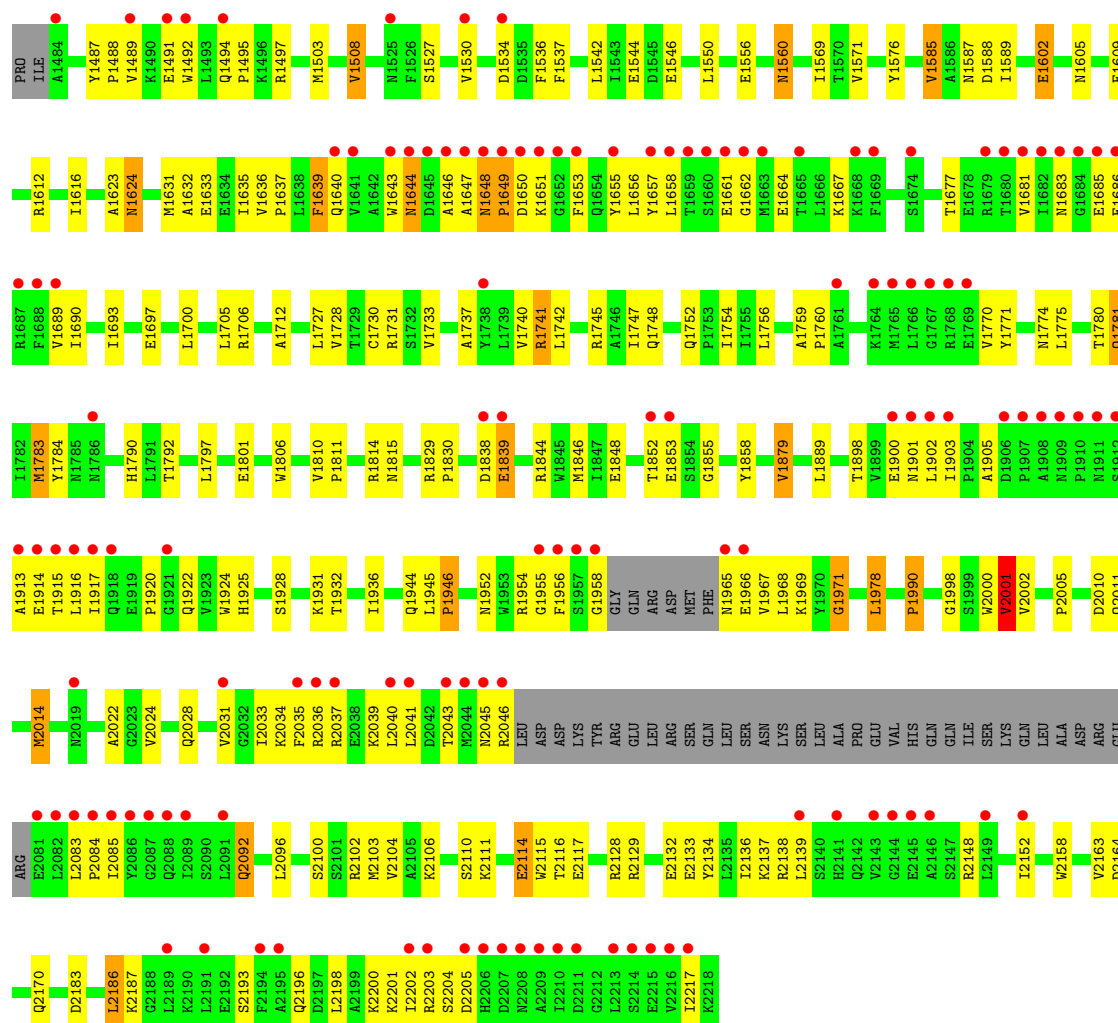
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: ACETYL-COA CARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.78Å 136.78Å 244.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.58 – 2.50 29.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.58-2.50) 98.4 (29.58-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.248 0.219 , 0.250	Depositor DCC
R_{free} test set	9060 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11229	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: D1L

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	0.42	0/5635	0.88	10/7634 (0.1%)
1	B	0.44	0/5614	0.91	16/7605 (0.2%)
All	All	0.43	0/11249	0.89	26/15239 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1647	ALA	N-CA-C	-13.77	96.54	113.20
1	A	1946	PRO	N-CA-C	-7.01	100.68	111.13
1	B	1946	PRO	N-CA-C	-6.82	99.43	110.40
1	A	1730	CYS	N-CA-C	-6.19	99.91	109.14
1	A	1644	ASN	N-CA-C	-6.17	104.18	111.03
1	B	1576	TYR	CA-C-N	6.16	126.62	119.47
1	B	1576	TYR	C-N-CA	6.16	126.62	119.47
1	B	1733	VAL	N-CA-C	5.99	117.22	108.53
1	A	1508	VAL	N-CA-C	5.98	116.64	110.36
1	A	1971	GLY	N-CA-C	-5.90	105.65	112.73
1	B	2001	VAL	N-CA-C	5.72	117.14	110.62
1	B	1990	PRO	N-CA-C	5.57	117.50	110.70
1	A	1712	ALA	N-CA-C	-5.56	105.13	111.14
1	B	1783	MET	N-CA-C	5.44	118.13	111.82
1	B	1971	GLY	N-CA-C	-5.40	106.25	112.73
1	A	1733	VAL	N-CA-C	5.33	116.99	108.89
1	B	1624	ASN	N-CA-C	5.27	116.01	108.74
1	A	1576	TYR	CA-C-N	5.21	125.26	119.32
1	A	1576	TYR	C-N-CA	5.21	125.26	119.32
1	B	1712	ALA	N-CA-C	-5.18	105.53	111.07
1	B	1648	ASN	CA-C-N	5.16	126.29	119.84
1	B	1648	ASN	C-N-CA	5.16	126.29	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1572	LYS	N-CA-C	-5.15	100.78	108.96
1	B	1585	VAL	CB-CA-C	-5.04	103.32	110.83
1	B	1616	ILE	CA-C-N	5.03	125.03	119.90
1	B	1616	ILE	C-N-CA	5.03	125.03	119.90

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	5515	0	5430	158	0
1	B	5495	0	5404	179	0
2	A	21	0	11	6	0
2	B	21	0	11	6	0
3	A	92	0	0	3	0
3	B	85	0	0	5	0
All	All	11229	0	10856	324	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 15.

All (324) 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:1494:GLN:HE21	1:A:1496:LYS:H	1.11	0.98
1:A:2014:MET:HG2	1:A:2109:ILE:HG22	1.45	0.98
1:A:1815:ASN:H	1:A:1944:GLN:HE22	1.06	0.97
1:B:1681:VAL:HA	1:B:1686:GLU:HA	1.51	0.90
1:A:2082:LEU:HD23	1:A:2082:LEU:H	1.38	0.88
1:B:1759:ALA:H	1:B:1774:ASN:HD21	1.20	0.87
1:B:1646:ALA:HB1	1:B:1648:ASN:O	1.77	0.85
1:A:2031:VAL:HG21	1:A:2091:LEU:HD23	1.60	0.84
2:A:3219:D1L:H13	1:B:1971:GLY:HA3	1.59	0.83
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1660:SER:O	1:A:1664:GLU:HG2	1.79	0.83
1:A:1781:GLN:HE21	1:A:1782:ILE:HG13	1.46	0.81
1:B:1658:LEU:HG	1:B:1690:ILE:HD11	1.64	0.80
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.29	0.79
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.48	0.79
1:A:1677:THR:HG22	1:A:1690:ILE:HA	1.66	0.78
1:B:2164:ASP:H	1:B:2170:GLN:NE2	1.82	0.77
1:B:1560:ASN:HD22	1:B:1560:ASN:H	1.34	0.76
1:A:1503:MET:HE3	1:A:1589:ILE:HG13	1.66	0.76
1:A:1508:VAL:HG21	1:A:1588:ASP:HA	1.68	0.75
1:B:1681:VAL:HG22	1:B:1686:GLU:HB3	1.69	0.74
1:B:2037:ARG:NH1	1:B:2041:LEU:HD22	2.04	0.72
1:B:2183:ASP:OD1	1:B:2187:LYS:HE3	1.89	0.72
1:A:1738:TYR:CD1	2:A:3219:D1L:H5	2.24	0.72
1:B:1759:ALA:H	1:B:1774:ASN:ND2	1.89	0.71
1:B:1954:ARG:HG3	1:B:1955:GLY:H	1.56	0.70
2:A:3219:D1L:CL14	1:B:1968:LEU:HD12	2.28	0.70
1:A:1738:TYR:OH	1:B:2002:VAL:HG12	1.91	0.70
1:B:2028:GLN:O	1:B:2031:VAL:HG12	1.90	0.70
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.57	0.70
1:B:1697:GLU:O	1:B:1700:LEU:HD13	1.92	0.68
1:A:2085:ILE:O	1:A:2089:ILE:HG13	1.94	0.67
1:B:2164:ASP:H	1:B:2170:GLN:HE22	1.41	0.67
1:A:1846:MET:HE1	1:A:1990:PRO:HB2	1.77	0.67
1:B:1737:ALA:O	1:B:1740:VAL:HG22	1.95	0.67
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	1.93	0.66
1:A:2022:ALA:HB3	1:A:2103:MET:HE2	1.77	0.66
1:B:1745:ARG:NH2	3:B:4037:HOH:O	2.29	0.66
1:B:1730:CYS:HA	1:B:1752:GLN:OE1	1.96	0.66
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.44	0.66
1:A:2197:ASP:OD2	1:A:2201:LYS:HE2	1.96	0.66
1:A:1663:MET:O	1:A:1667:LYS:HG3	1.97	0.64
1:A:2001:VAL:HG21	2:B:3219:D1L:H4	1.79	0.64
1:B:2137:LYS:HE3	3:B:4079:HOH:O	1.97	0.63
1:A:1745:ARG:NH2	3:A:4038:HOH:O	2.31	0.62
1:A:1768:ARG:H	1:A:1768:ARG:HD3	1.65	0.62
1:A:1968:LEU:HD23	2:B:3219:D1L:CL14	2.36	0.62
1:A:2046:ARG:C	1:A:2047:LEU:HD12	2.24	0.62
1:B:2083:LEU:HB3	1:B:2084:PRO:HD3	1.82	0.62
1:A:2083:LEU:HB3	1:A:2084:PRO:HD3	1.82	0.62
1:A:1511:PHE:HZ	1:A:1729:THR:HG21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1905:ALA:HB2	1:B:1913:ALA:C	2.25	0.61
1:A:1631:MET:HE2	1:B:2034:LYS:HB3	1.82	0.61
1:A:1956:PHE:CE1	1:A:1998:GLY:HA3	2.34	0.61
1:A:1956:PHE:HE1	1:A:1998:GLY:HA3	1.65	0.61
1:A:2192:GLU:O	1:A:2196:GLN:HG2	2.01	0.61
1:B:1781:GLN:H	1:B:1781:GLN:HE21	1.47	0.60
1:A:1987:ILE:CG2	1:A:2014:MET:HE3	2.32	0.59
1:A:2046:ARG:NH1	1:A:2047:LEU:HD11	2.17	0.59
1:B:1902:LEU:HD12	1:B:1915:THR:O	2.02	0.59
1:B:2033:ILE:HG22	1:B:2034:LYS:HD2	1.83	0.59
1:B:2022:ALA:HB3	1:B:2103:MET:HE2	1.84	0.59
1:B:1527:SER:O	1:B:1530:VAL:HG22	2.01	0.59
1:A:1571:VAL:O	1:A:1579:GLY:HA2	2.03	0.59
1:B:2110:SER:O	1:B:2111:LYS:HB3	2.02	0.58
1:B:2102:ARG:NH1	1:B:2106:LYS:HG3	2.18	0.58
1:A:1987:ILE:HG22	1:A:2014:MET:HE3	1.86	0.58
2:A:3219:D1L:CL14	1:B:1968:LEU:HA	2.40	0.58
1:B:1792:THR:HG23	3:B:4038:HOH:O	2.03	0.58
1:B:1681:VAL:HG22	1:B:1686:GLU:CB	2.34	0.58
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.39	0.58
2:A:3219:D1L:C4	1:B:2001:VAL:HG11	2.34	0.57
1:A:1630:GLY:C	1:A:1700:LEU:HD22	2.29	0.57
1:B:1901:ASN:HB3	1:B:1917:ILE:HB	1.85	0.57
1:A:1586:ALA:HB2	1:A:1621:LEU:HB2	1.86	0.57
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	1.84	0.57
1:B:1898:THR:HG22	1:B:1920:PRO:HA	1.85	0.57
1:A:1537:PHE:HD2	1:A:1571:VAL:HG13	1.70	0.57
1:A:2148:ARG:HG3	1:A:2148:ARG:HH11	1.69	0.57
1:B:1838:ASP:O	1:B:1839:GLU:HB2	2.05	0.57
1:B:1846:MET:HE1	1:B:1990:PRO:HB2	1.87	0.57
1:A:2001:VAL:HG21	2:B:3219:D1L:C4	2.34	0.56
1:A:2082:LEU:HD23	1:A:2082:LEU:N	2.15	0.56
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.41	0.56
1:A:1763:ASN:HD21	1:A:1771:TYR:H	1.53	0.56
1:B:1569:ILE:HG22	1:B:1571:VAL:HG23	1.88	0.56
1:B:1815:ASN:ND2	1:B:1944:GLN:HE22	2.02	0.56
1:A:2097:HIS:NE2	1:B:1631:MET:HG3	2.21	0.56
1:B:1902:LEU:HD11	1:B:1914:GLU:OE1	2.06	0.56
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.87	0.55
1:A:2097:HIS:CE1	1:B:1632:ALA:H	2.25	0.55
1:A:1884:LEU:HD13	1:A:2123:PHE:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1560:ASN:H	1:B:1560:ASN:ND2	2.01	0.55
1:A:2142:GLN:NE2	1:A:2151:LYS:HE2	2.22	0.55
1:B:2128:ARG:HE	1:B:2132:GLU:CD	2.15	0.55
1:B:2033:ILE:HG22	1:B:2034:LYS:CD	2.36	0.55
1:B:2100:SER:O	1:B:2104:VAL:HG23	2.06	0.55
1:A:1729:THR:HG22	1:A:1796:ASP:OD1	2.07	0.55
1:B:1903:ILE:HD12	1:B:1903:ILE:N	2.21	0.55
1:B:1966:GLU:HA	1:B:1966:GLU:OE1	2.05	0.54
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.89	0.54
1:A:1541:GLU:OE1	1:A:1555:ARG:HD3	2.07	0.54
1:B:1646:ALA:HB1	1:B:1648:ASN:C	2.33	0.54
1:A:1756:LEU:HD21	1:B:1968:LEU:HD13	1.90	0.54
1:B:1797:LEU:O	1:B:1801:GLU:HG3	2.08	0.54
1:A:1630:GLY:O	1:A:1700:LEU:HD22	2.08	0.53
1:A:1815:ASN:H	1:A:1944:GLN:NE2	1.90	0.53
1:B:1661:GLU:HG3	1:B:1662:GLY:N	2.23	0.53
1:B:1741:ARG:HD3	1:B:1741:ARG:C	2.34	0.53
1:B:1756:LEU:HD22	2:B:3219:D1L:H7	1.91	0.53
1:B:2193:SER:HA	1:B:2196:GLN:HB2	1.90	0.53
1:B:1922:GLN:HG2	1:B:1952:ASN:O	2.09	0.53
1:A:1630:GLY:O	1:A:1700:LEU:HB3	2.09	0.52
1:B:1900:GLU:OE1	1:B:1916:LEU:HD21	2.10	0.52
1:B:2000:TRP:CZ2	1:B:2014:MET:HE3	2.45	0.52
1:B:1741:ARG:HD3	1:B:1741:ARG:O	2.09	0.51
1:A:1494:GLN:NE2	1:A:1496:LYS:H	1.94	0.51
1:A:2043:THR:O	1:A:2047:LEU:HD13	2.10	0.51
1:A:2148:ARG:HG3	1:A:2148:ARG:NH1	2.26	0.51
1:A:2149:LEU:C	1:A:2149:LEU:HD13	2.35	0.51
1:A:2139:LEU:HD21	1:A:2189:LEU:HD23	1.93	0.51
1:B:1781:GLN:H	1:B:1781:GLN:NE2	2.08	0.51
1:A:1578:ARG:HG2	1:A:1578:ARG:HH11	1.75	0.51
1:A:1810:VAL:HG13	1:A:1811:PRO:HD2	1.92	0.51
1:B:2010:ASP:OD1	1:B:2148:ARG:HD3	2.11	0.51
1:B:1958:GLY:O	1:B:1965:ASN:ND2	2.44	0.51
1:B:2031:VAL:HG23	1:B:2035:PHE:HB3	1.93	0.51
1:A:1586:ALA:CB	1:A:1621:LEU:HB2	2.41	0.50
1:B:1661:GLU:HG3	1:B:1662:GLY:H	1.76	0.50
1:A:1968:LEU:HA	2:B:3219:D1L:CL14	2.48	0.50
1:A:2024:VAL:HG12	1:A:2025:LEU:HD13	1.93	0.50
1:B:1589:ILE:HG13	1:B:1589:ILE:O	2.11	0.50
1:B:1643:TRP:CE2	1:B:1649:PRO:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1824:LYS:HG3	1:A:1825:ASP:N	2.26	0.50
1:B:1546:GLU:H	1:B:1546:GLU:CD	2.19	0.50
1:B:1635:ILE:O	1:B:1639:PHE:HB3	2.10	0.50
1:B:1998:GLY:HA2	1:B:2001:VAL:CG1	2.41	0.50
1:A:1648:ASN:HB3	1:A:1651:LYS:HG2	1.93	0.50
1:A:1768:ARG:H	1:A:1768:ARG:CD	2.24	0.50
1:A:1781:GLN:NE2	1:A:1782:ILE:HG13	2.23	0.50
1:A:1605:ASN:ND2	1:A:1714:ALA:HB2	2.27	0.50
1:B:2136:ILE:CD1	1:B:2152:ILE:HG12	2.42	0.50
1:B:2133:GLU:O	1:B:2137:LYS:HG2	2.11	0.49
1:B:1587:ASN:ND2	1:B:1624:ASN:HD22	2.10	0.49
1:B:1853:GLU:CD	1:B:1853:GLU:H	2.20	0.49
1:B:2005:PRO:HD3	1:B:2014:MET:HG3	1.93	0.49
1:A:1669:PHE:C	1:A:1671:LYS:H	2.20	0.49
1:B:1646:ALA:C	1:B:1648:ASN:H	2.12	0.49
1:B:1790:HIS:HD2	3:B:4057:HOH:O	1.96	0.49
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.24	0.49
1:B:2045:ASN:HD22	1:B:2046:ARG:NH1	2.10	0.49
1:A:1730:CYS:O	1:A:1731:ARG:C	2.55	0.49
1:A:2047:LEU:HD12	1:A:2047:LEU:N	2.27	0.49
1:A:2148:ARG:O	1:A:2152:ILE:HG13	2.12	0.49
1:B:1646:ALA:C	1:B:1648:ASN:N	2.66	0.49
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.13	0.49
1:B:1492:TRP:HZ2	1:B:1556:GLU:CG	2.26	0.49
1:B:1664:GLU:CD	1:B:1667:LYS:HD3	2.38	0.49
1:A:1643:TRP:H	1:A:1643:TRP:CD1	2.31	0.49
1:A:1602:GLU:HG3	3:A:4023:HOH:O	2.13	0.48
1:B:1544:GLU:OE2	1:B:1602:GLU:OE2	2.31	0.48
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.28	0.48
1:A:1900:GLU:HB3	1:A:1916:LEU:HD11	1.94	0.48
1:A:2133:GLU:OE2	1:A:2148:ARG:NH2	2.45	0.48
1:B:1727:LEU:HD12	1:B:1747:ILE:O	2.14	0.48
1:A:1705:LEU:HD21	1:B:2024:VAL:HG22	1.95	0.48
1:A:2214:SER:C	1:A:2216:VAL:N	2.72	0.48
1:A:2031:VAL:CG2	1:A:2091:LEU:HD23	2.39	0.48
1:A:1664:GLU:OE2	1:A:1667:LYS:HD2	2.13	0.48
1:B:2043:THR:HG23	1:B:2046:ARG:CZ	2.43	0.48
1:B:1655:TYR:C	1:B:1656:LEU:HD12	2.38	0.48
1:B:1815:ASN:HD22	1:B:1944:GLN:HE22	1.62	0.48
1:A:2046:ARG:CZ	1:A:2047:LEU:HD11	2.44	0.47
1:A:2086:TYR:HA	1:A:2089:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1635:ILE:HG22	1:A:1635:ILE:O	2.14	0.47
1:B:1830:PRO:HB2	1:B:2116:THR:HG23	1.95	0.47
1:B:1503:MET:CE	1:B:1731:ARG:HH21	2.28	0.47
1:A:2158:TRP:CZ3	1:A:2186:LEU:HD13	2.50	0.47
1:A:2000:TRP:HB3	1:B:1705:LEU:HD13	1.97	0.47
1:B:1677:THR:CG2	1:B:1690:ILE:HD13	2.44	0.47
1:B:2045:ASN:C	1:B:2046:ARG:HD2	2.39	0.47
1:B:2198:LEU:O	1:B:2201:LYS:HB2	2.15	0.47
1:B:1508:VAL:HG21	1:B:1588:ASP:HA	1.96	0.47
1:B:1664:GLU:O	1:B:1667:LYS:HB2	2.14	0.47
1:A:1497:ARG:HD3	1:A:1510:ASP:OD1	2.14	0.47
1:B:1612:ARG:O	1:B:1814:ARG:NH2	2.48	0.47
1:B:1639:PHE:CD1	1:B:1639:PHE:C	2.91	0.47
1:B:1644:ASN:C	1:B:1646:ALA:H	2.23	0.47
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.97	0.47
1:B:2043:THR:O	1:B:2043:THR:HG22	2.15	0.47
1:B:2046:ARG:HD2	1:B:2046:ARG:N	2.29	0.47
1:A:1741:ARG:NH2	1:A:1934:GLN:NE2	2.63	0.47
1:A:2214:SER:C	1:A:2216:VAL:H	2.22	0.47
1:B:2035:PHE:HE1	1:B:2040:LEU:HA	1.80	0.47
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.50	0.47
1:A:2004:ASP:OD1	1:B:1706:ARG:HA	2.15	0.46
1:A:2082:LEU:H	1:A:2082:LEU:CD2	2.20	0.46
1:B:2200:LYS:HG3	1:B:2203:ARG:NH2	2.30	0.46
1:A:1592:LYS:O	1:A:1593:ILE:HG12	2.14	0.46
1:A:2001:VAL:HG11	2:B:3219:D1L:H4	1.97	0.46
1:B:1489:VAL:CG1	1:B:1497:ARG:HH12	2.28	0.46
1:B:1494:GLN:HB3	1:B:1495:PRO:CD	2.44	0.46
1:A:1578:ARG:HG2	1:A:1578:ARG:NH1	2.30	0.46
1:A:1620:TYR:HB3	1:A:1726:THR:HB	1.97	0.46
1:B:1602:GLU:HG3	3:B:4017:HOH:O	2.15	0.46
1:A:1582:PHE:CD2	1:A:1807:MET:HE1	2.51	0.46
1:A:2000:TRP:CD1	1:A:2000:TRP:C	2.94	0.46
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.16	0.46
2:A:3219:D1L:C13	1:B:1971:GLY:HA3	2.39	0.46
1:B:1640:GLN:HB3	1:B:1657:TYR:CZ	2.51	0.46
1:B:1852:THR:HG23	1:B:1855:GLY:N	2.31	0.46
1:A:1836:THR:HG22	1:A:1838:ASP:HB2	1.98	0.45
1:A:1511:PHE:CZ	1:A:1729:THR:HG21	2.48	0.45
1:A:1616:ILE:HD12	1:A:1813:LYS:HB3	1.98	0.45
1:B:1491:GLU:HG2	1:B:1492:TRP:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1915:THR:HG22	1:B:1916:LEU:N	2.31	0.45
1:A:1833:PHE:CZ	1:A:1845:TRP:HE3	2.34	0.45
1:A:2045:ASN:C	1:A:2047:LEU:H	2.25	0.45
1:A:2149:LEU:HD13	1:A:2149:LEU:O	2.15	0.45
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.96	0.45
1:B:2092:GLN:HE22	1:B:2096:LEU:HG	1.81	0.45
1:B:2035:PHE:HA	1:B:2039:LYS:HD2	1.98	0.45
1:A:1543:ILE:HD11	1:A:1553:VAL:HG11	1.98	0.45
1:A:2045:ASN:C	1:A:2047:LEU:N	2.73	0.45
1:B:1810:VAL:HG13	1:B:1811:PRO:HD2	1.97	0.45
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.17	0.45
1:A:2097:HIS:HE1	1:B:1632:ALA:H	1.64	0.45
1:B:1643:TRP:CD1	1:B:1649:PRO:HA	2.51	0.45
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.16	0.45
1:A:1966:GLU:OE1	1:A:1966:GLU:HA	2.16	0.45
1:B:2045:ASN:HB2	1:B:2046:ARG:NH1	2.31	0.45
1:B:1770:VAL:HG13	1:B:1771:TYR:CD1	2.52	0.45
1:B:1605:ASN:O	1:B:1609:GLU:HG3	2.17	0.45
1:B:2045:ASN:HD22	1:B:2046:ARG:HH12	1.65	0.45
1:B:2158:TRP:HZ3	1:B:2186:LEU:HD13	1.81	0.45
1:B:1494:GLN:HB3	1:B:1495:PRO:HD3	1.98	0.44
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.17	0.44
1:A:1924:TRP:HD1	1:A:1928:SER:HB2	1.82	0.44
1:A:2096:LEU:HB3	1:B:1693:ILE:HG13	2.00	0.44
1:B:1537:PHE:CD2	1:B:1571:VAL:HG22	2.52	0.44
1:B:1487:TYR:CD2	1:B:1488:PRO:HD2	2.52	0.44
1:B:1491:GLU:HG2	1:B:1492:TRP:CE3	2.53	0.44
1:B:1925:HIS:H	1:B:1928:SER:HG	1.65	0.44
1:B:2045:ASN:HB2	1:B:2046:ARG:HH11	1.83	0.44
1:A:1770:VAL:HG13	1:A:1907:PRO:O	2.18	0.44
1:B:1492:TRP:CZ2	1:B:1556:GLU:CG	3.01	0.44
1:A:1583:VAL:HG11	1:A:1607:VAL:CG1	2.48	0.44
1:A:1853:GLU:C	1:A:1855:GLY:H	2.26	0.44
1:B:1492:TRP:CZ2	1:B:1556:GLU:HG2	2.53	0.44
1:B:1635:ILE:O	1:B:1635:ILE:HG22	2.17	0.44
1:A:2187:LYS:O	1:A:2191:LEU:HG	2.18	0.43
1:A:1663:MET:HB3	1:A:1667:LYS:HE2	2.00	0.43
1:B:1643:TRP:NE1	1:B:1649:PRO:HB3	2.32	0.43
1:B:2011:GLN:O	1:B:2129:ARG:NH2	2.51	0.43
1:B:2158:TRP:CZ3	1:B:2186:LEU:HD13	2.54	0.43
1:A:1649:PRO:O	1:B:2085:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1677:THR:HG22	1:A:1689:VAL:O	2.19	0.43
1:A:1759:ALA:N	1:A:1760:PRO:CD	2.81	0.43
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	2.00	0.43
1:B:1508:VAL:CG2	1:B:1588:ASP:HA	2.48	0.43
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	2.01	0.43
1:B:1487:TYR:HA	1:B:1488:PRO:HD3	1.88	0.43
1:B:1677:THR:HA	1:B:1689:VAL:O	2.17	0.43
1:B:2139:LEU:N	1:B:2139:LEU:HD12	2.33	0.43
1:A:1693:ILE:HG13	1:B:2096:LEU:HB3	2.00	0.43
1:A:1877:VAL:CG1	1:A:1931:LYS:HD3	2.48	0.43
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.84	0.43
1:A:2081:GLU:OE1	1:A:2082:LEU:HD23	2.19	0.42
1:B:1728:VAL:HG21	1:B:1754:ILE:HD11	2.01	0.42
1:B:2005:PRO:HG2	1:B:2014:MET:HB2	2.01	0.42
1:A:1633:GLU:C	1:A:1635:ILE:H	2.27	0.42
1:A:1679:ARG:O	1:A:1679:ARG:HG3	2.18	0.42
1:B:1879:VAL:HG13	1:B:1931:LYS:HE2	2.01	0.42
1:B:1889:LEU:HA	1:B:1946:PRO:HD2	2.01	0.42
1:A:2199:ALA:O	1:A:2203:ARG:HG2	2.19	0.42
1:A:1537:PHE:CD2	1:A:1571:VAL:HG13	2.52	0.42
1:B:1852:THR:HG23	1:B:1855:GLY:H	1.83	0.42
1:B:2138:ARG:C	1:B:2139:LEU:HD12	2.43	0.42
1:A:1755:ILE:HD12	1:A:1758:GLY:HA2	2.02	0.42
1:A:1587:ASN:HB2	1:A:1623:ALA:O	2.20	0.42
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.20	0.42
1:A:2031:VAL:C	1:A:2033:ILE:H	2.28	0.42
1:B:1683:ASN:C	1:B:1685:GLU:H	2.27	0.42
1:B:1560:ASN:ND2	1:B:1560:ASN:N	2.68	0.42
1:B:1954:ARG:HG3	1:B:1955:GLY:N	2.30	0.42
1:A:1790:HIS:HD2	3:A:4053:HOH:O	2.03	0.42
1:A:2102:ARG:O	1:A:2106:LYS:HG2	2.20	0.42
1:B:1829:ARG:CZ	1:B:1858:TYR:HB3	2.49	0.42
1:B:1901:ASN:O	1:B:1917:ILE:N	2.53	0.42
1:B:2114:GLU:O	1:B:2115:TRP:C	2.63	0.42
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	2.02	0.41
1:A:1945:LEU:HA	1:A:1946:PRO:HD3	1.88	0.41
1:B:1775:LEU:HD12	1:B:1775:LEU:N	2.34	0.41
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	2.01	0.41
1:B:1677:THR:HG22	1:B:1689:VAL:O	2.20	0.41
1:A:1569:ILE:HG22	1:A:1571:VAL:HG22	2.02	0.41
1:A:1836:THR:C	1:A:1838:ASP:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:VAL:HG12	1:A:1734:GLY:N	2.34	0.41
1:A:1810:VAL:HA	1:A:1811:PRO:HD3	1.94	0.41
1:A:1948:MET:HA	1:A:1986:ILE:O	2.20	0.41
1:B:1966:GLU:O	1:B:1967:VAL:C	2.63	0.41
1:B:2092:GLN:C	1:B:2092:GLN:HE21	2.28	0.41
1:B:2163:VAL:HG13	1:B:2170:GLN:HE21	1.86	0.41
1:A:1996:ARG:O	1:A:1997:GLY:C	2.64	0.41
1:B:1664:GLU:OE1	1:B:1667:LYS:HD3	2.20	0.41
1:A:1655:TYR:CD1	1:A:1689:VAL:HG23	2.56	0.41
1:B:1936:ILE:HD13	1:B:1978:LEU:HD13	2.02	0.41
1:A:1601:ASP:OD1	1:A:1707:GLY:HA3	2.21	0.41
1:A:1605:ASN:HD22	1:A:1714:ALA:HB2	1.85	0.40
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.56	0.40
1:A:2041:LEU:HD13	1:A:2044:MET:HE2	2.01	0.40
1:A:2044:MET:HA	1:A:2086:TYR:CE2	2.56	0.40
1:B:1527:SER:O	1:B:1530:VAL:HG13	2.21	0.40
1:B:2202:ILE:C	1:B:2204:SER:H	2.28	0.40
1:A:1873:TRP:O	1:A:1874:ALA:C	2.65	0.40
1:A:1741:ARG:CZ	1:B:1969:LYS:HG2	2.51	0.40
1:B:1649:PRO:O	1:B:1651:LYS:N	2.54	0.40
1:B:2116:THR:HG22	1:B:2117:GLU:OE2	2.20	0.40
1:B:1932:THR:O	1:B:1936:ILE:HG13	2.22	0.40
1:A:1607:VAL:O	1:A:1610:TYR:HB3	2.22	0.40
1:A:2128:ARG:HE	1:A:2132:GLU:CD	2.29	0.40
1:B:1697:GLU:OE2	1:B:1697:GLU:HA	2.21	0.40
1:B:2036:ARG:O	1:B:2037:ARG:C	2.65	0.40
1:B:2134:TYR:O	1:B:2138:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	692/737 (94%)	628 (91%)	54 (8%)	10 (1%)	9	17
1	B	689/737 (94%)	619 (90%)	63 (9%)	7 (1%)	12	24
All	All	1381/1474 (94%)	1247 (90%)	117 (8%)	17 (1%)	10	20

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1766	LEU
1	A	2205	ASP
1	A	1683	ASN
1	A	1731	ARG
1	A	1997	GLY
1	A	2207	ASP
1	B	1644	ASN
1	B	1650	ASP
1	B	1839	GLU
1	A	1484	ALA
1	B	1534	ASP
1	A	1838	ASP
1	B	1649	PRO
1	B	2205	ASP
1	A	2032	GLY
1	B	2217	ILE
1	A	1767	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	579/628 (92%)	551 (95%)	28 (5%)	23	46
1	B	577/628 (92%)	556 (96%)	21 (4%)	31	58
All	All	1156/1256 (92%)	1107 (96%)	49 (4%)	26	52

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1502	LEU
1	A	1508	VAL
1	A	1536	PHE
1	A	1555	ARG
1	A	1571	VAL
1	A	1585	VAL
1	A	1602	GLU
1	A	1616	ILE
1	A	1618	ARG
1	A	1726	THR
1	A	1769	GLU
1	A	1791	LEU
1	A	1797	LEU
1	A	1823	THR
1	A	1843	VAL
1	A	1884	LEU
1	A	1924	TRP
1	A	1956	PHE
1	A	2014	MET
1	A	2035	PHE
1	A	2041	LEU
1	A	2045	ASN
1	A	2081	GLU
1	A	2082	LEU
1	A	2139	LEU
1	A	2152	ILE
1	A	2186	LEU
1	A	2192	GLU
1	B	1508	VAL
1	B	1536	PHE
1	B	1542	LEU
1	B	1550	LEU
1	B	1560	ASN
1	B	1585	VAL
1	B	1602	GLU
1	B	1639	PHE
1	B	1741	ARG
1	B	1742	LEU
1	B	1781	GLN
1	B	1879	VAL
1	B	1924	TRP
1	B	1945	LEU
1	B	1956	PHE

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Mol	Chain	Res	Type
1	B	1978	LEU
1	B	2001	VAL
1	B	2014	MET
1	B	2092	GLN
1	B	2114	GLU
1	B	2186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1517	GLN
1	A	1525	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1683	ASN
1	A	1744	GLN
1	A	1748	GLN
1	A	1752	GLN
1	A	1763	ASN
1	A	1781	GLN
1	A	1790	HIS
1	A	1815	ASN
1	A	1909	ASN
1	A	1911	ASN
1	A	1934	GLN
1	A	1944	GLN
1	A	2097	HIS
1	A	2131	ASN
1	A	2142	GLN
1	A	2196	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1522	GLN
1	B	1560	ASN
1	B	1581	GLN
1	B	1587	ASN
1	B	1605	ASN
1	B	1640	GLN
1	B	1644	ASN
1	B	1648	ASN

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Mol	Chain	Res	Type
1	B	1683	ASN
1	B	1748	GLN
1	B	1774	ASN
1	B	1781	GLN
1	B	1785	ASN
1	B	1786	ASN
1	B	1790	HIS
1	B	1815	ASN
1	B	1922	GLN
1	B	1934	GLN
1	B	2011	GLN
1	B	2045	ASN
1	B	2092	GLN
1	B	2142	GLN
1	B	2170	GLN
1	B	2178	ASN
1	B	2208	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	D1L	B	3219	-	22,22,22	0.81	1 (4%)	30,30,30	0.96	1 (3%)
2	D1L	A	3219	-	22,22,22	0.79	1 (4%)	30,30,30	0.97	2 (6%)

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	D1L	B	3219	-	-	2/12/12/12	0/2/2/2
2	D1L	A	3219	-	-	4/12/12/12	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3219	D1L	O1A-C1	-2.29	1.23	1.30
2	A	3219	D1L	O1A-C1	-2.21	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3219	D1L	O2-C2-C1	-3.14	107.36	111.34
2	A	3219	D1L	O2-C2-C1	-2.88	107.70	111.34
2	A	3219	D1L	C3-O2-C2	-2.16	114.88	118.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

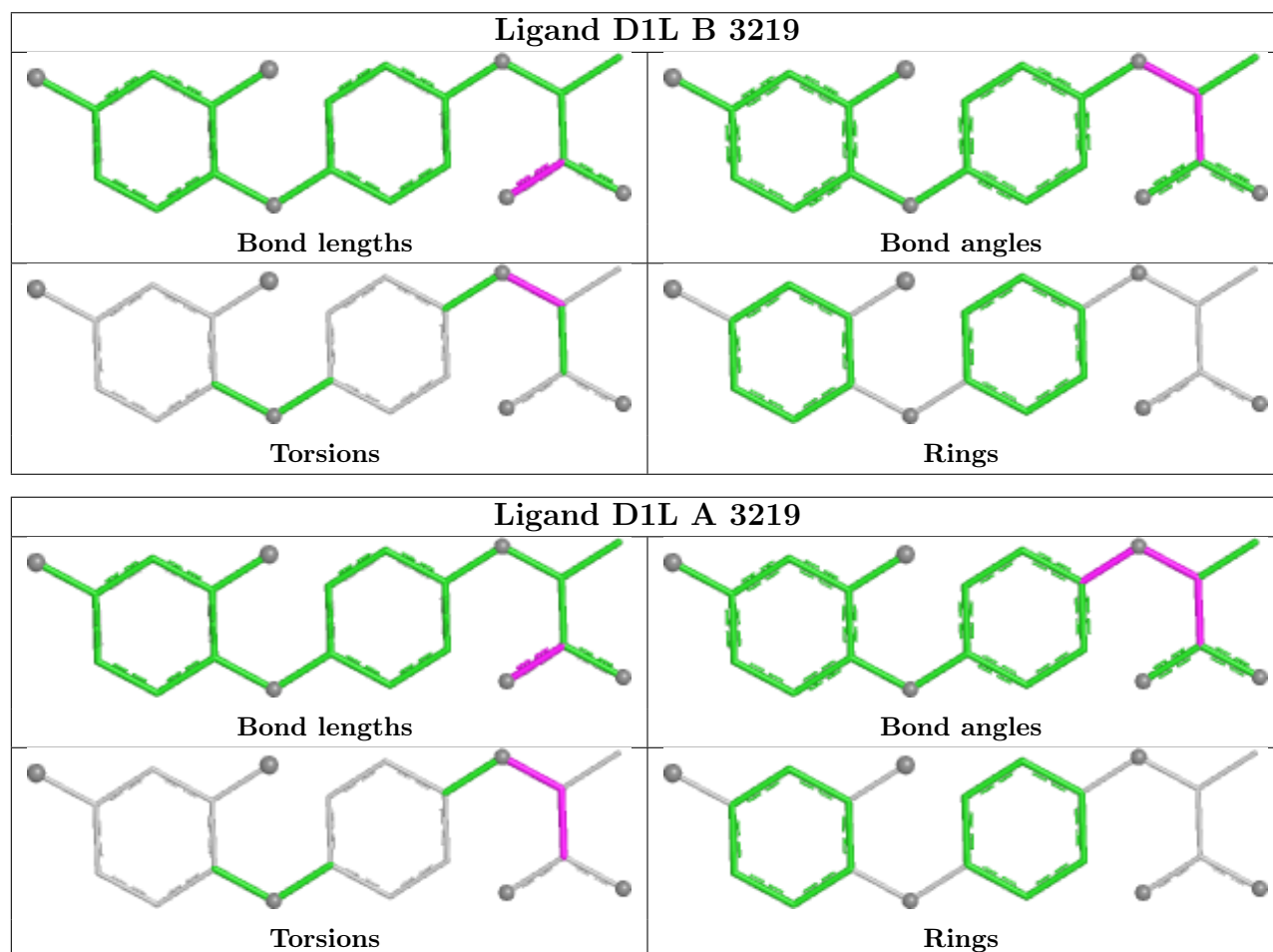
Mol	Chain	Res	Type	Atoms
2	A	3219	D1L	C1-C2-O2-C3
2	B	3219	D1L	C1-C2-O2-C3
2	A	3219	D1L	O1A-C1-C2-O2
2	A	3219	D1L	C2A-C2-O2-C3
2	B	3219	D1L	C2A-C2-O2-C3
2	A	3219	D1L	O1B-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3219	D1L	6	0
2	A	3219	D1L	6	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

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	698/737 (94%)	0.64	130 (18%) 3 2	21, 43, 100, 100	0
1	B	695/737 (94%)	0.66	128 (18%) 3 2	21, 44, 100, 100	0
All	All	1393/1474 (94%)	0.65	258 (18%) 3 2	21, 43, 100, 100	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1958	GLY	11.1
1	B	2207	ASP	6.7
1	A	1648	ASN	6.6
1	B	2206	HIS	6.4
1	B	2217	ILE	6.1
1	A	1682	ILE	6.1
1	A	1681	VAL	6.0
1	B	1681	VAL	5.9
1	B	1912	SER	5.7
1	A	2217	ILE	5.6
1	B	1913	ALA	5.5
1	B	1680	THR	5.4
1	B	2194	PHE	5.4
1	B	1958	GLY	5.3
1	B	2083	LEU	5.3
1	A	1646	ALA	5.2
1	B	1957	SER	5.2
1	A	1662	GLY	5.1
1	A	1965	ASN	5.1
1	A	1658	LEU	5.1
1	B	2041	LEU	5.1
1	B	1650	ASP	5.0
1	B	1484	ALA	4.8
1	B	1907	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	2085	ILE	4.8
1	B	2043	THR	4.8
1	A	1910	PRO	4.6
1	A	1659	THR	4.6
1	A	1902	LEU	4.6
1	A	1916	LEU	4.5
1	A	1660	SER	4.5
1	A	1955	GLY	4.4
1	B	1916	LEU	4.4
1	B	1915	THR	4.3
1	B	1965	ASN	4.3
1	A	1643	TRP	4.3
1	B	1649	PRO	4.3
1	B	2045	ASN	4.2
1	B	1658	LEU	4.2
1	A	2213	LEU	4.2
1	B	1646	ALA	4.2
1	A	1688	PHE	4.1
1	B	2035	PHE	4.1
1	A	1637	PRO	4.1
1	A	1685	GLU	4.1
1	B	1659	THR	4.1
1	B	1910	PRO	4.0
1	A	1956	PHE	4.0
1	A	2206	HIS	4.0
1	A	1482	PRO	4.0
1	A	1684	GLY	3.9
1	B	1766	LEU	3.9
1	B	2213	LEU	3.9
1	A	1647	ALA	3.9
1	A	2208	ASN	3.9
1	B	2046	ARG	3.9
1	B	2084	PRO	3.9
1	B	1908	ALA	3.9
1	B	1648	ASN	3.8
1	B	2044	MET	3.8
1	A	1655	TYR	3.8
1	B	2085	ILE	3.8
1	A	2215	GLU	3.8
1	A	1649	PRO	3.8
1	A	1663	MET	3.8
1	B	1769	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	2082	LEU	3.8
1	B	1900	GLU	3.8
1	A	2214	SER	3.7
1	A	1767	GLY	3.7
1	B	2081	GLU	3.7
1	A	1680	THR	3.7
1	B	1669	PHE	3.7
1	A	1666	LEU	3.7
1	B	1684	GLY	3.6
1	A	2041	LEU	3.6
1	A	1644	ASN	3.6
1	A	2081	GLU	3.6
1	B	1956	PHE	3.6
1	B	1853	GLU	3.6
1	A	1689	VAL	3.6
1	B	1647	ALA	3.6
1	B	2087	GLY	3.6
1	A	1673	ASN	3.5
1	B	1645	ASP	3.5
1	B	2036	ARG	3.5
1	A	2044	MET	3.5
1	A	1636	VAL	3.5
1	B	1764	LYS	3.5
1	B	2145	GLU	3.4
1	B	2152	ILE	3.4
1	A	1903	ILE	3.4
1	B	2089	ILE	3.4
1	A	1907	PRO	3.4
1	A	1483	ILE	3.4
1	A	1652	GLY	3.4
1	A	2204	SER	3.4
1	A	1645	ASP	3.3
1	A	2202	ILE	3.3
1	A	2205	ASP	3.3
1	A	1669	PHE	3.3
1	A	2211	ASP	3.3
1	A	2047	LEU	3.3
1	A	1642	ALA	3.3
1	A	1913	ALA	3.3
1	B	2040	LEU	3.3
1	B	2143	VAL	3.3
1	A	1762	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	2045	ASN	3.2
1	B	1657	TYR	3.2
1	A	1641	VAL	3.2
1	B	1489	VAL	3.2
1	B	2208	ASN	3.2
1	A	2046	ARG	3.2
1	A	1677	THR	3.2
1	A	1683	ASN	3.1
1	B	1955	GLY	3.1
1	A	1908	ALA	3.1
1	A	1904	PRO	3.1
1	A	1687	ARG	3.1
1	A	2201	LYS	3.1
1	B	1687	ARG	3.1
1	B	1682	ILE	3.1
1	B	1838	ASP	3.0
1	A	1911	ASN	3.0
1	B	1786	ASN	3.0
1	B	1767	GLY	3.0
1	A	1966	GLU	3.0
1	B	2210	ILE	3.0
1	A	1665	THR	3.0
1	B	2091	LEU	3.0
1	A	1657	TYR	3.0
1	B	1530	VAL	2.9
1	B	1765	MET	2.9
1	B	1655	TYR	2.9
1	A	2203	ARG	2.9
1	B	1651	LYS	2.9
1	B	1902	LEU	2.9
1	B	2191	LEU	2.9
1	B	1660	SER	2.8
1	A	2152	ILE	2.8
1	B	2209	ALA	2.8
1	B	2203	ARG	2.8
1	A	2043	THR	2.8
1	B	2146	ALA	2.8
1	B	1494	GLN	2.8
1	B	1906	ASP	2.8
1	A	1766	LEU	2.8
1	A	1671	LYS	2.8
1	B	1686	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1768	ARG	2.8
1	B	2037	ARG	2.8
1	A	1661	GLU	2.7
1	A	1686	GLU	2.7
1	A	1653	PHE	2.7
1	A	1635	ILE	2.7
1	A	1786	ASN	2.7
1	A	1674	SER	2.7
1	A	1912	SER	2.7
1	A	2207	ASP	2.7
1	A	1667	LYS	2.7
1	A	1763	ASN	2.7
1	B	1901	ASN	2.7
1	A	2216	VAL	2.7
1	A	2218	LYS	2.6
1	B	1679	ARG	2.6
1	B	1683	ASN	2.6
1	B	1909	ASN	2.6
1	A	2040	LEU	2.6
1	B	1534	ASP	2.6
1	A	1651	LYS	2.6
1	A	1764	LYS	2.6
1	A	1917	ILE	2.6
1	B	2031	VAL	2.6
1	B	1640	GLN	2.6
1	B	2195	ALA	2.6
1	B	2086	TYR	2.6
1	B	1652	GLY	2.6
1	B	1761	ALA	2.6
1	A	2042	ASP	2.6
1	B	2211	ASP	2.6
1	A	2038	GLU	2.6
1	A	1918	GLN	2.6
1	A	1915	THR	2.6
1	B	1688	PHE	2.5
1	B	2141	HIS	2.5
1	B	1911	ASN	2.5
1	A	1768	ARG	2.5
1	A	1679	ARG	2.5
1	B	1663	MET	2.5
1	B	1643	TRP	2.5
1	B	1839	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2198	LEU	2.4
1	B	2216	VAL	2.4
1	B	1668	LYS	2.4
1	B	2139	LEU	2.4
1	B	1653	PHE	2.4
1	A	2146	ALA	2.4
1	A	1759	ALA	2.4
1	B	1492	TRP	2.4
1	B	1685	GLU	2.4
1	A	1675	VAL	2.4
1	A	1836	THR	2.3
1	A	1650	ASP	2.3
1	B	2205	ASP	2.3
1	A	1901	ASN	2.3
1	A	2037	ARG	2.3
1	B	1674	SER	2.3
1	A	1823	THR	2.3
1	B	1665	THR	2.3
1	A	1957	SER	2.3
1	B	1918	GLN	2.3
1	B	2202	ILE	2.3
1	A	1678	GLU	2.3
1	B	1525	ASN	2.3
1	A	2089	ILE	2.3
1	A	1631	MET	2.3
1	A	1528	ALA	2.2
1	B	1644	ASN	2.2
1	B	1738	TYR	2.3
1	A	2200	LYS	2.2
1	B	1903	ILE	2.2
1	B	1914	GLU	2.2
1	B	1921	GLY	2.2
1	A	1527	SER	2.2
1	B	1641	VAL	2.2
1	B	2019	ASN	2.2
1	B	2189	LEU	2.2
1	B	2214	SER	2.2
1	A	2036	ARG	2.2
1	B	2088	GLN	2.2
1	B	1662	GLY	2.2
1	B	1661	GLU	2.2
1	B	1966	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1917	ILE	2.1
1	A	2039	LYS	2.1
1	A	1632	ALA	2.1
1	A	1638	LEU	2.1
1	A	1695	GLY	2.1
1	B	2149	LEU	2.1
1	A	1664	GLU	2.1
1	A	1668	LYS	2.1
1	A	1909	ASN	2.1
1	A	2082	LEU	2.1
1	B	1491	GLU	2.1
1	A	1832	ASP	2.1
1	A	1905	ALA	2.0
1	A	2083	LEU	2.0
1	A	1839	GLU	2.0
1	A	2145	GLU	2.0
1	B	2144	GLY	2.0
1	B	2215	GLU	2.0
1	A	1826	THR	2.0
1	B	1852	THR	2.0
1	B	1689	VAL	2.0
1	A	1692	THR	2.0
1	A	1906	ASP	2.0
1	A	1771	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

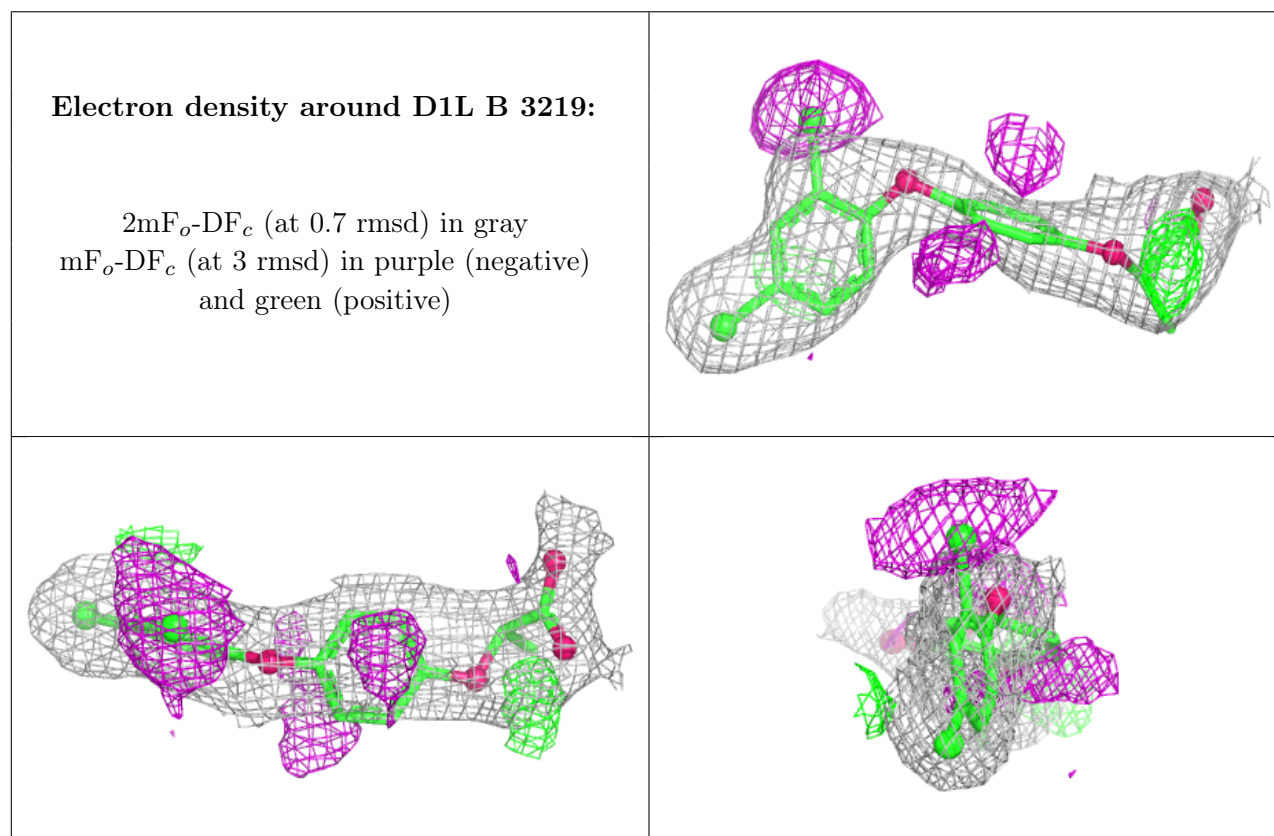
There are no oligosaccharides in this entry.

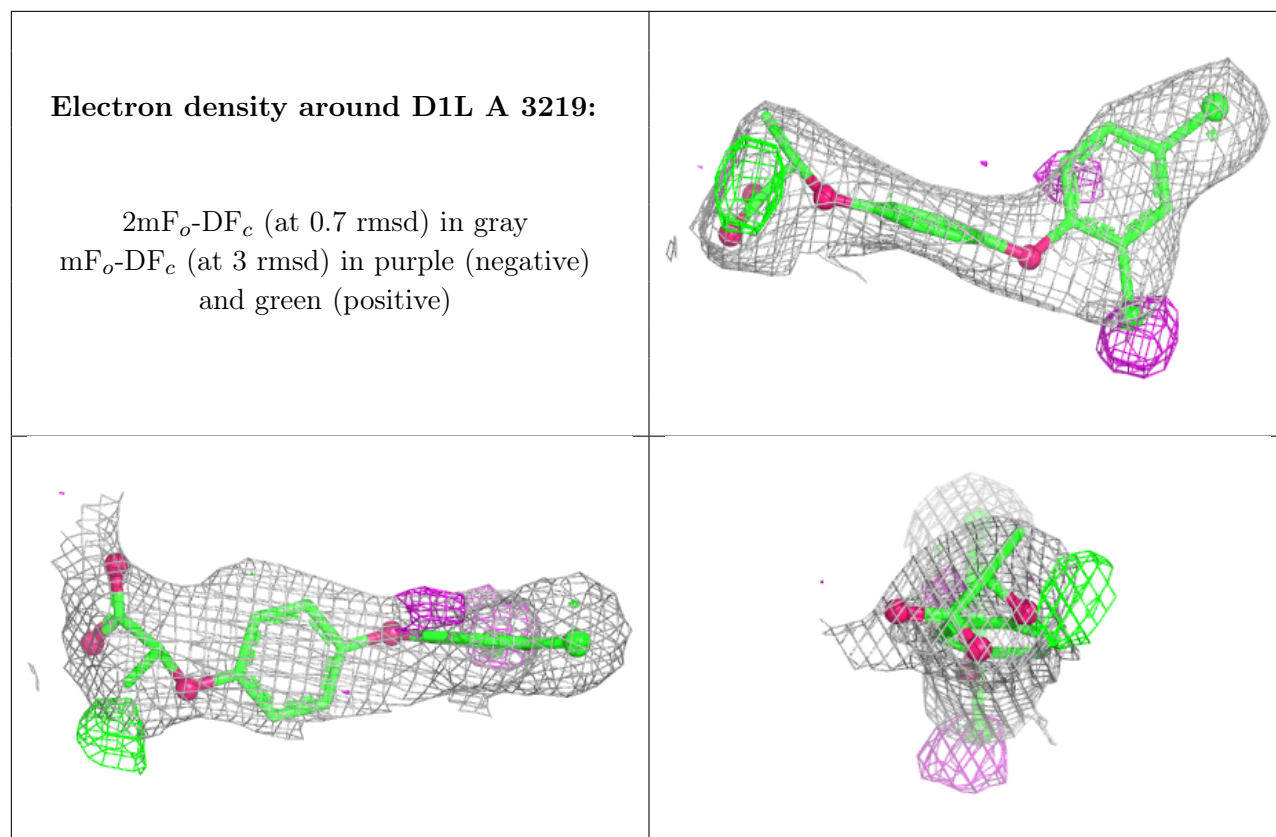
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	D1L	B	3219	21/21	0.81	0.23	73,78,80,89	0
2	D1L	A	3219	21/21	0.86	0.19	74,79,80,88	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.