



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:10 PM UTC

PDB ID : 5GUG / pdb_00005gug
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor large cytosolic domain with inositol 1,4,5-trisphosphate
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.
Deposited on : 2016-08-29
Resolution : 7.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

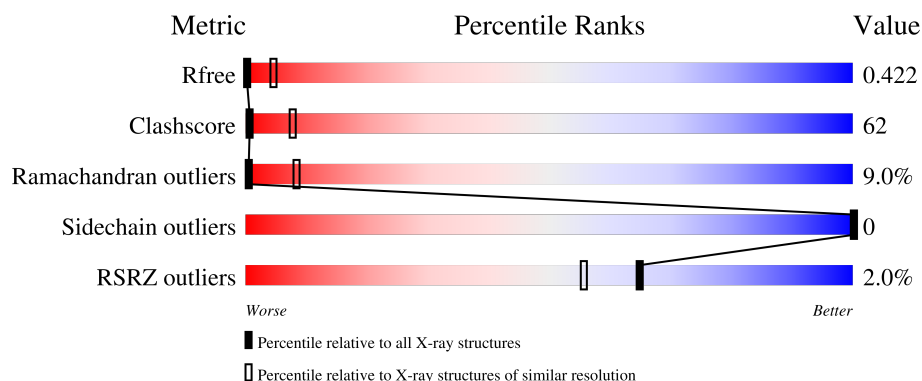
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.40 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	2217	2% 40% 32% 5% 22%
1	B	2217	2% 40% 32% 6% 22%

2 Entry composition [i](#)

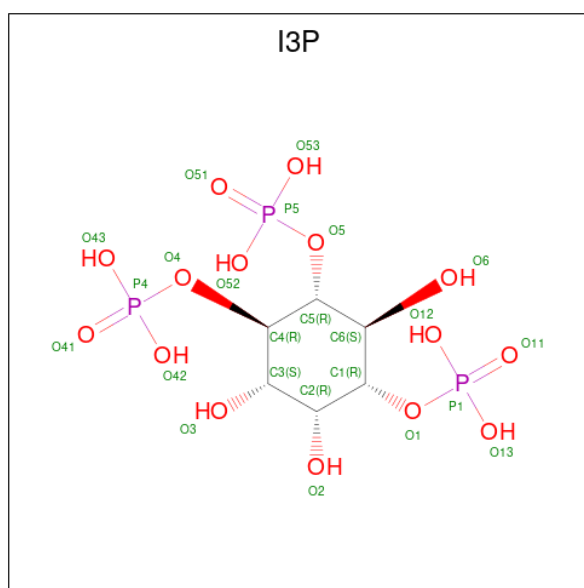
There are 2 unique types of molecules in this entry. The entry contains 25117 atoms, of which 7810 are hydrogens and 0 are deuteriums.

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 Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1721	Total	C	H	N	O	S	0	0	0
			12529	5147	3897	1746	1738	1			
1	B	1720	Total	C	H	N	O	S	0	0	0
			12522	5144	3895	1745	1737	1			

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: $C_6H_{15}O_{15}P_3$).

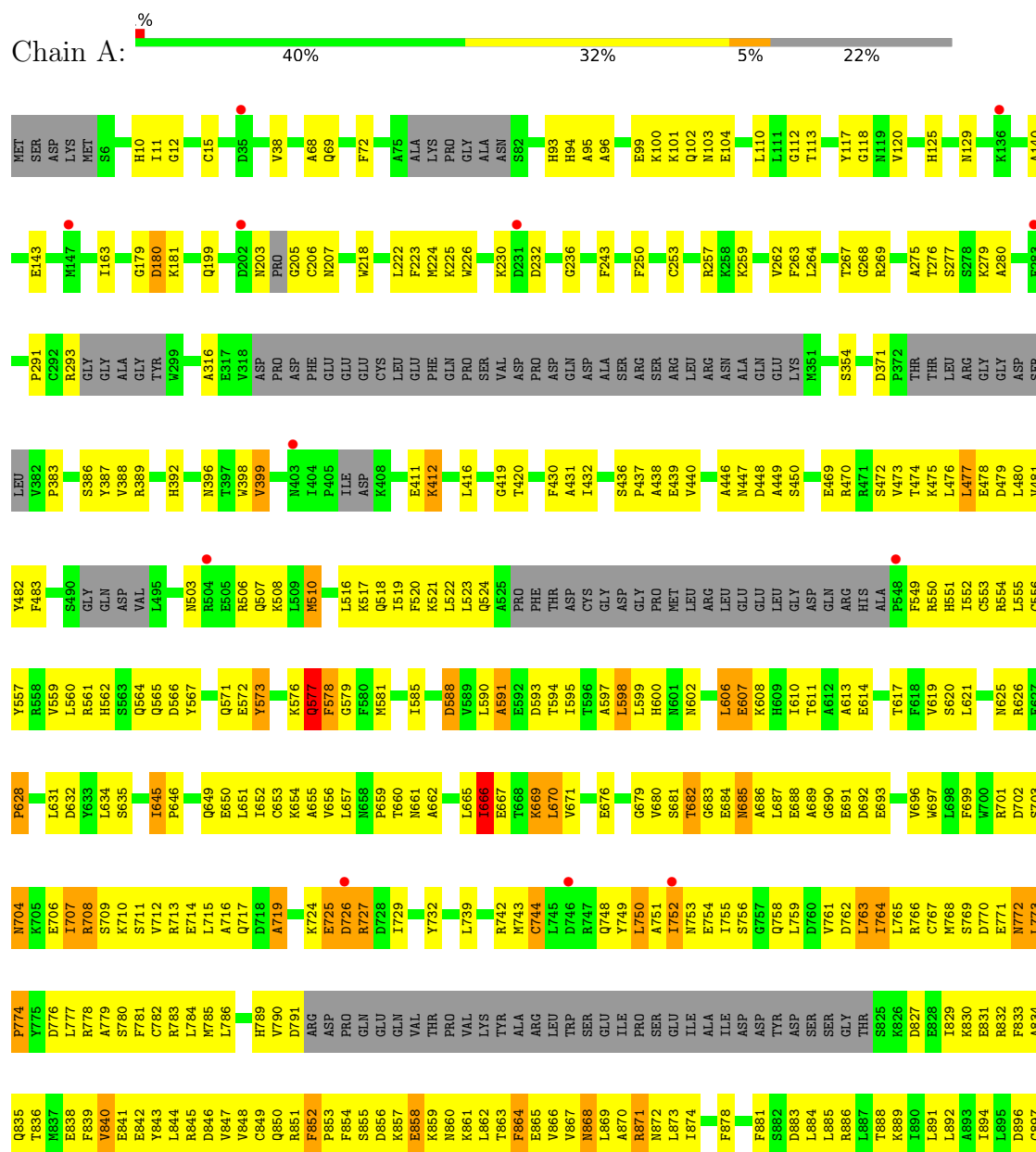


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			33	6	9	15	3		
2	B	1	Total	C	H	O	P	0	0
			33	6	9	15	3		

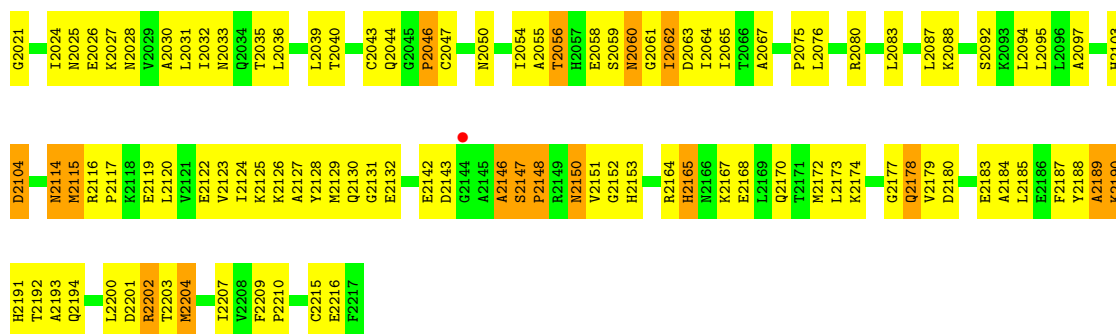
3 Residue-property plots

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.

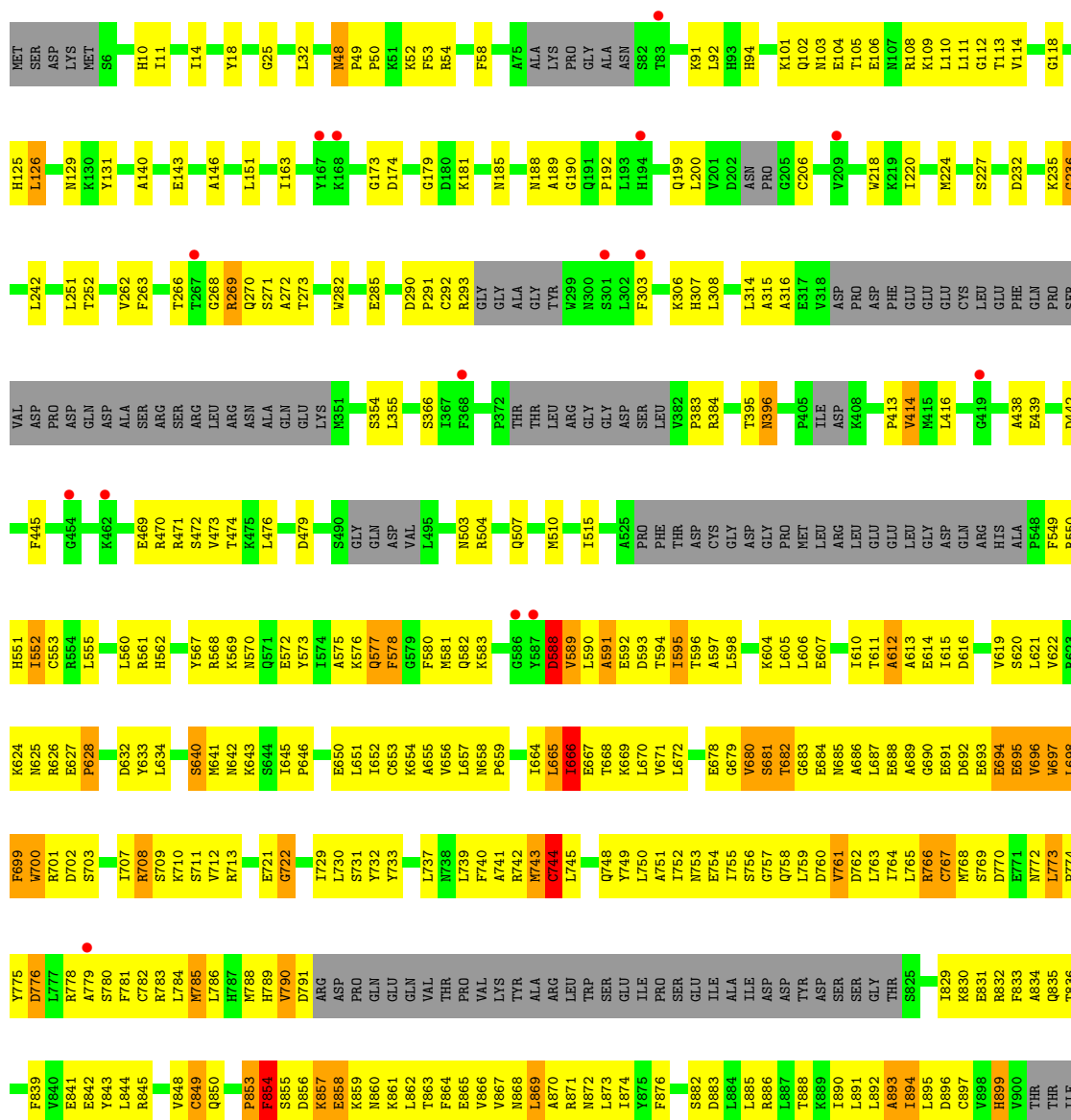
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1



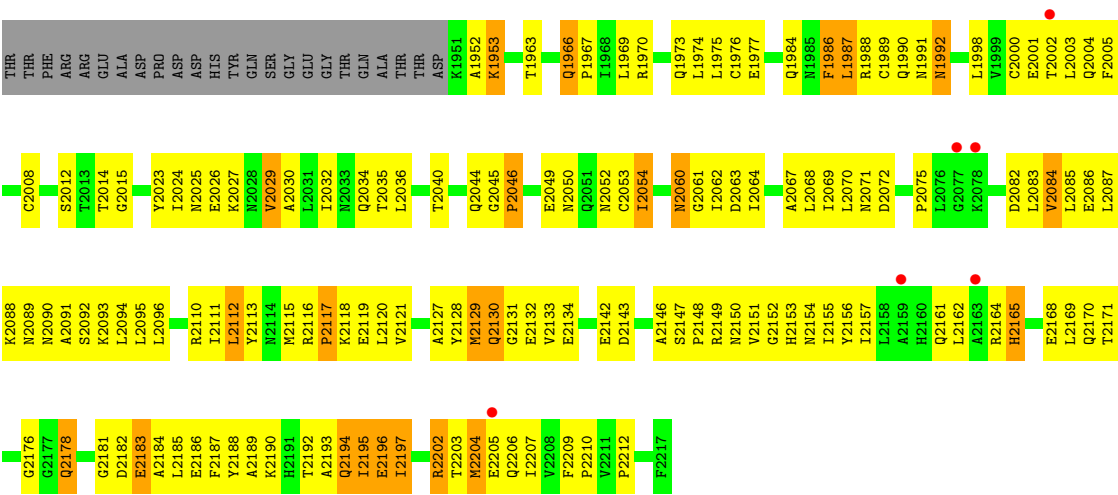




● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1



PHE	1965	F1041	K1116	I1179	Q1250	D1347	L1449	MET	ARG	L1662	GLU	GLY	F1856
PRO	M966	G1042	Q1117	R1182	N1261	D1350	F1453	PRO	ARG	L1663	ASP	GLU	K1857
ILE	V967	G1043	D1118	L1183	Q1262	F1351	F1453	SER	ASP	E1664	HIS	GLU	V1858
SER	M968	E1046	L1119	E1190	K1257	L1354	D1456	GLN	SER	E1665	LYS	ARG	F1859
LYS	D969	D1051	L1122	S1191	H1258	L1355	R1459	LYS	VAL	E1667	ALA	GLY	Y1860
MET	T970	L1052	V1126	A1192	E1269	Q1356	A1460	ALA	ALA	E1668	LEU	GLU	M1863
THR	K971	D1053	E1127	A1193	E1270	D1363	R1461	SER	ALA	C1671	VAL	ALA	K1864
LYS	L972	H1054	K1128	V1194	V1271	D1363	R1462	GLU	ALA	T1677	LEU	ALA	Q1867
GLY	K973	H1055	S1129	S1197	T1272	P1370	E1470	ILE	ALA	L1678	ILE	GLN	L1871
GLU	I974	G1056	E1130	R1198	H1275	H1376	A1471	VAL	ALA	R1679	LEU	VAL	K1872
ASN	E976	R1058	W1132	K1199	F1276	V1377	D1471	VAL	LYS	E1680	VAL	ASN	E1801
LYS	L977	T1059	V1133	Q1201	L1277	V1378	K1476	LEU	SER	M1681	ASN	ARG	G1802
GLY	L978	F1060	Y1134	Q1201	N1278	E1379	K1476	LEU	SER	M1682	VAL	ARG	G1802
SER	Q979	L1061	LYS	Q1202	N1279	E1380	E1480	ASP	ASP	T1683	VAL	TYR	N1805
ASN	I981	R1062	GLY	R1203	M1280	L1381	E1480	VAL	ALA	K1684	GLY	TYR	L1806
VAL	L982	V1063	GLN	Q1203	F1281	L1382	M1483	ALA	LYS	D1685	ASN	GLY	L1810
GLY	N983	L1064	PRO	G1209	Q1282	V1383	S1484	LYS	SER	R1686	ILE	ASN	L1810
ARG	V984	T1068	ASP	A1210	L1283	E1386	I1485	SER	ARG	E1687	ILE	ARG	N1813
SER	R985	D1071	GLU	H1211	C1284	G1387	I1486	ALA	ALA	GLY	PRO	ARG	A1814
ILE	L986	Y988	PRO	A1212	S1285	E1387	T1487	ILE	ILE	GLU	SER	SER	S1815
HIS	D987	MET	MET	V1213	E1286	K1388	T1488	ALA	ALA	LYS	GLY	GLY	S1816
GLY	Y988	Y1072	ASP	V1214	I1287	N1389	F1489	ILE	ILE	GLN	ARG	ARG	D1817
GLY	R989	F1073	ASP	L1215	N1288	E1397	S1492	ILE	PRO	ILE	ARG	ARG	R1818
GLU	I990	P1074	GLY	E1216	N1288	M1397	P1493	VAL	VAL	D1627	GLU	GLU	H1821
PHE	S991	L1075	ALA	L1217	R1290	L1400	P1493	ASP	ASP	V1628	LEU	LEU	E1822
LEU	C992	THR	SER	L1218	R1291	L1400	P1493	LEU	LEU	V1629	LEU	THR	S1823
PRO	L993	GLN	GLY	Q1219	V1292	D1403	P1493	ASP	SER	H1630	THR	SER	I1824
VAL	L994	VAL	GLU	I1220	Q1293	D1404	P1493	ASP	SER	P1632	PHE	SER	L1825
VAL	F997	L1080	ASN	F1221	H1294	D1404	P1493	GLN	GLN	E1633	GLY	GLY	L1826
LEU	K998	Q1081	HIS	Y1222	F1295	V1405	P1493	VAL	VAL	L1634	ASN	ASN	A1827
ARG	R999	L1082	LYS	E1223	F1295	V1406	P1493	VAL	ASN	L1635	GLY	GLY	I1828
GLY	D1002	F1084	LYS	K1224	E1300	E1417	P1493	THR	THR	F1636	LEU	PRO	A1829
GLY	S1008	R1085	THR	A1225	T1301	V1418	P1493	LEU	LEU	P1637	LEU	LEU	G1833
PHE	S1009	H1086	GLU	E1226	T1301	V1418	P1493	PHE	PHE	E1638	SER	SER	N1835
LEU	GLU	S1087	GLY	D1227	R1304	V1418	P1493	LEU	LEU	T1641	PRO	GLY	T1836
PRO	THR	S1088	THR	T1228	K1304	V1418	P1493	LEU	LEU	A1642	GLY	PRO	GLY
MET	THR	V1093	THR	K1229	K1310	Y1422	P1493	LYS	LYS	R1643	GLY	PRO	GLY
THR	SER	L1094	LYS	Q1231	F1311	Y1422	P1493	HIS	HIS	A1644	ALA	PRO	GLY
PRO	SER	Q1095	PRO	E1233	Q1312	L1426	P1493	ASN	ASN	R1645	LYS	SER	GLY
MET	GLY	A1096	PRO	I1233	Q1313	P1431	P1493	ILE	ILE	C1646	VAL	VAL	GLY
ALA	ASN	F1097	LEU	M1234	T1314	D1432	P1493	VAL	VAL	G1649	GLN	GLY	GLY
ALA	SER	K1098	LYS	R1235	I1315	T1433	P1493	GLN	GLN	G1650	GLY	GLY	GLY
ALA	SER	Q1099	HIS	L1236	V1316	E1434	P1493	LYS	LYS	F1651	PRO	PRO	GLY
PRO	GLN	Q1099	GLU	A1237	K1317	V1435	P1493	THR	THR	C1652	GLY	SER	GLY
GLU	GLY	V1100	SER	H1238	A1318	E1436	P1493	ALA	ALA	K1653	GLY	SER	GLY
GLY	GLY	Q1101	THR	E1239	C1326	F1436	P1493	LEU	LEU	K1654	GLY	SER	GLY
ASN	PRO	L1102	SER	F1240	Q1327	H1437	P1493	ASN	ASN	L1655	GLY	SER	GLY
VAL	SER	L1103	SER	L1241	D1328	K1438	P1493	TRP	TRP	L1656	PRO	SER	GLY
LYS	ASN	V1104	TYR	Q1242	N1329	E1439	P1493	LEU	LEU	K1657	LEU	SER	GLY
GLN	VAL	T1105	ASN	N1243	V1330	T1442	P1493	SER	SER	K1660	ARG	THR	ARG
ALA	PRO	S1106	TYR	C1245	Y1341	H1444	P1493	ALA	ALA	Q1661	GLN	SER	ARG
GLY	G1026	Q1107	ARG	A1246	Y1345	H1446	P1493	ALA	ALA	LEU	LEU	ARG	PHE
P960	D1029	K1113	VAL	G1247	Y1345	H1446	P1493	ALA	ALA	LEU	LEU	ARG	F1855
K962	I1040	Q1114	K1177	N1248	Y1345	H1446	P1493	ALA	ALA	LEU	LEU	ARG	F1855
		I1115	E1178	Q1249	N1346	H1446	P1493	ALA	ALA	LEU	LEU	ARG	F1855



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.99Å 223.49Å 319.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 7.40 49.49 – 7.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.49-7.40) 85.7 (49.49-7.40)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 7.37Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.356 , 0.416 0.361 , 0.422	Depositor DCC
R_{free} test set	526 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	159.4	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 700.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.23$, $\langle L^2 \rangle = 0.08$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	25117	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: I3P

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	1.01	13/8617 (0.2%)	1.11	25/11978 (0.2%)
1	B	0.99	11/8612 (0.1%)	1.08	21/11971 (0.2%)
All	All	1.00	24/17229 (0.1%)	1.09	46/23949 (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	A	0	8
1	B	0	9
All	All	0	17

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	GLN	CA-C	11.22	1.68	1.52
1	B	270	GLN	CD-NE2	-11.09	1.09	1.33
1	A	577	GLN	C-O	10.33	1.37	1.24
1	B	270	GLN	CD-OE1	-8.94	1.06	1.23
1	B	588	ASP	C-O	7.90	1.32	1.23

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	GLN	CA-C-N	12.85	144.83	121.70
1	A	577	GLN	C-N-CA	12.85	144.83	121.70
1	B	588	ASP	N-CA-C	10.31	129.24	107.70
1	A	578	PHE	N-CA-CB	8.83	125.51	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	553	CYS	N-CA-C	-8.20	99.48	110.55

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	GLU	Peptide
1	A	1375	ILE	Peptide
1	A	1380	LEU	Peptide
1	A	577	GLN	Peptide
1	A	588	ASP	Peptide

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	8632	3897	3899	762	0
1	B	8627	3895	3898	792	0
2	A	24	9	9	6	0
2	B	24	9	9	1	0
All	All	17307	7810	7815	1553	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 62.

The worst 5 of 1553 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:2020:LEU:O	1:A:2024:ILE:N	1.57	1.38
1:B:863:THR:O	1:B:867:VAL:N	1.72	1.21
1:A:1210:ALA:O	1:A:1214:VAL:CB	1.89	1.20
1:A:1125:ILE:O	1:A:1129:SER:CB	1.91	1.19
1:B:1682:MET:O	1:B:1686:ARG:N	1.78	1.16

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	1689/2217 (76%)	1219 (72%)	330 (20%)	140 (8%)	0	9
1	B	1688/2217 (76%)	1173 (70%)	350 (21%)	165 (10%)	0	7
All	All	3377/4434 (76%)	2392 (71%)	680 (20%)	305 (9%)	0	8

5 of 305 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	LEU
1	A	628	PRO
1	A	659	PRO
1	A	666	ILE
1	A	669	LYS

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	26/1980 (1%)	26 (100%)	0	100	100
1	B	26/1980 (1%)	26 (100%)	0	100	100
All	All	52/3960 (1%)	52 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	I3P	B	3000	-	24,24,24	1.17	2 (8%)	39,39,39	1.15	4 (10%)
2	I3P	A	3000	-	24,24,24	1.15	1 (4%)	39,39,39	1.13	4 (10%)

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	I3P	B	3000	-	-	0/15/39/39	0/1/1/1
2	I3P	A	3000	-	-	0/15/39/39	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3000	I3P	P5-O53	-2.30	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	I3P	P4-O42	-2.22	1.46	1.54
2	B	3000	I3P	P1-O13	-2.19	1.46	1.54

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3000	I3P	O13-P1-O12	2.52	117.24	107.80
2	A	3000	I3P	O1-P1-O11	-2.43	100.67	109.33
2	B	3000	I3P	O43-P4-O42	2.38	116.74	107.80
2	B	3000	I3P	O1-C1-C2	2.30	113.60	108.73
2	A	3000	I3P	O53-P5-O52	2.27	116.32	107.80

There are no chirality outliers.

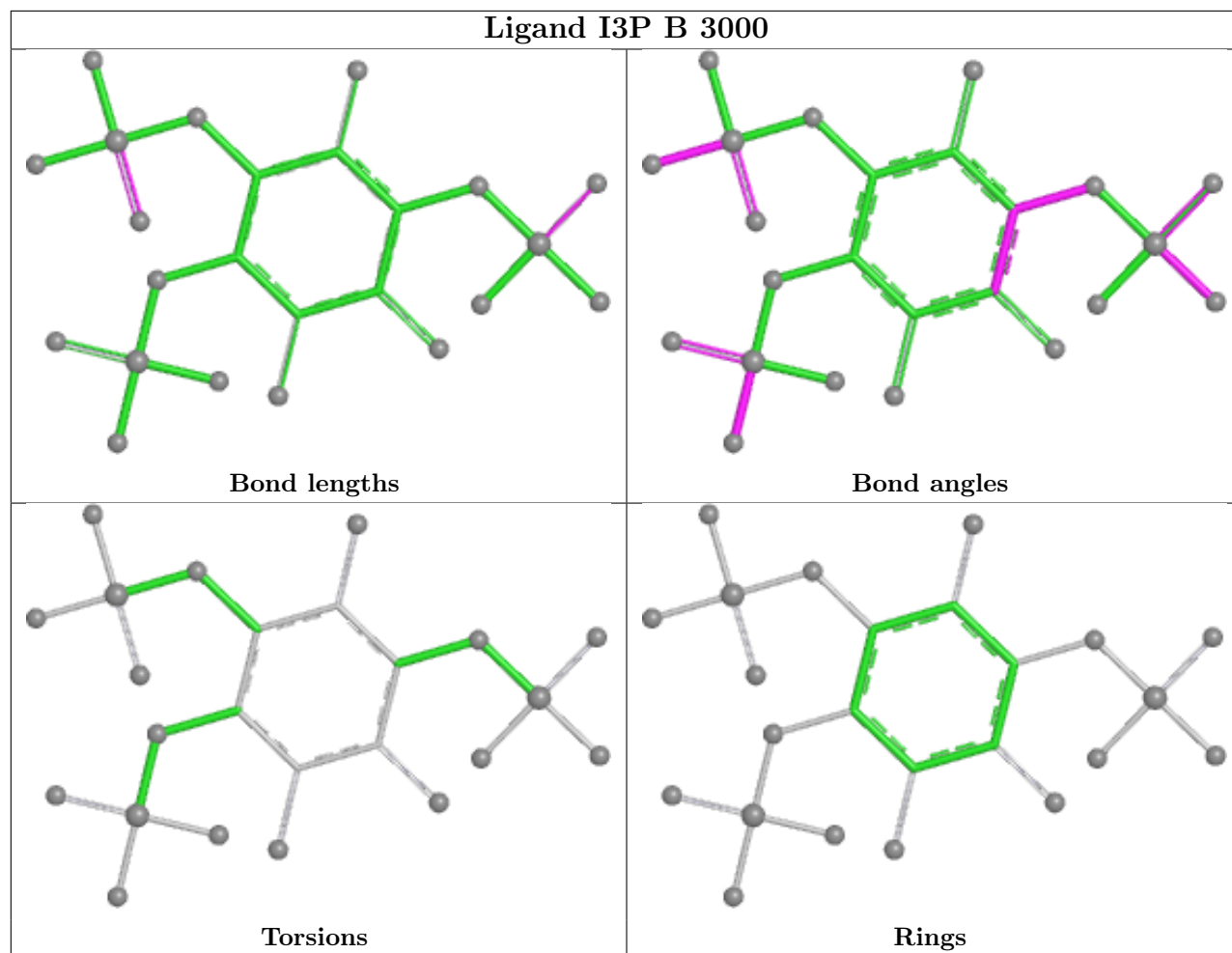
There are no torsion outliers.

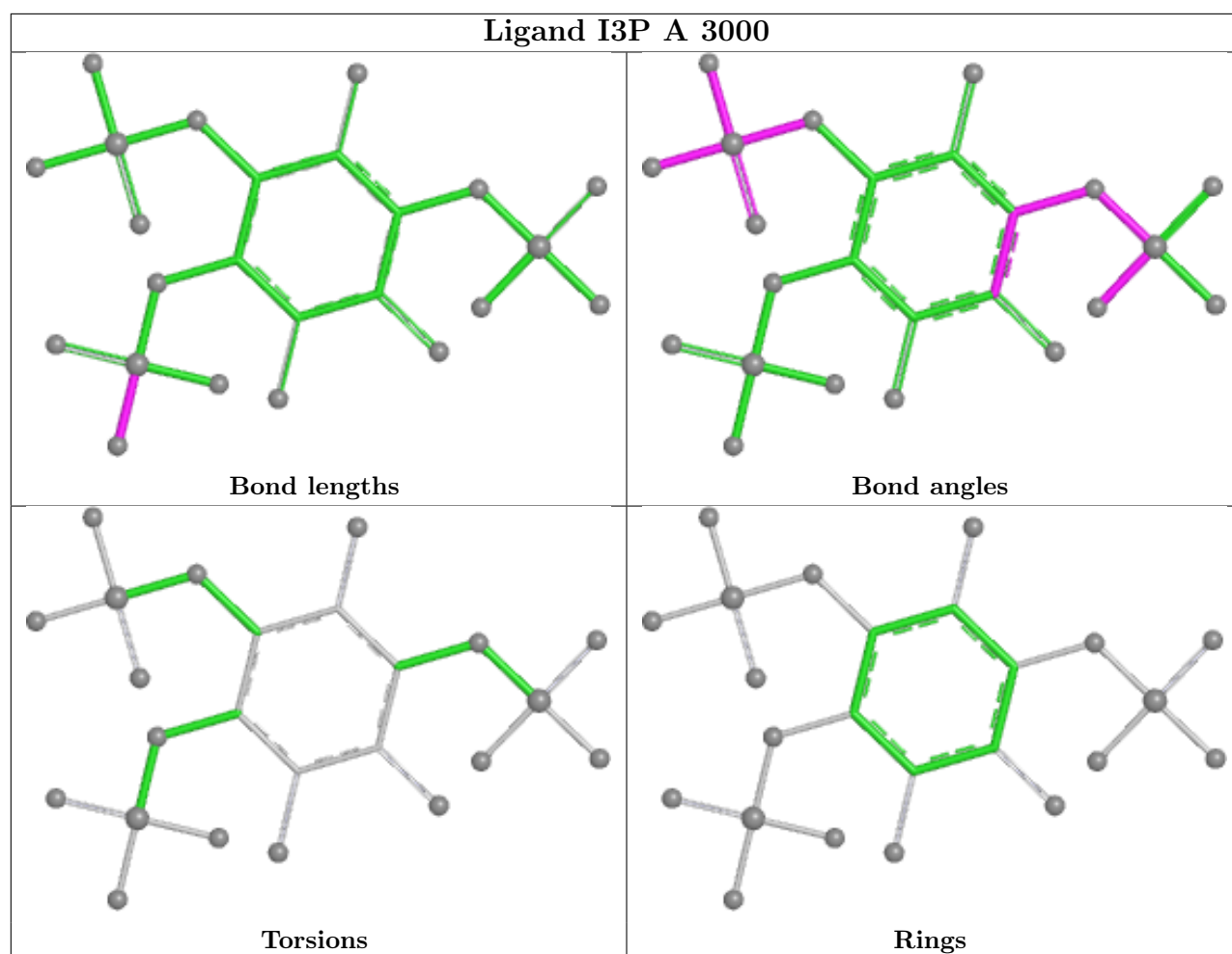
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3000	I3P	1	0
2	A	3000	I3P	6	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	1721/2217 (77%)	-0.40	26 (1%) 72 60	146, 167, 174, 184	0
1	B	1720/2217 (77%)	-0.38	44 (2%) 57 49	151, 166, 175, 192	0
All	All	3441/4434 (77%)	-0.39	70 (2%) 65 56	146, 166, 174, 192	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1444	ASN	6.5
1	B	1435	VAL	6.3
1	B	1443	SER	5.2
1	B	1438	LYS	5.0
1	A	548	PRO	4.8

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](#)

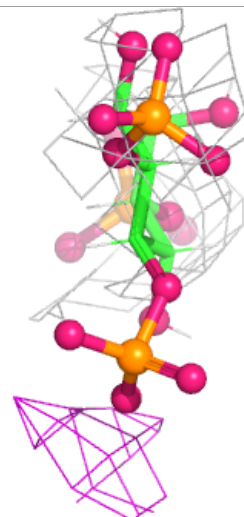
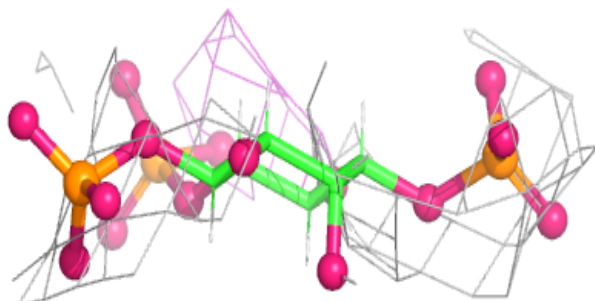
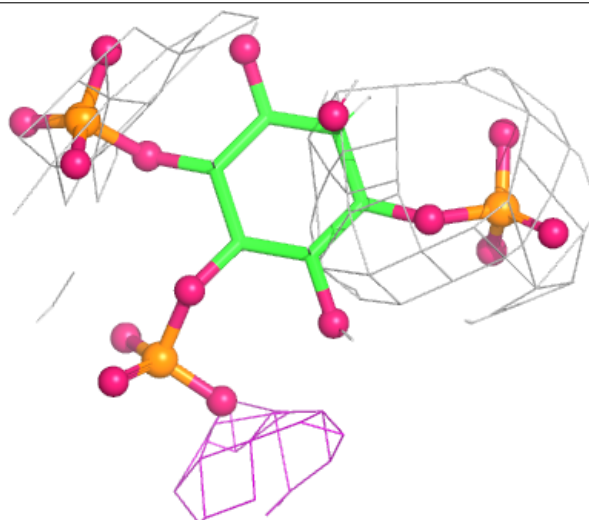
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

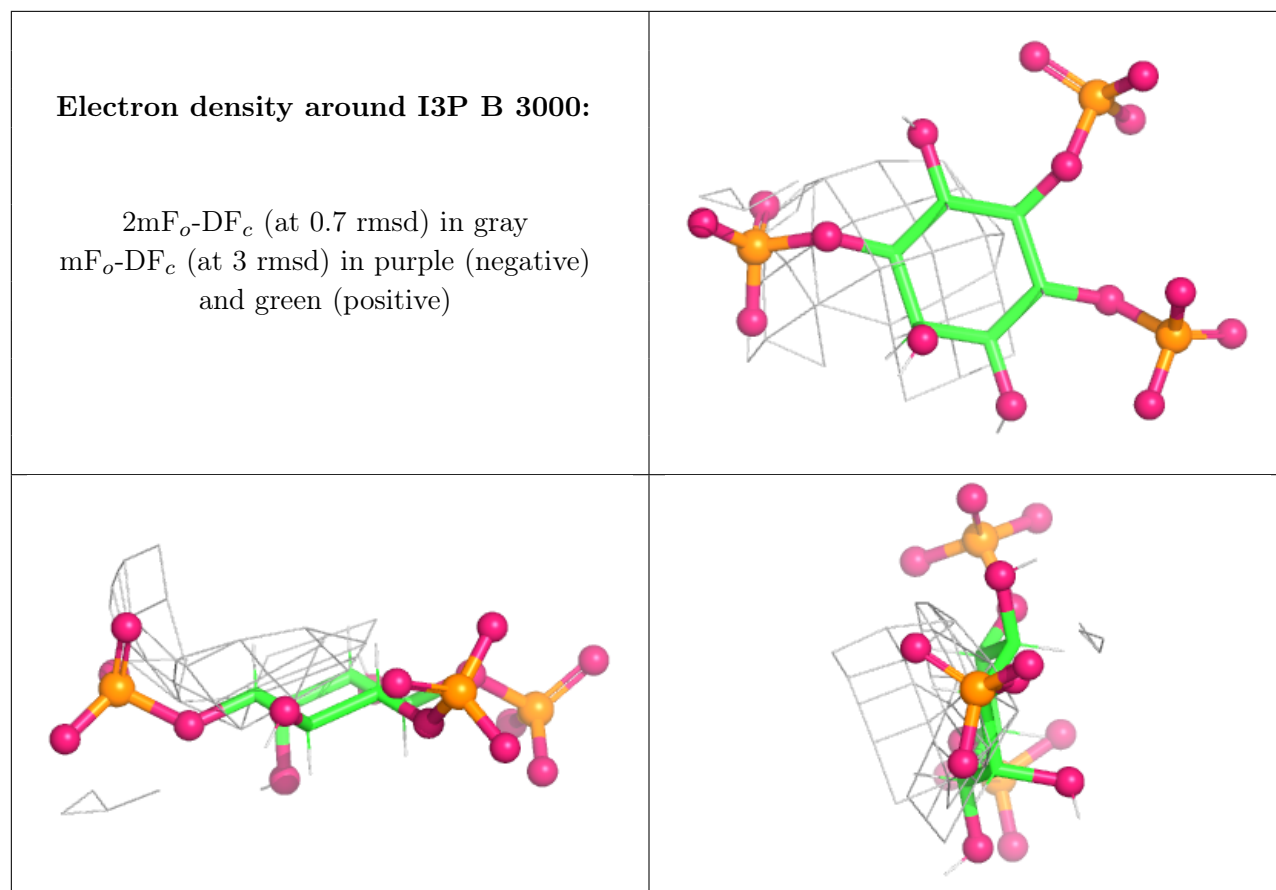
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	I3P	A	3000	24/24	0.81	0.12	169,172,172,172	0
2	I3P	B	3000	24/24	0.97	0.09	199,199,203,203	0

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 I3P A 3000:

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.