



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:39 AM UTC

PDB ID : 8UUD / pdb_00008uud
Title : BCX2627 complexed with human FVIIa and soluble Tissue Factor.
Authors : Krishnan, R.; Kotian, P.
Deposited on : 2023-11-01
Resolution : 2.40 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

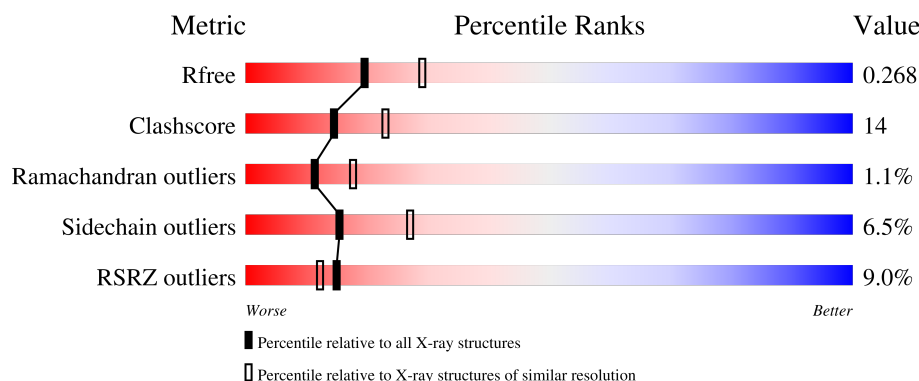
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	L	142	13% 74% 13% 6% 6%
2	H	254	9% 78% 17% 5%
3	T	75	% 83% 17%
4	U	116	9% 78% 19% .

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CA	L	204	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4848 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 VII light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	142	Total	C	N	O	S	0	0	0
			1134	683	189	247	15			

- Molecule 2 is a protein called Coagulation factor VII Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	254	Total	C	N	O	S	0	0	0
			1973	1253	351	356	13			

- Molecule 3 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	75	Total	C	N	O	S	0	0	0
			614	397	95	120	2			

- Molecule 4 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	U	116	Total	C	N	O	S	0	0	0
			940	593	155	189	3			

There are 4 discrepancies between the modelled and reference sequences:

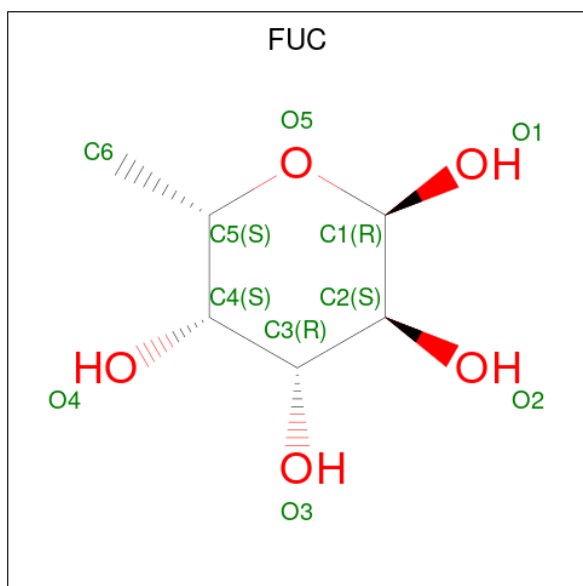
Chain	Residue	Modelled	Actual	Comment	Reference
U	?	-	LYS	deletion	UNP P13726
U	?	-	SER	deletion	UNP P13726
U	?	-	SER	deletion	UNP P13726
U	?	-	SER	deletion	UNP P13726

- Molecule 5 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).

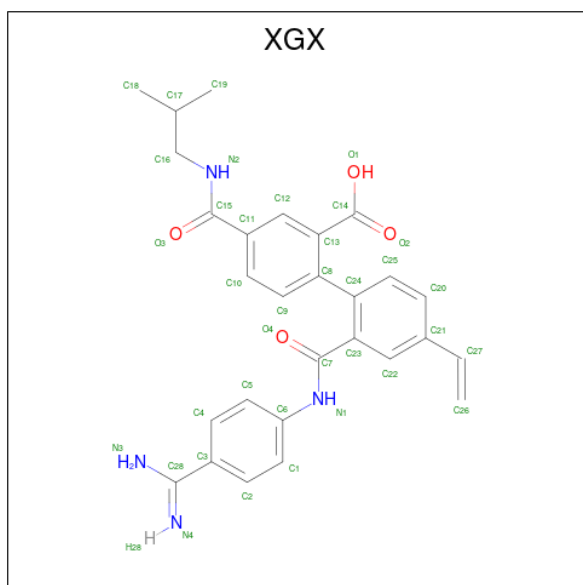


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	8	Total Ca 8 8	0	0
7	H	1	Total Ca 1 1	0	0

- Molecule 8 is (1P)-2'-[(4-carbamimidoylphenyl)carbamoyl]-4'-ethenyl-4-[(2-methylpropyl)carbamoyl][1,1'-biphenyl]-2-carboxylic acid (CCD ID: XGX) (formula: C₂₈H₂₈N₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C N O 36 28 4 4	0	0

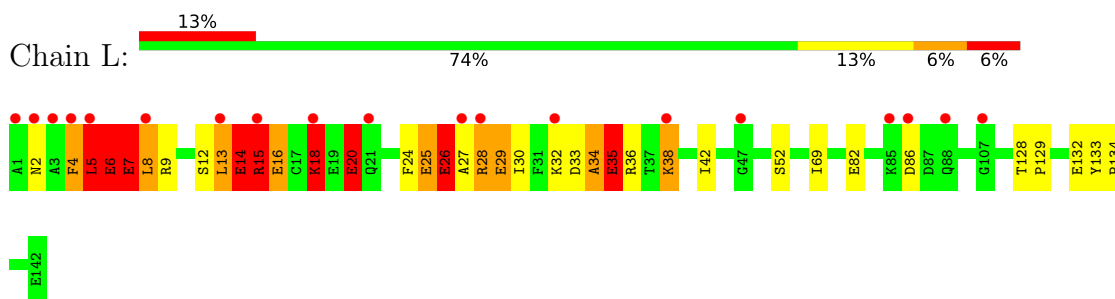
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	32	Total O 32 32	0	0
9	H	51	Total O 51 51	0	0
9	T	17	Total O 17 17	0	0
9	U	21	Total O 21 21	0	0

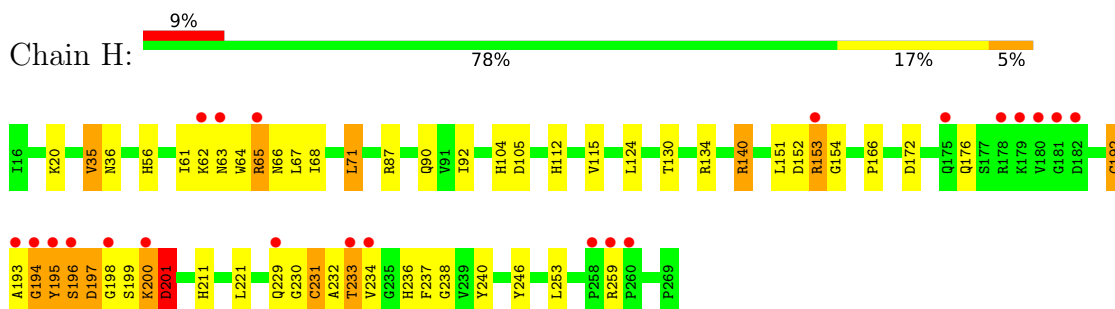
3 Residue-property plots

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.

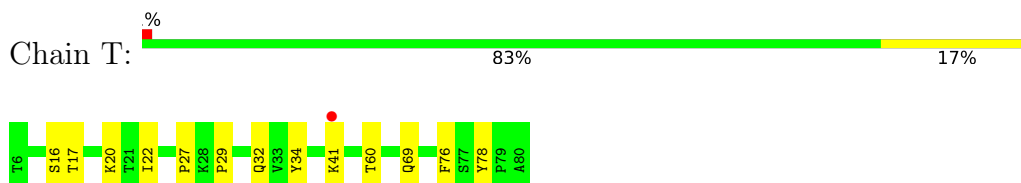
- Molecule 1: Factor VII light chain



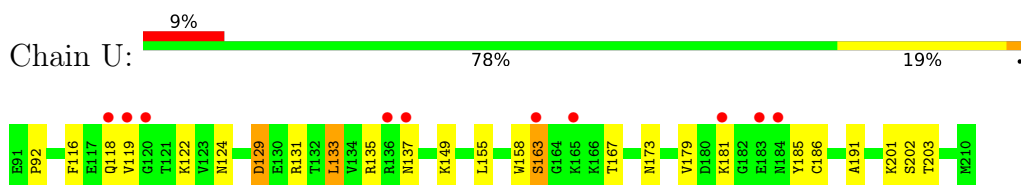
- Molecule 2: Coagulation factor VII Heavy Chain



- Molecule 3: Tissue factor



- Molecule 4: Tissue factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.49Å 82.87Å 126.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.09 – 2.40 47.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.0 (47.09-2.40) 90.0 (47.09-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.204 , 0.265 0.209 , 0.268	Depositor DCC
R_{free} test set	1290 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.8	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	0.93	EDS
Total number of atoms	4848	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CGU, BGC, XGX, CA, FUC

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	L	0.59	0/1028	1.02	0/1374
2	H	1.83	3/2016 (0.1%)	1.47	13/2734 (0.5%)
3	T	0.56	0/630	1.02	0/860
4	U	0.56	0/958	1.04	1/1299 (0.1%)
All	All	1.28	3/4632 (0.1%)	1.24	14/6267 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	20
2	H	0	2
All	All	0	22

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	35	VAL	C-N	44.68	1.91	1.33
2	H	231	CYS	C-N	44.42	1.95	1.33
2	H	192	CYS	C-N	43.77	1.94	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	231	CYS	O-C-N	-35.04	82.63	123.27
2	H	192	CYS	CA-C-N	20.31	158.26	121.70
2	H	192	CYS	C-N-CA	20.31	158.26	121.70
2	H	192	CYS	O-C-N	-16.22	103.70	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	195	TYR	N-CA-CB	10.23	127.90	110.50
2	H	201	ASP	CA-CB-CG	9.62	122.22	112.60
2	H	197	ASP	CA-CB-CG	7.40	120.00	112.60
2	H	35	VAL	O-C-N	-7.39	115.86	123.03
2	H	195	TYR	CA-C-O	-7.31	108.38	120.80
2	H	195	TYR	CA-CB-CG	-6.27	102.62	113.90
4	U	129	ASP	CA-CB-CG	5.64	118.24	112.60
2	H	112	HIS	CB-CA-C	5.37	119.39	110.90
2	H	211	HIS	CA-CB-CG	5.30	119.10	113.80
2	H	192	CYS	CA-C-O	-5.16	115.86	121.89

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	140	ARG	Sidechain
2	H	194	GLY	Peptide
1	L	13	LEU	Mainchain
1	L	14	CGU	Peptide,Mainchain
1	L	15	ARG	Mainchain
1	L	16	CGU	Mainchain
1	L	18	LYS	Peptide,Mainchain
1	L	20	CGU	Mainchain
1	L	24	PHE	Mainchain
1	L	26	CGU	Mainchain
1	L	28	ARG	Peptide,Mainchain,Sidechain
1	L	34	ALA	Peptide,Mainchain
1	L	35	CGU	Mainchain
1	L	5	LEU	Peptide
1	L	6	CGU	Peptide,Mainchain
1	L	7	CGU	Peptide

5.2 Too-close contacts ⓘ

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	L	1134	0	989	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1973	0	1940	82	0
3	T	614	0	598	9	0
4	U	940	0	912	11	0
5	L	11	0	10	0	0
6	L	10	0	10	0	0
7	H	1	0	0	0	0
7	L	8	0	0	0	0
8	H	36	0	0	1	0
9	H	51	0	0	2	0
9	L	32	0	0	5	0
9	T	17	0	0	0	0
9	U	21	0	0	2	0
All	All	4848	0	4459	129	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 14.

All (129) 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:H:193:ALA:HA	2:H:194:GLY:N	1.30	1.47
2:H:229:GLN:O	2:H:230:GLY:N	1.60	1.34
2:H:199:SER:N	2:H:200:LYS:O	1.59	1.33
2:H:35:VAL:C	2:H:36:ASN:N	1.91	1.29
1:L:26:CGU:HB3	9:L:310:HOH:O	1.13	1.28
2:H:198:GLY:C	2:H:200:LYS:O	1.76	1.27
2:H:231:CYS:C	2:H:232:ALA:N	1.95	1.25
2:H:192:CYS:C	2:H:193:ALA:N	1.94	1.23
2:H:193:ALA:CA	2:H:194:GLY:N	2.12	1.11
1:L:5:LEU:HB3	1:L:6:CGU:HA	1.43	0.98
2:H:233:THR:HB	2:H:236:HIS:HB2	1.43	0.96
2:H:199:SER:N	2:H:200:LYS:C	2.25	0.94
1:L:25:CGU:OE21	1:L:28:ARG:NH2	2.03	0.91
2:H:232:ALA:N	2:H:233:THR:C	2.29	0.90
2:H:193:ALA:C	2:H:237:PHE:HB3	1.97	0.89
2:H:193:ALA:HB3	2:H:240:TYR:HE2	1.44	0.82
2:H:193:ALA:O	2:H:238:GLY:N	2.12	0.81
2:H:166:PRO:HG2	2:H:195:TYR:C	2.07	0.79
2:H:231:CYS:O	2:H:232:ALA:N	2.17	0.78
2:H:195:TYR:N	2:H:196:SER:N	2.33	0.76
2:H:229:GLN:C	2:H:230:GLY:N	2.42	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:196:SER:O	2:H:197:ASP:OD1	2.04	0.76
2:H:195:TYR:HB3	2:H:237:PHE:HE1	1.50	0.76
2:H:199:SER:OG	2:H:200:LYS:C	2.32	0.72
2:H:231:CYS:CA	2:H:232:ALA:N	2.55	0.70
2:H:198:GLY:CA	2:H:200:LYS:O	2.40	0.70
1:L:4:PHE:O	1:L:5:LEU:HD13	1.92	0.69
1:L:14:CGU:OE21	1:L:14:CGU:HA	1.91	0.69
2:H:56:HIS:HD2	2:H:105:ASP:OD2	1.76	0.68
2:H:195:TYR:HB3	2:H:237:PHE:CE1	2.29	0.68
2:H:198:GLY:C	2:H:232:ALA:HB1	2.19	0.68
2:H:194:GLY:N	2:H:195:TYR:O	2.28	0.67
2:H:193:ALA:O	2:H:194:GLY:HA3	1.96	0.65
2:H:194:GLY:C	2:H:195:TYR:O	2.35	0.65
2:H:196:SER:O	2:H:197:ASP:CG	2.40	0.65
2:H:198:GLY:O	2:H:200:LYS:O	2.16	0.64
2:H:232:ALA:CA	2:H:233:THR:C	2.71	0.64
2:H:198:GLY:O	2:H:199:SER:N	2.31	0.64
2:H:196:SER:OG	2:H:197:ASP:N	2.31	0.63
2:H:193:ALA:CB	2:H:194:GLY:N	2.62	0.62
2:H:201:ASP:HB2	9:H:429:HOH:O	1.99	0.62
2:H:201:ASP:OD2	2:H:233:THR:C	2.42	0.62
2:H:233:THR:HB	2:H:236:HIS:CB	2.23	0.61
1:L:4:PHE:O	1:L:4:PHE:CD1	2.54	0.61
2:H:153:ARG:O	2:H:154:GLY:N	2.34	0.61
2:H:229:GLN:C	2:H:233:THR:HG21	2.26	0.60
1:L:5:LEU:HB3	1:L:6:CGU:CA	2.23	0.60
1:L:25:CGU:O	1:L:26:CGU:C	2.49	0.59
2:H:193:ALA:C	2:H:194:GLY:HA3	2.27	0.59
1:L:4:PHE:O	1:L:4:PHE:CG	2.56	0.58
1:L:4:PHE:HA	9:L:321:HOH:O	2.02	0.58
2:H:201:ASP:OD2	2:H:233:THR:O	2.22	0.58
3:T:20:LYS:HB2	4:U:133:LEU:HD13	1.87	0.57
1:L:26:CGU:CG	9:L:310:HOH:O	2.43	0.57
2:H:152:ASP:O	2:H:153:ARG:C	2.48	0.56
1:L:4:PHE:O	1:L:5:LEU:CD1	2.54	0.56
2:H:71:LEU:HD13	2:H:115:VAL:HG11	1.88	0.56
1:L:28:ARG:O	1:L:30:ILE:N	2.40	0.55
2:H:193:ALA:CB	2:H:240:TYR:HE2	2.15	0.55
2:H:63:ASN:C	2:H:65:ARG:H	2.14	0.55
2:H:35:VAL:HG12	2:H:67:LEU:HD13	1.88	0.54
2:H:199:SER:CA	2:H:200:LYS:C	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:193:ALA:CA	2:H:194:GLY:CA	2.85	0.54
1:L:26:CGU:CB	9:L:310:HOH:O	1.95	0.53
1:L:12:SER:OG	1:L:14:CGU:HB3	2.09	0.53
2:H:63:ASN:O	2:H:65:ARG:N	2.44	0.51
1:L:33:ASP:HB3	1:L:36:ARG:HD2	1.93	0.50
1:L:18:LYS:O	1:L:20:CGU:N	2.44	0.50
1:L:6:CGU:N	1:L:7:CGU:HB3	2.25	0.50
2:H:198:GLY:N	2:H:200:LYS:O	2.44	0.50
1:L:82:GLU:OE1	1:L:82:GLU:N	2.37	0.49
1:L:6:CGU:OE22	1:L:9:ARG:NH2	2.44	0.49
1:L:132:GLU:OE1	1:L:133:TYR:CE2	2.65	0.49
1:L:25:CGU:O	1:L:27:ALA:N	2.45	0.49
2:H:200:LYS:HG2	2:H:201:ASP:N	2.28	0.49
1:L:36:ARG:HH22	4:U:163:SER:HB3	1.78	0.49
3:T:60:THR:HG21	4:U:133:LEU:HD22	1.95	0.49
2:H:200:LYS:CG	2:H:201:ASP:N	2.75	0.48
2:H:35:VAL:CG1	2:H:67:LEU:HD13	2.44	0.48
2:H:172:ASP:O	2:H:176:GLN:HB3	2.14	0.48
2:H:104:HIS:HA	2:H:246:TYR:OH	2.14	0.48
2:H:90:GLN:HB2	9:H:418:HOH:O	2.13	0.48
2:H:92:ILE:HG21	2:H:253:LEU:HD13	1.94	0.48
3:T:27:PRO:HD2	3:T:34:TYR:OH	2.14	0.47
1:L:13:LEU:O	1:L:14:CGU:O	2.31	0.47
1:L:4:PHE:O	1:L:5:LEU:HB2	2.13	0.47
2:H:198:GLY:C	2:H:200:LYS:C	2.73	0.47
2:H:35:VAL:HG11	2:H:61:ILE:HD12	1.95	0.47
2:H:234:VAL:O	2:H:234:VAL:HG12	2.15	0.46
1:L:38:LYS:O	1:L:42:ILE:HG13	2.14	0.46
4:U:173:ASN:HB2	9:U:313:HOH:O	2.14	0.46
1:L:28:ARG:O	1:L:29:CGU:C	2.64	0.46
4:U:116:PHE:HA	4:U:124:ASN:O	2.15	0.46
2:H:166:PRO:HG2	2:H:195:TYR:O	2.16	0.45
2:H:56:HIS:HE1	8:H:302:XGX:O2	1.99	0.45
2:H:195:TYR:CA	2:H:196:SER:N	2.79	0.45
3:T:76:PHE:CD1	4:U:92:PRO:HG2	2.51	0.45
4:U:179:VAL:HB	4:U:185:TYR:CE2	2.52	0.45
2:H:193:ALA:HB1	2:H:194:GLY:CA	2.47	0.45
2:H:198:GLY:C	2:H:199:SER:N	2.75	0.45
2:H:198:GLY:HA2	2:H:234:VAL:HG23	1.99	0.45
3:T:29:PRO:HB2	3:T:32:GLN:O	2.18	0.44
1:L:69:ILE:HD11	3:T:17:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:231:CYS:C	2:H:232:ALA:C	2.85	0.44
2:H:231:CYS:C	2:H:232:ALA:CA	2.86	0.44
2:H:195:TYR:C	2:H:195:TYR:CD2	2.90	0.44
2:H:61:ILE:O	2:H:62:LYS:HG3	2.18	0.43
2:H:130:THR:O	2:H:134:ARG:HB3	2.18	0.43
2:H:151:LEU:O	2:H:154:GLY:N	2.52	0.43
3:T:69:GLN:NE2	3:T:69:GLN:HA	2.34	0.43
1:L:4:PHE:O	1:L:5:LEU:CB	2.67	0.43
1:L:129:PRO:HB3	1:L:134:PRO:HG3	2.01	0.43
2:H:199:SER:OG	2:H:200:LYS:HB2	2.18	0.42
4:U:191:ALA:HB3	4:U:202:SER:HB3	2.00	0.42
2:H:36:ASN:N	2:H:66:ASN:O	2.53	0.42
2:H:201:ASP:CG	2:H:233:THR:O	2.61	0.42
4:U:158:TRP:NE1	4:U:186:CYS:HB2	2.34	0.42
2:H:193:ALA:CB	2:H:240:TYR:CE2	2.99	0.41
3:T:16:SER:HA	3:T:20:LYS:O	2.20	0.41
4:U:203:THR:HG22	9:U:301:HOH:O	2.20	0.41
1:L:26:CGU:CD2	9:L:310:HOH:O	2.67	0.41
2:H:63:ASN:C	2:H:65:ARG:N	2.78	0.41
2:H:140:ARG:O	2:H:166:PRO:HA	2.21	0.41
4:U:155:LEU:O	4:U:167:THR:HA	2.21	0.41
1:L:34:ALA:O	1:L:35:CGU:C	2.68	0.41
2:H:124:LEU:HD23	2:H:221:LEU:HB2	2.03	0.41
2:H:35:VAL:HA	2:H:66:ASN:O	2.20	0.41
2:H:200:LYS:HG3	2:H:201:ASP:N	2.36	0.41
3:T:32:GLN:HA	3:T:78:TYR:O	2.21	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	L	130/142 (92%)	116 (89%)	10 (8%)	4 (3%)	3	3
2	H	238/254 (94%)	225 (94%)	12 (5%)	1 (0%)	30	43
3	T	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
4	U	112/116 (97%)	108 (96%)	3 (3%)	1 (1%)	14	22
All	All	553/587 (94%)	521 (94%)	26 (5%)	6 (1%)	11	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	5	LEU
1	L	15	ARG
2	H	64	TRP
1	L	4	PHE
1	L	8	LEU
4	U	137	ASN

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	L	114/114 (100%)	105 (92%)	9 (8%)	11	19
2	H	216/216 (100%)	205 (95%)	11 (5%)	21	37
3	T	70/70 (100%)	68 (97%)	2 (3%)	37	60
4	U	109/109 (100%)	98 (90%)	11 (10%)	7	11
All	All	509/509 (100%)	476 (94%)	33 (6%)	15	27

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ASN
1	L	8	LEU
1	L	15	ARG
1	L	18	LYS
1	L	32	LYS

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Mol	Chain	Res	Type
1	L	38	LYS
1	L	52	SER
1	L	86	ASP
1	L	128	THR
2	H	20	LYS
2	H	65	ARG
2	H	68	ILE
2	H	71	LEU
2	H	87	ARG
2	H	153	ARG
2	H	196	SER
2	H	200	LYS
2	H	201	ASP
2	H	233	THR
2	H	259	ARG
3	T	22	ILE
3	T	41	LYS
4	U	118	GLN
4	U	119	VAL
4	U	122	LYS
4	U	129	ASP
4	U	131	ARG
4	U	133	LEU
4	U	135	ARG
4	U	149	LYS
4	U	163	SER
4	U	181	LYS
4	U	201	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	21	GLN
1	L	57	ASN
1	L	66	GLN
2	H	36	ASN
2	H	56	HIS
2	H	120	HIS
2	H	171	GLN
2	H	214	HIS
3	T	69	GLN
4	U	96	ASN

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Mol	Chain	Res	Type
4	U	110	GLN
4	U	118	GLN
4	U	184	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	$\# Z > 2$
1	CGU	L	7	7,1	9,11,12	1.68	2 (22%)	10,14,16	0.97	1 (10%)
1	CGU	L	20	7,1	9,11,12	1.46	2 (22%)	10,14,16	1.29	2 (20%)
1	CGU	L	35	1	9,11,12	1.56	2 (22%)	10,14,16	1.38	3 (30%)
1	CGU	L	19	7,1	9,11,12	1.44	0	10,14,16	0.46	0
1	CGU	L	16	7,1	9,11,12	1.76	4 (44%)	10,14,16	1.00	1 (10%)
1	CGU	L	25	7,1	9,11,12	1.11	1 (11%)	10,14,16	0.94	1 (10%)
1	CGU	L	26	7,1	9,11,12	1.59	1 (11%)	10,14,16	0.95	1 (10%)
1	CGU	L	6	7,1	9,11,12	1.51	2 (22%)	10,14,16	0.92	1 (10%)
1	CGU	L	29	7,1	9,11,12	1.69	1 (11%)	10,14,16	1.17	1 (10%)
1	CGU	L	14	7,1	9,11,12	1.43	1 (11%)	10,14,16	0.50	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
1	CGU	L	7	7,1	-	10/13/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CGU	L	20	7,1	-	3/13/14/16	-
1	CGU	L	35	1	-	5/13/14/16	-
1	CGU	L	19	7,1	-	0/13/14/16	-
1	CGU	L	16	7,1	-	8/13/14/16	-
1	CGU	L	25	7,1	-	5/13/14/16	-
1	CGU	L	26	7,1	-	8/13/14/16	-
1	CGU	L	6	7,1	-	8/13/14/16	-
1	CGU	L	29	7,1	-	6/13/14/16	-
1	CGU	L	14	7,1	-	8/13/14/16	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	26	CGU	CG-CD2	3.08	1.56	1.52
1	L	29	CGU	CG-CD2	2.93	1.55	1.52
1	L	16	CGU	OE22-CD2	-2.83	1.21	1.30
1	L	7	CGU	CG-CD1	2.63	1.55	1.52
1	L	6	CGU	CG-CD1	2.49	1.55	1.52
1	L	35	CGU	CG-CD2	2.47	1.55	1.52
1	L	7	CGU	OE21-CD2	2.35	1.29	1.22
1	L	16	CGU	CG-CD2	2.33	1.55	1.52
1	L	14	CGU	CG-CD1	2.32	1.55	1.52
1	L	16	CGU	CG-CD1	2.28	1.55	1.52
1	L	16	CGU	O-C	2.21	1.28	1.20
1	L	6	CGU	CG-CD2	2.14	1.54	1.52
1	L	35	CGU	CG-CD1	2.09	1.54	1.52
1	L	20	CGU	CG-CD2	2.02	1.54	1.52
1	L	20	CGU	CG-CD1	2.02	1.54	1.52
1	L	25	CGU	CG-CD2	2.01	1.54	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	29	CGU	CB-CG-CD1	-2.91	107.20	113.11
1	L	20	CGU	CB-CG-CD2	-2.81	107.41	113.11
1	L	35	CGU	CB-CG-CD2	-2.64	107.74	113.11
1	L	20	CGU	CB-CA-C	-2.62	106.95	110.99
1	L	6	CGU	CB-CG-CD2	-2.40	108.23	113.11
1	L	26	CGU	CB-CG-CD2	2.39	117.97	113.11
1	L	25	CGU	CB-CG-CD2	2.37	117.92	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	7	CGU	CB-CG-CD2	-2.17	108.71	113.11
1	L	35	CGU	CB-CA-C	-2.14	107.69	110.99
1	L	16	CGU	CB-CG-CD2	-2.07	108.91	113.11
1	L	35	CGU	CB-CA-N	2.02	114.89	110.48

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L	6	CGU	O-C-CA-CB
1	L	6	CGU	C-CA-CB-CG
1	L	6	CGU	CA-CB-CG-CD1
1	L	6	CGU	CA-CB-CG-CD2
1	L	7	CGU	N-CA-CB-CG
1	L	14	CGU	O-C-CA-CB
1	L	14	CGU	N-CA-CB-CG
1	L	14	CGU	C-CA-CB-CG
1	L	14	CGU	CA-CB-CG-CD1
1	L	14	CGU	CA-CB-CG-CD2
1	L	16	CGU	N-CA-CB-CG
1	L	16	CGU	C-CA-CB-CG
1	L	16	CGU	CA-CB-CG-CD1
1	L	16	CGU	CA-CB-CG-CD2
1	L	16	CGU	OE21-CD2-CG-CD1
1	L	16	CGU	OE22-CD2-CG-CD1
1	L	25	CGU	N-CA-CB-CG
1	L	26	CGU	N-CA-CB-CG
1	L	26	CGU	C-CA-CB-CG
1	L	26	CGU	OE21-CD2-CG-CD1
1	L	26	CGU	OE22-CD2-CG-CD1
1	L	29	CGU	CA-CB-CG-CD1
1	L	35	CGU	CA-CB-CG-CD1
1	L	35	CGU	CA-CB-CG-CD2
1	L	35	CGU	OE11-CD1-CG-CD2
1	L	35	CGU	OE12-CD1-CG-CD2
1	L	7	CGU	CA-CB-CG-CD1
1	L	26	CGU	CA-CB-CG-CD1
1	L	29	CGU	N-CA-CB-CG
1	L	6	CGU	OE11-CD1-CG-CB
1	L	6	CGU	OE21-CD2-CG-CB
1	L	6	CGU	OE22-CD2-CG-CB
1	L	7	CGU	OE11-CD1-CG-CB

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Mol	Chain	Res	Type	Atoms
1	L	7	CGU	OE12-CD1-CG-CB
1	L	7	CGU	OE21-CD2-CG-CB
1	L	7	CGU	OE22-CD2-CG-CB
1	L	16	CGU	OE11-CD1-CG-CB
1	L	16	CGU	OE12-CD1-CG-CB
1	L	25	CGU	OE11-CD1-CG-CB
1	L	25	CGU	OE12-CD1-CG-CB
1	L	29	CGU	OE11-CD1-CG-CB
1	L	29	CGU	OE12-CD1-CG-CB
1	L	7	CGU	OE21-CD2-CG-CD1
1	L	7	CGU	OE22-CD2-CG-CD1
1	L	14	CGU	OE11-CD1-CG-CD2
1	L	14	CGU	OE12-CD1-CG-CD2
1	L	20	CGU	OE11-CD1-CG-CD2
1	L	7	CGU	C-CA-CB-CG
1	L	25	CGU	C-CA-CB-CG
1	L	35	CGU	N-CA-CB-CG
1	L	6	CGU	OE12-CD1-CG-CB
1	L	14	CGU	OE12-CD1-CG-CB
1	L	20	CGU	OE11-CD1-CG-CB
1	L	20	CGU	OE12-CD1-CG-CB
1	L	25	CGU	OE22-CD2-CG-CB
1	L	26	CGU	OE11-CD1-CG-CB
1	L	26	CGU	OE12-CD1-CG-CB
1	L	7	CGU	OE12-CD1-CG-CD2
1	L	26	CGU	OE12-CD1-CG-CD2
1	L	29	CGU	OE11-CD1-CG-CD2
1	L	29	CGU	OE12-CD1-CG-CD2

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	7	CGU	1	0
1	L	20	CGU	1	0
1	L	35	CGU	1	0
1	L	25	CGU	3	0
1	L	26	CGU	5	0
1	L	6	CGU	4	0
1	L	29	CGU	1	0
1	L	14	CGU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z > 2$
6	FUC	L	202	1	10,10,11	0.52	0	14,14,16	0.83	0
5	BGC	L	201	1	11,11,12	0.40	0	15,15,17	0.73	0
8	XGX	H	302	-	38,38,38	1.04	1 (2%)	49,53,53	0.74	1 (2%)

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
8	XGX	H	302	-	-	14/31/31/31	0/3/3/3
5	BGC	L	201	1	-	2/2/19/22	0/1/1/1
6	FUC	L	202	1	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	302	XGX	C15-N2	5.24	1.45	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	302	XGX	O2-C14-C13	-2.38	116.29	121.97

There are no chirality outliers.

All (16) torsion outliers are listed below:

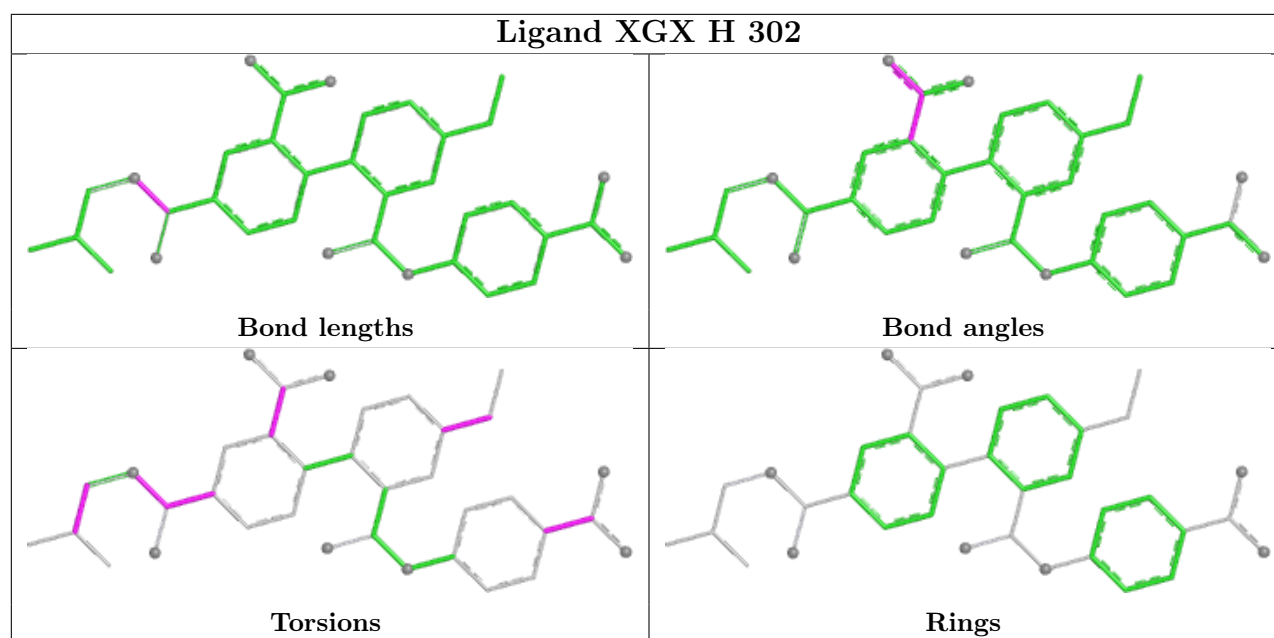
Mol	Chain	Res	Type	Atoms
8	H	302	XGX	C11-C15-N2-C16
8	H	302	XGX	O3-C15-N2-C16
8	H	302	XGX	N2-C16-C17-C19
5	L	201	BGC	O5-C5-C6-O6
8	H	302	XGX	N2-C16-C17-C18
5	L	201	BGC	C4-C5-C6-O6
8	H	302	XGX	C12-C13-C14-O2
8	H	302	XGX	C12-C13-C14-O1
8	H	302	XGX	C22-C21-C27-C26
8	H	302	XGX	C20-C21-C27-C26
8	H	302	XGX	C8-C13-C14-O1
8	H	302	XGX	C8-C13-C14-O2
8	H	302	XGX	C12-C11-C15-N2
8	H	302	XGX	C10-C11-C15-N2
8	H	302	XGX	C12-C11-C15-O3
8	H	302	XGX	N4-C28-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	302	XGX	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	10
4	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	158:TRP	C	163:SER	N	9.09
1	H	200:LYS	C	201:ASP	N	5.38
1	H	233:THR	C	234:VAL	N	5.01
1	H	195:TYR	C	196:SER	N	4.24
1	H	153:ARG	C	154:GLY	N	3.01
1	H	193:ALA	C	194:GLY	N	2.90
1	H	198:GLY	C	199:SER	N	2.75
1	H	229:GLN	C	230:GLY	N	2.42
1	H	231:CYS	C	232:ALA	N	1.95
1	H	192:CYS	C	193:ALA	N	1.94
1	H	35:VAL	C	36:ASN	N	1.91

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	L	132/142 (92%)	0.78	19 (14%) 6 4	20, 39, 86, 141	0
2	H	254/254 (100%)	0.08	22 (8%) 16 13	11, 24, 77, 101	0
3	T	75/75 (100%)	-0.18	1 (1%) 75 71	19, 27, 49, 59	0
4	U	116/116 (100%)	0.31	10 (8%) 16 13	20, 34, 78, 90	0
All	All	577/587 (98%)	0.25	52 (9%) 15 12	11, 30, 77, 141	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	233	THR	9.5
2	H	195	TYR	8.2
2	H	193	ALA	8.1
1	L	1	ALA	7.7
1	L	3	ALA	7.5
1	L	5	LEU	6.8
2	H	194	GLY	6.1
2	H	196	SER	5.7
1	L	18	LYS	5.6
1	L	4	PHE	5.4
2	H	200	LYS	5.3
1	L	15	ARG	5.0
1	L	2	ASN	4.8
1	L	21	GLN	4.2
1	L	32	LYS	4.0
2	H	65	ARG	3.4
1	L	38	LYS	3.2
2	H	62	LYS	3.2
2	H	153	ARG	3.2
4	U	137	ASN	3.2
2	H	234	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
4	U	181	LYS	3.0
1	L	47	GLY	2.8
2	H	178	ARG	2.8
4	U	136	ARG	2.8
4	U	163	SER	2.8
1	L	28	ARG	2.8
4	U	119	VAL	2.7
2	H	181	GLY	2.7
2	H	258	PRO	2.6
4	U	165	LYS	2.6
1	L	13	LEU	2.5
4	U	118	GLN	2.5
2	H	229	GLN	2.5
2	H	175	GLN	2.4
2	H	179	LYS	2.4
2	H	180	VAL	2.4
2	H	259	ARG	2.3
2	H	260	PRO	2.3
3	T	41	LYS	2.3
1	L	88	GLN	2.3
1	L	86	ASP	2.3
4	U	184	ASN	2.2
2	H	182	ASP	2.2
2	H	198	GLY	2.2
4	U	120	GLY	2.1
4	U	183	GLU	2.1
1	L	27	ALA	2.1
1	L	8	LEU	2.1
1	L	85	LYS	2.1
2	H	63	ASN	2.0
1	L	107	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CGU	L	7	12/13	0.42	0.37	87,113,126,139	0
1	CGU	L	19	12/13	0.55	0.23	87,105,115,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CGU	L	35	12/13	0.55	0.20	84,99,132,133	0
1	CGU	L	6	12/13	0.57	0.26	78,95,115,119	0
1	CGU	L	25	12/13	0.66	0.23	49,69,77,88	0
1	CGU	L	16	12/13	0.66	0.25	50,73,102,113	0
1	CGU	L	29	12/13	0.70	0.28	56,97,111,116	0
1	CGU	L	20	12/13	0.71	0.21	81,102,114,115	0
1	CGU	L	14	12/13	0.72	0.28	74,95,105,108	0
1	CGU	L	26	12/13	0.78	0.25	63,70,84,114	0

6.3 Carbohydrates [i](#)

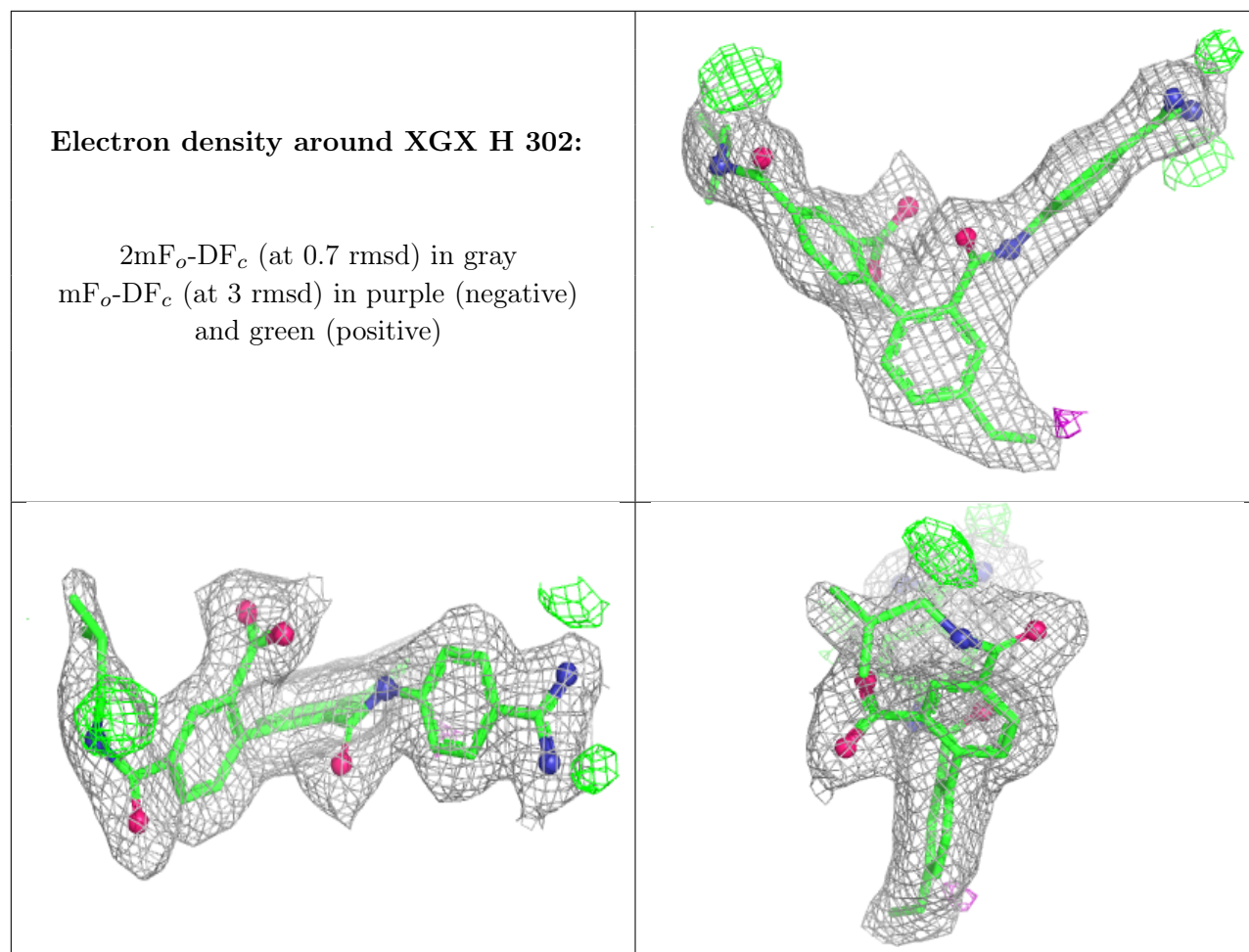
There are no oligosaccharides in this entry.

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
7	CA	L	204	1/1	0.44	0.45	123,123,123,123	0
7	CA	L	207	1/1	0.53	0.32	127,127,127,127	0
7	CA	L	205	1/1	0.62	0.30	103,103,103,103	0
7	CA	L	206	1/1	0.63	0.31	105,105,105,105	0
7	CA	L	209	1/1	0.63	0.22	107,107,107,107	0
7	CA	L	210	1/1	0.78	0.20	91,91,91,91	0
7	CA	L	208	1/1	0.87	0.10	87,87,87,87	0
6	FUC	L	202	10/11	0.87	0.10	40,44,45,45	0
7	CA	L	203	1/1	0.87	0.14	58,58,58,58	0
5	BGC	L	201	11/12	0.89	0.16	54,63,71,77	0
7	CA	H	301	1/1	0.93	0.07	43,43,43,43	0
8	XGX	H	302	36/36	0.93	0.10	19,25,65,67	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.