



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:31 AM BST

PDB ID : 2ZP0
Title : Human factor viia-tissue factor complexed with benzylsulfonamide-D-ile-gln-P-aminobenzamidine
Authors : Kadono, S.; Sakamoto, A.; Kikuchi, Y.; Oh-eda, M.; Yabuta, N.; Koga, T.; Hattori, K.; Shiraishi, T.; Haramura, M.; Kodama, H.
Deposited on : 2008-06-20
Resolution : 2.70 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 : 2.13.1
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) : 2.13.1

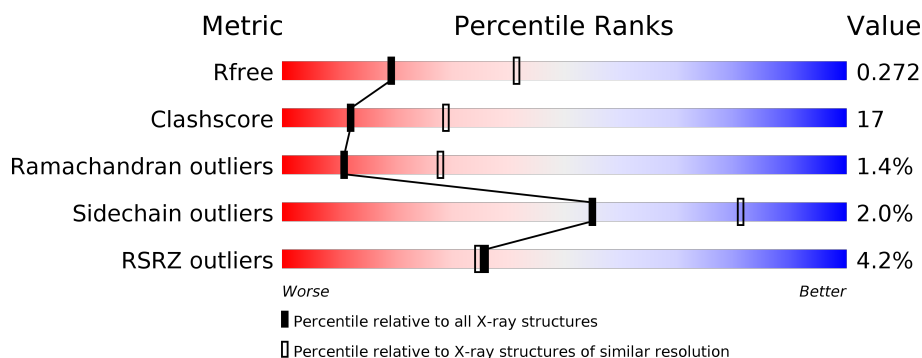
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	L	152	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>34%</div> <div>• 7%</div> </div> </div>
2	H	254	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>31%</div> <div>•</div> </div> </div>
3	T	218	<div> <div>6%</div> <div> <div></div> <div>57%</div> <div>28%</div> <div>• 12%</div> </div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5032 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
			Total	C	N	O	S			
1	L	142	1134	683	189	247	15	0	0	0

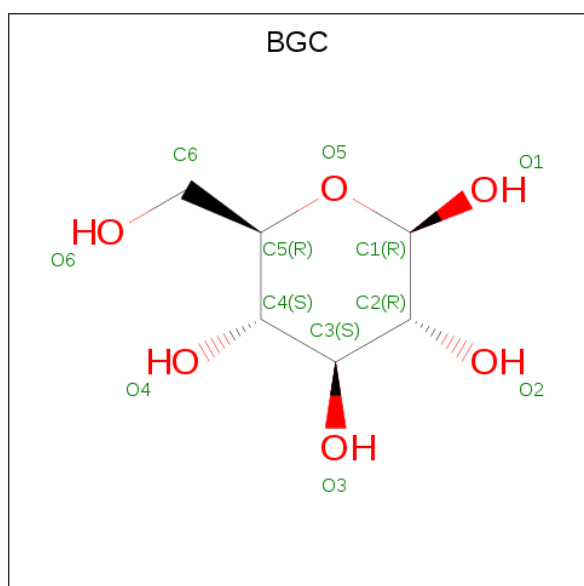
- Molecule 2 is a protein called Factor VII heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	254	1974	1253	351	357	13	0	0	0

- Molecule 3 is a protein called Tissue factor.

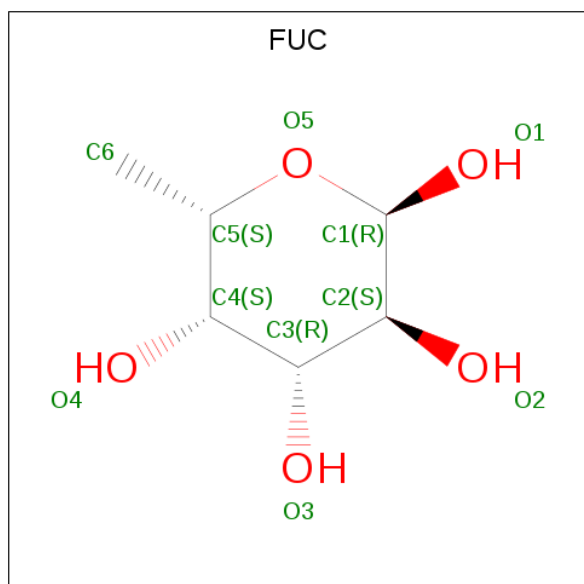
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	T	191	1557	993	251	308	5	0	0	0

- Molecule 4 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



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

- Molecule 5 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).

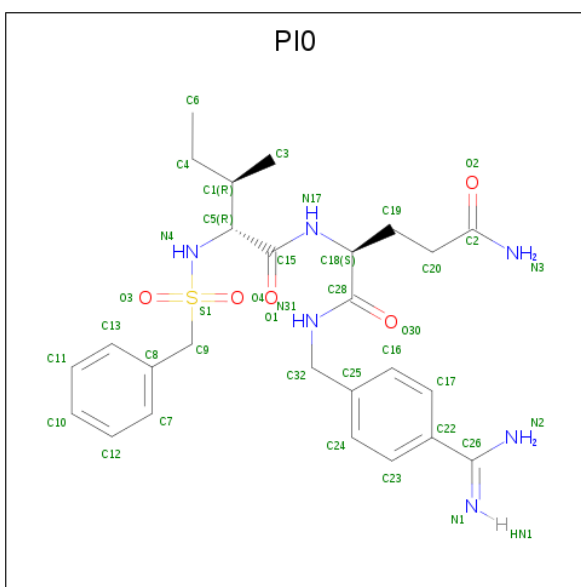


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is (2S)-N-[(4-carbamimidoylphenyl)methyl]-2-[(2R,3R)-3-methyl-2-(phenyl methylsulfonylamino)pentanoyl]amino]pentanediamide (three-letter code: PI0) (formula: $C_{26}H_{36}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	H	1	Total	C	N	O	S	0	0
			38	26	6	5	1		

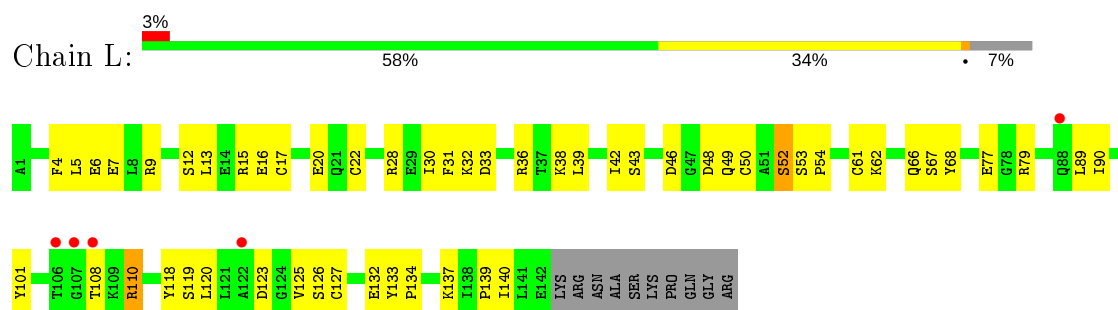
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	61	Total O 61 61	0	0
8	H	175	Total O 175 175	0	0
8	T	63	Total O 63 63	0	0

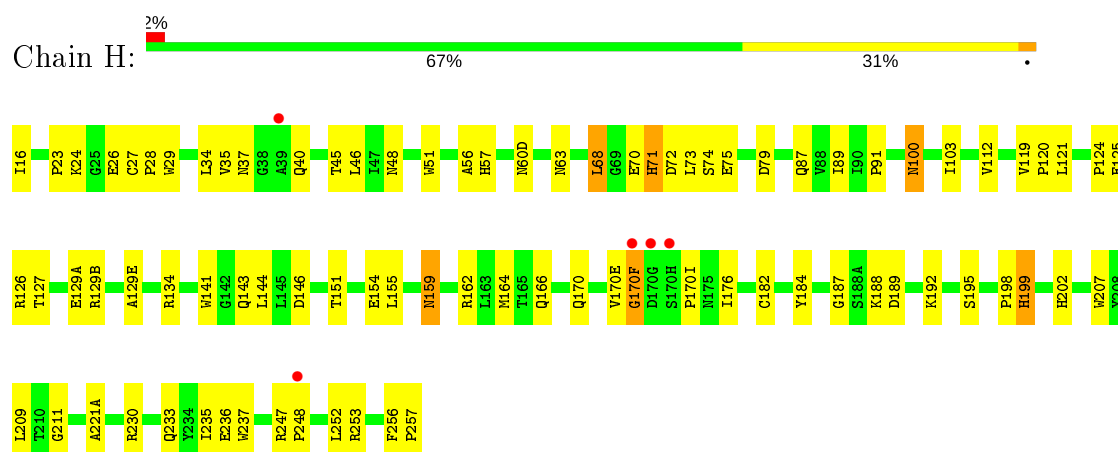
3 Residue-property plots [i](#)

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.

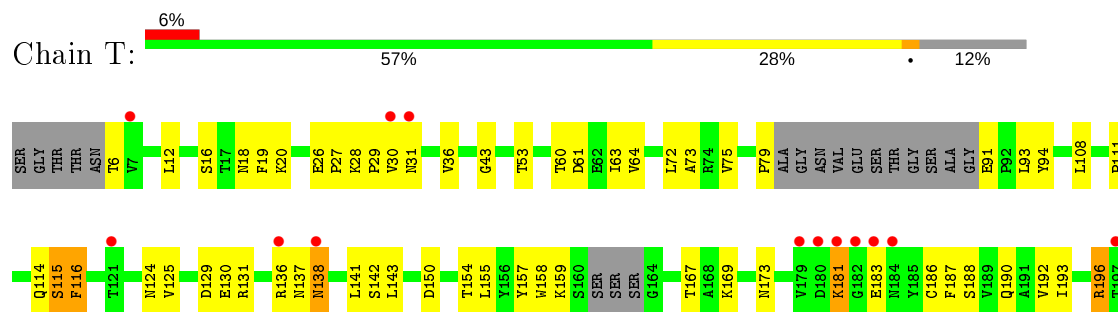
- Molecule 1: Factor VII light chain



- Molecule 2: Factor VII heavy chain



- Molecule 3: Tissue factor



V198	R200	T203	I204	V207	C209	GLY	GLN	GLU	LYS	GLY	GLU	PHE	ARG
M199	R201	S202	S205	E208	M210								

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.37Å 81.99Å 123.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.94 – 2.70 38.90 – 2.39	Depositor EDS
% Data completeness (in resolution range)	92.0 (14.94-2.70) 79.8 (38.90-2.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.39Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.218 , 0.306 0.197 , 0.272	Depositor DCC
R_{free} test set	1601 reflections (6.85%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5032	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: PI0, CA, BGC, CGU, 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	0.30	0/1028	0.58	0/1374
2	H	0.31	0/2024	0.63	1/2755 (0.0%)
3	T	0.32	0/1591	0.61	0/2163
All	All	0.31	0/4643	0.62	1/6292 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	H	199	HIS	N-CA-C	-5.59	95.90	111.00

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	L	1134	0	988	42	0
2	H	1974	0	1950	71	0
3	T	1557	0	1522	53	0
4	L	11	0	10	4	0
5	L	10	0	10	0	0
6	H	1	0	0	0	0
6	L	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	38	0	35	4	0
8	H	175	0	0	7	0
8	L	61	0	0	4	0
8	T	63	0	0	1	0
All	All	5032	0	4515	156	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 17.

All (156) 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:75:GLU:HB2	8:H:1144:HOH:O	1.81	0.79
1:L:120:LEU:HD12	1:L:126:SER:O	1.86	0.75
3:T:154:THR:HG22	3:T:169:LYS:HG2	1.66	0.75
2:H:170(E):VAL:HG12	2:H:170(F):GLY:N	2.01	0.75
2:H:46:LEU:HD22	2:H:68:LEU:HD22	1.70	0.71
3:T:60:THR:O	3:T:64:VAL:HG22	1.90	0.71
2:H:166:GLN:HB3	3:T:94:TYR:OH	1.92	0.70
2:H:170(E):VAL:HG12	2:H:170(F):GLY:H	1.57	0.69
2:H:45:THR:HG21	2:H:209:LEU:HD13	1.74	0.69
3:T:116:PHE:HA	3:T:124:ASN:O	1.93	0.68
1:L:13:LEU:HD12	1:L:17:CYS:HB2	1.77	0.67
2:H:87:GLN:HE22	2:H:247:ARG:H	1.42	0.67
1:L:101:TYR:CZ	2:H:125:GLU:HG3	2.30	0.66
2:H:46:LEU:HD22	2:H:68:LEU:CD2	2.26	0.66
3:T:108:LEU:HD11	3:T:193:ILE:HG12	1.78	0.66
2:H:146:ASP:HB2	8:H:1132:HOH:O	1.94	0.66
2:H:166:GLN:O	2:H:170:GLN:HG3	1.97	0.64
2:H:45:THR:OG1	2:H:198:PRO:HB3	1.97	0.64
1:L:140:ILE:HD11	2:H:26:GLU:HG3	1.80	0.63
2:H:24:LYS:NZ	2:H:79:ASP:OD2	2.31	0.63
3:T:136:ARG:HD3	3:T:141:LEU:HD21	1.81	0.62
3:T:108:LEU:HD22	3:T:143:LEU:HD21	1.81	0.62
3:T:26:GLU:HB3	3:T:27:PRO:HA	1.81	0.61
3:T:63:ILE:HD12	3:T:64:VAL:N	2.14	0.61
2:H:170(E):VAL:CG1	2:H:170(F):GLY:H	2.14	0.61
3:T:28:LYS:O	3:T:30:VAL:HG23	2.01	0.60
3:T:29:PRO:HG3	3:T:53:THR:O	2.01	0.60
3:T:72:LEU:HB3	8:T:260:HOH:O	2.02	0.60
2:H:176:ILE:HD13	2:H:182:CYS:SG	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:LEU:HD23	2:H:40:GLN:HA	1.85	0.58
2:H:170(E):VAL:CG1	2:H:170(F):GLY:N	2.66	0.58
1:L:12:SER:OG	1:L:15:ARG:HB3	2.03	0.58
2:H:121:LEU:HD23	2:H:209:LEU:HD13	1.86	0.57
2:H:37:ASN:HD21	2:H:60(D):ASN:HD22	1.50	0.57
1:L:38:LYS:O	1:L:42:ILE:HG23	2.05	0.57
2:H:184:TYR:CE1	2:H:188:LYS:HE2	2.39	0.57
2:H:143:GLN:H	2:H:143:GLN:CD	2.09	0.56
2:H:87:GLN:NE2	2:H:247:ARG:H	2.02	0.56
2:H:170(I):PRO:HD3	7:H:1001:PI0:H6B	1.89	0.55
1:L:33:ASP:OD2	1:L:36:ARG:HG3	2.06	0.55
1:L:6:CGU:HG	1:L:9:ARG:HD3	1.89	0.55
2:H:68:LEU:HD13	2:H:112:VAL:HG11	1.89	0.54
1:L:123:ASP:OD1	1:L:125:VAL:HG22	2.08	0.54
2:H:126:ARG:O	2:H:129(A):GLU:HG3	2.08	0.54
3:T:116:PHE:O	3:T:116:PHE:HD1	1.91	0.54
1:L:16:CGU:O	1:L:22:CYS:HB3	2.07	0.54
2:H:57:HIS:CE1	2:H:195:SER:HB3	2.43	0.53
3:T:155:LEU:O	3:T:167:THR:HA	2.09	0.53
2:H:27:CYS:N	2:H:28:PRO:CD	2.71	0.53
1:L:13:LEU:HA	1:L:30:ILE:HD13	1.90	0.53
3:T:108:LEU:CD2	3:T:143:LEU:HD11	2.39	0.53
3:T:129:ASP:HB2	3:T:173:ASN:ND2	2.24	0.53
3:T:159:LYS:HD3	3:T:183:GLU:HG3	1.91	0.52
3:T:131:ARG:HA	3:T:142:SER:HA	1.91	0.52
3:T:30:VAL:O	3:T:31:ASN:CB	2.57	0.52
2:H:202:HIS:HB2	2:H:207:TRP:CZ3	2.45	0.52
2:H:16:ILE:O	2:H:144:LEU:HA	2.10	0.52
1:L:89:LEU:HD13	8:L:1108:HOH:O	2.10	0.52
2:H:256:PHE:HA	2:H:257:PRO:C	2.30	0.51
3:T:192:VAL:HA	3:T:200:ARG:O	2.10	0.51
2:H:37:ASN:ND2	2:H:60(D):ASN:HD22	2.09	0.51
3:T:114:GLN:O	3:T:115:SER:HB3	2.09	0.51
2:H:56:ALA:HB2	2:H:103:ILE:O	2.10	0.51
2:H:46:LEU:HB2	2:H:68:LEU:HD21	1.93	0.51
1:L:49:GLN:HG3	4:L:1052:BGC:H6C1	1.93	0.51
3:T:30:VAL:O	3:T:31:ASN:HB2	2.10	0.50
2:H:195:SER:OG	7:H:1001:PI0:H32A	2.11	0.50
2:H:60(D):ASN:HB3	2:H:63:ASN:ND2	2.26	0.50
3:T:192:VAL:HG22	3:T:201:LYS:HG2	1.93	0.50
1:L:49:GLN:CG	4:L:1052:BGC:H6C1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:LYS:HE3	3:T:130:GLU:CD	2.32	0.49
3:T:150:ASP:O	3:T:193:ILE:HA	2.12	0.49
1:L:90:ILE:HB	8:L:1101:HOH:O	2.11	0.49
2:H:70:GLU:HB2	8:H:1033:HOH:O	2.12	0.49
3:T:31:ASN:O	3:T:79:PRO:C	2.51	0.49
2:H:129(E):ALA:HA	2:H:162:ARG:NH1	2.27	0.49
2:H:35:VAL:HG13	2:H:35:VAL:O	2.13	0.49
2:H:199:HIS:HB3	2:H:211:GLY:CA	2.43	0.49
3:T:158:TRP:CE2	3:T:186:CYS:HB2	2.47	0.48
2:H:126:ARG:HB3	8:H:1077:HOH:O	2.13	0.48
2:H:124:PRO:O	2:H:235:ILE:HD12	2.13	0.48
1:L:77:GLU:HB3	3:T:61:ASP:OD2	2.12	0.48
1:L:31:PHE:O	1:L:32:LYS:HB2	2.14	0.48
2:H:141:TRP:O	2:H:151:THR:HB	2.13	0.48
1:L:137:LYS:O	1:L:139:PRO:HD3	2.14	0.48
3:T:6:THR:OG1	3:T:93:LEU:HD12	2.13	0.48
3:T:157:TYR:HB3	3:T:187:PHE:CD1	2.49	0.47
1:L:52:SER:CB	4:L:1052:BGC:O2	2.63	0.47
1:L:132:GLU:HG2	1:L:133:TYR:CE2	2.50	0.47
1:L:48:ASP:OD1	1:L:50:CYS:HB2	2.14	0.47
1:L:39:LEU:HD12	1:L:42:ILE:HD11	1.96	0.47
3:T:116:PHE:HB3	3:T:125:VAL:HA	1.96	0.47
1:L:119:SER:O	1:L:127:CYS:HA	2.15	0.46
1:L:118:TYR:CE1	1:L:134:PRO:HB2	2.50	0.46
1:L:101:TYR:CE2	2:H:125:GLU:HG3	2.51	0.46
3:T:18:ASN:O	3:T:19:PHE:HB2	2.15	0.46
3:T:200:ARG:HH11	3:T:200:ARG:HB3	1.81	0.46
3:T:200:ARG:HG3	3:T:201:LYS:HG3	1.97	0.46
1:L:53:SER:N	1:L:54:PRO:CD	2.78	0.46
2:H:89:ILE:HG12	2:H:252:LEU:HD23	1.97	0.46
2:H:126:ARG:NH2	2:H:233:GLN:OE1	2.50	0.45
2:H:189:ASP:HB2	8:H:1013:HOH:O	2.16	0.45
3:T:12:LEU:N	3:T:12:LEU:HD12	2.32	0.45
3:T:63:ILE:C	3:T:63:ILE:HD12	2.37	0.45
2:H:23:PRO:HB2	2:H:26:GLU:OE2	2.17	0.45
2:H:60(D):ASN:CB	2:H:63:ASN:ND2	2.80	0.45
1:L:13:LEU:CD1	1:L:17:CYS:HB2	2.46	0.45
1:L:52:SER:O	1:L:53:SER:HB2	2.17	0.44
1:L:132:GLU:HG2	1:L:133:TYR:CD2	2.52	0.44
2:H:141:TRP:CZ2	2:H:155:LEU:HD13	2.53	0.44
3:T:137:ASN:O	3:T:138:ASN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:162:ARG:HD2	8:H:1047:HOH:O	2.17	0.44
3:T:136:ARG:HB3	3:T:141:LEU:HD21	1.98	0.44
3:T:36:VAL:HG22	3:T:75:VAL:HG22	2.00	0.44
2:H:202:HIS:HB2	2:H:207:TRP:CH2	2.53	0.44
3:T:155:LEU:HD12	3:T:188:SER:O	2.18	0.43
3:T:193:ILE:O	3:T:196:ARG:HB2	2.17	0.43
2:H:127:THR:O	2:H:129(B):ARG:HB3	2.19	0.43
1:L:66:GLN:O	1:L:67:SER:HB3	2.17	0.43
2:H:230:ARG:NH1	8:H:1108:HOH:O	2.52	0.43
2:H:71:HIS:O	2:H:154:GLU:HA	2.18	0.43
2:H:48:ASN:OD1	2:H:51:TRP:N	2.46	0.43
3:T:16:SER:HA	3:T:20:LYS:O	2.18	0.43
2:H:247:ARG:HG3	2:H:252:LEU:HD22	2.01	0.42
1:L:118:TYR:CZ	1:L:134:PRO:HB2	2.54	0.42
1:L:4:PHE:CE2	1:L:5:LEU:HG	2.53	0.42
2:H:72:ASP:C	2:H:74:SER:H	2.21	0.42
1:L:43:SER:HB3	3:T:206:PRO:HG3	2.01	0.42
1:L:49:GLN:HB3	4:L:1052:BGC:H6C1	2.00	0.42
1:L:110:ARG:HD2	1:L:110:ARG:C	2.40	0.42
3:T:108:LEU:HB2	3:T:202:SER:HB3	2.02	0.42
3:T:187:PHE:N	3:T:208:GLU:O	2.48	0.42
2:H:100:ASN:HA	2:H:100:ASN:HD22	1.65	0.42
2:H:166:GLN:HB3	3:T:94:TYR:CZ	2.55	0.42
1:L:20:CGU:HB2	8:L:1105:HOH:O	2.20	0.41
1:L:28:ARG:O	1:L:28:ARG:HD2	2.20	0.41
3:T:190:GLN:NE2	3:T:204:ASP:OD1	2.53	0.41
2:H:236:GLU:HG3	2:H:236:GLU:H	1.56	0.41
1:L:13:LEU:CA	1:L:30:ILE:HD13	2.50	0.41
2:H:187:GLY:HA2	2:H:221(A):ALA:O	2.19	0.41
2:H:87:GLN:NE2	2:H:247:ARG:HB2	2.36	0.41
2:H:134:ARG:HB2	3:T:43:GLY:O	2.20	0.41
3:T:72:LEU:HD12	3:T:73:ALA:H	1.85	0.41
1:L:46:ASP:OD2	1:L:66:GLN:N	2.49	0.41
1:L:61:CYS:SG	1:L:68:TYR:HB2	2.61	0.41
2:H:192:LYS:HD2	7:H:1001:PI0:C12	2.51	0.41
2:H:159:ASN:HD22	2:H:159:ASN:HA	1.66	0.41
2:H:170(I):PRO:HG2	7:H:1001:PI0:H3B	2.03	0.41
1:L:7:CGU:HG	8:L:1089:HOH:O	2.20	0.40
3:T:28:LYS:HD3	3:T:28:LYS:HA	1.75	0.40
2:H:91:PRO:HG3	2:H:237:TRP:CH2	2.55	0.40
3:T:181:LYS:HB3	3:T:181:LYS:HE3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:MET:CE	3:T:91:GLU:HB3	2.51	0.40
3:T:111:PRO:HB2	3:T:205:SER:HB3	2.03	0.40
2:H:119:VAL:CG1	2:H:120:PRO:HD2	2.52	0.40
2:H:37:ASN:OD1	2:H:63:ASN:ND2	2.51	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	130/152 (86%)	107 (82%)	21 (16%)	2 (2%)	10	26
2	H	252/254 (99%)	233 (92%)	15 (6%)	4 (2%)	9	24
3	T	185/218 (85%)	165 (89%)	18 (10%)	2 (1%)	14	34
All	All	567/624 (91%)	505 (89%)	54 (10%)	8 (1%)	11	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	108	THR
3	T	196	ARG
2	H	73	LEU
3	T	115	SER
1	L	79	ARG
2	H	71	HIS
2	H	248	PRO
2	H	170(F)	GLY

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	114/122 (93%)	112 (98%)	2 (2%)	59	83
2	H	216/216 (100%)	211 (98%)	5 (2%)	50	78
3	T	180/199 (90%)	177 (98%)	3 (2%)	60	84
All	All	510/537 (95%)	500 (98%)	10 (2%)	55	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	52	SER
1	L	110	ARG
2	H	29	TRP
2	H	68	LEU
2	H	100	ASN
2	H	159	ASN
2	H	253	ARG
3	T	116	PHE
3	T	138	ASN
3	T	181	LYS

Some 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	80	ASN
1	L	88	GLN
2	H	60(D)	ASN
2	H	87	GLN
2	H	100	ASN
2	H	159	ASN
2	H	202	HIS
2	H	239	GLN
3	T	31	ASN
3	T	118	GLN

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Mol	Chain	Res	Type
3	T	138	ASN
3	T	190	GLN

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	20	1,6	3,11,12	0.77	0	1,14,16	0.64	0
1	CGU	L	7	1,6	3,11,12	0.75	0	1,14,16	0.68	0
1	CGU	L	16	1,6	3,11,12	0.65	0	1,14,16	0.64	0
1	CGU	L	35	1	3,11,12	0.75	0	1,14,16	0.03	0
1	CGU	L	26	1,6	3,11,12	0.66	0	1,14,16	0.19	0
1	CGU	L	29	1,6	3,11,12	0.65	0	1,14,16	0.20	0
1	CGU	L	6	1,6	3,11,12	0.69	0	1,14,16	0.29	0
1	CGU	L	19	1,6	3,11,12	0.75	0	1,14,16	0.39	0
1	CGU	L	25	1,6	3,11,12	0.91	0	1,14,16	0.10	0
1	CGU	L	14	1,6	3,11,12	0.69	0	1,14,16	0.25	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	20	1,6	-	2/5/14/16	-
1	CGU	L	7	1,6	-	0/5/14/16	-
1	CGU	L	16	1,6	-	0/5/14/16	-
1	CGU	L	35	1	-	1/5/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CGU	L	26	1,6	-	0/5/14/16	-
1	CGU	L	29	1,6	-	0/5/14/16	-
1	CGU	L	6	1,6	-	2/5/14/16	-
1	CGU	L	19	1,6	-	0/5/14/16	-
1	CGU	L	25	1,6	-	0/5/14/16	-
1	CGU	L	14	1,6	-	0/5/14/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L	6	CGU	CA-CB-CG-CD1
1	L	6	CGU	CA-CB-CG-CD2
1	L	20	CGU	CA-CB-CG-CD1
1	L	35	CGU	C-CA-CB-CG
1	L	20	CGU	CA-CB-CG-CD2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	20	CGU	1	0
1	L	7	CGU	1	0
1	L	16	CGU	1	0
1	L	6	CGU	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
5	FUC	L	1060	1	10,10,11	0.54	0	14,14,16	0.77	0
4	BGC	L	1052	1	11,11,12	0.65	0	15,15,17	0.75	0
7	PI0	H	1001	-	38,39,39	1.22	1 (2%)	47,53,53	1.35	6 (12%)

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
5	FUC	L	1060	1	-	-	0/1/1/1
4	BGC	L	1052	1	-	1/2/19/22	0/1/1/1
7	PI0	H	1001	-	-	4/42/42/42	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	1001	PI0	S1-N4	5.39	1.70	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	1001	PI0	O3-S1-N4	-4.58	100.54	107.12
7	H	1001	PI0	O3-S1-C9	3.53	113.67	108.30
7	H	1001	PI0	C22-C26-N2	2.64	122.02	118.05
7	H	1001	PI0	O1-C15-N17	2.35	127.29	122.93
7	H	1001	PI0	C18-C28-N31	-2.29	111.93	116.54
7	H	1001	PI0	O4-S1-N4	-2.23	103.92	107.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1052	BGC	O5-C5-C6-O6
7	H	1001	PI0	C17-C22-C26-N2
7	H	1001	PI0	C23-C22-C26-N2

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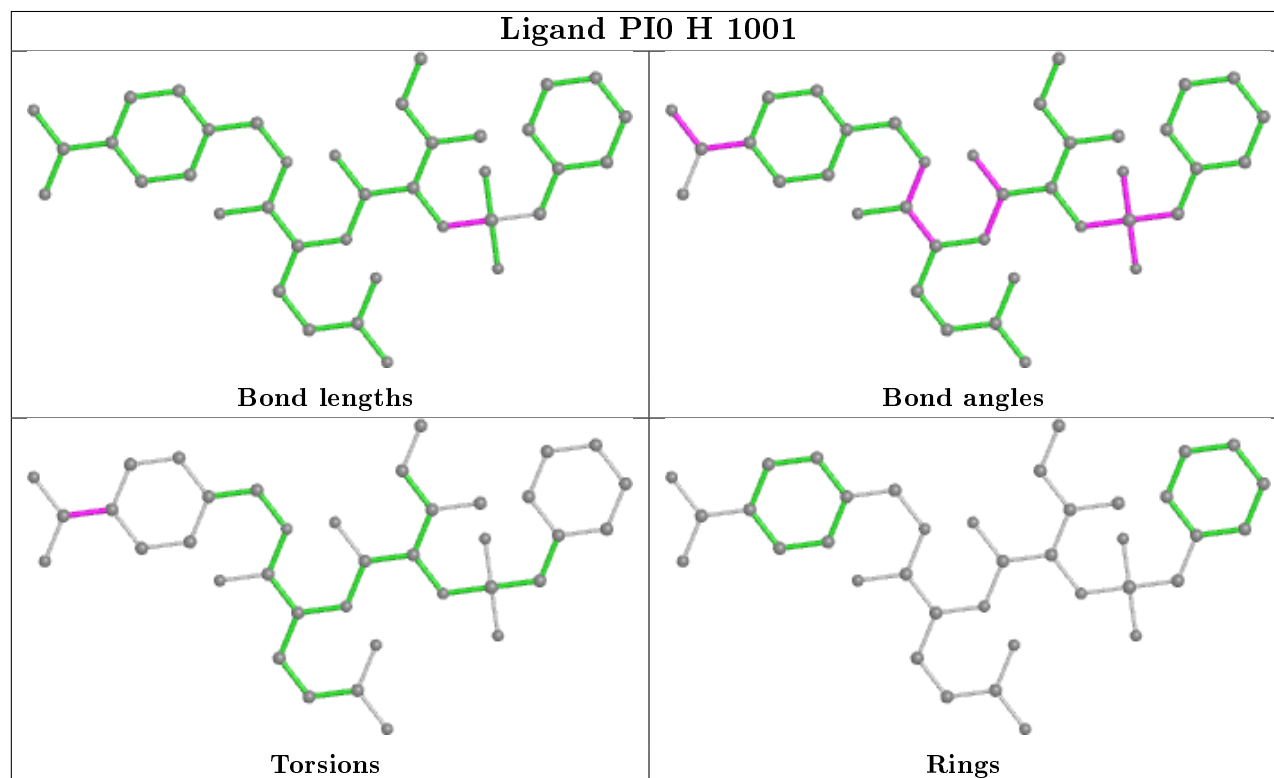
Mol	Chain	Res	Type	Atoms
7	H	1001	PI0	C17-C22-C26-N1
7	H	1001	PI0	C23-C22-C26-N1

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1052	BGC	4	0
7	H	1001	PI0	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	132/152 (86%)	-0.10	5 (3%) 40 39	9, 20, 37, 44	0
2	H	254/254 (100%)	-0.16	5 (1%) 65 67	1, 10, 32, 51	0
3	T	191/218 (87%)	-0.06	14 (7%) 15 13	2, 20, 46, 55	0
All	All	577/624 (92%)	-0.11	24 (4%) 36 35	1, 15, 41, 55	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	170(G)	ASP	5.1
2	H	170(F)	GLY	4.3
3	T	181	LYS	4.2
3	T	30	VAL	4.1
3	T	182	GLY	4.1
2	H	170(H)	SER	3.5
3	T	198	VAL	3.1
3	T	7	VAL	3.0
3	T	31	ASN	3.0
3	T	197	THR	2.9
1	L	122	ALA	2.8
1	L	107	GLY	2.7
3	T	183	GLU	2.7
1	L	106	THR	2.6
1	L	108	THR	2.5
2	H	39	ALA	2.4
3	T	136	ARG	2.2
3	T	179	VAL	2.2
3	T	180	ASP	2.1
2	H	248	PRO	2.1
3	T	121	THR	2.1
3	T	138	ASN	2.1
3	T	184	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	88	GLN	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	35	12/13	0.67	0.33	35,45,50,51	0
1	CGU	L	20	12/13	0.89	0.22	28,34,35,36	0
1	CGU	L	25	12/13	0.89	0.14	19,23,27,30	0
1	CGU	L	29	12/13	0.90	0.15	20,22,23,27	0
1	CGU	L	19	12/13	0.91	0.21	28,34,37,38	0
1	CGU	L	7	12/13	0.92	0.14	14,17,22,22	0
1	CGU	L	16	12/13	0.93	0.16	19,22,24,27	0
1	CGU	L	6	12/13	0.93	0.15	12,17,20,21	0
1	CGU	L	14	12/13	0.93	0.17	17,20,23,23	0
1	CGU	L	26	12/13	0.94	0.14	20,21,24,24	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.

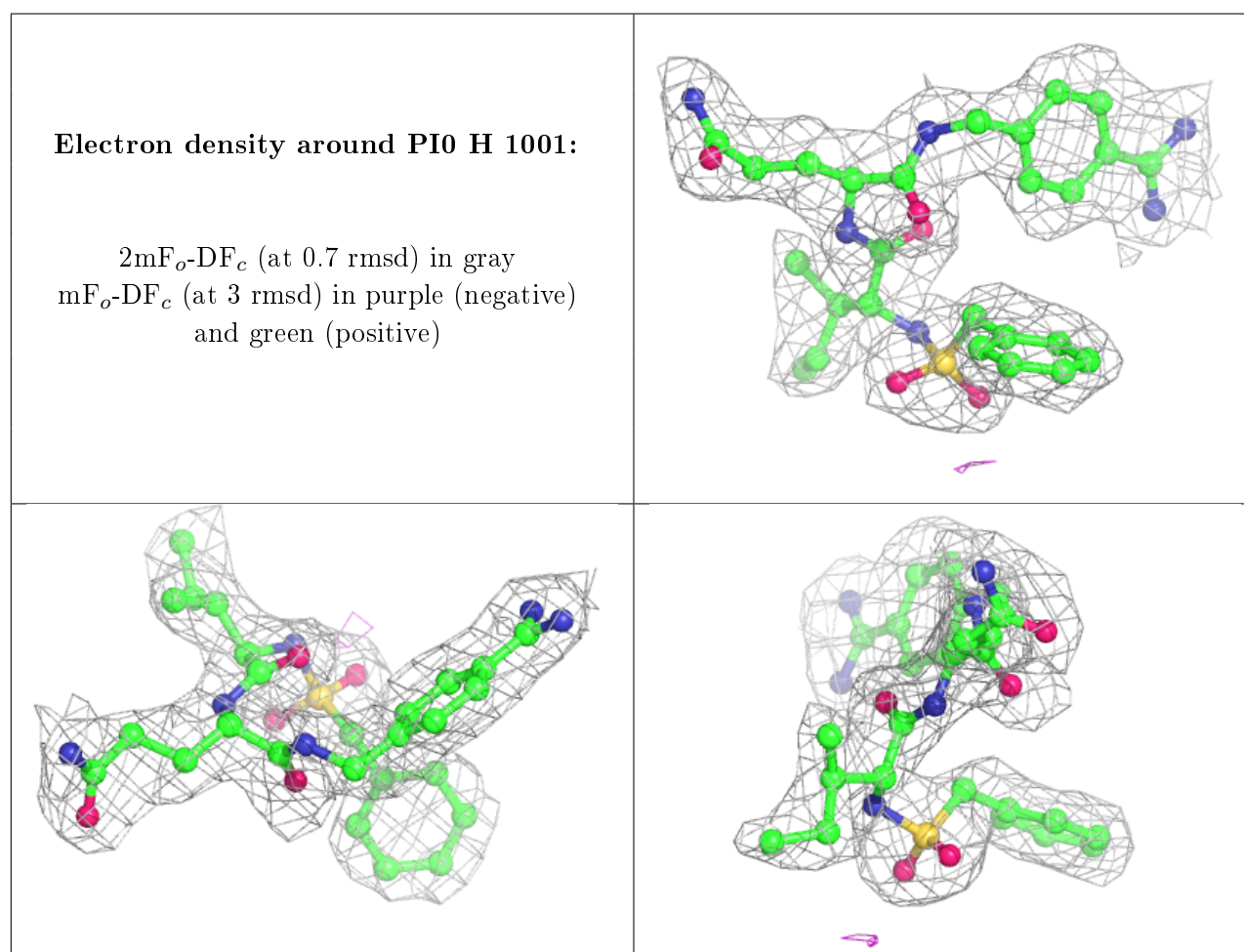
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BGC	L	1052	11/12	0.85	0.14	29,30,30,32	0
6	CA	L	508	1/1	0.87	0.23	53,53,53,53	0
6	CA	L	506	1/1	0.91	0.12	39,39,39,39	0
5	FUC	L	1060	10/11	0.94	0.18	23,25,27,27	0
7	PI0	H	1001	38/38	0.95	0.14	4,9,18,18	0
6	CA	L	509	1/1	0.95	0.20	32,32,32,32	0
6	CA	H	501	1/1	0.96	0.10	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CA	L	507	1/1	0.96	0.06	39,39,39,39	0
6	CA	L	504	1/1	0.97	0.20	36,36,36,36	0
6	CA	L	503	1/1	0.97	0.18	27,27,27,27	0
6	CA	L	502	1/1	0.97	0.08	21,21,21,21	0
6	CA	L	505	1/1	0.98	0.10	20,20,20,20	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 ⓘ

There are no such residues in this entry.