



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:38 AM UTC

PDB ID : 3ENS / pdb_00003ens
Title : Crystal structure of human FXA in complex with methyl (2Z)-3-[(3-chloro-1-H-indol-7-yl)amino]-2-cyano-3-{[(3S)-2-oxo-1-(2-oxo-2-pyrrolidin-1-ylethyl)azepan-3-yl]amino}acrylate
Authors : Klei, H.E.
Deposited on : 2008-09-25
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

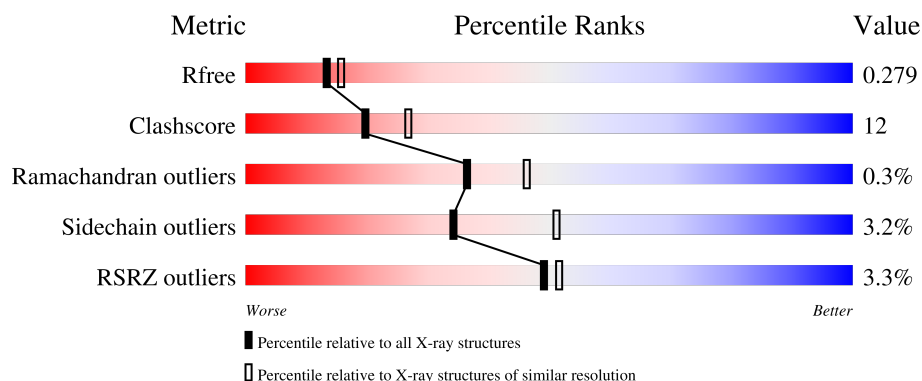
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	94	5% 66% 21% • 11%
1	C	94	6% 71% 16% • 11%
2	B	238	• 71% 28% •
2	D	238	3% 82% 16% •

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5432 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.

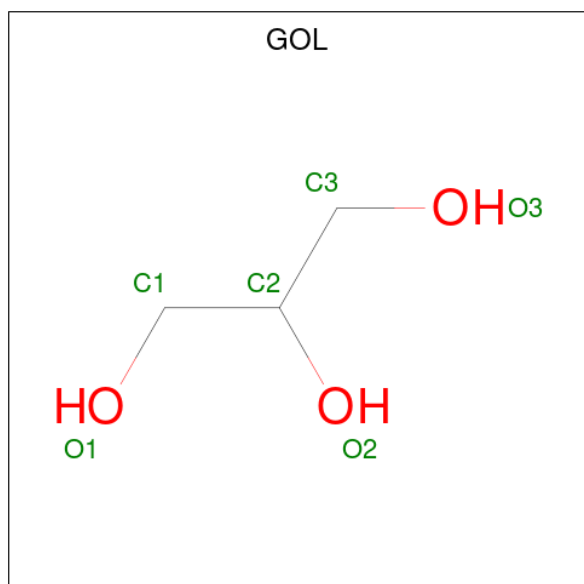
- Molecule 1 is a protein called Factor X light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	84	Total	C	N	O	S	0	0	0
			625	375	106	131	13			
1	C	84	Total	C	N	O	S	0	0	1
			610	366	104	127	13			

- Molecule 2 is a protein called Activated factor Xa heavy chain.

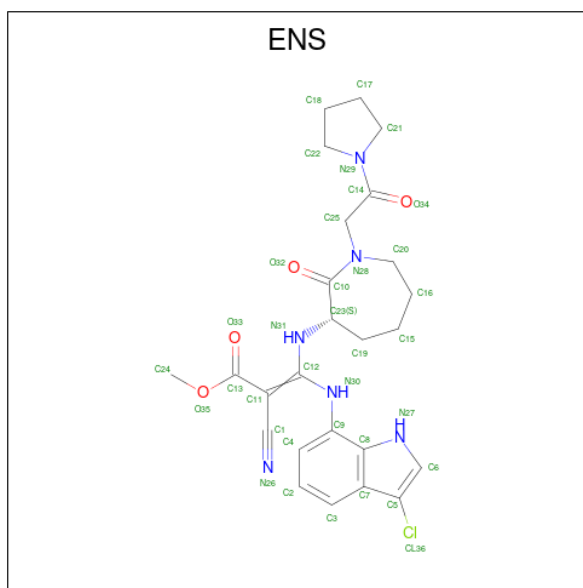
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1879	1183	329	353	14			
2	D	238	Total	C	N	O	S	0	0	0
			1864	1175	324	351	14			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is methyl (2Z)-3-[(3-chloro-1H-indol-7-yl)amino]-2-cyano-3-[[[(3S)-2-oxo-1-(2-oxo-2-pyrrolidin-1-ylethyl)azepan-3-yl]amino}acrylate (CCD ID: ENS) (formula: C₂₅H₂₉ClN₆O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0
			36	25	1	6	4	0
4	D	1	Total	C	Cl	N	O	0
			36	25	1	6	4	0

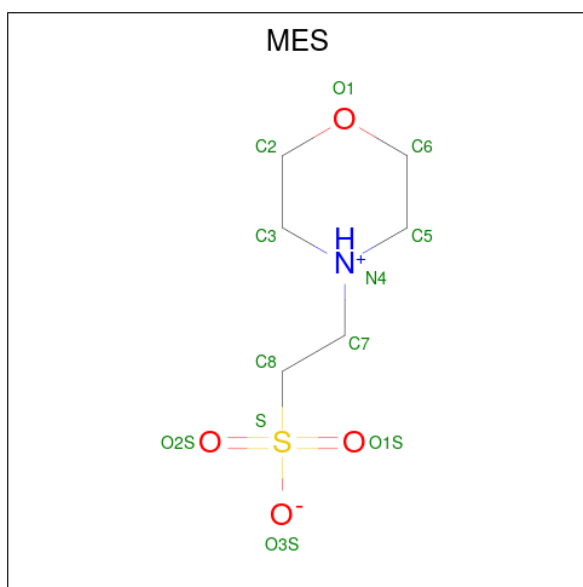
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

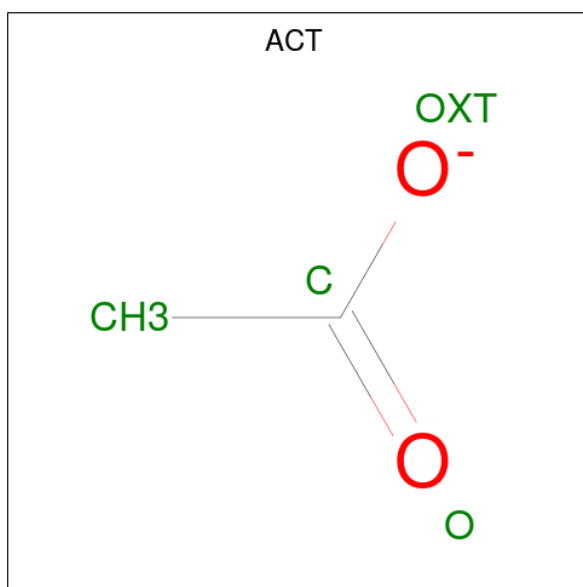
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

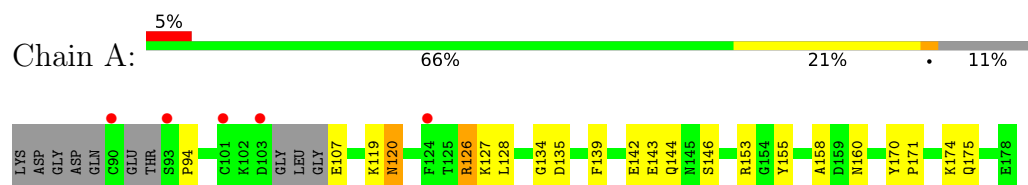
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	28	Total	O	0	0
			28	28		
9	B	126	Total	O	0	0
			126	126		
9	C	26	Total	O	0	0
			26	26		
9	D	124	Total	O	0	0
			124	124		

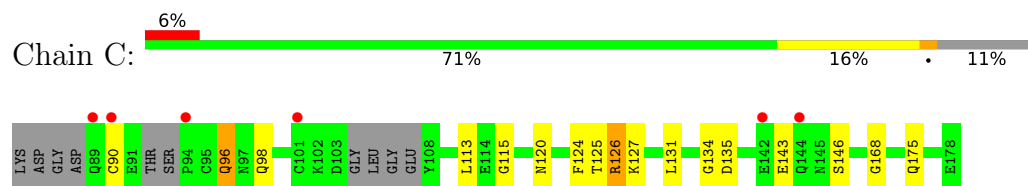
3 Residue-property plots [i](#)

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.

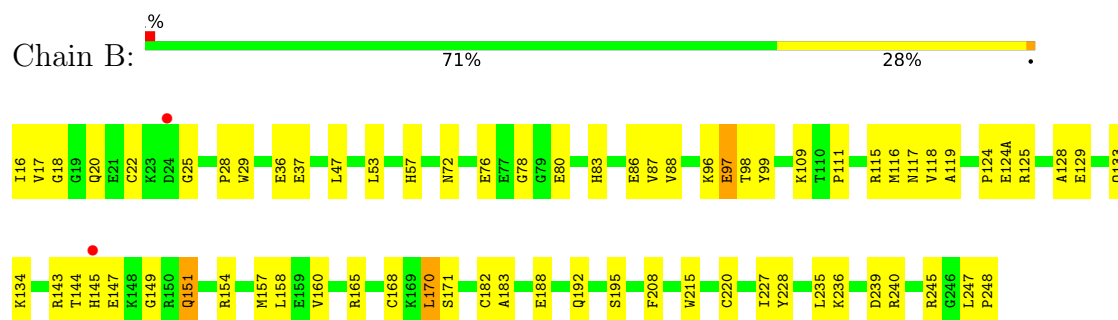
- Molecule 1: Factor X light chain



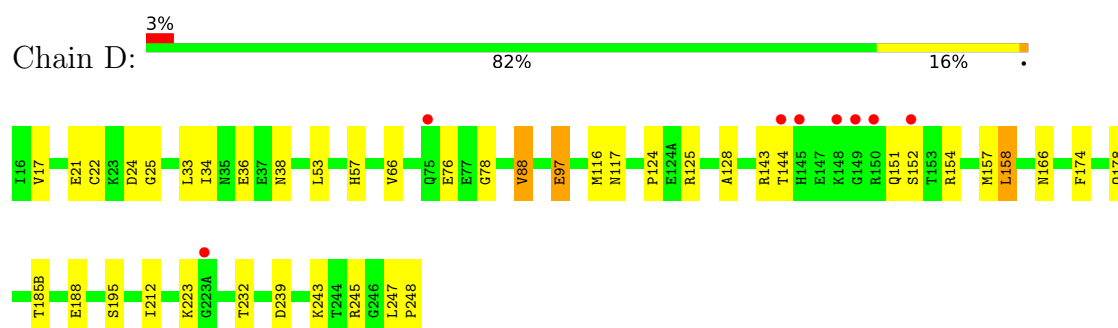
- Molecule 1: Factor X light chain



- Molecule 2: Activated factor Xa heavy chain



- Molecule 2: Activated factor Xa heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.31Å 78.86Å 73.85Å 90.00° 102.82° 90.00°	Depositor
Resolution (Å)	19.03 – 2.30 19.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.03-2.30) 97.1 (19.03-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.30Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.286 0.217 , 0.279	Depositor DCC
R_{free} test set	1000 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5432	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ENS, NA, CA, MES, ACT

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	0.34	0/633	0.75	0/850
1	C	0.34	0/618	0.80	2/830 (0.2%)
2	B	0.40	0/1918	0.77	2/2583 (0.1%)
2	D	0.40	0/1903	0.76	1/2566 (0.0%)
All	All	0.39	0/5072	0.77	5/6829 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	245	ARG	CB-CA-C	-5.38	109.39	115.79
2	B	160	VAL	CA-C-N	5.27	125.19	119.76
2	B	160	VAL	C-N-CA	5.27	125.19	119.76
1	C	168	GLY	CA-C-N	5.21	124.82	119.56
1	C	168	GLY	C-N-CA	5.21	124.82	119.56

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	625	0	550	20	0
1	C	610	0	533	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1879	0	1836	48	0
2	D	1864	0	1805	29	0
3	A	18	0	24	3	0
3	B	6	0	8	0	0
3	D	18	0	24	1	0
4	B	36	0	29	4	0
4	D	36	0	29	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	12	0	12	2	0
7	D	12	0	12	2	0
8	B	4	0	3	0	0
8	D	4	0	3	0	0
9	A	28	0	0	3	0
9	B	126	0	0	4	0
9	C	26	0	0	1	0
9	D	124	0	0	6	0
All	All	5432	0	4868	115	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 12.

All (115) 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)
2:D:24:ASP:HB3	2:D:116:MET:HE3	1.72	0.71
4:B:301:ENS:HN31	4:B:301:ENS:C4	2.03	0.71
2:D:232:THR:HG23	9:D:337:HOH:O	1.92	0.69
2:B:145:HIS:HB3	2:B:149:GLY:HA3	1.74	0.69
2:D:22:CYS:SG	2:D:157:MET:HG2	2.33	0.69
2:B:170:LEU:C	2:B:170:LEU:HD12	2.18	0.68
2:B:125:ARG:O	2:B:129:GLU:HG3	1.95	0.67
1:A:174:LYS:HB3	3:A:203:GOL:H31	1.78	0.66
2:D:36:GLU:H	2:D:36:GLU:CD	2.04	0.64
2:B:22:CYS:SG	2:B:157:MET:HG2	2.37	0.64
2:B:72:ASN:ND2	2:B:154:ARG:HD3	2.13	0.64
2:B:72:ASN:HD22	2:B:154:ARG:HD3	1.61	0.63
2:B:86:GLU:HB2	2:B:109:LYS:HG2	1.82	0.62
2:B:86:GLU:HG2	2:B:87:VAL:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLN:NE2	1:C:96:GLN:H	2.00	0.60
1:C:98:GLN:O	1:C:113:LEU:HD21	2.03	0.59
2:B:134:LYS:HE3	9:D:425:HOH:O	2.04	0.57
2:D:88:VAL:O	3:D:307:GOL:H11	2.05	0.57
2:D:158:LEU:HD11	2:D:188:GLU:HB3	1.86	0.56
2:B:47:LEU:HD11	2:B:53:LEU:HB2	1.87	0.56
2:B:18:GLY:HA3	2:B:188:GLU:HG2	1.88	0.56
1:A:158:ALA:HB1	9:A:221:HOH:O	2.05	0.55
2:D:239:ASP:O	2:D:243:LYS:HG2	2.06	0.55
2:D:34:ILE:HD12	2:D:38:ASN:HD22	1.72	0.55
2:B:57:HIS:CE1	2:B:195:SER:OG	2.60	0.55
2:B:195:SER:HB2	9:B:424:HOH:O	2.05	0.55
1:A:119:LYS:C	1:A:120:ASN:HD22	2.14	0.54
2:B:36:GLU:H	2:B:36:GLU:CD	2.15	0.54
2:D:143:ARG:HA	2:D:151:GLN:HA	1.90	0.54
2:B:192:GLN:HB2	4:B:301:ENS:O33	2.07	0.54
2:B:57:HIS:CE1	2:B:195:SER:HG	2.26	0.54
4:B:301:ENS:C4	4:B:301:ENS:N31	2.69	0.53
2:D:33:LEU:HD22	2:D:66:VAL:HG22	1.89	0.53
2:B:236:LYS:HG2	2:B:240:ARG:HH12	1.74	0.53
2:D:178:GLN:HG2	9:D:395:HOH:O	2.09	0.52
2:D:116:MET:O	2:D:117:ASN:HB2	2.09	0.52
2:B:116:MET:O	2:B:117:ASN:HB2	2.09	0.52
1:A:127:LYS:HE3	1:A:135:ASP:OD1	2.09	0.52
2:D:124:PRO:HB2	2:D:128:ALA:HB2	1.91	0.52
1:A:119:LYS:HG2	1:A:120:ASN:ND2	2.26	0.51
2:B:115:ARG:CZ	2:B:118:VAL:HG21	2.40	0.51
1:C:96:GLN:HG2	1:C:120:ASN:O	2.11	0.50
1:C:126:ARG:HB3	9:C:207:HOH:O	2.11	0.50
2:B:124:PRO:HB2	2:B:128:ALA:HB2	1.93	0.49
2:D:144:THR:CG2	2:D:152:SER:HB2	2.41	0.49
2:B:28:PRO:HB2	2:B:119:ALA:HB3	1.95	0.48
1:C:96:GLN:H	1:C:96:GLN:HE21	1.60	0.48
2:D:97:GLU:H	2:D:97:GLU:CD	2.21	0.48
1:A:174:LYS:HG3	3:A:203:GOL:H11	1.96	0.48
2:B:78:GLY:C	2:B:80:GLU:H	2.21	0.48
2:B:28:PRO:HD2	2:B:29:TRP:CE3	2.49	0.47
7:B:304:MES:H51	9:B:412:HOH:O	2.15	0.47
1:A:120:ASN:HD22	1:A:120:ASN:N	2.12	0.47
2:B:170:LEU:HD12	2:B:171:SER:N	2.30	0.47
1:A:155:TYR:CZ	1:A:171:PRO:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:LYS:HG2	2:B:240:ARG:NH1	2.29	0.47
2:B:124:PRO:HG3	2:B:208:PHE:HB3	1.96	0.47
2:B:183:ALA:HB3	2:B:228:TYR:CE1	2.50	0.46
2:B:16:ILE:O	2:B:144:THR:HA	2.15	0.46
2:B:170:LEU:C	2:B:170:LEU:CD1	2.88	0.46
1:A:160:ASN:OD1	1:A:160:ASN:C	2.58	0.46
2:B:98:THR:O	2:B:99:TYR:HB2	2.15	0.46
2:D:243:LYS:HD3	2:D:243:LYS:HA	1.67	0.46
1:C:115:GLY:HA2	1:C:125:THR:OG1	2.16	0.46
2:B:124:PRO:HD2	2:B:235:LEU:HD21	1.98	0.46
1:A:139:PHE:CD2	2:B:124(A):GLU:HG3	2.51	0.45
1:A:143:GLU:O	1:A:146:SER:HB3	2.16	0.45
1:A:170:TYR:CZ	2:B:115:ARG:HA	2.51	0.45
4:B:301:ENS:H23	4:B:301:ENS:C1	2.47	0.45
1:C:113:LEU:H	1:C:113:LEU:CD2	2.29	0.45
2:D:57:HIS:CE1	2:D:195:SER:OG	2.69	0.45
2:B:215:TRP:CE2	2:B:227:ILE:HG21	2.52	0.45
1:A:134:GLY:O	1:A:135:ASP:HB2	2.17	0.44
1:C:126:ARG:NH2	1:C:146:SER:OG	2.50	0.44
1:C:143:GLU:O	1:C:146:SER:HB3	2.17	0.44
2:D:185(B):THR:HA	2:D:223:LYS:HD2	2.00	0.44
7:D:304:MES:H81	9:D:418:HOH:O	2.16	0.44
1:A:119:LYS:HE2	2:D:174:PHE:CE1	2.53	0.43
2:B:97:GLU:CD	2:B:97:GLU:H	2.25	0.43
2:D:24:ASP:HB3	2:D:116:MET:CE	2.44	0.43
1:C:134:GLY:O	1:C:135:ASP:HB2	2.19	0.43
1:A:126:ARG:HB3	9:A:211:HOH:O	2.18	0.42
1:A:128:LEU:HB3	1:A:142:GLU:OE1	2.19	0.42
2:B:115:ARG:HG2	2:B:118:VAL:HB	2.01	0.42
1:C:175:GLN:HB3	2:D:25:GLY:O	2.19	0.42
2:D:125:ARG:NH2	9:D:432:HOH:O	2.53	0.42
2:B:147:GLU:HB2	2:B:220:CYS:HB2	2.01	0.42
1:C:113:LEU:N	1:C:113:LEU:HD22	2.34	0.42
1:A:153:ARG:O	1:A:153:ARG:HG3	2.19	0.42
2:B:72:ASN:HB2	2:B:154:ARG:HH21	1.85	0.42
2:B:96:LYS:HG3	9:B:393:HOH:O	2.20	0.42
2:B:245:ARG:HB3	9:B:386:HOH:O	2.20	0.42
1:C:124:PHE:N	1:C:124:PHE:CD2	2.87	0.42
2:D:57:HIS:CE1	2:D:195:SER:HG	2.36	0.42
2:B:83:HIS:HE1	2:B:111:PRO:O	2.03	0.41
1:C:124:PHE:N	1:C:124:PHE:HD2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLN:C	1:A:146:SER:N	2.78	0.41
2:B:17:VAL:O	2:B:188:GLU:HA	2.20	0.41
1:A:143:GLU:O	1:A:144:GLN:HB2	2.19	0.41
1:A:175:GLN:HB3	2:B:25:GLY:O	2.21	0.41
2:D:21:GLU:CD	2:D:154:ARG:HD2	2.45	0.41
7:D:304:MES:H31	9:D:418:HOH:O	2.19	0.41
3:A:203:GOL:H2	9:A:209:HOH:O	2.20	0.41
2:B:143:ARG:HA	2:B:151:GLN:HA	2.03	0.41
2:B:165:ARG:O	2:B:168:CYS:HB3	2.21	0.41
1:C:90:CYS:O	1:C:90:CYS:SG	2.79	0.41
2:D:17:VAL:HG22	2:D:144:THR:O	2.20	0.41
2:D:166:ASN:HD22	2:D:166:ASN:HA	1.64	0.41
2:B:168:CYS:HB2	2:B:182:CYS:HB2	1.97	0.40
2:D:247:LEU:HA	2:D:248:PRO:HD3	1.86	0.40
2:B:236:LYS:HD3	7:B:304:MES:O3S	2.22	0.40
1:C:127:LYS:HD3	1:C:131:LEU:O	2.22	0.40
2:D:76:GLU:C	2:D:78:GLY:H	2.29	0.40
2:B:247:LEU:HA	2:B:248:PRO:HD3	1.85	0.40
2:D:53:LEU:HD21	2:D:212:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	79/94 (84%)	72 (91%)	6 (8%)	1 (1%)	9	10
1	C	78/94 (83%)	75 (96%)	3 (4%)	0	100	100
2	B	236/238 (99%)	224 (95%)	11 (5%)	1 (0%)	30	38
2	D	236/238 (99%)	226 (96%)	10 (4%)	0	100	100
All	All	629/664 (95%)	597 (95%)	30 (5%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	PRO
2	B	76	GLU

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	71/80 (89%)	68 (96%)	3 (4%)	26	40
1	C	68/80 (85%)	66 (97%)	2 (3%)	37	55
2	B	201/202 (100%)	192 (96%)	9 (4%)	24	37
2	D	197/202 (98%)	194 (98%)	3 (2%)	57	75
All	All	537/564 (95%)	520 (97%)	17 (3%)	34	51

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	120	ASN
1	A	126	ARG
2	B	20	GLN
2	B	37	GLU
2	B	88	VAL
2	B	97	GLU
2	B	133	GLN
2	B	151	GLN
2	B	158	LEU
2	B	170	LEU
2	B	239	ASP
1	C	96	GLN
1	C	126	ARG
2	D	88	VAL
2	D	97	GLU
2	D	158	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	144	GLN
2	B	30	GLN
2	B	151	GLN
2	B	187	GLN
1	C	96	GLN
1	C	141	HIS
1	C	145	ASN
2	D	38	ASN
2	D	133	GLN
2	D	166	ASN
2	D	187	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\# Z > 2$
3	GOL	A	202	-	5,5,5	0.35	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	305	-	5,5,5	0.31	0	5,5,5	0.23	0
3	GOL	D	306	-	5,5,5	0.31	0	5,5,5	0.46	0
4	ENS	B	301	-	38,39,39	3.93	16 (42%)	45,54,54	1.68	9 (20%)
4	ENS	D	301	-	38,39,39	3.90	16 (42%)	45,54,54	1.65	9 (20%)
3	GOL	B	305	-	5,5,5	0.34	0	5,5,5	0.30	0
3	GOL	A	201	-	5,5,5	0.36	0	5,5,5	0.42	0
3	GOL	A	203	-	5,5,5	0.37	0	5,5,5	0.50	0
7	MES	B	304	-	12,12,12	2.25	1 (8%)	15,16,16	2.33	6 (40%)
8	ACT	D	308	-	3,3,3	0.78	0	3,3,3	1.37	0
7	MES	D	304	-	12,12,12	2.08	1 (8%)	15,16,16	2.26	6 (40%)
8	ACT	B	306	-	3,3,3	0.74	0	3,3,3	1.27	0
3	GOL	D	307	-	5,5,5	0.36	0	5,5,5	0.16	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
3	GOL	A	202	-	-	2/4/4/4	-
3	GOL	D	305	-	-	3/4/4/4	-
3	GOL	D	306	-	-	2/4/4/4	-
4	ENS	B	301	-	-	2/26/50/50	0/4/4/4
4	ENS	D	301	-	-	3/26/50/50	0/4/4/4
3	GOL	B	305	-	-	0/4/4/4	-
3	GOL	A	201	-	-	0/4/4/4	-
3	GOL	A	203	-	-	2/4/4/4	-
7	MES	B	304	-	-	1/6/14/14	0/1/1/1
7	MES	D	304	-	-	2/6/14/14	0/1/1/1
3	GOL	D	307	-	-	2/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	ENS	C1-N26	12.04	1.35	1.14
4	D	301	ENS	C1-N26	11.86	1.35	1.14
4	D	301	ENS	C23-C10	-10.20	1.39	1.53
4	B	301	ENS	C23-C10	-10.19	1.39	1.53
4	D	301	ENS	C1-C11	-8.85	1.24	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	ENS	C1-C11	-8.81	1.24	1.43
4	B	301	ENS	O32-C10	8.14	1.36	1.22
4	D	301	ENS	O32-C10	7.92	1.36	1.22
4	B	301	ENS	O33-C13	7.83	1.37	1.21
7	B	304	MES	C8-S	-7.50	1.67	1.77
4	D	301	ENS	O33-C13	7.47	1.36	1.21
7	D	304	MES	C8-S	-6.90	1.67	1.77
4	D	301	ENS	O34-C14	6.11	1.36	1.23
4	B	301	ENS	O34-C14	5.88	1.35	1.23
4	D	301	ENS	C11-C13	-4.53	1.36	1.47
4	B	301	ENS	C11-C13	-4.41	1.36	1.47
4	D	301	ENS	C10-N28	3.18	1.38	1.35
4	B	301	ENS	C7-C8	-3.16	1.37	1.41
4	D	301	ENS	C7-C8	-3.11	1.37	1.41
4	B	301	ENS	C10-N28	2.99	1.38	1.35
4	B	301	ENS	O35-C13	-2.81	1.27	1.33
4	D	301	ENS	C12-N31	2.79	1.39	1.34
4	D	301	ENS	O35-C13	-2.73	1.27	1.33
4	B	301	ENS	C12-N30	-2.63	1.30	1.35
4	B	301	ENS	C7-C5	-2.45	1.37	1.44
4	D	301	ENS	C7-C5	-2.43	1.37	1.44
4	B	301	ENS	C14-N29	-2.42	1.30	1.35
4	D	301	ENS	C9-N30	-2.28	1.37	1.41
4	D	301	ENS	C6-C5	2.26	1.39	1.36
4	B	301	ENS	C12-N31	2.22	1.38	1.34
4	B	301	ENS	C9-N30	-2.21	1.37	1.41
4	D	301	ENS	C14-N29	-2.18	1.31	1.35
4	B	301	ENS	C4-C9	2.10	1.43	1.39
4	D	301	ENS	C12-N30	-2.04	1.31	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	304	MES	C5-N4-C3	5.45	120.58	108.84
7	D	304	MES	C5-N4-C3	5.27	120.20	108.84
4	D	301	ENS	O35-C13-C11	4.47	119.29	111.47
4	B	301	ENS	C25-C14-N29	4.25	122.19	117.04
4	B	301	ENS	O35-C13-C11	4.14	118.71	111.47
7	B	304	MES	C7-N4-C3	3.91	121.65	111.24
7	D	304	MES	C7-N4-C3	3.77	121.28	111.24
4	D	301	ENS	C25-C14-N29	3.59	121.39	117.04
4	B	301	ENS	O32-C10-N28	-3.27	119.44	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	ENS	C8-N27-C6	-3.26	106.12	108.93
4	D	301	ENS	C8-N27-C6	-3.14	106.22	108.93
4	B	301	ENS	C3-C7-C8	3.06	122.59	119.14
4	D	301	ENS	O33-C13-C11	-3.06	118.93	125.14
4	D	301	ENS	O32-C10-N28	-3.00	119.70	122.55
4	B	301	ENS	O33-C13-C11	-2.97	119.12	125.14
4	B	301	ENS	C9-C8-N27	-2.81	127.63	130.39
4	D	301	ENS	C3-C7-C8	2.81	122.30	119.14
7	B	304	MES	C2-C3-N4	-2.78	105.89	110.12
7	D	304	MES	C6-C5-N4	-2.75	105.94	110.12
7	D	304	MES	C7-N4-C5	2.73	118.53	111.24
4	B	301	ENS	C23-N31-C12	2.60	128.61	121.27
7	B	304	MES	O2S-S-C8	2.46	110.44	106.73
7	B	304	MES	C7-N4-C5	2.45	117.76	111.24
7	B	304	MES	O3S-S-C8	2.31	110.53	106.00
4	D	301	ENS	C19-C23-C10	-2.31	108.70	111.65
7	D	304	MES	O3S-S-C8	2.27	110.45	106.00
4	B	301	ENS	C7-C8-N27	2.26	110.75	107.54
4	D	301	ENS	C9-C8-N27	-2.21	128.22	130.39
4	D	301	ENS	C7-C8-N27	2.09	110.51	107.54
7	D	304	MES	O1S-S-C8	2.01	109.76	106.73

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	GOL	O1-C1-C2-C3
3	A	203	GOL	O1-C1-C2-C3
3	D	306	GOL	O1-C1-C2-C3
3	D	307	GOL	O1-C1-C2-C3
4	B	301	ENS	C1-C11-C12-N30
4	B	301	ENS	C1-C11-C12-N31
4	D	301	ENS	C1-C11-C12-N30
4	D	301	ENS	C19-C23-N31-C12
7	B	304	MES	C8-C7-N4-C3
7	D	304	MES	C8-C7-N4-C3
3	A	202	GOL	O1-C1-C2-O2
3	A	203	GOL	O1-C1-C2-O2
3	D	305	GOL	C1-C2-C3-O3
3	D	306	GOL	O1-C1-C2-O2
3	D	307	GOL	O1-C1-C2-O2
7	D	304	MES	C8-C7-N4-C5

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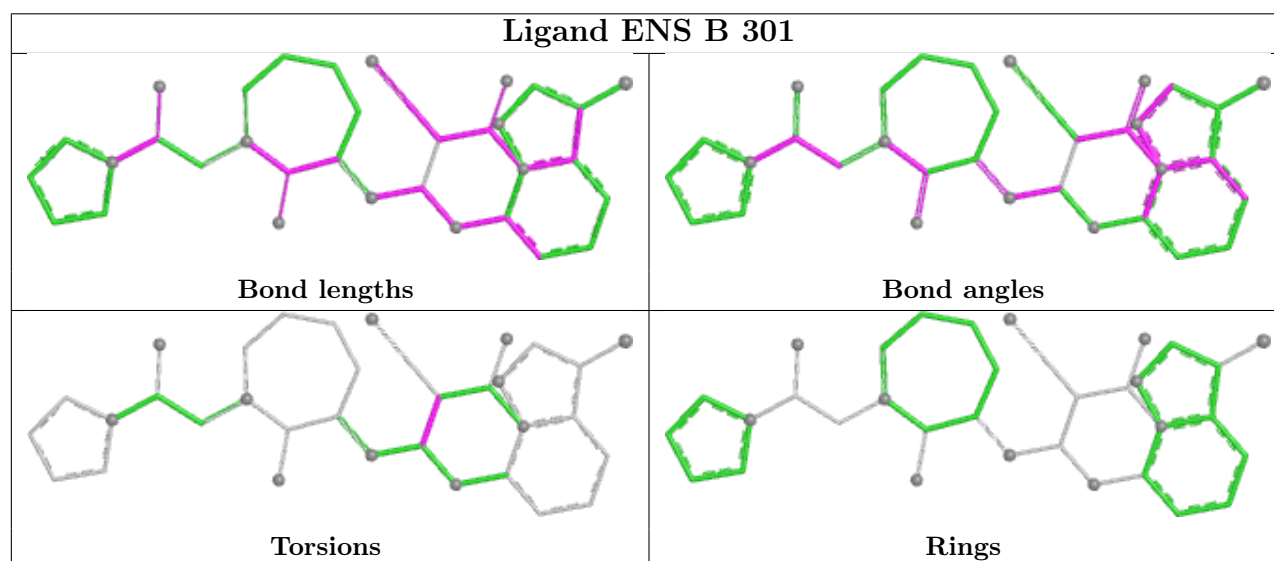
Mol	Chain	Res	Type	Atoms
3	D	305	GOL	O2-C2-C3-O3
4	D	301	ENS	C13-C11-C12-N31
3	D	305	GOL	O1-C1-C2-O2

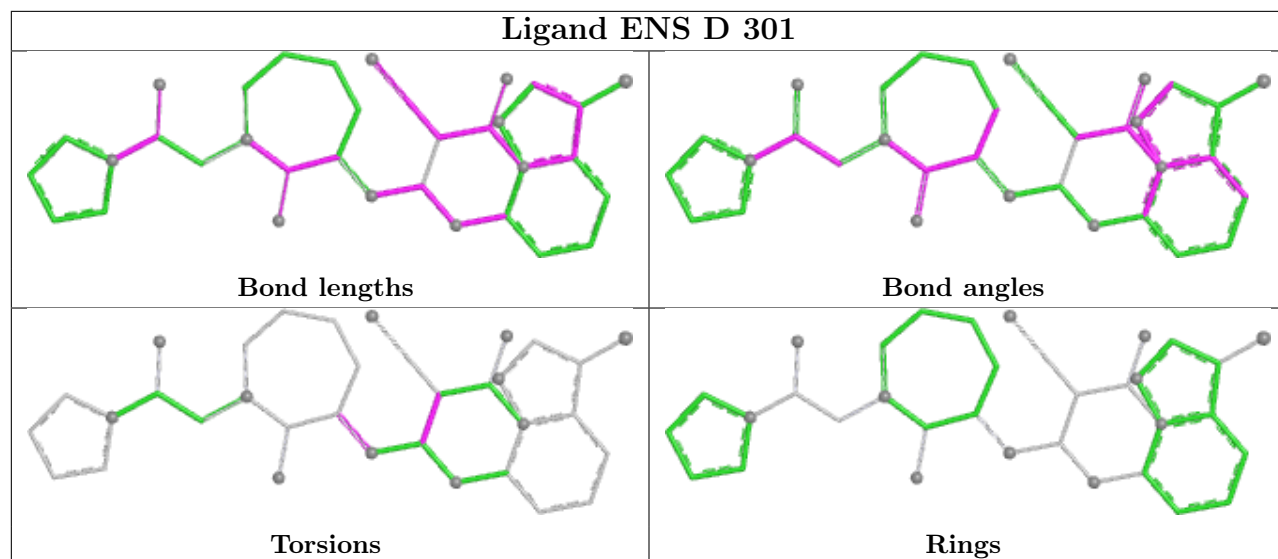
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	ENS	4	0
3	A	203	GOL	3	0
7	B	304	MES	2	0
7	D	304	MES	2	0
3	D	307	GOL	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.





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	84/94 (89%)	0.53	5 (5%) 27 29	21, 30, 52, 57	0
1	C	84/94 (89%)	0.65	6 (7%) 22 24	20, 32, 58, 63	0
2	B	238/238 (100%)	0.16	2 (0%) 82 83	20, 24, 35, 46	0
2	D	238/238 (100%)	0.32	8 (3%) 48 50	19, 24, 37, 43	0
All	All	644/664 (96%)	0.33	21 (3%) 49 51	19, 25, 44, 63	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	89	GLN	3.8
2	D	145	HIS	3.6
1	A	90	CYS	3.4
2	D	148	LYS	2.8
2	D	150	ARG	2.8
1	C	94	PRO	2.8
2	D	149	GLY	2.7
1	C	142	GLU	2.7
2	D	152	SER	2.7
1	A	101	CYS	2.6
1	C	90	CYS	2.5
2	D	144	THR	2.4
1	A	93	SER	2.3
1	A	103	ASP	2.3
1	A	124	PHE	2.2
2	B	24	ASP	2.2
1	C	144	GLN	2.1
2	D	75	GLN	2.1
2	B	145	HIS	2.1
2	D	223(A)	GLY	2.1
1	C	101	CYS	2.1

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](#)

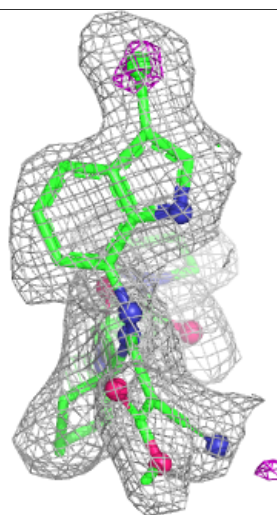
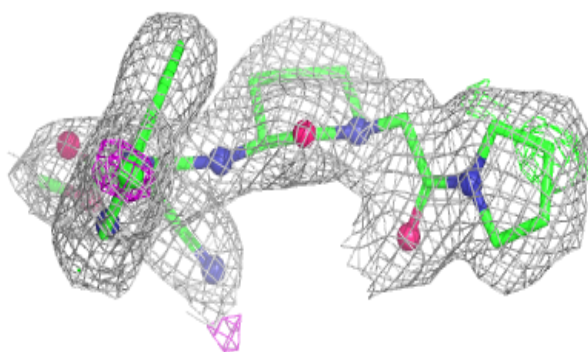
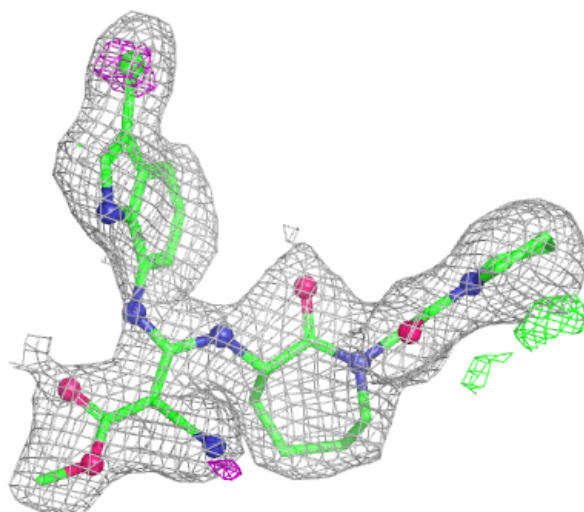
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	CA	D	302	1/1	0.58	0.19	45,45,45,45	0
6	NA	B	303	1/1	0.67	0.16	29,29,29,29	0
6	NA	D	303	1/1	0.76	0.11	31,31,31,31	0
5	CA	B	302	1/1	0.79	0.21	44,44,44,44	0
8	ACT	D	308	4/4	0.79	0.13	31,31,31,31	0
3	GOL	A	202	6/6	0.85	0.13	28,29,29,30	0
4	ENS	D	301	36/36	0.86	0.10	24,28,31,33	0
3	GOL	A	203	6/6	0.87	0.18	23,23,24,25	0
3	GOL	B	305	6/6	0.88	0.09	22,23,24,24	0
8	ACT	B	306	4/4	0.89	0.12	27,27,27,28	0
3	GOL	D	305	6/6	0.89	0.09	22,23,23,24	0
4	ENS	B	301	36/36	0.90	0.08	23,27,30,31	0
3	GOL	D	307	6/6	0.90	0.17	23,23,24,24	0
3	GOL	D	306	6/6	0.91	0.10	20,20,20,20	0
7	MES	D	304	12/12	0.93	0.10	20,21,23,24	0
7	MES	B	304	12/12	0.96	0.08	21,22,23,24	0
3	GOL	A	201	6/6	0.97	0.07	20,21,21,22	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.

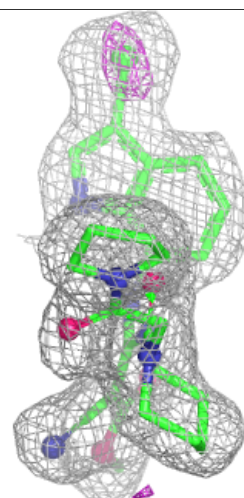
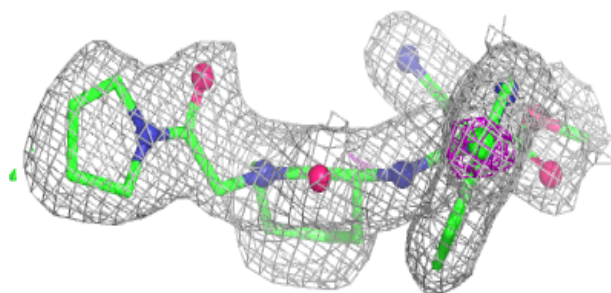
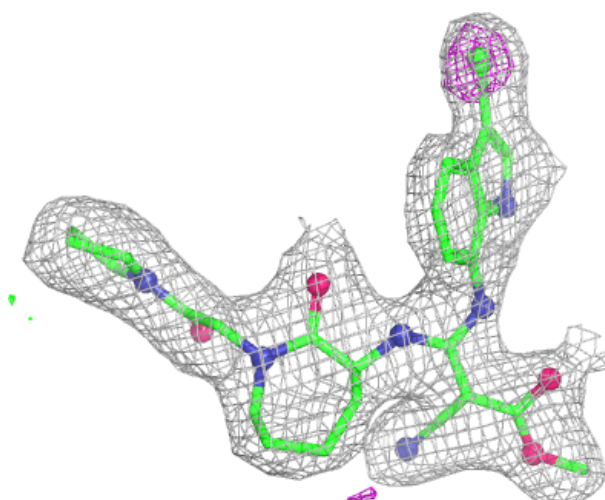
Electron density around ENS D 301:

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



Electron density around ENS B 301:

$2mF_o-DF_c$ (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.