



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:34 AM BST

PDB ID : 1E1F  
Title : Crystal structure of a Monocot (Maize ZMGlu1) beta-glucosidase in complex with p-Nitrophenyl-beta-D-thioglucoside  
Authors : Czjzek, M.; Cicek, M.; Bevan, D.R.; Henrissat, B.; Esen, A.  
Deposited on : 2000-05-03  
Resolution : 2.60 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.

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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 : 2.13.1  
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

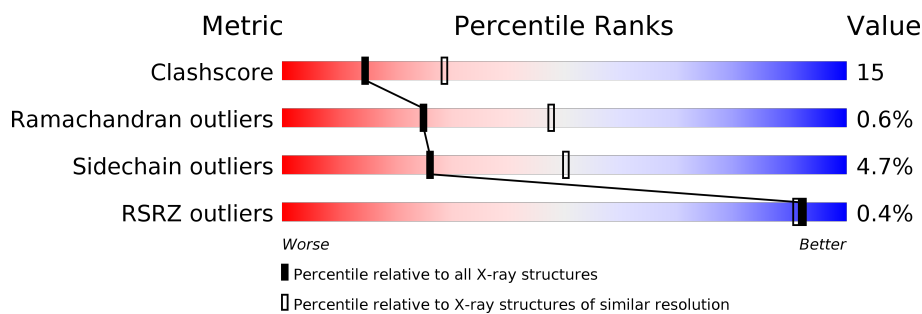
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	512	 72% 20% . .
1	B	512	 69% 24% . .

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	PSG	A	513[A]	-	-	-	X
2	PSG	A	513[B]	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PSG	B	513[A]	-	-	-	X
2	PSG	B	513[B]	X	-	-	X

## 2 Entry composition [i](#)

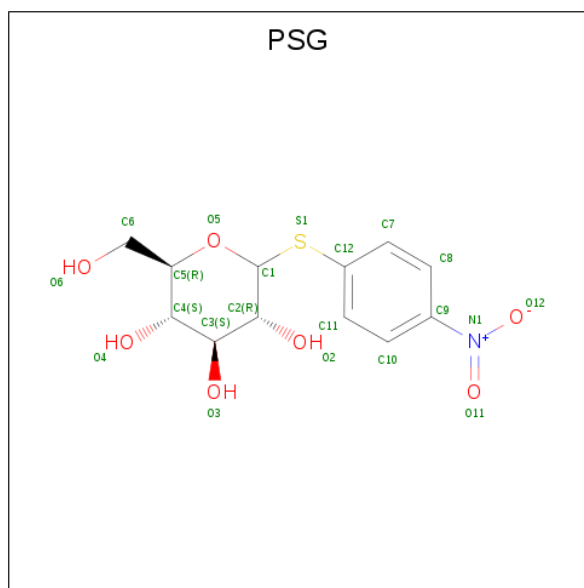
There are 3 unique types of molecules in this entry. The entry contains 8374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3967	2544	656	749	18			
1	B	490	Total	C	N	O	S	0	0	0
			3967	2544	656	749	18			

- Molecule 2 is 4-nitrophenyl 1-thio-beta-D-glucopyranoside (three-letter code: PSG) (formula: C<sub>12</sub>H<sub>15</sub>NO<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			42	24	2	14	2		
2	B	1	Total	C	N	O	S	0	1
			42	24	2	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total 174	O 174	0	0
3	B	182	Total 182	O 182	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.64Å 118.15Å 80.88Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	39.00 – 2.60 36.41 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.9 (39.00-2.60) 97.1 (36.41-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.58Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.199 , 0.252 0.196 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 28.2	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	0.92	EDS
Total number of atoms	8374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: PSG

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	0.38	0/4088	0.61	1/5550 (0.0%)
1	B	0.37	0/4088	0.60	0/5550
All	All	0.37	0/8176	0.61	1/11100 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	TRP	N-CA-C	-7.06	91.94	111.00

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	A	3967	0	3759	111	0
1	B	3967	0	3759	128	0
2	A	42	0	28	5	0
2	B	42	0	28	10	0
3	A	174	0	0	5	0
3	B	182	0	0	8	0
All	All	8374	0	7574	237	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 15.

All (237) 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:64:ILE:HD11	1:A:68:SER:H	1.06	1.14
1:B:464:GLU:OE1	2:B:513[A]:PSG:H62	1.49	1.13
1:B:64:ILE:HD11	1:B:68:SER:H	1.25	1.01
1:B:464:GLU:OE1	2:B:513[B]:PSG:H62	1.59	1.01
1:A:334:THR:HG21	1:A:380:TYR:H	1.28	0.95
1:B:458:SER:HA	3:B:2170:HOH:O	1.68	0.92
1:B:206:ALA:HB3	1:B:207:PRO:HD3	1.53	0.90
1:B:334:THR:HG21	1:B:380:TYR:H	1.35	0.89
1:A:376:ASN:HB2	1:A:377:PRO:HD2	1.55	0.87
1:A:206:ALA:HB3	1:A:207:PRO:HD3	1.58	0.86
2:A:513[B]:PSG:O12	3:A:2174:HOH:O	1.94	0.85
1:B:38:GLN:HA	3:B:2021:HOH:O	1.75	0.85
1:B:376:ASN:HD21	1:B:379:ILE:H	1.21	0.84
1:B:38:GLN:NE2	2:B:513[B]:PSG:O4	2.10	0.83
1:A:334:THR:HG22	1:A:380:TYR:O	1.82	0.79
1:A:64:ILE:HD11	1:A:68:SER:N	1.92	0.79
1:A:52:ASN:N	1:A:52:ASN:HD22	1.84	0.75
1:A:334:THR:CG2	1:A:380:TYR:H	2.00	0.73
1:B:334:THR:HG22	1:B:380:TYR:O	1.89	0.72
1:B:52:ASN:HD22	1:B:52:ASN:N	1.87	0.72
1:A:191:GLU:HG2	1:A:261:ASP:HB3	1.71	0.72
1:B:75:ASN:HB3	1:B:79:MET:HE3	1.73	0.71
1:A:334:THR:HG21	1:A:380:TYR:N	2.04	0.70
1:B:334:THR:HG21	1:B:380:TYR:N	2.05	0.70
1:B:464:GLU:OE1	2:B:513[B]:PSG:C6	2.35	0.70
1:B:191:GLU:HG2	1:B:261:ASP:HB3	1.74	0.70
1:B:376:ASN:ND2	1:B:379:ILE:H	1.89	0.70
1:A:383:PRO:HB2	1:A:440:THR:HG21	1.75	0.69
1:B:290:LEU:O	1:B:294:VAL:HG12	1.93	0.68
1:B:15:PRO:C	1:B:17:GLU:H	1.98	0.66
1:B:334:THR:CG2	1:B:380:TYR:H	2.09	0.65
1:B:376:ASN:C	1:B:376:ASN:HD22	1.99	0.64
1:A:38:GLN:O	1:A:462:ASN:HB2	1.98	0.64
1:A:21:ARG:O	1:A:23:TRP:O	2.16	0.64
1:A:75:ASN:HB3	1:A:79:MET:HE3	1.78	0.64
1:B:457:TRP:O	1:B:458:SER:HB2	1.98	0.63
1:B:463:PHE:HB3	3:B:2021:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PHE:CE2	1:A:234:ILE:HG23	2.35	0.62
1:A:376:ASN:HD21	1:A:379:ILE:H	1.47	0.62
1:B:75:ASN:HD21	1:B:78:HIS:HD2	1.46	0.62
1:A:53:TRP:NE1	1:A:206:ALA:HB2	2.15	0.61
1:B:206:ALA:CB	1:B:207:PRO:HD3	2.28	0.61
1:B:53:TRP:NE1	1:B:206:ALA:HB2	2.16	0.61
1:A:457:TRP:O	1:A:458:SER:HB2	1.99	0.61
1:B:376:ASN:HB2	1:B:377:PRO:CD	2.30	0.61
1:B:206:ALA:HB3	1:B:207:PRO:CD	2.30	0.60
1:A:290:LEU:O	1:A:294:VAL:HG12	2.01	0.60
1:A:191:GLU:OE2	2:A:513[A]:PSG:O2	2.16	0.60
1:B:189:PHE:CE2	1:B:234:ILE:HG23	2.36	0.60
1:A:303:ARG:HH11	1:A:303:ARG:HG2	1.66	0.60
1:A:419:LEU:HD13	1:A:424:ALA:HB2	1.84	0.60
1:B:162:LYS:O	1:B:166:GLU:HG3	2.03	0.58
1:A:431:LEU:O	1:A:435:GLN:HG3	2.03	0.58
1:A:232:HIS:CD2	1:A:311:PRO:HB2	2.38	0.58
1:B:191:GLU:CG	1:B:261:ASP:HB3	2.34	0.58
1:A:191:GLU:CG	1:A:261:ASP:HB3	2.32	0.58
1:A:275:LYS:HB3	1:A:275:LYS:NZ	2.19	0.58
1:B:459:LEU:O	1:B:476:VAL:HB	2.04	0.57
1:B:457:TRP:CZ2	2:B:513[B]:PSG:H3	2.39	0.57
1:A:334:THR:HG21	1:A:379:ILE:HA	1.86	0.57
1:B:308:GLU:CD	1:B:308:GLU:H	2.08	0.57
1:B:458:SER:HB3	1:B:474:GLY:HA2	1.85	0.57
1:A:52:ASN:H	1:A:52:ASN:HD22	1.48	0.57
1:B:334:THR:HG21	1:B:379:ILE:HA	1.87	0.57
1:A:480:ARG:HG2	1:A:480:ARG:HH11	1.69	0.57
1:B:275:LYS:NZ	1:B:275:LYS:HB3	2.20	0.57
1:A:64:ILE:CD1	1:A:68:SER:H	1.97	0.57
1:A:396:LYS:HE3	1:B:272:PHE:CD2	2.39	0.56
1:A:75:ASN:HB3	1:A:79:MET:CE	2.36	0.56
1:B:464:GLU:OE1	2:B:513[A]:PSG:C6	2.39	0.56
1:B:14:SER:HB2	1:B:15:PRO:HD2	1.87	0.55
1:B:291:GLU:HA	1:B:294:VAL:CG1	2.36	0.55
1:B:457:TRP:CE2	2:B:513[B]:PSG:H3	2.41	0.55
1:A:459:LEU:O	1:A:476:VAL:HB	2.06	0.55
1:A:162:LYS:O	1:A:166:GLU:HG3	2.07	0.55
1:A:376:ASN:ND2	1:A:379:ILE:H	2.03	0.55
1:B:193:GLN:NE2	1:B:197:SER:OG	2.40	0.55
1:B:19:PRO:HA	1:B:23:TRP:CZ3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:PRO:HG2	3:B:2012:HOH:O	2.07	0.55
1:A:284:ILE:HG13	1:A:302:MET:CE	2.37	0.54
1:B:52:ASN:ND2	1:B:52:ASN:N	2.55	0.54
1:A:376:ASN:C	1:A:376:ASN:HD22	2.09	0.54
1:A:482:ASN:O	1:A:485:THR:HG23	2.08	0.54
1:A:191:GLU:OE1	2:A:513[B]:PSG:S1	2.66	0.54
1:A:206:ALA:CB	1:A:207:PRO:HD3	2.33	0.54
1:A:394:LYS:NZ	1:A:395:ASN:HD21	2.05	0.54
1:A:36:ALA:O	1:A:40:GLU:HG3	2.08	0.54
1:A:52:ASN:H	1:A:52:ASN:ND2	2.06	0.54
1:B:90:MET:HE1	1:B:492:ALA:HA	1.90	0.54
1:A:381:MET:HE1	1:A:433:TYR:HA	1.89	0.54
1:A:376:ASN:HB2	1:A:377:PRO:CD	2.33	0.53
1:B:303:ARG:NH2	1:B:312:PHE:HA	2.24	0.53
1:B:199:SER:HB3	1:B:207:PRO:HD2	1.91	0.53
1:A:344:SER:HB2	1:A:345:PRO:HD2	1.89	0.53
1:A:458:SER:HB3	1:A:474:GLY:HA2	1.91	0.52
1:A:206:ALA:HB3	1:A:207:PRO:CD	2.36	0.52
1:A:427:ASP:OD2	1:A:430:ARG:HD2	2.09	0.52
1:B:156:PHE:O	1:B:230:ALA:HA	2.10	0.52
1:B:38:GLN:O	1:B:462:ASN:HB2	2.10	0.52
1:A:90:MET:HE1	1:A:475:ILE:HD12	1.90	0.52
1:A:193:GLN:NE2	1:A:197:SER:OG	2.43	0.52
1:A:303:ARG:HG2	1:A:303:ARG:NH1	2.25	0.52
1:B:99:ILE:HG23	1:B:122:TYR:CE2	2.44	0.52
1:B:442:LYS:HD3	1:B:442:LYS:O	2.10	0.52
1:A:191:GLU:OE2	2:A:513[B]:PSG:O2	2.27	0.52
1:B:303:ARG:HH22	1:B:312:PHE:HA	1.75	0.51
1:A:52:ASN:HD21	1:A:144:ASP:HA	1.76	0.51
1:B:52:ASN:H	1:B:52:ASN:HD22	1.58	0.51
1:A:476:VAL:CG1	1:A:486:ARG:HB2	2.40	0.50
1:A:330:LEU:HG	1:A:389:LEU:HD21	1.94	0.50
1:A:64:ILE:O	1:A:64:ILE:HG13	2.10	0.50
1:B:52:ASN:ND2	1:B:53:TRP:H	2.10	0.50
1:B:463:PHE:CE1	1:B:468:GLY:HA2	2.47	0.50
1:B:15:PRO:O	1:B:17:GLU:N	2.44	0.50
1:A:463:PHE:CE1	1:A:468:GLY:HA2	2.46	0.50
1:B:39:ILE:HG13	1:B:40:GLU:N	2.25	0.50
1:A:86:LEU:O	1:A:90:MET:HG3	2.11	0.49
1:A:147:GLN:HE21	1:A:151:GLU:HG3	1.76	0.49
1:A:189:PHE:CD2	1:A:234:ILE:HG23	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:PRO:C	1:B:17:GLU:N	2.66	0.49
1:B:307:ARG:HB3	1:B:308:GLU:OE2	2.13	0.49
1:B:56:PHE:CD1	1:B:206:ALA:O	2.66	0.49
1:A:207:PRO:HG3	3:A:2073:HOH:O	2.12	0.49
1:B:189:PHE:CD2	1:B:234:ILE:HG23	2.48	0.49
1:B:334:THR:CG2	1:B:380:TYR:N	2.74	0.49
1:B:482:ASN:O	1:B:485:THR:HG23	2.14	0.48
1:B:206:ALA:CB	1:B:207:PRO:CD	2.91	0.48
1:A:464:GLU:OE1	2:A:513[A]:PSG:H62	2.12	0.48
1:B:431:LEU:O	1:B:435:GLN:HG3	2.14	0.48
1:A:386:LEU:HD11	1:A:441:LEU:HD21	1.95	0.48
1:A:436:ARG:O	1:A:440:THR:HG23	2.14	0.48
1:A:458:SER:O	1:A:474:GLY:HA2	2.14	0.48
1:A:477:TYR:O	1:A:486:ARG:HA	2.14	0.48
1:A:75:ASN:OD1	1:A:79:MET:HE2	2.14	0.48
1:B:36:ALA:HA	1:B:40:GLU:HG3	1.96	0.48
1:A:199:SER:HB3	1:A:207:PRO:HD2	1.96	0.47
1:B:458:SER:O	1:B:474:GLY:HA2	2.14	0.47
1:A:312:PHE:CD2	1:B:345:PRO:HD3	2.49	0.47
1:A:173:LYS:HE2	3:A:2098:HOH:O	2.15	0.47
1:B:396:LYS:HE2	1:B:397:TYR:CZ	2.50	0.47
1:B:476:VAL:CG1	1:B:486:ARG:HB3	2.44	0.47
1:A:203:GLY:O	1:A:208:GLY:HA2	2.15	0.47
1:A:39:ILE:HG22	1:A:462:ASN:HB3	1.97	0.47
1:A:53:TRP:CE2	1:A:206:ALA:HB2	2.50	0.47
1:B:52:ASN:HD22	1:B:53:TRP:H	1.61	0.47
1:B:64:ILE:HD11	1:B:66:ASP:OD1	2.15	0.47
1:A:111:GLU:OE1	1:A:111:GLU:N	2.44	0.47
1:B:475:ILE:O	1:B:492:ALA:HB2	2.14	0.47
1:A:381:MET:HE2	1:A:433:TYR:HD2	1.80	0.47
1:A:381:MET:HE2	1:A:433:TYR:CD2	2.50	0.47
1:B:260:PHE:HE2	1:B:328:LEU:HG	1.80	0.47
1:B:29:THR:CG2	3:B:2150:HOH:O	2.62	0.46
1:B:52:ASN:ND2	1:B:52:ASN:H	2.13	0.46
1:A:90:MET:HE1	1:A:492:ALA:HA	1.97	0.46
1:B:64:ILE:HD11	1:B:68:SER:N	2.09	0.46
1:B:85:ARG:O	1:B:89:GLU:HG3	2.16	0.46
1:B:75:ASN:HD21	1:B:78:HIS:CD2	2.30	0.46
1:B:21:ARG:HB2	1:B:498:PHE:O	2.14	0.46
1:A:480:ARG:NH1	1:A:480:ARG:HG2	2.30	0.46
1:A:334:THR:CG2	1:A:380:TYR:N	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ARG:HB3	1:B:308:GLU:H	1.51	0.46
1:A:99:ILE:HG23	1:A:122:TYR:CE2	2.50	0.46
1:A:400:PRO:HD3	3:A:2149:HOH:O	2.16	0.46
1:B:51:SER:HB3	1:B:102:PRO:HG3	1.98	0.46
1:B:289:PHE:C	1:B:292:PRO:HD2	2.37	0.45
1:B:61:PRO:O	1:B:67:GLY:HA2	2.15	0.45
1:A:290:LEU:O	1:A:293:VAL:HG22	2.16	0.45
1:A:260:PHE:HE2	1:A:328:LEU:HG	1.80	0.45
1:A:296:GLY:O	1:A:318:LYS:HG2	2.17	0.45
1:B:64:ILE:HG13	1:B:64:ILE:O	2.16	0.45
1:A:51:SER:HB3	1:A:102:PRO:HG3	1.99	0.45
1:B:82:THR:O	1:B:86:LEU:HD22	2.17	0.45
1:A:275:LYS:HB3	1:A:275:LYS:HZ3	1.81	0.45
1:A:52:ASN:ND2	1:A:53:TRP:H	2.15	0.45
1:A:85:ARG:O	1:A:89:GLU:HG3	2.17	0.45
1:B:161:HIS:HA	1:B:233:ASN:OD1	2.16	0.45
1:B:122:TYR:O	1:B:126:ILE:HG13	2.16	0.44
1:B:232:HIS:HE1	3:B:2118:HOH:O	2.00	0.44
1:B:232:HIS:CD2	1:B:311:PRO:HB2	2.52	0.44
1:B:64:ILE:CD1	1:B:68:SER:H	2.12	0.44
1:A:14:SER:HB2	1:A:15:PRO:HD2	1.99	0.44
1:B:457:TRP:HE1	2:B:513[A]:PSG:H4O1	1.64	0.44
1:B:473:TYR:CZ	2:B:513[A]:PSG:H61	2.52	0.44
1:A:56:PHE:CD1	1:A:206:ALA:O	2.70	0.44
1:B:327:MET:HA	1:B:401:PRO:HG2	1.99	0.44
1:A:204:VAL:HG13	1:A:466:PHE:CD2	2.53	0.44
1:A:441:LEU:O	1:A:445:ILE:HG13	2.18	0.44
1:B:324:SER:O	1:B:325:TYR:HB3	2.18	0.44
1:B:412:VAL:HG12	3:B:2155:HOH:O	2.18	0.44
1:A:475:ILE:O	1:A:492:ALA:HB2	2.19	0.43
1:B:86:LEU:O	1:B:90:MET:HG3	2.18	0.43
1:A:156:PHE:HA	1:A:164:ILE:HG12	1.99	0.43
1:A:381:MET:HE1	1:A:433:TYR:CA	2.49	0.43
1:A:416:GLU:OE1	1:A:416:GLU:N	2.38	0.43
1:A:147:GLN:NE2	1:A:151:GLU:HG3	2.34	0.43
1:B:442:LYS:HD3	1:B:442:LYS:C	2.37	0.43
1:B:376:ASN:HB2	1:B:377:PRO:HD2	1.99	0.43
1:B:12:MET:HG3	1:B:12:MET:O	2.19	0.42
1:B:111:GLU:OE1	1:B:111:GLU:N	2.46	0.42
1:B:41:GLY:O	1:B:42:ALA:C	2.56	0.42
1:B:96:ARG:HA	1:B:137:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:HD23	1:B:441:LEU:HA	1.89	0.42
1:A:107:LYS:HD2	1:A:112:GLY:HA2	2.01	0.42
1:A:122:TYR:O	1:A:126:ILE:HG13	2.19	0.42
1:B:238:HIS:CE1	1:B:258:LEU:HD22	2.55	0.42
1:B:376:ASN:ND2	1:B:378:TRP:H	2.17	0.42
1:B:416:GLU:N	1:B:416:GLU:OE1	2.49	0.42
1:A:36:ALA:HA	1:A:40:GLU:HG3	2.02	0.42
1:B:143:TRP:N	1:B:143:TRP:CD1	2.86	0.42
1:B:110:LYS:HA	1:B:170:TYR:CE2	2.55	0.42
1:B:180:GLY:O	1:B:251:ARG:NH2	2.45	0.42
1:A:291:GLU:HA	1:A:294:VAL:CG1	2.49	0.41
1:B:290:LEU:O	1:B:293:VAL:HG22	2.20	0.41
1:A:180:GLY:O	1:A:251:ARG:NH2	2.52	0.41
1:A:23:TRP:O	1:A:24:PHE:O	2.38	0.41
1:B:141:PHE:CZ	1:B:143:TRP:HA	2.55	0.41
1:B:203:GLY:O	1:B:208:GLY:HA2	2.20	0.41
1:B:52:ASN:HD21	1:B:144:ASP:HA	1.85	0.41
1:A:206:ALA:CB	1:A:207:PRO:CD	2.96	0.41
1:B:371:GLY:HA3	1:B:381:MET:O	2.20	0.41
1:A:184:LYS:HE3	3:A:2101:HOH:O	2.20	0.41
1:A:312:PHE:CE2	1:B:345:PRO:HD3	2.56	0.41
1:B:154:GLY:O	1:B:157:LEU:HB2	2.20	0.41
1:B:14:SER:C	1:B:15:PRO:O	2.59	0.41
1:A:162:LYS:HE2	1:A:162:LYS:HB3	1.77	0.41
1:B:285:ASN:C	1:B:285:ASN:HD22	2.24	0.41
1:B:245:TYR:CD1	1:B:249:TYR:HB2	2.56	0.41
1:B:441:LEU:O	1:B:445:ILE:HG13	2.21	0.41
1:B:477:TYR:O	1:B:486:ARG:HA	2.20	0.41
1:A:307:ARG:HB3	1:A:308:GLU:H	1.53	0.40
1:B:12:MET:HG2	3:B:2004:HOH:O	2.21	0.40
1:B:291:GLU:HB3	1:B:292:PRO:HD3	2.03	0.40
1:A:394:LYS:HZ2	1:A:395:ASN:HD21	1.69	0.40
1:B:53:TRP:CE2	1:B:206:ALA:HB2	2.56	0.40
1:B:457:TRP:CZ2	2:B:513[A]:PSG:H3	2.56	0.40
1:A:107:LYS:HB2	1:A:112:GLY:HA3	2.04	0.40
1:B:52:ASN:ND2	1:B:53:TRP:N	2.70	0.40

There are no symmetry-related clashes.

## 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	488/512 (95%)	447 (92%)	38 (8%)	3 (1%)	25	47
1	B	488/512 (95%)	449 (92%)	36 (7%)	3 (1%)	25	47
All	All	976/1024 (95%)	896 (92%)	74 (8%)	6 (1%)	25	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ALA
1	B	206	ALA
1	B	13	LEU
1	A	458	SER
1	B	458	SER
1	A	24	PHE

### 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	423/441 (96%)	401 (95%)	22 (5%)	23	46
1	B	423/441 (96%)	405 (96%)	18 (4%)	29	54
All	All	846/882 (96%)	806 (95%)	40 (5%)	26	50

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	29	THR
1	A	52	ASN
1	A	64	ILE
1	A	75	ASN
1	A	86	LEU
1	A	204	VAL
1	A	252	ASP
1	A	285	ASN
1	A	286	LEU
1	A	307	ARG
1	A	308	GLU
1	A	315	ASP
1	A	316	GLU
1	A	328	LEU
1	A	330	LEU
1	A	376	ASN
1	A	419	LEU
1	A	451	VAL
1	A	459	LEU
1	A	462	ASN
1	A	486	ARG
1	B	29	THR
1	B	52	ASN
1	B	64	ILE
1	B	86	LEU
1	B	204	VAL
1	B	252	ASP
1	B	285	ASN
1	B	286	LEU
1	B	315	ASP
1	B	316	GLU
1	B	328	LEU
1	B	330	LEU
1	B	344	SER
1	B	361	GLU
1	B	376	ASN
1	B	386	LEU
1	B	459	LEU
1	B	462	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	20	GLN
1	A	52	ASN
1	A	59	ASN
1	A	147	GLN
1	A	193	GLN
1	A	232	HIS
1	A	276	GLN
1	A	376	ASN
1	A	395	ASN
1	A	462	ASN
1	A	481	ASN
1	A	499	ASN
1	B	52	ASN
1	B	59	ASN
1	B	78	HIS
1	B	124	ASN
1	B	193	GLN
1	B	232	HIS
1	B	276	GLN
1	B	376	ASN
1	B	395	ASN
1	B	481	ASN
1	B	499	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	PSG	A	513[B]	1	21,22,22	3.65	5 (23%)	29,31,31	2.34	5 (17%)
2	PSG	A	513[A]	-	21,22,22	1.54	5 (23%)	29,31,31	1.13	2 (6%)
2	PSG	B	513[A]	-	21,22,22	1.42	4 (19%)	29,31,31	1.34	4 (13%)
2	PSG	B	513[B]	1	21,22,22	3.65	5 (23%)	29,31,31	2.34	5 (17%)

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
2	PSG	A	513[B]	1	1/1/6/6	1/8/30/30	0/2/2/2
2	PSG	A	513[A]	-	-	1/8/30/30	0/2/2/2
2	PSG	B	513[A]	-	-	3/8/30/30	0/2/2/2
2	PSG	B	513[B]	1	1/1/6/6	1/8/30/30	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	513[B]	PSG	O11-N1	12.21	1.43	1.22
2	B	513[B]	PSG	O11-N1	12.18	1.43	1.22
2	B	513[B]	PSG	C12-S1	6.94	1.90	1.77
2	A	513[B]	PSG	C12-S1	6.92	1.90	1.77
2	B	513[B]	PSG	O2-C2	-6.16	1.28	1.43
2	A	513[B]	PSG	O2-C2	-6.15	1.28	1.43
2	B	513[B]	PSG	C1-S1	5.32	1.91	1.82
2	A	513[B]	PSG	C1-S1	5.31	1.91	1.82
2	B	513[A]	PSG	C7-C12	2.75	1.44	1.39
2	A	513[A]	PSG	C7-C12	2.69	1.44	1.39
2	A	513[A]	PSG	C12-S1	2.56	1.82	1.77
2	A	513[A]	PSG	C9-N1	2.49	1.51	1.45
2	B	513[A]	PSG	C9-N1	2.41	1.50	1.45
2	B	513[A]	PSG	C12-S1	2.36	1.82	1.77
2	A	513[B]	PSG	C9-N1	2.20	1.50	1.45
2	B	513[B]	PSG	C9-N1	2.18	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	513[A]	PSG	C1-S1	2.18	1.85	1.82
2	A	513[A]	PSG	C1-C2	2.06	1.57	1.53
2	B	513[A]	PSG	C1-S1	2.04	1.85	1.82

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	513[B]	PSG	C12-S1-C1	7.28	116.11	101.54
2	B	513[B]	PSG	C12-S1-C1	7.27	116.08	101.54
2	B	513[B]	PSG	C2-C1-S1	7.15	121.58	109.37
2	A	513[B]	PSG	C2-C1-S1	7.14	121.56	109.37
2	B	513[A]	PSG	C12-S1-C1	4.80	111.14	101.54
2	A	513[A]	PSG	C12-S1-C1	4.51	110.57	101.54
2	B	513[B]	PSG	O5-C1-S1	4.34	122.72	110.43
2	A	513[B]	PSG	O5-C1-S1	4.33	122.70	110.43
2	A	513[B]	PSG	O5-C1-C2	4.28	115.70	110.31
2	B	513[B]	PSG	O5-C1-C2	4.26	115.67	110.31
2	B	513[A]	PSG	C4-C3-C2	3.23	116.46	110.82
2	B	513[A]	PSG	C1-C2-C3	2.43	115.39	110.59
2	B	513[B]	PSG	C1-O5-C5	2.41	117.02	112.58
2	A	513[B]	PSG	C1-O5-C5	2.40	117.01	112.58
2	B	513[A]	PSG	C3-C4-C5	2.26	114.26	110.24
2	A	513[A]	PSG	C4-C3-C2	2.10	114.48	110.82

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	513[B]	PSG	C1
2	B	513[B]	PSG	C1

All (6) torsion outliers are listed below:

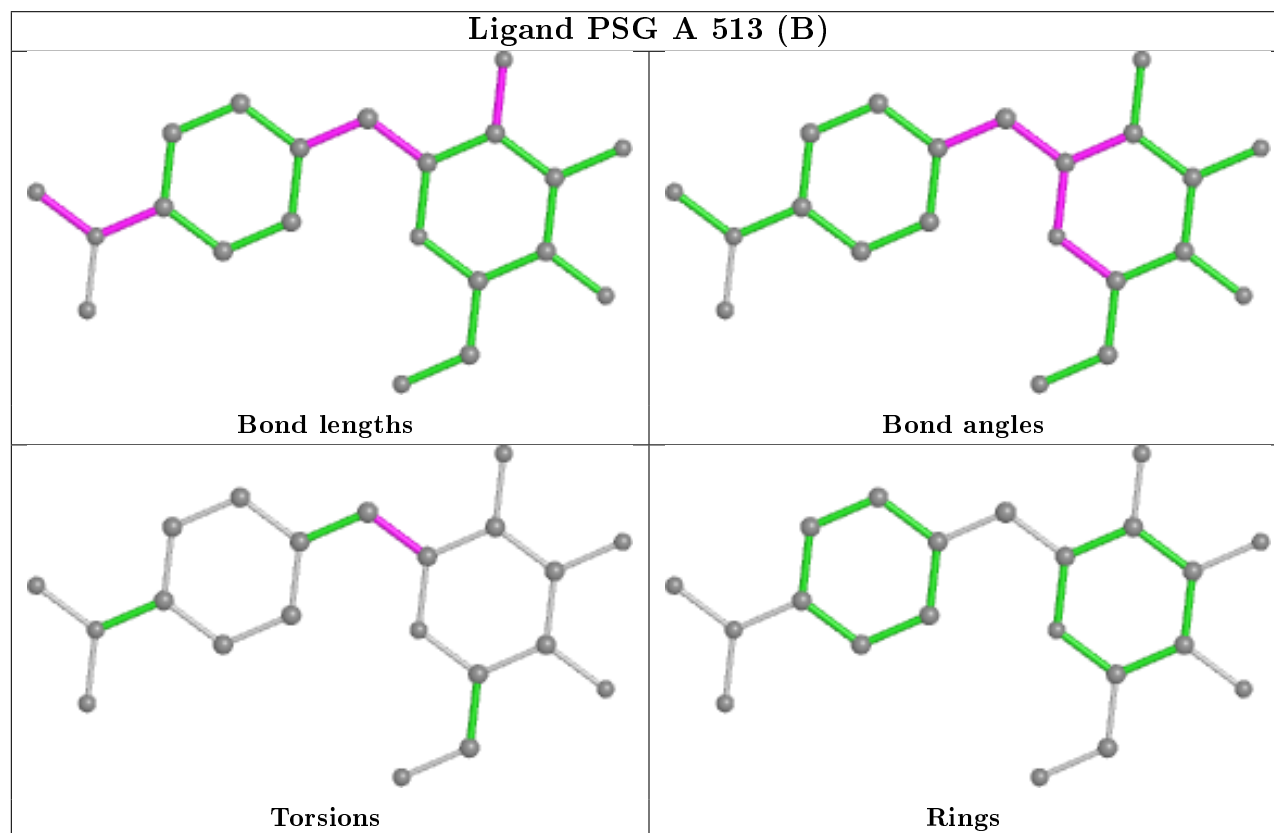
Mol	Chain	Res	Type	Atoms
2	A	513[B]	PSG	O5-C1-S1-C12
2	A	513[A]	PSG	O5-C1-S1-C12
2	B	513[A]	PSG	O5-C1-S1-C12
2	B	513[B]	PSG	O5-C1-S1-C12
2	B	513[A]	PSG	O5-C5-C6-O6
2	B	513[A]	PSG	C4-C5-C6-O6

There are no ring outliers.

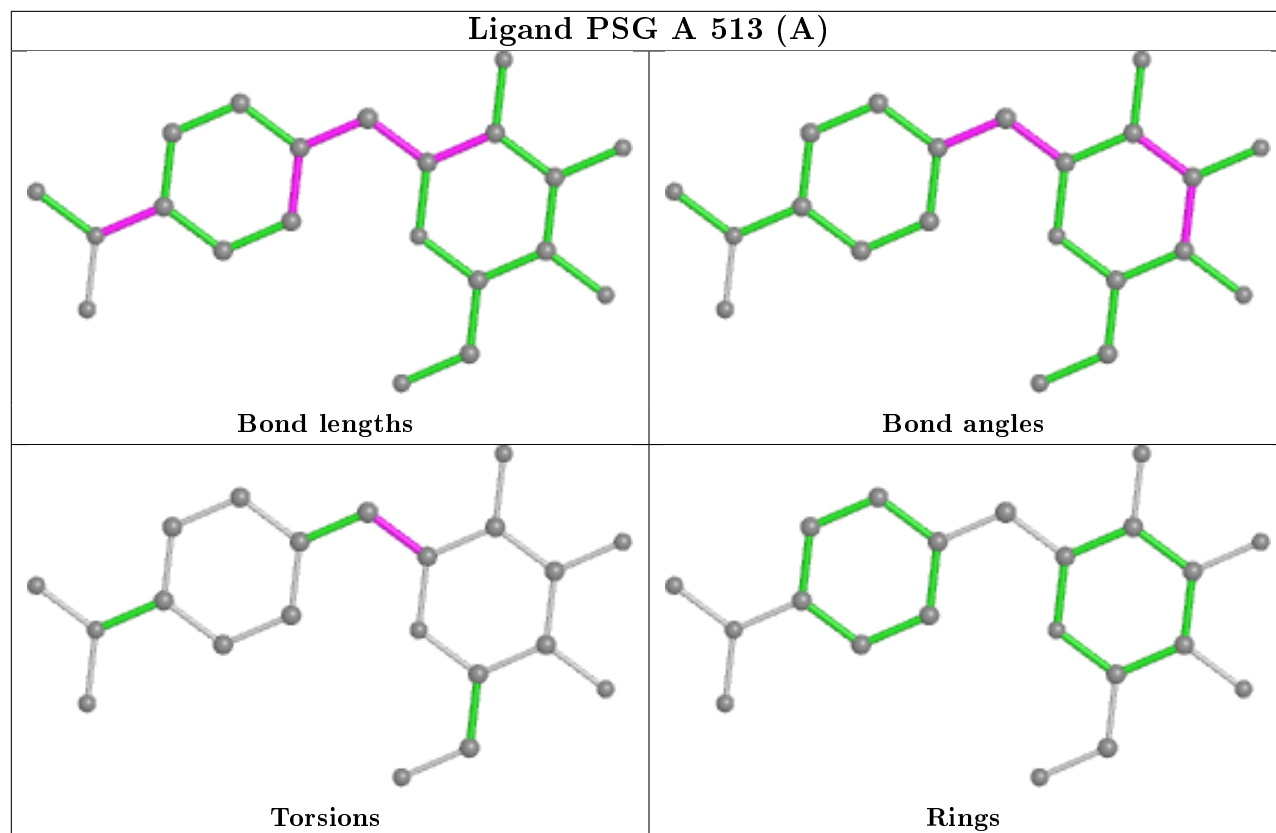
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	513[B]	PSG	3	0
2	A	513[A]	PSG	2	0
2	B	513[A]	PSG	5	0
2	B	513[B]	PSG	5	0

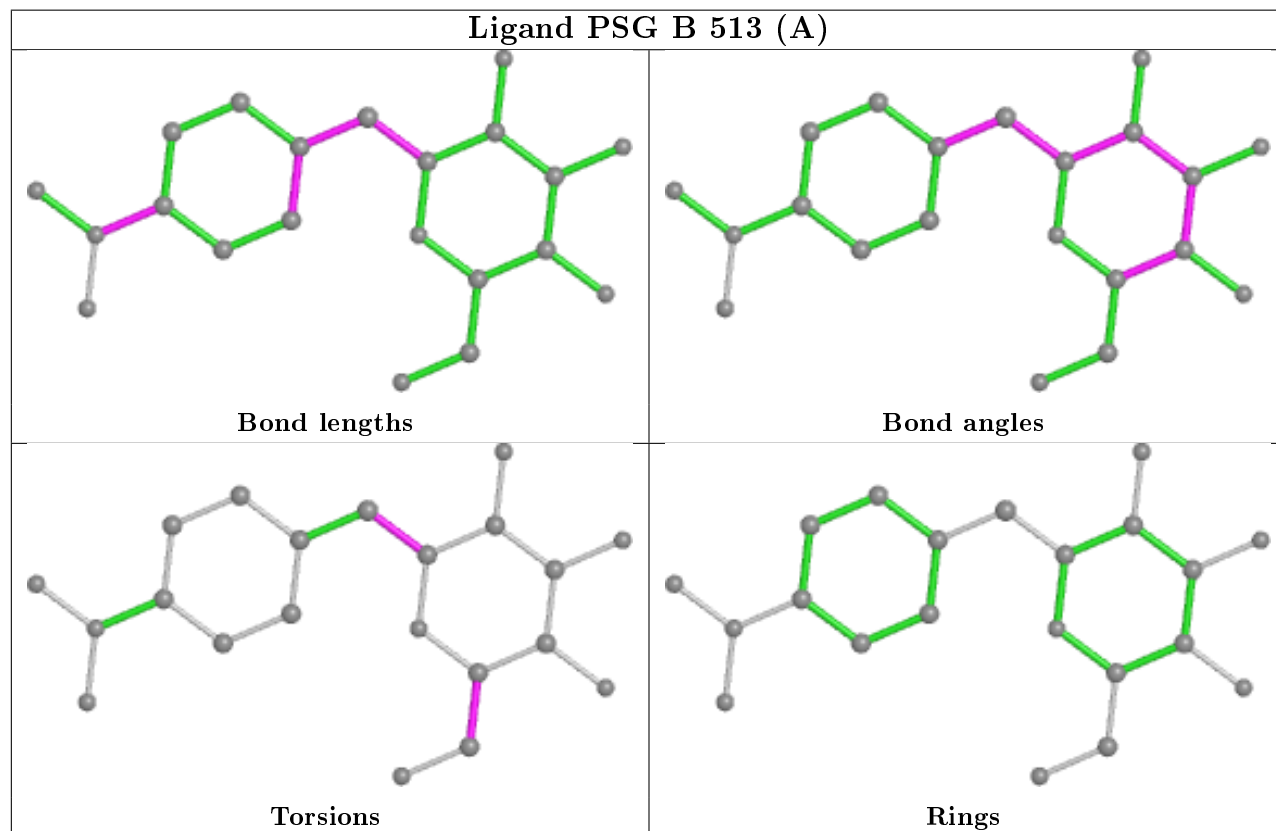
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

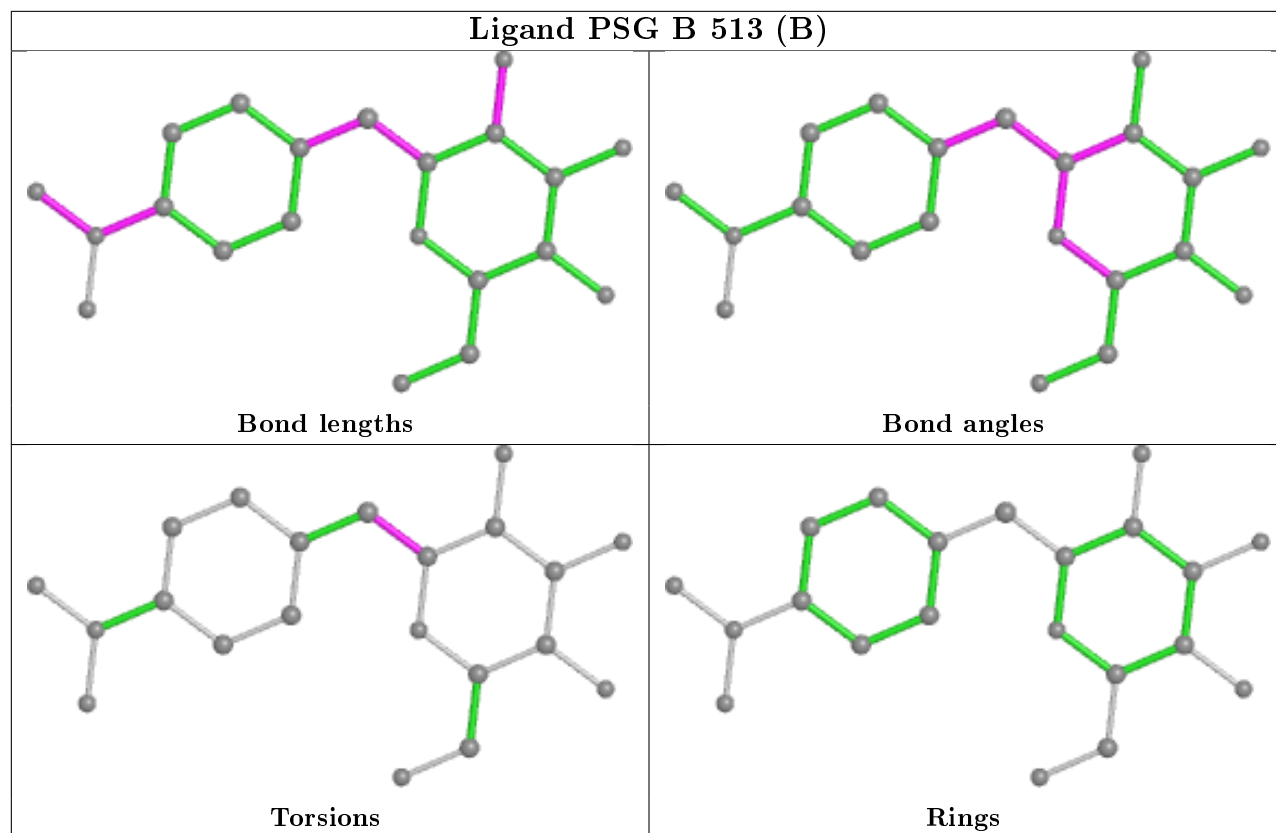


## Ligand PSG A 513 (A)



## Ligand PSG B 513 (A)





## 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	490/512 (95%)	-0.37	2 (0%) 92 91	6, 20, 43, 66	1 (0%)
1	B	490/512 (95%)	-0.37	2 (0%) 92 91	5, 17, 47, 77	1 (0%)
All	All	980/1024 (95%)	-0.37	4 (0%) 92 91	5, 18, 45, 77	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	12	MET	2.7
1	A	206	ALA	2.3
1	B	206	ALA	2.1
1	A	458	SER	2.1

### 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(Å <sup>2</sup> )	Q<0.9
2	PSG	A	513[B]	21/21	0.53	0.49	52,56,68,69	21

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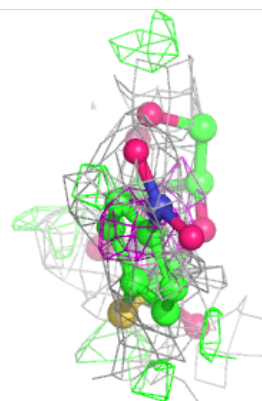
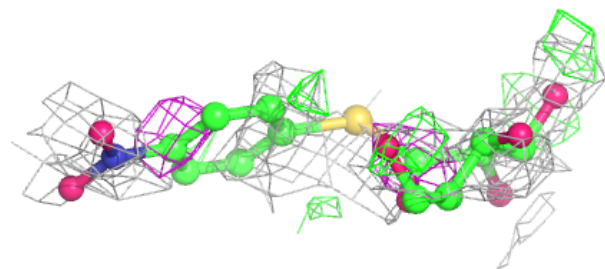
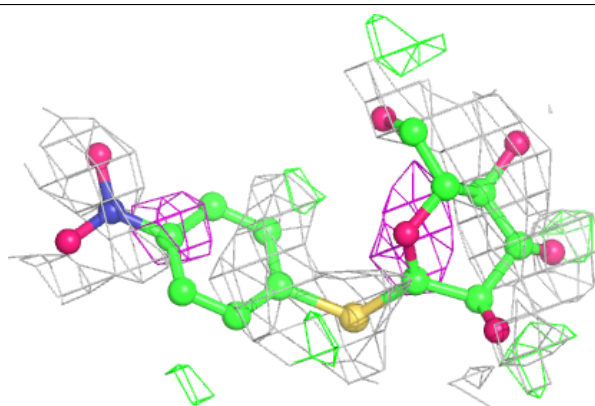
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PSG	A	513[A]	21/21	0.53	0.49	52,64,69,74	21
2	PSG	B	513[A]	21/21	0.64	0.44	48,52,67,69	21
2	PSG	B	513[B]	21/21	0.64	0.44	52,56,68,69	21

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 PSG A 513 (B):**

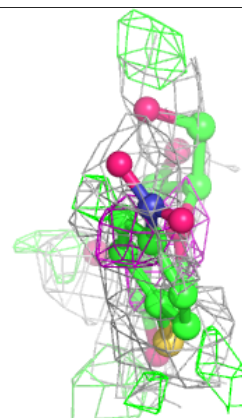
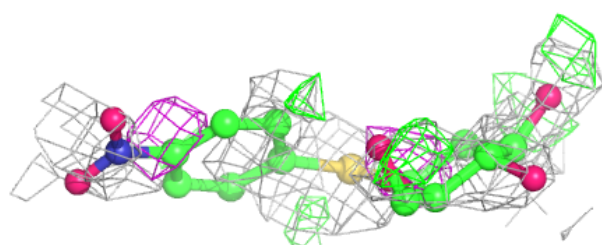
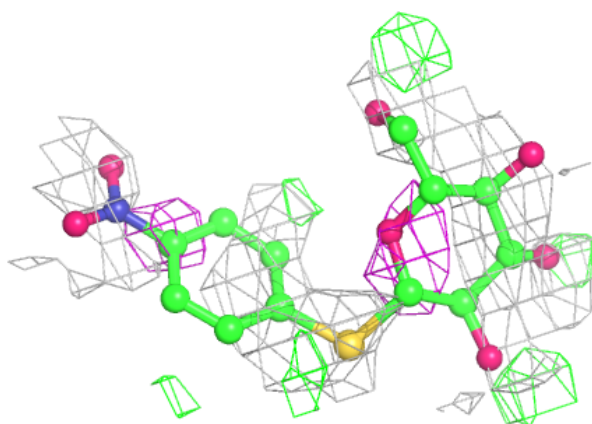
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



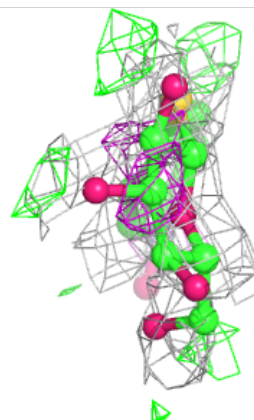
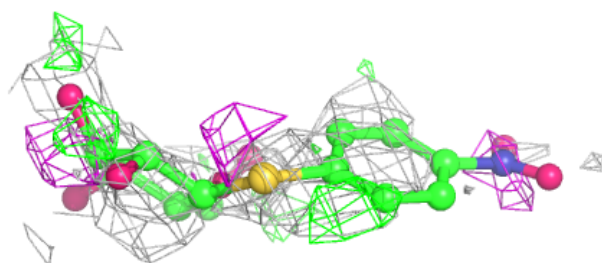
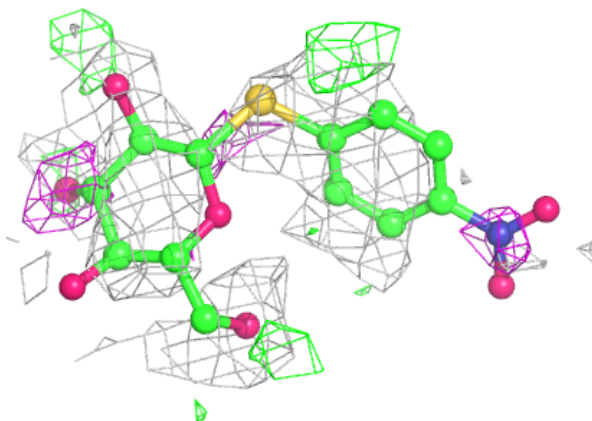


**Electron density around PSG A 513 (A):**

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

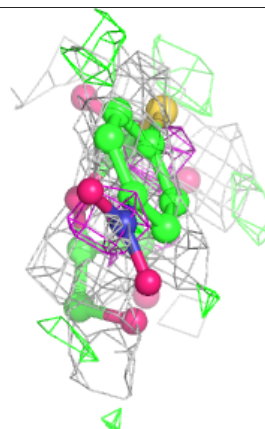
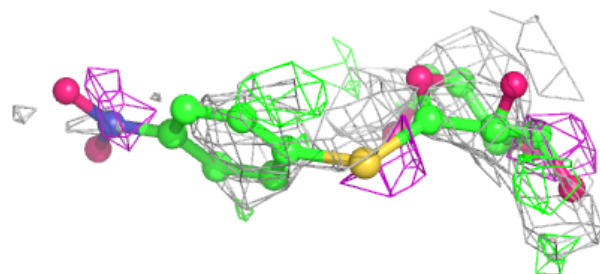
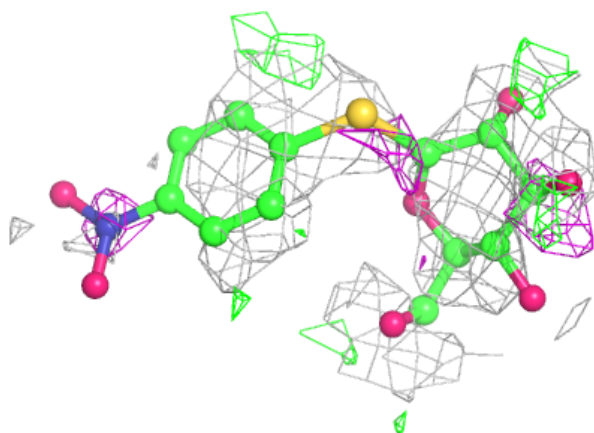
**Electron density around PSG B 513 (A):**

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



**Electron density around PSG B 513 (B):**

$2mF_o-DF_c$  (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.