



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 10:57 pm BST

PDB ID : 3ENS
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 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

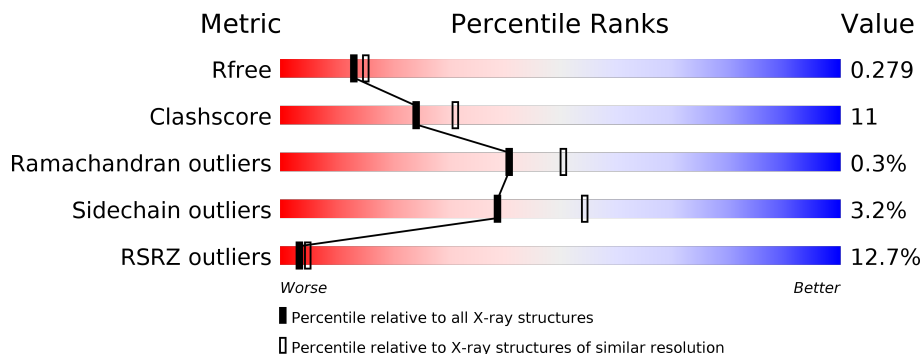
1 Overall quality at a glance i

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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	94	<div style="display: flex; align-items: center;"> <div style="width: 20%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">20% 66% 22% • 11%</p>
1	C	94	<div style="display: flex; align-items: center;"> <div style="width: 23%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">23% 72% 15% • 11%</p>
2	B	238	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">7% 71% 27% •</p>
2	D	238	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">11% 84% 15% •</p>

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
			Total	C	N	O	S			
1	A	84	Total 625	C 375	N 106	O 131	S 13	0	0	0
1	C	84	Total 610	C 366	N 104	O 127	S 13	0	0	1

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

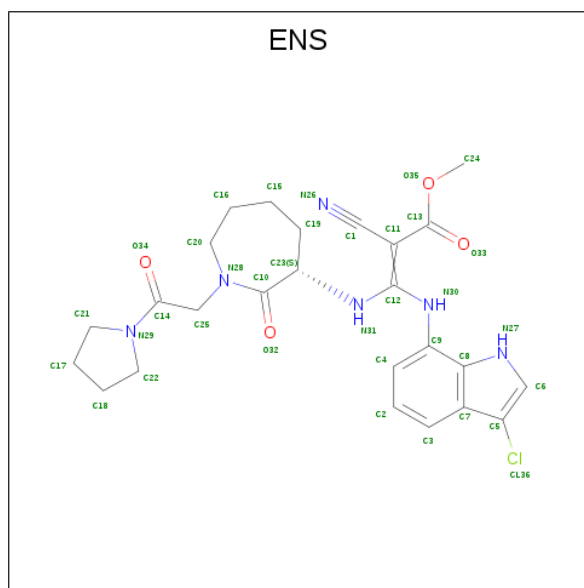
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	238	Total 1879	C 1183	N 329	O 353	S 14	0	0	0
2	D	238	Total 1864	C 1175	N 324	O 351	S 14	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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 (three-letter code: ENS) (formula: C₂₅H₂₉ClN₆O₄).



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

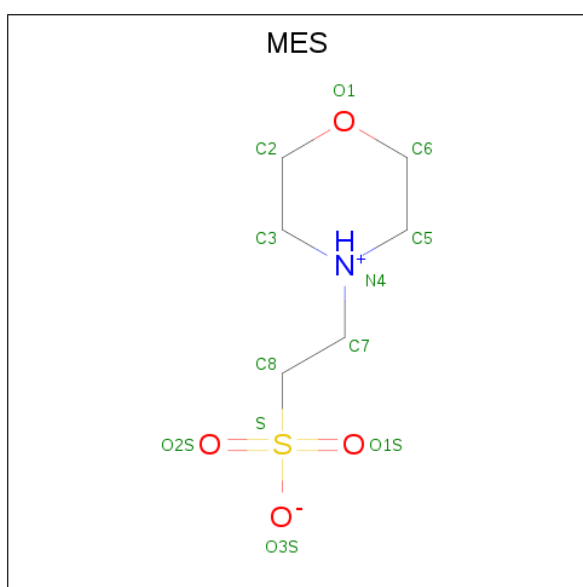
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

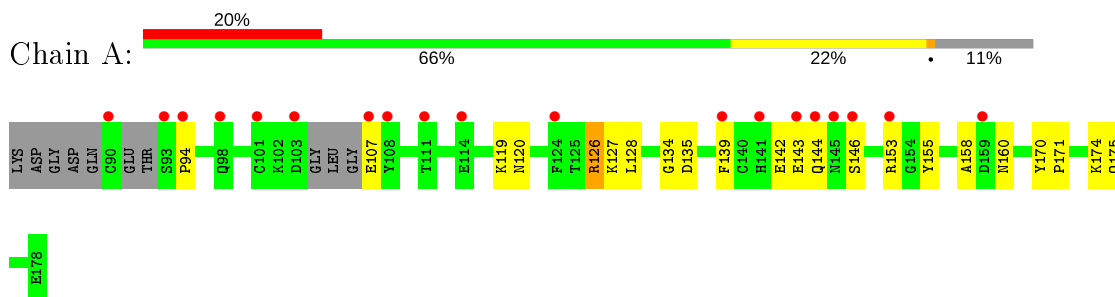
- Molecule 9 is water.

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

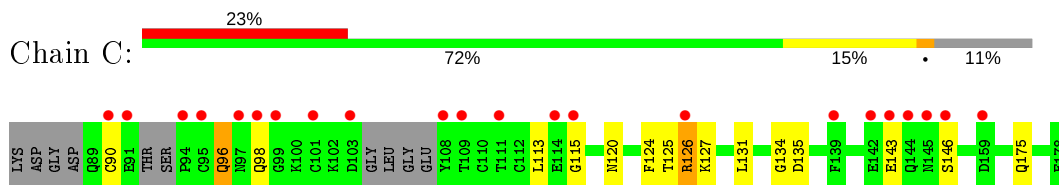
3 Residue-property plots [i](#)

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.

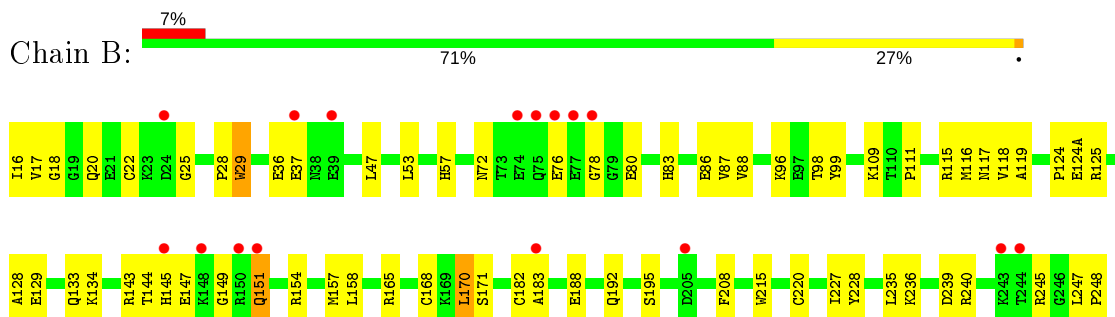
- Molecule 1: Factor X light chain



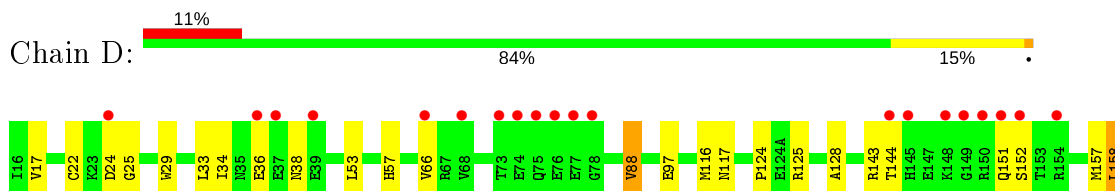
- Molecule 1: Factor X light chain

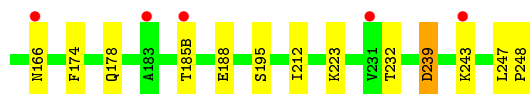


- Molecule 2: Activated factor Xa heavy chain



- 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) 97.3 (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)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.286 0.216 , 0.279	Depositor DCC
R_{free} test set	1000 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtrriage
Anisotropy	0.375	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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, NA, CA, ENS, 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	0.32	0/633	0.47	0/850
1	C	0.30	0/618	0.47	0/830
2	B	0.32	0/1918	0.52	0/2583
2	D	0.33	0/1903	0.51	0/2566
All	All	0.32	0/5072	0.50	0/6829

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	625	0	550	19	0
1	C	610	0	533	16	0
2	B	1879	0	1836	47	0
2	D	1864	0	1805	26	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	110	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 11.

All (110) 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)
4:B:301:ENS:C4	4:B:301:ENS:HN31	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: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: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:170:LEU:HD12	2:B:170:LEU:C	2.18	0.63
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
2:D:36:GLU:CD	2:D:36:GLU:H	2.04	0.60
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:195:SER:HB2	9:B:424:HOH:O	2.05	0.55
2:B:57:HIS:CE1	2:B:195:SER:OG	2.60	0.55
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:N31	4:B:301:ENS:C4	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
1:A:119:LYS:C	1:A:120:ASN:HD22	2.14	0.50
2:B:124:PRO:HB2	2:B:128:ALA:HB2	1.93	0.49
2:B:36:GLU:H	2:B:36:GLU:CD	2.15	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
2:D:24:ASP:HB3	2:D:116:MET:CE	2.44	0.48
1:C:96:GLN:H	1:C:96:GLN:HE21	1.60	0.48
1:A:174:LYS:HG3	3:A:203:GOL:H11	1.96	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
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:98:THR:O	2:B:99:TYR:HB2	2.15	0.46
2:D:243:LYS:HA	2:D:243:LYS:HD3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:GLY:C	2:B:80:GLU:H	2.21	0.43
1:C:134:GLY:O	1:C:135:ASP:HB2	2.19	0.43
2:D:97:GLU:H	2:D:97:GLU:CD	2.21	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
2:D:125:ARG:NH2	9:D:432:HOH:O	2.53	0.42
1:C:175:GLN:HB3	2:D:25:GLY:O	2.19	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:HG3	1:A:153:ARG:O	2.19	0.42
2:B:72:ASN:HB2	2:B:154:ARG:HH21	1.85	0.42
2:B:245:ARG:HB3	9:B:386:HOH:O	2.20	0.42
2:B:96:LYS:HG3	9:B:393: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:170:LEU:C	2:B:170:LEU:CD1	2.88	0.41
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
2:B:17:VAL:O	2:B:188:GLU:HA	2.20	0.41
1:A:160:ASN:C	1:A:160:ASN:OD1	2.58	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
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:SG	1:C:90:CYS:O	2.79	0.41
2:D:17:VAL:HG22	2:D:144:THR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 [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	79/94 (84%)	72 (91%)	6 (8%)	1 (1%)	12	12
1	C	78/94 (83%)	75 (96%)	3 (4%)	0	100	100
2	B	236/238 (99%)	224 (95%)	11 (5%)	1 (0%)	34	42
2	D	236/238 (99%)	226 (96%)	10 (4%)	0	100	100
All	All	629/664 (95%)	597 (95%)	30 (5%)	2 (0%)	41	50

All (2) Ramachandran outliers are listed below:

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

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	71/80 (89%)	69 (97%)	2 (3%)	43	60
1	C	68/80 (85%)	66 (97%)	2 (3%)	42	58
2	B	201/202 (100%)	192 (96%)	9 (4%)	27	39
2	D	197/202 (98%)	193 (98%)	4 (2%)	55	72
All	All	537/564 (95%)	520 (97%)	17 (3%)	39	54

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

Mol	Chain	Res	Type
1	A	107	GLU
1	A	126	ARG
2	B	20	GLN
2	B	29	TRP
2	B	37	GLU
2	B	88	VAL
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	29	TRP
2	D	88	VAL
2	D	158	LEU
2	D	239	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	151	GLN
2	D	166	ASN

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 carbohydrates 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	201	-	5,5,5	0.36	0	5,5,5	0.38	0
3	GOL	D	307	-	5,5,5	0.36	0	5,5,5	0.14	0
3	GOL	A	202	-	5,5,5	0.34	0	5,5,5	0.21	0
3	GOL	A	203	-	5,5,5	0.37	0	5,5,5	0.47	0
7	MES	B	304	-	12,12,12	2.20	1 (8%)	14,16,16	2.48	6 (42%)
8	ACT	B	306	-	1,3,3	1.37	0	0,3,3	0.00	-
7	MES	D	304	-	12,12,12	2.03	1 (8%)	14,16,16	2.40	6 (42%)
3	GOL	D	306	-	5,5,5	0.31	0	5,5,5	0.42	0
4	ENS	D	301	-	35,39,39	4.01	11 (31%)	37,54,54	1.59	8 (21%)
4	ENS	B	301	-	35,39,39	4.05	12 (34%)	37,54,54	1.62	8 (21%)
8	ACT	D	308	-	1,3,3	1.15	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	305	-	5,5,5	0.34	0	5,5,5	0.27	0
3	GOL	D	305	-	5,5,5	0.30	0	5,5,5	0.21	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	D	307	-	-	2/4/4/4	-
3	GOL	A	202	-	-	2/4/4/4	-
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	306	-	-	2/4/4/4	-
4	ENS	D	301	-	-	3/26/50/50	0/4/4/4
3	GOL	D	305	-	-	4/4/4/4	-
4	ENS	B	301	-	-	2/26/50/50	0/4/4/4
3	GOL	B	305	-	-	0/4/4/4	-
3	GOL	A	201	-	-	0/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	ENS	C1-N26	12.34	1.35	1.14
4	D	301	ENS	C1-N26	12.15	1.35	1.14
4	D	301	ENS	C23-C10	-9.96	1.39	1.53
4	B	301	ENS	C23-C10	-9.94	1.39	1.53
4	D	301	ENS	C1-C11	-9.75	1.24	1.43
4	B	301	ENS	C1-C11	-9.71	1.24	1.43
4	B	301	ENS	O32-C10	8.16	1.36	1.22
4	D	301	ENS	O32-C10	7.94	1.36	1.22
4	B	301	ENS	O33-C13	7.60	1.37	1.21
7	B	304	MES	C8-S	-7.34	1.67	1.77
4	D	301	ENS	O33-C13	7.25	1.36	1.21
7	D	304	MES	C8-S	-6.75	1.67	1.77
4	D	301	ENS	O34-C14	5.95	1.36	1.23
4	B	301	ENS	O34-C14	5.72	1.35	1.23
4	D	301	ENS	C11-C13	-4.52	1.36	1.47
4	B	301	ENS	C11-C13	-4.40	1.36	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	ENS	C10-N28	3.18	1.38	1.35
4	B	301	ENS	C10-N28	2.99	1.38	1.35
4	B	301	ENS	O35-C13	-2.74	1.27	1.33
4	D	301	ENS	O35-C13	-2.66	1.27	1.33
4	B	301	ENS	C12-N30	-2.36	1.30	1.34
4	B	301	ENS	C14-N29	-2.32	1.30	1.35
4	B	301	ENS	C4-C9	2.32	1.43	1.38
4	D	301	ENS	C4-C9	2.10	1.42	1.38
4	D	301	ENS	C14-N29	-2.09	1.31	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	304	MES	C5-N4-C3	5.22	120.58	108.83
7	D	304	MES	C5-N4-C3	5.05	120.20	108.83
4	D	301	ENS	O35-C13-C11	4.18	119.29	111.41
7	B	304	MES	C7-N4-C3	4.07	121.65	111.23
4	B	301	ENS	C25-C14-N29	4.06	122.19	117.08
7	D	304	MES	C7-N4-C3	3.93	121.28	111.23
4	B	301	ENS	O35-C13-C11	3.87	118.71	111.41
4	D	301	ENS	C25-C14-N29	3.42	121.39	117.08
4	B	301	ENS	O32-C10-N28	-3.27	119.44	122.55
4	D	301	ENS	O32-C10-N28	-3.00	119.70	122.55
4	D	301	ENS	O33-C13-C11	-2.98	118.93	125.17
7	B	304	MES	O3S-S-C8	2.94	110.53	105.77
7	B	304	MES	O2S-S-C8	2.93	110.44	106.92
7	D	304	MES	O3S-S-C8	2.89	110.45	105.77
4	B	301	ENS	O33-C13-C11	-2.89	119.12	125.17
7	D	304	MES	C7-N4-C5	2.85	118.53	111.23
4	D	301	ENS	C8-C9-N30	2.80	120.89	115.42
7	B	304	MES	C2-C3-N4	-2.78	105.89	110.10
7	D	304	MES	C6-C5-N4	-2.74	105.94	110.10
4	B	301	ENS	C23-N31-C12	2.74	128.61	121.12
7	B	304	MES	C7-N4-C5	2.55	117.76	111.23
4	B	301	ENS	C9-N30-C12	-2.45	120.92	125.95
4	B	301	ENS	C2-C3-C7	-2.38	117.59	120.89
7	D	304	MES	O1S-S-C8	2.37	109.76	106.92
4	B	301	ENS	C8-C9-N30	2.33	119.98	115.42
4	D	301	ENS	C19-C23-C10	-2.31	108.70	111.65
4	D	301	ENS	C2-C3-C7	-2.12	117.96	120.89
4	D	301	ENS	C23-N31-C12	2.12	126.90	121.12

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	304	MES	C8-C7-N4-C3
3	D	307	GOL	O1-C1-C2-C3
3	A	202	GOL	O1-C1-C2-C3
3	A	203	GOL	O1-C1-C2-C3
4	D	301	ENS	C1-C11-C12-N30
4	D	301	ENS	C19-C23-N31-C12
7	D	304	MES	C8-C7-N4-C3
3	D	306	GOL	O1-C1-C2-C3
4	B	301	ENS	C1-C11-C12-N30
4	B	301	ENS	C1-C11-C12-N31
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	307	GOL	O1-C1-C2-O2
3	D	306	GOL	O1-C1-C2-O2
7	D	304	MES	C8-C7-N4-C5
3	D	305	GOL	O2-C2-C3-O3
4	D	301	ENS	C13-C11-C12-N31
3	D	305	GOL	O1-C1-C2-C3
3	D	305	GOL	O1-C1-C2-O2

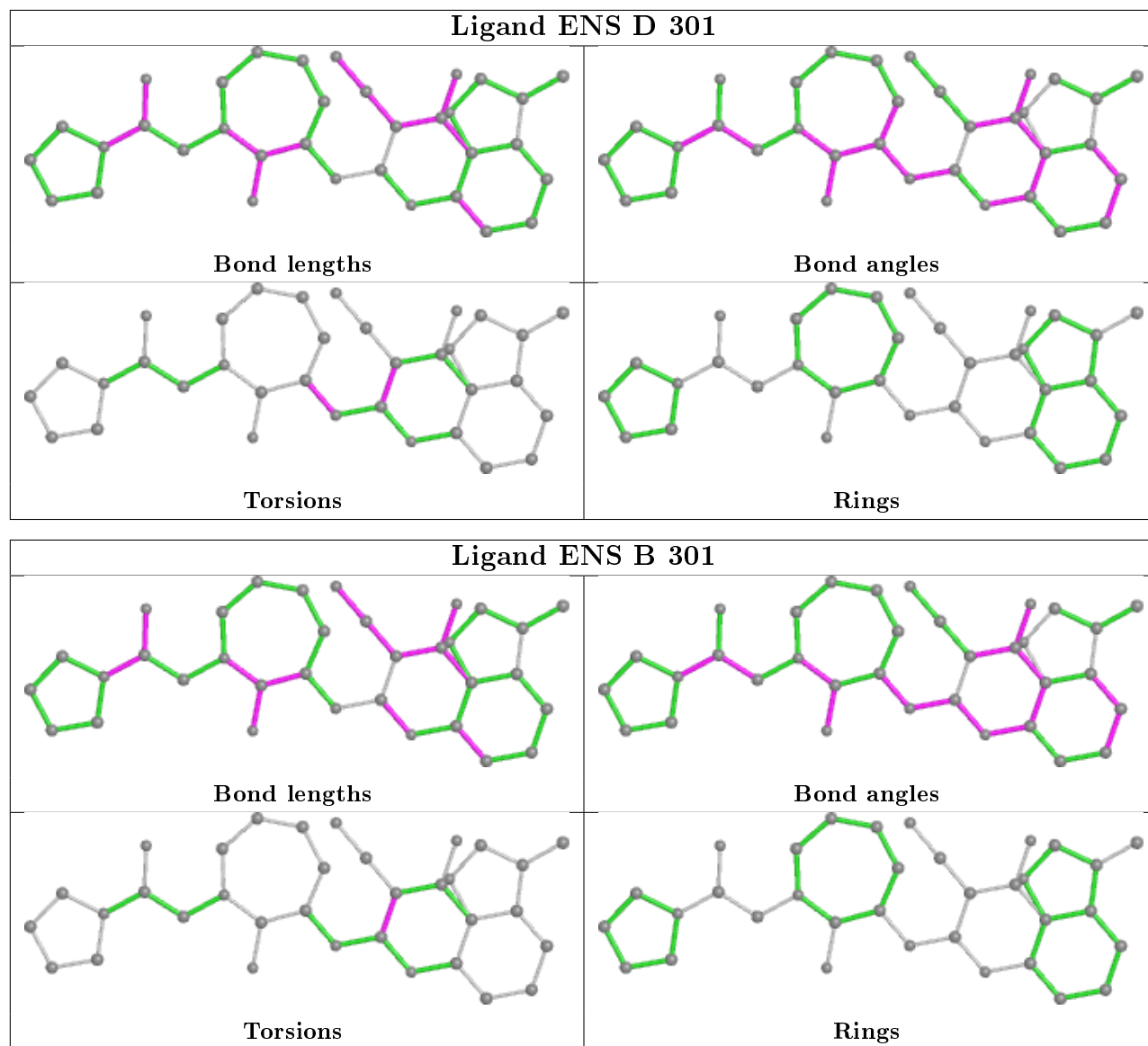
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	307	GOL	1	0
3	A	203	GOL	3	0
7	B	304	MES	2	0
7	D	304	MES	2	0
4	B	301	ENS	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	84/94 (89%)	1.01	19 (22%) 0 1	21, 30, 52, 57	0
1	C	84/94 (89%)	1.33	22 (26%) 0 0	20, 32, 58, 63	0
2	B	238/238 (100%)	0.60	16 (6%) 17 23	20, 24, 35, 46	0
2	D	238/238 (100%)	0.78	25 (10%) 6 8	19, 24, 37, 43	0
All	All	644/664 (96%)	0.82	82 (12%) 3 5	19, 25, 44, 63	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	CYS	7.7
2	D	148	LYS	5.8
2	D	145	HIS	5.7
1	A	101	CYS	5.3
2	D	150	ARG	4.7
1	C	144	GLN	4.6
1	C	98	GLN	4.5
1	C	108	TYR	4.5
2	D	149	GLY	4.4
1	A	107	GLU	4.3
1	A	144	GLN	4.2
2	D	76	GLU	4.1
1	C	94	PRO	4.0
1	C	114	GLU	4.0
1	C	103	ASP	3.9
2	D	77	GLU	3.7
1	C	146	SER	3.6
1	C	95	CYS	3.4
2	B	78	GLY	3.4
1	A	108	TYR	3.4
1	C	115	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	101	CYS	3.3
1	A	90	CYS	3.2
1	C	159	ASP	3.1
1	A	146	SER	3.0
2	D	144	THR	3.0
2	D	75	GLN	3.0
2	B	150	ARG	2.9
1	A	103	ASP	2.9
1	C	145	ASN	2.9
2	D	74	GLU	2.9
1	C	142	GLU	2.9
2	D	151	GLN	2.8
2	D	152	SER	2.8
2	B	151	GLN	2.8
2	D	39	GLU	2.7
1	A	94	PRO	2.7
2	D	37	GLU	2.7
2	B	75	GLN	2.7
2	B	145	HIS	2.7
1	A	141	HIS	2.7
2	B	77	GLU	2.7
2	B	74	GLU	2.6
1	A	114	GLU	2.6
2	D	243	LYS	2.6
1	C	139	PHE	2.6
2	B	37	GLU	2.6
1	C	111	THR	2.5
2	B	24	ASP	2.5
2	B	243	LYS	2.5
2	D	166	ASN	2.5
2	D	154	ARG	2.5
1	C	126	ARG	2.4
1	C	109	THR	2.4
1	A	93	SER	2.4
2	B	148	LYS	2.4
2	B	76	GLU	2.4
2	D	68	VAL	2.4
1	A	153	ARG	2.3
1	C	91	GLU	2.3
2	D	183	ALA	2.3
1	A	98	GLN	2.3
1	A	139	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	99	GLY	2.2
1	A	145	ASN	2.2
1	C	143	GLU	2.2
2	D	73	THR	2.2
1	A	159	ASP	2.2
2	B	205	ASP	2.2
2	D	66	VAL	2.1
1	C	97	ASN	2.1
2	B	39	GLU	2.1
2	D	24	ASP	2.1
2	D	231	VAL	2.1
1	A	124	PHE	2.1
2	D	78	GLY	2.1
1	A	111	THR	2.1
2	D	185(B)	THR	2.1
2	B	183	ALA	2.1
1	A	143	GLU	2.0
2	D	36	GLU	2.0
2	B	244	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CA	B	302	1/1	0.61	0.30	44,44,44,44	0
6	NA	B	303	1/1	0.63	0.19	29,29,29,29	0
5	CA	D	302	1/1	0.64	0.27	45,45,45,45	0
6	NA	D	303	1/1	0.69	0.18	31,31,31,31	0

Continued on next page...

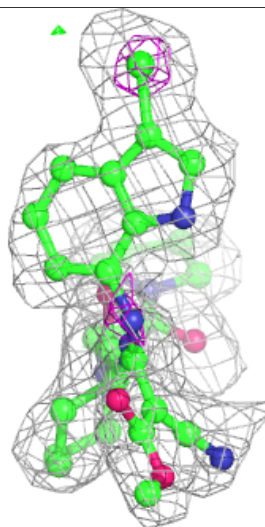
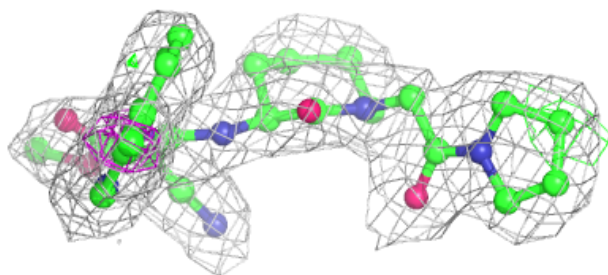
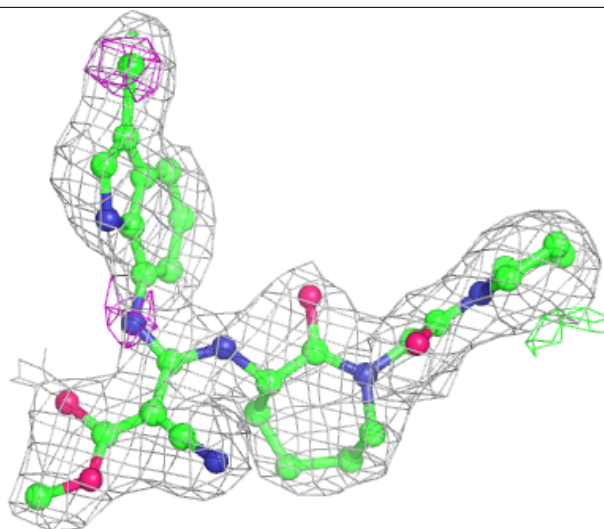
Continued from previous page...

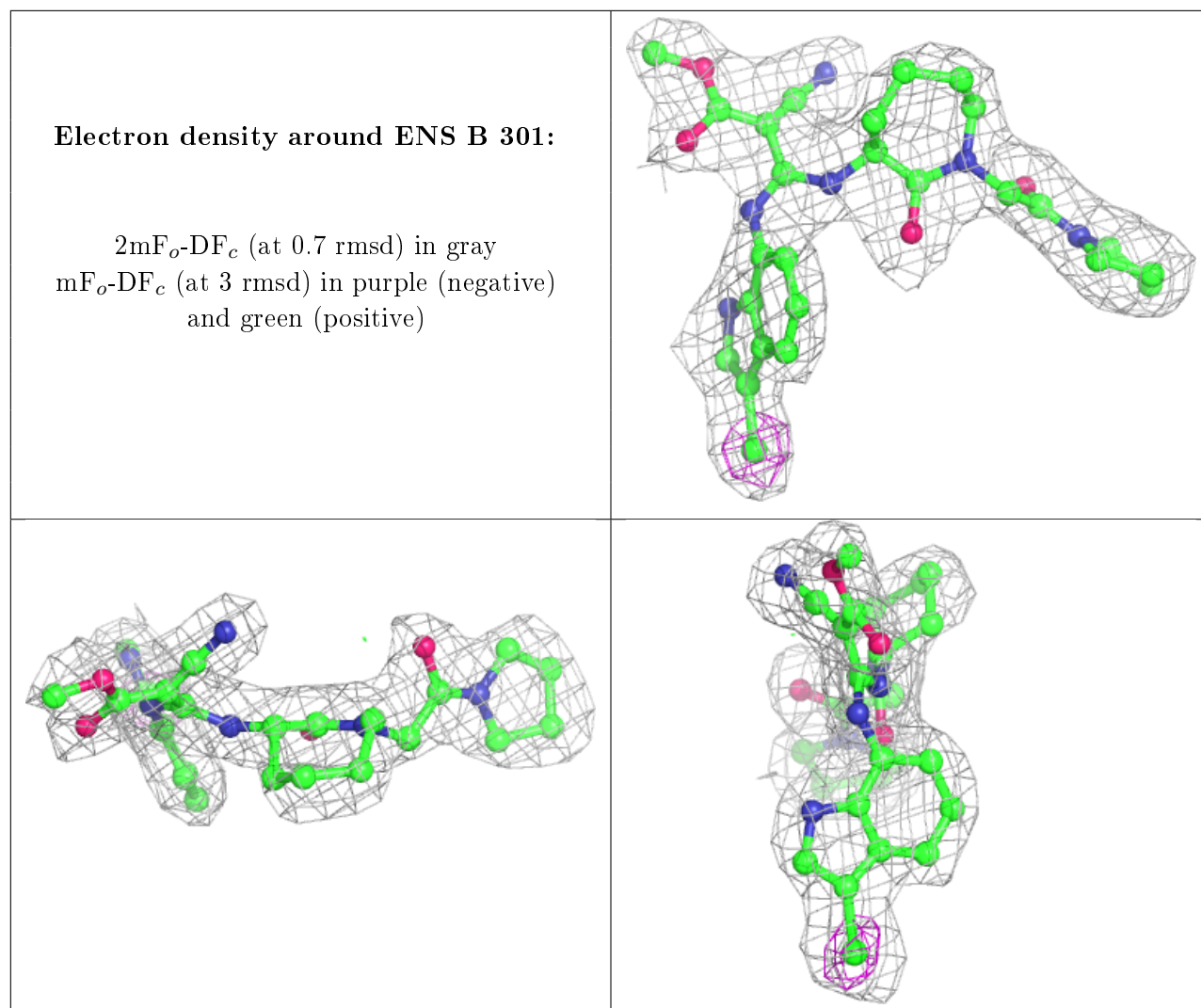
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	202	6/6	0.84	0.36	28,29,29,30	0
4	ENS	D	301	36/36	0.86	0.18	24,28,31,33	0
3	GOL	D	305	6/6	0.86	0.15	22,23,23,24	0
3	GOL	B	305	6/6	0.88	0.14	22,23,24,24	0
8	ACT	B	306	4/4	0.91	0.13	27,27,27,28	0
4	ENS	B	301	36/36	0.91	0.14	23,27,30,31	0
3	GOL	D	307	6/6	0.91	0.33	23,23,24,24	0
3	GOL	D	306	6/6	0.92	0.22	20,20,20,20	0
7	MES	D	304	12/12	0.92	0.18	20,21,23,24	0
3	GOL	A	203	6/6	0.93	0.31	23,23,24,25	0
8	ACT	D	308	4/4	0.93	0.15	31,31,31,31	0
7	MES	B	304	12/12	0.94	0.16	21,22,23,24	0
3	GOL	A	201	6/6	0.96	0.13	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)





6.5 Other polymers [i](#)

There are no such residues in this entry.