



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 08:42 PM EDT

PDB ID : 4ZJR  
Title : RORgamma in complex with inverse agonist 48  
Authors : Marcotte, D.J.  
Deposited on : 2015-04-29  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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

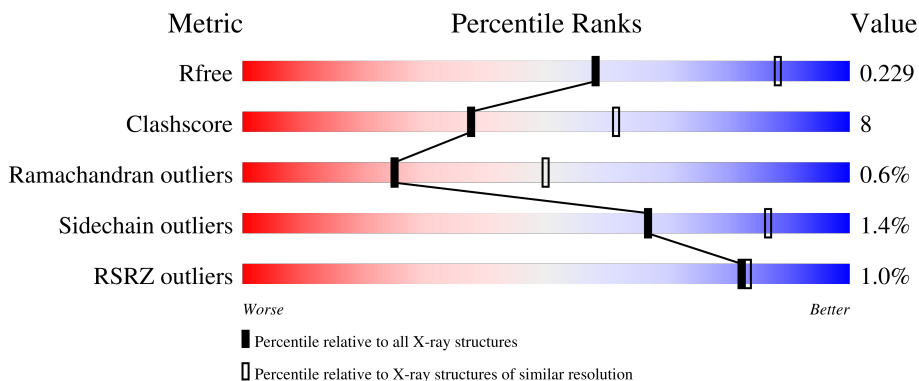
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


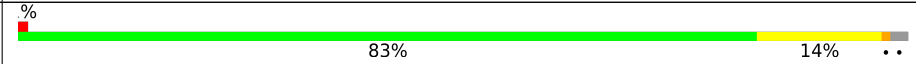
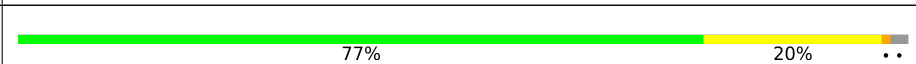

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	225	 2% 80% 15% ..
1	B	225	 % 83% 14% ..
1	C	225	 77% 20% ..
1	D	225	 76% 20% ..

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7293 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.

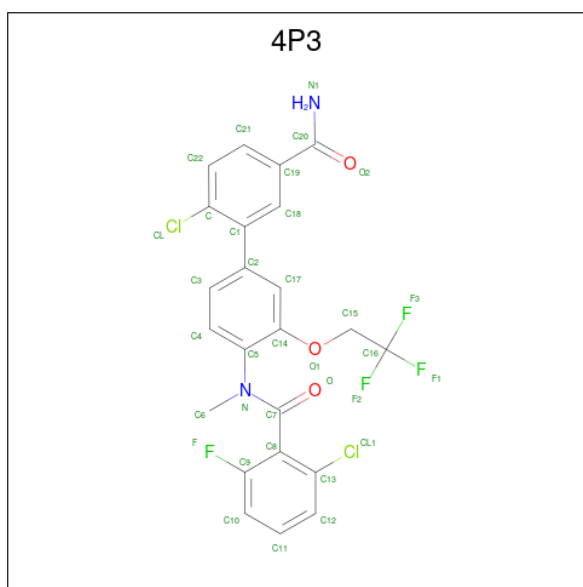
- Molecule 1 is a protein called Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	1747	1105	313	315	14	0	0	0
1	B	220	1771	1118	320	319	14	0	0	0
1	C	220	1770	1119	318	319	14	0	0	0
1	D	219	1761	1113	316	318	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P51449
A	0	SER	-	expression tag	UNP P51449
B	-1	GLY	-	expression tag	UNP P51449
B	0	SER	-	expression tag	UNP P51449
C	263	GLY	-	expression tag	UNP P51449
C	264	SER	-	expression tag	UNP P51449
D	-1	GLY	-	expression tag	UNP P51449
D	0	SER	-	expression tag	UNP P51449

- Molecule 2 is 6-chloro-4'-[(2-chloro-6-fluorobenzoyl)(methyl)amino]-3'-(2,2,2-trifluoroethoxy) biphenyl-3-carboxamide (three-letter code: 4P3) (formula: C<sub>23</sub>H<sub>16</sub>Cl<sub>2</sub>F<sub>4</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
2	A	1	Total	C	Cl	F	N	O	0	0
			34	23	2	4	2	3		
2	B	1	Total	C	Cl	F	N	O	0	0
			34	23	2	4	2	3		
2	C	1	Total	C	Cl	F	N	O	0	0
			34	23	2	4	2	3		
2	D	1	Total	C	Cl	F	N	O	0	0
			34	23	2	4	2	3		

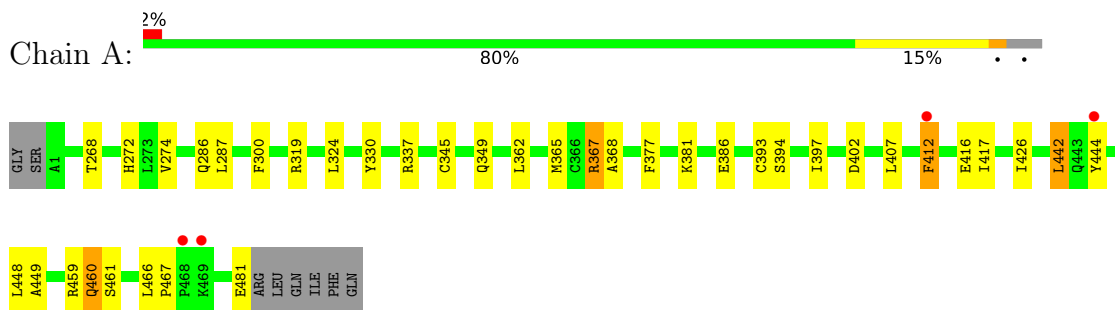
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	24	Total	O	0	0
			24	24		
3	C	28	Total	O	0	0
			28	28		
3	D	27	Total	O	0	0
			27	27		

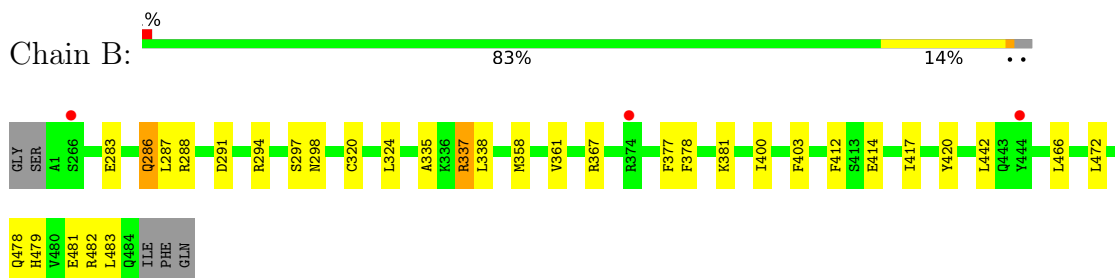
### 3 Residue-property plots [i](#)

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.

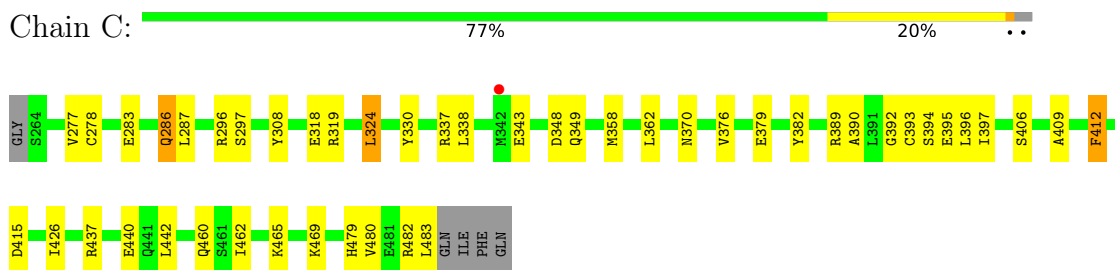
- Molecule 1: Nuclear receptor ROR-gamma



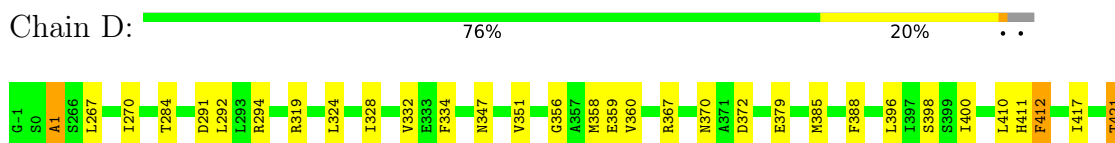
- Molecule 1: Nuclear receptor ROR-gamma



- Molecule 1: Nuclear receptor ROR-gamma



- Molecule 1: Nuclear receptor ROR-gamma





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.41Å 98.41Å 129.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.22 – 2.70 24.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (85.22-2.70) 100.0 (24.83-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.173 , 0.223 0.183 , 0.229	Depositor DCC
$R_{free}$ test set	1922 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 31.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.298 for -h,-k,l 0.034 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: 4P3

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	0.78	0/1781	0.90	6/2397 (0.3%)
1	B	0.81	0/1805	0.93	3/2430 (0.1%)
1	C	0.78	0/1804	0.93	4/2427 (0.2%)
1	D	0.78	0/1795	0.94	5/2414 (0.2%)
All	All	0.79	0/7185	0.92	18/9668 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	GLN	CB-CA-C	-8.37	93.65	110.40
1	C	287	LEU	N-CA-CB	7.78	125.96	110.40
1	A	367	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	319	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	367	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	C	287	LEU	N-CA-C	-5.82	95.29	111.00
1	D	1	ALA	N-CA-C	5.76	126.54	111.00
1	C	286	GLN	CB-CA-C	-5.65	99.10	110.40
1	D	437	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	337	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	337	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	402	ASP	CB-CG-OD2	-5.24	113.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	286	GLN	N-CA-C	5.20	125.03	111.00
1	B	288	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	473	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	319	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	D	430	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	337	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1	ALA	Peptide

## 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	1747	0	1731	25	0
1	B	1771	0	1746	22	0
1	C	1770	0	1751	29	0
1	D	1761	0	1750	33	0
2	A	34	0	16	0	0
2	B	34	0	16	3	0
2	C	34	0	16	1	0
2	D	34	0	16	7	0
3	A	29	0	0	0	0
3	B	24	0	0	0	0
3	C	28	0	0	1	0
3	D	27	0	0	0	0
All	All	7293	0	7042	109	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 8.

All (109) 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:C:286:GLN:HG3	1:C:330:TYR:CD2	2.09	0.88
1:D:324:LEU:HD11	1:D:358:MET:CE	2.17	0.74
1:D:324:LEU:HD11	1:D:358:MET:HE1	1.68	0.74
1:A:412:PHE:HE2	1:A:466:LEU:HD21	1.55	0.70
1:B:286:GLN:O	1:B:286:GLN:HG2	1.93	0.67
1:C:283:GLU:OE1	1:C:337:ARG:NH1	2.28	0.66
1:C:480:VAL:O	1:C:482:ARG:N	2.29	0.65
1:B:298:ASN:O	1:B:381:LYS:HB3	1.99	0.63
2:D:501:4P3:O1	2:D:501:4P3:H13	1.99	0.63
1:B:286:GLN:O	1:B:287:LEU:HG	2.00	0.62
1:B:324:LEU:HD22	2:B:501:4P3:CL1	2.35	0.62
1:A:412:PHE:HE2	1:A:466:LEU:CD2	2.13	0.62
1:A:412:PHE:CE1	1:A:416:GLU:HB3	2.35	0.61
1:A:287:LEU:O	1:A:367:ARG:NH2	2.32	0.61
1:A:286:GLN:HG3	1:A:330:TYR:CE2	2.36	0.61
1:C:392:GLY:O	1:D:456:LYS:HE2	2.01	0.60
1:A:481:GLU:HG2	1:A:481:GLU:O	2.01	0.59
1:C:277:VAL:HG22	1:C:338:LEU:CD2	2.34	0.57
1:D:454:LEU:CD1	1:D:463:LEU:HD21	2.33	0.57
1:C:296:ARG:NH2	3:C:601:HOH:O	2.23	0.57
1:D:291:ASP:O	1:D:292:LEU:C	2.43	0.57
1:B:320:CYS:SG	2:B:501:4P3:H12	2.45	0.56
1:D:454:LEU:HD21	1:D:462:ILE:HD11	1.87	0.55
1:C:426:ILE:HG21	1:C:442:LEU:HG	1.90	0.54
1:C:393:CYS:SG	2:C:501:4P3:H15	2.47	0.54
1:A:286:GLN:HB2	1:A:330:TYR:CD2	2.43	0.54
1:B:283:GLU:OE1	1:B:337:ARG:NH1	2.41	0.53
1:A:407:LEU:HD21	1:A:467:PRO:HG3	1.90	0.53
1:C:406:SER:O	1:C:409:ALA:HB3	2.08	0.53
1:C:396:LEU:O	1:C:397:ILE:C	2.44	0.53
1:D:411:HIS:O	1:D:459:ARG:NH2	2.42	0.53
1:D:360:VAL:HG13	1:D:421:THR:CG2	2.39	0.53
1:A:444:TYR:CE1	1:A:448:LEU:HD21	2.44	0.52
1:C:324:LEU:HD11	1:C:358:MET:HE1	1.91	0.52
1:C:343:GLU:OE1	1:C:343:GLU:N	2.41	0.52
1:C:392:GLY:O	1:D:456:LYS:CE	2.58	0.52
1:A:459:ARG:O	1:A:461:SER:N	2.42	0.52
1:D:270:ILE:HD13	1:D:448:LEU:HG	1.90	0.52
1:D:324:LEU:HD11	1:D:358:MET:HE3	1.92	0.52
1:D:417:ILE:O	1:D:421:THR:OG1	2.21	0.52
1:B:478:GLN:O	1:B:481:GLU:CB	2.59	0.51
1:C:308:TYR:OH	1:C:379:GLU:OE1	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:GLU:O	1:B:483:LEU:N	2.44	0.51
1:A:345:CYS:O	1:A:349:GLN:HG3	2.10	0.51
1:B:335:ALA:O	1:B:338:LEU:HB2	2.11	0.51
1:B:286:GLN:O	1:B:286:GLN:CG	2.57	0.50
1:D:328:ILE:O	1:D:332:VAL:HG23	2.11	0.50
1:B:403:PHE:CZ	1:B:472:LEU:HD13	2.46	0.50
1:C:389:ARG:O	1:C:390:ALA:C	2.50	0.50
1:D:396:LEU:HG	2:D:501:4P3:H16	1.93	0.49
1:C:286:GLN:HG3	1:C:330:TYR:CE2	2.47	0.49
1:D:347:ASN:O	1:D:351:VAL:HG23	2.13	0.49
1:D:359:GLU:HB3	1:D:472:LEU:HD21	1.94	0.48
1:A:412:PHE:CE2	1:A:466:LEU:HD21	2.40	0.48
1:C:412:PHE:HE1	1:C:462:ILE:HD12	1.79	0.48
1:D:410:LEU:HD12	1:D:412:PHE:CE1	2.48	0.47
1:B:291:ASP:OD1	1:B:294:ARG:NH2	2.46	0.47
1:A:459:ARG:O	1:A:460:GLN:C	2.51	0.47
1:D:370:ASN:OD1	1:D:372:ASP:N	2.47	0.47
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.74	0.47
1:C:278:CYS:SG	1:C:415:ASP:HB3	2.54	0.47
1:B:320:CYS:O	1:B:324:LEU:HB2	2.14	0.47
1:C:362:LEU:HD21	1:C:479:HIS:ND1	2.30	0.47
1:A:300:PHE:CZ	1:A:381:LYS:HB2	2.50	0.46
1:C:296:ARG:HD3	1:C:370:ASN:ND2	2.30	0.46
1:B:358:MET:HE3	1:B:361:VAL:CG1	2.46	0.46
1:C:462:ILE:O	1:C:465:LYS:N	2.47	0.45
1:D:291:ASP:O	1:D:294:ARG:N	2.50	0.45
1:C:376:VAL:O	1:C:382:TYR:HA	2.15	0.45
1:C:394:SER:O	1:C:395:GLU:C	2.52	0.45
1:A:426:ILE:HG21	1:A:442:LEU:HG	1.98	0.45
1:D:400:ILE:HD12	2:D:501:4P3:F	2.06	0.45
1:B:377:PHE:O	1:B:378:PHE:HB2	2.15	0.45
1:D:385:MET:SD	1:D:398:SER:HA	2.57	0.45
1:A:412:PHE:HE1	1:A:416:GLU:C	2.20	0.45
1:A:274:VAL:CG2	1:A:449:ALA:HB1	2.46	0.44
1:B:479:HIS:C	1:B:481:GLU:N	2.70	0.44
1:D:396:LEU:HD23	2:D:501:4P3:H15	1.98	0.44
1:D:476:CYS:O	1:D:480:VAL:HG23	2.18	0.44
1:D:454:LEU:CD2	1:D:462:ILE:HD11	2.48	0.43
1:A:274:VAL:HG22	1:A:449:ALA:HB1	2.00	0.43
1:C:362:LEU:HD21	1:C:479:HIS:CE1	2.53	0.43
1:C:482:ARG:O	1:C:483:LEU:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:GLY:HA3	1:D:425:LEU:HD23	1.99	0.43
1:D:388:PHE:CZ	2:D:501:4P3:H7	2.54	0.43
1:A:368:ALA:HB1	1:A:377:PHE:HB3	2.01	0.42
1:A:393:CYS:O	1:A:397:ILE:HG12	2.18	0.42
1:C:277:VAL:HG22	1:C:338:LEU:HD23	2.01	0.42
1:D:370:ASN:OD1	1:D:370:ASN:C	2.57	0.42
1:D:426:ILE:HG22	1:D:443:GLN:HB2	2.02	0.42
1:B:367:ARG:NE	1:B:414:GLU:OE2	2.52	0.42
1:D:284:THR:HG21	1:D:334:PHE:N	2.35	0.42
1:A:412:PHE:CD1	1:A:417:ILE:HG13	2.55	0.42
1:B:420:TYR:CE1	1:B:466:LEU:HD13	2.56	0.41
1:D:267:LEU:HD12	1:D:267:LEU:HA	1.93	0.41
1:D:319:ARG:NH1	1:D:379:GLU:OE2	2.53	0.41
1:A:268:THR:O	1:A:272:HIS:HB2	2.21	0.41
1:C:437:ARG:NH1	1:C:440:GLU:HB2	2.35	0.41
1:D:396:LEU:HD23	2:D:501:4P3:C11	2.51	0.41
1:B:324:LEU:HD11	1:B:358:MET:HE1	2.02	0.41
1:B:412:PHE:CD2	1:B:417:ILE:HG13	2.56	0.41
1:A:286:GLN:CG	1:A:330:TYR:CE2	3.04	0.41
1:B:400:ILE:HG21	2:B:501:4P3:F1	2.10	0.41
1:D:454:LEU:HD12	1:D:463:LEU:HD21	2.01	0.41
2:D:501:4P3:C3	2:D:501:4P3:CL	3.06	0.40
1:C:348:ASP:O	1:C:349:GLN:C	2.60	0.40
1:C:319:ARG:NH1	1:C:379:GLU:OE2	2.54	0.40
1:A:362:LEU:O	1:A:365:MET:HB2	2.22	0.40
1:B:479:HIS:C	1:B:481:GLU:H	2.24	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	215/225 (96%)	202 (94%)	12 (6%)	1 (0%)	29	54
1	B	218/225 (97%)	186 (85%)	30 (14%)	2 (1%)	17	40
1	C	218/225 (97%)	199 (91%)	17 (8%)	2 (1%)	17	40
1	D	217/225 (96%)	197 (91%)	20 (9%)	0	100	100
All	All	868/900 (96%)	784 (90%)	79 (9%)	5 (1%)	25	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	ARG
1	C	469	LYS
1	A	460	GLN
1	B	297	SER
1	C	460	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	189/200 (94%)	185 (98%)	4 (2%)	53	80
1	B	190/200 (95%)	189 (100%)	1 (0%)	88	96
1	C	191/200 (96%)	187 (98%)	4 (2%)	53	80
1	D	191/200 (96%)	189 (99%)	2 (1%)	76	91
All	All	761/800 (95%)	750 (99%)	11 (1%)	67	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	386	GLU
1	A	394	SER
1	A	412	PHE
1	A	442	LEU
1	B	442	LEU
1	C	297	SER

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Mol	Chain	Res	Type
1	C	318	GLU
1	C	324	LEU
1	C	412	PHE
1	D	412	PHE
1	D	421	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	ASN
1	A	453	HIS
1	C	441	GLN
1	D	453	HIS

### 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](#)

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	4P3	C	501	-	36,36,36	1.91	6 (16%)	52,53,53	2.00	13 (25%)
2	4P3	D	501	-	36,36,36	1.97	8 (22%)	52,53,53	1.65	13 (25%)
2	4P3	A	501	-	36,36,36	2.18	8 (22%)	52,53,53	1.61	13 (25%)
2	4P3	B	501	-	36,36,36	1.94	6 (16%)	52,53,53	1.72	12 (23%)

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	4P3	C	501	-	-	8/26/26/26	0/3/3/3
2	4P3	D	501	-	-	8/26/26/26	0/3/3/3
2	4P3	A	501	-	-	7/26/26/26	0/3/3/3
2	4P3	B	501	-	-	9/26/26/26	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	4P3	C8-C13	6.73	1.49	1.39
2	A	501	4P3	C8-C9	6.23	1.49	1.39
2	A	501	4P3	C8-C13	5.91	1.48	1.39
2	A	501	4P3	C5-N	-5.52	1.37	1.44
2	B	501	4P3	C8-C13	5.25	1.47	1.39
2	C	501	4P3	C5-C14	5.02	1.48	1.40
2	C	501	4P3	C8-C9	4.73	1.46	1.39
2	B	501	4P3	C5-N	-4.72	1.38	1.44
2	B	501	4P3	C8-C9	4.62	1.46	1.39
2	A	501	4P3	C1-C	4.52	1.48	1.39
2	D	501	4P3	C5-N	-4.41	1.38	1.44
2	B	501	4P3	C1-C	4.40	1.47	1.39
2	D	501	4P3	C8-C13	4.17	1.46	1.39
2	B	501	4P3	C5-C14	4.16	1.47	1.40
2	D	501	4P3	C1-C	3.88	1.46	1.39
2	D	501	4P3	O2-C20	-3.62	1.17	1.24
2	D	501	4P3	C5-C14	3.62	1.46	1.40
2	D	501	4P3	C8-C9	3.42	1.44	1.39
2	B	501	4P3	C-CL	3.25	1.81	1.73
2	A	501	4P3	C5-C14	3.23	1.45	1.40
2	C	501	4P3	C1-C	3.06	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	4P3	C7-N	-2.90	1.30	1.36
2	D	501	4P3	C19-C20	-2.77	1.46	1.50
2	C	501	4P3	C13-CL1	2.29	1.79	1.73
2	A	501	4P3	C-CL	2.24	1.79	1.73
2	D	501	4P3	C4-C5	-2.14	1.36	1.39
2	A	501	4P3	C13-CL1	2.11	1.78	1.73
2	C	501	4P3	C5-N	-2.07	1.41	1.44

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	4P3	C13-C8-C7	7.96	130.72	121.19
2	C	501	4P3	C8-C13-CL1	4.36	125.28	119.59
2	B	501	4P3	C19-C20-N1	4.34	122.95	117.75
2	B	501	4P3	O1-C14-C5	4.20	122.72	116.28
2	C	501	4P3	C1-C-CL	-4.04	114.96	120.75
2	B	501	4P3	C13-C8-C7	3.94	125.90	121.19
2	C	501	4P3	C19-C20-N1	3.71	122.20	117.75
2	D	501	4P3	C21-C19-C18	3.61	123.50	119.24
2	D	501	4P3	C4-C5-N	3.59	123.37	118.74
2	D	501	4P3	C13-C8-C7	3.57	125.46	121.19
2	D	501	4P3	C6-N-C5	-3.51	111.80	116.72
2	A	501	4P3	C8-C13-CL1	3.50	124.17	119.59
2	A	501	4P3	C10-C9-C8	-3.50	117.33	123.58
2	B	501	4P3	C6-N-C7	3.42	125.44	118.71
2	D	501	4P3	C6-N-C7	3.31	125.23	118.71
2	A	501	4P3	O-C7-C8	3.11	125.86	119.43
2	C	501	4P3	C10-C9-C8	-2.96	118.29	123.58
2	C	501	4P3	O2-C20-N1	-2.95	118.39	122.58
2	A	501	4P3	C15-O1-C14	2.90	124.75	117.67
2	A	501	4P3	F-C9-C8	2.89	122.51	118.01
2	D	501	4P3	C19-C20-N1	2.87	121.19	117.75
2	A	501	4P3	F3-C16-C15	-2.82	101.33	111.89
2	B	501	4P3	C17-C2-C1	-2.68	116.17	120.61
2	D	501	4P3	C18-C1-C2	2.62	123.46	118.58
2	C	501	4P3	C22-C-CL	2.60	123.63	118.41
2	B	501	4P3	C4-C5-N	2.60	122.09	118.74
2	B	501	4P3	O2-C20-N1	-2.58	118.91	122.58
2	C	501	4P3	C6-N-C7	2.48	123.60	118.71
2	C	501	4P3	F-C9-C10	2.45	124.06	118.59
2	B	501	4P3	C15-O1-C14	-2.45	111.69	117.67
2	C	501	4P3	C15-O1-C14	2.38	123.47	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	4P3	C6-N-C7	2.32	123.28	118.71
2	B	501	4P3	C2-C1-C	-2.32	119.63	123.53
2	A	501	4P3	F1-C16-F3	2.28	114.81	106.43
2	A	501	4P3	C8-C7-N	-2.26	114.03	117.72
2	C	501	4P3	C4-C5-N	2.24	121.63	118.74
2	D	501	4P3	C2-C1-C	-2.21	119.80	123.53
2	A	501	4P3	C6-N-C5	2.19	119.77	116.72
2	B	501	4P3	O1-C14-C17	-2.18	118.57	123.58
2	D	501	4P3	C15-O1-C14	2.17	122.97	117.67
2	D	501	4P3	C21-C19-C20	-2.16	115.26	121.04
2	A	501	4P3	C3-C2-C17	2.13	121.18	118.16
2	D	501	4P3	C10-C9-C8	-2.10	119.82	123.58
2	C	501	4P3	C3-C2-C17	2.08	121.10	118.16
2	B	501	4P3	C1-C-CL	-2.07	117.78	120.75
2	B	501	4P3	O1-C15-C16	2.07	112.86	108.15
2	C	501	4P3	C12-C13-C8	-2.07	119.11	121.86
2	A	501	4P3	C3-C2-C1	-2.05	117.59	120.91
2	D	501	4P3	C14-C5-N	-2.05	118.02	119.94
2	D	501	4P3	O-C7-N	2.04	124.56	121.47
2	A	501	4P3	C10-C11-C12	2.03	123.13	120.25

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	4P3	O1-C15-C16-F3
2	B	501	4P3	O1-C15-C16-F1
2	B	501	4P3	O-C7-N-C5
2	C	501	4P3	O1-C15-C16-F3
2	C	501	4P3	O1-C15-C16-F1
2	C	501	4P3	C4-C5-N-C6
2	B	501	4P3	O1-C15-C16-F2
2	C	501	4P3	O1-C15-C16-F2
2	B	501	4P3	O-C7-N-C6
2	A	501	4P3	O1-C15-C16-F2
2	C	501	4P3	O-C7-N-C5
2	B	501	4P3	C8-C7-N-C6
2	B	501	4P3	C8-C7-N-C5
2	A	501	4P3	O1-C15-C16-F3
2	D	501	4P3	C18-C19-C20-O2
2	D	501	4P3	C21-C19-C20-O2
2	D	501	4P3	C18-C19-C20-N1

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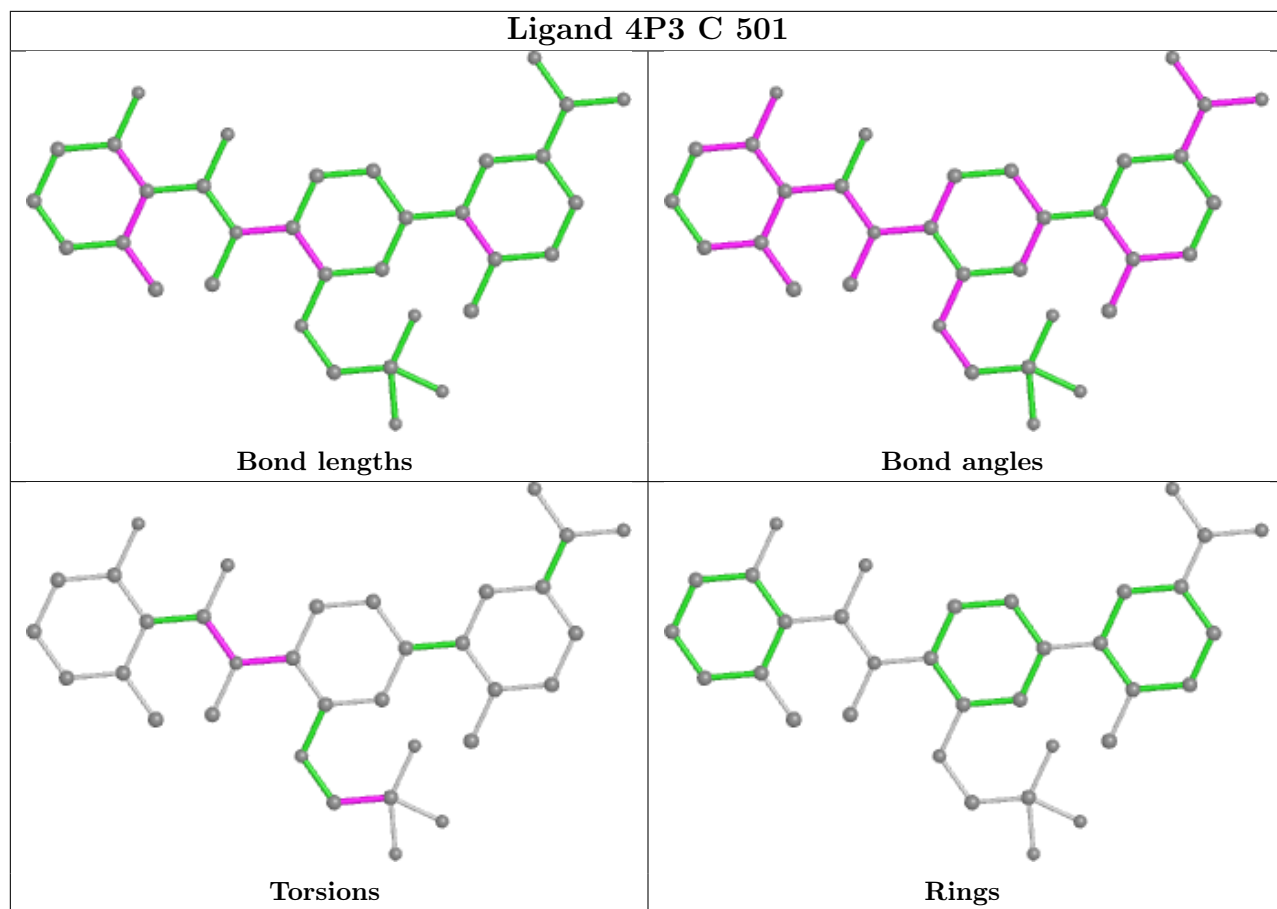
Mol	Chain	Res	Type	Atoms
2	B	501	4P3	C5-C14-O1-C15
2	A	501	4P3	O1-C15-C16-F1
2	D	501	4P3	C21-C19-C20-N1
2	B	501	4P3	C17-C14-O1-C15
2	D	501	4P3	C4-C5-N-C6
2	C	501	4P3	O-C7-N-C6
2	A	501	4P3	O-C7-N-C5
2	A	501	4P3	C8-C7-N-C5
2	C	501	4P3	C8-C7-N-C5
2	A	501	4P3	C4-C5-N-C6
2	D	501	4P3	C8-C7-N-C6
2	A	501	4P3	C14-C5-N-C7
2	C	501	4P3	C14-C5-N-C7
2	D	501	4P3	C14-C5-N-C7
2	D	501	4P3	C14-C5-N-C6

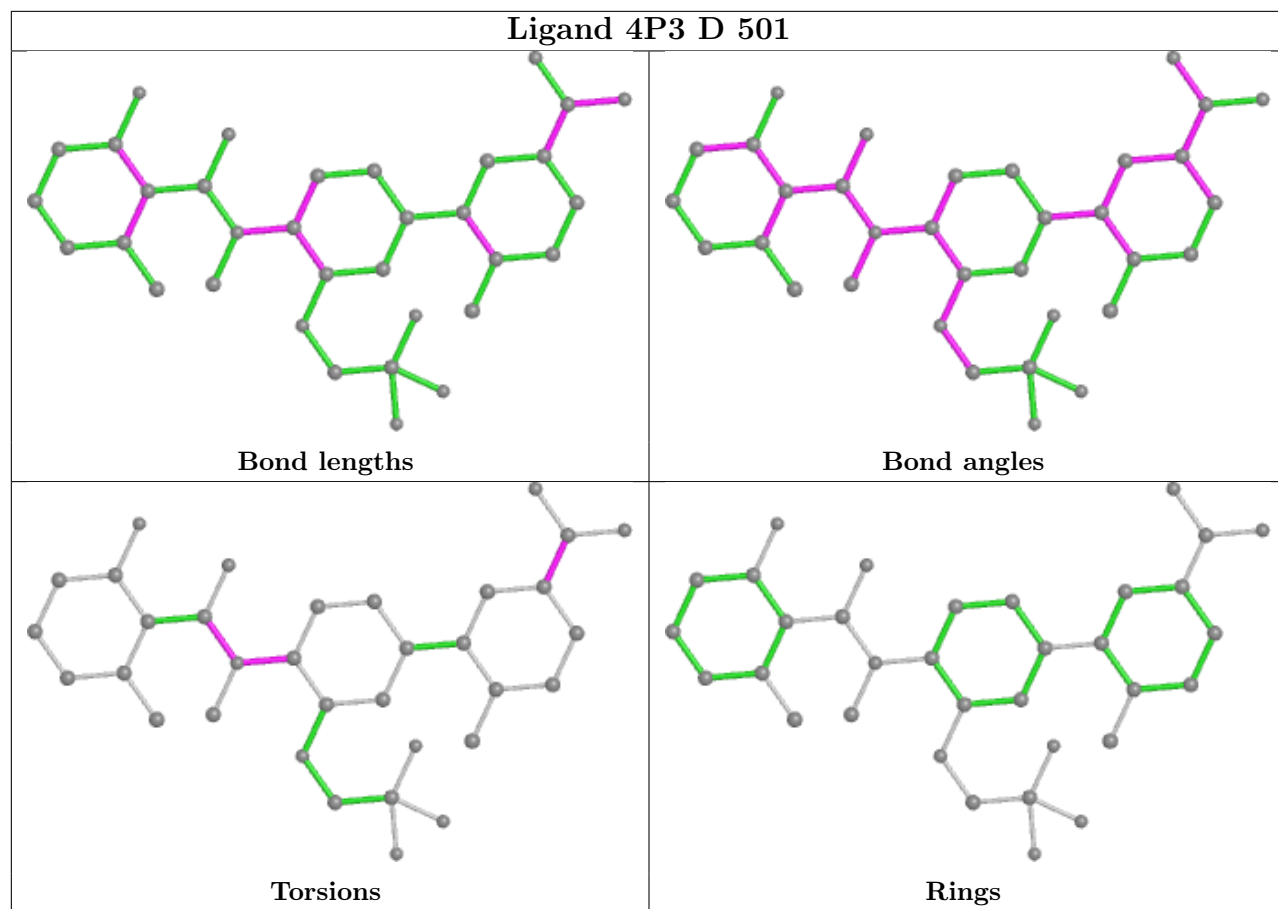
There are no ring outliers.

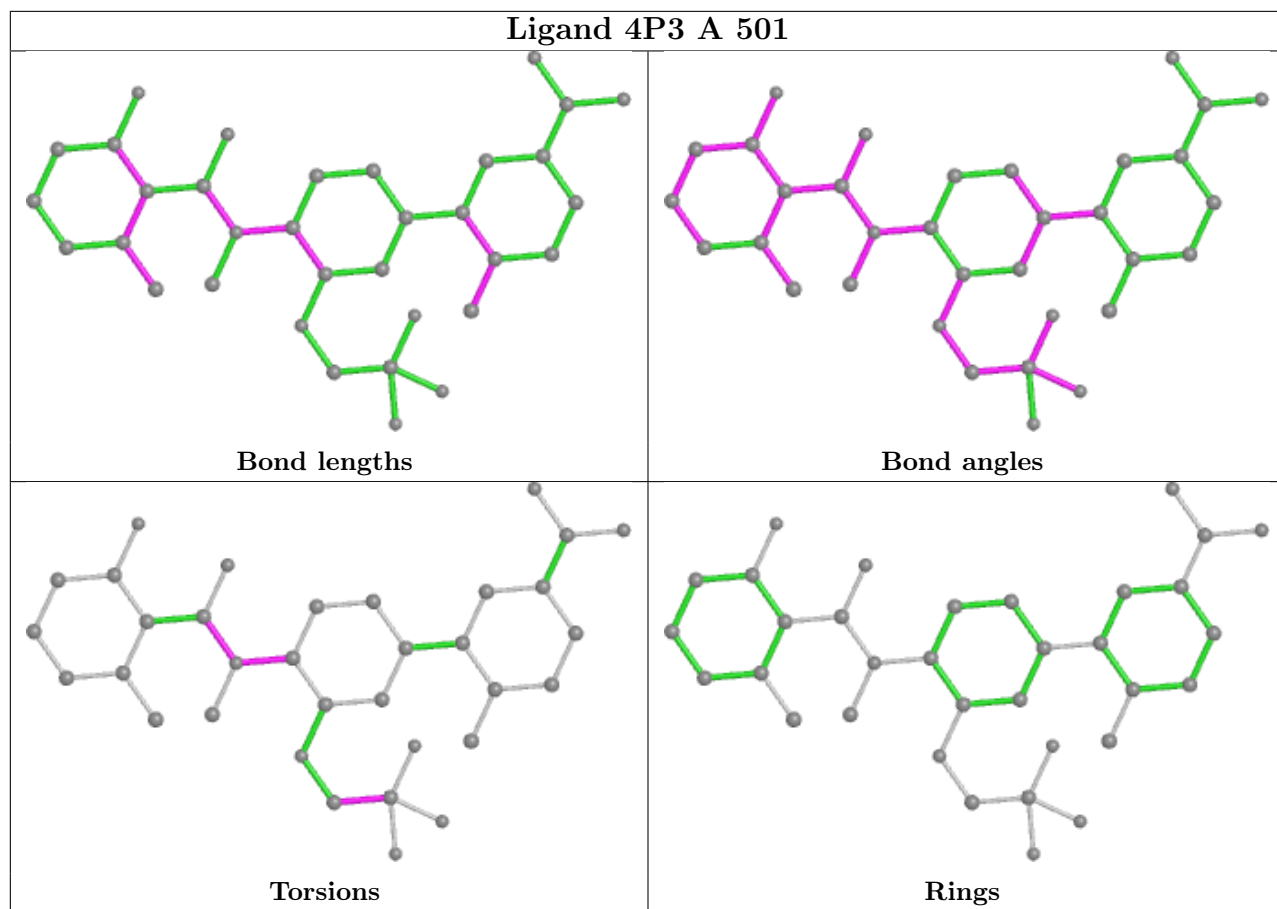
3 monomers are involved in 11 short contacts:

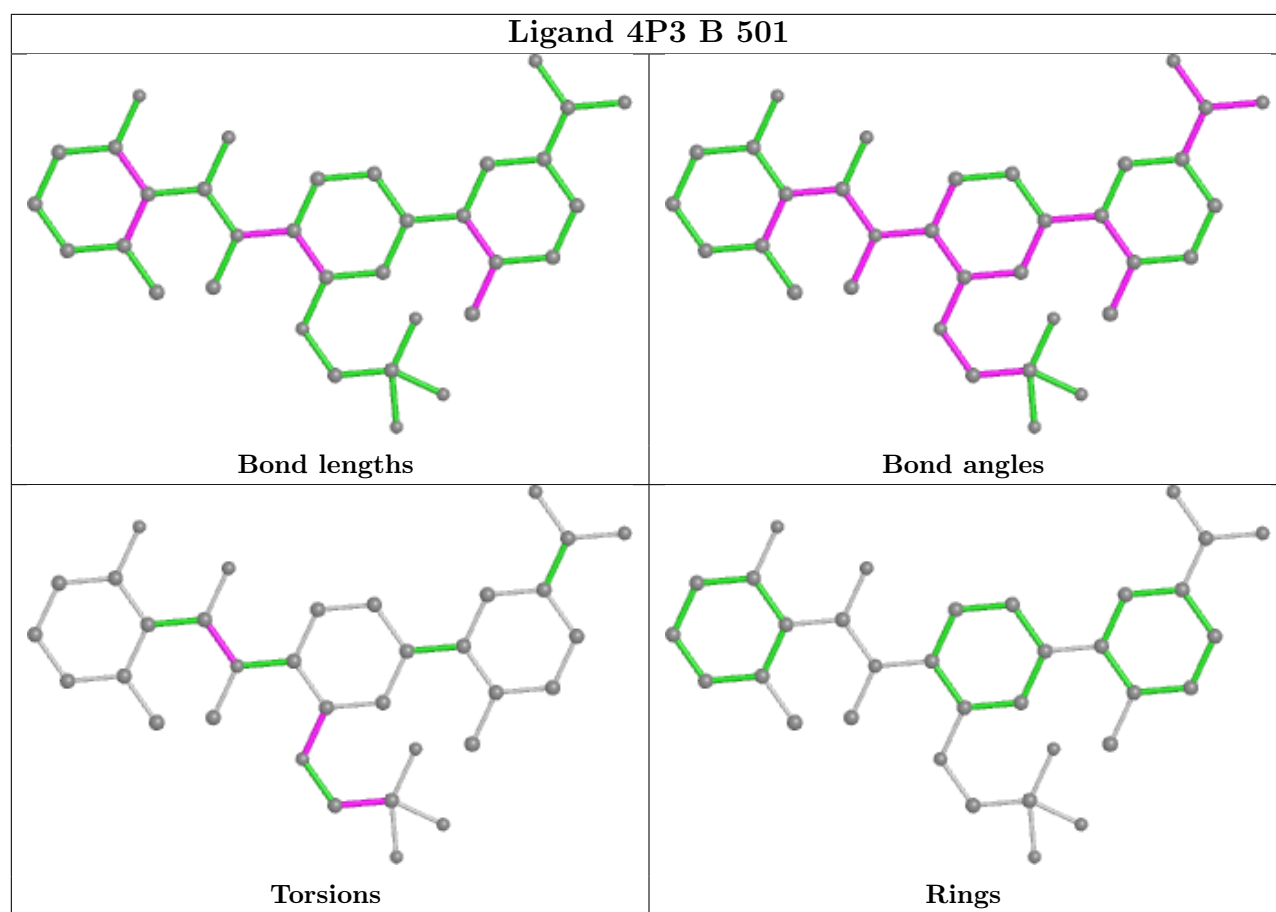
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	4P3	1	0
2	D	501	4P3	7	0
2	B	501	4P3	3	0

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	217/225 (96%)	0.34	4 (1%) 68 70	33, 48, 74, 102	0
1	B	220/225 (97%)	0.36	3 (1%) 75 77	24, 47, 72, 104	0
1	C	220/225 (97%)	0.35	1 (0%) 91 92	28, 49, 77, 99	0
1	D	219/225 (97%)	0.35	1 (0%) 91 92	27, 48, 77, 101	0
All	All	876/900 (97%)	0.35	9 (1%) 82 83	24, 48, 76, 104	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	SER	3.2
1	D	478	GLN	3.1
1	B	374	ARG	2.8
1	A	469	LYS	2.4
1	B	444	TYR	2.3
1	A	468	PRO	2.2
1	C	342	MET	2.1
1	A	412	PHE	2.1
1	A	444	TYR	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](#)

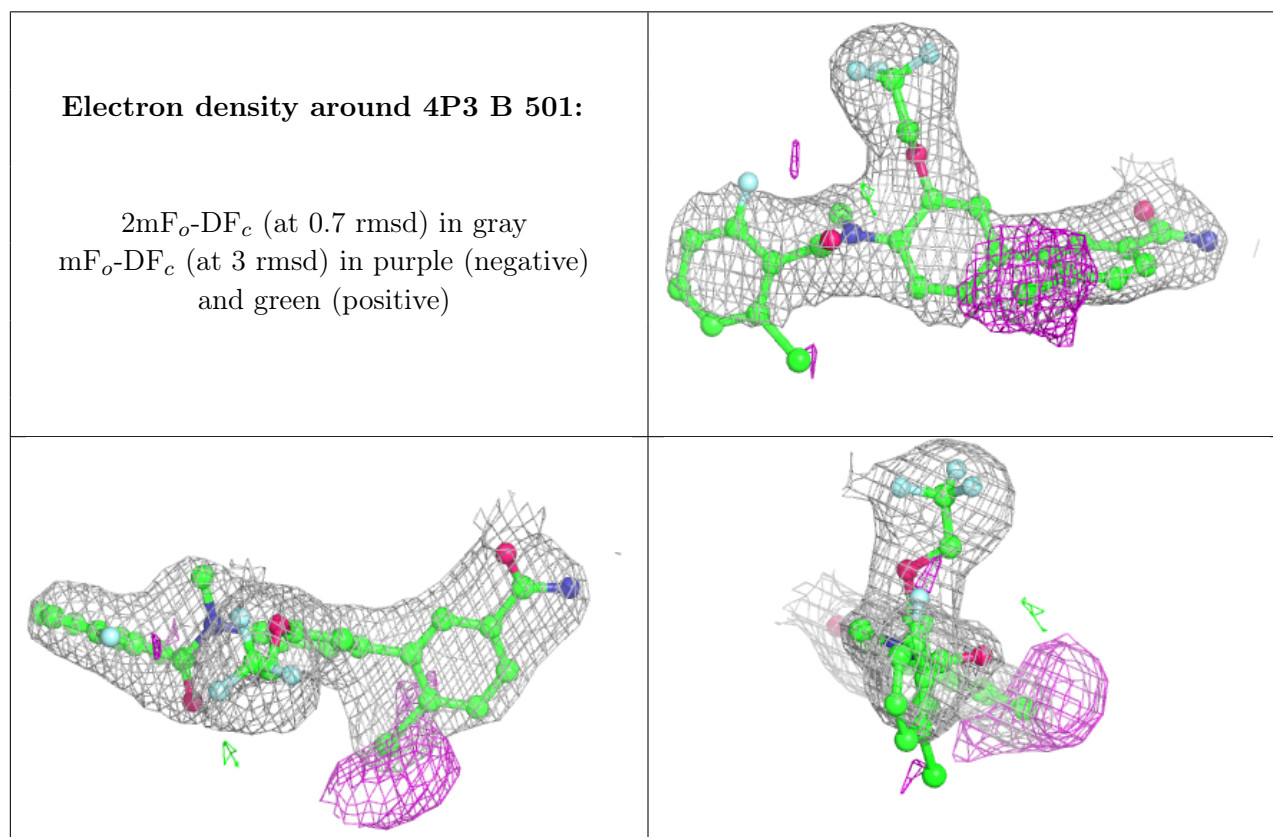
There are no monosaccharides in this entry.

## 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	4P3	B	501	34/34	0.95	0.27	39,49,87,130	0
2	4P3	D	501	34/34	0.96	0.25	37,52,93,134	0
2	4P3	C	501	34/34	0.97	0.27	40,51,70,85	0
2	4P3	A	501	34/34	0.97	0.22	33,43,52,70	0

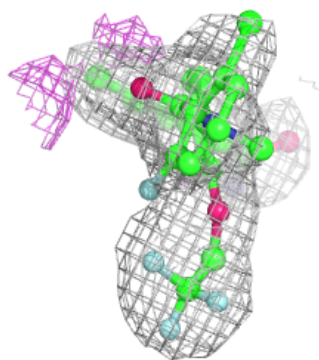
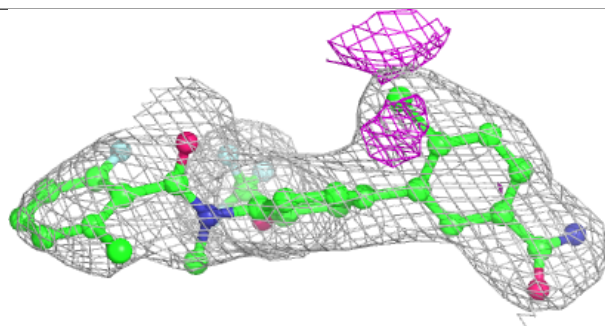
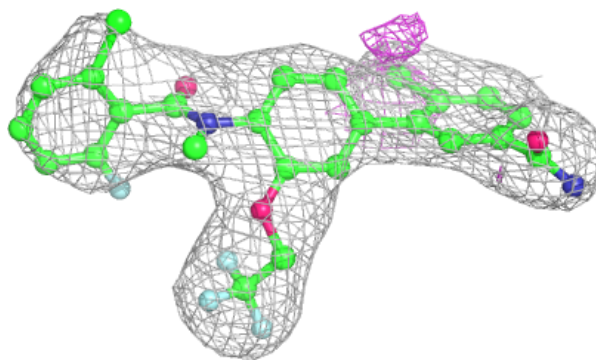
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



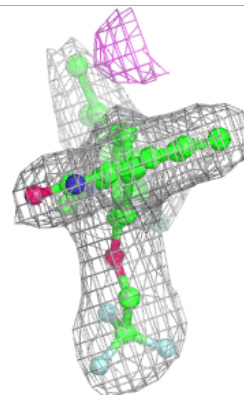
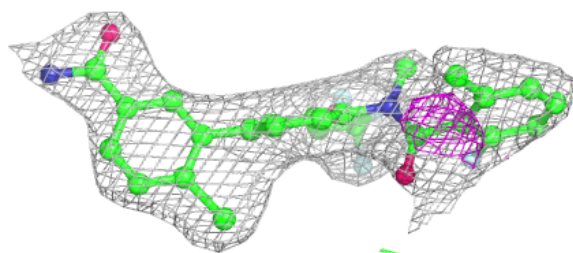
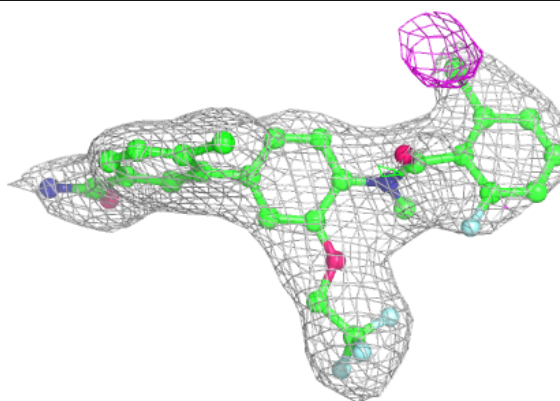


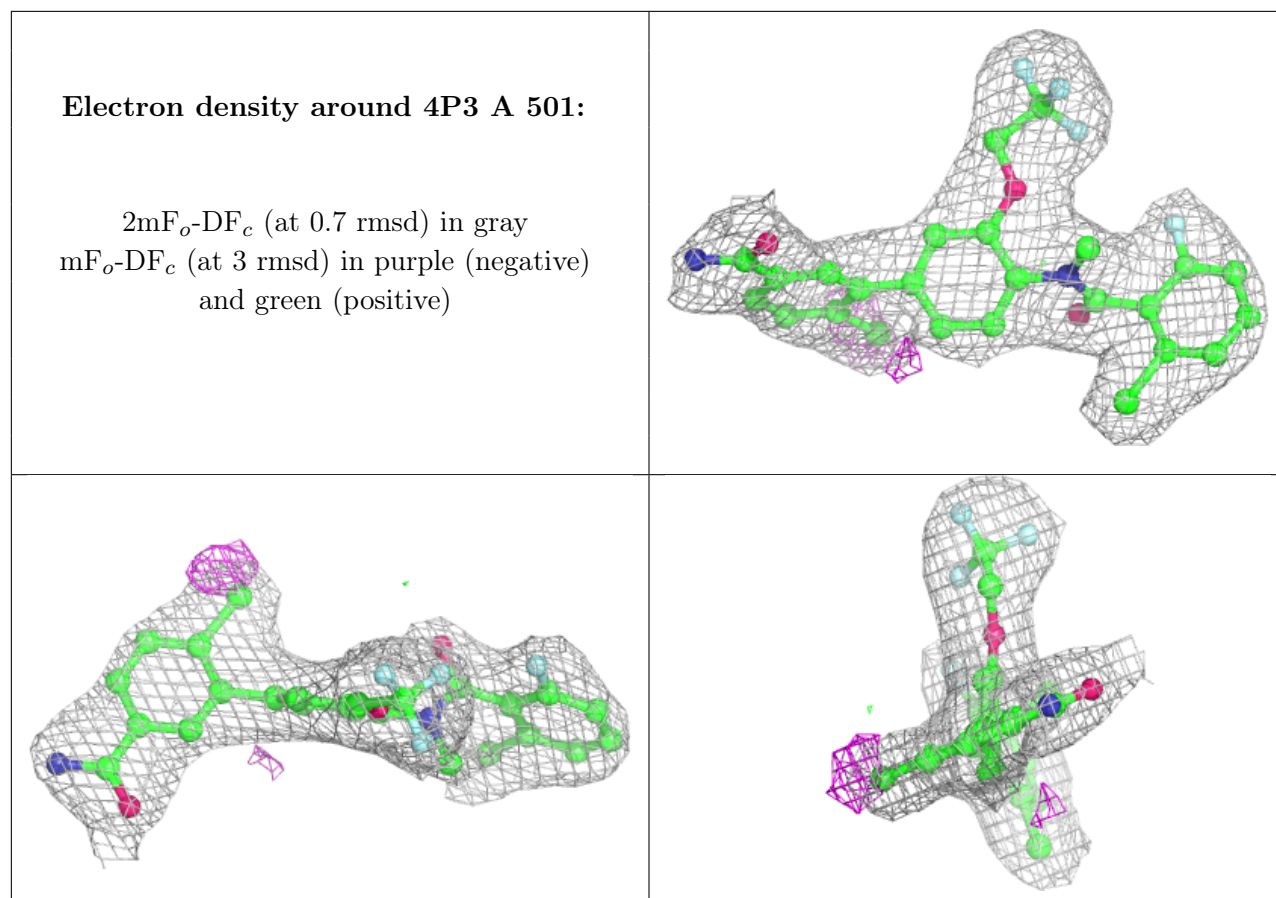
**Electron density around 4P3 D 501:**

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

**Electron density around 4P3 C 501:**

$2mF_o-DF_c$  (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.