



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:19 PM UTC

PDB ID : 4FYG / pdb_00004fyg
Title : Structural basis for substrate recognition by a novel Legionella phosphoinositide phosphatase
Authors : Hsu, F.S.; Zhu, W.; Brennan, L.; Tao, L.; Luo, Z.Q.; Mao, Y.
Deposited on : 2012-07-04
Resolution : 2.82 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

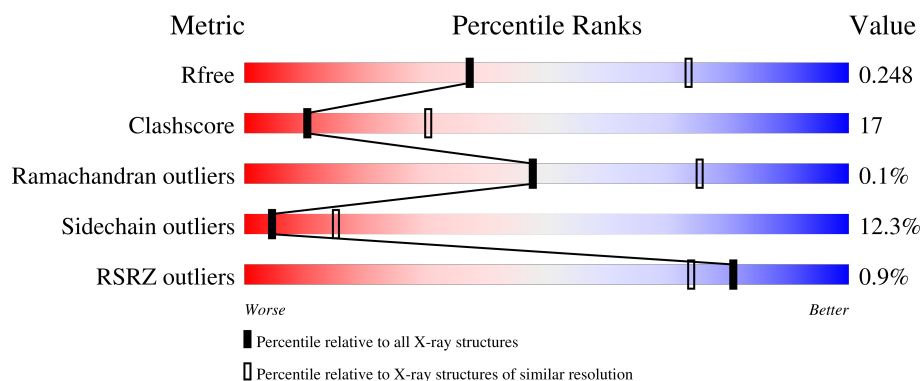
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 ≥ 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	761	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5968 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.

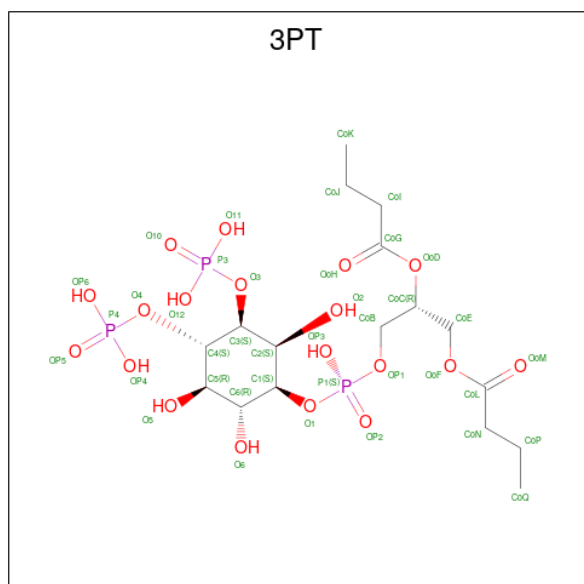
- Molecule 1 is a protein called SidF, inhibitor of growth family, member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	743	5923	3680	1059	1165	19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q5ZSD5
A	645	SER	CYS	engineered mutation	UNP Q5ZSD5

- Molecule 2 is (2R)-3-{[(S)-hydroxy{[(1S,2R,3R,4S,5S,6S)-2,3,6-trihydroxy-4,5-bis(phosphonooxy)cyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl dibutanoate (CCD ID: 3PT) (formula: C₁₇H₃₃O₁₉P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	39	17	19	3	0	0

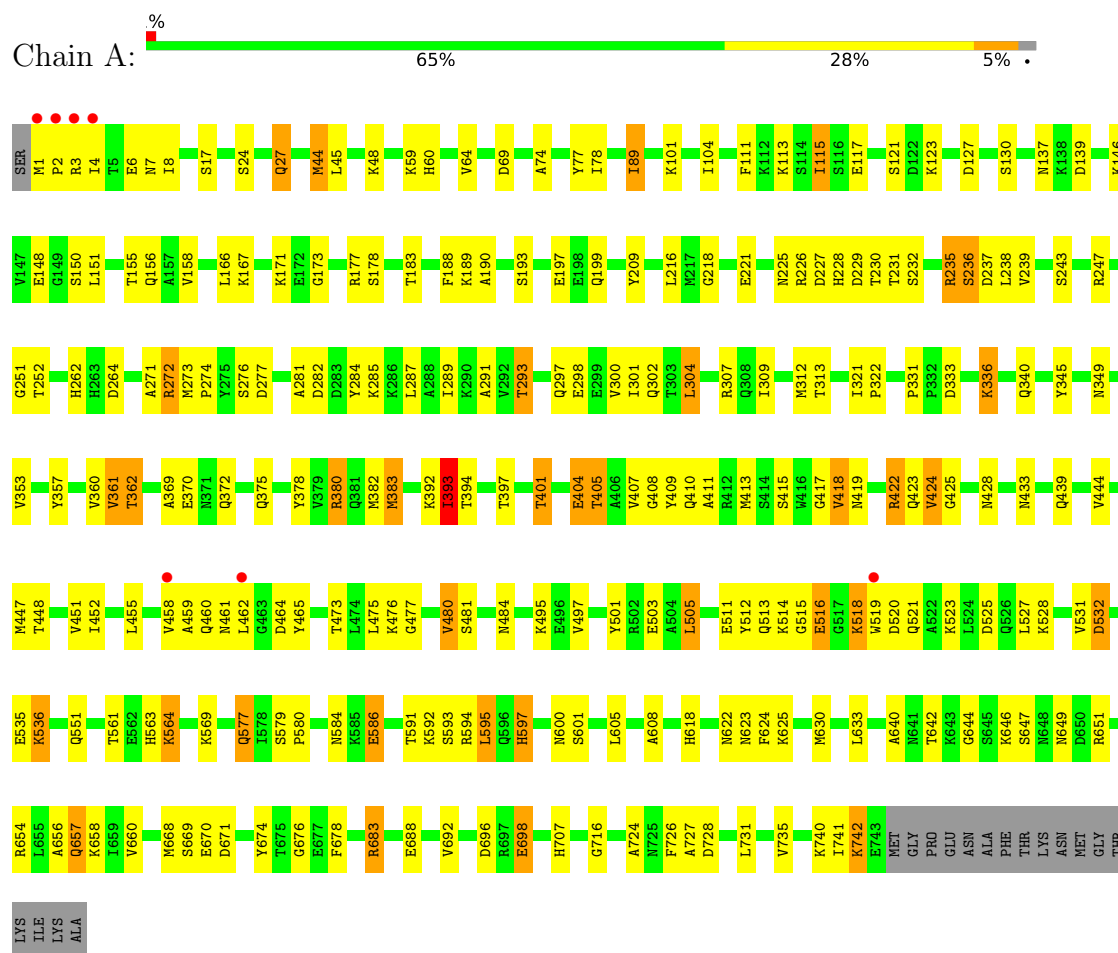
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		

3 Residue-property plots

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: SidF, inhibitor of growth family, member 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.23Å 114.83Å 124.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.58 – 2.82 36.58 – 2.82	Depositor EDS
% Data completeness (in resolution range)	96.0 (36.58-2.82) 96.0 (36.58-2.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.179 , 0.252 (Not available) , 0.248	Depositor DCC
R_{free} test set	1253 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.587	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5968	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 3PT

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	0.93	1/6028 (0.0%)	1.09	15/8122 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	HIS	CG-CD2	5.31	1.41	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	THR	CB-CA-C	-7.49	97.93	109.99
1	A	644	GLY	N-CA-C	6.92	121.12	110.88
1	A	383	MET	N-CA-C	-6.40	104.30	111.28
1	A	649	ASN	N-CA-C	-6.00	107.78	114.62
1	A	393	ILE	N-CA-CB	-5.99	105.24	112.07
1	A	370	GLU	N-CA-C	-5.87	103.81	111.74
1	A	461	ASN	N-CA-C	5.54	118.16	111.40
1	A	623	ASN	CA-C-N	-5.49	113.86	122.65
1	A	623	ASN	C-N-CA	-5.49	113.86	122.65
1	A	495	LYS	N-CA-C	5.36	116.81	111.07
1	A	369	ALA	N-CA-C	-5.19	104.88	111.11
1	A	551	GLN	N-CA-C	-5.19	105.70	111.36
1	A	331	PRO	CA-C-N	5.09	124.88	119.28
1	A	331	PRO	C-N-CA	5.09	124.88	119.28
1	A	726	PHE	N-CA-C	5.04	117.46	109.50

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	5923	0	5809	201	0
2	A	39	0	28	2	0
3	A	6	0	0	1	0
All	All	5968	0	5837	201	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 17.

All (201) 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:516:GLU:HA	1:A:519:TRP:CE3	1.43	1.49
1:A:516:GLU:HB2	1:A:519:TRP:CZ3	1.71	1.25
1:A:516:GLU:HA	1:A:519:TRP:CD2	1.77	1.19
1:A:741:ILE:O	1:A:742:LYS:HD2	1.41	1.17
1:A:516:GLU:CA	1:A:519:TRP:CE3	2.33	1.10
1:A:516:GLU:CB	1:A:519:TRP:CZ3	2.36	1.09
1:A:515:GLY:C	1:A:519:TRP:CE2	2.30	1.09
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.08	1.07
1:A:741:ILE:C	1:A:742:LYS:HD2	1.83	1.04
1:A:422:ARG:NH1	1:A:618:HIS:O	1.90	1.04
1:A:178:SER:HB3	1:A:231:THR:HG23	1.47	0.96
1:A:516:GLU:N	1:A:519:TRP:CE2	2.36	0.94
1:A:515:GLY:CA	1:A:519:TRP:NE1	2.30	0.93
1:A:1:MET:N	1:A:2:PRO:HD2	1.83	0.93
1:A:516:GLU:HA	1:A:519:TRP:CZ3	2.04	0.93
1:A:424:VAL:CG1	1:A:428:ASN:HB3	1.99	0.93
1:A:516:GLU:CA	1:A:519:TRP:CZ3	2.52	0.92
1:A:190:ALA:H	1:A:199:GLN:HE21	1.10	0.91
1:A:515:GLY:C	1:A:519:TRP:NE1	2.30	0.90
1:A:622:ASN:HD22	1:A:625:LYS:HE3	1.39	0.87
1:A:1:MET:H2	1:A:2:PRO:HD2	1.38	0.86
1:A:1:MET:N	1:A:2:PRO:CD	2.37	0.86
1:A:516:GLU:CA	1:A:519:TRP:CD2	2.55	0.85
1:A:424:VAL:HG13	1:A:428:ASN:HB3	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ARG:HH11	1:A:297:GLN:HE22	1.21	0.84
1:A:515:GLY:O	1:A:519:TRP:CD1	2.30	0.84
1:A:740:LYS:NZ	2:A:801:3PT:OP4	2.15	0.79
1:A:236:SER:O	1:A:277:ASP:OD1	2.01	0.78
1:A:515:GLY:O	1:A:519:TRP:CG	2.35	0.78
1:A:516:GLU:N	1:A:519:TRP:CZ2	2.52	0.78
1:A:683:ARG:HH11	1:A:696:ASP:CG	1.92	0.78
1:A:6:GLU:HG3	1:A:7:ASN:N	1.99	0.78
1:A:235:ARG:HB3	1:A:274:PRO:HA	1.66	0.76
1:A:741:ILE:O	1:A:742:LYS:CD	2.30	0.76
1:A:515:GLY:N	1:A:519:TRP:NE1	2.33	0.76
1:A:380:ARG:HG3	1:A:380:ARG:NH1	1.87	0.76
1:A:481:SER:HA	1:A:484:ASN:HB2	1.69	0.76
1:A:528:LYS:O	1:A:532:ASP:OD2	2.05	0.74
1:A:515:GLY:H	1:A:519:TRP:NE1	1.85	0.74
1:A:304:LEU:HB2	1:A:353:VAL:HG21	1.70	0.73
1:A:127:ASP:H	1:A:137:ASN:HD21	1.36	0.72
1:A:362:THR:HG22	1:A:417:GLY:HA3	1.70	0.72
1:A:424:VAL:HG13	1:A:428:ASN:CB	2.19	0.72
1:A:515:GLY:C	1:A:519:TRP:CD1	2.68	0.72
1:A:516:GLU:CB	1:A:519:TRP:CH2	2.72	0.71
1:A:394:THR:HG22	1:A:404:GLU:HG3	1.72	0.71
1:A:516:GLU:HB2	1:A:519:TRP:HZ3	1.52	0.71
1:A:178:SER:HB3	1:A:231:THR:CG2	2.21	0.70
1:A:515:GLY:H	1:A:519:TRP:HE1	1.38	0.70
1:A:302:GLN:HE21	1:A:394:THR:H	1.37	0.70
1:A:740:LYS:O	1:A:742:LYS:HD3	1.93	0.69
1:A:515:GLY:C	1:A:519:TRP:CD2	2.71	0.69
1:A:190:ALA:H	1:A:199:GLN:NE2	1.89	0.69
1:A:424:VAL:H	1:A:433:ASN:HD21	1.37	0.69
1:A:1:MET:HB3	1:A:225:ASN:HB3	1.75	0.67
1:A:424:VAL:HG11	1:A:428:ASN:HB3	1.74	0.67
1:A:515:GLY:N	1:A:519:TRP:HE1	1.93	0.66
1:A:1:MET:H3	1:A:2:PRO:CD	2.07	0.66
1:A:579:SER:HB3	1:A:580:PRO:CD	2.25	0.66
1:A:683:ARG:NH1	1:A:696:ASP:CG	2.54	0.66
1:A:199:GLN:OE1	1:A:252:THR:HG22	1.95	0.65
1:A:380:ARG:HH11	1:A:380:ARG:CG	1.96	0.65
1:A:462:LEU:HD21	1:A:594:ARG:NH1	2.12	0.65
1:A:515:GLY:CA	1:A:519:TRP:CE2	2.78	0.65
1:A:232:SER:HB2	1:A:647:SER:HB2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:GLY:CA	1:A:519:TRP:HE1	2.11	0.64
1:A:409:TYR:CE2	1:A:411:ALA:HB2	2.32	0.64
1:A:151:LEU:O	1:A:155:THR:HG23	1.98	0.63
1:A:209:TYR:O	1:A:226:ARG:NH1	2.31	0.62
1:A:272:ARG:NH1	1:A:297:GLN:HE22	1.95	0.62
1:A:312:MET:HE1	1:A:345:TYR:CE2	2.34	0.62
1:A:173:GLY:O	1:A:177:ARG:HB2	1.98	0.62
1:A:380:ARG:HB2	1:A:413:MET:SD	2.39	0.61
1:A:418:VAL:HG21	1:A:624:PHE:CE2	2.36	0.61
1:A:654:ARG:HH21	1:A:657:GLN:HE22	1.48	0.61
1:A:372:GLN:HE22	1:A:651:ARG:HH12	1.50	0.59
1:A:584:ASN:ND2	1:A:586:GLU:H	2.00	0.59
1:A:178:SER:CB	1:A:231:THR:HG23	2.27	0.59
1:A:228:HIS:HD2	1:A:230:THR:H	1.49	0.59
1:A:579:SER:HB3	1:A:580:PRO:HD2	1.84	0.59
1:A:372:GLN:NE2	1:A:651:ARG:HH12	2.01	0.59
1:A:1:MET:H3	1:A:2:PRO:HD2	1.67	0.58
1:A:304:LEU:HD13	1:A:640:ALA:HB3	1.85	0.58
1:A:515:GLY:HA2	1:A:519:TRP:NE1	2.19	0.58
1:A:333:ASP:HB3	1:A:336:LYS:HG2	1.85	0.57
1:A:516:GLU:N	1:A:519:TRP:CD2	2.69	0.57
1:A:515:GLY:N	1:A:519:TRP:CD1	2.72	0.56
1:A:251:GLY:HA2	1:A:262:HIS:CD2	2.40	0.56
1:A:282:ASP:OD2	1:A:284:TYR:HB2	2.05	0.56
1:A:216:LEU:C	1:A:218:GLY:H	2.12	0.56
1:A:302:GLN:HG3	1:A:393:ILE:HG23	1.88	0.56
1:A:77:TYR:HE1	1:A:155:THR:CG2	2.19	0.56
1:A:378:TYR:O	1:A:382:MET:HG2	2.05	0.56
1:A:6:GLU:HG3	1:A:7:ASN:H	1.70	0.56
1:A:521:GLN:O	1:A:525:ASP:OD2	2.24	0.56
1:A:264:ASP:OD1	1:A:307:ARG:NH1	2.40	0.55
1:A:237:ASP:C	1:A:237:ASP:OD2	2.48	0.55
1:A:515:GLY:H	1:A:519:TRP:CD1	2.23	0.55
1:A:622:ASN:HD22	1:A:625:LYS:CE	2.16	0.55
1:A:622:ASN:HA	1:A:625:LYS:HE3	1.88	0.55
1:A:113:LYS:O	1:A:117:GLU:HG3	2.07	0.55
1:A:383:MET:HE2	1:A:411:ALA:HB1	1.88	0.55
1:A:77:TYR:OH	1:A:155:THR:HG21	2.08	0.54
1:A:188:PHE:CD2	1:A:698:GLU:HG2	2.42	0.54
1:A:252:THR:HG23	1:A:262:HIS:NE2	2.23	0.54
1:A:448:THR:HG22	1:A:605:LEU:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:TYR:CD1	1:A:512:TYR:O	2.61	0.53
1:A:24:SER:O	1:A:27:GLN:HG3	2.09	0.53
1:A:111:PHE:O	1:A:115:ILE:HG13	2.07	0.53
1:A:654:ARG:NH2	1:A:728:ASP:OD1	2.38	0.53
1:A:678:PHE:O	1:A:683:ARG:NH2	2.42	0.53
1:A:407:VAL:HG12	1:A:408:GLY:O	2.09	0.53
1:A:272:ARG:HA	3:A:905:HOH:O	2.09	0.52
1:A:74:ALA:O	1:A:78:ILE:HG12	2.09	0.52
1:A:397:THR:OG1	1:A:401:THR:HB	2.10	0.51
1:A:422:ARG:HG2	1:A:423:GLN:N	2.26	0.51
1:A:465:TYR:HA	1:A:577:GLN:NE2	2.25	0.51
1:A:362:THR:H	1:A:372:GLN:NE2	2.09	0.51
1:A:656:ALA:O	1:A:660:VAL:HG23	2.11	0.50
1:A:247:ARG:CZ	1:A:307:ARG:HG3	2.41	0.50
1:A:516:GLU:CA	1:A:519:TRP:CH2	2.92	0.50
1:A:696:ASP:HB3	1:A:727:ALA:HB2	1.94	0.50
1:A:527:LEU:O	1:A:531:VAL:HG23	2.12	0.50
1:A:230:THR:O	1:A:243:SER:HA	2.12	0.50
1:A:512:TYR:CD1	1:A:512:TYR:C	2.90	0.50
1:A:273:MET:HE1	1:A:375:GLN:HA	1.94	0.50
1:A:237:ASP:OD2	1:A:237:ASP:O	2.30	0.49
1:A:444:VAL:O	1:A:448:THR:HG23	2.12	0.49
1:A:380:ARG:NH1	1:A:380:ARG:CG	2.63	0.49
1:A:515:GLY:HA2	1:A:519:TRP:CE2	2.48	0.49
1:A:272:ARG:HH11	1:A:297:GLN:NE2	2.02	0.49
1:A:458:VAL:O	1:A:458:VAL:CG1	2.61	0.49
1:A:591:THR:O	1:A:595:LEU:HD22	2.13	0.49
1:A:584:ASN:HD22	1:A:586:GLU:H	1.61	0.48
1:A:597:HIS:O	1:A:601:SER:HB3	2.14	0.48
1:A:127:ASP:N	1:A:137:ASN:HD21	2.08	0.48
1:A:216:LEU:C	1:A:218:GLY:N	2.69	0.48
1:A:669:SER:C	1:A:671:ASP:H	2.20	0.48
1:A:2:PRO:HG2	1:A:45:LEU:HD21	1.94	0.48
1:A:579:SER:CB	1:A:580:PRO:CD	2.91	0.48
1:A:235:ARG:NH1	1:A:271:ALA:O	2.46	0.48
1:A:455:LEU:O	1:A:459:ALA:N	2.44	0.48
1:A:189:LYS:HE2	1:A:193:SER:OG	2.14	0.47
1:A:155:THR:O	1:A:156:GLN:C	2.56	0.47
1:A:304:LEU:CB	1:A:353:VAL:HG21	2.39	0.47
1:A:291:ALA:HB2	1:A:505:LEU:HD22	1.96	0.47
1:A:511:GLU:HA	1:A:514:LYS:HD2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ARG:HG2	1:A:724:ALA:O	2.15	0.47
1:A:2:PRO:HG2	1:A:45:LEU:CD2	2.45	0.47
1:A:447:MET:O	1:A:451:VAL:HG23	2.15	0.46
1:A:646:LYS:NZ	2:A:801:3PT:OP5	2.45	0.46
1:A:229:ASP:O	1:A:230:THR:C	2.58	0.46
1:A:89:ILE:HD11	1:A:101:LYS:HG2	1.98	0.46
1:A:535:GLU:O	1:A:536:LYS:C	2.59	0.46
1:A:289:ILE:O	1:A:293:THR:HG23	2.16	0.46
1:A:321:ILE:O	1:A:322:PRO:C	2.59	0.46
1:A:1:MET:O	1:A:227:ASP:CG	2.58	0.46
1:A:501:TYR:HE1	1:A:531:VAL:HG13	1.81	0.45
1:A:448:THR:O	1:A:452:ILE:HG12	2.17	0.45
1:A:190:ALA:N	1:A:199:GLN:HE21	1.94	0.45
1:A:289:ILE:O	1:A:293:THR:CG2	2.65	0.45
1:A:451:VAL:O	1:A:455:LEU:HG	2.17	0.45
1:A:516:GLU:HB3	1:A:519:TRP:CH2	2.50	0.45
1:A:77:TYR:CE1	1:A:155:THR:CG2	3.00	0.45
1:A:362:THR:HG21	1:A:419:ASN:OD1	2.18	0.45
1:A:104:ILE:HD12	1:A:158:VAL:HG13	1.99	0.44
1:A:287:LEU:HD11	1:A:531:VAL:HG11	1.99	0.44
1:A:304:LEU:HD13	1:A:640:ALA:CB	2.47	0.44
1:A:123:LYS:HG2	1:A:139:ASP:HB3	1.99	0.44
1:A:633:LEU:HA	1:A:633:LEU:HD12	1.72	0.44
1:A:302:GLN:HA	1:A:393:ILE:HG13	1.99	0.44
1:A:592:LYS:HE3	1:A:592:LYS:HB2	1.76	0.44
1:A:291:ALA:HB2	1:A:505:LEU:CD2	2.48	0.43
1:A:674:TYR:CZ	1:A:676:GLY:HA2	2.53	0.43
1:A:563:HIS:O	1:A:564:LYS:C	2.61	0.43
1:A:480:VAL:O	1:A:480:VAL:HG13	2.18	0.43
1:A:475:LEU:C	1:A:477:GLY:N	2.75	0.43
1:A:422:ARG:HG2	1:A:423:GLN:H	1.84	0.43
1:A:44:MET:HE3	1:A:44:MET:HB3	1.78	0.43
1:A:281:ALA:HB1	1:A:285:LYS:HB3	2.01	0.42
1:A:380:ARG:CB	1:A:413:MET:SD	3.07	0.42
1:A:357:TYR:HA	1:A:642:THR:O	2.19	0.42
1:A:237:ASP:O	1:A:237:ASP:CG	2.62	0.42
1:A:707:HIS:CD2	1:A:716:GLY:H	2.37	0.42
1:A:608:ALA:CB	1:A:630:MET:HE2	2.50	0.41
1:A:741:ILE:O	1:A:742:LYS:NZ	2.51	0.41
1:A:668:MET:HE2	1:A:668:MET:HB3	1.90	0.41
1:A:1:MET:H3	1:A:2:PRO:HD3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:VAL:HG22	1:A:372:GLN:HE21	1.86	0.41
1:A:69:ASP:OD1	1:A:69:ASP:C	2.62	0.41
1:A:301:ILE:HG12	1:A:409:TYR:CD1	2.56	0.41
1:A:731:LEU:HD23	1:A:731:LEU:HA	1.93	0.41
1:A:235:ARG:O	1:A:276:SER:HB2	2.20	0.41
1:A:345:TYR:O	1:A:349:ASN:HB2	2.21	0.41
1:A:514:LYS:HB3	1:A:518:LYS:HB2	2.02	0.41
1:A:189:LYS:HE3	1:A:197:GLU:O	2.21	0.41
1:A:424:VAL:HG13	1:A:425:GLY:N	2.36	0.40
1:A:600:ASN:O	1:A:601:SER:C	2.62	0.40
1:A:422:ARG:CG	1:A:423:GLN:N	2.84	0.40
1:A:3:ARG:HD3	1:A:3:ARG:HA	1.82	0.40
1:A:669:SER:C	1:A:671:ASP:N	2.80	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	741/761 (97%)	690 (93%)	50 (7%)	1 (0%)	48 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	LYS

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	640/654 (98%)	561 (88%)	79 (12%)	4 15

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	8	ILE
1	A	17	SER
1	A	27	GLN
1	A	44	MET
1	A	48	LYS
1	A	59	LYS
1	A	64	VAL
1	A	89	ILE
1	A	115	ILE
1	A	121	SER
1	A	130	SER
1	A	146	LYS
1	A	148	GLU
1	A	150	SER
1	A	166	LEU
1	A	167	LYS
1	A	171	LYS
1	A	183	THR
1	A	221	GLU
1	A	235	ARG
1	A	236	SER
1	A	238	LEU
1	A	239	VAL
1	A	272	ARG
1	A	293	THR
1	A	298	GLU
1	A	300	VAL
1	A	304	LEU
1	A	309	ILE
1	A	313	THR
1	A	336	LYS
1	A	340	GLN
1	A	360	VAL
1	A	361	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	362	THR
1	A	380	ARG
1	A	392	LYS
1	A	393	ILE
1	A	401	THR
1	A	404	GLU
1	A	405	THR
1	A	410	GLN
1	A	415	SER
1	A	418	VAL
1	A	422	ARG
1	A	424	VAL
1	A	439	GLN
1	A	460	GLN
1	A	464	ASP
1	A	473	THR
1	A	480	VAL
1	A	497	VAL
1	A	503	GLU
1	A	505	LEU
1	A	513	GLN
1	A	516	GLU
1	A	518	LYS
1	A	520	ASP
1	A	523	LYS
1	A	532	ASP
1	A	536	LYS
1	A	561	THR
1	A	564	LYS
1	A	569	LYS
1	A	577	GLN
1	A	586	GLU
1	A	593	SER
1	A	595	LEU
1	A	597	HIS
1	A	657	GLN
1	A	658	LYS
1	A	670	GLU
1	A	683	ARG
1	A	688	GLU
1	A	692	VAL
1	A	698	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	735	VAL
1	A	742	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	28	HIS
1	A	137	ASN
1	A	175	ASN
1	A	180	ASN
1	A	199	GLN
1	A	228	HIS
1	A	242	ASN
1	A	297	GLN
1	A	302	GLN
1	A	319	ASN
1	A	359	GLN
1	A	365	GLN
1	A	371	ASN
1	A	372	GLN
1	A	375	GLN
1	A	381	GLN
1	A	433	ASN
1	A	454	ASN
1	A	530	GLN
1	A	550	ASN
1	A	584	ASN
1	A	597	HIS
1	A	618	HIS
1	A	619	HIS
1	A	622	ASN
1	A	657	GLN
1	A	691	ASN
1	A	703	GLN
1	A	706	HIS

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	3PT	A	801	-	39,39,39	1.31	2 (5%)	54,57,57	1.67	12 (22%)

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	3PT	A	801	-	-	16/36/60/60	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	3PT	O0D-C0G	5.03	1.48	1.34
2	A	801	3PT	O0F-C0L	4.98	1.47	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	3PT	O0D-C0G-C0I	5.24	122.83	111.48
2	A	801	3PT	C0C-O0D-C0G	3.56	126.31	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	3PT	O0F-C0L-C0N	3.38	122.14	111.83
2	A	801	3PT	O3-P3-O10	-3.04	98.50	109.33
2	A	801	3PT	O0F-C0L-O0M	-2.60	117.12	123.63
2	A	801	3PT	O0D-C0G-O0H	-2.44	117.99	123.70
2	A	801	3PT	O1-C1-C6	-2.41	103.62	108.73
2	A	801	3PT	O5-C5-C4	-2.35	103.91	109.94
2	A	801	3PT	C5-C6-C1	2.35	115.01	109.68
2	A	801	3PT	O5-C5-C6	-2.28	105.01	110.38
2	A	801	3PT	C5-C4-C3	2.25	116.78	111.72
2	A	801	3PT	C0E-O0F-C0L	2.10	124.80	117.12

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	3PT	O0H-C0G-O0D-C0C
2	A	801	3PT	C0B-OP1-P1-OP2
2	A	801	3PT	C0B-OP1-P1-O1
2	A	801	3PT	C1-O1-P1-OP1
2	A	801	3PT	C1-O1-P1-OP2
2	A	801	3PT	C0C-C0E-O0F-C0L
2	A	801	3PT	C0I-C0G-O0D-C0C
2	A	801	3PT	C0N-C0L-O0F-C0E
2	A	801	3PT	O0M-C0L-O0F-C0E
2	A	801	3PT	C0G-C0I-C0J-C0K
2	A	801	3PT	C0L-C0N-C0P-C0Q
2	A	801	3PT	O0D-C0C-C0E-O0F
2	A	801	3PT	C0B-C0C-C0E-O0F
2	A	801	3PT	C0B-OP1-P1-OP3
2	A	801	3PT	C0B-C0C-O0D-C0G
2	A	801	3PT	C4-O4-P4-OP5

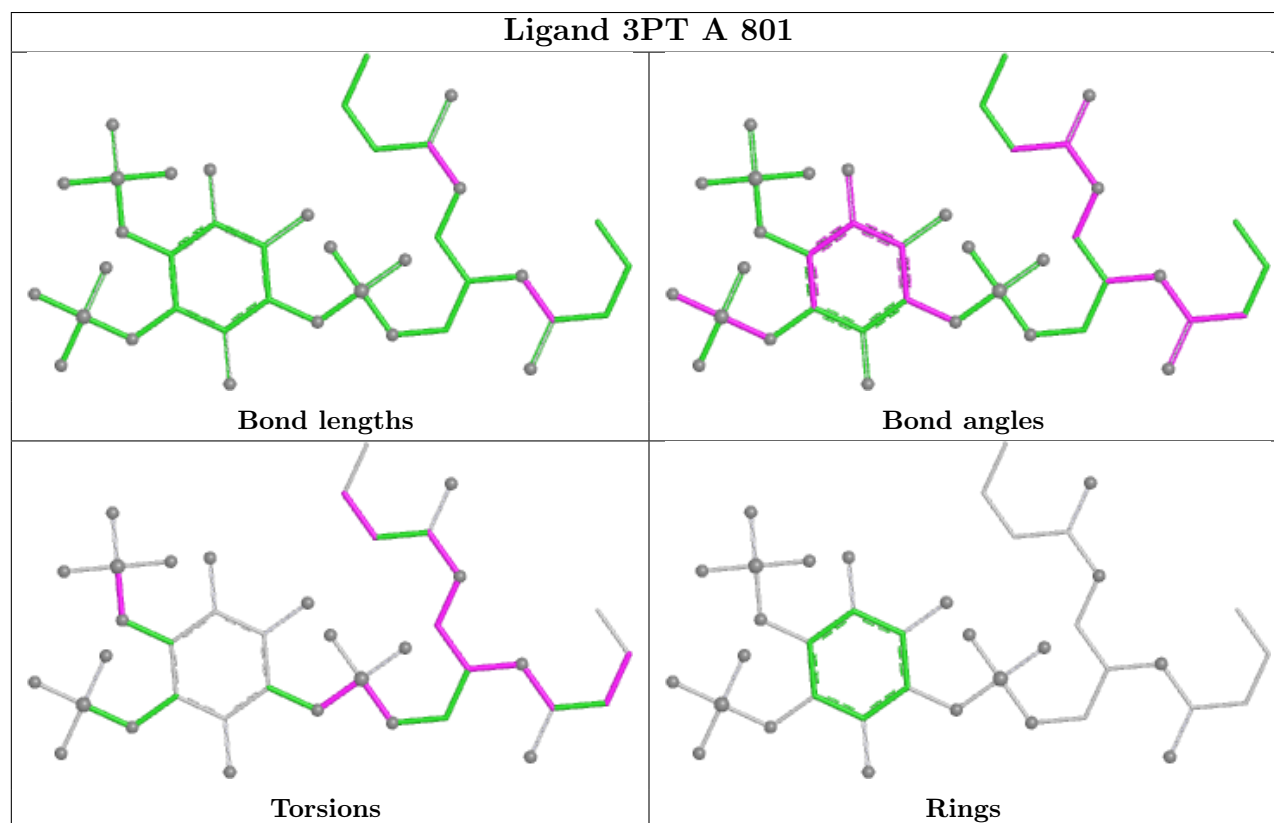
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	3PT	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, 95th 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 ²)	Q<0.9
1	A	743/761 (97%)	-0.52	7 (0%)	81 74	35, 65, 110, 142	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	PRO	4.3
1	A	462	LEU	4.0
1	A	4	ILE	3.3
1	A	1	MET	2.9
1	A	458	VAL	2.7
1	A	519	TRP	2.3
1	A	3	ARG	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](#)

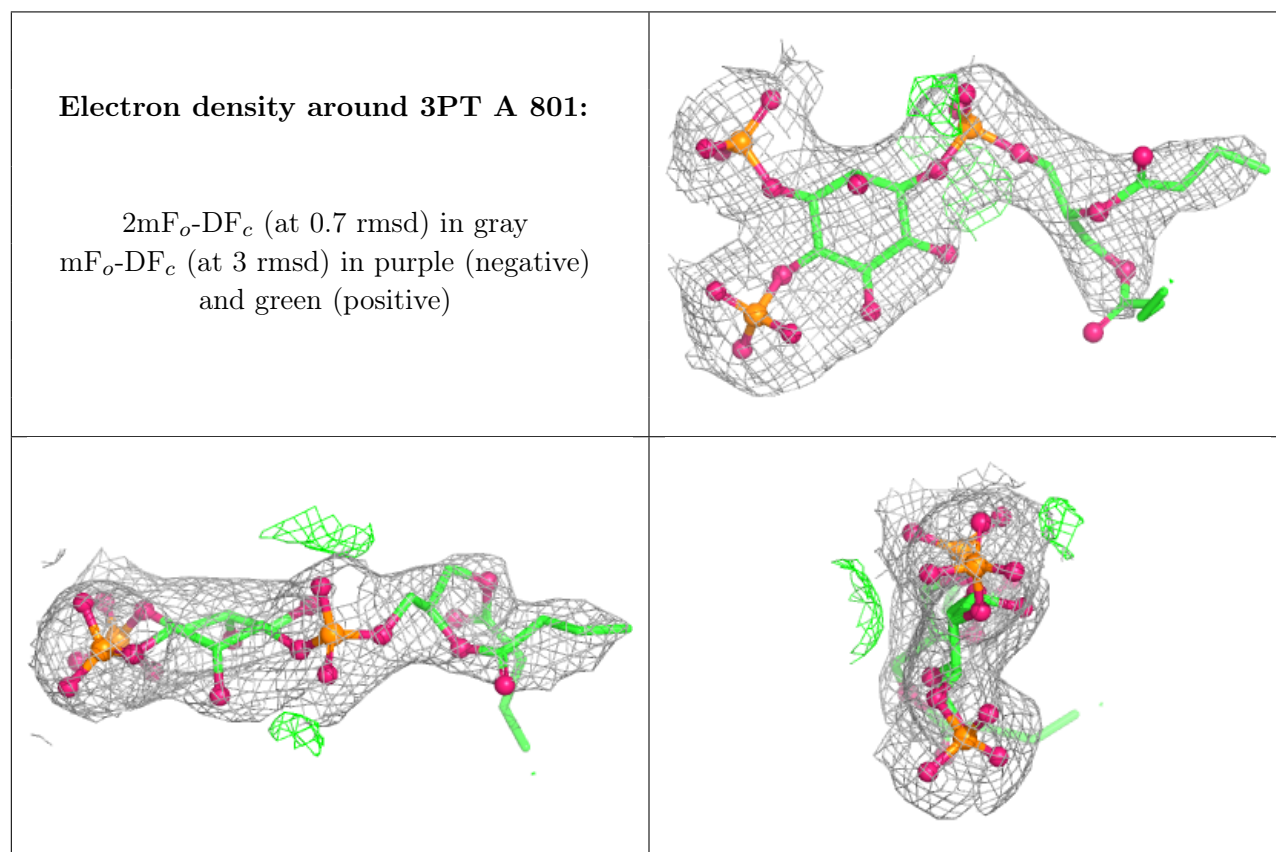
There are no oligosaccharides in this entry.

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, 95th 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 ²)	Q<0.9
2	3PT	A	801	39/39	0.97	0.08	51,68,113,123	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.