



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:42 PM UTC

PDB ID : 8FIU / pdb_00008fiu
Title : Potent long-acting inhibitors targeting HIV-1 capsid based on a versatile quinazolin-4-one scaffold
Authors : Nolte, R.T.
Deposited on : 2022-12-16
Resolution : 1.56 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

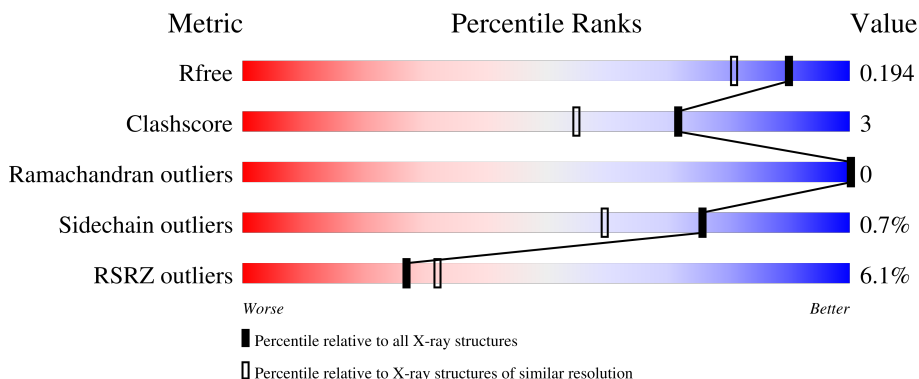
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	232	2% 88% 6% 6%
1	B	232	6% 85% 7% 8%
1	C	232	9% 87% 7% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11403 atoms, of which 5253 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.

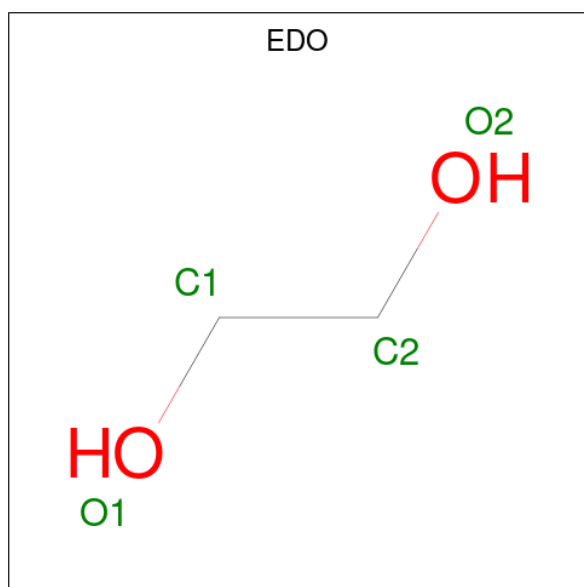
- Molecule 1 is a protein called HIV-1 capsid.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	219	Total	C	H	N	O	S	0	5	0
			3430	1079	1722	296	317	16			
1	B	214	Total	C	H	N	O	S	0	3	0
			3314	1046	1655	288	311	14			
1	C	219	Total	C	H	N	O	S	0	5	0
			3425	1080	1720	296	314	15			

There are 15 discrepancies between the modelled and reference sequences:

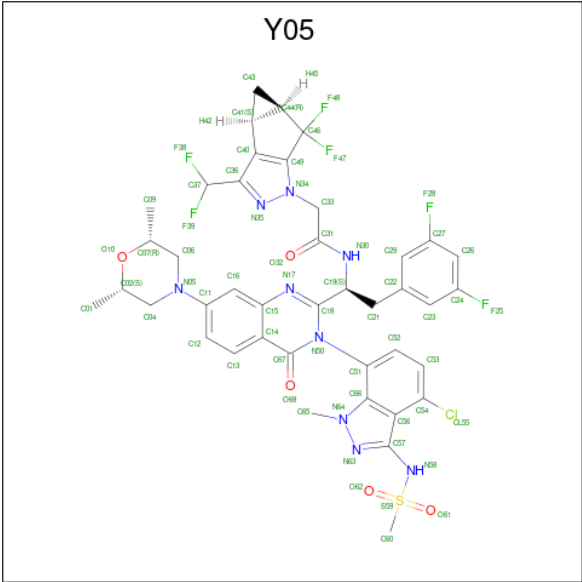
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP B6DRA0
A	14	CYS	ALA	conflict	UNP B6DRA0
A	45	CYS	GLU	conflict	UNP B6DRA0
A	184	ALA	TRP	conflict	UNP B6DRA0
A	185	ALA	MET	conflict	UNP B6DRA0
B	0	MET	-	initiating methionine	UNP B6DRA0
B	14	CYS	ALA	conflict	UNP B6DRA0
B	45	CYS	GLU	conflict	UNP B6DRA0
B	184	ALA	TRP	conflict	UNP B6DRA0
B	185	ALA	MET	conflict	UNP B6DRA0
C	0	MET	-	initiating methionine	UNP B6DRA0
C	14	CYS	ALA	conflict	UNP B6DRA0
C	45	CYS	GLU	conflict	UNP B6DRA0
C	184	ALA	TRP	conflict	UNP B6DRA0
C	185	ALA	MET	conflict	UNP B6DRA0

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is N-[(1S)-1-{(3P)-3-{4-chloro-3-[(methanesulfonyl)amino]-1-methyl-1H-indazol-7-yl}-7-[(2R,6S)-2,6-dimethylmorpholin-4-yl]-4-oxo-3,4-dihydroquinazolin-2-yl}-2-(3,5-difluorophenyl)ethyl]-2-[(3bS,4aR)-3-(difluoromethyl)-5,5-difluoro-3b,4,4a,5-tetrahydro-1H-cyclopropa[3,4]cyclopenta[1,2-c]pyrazol-1-yl]acetamide (CCD ID: Y05) (formula: C₄₁H₃₈ClF₆N₉O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	H	N	O	S	0	0
			101	41	1	6	38	9	5	1		
3	B	1	Total	C	Cl	F	H	N	O	S	0	0
			101	41	1	6	38	9	5	1		
3	C	1	Total	C	Cl	F	H	N	O	S	0	0
			101	41	1	6	38	9	5	1		

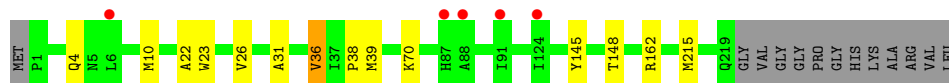
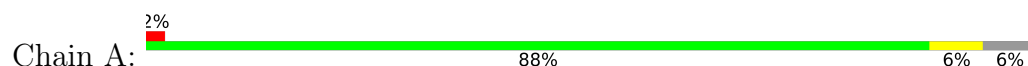
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	289	Total O	0	0
			289 289		
4	B	266	Total O	0	0
			266 266		
4	C	306	Total O	0	0
			306 306		

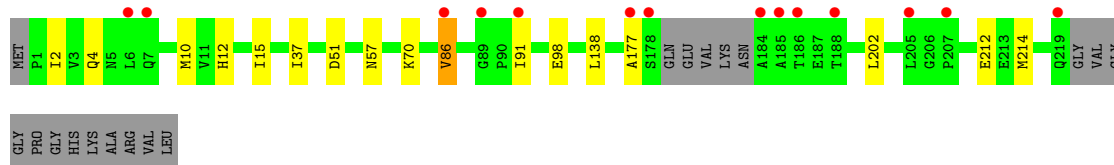
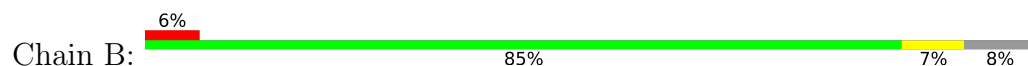
3 Residue-property plots [i](#)

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.

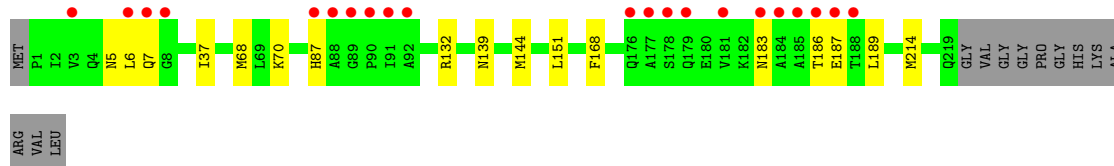
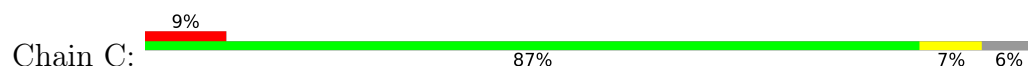
- Molecule 1: HIV-1 capsid



- Molecule 1: HIV-1 capsid



- Molecule 1: HIV-1 capsid



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	156.20Å 156.20Å 56.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.18 – 1.56 35.18 – 1.56	Depositor EDS
% Data completeness (in resolution range)	87.5 (35.18-1.56) 87.6 (35.18-1.56)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.56Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.161 , 0.194 0.161 , 0.194	Depositor DCC
R_{free} test set	1945 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11403	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 33.27 % 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 8.2196e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: EDO, Y05

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	0.73	0/1764	0.71	0/2398
1	B	0.74	0/1703	0.73	0/2316
1	C	0.83	1/1761 (0.1%)	0.80	0/2395
All	All	0.77	1/5228 (0.0%)	0.75	0/7109

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	214	MET	SD-CE	-5.46	1.65	1.79

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	1708	1722	1718	10	0
1	B	1659	1655	1657	12	0
1	C	1705	1720	1718	13	0
2	A	12	18	18	0	0
2	B	8	12	12	0	0
2	C	8	12	12	0	0
3	A	63	38	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	63	38	0	1	0
3	C	63	38	0	1	0
4	A	289	0	0	2	2
4	B	266	0	0	2	2
4	C	306	0	0	4	0
All	All	6150	5253	5135	34	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 3.

All (34) 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:C:68[B]:MET:HE1	1:C:144:MET:HE3	1.37	1.04
1:C:183:ASN:OD1	4:C:401:HOH:O	1.78	0.98
1:B:212:GLU:OE2	4:B:401:HOH:O	2.03	0.75
1:B:202:LEU:HD22	1:B:214:MET:HE3	1.70	0.73
1:A:145:TYR:OH	4:A:401:HOH:O	2.06	0.73
1:C:70:LYS:HD2	3:C:303:Y05:F47	1.85	0.65
1:B:37:ILE:HD12	1:B:138:LEU:HB3	1.83	0.61
1:C:186:THR:O	1:C:187:GLU:C	2.43	0.60
1:A:70:LYS:HD2	3:A:304:Y05:F47	1.92	0.59
1:B:202:LEU:HD22	1:B:214:MET:CE	2.35	0.56
1:B:2:ILE:HG22	1:B:10:MET:HE3	1.90	0.54
1:A:4:GLN:HG2	1:A:10:MET:SD	2.47	0.54
1:C:186:THR:HG21	4:C:495:HOH:O	2.09	0.53
1:B:15[B]:ILE:HD11	1:B:51:ASP:CB	2.39	0.52
1:A:23:TRP:O	1:A:26[B]:VAL:HG22	2.11	0.51
1:B:4:GLN:HG3	1:B:10:MET:SD	2.51	0.51
1:B:70:LYS:HD2	3:B:303:Y05:F47	2.02	0.50
1:B:86:VAL:HG22	1:B:98:GLU:HB2	1.95	0.49
1:C:151:LEU:HD23	1:C:189[A]:LEU:HD21	1.95	0.49
1:B:177:ALA:HB2	4:B:543:HOH:O	2.13	0.48
1:A:31:ALA:O	1:A:36[B]:VAL:HG21	2.16	0.45
1:A:162:ARG:HG3	1:A:215:MET:CE	2.46	0.45
1:C:132:ARG:HD2	4:C:406:HOH:O	2.17	0.44
1:C:168:PHE:HE1	1:C:186:THR:HG22	1.82	0.44
1:C:6:LEU:HA	1:C:7:GLN:HA	1.76	0.44
1:A:26[B]:VAL:HG11	1:A:39[B]:MET:HG2	2.00	0.43
1:A:22:ALA:O	1:A:26[B]:VAL:HG13	2.18	0.43
1:C:144:MET:HE2	1:C:144:MET:HB2	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:HD13	1:C:139:ASN:OD1	2.19	0.43
1:C:68[B]:MET:HG2	4:C:493:HOH:O	2.18	0.43
1:A:38:PRO:HG3	1:B:57:ASN:HB3	2.01	0.42
1:A:148:THR:HG22	4:A:507:HOH:O	2.19	0.42
1:B:2:ILE:HD13	1:B:12:HIS:HA	2.01	0.42
1:C:5:ASN:OD1	1:C:5:ASN:C	2.63	0.41

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)
4:A:588:HOH:O	4:B:522:HOH:O[3_665]	1.80	0.40
4:A:553:HOH:O	4:B:553:HOH:O[1_554]	1.95	0.25

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	222/232 (96%)	221 (100%)	1 (0%)	0	100	100
1	B	213/232 (92%)	212 (100%)	1 (0%)	0	100	100
1	C	222/232 (96%)	219 (99%)	3 (1%)	0	100	100
All	All	657/696 (94%)	652 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	188/194 (97%)	186 (99%)	2 (1%)	65	43
1	B	180/194 (93%)	178 (99%)	2 (1%)	65	43
1	C	186/194 (96%)	185 (100%)	1 (0%)	81	68
All	All	554/582 (95%)	549 (99%)	5 (1%)	76	51

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36[A]	VAL
1	A	36[B]	VAL
1	B	86	VAL
1	B	91	ILE
1	C	87	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	87	HIS
1	A	179	GLN
1	B	21	ASN
1	B	84	HIS
1	C	84	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	303	-	3,3,3	0.37	0	2,2,2	0.66	0
2	EDO	A	301	-	3,3,3	0.70	0	2,2,2	0.28	0
2	EDO	B	302	-	3,3,3	0.41	0	2,2,2	0.58	0
3	Y05	A	304	-	68,71,71	1.66	9 (13%)	92,112,112	1.89	25 (27%)
2	EDO	A	302	-	3,3,3	0.55	0	2,2,2	0.44	0
2	EDO	B	301	-	3,3,3	0.28	0	2,2,2	0.64	0
3	Y05	C	303	-	68,71,71	1.65	13 (19%)	92,112,112	1.90	20 (21%)
2	EDO	C	302	-	3,3,3	0.66	0	2,2,2	0.21	0
2	EDO	C	301	-	3,3,3	0.27	0	2,2,2	0.54	0
3	Y05	B	303	-	68,71,71	1.34	9 (13%)	92,112,112	1.61	17 (18%)

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	EDO	A	303	-	-	0/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-
2	EDO	B	302	-	-	1/1/1/1	-
3	Y05	A	304	-	-	0/29/66/66	0/9/9/9
2	EDO	A	302	-	-	0/1/1/1	-
2	EDO	B	301	-	-	0/1/1/1	-
3	Y05	C	303	-	-	0/29/66/66	0/9/9/9
2	EDO	C	302	-	-	0/1/1/1	-
2	EDO	C	301	-	-	0/1/1/1	-
3	Y05	B	303	-	-	3/29/66/66	0/9/9/9

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	304	Y05	O10-C02	-5.17	1.35	1.44
3	C	303	Y05	C66-N64	5.10	1.40	1.37
3	A	304	Y05	C41-C44	4.65	1.58	1.51
3	A	304	Y05	N64-N63	4.25	1.42	1.36
3	A	304	Y05	F47-C46	-4.20	1.29	1.36
3	C	303	Y05	C19-C18	-3.81	1.47	1.51
3	C	303	Y05	C18-N17	3.81	1.33	1.29
3	C	303	Y05	C41-C44	3.78	1.57	1.51
3	C	303	Y05	O10-C02	-3.60	1.38	1.44
3	B	303	Y05	C18-N17	3.33	1.32	1.29
3	C	303	Y05	N64-N63	3.27	1.41	1.36
3	B	303	Y05	F47-C46	-2.94	1.31	1.36
3	A	304	Y05	C19-N30	-2.91	1.39	1.45
3	C	303	Y05	O10-C07	-2.87	1.39	1.44
3	C	303	Y05	C12-C13	2.80	1.43	1.38
3	B	303	Y05	O61-S59	2.61	1.47	1.43
3	B	303	Y05	N64-N63	2.57	1.40	1.36
3	B	303	Y05	C06-N05	-2.56	1.41	1.46
3	A	304	Y05	O61-S59	2.51	1.47	1.43
3	B	303	Y05	O62-S59	2.50	1.47	1.43
3	C	303	Y05	F25-C24	-2.48	1.30	1.36
3	A	304	Y05	C11-N05	2.38	1.45	1.38
3	A	304	Y05	C31-N30	2.37	1.39	1.34
3	C	303	Y05	C40-C36	-2.36	1.35	1.42
3	B	303	Y05	O10-C02	-2.28	1.40	1.44
3	B	303	Y05	C53-C52	2.26	1.42	1.38
3	B	303	Y05	C41-C44	2.25	1.55	1.51
3	C	303	Y05	C18-N50	2.21	1.42	1.39
3	A	304	Y05	C52-C51	-2.08	1.36	1.39
3	C	303	Y05	C66-C51	2.07	1.43	1.40
3	C	303	Y05	C31-N30	2.04	1.38	1.34

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	Y05	C66-N64-N63	9.22	115.48	110.95
3	B	303	Y05	C66-N64-N63	5.59	113.70	110.95
3	A	304	Y05	C41-C43-C44	5.56	63.93	60.51
3	C	303	Y05	C36-N35-N34	-5.23	101.86	108.50
3	A	304	Y05	O62-S59-N58	5.07	117.08	106.83
3	A	304	Y05	N50-C18-N17	-4.45	120.36	124.21
3	C	303	Y05	C41-C43-C44	4.26	63.13	60.51
3	A	304	Y05	F39-C37-F38	-4.17	89.98	105.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	Y05	C27-C26-C24	3.83	121.66	116.08
3	A	304	Y05	C23-C24-C26	-3.78	118.90	123.50
3	B	303	Y05	C23-C24-C26	-3.73	118.97	123.50
3	C	303	Y05	C16-C11-N05	-3.69	117.35	121.33
3	A	304	Y05	C52-C51-N50	3.68	125.94	118.61
3	B	303	Y05	O62-S59-N58	3.60	114.11	106.83
3	C	303	Y05	O62-S59-O61	-3.59	114.05	118.87
3	A	304	Y05	C43-C41-C44	-3.50	57.09	59.26
3	A	304	Y05	C66-N64-N63	3.43	112.64	110.95
3	A	304	Y05	C36-N35-N34	-3.39	104.20	108.50
3	B	303	Y05	F25-C24-C26	3.34	123.03	118.28
3	C	303	Y05	C22-C23-C24	3.31	121.64	118.75
3	C	303	Y05	C52-C51-N50	3.23	125.05	118.61
3	C	303	Y05	O62-S59-N58	3.17	113.23	106.83
3	C	303	Y05	N58-C57-N63	3.09	125.28	119.03
3	A	304	Y05	N58-C57-N63	3.06	125.24	119.03
3	B	303	Y05	N50-C18-N17	-3.05	121.57	124.21
3	B	303	Y05	C36-N35-N34	-3.01	104.69	108.50
3	A	304	Y05	C15-N17-C18	2.95	121.54	117.46
3	A	304	Y05	C01-C02-C04	-2.85	105.23	112.39
3	B	303	Y05	F39-C37-F38	-2.83	94.95	105.44
3	C	303	Y05	C46-C44-C41	2.81	110.53	108.40
3	A	304	Y05	C29-C22-C23	2.77	122.77	119.01
3	C	303	Y05	C43-C44-C41	-2.75	58.08	60.23
3	B	303	Y05	C56-C54-CL55	2.72	123.12	119.62
3	B	303	Y05	C27-C26-C24	2.61	119.88	116.08
3	B	303	Y05	C52-C51-N50	2.60	123.78	118.61
3	C	303	Y05	C14-C15-N17	-2.56	119.84	122.41
3	B	303	Y05	C41-C43-C44	2.52	62.06	60.51
3	A	304	Y05	C56-C54-CL55	2.50	122.84	119.62
3	C	303	Y05	C06-N05-C11	2.49	121.58	116.42
3	A	304	Y05	O32-C31-N30	-2.47	118.77	122.95
3	C	303	Y05	C65-N64-C66	-2.44	126.16	130.11
3	A	304	Y05	C21-C22-C29	-2.42	116.27	120.43
3	A	304	Y05	O61-S59-N58	-2.39	102.00	106.83
3	B	303	Y05	C22-C29-C27	-2.38	116.68	118.75
3	C	303	Y05	C14-C67-N50	2.38	117.94	114.69
3	A	304	Y05	C16-C11-N05	-2.37	118.77	121.33
3	B	303	Y05	O10-C07-C09	2.37	111.31	106.88
3	C	303	Y05	C12-C13-C14	-2.34	117.00	120.86
3	B	303	Y05	C12-C11-N05	-2.31	118.19	121.39
3	A	304	Y05	O62-S59-C60	-2.25	104.71	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	Y05	C21-C19-C18	-2.23	107.12	110.88
3	B	303	Y05	F39-C37-C36	-2.22	106.04	110.00
3	A	304	Y05	C07-O10-C02	-2.20	108.86	112.12
3	C	303	Y05	O10-C02-C01	-2.18	102.79	106.88
3	A	304	Y05	C46-C44-C41	2.16	110.03	108.40
3	A	304	Y05	C14-C15-N17	-2.14	120.26	122.41
3	C	303	Y05	C23-C24-C26	-2.11	120.94	123.50
3	B	303	Y05	C66-C56-C54	2.08	120.93	118.10
3	C	303	Y05	C18-C19-N30	2.04	113.14	108.69
3	A	304	Y05	O32-C31-C33	2.01	124.53	121.02
3	C	303	Y05	C56-C54-CL55	2.00	122.20	119.62
3	B	303	Y05	O62-S59-C60	-2.00	105.09	108.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	303	Y05	N35-C36-C37-F39
3	B	303	Y05	C40-C36-C37-F39
3	B	303	Y05	N35-C36-C37-F38
2	B	302	EDO	O1-C1-C2-O2

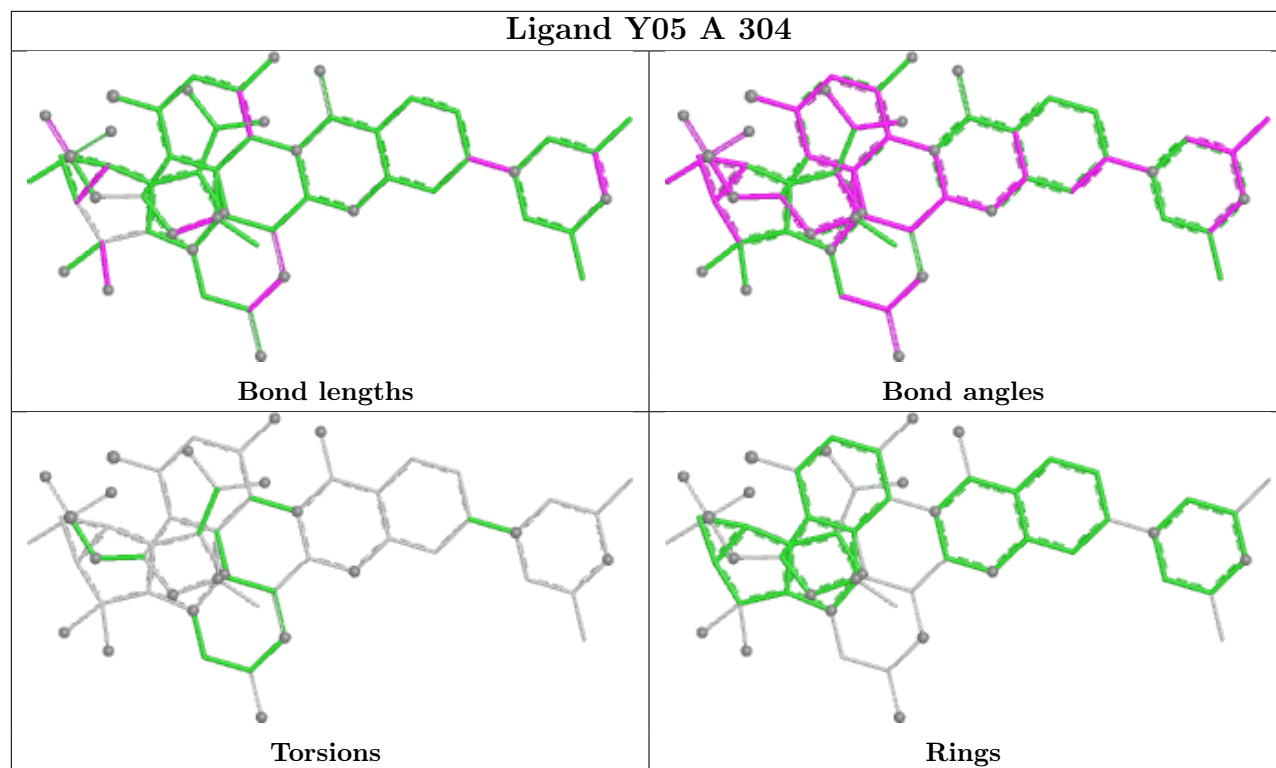
There are no ring outliers.

3 monomers are involved in 3 short contacts:

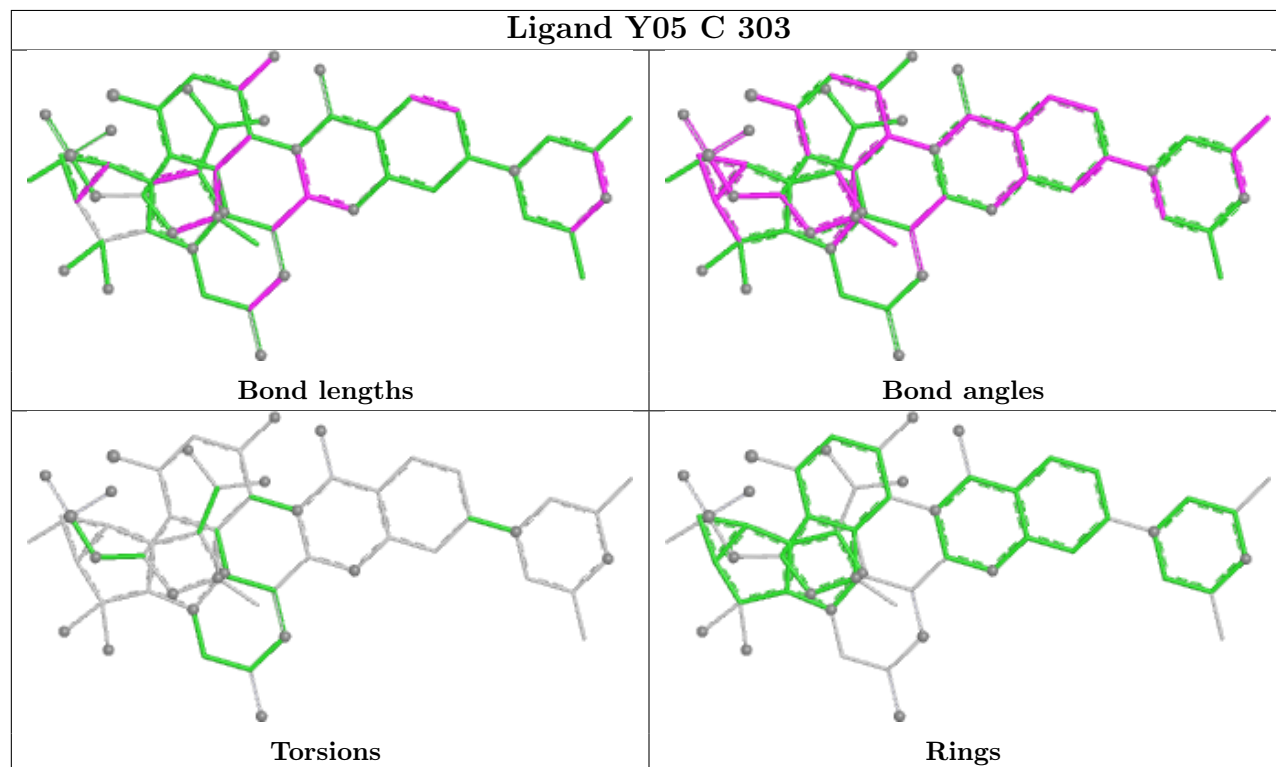
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	Y05	1	0
3	C	303	Y05	1	0
3	B	303	Y05	1	0

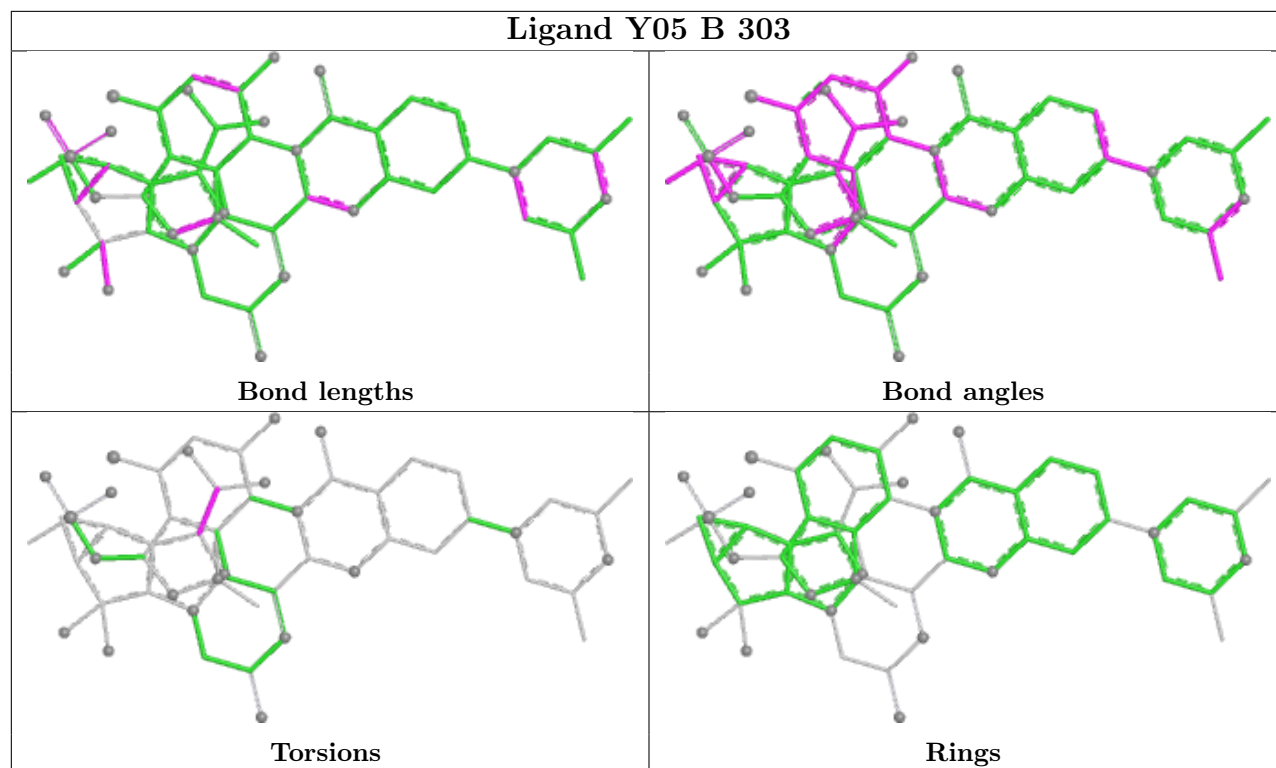
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 Y05 A 304



Ligand Y05 C 303





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	219/232 (94%)	0.01	5 (2%) 61 69	16, 35, 68, 84	5 (2%)
1	B	214/232 (92%)	0.07	14 (6%) 25 29	18, 34, 72, 95	3 (1%)
1	C	219/232 (94%)	0.22	21 (9%) 13 15	15, 32, 90, 126	5 (2%)
All	All	652/696 (93%)	0.10	40 (6%) 27 32	15, 34, 76, 126	13 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	LEU	6.5
1	C	184	ALA	4.7
1	B	184	ALA	4.5
1	C	181	VAL	4.1
1	B	6	LEU	3.9
1	C	92	ALA	3.8
1	C	8	GLY	3.7
1	C	91	ILE	3.7
1	C	177	ALA	3.5
1	C	183	ASN	3.5
1	C	188	THR	3.4
1	C	185	ALA	3.3
1	C	3	VAL	3.2
1	B	188	THR	3.0
1	C	7	GLN	3.0
1	C	186	THR	3.0
1	C	178	SER	3.0
1	C	187	GLU	2.9
1	B	91	ILE	2.9
1	B	185	ALA	2.8
1	C	88	ALA	2.8
1	C	176	GLN	2.8
1	B	86	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	186	THR	2.7
1	A	6	LEU	2.7
1	C	90	PRO	2.6
1	B	178	SER	2.5
1	C	89	GLY	2.5
1	B	7	GLN	2.4
1	C	87	HIS	2.4
1	C	179	GLN	2.4
1	A	87	HIS	2.3
1	A	91	ILE	2.3
1	A	124	ILE	2.3
1	B	207	PRO	2.2
1	B	219	GLN	2.2
1	A	88	ALA	2.1
1	B	89	GLY	2.1
1	B	177	ALA	2.1
1	B	205	LEU	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	EDO	A	301	4/4	0.83	0.14	27,49,67,67	0
2	EDO	A	302	4/4	0.83	0.16	59,71,77,85	0
2	EDO	C	302	4/4	0.83	0.15	43,60,72,72	0
2	EDO	B	301	4/4	0.91	0.12	35,47,54,65	0
2	EDO	A	303	4/4	0.92	0.09	39,48,58,58	0
2	EDO	B	302	4/4	0.94	0.09	32,41,49,53	0

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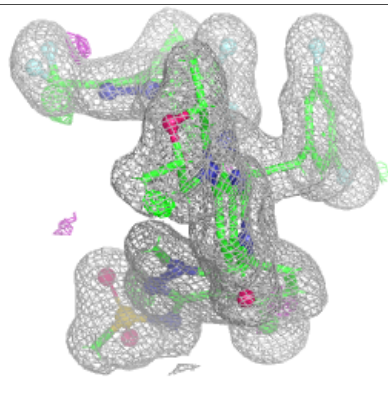
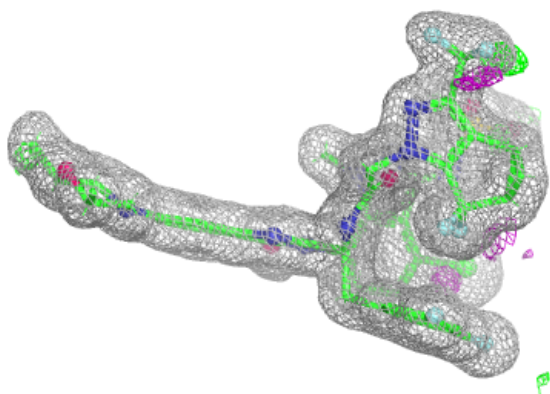
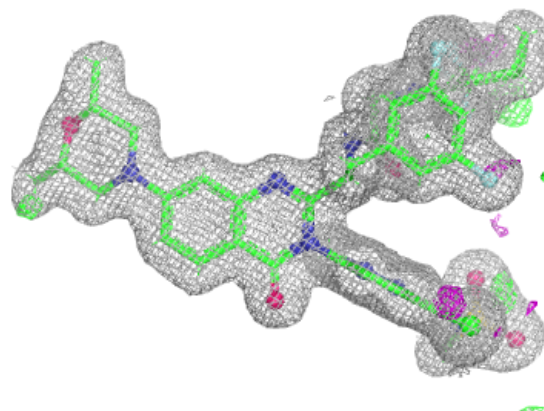
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	C	301	4/4	0.95	0.10	31,43,59,71	0
3	Y05	A	304	63/63	0.98	0.05	18,26,45,54	0
3	Y05	B	303	63/63	0.98	0.06	19,27,45,51	0
3	Y05	C	303	63/63	0.98	0.05	17,24,40,49	0

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.

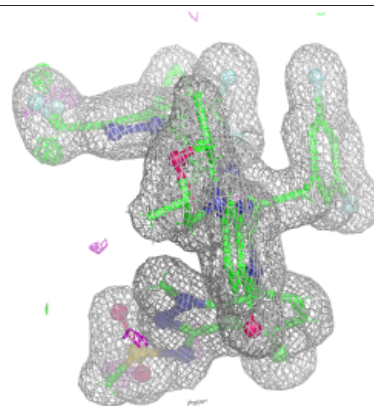
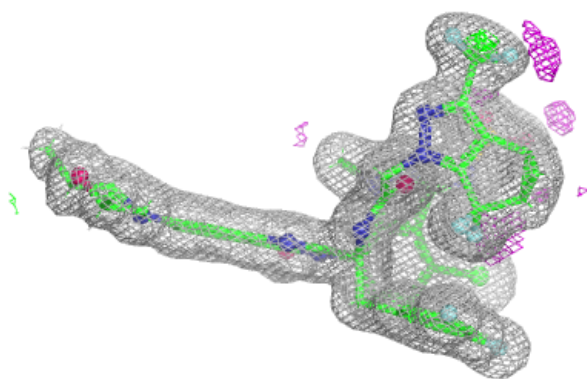
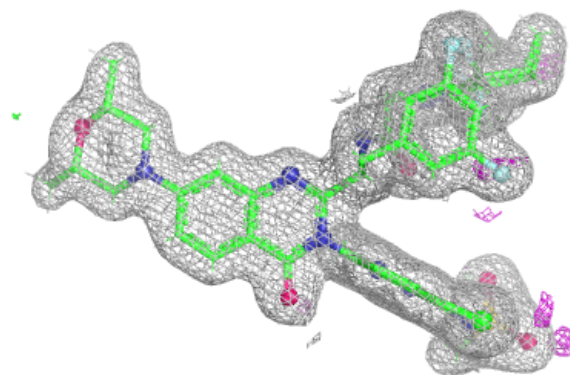
Electron density around Y05 A 304:

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

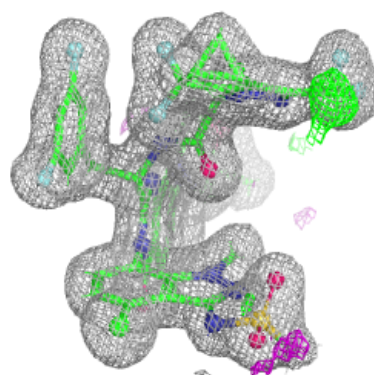
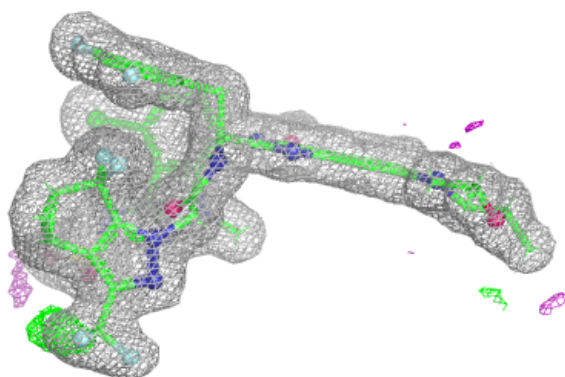
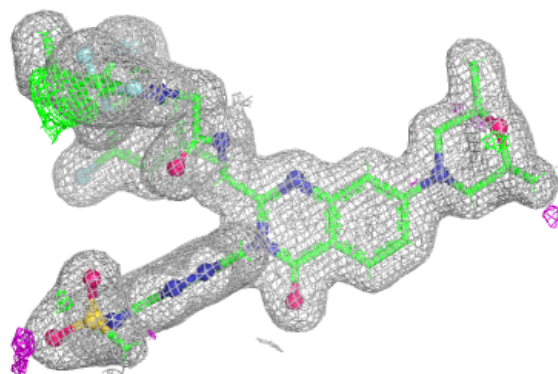


Electron density around Y05 B 303:

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

**Electron density around Y05 C 303:**

$2mF_o-DF_c$ (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.