



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:18 am BST

PDB ID : 5O6Y
Title : Crystal structure of the Bc1960 peptidoglycan N-acetylglucosamine deacetylase in complex with 4-naphthalen-1-yl- {N}-oxidanyl-benzamide
Authors : Fadoulglou, V.E.; Kotsifaki, D.; Kokkinidis, M.
Deposited on : 2017-06-07
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

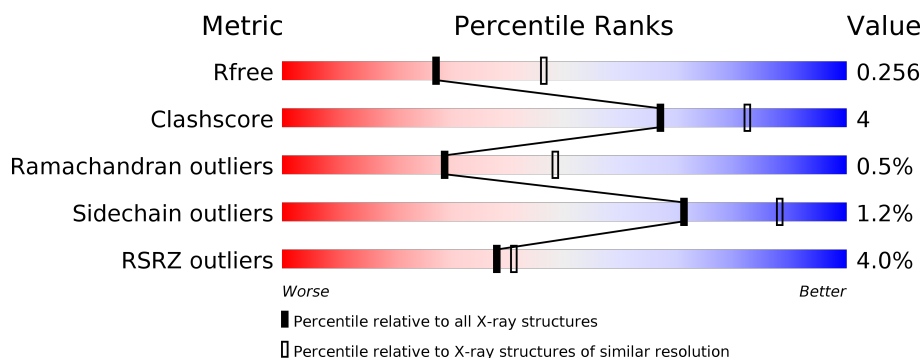
1 Overall quality at a glance ⓘ

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	214	<div> <div>3%</div> <div>92%</div> <div>8%</div> </div>
2	B	214	<div> <div>3%</div> <div>86%</div> <div>13%</div> </div>
2	C	214	<div> <div>5%</div> <div>89%</div> <div>11%</div> </div>
2	D	214	<div> <div>5%</div> <div>90%</div> <div>9%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	5YA	A	304[B]	-	-	-	X
4	5YA	D	302[B]	-	-	-	X
6	PEG	A	308	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 7815 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 Peptidoglycan N-acetylglucosamine deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1710	1105	288	315	2			

- Molecule 2 is a protein called Peptidoglycan N-acetylglucosamine deacetylase.

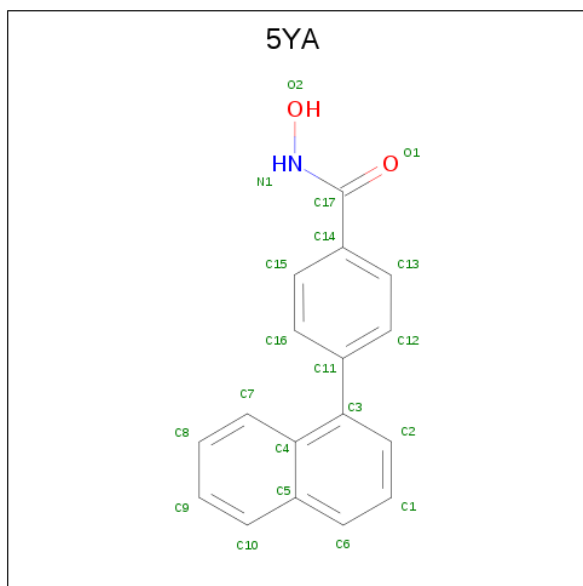
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	1	0
			1715	1107	288	318	2			
2	C	214	Total	C	N	O	S	0	0	0
			1700	1099	282	317	2			
2	D	214	Total	C	N	O	S	0	1	0
			1693	1092	282	317	2			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 4-naphthalen-1-yl- {N}-oxidanyl-benzamide (three-letter code: 5YA) (formula: C₁₇H₁₃NO₂).



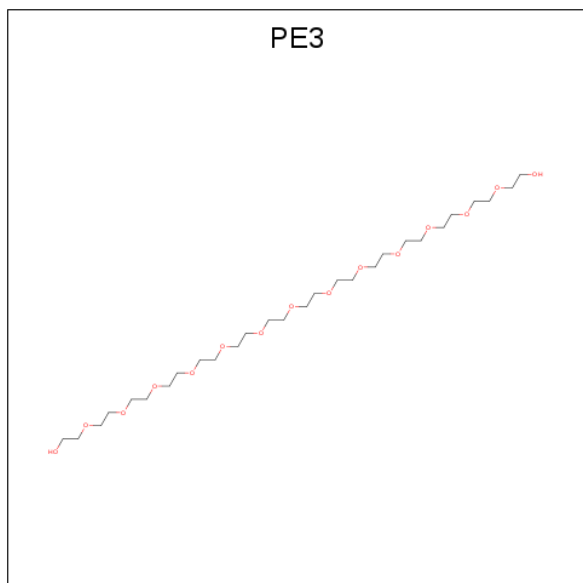
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 20 17 1 2	0	1
4	B	1	Total C N O 20 17 1 2	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	1
			20	17	1	2		
4	D	1	Total	C	N	O	0	1
			20	17	1	2		

- Molecule 5 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1,41-DIOL (three-letter code: PE3) (formula: C₂₈H₅₈O₁₅).



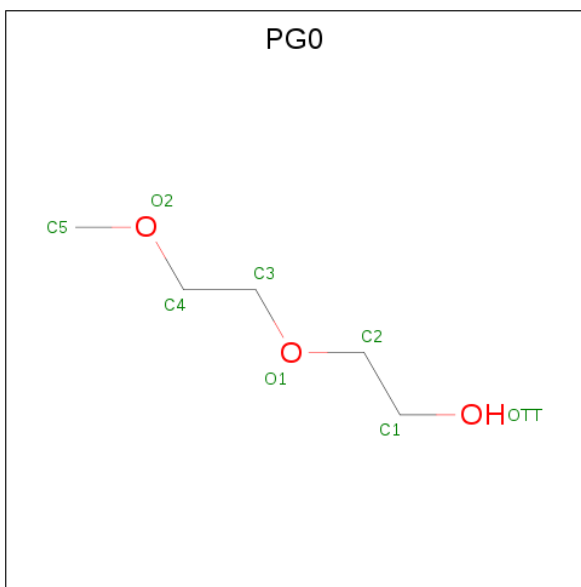
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			5	3	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			5	4	1		
6	D	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 7 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: C₅H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	5	3		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	9	Total	Na	0	0
			9	9		
8	A	7	Total	Na	0	0
			7	7		
8	D	1	Total	Na	0	0
			1	1		
8	C	4	Total	Na	0	0
			4	4		

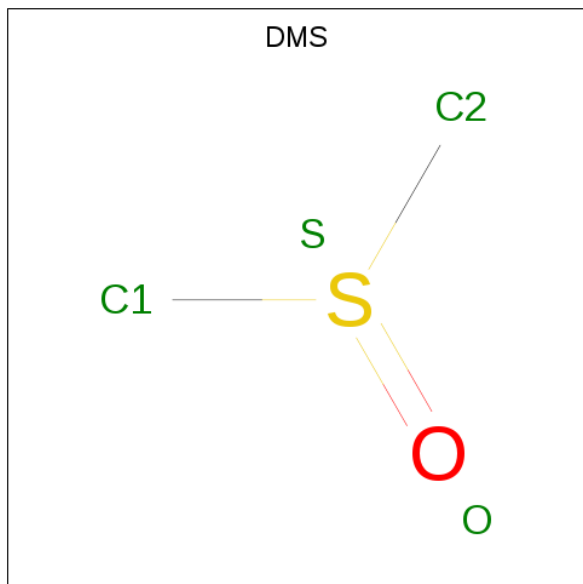
- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	Cl	0	0
			2	2		
9	A	1	Total	Cl	0	0
			1	1		
9	D	1	Total	Cl	0	0
			1	1		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Zn	0	1
			1	1		
10	D	2	Total	Zn	0	1
			2	2		
10	C	1	Total	Zn	0	1
			1	1		

- Molecule 11 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	O	S	0	0
			4	2	1	1		
11	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	196	Total	O	0	0
			196	196		
12	B	190	Total	O	0	0
			190	190		
12	C	191	Total	O	0	0
			191	191		
12	D	171	Total	O	0	0
			171	171		

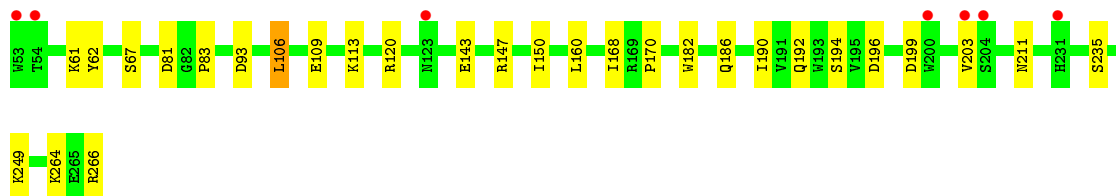
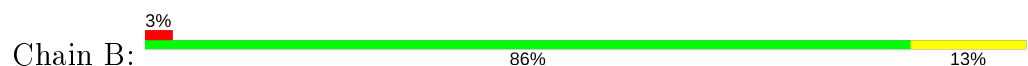
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

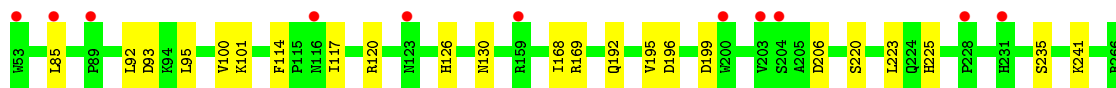
- Molecule 1: Peptidoglycan N-acetylglucosamine deacetylase



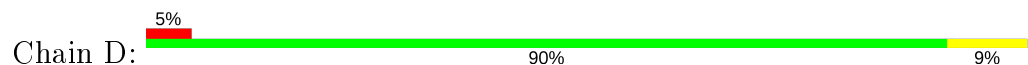
- Molecule 2: Peptidoglycan N-acetylglucosamine deacetylase



- Molecule 2: Peptidoglycan N-acetylglucosamine deacetylase



- Molecule 2: Peptidoglycan N-acetylglucosamine deacetylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.04Å 93.04Å 243.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.52 – 2.50 46.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.52-2.50) 99.3 (46.52-2.50)	Depositor EDS
R_{merge}	0.56	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.196 , 0.254 0.196 , 0.256	Depositor DCC
R_{free} test set	1888 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	-4.8	Xtriage
Anisotropy	-9.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7815	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.07 % 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 9.9718e-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: ZN, CL, NA, PXU, PE3, 5YA, DMS, SO4, PG0, PEG

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	0.24	0/1757	0.41	0/2387
2	B	0.24	0/1755	0.42	0/2382
2	C	0.25	0/1736	0.41	0/2356
2	D	0.25	0/1728	0.42	0/2344
All	All	0.24	0/6976	0.41	0/9469

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	1710	0	1681	13	0
2	B	1715	0	1683	16	0
2	C	1700	0	1664	14	0
2	D	1693	0	1647	10	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
3	C	20	0	0	0	0
3	D	5	0	0	0	0
4	A	20	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	0	1	0
4	C	20	0	0	1	0
4	D	20	0	0	2	0
5	A	4	0	4	1	0
5	C	5	0	4	2	0
6	A	20	0	27	1	0
6	B	18	0	21	3	0
6	C	12	0	14	1	0
6	D	20	0	27	3	0
7	A	8	0	12	2	0
8	A	7	0	0	0	0
8	B	9	0	0	0	0
8	C	4	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	D	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	2	0	0	0	0
11	B	8	0	12	0	0
12	A	196	0	0	1	0
12	B	190	0	0	0	0
12	C	191	0	0	0	0
12	D	171	0	0	2	0
All	All	7815	0	6796	54	0

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

All (54) 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)
6:D:306:PEG:H21	12:D:448:HOH:O	1.55	1.04
2:B:93:ASP:OD1	2:B:120:ARG:NH2	2.23	0.71
6:D:306:PEG:C2	12:D:448:HOH:O	2.22	0.70
2:B:83:PRO:HD3	2:B:106:LEU:HG	1.79	0.63
2:D:157:LEU:HD23	2:D:165:PRO:HG2	1.82	0.61
2:D:93:ASP:OD2	2:D:120:ARG:NH2	2.32	0.61
2:C:114:PHE:HB3	2:C:117:ILE:HD12	1.85	0.59
2:C:130:ASN:HB3	2:C:168:ILE:HG12	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:ASP:O	2:B:211:ASN:ND2	2.36	0.58
2:C:195:VAL:HA	5:C:307:PE3:H352	1.86	0.57
1:A:66:PHE:HE2	5:A:305:PE3:H231	1.71	0.55
2:C:196:ASP:H	5:C:307:PE3:H352	1.72	0.54
2:B:182:TRP:HB2	6:B:306:PEG:H21	1.89	0.54
2:B:81:ASP:OD1	4:B:302[B]:5YA:O2	2.26	0.53
2:C:225:HIS:NE2	4:C:305[B]:5YA:O1	2.40	0.53
2:B:143:GLU:OE1	2:B:147:ARG:NH1	2.39	0.53
1:A:135:HIS:NE2	4:A:304[B]:5YA:O2	2.37	0.53
2:C:93:ASP:OD1	2:C:120:ARG:NH2	2.39	0.52
2:D:199:ASP:HB2	2:D:235:SER:HB2	1.91	0.52
1:A:176:LEU:HD23	6:A:307:PEG:H31	1.92	0.51
2:C:85:LEU:HD23	2:C:117:ILE:HD11	1.92	0.51
2:B:186:GLN:HB3	2:B:266:ARG:NH1	2.26	0.51
2:C:199:ASP:OD1	2:C:225:HIS:ND1	2.44	0.51
2:C:206:ASP:OD1	2:C:241:LYS:NZ	2.45	0.50
2:C:199:ASP:HB2	2:C:235:SER:HB2	1.95	0.49
2:C:169:ARG:NH1	2:C:223:LEU:HD23	2.28	0.48
1:A:142:ASN:HA	7:A:309:PG0:H31	1.95	0.47
2:D:101:LYS:HE3	2:D:125:GLY:HA3	1.96	0.47
2:D:172:TYR:HA	4:D:302[B]:5YA:C15	2.45	0.47
1:A:143:GLU:HB2	7:A:309:PG0:H12	1.97	0.47
2:B:150:ILE:HD12	2:B:168:ILE:HD13	1.97	0.46
2:D:247:LYS:HZ3	6:D:304:PEG:H32	1.81	0.46
1:A:186:GLN:O	1:A:266:ARG:HD2	2.16	0.46
2:D:197:THR:HB	2:D:208:ILE:HG23	1.98	0.45
2:D:223:LEU:HD21	4:D:302[B]:5YA:C13	2.47	0.45
2:C:220:SER:HA	6:C:309:PEG:H31	1.98	0.44
2:B:61:LYS:HD2	2:B:62:TYR:CZ	2.53	0.44
1:A:81:ASP:OD1	4:A:304[B]:5YA:O2	2.36	0.44
2:B:170:PRO:HD3	2:B:190:ILE:HG23	2.01	0.43
1:A:150:ILE:HD12	1:A:168:ILE:HD13	2.01	0.43
1:A:147:ARG:NH2	12:A:411:HOH:O	2.52	0.42
2:D:57:SER:HB2	2:D:61:LYS:HE2	2.01	0.42
2:B:120:ARG:HB2	6:B:308:PEG:H22	2.02	0.42
1:A:56:PHE:HE2	2:B:249:LYS:HE3	1.85	0.42
1:A:56:PHE:O	1:A:59:VAL:HG22	2.19	0.42
2:B:199:ASP:HB2	2:B:235:SER:HB2	2.02	0.42
2:C:101:LYS:HA	2:C:126:HIS:CE1	2.55	0.42
2:D:246:LEU:HD12	2:D:246:LEU:HA	1.92	0.41
2:B:67:SER:HB3	2:B:194[A]:SER:OG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:N	1:A:116:ASN:OD1	2.51	0.41
2:C:95:LEU:HB3	2:C:100:VAL:O	2.20	0.40
1:A:80:ASP:OD1	1:A:105:PHE:HB2	2.22	0.40
2:B:109:GLU:O	2:B:113:LYS:HG3	2.20	0.40
2:B:264:LYS:N	6:B:307:PEG:O4	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/214 (99%)	204 (96%)	7 (3%)	1 (0%)	29	48
2	B	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	29	48
2	C	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	29	48
2	D	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	29	48
All	All	846/856 (99%)	811 (96%)	31 (4%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	192	GLN
2	C	192	GLN
2	D	192	GLN
1	A	192	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/186 (99%)	184 (100%)	0	100	100
2	B	183/185 (99%)	180 (98%)	3 (2%)	62	84
2	C	180/185 (97%)	179 (99%)	1 (1%)	86	95
2	D	178/185 (96%)	173 (97%)	5 (3%)	43	70
All	All	725/741 (98%)	716 (99%)	9 (1%)	71	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	106	LEU
2	B	160	LEU
2	B	203	VAL
2	C	92	LEU
2	D	114	PHE
2	D	117	ILE
2	D	155	GLU
2	D	198	VAL
2	D	246	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	PXU	D	171	2	6,8,9	1.27	1 (16%)	4,11,13	1.03	0
2	PXU	B	171	2	6,8,9	1.27	1 (16%)	4,11,13	0.89	0
2	PXU	C	171	2	6,8,9	1.27	0	4,11,13	0.96	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	PXU	D	171	2	-	0/0/12/15	0/1/1/1
2	PXU	B	171	2	-	0/0/12/15	0/1/1/1
2	PXU	C	171	2	-	0/0/12/15	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	171	PXU	O-C	2.03	1.26	1.19
2	D	171	PXU	O-C	2.02	1.26	1.19

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 29 are monoatomic - leaving 29 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	$\# Z > 2$
4	5YA	D	302[B]	-	22,22,22	0.69	0	30,30,30	0.55	0
3	SO4	C	302	-	4,4,4	0.15	0	6,6,6	0.07	0
6	PEG	D	304	-	6,6,6	0.48	0	5,5,5	0.45	0
4	5YA	C	305[B]	-	22,22,22	0.68	0	30,30,30	0.59	0
11	DMS	B	304	-	3,3,3	0.65	0	3,3,3	0.42	0
4	5YA	B	302[B]	-	22,22,22	0.68	0	30,30,30	0.70	0
6	PEG	D	306	-	5,5,6	0.52	0	4,4,5	0.42	0
3	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.05	0
6	PEG	D	305	-	6,6,6	0.49	0	5,5,5	0.47	0
3	SO4	A	302	-	4,4,4	0.13	0	6,6,6	0.04	0
3	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.07	0
4	5YA	A	304[B]	-	22,22,22	0.70	0	30,30,30	0.73	0
11	DMS	B	305	-	3,3,3	0.66	0	3,3,3	0.49	0
3	SO4	C	304	-	4,4,4	0.10	0	6,6,6	0.13	0
3	SO4	C	301	-	4,4,4	0.15	0	6,6,6	0.06	0
6	PEG	C	308	-	6,6,6	0.48	0	5,5,5	0.46	0
7	PG0	A	309	-	7,7,7	0.47	0	6,6,6	0.38	0
3	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.06	0
6	PEG	B	308	-	5,5,6	0.53	0	4,4,5	0.33	0
6	PEG	B	306	-	5,5,6	0.54	0	4,4,5	0.37	0
6	PEG	B	307	-	5,5,6	0.54	0	4,4,5	0.43	0
3	SO4	D	301	-	4,4,4	0.13	0	6,6,6	0.04	0
5	PE3	A	305	-	3,3,42	0.48	0	2,2,41	0.49	0
6	PEG	A	307	-	6,6,6	0.48	0	5,5,5	0.45	0
6	PEG	C	309	-	4,4,6	0.60	0	3,3,5	0.23	0
5	PE3	C	307	-	4,4,42	0.41	0	3,3,41	0.40	0
3	SO4	A	301	-	4,4,4	0.15	0	6,6,6	0.07	0
6	PEG	A	306	-	6,6,6	0.48	0	5,5,5	0.46	0
6	PEG	A	308	-	5,5,6	0.54	0	4,4,5	0.43	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	5YA	D	302[B]	-	-	0/10/10/10	0/3/3/3
6	PEG	C	308	-	-	1/4/4/4	-
6	PEG	A	307	-	-	2/4/4/4	-
6	PEG	C	309	-	-	1/2/2/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG0	A	309	-	-	2/5/5/5	-
4	5YA	A	304[B]	-	-	0/10/10/10	0/3/3/3
5	PE3	C	307	-	-	1/2/2/40	-
6	PEG	D	304	-	-	2/4/4/4	-
6	PEG	B	306	-	-	2/3/3/4	-
6	PEG	B	307	-	-	0/3/3/4	-
6	PEG	D	305	-	-	0/4/4/4	-
4	5YA	B	302[B]	-	-	8/10/10/10	0/3/3/3
6	PEG	D	306	-	-	2/3/3/4	-
4	5YA	C	305[B]	-	-	0/10/10/10	0/3/3/3
6	PEG	B	308	-	-	2/3/3/4	-
6	PEG	A	306	-	-	1/4/4/4	-
5	PE3	A	305	-	-	1/1/1/40	-
6	PEG	A	308	-	-	0/3/3/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	309	PG0	O1-C3-C4-O2
6	A	306	PEG	O1-C1-C2-O2
6	C	309	PEG	C4-C3-O2-C2
4	B	302[B]	5YA	C13-C14-C17-N1
6	D	306	PEG	C1-C2-O2-C3
6	B	308	PEG	O2-C3-C4-O4
6	D	306	PEG	C4-C3-O2-C2
6	B	306	PEG	C4-C3-O2-C2
5	C	307	PE3	C36-C35-O34-C33
6	B	308	PEG	C4-C3-O2-C2
6	D	304	PEG	C1-C2-O2-C3
7	A	309	PG0	C1-C2-O1-C3
6	B	306	PEG	O2-C3-C4-O4
5	A	305	PE3	O22-C23-C24-O25
6	D	304	PEG	O2-C3-C4-O4
6	A	307	PEG	O2-C3-C4-O4
4	B	302[B]	5YA	C15-C14-C17-N1
4	B	302[B]	5YA	C13-C14-C17-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	302[B]	5YA	C16-C11-C3-C2
4	B	302[B]	5YA	C12-C11-C3-C2
4	B	302[B]	5YA	C12-C11-C3-C4
6	A	307	PEG	C4-C3-O2-C2
4	B	302[B]	5YA	C16-C11-C3-C4
6	C	308	PEG	C1-C2-O2-C3
4	B	302[B]	5YA	C15-C14-C17-O1

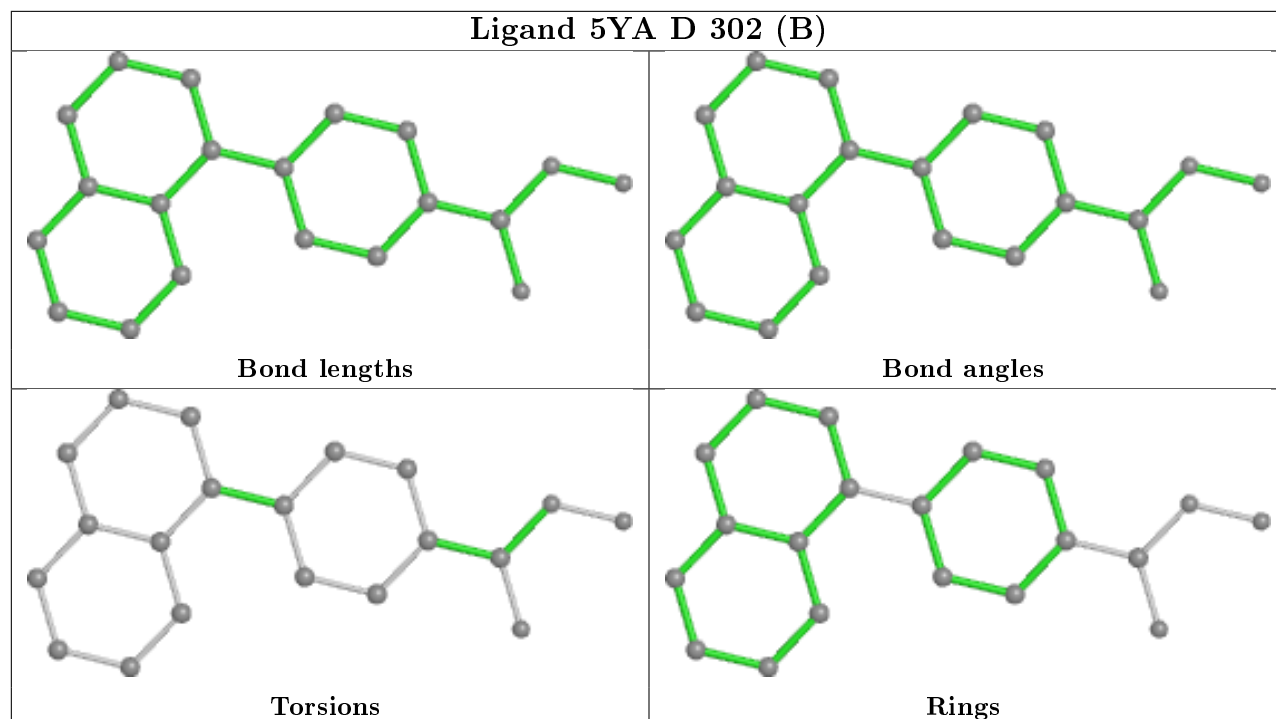
There are no ring outliers.

14 monomers are involved in 19 short contacts:

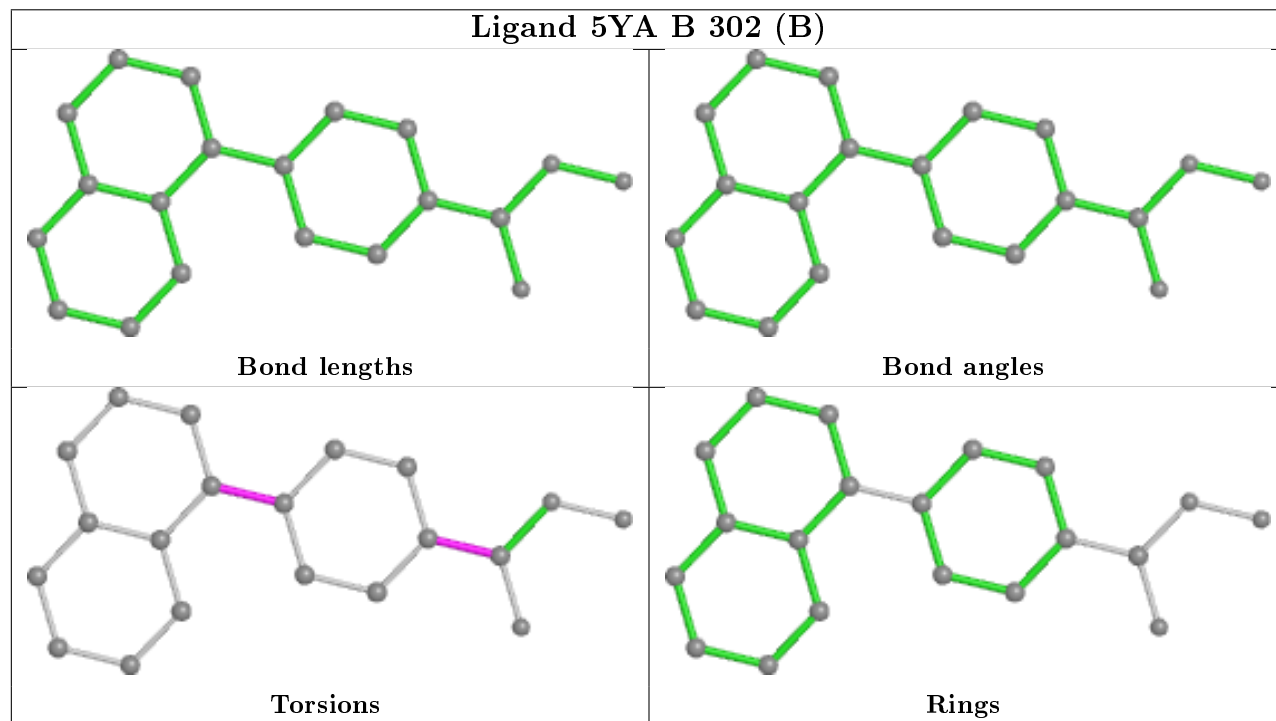
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302[B]	5YA	2	0
6	D	304	PEG	1	0
4	C	305[B]	5YA	1	0
4	B	302[B]	5YA	1	0
6	D	306	PEG	2	0
4	A	304[B]	5YA	2	0
7	A	309	PG0	2	0
6	B	308	PEG	1	0
6	B	306	PEG	1	0
6	B	307	PEG	1	0
5	A	305	PE3	1	0
6	A	307	PEG	1	0
6	C	309	PEG	1	0
5	C	307	PE3	2	0

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.

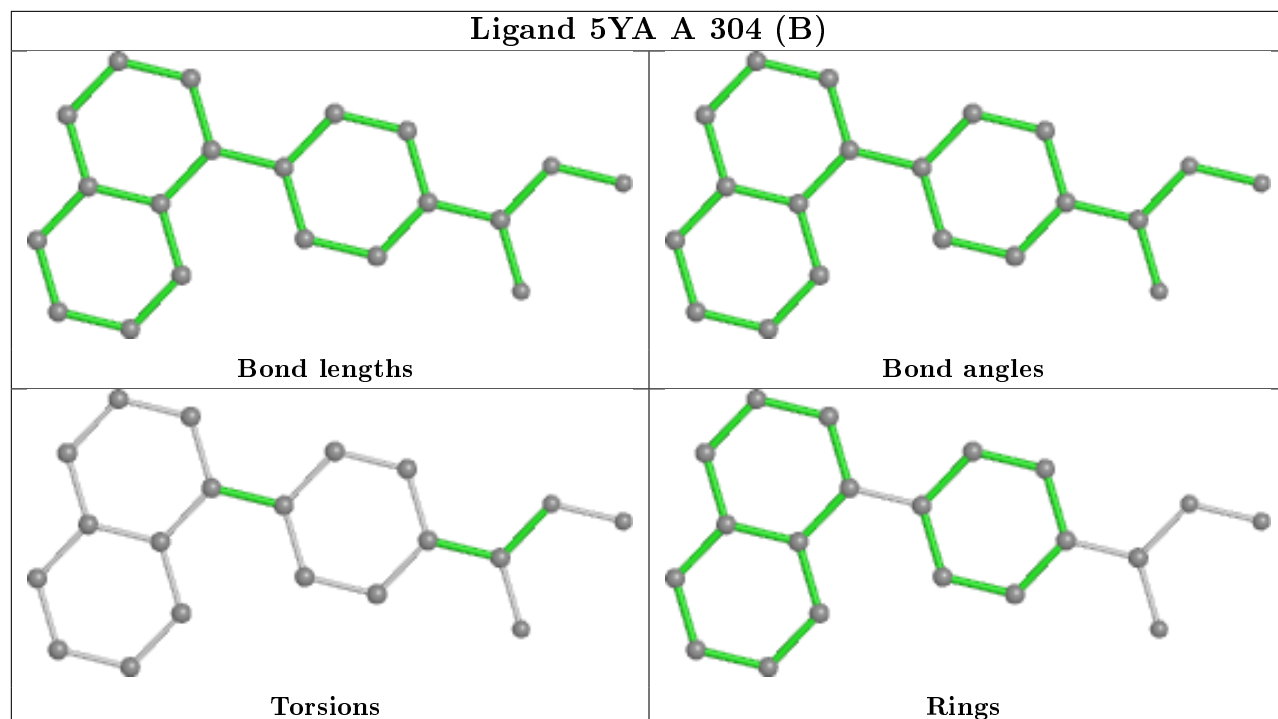
Ligand 5YA D 302 (B)



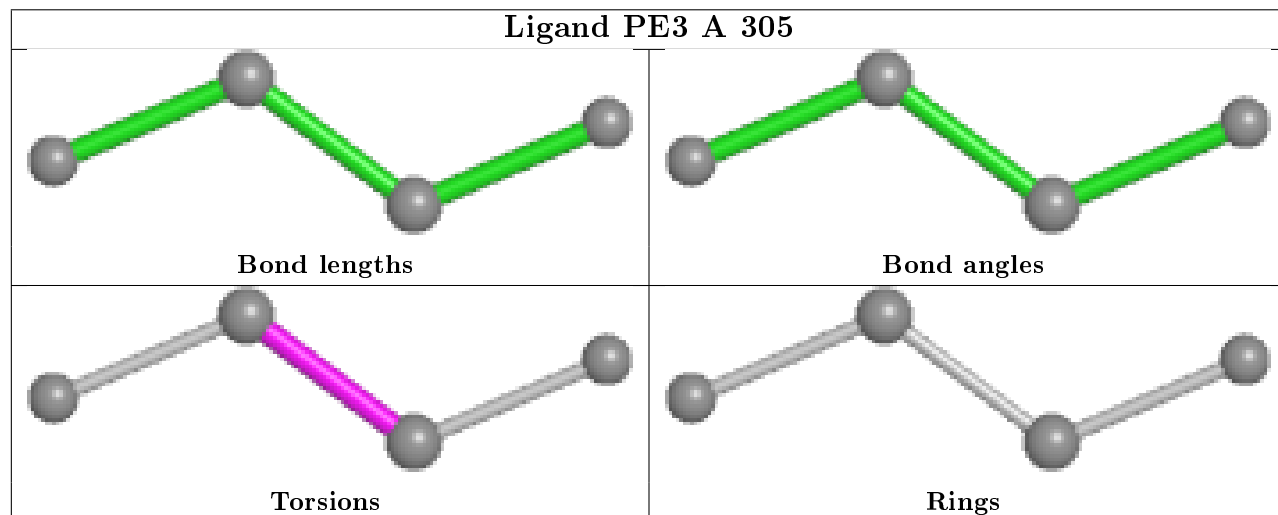
Ligand 5YA B 302 (B)



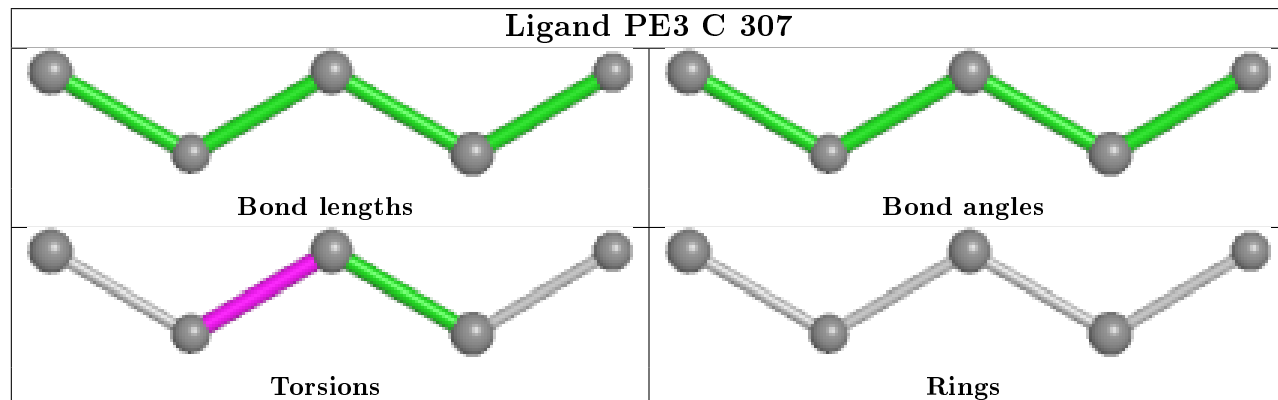
Ligand 5YA A 304 (B)



Ligand PE3 A 305



Ligand PE3 C 307



5.7 Other polymers

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	214/214 (100%)	0.27	6 (2%)	53	56	4, 15, 38, 53	0
2	B	213/214 (99%)	0.25	7 (3%)	46	50	4, 13, 35, 50	0
2	C	213/214 (99%)	0.38	11 (5%)	27	29	5, 15, 38, 62	0
2	D	213/214 (99%)	0.54	10 (4%)	31	33	7, 21, 43, 59	0
All	All	853/856 (99%)	0.36	34 (3%)	38	41	4, 16, 40, 62	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	53	TRP	4.8
2	B	231	HIS	4.6
1	A	53	TRP	4.3
2	B	53	TRP	4.3
2	D	200	TRP	3.3
2	D	233	GLN	3.2
2	D	231	HIS	3.0
2	D	159	ARG	2.9
2	B	204	SER	2.9
2	D	155	GLU	2.8
2	D	202	GLY	2.7
2	C	200	TRP	2.6
2	C	123	ASN	2.6
2	D	85	LEU	2.6
2	B	203	VAL	2.5
1	A	206	ASP	2.5
2	C	85	LEU	2.5
2	D	230	GLY	2.5
2	B	200	TRP	2.5
2	C	89	PRO	2.5
2	C	231	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	231	HIS	2.4
2	C	203	VAL	2.4
1	A	159	ARG	2.4
2	B	123	ASN	2.3
2	C	159	ARG	2.3
1	A	123	ASN	2.2
1	A	203	VAL	2.2
2	D	203	VAL	2.1
2	B	54	THR	2.1
2	C	228	PRO	2.1
2	D	116	ASN	2.1
2	C	204	SER	2.0
2	C	116	ASN	2.0

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

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
2	PXU	D	171	8/9	0.92	0.15	11,15,17,20	0
2	PXU	B	171	8/9	0.92	0.19	3,9,10,13	0
2	PXU	C	171	8/9	0.95	0.15	5,7,15,24	1

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	A	308	6/7	0.59	0.44	47,49,52,53	6
4	5YA	A	304[B]	20/20	0.66	0.53	4,43,48,48	20

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	CL	A	317	1/1	0.67	0.23	59,59,59,59	0
8	NA	B	311	1/1	0.68	0.22	44,44,44,44	0
7	PG0	A	309	8/8	0.68	0.38	4,23,28,30	8
3	SO4	A	303	5/5	0.73	0.33	44,64,64,72	0
6	PEG	B	308	6/7	0.75	0.32	32,40,48,48	6
4	5YA	C	305[B]	20/20	0.75	0.35	25,52,57,57	20
4	5YA	B	302[B]	20/20	0.76	0.40	11,40,49,51	20
4	5YA	D	302[B]	20/20	0.77	0.42	26,52,55,57	20
6	PEG	B	306	6/7	0.77	0.27	26,37,39,40	6
6	PEG	A	307	7/7	0.78	0.29	20,27,33,34	7
6	PEG	B	307	6/7	0.81	0.37	31,32,39,41	6
6	PEG	A	306	7/7	0.81	0.23	24,28,34,36	7
9	CL	B	319	1/1	0.81	0.12	79,79,79,79	0
8	NA	B	315	1/1	0.83	0.15	52,52,52,52	0
5	PE3	A	305	4/43	0.83	0.24	17,17,25,28	4
3	SO4	D	301	5/5	0.84	0.36	71,72,78,84	0
3	SO4	C	303	5/5	0.84	0.22	61,67,71,71	0
11	DMS	B	304	4/4	0.87	0.27	38,44,47,53	0
6	PEG	C	308	7/7	0.87	0.28	25,32,38,39	7
6	PEG	C	309	5/7	0.88	0.24	5,13,16,16	5
6	PEG	D	304	7/7	0.89	0.20	24,31,36,36	0
8	NA	B	314	1/1	0.89	0.30	29,29,29,29	0
8	NA	C	310	1/1	0.89	0.15	36,36,36,36	0
9	CL	D	309	1/1	0.89	0.08	66,66,66,66	0
6	PEG	D	305	7/7	0.90	0.21	23,27,35,37	7
3	SO4	C	302	5/5	0.90	0.34	72,75,77,82	0
3	SO4	B	301	5/5	0.90	0.25	60,66,69,69	0
11	DMS	B	305	4/4	0.90	0.20	17,21,22,28	4
8	NA	A	314	1/1	0.91	0.12	37,37,37,37	0
8	NA	B	317	1/1	0.91	0.11	36,36,36,36	0
3	SO4	A	302	5/5	0.92	0.29	53,55,57,62	0
8	NA	A	315	1/1	0.92	0.14	32,32,32,32	0
8	NA	B	312	1/1	0.92	0.10	29,29,29,29	0
8	NA	B	310	1/1	0.93	0.29	28,28,28,28	0
5	PE3	C	307	5/43	0.93	0.22	17,19,23,28	5
8	NA	A	312	1/1	0.94	0.12	9,9,9,9	0
8	NA	A	310	1/1	0.94	0.15	5,5,5,5	0
3	SO4	A	301	5/5	0.94	0.19	24,36,40,41	0
8	NA	A	316	1/1	0.94	0.14	38,38,38,38	0
8	NA	C	312	1/1	0.94	0.18	36,36,36,36	0
8	NA	C	313	1/1	0.94	0.14	24,24,24,24	0
6	PEG	D	306	6/7	0.95	0.23	6,13,16,20	6

Continued on next page...

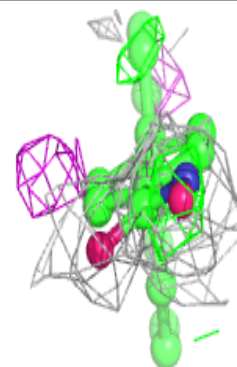
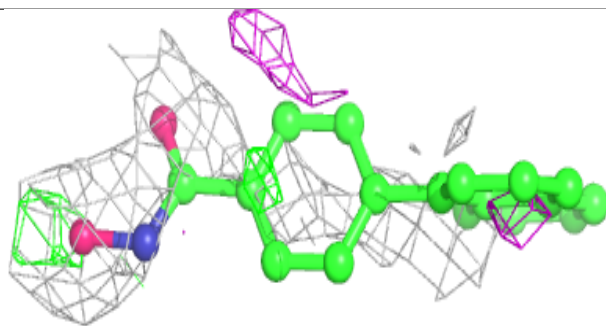
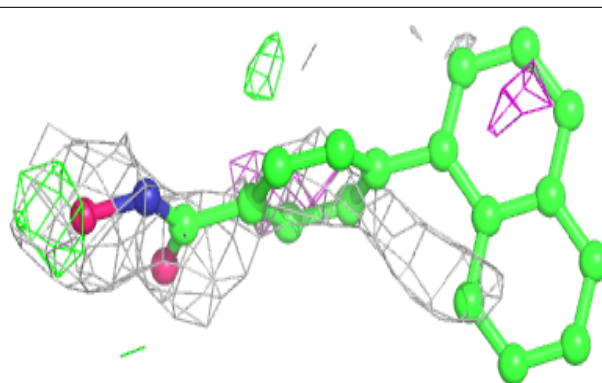
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NA	B	316	1/1	0.95	0.09	38,38,38,38	0
8	NA	C	311	1/1	0.96	0.16	39,39,39,39	0
8	NA	B	313	1/1	0.96	0.16	31,31,31,31	0
10	ZN	B	303[A]	1/1	0.97	0.15	19,19,19,19	1
8	NA	A	311	1/1	0.97	0.13	10,10,10,10	0
8	NA	D	307	1/1	0.97	0.17	19,19,19,19	0
8	NA	B	309	1/1	0.97	0.14	10,10,10,10	0
10	ZN	D	303[A]	1/1	0.98	0.05	33,33,33,33	1
10	ZN	C	306[A]	1/1	0.98	0.08	26,26,26,26	1
9	CL	B	318	1/1	0.98	0.08	27,27,27,27	0
3	SO4	C	301	5/5	0.98	0.19	9,14,21,28	0
3	SO4	C	304	5/5	0.98	0.21	45,45,46,52	0
8	NA	A	313	1/1	0.99	0.11	9,9,9,9	0
10	ZN	D	308	1/1	0.99	0.09	34,34,34,34	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.

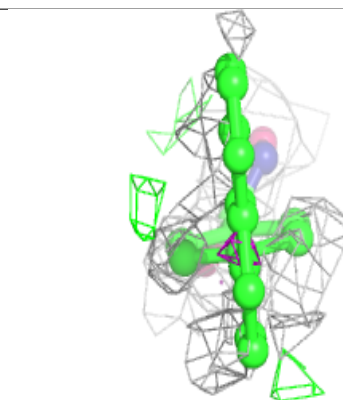
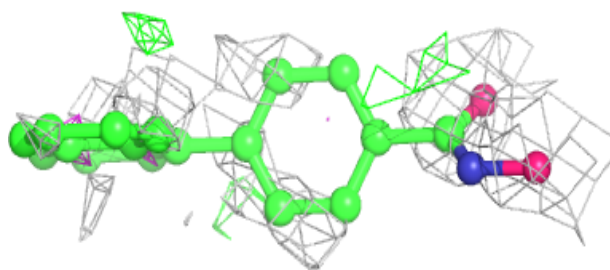
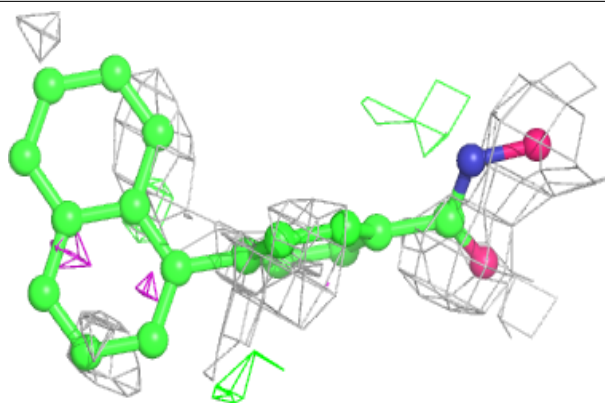
Electron density around 5YA A 304 (B):

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

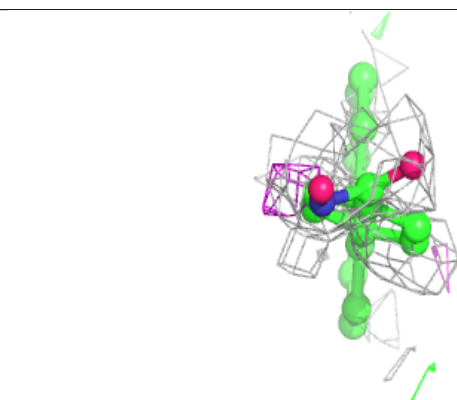
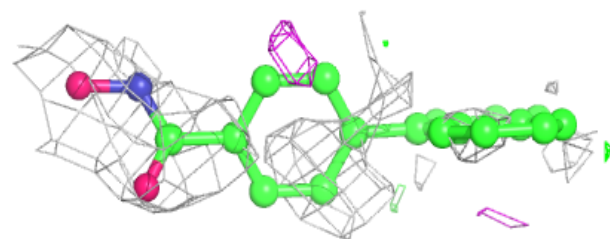
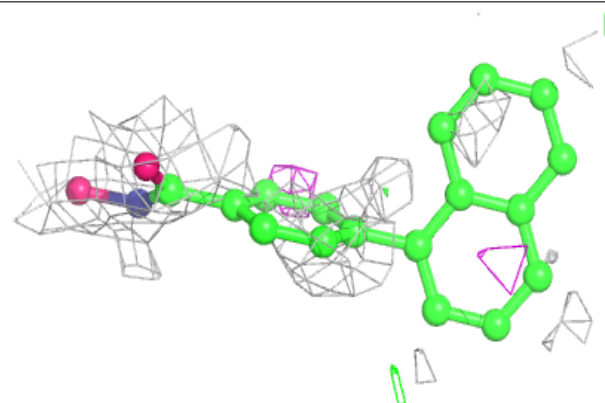


Electron density around 5YA B 302 (B):

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

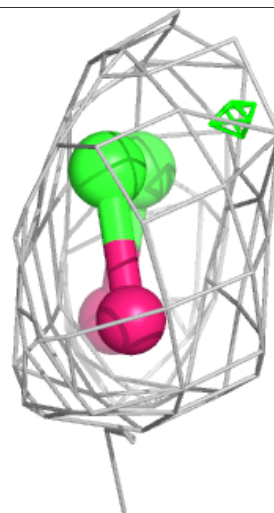
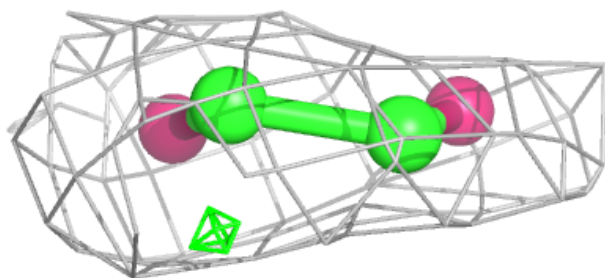
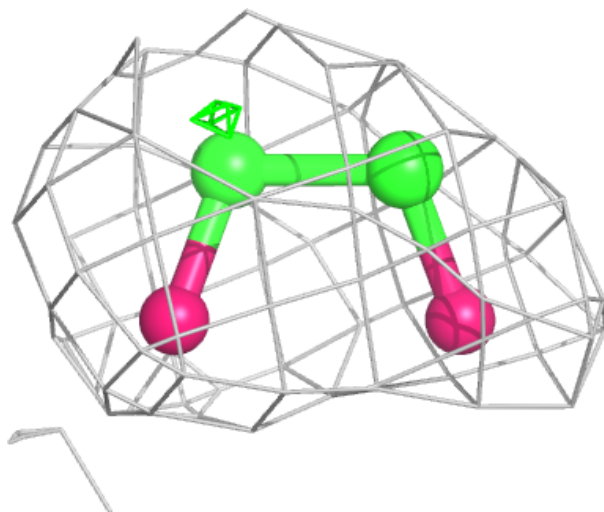
**Electron density around 5YA D 302 (B):**

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



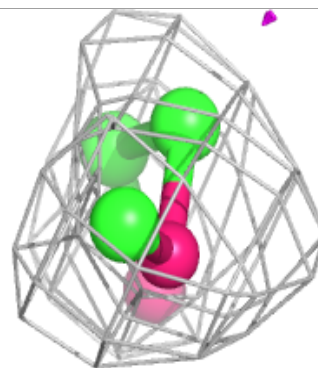
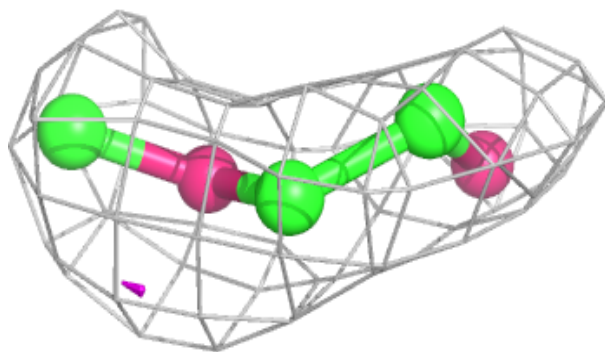
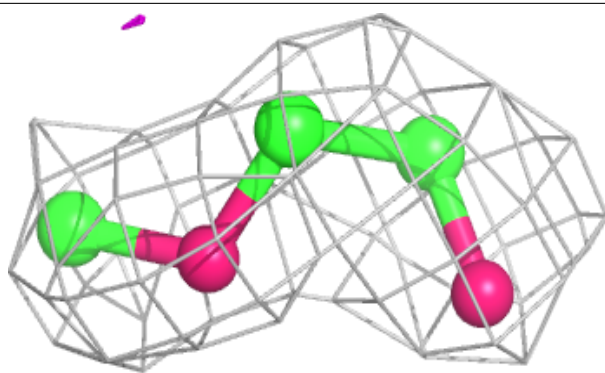
Electron density around PE3 A 305:

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



Electron density around PE3 C 307:

$2mF_o-DF_c$ (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.