



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2025 – 03:22 PM JST

PDB ID : 8Z9I / pdb\_00008z9i  
Title : Crystal structure of RaTG13 RBD bound to Rhinolophus affinis ACE2  
Authors : Lan, J.; Wang, C.H.  
Deposited on : 2024-04-23  
Resolution : 3.01 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:

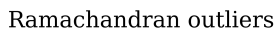
MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

**i**

## X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.



R <sub>free</sub>
Clashscore
Ramachandran outliers
Sidechain outliers
RSRZ outliers

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.

1	E	196	3%	74%	25%
1	O	196	%	74%	24%
2	A	597	%	70%	29%
2	F	597	%	72%	27%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12916 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.

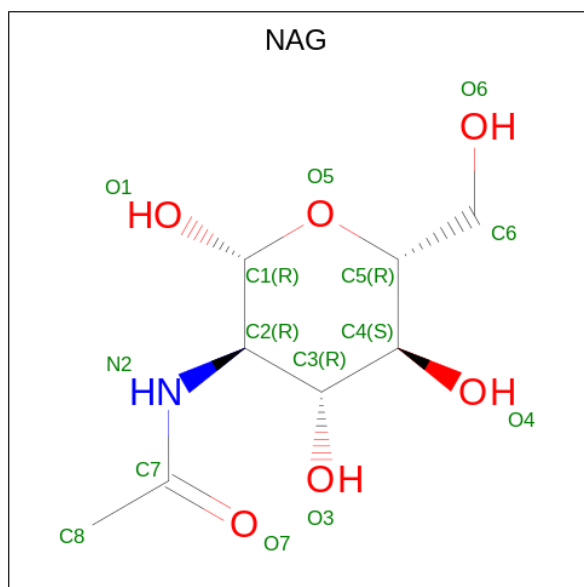
- Molecule 1 is a protein called RaTG13 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	195	Total	C	N	O	S	0	0	0
			1550	996	257	289	8			
1	E	196	Total	C	N	O	S	0	0	0
			1560	1002	260	290	8			

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	596	Total	C	N	O	S	0	0	0
			4886	3121	816	919	30			
2	F	597	Total	C	N	O	S	0	0	0
			4894	3125	817	922	30			

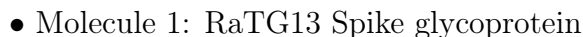
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	O	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			12	6	1	5		

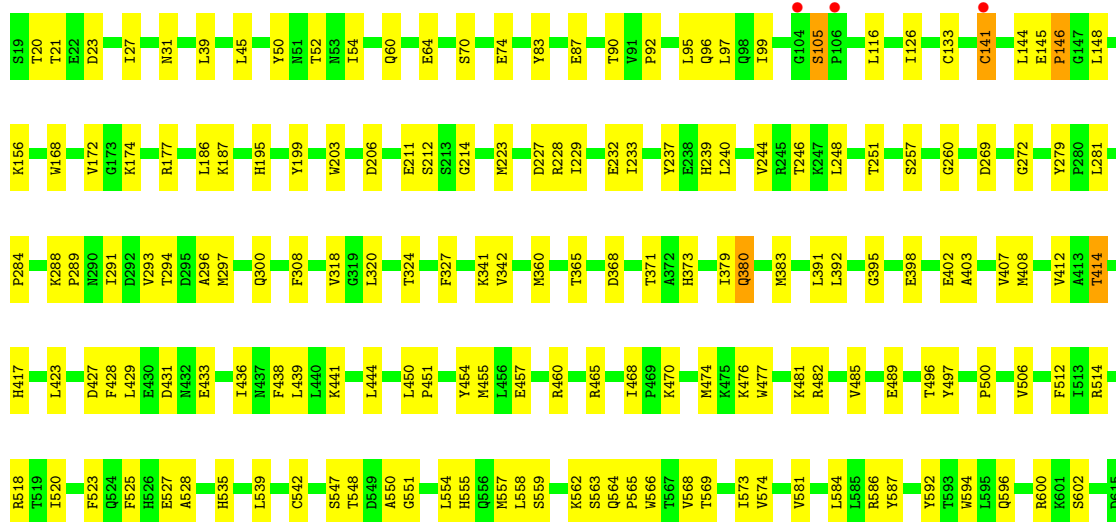


- Molecule 1: RaTG13 Spike glycoprotein





● Molecule 2: Angiotensin-converting enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.92Å 273.39Å 165.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.65 – 3.01 28.65 – 3.01	Depositor EDS
% Data completeness (in resolution range)	97.5 (28.65-3.01) 97.4 (28.65-3.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, $R_{free}$	0.194 , 0.238 0.198 , 0.243	Depositor DCC
$R_{free}$ test set	2248 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	E	0.59	1/1606 (0.1%)	0.80	2/2186 (0.1%)
1	O	0.48	0/1595	0.76	1/2171 (0.0%)
2	A	0.48	0/5028	0.72	5/6824 (0.1%)
2	F	0.49	1/5036 (0.0%)	0.73	1/6835 (0.0%)
All	All	0.50	2/13265 (0.0%)	0.74	9/18016 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	517	LEU	CG-CD1	-8.22	1.25	1.52
2	F	105	SER	C-N	7.58	1.51	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	517	LEU	CD1-CG-CD2	-8.10	92.98	110.80
2	A	211	GLU	CA-C-N	7.98	136.78	121.54
2	A	211	GLU	C-N-CA	7.98	136.78	121.54
1	E	480	CYS	CA-CB-SG	-5.99	100.63	114.40
1	O	369	TYR	CA-CB-CG	-5.81	103.44	113.90
2	F	141	CYS	CA-CB-SG	5.55	127.17	114.40
2	A	478	TRP	CA-CB-CG	-5.44	103.26	113.60
2	A	210	GLU	CA-C-N	-5.07	112.55	120.81
2	A	210	GLU	C-N-CA	-5.07	112.55	120.81

There are no chirality outliers.

There are no planarity outliers.

## 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	E	1560	0	1477	47	0
1	O	1550	0	1469	35	0
2	A	4886	0	4664	120	0
2	F	4894	0	4668	115	0
3	E	12	0	9	2	0
3	O	14	0	13	0	0
All	All	12916	0	12300	310	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 12.

All (310) 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:F:457:GLU:OE2	2:F:460:ARG:NH1	1.71	1.22
2:F:460:ARG:HH22	2:F:512:PHE:HB2	1.08	1.09
2:F:460:ARG:NH2	2:F:512:PHE:HB2	1.78	0.98
1:O:361:CYS:SG	1:O:362:VAL:N	2.44	0.90
1:E:392:PHE:CD2	1:E:517:LEU:HD21	2.09	0.87
2:A:288:LYS:NZ	2:A:431:ASP:OD2	2.10	0.85
1:E:392:PHE:HD2	1:E:517:LEU:HD21	1.42	0.82
1:O:393:THR:HG21	1:O:518:LEU:HB2	1.60	0.81
2:F:90:THR:HG22	2:F:92:PRO:HD2	1.62	0.81
1:O:393:THR:HG21	1:O:518:LEU:H	1.48	0.79
2:F:288:LYS:NZ	2:F:431:ASP:OD2	2.16	0.78
2:F:402:GLU:HG3	2:F:514:ARG:HG3	1.65	0.78
3:E:601:NAG:C3	3:E:601:NAG:N2	2.46	0.78
2:F:229:ILE:HG23	2:F:581:VAL:HG11	1.65	0.77
2:A:134:LYS:HG3	2:A:135:PRO:HD2	1.65	0.77
1:E:392:PHE:CD2	1:E:515:PHE:HB3	2.20	0.76
1:E:392:PHE:HD2	1:E:517:LEU:CD2	2.00	0.75
1:O:493:TYR:OH	2:F:31:ASN:ND2	2.21	0.74
2:A:107:VAL:HG21	2:A:193:GLY:HA3	1.68	0.74
2:F:50:TYR:CE1	2:F:54:ILE:HG13	2.21	0.74
2:A:477:TRP:CE3	2:A:500:PRO:HG3	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:520:ILE:HG12	2:F:581:VAL:HG12	1.70	0.73
2:F:527:GLU:OE2	2:F:586:ARG:NH1	2.22	0.72
2:A:31:ASN:ND2	1:E:493:TYR:OH	2.23	0.72
1:E:390:LEU:HB3	1:E:392:PHE:CE1	2.24	0.72
2:A:43:SER:HA	2:A:65:ALA:HB1	1.70	0.72
2:F:233:ILE:HD13	2:F:450:LEU:HD13	1.71	0.71
1:O:487:ASN:OD1	2:F:83:TYR:OH	2.09	0.71
2:F:474:MET:HE1	2:F:500:PRO:HD3	1.73	0.71
2:A:373:HIS:CD2	2:A:412:VAL:HG21	2.27	0.70
2:F:293:VAL:HG11	2:F:423:LEU:HB3	1.73	0.69
2:A:52:THR:HA	2:A:342:VAL:HG23	1.74	0.69
1:E:353:TRP:O	1:E:466:ARG:NH2	2.27	0.67
2:F:324:THR:HG23	2:F:327:PHE:H	1.59	0.66
2:A:403:ALA:O	2:A:407:VAL:HG23	1.96	0.66
2:F:50:TYR:HE1	2:F:54:ILE:HG13	1.60	0.66
2:A:232:GLU:OE1	2:F:596:GLN:NE2	2.27	0.66
2:F:308:PHE:HZ	2:F:360:MET:HE3	1.60	0.66
1:O:335:LEU:HA	1:O:362:VAL:O	1.95	0.66
1:E:361:CYS:SG	1:E:362:VAL:N	2.68	0.65
2:A:52:THR:O	2:A:340:ARG:NH1	2.30	0.64
2:F:318:VAL:O	2:F:551:GLY:HA3	1.97	0.64
1:E:438:SER:HB2	1:E:509:ARG:HG3	1.79	0.64
2:A:84:PRO:HB2	2:A:87:GLU:HG3	1.78	0.64
2:F:144:LEU:HA	2:F:148:LEU:HB2	1.79	0.64
1:O:333:THR:O	1:O:333:THR:OG1	2.13	0.64
2:F:455:MET:HE2	2:F:485:VAL:HG21	1.78	0.64
1:E:356:LYS:HD3	1:E:358:ILE:HD13	1.81	0.63
2:F:564:GLN:OE1	2:F:569:THR:HG22	1.99	0.63
2:A:457:GLU:OE2	2:A:460:ARG:NH1	2.32	0.63
2:F:320:LEU:HD13	2:F:380:GLN:HG2	1.80	0.63
2:F:539:LEU:HD23	2:F:587:TYR:HB2	1.80	0.62
2:F:407:VAL:HG21	2:F:525:PHE:HB2	1.80	0.62
2:A:90:THR:HG22	2:A:92:PRO:HD2	1.79	0.62
2:A:137:ASN:ND2	2:A:140:GLU:HG2	2.14	0.62
2:F:392:LEU:HD13	2:F:563:SER:HA	1.82	0.61
1:O:350:VAL:HG22	1:O:422:ASN:HB3	1.83	0.61
2:A:294:THR:HG23	2:A:365:THR:HA	1.81	0.61
2:A:77:SER:OG	2:A:100:LEU:O	2.16	0.61
2:A:261:CYS:HB2	2:A:488:VAL:HB	1.82	0.60
2:F:251:THR:HG21	2:F:281:LEU:HD22	1.81	0.60
2:A:493:HIS:ND1	2:A:499:ASP:OD2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:247:LYS:HB2	2:A:282:THR:HG22	1.85	0.59
2:A:527:GLU:OE2	2:A:586:ARG:NH1	2.34	0.59
2:F:211:GLU:HG3	2:F:214:GLY:H	1.68	0.59
2:F:211:GLU:OE1	2:F:214:GLY:HA2	2.03	0.58
2:A:137:ASN:HD22	2:A:140:GLU:HG2	1.68	0.58
2:F:373:HIS:CD2	2:F:412:VAL:HG21	2.39	0.58
2:F:187:LYS:HD2	2:F:199:TYR:CZ	2.38	0.58
2:F:187:LYS:HD2	2:F:199:TYR:CE1	2.39	0.57
1:O:371:SER:OG	1:O:373:SER:OG	2.20	0.57
2:A:320:LEU:HD13	2:A:380:GLN:HG2	1.86	0.57
2:A:489:GLU:OE2	2:A:489:GLU:N	2.30	0.57
2:F:291:ILE:HD13	2:F:438:PHE:HA	1.86	0.57
1:O:393:THR:CG2	1:O:518:LEU:H	2.18	0.57
2:A:288:LYS:HE3	2:A:433:GLU:OE1	2.05	0.57
1:E:336:CYS:HB2	1:E:363:ALA:HB2	1.87	0.57
1:O:393:THR:HG21	1:O:518:LEU:N	2.18	0.56
1:E:393:THR:HA	1:E:522:ALA:HA	1.87	0.56
2:F:457:GLU:OE2	2:F:460:ARG:CZ	2.49	0.56
2:F:174:LYS:NZ	2:F:496:THR:OG1	2.38	0.56
1:E:390:LEU:HD23	1:E:392:PHE:HZ	1.70	0.56
2:F:246:THR:HG21	2:F:602:SER:OG	2.05	0.56
2:A:157:ASP:O	2:A:161:ARG:HG3	2.05	0.56
2:F:294:THR:HG23	2:F:365:THR:HA	1.88	0.56
1:E:343:ASN:ND2	3:E:601:NAG:O5	2.39	0.56
2:A:132:VAL:HG11	2:A:148:LEU:HD11	1.88	0.56
2:A:144:LEU:HA	2:A:148:LEU:HB2	1.89	0.55
2:F:240:LEU:O	2:F:244:VAL:HG23	2.06	0.55
2:F:133:CYS:HA	2:F:141:CYS:HA	1.88	0.55
2:A:83:TYR:OH	1:E:487:ASN:OD1	2.14	0.55
1:E:392:PHE:CD2	1:E:517:LEU:CD2	2.81	0.55
1:O:393:THR:HA	1:O:522:ALA:HA	1.89	0.55
2:A:157:ASP:HB3	2:A:160:GLU:HB2	1.89	0.55
1:O:439:LYS:HD3	1:O:499:PRO:HA	1.87	0.55
2:A:211:GLU:CG	2:A:214:GLY:H	2.20	0.54
1:E:335:LEU:HA	1:E:362:VAL:O	2.07	0.54
1:O:431:GLY:HA2	1:O:515:PHE:CD2	2.42	0.54
2:F:557:MET:HB2	2:F:573:ILE:HD11	1.89	0.54
1:E:359:SER:HA	1:E:524:VAL:HG22	1.88	0.54
1:O:336:CYS:N	1:O:361:CYS:SG	2.80	0.54
2:A:532:ILE:HD11	2:A:553:LYS:HD2	1.90	0.54
2:A:246:THR:HA	2:A:249:MET:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:532:ILE:CD1	2:A:553:LYS:HD2	2.37	0.54
1:E:399:SER:HA	1:E:510:VAL:O	2.09	0.53
2:F:269:ASP:OD1	2:F:272:GLY:N	2.40	0.53
2:A:455:MET:HE1	2:A:481:LYS:HE2	1.90	0.53
2:F:395:GLY:O	2:F:562:LYS:HD3	2.09	0.53
2:A:37:GLU:OE1	2:A:393:ARG:NH2	2.40	0.53
2:A:56:ASP:O	2:A:59:VAL:HG12	2.09	0.53
2:A:231:THR:HA	2:A:234:LYS:HG3	1.91	0.53
1:E:371:SER:OG	1:E:373:SER:OG	2.27	0.52
2:A:554:LEU:O	2:A:558:LEU:HG	2.08	0.52
2:F:156:LYS:HD3	2:F:281:LEU:HD21	1.90	0.52
2:A:197:GLU:HG2	2:A:201:ASP:OD2	2.10	0.52
1:O:358:ILE:HB	1:O:395:VAL:HB	1.91	0.52
2:A:211:GLU:HG3	2:A:214:GLY:H	1.75	0.52
2:F:168:TRP:CZ3	2:F:172:VAL:HG21	2.45	0.52
2:F:414:THR:HG22	2:F:417:HIS:H	1.75	0.52
2:F:145:GLU:HB3	2:F:146:PRO:HD3	1.92	0.51
2:F:177:ARG:HD3	2:F:497:TYR:O	2.10	0.51
2:A:527:GLU:HA	2:A:539:LEU:HD11	1.91	0.51
1:O:393:THR:HG21	1:O:518:LEU:CB	2.34	0.51
2:A:135:PRO:HD3	2:A:163:TRP:CD1	2.47	0.50
2:A:177:ARG:O	2:A:181:GLU:HG3	2.11	0.50
2:A:332:MET:HE2	2:A:336:PRO:HB3	1.93	0.50
2:A:594:TRP:O	2:A:597:GLU:HG2	2.12	0.50
2:F:54:ILE:HG22	2:F:341:LYS:O	2.12	0.50
1:E:337:PRO:HD2	1:E:358:ILE:HG23	1.94	0.50
2:F:237:TYR:CE1	2:F:451:PRO:HG2	2.46	0.50
2:A:233:ILE:HD11	2:A:581:VAL:HG11	1.94	0.50
2:A:450:LEU:HB2	2:A:451:PRO:HD3	1.92	0.50
2:F:116:LEU:HB2	2:F:186:LEU:HD13	1.94	0.50
2:F:477:TRP:CE3	2:F:500:PRO:HG3	2.47	0.50
1:E:517:LEU:N	1:E:517:LEU:HD23	2.26	0.49
2:F:237:TYR:CZ	2:F:451:PRO:HG2	2.47	0.49
2:F:468:ILE:HG12	2:F:476:LYS:HG2	1.94	0.49
2:A:187:LYS:HE3	2:A:509:ASP:OD1	2.13	0.49
2:A:212:SER:HB3	2:A:215:SER:OG	2.12	0.49
1:E:336:CYS:SG	1:E:358:ILE:HG22	2.51	0.49
1:E:363:ALA:O	1:E:526:GLY:HA2	2.13	0.49
2:A:363:LYS:HB2	2:A:365:THR:HG23	1.94	0.49
2:F:482:ARG:NH2	2:F:489:GLU:OE1	2.41	0.49
1:O:435:ALA:HA	1:O:509:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:332:MET:SD	2:A:342:VAL:HG21	2.52	0.49
2:F:60:GLN:O	2:F:64:GLU:HG2	2.12	0.49
2:A:130:GLY:O	2:A:143:LEU:HD22	2.12	0.49
2:A:132:VAL:CG1	2:A:148:LEU:HD11	2.43	0.49
2:F:52:THR:O	2:F:342:VAL:HG12	2.13	0.48
1:O:359:SER:OG	1:O:394:ASN:OD1	2.23	0.48
2:A:200:GLY:O	2:A:204:ARG:HG3	2.14	0.48
2:F:229:ILE:HG21	2:F:520:ILE:HD11	1.96	0.48
2:F:296:ALA:O	2:F:300:GLN:HG3	2.13	0.48
2:F:239:HIS:HD2	2:F:592:TYR:HE1	1.60	0.48
1:E:362:VAL:HA	1:E:525:CYS:O	2.12	0.48
2:A:107:VAL:CG2	2:A:193:GLY:HA3	2.40	0.48
2:A:265:HIS:CE1	2:A:490:PRO:HB3	2.49	0.47
1:O:369:TYR:HD1	1:O:369:TYR:HA	1.33	0.47
1:E:359:SER:HA	1:E:524:VAL:CG2	2.44	0.47
2:A:221:GLN:NE2	2:F:600:ARG:O	2.40	0.47
1:E:337:PRO:HG2	1:E:356:LYS:HE3	1.97	0.47
1:O:417:LYS:HD2	1:O:455:LEU:HD12	1.96	0.47
2:F:284:PRO:HG2	2:F:436:ILE:HG22	1.96	0.47
2:F:527:GLU:CD	2:F:586:ARG:HH12	2.22	0.47
2:F:592:TYR:O	2:F:596:GLN:HG3	2.15	0.47
1:E:380:TYR:O	1:E:430:THR:HA	2.15	0.47
2:F:279:TYR:CD1	2:F:441:LYS:HG3	2.50	0.47
1:O:354:ASN:O	1:O:398:ASP:HA	2.15	0.47
1:O:379:CYS:SG	1:O:384:PRO:HG3	2.55	0.47
2:F:126:ILE:HG22	2:F:172:VAL:HG13	1.96	0.47
2:F:70:SER:O	2:F:74:GLU:HG3	2.15	0.46
2:A:50:TYR:CZ	2:A:54:ILE:HG23	2.50	0.46
2:A:528:ALA:O	2:A:531:ARG:HB2	2.15	0.46
1:E:362:VAL:HG21	1:E:527:HIS:ND1	2.30	0.46
2:F:408:MET:HE2	2:F:554:LEU:HD22	1.97	0.46
2:A:549:ASP:OD1	2:A:549:ASP:N	2.49	0.46
2:F:535:HIS:CD2	2:F:542:CYS:HB2	2.51	0.46
2:A:318:VAL:O	2:A:551:GLY:HA3	2.15	0.46
2:F:470:LYS:HB2	2:F:470:LYS:HE2	1.74	0.46
2:F:227:ASP:OD1	2:F:454:TYR:OH	2.30	0.46
2:A:52:THR:O	2:A:53:ASN:HB2	2.15	0.46
1:O:364:ASP:OD2	1:O:366:SER:OG	2.32	0.46
2:A:335:GLU:HG3	2:A:336:PRO:HD2	1.98	0.46
2:A:564:GLN:OE1	2:A:569:THR:HG22	2.15	0.46
2:A:585:LEU:HA	2:A:585:LEU:HD23	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:547:SER:O	2:F:548:THR:HB	2.15	0.45
2:A:204:ARG:HD2	2:A:222:LEU:HD23	1.98	0.45
1:O:393:THR:HG23	1:O:394:ASN:N	2.31	0.45
2:A:331:SER:HB3	2:A:358:ILE:O	2.17	0.45
1:O:462:LYS:HE2	1:O:462:LYS:HB2	1.55	0.45
2:F:380:GLN:HE21	2:F:380:GLN:HB2	1.53	0.45
2:F:535:HIS:CE1	2:F:542:CYS:HA	2.52	0.45
2:A:30:ASP:OD2	1:E:417:LYS:NZ	2.49	0.45
2:F:45:LEU:HD12	2:F:45:LEU:HA	1.87	0.45
2:A:263:PRO:HA	2:A:488:VAL:O	2.17	0.45
2:F:21:THR:HG21	2:F:87:GLU:HG3	1.98	0.45
2:F:320:LEU:HB3	2:F:380:GLN:OE1	2.17	0.45
2:F:547:SER:HB3	2:F:550:ALA:HB3	1.99	0.45
2:F:554:LEU:O	2:F:558:LEU:HG	2.16	0.45
2:A:417:HIS:O	2:A:420:THR:HG22	2.16	0.45
2:F:477:TRP:CZ2	2:F:481:LYS:HE2	2.52	0.45
2:F:528:ALA:HB2	2:F:574:VAL:HG12	1.97	0.45
2:A:442:GLN:NE2	2:A:587:TYR:OH	2.48	0.45
2:F:403:ALA:HA	2:F:518:ARG:HG3	1.98	0.45
2:F:427:ASP:O	2:F:429:LEU:N	2.49	0.45
2:A:478:TRP:HA	2:A:478:TRP:CE3	2.50	0.45
1:E:356:LYS:HD3	1:E:358:ILE:CD1	2.45	0.44
1:E:398:ASP:OD2	1:E:423:TYR:OH	2.34	0.44
2:A:32:PHE:HD1	2:A:76:GLN:HG3	1.82	0.44
2:A:392:LEU:HD13	2:A:563:SER:HA	2.00	0.44
1:E:392:PHE:CE2	1:E:515:PHE:HB3	2.52	0.44
2:F:96:GLN:HB3	2:F:391:LEU:HD12	1.97	0.44
2:A:430:GLU:OE1	2:A:541:LYS:NZ	2.32	0.44
2:F:368:ASP:HA	2:F:371:THR:HB	1.98	0.44
2:F:455:MET:HB3	2:F:455:MET:HE3	1.54	0.44
1:O:340:GLU:O	1:O:344:ALA:HB2	2.17	0.44
1:E:376:THR:HG23	1:E:378:LYS:HZ3	1.82	0.44
2:F:95:LEU:O	2:F:99:ILE:HG13	2.17	0.44
2:F:565:PRO:O	2:F:568:VAL:N	2.49	0.44
2:A:229:ILE:HG23	2:A:581:VAL:CG1	2.48	0.44
1:E:384:PRO:HA	1:E:387:LEU:HG	1.99	0.44
1:E:517:LEU:CD2	1:E:517:LEU:N	2.78	0.44
2:A:122:ALA:O	2:A:126:ILE:HG13	2.18	0.44
2:A:402:GLU:HB3	2:A:518:ARG:HD2	2.00	0.44
2:A:520:ILE:HG21	2:A:579:MET:HB3	2.00	0.43
2:A:315:PHE:HE1	2:A:408:MET:HE3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:86:GLU:CD	2:A:86:GLU:H	2.26	0.43
2:A:227:ASP:O	2:A:231:THR:HG23	2.18	0.43
1:O:456:PHE:CE1	2:F:27:ILE:HG23	2.53	0.43
2:A:332:MET:HE3	2:A:332:MET:HB2	1.84	0.43
2:A:573:ILE:HG21	2:A:573:ILE:HD13	1.50	0.43
2:F:557:MET:CB	2:F:573:ILE:HD11	2.48	0.43
2:A:45:LEU:HA	2:A:45:LEU:HD12	1.57	0.43
2:A:322:ASN:OD1	2:A:322:ASN:N	2.49	0.43
1:E:516:GLU:C	1:E:517:LEU:HD23	2.44	0.43
1:O:517:LEU:H	1:O:517:LEU:HD23	1.83	0.43
2:A:140:GLU:O	2:A:140:GLU:HG3	2.18	0.43
2:A:600:ARG:NH1	2:A:601:LYS:HE2	2.33	0.43
1:E:336:CYS:SG	1:E:358:ILE:CG2	3.07	0.43
2:F:95:LEU:HA	2:F:95:LEU:HD23	1.76	0.42
2:F:297:MET:HE1	2:F:365:THR:O	2.20	0.42
2:F:523:PHE:CD1	2:F:584:LEU:HD12	2.54	0.42
2:A:103:SER:O	2:A:105:SER:N	2.41	0.42
2:A:85:LEU:CD1	2:A:101:GLN:HE22	2.32	0.42
2:A:155:SER:HB3	2:A:161:ARG:HG2	2.01	0.42
1:E:425:LEU:HD23	1:E:425:LEU:HA	1.85	0.42
1:O:480:CYS:O	1:O:481:ASN:C	2.63	0.42
2:A:294:THR:O	2:A:298:VAL:HG23	2.20	0.42
1:O:377:PHE:C	1:O:378:LYS:HD3	2.44	0.42
1:O:382:VAL:HG11	1:O:387:LEU:HD21	2.01	0.42
2:A:402:GLU:O	2:A:406:GLU:HG2	2.19	0.42
2:F:439:LEU:HA	2:F:439:LEU:HD23	1.65	0.42
2:F:555:HIS:O	2:F:559:SER:OG	2.37	0.42
1:O:401:VAL:HG22	1:O:509:ARG:HG2	2.01	0.42
2:A:171:GLU:O	2:A:175:GLN:NE2	2.45	0.42
2:A:457:GLU:HG2	2:A:513:ILE:HB	2.02	0.42
2:F:20:THR:O	2:F:23:ASP:HB2	2.19	0.42
1:E:400:PHE:HZ	1:E:410:ILE:HD12	1.85	0.42
2:F:39:LEU:HD23	2:F:39:LEU:HA	1.85	0.42
1:O:492:LEU:O	1:O:493:TYR:HD1	2.02	0.42
1:E:398:ASP:O	1:E:511:VAL:HA	2.18	0.42
2:A:474:MET:HE1	2:A:499:ASP:HB2	2.01	0.42
2:F:97:LEU:HD23	2:F:97:LEU:HA	1.78	0.42
2:F:379:ILE:O	2:F:383:MET:HG3	2.20	0.41
2:A:351:LEU:HD12	2:A:351:LEU:H	1.85	0.41
2:F:257:SER:HB3	2:F:260:GLY:HA3	2.02	0.41
2:F:408:MET:CE	2:F:554:LEU:HD22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:335:GLU:O	2:A:337:GLY:N	2.52	0.41
2:A:477:TRP:CZ3	2:A:500:PRO:HG3	2.55	0.41
2:A:611:SER:OG	2:A:614:SER:HB3	2.20	0.41
2:F:228:ARG:O	2:F:232:GLU:HG3	2.20	0.41
2:A:287:GLN:OE1	2:A:287:GLN:HA	2.19	0.41
2:A:360:MET:HE2	2:A:375:GLU:HG3	2.03	0.41
2:A:429:LEU:HD23	2:A:429:LEU:HA	1.92	0.41
1:E:421:TYR:CD1	1:E:457:ARG:HB3	2.55	0.41
2:F:206:ASP:OD2	2:F:398:GLU:HG2	2.20	0.41
2:F:476:LYS:HD2	2:F:476:LYS:HA	1.74	0.41
1:O:438:SER:OG	1:O:442:ASP:OD2	2.36	0.41
2:A:157:ASP:HB3	2:A:160:GLU:CB	2.51	0.41
1:E:387:LEU:HA	1:E:390:LEU:HD22	2.03	0.41
1:E:431:GLY:HA2	1:E:515:PHE:CD2	2.55	0.41
1:E:517:LEU:HA	1:E:517:LEU:HD22	1.51	0.41
2:F:223:MET:HE1	2:F:465:ARG:HH22	1.85	0.41
2:F:248:LEU:HA	2:F:248:LEU:HD23	1.70	0.41
2:A:110:GLU:O	2:A:114:LYS:HG3	2.21	0.41
2:A:155:SER:O	2:A:161:ARG:NH1	2.45	0.41
1:E:390:LEU:HB3	1:E:392:PHE:CZ	2.55	0.41
2:A:226:VAL:HG22	2:A:516:TYR:CD2	2.56	0.41
2:F:92:PRO:O	2:F:96:GLN:HG3	2.21	0.41
2:F:284:PRO:HB3	2:F:594:TRP:CH2	2.56	0.41
2:F:308:PHE:CZ	2:F:360:MET:HE3	2.47	0.41
2:F:460:ARG:HE	2:F:506:VAL:HG22	1.86	0.41
2:F:565:PRO:O	2:F:566:TRP:C	2.64	0.41
2:A:176:LEU:HD23	2:A:176:LEU:HA	1.93	0.41
2:A:352:GLY:O	2:A:353:LYS:C	2.63	0.40
2:A:557:MET:HB2	2:A:573:ILE:HG13	2.02	0.40
2:A:50:TYR:CD1	2:A:50:TYR:C	3.00	0.40
2:F:203:TRP:HZ3	2:F:460:ARG:HH11	1.68	0.40
2:A:97:LEU:HD23	2:A:97:LEU:HA	1.90	0.40
2:A:492:PRO:HD3	2:A:613:TYR:CD2	2.56	0.40
1:E:462:LYS:HB2	1:E:462:LYS:HE2	1.92	0.40
2:F:444:LEU:HD23	2:F:444:LEU:HA	1.89	0.40
2:F:523:PHE:CE1	2:F:584:LEU:HD12	2.56	0.40
2:A:135:PRO:HD3	2:A:163:TRP:NE1	2.37	0.40
2:A:229:ILE:HG23	2:A:581:VAL:HG11	2.02	0.40
2:A:346:PRO:HG3	2:A:360:MET:HG3	2.04	0.40
2:A:369:PHE:HZ	2:A:421:MET:HE1	1.86	0.40
2:A:521:PHE:O	2:A:522:GLU:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:288:LYS:HE3	2:F:433:GLU:OE1	2.21	0.40
2:A:402:GLU:HB3	2:A:518:ARG:CD	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	E	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	25	59
1	O	193/196 (98%)	180 (93%)	11 (6%)	2 (1%)	13	44
2	A	594/597 (100%)	563 (95%)	26 (4%)	5 (1%)	16	49
2	F	595/597 (100%)	564 (95%)	25 (4%)	6 (1%)	13	44
All	All	1576/1586 (99%)	1491 (95%)	71 (4%)	14 (1%)	14	47

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	481	ASN
2	A	53	ASN
2	A	146	PRO
2	F	146	PRO
2	F	212	SER
2	F	289	PRO
2	A	212	SER
1	E	520	ALA
2	F	428	PHE
2	A	213	SER
1	O	482	GLY
2	A	104	GLY
2	F	195	HIS

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Mol	Chain	Res	Type
2	F	105	SER

### 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	E	168/168 (100%)	168 (100%)	0	100	100
1	O	167/168 (99%)	167 (100%)	0	100	100
2	A	531/532 (100%)	529 (100%)	2 (0%)	89	95
2	F	532/532 (100%)	530 (100%)	2 (0%)	89	95
All	All	1398/1400 (100%)	1394 (100%)	4 (0%)	91	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	231	THR
2	A	401	HIS
2	F	380	GLN
2	F	414	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	388	ASN
2	A	31	ASN
2	A	33	ASN
2	A	76	GLN
2	A	96	GLN
2	A	98	GLN
2	A	101	GLN
2	A	121	ASN
2	A	137	ASN
2	A	139	GLN
2	A	305	ASN

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Mol	Chain	Res	Type
2	A	330	ASN
2	A	442	GLN
2	A	540	HIS
2	A	599	ASN
2	F	31	ASN
2	F	33	ASN
2	F	34	HIS
2	F	76	GLN
2	F	239	HIS
2	F	255	HIS
2	F	345	HIS
2	F	374	HIS
2	F	380	GLN
2	F	526	HIS
2	F	535	HIS
2	F	596	GLN
2	F	599	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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
3	NAG	E	601	-	10,10,15	0.33	0	11,11,21	0.70	0
3	NAG	O	601	1	14,14,15	0.50	0	17,19,21	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	601	-	-	0/8/8/26	-
3	NAG	O	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

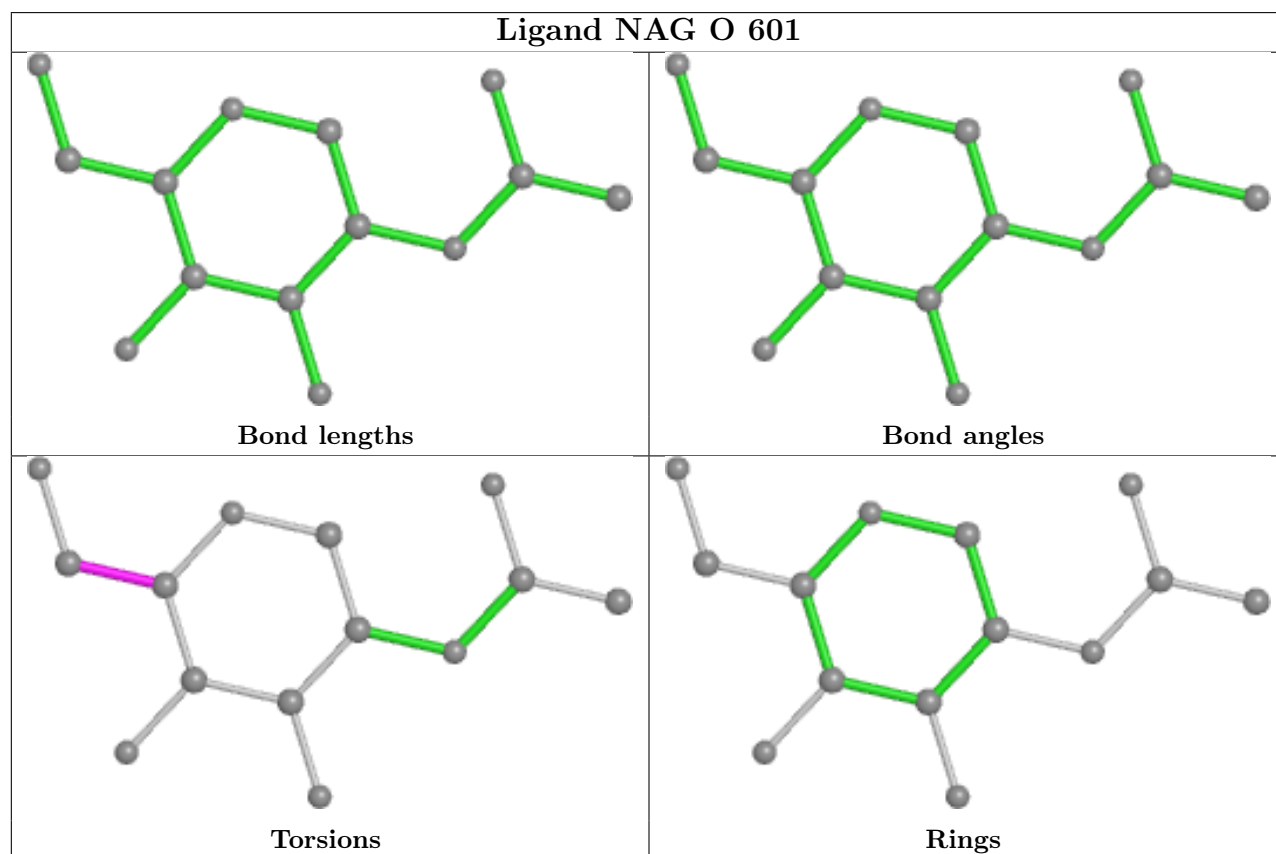
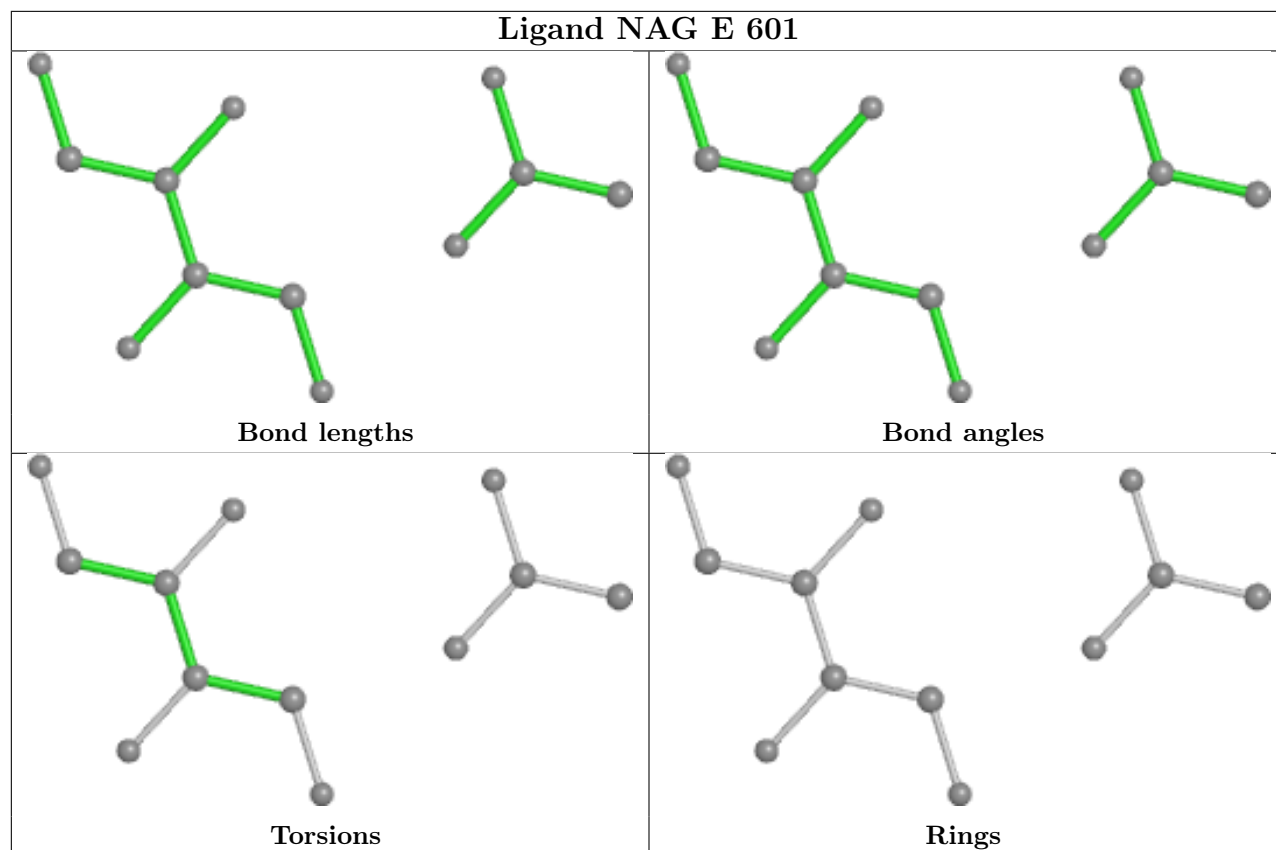
Mol	Chain	Res	Type	Atoms
3	O	601	NAG	C4-C5-C6-O6
3	O	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	NAG	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](#)

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	E	196/196 (100%)	-0.35	6 (3%) 51 31	34, 53, 95, 117	0
1	O	195/196 (99%)	-0.34	2 (1%) 79 61	36, 58, 102, 165	0
2	A	596/597 (99%)	-0.53	3 (0%) 87 75	27, 55, 97, 155	0
2	F	597/597 (100%)	-0.58	3 (0%) 87 75	28, 51, 88, 132	0
All	All	1584/1586 (99%)	-0.50	14 (0%) 81 63	27, 53, 96, 165	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	517	LEU	3.8
2	A	338	ASP	3.8
1	O	369	TYR	3.2
2	F	141	CYS	3.2
2	A	578	ASN	3.1
2	F	106	PRO	3.0
1	O	517	LEU	2.9
1	E	486	LEU	2.9
2	F	104	GLY	2.7
1	E	392	PHE	2.6
1	E	518	LEU	2.4
1	E	480	CYS	2.3
2	A	339	GLY	2.3
1	E	528	HIS	2.2

### 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](#)

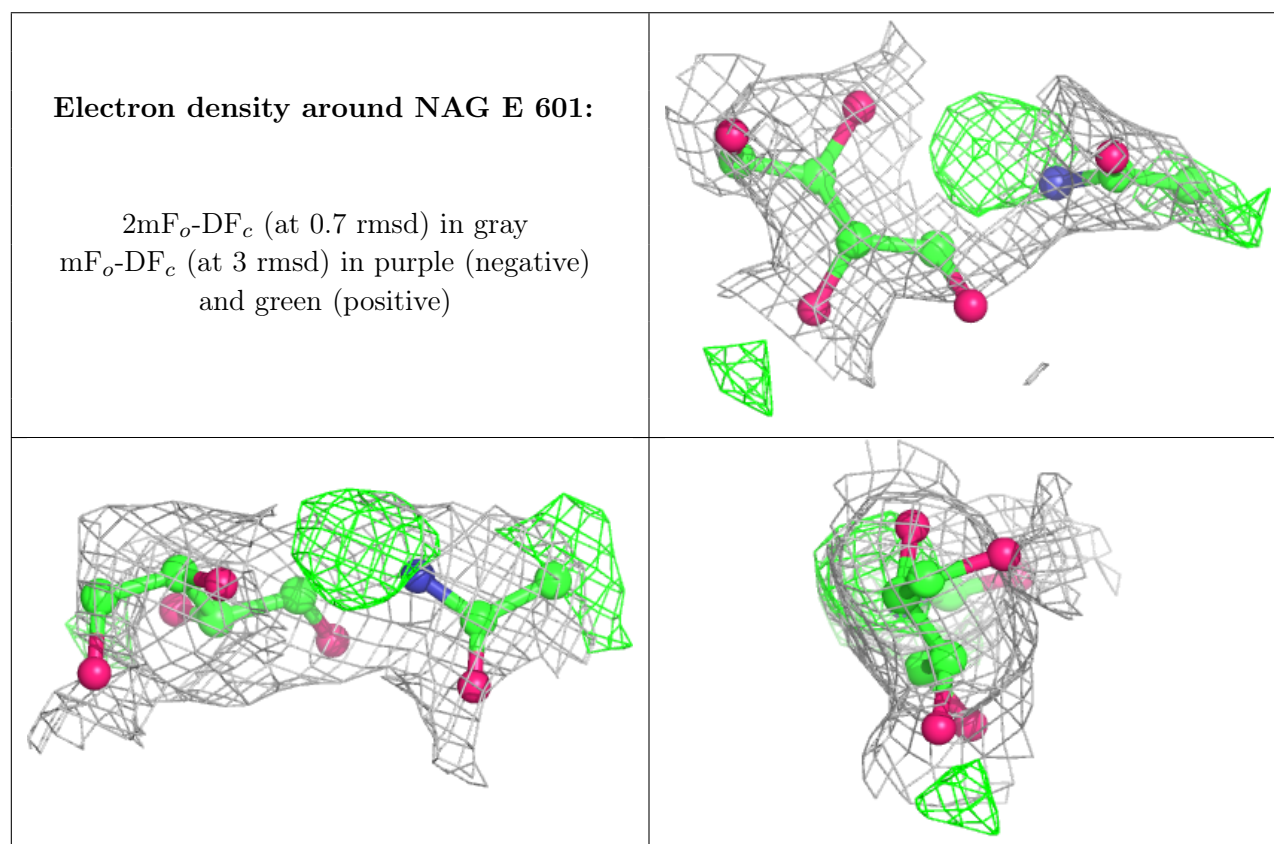
There are no monosaccharides in this entry.

## 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.

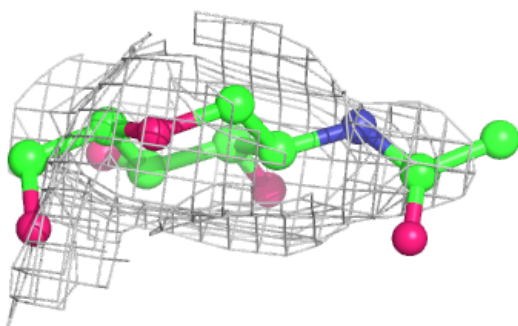
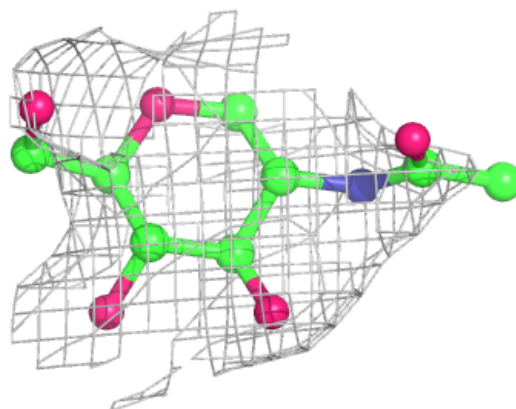
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	601	12/15	0.69	0.16	94,101,107,107	0
3	NAG	O	601	14/15	0.81	0.12	101,106,126,132	0

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 NAG O 601:**

$2mF_o-DF_c$  (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.