



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 04:53 PM EDT

PDB ID : 1ZVR
Title : Crystal Structure of MTMR2 in complex with phosphatidylinositol 3,5-bisphosphate
Authors : Begley, M.J.; Taylor, G.S.; Brock, M.A.; Ghosh, P.; Woods, V.L.; Dixon, J.E.
Deposited on : 2005-06-02
Resolution : 1.98 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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

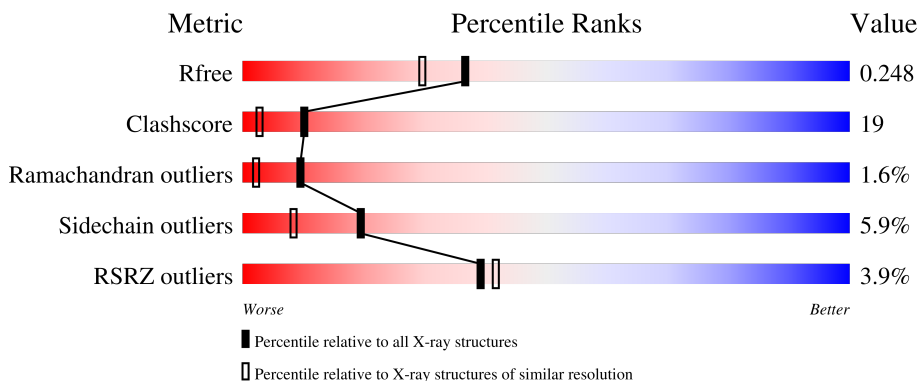
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	528	 4% 58% 33% 6% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4646 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 Myotubularin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	514	4197	2684	730	765	18	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

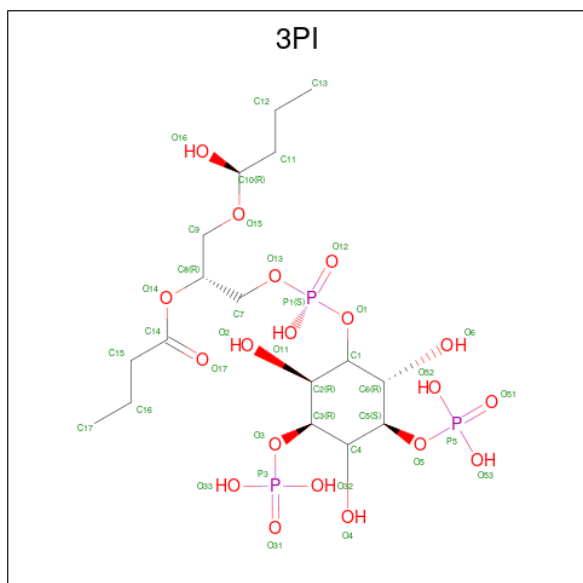
Chain	Residue	Modelled	Actual	Comment	Reference
A	70	MET	-	cloning artifact	UNP Q13614
A	71	ALA	-	cloning artifact	UNP Q13614
A	72	SER	-	cloning artifact	UNP Q13614
A	417	SER	CYS	engineered mutation	UNP Q13614
A	587	ALA	-	cloning artifact	UNP Q13614
A	588	ALA	-	cloning artifact	UNP Q13614
A	589	ALA	-	cloning artifact	UNP Q13614
A	590	LEU	-	cloning artifact	UNP Q13614
A	591	GLU	-	cloning artifact	UNP Q13614
A	592	HIS	-	expression tag	UNP Q13614
A	593	HIS	-	expression tag	UNP Q13614
A	594	HIS	-	expression tag	UNP Q13614
A	595	HIS	-	expression tag	UNP Q13614
A	596	HIS	-	expression tag	UNP Q13614
A	597	HIS	-	expression tag	UNP Q13614

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is (1S)-2-(1-HYDROXYBUTOXY)-1-[[[(HYDROXY){[(2R,3S,5R,6S)-2,4,6-TRI HYDROXY-3,5-BIS(PHOSPHONOXY)CYCLOHEXYL]OXY}PHOSPHORYL)OXY]M ETHYL}ETHYL BUTYRATE (three-letter code: 3PI) (formula: C₁₇H₃₅O₁₉P₃).



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

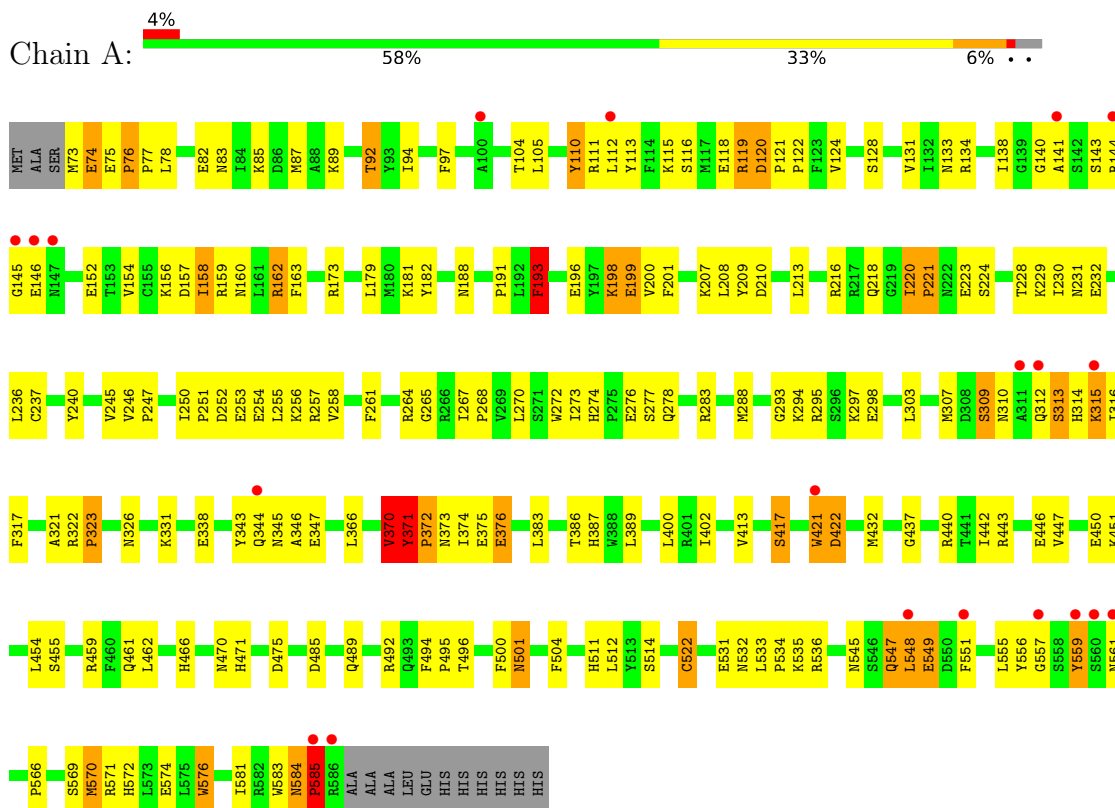
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	398	398	398	0	0

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: Myotubularin-related protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	66.18Å 66.18Å 262.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.98 46.80 – 1.98	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-1.98) 89.1 (46.80-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 1.98Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.252 0.223 , 0.248	Depositor DCC
R_{free} test set	4050 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtrriage
Anisotropy	0.543	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4646	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 3PI, EDO

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	0.75	8/4308 (0.2%)	1.20	40/5839 (0.7%)

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	A	1	13

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	PRO	N-CD	12.86	1.65	1.47
1	A	372	PRO	N-CD	11.32	1.63	1.47
1	A	221	PRO	N-CD	10.46	1.62	1.47
1	A	373	ASN	C-N	-7.31	1.17	1.34
1	A	120	ASP	C-O	6.72	1.36	1.23
1	A	495	PRO	N-CD	5.73	1.55	1.47
1	A	371	TYR	C-O	5.65	1.34	1.23
1	A	75	GLU	C-N	5.17	1.44	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	ASP	CB-CG-OD2	-13.20	106.42	118.30
1	A	121	PRO	CA-N-CD	-11.55	95.33	111.50
1	A	584	ASN	C-N-CD	11.32	152.17	128.40
1	A	75	GLU	C-N-CD	10.98	151.46	128.40
1	A	322	ARG	C-N-CD	10.83	151.14	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ASP	CA-C-N	10.76	147.23	117.10
1	A	76	PRO	C-N-CD	10.55	150.55	128.40
1	A	372	PRO	CA-N-CD	-10.12	97.33	111.50
1	A	121	PRO	C-N-CD	9.89	149.18	128.40
1	A	221	PRO	CA-N-CD	-9.43	98.30	111.50
1	A	371	TYR	CB-CA-C	9.09	128.58	110.40
1	A	157	ASP	CB-CG-OD1	8.70	126.13	118.30
1	A	120	ASP	O-C-N	-8.60	104.75	121.10
1	A	371	TYR	O-C-N	-8.53	104.89	121.10
1	A	121	PRO	N-CA-CB	8.41	113.39	103.30
1	A	585	PRO	CA-N-CD	-8.24	99.97	111.50
1	A	559	TYR	CB-CG-CD1	-8.02	116.19	121.00
1	A	494	PHE	C-N-CD	7.89	144.98	128.40
1	A	371	TYR	CA-C-N	7.37	137.73	117.10
1	A	585	PRO	O-C-N	-7.25	111.10	122.70
1	A	110	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	A	323	PRO	CA-N-CD	-6.91	101.83	111.50
1	A	77	PRO	CA-N-CD	-6.85	101.91	111.50
1	A	422	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	A	76	PRO	CA-N-CD	-6.44	102.49	111.50
1	A	576	TRP	O-C-N	-6.34	112.55	122.70
1	A	370	VAL	CA-CB-CG1	6.33	120.40	110.90
1	A	220	ILE	CA-C-N	6.15	134.32	117.10
1	A	122	PRO	CA-N-CD	-6.04	103.04	111.50
1	A	495	PRO	CA-N-CD	-5.99	103.12	111.50
1	A	371	TYR	CA-CB-CG	5.93	124.67	113.40
1	A	494	PHE	CB-CG-CD2	5.92	124.94	120.80
1	A	120	ASP	CA-C-O	-5.86	107.79	120.10
1	A	372	PRO	N-CA-CB	5.40	109.78	103.30
1	A	193	PHE	CD1-CG-CD2	-5.38	111.30	118.30
1	A	120	ASP	CB-CA-C	5.35	121.10	110.40
1	A	317	PHE	CB-CG-CD1	5.29	124.50	120.80
1	A	121	PRO	O-C-N	5.12	130.83	121.10
1	A	92	THR	O-C-N	-5.07	114.58	122.70
1	A	220	ILE	O-C-N	-5.03	111.55	121.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	371	TYR	CA

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	TYR	Sidechain
1	A	193	PHE	Sidechain
1	A	220	ILE	Mainchain
1	A	314	HIS	Peptide,Mainchain
1	A	370	VAL	Mainchain
1	A	371	TYR	Peptide,Mainchain
1	A	387	HIS	Mainchain
1	A	417	SER	Mainchain
1	A	422	ASP	Sidechain
1	A	522	CYS	Mainchain
1	A	585	PRO	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4197	0	4121	157	5
2	A	12	0	18	1	0
3	A	39	0	27	3	0
4	A	398	0	0	25	3
All	All	4646	0	4166	159	8

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 19.

All (159) 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:559:TYR:CD2	1:A:561:ASN:O	2.08	1.06
1:A:231:ASN:ND2	1:A:237:CYS:H	1.59	1.01
1:A:232:GLU:CB	4:A:1427:HOH:O	2.13	0.96
3:A:3632:3PI:H91	4:A:1250:HOH:O	1.66	0.95
1:A:559:TYR:HD2	1:A:561:ASN:O	1.51	0.93
1:A:231:ASN:HD21	1:A:237:CYS:H	1.18	0.91
1:A:216:ARG:NH1	4:A:1523:HOH:O	2.05	0.87
1:A:310:ASN:O	1:A:313:SER:OG	1.94	0.84
1:A:232:GLU:HB2	4:A:1427:HOH:O	1.71	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD11	1:A:112:LEU:HD11	1.59	0.84
1:A:374:ILE:HD11	1:A:581:ILE:HD13	1.64	0.79
1:A:74:GLU:HG3	1:A:104:THR:HB	1.63	0.78
1:A:274:HIS:HD2	1:A:277:SER:H	1.30	0.78
3:A:3632:3PI:H8	4:A:1465:HOH:O	1.83	0.77
1:A:559:TYR:CE2	1:A:561:ASN:O	2.39	0.76
1:A:198:LYS:HE3	4:A:1463:HOH:O	1.85	0.75
1:A:231:ASN:HD22	1:A:236:LEU:HB3	1.52	0.73
1:A:76:PRO:HB3	1:A:113:TYR:CG	2.24	0.72
1:A:232:GLU:HB3	4:A:1427:HOH:O	1.79	0.72
1:A:570:MET:HE3	1:A:570:MET:HA	1.71	0.71
1:A:216:ARG:HG2	1:A:216:ARG:HH11	1.55	0.70
1:A:496:THR:HG22	1:A:555:LEU:HB3	1.72	0.70
1:A:402:ILE:HG23	1:A:413:VAL:HG21	1.75	0.69
1:A:141:ALA:HA	4:A:1184:HOH:O	1.93	0.68
1:A:370:VAL:HG22	1:A:581:ILE:HD11	1.75	0.68
1:A:274:HIS:CD2	1:A:277:SER:H	2.12	0.68
1:A:251:PRO:HG2	1:A:254:GLU:HB2	1.77	0.67
1:A:570:MET:HA	1:A:570:MET:CE	2.25	0.67
1:A:310:ASN:HB3	4:A:1044:HOH:O	1.94	0.66
1:A:201:PHE:HB2	4:A:1466:HOH:O	1.97	0.65
1:A:208:LEU:HD21	1:A:446:GLU:HB2	1.79	0.65
1:A:74:GLU:HA	1:A:115:LYS:HE2	1.78	0.64
1:A:94:ILE:HD12	1:A:162:ARG:HD2	1.81	0.63
1:A:247:PRO:HB2	1:A:250:ILE:HG12	1.82	0.62
1:A:370:VAL:HG22	1:A:581:ILE:CD1	2.29	0.62
1:A:138:ILE:HD11	1:A:152:GLU:HB2	1.82	0.61
1:A:315:LYS:HG3	1:A:316:ILE:H	1.66	0.60
1:A:338:GLU:HB3	1:A:343:TYR:CD1	2.37	0.60
1:A:105:LEU:HD11	1:A:112:LEU:CD1	2.30	0.59
1:A:138:ILE:HD11	1:A:152:GLU:CB	2.32	0.59
1:A:199:GLU:HG2	1:A:201:PHE:CE1	2.38	0.59
1:A:389:LEU:HB3	1:A:570:MET:HE1	1.84	0.59
1:A:273:ILE:HD11	1:A:278:GLN:HG3	1.85	0.58
1:A:82:GLU:OE2	1:A:111:ARG:HG2	2.03	0.58
1:A:133:ASN:HD21	1:A:156:LYS:HE3	1.69	0.58
1:A:470:ASN:HB3	4:A:1121:HOH:O	2.03	0.57
1:A:532:ASN:OD1	1:A:535:LYS:HB2	2.03	0.57
1:A:115:LYS:HD2	1:A:124:VAL:HG22	1.86	0.57
1:A:116:SER:OG	1:A:118:GLU:HB2	2.04	0.57
1:A:218:GLN:HE22	1:A:272:TRP:HA	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ARG:HG3	1:A:443:ARG:HH21	1.70	0.57
1:A:459:ARG:NH2	3:A:3632:3PI:O51	2.38	0.57
1:A:459:ARG:HD3	4:A:1071:HOH:O	2.05	0.57
1:A:216:ARG:NH1	1:A:216:ARG:HG2	2.20	0.57
1:A:119:ARG:HH21	1:A:119:ARG:HG2	1.69	0.56
1:A:216:ARG:HG2	4:A:1523:HOH:O	2.04	0.56
1:A:231:ASN:ND2	1:A:237:CYS:N	2.42	0.56
1:A:134:ARG:HG2	1:A:471:HIS:CD2	2.40	0.56
1:A:196:GLU:O	1:A:198:LYS:HD2	2.05	0.56
1:A:569:SER:HB3	1:A:572:HIS:HD2	1.71	0.56
1:A:274:HIS:CD2	1:A:276:GLU:H	2.24	0.55
1:A:173:ARG:NH2	4:A:1521:HOH:O	2.39	0.55
1:A:94:ILE:HD12	1:A:162:ARG:CD	2.37	0.55
1:A:531:GLU:O	1:A:536:ARG:HD3	2.06	0.55
1:A:344:GLN:C	1:A:346:ALA:H	2.10	0.55
1:A:569:SER:HB3	1:A:572:HIS:CD2	2.42	0.54
1:A:112:LEU:HD13	1:A:179:LEU:HD21	1.89	0.54
1:A:315:LYS:HD2	1:A:345:ASN:HA	1.90	0.54
1:A:119:ARG:HG2	1:A:119:ARG:NH2	2.23	0.53
1:A:256:LYS:NZ	4:A:1484:HOH:O	2.40	0.53
1:A:556:TYR:CG	1:A:557:GLY:N	2.77	0.53
1:A:74:GLU:HG3	1:A:104:THR:CB	2.34	0.53
1:A:437:GLY:HA2	1:A:440:ARG:NH2	2.24	0.52
1:A:210:ASP:HB3	1:A:213:LEU:HB2	1.92	0.52
1:A:231:ASN:HD21	1:A:237:CYS:N	1.99	0.52
1:A:254:GLU:OE1	4:A:1105:HOH:O	2.19	0.52
1:A:257:ARG:NE	4:A:1477:HOH:O	2.42	0.52
1:A:442:ILE:O	1:A:446:GLU:HG3	2.09	0.52
1:A:140:GLY:O	1:A:143:SER:HB2	2.10	0.52
1:A:307:MET:SD	1:A:345:ASN:HB3	2.50	0.52
1:A:73:MET:N	4:A:1333:HOH:O	2.42	0.51
1:A:446:GLU:OE2	1:A:545:ASN:ND2	2.43	0.51
1:A:443:ARG:NH2	1:A:548:LEU:HD11	2.25	0.51
1:A:119:ARG:HH21	1:A:119:ARG:CG	2.24	0.51
1:A:94:ILE:HB	1:A:162:ARG:HD2	1.93	0.51
1:A:370:VAL:CG2	1:A:581:ILE:HD11	2.40	0.50
1:A:462:LEU:HG	1:A:475:ASP:HB3	1.93	0.50
1:A:228:THR:OG1	1:A:252:ASP:OD1	2.22	0.50
1:A:97:PHE:CD1	1:A:585:PRO:HD3	2.46	0.50
1:A:199:GLU:HG3	1:A:200:VAL:N	2.26	0.50
1:A:74:GLU:HB2	1:A:115:LYS:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ASN:ND2	1:A:236:LEU:HB3	2.26	0.50
1:A:257:ARG:NH2	4:A:1218:HOH:O	2.45	0.50
1:A:82:GLU:HB2	1:A:193:PHE:HZ	1.76	0.49
1:A:181:LYS:HA	1:A:188:ASN:ND2	2.27	0.49
1:A:274:HIS:HD2	1:A:277:SER:N	2.05	0.49
1:A:237:CYS:HB2	1:A:265:GLY:O	2.13	0.48
1:A:245:VAL:HB	1:A:270:LEU:HB3	1.95	0.48
1:A:512:LEU:HD21	2:A:1878:EDO:H11	1.94	0.48
1:A:253:GLU:O	1:A:256:LYS:HB2	2.14	0.48
1:A:442:ILE:HG12	1:A:500:PHE:HB3	1.96	0.48
1:A:443:ARG:HH22	1:A:548:LEU:HD11	1.79	0.48
1:A:584:ASN:ND2	4:A:1487:HOH:O	2.47	0.48
1:A:209:TYR:CD1	1:A:447:VAL:HG13	2.49	0.47
1:A:82:GLU:HB2	1:A:193:PHE:CZ	2.49	0.47
1:A:159:ARG:HD3	1:A:583:TRP:CE2	2.49	0.47
1:A:128:SER:O	1:A:131:VAL:HG22	2.14	0.47
1:A:547:GLN:O	1:A:549:GLU:HG2	2.14	0.47
1:A:501:ASN:O	1:A:504:PHE:HB3	2.15	0.47
1:A:485:ASP:O	1:A:489:GLN:HG2	2.15	0.46
1:A:76:PRO:HB3	1:A:113:TYR:CD2	2.50	0.46
1:A:229:LYS:HG3	4:A:1294:HOH:O	2.16	0.46
1:A:313:SER:HA	4:A:1044:HOH:O	2.16	0.46
1:A:245:VAL:HG11	1:A:270:LEU:HD23	1.97	0.46
1:A:87:MET:CE	1:A:89:LYS:HE3	2.46	0.46
1:A:323:PRO:HD2	1:A:326:ASN:ND2	2.31	0.46
1:A:331:LYS:HE2	4:A:1187:HOH:O	2.15	0.46
1:A:389:LEU:HB3	1:A:570:MET:CE	2.44	0.46
1:A:94:ILE:HD12	1:A:162:ARG:NE	2.31	0.45
1:A:85:LYS:HE3	1:A:182:TYR:CE2	2.50	0.45
1:A:224:SER:HB3	1:A:309:SER:OG	2.16	0.45
1:A:400:LEU:HD11	1:A:566:PRO:O	2.16	0.45
1:A:432:MET:HE3	1:A:451:LYS:HE3	1.98	0.45
1:A:547:GLN:HB2	4:A:1445:HOH:O	2.15	0.45
1:A:92:THR:O	1:A:163:PHE:HA	2.16	0.45
1:A:191:PRO:HG2	1:A:196:GLU:OE1	2.16	0.45
1:A:258:VAL:HG12	1:A:267:ILE:HG22	1.98	0.45
1:A:450:GLU:HA	1:A:454:LEU:HD12	1.99	0.45
1:A:489:GLN:HE22	1:A:574:GLU:H	1.63	0.45
1:A:511:HIS:HA	1:A:514:SER:OG	2.18	0.44
1:A:492:ARG:HA	1:A:492:ARG:HD2	1.82	0.44
1:A:218:GLN:HE21	1:A:273:ILE:HG22	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:VAL:HA	1:A:160:ASN:OD1	2.18	0.43
1:A:198:LYS:HD2	1:A:198:LYS:N	2.34	0.43
1:A:501:ASN:HD21	1:A:551:PHE:HA	1.83	0.43
1:A:533:LEU:N	1:A:534:PRO:CD	2.82	0.42
1:A:321:ALA:HB3	1:A:417:SER:HB3	2.00	0.42
1:A:461:GLN:HA	1:A:466:HIS:CD2	2.54	0.42
1:A:138:ILE:HD11	1:A:152:GLU:HB3	2.00	0.42
1:A:569:SER:CB	1:A:572:HIS:HD2	2.32	0.42
1:A:261:PHE:O	1:A:288:MET:HG2	2.18	0.42
1:A:501:ASN:ND2	1:A:504:PHE:H	2.18	0.42
1:A:254:GLU:O	1:A:257:ARG:HB2	2.20	0.42
1:A:383:LEU:HD21	1:A:389:LEU:CD1	2.50	0.42
1:A:383:LEU:HD21	1:A:389:LEU:HD12	2.00	0.41
1:A:268:PRO:HA	1:A:283:ARG:O	2.19	0.41
1:A:274:HIS:CD2	1:A:276:GLU:HB3	2.55	0.41
1:A:303:LEU:HD22	1:A:343:TYR:CD2	2.54	0.41
1:A:501:ASN:ND2	1:A:501:ASN:H	2.18	0.41
1:A:501:ASN:C	1:A:501:ASN:HD22	2.24	0.41
1:A:255:LEU:C	1:A:257:ARG:N	2.73	0.41
1:A:87:MET:HE1	1:A:89:LYS:HE3	2.03	0.41
1:A:133:ASN:ND2	1:A:156:LYS:HE3	2.33	0.41
1:A:230:ILE:HG12	1:A:230:ILE:O	2.20	0.41
1:A:294:LYS:HD2	4:A:1469:HOH:O	2.21	0.40
1:A:366:LEU:HA	1:A:386:THR:HG21	2.03	0.40
1:A:78:LEU:HD22	1:A:82:GLU:HG2	2.02	0.40
1:A:246:VAL:HB	1:A:247:PRO:CD	2.51	0.40
1:A:264:ARG:HD3	1:A:421:TRP:CH2	2.56	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1018:HOH:O	4:A:1399:HOH:O[4_464]	0.35	1.85
1:A:295:ARG:N	1:A:312:GLN:NE2[6_465]	0.97	1.23
1:A:294:LYS:C	1:A:312:GLN:NE2[6_465]	1.56	0.64
4:A:1165:HOH:O	4:A:1165:HOH:O[8_775]	1.73	0.47
1:A:376:GLU:OE2	1:A:571:ARG:NH2[8_775]	2.04	0.16
1:A:294:LYS:CA	1:A:312:GLN:NE2[6_465]	2.06	0.14
4:A:1476:HOH:O	4:A:1476:HOH:O[8_775]	2.14	0.06
1:A:145:GLY:N	1:A:223:GLU:OE2[8_675]	2.16	0.04

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	512/528 (97%)	479 (94%)	25 (5%)	8 (2%)	9 2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	GLY
1	A	313	SER
1	A	548	LEU
1	A	315	LYS
1	A	576	TRP
1	A	522	CYS
1	A	547	GLN
1	A	158	ILE

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	457/467 (98%)	430 (94%)	27 (6%)	19 8

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	A	83	ASN
1	A	119	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	120	ASP
1	A	144	ARG
1	A	146	GLU
1	A	158	ILE
1	A	162	ARG
1	A	198	LYS
1	A	199	GLU
1	A	207	LYS
1	A	221	PRO
1	A	240	TYR
1	A	297	LYS
1	A	298	GLU
1	A	309	SER
1	A	347	GLU
1	A	370	VAL
1	A	371	TYR
1	A	372	PRO
1	A	375	GLU
1	A	376	GLU
1	A	421	TRP
1	A	455	SER
1	A	501	ASN
1	A	549	GLU
1	A	570	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	133	ASN
1	A	188	ASN
1	A	218	GLN
1	A	231	ASN
1	A	274	HIS
1	A	416	HIS
1	A	489	GLN
1	A	501	ASN
1	A	545	ASN
1	A	572	HIS
1	A	584	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	EDO	A	1879	-	3,3,3	0.68	0	2,2,2	0.11	0
2	EDO	A	1878	-	3,3,3	0.70	0	2,2,2	0.14	0
3	3PI	A	3632	-	39,39,39	3.48	15 (38%)	52,57,57	1.87	10 (19%)
2	EDO	A	1880	-	3,3,3	0.62	0	2,2,2	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	1879	-	-	1/1/1/1	-
2	EDO	A	1878	-	-	1/1/1/1	-
3	3PI	A	3632	-	-	14/36/60/60	0/1/1/1
2	EDO	A	1880	-	-	1/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3632	3PI	O16-C10	-12.44	1.04	1.39
3	A	3632	3PI	O15-C10	10.60	1.58	1.40
3	A	3632	3PI	C2-C3	5.22	1.66	1.52
3	A	3632	3PI	O14-C8	5.22	1.59	1.46
3	A	3632	3PI	C6-C1	4.47	1.64	1.52
3	A	3632	3PI	O6-C6	-4.04	1.33	1.43
3	A	3632	3PI	C2-C1	3.89	1.62	1.52
3	A	3632	3PI	C4-C5	3.67	1.62	1.52
3	A	3632	3PI	O2-C2	3.31	1.50	1.43
3	A	3632	3PI	O14-C14	2.98	1.42	1.34
3	A	3632	3PI	C4-C3	2.70	1.59	1.52
3	A	3632	3PI	C11-C10	-2.66	1.45	1.50
3	A	3632	3PI	C6-C5	2.57	1.59	1.52
3	A	3632	3PI	O4-C4	-2.49	1.37	1.43
3	A	3632	3PI	P3-O31	2.29	1.57	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3632	3PI	O15-C9-C8	6.53	126.66	110.90
3	A	3632	3PI	O15-C10-C11	-5.55	92.27	109.49
3	A	3632	3PI	O16-C10-C11	4.83	118.06	109.12
3	A	3632	3PI	C8-O14-C14	3.51	126.42	117.79
3	A	3632	3PI	O14-C8-C7	2.98	119.21	108.40
3	A	3632	3PI	O14-C14-O17	2.79	130.46	123.70
3	A	3632	3PI	P1-O1-C1	2.60	128.88	119.41
3	A	3632	3PI	C13-C12-C11	-2.47	101.34	113.29
3	A	3632	3PI	C9-C8-C7	-2.36	106.20	111.79
3	A	3632	3PI	C6-C5-C4	2.28	114.14	110.85

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3632	3PI	C11-C10-O15-C9
3	A	3632	3PI	O16-C10-O15-C9
2	A	1878	EDO	O1-C1-C2-O2
2	A	1879	EDO	O1-C1-C2-O2
2	A	1880	EDO	O1-C1-C2-O2
3	A	3632	3PI	C7-O13-P1-O1
3	A	3632	3PI	C7-C8-O14-C14
3	A	3632	3PI	C2-C3-O3-P3

Continued on next page...

Continued from previous page...

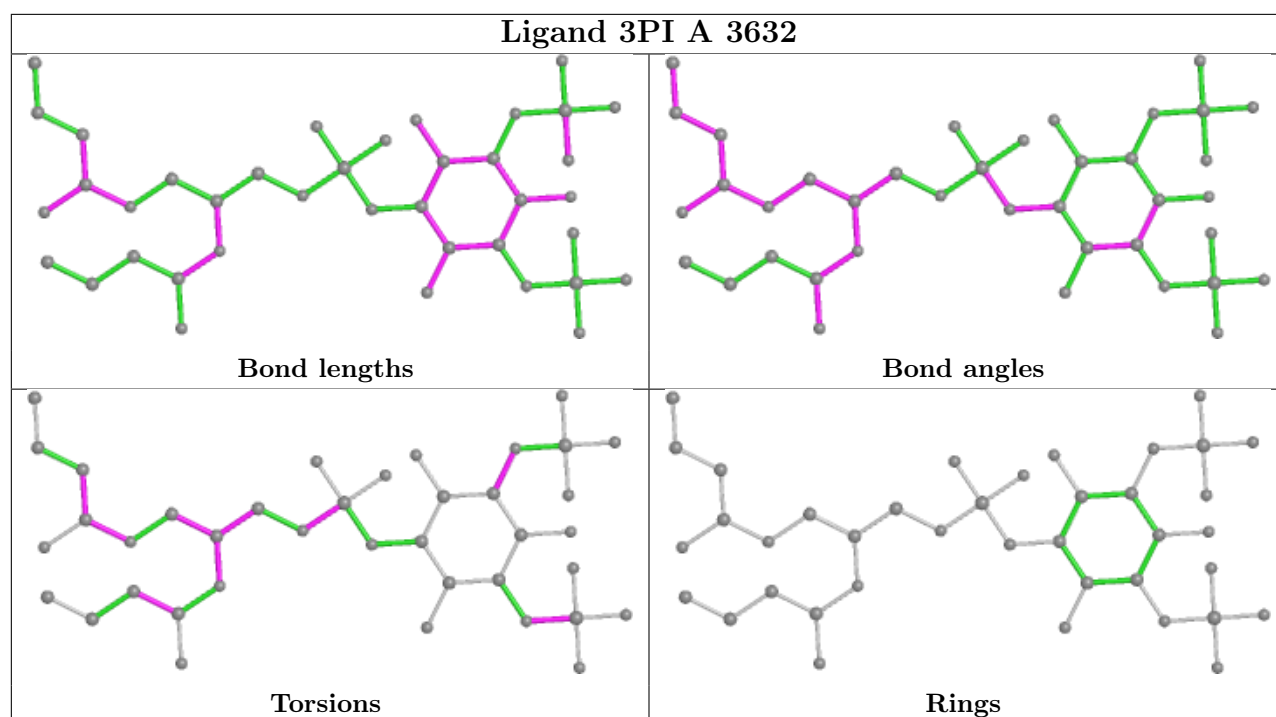
Mol	Chain	Res	Type	Atoms
3	A	3632	3PI	O13-C7-C8-C9
3	A	3632	3PI	C4-C3-O3-P3
3	A	3632	3PI	C7-O13-P1-O11
3	A	3632	3PI	O16-C10-C11-C12
3	A	3632	3PI	O13-C7-C8-O14
3	A	3632	3PI	C7-C8-C9-O15
3	A	3632	3PI	O14-C14-C15-C16
3	A	3632	3PI	C5-O5-P5-O52
3	A	3632	3PI	C7-O13-P1-O12

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1878	EDO	1	0
3	A	3632	3PI	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 [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	373:ASN	C	374:ILE	N	1.17

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	514/528 (97%)	0.44	20 (3%) 39 42	24, 44, 72, 96	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	ALA	10.7
1	A	141	ALA	5.1
1	A	559	TYR	4.5
1	A	312	GLN	4.2
1	A	560	SER	4.0
1	A	548	LEU	3.3
1	A	561	ASN	3.3
1	A	585	PRO	3.3
1	A	557	GLY	3.3
1	A	315	LYS	2.7
1	A	421	TRP	2.4
1	A	551	PHE	2.4
1	A	146	GLU	2.3
1	A	145	GLY	2.3
1	A	586	ARG	2.2
1	A	144	ARG	2.1
1	A	147	ASN	2.1
1	A	100	ALA	2.0
1	A	344	GLN	2.0
1	A	112	LEU	2.0

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](#)

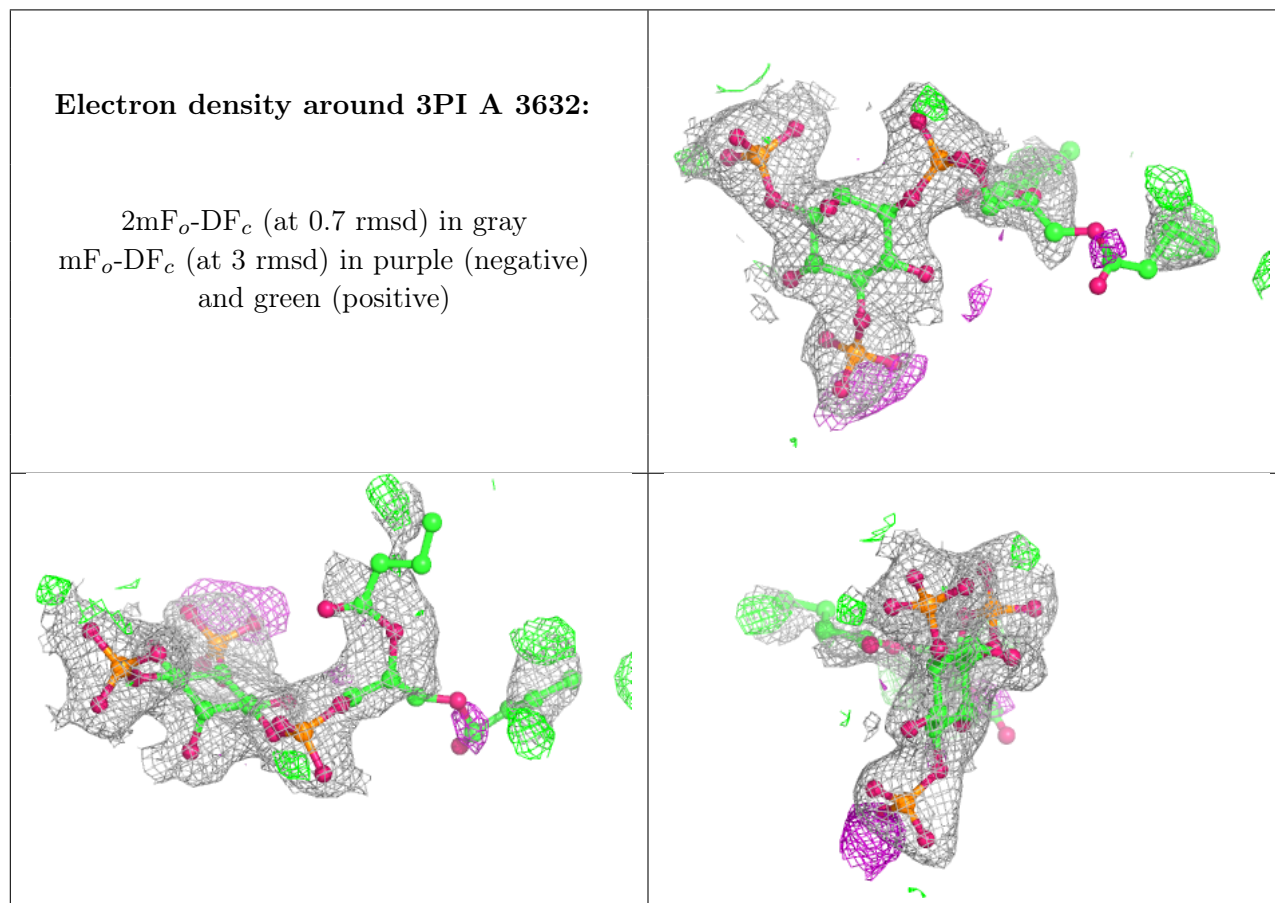
There are no monosaccharides in this entry.

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, 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(\AA^2)	Q<0.9
2	EDO	A	1880	4/4	0.77	0.19	51,51,52,52	0
2	EDO	A	1879	4/4	0.87	0.18	51,54,54,55	0
3	3PI	A	3632	39/39	0.92	0.18	30,64,94,96	3
2	EDO	A	1878	4/4	0.95	0.14	25,33,35,37	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 [i](#)

There are no such residues in this entry.