



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:18 AM UTC

PDB ID : 6OJD / pdb_00006ojd
Title : A high-resolution crystal structure of covalent complex of NocB thioesterase domain with fluorophosphonate nocardicin G analog
Authors : Patel, K.D.; Gulick, A.M.
Deposited on : 2019-04-11
Resolution : 1.99 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

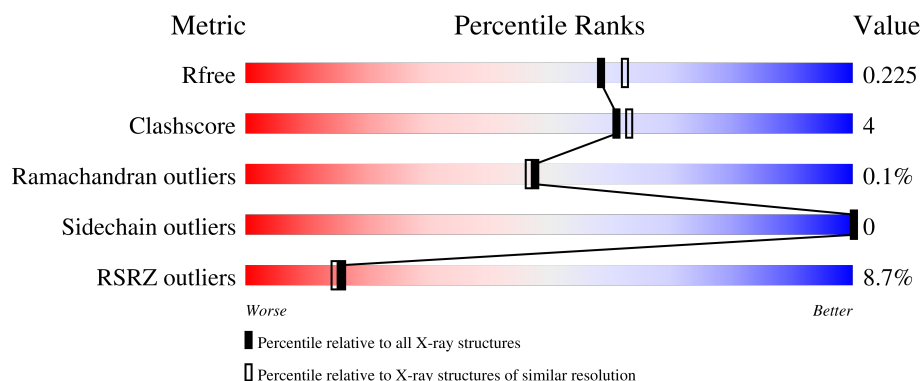
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	257	3% 80% 8% 12%
1	B	257	7% 82% 6% 12%
1	C	257	9% 78% 9% 13%
1	D	257	11% 79% 7% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13603 atoms, of which 6445 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 NocB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	H	N	O	S	0	0	0
			3303	1061	1618	307	314	3			
1	B	226	Total	C	H	N	O	S	0	0	0
			3260	1048	1595	305	309	3			
1	C	224	Total	C	H	N	O	S	0	0	0
			3182	1030	1554	297	298	3			
1	D	222	Total	C	H	N	O	S	0	0	0
			3114	1012	1512	290	297	3			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1669	MET	-	initiating methionine	UNP Q5J1Q6
A	1670	GLY	-	expression tag	UNP Q5J1Q6
A	1671	SER	-	expression tag	UNP Q5J1Q6
A	1672	SER	-	expression tag	UNP Q5J1Q6
A	1673	HIS	-	expression tag	UNP Q5J1Q6
A	1674	HIS	-	expression tag	UNP Q5J1Q6
A	1675	HIS	-	expression tag	UNP Q5J1Q6
A	1676	HIS	-	expression tag	UNP Q5J1Q6
A	1677	HIS	-	expression tag	UNP Q5J1Q6
A	1678	HIS	-	expression tag	UNP Q5J1Q6
A	1679	SER	-	expression tag	UNP Q5J1Q6
A	1680	SER	-	expression tag	UNP Q5J1Q6
A	1681	GLY	-	expression tag	UNP Q5J1Q6
A	1682	LEU	-	expression tag	UNP Q5J1Q6
A	1683	VAL	-	expression tag	UNP Q5J1Q6
A	1684	PRO	-	expression tag	UNP Q5J1Q6
A	1685	ARG	-	expression tag	UNP Q5J1Q6
A	1686	GLY	-	expression tag	UNP Q5J1Q6
A	1687	SER	-	expression tag	UNP Q5J1Q6
A	1688	HIS	-	expression tag	UNP Q5J1Q6
A	1689	MET	-	expression tag	UNP Q5J1Q6

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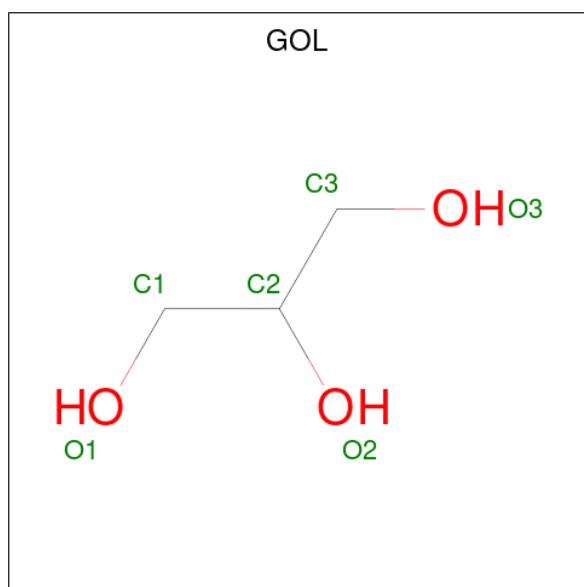
Chain	Residue	Modelled	Actual	Comment	Reference
B	1669	MET	-	initiating methionine	UNP Q5J1Q6
B	1670	GLY	-	expression tag	UNP Q5J1Q6
B	1671	SER	-	expression tag	UNP Q5J1Q6
B	1672	SER	-	expression tag	UNP Q5J1Q6
B	1673	HIS	-	expression tag	UNP Q5J1Q6
B	1674	HIS	-	expression tag	UNP Q5J1Q6
B	1675	HIS	-	expression tag	UNP Q5J1Q6
B	1676	HIS	-	expression tag	UNP Q5J1Q6
B	1677	HIS	-	expression tag	UNP Q5J1Q6
B	1678	HIS	-	expression tag	UNP Q5J1Q6
B	1679	SER	-	expression tag	UNP Q5J1Q6
B	1680	SER	-	expression tag	UNP Q5J1Q6
B	1681	GLY	-	expression tag	UNP Q5J1Q6
B	1682	LEU	-	expression tag	UNP Q5J1Q6
B	1683	VAL	-	expression tag	UNP Q5J1Q6
B	1684	PRO	-	expression tag	UNP Q5J1Q6
B	1685	ARG	-	expression tag	UNP Q5J1Q6
B	1686	GLY	-	expression tag	UNP Q5J1Q6
B	1687	SER	-	expression tag	UNP Q5J1Q6
B	1688	HIS	-	expression tag	UNP Q5J1Q6
B	1689	MET	-	expression tag	UNP Q5J1Q6
C	1669	MET	-	initiating methionine	UNP Q5J1Q6
C	1670	GLY	-	expression tag	UNP Q5J1Q6
C	1671	SER	-	expression tag	UNP Q5J1Q6
C	1672	SER	-	expression tag	UNP Q5J1Q6
C	1673	HIS	-	expression tag	UNP Q5J1Q6
C	1674	HIS	-	expression tag	UNP Q5J1Q6
C	1675	HIS	-	expression tag	UNP Q5J1Q6
C	1676	HIS	-	expression tag	UNP Q5J1Q6
C	1677	HIS	-	expression tag	UNP Q5J1Q6
C	1678	HIS	-	expression tag	UNP Q5J1Q6
C	1679	SER	-	expression tag	UNP Q5J1Q6
C	1680	SER	-	expression tag	UNP Q5J1Q6
C	1681	GLY	-	expression tag	UNP Q5J1Q6
C	1682	LEU	-	expression tag	UNP Q5J1Q6
C	1683	VAL	-	expression tag	UNP Q5J1Q6
C	1684	PRO	-	expression tag	UNP Q5J1Q6
C	1685	ARG	-	expression tag	UNP Q5J1Q6
C	1686	GLY	-	expression tag	UNP Q5J1Q6
C	1687	SER	-	expression tag	UNP Q5J1Q6
C	1688	HIS	-	expression tag	UNP Q5J1Q6
C	1689	MET	-	expression tag	UNP Q5J1Q6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1669	MET	-	initiating methionine	UNP Q5J1Q6
D	1670	GLY	-	expression tag	UNP Q5J1Q6
D	1671	SER	-	expression tag	UNP Q5J1Q6
D	1672	SER	-	expression tag	UNP Q5J1Q6
D	1673	HIS	-	expression tag	UNP Q5J1Q6
D	1674	HIS	-	expression tag	UNP Q5J1Q6
D	1675	HIS	-	expression tag	UNP Q5J1Q6
D	1676	HIS	-	expression tag	UNP Q5J1Q6
D	1677	HIS	-	expression tag	UNP Q5J1Q6
D	1678	HIS	-	expression tag	UNP Q5J1Q6
D	1679	SER	-	expression tag	UNP Q5J1Q6
D	1680	SER	-	expression tag	UNP Q5J1Q6
D	1681	GLY	-	expression tag	UNP Q5J1Q6
D	1682	LEU	-	expression tag	UNP Q5J1Q6
D	1683	VAL	-	expression tag	UNP Q5J1Q6
D	1684	PRO	-	expression tag	UNP Q5J1Q6
D	1685	ARG	-	expression tag	UNP Q5J1Q6
D	1686	GLY	-	expression tag	UNP Q5J1Q6
D	1687	SER	-	expression tag	UNP Q5J1Q6
D	1688	HIS	-	expression tag	UNP Q5J1Q6
D	1689	MET	-	expression tag	UNP Q5J1Q6

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



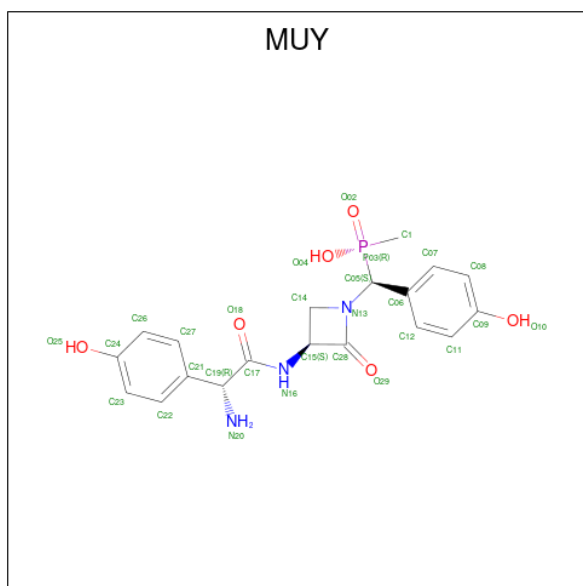
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			13	3	7	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			11	3	5	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			12	3	6	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is (R)-[(S)-[(3S)-3-{[(2R)-2-amino-2-(4-hydroxyphenyl)acetyl]amino}-2-oxazetidin-1-yl](4-hydroxyphenyl)methyl]methylphosphinic acid (CCD ID: MUY) (formula: $C_{19}H_{22}N_3O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	
			47	18	19	3	6	1	
3	B	1	Total	C	H	N	O	P	
			47	18	19	3	6	1	
3	C	1	Total	C	H	N	O	P	
			47	18	19	3	6	1	
3	D	1	Total	C	H	N	O	P	
			47	18	19	3	6	1	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca		
			2	2	0	0
4	B	1	Total	Ca		
			1	1	0	0
4	C	1	Total	Ca		
			1	1	0	0

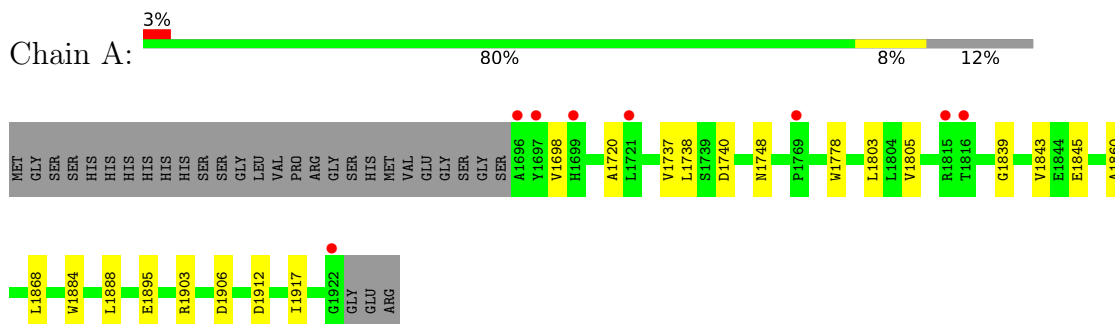
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O		
			112	112	0	0
5	B	100	Total	O		
			100	100	0	0
5	C	98	Total	O		
			98	98	0	0
5	D	80	Total	O		
			80	80	0	0

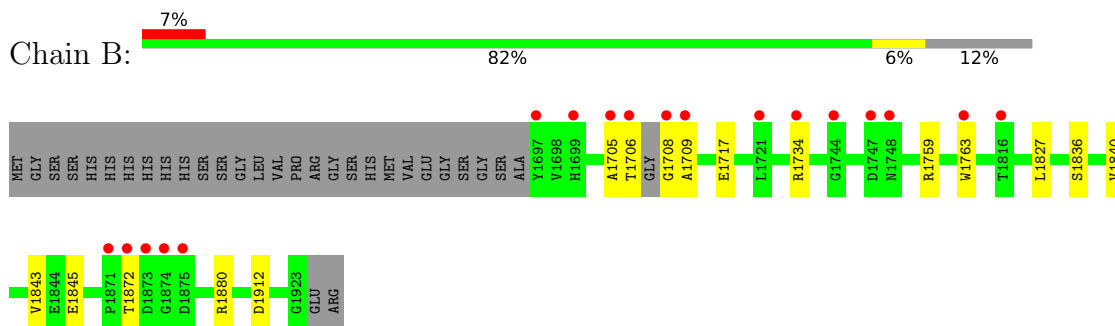
3 Residue-property plots [i](#)

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.

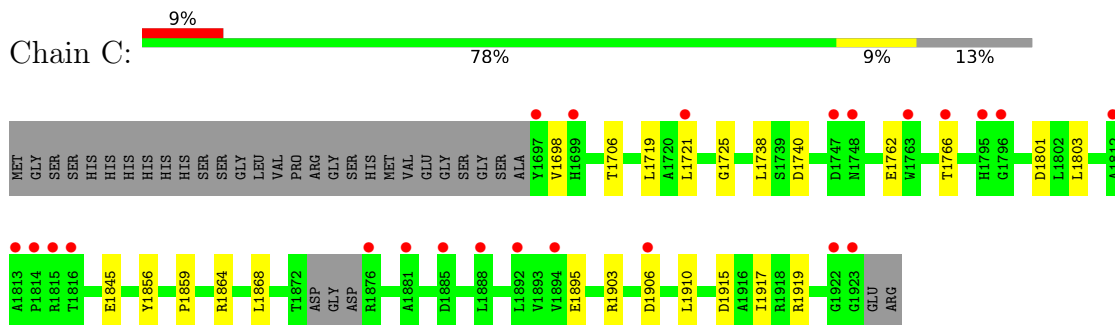
• Molecule 1: NocB



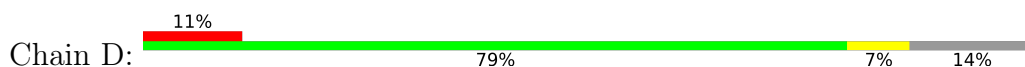
• Molecule 1: NocB

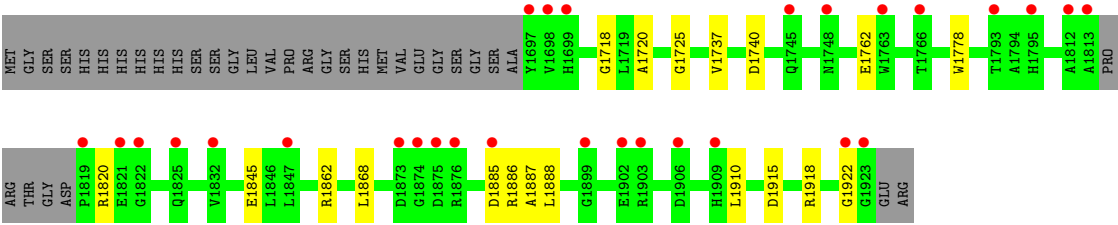


• Molecule 1: NocB



• Molecule 1: NocB





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.68Å 78.56Å 146.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.55 – 1.99 41.55 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.8 (41.55-1.99) 97.9 (41.55-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.188 , 0.225 0.191 , 0.225	Depositor DCC
R_{free} test set	2005 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.666	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13603	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0325e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/1727	0.53	0/2368
1	B	0.43	0/1705	0.51	0/2337
1	C	0.44	0/1668	0.50	0/2290
1	D	0.39	0/1641	0.52	0/2252
All	All	0.42	0/6741	0.51	0/9247

There are no bond length outliers.

There are no bond angle outliers.

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	A	1685	1618	1617	15	0
1	B	1665	1595	1594	13	1
1	C	1628	1554	1553	17	0
1	D	1602	1512	1511	13	0
2	A	24	31	32	2	0
2	B	24	29	29	4	0
2	C	18	22	21	0	0
2	D	6	8	8	1	0
3	A	28	19	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	19	0	0	0
3	C	28	19	0	0	0
3	D	28	19	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	112	0	0	2	1
5	B	100	0	0	2	0
5	C	98	0	0	2	1
5	D	80	0	0	2	1
All	All	7158	6445	6365	55	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (55) 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:1748:ASN:ND2	5:A:2201:HOH:O	1.91	1.00
1:D:1915:ASP:OD1	1:D:1918:ARG:NH2	1.95	0.99
1:A:1860:ALA:HB3	1:D:1888:LEU:HD23	1.65	0.79
1:C:1864:ARG:NH1	5:C:2201:HOH:O	2.14	0.79
1:D:1820:ARG:NH1	5:D:2101:HOH:O	2.17	0.75
1:C:1903:ARG:HD2	1:C:1906:ASP:OD2	1.89	0.72
1:B:1709:ALA:HB2	1:B:1734:ARG:NH2	2.04	0.72
1:D:1725:GLY:HA3	1:D:1910:LEU:HD21	1.82	0.62
1:C:1762:GLU:O	1:C:1766:THR:HG23	1.99	0.61
1:C:1868:LEU:HD22	1:C:1895:GLU:HB2	1.84	0.60
5:B:2201:HOH:O	1:C:1919:ARG:NH2	2.36	0.59
1:C:1725:GLY:HA3	1:C:1910:LEU:HD21	1.86	0.58
1:B:1708:GLY:HA2	2:B:2106:GOL:C3	2.34	0.58
1:C:1719:LEU:HB3	1:C:1721:LEU:HD13	1.85	0.57
1:C:1801:ASP:CG	1:C:1864:ARG:HH12	2.16	0.54
1:B:1872:THR:HG21	5:B:2209:HOH:O	2.09	0.52
1:A:1912:ASP:CB	5:A:2295:HOH:O	2.58	0.52
1:C:1915:ASP:HB3	1:C:1919:ARG:HH12	1.75	0.52
1:B:1708:GLY:N	1:B:1734:ARG:H	2.09	0.50
1:C:1698:VAL:HG22	1:C:1738:LEU:HD22	1.92	0.50
1:C:1803:LEU:HD21	1:C:1917:ILE:HG12	1.93	0.50
1:A:1720:ALA:HB1	1:A:1737:VAL:HB	1.94	0.49
1:A:1803:LEU:HD21	1:A:1917:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1860:ALA:HB2	1:D:1887:ALA:HB1	1.94	0.48
1:A:1903:ARG:HD3	1:A:1906:ASP:OD2	2.13	0.48
1:B:1836:SER:O	1:B:1840:VAL:HG23	2.13	0.48
1:D:1740:ASP:OD2	1:D:1845:GLU:OE2	2.33	0.47
1:D:1868:LEU:HD12	1:D:1868:LEU:N	2.29	0.47
1:A:1740:ASP:OD2	1:A:1845:GLU:OE2	2.34	0.46
1:A:1698:VAL:HG22	1:A:1738:LEU:HD22	1.98	0.46
1:B:1708:GLY:CA	2:B:2106:GOL:H2	2.46	0.46
1:D:1885:ASP:OD1	1:D:1886:ARG:N	2.49	0.45
1:C:1721:LEU:HD12	5:C:2244:HOH:O	2.17	0.45
1:D:1718:GLY:HA3	1:D:1845:GLU:HG2	1.99	0.45
1:B:1705:ALA:O	1:B:1706:THR:C	2.59	0.44
1:B:1708:GLY:HA2	2:B:2106:GOL:H32	1.99	0.44
1:D:1778:TRP:CH2	2:D:2002:GOL:H2	2.52	0.44
1:A:1778:TRP:HA	1:A:1805:VAL:HB	2.00	0.43
1:A:1839:GLY:O	1:A:1843:VAL:HG23	2.18	0.43
1:D:1762:GLU:OE1	5:D:2102:HOH:O	2.20	0.43
1:C:1801:ASP:CG	1:C:1864:ARG:NH1	2.77	0.43
1:D:1720:ALA:HB1	1:D:1737:VAL:HB	2.00	0.42
2:B:2105:GOL:O3	1:C:1706:THR:OG1	2.36	0.42
1:B:1709:ALA:HB2	1:B:1734:ARG:HH21	1.81	0.42
1:B:1827:LEU:HD12	1:B:1843:VAL:HG22	2.02	0.42
1:C:1740:ASP:OD2	1:C:1845:GLU:OE2	2.38	0.42
2:A:2105:GOL:H31	1:D:1862:ARG:HE	1.85	0.41
1:C:1856:TYR:OH	1:C:1859:PRO:HD3	2.20	0.41
1:A:1868:LEU:HA	1:A:1895:GLU:O	2.21	0.41
1:A:1868:LEU:HD12	1:A:1868:LEU:N	2.35	0.41
1:A:1884:TRP:O	2:A:2107:GOL:H32	2.21	0.41
1:C:1803:LEU:CD2	1:C:1917:ILE:HG23	2.50	0.41
1:B:1717:GLU:O	1:B:1845:GLU:HG2	2.22	0.40
1:B:1759:ARG:HE	1:B:1763:TRP:NE1	2.19	0.40
1:A:1888:LEU:HD21	1:B:1880:ARG:HH12	1.86	0.40

All (2) 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)
1:B:1912:ASP:OD1	5:A:2201:HOH:O[4_555]	1.84	0.36
5:C:2252:HOH:O	5:D:2128:HOH:O[2_565]	2.14	0.06

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	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
1	B	222/257 (86%)	214 (96%)	8 (4%)	0	100	100
1	C	220/257 (86%)	215 (98%)	5 (2%)	0	100	100
1	D	218/257 (85%)	211 (97%)	6 (3%)	1 (0%)	24	21
All	All	885/1028 (86%)	860 (97%)	24 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1922	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	168/204 (82%)	168 (100%)	0	100	100
1	B	165/204 (81%)	165 (100%)	0	100	100
1	C	158/204 (78%)	158 (100%)	0	100	100
1	D	154/204 (76%)	154 (100%)	0	100	100
All	All	645/816 (79%)	645 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1811	ASN
1	A	1855	GLN
1	B	1855	GLN
1	C	1909	HIS
1	D	1909	HIS

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](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

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	GOL	A	2101	-	5,5,5	1.13	0	5,5,5	1.30	1 (20%)
2	GOL	C	2101	-	5,5,5	0.87	0	5,5,5	1.23	1 (20%)
2	GOL	B	2104	-	5,5,5	0.82	0	5,5,5	1.12	1 (20%)
3	MUY	B	2102	1	24,30,31	3.10	5 (20%)	29,43,46	1.53	5 (17%)
2	GOL	C	2105	-	5,5,5	0.77	0	5,5,5	0.91	0
2	GOL	A	2106	-	5,5,5	0.59	0	5,5,5	0.80	0
2	GOL	A	2107	-	5,5,5	0.70	0	5,5,5	0.94	0
3	MUY	A	2102	1	24,30,31	3.02	6 (25%)	29,43,46	1.37	6 (20%)
2	GOL	B	2101	-	5,5,5	0.64	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MUY	D	2001	1	24,30,31	2.98	7 (29%)	29,43,46	1.12	3 (10%)
2	GOL	A	2105	-	5,5,5	0.60	0	5,5,5	0.91	0
2	GOL	D	2002	-	5,5,5	0.79	0	5,5,5	1.04	0
2	GOL	C	2104	4	5,5,5	0.75	0	5,5,5	0.88	0
3	MUY	C	2102	1	24,30,31	3.15	6 (25%)	29,43,46	1.33	6 (20%)
2	GOL	B	2105	4	5,5,5	0.64	0	5,5,5	0.97	0
2	GOL	B	2106	-	5,5,5	0.60	0	5,5,5	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	2101	-	-	4/4/4/4	-
2	GOL	C	2101	-	-	2/4/4/4	-
2	GOL	B	2104	-	-	2/4/4/4	-
3	MUY	B	2102	1	-	2/18/36/38	0/3/3/3
2	GOL	C	2105	-	-	4/4/4/4	-
2	GOL	A	2106	-	-	2/4/4/4	-
2	GOL	A	2107	-	-	4/4/4/4	-
3	MUY	A	2102	1	-	2/18/36/38	0/3/3/3
2	GOL	B	2101	-	-	3/4/4/4	-
3	MUY	D	2001	1	-	2/18/36/38	0/3/3/3
2	GOL	A	2105	-	-	3/4/4/4	-
2	GOL	D	2002	-	-	2/4/4/4	-
2	GOL	C	2104	4	-	2/4/4/4	-
3	MUY	C	2102	1	-	3/18/36/38	0/3/3/3
2	GOL	B	2105	4	-	2/4/4/4	-
2	GOL	B	2106	-	-	3/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2102	MUY	C21-C19	-9.94	1.41	1.52
3	C	2102	MUY	C21-C19	-9.12	1.42	1.52
3	C	2102	MUY	C06-C05	-9.00	1.43	1.52
3	A	2102	MUY	C21-C19	-8.75	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2001	MUY	C06-C05	-8.55	1.44	1.52
3	D	2001	MUY	C21-C19	-8.55	1.43	1.52
3	A	2102	MUY	C06-C05	-8.11	1.44	1.52
3	B	2102	MUY	C06-C05	-7.89	1.44	1.52
3	C	2102	MUY	C14-N13	5.35	1.54	1.47
3	B	2102	MUY	C15-C28	-5.11	1.43	1.54
3	A	2102	MUY	C15-C28	-4.69	1.43	1.54
3	D	2001	MUY	C15-C28	-4.54	1.44	1.54
3	A	2102	MUY	C14-N13	4.22	1.52	1.47
3	B	2102	MUY	C14-N13	4.07	1.52	1.47
3	C	2102	MUY	C15-C28	-3.64	1.46	1.54
3	D	2001	MUY	O29-C28	3.62	1.28	1.22
3	A	2102	MUY	O29-C28	3.53	1.28	1.22
3	D	2001	MUY	C14-N13	3.46	1.51	1.47
3	C	2102	MUY	C28-N13	-3.36	1.31	1.35
3	A	2102	MUY	C26-C27	3.22	1.44	1.38
3	D	2001	MUY	C28-N13	-2.80	1.32	1.35
3	C	2102	MUY	C26-C27	2.49	1.42	1.38
3	B	2102	MUY	O29-C28	2.41	1.26	1.22
3	D	2001	MUY	C26-C27	2.16	1.42	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2102	MUY	C14-N13-C28	-4.21	92.85	95.78
3	A	2102	MUY	C14-N13-C28	-3.76	93.16	95.78
3	C	2102	MUY	C14-N13-C28	-3.36	93.44	95.78
3	B	2102	MUY	C21-C19-C17	3.31	118.76	111.76
3	C	2102	MUY	C07-C06-C05	3.09	126.24	120.38
3	B	2102	MUY	C15-C28-N13	3.02	95.74	91.94
3	C	2102	MUY	C15-C28-N13	2.81	95.48	91.94
3	D	2001	MUY	C14-N13-C28	-2.76	93.86	95.78
3	A	2102	MUY	C07-C06-C05	2.63	125.37	120.38
3	D	2001	MUY	C07-C06-C05	2.46	125.04	120.38
3	B	2102	MUY	C07-C06-C05	2.42	124.96	120.38
3	A	2102	MUY	O29-C28-N13	-2.35	129.86	131.82
3	A	2102	MUY	C15-C28-N13	2.34	94.89	91.94
3	D	2001	MUY	C15-C28-N13	2.26	94.80	91.94
3	B	2102	MUY	C11-C12-C06	2.26	123.44	121.18
2	A	2101	GOL	C3-C2-C1	-2.25	103.54	111.80
2	C	2101	GOL	C3-C2-C1	-2.21	103.67	111.80
3	C	2102	MUY	O29-C28-N13	-2.18	130.00	131.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2102	MUY	C28-C15-N16	2.08	121.23	115.32
3	A	2102	MUY	C21-C19-C17	2.08	116.16	111.76
3	C	2102	MUY	C21-C19-C17	2.05	116.10	111.76
2	B	2104	GOL	C3-C2-C1	-2.01	104.44	111.80
3	C	2102	MUY	C12-C06-C05	-2.00	116.58	120.38

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2101	GOL	O1-C1-C2-C3
2	A	2106	GOL	C1-C2-C3-O3
2	A	2107	GOL	C1-C2-C3-O3
2	B	2104	GOL	O1-C1-C2-C3
2	C	2101	GOL	O1-C1-C2-C3
2	D	2002	GOL	O1-C1-C2-C3
3	A	2102	MUY	C06-C05-N13-C14
3	C	2102	MUY	C06-C05-N13-C14
2	A	2101	GOL	C1-C2-C3-O3
2	A	2105	GOL	O1-C1-C2-C3
2	A	2107	GOL	O1-C1-C2-C3
2	B	2101	GOL	O1-C1-C2-C3
2	B	2105	GOL	O1-C1-C2-C3
2	B	2106	GOL	O1-C1-C2-C3
2	B	2106	GOL	C1-C2-C3-O3
2	C	2104	GOL	O1-C1-C2-C3
2	C	2105	GOL	O1-C1-C2-C3
2	C	2105	GOL	C1-C2-C3-O3
2	A	2101	GOL	O1-C1-C2-O2
2	A	2101	GOL	O2-C2-C3-O3
2	A	2105	GOL	O1-C1-C2-O2
2	B	2104	GOL	O1-C1-C2-O2
2	D	2002	GOL	O1-C1-C2-O2
2	A	2106	GOL	O2-C2-C3-O3
2	A	2107	GOL	O1-C1-C2-O2
2	A	2107	GOL	O2-C2-C3-O3
2	B	2105	GOL	O1-C1-C2-O2
2	C	2101	GOL	O1-C1-C2-O2
2	C	2105	GOL	O2-C2-C3-O3
2	C	2104	GOL	O1-C1-C2-O2
3	C	2102	MUY	C28-C15-N16-C17
3	D	2001	MUY	C28-C15-N16-C17

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Mol	Chain	Res	Type	Atoms
2	B	2106	GOL	O1-C1-C2-O2
2	C	2105	GOL	O1-C1-C2-O2
2	B	2101	GOL	O1-C1-C2-O2
3	A	2102	MUY	C28-C15-N16-C17
3	B	2102	MUY	C28-C15-N16-C17
3	B	2102	MUY	C06-C05-N13-C28
3	C	2102	MUY	C06-C05-N13-C28
3	D	2001	MUY	C06-C05-N13-C28
2	A	2105	GOL	C1-C2-C3-O3
2	B	2101	GOL	O2-C2-C3-O3

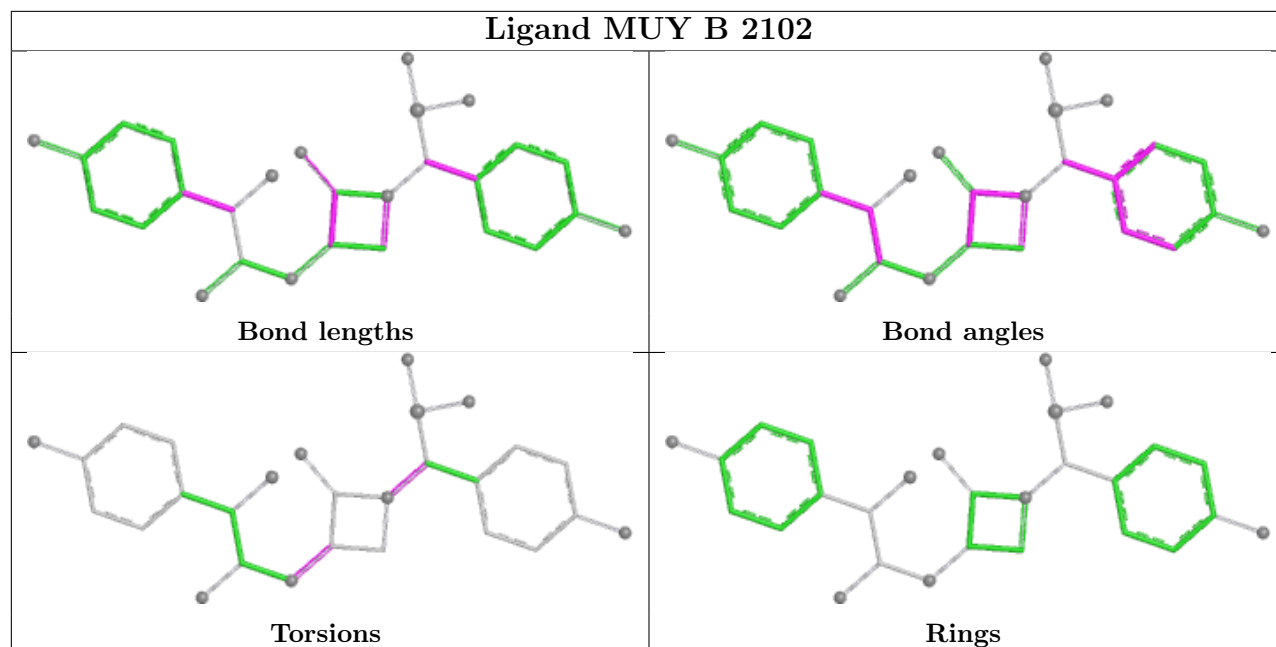
There are no ring outliers.

5 monomers are involved in 7 short contacts:

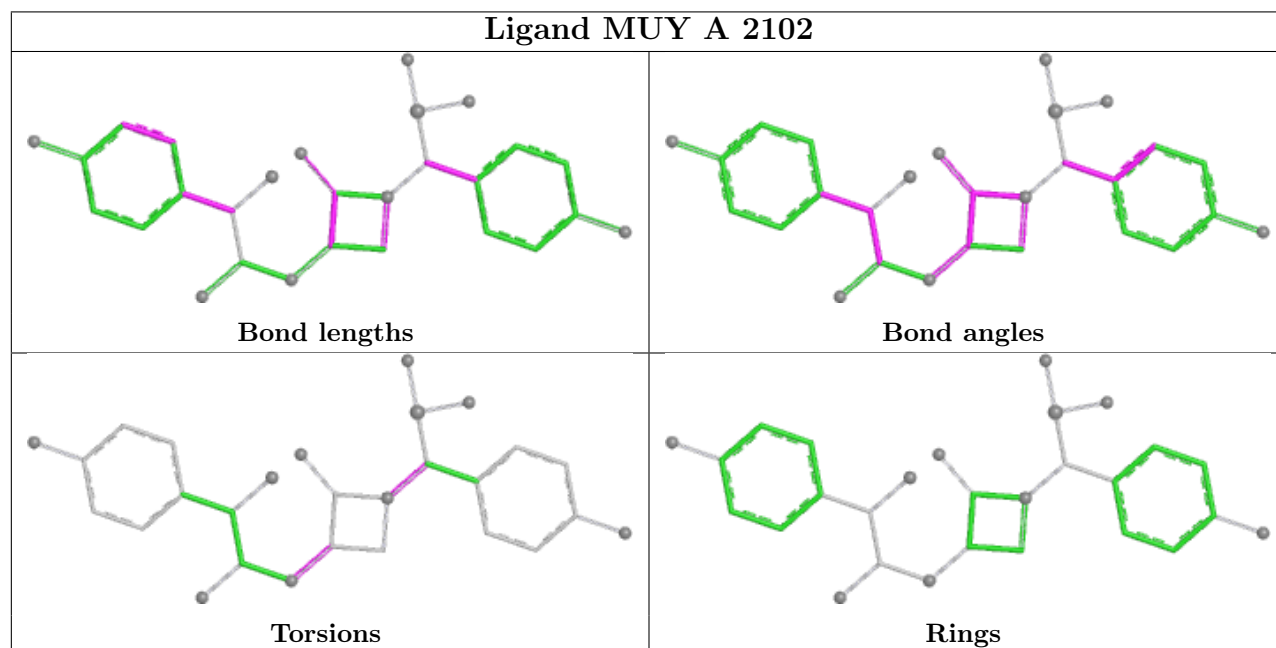
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2107	GOL	1	0
2	A	2105	GOL	1	0
2	D	2002	GOL	1	0
2	B	2105	GOL	1	0
2	B	2106	GOL	3	0

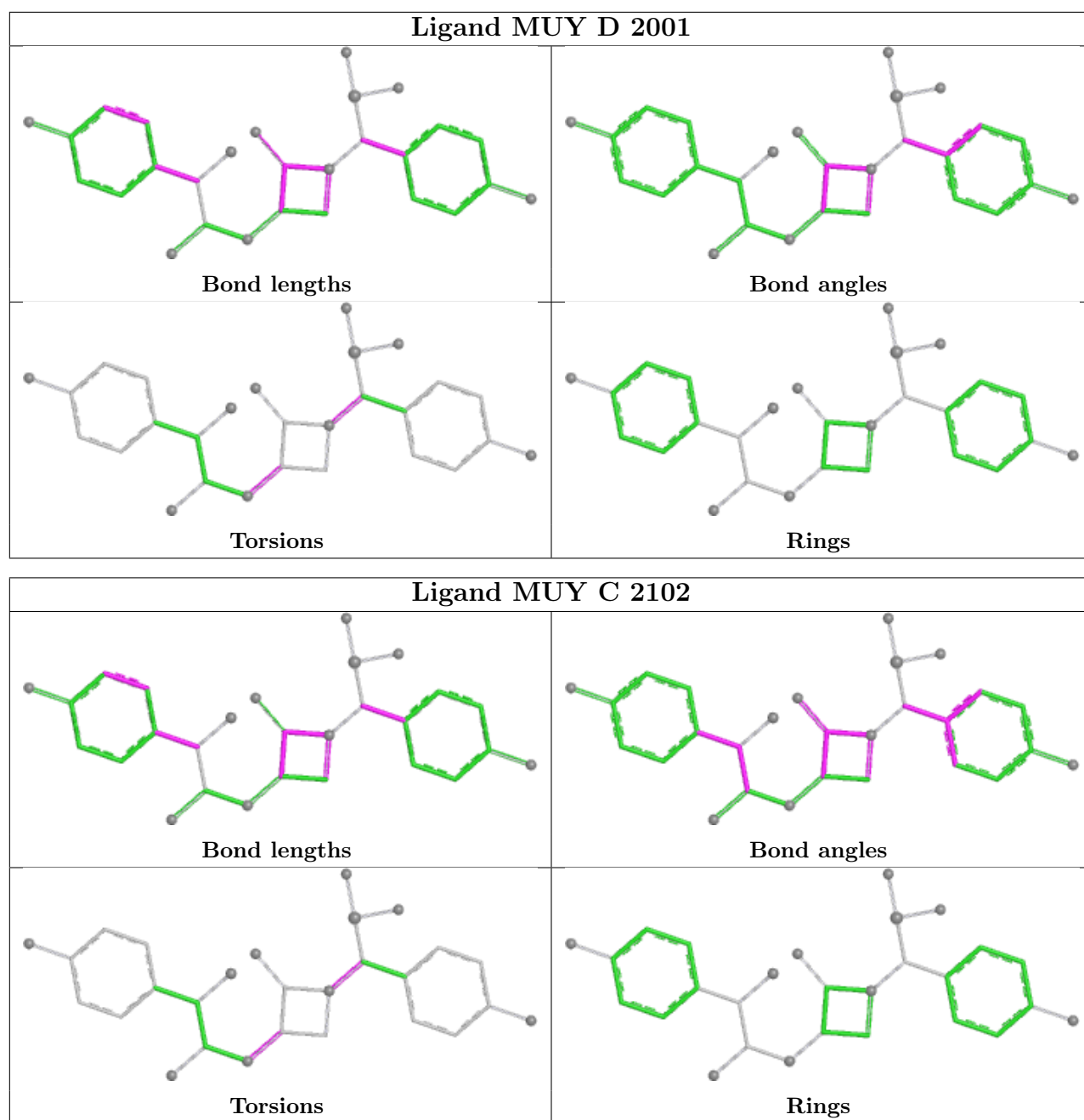
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand MUY B 2102



Ligand MUY A 2102





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	227/257 (88%)	0.42	8 (3%) 47 46	18, 33, 65, 85	0
1	B	226/257 (87%)	0.59	18 (7%) 18 17	20, 33, 64, 140	0
1	C	224/257 (87%)	0.62	23 (10%) 12 11	20, 35, 70, 100	0
1	D	222/257 (86%)	0.92	29 (13%) 7 6	22, 39, 74, 117	0
All	All	899/1028 (87%)	0.63	78 (8%) 16 15	18, 35, 72, 140	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1813	ALA	7.9
1	D	1875	ASP	6.0
1	D	1874	GLY	5.8
1	B	1873	ASP	5.7
1	D	1698	VAL	4.3
1	D	1822	GLY	4.3
1	C	1816	THR	4.3
1	B	1697	TYR	4.2
1	A	1816	THR	4.0
1	C	1697	TYR	4.0
1	D	1876	ARG	3.9
1	C	1876	ARG	3.7
1	D	1825	GLN	3.7
1	A	1696	ALA	3.7
1	B	1816	THR	3.6
1	D	1763	TRP	3.6
1	C	1795	HIS	3.6
1	D	1821	GLU	3.4
1	B	1709	ALA	3.4
1	C	1748	ASN	3.4
1	A	1697	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	1873	ASP	3.3
1	C	1763	TRP	3.3
1	B	1872	THR	3.2
1	D	1923	GLY	3.2
1	C	1888	LEU	3.1
1	C	1796	GLY	3.1
1	C	1721	LEU	3.0
1	D	1819	PRO	3.0
1	B	1875	ASP	3.0
1	C	1812	ALA	3.0
1	B	1763	TRP	2.9
1	C	1906	ASP	2.9
1	C	1923	GLY	2.9
1	D	1903	ARG	2.8
1	D	1899	GLY	2.8
1	A	1815	ARG	2.8
1	D	1766	THR	2.8
1	B	1748	ASN	2.7
1	B	1699	HIS	2.7
1	D	1909	HIS	2.7
1	C	1766	THR	2.7
1	C	1922	GLY	2.6
1	B	1871	PRO	2.6
1	B	1708	GLY	2.6
1	D	1922	GLY	2.6
1	A	1721	LEU	2.5
1	C	1885	ASP	2.5
1	B	1744	GLY	2.5
1	B	1874	GLY	2.5
1	A	1699	HIS	2.5
1	C	1747	ASP	2.5
1	C	1813	ALA	2.5
1	D	1812	ALA	2.4
1	D	1748	ASN	2.4
1	D	1699	HIS	2.4
1	D	1745	GLN	2.4
1	A	1922	GLY	2.4
1	D	1847	LEU	2.3
1	D	1832	VAL	2.3
1	D	1885	ASP	2.3
1	D	1906	ASP	2.3
1	C	1881	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1706	THR	2.3
1	D	1697	TYR	2.3
1	C	1892	LEU	2.2
1	C	1814	PRO	2.2
1	B	1705	ALA	2.2
1	C	1699	HIS	2.2
1	B	1721	LEU	2.2
1	B	1747	ASP	2.1
1	A	1769	PRO	2.1
1	B	1734	ARG	2.1
1	D	1795	HIS	2.1
1	D	1902	GLU	2.1
1	C	1894	VAL	2.1
1	C	1815	ARG	2.0
1	D	1793	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	GOL	B	2106	6/6	0.77	0.13	59,71,82,84	0
2	GOL	B	2104	6/6	0.79	0.18	50,67,80,80	14
2	GOL	A	2107	6/6	0.83	0.17	32,58,83,89	0
2	GOL	C	2105	6/6	0.83	0.15	67,84,101,101	0
2	GOL	A	2106	6/6	0.84	0.16	39,68,88,95	0
2	GOL	D	2002	6/6	0.86	0.09	51,62,66,66	0
2	GOL	C	2101	6/6	0.87	0.13	50,63,76,76	0
2	GOL	A	2105	6/6	0.87	0.13	62,75,87,87	0

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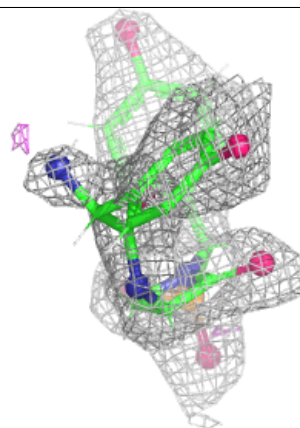
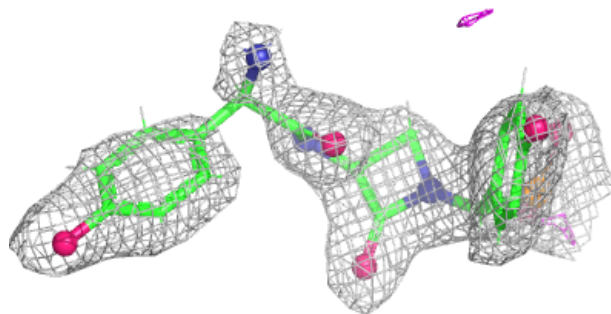
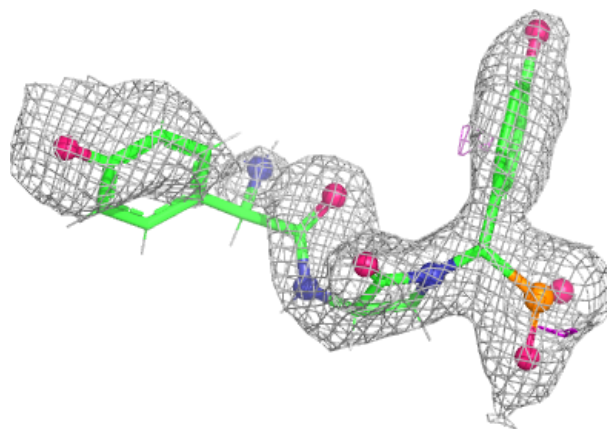
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	2101	6/6	0.87	0.17	46,75,97,97	0
2	GOL	A	2101	6/6	0.90	0.13	34,44,52,52	0
2	GOL	C	2104	6/6	0.90	0.13	26,34,42,42	0
4	CA	A	2103	1/1	0.91	0.09	66,66,66,66	0
2	GOL	B	2105	6/6	0.92	0.10	26,32,39,39	0
3	MUY	D	2001	28/29	0.93	0.13	25,72,98,103	0
3	MUY	B	2102	28/29	0.94	0.09	19,34,46,52	0
3	MUY	C	2102	28/29	0.94	0.09	21,38,71,89	0
3	MUY	A	2102	28/29	0.95	0.09	16,36,58,84	0
4	CA	B	2103	1/1	0.95	0.05	25,25,25,25	0
4	CA	C	2103	1/1	0.96	0.07	27,27,27,27	0
4	CA	A	2104	1/1	0.97	0.06	49,49,49,49	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.

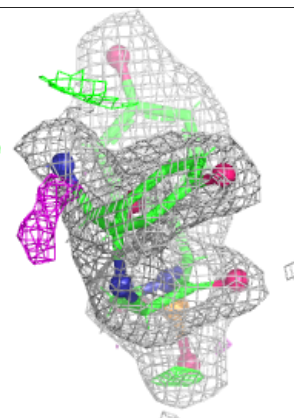
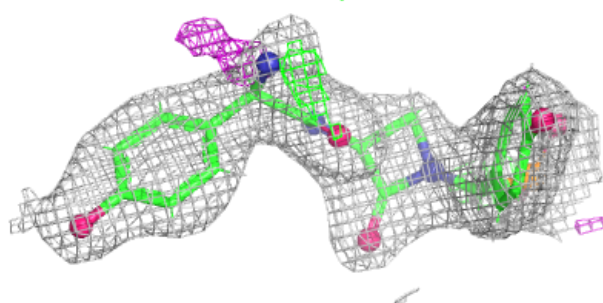
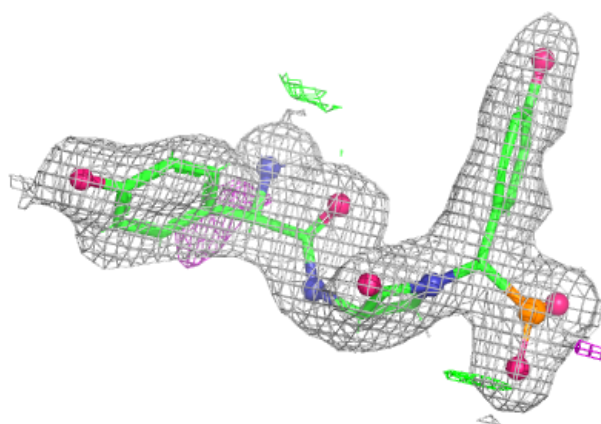
Electron density around MUY D 2001:

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

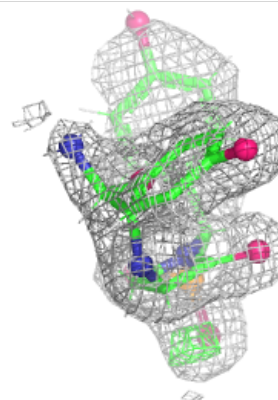
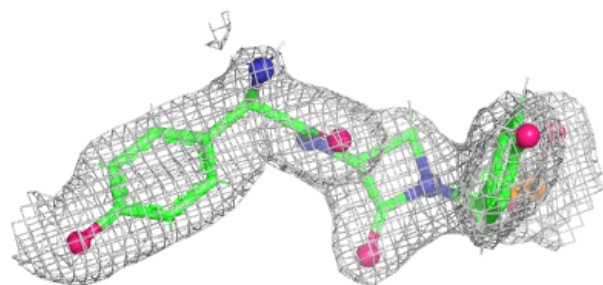
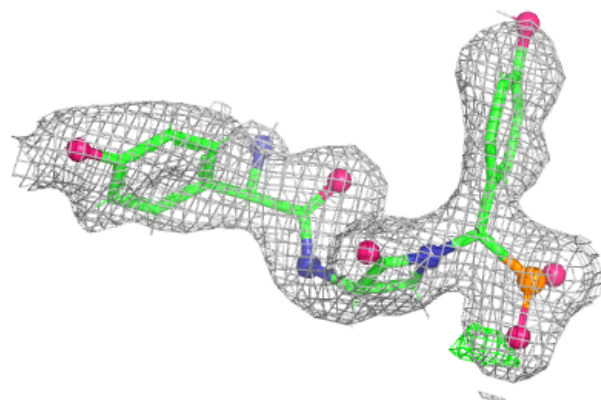


Electron density around MUY B 2102:

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

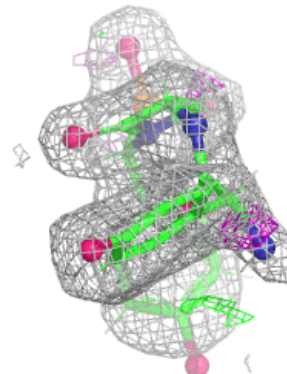
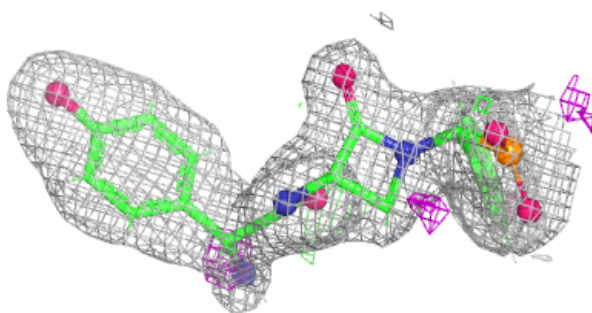
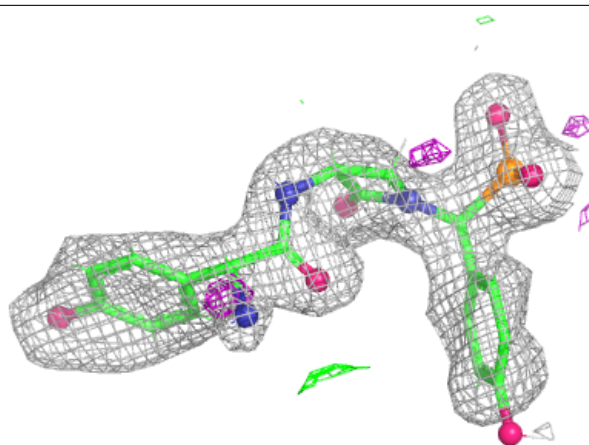
**Electron density around MUY C 2102:**

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



Electron density around MUY A 2102:

$2mF_o - DF_c$ (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.