Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2022 – 04:10 pm BST

PDB ID	:	6TKY
Title	:	Crystal structure of the DHR2 domain of DOCK10 in complex with CDC42
Authors	:	Barford, D.; Fan, D.; Cronin, N.; Yang, J.
Deposited on	:	2019-11-29
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

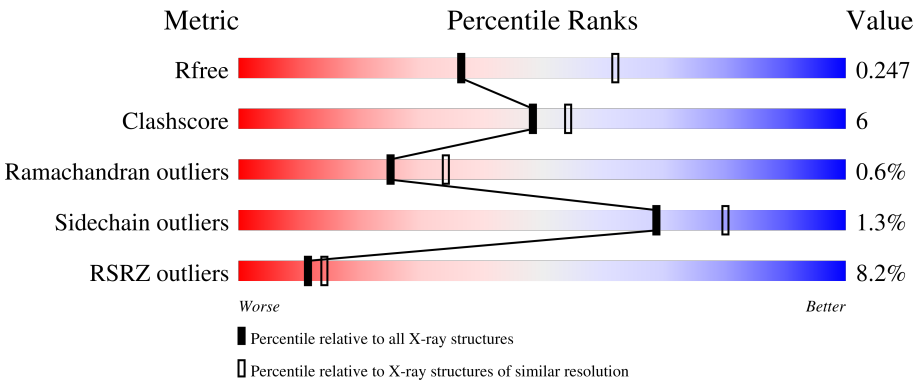
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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

Mol	Chain	Length	Quality of chain
1	B	457	8% 79% 12% 9%
2	C	188	5% 81% 13% 6%
2	D	188	7% 77% 18% 5%
3	A	458	9% 76% 14% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	2202	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9543 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 Dedicator of cytokinesis protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	416	3316	2119	555	625	17	0	0	0

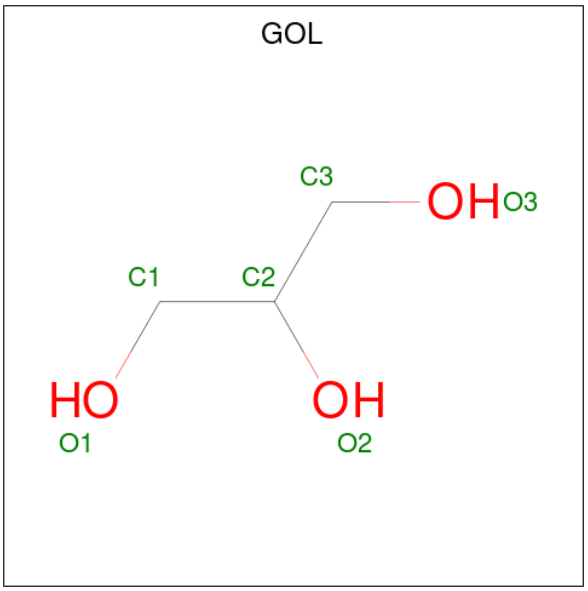
- Molecule 2 is a protein called Cell division control protein 42 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	177	1327	855	212	254	6	0	0	0
2	D	178	1323	851	209	257	6	0	0	0

- Molecule 3 is a protein called Dedicator of cytokinesis protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	417	3328	2135	559	617	17	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	D	1	6	3	3	0	0
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	A	1	6	3	3	0	0

- Molecule 5 is water.

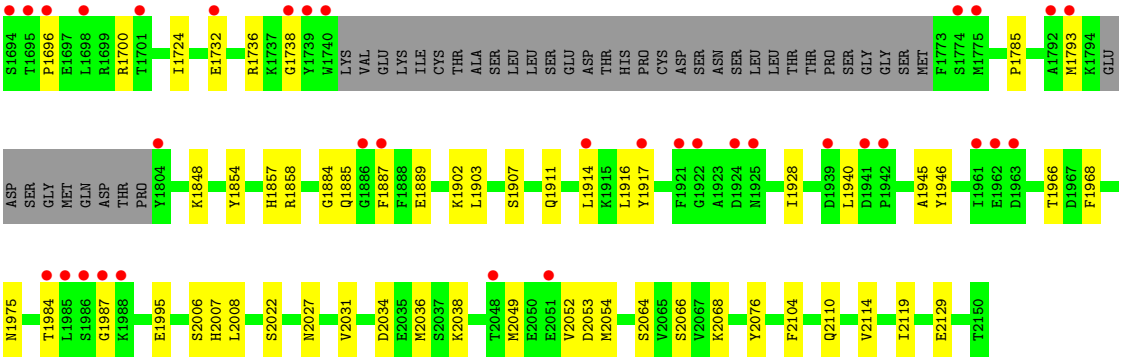
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	97	97	97	0	0
			Total	O		
5	C	31	31	31	0	0
			Total	O		
5	D	29	29	29	0	0
			Total	O		
5	A	74	74	74	0	0

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.

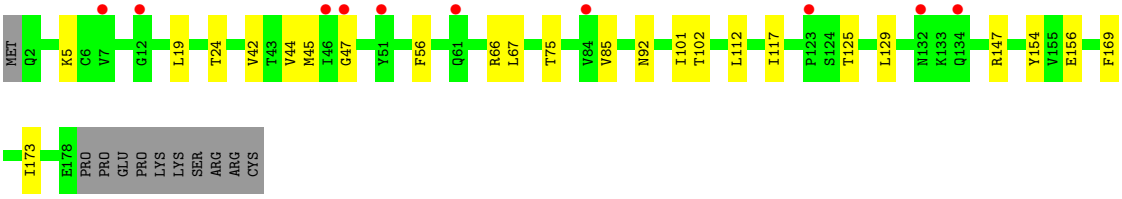
• Molecule 1: Dedicator of cytokinesis protein 10

Chain B:



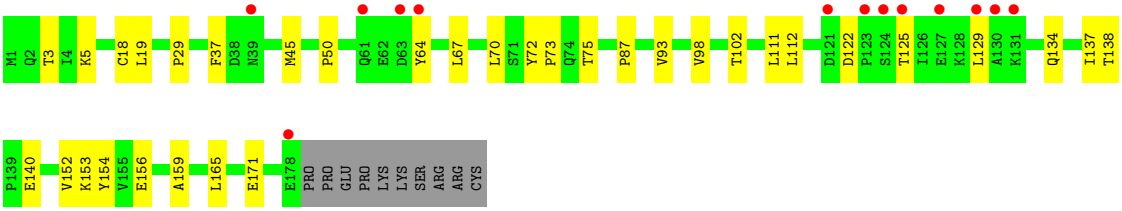
• Molecule 2: Cell division control protein 42 homolog

Chain C:



• Molecule 2: Cell division control protein 42 homolog

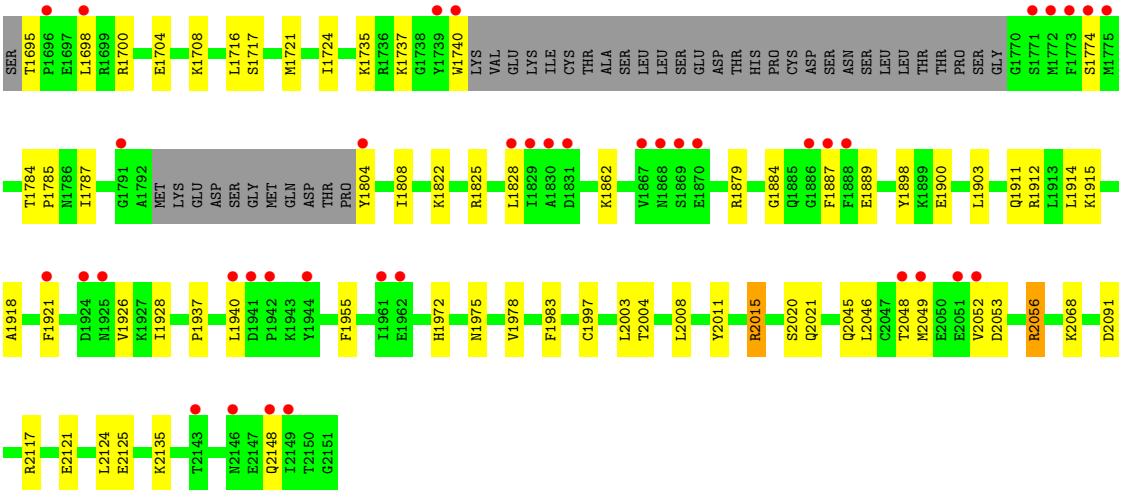
Chain D:



• Molecule 3: Dedicator of cytokinesis protein 10

Chain A:

9%
76%
14%
9%


SER T1695 P1696 E1697 L1698 R1699 R1700 E1704 K1708 L1716 S1717 M1721 I1724 K1735 R1736 K1737 G1738 Y1739 W1740 LYS VAL GLU LYS ILE CYS THR ALA SER LEU LEU LEU SER GLU ASP THR HIS PRO CYS ASP SER ASN SER LEU LEU THR THR PRO SER GLY G1770 S1771 M1772 F1773 S1774 M1775
T1784 P1785 N1786 I1787 G1791 A1792 MET LYS GLU ASP SER GLY MET GLN ASP THR PRO Y1804 I1808 K1822 R1825 L1828 I1829 A1830 D1831 K1862 V1867 N1868 S1869 E1870 R1879 G1884 Q1885 G1886 F1887 F1888 E1889 Y1898 K1899 E1900 L1903 Q1911 R1912 L1913 L1914 K1915
A1918 F1921 D1924 N1925 V1926 K1927 I1928 P1937 L1940 D1941 P1942 K1943 Y1944 F1955 I1961 E1962 H1972 N1975 V1978 F1983 C1997 L2003 T2004 L2008 Y2011 R2015 S2020 Q2021 Q2045 L2046 C2047 T2048 M2049 E2050 E2051 V2052 D2053 R2056 K2068 D2091
R2117 E2121 L2124 E2125 K2135 T2143 N2146 E2147 Q2148 I2149 T2150 G2151

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	96.90Å 96.90Å 310.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.55 29.83 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.83-2.55) 99.9 (29.83-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.188 , 0.246 0.188 , 0.247	Depositor DCC
R_{free} test set	2495 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9543	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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 (i)

5.1 Standard geometry (i)

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

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	B	0.44	0/3382	0.56	0/4570
2	C	0.42	0/1357	0.57	1/1859 (0.1%)
2	D	0.42	0/1353	0.58	0/1856
3	A	0.45	0/3397	0.58	1/4589 (0.0%)
All	All	0.44	0/9489	0.57	2/12874 (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})
3	A	2015	ARG	NE-CZ-NH2	-5.39	117.61	120.30
2	C	19	LEU	CA-CB-CG	5.34	127.58	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	B	3316	0	3195	36	0
2	C	1327	0	1290	17	0
2	D	1323	0	1268	21	0
3	A	3328	0	3234	42	0
4	A	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	6	0	8	0	0
5	A	74	0	0	5	0
5	B	97	0	0	1	0
5	C	31	0	0	3	0
5	D	29	0	0	0	0
All	All	9543	0	9011	109	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 6.

All (109) 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)
3:A:2015:ARG:NH2	5:A:2301:HOH:O	2.03	0.90
3:A:1695:THR:HB	3:A:1698:LEU:HD12	1.58	0.84
3:A:1975:ASN:HB3	3:A:2008:LEU:HD23	1.64	0.79
1:B:2054:MET:HE1	1:B:2119:ILE:HA	1.67	0.76
2:C:85:VAL:HG13	2:C:129:LEU:HD11	1.70	0.74
3:A:2121:GLU:HA	3:A:2124:LEU:HD12	1.72	0.72
3:A:1735:LYS:NZ	5:A:2304:HOH:O	2.24	0.70
3:A:1918:ALA:HB2	3:A:1926:VAL:HG11	1.73	0.70
3:A:2148:GLN:NE2	5:A:2303:HOH:O	2.22	0.70
2:C:44:VAL:HG11	2:C:173:ILE:HD11	1.74	0.69
2:C:5:LYS:NZ	5:C:202:HOH:O	2.22	0.67
1:B:1902:LYS:NZ	5:B:2201:HOH:O	2.25	0.66
3:A:1695:THR:CB	3:A:1698:LEU:HD12	2.27	0.64
1:B:2049:MET:HE3	1:B:2052:VAL:HA	1.80	0.62
1:B:2036:MET:HE1	2:D:37:PHE:CZ	2.35	0.61
1:B:1966:THR:HG22	1:B:1968:PHE:N	2.15	0.61
1:B:1966:THR:HG22	1:B:1968:PHE:H	1.67	0.59
1:B:1907:SER:O	1:B:1911:GLN:HG2	2.04	0.58
3:A:2045:GLN:O	3:A:2048:THR:HG22	2.03	0.57
2:D:111:LEU:HD23	2:D:152:VAL:HB	1.85	0.57
2:C:5:LYS:HG3	2:C:56:PHE:CE1	2.39	0.57
1:B:2068:LYS:HD2	2:D:64:TYR:CE1	2.39	0.57
3:A:2117:ARG:NH2	5:A:2307:HOH:O	2.38	0.56
3:A:1914:LEU:HD13	3:A:1928:ILE:HG12	1.87	0.55
2:C:44:VAL:HG11	2:C:173:ILE:CD1	2.36	0.54
1:B:2054:MET:CE	1:B:2119:ILE:HA	2.36	0.54
1:B:2049:MET:CE	1:B:2053:ASP:H	2.21	0.54
3:A:1785:PRO:HD2	3:A:2008:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:LYS:HG2	2:D:75:THR:HA	1.91	0.53
2:C:92:ASN:OD1	5:C:201:HOH:O	2.19	0.52
2:C:24:THR:HG22	2:C:42:VAL:HB	1.90	0.52
3:A:2015:ARG:NH1	5:A:2310:HOH:O	2.43	0.52
2:D:140:GLU:H	2:D:140:GLU:CD	2.13	0.52
1:B:1984:THR:HB	1:B:1995:GLU:HG3	1.92	0.51
3:A:2049:MET:HE3	3:A:2052:VAL:HA	1.92	0.51
3:A:1716:LEU:HD13	3:A:1822:LYS:HB3	1.91	0.51
2:D:67:LEU:HD12	2:D:70:LEU:HD12	1.91	0.51
2:C:85:VAL:HG12	2:C:85:VAL:O	2.11	0.51
1:B:1914:LEU:HD13	1:B:1928:ILE:HG12	1.92	0.50
1:B:1736:ARG:NH1	1:B:1793:MET:HB3	2.27	0.50
1:B:2036:MET:HE3	1:B:2076:TYR:HD2	1.76	0.50
1:B:1916:LEU:HD23	1:B:1917:TYR:CE2	2.47	0.50
3:A:1804:TYR:HA	3:A:1808:ILE:HD12	1.94	0.50
1:B:1854:TYR:CZ	1:B:1858:ARG:HD2	2.46	0.49
2:C:85:VAL:HG11	2:C:125:THR:CG2	2.43	0.49
1:B:1696:PRO:HG3	1:B:1793:MET:HG3	1.95	0.49
2:C:5:LYS:HD3	2:C:75:THR:HA	1.94	0.49
2:D:153:LYS:HD2	2:D:171:GLU:HG2	1.95	0.48
2:C:45:MET:HG2	3:A:1903:LEU:HD12	1.94	0.48
2:C:66:ARG:NH1	3:A:2125:GLU:OE2	2.47	0.48
1:B:1785:PRO:HD2	1:B:2008:LEU:HD12	1.95	0.48
2:C:169:PHE:O	2:C:173:ILE:HD12	2.14	0.48
1:B:1975:ASN:HB3	1:B:2008:LEU:HD23	1.96	0.47
3:A:1955:PHE:HB2	3:A:1978:VAL:HB	1.95	0.47
1:B:2129:GLU:HG2	2:D:67:LEU:CD1	2.44	0.47
1:B:1940:LEU:HD22	1:B:1946:TYR:CE2	2.49	0.47
3:A:1695:THR:HB	3:A:1698:LEU:CD1	2.39	0.47
3:A:1740:TRP:CE3	3:A:1774:SER:HA	2.50	0.47
1:B:1724:ILE:HA	1:B:1724:ILE:HD12	1.72	0.47
1:B:1732:GLU:O	1:B:1736:ARG:HG3	2.15	0.46
3:A:2121:GLU:HA	3:A:2124:LEU:CD1	2.44	0.46
3:A:1898:TYR:CZ	3:A:2015:ARG:HG2	2.51	0.46
2:C:117:ILE:HG21	2:C:156:GLU:HB3	1.98	0.46
3:A:2003:LEU:HD23	3:A:2021:GLN:HB3	1.97	0.46
3:A:1915:LYS:HA	3:A:1915:LYS:HD3	1.74	0.45
3:A:1900:GLU:OE2	3:A:1912:ARG:NH1	2.50	0.45
2:D:19:LEU:HD11	2:D:165:LEU:HD13	1.99	0.45
3:A:2046:LEU:HD21	3:A:2056:ARG:HE	1.82	0.45
3:A:2135:LYS:HB3	3:A:2135:LYS:HE2	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:PRO:HA	2:D:137:ILE:HD11	2.00	0.44
1:B:1903:LEU:HD23	1:B:1903:LEU:HA	1.78	0.44
1:B:2053:ASP:OD2	2:D:3:THR:OG1	2.36	0.43
3:A:1784:THR:O	3:A:1787:ILE:HG13	2.18	0.43
1:B:2006:SER:HG	1:B:2007:HIS:CE1	2.35	0.43
3:A:1721:MET:O	3:A:1724:ILE:HG22	2.18	0.43
1:B:2068:LYS:HD2	2:D:64:TYR:HE1	1.83	0.43
2:D:122:ASP:OD2	2:D:125:THR:OG1	2.30	0.43
1:B:2036:MET:HE3	1:B:2076:TYR:CD2	2.54	0.43
1:B:2064:SER:HB3	1:B:2104:PHE:HZ	1.83	0.43
3:A:2008:LEU:O	3:A:2011:TYR:HB2	2.19	0.43
1:B:2049:MET:HE1	1:B:2053:ASP:H	1.83	0.42
1:B:2064:SER:HB3	1:B:2104:PHE:CZ	2.54	0.42
2:D:29:PRO:HD3	2:D:159:ALA:O	2.19	0.42
3:A:1828:LEU:HD11	3:A:1972:HIS:CE1	2.54	0.42
3:A:1937:PRO:HA	3:A:1940:LEU:HD22	2.00	0.42
1:B:2027:ASN:O	1:B:2031:VAL:HG23	2.20	0.42
1:B:2049:MET:HE3	1:B:2053:ASP:H	1.83	0.42
3:A:1717:SER:OG	3:A:1825:ARG:NE	2.52	0.42
1:B:2034:ASP:O	1:B:2038:LYS:HD2	2.18	0.42
3:A:1704:GLU:O	3:A:1708:LYS:HD3	2.20	0.42
2:D:93:VAL:HG11	2:D:112:LEU:HD11	2.01	0.41
3:A:1862:LYS:HA	3:A:1862:LYS:HD2	1.85	0.41
2:D:154:TYR:CZ	2:D:156:GLU:HG3	2.55	0.41
2:D:45:MET:HE2	2:D:50:PRO:HA	2.02	0.41
2:D:138:THR:HB	2:D:140:GLU:OE1	2.20	0.41
3:A:1879:ARG:HD2	3:A:1879:ARG:C	2.41	0.41
2:C:147:ARG:NH1	5:C:206:HOH:O	2.49	0.41
2:D:72:TYR:N	2:D:73:PRO:CD	2.84	0.41
2:D:98:VAL:O	2:D:102:THR:OG1	2.34	0.41
3:A:2004:THR:HB	3:A:2020:SER:HB3	2.03	0.41
2:C:112:LEU:HB3	2:C:154:TYR:HD1	1.86	0.41
2:D:129:LEU:HB3	2:D:134:GLN:O	2.20	0.40
3:A:1911:GLN:NE2	3:A:1915:LYS:HE2	2.36	0.40
1:B:2110:GLN:O	1:B:2114:VAL:HG23	2.22	0.40
2:C:101:ILE:HG13	2:C:102:THR:N	2.36	0.40
1:B:1887:PHE:CG	1:B:1945:ALA:HB2	2.57	0.40
3:A:1983:PHE:O	3:A:1997:CYS:HB2	2.20	0.40
3:A:2049:MET:CE	3:A:2053:ASP:H	2.35	0.40
3:A:1887:PHE:HB3	3:A:1921:PHE:CZ	2.57	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	B	410/457 (90%)	394 (96%)	12 (3%)	4 (1%)	15	22
2	C	175/188 (93%)	164 (94%)	10 (6%)	1 (1%)	25	34
2	D	176/188 (94%)	172 (98%)	4 (2%)	0	100	100
3	A	411/458 (90%)	401 (98%)	8 (2%)	2 (0%)	29	40
All	All	1172/1291 (91%)	1131 (96%)	34 (3%)	7 (1%)	25	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1738	GLY
2	C	47	GLY
1	B	1987	GLY
3	A	1889	GLU
1	B	1889	GLU
1	B	1884	GLY
3	A	1884	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	B	346/411 (84%)	340 (98%)	6 (2%)	60	75
2	C	143/168 (85%)	142 (99%)	1 (1%)	84	90
2	D	141/168 (84%)	140 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	347/411 (84%)	342 (99%)	5 (1%)	67 79
All	All	977/1158 (84%)	964 (99%)	13 (1%)	69 80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1700	ARG
1	B	1848	LYS
1	B	1857	HIS
1	B	1885	GLN
1	B	2022	SER
1	B	2066	SER
2	C	67	LEU
2	D	18	CYS
3	A	1700	ARG
3	A	1737	LYS
3	A	2056	ARG
3	A	2068	LYS
3	A	2091	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	104	HIS
3	A	1911	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	2201	-	5,5,5	0.94	0	5,5,5	0.99	0
4	GOL	D	201	-	5,5,5	1.23	0	5,5,5	0.94	0
4	GOL	A	2202	-	5,5,5	0.97	0	5,5,5	0.93	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
4	GOL	A	2201	-	-	3/4/4/4	-
4	GOL	D	201	-	-	4/4/4/4	-
4	GOL	A	2202	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

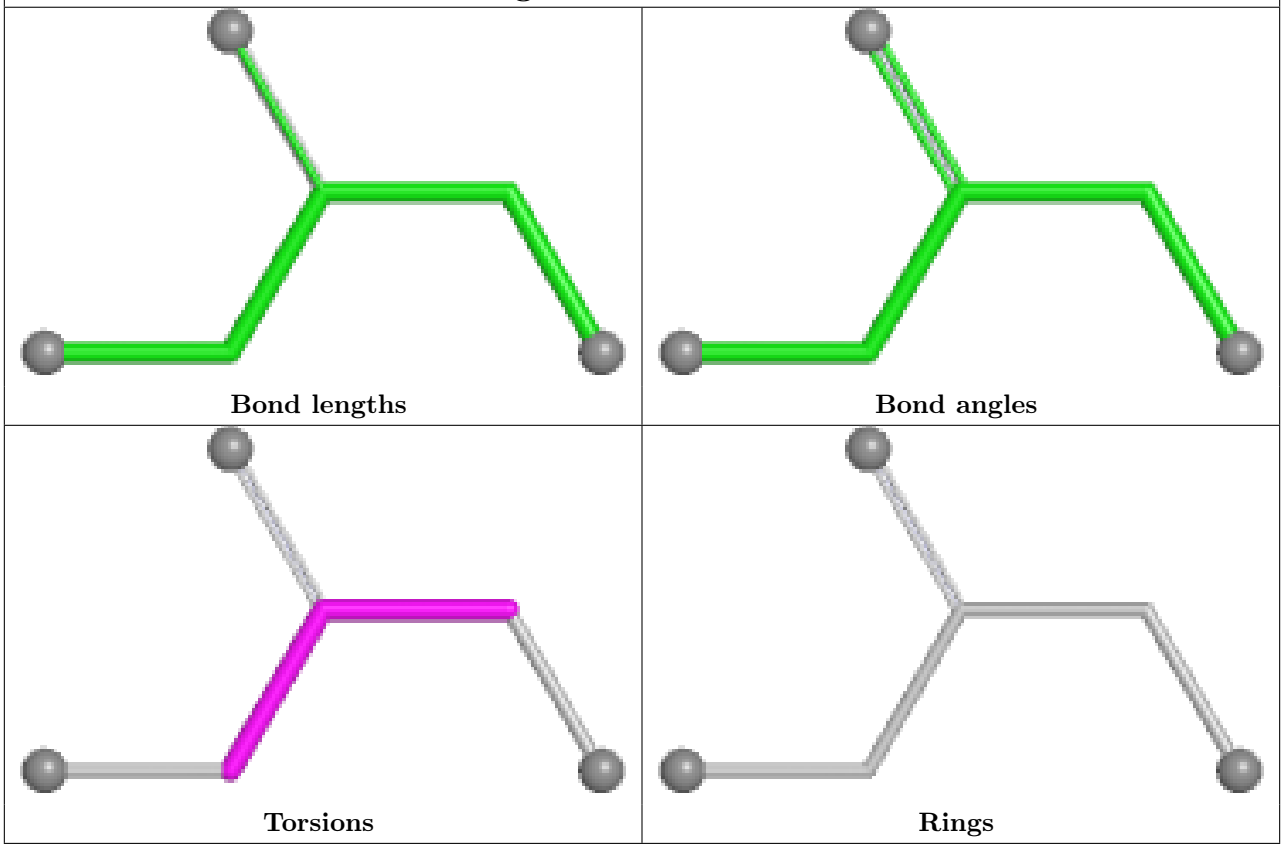
Mol	Chain	Res	Type	Atoms
4	D	201	GOL	O1-C1-C2-C3
4	D	201	GOL	C1-C2-C3-O3
4	D	201	GOL	O2-C2-C3-O3
4	A	2201	GOL	O1-C1-C2-C3
4	A	2202	GOL	C1-C2-C3-O3
4	A	2201	GOL	O1-C1-C2-O2
4	A	2202	GOL	O2-C2-C3-O3
4	A	2201	GOL	C1-C2-C3-O3
4	D	201	GOL	O1-C1-C2-O2

There are no ring outliers.

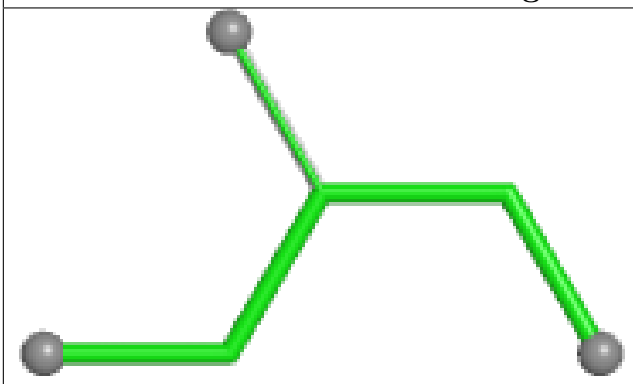
No monomer is involved in short contacts.

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.

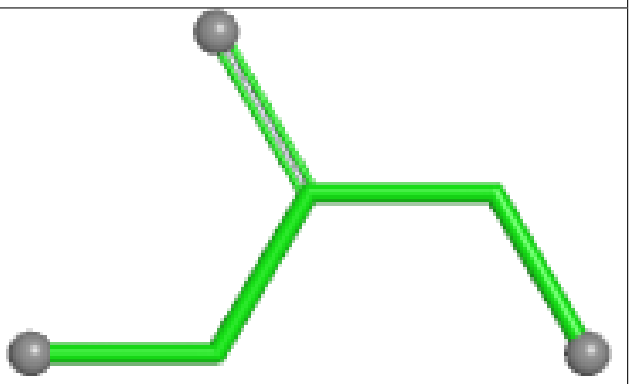
Ligand GOL A 2201



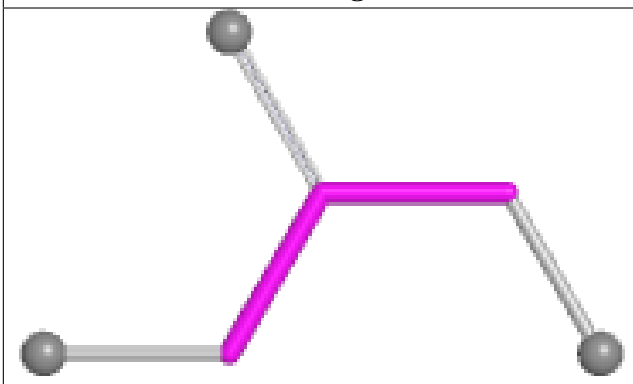
Ligand GOL D 201



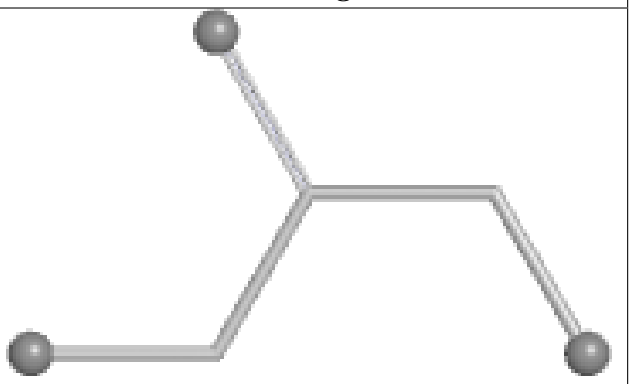
Bond lengths



Bond angles

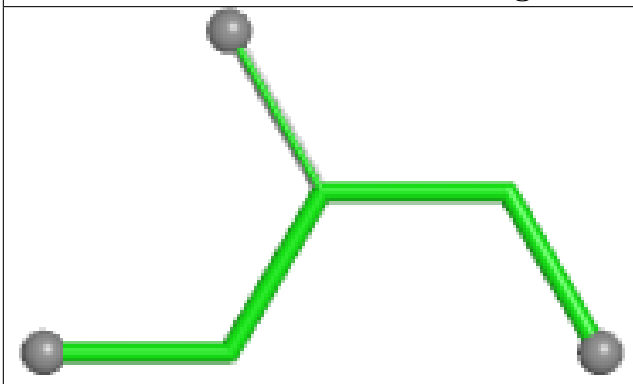


Torsions

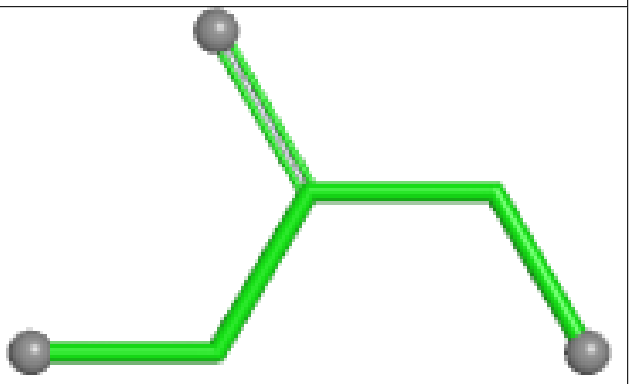


Rings

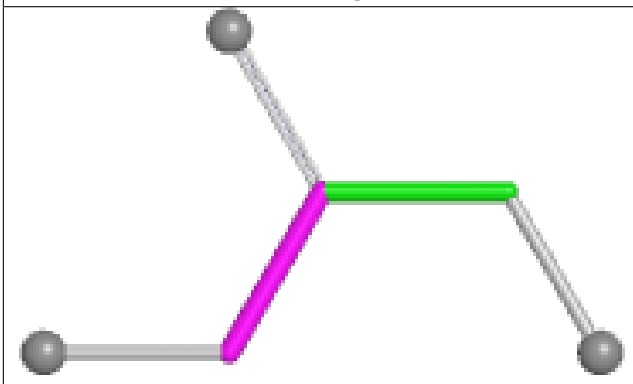
Ligand GOL A 2202



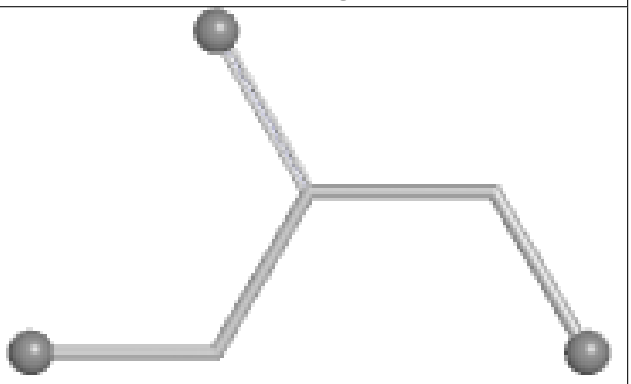
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	B	416/457 (91%)	0.48	35 (8%)	11	13	27, 42, 69, 79	0
2	C	177/188 (94%)	0.43	10 (5%)	24	29	30, 49, 67, 72	0
2	D	178/188 (94%)	0.47	13 (7%)	15	18	28, 41, 71, 83	0
3	A	417/458 (91%)	0.52	39 (9%)	8	10	24, 41, 70, 88	0
All	All	1188/1291 (92%)	0.48	97 (8%)	11	14	24, 43, 70, 88	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1696	PRO	5.7
3	A	2148	GLN	4.9
2	D	131	LYS	4.7
3	A	1944	TYR	4.6
1	B	1793	MET	4.5
3	A	1739	TYR	4.4
3	A	1740	TRP	4.3
2	D	130	ALA	4.2
2	D	127	GLU	4.0
3	A	1696	PRO	3.9
1	B	1774	SER	3.9
1	B	1914	LEU	3.9
3	A	1941	ASP	3.8
3	A	2048	THR	3.8
1	B	1921	PHE	3.7
3	A	2146	ASN	3.7
1	B	1792	ALA	3.6
2	C	51	TYR	3.6
1	B	1740	TRP	3.6
1	B	1925	ASN	3.5
3	A	1774	SER	3.4

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Mol	Chain	Res	Type	RSRZ
3	A	1698	LEU	3.4
1	B	1942	PRO	3.3
3	A	1886	GLY	3.3
3	A	1925	ASN	3.3
1	B	2048	THR	3.3
1	B	2051	GLU	3.3
1	B	1739	TYR	3.3
1	B	1701	THR	3.2
3	A	1804	TYR	3.2
2	D	125	THR	3.2
2	C	84	VAL	3.1
3	A	1887	PHE	3.0
2	D	178	GLU	3.0
3	A	2051	GLU	3.0
3	A	1869	SER	3.0
1	B	1698	LEU	3.0
1	B	1963	ASP	2.9
2	C	134	GLN	2.9
1	B	1775	MET	2.9
3	A	1773	PHE	2.9
1	B	1922	GLY	2.8
3	A	1942	PRO	2.8
1	B	1941	ASP	2.8
1	B	1985	LEU	2.8
2	D	124	SER	2.8
3	A	1921	PHE	2.8
3	A	1775	MET	2.8
1	B	1732	GLU	2.8
1	B	1738	GLY	2.8
3	A	1830	ALA	2.7
3	A	1924	ASP	2.7
1	B	1695	THR	2.7
3	A	1961	ILE	2.7
3	A	2052	VAL	2.6
3	A	1870	GLU	2.6
2	D	129	LEU	2.6
1	B	1984	THR	2.5
1	B	1962	GLU	2.5
3	A	1771	SER	2.5
3	A	1828	LEU	2.5
1	B	1887	PHE	2.5
2	C	47	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	1867	VAL	2.5
1	B	1961	ILE	2.4
3	A	1888	PHE	2.4
2	D	123	PRO	2.4
3	A	2143	THR	2.4
3	A	1962	GLU	2.4
3	A	1868	ASN	2.4
1	B	1986	SER	2.4
2	D	61	GLN	2.4
3	A	1791	GLY	2.4
1	B	1917	TYR	2.4
3	A	1940	LEU	2.4
2	C	61	GLN	2.3
2	C	7	VAL	2.3
3	A	2149	ILE	2.3
1	B	1886	GLY	2.3
2	C	132	ASN	2.3
2	D	39	ASN	2.3
2	C	12	GLY	2.2
3	A	2049	MET	2.2
3	A	1772	MET	2.2
1	B	1987	GLY	2.2
2	D	64	TYR	2.2
2	C	123	PRO	2.1
1	B	1694	SER	2.1
2	D	63	ASP	2.1
1	B	1939	ASP	2.1
1	B	1988	LYS	2.1
1	B	1804	TYR	2.1
1	B	1924	ASP	2.1
3	A	1829	ILE	2.1
3	A	1831	ASP	2.1
2	C	46	ILE	2.1
2	D	121	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

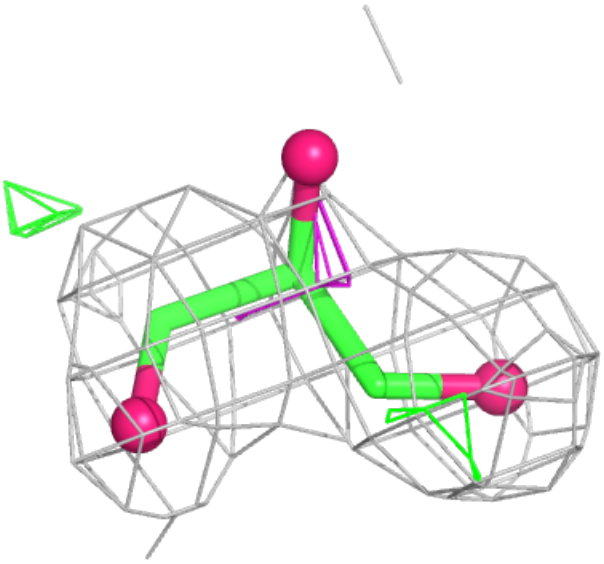
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

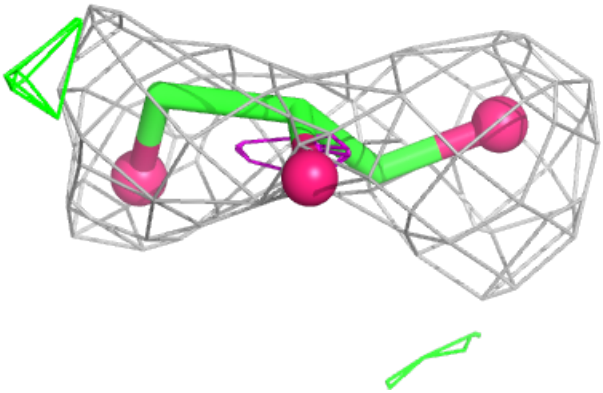
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	D	201	6/6	0.74	0.31	38,49,54,59	0
4	GOL	A	2202	6/6	0.79	0.45	68,73,74,79	0
4	GOL	A	2201	6/6	0.84	0.48	56,57,68,75	0

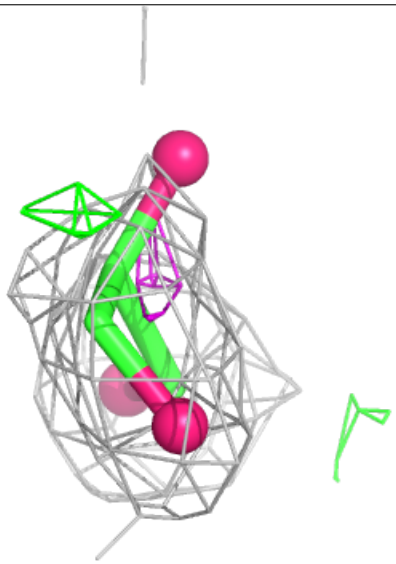
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GOL D 201:

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

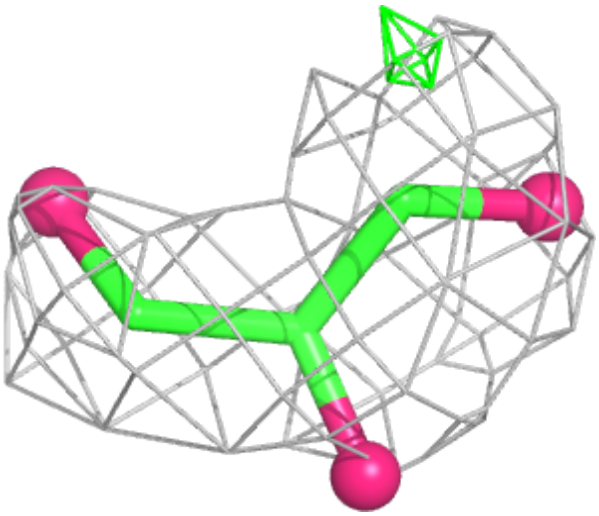


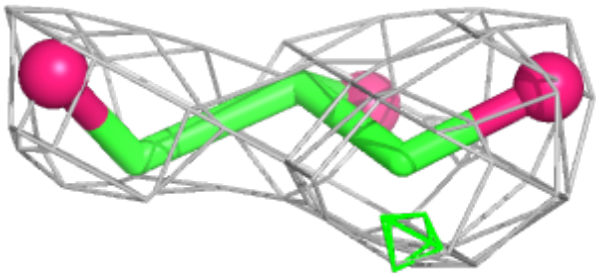


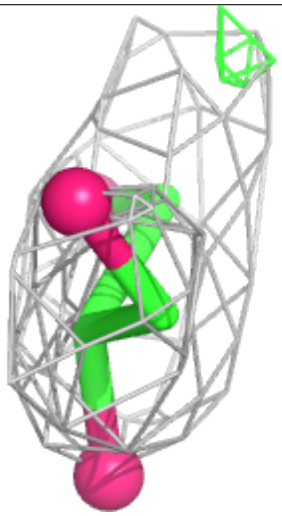


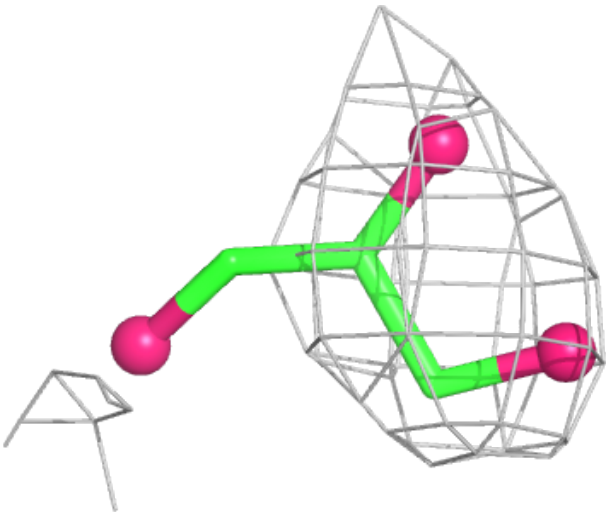
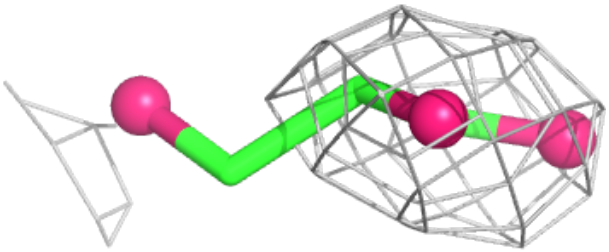
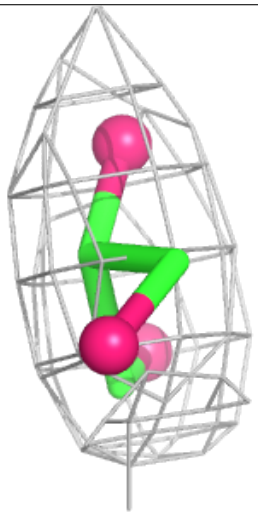
Electron density around GOL A 2202:

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







Electron density around GOL A 2201: 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.