



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 01:53 PM EDT

PDB ID : 1Z8J  
Title : Crystal structure of the thrombin mutant G193P bound to PPACK  
Authors : Bobofchak, K.M.; Pineda, A.O.; Mathews, F.S.; Di Cera, E.  
Deposited on : 2005-03-30  
Resolution : 2.00 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](mailto: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 : 2.23.2  
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) : 2.23.2

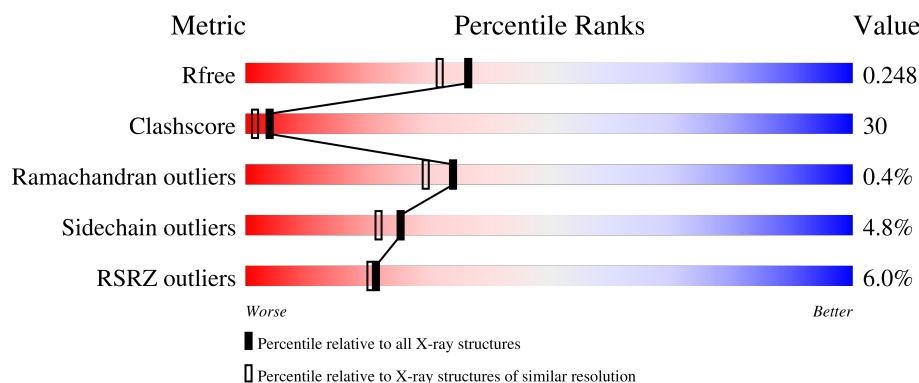
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	40	<div> <div>8%</div> <div>50%</div> <div>45%</div> <div>5%</div> </div>
2	B	259	<div> <div>5%</div> <div>64%</div> <div>26%</div> <div>• 6%</div> </div>

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
5	NAG	B	600	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2592 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 Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	40	Total	C	N	O	S	0	0	0
			327	206	53	67	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1968	1260	345	349	14			

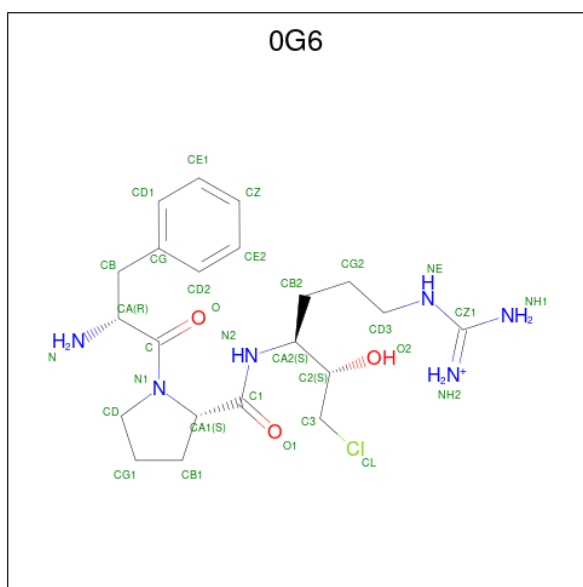
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	193	PRO	GLY	engineered mutation	UNP P00734

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	2	Total	Zn	0	0
			2	2		

- Molecule 4 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (three-letter code: 0G6) (formula: C<sub>21</sub>H<sub>34</sub>ClN<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			30	21	6	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

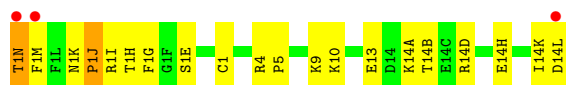
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	56	Total 56	O 56	0	0
7	B	193	Total 193	O 193	0	0

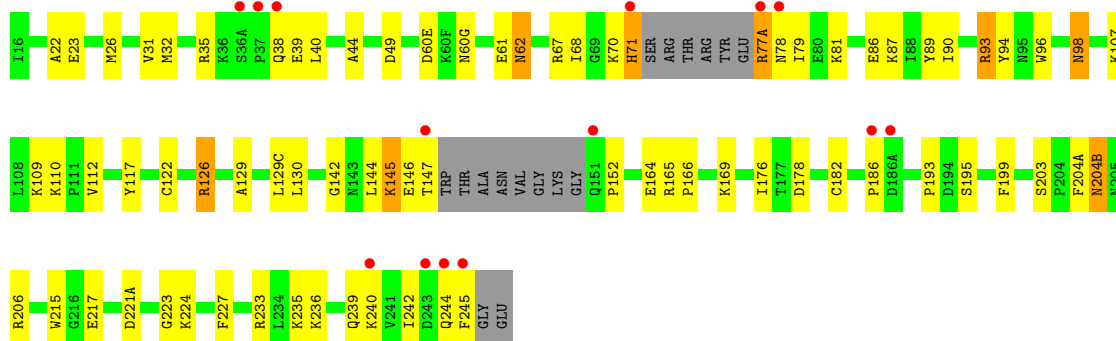
### 3 Residue-property plots [i](#)

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: Thrombin light chain



- Molecule 2: Thrombin heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.71Å 73.55Å 90.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 37.46 – 1.69	Depositor EDS
% Data completeness (in resolution range)	97.9 (40.00-2.00) 86.2 (37.46-1.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.07 (at 1.70Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.205 , 0.246 0.210 , 0.248	Depositor DCC
$R_{free}$ test set	1116 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2592	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, OG6, NAG, ZN

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	0.65	1/333 (0.3%)	0.91	0/444
2	B	0.38	0/2019	0.68	1/2729 (0.0%)
All	All	0.43	1/2352 (0.0%)	0.71	1/3173 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1(J)	PRO	N-CD	5.31	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	199	PHE	N-CA-C	-5.22	96.89	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	A	327	0	313	23	1
2	B	1968	0	1946	115	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	0	30	10	0
5	B	14	0	12	13	0
6	B	1	0	0	0	0
7	A	56	0	0	4	5
7	B	193	0	0	25	3
All	All	2592	0	2301	139	6

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 30.

All (139) 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)
5:B:600:NAG:C5	5:B:600:NAG:C6	1.74	1.62
5:B:600:NAG:O3	5:B:600:NAG:C3	1.68	1.41
2:B:23:GLU:N	2:B:26:MET:HE3	1.68	1.08
2:B:23:GLU:H	2:B:26:MET:HE3	0.97	1.07
2:B:93:ARG:HH11	2:B:93:ARG:HG3	1.16	1.06
2:B:240:LYS:O	2:B:244:GLN:HB2	1.60	1.02
2:B:23:GLU:H	2:B:26:MET:CE	1.73	1.01
2:B:60(G):ASN:ND2	5:B:600:NAG:C2	2.25	0.98
2:B:195:SER:CB	4:B:301:OG6:C2	2.40	0.98
2:B:60(G):ASN:CG	5:B:600:NAG:C1	2.36	0.92
2:B:61:GLU:HG2	2:B:87:LYS:HA	1.55	0.87
2:B:71:HIS:HE1	7:B:337:HOH:O	1.56	0.87
2:B:32:MET:CE	7:B:472:HOH:O	2.24	0.85
2:B:110:LYS:HE3	7:B:509:HOH:O	1.74	0.85
5:B:600:NAG:C6	5:B:600:NAG:C4	2.55	0.84
2:B:60(E):ASP:HB3	7:B:405:HOH:O	1.77	0.84
2:B:22:ALA:HA	2:B:26:MET:HE1	1.60	0.82
1:A:14(K):ILE:O	1:A:14(L):ASP:O	1.97	0.82
2:B:93:ARG:HG3	2:B:93:ARG:NH1	1.95	0.81
2:B:70:LYS:NZ	7:B:501:HOH:O	2.15	0.80
2:B:32:MET:HE1	7:B:472:HOH:O	1.80	0.79
2:B:217:GLU:HB2	2:B:224:LYS:HE2	1.63	0.79
2:B:165:ARG:NE	7:B:484:HOH:O	2.11	0.78
2:B:71:HIS:ND1	2:B:71:HIS:N	2.30	0.78
2:B:126:ARG:CG	2:B:126:ARG:HH11	1.97	0.78
2:B:129:ALA:O	2:B:130:LEU:HB2	1.84	0.76
2:B:178:ASP:HB2	2:B:233:ARG:HH11	1.50	0.75
2:B:178:ASP:HB2	2:B:233:ARG:NH1	2.03	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60(G):ASN:ND2	5:B:600:NAG:H2	2.02	0.72
2:B:165:ARG:HH12	2:B:169:LYS:HE2	1.53	0.72
2:B:165:ARG:HH22	2:B:169:LYS:HZ3	1.40	0.70
2:B:60(G):ASN:ND2	5:B:600:NAG:O5	2.24	0.70
2:B:22:ALA:HA	2:B:26:MET:CE	2.21	0.69
2:B:71:HIS:CD2	7:B:477:HOH:O	2.46	0.69
2:B:195:SER:HB2	4:B:301:OG6:C2	2.21	0.69
1:A:1(M):PHE:HE1	2:B:235:LYS:HG2	1.57	0.69
2:B:195:SER:OG	4:B:301:OG6:CA2	2.41	0.68
2:B:32:MET:HE3	7:B:472:HOH:O	1.92	0.67
2:B:93:ARG:HH11	2:B:93:ARG:CG	2.01	0.67
2:B:142:GLY:HA2	2:B:193:PRO:HD2	1.78	0.66
1:A:14(K):ILE:HD13	1:A:14(K):ILE:N	2.10	0.65
2:B:87:LYS:NZ	7:B:554:HOH:O	2.25	0.65
2:B:165:ARG:HH12	2:B:169:LYS:CE	2.09	0.64
2:B:145:LYS:HD2	2:B:146:GLU:O	1.98	0.64
1:A:1(M):PHE:CE1	2:B:235:LYS:HG2	2.33	0.63
2:B:178:ASP:CB	2:B:233:ARG:HH11	2.12	0.63
2:B:169:LYS:HD2	7:B:434:HOH:O	1.99	0.63
1:A:1(M):PHE:CZ	2:B:239:GLN:OE1	2.52	0.63
2:B:60(G):ASN:OD1	5:B:600:NAG:C1	2.47	0.63
2:B:169:LYS:CD	7:B:434:HOH:O	2.46	0.63
2:B:240:LYS:O	2:B:244:GLN:CB	2.42	0.63
2:B:98:ASN:HD22	2:B:98:ASN:H	1.47	0.63
2:B:165:ARG:HH22	2:B:169:LYS:NZ	1.96	0.62
2:B:217:GLU:HB2	2:B:224:LYS:CE	2.30	0.61
2:B:62:ASN:HD22	2:B:62:ASN:H	1.50	0.59
1:A:14(D):ARG:O	1:A:14(H):GLU:CG	2.52	0.58
2:B:126:ARG:HH11	2:B:126:ARG:HG3	1.68	0.58
1:A:14(A):LYS:HG3	1:A:14(B):THR:HG23	1.85	0.58
2:B:165:ARG:HB3	2:B:166:PRO:HD3	1.85	0.58
5:B:600:NAG:O6	7:B:519:HOH:O	2.16	0.57
2:B:126:ARG:HG2	2:B:126:ARG:NH1	2.19	0.57
2:B:62:ASN:H	2:B:62:ASN:ND2	2.03	0.57
2:B:195:SER:OG	4:B:301:OG6:C3	2.49	0.57
2:B:195:SER:OG	4:B:301:OG6:CB2	2.53	0.56
4:B:301:OG6:HD3	4:B:301:OG6:CD1	2.35	0.56
2:B:144:LEU:HD21	2:B:152:PRO:HB3	1.87	0.56
2:B:145:LYS:HE3	2:B:147:THR:HG22	1.86	0.56
2:B:67:ARG:HG3	2:B:67:ARG:HH11	1.71	0.56
2:B:178:ASP:O	2:B:233:ARG:HD3	2.05	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ARG:HH12	2:B:169:LYS:NZ	2.05	0.54
2:B:126:ARG:CG	2:B:126:ARG:NH1	2.60	0.54
1:A:14(D):ARG:O	1:A:14(H):GLU:HG2	2.08	0.54
5:B:600:NAG:O3	5:B:600:NAG:C4	2.54	0.52
2:B:77(A):ARG:N	7:B:496:HOH:O	2.41	0.52
2:B:93:ARG:NH1	2:B:93:ARG:CG	2.66	0.52
2:B:176:ILE:HD12	2:B:227:PHE:CE2	2.44	0.52
2:B:165:ARG:HH12	2:B:169:LYS:HZ1	1.57	0.51
1:A:1(K):ASN:OD1	1:A:1(J):PRO:HD2	2.10	0.51
2:B:195:SER:CB	4:B:301:OG6:C3	2.89	0.51
2:B:87:LYS:HD2	2:B:89:TYR:CZ	2.45	0.51
2:B:39:GLU:OE2	7:B:385:HOH:O	2.19	0.50
1:A:1(N):THR:N	7:A:537:HOH:O	2.44	0.50
2:B:107:LYS:HZ2	2:B:245:PHE:HZ	1.57	0.49
2:B:215:TRP:HA	4:B:301:OG6:HG21	1.93	0.49
2:B:98:ASN:H	2:B:98:ASN:ND2	2.09	0.49
2:B:236:LYS:HG2	7:B:419:HOH:O	2.13	0.48
2:B:71:HIS:CE1	7:B:337:HOH:O	2.42	0.47
2:B:67:ARG:HA	2:B:81:LYS:O	2.15	0.47
2:B:93:ARG:HD2	7:B:531:HOH:O	2.13	0.47
2:B:169:LYS:HG3	7:B:433:HOH:O	2.14	0.47
1:A:1(M):PHE:CE1	2:B:239:GLN:OE1	2.68	0.47
2:B:35:ARG:O	2:B:38:GLN:HA	2.14	0.47
2:B:62:ASN:ND2	2:B:62:ASN:N	2.62	0.47
2:B:217:GLU:CB	2:B:224:LYS:HE2	2.39	0.47
2:B:94:TYR:CZ	2:B:96:TRP:HB3	2.50	0.47
2:B:98:ASN:HD22	2:B:98:ASN:N	2.07	0.47
2:B:186:PRO:HG3	2:B:223:GLY:N	2.29	0.46
1:A:10:LYS:NZ	7:A:441:HOH:O	2.47	0.46
2:B:204(B):ASN:ND2	2:B:206:ARG:H	2.13	0.46
2:B:22:ALA:CA	2:B:26:MET:CE	2.91	0.46
2:B:67:ARG:HG3	2:B:67:ARG:NH1	2.30	0.46
2:B:86:GLU:HB2	2:B:109:LYS:HA	1.97	0.46
1:A:14(D):ARG:O	1:A:14(H):GLU:HG3	2.15	0.46
2:B:61:GLU:HG2	2:B:87:LYS:CA	2.38	0.46
2:B:186:PRO:HG3	2:B:223:GLY:H	1.81	0.46
2:B:204(B):ASN:C	2:B:204(B):ASN:HD22	2.18	0.45
4:B:301:OG6:HD3	4:B:301:OG6:HD1	1.97	0.45
1:A:1:CYS:O	2:B:122:CYS:SG	2.75	0.45
2:B:165:ARG:NH1	2:B:169:LYS:HE2	2.28	0.45
2:B:165:ARG:HH11	2:B:165:ARG:HG2	1.81	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:CYS:C	2:B:122:CYS:SG	2.95	0.45
1:A:1(G):PHE:CD1	2:B:242:ILE:HD13	2.51	0.45
1:A:14(K):ILE:C	1:A:14(L):ASP:O	2.55	0.45
2:B:126:ARG:HH11	2:B:126:ARG:HG2	1.74	0.45
2:B:164:GLU:H	2:B:164:GLU:CD	2.19	0.45
2:B:40:LEU:HD21	7:B:341:HOH:O	2.16	0.44
2:B:87:LYS:HD2	2:B:89:TYR:OH	2.17	0.44
2:B:98:ASN:ND2	2:B:98:ASN:N	2.66	0.44
5:B:600:NAG:C6	5:B:600:NAG:O5	2.59	0.44
5:B:600:NAG:C3	5:B:600:NAG:HO3	2.12	0.44
1:A:1(H):THR:HB	2:B:242:ILE:O	2.18	0.43
1:A:1(E):SER:H	2:B:49:ASP:CG	2.22	0.43
2:B:81:LYS:HE3	2:B:112:VAL:HG12	2.01	0.42
2:B:215:TRP:CE3	4:B:301:OG6:HD2	2.54	0.42
2:B:245:PHE:HB2	7:B:548:HOH:O	2.19	0.42
5:B:600:NAG:H83	7:B:400:HOH:O	2.20	0.42
2:B:40:LEU:C	2:B:40:LEU:HD23	2.40	0.42
2:B:129(C):LEU:HD21	2:B:203:SER:HA	2.01	0.41
2:B:204(A):PHE:HD2	7:B:418:HOH:O	2.03	0.41
1:A:9:LYS:HE3	7:A:465:HOH:O	2.20	0.41
2:B:23:GLU:OE2	7:B:356:HOH:O	2.22	0.41
2:B:68:ILE:O	2:B:81:LYS:N	2.52	0.41
1:A:1(K):ASN:HA	1:A:1(J):PRO:HD3	1.83	0.41
2:B:79:ILE:HD11	2:B:117:TYR:CD2	2.56	0.41
1:A:13:GLU:OE1	7:A:458:HOH:O	2.22	0.41
2:B:87:LYS:CD	2:B:89:TYR:CZ	3.04	0.40
2:B:221(A):ASP:HA	7:B:328:HOH:O	2.21	0.40
1:A:4:ARG:HA	1:A:5:PRO:HD3	1.98	0.40
2:B:31:VAL:HB	2:B:44:ALA:HB3	2.03	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:537:HOH:O	7:A:547:HOH:O[4_465]	0.48	1.72
7:A:528:HOH:O	7:A:538:HOH:O[4_565]	0.56	1.64
7:A:552:HOH:O	7:B:533:HOH:O[1_655]	0.59	1.61
7:B:515:HOH:O	7:B:517:HOH:O[1_655]	1.54	0.66
7:A:518:HOH:O	7:B:533:HOH:O[1_655]	1.99	0.21
1:A:1(N):THR:N	7:A:547:HOH:O[4_465]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	38/40 (95%)	34 (90%)	4 (10%)	0	100	100
2	B	237/259 (92%)	227 (96%)	9 (4%)	1 (0%)	34	30
All	All	275/299 (92%)	261 (95%)	13 (5%)	1 (0%)	34	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	78	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	A	36/36 (100%)	34 (94%)	2 (6%)	21	17
2	B	214/226 (95%)	204 (95%)	10 (5%)	26	22
All	All	250/262 (95%)	238 (95%)	12 (5%)	25	22

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1(N)	THR
1	A	1(I)	ARG
2	B	62	ASN
2	B	71	HIS
2	B	77(A)	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	90	ILE
2	B	93	ARG
2	B	98	ASN
2	B	126	ARG
2	B	145	LYS
2	B	182	CYS
2	B	204(B)	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	38	GLN
2	B	62	ASN
2	B	71	HIS
2	B	98	ASN
2	B	131	GLN
2	B	143	ASN
2	B	151	GLN
2	B	204(B)	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	NAG	B	600	2	14,14,15	5.29	9 (64%)	17,19,21	3.63	10 (58%)
4	OG6	B	301	2	30,31,32	1.19	1 (3%)	37,41,42	0.59	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
5	NAG	B	600	2	-	2/6/23/26	0/1/1/1
4	OG6	B	301	2	-	4/31/41/43	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	NAG	O3-C3	10.89	1.68	1.43
5	B	600	NAG	O5-C5	7.91	1.59	1.43
5	B	600	NAG	O4-C4	7.48	1.60	1.43
5	B	600	NAG	C6-C5	6.82	1.74	1.51
5	B	600	NAG	C1-C2	-6.40	1.42	1.52
4	B	301	OG6	O2-C2	-6.08	1.26	1.43
5	B	600	NAG	C7-N2	4.41	1.49	1.34
5	B	600	NAG	O7-C7	4.33	1.33	1.23
5	B	600	NAG	O5-C1	3.49	1.49	1.43
5	B	600	NAG	O6-C6	-3.19	1.29	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	NAG	C1-O5-C5	-10.19	98.38	112.19
5	B	600	NAG	C2-N2-C7	-5.01	115.78	122.90
5	B	600	NAG	C1-C2-N2	4.01	117.34	110.49
5	B	600	NAG	C6-C5-C4	-3.93	103.80	113.00
5	B	600	NAG	O4-C4-C3	-3.55	102.15	110.35
5	B	600	NAG	O5-C5-C6	-3.34	101.97	107.20
5	B	600	NAG	O5-C1-C2	3.31	116.52	111.29

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	NAG	O3-C3-C4	-3.10	103.18	110.35
5	B	600	NAG	C4-C3-C2	-2.45	107.43	111.02
5	B	600	NAG	O4-C4-C5	2.25	114.89	109.30

There are no chirality outliers.

All (6) torsion outliers are listed below:

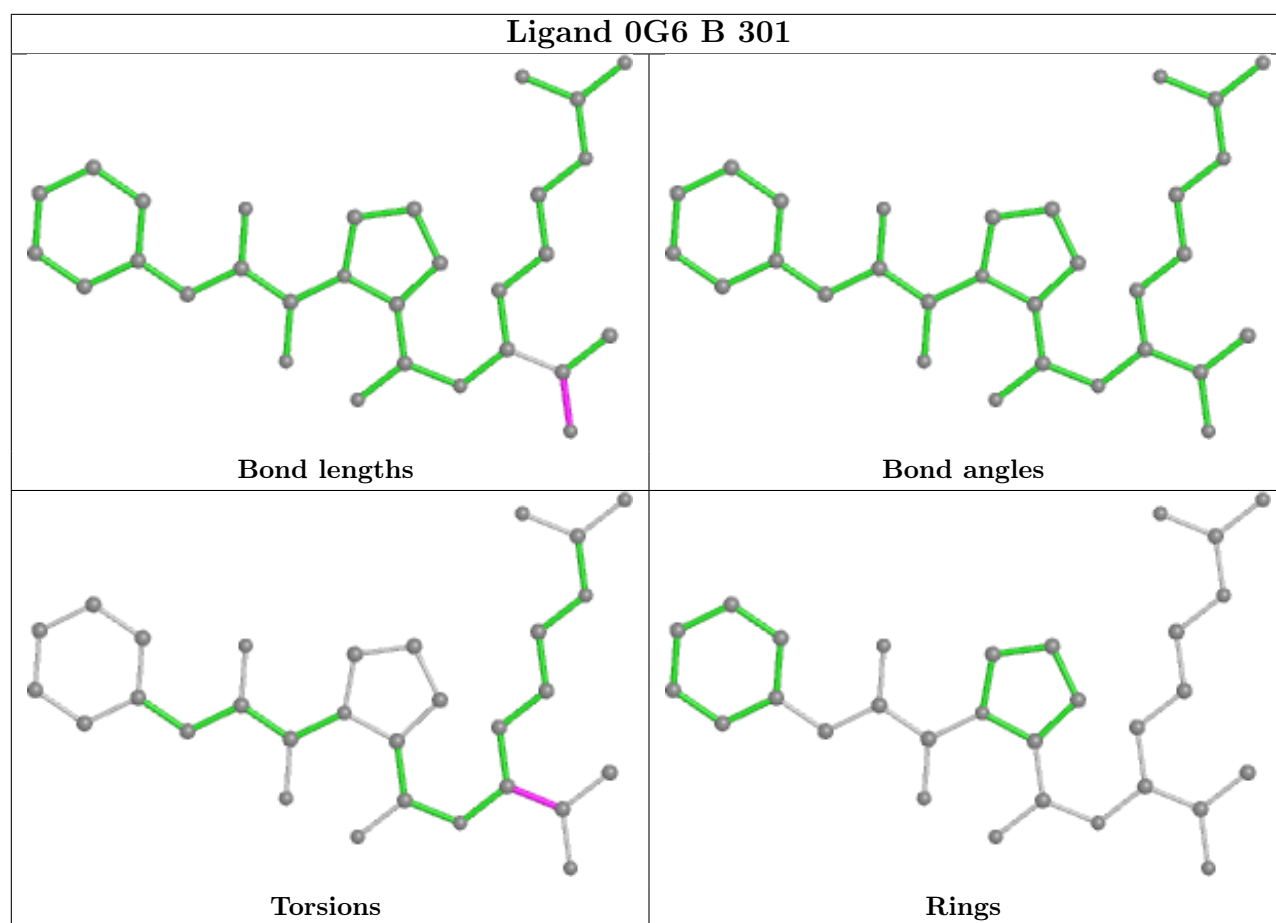
Mol	Chain	Res	Type	Atoms
4	B	301	0G6	O2-C2-CA2-N2
4	B	301	0G6	C3-C2-CA2-N2
4	B	301	0G6	O2-C2-CA2-CB2
5	B	600	NAG	C8-C7-N2-C2
5	B	600	NAG	O7-C7-N2-C2
4	B	301	0G6	C3-C2-CA2-CB2

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	600	NAG	13	0
4	B	301	0G6	10	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	40/40 (100%)	-0.04	3 (7%) 14 13	23, 34, 60, 68	0
2	B	243/259 (93%)	0.10	14 (5%) 23 22	21, 32, 57, 80	0
All	All	283/299 (94%)	0.08	17 (6%) 21 20	21, 33, 58, 80	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	245	PHE	6.2
2	B	77(A)	ARG	6.0
1	A	14(L)	ASP	5.6
2	B	71	HIS	4.8
2	B	78	ASN	4.0
2	B	244	GLN	3.8
2	B	151	GLN	3.8
2	B	186(A)	ASP	3.2
2	B	186	PRO	3.1
2	B	36(A)	SER	2.8
1	A	1(N)	THR	2.6
2	B	147	THR	2.6
2	B	37	PRO	2.4
1	A	1(M)	PHE	2.3
2	B	38	GLN	2.2
2	B	240	LYS	2.1
2	B	243	ASP	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

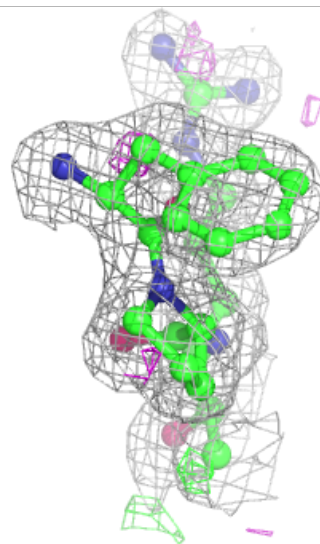
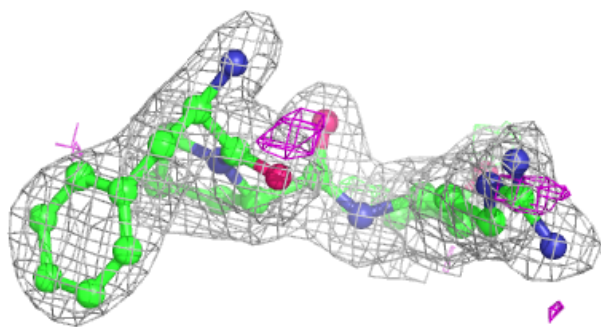
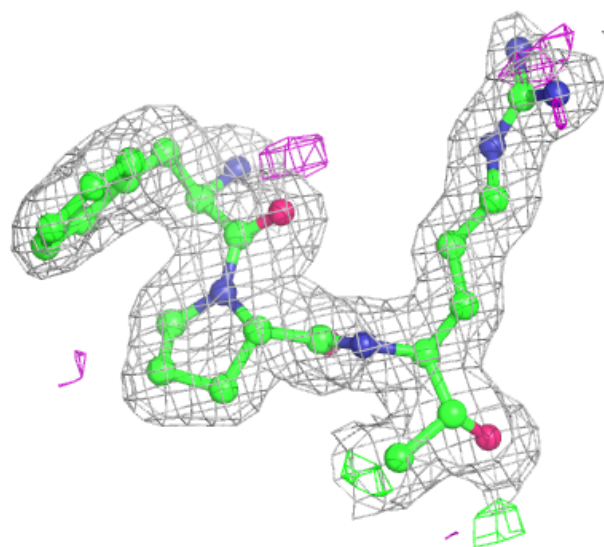
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	600	14/15	0.73	0.18	52,55,57,58	0
3	ZN	A	15	1/1	0.90	0.09	30,30,30,30	0
4	OG6	B	301	30/31	0.91	0.13	22,28,37,40	0
3	ZN	B	1	1/1	0.97	0.04	42,42,42,42	0
3	ZN	B	4	1/1	0.97	0.04	62,62,62,62	0
6	NA	B	601	1/1	0.98	0.13	36,36,36,36	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 0G6 B 301:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.