



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 11:36 PM EDT

PDB ID : 4QEB  
Title : Dcps in complex with covalent inhibitor targeting Tyrosine  
Authors : Liu, S.  
Deposited on : 2014-05-15  
Resolution : 3.21 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 types of validation reports are described at

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

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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 : 2.35.1  
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) : 2.35.1

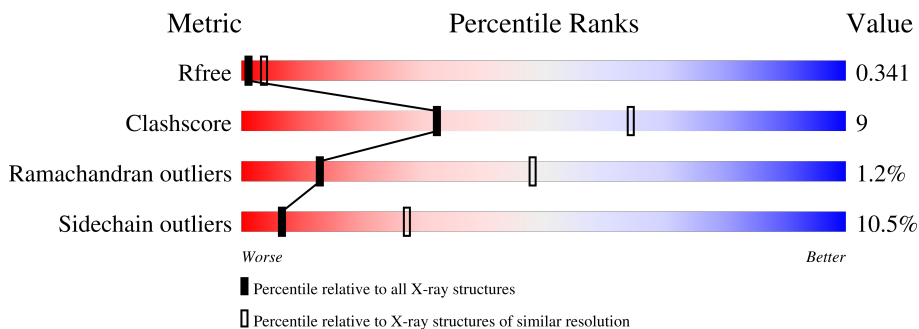
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	
1	C	337	
1	D	337	

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
2	PO4	B	402	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9617 atoms, of which 13 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 m7GpppX diphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2377	1523	425	426	3	0	0	0
1	B	288	2384	1526	427	428	3	0	0	0
1	C	289	2389	1529	427	430	3	0	0	0
1	D	292	2411	1542	430	436	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

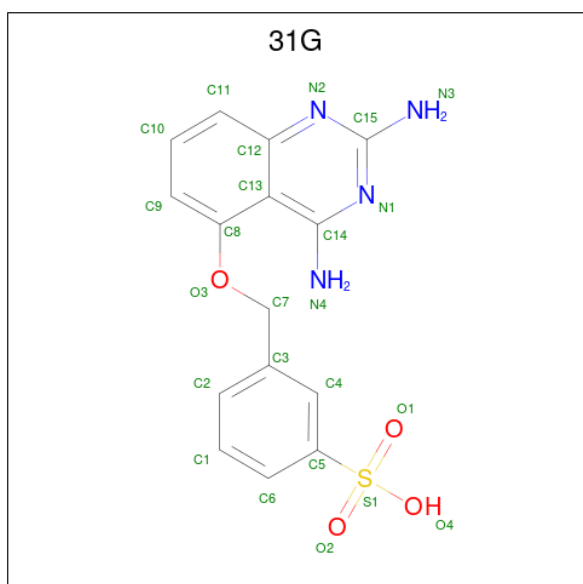
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q96C86
B	1	GLY	-	expression tag	UNP Q96C86
C	1	GLY	-	expression tag	UNP Q96C86
D	1	GLY	-	expression tag	UNP Q96C86

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



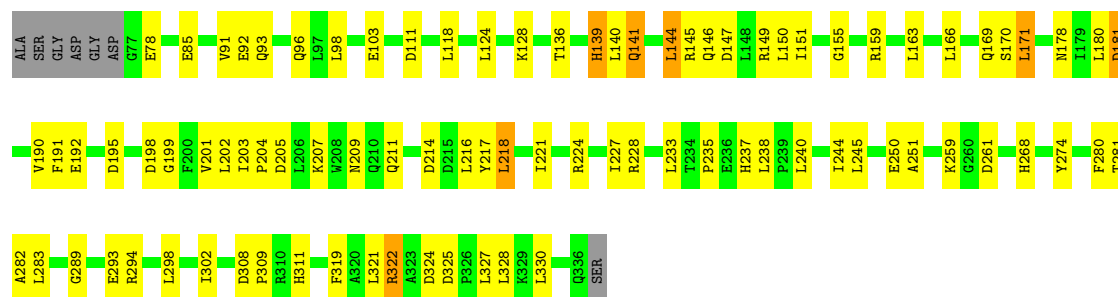
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 3-[(2,4-diaminoquinazolin-5-yl)oxy]methyl}benzenesulfonic acid (three-letter code: 31G) (formula: C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>O<sub>4</sub>S).



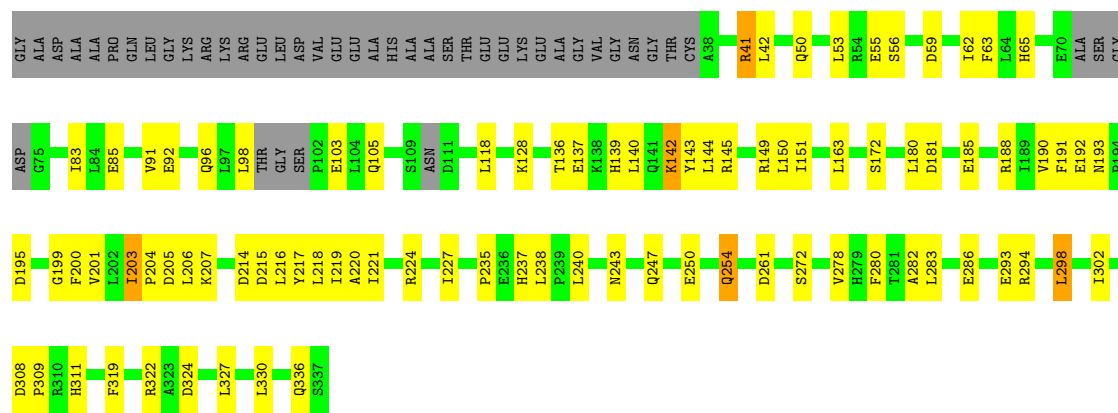
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
3	B	1	36	15	13	4	3	1	13	0





- Molecule 1: m7GpppX diphosphatase

Chain D: 61% 25% 13%





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.25Å 105.23Å 139.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.89 – 3.21 82.03 – 3.21	Depositor EDS
% Data completeness (in resolution range)	83.2 (33.89-3.21) 83.4 (82.03-3.21)	Depositor EDS
$R_{merge}$	0.32	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 3.19Å)	Xtrriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.211 , 0.276 0.276 , 0.341	Depositor DCC
$R_{free}$ test set	1069 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtrriage
Anisotropy	0.752	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 84.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	0.036 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9617	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1064e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 31G, PO4

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	0.56	0/2432	0.78	0/3298
1	B	0.54	0/2440	0.75	1/3311 (0.0%)
1	C	0.52	0/2446	0.76	0/3318
1	D	0.53	0/2466	0.77	1/3342 (0.0%)
All	All	0.54	0/9784	0.76	2/13269 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	ASN	N-CA-C	-5.07	97.32	111.00
1	B	193	ASN	N-CA-C	-5.03	97.42	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	2377	0	2384	44	0
1	B	2384	0	2388	55	0
1	C	2389	0	2391	47	0
1	D	2411	0	2406	40	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	4	0
2	C	5	0	0	1	0
3	B	23	13	13	2	0
All	All	9604	13	9582	168	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 9.

All (168) 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)
1:A:146:GLN:HG3	1:A:324:ASP:HB3	1.63	0.80
1:A:243:ASN:O	1:A:247:GLN:HB2	1.85	0.74
1:C:57:ALA:HB1	1:D:215:ASP:HB3	1.68	0.74
1:B:277:HIS:HE1	2:B:402:PO4:O4	1.70	0.73
1:B:62:ILE:HD12	1:B:64:LEU:HD11	1.75	0.69
1:B:243:ASN:O	1:B:247:GLN:HB2	1.93	0.67
1:B:205:ASP:OD2	1:B:207:LYS:HG2	1.95	0.67
1:A:94:VAL:HG11	1:B:62:ILE:HD11	1.78	0.66
1:C:141:GLN:HA	1:C:144:LEU:HB2	1.77	0.65
1:A:41:ARG:HG3	1:A:42:LEU:N	2.10	0.64
1:A:224:ARG:HD3	1:A:227:ILE:HD11	1.78	0.64
1:C:224:ARG:HD3	1:C:227:ILE:HD11	1.80	0.62
1:C:244:ILE:O	1:C:280:PHE:HZ	1.81	0.62
1:D:41:ARG:HD2	1:D:42:LEU:H	1.65	0.61
1:A:203:ILE:HG13	1:A:204:PRO:HD2	1.82	0.61
1:D:224:ARG:HD3	1:D:227:ILE:HD11	1.80	0.61
1:B:191:PHE:CZ	1:D:254:GLN:HB2	2.36	0.61
1:B:56:SER:HB3	1:B:61:ILE:HG22	1.82	0.60
1:B:217:TYR:CD1	1:B:281:THR:HG22	2.36	0.60
1:A:244:ILE:O	1:A:280:PHE:HZ	1.85	0.60
1:B:180:LEU:HD21	1:B:221:ILE:HG22	1.84	0.59
1:B:224:ARG:HD3	1:B:227:ILE:HD11	1.83	0.59
1:C:198:ASP:HA	1:C:240:LEU:HB2	1.85	0.58
1:A:60:LYS:HG2	1:B:86:LYS:O	2.04	0.58
1:B:113:TYR:HE1	3:B:401:31G:O2	1.85	0.58
1:C:147:ASP:HB3	1:C:149:ARG:HH12	1.68	0.58
1:C:41:ARG:HH12	1:C:42:LEU:HD22	1.68	0.57
1:B:113:TYR:CE1	3:B:401:31G:O2	2.57	0.57
1:B:85:GLU:HB3	1:B:128:LYS:HB3	1.87	0.57
1:D:327:LEU:HA	1:D:330:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD13	1:B:283:LEU:HD11	1.87	0.56
1:B:191:PHE:CE2	1:D:254:GLN:HB2	2.40	0.56
1:B:327:LEU:HA	1:B:330:LEU:HD12	1.87	0.56
1:B:209:ASN:HD22	1:B:211:GLN:HE21	1.53	0.56
1:D:85:GLU:HB3	1:D:128:LYS:HB3	1.87	0.56
1:A:240:LEU:O	1:A:244:ILE:HD12	2.06	0.56
1:A:271:PRO:HD2	1:A:274:TYR:HE1	1.70	0.56
1:A:85:GLU:HB3	1:A:128:LYS:HB3	1.87	0.55
1:A:215:ASP:HB3	1:B:57:ALA:HB1	1.88	0.55
1:C:180:LEU:HD21	1:C:221:ILE:HG22	1.88	0.55
1:C:85:GLU:HB3	1:C:128:LYS:HB3	1.88	0.55
1:D:137:GLU:HA	1:D:140:LEU:HD12	1.88	0.55
1:C:327:LEU:HA	1:C:330:LEU:HD12	1.88	0.55
1:C:191:PHE:CD2	1:C:251:ALA:HB2	2.42	0.55
1:C:209:ASN:HD22	1:C:211:GLN:HE21	1.55	0.55
1:A:202:LEU:HA	1:A:219:ILE:O	2.07	0.54
1:A:220:ALA:HB2	1:A:280:PHE:HE1	1.73	0.54
1:B:222:CYS:HB2	1:B:240:LEU:HD11	1.90	0.54
1:B:277:HIS:CE1	2:B:402:PO4:O4	2.55	0.54
1:D:50:GLN:HE21	1:D:65:HIS:HE1	1.56	0.54
1:A:271:PRO:HD2	1:A:274:TYR:CE1	2.42	0.54
1:C:178:ASN:HA	1:C:181:ASP:OD1	2.08	0.54
1:C:268:HIS:HB2	2:C:401:PO4:O2	2.08	0.53
1:C:163:LEU:HD11	1:C:228:ARG:NH1	2.24	0.53
1:B:178:ASN:HA	1:B:181:ASP:OD1	2.09	0.53
1:A:149:ARG:HH21	1:B:259:LYS:NZ	2.07	0.53
1:A:327:LEU:HA	1:A:330:LEU:HD12	1.89	0.53
1:B:268:HIS:HB2	2:B:402:PO4:O2	2.08	0.53
1:A:191:PHE:HB3	1:A:202:LEU:HB3	1.90	0.53
1:B:56:SER:HB3	1:B:61:ILE:CG2	2.39	0.53
1:B:188:ARG:NH1	1:B:206:LEU:HG	2.23	0.53
1:A:192:GLU:HG3	1:A:201:VAL:HG22	1.91	0.52
1:C:58:ARG:HD3	1:D:286:GLU:O	2.10	0.52
1:A:94:VAL:HG11	1:B:62:ILE:CD1	2.39	0.52
1:D:180:LEU:HD21	1:D:221:ILE:HG22	1.91	0.52
1:D:56:SER:HB3	1:D:59:ASP:HB2	1.91	0.52
1:C:192:GLU:HG3	1:C:201:VAL:HG22	1.92	0.51
1:D:192:GLU:HG3	1:D:201:VAL:HG22	1.92	0.51
1:A:50:GLN:HE21	1:A:65:HIS:CE1	2.28	0.51
1:C:54:ARG:HG2	1:C:145:ARG:HB2	1.92	0.51
1:C:150:LEU:HD13	1:D:283:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HD2	1:B:86:LYS:HD2	1.92	0.51
1:B:293:GLU:O	1:B:319:PHE:HA	2.11	0.51
1:A:180:LEU:HD21	1:A:221:ILE:HG22	1.91	0.51
1:B:190:VAL:HG23	1:B:204:PRO:HD3	1.92	0.51
1:B:238:LEU:HD22	1:B:302:ILE:HG23	1.92	0.51
1:C:233:LEU:HA	1:C:237:HIS:ND1	2.26	0.50
1:A:145:ARG:HG2	1:A:145:ARG:HH11	1.76	0.50
1:D:185:GLU:HG2	1:D:188:ARG:HD3	1.93	0.50
1:C:39:PRO:HA	1:D:105:GLN:HG2	1.93	0.50
1:C:283:LEU:HD11	1:D:150:LEU:HD13	1.94	0.50
1:B:233:LEU:HB3	1:B:305:LEU:HD11	1.94	0.49
1:A:191:PHE:HB2	1:A:251:ALA:HB1	1.95	0.49
1:A:195:ASP:O	1:A:199:GLY:HA3	2.13	0.49
1:B:192:GLU:HG3	1:B:201:VAL:HG22	1.94	0.49
1:A:293:GLU:O	1:A:319:PHE:HA	2.11	0.49
1:B:138:LYS:NZ	1:B:141:GLN:HE22	2.11	0.49
1:C:238:LEU:HD22	1:C:302:ILE:HG23	1.93	0.49
1:A:267:LEU:HD12	1:A:301:VAL:HG21	1.95	0.49
1:D:142:LYS:HD2	1:D:322:ARG:HH21	1.77	0.49
1:C:293:GLU:O	1:C:319:PHE:HA	2.13	0.49
1:C:147:ASP:HB3	1:C:149:ARG:NH1	2.27	0.48
1:D:55:GLU:HG3	1:D:62:ILE:HD12	1.94	0.48
1:C:268:HIS:HE2	1:C:289:GLY:CA	2.26	0.48
1:A:268:HIS:HE2	1:A:289:GLY:CA	2.25	0.48
1:B:163:LEU:HD11	1:B:228:ARG:NH1	2.29	0.48
1:D:50:GLN:HE21	1:D:65:HIS:CE1	2.31	0.48
1:D:63:PHE:CD2	1:D:83:ILE:HD12	2.49	0.48
1:D:203:ILE:N	1:D:203:ILE:HD13	2.29	0.48
1:A:63:PHE:CD2	1:A:83:ILE:HD12	2.50	0.47
1:B:235:PRO:HG2	1:B:309:PRO:HB3	1.97	0.47
1:C:204:PRO:HA	1:C:218:LEU:HA	1.97	0.46
1:A:238:LEU:HD22	1:A:302:ILE:HG23	1.96	0.46
1:B:53:LEU:HD23	1:B:144:LEU:HB2	1.96	0.46
1:C:235:PRO:HG2	1:C:309:PRO:HB3	1.97	0.46
1:D:238:LEU:HD22	1:D:302:ILE:HG23	1.97	0.46
1:A:216:LEU:HB3	1:A:282:ALA:HB2	1.97	0.46
1:D:293:GLU:O	1:D:319:PHE:HA	2.14	0.46
1:A:137:GLU:HA	1:A:140:LEU:HD12	1.97	0.46
1:C:141:GLN:HE21	1:C:144:LEU:HD13	1.81	0.46
1:D:41:ARG:HD2	1:D:42:LEU:HG	1.98	0.46
1:C:190:VAL:HG23	1:C:204:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:GLN:O	1:C:171:LEU:HD22	2.15	0.46
1:C:155:GLY:O	1:C:159:ARG:HG3	2.16	0.46
1:D:195:ASP:O	1:D:199:GLY:HA3	2.16	0.46
1:D:243:ASN:O	1:D:247:GLN:HB2	2.17	0.45
1:D:201:VAL:HG12	1:D:203:ILE:CD1	2.46	0.45
1:C:93:GLN:HB3	1:C:124:LEU:HD21	1.99	0.45
1:C:195:ASP:O	1:C:199:GLY:HA3	2.16	0.45
1:C:308:ASP:HB3	1:C:311:HIS:HB2	1.98	0.45
1:A:47:PHE:O	1:B:99:THR:HG22	2.16	0.45
1:D:191:PHE:CD2	1:D:200:PHE:CZ	3.04	0.45
1:D:220:ALA:HB2	1:D:280:PHE:HE1	1.81	0.45
1:D:216:LEU:HB3	1:D:282:ALA:HB2	1.98	0.45
1:B:277:HIS:HE1	2:B:402:PO4:P	2.39	0.45
1:D:191:PHE:HD2	1:D:200:PHE:CZ	2.35	0.45
1:A:185:GLU:HG2	1:A:188:ARG:HD3	1.97	0.45
1:B:200:PHE:HE2	1:B:202:LEU:HB2	1.82	0.45
1:B:171:LEU:HD21	1:B:173:ILE:HG23	1.98	0.45
1:C:41:ARG:NH1	1:C:42:LEU:HD22	2.30	0.45
1:C:216:LEU:HB3	1:C:282:ALA:HB2	1.99	0.45
1:B:53:LEU:HA	1:B:144:LEU:HD12	1.98	0.44
1:C:205:ASP:OD2	1:C:207:LYS:HE2	2.16	0.44
1:B:80:ALA:HB2	1:B:133:TYR:HD1	1.83	0.44
1:A:308:ASP:HB3	1:A:311:HIS:HB2	1.98	0.44
1:C:322:ARG:HH21	1:C:325:ASP:HA	1.83	0.44
1:B:195:ASP:O	1:B:199:GLY:HA3	2.18	0.44
1:B:308:ASP:HB3	1:B:311:HIS:HB2	1.99	0.44
1:B:216:LEU:HB3	1:B:282:ALA:HB2	2.00	0.44
1:A:146:GLN:HE21	1:A:323:ALA:HB3	1.83	0.44
1:B:201:VAL:HG12	1:B:203:ILE:HG23	1.99	0.43
1:C:166:LEU:HA	1:C:169:GLN:HE21	1.83	0.43
1:C:217:TYR:CD1	1:C:281:THR:HG22	2.54	0.43
1:B:204:PRO:HA	1:B:218:LEU:HA	2.00	0.42
1:B:54:ARG:H	1:B:63:PHE:HB2	1.84	0.42
1:B:240:LEU:O	1:B:244:ILE:HG13	2.19	0.42
1:D:308:ASP:HB3	1:D:311:HIS:HB2	2.00	0.42
1:A:206:LEU:HA	1:B:108:PHE:HZ	1.84	0.42
1:C:136:THR:HG23	1:C:139:HIS:H	1.84	0.42
1:C:202:LEU:HD11	1:C:218:LEU:HB3	2.01	0.42
1:D:205:ASP:OD1	1:D:207:LYS:HB2	2.20	0.42
1:A:56:SER:HB3	1:A:59:ASP:HB2	2.02	0.42
1:C:54:ARG:H	1:C:63:PHE:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:PRO:HA	1:A:218:LEU:HA	2.02	0.42
1:A:253:LEU:HD13	1:A:259:LYS:HA	2.02	0.41
1:A:175:TRP:HB2	1:B:110:ASN:ND2	2.35	0.41
1:B:271:PRO:HD2	1:B:274:TYR:HE1	1.85	0.41
1:A:41:ARG:NH2	1:A:42:LEU:HD12	2.35	0.41
1:C:259:LYS:NZ	1:D:149:ARG:HH21	2.18	0.41
1:D:53:LEU:HD13	1:D:143:TYR:HB2	2.01	0.41
1:D:235:PRO:HG2	1:D:309:PRO:HB3	2.03	0.41
1:B:197:SER:O	1:B:240:LEU:HD13	2.21	0.40
1:D:190:VAL:HG23	1:D:204:PRO:HD3	2.03	0.40
1:D:237:HIS:O	1:D:240:LEU:HB3	2.22	0.40
1:D:278:VAL:HG11	1:D:298:LEU:HD12	2.03	0.40
1:B:110:ASN:O	1:B:113:TYR:HB2	2.20	0.40
1:C:228:ARG:HB3	1:C:274:TYR:HB3	2.04	0.40
1:C:321:LEU:HB2	1:C:328:LEU:HD13	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	281/337 (83%)	251 (89%)	27 (10%)	3 (1%)	14	50
1	B	284/337 (84%)	257 (90%)	24 (8%)	3 (1%)	14	50
1	C	285/337 (85%)	260 (91%)	21 (7%)	4 (1%)	11	45
1	D	284/337 (84%)	254 (89%)	26 (9%)	4 (1%)	11	45
All	All	1134/1348 (84%)	1022 (90%)	98 (9%)	14 (1%)	13	48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	91	VAL
1	A	174	GLN
1	C	46	GLY
1	C	91	VAL
1	C	146	GLN
1	B	41	ARG
1	B	288	PRO
1	D	91	VAL
1	D	206	LEU
1	B	170	SER
1	D	172	SER
1	C	40	VAL
1	D	336	GLN

### 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	261/294 (89%)	234 (90%)	27 (10%)	7 28
1	B	262/294 (89%)	234 (89%)	28 (11%)	6 26
1	C	262/294 (89%)	233 (89%)	29 (11%)	6 25
1	D	264/294 (90%)	238 (90%)	26 (10%)	8 30
All	All	1049/1176 (89%)	939 (90%)	110 (10%)	7 27

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	48	ARG
1	A	54	ARG
1	A	64	LEU
1	A	78	GLU
1	A	92	GLU
1	A	93	GLN
1	A	96	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	98	LEU
1	A	106	LEU
1	A	109	SER
1	A	112	ILE
1	A	118	LEU
1	A	145	ARG
1	A	151	ILE
1	A	163	LEU
1	A	181	ASP
1	A	202	LEU
1	A	214	ASP
1	A	217	TYR
1	A	218	LEU
1	A	219	ILE
1	A	250	GLU
1	A	294	ARG
1	A	298	LEU
1	A	322	ARG
1	A	324	ASP
1	B	45	SER
1	B	55	GLU
1	B	60	LYS
1	B	96	GLN
1	B	98	LEU
1	B	118	LEU
1	B	123	GLN
1	B	140	LEU
1	B	144	LEU
1	B	145	ARG
1	B	146	GLN
1	B	147	ASP
1	B	151	ILE
1	B	161	ILE
1	B	168	SER
1	B	171	LEU
1	B	181	ASP
1	B	205	ASP
1	B	206	LEU
1	B	218	LEU
1	B	245	LEU
1	B	250	GLU
1	B	254	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	261	ASP
1	B	294	ARG
1	B	298	LEU
1	B	322	ARG
1	B	324	ASP
1	C	41	ARG
1	C	42	LEU
1	C	50	GLN
1	C	60	LYS
1	C	78	GLU
1	C	92	GLU
1	C	96	GLN
1	C	98	LEU
1	C	103	GLU
1	C	111	ASP
1	C	118	LEU
1	C	139	HIS
1	C	140	LEU
1	C	141	GLN
1	C	144	LEU
1	C	151	ILE
1	C	170	SER
1	C	171	LEU
1	C	181	ASP
1	C	203	ILE
1	C	214	ASP
1	C	218	LEU
1	C	245	LEU
1	C	250	GLU
1	C	261	ASP
1	C	294	ARG
1	C	298	LEU
1	C	322	ARG
1	C	324	ASP
1	D	41	ARG
1	D	92	GLU
1	D	96	GLN
1	D	98	LEU
1	D	103	GLU
1	D	118	LEU
1	D	136	THR
1	D	139	HIS

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Mol	Chain	Res	Type
1	D	142	LYS
1	D	144	LEU
1	D	145	ARG
1	D	151	ILE
1	D	163	LEU
1	D	181	ASP
1	D	203	ILE
1	D	214	ASP
1	D	217	TYR
1	D	218	LEU
1	D	219	ILE
1	D	250	GLU
1	D	254	GLN
1	D	261	ASP
1	D	272	SER
1	D	294	ARG
1	D	298	LEU
1	D	324	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	107	GLN
1	A	146	GLN
1	B	107	GLN
1	B	141	GLN
1	B	193	ASN
1	B	211	GLN
1	B	277	HIS
1	C	110	ASN
1	C	169	GLN
1	C	211	GLN
1	C	262	HIS
1	D	65	HIS
1	D	69	ASN
1	D	146	GLN
1	D	169	GLN
1	D	249	GLN
1	D	254	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands 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
2	PO4	B	402	-	4,4,4	2.68	2 (50%)	6,6,6	1.00	0
2	PO4	C	401	-	4,4,4	1.89	1 (25%)	6,6,6	1.10	1 (16%)
2	PO4	A	402	-	4,4,4	2.49	1 (25%)	6,6,6	0.19	0
2	PO4	A	401	-	4,4,4	2.48	1 (25%)	6,6,6	1.32	1 (16%)
3	31G	B	401	1	22,25,26	0.38	0	33,35,38	1.73	6 (18%)

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	31G	B	401	1	-	2/9/9/11	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	PO4	P-O1	4.25	1.60	1.50
2	A	402	PO4	P-O1	4.13	1.60	1.50
2	A	401	PO4	P-O1	4.02	1.60	1.50
2	B	402	PO4	P-O3	2.06	1.60	1.54
2	C	401	PO4	P-O3	2.05	1.60	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	31G	C7-O3-C8	5.20	124.86	117.56
3	B	401	31G	O3-C7-C3	4.20	121.75	109.16
3	B	401	31G	O2-S1-C5	3.48	112.50	104.58
3	B	401	31G	C8-C13-C14	3.43	129.10	127.36
3	B	401	31G	C14-C13-C12	-3.23	112.65	114.86
2	A	401	PO4	O4-P-O3	2.68	116.58	107.97
2	C	401	PO4	O3-P-O2	2.40	115.67	107.97
3	B	401	31G	O3-C8-C13	-2.06	110.79	117.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	31G	C13-C8-O3-C7
3	B	401	31G	C9-C8-O3-C7

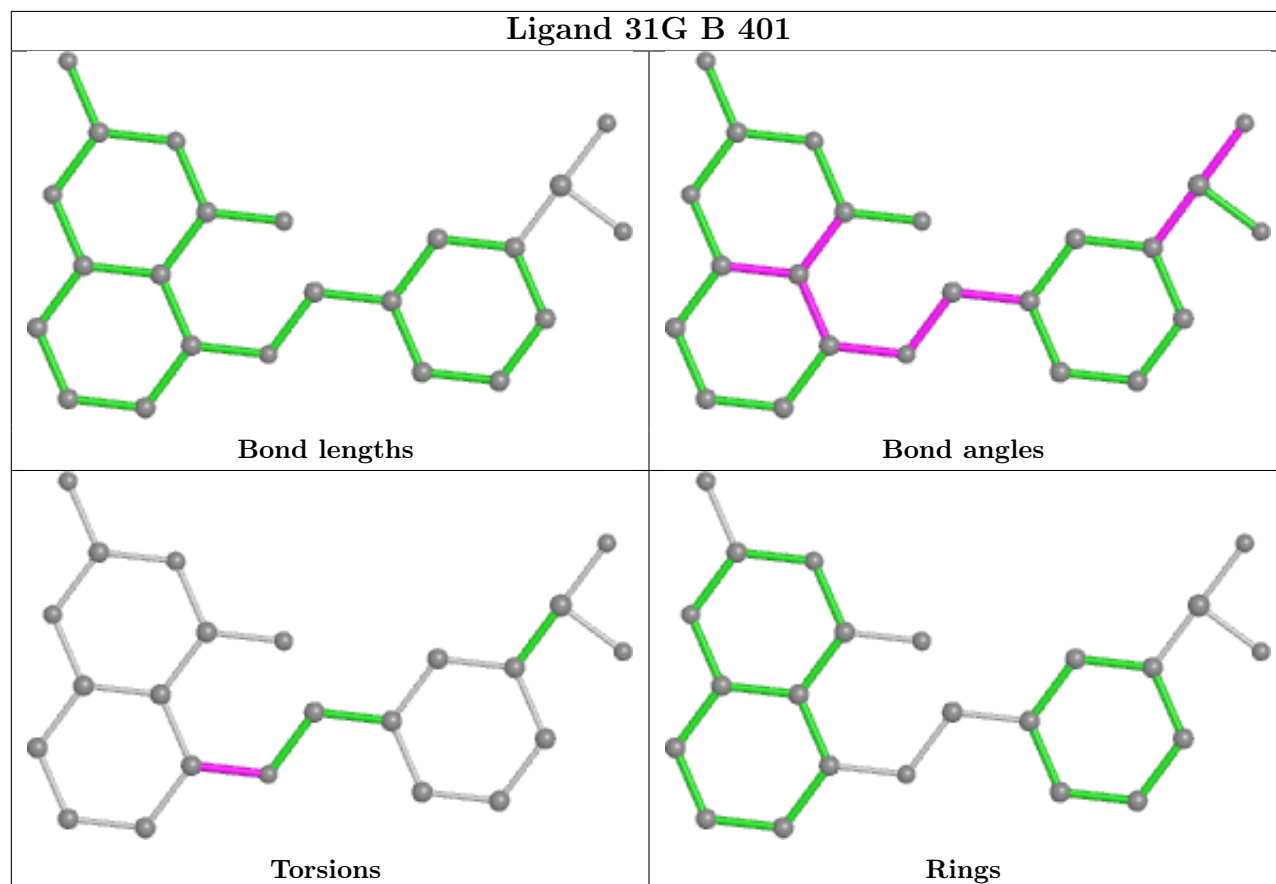
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	PO4	4	0
2	C	401	PO4	1	0
3	B	401	31G	2	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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

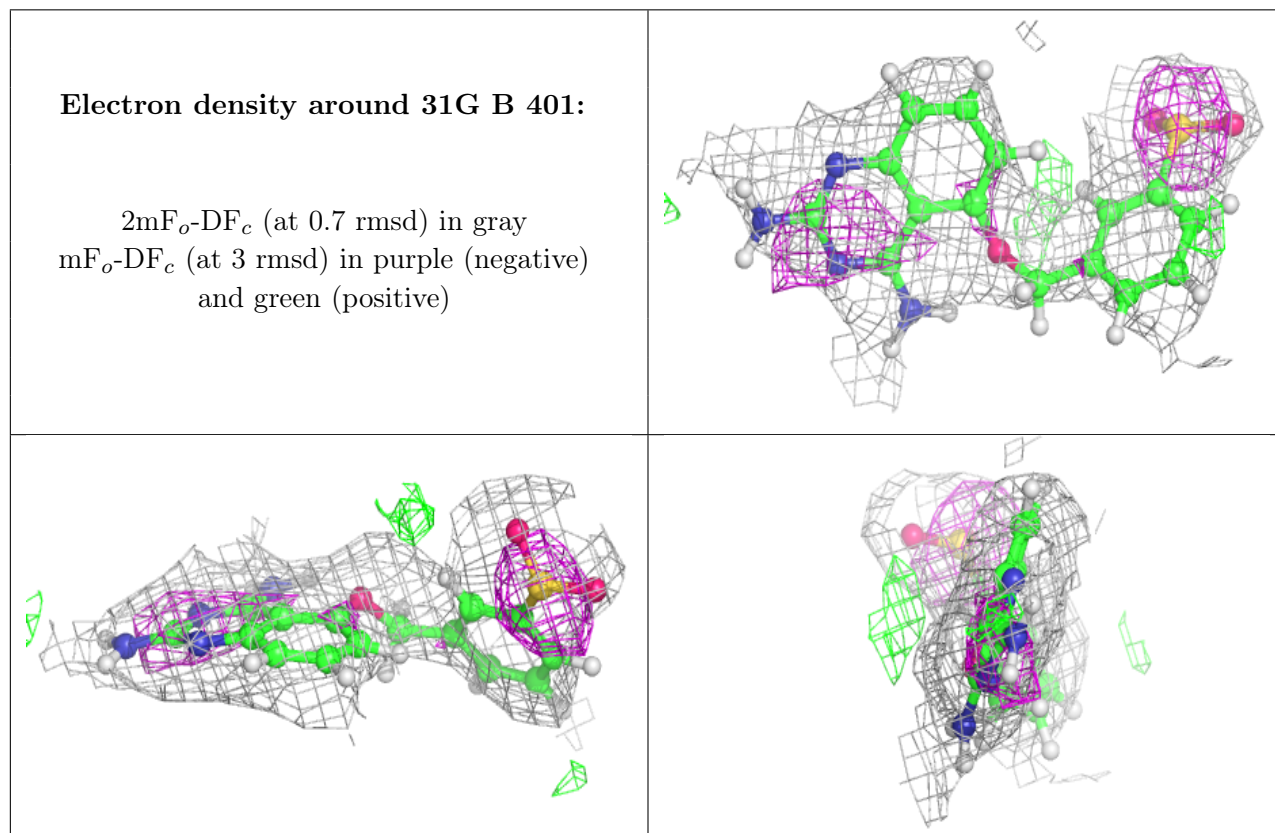
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.